

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
Primary Metabolites (PM)				
1,2,4-benzenetriol	1079.549(1400.131)	1012.135(991.038)	1219.986(1622.134)	1003.791(974.943)
1-methylgalactose NIST	10405.216(25620.129)	6749.551(12633.562)	9280.083(19819.358)	7326.91(14383.141)
2-aminobutyric acid	6778.127(2312.798)	6819.584(2333.931)	6538.875(2122.79)	6681.09(2450.474)
2-deoxytetronic acid	3802(1871.5)	3811.933(1810.183)	3405.014(1336.781)	3496.373(1349.925)
2-hydroxybutanoic acid	37828.971(19975.01)	35735.831(20029.106)	35074.056(19703.304)	33061.194(17514.433)
2-hydroxyvaleric acid	4237.382(2334.07)	4287.303(2132.918)	4003.222(1997.14)	4230.507(2200.495)
2-ketoisocaproic acid	18813.069(5556.745)	19149.258(6078.798)	17882.208(5701.625)	18095.209(5592.465)
3-hydroxybutyric acid	39212.265(52464.62)	34152(42085.017)	40661.653(58622.991)	35564.567(37757.331)
4-hydroxybutyric acid	2256.422(736.812)	2269.843(849.082)	2271.958(777.963)	2256.269(835.419)
adipic acid	2895.686(1583.539)	2847.101(1343.166)	3036.819(1790.081)	2859.149(1326.626)
alanine	73245.52(30295.714)	75399.281(33101.158)	73297.403(29228.707)	76971.896(35025.025)
alloxanoic acid	2006.5(1375.468)	1837.64(1056.367)	1910.056(1352.394)	1729.866(1008.286)
alpha-ketoglutarate	1657.627(531.612)	1527.562(557.531)	1568.597(485.248)	1502.254(536.214)
aminomalonate	3619.186(1973.13)	2911.888(1665.318)	3724.167(2146.781)	3059.761(1777.82)
arachidic acid	4924.814(2338.338)	4808.124(2355.798)	4992.903(2595.024)	4769.925(2184.92)
behenic acid	2886.951(836.07)	3031.506(992.687)	2889.347(920.857)	3044.09(951.682)
benzoic acid	17834.373(6150.942)	17061.82(6244.429)	17735.486(6186.192)	17418.731(6079.543)
beta-alanine	1309.833(728.789)	1377.112(890.61)	1245.958(556.16)	1391.507(984.314)
capric acid	1629.931(794.154)	1873.809(1125.953)	1659.306(869.109)	1926.597(1199.193)
caprylic acid	5704.039(1875.061)	5854.764(2939.166)	5768.153(1874.782)	5987.373(3013.043)
citric acid	41473.245(20630.652)	41135.135(19465.808)	42914.653(22662.022)	43440.642(20818.822)
citrulline	4478.147(1507.009)	4592.506(1393.12)	4498.722(1671.082)	4685.075(1358.663)
conduritol-beta-exopoxide	1309.863(794.473)	1296.146(815.46)	1439.264(869.208)	1299.627(854.864)
creatine	7813.647(4623.762)	7540.27(4234.565)	7484.681(4610.221)	7697.672(4194.764)
creatinine	8228.716(4668.248)	8192.91(4583.811)	8071.514(4793.075)	8733.493(4284.52)
erythritol	7881.353(18212.112)	8811.472(35942.446)	7359.583(16455.919)	8897.06(40653.41)
fructose	2597.775(3830.73)	2215.82(2366.76)	2047.014(2353.022)	2276.851(2639.361)
fumaric acid	9386.029(3097.763)	9434.101(2971.299)	9300.639(3300.011)	9383.06(3025.01)
gluconic acid	783.971(293.026)	776.438(203.662)	808.403(326.755)	812.418(190.038)
glucose	388539.039(113173.178)	378196.978(110227.014)	381069.236(112778.529)	386519.015(103390.2)
glucose-1-phosphate	2858.431(1035.667)	2901.236(1183.342)	2806.708(931.937)	2919.687(1297.013)
glucuronic acid	1283.441(842.594)	1067.326(518.171)	1182.639(562.989)	1090.776(561.713)
glutamic acid	8913.157(3993.644)	8273.382(4085.076)	8536.792(3830.733)	8214.761(4266.633)
glutamine	30937.275(21124.794)	32325.416(15805.25)	31662.556(22695.996)	34107.239(16505.65)
glutaric acid	568.461(206.452)	532.449(209.713)	573.208(220.796)	535.06(202.663)
glyceric acid	10747.598(4862.652)	9509.18(4092.259)	10589.486(4595.623)	9543.403(4305.927)
glycerol	94812.804(37180.866)	95386.449(35827.521)	100344.306(37690.486)	99697.985(36613.08)
glycerol-alpha-phosphate	970.676(374.848)	952.978(388.821)	991.222(373.441)	959.343(403.965)
glycine	68370.147(24574.146)	66183.809(20178.354)	73137.5(26791.978)	69909.254(20799.518)
glycolic acid	6131.461(2349.621)	6039.528(2582.552)	6211.681(2417.159)	6016.627(2773.779)
heptadecanoic acid	4659.657(1498.193)	4722.045(1568.799)	4736.75(1623.265)	4662.478(1570.389)
hydroxycarbamate NIST	9159.343(4227.978)	9278.079(4002.355)	9397.375(4421.922)	9357.597(4099.154)
indole-3-acetate	2888.461(1569.254)	2930.517(2502.67)	2828.514(1675.344)	3057.955(2831.206)
indole-3-lactate	1920.853(610.853)	2047.753(765.819)	1834.125(531.593)	1942.627(629.712)
indole-3-propionic acid	1758.569(1386.393)	2146.528(1481.229)	1732.056(994.58)	2217.716(1584.021)
isoleucine	42005.147(16265.503)	42337.787(14176.603)	39405.694(14415.12)	41216.806(14003.215)
isopropylbenzene	16849.167(16235.754)	16249.494(18003.148)	18402.083(17917.397)	16790.97(20151.387)

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Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
isothreononic acid	1867.461(718.975)	1810.944(701.346)	1844.194(735.944)	1898.612(674.425)
lactic acid	192717.833(119615.393)	173890.775(103094.546)	180763.528(111652.076)	162160.896(91976.988)
lauric acid	8363.078(12244.741)	10000.079(13605.883)	9131(14384.754)	11053.09(15461.218)
leucine	70058.255(22610.471)	77074.056(24098.618)	67000.458(22724.459)	75390(24758.076)
levoglucosan	1659.137(1216.05)	1870.697(1782.358)	1726.236(1329.44)	1800.09(1389.732)
linoleic acid	1164.52(386.052)	1194.708(500.78)	1203.625(364.979)	1207.209(520.374)
lysine	15344.127(10811.81)	15204.719(7437.624)	15836.986(10789.329)	15994.418(7552.007)
lysine	18427.5(13565.891)	18658(9668.614)	19624.056(13111.026)	19306.612(9738.677)
lyxitol	3098.794(1031.473)	3248.989(1189.283)	3096.708(970.26)	3127.582(1000.34)
maleic acid	878.186(349.551)	788.416(361.008)	874.556(374.467)	809.09(349.401)
maleimide	8053.353(10208.802)	6862.888(5737.055)	8891.208(11955.832)	6344.701(3004.902)
malic acid	1120.422(375.058)	1096.719(407.251)	1105.236(362.52)	1111.716(361.939)
maltose	1438.294(1117.335)	1611.483(3326.737)	1404.944(780.681)	1754.448(3794.843)
mannitol	7384.294(34427.962)	2531.82(2424.356)	9210.819(40878.375)	2354.657(1910.561)
mannose	23546.755(8923.898)	30536.393(70206.191)	22653.167(9106.751)	33367.104(80635.606)
methionine	2349.51(1025.929)	2403.135(919.059)	2337.778(1119.461)	2507.567(850.817)
myo-inositol	21222.363(6524.406)	20873.449(7257.918)	21375.847(6329.61)	20822.343(7312.203)
myristic acid	2466.971(764.975)	2620.674(814.52)	2514.778(810.279)	2671.358(814.573)
N-acetylornithine	2287.627(630.487)	2420.708(709.39)	2296.653(679.83)	2434.06(749.283)
N-acetylputrescine	2335.549(2188.271)	2392.753(2148.301)	2130.389(1024.341)	2557.403(2426.534)
nicotinic acid	22012.588(31343.256)	23151.326(37119.635)	22864.819(32433.543)	26788.985(40997.646)
ornithine	22444.167(16004.833)	23350.124(11618.996)	22788.375(16240.437)	24179.194(11856.253)
oxalic acid	38138.853(34967.284)	31155.685(23852.651)	35563.861(35006.662)	30009.03(24888.703)
oxoproline	148843.422(35478.319)	149227.169(31627.972)	147583.903(40185.571)	149267.433(32922.76)
palmitic acid	83826.745(26436.792)	87530.236(29254.435)	85898.806(28513.631)	85002.239(28878.676)
palmitoleic acid	620.618(273.823)	620.933(267.671)	654.528(303.431)	620.821(255.343)
pelargonic acid	29902.833(10040.315)	30430.506(13250.889)	30961.722(10552.778)	30450.269(12658.324)
pentadecanoic acid	10300.402(2114.862)	10098.079(2516.636)	10283.056(2261.178)	10342.313(2451.259)
phenylalanine	21140.618(6021.369)	22473.629(6495.431)	20492.139(5953.159)	22896.507(6363.749)
phosphate	62360.137(25668.008)	60891.899(24903.713)	67682.625(26025.372)	64793.806(25638.342)
phthalic acid	6103.99(2526.222)	6071.337(3064.102)	6283.014(2757.299)	6236.478(3381.886)
proline	10358.696(7248.838)	10114.865(6954.499)	10278.653(7595.157)	9602.463(6087.033)
pseudo uridine	2775.873(653.848)	2855.146(716.503)	2839.042(677.462)	2909.299(750.373)
pyrrole-2-carboxylic acid	6415.049(4040.235)	5793.022(3390.2)	6070.722(3862.072)	5839.91(3286.061)
pyruvic acid	11489.667(4788.685)	10820.404(3860.672)	11843.722(4927.602)	10898.537(3981.009)
quinic acid	1272.48(1447.647)	1600.753(1769.131)	1207.264(1395.694)	1627.761(1726.716)
ribonic acid	873.931(245.494)	868.337(240.982)	878.722(246.588)	867.343(256.395)
ribose	2038.549(602.463)	2037.371(644.28)	1952.694(588.947)	2069.731(671.325)
salicylic acid	4293.333(14512.238)	2853.427(9490.954)	4624.556(16288.869)	3082.567(10830.814)
serine	37492.01(17259.952)	38555.775(15218.55)	39316.236(19150.177)	40813.806(15539.561)
stearic acid	378059.412(154306.997)	405425.36(162088.008)	392137.014(173120.537)	389522.836(144375.349)
succinic acid	2428.686(828.589)	2106.888(729.61)	2445.069(869.246)	2112.403(771.778)
sucrose	671.637(698.395)	613.989(381.592)	744.056(789.835)	635.194(402.983)
tagatose	4063.725(4123.989)	3589.213(2553.245)	3440.903(2751.873)	3661.881(2813.897)
threitol	1452.196(807.611)	1395.584(582.087)	1511.361(901.417)	1392.925(611.212)
threononic acid	8560.99(4195.661)	7285.618(3051.907)	8602.167(4062.708)	7531(3287.101)
threonine	13282.686(4817.033)	14237.438(5929.372)	13235.931(5140.448)	15006.119(6365.817)
trans-4-hydroxyproline	1700(1224.851)	1418.764(658.035)	1794.542(1357.079)	1371.925(553.495)

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Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
tryptophan	21152.706(10249.693)	21495.079(8899.268)	20616.319(9846.47)	21355.015(8793.98)
tyrosine	42719.343(12721.061)	44217.124(10941.659)	41085.653(12684.991)	44149.269(9748.327)
urea	785114.216(265741.232)	831665.056(279983.579)	754943.208(248424.764)	838122.119(274463.33)
uric acid	32108.833(16219.644)	33489.944(17068.328)	29210.222(15439.048)	29761.881(13946.09)
valine	79110.618(21747.997)	82792.506(32138.457)	75807.153(20507.272)	81418.313(34557.102)
Biogenic Amines (BA)				
(2R)-3-Hydroxyisovalerylcarnitine	1880.687(1046.064)	1825.6(555.898)	1736.25(759.31)	1762.654(565.708)
(3-Carboxypropyl)trimethylammonium cation	16403.7(5302.415)	17555.878(5550.678)	15580.716(5251.357)	16940.727(5053.444)
(R)-Butyrylcarnitine	34078.718(15321.062)	37105.876(16533.628)	34088.945(16762.288)	36207.842(16171.868)
.beta.-Phenyl-.gamma.-aminobutyric acid	869.907(2440.04)	709.92(241.154)	643.618(301.777)	721.387(263.381)
.epsilon.-Caprolactam	87755.933(68018.05)	89742.427(68532.183)	86328.183(70251.29)	85416.594(66739.158)
1,2-Dimethylimidazole	1819.366(2845.633)	1694.49(1032.734)	2037.18(3377.863)	1762.948(1162.502)
1-Acetyl-3-piperidinamine	1839.3(818.798)	1738.972(605.781)	1852.274(813.83)	1703.792(523.936)
1-Acetyl-4-piperidinamine	2047.585(2838.897)	1533.704(815.512)	1979.034(2088.427)	1536.323(805.703)
1-Methyladenosine A	4344.676(1038.43)	4455.103(1138.778)	4429.169(1077.875)	4439.09(1166.254)
1-Methyl-L-histidine	22958.602(14651.539)	23284.637(14336.386)	22354.704(14663.536)	23572.374(14325.805)
1-Methylnicotinamide	14470.114(11101.857)	14251.823(7589.804)	14418.734(9495.696)	14476.406(7942.219)
1-Monostearin	2115.305(1451.321)	2830.121(4236.602)	2177.064(1526.767)	2601.232(2151.589)
1-Oleoyl-2-acetyl-sn-glycerol	9191.209(8932.606)	14964.193(39026.124)	9841.135(10395.606)	16928.701(44698.374)
1-Oleoyl-sn-glycero-3-phosphoethanolamine	6355.005(5324.408)	6525.509(3772.709)	6095.835(5637.756)	6338.457(3307.175)
1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	6410.996(4032.932)	6606.582(3360.162)	6517.585(4263.178)	6682.955(3226.653)
1-Phenylpyrrolidine	143.457(290.638)	117.902(39.385)	160.128(346.32)	120.76(41.362)
1-Stearoyl-2-arachidonoyl-sn-glycero-3-phospho-(1'-myo-inositol)	1329.25(881.122)	1346.97(825.295)	1412.649(948.673)	1375.1(847.811)
1-Stearoyl-2-arachidonoyl-sn-glycero-3-phosphoserine	1894.838(2682.073)	1778.287(2056.277)	1856.246(2611.087)	1935.426(2038.887)
1-Stearoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	6094.917(4604.091)	5803.43(2687.326)	6235.181(4995.225)	5778.688(2431.299)
2,2',2''-Nitrilotriethanol	4650.025(6102.206)	5725.159(8642.651)	5320.019(7154.417)	6576.946(9784.759)
2,2-Bishydroxymethyl]-2,2',2''-nitrilotriethanol	661.365(1011.212)	683.907(582.601)	729.049(1200.747)	729.169(650.841)
2,6-Diaminopimelic acid	658.783(580.92)	497.274(446.965)	678.564(585.353)	508.356(456.288)
2-Amino-1-phenylethanol	50064.106(14796.501)	51939.812(12195.207)	48749.621(14343.952)	52299.921(13191.029)
2-Hydroxyibuprofen	3646.161(11203.95)	2794.402(8390.204)	2716.27(5046.864)	2665.938(9448.507)
2-Indolinone	22360.698(11782.007)	25707.648(13967.826)	23360.713(12417.222)	25395.462(14495.492)
2-Methylbutyryl-L-carnitine	15742.272(6758.335)	19766.912(10894.625)	14167.581(6470.11)	17337.175(7188.976)
3-(1-Pyrazolyl)-alanine	358.412(1009.805)	338.461(595.673)	321.331(714.353)	400.74(672.044)
3,4-Dimethoxybenzaldehyde	2111.85(1817.258)	2433.796(3874.558)	2231.388(2013.467)	2447.356(4335.605)
3,5-Dihydroxyphenylglycine	1521.258(1937.934)	1263.783(1225.374)	1742.967(2202.951)	1342.855(1314.494)
3-Amino-1-propanol	14759.177(17371.398)	11356.849(7175.122)	15972.716(19546.631)	10627.843(6034.141)
3-Aminoquinoline	2768.697(3284.974)	3229.232(3720.884)	2992.714(3269.222)	3676.498(3966.221)
3-Cysteinylacetaminophen	85.628(278.461)	31.56(22.915)	86.812(304.878)	32.108(22.791)
3-Dehydrocarnitine	2713.916(1241.044)	2870.766(1231.212)	2693.857(1322.487)	2599.336(925.909)
3-Hydroxybutyrylcarnitine	3061.608(2849.628)	2805.221(2351.317)	3310.658(3136.113)	2772.17(1938.867)
3-Hydroxyyleylcarnitine	1499.787(2022.956)	1253.212(1804.396)	1372.661(1923.433)	1130.92(1716.403)
3-Hydroxypyridine	1971.739(3569.602)	3209.464(4987.632)	1482.697(2804.788)	3347.393(5367.51)
3-Methylglutaryl-L-carnitine	575.563(258.16)	1052.615(1965.769)	572.823(284.547)	659.9(336.824)
3-Methylxanthine	555.738(650.872)	522.536(446.424)	602.522(690.615)	568.763(477.615)
3-Pyridinemethanol	1549.304(1050.899)	1769.148(2316.24)	1582.528(1146.057)	1835.908(2625.598)
4,5,7-Trihydroxyisoflavone	507.397(2564.172)	124.958(731.854)	561.595(2843.781)	153.911(841.29)
4-Acetamidobutyric acid	3471.712(2342.69)	3727.521(2854.822)	3615.048(2473.068)	3939.109(3184.595)
4-Aminomethylcyclohexanecarboxylic acid;	1589.572(3239.52)	1326.667(747.566)	1401.408(1985.592)	1323.682(729.624)

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4-Fluoro-.alpha.-pyrrolidinobutiophenone	532.638(610.097)	458.298(230.627)	554.359(649.079)	459.133(227.638)
4'-Methyl-N-methylhexanophenone	2337.883(2599.719)	2483.552(2368.085)	2417.654(2633.99)	2642.039(2537.353)
4-Pyridoxic acid;	9506.692(32185.74)	3611.761(6927.589)	10060.296(36968.279)	3804.289(7433.485)
5'-S-Methyl-5'-thioadenosine	2295.417(2441.494)	2541.641(1775.543)	2469.835(2761.965)	2655.655(1832.667)
5'-S-Methylthioadenosine	2232.692(2448.886)	2396.981(1900.293)	2370.237(2777.789)	2481.076(1983.511)
6-Hydroxyflavone	1191.845(6678.29)	403.876(528.261)	1481.81(7954.915)	353.353(409.453)
6-Methoxynaphthaleneacetic acid	7862.951(2449.945)	9327.172(12784.412)	8185.531(2515.823)	8105.686(2065.758)
7.alpha.-Hydroxy-3-oxo-4-cholestenic acid	7832.128(4085.847)	7971.016(3525.274)	7988.535(4451.445)	7856.561(3289.14)
7-Hydroxywarfarin	256.276(1326.793)	125.152(55.26)	316.435(1586.026)	120.883(52.118)
7-Methylguanosine	2894.162(982.806)	3126.746(1088.991)	2980.301(1011.499)	3171.08(1170.041)
Acetazolamide	111.881(1032.576)	10.68(5.05)	10.574(6.06)	10.878(4.95)
Acetaminophen	8598.401(25412.26)	1888.819(3095.431)	8664.723(27961.761)	1954.635(3481.327)
Acetyl-DL-carnitine	4040.595(1781.273)	3886.498(1192.6)	4161.284(1862.636)	3932.342(1212.884)
Acyclovir	10042.642(38991.986)	102.244(109.125)	13378.101(45628.802)	99.14(108.798)
Adenosine	476.693(252.498)	554.001(724.574)	477.541(212.691)	611.275(821.588)
Ala-Ile	1117.937(531.714)	1022.708(379.234)	1153.66(538.781)	1022.593(369.487)
Albendazole	1404.595(9285.314)	342.564(133.753)	1876.415(11095.377)	355.058(141.429)
Albendazole sulfoxide	556.474(1732.254)	706.284(5840.411)	658.421(2024.354)	911.792(6718.083)
alpha-Methylhistidine;	18823.314(15559.922)	19428.048(15625.399)	18017.263(14601.37)	20347.68(16173.525)
Alprazolam	219.224(700.569)	79.36(42.975)	209.565(755.994)	76.592(43.888)
Aminodiphenylmethane	10035.44(39641.241)	4831.419(12787.502)	7128.186(14760.998)	5206.398(14422.701)
Androstan-3-ol-17-one 3-glucuronide	1018.393(816.112)	997.46(700.178)	954.271(739.508)	898.382(668.913)
Arginine	66971.722(30497.565)	63686.741(31676.786)	70541.746(33026.077)	66753.473(27292.861)
Atenolol	2831.445(26482.196)	235.929(152.586)	228.711(127.871)	242.031(156.639)
Atorvastatin	310.188(170.392)	307.876(96.997)	329.376(192.18)	309.451(103.349)
Avobenzon	1620.013(901.713)	2204.034(6233.272)	1625.707(809.631)	1517.537(583.705)
Benthiavalicarb-isopropyl	397.898(475.323)	338.666(425.872)	387.129(452.525)	343.498(481.04)
Benzophenone-3	79.42(118.399)	152.05(480.887)	94.023(138.386)	176.503(548.803)
Betaine	1396162.001(400978.201)	1465520.587(366608.787)	1356785.522(423707.652)	1417694.595(341114.75)
Betaine aldehyde cation	14682.235(107622.215)	56.189(19.083)	20851.707(128492.149)	56.738(19.839)
Betonicine	5018.889(9595.989)	5425.561(9356.727)	4242.1(6533.329)	6202.06(10533.221)
Biliverden	37882.387(29682.943)	38990.463(24851.237)	35273.646(28537.043)	35664.215(20507.162)
Borrelidin	1800.784(4109.912)	1698.556(4228.984)	1876.809(4290.433)	1452.819(3956.247)
Bradykinin	2350.694(4905.075)	2102.181(4523.581)	2055.799(4093.04)	2277.815(4790.793)
Caffeine	46358.68(97388.926)	86219.943(115602.167)	41207.184(95909.44)	92115.413(118321.704)
Carbamazepine	424.616(1432.071)	11883.366(108750.28)	375.298(1107.091)	15626.683(125106.825)
Carnitine	1001164.333(283021.215)	1045982.351(310270.412)	970340.809(286347.389)	1001183.088(275670.844)
Choline cation	254611.526(57164.648)	282373.342(63913.774)	256045.629(58199.308)	280565.281(62246.483)
cis-10,11-Dihydroxy-10,11-dihydrocarbamazepine	525.109(153.075)	959.717(3818.829)	547.058(164.975)	1094.893(4391.718)
Citrulline	19901.677(6196.281)	21504.169(6882.343)	20450.559(6314.125)	22463.956(7168.386)
Codeine-6-.beta.-D-glucuronide	774.993(5522.859)	232.532(91.583)	1020.604(6604.132)	235.304(100.647)
Coniferylaldehyde	765.911(462.54)	787.668(824.323)	768.803(350.473)	835.32(940.869)
Cotinine N-.beta.-D-glucuronide	76.449(283.47)	46.197(159.887)	57.743(224.767)	31.424(55.891)
Creatine	217981.51(118303.317)	203650.285(97913.88)	239445.001(122895.866)	224296.739(95276.546)
Creatinine	1006729.671(287698.034)	1029213.304(254200.686)	968014.1(297487.798)	1005188.696(241774.03)
Cyclo(Leu-Pro)	2228.564(1706.261)	2027.347(1104.514)	2361.372(1874.821)	2002.407(1032.619)
D-.alpha.-Cyclohexylglycine	6326.782(6206.867)	8327.262(8211.34)	6963.999(6970.157)	8208.176(8697.467)
Decanoyl-L-carnitine	42146.5(48589.406)	42071.952(30458.853)	41378.73(53905.48)	44599.02(33313.09)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
D-erythro-Sphingosine-1-phosphate	7295.174(3378.972)	7543.128(3687.008)	7215.842(3142.458)	8064.372(3531.397)
Dexpanthenol	1546.048(2341.347)	2108.653(3911.294)	1339.362(633.825)	2386.132(4460.192)
D-Fructose	34526.336(8214.427)	34866.41(9180.115)	35258.4(7984.551)	35466.161(9360.386)
Diazepam	370.721(2360.704)	46.476(76.296)	354.102(2509.34)	48.869(87.424)
Dinor-12-oxophytodienoic acid	525.23(862.885)	416.42(194.711)	602.168(1019.314)	425.507(195.769)
Diphenhydramine	2585.349(6127.955)	3178.366(14715.458)	2336.057(3983.41)	3707.339(16925.362)
DL-Indole-3-lactic acid	37199.448(18913.594)	35604.136(12065.446)	37363.886(20753.868)	35327.001(12981.249)
D-Pyroglutamic acid	121612.569(22366.016)	123013.056(24064.978)	123418.191(24064.122)	125690.461(24817.147)
D-Turanose	525.908(351.452)	631.074(581.896)	520.138(265.379)	609.634(488.419)
Ergothioneine	767.24(1494.771)	719.663(431.749)	641.187(444.426)	742.568(450.052)
Esomeprazole	2660.51(10721.074)	1307.945(4540.326)	3400.906(12758.474)	1477.047(5219.404)
Ethiolat	11862.296(20760.107)	9779.989(18228.881)	11694.874(22626.1)	10043.125(20657.08)
Ethylidethanolamine	734.979(766.768)	727.196(595.857)	782.081(892.314)	784.328(667.115)
Ethylenediaminetetraacetic acid	663091.766(891136.229)	496339.244(788805.165)	707188.787(939588.255)	525798.856(819400.236)
Ezetimibe	223.611(238.157)	234.24(306.197)	237.685(276.619)	238.293(346.126)
Fexofenadine	450.355(238.197)	841.091(3125.726)	445.615(146.548)	979.139(3591.011)
Gabapentin	62080.105(201779.015)	5287.117(32734.04)	65249.893(197458.731)	1736.245(1006.505)
Glaucine	860.63(2849.169)	574.959(169.559)	1011.561(3402.675)	575.815(174.676)
Glutamic acid	7933.975(3124.287)	7180.498(3426.266)	7685.959(2912.252)	6790.446(2759.596)
Glutamine	101505.785(19190.477)	102907.791(20574.24)	103011.688(20506.373)	105238.609(21074.201)
Glycocholic acid	4874.144(5532.195)	3707.728(3340.534)	4835.094(5666.975)	3839.337(3220.547)
Glycodeoxycholic acid	16574.334(17400.385)	14780.84(19064.118)	15665.2(16876.362)	14124.624(16898.648)
Gly-Pro-Arg	586.043(2198.483)	428.808(1170.147)	394.694(2029.309)	440.56(1188.759)
Guanidine	5493.87(8781.142)	4475.798(4190.121)	6162.546(10314.276)	4770.688(4754.17)
Guanine	6226.314(23441.739)	279.003(1082.414)	8246.388(27387.081)	169.027(155.108)
Heptadecaphing-4-enine	5557.437(4651.009)	5538.189(4468.342)	5527.139(4907.465)	5161.482(4445.015)
Hexanoyl-L-carnitine	8996.499(13556.537)	8356.705(5002.169)	9402.717(15859.832)	8656.44(5504.128)
H-gamma-glutamyl-glutamine	2339.192(1792.988)	2006.339(1305.502)	2544.089(1995.762)	2084.667(1260.692)
Histidine	49555.943(23320.509)	53178.919(21745.875)	49244.588(24505.38)	54934.704(20736.674)
Homoarginine;	3381.815(2097.316)	3026.593(2160.863)	3437.227(2173.842)	3116.108(1905.262)
H-Pro-Hyp-OH	2228.15(1753.581)	1756.456(871.446)	2360.853(1986.558)	1739.039(885.645)
Hydroxybupropion	884.813(2016.341)	1883.832(8028.514)	966.47(2225.998)	1326.55(4137.981)
Hypoxanthine	31281.328(19491.261)	30486.398(22288.554)	31017.305(20197.579)	28804.254(15185.823)
Ile-Glu-Arg	365.728(1522.667)	320.225(998.515)	286.888(1615.263)	371.056(1124.937)
Indole-3-propionic acid	1220.413(1004.075)	1438.512(994.93)	1294.439(896.394)	1450.489(959.941)
Irbesartan	34111.466(330125.328)	1632.597(1008.364)	48237.142(394834.653)	1665.958(1152.085)
Isoleucine	15404.33(5244.539)	15607.18(5393.939)	14827.325(5014.375)	15178.898(5537.463)
Isopentenyladenine	1014642.651(399845.125)	1046922.522(370983.691)	1031908.219(421699.096)	1056127.36(345968.422)
Isopropylamine	4749.851(1414.044)	5211.39(1333.561)	4813.12(1502.012)	5179.224(1250.988)
Kynurenine	2125.376(754.54)	2313.805(749.317)	2055.529(729.308)	2285.971(712.949)
Lamotrigine;	2244.641(22565.331)	18.464(16.389)	3201.952(26989.449)	18.54(17.344)
Lansoprazole	736.475(4048.63)	2665.031(13708.313)	987.707(4814.561)	2829.094(14792.141)
Lauric acid diethanolamide	413.111(567.669)	345.335(216.443)	448.33(666.531)	327.439(204.242)
Lauroyl-L-carnitine	5784.303(4911.391)	6763.368(3908.375)	5731.635(5283.284)	6696.194(3998.479)
L-Carnitine	16079.975(4595.436)	15890.768(4307.224)	15793.384(4678.999)	15559.285(4194.778)
L-Citrulline	20161.291(5985.134)	21758.529(6402.073)	20674.288(6096.622)	22617.585(6585.22)
L-Cysteine-glutathione disulfide	1116.696(1162.972)	1224.484(1444.167)	1216.194(1224.408)	1353.062(1496.972)
L-Cystine	2137.312(1969.911)	2271.747(2210.344)	2310.258(1847.501)	2449.457(2214.124)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
Levocetirizine;	9007.024(38087.67)	5404.405(22513.101)	9755.004(42513.045)	6447.278(25353.913)
Linoleoylcarnitine	6028.057(4694.504)	6937.757(5240.418)	5890.895(4970.782)	7324.182(4782.704)
L-Leucine, methyl ester	936.172(1279.128)	734.385(675.979)	844.02(959.174)	727.712(723.551)
Losartan	1124.145(6579.061)	2289.546(19221.441)	255.822(125.143)	2942.867(22113.406)
L-Threonine	6399.383(2197.795)	6434.59(1928.87)	6569.693(2432.17)	6582.749(1953.44)
L-Tyrosine	3214.55(1382.508)	3345.219(1261.579)	3191.419(1464.291)	3283.667(1355.218)
Lysine	24048.561(14481.217)	23142.646(14133.037)	26085.381(16010.536)	24289.949(13450.24)
Matrine	2325.219(12579.91)	500.431(207.181)	3144.599(15002.584)	513.737(206.412)
Mefenorex	622.656(716.718)	3807.946(26441.59)	634.16(803.491)	668.885(826.358)
Meloxicam	28306.258(195269.072)	12851.881(121675.611)	17836.666(151075.883)	17003.109(139981.187)
Meprobamate	1573.996(3579.443)	932.297(1488.818)	1271.328(2301.477)	921.028(1674.405)
Metformin	7135.099(48045.124)	3475.203(23828.338)	9863.786(57367.973)	4323.549(27408.303)
Methacholine cation	56501.078(33409.327)	67485.057(42836.21)	59647.284(34908.691)	64433.74(23560.197)
Methionine	6161.544(1634.068)	6223.87(1770.355)	6036.444(1672.884)	6246.537(1851.937)
Methioninesulfoxide	753.827(372.4)	693.081(379.811)	768.805(401.695)	731.508(415.592)
Methylgallate	139.383(458.151)	67.958(251.269)	159.529(526.421)	72.307(280.953)
Metoprolol	897.413(4862.805)	234.563(653.184)	1006.345(5713.033)	260.193(750.546)
Metoprolol acid	7786.566(33910.371)	535.074(2767.371)	5313.31(28575.468)	635.6(3182.653)
Milnacipran	276.882(1331.735)	148.067(53.863)	339.641(1591.763)	151.333(53.12)
Modafinil	1075.48(6709.26)	71.168(24.162)	856.222(5843.393)	70.136(24.567)
Modafinil acid	131.611(721.079)	24.78(13.35)	89.453(410.063)	23.701(13.311)
Montelukast-1,2-diol	75.941(301.129)	84.645(479.266)	68.948(274.135)	98.954(550.468)
Moxonidine	3500.133(2726.862)	3040.75(1987.891)	3494.77(2782.516)	3129.874(1890.894)
N-(3-(Aminomethyl)benzyl)acetamidine	20921.024(28034.826)	18034.449(15522.733)	21426.169(26692.226)	18342.407(16707.634)
N-.alpha.-Acetyl-L-arginine	3082.187(1181.981)	3213.461(1045.445)	3045.215(1184.893)	3232.865(1091.37)
N.alpha.-Methyl-L-lysine	29306.073(114182.748)	13134.602(36620.029)	27616.816(101350.581)	9580.597(6849.304)
N.epsilon.-Acetyl-L-lysine	2453.841(2107.986)	2280.92(1269.094)	2602.365(2447.778)	2358.717(1430.008)
N.epsilon.-Methyl-L-lysine	8975.039(6927.428)	8793.019(6711.352)	9268.888(7015.526)	9284.578(7186.447)
N8-Acetylspermidine	3001.558(1211.178)	2900.086(896.957)	2881.329(1046.705)	2851.314(833.99)
N-Acetylaniline	707.391(950.515)	582.675(496.092)	792.246(1091.701)	619.1(511.521)
N-Acetyl-D-norleucine	3757.634(3749.095)	3860.092(3382.148)	4143.693(3978.725)	4142.792(3707.786)
N-Acetylhistidine	1008.892(648.298)	1039.722(610.487)	1029.937(698.38)	1051.991(674.644)
N-Acetyl-L-carnosine	2954.051(1639.621)	2926.55(1628.741)	2355.911(950.184)	2451.763(1167.01)
Naproxen	3476.065(13446.579)	4450.949(22153.769)	2032.557(7784.078)	5543.465(25430.423)
NEPSILON,NEPSILON,NEPSILON-TRIMETHYLLYSINE	13358.236(4821.32)	15219.514(11953.152)	12581.416(4428.925)	13549.071(6450.745)
N-Methylhistidine	35730.75(37645.645)	33537.29(29498.297)	30230.148(33903.282)	32150.208(28181.793)
N-Methylproline	11656.687(9296.226)	11510.001(9904.91)	11753.456(9333.458)	11857.717(10588.637)
Norleucine	15444.661(6060.568)	15678.34(4128.345)	14637.073(4788.935)	15362.688(4038.533)
Nudifloramide	64111.911(56284.553)	63703.328(37012.76)	58887.733(33435.743)	63376.868(34799.728)
Octanoylcarnitine	46353.596(55972.637)	47100.775(29066.033)	47144.841(64211.055)	49577.747(31693.746)
Oleoyl-L-carnitine	10823.414(8463.672)	11676.244(8434.192)	10729.659(8590.403)	12310.139(8440.117)
Omeprazole sulfone	4929.053(23929.418)	1843.877(13957.834)	6301.035(28062.735)	2096.193(15907.146)
Omeprazole sulfone N-oxide	1165.746(5101.882)	421.937(2441.309)	1400.94(5908.665)	450.787(2744.995)
Ondansetron	365.61(1271.909)	240.115(62.33)	430.734(1519.455)	243.04(68.123)
Ornithine	3959.933(2287.816)	4022.624(2665.327)	4128.265(2438.596)	4207.488(2640.386)
p-Acetamidophenyl .beta.-D-glucuronide	766.028(3177.057)	171.088(73.211)	854.182(3679.025)	171.801(71.797)
Palmitamide	3270.611(17777.123)	1962.253(8761.313)	4316.593(21213.234)	2315.319(10069.12)
Pantoprazole	898.088(8152.763)	16270.845(118825.791)	1249.917(9750.392)	15650.814(128427.894)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
Pantothenic acid	10030.786(7968.504)	8465.694(5284.919)	10126.233(8359.344)	8677.218(5145.136)
Penciclovir	615.263(2184.586)	280.151(80.439)	747.499(2600.119)	284.949(82.361)
Phenylacetylglutamine	31218.152(22442.043)	34681.21(38768.962)	32853.447(24164.403)	36131.129(43000.834)
Phenylacetyl-L-glutamine	14884.784(10785.176)	16607.075(17719.928)	15603.194(11631.592)	17446.503(19744.39)
Phenylalanine	55973.85(16422.42)	58120.533(13302.726)	54542.869(15990.617)	58589.269(14424.404)
Pipecolic acid	425.09(586.911)	426.157(508.716)	422.322(411.915)	466.253(576.586)
Piperine	5718.294(8337.056)	7720.583(10963.746)	5437.646(7527.174)	6841.21(7360.472)
Prazepam	288.862(1542.242)	137.608(93.414)	357.083(1843.726)	135.971(95.239)
Proline	14486.098(6367.337)	14482.522(5997.29)	14411.268(7109.856)	13721.924(5754.6)
Propionylcarnitine	68344.79(23209.488)	71041.55(26326.498)	65475.827(22787.033)	65045.673(20218.858)
Pyrantel	372.256(111.716)	1129.226(7044.272)	384.923(119.14)	1372.434(8103.556)
Pyridoxal	1642.179(3991.664)	946.29(438.171)	1926.346(4738.724)	966.128(487.166)
Pyridoxine;	1022.88(4388.483)	435.057(382.972)	1291.631(5232.132)	402.065(337.933)
Quetiapine	369.86(1339.4)	222.872(66.167)	255.71(234.5)	224.248(71.778)
Quetiapine sulfoxide	650.477(4802.113)	136.563(42.808)	205.765(560.74)	136.638(46.732)
R-(-)-O-Desmethylvenlafaxine	592.445(3164.213)	410.727(1880.497)	790.269(3775.065)	263.649(936.258)
rac-4-Sulfoxypropranolol	202.948(514.821)	151.335(57.243)	162.535(82.087)	153.516(60.927)
Ranitidine	2507.731(13468.136)	205.008(53.061)	2017.312(11803.676)	206.538(53.841)
Ranitidine N-oxide	713.593(4219.564)	62.623(17.85)	390.958(1801.266)	62.105(18.285)
Ranitidine-S-oxide	213.634(515.841)	132.212(90.781)	145.129(175.128)	133.881(98.329)
Scopoletin	591.68(2509.742)	178.452(414.272)	688.798(2864.176)	192.277(467.346)
SDMA	9500.368(2703.971)	10370.308(2765.049)	9808.401(2760.319)	10599.213(2673.464)
Serotonin	18189.163(41222.489)	14668.474(23684.703)	14353.675(19998.499)	13363.044(17156.067)
Ser-Tyr-Lys	193.809(988.093)	91.613(175.965)	184.445(1115.822)	104.226(200.316)
Stachydrine	563959.448(691819.57)	612164.26(685817.817)	587518.508(706098.216)	653922.988(726897.281)
Sulfamethoxazole	41.919(48.984)	4622.278(43440.039)	41.835(43.623)	6101.074(49975.795)
Tapentadol-.beta.-D-glucuronide	221.214(1394.74)	127.85(761.689)	41.736(24.102)	147.58(875.506)
Tauroursodeoxycholic acid	2706.846(6111.732)	1545.619(2380.983)	2678.948(5486.303)	1274.586(1130.138)
Telmisartan	4699.894(41335.897)	3856.6(30518.071)	6481.819(49436.552)	4898.127(35109.147)
Temazepam	279.199(1061.022)	153.782(115.023)	342.847(1265.834)	146.924(65.02)
Testosterone	3622.17(4140.278)	4445.438(4912.789)	3663.498(4396.175)	4590.956(5246.58)
Theanine;	1819.454(2742.739)	1366.781(1424.619)	2138.05(3146.371)	1493.761(1527.77)
Theobromine	43840.022(50239.28)	50274.237(39008.573)	42746.307(46884.552)	53954.352(39621.193)
threo-Dihydrobupropion	959.671(1263.114)	899.034(1318.122)	970.564(1208.202)	898.166(1350.257)
Thr-Ile-Arg	334.018(1580.162)	174.397(391.703)	299.942(1746.529)	188.59(438.92)
Ticlopidine	228.217(1202.183)	52.712(180.862)	277.805(1397.262)	45.125(168.628)
Topiramate	883.512(3767.87)	360.884(470.487)	1085.88(4482.725)	366.228(537.766)
Toradol	356.538(2066.064)	150.603(104.488)	455.463(2469.352)	148.593(102.035)
trans-3'-Hydroxycotinine	2268.615(10601.908)	1686.299(5203.465)	1233.236(3119.976)	1359.612(4030.731)
Trazodone	2672.469(13819.619)	206.455(55.025)	3739.443(16447.77)	208.643(57.472)
Tri-2-ethylhexyl trimellitate	6954.814(58249.323)	2150.885(4550.116)	1221.862(1696.585)	2565.286(5161.634)
Trigonelline	62593.319(128404.523)	87574.388(113723.624)	66818.372(143147.881)	94052.01(122519.557)
Trileptal	378.242(124.735)	1737.665(13037.79)	392.867(128.704)	2189.462(14998.322)
Trimethoprim	234.855(71.982)	2512.23(21564.074)	240.288(76.487)	3245.027(24808.634)
Trimethylamine-N-oxide	22496.762(34083.237)	15784.326(13954.105)	25028.914(38657.129)	14414.784(10594.282)
Triptolide	572.071(359.723)	709.428(1341.517)	608.313(410.976)	757.077(1539.512)
Tryptophan	15719.222(4762.968)	15591.457(4927.165)	15508.626(4851.561)	15048.978(5005.799)
Tyrosine	6484.429(2346.848)	6649.41(2125.156)	6372.675(2355.791)	6620.619(2272.411)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
Urea	128763.489(48161.656)	135736.88(41188.088)	128773.302(50486.088)	132146.779(38578.177)
Urocanic acid;	20103.21(25401.881)	20113.659(16158.372)	21750.5(29758.063)	21866.059(18012.708)
Usnic acid	6421.074(38109.236)	5909.508(26905.817)	2771.907(1725.232)	6767.755(30846.452)
Complex Lipids (CL)				
AC (10:0)	14300.667(14495.722)	14592.903(12632.497)	14299.18(15986.705)	15304.621(13912.854)
AC (10:1)	7852.356(5661.808)	8700.584(5463.897)	7704.051(6028.18)	8895.645(5924.822)
AC (12:0)	6801.104(4854.843)	7472.708(4034.354)	6652.962(5029.517)	7433.406(3978.211)
AC (12:1)	5342.259(2975.805)	5782.079(2495.997)	5250.448(3005.47)	5779.664(2466.414)
AC (14:1)	7653.305(5643.002)	7865.258(4525.933)	7670.8(5957.272)	7876.844(4540.047)
AC (14:2)	4537.778(3261.62)	5105.633(2880.79)	4533.971(3556.58)	5111.986(2806.317)
AC (16:0)	10907.214(3516.947)	10958.197(3206.646)	10240.456(3053.947)	10630.098(2958.93)
AC (18:0)	4409.46(1523.433)	4658.607(1398.628)	4241.255(1498.351)	4527.743(1288.803)
AC (18:1)	15169.411(6563.264)	14716.482(4589.592)	14552.69(6291.98)	14539.384(4595.967)
AC (18:2)	9086.774(4258.756)	9507.785(3723.066)	8473.128(4008.707)	9215.757(3414.944)
AC (8:0)	5424.664(7636.621)	5324.659(5489.183)	5578.054(8810.926)	5661.698(6126.403)
CE (14:0)	483.105(328.13)	550.26(299.965)	517.754(354.457)	566.25(294.07)
CE (16:0)	6284.196(5322.107)	5971.764(4027.806)	6640.605(5705.632)	6052.502(3655.343)
CE (16:1)	44723.031(22333.233)	45240.669(19130.581)	46466.245(21911.29)	44961.974(18550.491)
CE (18:0)	3286.85(1793.581)	3220.682(1502.875)	3248.724(1768.19)	3255.714(1566.484)
CE (18:1)	32176.362(13035.556)	33019.476(10977.599)	33329.958(13182.182)	33803.223(10306.817)
CE (18:2)	360370.43(102450.354)	395504.729(97524.484)	365905.916(104757.775)	408420.872(96560.058)
CE (18:3)	13226.28(5296.356)	16158.621(6188.509)	13538.692(5308.083)	16026.716(5476.892)
CE (20:2)	7353.518(4456.574)	8560.232(3729.559)	7480.067(4723.572)	8876.919(3620.926)
CE (20:3)	65342.381(23690.393)	72249.761(24364.326)	66916.365(23589.777)	74083.382(23946.671)
CE (20:4)	760763.777(278873.716)	769431.808(251914.063)	774727.643(270809.091)	762789.124(215866.426)
CE (20:5)	17407.549(19917.453)	12423.777(8256.741)	19104.609(22573.844)	12828.237(8956.276)
CE (22:2)	686.936(506.637)	714.698(520.067)	676.49(502.562)	745.29(543.744)
CE (22:6)	132582.468(60465.938)	114384.853(39714.847)	139199.071(65068.192)	118510.435(39055.205)
Ceramide (d34:1) - ESI(+)	7991.308(2279.1)	7701.808(1766.753)	7687.199(2250.215)	7834.529(1868.036)
Ceramide (d36:1) - ESI(+)	5055.887(1639.5)	4781.199(1246.336)	4945.072(1449.706)	4913.929(1227.46)
Ceramide (d38:1) - ESI(+)	6696.998(1780.221)	6981.944(1458.36)	6664.704(1627.166)	7112.106(1389.354)
Ceramide (d40:1)	21686.844(5740.739)	23489.285(4735.334)	21422.451(5095.414)	23401.997(4615.503)
Ceramide (d41:1) - ESI (+)	6918.214(1876.08)	7517.217(1659.079)	6992.447(1758.751)	7645.828(1704.017)
Ceramide (d42:1) - ESI (+)	71508.239(18019.881)	78197.952(14457.978)	70141.421(16527.622)	77355.897(13980.101)
Ceramide (d42:2) A - ESI (+)	19273.129(4975.246)	18114.439(3325.542)	18658.838(4645.216)	18167.611(3294.727)
Ceramide (d42:2) B - ESI (+)	14981.161(4149.123)	17174.124(4245.274)	15071.338(4164.235)	17288.064(4089.868)
Ceramide (d32:1)	3595.683(1323.517)	3755.63(977.806)	3473.329(1135.936)	3749.235(876.773)
Ceramide (d33:1)	2916.634(935.773)	3016.705(807.728)	2905.891(954.228)	3011.126(830.753)
Ceramide (d34:0)	4886.997(2053.157)	4687(1716.579)	4705.485(1904.271)	4578.351(1702.528)
Ceramide (d34:1) - ESI(-)	18074.154(4880.408)	17694.653(3936.635)	16797.099(3886.53)	17358.862(3879.255)
Ceramide (d34:2)	3094.181(847.888)	3030.248(713.119)	3059.406(823.881)	3103.748(732.199)
Ceramide (d36:1) - ESI(-)	1637.345(721.82)	1539.002(608.946)	1547.936(631.269)	1516.191(611.004)
Ceramide (d38:1) - ESI(-)	11993.384(4407.452)	12156.053(3738.061)	11661.638(4066.525)	12037.971(3600.075)
Ceramide (d39:1)	6299.483(2739.989)	6979.275(2440.541)	6280.654(2642.502)	6928.753(2492.845)
Ceramide (d40:0)	1765.181(1227.484)	1564.678(901.085)	1775.733(1264.199)	1479.739(772.332)
Ceramide (d40:2)	6057.125(4179.286)	6235.898(4315.18)	5995.39(4515.358)	6101.231(4353.501)
Ceramide (d41:1) - ESI(-)	42041.811(15059.383)	46380.145(13427.707)	41060.244(14002.301)	45628.819(13367.535)
Ceramide (d42:0)	11948.609(7113.944)	11294.104(4976.297)	11987.369(7448.888)	10658.27(4389.341)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
Ceramide (d42:1) - ESI(-)	136674.648(44023.767)	149770.415(39576.94)	131275.247(38296.961)	146093.73(38714.63)
Ceramide (d42:2) A - ESI(-)	49252.166(17827.101)	47220.491(13180.04)	45881.62(14014.478)	45775.601(12303.101)
Ceramide (d42:2) B - ESI(-)	37317.754(16468.604)	35789.863(11255.565)	34603.652(14003.87)	34888.751(10464.998)
Ceramide (d43:1)	2528.23(1370.14)	2789.752(1196.521)	2524.053(1366.934)	2658.272(1055.678)
Ceramide (d44:1)	846.904(541.153)	822.512(399.283)	766.114(383.948)	766.223(335.297)
Cholesterol	266952.992(63543.111)	283483.733(67507.559)	259126.592(62668.048)	282785.483(70992.096)
DG (32:0)	2029.32(748.253)	1982.392(914.732)	1876.907(663.523)	1834.096(743.093)
DG (32:1)	5251.897(3457.449)	4947.61(2880.584)	4839.272(3261.309)	4417.438(2663.105)
DG (34:1)	1041.038(494.395)	999.382(487.017)	957.669(477.567)	926.246(447.834)
DG (34:2)	32528.392(13807.47)	30539.842(13070.979)	29395.286(12112.58)	28013.19(12155.434)
DG (34:3)	5185.782(3045.124)	4572.847(2077.17)	4934.302(2970.925)	4487.862(2240.726)
DG (36:1)	6350.769(3167.505)	6121.406(3281.803)	5774.621(2635.876)	5434.807(2715.326)
DG (36:2)	55205.662(20357.43)	49677.788(17704.742)	52703.881(20071.649)	46096.408(15020.654)
DG (36:3)	70925.903(27194.121)	65340.022(22354.965)	66885.539(26880.219)	62128.554(20637.751)
DG (36:4) A	16838.454(8807.583)	16004.561(7408.839)	15646.998(8185.164)	15562.018(6792.317)
DG (36:4) B	4169.876(3637.695)	3516.148(2613.304)	3898.521(3366.237)	3094.96(2394.278)
DG (36:5)	2206.156(1211.632)	2086.253(902.788)	2013.999(1107.932)	2061.556(899.951)
DG (38:5)	10566.304(4064.74)	10089.518(3680.913)	9992.912(3910.752)	9028.535(2964.831)
DG (38:6)	6169.284(3104.712)	5407.065(2535.955)	5872.225(2936.044)	4956.003(2363.195)
FA (10:0) (capric acid)	1604.441(1050.232)	1407.005(1073.102)	1560.414(987.235)	1389.12(1089.533)
FA (12:0) (lauric acid)	8080.776(5386.504)	8269.26(5625.99)	7817.814(5729.118)	8256.763(6226.421)
FA (14:0) (myristic acid)	46315.443(13985.33)	46285.78(10922.906)	47112.249(14211.236)	46853.296(11340.191)
FA (14:1) (physeteric acid)	5158.99(3232.701)	4681.581(1944.979)	5675.279(3405.73)	4939.859(1863.019)
FA (15:0) (pentadecylic acid)	10544.8(2976.688)	10266.457(2239.062)	10445.753(2875.65)	10166.415(2277.093)
FA (16:1) (palmitoleic acid)	87362.569(45359.632)	76933.028(35142.058)	94190.824(42663.898)	81229.717(35498.966)
FA (17:0) (margaric acid)	22117.789(4474.162)	21235.84(3887.35)	21808.81(4648.64)	21042.005(4049.927)
FA (18:1) (oleic acid)	1454192.087(480456.365)	1349284.059(394857.372)	1514940.428(454631.23)	1371889.761(394848.646)
FA (18:2) (linoleic acid)	573453.977(197151.585)	559405.212(162215.142)	585206.405(180559.916)	569154.315(153284.183)
FA (18:3) (linolenic acid)	52408.007(25261.774)	49568.813(16119.839)	51000.998(19313.505)	51302.963(15495.082)
FA (20:1) (eicosenoic acid)	18300.811(5932.05)	17239.139(4691.897)	18874.442(6071.433)	17346.67(4535.503)
FA (20:2) (eicosadienoic acid)	9414.386(2783.824)	9398.564(2656.075)	9649.009(2661.535)	9583.691(2575.188)
FA (20:3) (eicosatrienoic acid)	2064.852(782.798)	2106.53(696.017)	2092.753(748.261)	2033.302(662.201)
FA (20:3) (homo-gamma-linolenic acid)	9019.322(2564.168)	9232.52(2388.112)	9003.087(2432.207)	9053.404(2381.869)
FA (20:4) (arachidonic acid)	43084.156(11307.632)	45485.009(12124.954)	41194.285(10661.025)	43026.798(9467.557)
FA (20:5) (eicosapentaenoic acid)	7210.305(8172.735)	5310.154(4416.295)	6853.569(8590.614)	5238.719(4843.886)
FA (22:0) (behenic acid)	4796.588(1883.561)	4776.335(2235.782)	4558.918(1650.069)	4565.138(1731.25)
FA (22:6) (docosahexaenoic acid)	35785.158(23581.553)	31506.346(14537.092)	36424.522(25779.108)	31812.444(15865.045)
FA (24:0) (lignoceric acid)	9002.74(3316.901)	9144.823(3857.725)	8443.659(2750.451)	8653.491(3064.249)
FA (24:1) (nervonic acid)	3404.095(1062.601)	3216.118(871.277)	3222.997(823.848)	3107.598(848.043)
Gal-Gal-Cer (d18:1/16:0)/Lactosylceramide (d18:1/16:0)	37250.999(11809.088)	37236.749(10987.775)	36441.158(12453.56)	37090.618(11161.394)
GlcCer (d38:1)	3730.008(1287.974)	3948.513(1065.45)	3672.435(1216.352)	3940.785(1040.384)
GlcCer (d40:1) - ESI(-)	22073.89(7846.193)	22731.523(6665.458)	21197.084(7708.24)	22296.642(6309.151)
GlcCer (d41:1)	12088.153(4455.943)	12743.895(4333.197)	11654.937(4140.417)	12390.181(3955.261)
GlcCer (d42:1) - ESI(-)	25575.096(9070.161)	26263.818(7929.532)	24105.616(8565.355)	25349.459(6949.024)
GlcCer (d42:2) - ESI(-)	19888.456(7749.181)	17973.465(6288.748)	18678.346(6996.248)	17368.677(5282.948)
GlcCer (d14:1(4E)/20:0(2OH))	6302.067(3492.07)	6460.128(3125.454)	6498.705(3668.466)	6436.079(3158.302)
GlcCer (d34:1)	7468.445(3751.415)	8251.003(4419.557)	6935.992(3609.829)	8118.449(4638.314)
GlcCer (d40:1) - ESI(+)	4100.143(1480.243)	4234.688(1219.049)	4066.633(1476.06)	4231.376(1212.092)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
GlcCer (d42:1) - ESI(+)	17983.989(6028.82)	18240.869(5395.163)	17508.557(6212.084)	17779.495(4934.506)
GlcCer (d42:2) - ESI(+)	13729.159(5608.295)	12051.673(4176.986)	13382.165(5620)	12032.955(3833.784)
Lactosylceramide (d18:1/24:1(15Z))	2755.733(1184.633)	2537.724(815.608)	2706.015(1061.845)	2538.341(810.176)
LPC (14:0) - ESI(-)	1816.114(1007.334)	2045.03(925.463)	1806.548(974.751)	1983.11(915.949)
LPC (16:0) - ESI(-)	224092.722(72172.597)	240419.333(71704.173)	210628.888(62974.918)	229102.383(66473.46)
LPC (16:1) - ESI(-)	3256.883(1286.541)	3465.425(1194.712)	3230.526(1270.007)	3355.22(1189.375)
LPC (17:1)	2907.335(879.847)	2996.073(1096.874)	2853.821(865.494)	2872.984(1044.8)
LPC (18:0) A - ESI(-)	7418.389(3009.415)	8077.783(2590.056)	7053.492(2810.519)	7812.018(2599.199)
LPC (18:0) B - ESI(-)	99494.905(36134.374)	108242.985(32910.725)	94247.037(33404.908)	104492.539(33092.3)
LPC (18:1) - ESI(-)	47798.748(19375.801)	51591.653(19211.667)	45171.37(18891.253)	49476.855(18392.004)
LPC (18:2) - ESI(-)	60906.166(28020.858)	71522.652(31446.609)	55570.296(24563.184)	70307.404(30731.739)
LPC (20:0)	2602.173(1120.102)	2667.429(891.909)	2537.269(1076.668)	2657.007(901.485)
LPC (20:1) - ESI(-)	3013.633(1298.505)	2917.096(1050.301)	2949.314(1165.903)	2882.011(1092.87)
LPC (20:1) - ESI(+)	713.456(419.647)	654.494(268.413)	667.442(370.369)	640.514(265.426)
LPC (20:2) - ESI(-)	4059.133(1281.292)	4450.809(1469.606)	3913.556(1120.135)	4415.508(1530.112)
LPC (20:2) - ESI(+)	518.937(285.076)	598.846(314.265)	489.388(255.973)	591.929(320.009)
LPC (20:3) - ESI(-)	3582.326(1705.034)	4021.253(1564.565)	3377.067(1587.043)	3778.861(1520.097)
LPC (22:4)	1706.729(976.366)	1894.898(1004.387)	1482.79(851.308)	1675.62(753.05)
LPC (22:5) - ESI(-)	675.167(447.702)	664.823(383.062)	588.229(365.946)	625.645(378.889)
LPC (22:6)	18296.637(8748.95)	17120.89(7390.865)	17892.205(8795.155)	17059.345(7938.417)
LPC (o-16:0)	7726.959(3135.329)	8366.675(3289.673)	6972.434(2368.186)	8002.555(3166.715)
LPC (p-16:0)/LPC (o-16:1)	10752.235(4110.82)	11778.247(4172.532)	9871.584(3425.003)	11229.396(3803.267)
LPC (p-18:0)/LPC (o-18:1)	5609.615(1996.592)	5649.593(2083.157)	5320.569(1820.383)	5448.102(2139.783)
LPC (14:0) - ESI(+)	12225.274(5163.537)	14568.798(5062.405)	12327.159(4956.072)	14298.088(5037.991)
LPC (15:0)	12084.127(4819.914)	12943.535(4361.419)	11797.995(4420.944)	12914.474(4391.999)
LPC (16:0) - ESI(+)	1926106.937(412946.468)	2025455.264(509547.986)	1845303.056(386878.744)	1953940.844(488040.87)
LPC (16:1) - ESI(+)	18357.864(6537.325)	19256.04(6089.078)	18102.21(5252.964)	19005.283(6187.711)
LPC (18:0) - ESI(+)	597884.618(199525.827)	642665.246(221367.761)	575304.178(190861.694)	627007.336(232772.768)
LPC (18:1) - ESI(+)	267553.679(104625.2)	280752.212(113394.873)	250815.703(90364.26)	265656.896(100100.885)
LPC (18:2) - ESI(+)	453109.903(200728.084)	547483.468(267853.354)	411754.083(175401.553)	530079.324(250479.673)
LPC (18:3)	3781.745(1556.029)	4762.878(2448.244)	3586.936(1415.53)	4529.316(1778.483)
LPC (20:3) - ESI(+)	18658.988(7504.447)	20830.978(7040.033)	17363.957(6484.747)	19646.263(5900.561)
LPC (20:4)	92588.56(39171.901)	99801.287(39143.693)	83115.248(29224.178)	91499.708(29535.203)
LPC (20:5)	8554.056(10259.538)	6693.724(5097.151)	8602.432(11112.606)	6635.493(5583.273)
LPC (22:5) - ESI(+)	4133.499(2034.537)	4006.158(1626.825)	3743.911(1786.148)	3766.871(1528.189)
LPE (16:0)	3007.892(1492.945)	3345.916(1755.537)	2828.742(1357.831)	3246.499(1691.23)
LPE (18:2) - ESI(-)	4521.977(2417.216)	5517.915(3099.215)	4201.716(2091.519)	5649.956(3201.503)
LPE (20:4) - ESI(-)	3411.332(1579.491)	3835.167(1358.006)	3242.724(1471.892)	3781.322(1408.073)
LPE (22:6)	2511.314(1103.103)	2584.869(1142.272)	2513.448(1167.059)	2639.765(1167.794)
LPE (18:0)	2976.4(935.468)	3330.697(987.882)	2976.72(914.575)	3291.538(1032.858)
LPE (18:2) - ESI(+)	3940.782(1604.285)	4738.299(2407.019)	3705.225(1546.128)	4828.722(2527.474)
LPE (20:4) - ESI(+)	3205.181(1241.82)	3617.274(1320.76)	3131.703(1232.432)	3563.497(1232.696)
PC (16:0/9:0(CHO))	4327.064(2722.879)	4282.307(2603.353)	4063.458(2415.238)	4088.188(2455.075)
PC (32:0) - ESI(-)	14490.961(3964.7)	14558.291(3478.332)	14173.518(3865.137)	14514.44(3524.546)
PC (32:1) - ESI(-)	14447.376(7522.552)	14662.134(6394.392)	15141.45(7626.112)	14641.654(6148.462)
PC (32:2) - ESI(-)	13463.361(6508.264)	16204.369(5624.383)	14050.917(5985.079)	16666.589(5393.249)
PC (33:1) - ESI(-)	2353.684(1083.204)	2374.083(853.644)	2445.074(1104.637)	2361.716(832.373)
PC (33:2) - ESI(-)	3860.198(1605.855)	4336.55(1397.757)	4062.384(1595.616)	4497.506(1396.348)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
PC (34:0) - ESI(-)	8251.523(2184.754)	8469.609(1811.655)	8053.581(2009.851)	8465.187(1814.817)
PC (34:2) - ESI(-)	240630.097(60351.691)	258867.547(56457.148)	237975.775(58150.543)	260900.337(57213.603)
PC (34:3)	16244.273(6359.067)	18088.554(6094.852)	16619.89(6500.646)	18691.548(6145.103)
PC (34:4) - ESI(-)	3988.556(2296.794)	4598.624(1731.583)	4259(2366.311)	4641.965(1743.509)
PC (35:1) - ESI(-)	3093.959(1098.086)	3051.722(977.026)	3114.587(1111.442)	2990.347(962.299)
PC (35:2)	9207.837(2691.891)	9716.991(2633.897)	9074.375(2713.072)	9977.682(2615.637)
PC (35:4) - ESI(-)	2567.664(1136.268)	2622.666(936.586)	2598.481(1176.03)	2585.304(775.291)
PC (36:1) - ESI(-)	60700.134(17787.723)	61602.252(15986.223)	60443.364(17987.433)	61466.942(16301.303)
PC (36:3) A - ESI(-)	78001.315(26248.654)	80601.946(20165.252)	76566.024(25173.844)	80141.523(19892.495)
PC (36:3) B - ESI(-)	80122.729(25240.712)	84455.963(19138.885)	79575.825(24715.727)	83766.047(19227.98)
PC (36:4) A - ESI(-)	50001.555(19418.961)	58881.412(19057.435)	49070.262(18583.73)	60741.165(19396.955)
PC (36:4) B - ESI(-)	165608.498(45603.524)	172562.505(36378.869)	161991.938(43674.505)	170395.971(35833.334)
PC (36:5) A	2138.31(1339.816)	2567.216(1605.787)	2117.074(1258.51)	2799.54(1649.863)
PC (36:5) B	41857.83(35378.719)	33407.87(22725.882)	39725.734(31438.644)	33188.832(24114.183)
PC (37:2) - ESI(-)	1427.867(571.478)	1549.892(656.208)	1435.635(578.748)	1615.775(681.224)
PC (37:3)	19429.669(8642.077)	20766.774(7555.42)	19976.601(8593.197)	21666.748(7553.164)
PC (37:4) - ESI(-)	3610.43(1262.482)	3600.739(1164.94)	3505.437(1289.633)	3567.025(1181.887)
PC (38:2)	4724.469(1540.569)	4816.371(1178.537)	4783.461(1545.779)	4933.012(1212.134)
PC (38:3) - ESI(-)	29648.655(10260.002)	31432.948(7745.999)	29658.427(10093.354)	30947.485(7542.327)
PC (38:4) A - ESI(-)	57986.619(17566.019)	60883.346(16516.825)	57004.694(17456.97)	60297.426(17078.597)
PC (38:5) A - ESI(-)	19182.481(6029.043)	19166.914(4819.422)	18676.833(5687.059)	18966.356(4798.877)
PC (38:5) B - ESI(-)	12329.808(8869.88)	10448.295(4369.029)	12064.361(8160.002)	10504.881(4619.341)
PC (38:6) - ESI(-)	75564.438(34561.384)	68827.018(26086.774)	75541.752(33241.58)	68594.619(26922.203)
PC (39:6)	18191.534(9715.309)	16532.441(6454.175)	20136.065(10343.655)	17559.66(6586.754)
PC (40:4) - ESI(-)	3651.767(1838.864)	3888.447(1301.818)	3545.995(1888.218)	3778.623(1260.441)
PC (40:5) A - ESI(-)	4364.652(1888.948)	4187.943(1433.041)	4197.852(1807.296)	4159.711(1422.71)
PC (40:5) B - ESI(-)	1949.867(1019.491)	2160.184(912.295)	1965.854(1071.325)	2061.666(780.046)
PC (40:6) B	20657.541(8269.246)	18554.405(6543.511)	20500.278(7688.845)	18505.132(6694.103)
PC (40:7) - ESI(-)	2669.718(1393.762)	2433.114(925.635)	2687.754(1387.038)	2469.947(915.054)
PC (40:8) - ESI(-)	2630.788(1139.643)	2734.932(900.85)	2529.097(1022.741)	2689.323(903.241)
PC (42:5)	3139.766(1127.172)	3024.694(1140.962)	3350.413(1008.909)	3183.849(1178.252)
PC (42:6)	2237.693(1216.735)	2297.879(1311.502)	2395.646(1254.694)	2328.609(1331.271)
PC (o-32:0) - ESI(-)	2806.219(868.036)	2847.252(794.141)	2704.901(854.074)	2839.836(808.911)
PC (p-32:0)/PC (o-32:1) - ESI(-)	2338.644(927.886)	2365.854(804.708)	2198.427(840.691)	2327.428(708.201)
PC (p-32:0)/PC (o-32:1) - ESI(+)	29152.037(7872.188)	30771.998(7341.47)	28791.902(7290.532)	31452.394(7114.976)
PC (p-34:1)/PC (o-34:2) A	4520.84(2258.236)	5300.943(2014.065)	4423.379(2326.169)	5437.238(2111.38)
PC (p-34:1)/PC (o-34:2) B	2874.162(1241.363)	2975.868(1271.407)	2840.858(1220.775)	3051.915(1202.753)
PC (p-34:2)/PC (o-34:3) - ESI(-)	13080.94(4655.151)	15147.291(4618.811)	12892.841(4865.648)	15380.58(4804.902)
PC (p-36:1)/PC (o-36:2)	1579.393(1039.658)	1842.803(957.813)	1526.708(1086.379)	1895.22(1014.876)
PC (p-36:3)/PC (o-36:4) - ESI(-)	21432.678(7961.51)	23318.595(6892.306)	20094.728(7800.44)	22439.049(5928.081)
PC (p-36:3)/PC (o-36:4) - ESI(+)	227889.598(84207.01)	254677.838(68833.936)	218750.994(79336.03)	250260.239(66263.843)
PC (p-36:4)/PC (o-36:5) - ESI(-)	12136.93(5243.46)	13380.29(4590.962)	11209.419(4598.339)	12873.218(4180.114)
PC (p-38:3)/PC (o-38:4) - ESI(-)	7180.199(2581.694)	8011.26(2278.842)	6875.31(2520.292)	7818.047(2159.075)
PC (p-38:4)/PC (o-38:5) A	16408.903(5205.505)	17597.828(4431.343)	15828.761(5468.838)	17257.046(4153.423)
PC (p-38:4)/PC (o-38:5) B	2559.33(1097.47)	2769.763(1152.827)	2456.79(1084.768)	2618.333(1025.333)
PC (p-38:5)/PC (o-38:6)	1297.362(880.416)	1291.415(783.351)	1279.173(752.065)	1286.904(829.333)
PC (p-40:1)/PC (o-40:2)	1485.155(608.109)	1292.088(473.435)	1494.473(632.47)	1309.365(478.286)
PC (p-40:3)/PC (o-40:4)	1750.816(685.913)	1868.47(638.755)	1709.895(678.64)	1814.465(639.48)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
PC (p-40:4)/PC (o-40:5) - ESI(-)	1855.515(641.097)	1784.499(529.196)	1816.722(663.909)	1767.847(538.828)
PC (p-40:7)/PC (o-40:8)	12784.77(9315.863)	11294.973(6789.332)	14104.589(8777.856)	12457.324(6433.103)
PC (p-42:3)/PC (o-42:4)	4785.842(1784.509)	5178.399(1630.148)	4717.303(1763.415)	5127.617(1512.806)
PC (p-42:4)/PC (o-42:5) - ESI(-)	2268.307(909.076)	2270.498(870.57)	2194.447(934.078)	2241.394(850.209)
PC (p-42:5)/PC (o-42:6)	618.687(355.575)	610.366(274.685)	607.345(377.235)	581.2(268.483)
PC (p-44:4)/PC (o-44:5) - ESI(-)	2845.694(1045.311)	2893.365(908.463)	2771.075(1020.627)	2855.548(932.176)
PC (p-44:5)/PC (o-44:6)	3310.494(1275.999)	3174.484(993.019)	3381.333(1340.399)	3219.029(969.884)
PC 34:4e	6443.081(2515.863)	7999.075(2933.128)	6516.076(2412.817)	8349.359(2908.212)
PC 38:7e	16964.282(13526.498)	15342.968(9446.371)	17136.82(13560.53)	15811.988(10420.609)
PC 40:5e	12165.024(3482.196)	12677.876(3009.874)	12168.625(3744.067)	12594.987(2717.054)
PC 40:6e	22316.948(7430.313)	21474.846(6189.986)	22072.534(7682.321)	21356.415(5856.757)
PC (28:0)	3246.565(4662.849)	3239.16(2348.658)	3627.569(5348.607)	3183.558(2184.545)
PC (30:0)	158777.616(83572.094)	179096.713(65617.314)	168743.529(90634.233)	178533.126(59846.758)
PC (31:0)	10922.351(4521.628)	11042.588(3052.892)	11579.689(4762.557)	11515.423(3114.079)
PC (31:1)	1677.788(1455.465)	1660.939(915.401)	1878.221(1600.447)	1764.88(950.338)
PC (32:0) - ESI(+)	256268.716(58170.605)	250135.791(53964.518)	257737.991(58248.811)	252341.298(49340.284)
PC (32:1) - ESI(+)	239846.485(124170.713)	249536.641(113064.066)	256265.278(131558.123)	254543.335(118029.568)
PC (32:2) - ESI(+)	56756.644(28246.729)	67703.831(25937.146)	61281.052(25930.591)	72298.473(25007.78)
PC (33:0)	10952.596(5641.864)	11592.978(3878.492)	11587.264(5855.338)	11988.418(3933.779)
PC (33:1) - ESI(+)	53543.632(20928.978)	53553.558(13337.174)	57061.868(21666.224)	55115.812(13475.168)
PC (33:2) - ESI(+)	78531.369(27527.116)	87270.676(25504.3)	83522.469(27977.154)	93784.229(23994.517)
PC (34:0) - ESI(+)	56673.124(14226.497)	56575.078(11243.201)	56978.355(13113.206)	57245.93(10988.946)
PC (34:1)	4013338.964(720952.007)	4067426.422(727466.087)	4097795.071(686391.117)	4072387.886(668154.082)
PC (34:2) - ESI(+)	8298954.78(1436737.757)	8880671.15(1333757.007)	8418099.742(1517545.767)	9131469.985(1282337.625)
PC (34:3) A	97711.278(31702.813)	106631.972(39043.209)	103128.289(28956.558)	112048.788(37578.688)
PC (34:3) B	108771.059(36242.03)	128990.918(46188.814)	116006.756(36977.04)	137512.831(45224.383)
PC (34:3) C	86598.612(39702.386)	108697.965(49708.994)	90974.287(44406.274)	112006.398(49285.341)
PC (34:4) - ESI(+)	17218.357(9083.701)	20014.966(7594.249)	18765.38(9434.486)	20817.07(7544.067)
PC (35:1) - ESI(+)	46139.315(13080.522)	45638.931(9232.36)	48062.7(13479.237)	46489.793(9024.083)
PC (35:2) A	109536.799(36351.893)	103212.896(30675.48)	115910.298(36351.794)	104178.68(32765.995)
PC (35:2) B	131176.614(32124.982)	137458.977(30973.043)	136153.641(31409.779)	144620.016(29535.737)
PC (35:3)	40372.126(10564.132)	44343.372(11336.707)	42224.005(10290.336)	46715.552(10847.772)
PC (35:4) - ESI(+)	22778.31(8961.192)	23974.006(6756.722)	24298.305(9278.648)	25055.909(6516.302)
PC (36:1) - ESI(+)	656088.196(185659.526)	660392.494(148989.452)	684314.568(191032.324)	670588.694(154080.891)
PC (36:2)	4529060.48(909760.507)	4996033.975(881985.183)	4659485.5(885858.543)	5202361.202(878003.988)
PC (36:3) A - ESI(+)	1277000.345(445850.9)	1366182.069(370360.325)	1306783.59(413360.001)	1413698.006(377268.745)
PC (36:3) B - ESI(+)	1639032.954(502617.113)	1716418.049(393778.108)	1656786.979(497457.461)	1754675.994(417736.798)
PC (36:4) A - ESI(+)	344228.244(141889.724)	433150.27(175314.159)	352156.763(135378.468)	460327.086(179157.48)
PC (36:4) B - ESI(+)	254789.338(417790.093)	206974.331(69274.833)	290186.954(490075.248)	211942.437(72849.794)
PC (36:4) C - ESI(+)	3945315.162(980469.466)	4037185.749(932394.375)	4017345.587(950229.435)	4041263.953(904180.707)
PC (36:5) C	63676.772(293144.05)	37777.207(75598.623)	75066.456(344291.891)	36454.358(71241.705)
PC (36:5) D	466335.725(583640.353)	328794.138(256617.495)	522920.29(662773.132)	349071.021(285083.822)
PC (36:5)A	10087.21(5302.765)	12082.737(6355.171)	10537.385(5204.716)	13178.345(6561.16)
PC (36:6)	7517.927(4687.721)	7514.303(3539.182)	8522.707(4868.049)	8177.996(3691.057)
PC (37:2) - ESI(+)	12948.098(3497.278)	14134.187(3647.086)	13382.403(3420.515)	14766.724(3764.208)
PC (37:4) - ESI(+)	51981.159(19322.358)	49132.105(16397.252)	55140.179(19721.563)	49171.954(15891.326)
PC (37:5)	36908.954(34432.55)	28967.669(14940.073)	40739.105(38835.732)	30400.788(16224.117)
PC (37:6)	9891.772(5465.158)	8696.041(4047.719)	11125.227(5788.227)	9452.384(4154.234)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
PC (38:3) - ESI(+)	545962.223(199887.214)	581406.422(170804.445)	563669.536(203120.777)	586858.299(174007.685)
PC (38:4) A - ESI(+)	129827.943(52570.47)	130649.431(33178.708)	136588.525(56450.574)	134821.392(33538.443)
PC (38:4) B - ESI(+)	138945.853(49865.612)	150899.97(43419.782)	139468.52(48409.776)	148559.57(42347.703)
PC (38:4) C - ESI(+)	2313829.998(565304.201)	2391882.015(574272.595)	2369459.874(544941.787)	2417067.78(566241.852)
PC (38:5) A	732724.247(176405.92)	721011.877(165292.616)	749250.346(174332.641)	726361.694(164347.65)
PC (38:5) B - ESI(+)	385628.57(330057.265)	324021.431(136699.566)	421681.473(375952.014)	336941.192(149353.949)
PC (38:6) A - ESI(+)	122703.865(38145.153)	135842.09(35120.916)	127714.075(38815.023)	139468.196(35495.718)
PC (38:6) B - ESI(+)	3683483.214(1066200.996)	3373471.275(825187.655)	3837736.421(1126227.192)	3485281.204(837697.48)
PC (38:7)	9067.129(4522.378)	8494.519(3671.831)	10063.09(4613.949)	9197.56(3668.259)
PC (39:4)	4951.364(1392.551)	4980.401(1209.519)	5161.287(1412.986)	5084.381(1196.739)
PC (40:4) - ESI(+)	40710.749(17107.156)	43768.486(14761.039)	39908.33(17452.64)	42287.995(13584.315)
PC (40:5) A - ESI(+)	160984.496(51414.716)	153215.298(48927.121)	163977.645(53826.665)	154048.446(52495.588)
PC (40:5) B - ESI(+)	39290.673(16831.51)	43514.802(16159.023)	39626.637(17297.008)	43357.103(15760.681)
PC (40:6) A	26324.155(8352.257)	26286.775(7120.512)	27429.399(8246.52)	27065.817(7139.141)
PC (40:6)B	523343.738(235330.416)	448154.607(162581.361)	562604.084(254764.122)	467455.297(167059.509)
PC (40:7) A - ESI(+)	14123.954(4521.843)	15295.102(4113.716)	14194.433(4112.738)	15377.362(4186.091)
PC (40:7) B - ESI(+)	294687.493(123648.862)	260986.662(85720.284)	310043.863(123498.525)	274436.004(85433.318)
PC (40:8) - ESI(+)	15239.14(4848.028)	15297.801(4079.753)	15552.704(4225.795)	15705.297(4292.469)
PC (42:10)	2726.931(1374.175)	2509.831(1360.724)	2807.197(1358.449)	2557.702(1471.573)
PC (o-32:0) - ESI(+)	33066.939(8835.009)	34463.696(8408.236)	32634.257(8847.324)	35119.871(8361.956)
PC (o-34:0)	4253.752(1544.24)	4625.498(1473.237)	4254.556(1486.614)	4787.885(1516.673)
PC (p-32:1)/PC (o-32:2)	7732.065(2525.44)	8442.017(2078.799)	7658.733(2098.63)	8519.511(2085.491)
PC (p-34:1)/PC (o-34:2)	90514.308(41518.544)	112732.145(42037.713)	90362.3(43840.811)	118159.371(43883.945)
PC (p-34:2)/PC (o-34:3) - ESI(+)	134516.098(48579.028)	167161.547(53529.226)	136366.181(49093.247)	173386.082(53513.378)
PC (p-36:1)/PC (o-36:2) B	4576.41(1860.937)	4990.913(1761.819)	4686.759(1871.805)	5235.944(1736.014)
PC (p-36:2)/PC (o-36:3)	18401.743(7473.236)	22260.671(8493.763)	18848.555(7606.071)	23242.285(8689.103)
PC (p-36:4)/PC (o-36:5) - ESI(+)	222255.821(73873.841)	244403.223(62140.636)	213961.102(65308.437)	240147.53(55991.321)
PC (p-36:5)/PC (o-36:6)	43163.98(47010.214)	35793.982(29043.548)	43196.944(47713.695)	35753.832(31191.928)
PC (p-38:3)/PC (o-38:4) A - ESI(+)	23415.263(7747.924)	26268.221(7020.386)	23132.94(7893.985)	25693.398(6251.518)
PC (p-38:3)/PC (o-38:4) B - ESI(+)	60681.832(24417.325)	68924.225(21887.47)	59401.39(24899.037)	68257.213(21742.315)
PC (p-38:4)/PC (o-38:5) A	244736.068(73932.864)	253186.358(52211.505)	241258.162(73545.028)	251216.834(48379.253)
PC (p-38:4)/PC (o-38:5) B	46348.51(17350.154)	52251.201(14810.562)	45822.847(17680.613)	51798.501(13880.981)
PC (p-38:5)/PC (o-38:6) A	47602.588(24906.045)	44907.468(17837.495)	48165.106(23970.811)	46178.478(18332.548)
PC (p-38:5)/PC (o-38:6) B	60693.148(18465.69)	63136.031(15203.868)	61419.069(17813.941)	64316.344(14030.843)
PC (p-38:6)/PC (o-38:7)	38202.501(19743.59)	36368.564(13760.086)	38853.179(19547.248)	37243.933(14318.613)
PC (p-40:4)/PC (o-40:5) - ESI(+)	17184.561(5389.491)	17672.249(4621.409)	17091.52(5725.53)	17547.731(4356.749)
PC (p-40:6)/PC (o-40:7) A	40200.774(19957.817)	35888.168(13738.726)	41534.712(18886.27)	37069.642(14321.062)
PC (p-40:6)/PC (o-40:7) B	13510.106(6889.457)	13100.064(5544.826)	13963.862(7043.192)	13685.693(5731.919)
PC (p-42:4)/PC (o-42:5) - ESI(+)	12900.718(4496.163)	12896.037(3917.285)	12960.829(4885.885)	12882.917(3559.204)
PC (p-42:5)/PC (o-42:6) A	10237.461(3726.694)	10713.657(3758.542)	10263.989(3735.885)	10641.522(3407.914)
PC (p-42:5)/PC (o-42:6) B	3974.188(1415.292)	3956.085(1237.45)	4073.113(1509.236)	4103.264(1204.198)
PC (p-44:4)/PC (o-44:5) - ESI(+)	14453.858(5455.893)	14223.731(4628.827)	14264.516(5559.845)	14295.85(4388.886)
PE (34:1)	1935.048(1193.975)	1997.27(1266.931)	1940.194(1173.534)	1969.02(1276.846)
PE (34:2) - ESI(-)	2982.653(1876.385)	3405.593(2151.45)	3029.793(1764.276)	3459.196(2123.934)
PE (36:1) - ESI(-)	418.862(181.396)	445.435(181.825)	428.886(176.713)	435.757(175.15)
PE (36:2)	7905.774(4135.38)	8803.532(4225.603)	7732.053(3516.886)	8864.748(4103.972)
PE (36:3)	2026.786(1248.378)	2279.738(1430.26)	1955.058(975.455)	2312.145(1448.017)
PE (36:4) - ESI(-)	2941.499(1644.752)	3164.472(1950.982)	3029.575(1641.817)	3130.314(1951.074)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
PE (38:2)	629.602(222.186)	682.787(206.229)	631.364(228.296)	669.438(196.116)
PE (38:6) - ESI(-)	7437.759(5142.646)	7356.489(4624.489)	8012.329(5306.57)	7427.759(4778.33)
PE (p-34:1)/PE (o-34:2) - ESI(-)	2025.04(785.489)	2051.91(695.945)	1973.582(738.517)	2059.683(685.308)
PE (p-34:2)/PE (o-34:3)	3040.334(1576.283)	3609.46(1747.103)	2882.224(1449.324)	3661.438(1859.658)
PE (p-36:1)/PE (o-36:2) - ESI(-)	2760.373(1320.05)	3068.12(1351.566)	2635.577(1273.389)	3006.465(1281.886)
PE (p-36:2)/PE (o-36:3) - ESI(-)	5957.994(2773.012)	6972.062(2936.918)	5688.236(2599.885)	6988.788(3104.579)
PE (p-36:4)/PE (o-36:5) - ESI(-)	15261.909(9626.399)	15928.908(8581.977)	13935.692(7710.994)	15318.456(7991.015)
PE (p-36:5)/PE (o-36:6)	2102.097(2962.828)	1485.236(2041.939)	1789.331(2236.012)	1462.848(2221.901)
PE (p-38:3)/PE (o-38:4)	1340.345(687.934)	1513.805(782.147)	1283.123(668.687)	1460.129(771.765)
PE (p-38:5)/PE (o-38:6) - ESI(-)	11786.825(6628.023)	12149.489(5341.659)	11040.293(5570.985)	11907.516(5099.043)
PE (p-38:6)/PE (o-38:7)	7532.92(4292.66)	7188.888(3364.912)	7276.368(3883.07)	7078.837(3513.041)
PE (p-40:4)/PE (o-40:5)	3399.555(1897.801)	3410.027(1799.437)	3305.616(1812.216)	3332.351(1602.38)
PE (34:2) - ESI(+)	8757.929(6410.569)	9879.682(7371.827)	9220.507(6694.552)	9966.166(7816.693)
PE (36:1) - ESI(+)	3379.71(1611.842)	3316.561(1592.325)	3263.487(1446.003)	3237.931(1493.842)
PE (36:4) - ESI(+)	14739.008(7468.332)	15255.178(7705.241)	15753.285(7583.178)	15504.53(7845.412)
PE (38:4)	39570.697(19154.594)	40390.086(15772.1)	41121.491(18723.161)	41293.918(15461.624)
PE (38:6) - ESI(+)	20257.66(12022.688)	19884.696(11866.824)	23154.655(12574.001)	20815.727(12437.645)
PE (p-34:1)/PE (o-34:2) - ESI(+)	2742.254(1098.637)	2862.174(974.659)	2672.766(988.62)	2874.238(962.614)
PE (p-36:1)/PE (o-36:2) - ESI(+)	2454.413(1024.933)	2762.367(992.448)	2409.249(954.259)	2777.374(951.171)
PE (p-36:2)/PE (o-36:3) - ESI(+)	8991.903(3876.705)	11041.406(4021.531)	8785.477(3533.158)	11426.737(4221.509)
PE (p-36:4)/PE (o-36:5) - ESI(+)	29345.071(18055.185)	30532.635(14508.762)	26863.725(13494.708)	30216.432(14178.163)
PE (p-38:4)/PE (o-38:5)	42614.164(20321.576)	46103.9(17411.189)	40822.867(18224.537)	45964.889(16706.401)
PE (p-38:5)/PE (o-38:6) - ESI(+)	24747.834(11095.999)	26262.641(9101.812)	23571.321(8663.977)	26241.401(8898.027)
PE (p-40:4)/PE (o-40:5) A	2896.209(2724.733)	2989.973(2175.181)	2689.895(2373.18)	2967.712(1955.17)
PE (p-40:4)/PE (o-40:5) B	3708.007(1951.993)	3692.493(1528.458)	3694.774(1901.318)	3668.946(1409.857)
PE (p-40:5)/PE (o-40:6)	6740.897(2550.286)	6806.706(1987.436)	6474.732(2366.006)	6819.497(1911.385)
PG (34:0)/PG (17:0/17:0)	76853.368(21921.357)	85280.313(20224.124)	75357.297(22903.419)	85157.322(20327.055)
PI (38:4)/PI (18:0-20:4)	120817.481(39400.359)	124008.066(31642.823)	120581.869(37338.394)	122380.788(30748.13)
SM (d30:1) - ESI(-)	1704.845(1134.453)	1947.17(774.108)	1741.938(1093.709)	1972.955(715.8)
SM (d32:0) - ESI(-)	1032.341(809.55)	1064.49(657.551)	1053.879(858.514)	1017.411(603.003)
SM (d32:1) - ESI(-)	44492.705(15861.723)	49754.267(12913.605)	44727.747(15016.049)	49684.296(12615.847)
SM (d32:2) - ESI(-)	3030.003(1334.652)	3230.614(1251.27)	3226.202(1351.425)	3409.244(1299.318)
SM (d33:1) - ESI(-)	22975.489(8246.125)	25365.753(7028.514)	22644.729(8358.501)	25229.246(7270.357)
SM (d34:0) - ESI(-)	4927.976(1784.951)	5032.83(1672.907)	4794.344(1692.618)	5037.227(1704.116)
SM (d34:1) - ESI(-)	155715.48(39317.352)	163369.808(34296.98)	150308.85(36641.578)	162587.859(33725.445)
SM (d34:2) - ESI(-)	57475.881(14166.69)	60371.724(13403.338)	57244.429(13620.13)	61368.681(13998.656)
SM (d36:0) - ESI(-)	1066.803(653.242)	879.715(483.034)	1014.529(570.255)	793.512(407.436)
SM (d36:1) - ESI(-)	36132.26(10486.124)	36986.044(8862.176)	34995.042(8656.887)	36417.919(8481.388)
SM (d36:2) - ESI(-)	5807.249(1805.715)	5799.331(1630.41)	5775.03(1738.188)	5779.314(1601.4)
SM (d36:3) - ESI(-)	1713.798(653.047)	1804.421(563.54)	1757.144(685.763)	1812.821(597.69)
SM (d37:1)	2411.418(1019.95)	2404.494(818.507)	2444.066(950.289)	2409.022(763.946)
SM (d38:0)	696.441(811.576)	522.617(447.127)	700.134(856.544)	478.008(462.61)
SM (d38:2) - ESI(-)	4790.522(1380.077)	4974.002(1318.512)	4778.59(1309.009)	5107.688(1365.518)
SM (d39:1) - ESI(-)	12841.047(4278.992)	14353.601(3784.665)	13016.383(4211.156)	14492.537(3819.146)
SM (d39:2)	12449.201(3511.981)	12954.634(3279.589)	13477.133(3201.714)	13842.164(2925.889)
SM (d40:1) - ESI(-)	46897.381(13275.565)	50082.888(10695.858)	46399.113(12523.495)	49650.664(10908.118)
SM (d40:2) A - ESI(-)	12273.795(4442.543)	12319.223(4118.364)	11967.871(3692.789)	12241.65(3901.865)
SM (d40:2) B - ESI(-)	17613.206(5158.79)	18864.027(4350.959)	17746.067(4989.101)	19207.058(4516.62)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
SM (d40:3)	1079.194(398.684)	1151.905(387.017)	1050.49(391.197)	1191.378(407.458)
SM (d41:1) - ESI(-)	11075.677(11704.719)	13579.641(12424.293)	10616.592(11274.003)	13795.881(11975.701)
SM (d41:2) - ESI(-)	10157.654(3759.068)	10335.005(4166.592)	10404.338(3672.889)	10507.896(4378.528)
SM (d42:0) - ESI(+)	631.117(319.733)	572.32(282.695)	622.379(298.174)	537.076(274.555)
SM (d42:0) - ESI(-)	2435.513(802.742)	2325.825(740.385)	2470.148(793.653)	2287.991(787.949)
SM (d42:1) - ESI(-)	74113.422(22000.912)	76751.556(18783.673)	72184.156(20435.816)	74908.652(18692.96)
SM (d42:3) - ESI(-)	45369.2(13437.893)	44941.003(10551.682)	44198.136(12142.453)	45334.226(10354.542)
SM (d43:1) - ESI(-)	1610.475(804.178)	1785.517(763.855)	1618.018(814.733)	1667.998(676)
SM (d43:2) - ESI(-)	6637.877(3329.003)	6677.809(2804.014)	6613.861(3155.233)	6397.93(2458.095)
SM (d44:2)	3401.174(1320.178)	2954.684(961.942)	3395.111(1198.217)	2970.944(987.86)
SM (d41:3)	17542.807(4858.342)	18495.055(4033.934)	17960.03(4846.253)	18787.425(3742.284)
SM (d30:1) - ESI(+)	4627.855(3294.462)	5081.766(2205.718)	5028.808(3462.684)	5291.701(2009.151)
SM (d32:0) - ESI(+)	4527.417(2257.972)	4461.163(1515.584)	4874.777(2374.938)	4638.532(1513.107)
SM (d32:1) - ESI(+)	127487.665(50390.527)	141586.567(42157.93)	136372.342(49199.774)	147059.917(42153.968)
SM (d32:2) - ESI(+)	8419.355(3072.987)	8850.662(2752.191)	9261.809(3018.86)	9547.077(2585.789)
SM (d33:1) - ESI(+)	78897.543(30030.413)	81545.929(24155.104)	83598.798(30549.918)	85232.023(24689.826)
SM (d34:0) - ESI(+)	77128.042(21734.185)	77407.547(19252.704)	79148.787(20897.091)	80066.77(18722.585)
SM (d34:1) - ESI(+)	1815521.625(427328.564)	1839477.475(326129.156)	1828329.791(428344.536)	1881662.975(305967.847)
SM (d34:2) - ESI(+)	169414.754(41285.046)	172230.478(39764.32)	177731.172(39450.959)	181137.089(38632.856)
SM (d36:0) - ESI(+)	18743.046(8907.96)	15332.243(6070.249)	18843.91(8196.485)	15312.391(6112.929)
SM (d36:1) - ESI(+)	282139.394(75455.508)	277277.338(58280.773)	286717.136(68048.084)	283125.157(50994.077)
SM (d36:2) - ESI(+)	637435.743(182402.554)	634824.46(155709.619)	648968.61(164665.017)	658143.625(148372.072)
SM (d36:3) - ESI(+)	6491.66(2413.088)	6629.303(2061.528)	6979.774(2511.247)	7017.571(2071.407)
SM (d38:1)	224074.217(52840.443)	238184.289(46405.144)	233237.845(47492.938)	244612.794(44373.49)
SM (d38:2) - ESI(+)	102238.769(23254.677)	103697.728(23384.632)	106659.856(22123.4)	109042.026(21335.321)
SM (d39:1) - ESI(+)	55126.946(19385.078)	60979.282(17058.805)	59429.032(18852.674)	63790.017(17030.253)
SM (d40:0)	8519.977(3597.278)	7725.238(2745.348)	8866.396(3724.585)	7636.915(2899.059)
SM (d40:1) - ESI(+)	357194.17(87098.783)	373303.076(69403.177)	363600.727(79860.724)	376764.167(65965.404)
SM (d40:2) A - ESI(+)	192003.867(74381.653)	206939.521(72862.228)	197726.627(74937.129)	215299.681(75251.437)
SM (d40:2) B - ESI(+)	235158.05(59785.384)	255298.203(57750.75)	245271.672(56923.439)	266399.439(54255.607)
SM (d41:1) - ESI(+)	136526.853(38416.919)	143873.721(36214.448)	143360.216(37159.026)	147377.748(35202.988)
SM (d41:2) A - ESI(+)	41382.821(14921.589)	40584.006(12105.041)	43803.632(15241.692)	42626.808(11718.251)
SM (d41:2) B - ESI(+)	65492.772(20330.14)	72077.791(21032.207)	70731.196(19417.519)	77074.321(20042.703)
SM (d42:1) - ESI(+)	227228.943(65564.52)	235888.054(53178.336)	229198.281(66687.672)	234400.426(53184.15)
SM (d42:2)	552276.944(187216.547)	490026.241(121909.07)	554709.294(182209.049)	499090.359(116944.768)
SM (d42:3) - ESI(+)	360096.856(99212.364)	348735.256(79546.208)	369329.425(97539.146)	363893.997(72446.491)
SM (d43:1) - ESI(+)	6015.056(2273.428)	6198.991(2041.865)	6204.102(2326.495)	6117.228(1928.598)
SM (d43:2) - ESI(+)	14891.052(6807.646)	13945.815(5754.744)	15587.392(7127.791)	14090.14(5552.322)
TG (55:6)	10089.48(6268.964)	8140.342(3509.246)	10618.261(7123.437)	7813.759(3404.847)
TAG (58:7)/TAG (18:1/18:1/22:5)	17350.361(7968.934)	16648.95(5845.672)	17642.412(8739.651)	16064.8(5748.474)
TG (60:12)	6594.761(13689.356)	3710.704(4070.071)	7831.422(15989.851)	3920.165(4474.049)
TG (53:5)	10973.54(5251.608)	10286.984(3942.7)	10685.391(5107.823)	10116.072(3418.881)
TG (60:11)	8428.304(11674.572)	5497.847(3845.608)	9546.81(13530.976)	5506.312(3912.515)
TG (40:0)	6969.903(22773.737)	5975.792(11932.991)	5366.541(12887.212)	6134.296(13304.798)
TG (40:1)	1931.434(4239.428)	2087.013(3783.783)	1582.02(2660.445)	2140.263(4173.486)
TG (42:0)	9234.522(21761.184)	8844.978(15901.608)	7560.81(14465.31)	9004.003(17596.082)
TG (42:1)	6797.568(17520.658)	7739.975(16319.178)	5616.372(10985.062)	7542.464(16998.656)
TG (42:2)	2571.971(5933.309)	3829.423(10795.773)	2203.121(3842.725)	3854.495(11684.619)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
TG (42:3)	591.158(714.913)	671.443(879.22)	543.039(624.657)	667.857(910.252)
TG (44:0)	19087.048(32238.546)	17886.319(25507.344)	16866.3(27378.177)	16999.68(26581.255)
TG (44:1)	18788.092(29782.097)	19478.318(28152.179)	16881.987(23775.499)	18816.535(29572.076)
TG (44:2)	8060.679(14384.219)	10064.354(23367.775)	6958.338(11163.511)	10584.424(26138.23)
TG (46:0)	2913.683(2889.773)	3210.711(2865.495)	2633.088(2657.701)	3022.861(2847.843)
TG (46:1)	78988.174(99974.002)	74842.169(86950.751)	73527.42(94024.564)	67406.911(82723.716)
TG (46:2)	34399.438(37849.21)	37666.18(47712.032)	32184.39(35761.877)	36569.847(51554.153)
TG (46:3) A	601.482(563.369)	733.247(1466.526)	541.566(491.284)	783.319(1666.273)
TG (46:3) B	5520.005(7775.947)	5107.884(7131.762)	4751.972(6081.917)	5340.125(7936.867)
TG (46:4) A	1736.197(1706.675)	2452.533(7382.425)	1571.274(1434.583)	2689.604(8429.38)
TG (46:4) B	1520.942(1603.93)	2160.803(6838.834)	1363.537(1358.418)	2381.213(7803.968)
TG (46:5)	350.027(264.398)	426.476(1213.469)	326.444(238.678)	470.062(1385.206)
TG (48:0)	59633.947(40059.321)	72255.424(51804.827)	56646.378(39295.717)	70024.672(52229.989)
TG (48:1)	445353.036(404942.517)	421062.403(327886.505)	412944.557(383735.571)	379546.827(287273.446)
TG (48:2)	232753.491(212433.045)	215309.555(160839.721)	223287.825(211409.198)	198900.58(150604.766)
TG (48:3)	66257.783(45379.776)	68608.011(52545.382)	63809.422(43231.229)	65745.352(52409.463)
TG (48:4) A	14636.937(12229.537)	16489.544(19911.708)	13975.86(11673.51)	16013.507(20807.177)
TG (48:4) B	10569.309(10549.743)	12439.978(18504.13)	9774.202(10123.516)	11658.077(19127.757)
TG (48:5)	2394.932(2124.793)	2607.435(2613.644)	2321.835(2169.799)	2554.014(2691.21)
TG (48:6)	731.456(341.644)	1120.169(4094.332)	735.053(362.762)	1248.354(4683.687)
TG (49:0)	5475.884(3437.407)	5547.724(2851.467)	5219.237(3275.43)	5313.1(2932.212)
TG (49:1)	38039.35(31682.085)	32431.609(18199.476)	35461.279(30090.794)	30042.222(16962.334)
TG (49:2)	5347.71(2994.124)	4908.392(3180.31)	5284.331(2880.868)	4910.13(3450.395)
TG (49:3)	8782.798(5619.053)	8058.518(3765.588)	8602.413(5371.364)	8056.122(3929.513)
TG (50:0)	28294.36(17765.307)	35864.991(22391.136)	26737.748(17017.073)	33243.52(20485.763)
TG (50:1)	295740.881(378872.38)	268871.222(259991.973)	283860.844(350257.099)	241553.582(258746.168)
TG (50:2)	1473341.655(765417.549)	1337335.537(606243.723)	1396824.909(729547.499)	1257985.029(574862.635)
TG (50:3) A	599554.098(373888.427)	538070.653(271710.362)	578201.298(358127.789)	515201.921(266481.825)
TG (50:3) B	1463.989(2654.267)	1979.068(6822.777)	1490.21(2747.56)	2269.534(7783.442)
TG (50:4)	113705.603(61749.855)	111373.426(49803.428)	108601.458(55033.535)	110330.359(48106.23)
TG (50:5)	18164.523(11639.543)	17487.784(9234.201)	17437.444(10448.935)	17542.815(8919.388)
TG (50:6)	2907.741(1946.11)	2679.302(1733.966)	2917.163(1969.149)	2626.251(1822.35)
TG (51:2)	92658.55(49837.791)	81298.301(33345.525)	88644.76(46745.452)	76313.994(30285.369)
TG (51:3)	73828.122(33989.875)	68061.653(24068.889)	70084.162(29641.3)	65950.35(22204.849)
TG (51:4)	20600.271(10073.4)	19733.727(8062.558)	19502.825(8653.773)	19752.067(7808.805)
TG (51:5)	3397.515(1704.001)	3356.461(1275.262)	3291.237(1492.907)	3360.513(1180.21)
TG (52:1)	273344.812(258320.644)	254133.337(220416.288)	227065.38(199122.882)	215185.613(194263.196)
TG (52:2)	3924538.986(1182333.569)	3636556.102(1122279.122)	3768364.854(1099628.234)	3436434.472(1007005.155)
TG (52:3)	4416231.615(1252804.656)	4180937.847(1101985.633)	4199674.991(1183957.428)	4057679.469(1019804.465)
TG (52:4)	133068.448(44192.17)	130479.658(39344.454)	126352.449(42083.066)	129251.411(37900.358)
TG (52:5)	197791.574(102954.234)	174359.995(84000.915)	188217.153(97375.415)	170162.202(67877.07)
TG (52:6)	25178.432(15261.735)	23719.028(10920.524)	24662.199(13887.622)	22725.563(10345.977)
TG (53:0)	1583.982(681.915)	1815.471(661.05)	1594.348(752.808)	1804.08(672.071)
TG (53:1)	5936.774(4668.413)	5776.819(3671.696)	5445.202(4000.772)	5170.883(3349.695)
TG (53:2)	55792.745(24993.696)	51317.499(21651.56)	53435.252(23073.739)	47192.778(17319.808)
TG (53:3)	73056.718(28445.208)	67703.814(23631.61)	70038.964(26227.57)	64558.692(18876.147)
TG (53:4)	46389.39(19729.068)	43856.196(15698.609)	45059.64(18992.915)	42639.927(13631.342)
TG (54:1)	29942.881(33162.778)	29095.13(22321.153)	23372.449(14886.461)	25893.09(19302.326)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
TG (54:2)	321515.5(253928.808)	286249.499(201970.532)	272775.075(155956.486)	248260.886(151416.82)
TG (54:3)	1412729.685(654867.912)	1276837.39(524744.236)	1326143.056(537873.167)	1201773.944(430758.739)
TG (54:4)	1525311.494(686168.793)	1377217.291(578506.358)	1428692.291(658070.149)	1310971.798(477314.851)
TG (54:5) A	886580.788(456096.063)	802522.834(352287.756)	829669.398(458056.817)	770422.494(295087.83)
TG (54:5) B	262000.181(111804.806)	243734.88(92887.319)	246470.56(97593.421)	220769.995(79245.363)
TG (54:6) A	199405.641(130496.852)	176401.555(94248.554)	188477.062(133217.914)	171595.941(78375.698)
TG (54:6) B	1358.531(998.464)	1341.842(782.147)	1271.477(992.345)	1356.734(732.422)
TG (54:6) C	156170.234(80514.484)	137719.361(62448.4)	149032.02(69075.362)	126494.779(50961.587)
TG (54:7) A	49122.361(41128.683)	44915.907(27315.049)	46528.908(41940.085)	44917.947(25113.962)
TG (54:7) B	43061.59(27306.858)	34198.973(17471.92)	43732.939(29760.111)	32296.045(16095.635)
TG (54:8)	7077.455(4680.131)	6400.128(3571.251)	7293.169(4891.851)	6104.244(3149.695)
TG (54:9)	965.383(952.873)	800.15(740.888)	1118.466(1027.977)	833.562(828.393)
TG (55:1)	2381.308(1476.992)	2293.733(1193.428)	2159.599(1208.603)	2084.107(1008.765)
TG (55:2)	3209.3(1454.698)	3026.046(1288.231)	3034.168(1311.937)	2784.835(1101.838)
TG (56:1)	8425.454(9238.656)	8724.83(13724.801)	7159.574(8184.624)	6856.677(5945.118)
TG (56:10)	3107.113(3323.17)	2681.061(1812.641)	3522.679(3729.117)	2724.639(1890.743)
TG (56:2)	12956.986(10569.613)	12163.693(13180.75)	11547.417(9211.255)	10159.27(7087.405)
TG (56:3)	30313.86(19743.679)	27075.315(20697.58)	27887.522(18193.363)	23433.262(13258.936)
TG (56:4)	52216.171(23781.081)	49073.426(20687.965)	50726.706(24292.856)	46878.52(18714.874)
TG (56:5) A	53791.601(25940.471)	48027.297(18998.273)	50499.723(24773.705)	43962.011(15967.169)
TG (56:5) B	56496.764(28288.186)	50801.304(20794.293)	52700.992(25050.493)	45780.962(15711.276)
TG (56:5) C	113050.899(43777.393)	107344.31(43874.117)	110759.221(46991.808)	102525.692(40194.12)
TG (56:6)	257540.767(82209.876)	233475.447(74511.483)	247768.718(77523.926)	216721.854(59967.74)
TG (56:7) A	847.239(514.565)	783.159(401.886)	809.886(444.189)	737.903(404.859)
TG (56:7) B	187264.223(134086.996)	142003.825(96398.78)	199255.168(150216.195)	136094.6(95356.661)
TG (56:8) A	48927.531(26901.231)	42661.135(18087.989)	48460.43(28330.769)	41241.651(17049.738)
TG (56:8) B	88914.046(72816.031)	66492.66(53152.85)	95506.578(81848.551)	64933.259(53859.705)
TG (56:9)	16134.849(11093.145)	13921.157(6903.286)	17113.136(12041.655)	13653.569(6683.489)
TG (57:1)	1925.193(905.225)	1863.322(943.086)	1799.662(828.566)	1695.476(767.306)
TG (57:2)	2561.985(1153.018)	2479.474(1287.033)	2354.363(992.929)	2217.816(949.567)
TG (58:1)	6517.314(7345.499)	6747.301(10399.217)	5867.012(7243.153)	5136.303(4122.358)
TG (58:10)	19441.101(14120.814)	16598.368(8410.925)	20720.386(15648.293)	16503.089(8469.218)
TG (58:2)	10622.347(16674.782)	10834.266(23253.565)	9540.797(16741.937)	7660.389(9265.011)
TG (58:3)	6147.029(9675.465)	5932.174(10911.709)	5656.27(10073.707)	4465.516(4635.348)
TG (58:4)	3243.624(2529.139)	2899.892(2258.659)	3126.268(2695.788)	2655.21(2009.437)
TG (58:5)	3750.517(1804.936)	3824.305(1507.07)	3735.783(1894.391)	3688.34(1418.742)
TG (58:6)	14653.583(5134.288)	13533.44(3981.36)	14281.308(4839.397)	12750.519(3470.825)
TG (58:8)	61621.544(53618.106)	44303.591(28847.455)	64812.49(56697.219)	42434.62(24878.919)
TG (58:9)	45461.573(35467.981)	34450.345(20298.576)	48212.448(38602.355)	33687.789(18971.409)
TG (59:2)	1491.779(1048.687)	1415.968(980.975)	1335.284(749.673)	1244.29(609.866)
TG (59:3)	1482.159(789.741)	1388.449(810.7)	1407.147(698.83)	1273.949(610.407)
TG (60:1)	2548.677(2775.351)	2609.795(3662.099)	2380.665(2872.92)	2089.792(1817.214)
TG (60:2)	5106.678(6459.935)	5391.177(12127.075)	4637.255(5088.102)	4114.618(5785.42)
TG (60:3)	3356.443(4588.274)	3498.227(6192.138)	3132.217(4805.77)	2631.123(2498.163)
TG (60:4)	1479.004(1459.393)	1489.448(1601.775)	1415.878(1531.614)	1264.185(1005.741)
TG (60:6)	1058.884(479.188)	956.092(409.713)	1043.772(455.724)	921.05(418.144)
TG (62:1)	1025.712(1380.888)	981.286(1057.831)	994.782(1496.735)	859.475(551.843)
TG (62:2)	1814.769(2212.815)	1781.426(2417.302)	1782.514(2388.615)	1471.359(1405.363)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
TG (62:3)	571.887(485.151)	559.893(537.266)	599.577(541.896)	519.154(519.164)
TG (62:4)	547.101(334.64)	613.733(374.856)	537.383(359.013)	571.537(297.461)
TG (64:2)	864.662(732.038)	883.063(767.604)	852.086(716.207)	760.911(506.986)
TG (64:3)	552.787(234.996)	552.569(261.395)	538.92(231.867)	541.498(241.639)
Oxylipins (OL)				
10-nitrolinoleic acid	0.186(0.36)	0.149(0.221)	0.159(0.327)	0.141(0.219)
10-nitrooleic acid	5.022(4.039)	4.734(2.95)	5.063(4.384)	4.444(2.475)
11(12)-epoxy-5,8,14,17- eicosatetraenoic acid	0.045(0.051)	0.046(0.062)	0.052(0.054)	0.043(0.062)
11,12-Dihydroxyicosa-5,8,14-trienoic acid	0.729(0.365)	0.798(0.415)	0.688(0.328)	0.748(0.37)
11,12-Epoxyeicosa-5,8,14-trienoic acid	0.298(0.235)	0.25(0.225)	0.273(0.221)	0.235(0.213)
11-Hydroxy-14,15-epoxyeicosatrienoic acid	0.137(0.271)	0.236(0.486)	0.145(0.302)	0.208(0.493)
11-Hydroxy-arachidonic acid	0.954(0.559)	0.918(0.459)	0.987(0.593)	0.932(0.429)
12(13)-epoxy-9,15-octadecadienoic acid	0.131(0.14)	0.155(0.255)	0.093(0.079)	0.159(0.284)
12,13-dihydroxyoctadec-9-enoic acid	3.714(2.623)	4.151(2.308)	3.648(2.615)	4.042(1.846)
12,13-dihydroxyoctadeca-9,15-dienoic acid	0.107(0.148)	0.111(0.152)	0.12(0.157)	0.127(0.167)
12,13-epoxy-9-octadecenoic acid	2.678(3.381)	3.027(3.742)	2.24(2.216)	2.801(3.104)
12-Hydroxy-5,8,10,14,17-eicosapentaenoic acid	1.953(2.755)	1.117(1.211)	2.132(2.957)	1.226(1.308)
12-Hydroxy-5,8,10,14-eicosatetraenoic acid	17.204(15.381)	15.752(12.397)	17.655(15.309)	16.334(11.497)
13-hydroxyoctadeca-9,11,15-trienoic acid	0.935(0.885)	0.869(0.593)	0.804(0.536)	0.9(0.626)
13-Hydroxyoctadecadienoic acid	19.586(7.961)	19.825(7.897)	19.549(8.022)	19.806(7.067)
13-ketooctadeca-9,11-dienoic acid	11.779(7.152)	12.915(7.243)	11.241(7.005)	12.197(7.172)
14(15)-epoxy-5,8,11,17-eicosatetraenoic acid	0.234(0.427)	0.211(0.435)	0.185(0.259)	0.222(0.481)
14,15-dihydroxyeicosa-5,8,11,17-tetraenoic acid	0.445(0.453)	0.503(0.551)	0.44(0.469)	0.439(0.394)
14,15-dihydroxyeicosa-5,8,11-trienoic acid	0.816(0.427)	0.868(0.394)	0.768(0.397)	0.812(0.344)
14-hydroxydocosa-4,7,10,12,16,19-hexaenoic acid	13.05(14.814)	10.01(9.899)	14.349(15.523)	10.753(9.705)
15(16)-epoxy-9,12-octadecadienoic acid	0.221(0.211)	0.382(0.521)	0.212(0.191)	0.392(0.543)
15,16-dihydroxyoctadeca-9,12-dienoic acid	11.678(8.843)	12.862(6.666)	11.008(7.506)	13.369(6.958)
15-Deoxy-delta-12,14-Prostaglandin J2	0.043(0.036)	0.05(0.053)	0.041(0.03)	0.05(0.055)
15-hydroxyeicosa-5,8,11,13,17-pentaenoic acid	0.387(0.417)	0.288(0.303)	0.405(0.453)	0.256(0.293)
15-hydroxyeicosa-5,8,11,13-tetraenoic acid	3.04(1.536)	2.905(1.282)	3.08(1.537)	2.967(1.282)
15-ketoeicosa-5,8,11,13-tetraenoic acid	0.159(0.211)	0.167(0.276)	0.165(0.197)	0.166(0.296)
15-Keto-prostaglandin E2	0.319(0.368)	0.405(0.635)	0.345(0.405)	0.364(0.637)
16(17)-epoxy-4,7,10,13,19-docosapentaenoic acid	0.189(0.199)	0.159(0.206)	0.168(0.185)	0.138(0.134)
17,18-dihydroxyeicosa-5,8,11,14-tetraenoic acid	6.057(5.778)	4.785(3.299)	6.143(6.338)	4.677(3.081)
17,18-Epoxy-5,8,11,14-eicosatetraenoic acid	0.09(0.188)	0.122(0.18)	0.079(0.152)	0.106(0.148)
17-hydroxy-4,7,10,13,15,19-docosahexaenoic acid	1.382(0.957)	1.263(1.094)	1.371(0.977)	1.199(0.823)
18-(3-ethyloxiran-2-yl)octadeca-4,7,10,13,16-pentaenoic acid	0.406(0.383)	0.403(0.512)	0.376(0.277)	0.402(0.553)
19,20-dihydroxydocosa-4,7,10,13,16-pentaenoic acid	1.929(1.019)	1.91(1)	1.977(1.018)	1.94(0.997)
20-Hydroxyarachidonic acid	4.005(8.301)	3.874(6.762)	4.335(9.226)	4.269(7.105)
4-hydroxydocosa-5,7,10,13,16,19-hexaenoic acid	0.763(0.83)	0.673(0.657)	0.798(0.865)	0.66(0.67)
5,15-dihydroxyeicosa-6,8,11,13-tetraenoic acid	0.038(0.055)	0.053(0.095)	0.039(0.055)	0.059(0.106)
5,6,15-trihydroxyeicosa-7,9,11,13-tetraenoic acid	0.157(0.194)	0.207(0.32)	0.152(0.189)	0.197(0.309)
5,6-dihydroxyeicosa-8,11,14-trienoic acid	0.665(0.513)	0.709(0.521)	0.59(0.446)	0.596(0.354)
5-Hydroxy-6,8,11,14,17-eicosapentaenoic acid	0.954(0.728)	0.874(0.675)	1.002(0.759)	0.874(0.721)
5-Hydroxy-6,8,11,14-eicosatetraenoic acid	3.249(2.155)	3.575(2.057)	3.286(2.245)	3.461(1.99)
5-ketoeicosa-6,8,11,14-tetraenoic acid	0.116(0.104)	0.137(0.127)	0.121(0.108)	0.128(0.117)
6-Ketoprostaglandin F1 alpha	0.111(0.191)	0.091(0.14)	0.117(0.178)	0.087(0.139)
6-trans-Leukotriene B4	0.046(0.066)	0.051(0.099)	0.045(0.071)	0.056(0.11)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Female ME/CFS (n=75)	Female Control (n=69)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
8,15-dihydroxyeicosa-5,9,11,13-tetraenoic acid	0.121(0.272)	0.115(0.202)	0.128(0.312)	0.109(0.191)
8,9-dihydroxyeicosa-5,11,14-trienoic acid	0.391(0.311)	0.373(0.243)	0.35(0.264)	0.337(0.197)
8,9-Epoxyeicosa-5,11,14-trienoic acid	0.627(0.483)	0.848(0.762)	0.563(0.448)	0.783(0.635)
8-hydroxyeicosa-5,9,11,14-tetraenoic acid	0.707(0.521)	0.693(0.505)	0.744(0.563)	0.648(0.43)
9(10)-epoxy-12,15-octadecadienoic acid	1.238(2.543)	1.495(3.452)	1.472(2.98)	1.232(2.343)
9(10)-epoxy-12Z-octadecenoic acid	0.778(0.586)	0.789(0.455)	0.689(0.388)	0.808(0.465)
9,10-dihydroxyoctadec-12-enoic acid	3.994(2.996)	4.527(2.771)	3.862(3.199)	4.57(2.863)
9,10-dihydroxyoctadeca-12,15-dienoic acid	0.195(0.127)	0.233(0.156)	0.18(0.123)	0.253(0.164)
9,10-Epoxy stearic acid	2.482(2.294)	2.68(2.248)	2.416(2.099)	2.472(2.177)
9,11,15-trihydroxy-5,13,1Z-prostatrienoic acid	0.022(0.082)	0.033(0.09)	0.023(0.096)	0.031(0.086)
9,12,13-trihydroxyoctadec-10-enoic acid	6.746(3.013)	7.161(3.062)	6.492(2.67)	7.125(3.057)
9-Hydroxy-5,7,11,14,17-icosapentaenoic acid	0.259(0.225)	0.218(0.148)	0.259(0.222)	0.221(0.149)
9-hydroxyeicosa-5,7,11,14-tetraenoic acid	0.366(0.266)	0.386(0.267)	0.347(0.258)	0.354(0.23)
9-Hydroxylinoleic acid	9.759(4.207)	10.407(3.998)	9.884(4.493)	10.535(3.833)
9-hydroxyoctadeca-10,12,15-trienoic acid	0.602(0.484)	0.715(0.595)	0.553(0.466)	0.77(0.639)
9-ketooctadeca-10,12-dienoic acid	1.218(0.86)	1.249(0.847)	1.184(0.863)	1.15(0.836)
9-nitrooleic acid	0.611(0.737)	0.692(0.676)	0.667(0.837)	0.591(0.564)
9S,10R-dihydroxy-stearic acid	2.561(1.966)	2.883(2.166)	2.623(2.19)	2.929(2.17)
Leukotriene B4	0.079(0.051)	0.099(0.087)	0.083(0.053)	0.086(0.05)
Leukotriene B5	0.01(0.015)	0.012(0.018)	0.01(0.016)	0.012(0.018)
Prostaglandin D2	0.336(0.565)	0.54(0.959)	0.285(0.479)	0.593(0.945)
Prostaglandin E1	0.02(0.021)	0.019(0.026)	0.018(0.021)	0.019(0.027)
Prostaglandin E2	0.057(0.126)	0.052(0.08)	0.064(0.146)	0.05(0.084)
Prostaglandin E3	0.185(0.427)	0.14(0.232)	0.146(0.26)	0.159(0.256)
Prostaglandin F2a	0.83(0.921)	0.952(0.717)	0.802(0.998)	0.912(0.611)
Resolvin D1	0.147(0.362)	0.162(0.194)	0.113(0.158)	0.149(0.178)
Thromboxane B2	1.893(2.013)	2.178(4.62)	1.952(2.115)	2.372(5.278)
trans-12,13-epoxy-11-oxo-trans-9-octadecenoic acid	1.085(0.917)	1.082(0.66)	0.973(0.585)	1.072(0.653)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
Primary Metabolites (PM)				
1,2,4-benzenetriol	1079.549(1400.131)	1012.135(991.038)	742.5(467.772)	1037.545(1061.824)
1-methylgalactose NIST	10405.216(25620.129)	6749.551(12633.562)	13105.533(36244.524)	4991.227(3787.963)
2-aminobutyric acid	6778.127(2312.798)	6819.584(2333.931)	7352.333(2667.15)	7241.364(1925.267)
2-deoxytetronic acid	3802(1871.5)	3811.933(1810.183)	4754.767(2548.144)	4772.955(2592.052)
2-hydroxybutanoic acid	37828.971(19975.01)	35735.831(20029.106)	44440.767(19367.184)	43881.318(24993.048)
2-hydroxyvaleric acid	4237.382(2334.07)	4287.303(2132.918)	4799.367(2957.312)	4460.273(1950.384)
2-ketoisocaproic acid	18813.069(5556.745)	19149.258(6078.798)	21047.133(4542.494)	22359.318(6496.982)
3-hydroxybutyric acid	39212.265(52464.62)	34152(42085.017)	35733.733(33982.447)	29850.091(53997.176)
4-hydroxybutyric acid	2256.422(736.812)	2269.843(849.082)	2219.133(637.934)	2311.182(908.418)
adipic acid	2895.686(1583.539)	2847.101(1343.166)	2556.967(848.514)	2810.409(1423.696)
alanine	73245.52(30295.714)	75399.281(33101.158)	73121(33240.851)	70609.955(26533.394)
alloxanoic acid	2006.5(1375.468)	1837.64(1056.367)	2237.967(1425.74)	2165.864(1153.744)
alpha-ketoglutarate	1657.627(531.612)	1527.562(557.531)	1871.3(583.844)	1604.636(625.02)
aminomalonate	3619.186(1973.13)	2911.888(1665.318)	3367.233(1477.467)	2461.545(1185.624)
arachidic acid	4924.814(2338.338)	4808.124(2355.798)	4761.4(1586.479)	4924.455(2869.459)
behenic acid	2886.951(836.07)	3031.506(992.687)	2881.2(598.633)	2993.182(1131.761)
benzoic acid	17834.373(6150.942)	17061.82(6244.429)	18071.7(6163.721)	15974.864(6752.184)
beta-alanine	1309.833(728.789)	1377.112(890.61)	1463.133(1028.63)	1333.273(525.477)
capric acid	1629.931(794.154)	1873.809(1125.953)	1559.433(583.025)	1713.045(870.035)
caprylic acid	5704.039(1875.061)	5854.764(2939.166)	5550.167(1898.669)	5450.909(2727.835)
citric acid	41473.245(20630.652)	41135.135(19465.808)	38013.867(14403.206)	34113.818(12532.075)
citrulline	4478.147(1507.009)	4592.506(1393.12)	4428.767(1034.018)	4310.591(1490.17)
conduritol-beta-exopoxide	1309.863(794.473)	1296.146(815.46)	999.3(455.193)	1285.545(699.734)
creatine	7813.647(4623.762)	7540.27(4234.565)	8603.167(4637.781)	7060.909(4418.151)
creatinine	8228.716(4668.248)	8192.91(4583.811)	8606(4409.523)	6546.591(5155.764)
erythritol	7881.353(18212.112)	8811.472(35942.446)	9133.6(22133.243)	8550.818(14805.823)
fructose	2597.775(3830.73)	2215.82(2366.76)	3919.6(5915.381)	2029.955(1237.433)
fumaric acid	9386.029(3097.763)	9434.101(2971.299)	9590.967(2587.965)	9589.545(2864.12)
gluconic acid	783.971(293.026)	776.438(203.662)	725.333(180.568)	666.864(208.811)
glucose	388539.039(113173.178)	378196.978(110227.014)	406466.567(114004.975)	352852.591(128158.886)
glucose-1-phosphate	2858.431(1035.667)	2901.236(1183.342)	2982.567(1259.644)	2845.045(759.257)
glucuronic acid	1283.441(842.594)	1067.326(518.171)	1525.367(1269.199)	995.909(355.541)
glutamic acid	8913.157(3993.644)	8273.382(4085.076)	9816.433(4292.34)	8451.909(3559.859)
glutamine	30937.275(21124.794)	32325.416(15805.25)	29196.6(16989.341)	26898.955(12231.057)
glutaric acid	568.461(206.452)	532.449(209.713)	557.067(169.993)	524.5(234.781)
glyceric acid	10747.598(4862.652)	9509.18(4092.259)	11127.067(5516.625)	9404.955(3448.089)
glycerol	94812.804(37180.866)	95386.449(35827.521)	81537.2(32838.773)	82255.864(30429.52)
glycerol-alpha-phosphate	970.676(374.848)	952.978(388.821)	921.367(379.96)	933.591(346.587)
glycine	68370.147(24574.146)	66183.809(20178.354)	56928.5(12407.6)	54838.136(12939.173)
glycolic acid	6131.461(2349.621)	6039.528(2582.552)	5938.933(2206.481)	6109.273(1939.393)
heptadecanoic acid	4659.657(1498.193)	4722.045(1568.799)	4474.633(1147.165)	4903.455(1586.455)
hydroxycarbamate NIST	9159.343(4227.978)	9278.079(4002.355)	8588.067(3729.171)	9035.909(3772.975)
indole-3-acetate	2888.461(1569.254)	2930.517(1502.67)	3032.333(1293.983)	2542.409(918.984)
indole-3-lactate	1920.853(610.853)	2047.753(765.819)	2129(737.703)	2367.909(1033.791)
indole-3-propionic acid	1758.569(1386.393)	2146.528(1481.229)	1822.2(2065.53)	1929.727(1114.829)
isoleucine	42005.147(16265.503)	42337.787(14176.603)	48243.833(18858.439)	45751.682(14480.461)
isopropylbenzene	16849.167(16235.754)	16249.494(18003.148)	13122.167(10569.752)	14600.455(8840.735)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
isothreonine acid	1867.461(718.975)	1810.944(701.346)	1923.3(685.372)	1543.955(729.734)
lactic acid	192717.833(119615.393)	173890.775(103094.546)	221408.167(134550.285)	209613.591(127179.843)
lauric acid	8363.078(12244.741)	10000.079(13605.883)	6520.067(3256.506)	6793.182(3183.059)
leucine	70058.255(22610.471)	77074.056(24098.618)	77396.967(20911.301)	82202.773(21691.79)
levoglucosan	1659.137(1216.05)	1870.697(1782.358)	1498.1(886.062)	2085.727(2679.176)
linoleic acid	1164.52(386.052)	1194.708(500.78)	1070.667(424.282)	1156.636(444.772)
lysine	15344.127(10811.81)	15204.719(7437.624)	14161.267(10957.394)	12799.727(6671.938)
lysine	18427.5(13565.891)	18658(9668.614)	15555.767(14422.268)	16682.682(9393.094)
lyxitol	3098.794(1031.473)	3248.989(1189.283)	3103.8(1183.462)	3618.727(1609.89)
maleic acid	878.186(349.551)	788.416(361.008)	886.9(286.57)	725.455(396.146)
maleimide	8053.353(10208.802)	6862.888(5737.055)	6042.5(2661.724)	8441(10299.541)
malic acid	1120.422(375.058)	1096.719(407.251)	1156.867(407.694)	1051.045(529.516)
maltose	1438.294(1117.335)	1611.483(3326.737)	1518.333(1687.153)	1176.091(923.678)
mannitol	7384.294(34427.962)	2531.82(2424.356)	3000.633(2954.186)	3071.364(3571.028)
mannose	23546.755(8923.898)	30536.393(70206.191)	25691.367(8220.081)	21915.591(10764.775)
methionine	2349.51(1025.929)	2403.135(919.059)	2377.667(772.261)	2085.091(1060.058)
myo-inositol	21222.363(6524.406)	20873.449(7257.918)	20854(7068.743)	21029.091(7257.152)
myristic acid	2466.971(764.975)	2620.674(814.52)	2352.233(641.368)	2466.318(813.394)
N-acetylmethionine	2287.627(630.487)	2420.708(709.39)	2265.967(502.235)	2380.045(584.82)
N-acetylputrescine	2335.549(2188.271)	2392.753(2148.301)	2827.933(3708.515)	1891.318(696.145)
nicotinic acid	22012.588(31343.256)	23151.326(37119.635)	19967.233(28981.09)	12073(17905.092)
ornithine	22444.167(16004.833)	23350.124(11618.996)	21618.067(15664.852)	20825.227(10726.293)
oxalic acid	38138.853(34967.284)	31155.685(23852.651)	44318.833(34672.125)	34647.773(20502.725)
oxoproline	148843.422(35478.319)	149227.169(31627.972)	151866.267(20413.814)	149104.545(28022.56)
palmitic acid	83826.745(26436.792)	87530.236(29254.435)	78853.8(20183.079)	95229.136(29710.987)
palmitoleic acid	620.618(273.823)	620.933(267.671)	539.233(161.287)	621.273(308.745)
pelargonic acid	29902.833(10040.315)	30430.506(13250.889)	27361.5(8305.543)	30370.318(15237.921)
pentadecanoic acid	10300.402(2114.862)	10098.079(2516.636)	10342.033(1748.35)	9354.273(2624.098)
phenylalanine	21140.618(6021.369)	22473.629(6495.431)	22696.967(5996.417)	21185.773(6871.203)
phosphate	62360.137(25668.008)	60891.899(24903.713)	49586.167(19929.948)	49008.818(18344.709)
phthalic acid	6103.99(2526.222)	6071.337(3064.102)	5674.333(1828.173)	5568.409(1745.246)
proline	10358.696(7248.838)	10114.865(6954.499)	10550.8(6458.906)	11675.364(9101.36)
pseudo uridine	2775.873(653.848)	2855.146(716.503)	2624.267(575.854)	2690.227(586.367)
pyrrole-2-carboxylic acid	6415.049(4040.235)	5793.022(3390.2)	7241.433(4396.871)	5650.227(3767.956)
pyruvic acid	11489.667(4788.685)	10820.404(3860.672)	10639.933(4399.941)	10582.455(3545.42)
quinic acid	1272.48(1447.647)	1600.753(1769.131)	1429(1579.146)	1518.5(1932.734)
ribonic acid	873.931(245.494)	868.337(240.982)	862.433(246.645)	871.364(191.653)
ribose	2038.549(602.463)	2037.371(644.28)	2244.6(593.871)	1938.818(556.346)
salicylic acid	4293.333(14512.238)	2853.427(9490.954)	3498.4(9108.574)	2155.591(2848.722)
serine	37492.01(17259.952)	38555.775(15218.55)	33113.867(10563.558)	31679.045(12074.469)
stearic acid	378059.412(154306.997)	405425.36(162088.008)	344273.167(88753.876)	453855.773(203272.896)
succinic acid	2428.686(828.589)	2106.888(729.61)	2389.367(734.142)	2090.091(598.59)
sucrose	671.637(698.395)	613.989(381.592)	497.833(356.559)	549.409(306.587)
tagatose	4063.725(4123.989)	3589.213(2553.245)	5558.5(6116.983)	3367.909(1537.732)
threitol	1452.196(807.611)	1395.584(582.087)	1310.2(502.671)	1403.682(495.623)
threonine acid	8560.99(4195.661)	7285.618(3051.907)	8462.167(4569.948)	6538.318(2072.396)
threonine	13282.686(4817.033)	14237.438(5929.372)	13394.9(4012.612)	11896.455(3512.857)
trans-4-hydroxyproline	1700(1224.851)	1418.764(658.035)	1473.1(800.435)	1561.409(907.394)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
tryptophan	21152.706(10249.693)	21495.079(8899.268)	22440.033(11228.94)	21921.636(9411.156)
tyrosine	42719.343(12721.061)	44217.124(10941.659)	46640.2(12129.286)	44423.773(14246.354)
urea	785114.216(265741.232)	831665.056(279983.579)	857524.633(295241.831)	812000.364(302001.423)
uric acid	32108.833(16219.644)	33489.944(17068.328)	39065.5(16178.005)	44843.591(20740.081)
valine	79110.618(21747.997)	82792.506(32138.457)	87038.933(22924.252)	86977.545(23467.177)
Biogenic Amines (BA)				
(2R)-3-Hydroxyisovalerylcarnitine	1880.687(1046.064)	1825.6(555.898)	2216.153(1479.725)	2020.16(485.95)
(3-Carboxypropyl)trimethylammonium cation	16403.7(5302.415)	17555.878(5550.678)	18315.149(4992.706)	19457.256(6639.8)
(R)-Butyrylcarnitine	34078.718(15321.062)	37105.876(16533.628)	34054.963(11538.003)	39881.617(17704.327)
.beta.-Phenyl-.gamma.-aminobutyric acid	869.907(2440.04)	709.92(241.154)	1395.481(4429.338)	674.478(152.987)
.epsilon.-Caprolactam	87755.933(68018.05)	89742.427(68532.183)	91071.996(63510.75)	103113.184(73798.78)
1,2-Dimethylimidazole	1819.366(2845.633)	1694.49(1032.734)	1313.473(387.35)	1482.894(382.59)
1-Acetyl-3-piperidinamine	1839.3(818.798)	1738.972(605.781)	1809.168(842.991)	1847.71(814.279)
1-Acetyl-4-piperidinamine	2047.585(2838.897)	1533.704(815.512)	2206.801(4128.195)	1525.61(864.511)
1-Methyladenosine A	4344.676(1038.43)	4455.103(1138.778)	4148.434(927.249)	4504.597(1073.83)
1-Methyl-L-histidine	22958.602(14651.539)	23284.637(14336.386)	24361.203(14767.623)	22395.266(14669.359)
1-Methylnicotinamide	14470.114(11101.857)	14251.823(7589.804)	14589.447(14339.977)	13557.656(6497.407)
1-Monostearin	2115.305(1451.321)	2830.121(4236.602)	1971.864(1270.58)	3537.597(7784.916)
1-Oleoyl-2-acetyl-sn-glycerol	9191.209(8932.606)	14964.193(39026.124)	7681.703(3487.146)	8892.076(5409.579)
1-Oleoyl-sn-glycero-3-phosphoethanolamine	6355.005(5324.408)	6525.509(3772.709)	6956.948(4541.941)	7103.671(4996.319)
1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	6410.996(4032.932)	6606.582(3360.162)	6163.435(3492.196)	6370.52(3815.333)
1-Phenylpyrrolidine	143.457(290.638)	117.902(39.385)	104.738(33.627)	109.069(31.742)
1-Stearoyl-2-arachidonoyl-sn-glycero-3-phospho-(1'-myo-inositol)	1329.25(881.122)	1346.97(825.295)	1135.548(673.987)	1260.022(763.463)
1-Stearoyl-2-arachidonoyl-sn-glycero-3-phosphoserine	1894.838(2682.073)	1778.287(2056.277)	1984.471(2882.826)	1292.586(2080.799)
1-Stearoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	6094.917(4604.091)	5803.43(2687.326)	5769.144(3586.285)	5879.906(3426.172)
2,2',2''-Nitrilotriethanol	4650.025(6102.206)	5725.159(8642.651)	3093.909(1373.507)	3092.362(1222.395)
2,2-Bishydroxymethyl]-2,2',2''-nitrilotriethanol	661.365(1011.212)	683.907(582.601)	504.164(167.032)	544.009(244.754)
2,6-Diaminopimelic acid	658.783(580.92)	497.274(446.965)	612.84(577.376)	463.019(425.204)
2-Amino-1-phenylethanol	50064.106(14796.501)	51939.812(12195.207)	53117.104(15609.813)	50826.745(8569.221)
2-Hydroxyibuprofen	3646.161(11203.95)	2794.402(8390.204)	5805.907(18963.666)	3191.473(3646.479)
2-Indolinone	22360.698(11782.007)	25707.648(13967.826)	20038.083(9954.332)	26672.588(12457.185)
2-Methylbutyryl-L-carnitine	15742.272(6758.335)	19766.912(10894.625)	19399.619(6037.212)	27277.009(16122.643)
3-(1-Pyrazolyl)-alanine	358.412(1009.805)	338.461(595.673)	444.536(1499.442)	145.964(107.017)
3,4-Dimethoxybenzaldehyde	2111.85(1817.258)	2433.796(3874.558)	1834.215(1232.77)	2391.884(1909.925)
3,5-Dihydroxyphenylglycine	1521.258(1937.934)	1263.783(1225.374)	1006.321(944.252)	1019.377(876.383)
3-Amino-1-propanol	14759.177(17371.398)	11356.849(7175.122)	11940.636(10489.283)	13610.142(9745.729)
3-Aminoquinoline	2768.697(3284.974)	3229.232(3720.884)	2248.4(3315.861)	1846.773(2416.041)
3-Cysteinylacetaminophen	85.628(278.461)	31.56(22.915)	82.88(208.911)	29.864(23.752)
3-Dehydrocarnitine	2713.916(1241.044)	2870.766(1231.212)	2760.503(1046.042)	3709.729(1647.21)
3-Hydroxybutyrylcarnitine	3061.608(2849.628)	2805.221(2351.317)	2483.169(1959.092)	2907.379(3379.792)
3-Hydroxyyleylcarnitine	1499.787(2022.956)	1253.212(1804.396)	1795.047(2242.635)	1631.204(2049.684)
3-Hydroxypyridine	1971.739(3569.602)	3209.464(4987.632)	3107.58(4774.692)	2783.136(3641.25)
3-Methylglutaryl-L-carnitine	575.563(258.16)	1052.615(1965.769)	581.926(186.861)	2266.461(3737.928)
3-Methylxanthine	555.738(650.872)	522.536(446.424)	447.077(542.331)	379.653(297.53)
3-Pyridinemethanol	1549.304(1050.899)	1769.148(2316.24)	1472.138(798.518)	1562.799(826.931)
4,5,7-Trihydroxyisoflavone	507.397(2564.172)	124.958(731.854)	381.52(1786.633)	35.467(27.31)
4-Acetamidobutyric acid	3471.712(2342.69)	3727.521(2854.822)	3138.805(2005.327)	3073.521(1261.264)
4-Aminomethylcyclohexanecarboxylic acid;	1589.572(3239.52)	1326.667(747.566)	2026.6(5105.699)	1335.892(818.481)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
4-Fluoro-.alpha.-pyrrolidinobutiophenone	532.638(610.097)	458.298(230.627)	482.19(514.486)	455.718(245.117)
4'-Methyl-N-methylhexanophenone	2337.883(2599.719)	2483.552(2368.085)	2152.606(2551.192)	1993.683(1700.874)
4-Pyridoxic acid;	9506.692(32185.74)	3611.761(6927.589)	8220.902(16890.138)	3016.675(5158.128)
5'-S-Methyl-5'-thioadenosine	2295.417(2441.494)	2541.641(1775.543)	1890.319(1403.725)	2189.236(1572.54)
5'-S-Methylthioadenosine	2232.692(2448.886)	2396.981(1900.293)	1913.232(1406.276)	2137.052(1630.408)
6-Hydroxyflavone	1191.845(6678.29)	403.876(528.261)	518.379(1097.162)	560.039(783.568)
6-Methoxynaphthaleneacetic acid	7862.951(2449.945)	9327.172(12784.412)	7113.733(2144.366)	13102.675(25676.836)
7.alpha.-Hydroxy-3-oxo-4-cholestenoic acid	7832.128(4085.847)	7971.016(3525.274)	7468.86(3109.447)	8324.788(4240.242)
7-Hydroxywarfarin	256.276(1326.793)	125.152(55.26)	116.55(56.018)	138.344(63.514)
7-Methylguanosine	2894.162(982.806)	3126.746(1088.991)	2694.095(896.384)	2989.712(795.094)
Acetazolamide	111.881(1032.576)	10.68(5.05)	347.176(1882.338)	10.069(5.423)
Acetaminophen	8598.401(25412.26)	1888.819(3095.431)	8444.362(18580.227)	1685.388(1372.342)
Acetyl-DL-carnitine	4040.595(1781.273)	3886.498(1192.6)	3760.285(1568.718)	3744.798(1143.026)
Acyclovir	10042.642(38991.986)	102.244(109.125)	2295.767(12376.951)	111.839(112.139)
Adenosine	476.693(252.498)	554.001(724.574)	474.724(331.211)	376.975(167.302)
Ala-Ile	1117.937(531.714)	1022.708(379.234)	1034.968(513.869)	1023.066(417.073)
Albendazole	1404.595(9285.314)	342.564(133.753)	308.753(93.125)	303.945(99.669)
Albendazole sulfoxide	556.474(1732.254)	706.284(5840.411)	319.695(648.762)	71.077(95.162)
alpha-Methylhistidine;	18823.314(15559.922)	19428.048(15625.399)	20695.432(17703.776)	16585.549(13746.526)
Alprazolam	219.224(700.569)	79.36(42.975)	241.657(561.562)	87.916(39.751)
Aminodiphenylmethane	10035.44(39641.241)	4831.419(12787.502)	16787.772(68991.233)	3672.393(5242.794)
Androstan-3-ol-17-one 3-glucuronide	1018.393(816.112)	997.46(700.178)	1167.323(968.235)	1303.702(721.195)
Arginine	66971.722(30497.565)	63686.741(31676.786)	58680.054(21893.801)	54207.753(41849.9)
Atenolol	2831.445(26482.196)	235.929(152.586)	8876.504(48274.063)	217.071(141.065)
Atorvastatin	310.188(170.392)	307.876(96.997)	265.621(91.484)	303.006(75.916)
Avobenzone	1620.013(901.713)	2204.034(6233.272)	1606.788(1101.309)	4325.933(12543.351)
Benthiavalicarb-isopropyl	397.898(475.323)	338.666(425.872)	422.91(531.603)	323.732(173.396)
Benzophenone-3	79.42(118.399)	152.05(480.887)	45.504(25.274)	76.466(105.947)
Betaine	1396162.001(400978.201)	1465520.587(366608.787)	1487617.048(330781.755)	1613346.38(409960.194)
Betaine aldehyde cation	14682.235(107622.215)	56.189(19.083)	353.14(1704.805)	54.492(16.838)
Betonicine	5018.889(9595.989)	5425.561(9356.727)	6823.043(14396.209)	3025.475(3011.925)
Biliverden	37882.387(29682.943)	38990.463(24851.237)	43941.398(31844.437)	49271.595(33601.845)
Borrelidin	1800.784(4109.912)	1698.556(4228.984)	1624.211(3717.448)	2458.108(5005.844)
Bradykinin	2350.694(4905.075)	2102.181(4523.581)	3035.61(6439.022)	1559.314(3617.7)
Caffeine	46358.68(97388.926)	86219.943(115602.167)	58323.446(101321.084)	67997.582(107285.396)
Carbamazepine	424.616(1432.071)	11883.366(108750.28)	539.159(2013.135)	313.112(551.69)
Carnitine	1001164.333(283021.215)	1045982.351(310270.412)	1072754.451(265918.791)	1184452.8(372756.681)
Choline cation	254611.526(57164.648)	282373.342(63913.774)	251280.707(55478.214)	287961.893(70052.064)
cis-10,11-Dihydroxy-10,11-dihydrocarbamazepine	525.109(153.075)	959.717(3818.829)	474.129(106.838)	541.899(169.458)
Citrulline	19901.677(6196.281)	21504.169(6882.343)	18626.854(5812.245)	18537.558(4959.491)
Codeine-6-.beta.-D-glucuronide	774.993(5522.859)	232.532(91.583)	204.544(67.41)	223.963(55.908)
Coniferylaldehyde	765.911(462.54)	787.668(824.323)	759.192(660.787)	640.38(159.462)
Cotinine N-.beta.-D-glucuronide	76.449(283.47)	46.197(159.887)	119.894(388.398)	91.857(309.006)
Creatine	217981.51(118303.317)	203650.285(97913.88)	168130.821(90371.637)	139833.974(77604.487)
Creatinine	1006729.671(287698.034)	1029213.304(254200.686)	1096649.707(244986.626)	1103471.185(282335.148)
Cyclo(Leu-Pro)	2228.564(1706.261)	2027.347(1104.514)	1920.108(1199.64)	2104.435(1326.657)
D-.alpha.-Cyclohexylglycine	6326.782(6206.867)	8327.262(8211.34)	4846.795(3573.209)	8695.348(6650.099)
Decanoyl-L-carnitine	42146.5(48589.406)	42071.952(30458.853)	43929.706(33843.773)	34261.014(17509.83)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
D-erythro-Sphingosine-1-phosphate	7295.174(3378.972)	7543.128(3687.008)	7479.43(3924.057)	5932.01(3771.74)
Dexpanthenol	1546.048(2341.347)	2108.653(3911.294)	2026.092(4164.98)	1250.989(588.431)
D-Fructose	34526.336(8214.427)	34866.41(9180.115)	32826.06(8617.741)	33012.635(8535.76)
Diazepam	370.721(2360.704)	46.476(76.296)	409.32(2010.804)	39.081(14.492)
Dinor-12-oxophytodienoic acid	525.23(862.885)	416.42(194.711)	346.537(159.282)	388.334(193.145)
Diphenhydramine	2585.349(6127.955)	3178.366(14715.458)	3164.351(9467.176)	1543.357(247.978)
DL-Indole-3-lactic acid	37199.448(18913.594)	35604.136(12065.446)	36817.529(14023.849)	36460.735(8849.131)
D-Pyroglutamic acid	121612.569(22366.016)	123013.056(24064.978)	117418.865(17444.755)	114737.442(19860.385)
D-Turanose	525.908(351.452)	631.074(581.896)	539.308(503.012)	697.345(817.216)
Ergothioneine	767.24(1494.771)	719.663(431.749)	1060.01(2646.243)	648.864(369.92)
Esomeprazole	2660.51(10721.074)	1307.945(4540.326)	940.882(1089.34)	785.266(268.594)
Ethiolat	11862.296(20760.107)	9779.989(18228.881)	12251.146(15922.411)	8966.66(6778.225)
Ethylidethanolamine	734.979(766.768)	727.196(595.857)	625.582(311.265)	550.606(203.917)
Ethylenediaminetetraacetic acid	663091.766(891136.229)	496339.244(788805.165)	560672.877(771465.86)	405282.259(695244.459)
Ezetimibe	223.611(238.157)	234.24(306.197)	190.923(100.856)	221.715(122.08)
Fexofenadine	450.355(238.197)	841.091(3125.726)	461.362(376.699)	414.397(109.942)
Gabapentin	62080.105(201779.015)	5287.117(32734.04)	54718.015(214648.278)	16262.541(66113.057)
Glaucine	860.63(2849.169)	574.959(169.559)	510.08(130.422)	572.313(156.493)
Glutamic acid	7933.975(3124.287)	7180.498(3426.266)	8510.012(3553.203)	8386.114(4841.512)
Glutamine	101505.785(19190.477)	102907.791(20574.24)	98008.205(15454.429)	95703.445(17465.874)
Glycocholic acid	4874.144(5532.195)	3707.728(3340.534)	4964.843(5295.367)	3300.934(3738.019)
Glycodeoxycholic acid	16574.334(17400.385)	14780.84(19064.118)	18685.87(18675.775)	16809.144(24970.091)
Gly-Pro-Arg	586.043(2198.483)	428.808(1170.147)	1030.467(2528.87)	392.486(1136.9)
Guanidine	5493.87(8781.142)	4475.798(4190.121)	3940.816(2612.878)	3564.317(1070.149)
Guanine	6226.314(23441.739)	279.003(1082.414)	1534.53(7790.221)	618.926(2174.504)
Heptadecaphing-4-enine	5557.437(4651.009)	5538.189(4468.342)	5627.805(4067.451)	6702.555(4438.514)
Hexanoyl-L-carnitine	8996.499(13556.537)	8356.705(5002.169)	8053.024(5313.882)	7430.25(2863.103)
H-gamma-glutamyl-glutamine	2339.192(1792.988)	2006.339(1305.502)	1863.303(1081.189)	1764.231(1439.13)
Histidine	49555.943(23320.509)	53178.919(21745.875)	50279.091(20666.114)	47751.945(24317.713)
Homoarginine;	3381.815(2097.316)	3026.593(2160.863)	3253.114(1935.796)	2749.911(2846.298)
H-Pro-Hyp-OH	2228.15(1753.581)	1756.456(871.446)	1919.935(987.366)	1810.289(843.778)
Hydroxybupropion	884.813(2016.341)	1883.832(8028.514)	695.159(1429.329)	3606.341(14643.461)
Hypoxanthine	31281.328(19491.261)	30486.398(22288.554)	31894.543(18046.395)	35685.752(36498.809)
Ile-Glu-Arg	365.728(1522.667)	320.225(998.515)	548.839(1287.857)	163.108(392.16)
Indole-3-propionic acid	1220.413(1004.075)	1438.512(994.93)	1048.48(1217.539)	1401.494(1119.532)
Irbesartan	34111.466(330125.328)	1632.597(1008.364)	1303.444(269.683)	1529.481(244.582)
Isoleucine	15404.33(5244.539)	15607.18(5393.939)	16744.473(5599.589)	16930.963(4800.484)
Isopentenyladenine	1014642.651(399845.125)	1046922.522(370983.691)	974541.979(346896.356)	1018471.203(447527.278)
Isopropylamine	4749.851(1414.044)	5211.39(1333.561)	4602.906(1194.634)	5310.815(1590.676)
Kynurenine	2125.376(754.54)	2313.805(749.317)	2287.602(798.757)	2399.838(864.647)
Lamotrigine;	2244.641(22565.331)	18.464(16.389)	21.207(17.446)	18.228(13.363)
Lansoprazole	736.475(4048.63)	2665.031(13708.313)	152.966(606.74)	2157.927(9897.333)
Lauric acid diethanolamide	413.111(567.669)	345.335(216.443)	331.313(185.283)	400.649(247.413)
Lauroyl-L-carnitine	5784.303(4911.391)	6763.368(3908.375)	5906.628(3991.35)	6970.996(3697.297)
L-Carnitine	16079.975(4595.436)	15890.768(4307.224)	16745.605(4396.915)	16915.351(4585.871)
L-Citrulline	20161.291(5985.134)	21758.529(6402.073)	18969.814(5632.898)	19103.265(5057.045)
L-Cysteine-glutathione disulfide	1116.696(1162.972)	1224.484(1444.167)	885.604(985.658)	827.062(1212.613)
L-Cystine	2137.312(1969.911)	2271.747(2210.344)	1735.631(2208.461)	1722.462(2155.587)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
Levocetirizine;	9007.024(38087.67)	5404.405(22513.101)	7269.781(25502.991)	2180.98(9095.237)
Linoleoylcarnitine	6028.057(4694.504)	6937.757(5240.418)	6346.627(4037.73)	5743.351(6436.512)
L-Leucine, methyl ester	936.172(1279.128)	734.385(675.979)	1150.202(1821.508)	755.012(515.461)
Losartan	1124.145(6579.061)	2289.546(19221.441)	3140.895(11879.237)	270.189(131.167)
L-Threonine	6399.383(2197.795)	6434.59(1928.87)	6003.824(1480.482)	5976.646(1817.305)
L-Tyrosine	3214.55(1382.508)	3345.219(1261.579)	3268.273(1191.538)	3535.471(914.006)
Lysine	24048.561(14481.217)	23142.646(14133.037)	19317.883(8558.758)	19596.435(15871.555)
Matrine	2325.219(12579.91)	500.431(207.181)	422.143(164.006)	459.304(208.897)
Mefenorex	622.656(716.718)	3807.946(26441.59)	595.937(466.432)	13510.497(53201.397)
Meloxicam	28306.258(195269.072)	12851.881(121675.611)	52622.731(273406.929)	20.812(20.718)
Meprobamate	1573.996(3579.443)	932.297(1488.818)	2276.967(5504.175)	967.128(668.927)
Metformin	7135.099(48045.124)	3475.203(23828.338)	797.504(248.925)	853.039(281.844)
Methacholine cation	56501.078(33409.327)	67485.057(42836.21)	49193.762(28844.926)	76916.401(76696.421)
Methionine	6161.544(1634.068)	6223.87(1770.355)	6452.099(1526.628)	6153.806(1527.667)
Methioninesulfoxide	753.827(372.4)	693.081(379.811)	719.037(296.389)	574.306(201.898)
Methylgallate	139.383(458.151)	67.958(251.269)	92.591(233.625)	54.513(124.446)
Metoprolol	897.413(4862.805)	234.563(653.184)	644.411(1749.197)	155.342(47.167)
Metoprolol acid	7786.566(33910.371)	535.074(2767.371)	13530.901(43913.642)	224.357(75.422)
Milnacipran	276.882(1331.735)	148.067(53.863)	131.117(45.911)	137.972(56.141)
Modafinil	1075.48(6709.26)	71.168(24.162)	1584.725(8476.699)	74.36(23.117)
Modafinil acid	131.611(721.079)	24.78(13.35)	229.527(1164.351)	28.115(13.217)
Montelukast-1,2-diol	75.941(301.129)	84.645(479.266)	92.183(360.641)	40.416(63.232)
Moxonidine	3500.133(2726.862)	3040.75(1987.891)	3512.588(2637.755)	2765.278(2288.019)
N-(3-(Aminomethyl)benzyl)acetamidine	20921.024(28034.826)	18034.449(15522.733)	19747.783(31368.924)	17082.579(11372.308)
N-.alpha.-Acetyl-L-arginine	3082.187(1181.981)	3213.461(1045.445)	3168.06(1190.142)	3153.484(909.352)
N.alpha.-Methyl-L-lysine	29306.073(114182.748)	13134.602(36620.029)	33229.507(141404.266)	24119.706(73255.747)
N.epsilon.-Acetyl-L-lysine	2453.841(2107.986)	2280.92(1269.094)	2108.882(867.284)	2040.458(470.561)
N.epsilon.-Methyl-L-lysine	8975.039(6927.428)	8793.019(6711.352)	8292.549(6781.832)	7273.656(4787.515)
N8-Acetylspermidine	3001.558(1211.178)	2900.086(896.957)	3280.799(1509.793)	3050.834(1076.603)
N-Acetylaniline	707.391(950.515)	582.675(496.092)	510.307(440.215)	470.09(436.636)
N-Acetyl-D-norleucine	3757.634(3749.095)	3860.092(3382.148)	2860.983(3022.584)	2986.29(1886.514)
N-Acetylhistidine	1008.892(648.298)	1039.722(610.487)	960.013(520.722)	1001.798(354.107)
N-Acetyl-L-carnosine	2954.051(1639.621)	2926.55(1628.741)	4343.277(2037.336)	4394.072(1977.762)
Naproxen	3476.065(13446.579)	4450.949(22153.769)	6828.729(21324.608)	1074.083(948.624)
NEPSILON,NEPSILON,NEPSILON-TRIMETHYLLYSINE	13358.236(4821.32)	15219.514(11953.152)	15162.463(5272.414)	20382.701(20875.919)
N-Methylhistidine	35730.75(37645.645)	33537.29(29498.297)	48506.34(43091.365)	37824.633(33591.229)
N-Methylproline	11656.687(9296.226)	11510.001(9904.91)	11431.935(9358.647)	10435.242(7514.82)
Norleucine	15444.661(6060.568)	15678.34(4128.345)	17320.35(8087.398)	16653.99(4344.55)
Nudifloramide	64111.911(56284.553)	63703.328(37012.76)	76245.487(88924.622)	64712.387(44054.616)
Octanoylcarnitine	46353.596(55972.637)	47100.775(29066.033)	44515.865(29817.486)	39444.681(17158.127)
Oleoyl-L-carnitine	10823.414(8463.672)	11676.244(8434.192)	11041.169(8296.771)	9716.931(8299.466)
Omeprazole sulfone	4929.053(23929.418)	1843.877(13957.834)	1742.513(8252.115)	1063.989(4185.411)
Omeprazole sulfone N-oxide	1165.746(5101.882)	421.937(2441.309)	619.489(2330.734)	332.765(1098.976)
Ondansetron	365.61(1271.909)	240.115(62.33)	214.354(50.086)	231.076(39.312)
Ornithine	3959.933(2287.816)	4022.624(2665.327)	3568.97(1869.763)	3451.224(2722.453)
p-Acetamidophenyl .beta.-D-glucuronide	766.028(3177.057)	171.088(73.211)	561.283(1491.047)	168.884(79.134)
Palmitamide	3270.611(17777.123)	1962.253(8761.313)	841.234(872.513)	870.961(440.581)
Pantoprazole	898.088(8152.763)	16270.845(118825.791)	80.935(57.003)	18187.304(84924.38)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
Pantothenic acid	10030.786(7968.504)	8465.694(5284.919)	9809.103(7101.967)	7811.894(5772.281)
Penciclovir	615.263(2184.586)	280.151(80.439)	308.135(294.352)	265.322(73.998)
Phenylacetylglutamine	31218.152(22442.043)	34681.21(38768.962)	27420.047(17582.075)	30199.641(21041.081)
Phenylacetyl-L-glutamine	14884.784(10785.176)	16607.075(17719.928)	13216.22(8436.638)	14012.479(8810.894)
Phenylalanine	55973.85(16422.42)	58120.533(13302.726)	59297.418(17189.557)	56671.711(9124.259)
Pipecolic acid	425.09(586.911)	426.157(508.716)	431.518(877.242)	302.227(121.702)
Piperine	5718.294(8337.056)	7720.583(10963.746)	6370.124(10079.811)	10438.647(18064.942)
Prazepam	288.862(1542.242)	137.608(93.414)	130.413(68.935)	142.665(89.484)
Proline	14486.098(6367.337)	14482.522(5997.29)	14659.894(4262.202)	16833.462(6254.299)
Propionylcarnitine	68344.79(23209.488)	71041.55(26326.498)	75008.185(23173.021)	89574.261(34012.594)
Pyrantel	372.256(111.716)	1129.226(7044.272)	342.836(86.954)	377.493(85.041)
Pyridoxal	1642.179(3991.664)	946.29(438.171)	982.176(620.401)	884.975(226.448)
Pyridoxine;	1022.88(4388.483)	435.057(382.972)	398.684(340.458)	537.032(492.771)
Quetiapine	369.86(1339.4)	222.872(66.167)	634.982(2421.885)	218.621(45.738)
Quetiapine sulfoxide	650.477(4802.113)	136.563(42.808)	1683.355(8722.602)	136.332(28.26)
R(-)-O-Desmethylvenlafaxine	592.445(3164.213)	410.727(1880.497)	132.984(43.917)	865.333(3450.186)
rac-4-Sulfoxypropranolol	202.948(514.821)	151.335(57.243)	296.812(933.899)	144.592(44.507)
Ranitidine	2507.731(13468.136)	205.008(53.061)	3646.768(16884.028)	200.279(51.505)
Ranitidine N-oxide	713.593(4219.564)	62.623(17.85)	1462.938(7212.987)	64.225(16.737)
Ranitidine-S-oxide	213.634(515.841)	132.212(90.781)	372.742(891.461)	127.054(63.583)
Scopoletin	591.68(2509.742)	178.452(414.272)	366.114(1387.719)	135.721(167.27)
SDMA	9500.368(2703.971)	10370.308(2765.049)	8784.935(2463.706)	9662.784(2984.059)
Serotonin	18189.163(41222.489)	14668.474(23684.703)	27097.392(68656.868)	18703.44(37627.043)
Ser-Tyr-Lys	193.809(988.093)	91.613(175.965)	215.559(610.064)	52.627(33.116)
Stachydrine	563959.448(691819.57)	612164.26(685817.817)	509241.63(665509.328)	483091.828(533375.278)
Sulfamethoxazole	41.919(48.984)	4622.278(43440.039)	42.114(60.452)	51.453(64.423)
Tapentadol-.beta.-D-glucuronide	221.214(1394.74)	127.85(761.689)	638.067(2521.067)	66.867(90.138)
Tauroursodeoxycholic acid	2706.846(6111.732)	1545.619(2380.983)	2771.642(7467.22)	2383.357(4356.385)
Telmisartan	4699.894(41335.897)	3856.6(30518.071)	561.231(207.047)	637.336(209.82)
Temazepam	279.199(1061.022)	153.782(115.023)	131.371(55.789)	174.98(204.841)
Testosterone	3622.17(4140.278)	4445.438(4912.789)	3526.184(3539.749)	3995.656(3766.305)
Theanine;	1819.454(2742.739)	1366.781(1424.619)	1079.488(1156.863)	974.3(970.032)
Theobromine	43840.022(50239.28)	50274.237(39008.573)	46380.263(58049.085)	38899.333(35511.114)
threo-Dihydrobupropion	959.671(1263.114)	899.034(1318.122)	934.373(1403.161)	901.716(1243.618)
Thr-Ile-Arg	334.018(1580.162)	174.397(391.703)	413.161(1122.966)	130.527(181.492)
Ticlopidine	228.217(1202.183)	52.712(180.862)	113.045(523.142)	76.163(217.135)
Topiramate	883.512(3767.87)	360.884(470.487)	413.497(620.452)	344.367(122.878)
Toradol	356.538(2066.064)	150.603(104.488)	126.775(63.646)	156.815(114.02)
trans-3'-Hydroxycotinine	2268.615(10601.908)	1686.299(5203.465)	4673.366(18723.658)	2696.057(7842.329)
Trazodone	2672.469(13819.619)	206.455(55.025)	194.336(89.539)	199.693(47.225)
Tri-2-ethylhexyl trimellitate	6954.814(58249.323)	2150.885(4550.116)	20270.058(106147.287)	870.01(683.104)
Trigonelline	62593.319(128404.523)	87574.388(113723.624)	52780.293(86138.21)	67552.649(79770.613)
Trileptal	378.242(124.735)	1737.665(13037.79)	344.273(109.505)	341.202(87.944)
Trimethoprim	234.855(71.982)	2512.23(21564.074)	222.236(59.463)	247.22(56.674)
Trimethylamine-N-oxide	22496.762(34083.237)	15784.326(13954.105)	16615.634(19022.479)	20017.457(21030.643)
Triptolide	572.071(359.723)	709.428(1341.517)	487.897(172.496)	562.15(187.996)
Tryptophan	15719.222(4762.968)	15591.457(4927.165)	16208.348(4590.48)	17268.208(4363.797)
Tyrosine	6484.429(2346.848)	6649.41(2125.156)	6743.986(2343.539)	6738.398(1629.213)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
Urea	128763.489(48161.656)	135736.88(41188.088)	128740.698(43060.26)	146833.554(47651.964)
Urocanic acid;	20103.21(25401.881)	20113.659(16158.372)	16277.246(8743.394)	14697.149(5539.213)
Usnic acid	6421.074(38109.236)	5909.508(26905.817)	14896.56(69459.594)	3256.747(4748.431)
Complex Lipids (CL)				
AC (10:0)	14300.667(14495.722)	14592.903(12632.497)	14304.284(10224.154)	12288.294(6811.885)
AC (10:1)	7852.356(5661.808)	8700.584(5463.897)	8213.231(4726.31)	8068.959(3635.011)
AC (12:0)	6801.104(4854.843)	7472.708(4034.354)	7161.583(4461.614)	7599.974(4309.822)
AC (12:1)	5342.259(2975.805)	5782.079(2495.997)	5565.666(2940.647)	5789.9(2652.02)
AC (14:1)	7653.305(5643.002)	7865.258(4525.933)	7610.733(4887.504)	7827.739(4591.044)
AC (14:2)	4537.778(3261.62)	5105.633(2880.79)	4547.041(2451.901)	5085.062(3183.104)
AC (16:0)	10907.214(3516.947)	10958.197(3206.646)	12529.657(4062.832)	12020.615(3789.727)
AC (18:0)	4409.46(1523.433)	4658.607(1398.628)	4818.758(1531.186)	5082.356(1672.108)
AC (18:1)	15169.411(6563.264)	14716.482(4589.592)	16670.1(7066.335)	15289.944(4633.514)
AC (18:2)	9086.774(4258.756)	9507.785(3723.066)	10579.98(4543.181)	10453.403(4548.995)
AC (8:0)	5424.664(7636.621)	5324.659(5489.183)	5051.415(3488.917)	4233.297(2281.491)
CE (14:0)	483.105(328.13)	550.26(299.965)	398.792(237.464)	498.482(320.195)
CE (16:0)	6284.196(5322.107)	5971.764(4027.806)	5416.936(4207.504)	5710.329(5150.448)
CE (16:1)	44723.031(22333.233)	45240.669(19130.581)	40481.212(23152.954)	46143.111(21363.158)
CE (18:0)	3286.85(1793.581)	3220.682(1502.875)	3379.625(1881.442)	3107.244(1303.777)
CE (18:1)	32176.362(13035.556)	33019.476(10977.599)	29369.279(12439.441)	30481.628(12865.088)
CE (18:2)	360370.43(102450.354)	395504.729(97524.484)	346900.748(96985.256)	353681.03(90607.595)
CE (18:3)	13226.28(5296.356)	16158.621(6188.509)	12466.078(5278.865)	16585.743(8232.324)
CE (20:2)	7353.518(4456.574)	8560.232(3729.559)	7045.581(3784.452)	7534.769(3979.312)
CE (20:3)	65342.381(23690.393)	72249.761(24364.326)	61512.354(23895.339)	66312.322(25346.564)
CE (20:4)	760763.777(278873.716)	769431.808(251914.063)	726785.037(299621.635)	790941.454(349981.263)
CE (20:5)	17407.549(19917.453)	12423.777(8256.741)	13278.036(10259.439)	11114.096(5374.717)
CE (22:2)	686.936(506.637)	714.698(520.067)	712.355(524.213)	615.637(431.426)
CE (22:6)	132582.468(60465.938)	114384.853(39714.847)	116482.07(44378.479)	101025.826(39811.332)
Ceramide (d34:1) - ESI(+)	7991.308(2279.1)	7701.808(1766.753)	8731.306(2213.355)	7272.043(1338.049)
Ceramide (d36:1) - ESI(+)	5055.887(1639.5)	4781.199(1246.336)	5325.535(2032.287)	4351.407(1238.385)
Ceramide (d38:1) - ESI(+)	6696.998(1780.221)	6981.944(1458.36)	6775.581(2136.414)	6560.467(1627.061)
Ceramide (d40:1)	21686.844(5740.739)	23489.285(4735.334)	22330.201(7130.91)	23771.933(5214.261)
Ceramide (d41:1) - ESI (+)	6918.214(1876.08)	7517.217(1659.079)	6737.579(2156.907)	7100.762(1464.764)
Ceramide (d42:1) - ESI (+)	71508.239(18019.881)	78197.952(14457.978)	74834.162(21160.412)	80924.605(15962.261)
Ceramide (d42:2) A - ESI (+)	19273.129(4975.246)	18114.439(3325.542)	20767.903(5498.018)	17942.265(3500.693)
Ceramide (d42:2) B - ESI (+)	14981.161(4149.123)	17174.124(4245.274)	14761.732(4174.526)	16805.176(4803.723)
Ceramide (d32:1)	3595.683(1323.517)	3755.63(977.806)	3893.41(1681.704)	3776.339(1277.115)
Ceramide (d33:1)	2916.634(935.773)	3016.705(807.728)	2942.778(904.581)	3034.769(747.137)
Ceramide (d34:0)	4886.997(2053.157)	4687(1716.579)	5328.675(2353.493)	5038.817(1756.365)
Ceramide (d34:1) - ESI(-)	18074.154(4880.408)	17694.653(3936.635)	21181.657(5672.547)	18781.979(4018.654)
Ceramide (d34:2)	3094.181(847.888)	3030.248(713.119)	3178.801(912.631)	2792.248(603.107)
Ceramide (d36:1) - ESI(-)	1637.345(721.82)	1539.002(608.946)	1854.908(879.827)	1612.868(611.104)
Ceramide (d38:1) - ESI(-)	11993.384(4407.452)	12156.053(3738.061)	12800.634(5130.013)	12538.413(4226.451)
Ceramide (d39:1)	6299.483(2739.989)	6979.275(2440.541)	6345.302(3011)	7142.867(2313.623)
Ceramide (d40:0)	1765.181(1227.484)	1564.678(901.085)	1739.503(1153.507)	1839.717(1212.59)
Ceramide (d40:2)	6057.125(4179.286)	6235.898(4315.18)	6207.346(3283.457)	6671.962(4263.527)
Ceramide (d41:1) - ESI(-)	42041.811(15059.383)	46380.145(13427.707)	44430.29(17393.967)	48813.011(13659.64)
Ceramide (d42:0)	11948.609(7113.944)	11294.104(4976.297)	11854.292(6342.721)	13352.996(6212.231)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
Ceramide (d42:1) - ESI(-)	136674.648(44023.767)	149770.415(39576.94)	149813.191(54068.674)	161675.872(40939.304)
Ceramide (d42:2) A - ESI(-)	49252.166(17827.101)	47220.491(13180.04)	57453.828(23064.842)	51899.184(15072.465)
Ceramide (d42:2) B - ESI(-)	37317.754(16468.604)	35789.863(11255.565)	43922.069(20084.189)	38707.75(13373.343)
Ceramide (d43:1)	2528.23(1370.14)	2789.752(1196.521)	2538.392(1401.305)	3215.499(1522.097)
Ceramide (d44:1)	846.904(541.153)	822.512(399.283)	1043.492(779.49)	1004.782(528.397)
Cholesterol	266952.992(63543.111)	283483.733(67507.559)	285997.23(62624.153)	285744.734(56226.102)
DG (32:0)	2029.32(748.253)	1982.392(914.732)	2400.192(821.835)	2462.589(1230.819)
DG (32:1)	5251.897(3457.449)	4947.61(2880.584)	6255.949(3763.84)	6664.355(2949.793)
DG (34:1)	1041.038(494.395)	999.382(487.017)	1243.903(483.107)	1236.201(542.847)
DG (34:2)	32528.392(13807.47)	30539.842(13070.979)	40152.283(14881.321)	38721.383(12836.446)
DG (34:3)	5185.782(3045.124)	4572.847(2077.17)	5797.716(3186.568)	4848.035(1435.431)
DG (36:1)	6350.769(3167.505)	6121.406(3281.803)	7752.728(3894.885)	8344.677(3987.05)
DG (36:2)	55205.662(20357.43)	49677.788(17704.742)	61293.329(20082.532)	61274.639(20941.988)
DG (36:3)	70925.903(27194.121)	65340.022(22354.965)	80757.457(25808.489)	75739.062(24968.809)
DG (36:4) A	16838.454(8807.583)	16004.561(7408.839)	19737.663(9707.678)	17437.56(9172.99)
DG (36:4) B	4169.876(3637.695)	3516.148(2613.304)	4830.172(4215.821)	4879.996(2879.032)
DG (36:5)	2206.156(1211.632)	2086.253(902.788)	2673.737(1340.431)	2166.224(929.58)
DG (38:5)	10566.304(4064.74)	10089.518(3680.913)	11961.559(4159.269)	13525.081(3734.743)
DG (38:6)	6169.284(3104.712)	5407.065(2535.955)	6892.129(3426.167)	6867.647(2579.977)
FA (10:0) (capric acid)	1604.441(1050.232)	1407.005(1073.102)	1711.573(1201.227)	1464.917(1041.863)
FA (12:0) (lauric acid)	8080.776(5386.504)	8269.26(5625.99)	8720.65(4467.889)	8309.724(3064.579)
FA (14:0) (myristic acid)	46315.443(13985.33)	46285.78(10922.906)	44376.55(13454.821)	44448.11(9461.115)
FA (14:1) (physeteric acid)	5158.99(3232.701)	4681.581(1944.979)	3902.687(2378.069)	3845.25(2014.051)
FA (15:0) (pentadecylic acid)	10544.8(2976.688)	10266.457(2239.062)	10785.814(3247.999)	10590.402(2131.781)
FA (16:1) (palmitoleic acid)	87362.569(45359.632)	76933.028(35142.058)	70747.149(48110.445)	63019.939(30760.838)
FA (17:0) (margaric acid)	22117.789(4474.162)	21235.84(3887.35)	22869.638(3991.423)	21863.498(3317.04)
FA (18:1) (oleic acid)	1454192.087(480456.365)	1349284.059(394857.372)	1306371.124(516584.708)	1276084.64(395433.334)
FA (18:2) (linoleic acid)	573453.977(197151.585)	559405.212(162215.142)	544856.4(233611.766)	527836.688(188942.371)
FA (18:3) (linolenic acid)	52408.007(25261.774)	49568.813(16119.839)	55831.729(36074.175)	43953.469(17195.239)
FA (20:1) (eicosenoic acid)	18300.811(5932.05)	17239.139(4691.897)	16904.974(5422.633)	16890.944(5270.901)
FA (20:2) (eicosadienoic acid)	9414.386(2783.824)	9398.564(2656.075)	8843.47(3032.234)	8799.106(2886.371)
FA (20:3) (eicosatrienoic acid)	2064.852(782.798)	2106.53(696.017)	1996.96(870.894)	2343.651(765.021)
FA (20:3) (homo-gamma-linolenic acid)	9019.322(2564.168)	9232.52(2388.112)	9058.827(2904.539)	9812.517(2371.855)
FA (20:4) (arachidonic acid)	43084.156(11307.632)	45485.009(12124.954)	47682.842(11690.665)	53444.932(16109.434)
FA (20:5) (eicosapentaenoic acid)	7210.305(8172.735)	5310.154(4416.295)	8078.364(7113.727)	5541.467(2672.217)
FA (22:0) (behenic acid)	4796.588(1883.561)	4776.335(2235.782)	5374.917(2287.009)	5460.211(3363.174)
FA (22:6) (docosahexaenoic acid)	35785.158(23581.553)	31506.346(14537.092)	34229.371(17390.242)	30515.171(9235.535)
FA (24:0) (lignoceric acid)	9002.74(3316.901)	9144.823(3857.725)	10363.172(4148.816)	10735.801(5526.953)
FA (24:1) (nervonic acid)	3404.095(1062.601)	3216.118(871.277)	3844.766(1415.216)	3567.518(872.473)
Gal-Gal-Cer (d18:1/16:0)/Lactosylceramide (d18:1/16:0)	37250.999(11809.088)	37236.749(10987.775)	39221.61(9988.658)	37709.938(10657.275)
GlcCer (d38:1)	3730.008(1287.974)	3948.513(1065.45)	3870.099(1460.396)	3973.536(1169.578)
GlcCer (d40:1) - ESI(-)	22073.89(7846.193)	22731.523(6665.458)	24207.449(7897.39)	24139.711(7707.882)
GlcCer (d41:1)	12088.153(4455.943)	12743.895(4333.197)	13142.311(5064.807)	13889.254(5329.775)
GlcCer (d42:1) - ESI(-)	25575.096(9070.161)	26263.818(7929.532)	29150.83(9409.836)	29224.6(10141.294)
GlcCer (d42:2) - ESI(-)	19888.456(7749.181)	17973.465(6288.748)	22833.056(8776.62)	19931.828(8674.401)
GlcCer (d14:1(4E)/20:0(2OH))	6302.067(3492.07)	6460.128(3125.454)	5823.58(3024.058)	6538.001(3091.453)
GlcCer (d34:1)	7468.445(3751.415)	8251.003(4419.557)	8764.08(3833.514)	8680.226(3690.26)
GlcCer (d40:1) - ESI(+)	4100.143(1480.243)	4234.688(1219.049)	4181.685(1512.505)	4245.413(1271.567)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
GlcCer (d42:1) - ESI(+)	17983.989(6028.82)	18240.869(5395.163)	19140.873(5484.236)	19734.842(6590.648)
GlcCer (d42:2) - ESI(+)	13729.159(5608.295)	12051.673(4176.986)	14573.512(5583.067)	12112.285(5246.402)
Lactosylceramide (d18:1/24:1(15Z))	2755.733(1184.633)	2537.724(815.608)	2876.713(1454.383)	2535.727(853.264)
LPC (14:0) - ESI(-)	1816.114(1007.334)	2045.03(925.463)	1839.392(1099.666)	2245.535(950.128)
LPC (16:0) - ESI(-)	224092.722(72172.597)	240419.333(71704.173)	256854.719(83114.403)	277064.698(77293.971)
LPC (16:1) - ESI(-)	3256.883(1286.541)	3465.425(1194.712)	3321.019(1345.811)	3822.279(1168.9)
LPC (17:1)	2907.335(879.847)	2996.073(1096.874)	3037.551(915.572)	3394.649(1191.042)
LPC (18:0) A - ESI(-)	7418.389(3009.415)	8077.783(2590.056)	8306.305(3330.475)	8938.356(2422.212)
LPC (18:0) B - ESI(-)	99494.905(36134.374)	108242.985(32910.725)	112264.719(39798.755)	120387.288(29907.213)
LPC (18:1) - ESI(-)	47798.748(19375.801)	51591.653(19211.667)	54192.035(19358.272)	58439.57(20648.312)
LPC (18:2) - ESI(-)	60906.166(28020.858)	71522.652(31446.609)	73890.117(31899.667)	75457.741(34146.137)
LPC (20:0)	2602.173(1120.102)	2667.429(891.909)	2760.108(1224.082)	2701.178(881.013)
LPC (20:1) - ESI(-)	3013.633(1298.505)	2917.096(1050.301)	3170.145(1587.396)	3030.706(913.737)
LPC (20:1) - ESI(+)	713.456(419.647)	654.494(268.413)	825.423(510.424)	699.765(279.592)
LPC (20:2) - ESI(-)	4059.133(1281.292)	4450.809(1469.606)	4413.372(1573.531)	4565.117(1281.303)
LPC (20:2) - ESI(+)	518.937(285.076)	598.846(314.265)	590.84(340.026)	621.246(301.34)
LPC (20:3) - ESI(-)	3582.326(1705.034)	4021.253(1564.565)	4081.79(1899.384)	4806.142(1477.554)
LPC (22:4)	1706.729(976.366)	1894.898(1004.387)	2251.648(1058.406)	2604.942(1358.714)
LPC (22:5) - ESI(-)	675.167(447.702)	664.823(383.062)	886.715(554.24)	791.686(377.634)
LPC (22:6)	18296.637(8748.95)	17120.89(7390.865)	19280.755(8703.872)	17320.179(5402.133)
LPC (o-16:0)	7726.959(3135.329)	8366.675(3289.673)	9562.972(3966.252)	9545.73(3480.232)
LPC (p-16:0)/LPC (o-16:1)	10752.235(4110.82)	11778.247(4172.532)	12895.152(4859.04)	13555.48(4879.159)
LPC (p-18:0)/LPC (o-18:1)	5609.615(1996.592)	5649.593(2083.157)	6312.961(2252.03)	6302.042(1780.572)
LPC (14:0) - ESI(+)	12225.274(5163.537)	14568.798(5062.405)	11977.356(5718.762)	15445.385(5165.213)
LPC (15:0)	12084.127(4819.914)	12943.535(4361.419)	12780.381(5698.997)	13037.637(4366.256)
LPC (16:0) - ESI(+)	1926106.937(412946.468)	2025455.264(509547.986)	2122729.714(414415.433)	2257025.766(520385.84)
LPC (16:1) - ESI(+)	18357.864(6537.325)	19256.04(6089.078)	18979.953(9013.425)	20068.018(5828.219)
LPC (18:0) - ESI(+)	597884.618(199525.827)	642665.246(221367.761)	652830.354(212542.515)	693367.052(174842.328)
LPC (18:1) - ESI(+)	267553.679(104625.2)	280752.212(113394.873)	308282.753(125723.885)	329632.285(140448.722)
LPC (18:2) - ESI(+)	453109.903(200728.084)	547483.468(267853.354)	553742.399(224834.804)	603839.746(318018.732)
LPC (18:3)	3781.745(1556.029)	4762.878(2448.244)	4255.782(1792.563)	5519.175(3871.826)
LPC (20:3) - ESI(+)	18658.988(7504.447)	20830.978(7040.033)	21810.228(8898.33)	24667.198(9011.821)
LPC (20:4)	92588.56(39171.901)	99801.287(39143.693)	115640.286(50009.696)	126682.589(53164.432)
LPC (20:5)	8554.056(10259.538)	6693.724(5097.151)	8436.341(7975.092)	6882.284(3136.558)
LPC (22:5) - ESI(+)	4133.499(2034.537)	4006.158(1626.825)	5081.496(2307.922)	4780.993(1730.992)
LPE (16:0)	3007.892(1492.945)	3345.916(1755.537)	3443.824(1727.622)	3667.836(1958.6)
LPE (18:2) - ESI(-)	4521.977(2417.216)	5517.915(3099.215)	5301.279(2967.128)	5090.353(2770.4)
LPE (20:4) - ESI(-)	3411.332(1579.491)	3835.167(1358.006)	3821.613(1774.902)	4009.519(1196.108)
LPE (22:6)	2511.314(1103.103)	2584.869(1142.272)	2506.121(947.775)	2407.111(1062.591)
LPE (18:0)	2976.4(935.468)	3330.697(987.882)	2975.619(1000.622)	3457.5(835.551)
LPE (18:2) - ESI(+)	3940.782(1604.285)	4738.299(2407.019)	4513.971(1624.136)	4445.501(1993.594)
LPE (20:4) - ESI(+)	3205.181(1241.82)	3617.274(1320.76)	3383.978(1267.399)	3791.41(1594.759)
PC (16:0/9:0(CHO))	4327.064(2722.879)	4282.307(2603.353)	4968.504(3315.67)	4910.879(3014.302)
PC (32:0) - ESI(-)	14490.961(3964.7)	14558.291(3478.332)	15263.408(4162.383)	14700.287(3404.682)
PC (32:1) - ESI(-)	14447.376(7522.552)	14662.134(6394.392)	12758.462(7105.05)	14728.451(7297.961)
PC (32:2) - ESI(-)	13463.361(6508.264)	16204.369(5624.383)	12033.643(7553.981)	14707.656(6218.337)
PC (33:1) - ESI(-)	2353.684(1083.204)	2374.083(853.644)	2131.3(1012.513)	2414.131(939.724)
PC (33:2) - ESI(-)	3860.198(1605.855)	4336.55(1397.757)	3368.212(1547.831)	3815.359(1300.496)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
PC (34:0) - ESI(-)	8251.523(2184.754)	8469.609(1811.655)	8733.18(2533.887)	8483.927(1845.942)
PC (34:2) - ESI(-)	240630.097(60351.691)	258867.547(56457.148)	247088.946(65989.688)	252285.178(54764.773)
PC (34:3)	16244.273(6359.067)	18088.554(6094.852)	15330.272(6007.704)	16136.002(5630.699)
PC (34:4) - ESI(-)	3988.556(2296.794)	4598.624(1731.583)	3330.478(2005.054)	4458.283(1726.963)
PC (35:1) - ESI(-)	3093.959(1098.086)	3051.722(977.026)	3043.764(1081.863)	3250.46(1021.62)
PC (35:2)	9207.837(2691.891)	9716.991(2633.897)	9532.595(2656.684)	8872.848(2574.126)
PC (35:4) - ESI(-)	2567.664(1136.268)	2622.666(936.586)	2492.677(1048.406)	2743.646(1351.27)
PC (36:1) - ESI(-)	60700.134(17787.723)	61602.252(15986.223)	61324.941(17578.546)	62040.398(15296.844)
PC (36:3) A - ESI(-)	78001.315(26248.654)	80601.946(20165.252)	81493.858(28847.298)	82092.84(21459.655)
PC (36:3) B - ESI(-)	80122.729(25240.712)	84455.963(19138.885)	81453.529(26862.449)	86689.976(19139.009)
PC (36:4) A - ESI(-)	50001.555(19418.961)	58881.412(19057.435)	52267.702(21480.43)	52859.354(16963.772)
PC (36:4) B - ESI(-)	165608.498(45603.524)	172562.505(36378.869)	174408.792(49658.16)	179577.946(38130.404)
PC (36:5) A	2138.31(1339.816)	2567.216(1605.787)	2189.983(1541.952)	1814.926(1203.75)
PC (36:5) B	41857.83(35378.719)	33407.87(22725.882)	47045.93(43693.834)	34117.138(17993.151)
PC (37:2) - ESI(-)	1427.867(571.478)	1549.892(656.208)	1408.964(562.641)	1336.555(526.791)
PC (37:3)	19429.669(8642.077)	20766.774(7555.42)	18098.801(8761.691)	17852.572(6955.697)
PC (37:4) - ESI(-)	3610.43(1262.482)	3600.739(1164.94)	3865.914(1175.379)	3709.906(1129.303)
PC (38:2)	4724.469(1540.569)	4816.371(1178.537)	4580.92(1544.406)	4438.677(996.639)
PC (38:3) - ESI(-)	29648.655(10260.002)	31432.948(7745.999)	29624.875(10831.337)	33004.923(8368.738)
PC (38:4) A - ESI(-)	57986.619(17566.019)	60883.346(16516.825)	60375.971(17898.448)	62780.612(14774.114)
PC (38:5) A - ESI(-)	19182.481(6029.043)	19166.914(4819.422)	20412.89(6733.556)	19816.339(4946.775)
PC (38:5) B - ESI(-)	12329.808(8869.88)	10448.295(4369.029)	12975.729(10525.834)	10265.063(3529.805)
PC (38:6) - ESI(-)	75564.438(34561.384)	68827.018(26086.774)	75619.639(38181.774)	69579.548(23778.393)
PC (39:6)	18191.534(9715.309)	16532.441(6454.175)	13459.844(5802.603)	13206.209(4768.915)
PC (40:4) - ESI(-)	3651.767(1838.864)	3888.447(1301.818)	3909.143(1715.993)	4244.068(1400.298)
PC (40:5) A - ESI(-)	4364.652(1888.948)	4187.943(1433.041)	4770.531(2049.396)	4279.36(1497.875)
PC (40:5) B - ESI(-)	1949.867(1019.491)	2160.184(912.295)	1910.966(896.617)	2479.194(1218.116)
PC (40:6) B	20657.541(8269.246)	18554.405(6543.511)	21040.215(9670.584)	18713.955(6184.276)
PC (40:7) - ESI(-)	2669.718(1393.762)	2433.114(925.635)	2625.831(1432.89)	2313.846(972.287)
PC (40:8) - ESI(-)	2630.788(1139.643)	2734.932(900.85)	2878.238(1371.79)	2882.618(898.713)
PC (42:5)	3139.766(1127.172)	3024.694(1140.962)	2627.191(1248.213)	2509.332(843.894)
PC (42:6)	2237.693(1216.735)	2297.879(1311.502)	1853.339(1040.649)	2198.375(1271.775)
PC (o-32:0) - ESI(-)	2806.219(868.036)	2847.252(794.141)	3052.76(866.282)	2871.266(762.942)
PC (p-32:0)/PC (o-32:1) - ESI(-)	2338.644(927.886)	2365.854(804.708)	2679.84(1050.529)	2490.279(1071.344)
PC (p-32:0)/PC (o-32:1) - ESI(+)	29152.037(7872.188)	30771.998(7341.47)	30028.365(9213.253)	28568.812(7803.221)
PC (p-34:1)/PC (o-34:2) A	4520.84(2258.236)	5300.943(2014.065)	4757.993(2102.423)	4859.606(1626.867)
PC (p-34:1)/PC (o-34:2) B	2874.162(1241.363)	2975.868(1271.407)	2955.203(1307.817)	2729.62(1477.495)
PC (p-34:2)/PC (o-34:3) - ESI(-)	13080.94(4655.151)	15147.291(4618.811)	13538.65(4139.591)	14391.877(3967.502)
PC (p-36:1)/PC (o-36:2)	1579.393(1039.658)	1842.803(957.813)	1707.593(920.629)	1673.072(739.313)
PC (p-36:3)/PC (o-36:4) - ESI(-)	21432.678(7961.51)	23318.595(6892.306)	24688.357(7510.221)	26166.647(8952.3)
PC (p-36:3)/PC (o-36:4) - ESI(+)	227889.598(84207.01)	254677.838(68833.936)	250126.868(92689.597)	268982.446(76530.895)
PC (p-36:4)/PC (o-36:5) - ESI(-)	12136.93(5243.46)	13380.29(4590.962)	14393.873(6063.86)	15022.239(5522.478)
PC (p-38:3)/PC (o-38:4) - ESI(-)	7180.199(2581.694)	8011.26(2278.842)	7922.095(2620.948)	8636.903(2587.55)
PC (p-38:4)/PC (o-38:5) A	16408.903(5205.505)	17597.828(4431.343)	17820.582(4259.592)	18701.309(5190.175)
PC (p-38:4)/PC (o-38:5) B	2559.33(1097.47)	2769.763(1152.827)	2808.843(1106.312)	3260.105(1412.566)
PC (p-38:5)/PC (o-38:6)	1297.362(880.416)	1291.415(783.351)	1341.621(1148.57)	1306.021(628.98)
PC (p-40:1)/PC (o-40:2)	1485.155(608.109)	1292.088(473.435)	1462.481(553.862)	1236.145(464.308)
PC (p-40:3)/PC (o-40:4)	1750.816(685.913)	1868.47(638.755)	1850.389(704.887)	2043.343(619.095)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
PC (p-40:4)/PC (o-40:5) - ESI(-)	1855.515(641.097)	1784.499(529.196)	1949.912(581.6)	1838.42(505.562)
PC (p-40:7)/PC (o-40:8)	12784.77(9315.863)	11294.973(6789.332)	9573.21(9944.436)	7531.17(6686.616)
PC (p-42:3)/PC (o-42:4)	4785.842(1784.509)	5178.399(1630.148)	4952.621(1854.587)	5342.838(1997.141)
PC (p-42:4)/PC (o-42:5) - ESI(-)	2268.307(909.076)	2270.498(870.57)	2448.033(832.681)	2364.737(949.186)
PC (p-42:5)/PC (o-42:6)	618.687(355.575)	610.366(274.685)	646.286(300.455)	704.809(279.735)
PC (p-44:4)/PC (o-44:5) - ESI(-)	2845.694(1045.311)	2893.365(908.463)	3027.265(1099.475)	3015.819(836.508)
PC (p-44:5)/PC (o-44:6)	3310.494(1275.999)	3174.484(993.019)	3138.119(1105.716)	3030.243(1076.533)
PC 34:4e	6443.081(2515.863)	7999.075(2933.128)	6265.46(2786.167)	6864.822(2784.41)
PC 38:7e	16964.282(13526.498)	15342.968(9446.371)	16544.441(13664.894)	13824.238(5068.143)
PC 40:5e	12165.024(3482.196)	12677.876(3009.874)	12156.263(2800.976)	12946.278(3876.998)
PC 40:6e	22316.948(7430.313)	21474.846(6189.986)	22911.69(6865.962)	21858.337(7312.84)
PC (28:0)	3246.565(4662.849)	3239.16(2348.658)	2319.456(2047.457)	3419.203(2870.489)
PC (30:0)	158777.616(83572.094)	179096.713(65617.314)	134527.229(57552.582)	180921.663(83317.035)
PC (31:0)	10922.351(4521.628)	11042.588(3052.892)	9322.83(3444.162)	9511.503(2302.278)
PC (31:1)	1677.788(1455.465)	1660.939(915.401)	1190.067(862.691)	1324.367(711.207)
PC (32:0) - ESI(+)	256268.716(58170.605)	250135.791(53964.518)	252693.482(58815.308)	242994.15(67734.773)
PC (32:1) - ESI(+)	239846.485(124170.713)	249536.641(113064.066)	199894.088(94497.866)	233324.489(96006.991)
PC (32:2) - ESI(+)	56756.644(28246.729)	67703.831(25937.146)	45747.251(30984.152)	52825.941(23680.951)
PC (33:0)	10952.596(5641.864)	11592.978(3878.492)	9408.237(4832.541)	10312.507(3477.739)
PC (33:1) - ESI(+)	53543.632(20928.978)	53553.558(13337.174)	44982.592(16376.287)	48494.832(11798.772)
PC (33:2) - ESI(+)	78531.369(27527.116)	87270.676(25504.3)	66386.357(22506.876)	66179.171(17944.435)
PC (34:0) - ESI(+)	56673.124(14226.497)	56575.078(11243.201)	55930.398(16856.304)	54402.796(12049.128)
PC (34:1)	4013338.964(720952.007)	4067426.422(727466.087)	3807829.103(772533.633)	4051360.726(912477.724)
PC (34:2) - ESI(+)	8298954.78(1436737.757)	8880671.15(1333757.007)	8009035.373(1191638.206)	8068560.636(1188330.124)
PC (34:3) A	97711.278(31702.813)	106631.972(39043.209)	84529.885(34636.865)	89091.807(39417.08)
PC (34:3) B	108771.059(36242.03)	128990.918(46188.814)	91164.199(27797.142)	101396.149(38586.988)
PC (34:3) C	86598.612(39702.386)	108697.965(49708.994)	75951.137(21974.678)	97984.941(50767.182)
PC (34:4) - ESI(+)	17218.357(9083.701)	20014.966(7594.249)	13453.933(6967.576)	17417.677(7336.924)
PC (35:1) - ESI(+)	46139.315(13080.522)	45638.931(9232.36)	41459.078(10896.604)	42883.759(9581.456)
PC (35:2) A	109536.799(36351.893)	103212.896(30675.48)	94027.949(31874.332)	100085.598(23028.225)
PC (35:2) B	131176.614(32124.982)	137458.977(30973.043)	119065.848(31085.946)	114270.85(23658.334)
PC (35:3)	40372.126(10564.132)	44343.372(11336.707)	35865.887(9999.311)	36662.028(9497.255)
PC (35:4) - ESI(+)	22778.31(8961.192)	23974.006(6756.722)	19079.655(6980.574)	20470.702(6462.17)
PC (36:1) - ESI(+)	656088.196(185659.526)	660392.494(148989.452)	587404.023(154102.201)	627376.228(128997.811)
PC (36:2)	4529060.48(909760.507)	4996033.975(881985.183)	4211692.931(903186.615)	4327926.764(476276.167)
PC (36:3) A - ESI(+)	1277000.345(445850.9)	1366182.069(370360.325)	1204527.783(516992.597)	1212320.94(306902.701)
PC (36:3) B - ESI(+)	1639032.954(502617.113)	1716418.049(393778.108)	1595831.492(520981.85)	1592535.179(276748.936)
PC (36:4) A - ESI(+)	344228.244(141889.724)	433150.27(175314.159)	324935.514(157371.936)	345149.151(130634.465)
PC (36:4) B - ESI(+)	254789.338(417790.093)	206974.331(69274.833)	168655.141(82504.342)	190887.131(54600.311)
PC (36:4) C - ESI(+)	3945315.162(980469.466)	4037185.749(932394.375)	3770041.129(1046223.193)	4023980.133(1042196.2)
PC (36:5) C	63676.772(293144.05)	37777.207(75598.623)	35961.874(82637.482)	42060.718(90105.09)
PC (36:5) D	466335.725(583640.353)	328794.138(256617.495)	328646.617(282542.953)	263135.658(107530.626)
PC (36:5)A	10087.21(5302.765)	12082.737(6355.171)	8991.784(5467.663)	8535.056(4024.666)
PC (36:6)	7517.927(4687.721)	7514.303(3539.182)	5072.96(3119.115)	5365.199(1768.116)
PC (37:2) - ESI(+)	12948.098(3497.278)	14134.187(3647.086)	11891.289(3512.971)	12085.972(2300.68)
PC (37:4) - ESI(+)	51981.159(19322.358)	49132.105(16397.252)	44294.212(16164.247)	49003.07(18357.963)
PC (37:5)	36908.954(34432.55)	28967.669(14940.073)	27588.92(17283.673)	24327.094(8409.348)
PC (37:6)	9891.772(5465.158)	8696.041(4047.719)	6890.365(2953.421)	6246.927(2456.317)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
PC (38:3) - ESI(+)	545962.223(199887.214)	581406.422(170804.445)	502874.429(188115.354)	563752.727(162801.855)
PC (38:4) A - ESI(+)	129827.943(52570.47)	130649.431(33178.708)	113377.194(37599.238)	117140.224(28716.98)
PC (38:4) B - ESI(+)	138945.853(49865.612)	150899.97(43419.782)	137674.029(54084.911)	158478.41(46996.215)
PC (38:4) C - ESI(+)	2313829.998(565304.201)	2391882.015(574272.595)	2178463.964(599975.838)	2310328.11(606482.831)
PC (38:5) A	732724.247(176405.92)	721011.877(165292.616)	692510.741(177868.353)	703688.662(171227.462)
PC (38:5) B - ESI(+)	385628.57(330057.265)	324021.431(136699.566)	297899.839(144961.97)	282186.016(71340.288)
PC (38:6) A - ESI(+)	122703.865(38145.153)	135842.09(35120.916)	110512.355(34062.971)	124100.415(31890.776)
PC (38:6) B - ESI(+)	3683483.214(1066200.996)	3373471.275(825187.655)	3308133.746(802249.627)	3011420.074(682021.451)
PC (38:7)	9067.129(4522.378)	8494.519(3671.831)	6643.623(3241.473)	6218.005(2668.734)
PC (39:4)	4951.364(1392.551)	4980.401(1209.519)	4440.55(1217.731)	4643.705(1217.911)
PC (40:4) - ESI(+)	40710.749(17107.156)	43768.486(14761.039)	42663.302(16356.582)	48562.457(17576.609)
PC (40:5) A - ESI(+)	160984.496(51414.716)	153215.298(48927.121)	153701.168(45022.035)	150517.483(35932.021)
PC (40:5) B - ESI(+)	39290.673(16831.51)	43514.802(16159.023)	38473.161(15894.973)	44025.445(17787.819)
PC (40:6) A	26324.155(8352.257)	26286.775(7120.512)	23634.728(8121.937)	23764.161(6603.153)
PC (40:6)B	523343.738(235330.416)	448154.607(162581.361)	427810.229(142555.352)	385657.136(132065.673)
PC (40:7) A - ESI(+)	14123.954(4521.843)	15295.102(4113.716)	13952.454(5466.208)	15028.736(3957.139)
PC (40:7) B - ESI(+)	294687.493(123648.862)	260986.662(85720.284)	257320.328(117772.802)	217436.412(72618.439)
PC (40:8) - ESI(+)	15239.14(4848.028)	15297.801(4079.753)	14476.135(6122.24)	13978.291(3019.574)
PC (42:10)	2726.931(1374.175)	2509.831(1360.724)	2531.617(1415.798)	2354.819(927.021)
PC (o-32:0) - ESI(+)	33066.939(8835.009)	34463.696(8408.236)	34119.797(8865.124)	32338.938(8404.113)
PC (o-34:0)	4253.752(1544.24)	4625.498(1473.237)	4251.794(1703.095)	4099.673(1209.919)
PC (p-32:1)/PC (o-32:2)	7732.065(2525.44)	8442.017(2078.799)	7910.504(3383.972)	8191.083(2087.48)
PC (p-34:1)/PC (o-34:2)	90514.308(41518.544)	112732.145(42037.713)	90884.196(35928.824)	95158.27(29994.724)
PC (p-34:2)/PC (o-34:3) - ESI(+)	134516.098(48579.028)	167161.547(53529.226)	130014.23(47822.804)	147005.911(49558.404)
PC (p-36:1)/PC (o-36:2) B	4576.41(1860.937)	4990.913(1761.819)	4307.895(1837.538)	4197.481(1642.081)
PC (p-36:2)/PC (o-36:3)	18401.743(7473.236)	22260.671(8493.763)	17314.501(7146.789)	19082.113(7114.945)
PC (p-36:4)/PC (o-36:5) - ESI(+)	222255.821(73873.841)	244403.223(62140.636)	242439.639(89502.675)	258183.564(78912.006)
PC (p-36:5)/PC (o-36:6)	43163.98(47010.214)	35793.982(29043.548)	43083.765(46051.211)	35923.993(21264.091)
PC (p-38:3)/PC (o-38:4) A - ESI(+)	23415.263(7747.924)	26268.221(7020.386)	24102.249(7465.869)	28129.553(9009.63)
PC (p-38:3)/PC (o-38:4) B - ESI(+)	60681.832(24417.325)	68924.225(21887.47)	63797.576(23315.526)	71084.075(22755.644)
PC (p-38:4)/PC (o-38:5) A	244736.068(73932.864)	253186.358(52211.505)	253198.973(75445.49)	259563.862(64014.349)
PC (p-38:4)/PC (o-38:5) B	46348.51(17350.154)	52251.201(14810.562)	47627.623(16741.534)	53717.086(17796.507)
PC (p-38:5)/PC (o-38:6) A	47602.588(24906.045)	44907.468(17837.495)	46233.794(27430.939)	40791.817(15837.344)
PC (p-38:5)/PC (o-38:6) B	60693.148(18465.69)	63136.031(15203.868)	58926.741(20171.535)	59314.065(18371.793)
PC (p-38:6)/PC (o-38:7)	38202.501(19743.59)	36368.564(13760.086)	36619.184(20463.261)	33534.038(11628.77)
PC (p-40:4)/PC (o-40:5) - ESI(+)	17184.561(5389.491)	17672.249(4621.409)	17410.96(4549.737)	18075.452(5491.996)
PC (p-40:6)/PC (o-40:7) A	40200.774(19957.817)	35888.168(13738.726)	36954.859(22360.938)	32062.44(11105.695)
PC (p-40:6)/PC (o-40:7) B	13510.106(6889.457)	13100.064(5544.826)	12405.966(6481.044)	11203.745(4502.511)
PC (p-42:4)/PC (o-42:5) - ESI(+)	12900.718(4496.163)	12896.037(3917.285)	12754.45(3435.607)	12938.521(5007.842)
PC (p-42:5)/PC (o-42:6) A	10237.461(3726.694)	10713.657(3758.542)	10172.91(3767.066)	10947.237(4814.118)
PC (p-42:5)/PC (o-42:6) B	3974.188(1415.292)	3956.085(1237.45)	3733.472(1142.554)	3479.506(1252.076)
PC (p-44:4)/PC (o-44:5) - ESI(+)	14453.858(5455.893)	14223.731(4628.827)	14914.59(5257.409)	13990.202(5447.096)
PE (34:1)	1935.048(1193.975)	1997.27(1266.931)	1922.526(1262.798)	2088.749(1260.706)
PE (34:2) - ESI(-)	2982.653(1876.385)	3405.593(2151.45)	2867.947(2153.222)	3232.022(2283.173)
PE (36:1) - ESI(-)	418.862(181.396)	445.435(181.825)	394.47(193.221)	476.773(203.336)
PE (36:2)	7905.774(4135.38)	8803.532(4225.603)	8328.494(5401.93)	8605.309(4699.84)
PE (36:3)	2026.786(1248.378)	2279.738(1430.26)	2201.323(1753.452)	2174.804(1400.564)
PE (36:4) - ESI(-)	2941.499(1644.752)	3164.472(1950.982)	2727.181(1659.941)	3275.078(1994.651)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
PE (38:2)	629.602(222.186)	682.787(206.229)	625.315(210.258)	726.012(236.051)
PE (38:6) - ESI(-)	7437.759(5142.646)	7356.489(4624.489)	6039.64(4500.327)	7125.711(4187.612)
PE (p-34:1)/PE (o-34:2) - ESI(-)	2025.04(785.489)	2051.91(695.945)	2150.254(890.571)	2026.74(746.259)
PE (p-34:2)/PE (o-34:3)	3040.334(1576.283)	3609.46(1747.103)	3425.067(1818.788)	3441.15(1343.908)
PE (p-36:1)/PE (o-36:2) - ESI(-)	2760.373(1320.05)	3068.12(1351.566)	3064.044(1403.021)	3267.766(1574.172)
PE (p-36:2)/PE (o-36:3) - ESI(-)	5957.994(2773.012)	6972.062(2936.918)	6614.407(3104.076)	6917.904(2378.957)
PE (p-36:4)/PE (o-36:5) - ESI(-)	15261.909(9626.399)	15928.908(8581.977)	18489.037(12771.445)	17905.612(10235.869)
PE (p-36:5)/PE (o-36:6)	2102.097(2962.828)	1485.236(2041.939)	2863.162(4197.256)	1557.732(1341.719)
PE (p-38:3)/PE (o-38:4)	1340.345(687.934)	1513.805(782.147)	1479.584(725.327)	1687.613(809.239)
PE (p-38:5)/PE (o-38:6) - ESI(-)	11786.825(6628.023)	12149.489(5341.659)	13603.388(8523.127)	12933.022(6132.057)
PE (p-38:6)/PE (o-38:7)	7532.92(4292.66)	7188.888(3364.912)	8157.198(5177.597)	7545.245(2881.175)
PE (p-40:4)/PE (o-40:5)	3399.555(1897.801)	3410.027(1799.437)	3628.141(2106.633)	3661.55(2357.67)
PE (34:2) - ESI(+)	8757.929(6410.569)	9879.682(7371.827)	7632.324(5605.642)	9599.64(5858.139)
PE (36:1) - ESI(+)	3379.71(1611.842)	3316.561(1592.325)	3662.52(1957.017)	3571.172(1895.091)
PE (36:4) - ESI(+)	14739.008(7468.332)	15255.178(7705.241)	12270.933(6672.071)	14447.752(7358.067)
PE (38:4)	39570.697(19154.594)	40390.086(15772.1)	35797.097(19983.436)	37463.39(16790.23)
PE (38:6) - ESI(+)	20257.66(12022.688)	19884.696(11866.824)	13208.306(6582.466)	16869.926(9428.463)
PE (p-34:1)/PE (o-34:2) - ESI(+)	2742.254(1098.637)	2862.174(974.659)	2911.341(1333.048)	2823.109(1036.114)
PE (p-36:1)/PE (o-36:2) - ESI(+)	2454.413(1024.933)	2762.367(992.448)	2564.311(1190.111)	2713.77(1140.048)
PE (p-36:2)/PE (o-36:3) - ESI(+)	8991.903(3876.705)	11041.406(4021.531)	9494.206(4636.704)	9793.668(3052.8)
PE (p-36:4)/PE (o-36:5) - ESI(+)	29345.071(18055.185)	30532.635(14508.762)	35383.013(25322.79)	31556.53(15854.325)
PE (p-38:4)/PE (o-38:5)	42614.164(20321.576)	46103.9(17411.189)	46972.987(24498.228)	46554.029(19964.508)
PE (p-38:5)/PE (o-38:6) - ESI(+)	24747.834(11095.999)	26262.641(9101.812)	27610.681(15320.481)	26331.421(9963.269)
PE (p-40:4)/PE (o-40:5) A	2896.209(2724.733)	2989.973(2175.181)	3398.239(3429.56)	3062.06(2829.321)
PE (p-40:4)/PE (o-40:5) B	3708.007(1951.993)	3692.493(1528.458)	3740.207(2103.555)	3768.74(1900.642)
PE (p-40:5)/PE (o-40:6)	6740.897(2550.286)	6806.706(1987.436)	7388.568(2892.277)	6765.288(2266.793)
PG (34:0)/PG (17:0/17:0)	76853.368(21921.357)	85280.313(20224.124)	80493.808(19195.823)	85678.567(20378.055)
PI (38:4)/PI (18:0-20:4)	120817.481(39400.359)	124008.066(31642.823)	121390.805(44702.266)	129277.347(34643.533)
SM (d30:1) - ESI(-)	1704.845(1134.453)	1947.17(774.108)	1614.585(1242.928)	1863.674(954.282)
SM (d32:0) - ESI(-)	1032.341(809.55)	1064.49(657.551)	979.933(686.425)	1216.938(807.716)
SM (d32:1) - ESI(-)	44492.705(15861.723)	49754.267(12913.605)	43920.769(18017.314)	49980.838(14159.591)
SM (d32:2) - ESI(-)	3030.003(1334.652)	3230.614(1251.27)	2552.585(1182.446)	2652.193(879.559)
SM (d33:1) - ESI(-)	22975.489(8246.125)	25365.753(7028.514)	23780.337(8047.678)	25807.776(6325.893)
SM (d34:0) - ESI(-)	4927.976(1784.951)	5032.83(1672.907)	5253.149(1984.636)	5018.593(1607.857)
SM (d34:1) - ESI(-)	155715.48(39317.352)	163369.808(34296.98)	168871.615(43024.9)	165901.833(36831.034)
SM (d34:2) - ESI(-)	57475.881(14166.69)	60371.724(13403.338)	58039.082(15647.963)	57143.485(10939.005)
SM (d36:0) - ESI(-)	1066.803(653.242)	879.715(483.034)	1194.004(818.479)	1158.849(602.847)
SM (d36:1) - ESI(-)	36132.26(10486.124)	36986.044(8862.176)	38899.489(13766.352)	38825.686(9996.914)
SM (d36:2) - ESI(-)	5807.249(1805.715)	5799.331(1630.41)	5885.647(1989.529)	5864.148(1760.527)
SM (d36:3) - ESI(-)	1713.798(653.047)	1804.421(563.54)	1608.324(562.31)	1777.223(446.756)
SM (d37:1)	2411.418(1019.95)	2404.494(818.507)	2331.972(1186.471)	2389.831(996.191)
SM (d38:0)	696.441(811.576)	522.617(447.127)	687.455(703.572)	667.066(366.14)
SM (d38:2) - ESI(-)	4790.522(1380.077)	4974.002(1318.512)	4819.556(1563.18)	4541.111(1070.145)
SM (d39:1) - ESI(-)	12841.047(4278.992)	14353.601(3784.665)	12414.395(4483.9)	13903.713(3726.042)
SM (d39:2)	12449.201(3511.981)	12954.634(3279.589)	9947.898(2966.294)	10080.729(2701.081)
SM (d40:1) - ESI(-)	46897.381(13275.565)	50082.888(10695.858)	48109.832(15111.068)	51482.472(10102.847)
SM (d40:2) A - ESI(-)	12273.795(4442.543)	12319.223(4118.364)	13018.212(5895.037)	12570.412(4851.714)
SM (d40:2) B - ESI(-)	17613.206(5158.79)	18864.027(4350.959)	17289.91(5626.146)	17753.258(3641.515)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
SM (d40:3)	1079.194(398.684)	1151.905(387.017)	1149.041(414.719)	1024.09(283.58)
SM (d41:1) - ESI(-)	11075.677(11704.719)	13579.641(12424.293)	12192.786(12824.811)	12879.432(14073.923)
SM (d41:2) - ESI(-)	10157.654(3759.068)	10335.005(4166.592)	9557.389(3960.061)	9775.169(3425.035)
SM (d42:0) - ESI(+)	631.117(319.733)	572.32(282.695)	652.379(371.709)	686.442(284.971)
SM (d42:0) - ESI(-)	2435.513(802.742)	2325.825(740.385)	2351.234(832.029)	2448.334(558.062)
SM (d42:1) - ESI(-)	74113.422(22000.912)	76751.556(18783.673)	78807.969(25168.668)	82719.057(18246.025)
SM (d42:3) - ESI(-)	45369.2(13437.893)	44941.003(10551.682)	48218.789(16038.226)	43667.711(11335.064)
SM (d43:1) - ESI(-)	1610.475(804.178)	1785.517(763.855)	1592.12(791.256)	2166.055(915.104)
SM (d43:2) - ESI(-)	6637.877(3329.003)	6677.809(2804.014)	6696.314(3775.834)	7584.084(3636.587)
SM (d44:2)	3401.174(1320.178)	2954.684(961.942)	3415.928(1601.631)	2902.033(893.587)
SM (d41:3)	17542.807(4858.342)	18495.055(4033.934)	16527.565(4817.077)	17548.333(4842.736)
SM (d30:1) - ESI(+)	4627.855(3294.462)	5081.766(2205.718)	3652.203(2648.807)	4401.976(2692.374)
SM (d32:0) - ESI(+)	4527.417(2257.972)	4461.163(1515.584)	3682.177(1698.839)	3886.828(1408.425)
SM (d32:1) - ESI(+)	127487.665(50390.527)	141586.567(42157.93)	105868.284(47317.742)	123863.338(37889.321)
SM (d32:2) - ESI(+)	8419.355(3072.987)	8850.662(2752.191)	6369.383(2110.37)	6595.601(1985.036)
SM (d33:1) - ESI(+)	78897.543(30030.413)	81545.929(24155.104)	67457.824(25763.753)	69610.008(18148.263)
SM (d34:0) - ESI(+)	77128.042(21734.185)	77407.547(19252.704)	72210.897(23280.32)	68796.729(18834.64)
SM (d34:1) - ESI(+)	1815521.625(427328.564)	1839477.475(326129.156)	1784355.088(430500.205)	1702876.808(358785.295)
SM (d34:2) - ESI(+)	169414.754(41285.046)	172230.478(39764.32)	149178.135(39155.163)	143390.023(28536.708)
SM (d36:0) - ESI(+)	18743.046(8907.96)	15332.243(6070.249)	18497.609(10593.099)	15396.526(6078.054)
SM (d36:1) - ESI(+)	282139.394(75455.508)	277277.338(58280.773)	271000.224(91366.868)	258341.543(75770.475)
SM (d36:2) - ESI(+)	637435.743(182402.554)	634824.46(155709.619)	609372.433(220346.568)	559314.781(158419.266)
SM (d36:3) - ESI(+)	6491.66(2413.088)	6629.303(2061.528)	5303.916(1662.699)	5372.054(1467.429)
SM (d38:1)	224074.217(52840.443)	238184.289(46405.144)	201776.054(59116.355)	217368.176(47785.659)
SM (d38:2) - ESI(+)	102238.769(23254.677)	103697.728(23384.632)	91480.79(22758.592)	86392.382(21671.092)
SM (d39:1) - ESI(+)	55126.946(19385.078)	60979.282(17058.805)	44658.537(16713.1)	51877.857(13963.345)
SM (d40:0)	8519.977(3597.278)	7725.238(2745.348)	7677.025(3167.843)	8011.238(2212.435)
SM (d40:1) - ESI(+)	357194.17(87098.783)	373303.076(69403.177)	341604.881(102437.243)	362095.736(80274.56)
SM (d40:2) A - ESI(+)	192003.867(74381.653)	206939.521(72862.228)	178078.484(72349.431)	179868.527(58152.864)
SM (d40:2) B - ESI(+)	235158.05(59785.384)	255298.203(57750.75)	210548.235(60355.748)	219351.346(55114.116)
SM (d41:1) - ESI(+)	136526.853(38416.919)	143873.721(36214.448)	119899.005(36867.559)	132527.346(37975.354)
SM (d41:2) A - ESI(+)	41382.821(14921.589)	40584.006(12105.041)	35492.179(12478.446)	33969.219(11162.26)
SM (d41:2) B - ESI(+)	65492.772(20330.14)	72077.791(21032.207)	52745.939(16747.156)	55898.553(15520.632)
SM (d42:1) - ESI(+)	227228.943(65564.52)	235888.054(53178.336)	222436.887(63597.422)	240705.135(54179.07)
SM (d42:2)	552276.944(187216.547)	490026.241(121909.07)	546358.226(201991.029)	460675.764(135621.859)
SM (d42:3) - ESI(+)	360096.856(99212.364)	348735.256(79546.208)	337630.936(101307.266)	299649.811(83353.79)
SM (d43:1) - ESI(+)	6015.056(2273.428)	6198.991(2041.865)	5555.044(2105.178)	6463.747(2405.808)
SM (d43:2) - ESI(+)	14891.052(6807.646)	13945.815(5754.744)	13196.624(5716.2)	13478.476(6491.555)
TG (55:6)	10089.48(6268.964)	8140.342(3509.246)	8802.778(3134.839)	9197.851(3716.421)
TAG (58:7)/TAG (18:1/18:1/22:5)	17350.361(7968.934)	16648.95(5845.672)	16639.702(5743.219)	18540.485(5893.952)
TG (60:12)	6594.761(13689.356)	3710.704(4070.071)	3585.552(3335.897)	3032.451(2280.041)
TG (53:5)	10973.54(5251.608)	10286.984(3942.7)	11674.703(5613.463)	10840.413(5368.36)
TG (60:11)	8428.304(11674.572)	5497.847(3845.608)	5706.605(3743.089)	5470.435(3713.245)
TG (40:0)	6969.903(22773.737)	5975.792(11932.991)	10871.416(37277.846)	5462.54(5759.558)
TG (40:1)	1931.434(4239.428)	2087.013(3783.783)	2781.675(6677.307)	1914.582(2145.639)
TG (42:0)	9234.522(21761.184)	8844.978(15901.608)	13307.221(33494.34)	8330.04(8659.705)
TG (42:1)	6797.568(17520.658)	7739.975(16319.178)	9671.813(27713.589)	8379.533(14255.854)
TG (42:2)	2571.971(5933.309)	3829.423(10795.773)	3469.506(9272.753)	3748.236(7445.047)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
TG (42:3)	591.158(714.913)	671.443(879.22)	708.25(899.383)	683.053(790.865)
TG (44:0)	19087.048(32238.546)	17886.319(25507.344)	24490.87(41856.21)	20757.338(22009.867)
TG (44:1)	18788.092(29782.097)	19478.318(28152.179)	23426.281(41047.033)	21621.234(23479.509)
TG (44:2)	8060.679(14384.219)	10064.354(23367.775)	10743.044(20194.658)	8380.317(10487.693)
TG (46:0)	2913.683(2889.773)	3210.711(2865.495)	3596.463(3339.855)	3818.989(2907.059)
TG (46:1)	78988.174(99974.002)	74842.169(86950.751)	92276.008(113786.144)	98918.242(97696.155)
TG (46:2)	34399.438(37849.21)	37666.18(47712.032)	39789.39(42673.591)	41216.21(33094.939)
TG (46:3) A	601.482(563.369)	733.247(1466.526)	747.28(697.175)	571.11(354.662)
TG (46:3) B	5520.005(7775.947)	5107.884(7131.762)	7388.887(10758.099)	4355.864(3462.121)
TG (46:4) A	1736.197(1706.675)	2452.533(7382.425)	2137.511(2213.628)	1684.875(979.075)
TG (46:4) B	1520.942(1603.93)	2160.803(6838.834)	1903.962(2062.248)	1447.092(1031.978)
TG (46:5)	350.027(264.398)	426.476(1213.469)	407.412(315.649)	285.338(153.895)
TG (48:0)	59633.947(40059.321)	72255.424(51804.827)	66903.697(41634.01)	79478.814(50971.025)
TG (48:1)	445353.036(404942.517)	421062.403(327886.505)	524213.67(449533.987)	555493.791(414420.584)
TG (48:2)	232753.491(212433.045)	215309.555(160839.721)	255786.613(216764.761)	268443.377(184286.697)
TG (48:3)	66257.783(45379.776)	68608.011(52545.382)	72215.461(50509.48)	77877.575(53186.217)
TG (48:4) A	14636.937(12229.537)	16489.544(19911.708)	16245.558(13562.432)	18030.998(17055.356)
TG (48:4) B	10569.309(10549.743)	12439.978(18504.13)	12504.071(11469.438)	14971.849(16495.296)
TG (48:5)	2394.932(2124.793)	2607.435(2613.644)	2572.8(2035.771)	2780.416(2398.568)
TG (48:6)	731.456(341.644)	1120.169(4094.332)	722.702(289.312)	705.093(184.872)
TG (49:0)	5475.884(3437.407)	5547.724(2851.467)	6100.391(3788.603)	6307.46(2485.905)
TG (49:1)	38039.35(31682.085)	32431.609(18199.476)	44312.657(34999.664)	40168.672(20279.081)
TG (49:2)	5347.71(2994.124)	4908.392(3180.31)	5501.932(3300.177)	4902.763(2149.578)
TG (49:3)	8782.798(5619.053)	8058.518(3765.588)	9221.733(6256.187)	8066.278(3265.39)
TG (50:0)	28294.36(17765.307)	35864.991(22391.136)	32082.118(19239.608)	44353.561(26478.113)
TG (50:1)	295740.881(378872.38)	268871.222(259991.973)	324648.971(446178.44)	357328.342(249774.674)
TG (50:2)	1473341.655(765417.549)	1337335.537(606243.723)	1659532.403(829820.745)	1594280.037(647567.882)
TG (50:3) A	599554.098(373888.427)	538070.653(271710.362)	651512.576(411480.486)	612121.785(281795.546)
TG (50:3) B	1463.989(2654.267)	1979.068(6822.777)	1400.186(2455.795)	1038.515(809.914)
TG (50:4)	113705.603(61749.855)	111373.426(49803.428)	126125.687(75277.714)	114750.977(56083.861)
TG (50:5)	18164.523(11639.543)	17487.784(9234.201)	19933.75(14173.046)	17309.587(10422.837)
TG (50:6)	2907.741(1946.11)	2679.302(1733.966)	2884.817(1921.776)	2851.086(1436.465)
TG (51:2)	92658.55(49837.791)	81298.301(33345.525)	102425.44(56318.197)	97437.964(38234.191)
TG (51:3)	73828.122(33989.875)	68061.653(24068.889)	82938.425(41964.237)	74898.254(28861.793)
TG (51:4)	20600.271(10073.4)	19733.727(8062.558)	23270.722(12671.588)	19674.341(9041.132)
TG (51:5)	3397.515(1704.001)	3356.461(1275.262)	3656.126(2140.47)	3343.341(1577.736)
TG (52:1)	273344.812(258320.644)	254133.337(220416.288)	385958.096(343150.582)	380249.778(255901.526)
TG (52:2)	3924538.986(1182333.569)	3636556.102(1122279.122)	4304562.707(1305332.999)	4284568.998(1252064.19)
TG (52:3)	4416231.615(1252804.656)	4180937.847(1101985.633)	4943186.066(1278613.496)	4580060.216(1280748.182)
TG (52:4)	133068.448(44192.17)	130479.658(39344.454)	149410.712(45631.61)	134456.837(44467.248)
TG (52:5)	197791.574(102954.234)	174359.995(84000.915)	221089.331(113787.339)	187952.848(123930.287)
TG (52:6)	25178.432(15261.735)	23719.028(10920.524)	26434.601(18387.355)	26935.963(12326.041)
TG (53:0)	1583.982(681.915)	1815.471(661.05)	1558.757(477.059)	1852.357(638.551)
TG (53:1)	5936.774(4668.413)	5776.819(3671.696)	7132.934(5901.455)	7738.895(4054.487)
TG (53:2)	55792.745(24993.696)	51317.499(21651.56)	61529.31(28763.169)	64673.739(28506.202)
TG (53:3)	73056.718(28445.208)	67703.814(23631.61)	80399.918(32547.588)	77888.018(33481.67)
TG (53:4)	46389.39(19729.068)	43856.196(15698.609)	49625.115(21404.389)	47794.59(20989.819)
TG (54:1)	29942.881(33162.778)	29095.13(22321.153)	45930.932(54266.538)	39463.641(28219.587)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
TG (54:2)	321515.5(253928.808)	286249.499(201970.532)	440117.203(381933.248)	409260.248(286155.043)
TG (54:3)	1412729.685(654867.912)	1276837.39(524744.236)	1623423.817(851645.459)	1519899.979(713284.681)
TG (54:4)	1525311.494(686168.793)	1377217.291(578506.358)	1760418.221(707219.698)	1591726.506(803792.174)
TG (54:5) A	886580.788(456096.063)	802522.834(352287.756)	1025065.173(427497.763)	906466.793(489401.587)
TG (54:5) B	262000.181(111804.806)	243734.88(92887.319)	299788.926(135038.285)	318097.363(96574.507)
TG (54:6) A	199405.641(130496.852)	176401.555(94248.554)	225998.516(121666.969)	191962.588(134808.348)
TG (54:6) B	1358.531(998.464)	1341.842(782.147)	1570.362(998.026)	1293.618(944.161)
TG (54:6) C	156170.234(80514.484)	137719.361(62448.4)	173539.888(102538.702)	174065.629(81507.228)
TG (54:7) A	49122.361(41128.683)	44915.907(27315.049)	55433.098(39043.891)	44909.3(34205.411)
TG (54:7) B	43061.59(27306.858)	34198.973(17471.92)	41427.972(20491.371)	40360.834(20569.824)
TG (54:8)	7077.455(4680.131)	6400.128(3571.251)	6552.552(4150.332)	7358.226(4649.884)
TG (54:9)	965.383(952.873)	800.15(740.888)	592.879(606.119)	691.956(316.62)
TG (55:1)	2381.308(1476.992)	2293.733(1193.428)	2920.799(1903.01)	2972.521(1491.511)
TG (55:2)	3209.3(1454.698)	3026.046(1288.231)	3635.453(1704.304)	3807.112(1548.074)
TG (56:1)	8425.454(9238.656)	8724.83(13724.801)	11505.762(10956.361)	14774.086(25693.106)
TG (56:10)	3107.113(3323.17)	2681.061(1812.641)	2095.903(1680.467)	2539.949(1566.405)
TG (56:2)	12956.986(10569.613)	12163.693(13180.75)	16386.937(12849.427)	18654.205(23200.288)
TG (56:3)	30313.86(19743.679)	27075.315(20697.58)	36217.951(22324.807)	38868.629(32329.305)
TG (56:4)	52216.171(23781.081)	49073.426(20687.965)	55840.537(22467.404)	56180.741(25306.504)
TG (56:5) A	53791.601(25940.471)	48027.297(18998.273)	61801.837(27374.552)	61191.078(22268.531)
TG (56:5) B	56496.764(28288.186)	50801.304(20794.293)	65733.144(33645.995)	67057.648(26692.101)
TG (56:5) C	113050.899(43777.393)	107344.31(43874.117)	118627.317(34824.732)	122947.456(52182.386)
TG (56:6)	257540.767(82209.876)	233475.447(74511.483)	281319.421(89579.965)	287725.177(91307.651)
TG (56:7) A	847.239(514.565)	783.159(401.886)	938.132(655.262)	929.7(363.376)
TG (56:7) B	187264.223(134086.996)	142003.825(96398.78)	158086.258(77277.145)	161138.457(99617.435)
TG (56:8) A	48927.531(26901.231)	42661.135(18087.989)	50064.144(23467.331)	47257.557(20897.699)
TG (56:8) B	88914.046(72816.031)	66492.66(53152.85)	72872.217(40508.64)	71542.152(51749.829)
TG (56:9)	16134.849(11093.145)	13921.157(6903.286)	13754.351(8034.258)	14787.636(7681.834)
TG (57:1)	1925.193(905.225)	1863.322(943.086)	2230.651(1020.533)	2406.822(1238.998)
TG (57:2)	2561.985(1153.018)	2479.474(1287.033)	3067.197(1362.234)	3326.747(1811.417)
TG (58:1)	6517.314(7345.499)	6747.301(10399.217)	8099.715(7474.558)	11963.869(19532.172)
TG (58:10)	19441.101(14120.814)	16598.368(8410.925)	16328.172(8901.342)	16906.89(8417.462)
TG (58:2)	10622.347(16674.782)	10834.266(23253.565)	13254.119(16491.06)	21111.582(44118.983)
TG (58:3)	6147.029(9675.465)	5932.174(10911.709)	7341.209(8673.779)	10681.352(20516.14)
TG (58:4)	3243.624(2529.139)	2899.892(2258.659)	3529.189(2082.371)	3692.194(2838.546)
TG (58:5)	3750.517(1804.936)	3824.305(1507.07)	3786.371(1595.824)	4264.572(1727.481)
TG (58:6)	14653.583(5134.288)	13533.44(3981.36)	15559.451(5777.052)	16068.613(4533.944)
TG (58:8)	61621.544(53618.106)	44303.591(28847.455)	53856.909(45196.344)	50355.497(39213.793)
TG (58:9)	45461.573(35467.981)	34450.345(20298.576)	38767.777(25681.665)	36919.574(24471.402)
TG (59:2)	1491.779(1048.687)	1415.968(980.975)	1872.583(1503.685)	1971.88(1601.089)
TG (59:3)	1482.159(789.741)	1388.449(810.7)	1664.691(965.689)	1759.21(1206.118)
TG (60:1)	2548.677(2775.351)	2609.795(3662.099)	2957.506(2521.105)	4293.616(6636.964)
TG (60:2)	5106.678(6459.935)	5391.177(12127.075)	6248.941(8977.588)	9524.796(22615.929)
TG (60:3)	3356.443(4588.274)	3498.227(6192.138)	3902.058(4033.732)	6305.992(11703.269)
TG (60:4)	1479.004(1459.393)	1489.448(1601.775)	1632.611(1277.701)	2218.869(2677.546)
TG (60:6)	1058.884(479.188)	956.092(409.713)	1095.657(538.542)	1069.564(367.672)
TG (62:1)	1025.712(1380.888)	981.286(1057.831)	1100.973(1066.149)	1375.722(1920.844)
TG (62:2)	1814.769(2212.815)	1781.426(2417.302)	1893.257(1745.858)	2785.453(4208.202)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
TG (62:3)	571.887(485.151)	559.893(537.266)	504.508(303.591)	691.811(585.866)
TG (62:4)	547.101(334.64)	613.733(374.856)	570.749(270.285)	750.37(544.243)
TG (64:2)	864.662(732.038)	883.063(767.604)	895.264(780.971)	1278.603(1231.454)
TG (64:3)	552.787(234.996)	552.569(261.395)	586.53(243.089)	588.42(321.354)
Oxylipins (OL)				
10-nitrolinoleic acid	0.186(0.36)	0.149(0.221)	0.251(0.429)	0.172(0.231)
10-nitrooleic acid	5.022(4.039)	4.734(2.95)	4.925(3.125)	5.642(4.04)
11(12)-epoxy-5,8,14,17- eicosatetraenoic acid	0.045(0.051)	0.046(0.062)	0.026(0.033)	0.057(0.062)
11,12-Dihydroxyicosa-5,8,14-trienoic acid	0.729(0.365)	0.798(0.415)	0.828(0.43)	0.956(0.51)
11,12-Epoxyeicosa-5,8,14-trienoic acid	0.298(0.235)	0.25(0.225)	0.357(0.26)	0.298(0.257)
11-Hydroxy-14,15-epoxyeicosatrienoic acid	0.137(0.271)	0.236(0.486)	0.119(0.181)	0.327(0.463)
11-Hydroxy-arachidonic acid	0.954(0.559)	0.918(0.459)	0.874(0.468)	0.873(0.552)
12(13)-epoxy-9,15-octadecadienoic acid	0.131(0.14)	0.155(0.255)	0.224(0.2)	0.146(0.135)
12,13-dihydroxyoctadec-9-enoic acid	3.714(2.623)	4.151(2.308)	3.873(2.679)	4.493(3.412)
12,13-dihydroxyoctadeca-9,15-dienoic acid	0.107(0.148)	0.111(0.152)	0.077(0.119)	0.06(0.077)
12,13-epoxy-9-octadecenoic acid	2.678(3.381)	3.027(3.742)	3.723(5.106)	3.736(5.303)
12-Hydroxy-5,8,10,14,17-eicosapentaenoic acid	1.953(2.755)	1.117(1.211)	1.527(2.182)	0.773(0.762)
12-Hydroxy-5,8,10,14-eicosatetraenoic acid	17.204(15.381)	15.752(12.397)	16.128(15.755)	13.926(15.033)
13-hydroxyoctadeca-9,11,15-trienoic acid	0.935(0.885)	0.869(0.593)	1.247(1.37)	0.772(0.473)
13-Hydroxyoctadecadienoic acid	19.586(7.961)	19.825(7.897)	19.673(7.942)	19.885(10.275)
13-ketooctadeca-9,11-dienoic acid	11.779(7.152)	12.915(7.243)	13.064(7.45)	15.166(7.158)
14(15)-epoxy-5,8,11,17-eicosatetraenoic acid	0.234(0.427)	0.211(0.435)	0.353(0.67)	0.178(0.248)
14,15-dihydroxyeicosa-5,8,11,17-tetraenoic acid	0.445(0.453)	0.503(0.551)	0.455(0.42)	0.705(0.862)
14,15-dihydroxyeicosa-5,8,11-trienoic acid	0.816(0.427)	0.868(0.394)	0.931(0.478)	1.042(0.491)
14-hydroxydocosa-4,7,10,12,16,19-hexaenoic acid	13.05(14.814)	10.01(9.899)	9.949(12.661)	7.68(10.364)
15(16)-epoxy-9,12-octadecadienoic acid	0.221(0.211)	0.382(0.521)	0.242(0.256)	0.351(0.455)
15,16-dihydroxyoctadeca-9,12-dienoic acid	11.678(8.843)	12.862(6.666)	13.275(11.413)	11.275(5.498)
15-Deoxy-delta-12,14-Prostaglandin J2	0.043(0.036)	0.05(0.053)	0.049(0.048)	0.047(0.049)
15-hydroxyeicosa-5,8,11,13,17-pentaenoic acid	0.387(0.417)	0.288(0.303)	0.344(0.317)	0.387(0.317)
15-hydroxyeicosa-5,8,11,13-tetraenoic acid	3.04(1.536)	2.905(1.282)	2.942(1.555)	2.711(1.289)
15-ketoeicosa-5,8,11,13-tetraenoic acid	0.159(0.211)	0.167(0.276)	0.145(0.244)	0.17(0.202)
15-Keto-prostaglandin E2	0.319(0.368)	0.405(0.635)	0.258(0.253)	0.531(0.627)
16(17)-epoxy-4,7,10,13,19-docosapentaenoic acid	0.189(0.199)	0.159(0.206)	0.239(0.226)	0.224(0.343)
17,18-dihydroxyeicosa-5,8,11,14-tetraenoic acid	6.057(5.778)	4.785(3.299)	5.853(4.234)	5.125(3.967)
17,18-Epoxy-5,8,11,14-eicosatetraenoic acid	0.09(0.188)	0.122(0.18)	0.114(0.256)	0.173(0.255)
17-hydroxy-4,7,10,13,15,19-docosahexaenoic acid	1.382(0.957)	1.263(1.094)	1.408(0.922)	1.463(1.698)
18-(3-ethyloxiran-2-yl)octadeca-4,7,10,13,16-pentaenoic acid	0.406(0.383)	0.403(0.512)	0.476(0.562)	0.406(0.366)
19,20-dihydroxydocosa-4,7,10,13,16-pentaenoic acid	1.929(1.019)	1.91(1)	1.814(1.027)	1.815(1.027)
20-Hydroxyarachidonic acid	4.005(8.301)	3.874(6.762)	3.217(5.556)	2.633(5.511)
4-hydroxydocosa-5,7,10,13,16,19-hexaenoic acid	0.763(0.83)	0.673(0.657)	0.679(0.748)	0.714(0.627)
5,15-dihydroxyeicosa-6,8,11,13-tetraenoic acid	0.038(0.055)	0.053(0.095)	0.037(0.056)	0.033(0.044)
5,6,15-trihydroxyeicosa-7,9,11,13-tetraenoic acid	0.157(0.194)	0.207(0.32)	0.169(0.207)	0.239(0.359)
5,6-dihydroxyeicosa-8,11,14-trienoic acid	0.665(0.513)	0.709(0.521)	0.845(0.618)	1.064(0.765)
5-Hydroxy-6,8,11,14,17-eicosapentaenoic acid	0.954(0.728)	0.874(0.675)	0.84(0.643)	0.875(0.519)
5-Hydroxy-6,8,11,14-eicosatetraenoic acid	3.249(2.155)	3.575(2.057)	3.162(1.957)	3.932(2.264)
5-ketoeicosa-6,8,11,14-tetraenoic acid	0.116(0.104)	0.137(0.127)	0.105(0.095)	0.166(0.154)
6-Ketoprostaglandin F1 alpha	0.111(0.191)	0.091(0.14)	0.095(0.221)	0.104(0.149)
6-trans-Leukotriene B4	0.046(0.066)	0.051(0.099)	0.048(0.053)	0.036(0.053)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	Male ME/CFS (n=31)	Male Control (n=22)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
8,15-dihydroxyeicosa-5,9,11,13-tetraenoic acid	0.121(0.272)	0.115(0.202)	0.103(0.142)	0.137(0.236)
8,9-dihydroxyeicosa-5,11,14-trienoic acid	0.391(0.311)	0.373(0.243)	0.49(0.39)	0.484(0.334)
8,9-Epoxyeicosa-5,11,14-trienoic acid	0.627(0.483)	0.848(0.762)	0.781(0.535)	1.054(1.059)
8-hydroxyeicosa-5,9,11,14-tetraenoic acid	0.707(0.521)	0.693(0.505)	0.617(0.398)	0.837(0.683)
9(10)-epoxy-12,15-octadecadienoic acid	1.238(2.543)	1.495(3.452)	0.68(0.596)	2.319(5.687)
9(10)-epoxy-12Z-octadecenoic acid	0.778(0.586)	0.789(0.455)	0.991(0.871)	0.73(0.429)
9,10-dihydroxyoctadec-12-enoic acid	3.994(2.996)	4.527(2.771)	4.31(2.465)	4.392(2.521)
9,10-dihydroxyoctadeca-12,15-dienoic acid	0.195(0.127)	0.233(0.156)	0.23(0.131)	0.172(0.109)
9,10-Epoxy stearic acid	2.482(2.294)	2.68(2.248)	2.639(2.737)	3.33(2.391)
9,11,15-trihydroxy-5,13,1Z-prostatrienoic acid	0.022(0.082)	0.033(0.09)	0.018(0.026)	0.039(0.105)
9,12,13-trihydroxyoctadec-10-enoic acid	6.746(3.013)	7.161(3.062)	7.35(3.685)	7.274(3.146)
9-Hydroxy-5,7,11,14,17-icosapentaenoic acid	0.259(0.225)	0.218(0.148)	0.26(0.235)	0.209(0.147)
9-hydroxyeicosa-5,7,11,14-tetraenoic acid	0.366(0.266)	0.386(0.267)	0.412(0.284)	0.489(0.346)
9-Hydroxylinoleic acid	9.759(4.207)	10.407(3.998)	9.461(3.48)	10.005(4.55)
9-hydroxyoctadeca-10,12,15-trienoic acid	0.602(0.484)	0.715(0.595)	0.721(0.513)	0.539(0.387)
9-ketooctadeca-10,12-dienoic acid	1.218(0.86)	1.249(0.847)	1.297(0.861)	1.561(0.823)
9-nitrooleic acid	0.611(0.737)	0.692(0.676)	0.479(0.391)	1.009(0.889)
9S,10R-dihydroxy-stearic acid	2.561(1.966)	2.883(2.166)	2.414(1.3)	2.741(2.201)
Leukotriene B4	0.079(0.051)	0.099(0.087)	0.069(0.047)	0.139(0.148)
Leukotriene B5	0.01(0.015)	0.012(0.018)	0.01(0.013)	0.009(0.017)
Prostaglandin D2	0.336(0.565)	0.54(0.959)	0.459(0.726)	0.374(1.005)
Prostaglandin E1	0.02(0.021)	0.019(0.026)	0.023(0.022)	0.019(0.023)
Prostaglandin E2	0.057(0.126)	0.052(0.08)	0.038(0.05)	0.058(0.066)
Prostaglandin E3	0.185(0.427)	0.14(0.232)	0.28(0.673)	0.079(0.115)
Prostaglandin F2a	0.83(0.921)	0.952(0.717)	0.896(0.714)	1.078(0.987)
Resolvin D1	0.147(0.362)	0.162(0.194)	0.228(0.619)	0.204(0.237)
Thromboxane B2	1.893(2.013)	2.178(4.62)	1.753(1.77)	1.569(0.863)
trans-12,13-epoxy-11-oxo-trans-9-octadecenoic acid	1.085(0.917)	1.082(0.66)	1.353(1.407)	1.114(0.694)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
Primary Metabolites (PM)				
1,2,4-benzenetriol	1079.549(1400.131)	1012.135(991.038)	1002.294(1446.43)	1013(996.75)
1-methylgalactose NIST	10405.216(25620.129)	6749.551(12633.562)	9639.456(25578.02)	6826.651(12840.65)
2-aminobutyric acid	6778.127(2312.798)	6819.584(2333.931)	6947.426(2457.48)	6853.965(2362.536)
2-deoxytetronic acid	3802(1871.5)	3811.933(1810.183)	4136.647(1892.756)	3851.767(1815.416)
2-hydroxybutanoic acid	37828.971(19975.01)	35735.831(20029.106)	40403.824(21082.852)	35550.186(20212.41)
2-hydroxyvaleric acid	4237.382(2334.07)	4287.303(2132.918)	4376(2466.058)	4307.965(2155.877)
2-ketoisocaproic acid	18813.069(5556.745)	19149.258(6078.798)	19437.824(5839.105)	19111.605(6066.511)
3-hydroxybutyric acid	39212.265(52464.62)	34152(42085.017)	47151.324(61640.069)	34644.686(42734.988)
4-hydroxybutyric acid	2256.422(736.812)	2269.843(849.082)	2329.868(748.029)	2256.988(857.976)
adipic acid	2895.686(1583.539)	2847.101(1343.166)	2937.044(1688.932)	2856.442(1357.957)
alanine	73245.52(30295.714)	75399.281(33101.158)	69742.426(30239.563)	74847.57(33516.509)
alloxanoic acid	2006.5(1375.468)	1837.64(1056.367)	2001.853(1303.393)	1832.198(1059.848)
alpha-ketoglutarate	1657.627(531.612)	1527.562(557.531)	1660.176(533.451)	1544.233(552.207)
aminomalonate	3619.186(1973.13)	2911.888(1665.318)	3531.279(1803.841)	2949.116(1674.386)
arachidic acid	4924.814(2338.338)	4808.124(2355.798)	4976.015(2288.031)	4799.756(2320.373)
behenic acid	2886.951(836.07)	3031.506(992.687)	2896.779(911.452)	3051.674(1002.272)
benzoic acid	17834.373(6150.942)	17061.82(6244.429)	17951.088(6555.996)	17204.547(6268.506)
beta-alanine	1309.833(728.789)	1377.112(890.61)	1354.279(751.62)	1378.314(898.302)
capric acid	1629.931(794.154)	1873.809(1125.953)	1717.574(849.397)	1863.744(1136.127)
caprylic acid	5704.039(1875.061)	5854.764(2939.166)	5700.471(1999.195)	5865.64(2982.179)
citric acid	41473.245(20630.652)	41135.135(19465.808)	41179.353(18335.064)	41220.093(19676.169)
citrulline	4478.147(1507.009)	4592.506(1393.12)	4419.206(1367.037)	4624.5(1405.977)
conduritol-beta-exopoxide	1309.863(794.473)	1296.146(815.46)	1272.441(740.555)	1309.209(826.609)
creatine	7813.647(4623.762)	7540.27(4234.565)	7800.397(4490.2)	7663.07(4255.072)
creatinine	8228.716(4668.248)	8192.91(4583.811)	8038.088(4635.892)	8315.093(4603.393)
erythritol	7881.353(18212.112)	8811.472(35942.446)	8728.588(20951.725)	8912.953(36563.641)
fructose	2597.775(3830.73)	2215.82(2366.76)	2974.118(4455.038)	2048.233(1719.954)
fumaric acid	9386.029(3097.763)	9434.101(2971.299)	9307.059(3078.13)	9442.756(3017.205)
gluconic acid	783.971(293.026)	776.438(203.662)	788.294(322.547)	779.826(202.775)
glucose	388539.039(113173.178)	378196.978(110227.014)	372105.956(111571.311)	375136.081(110684.535)
glucose-1-phosphate	2858.431(1035.667)	2901.236(1183.342)	2823.221(1092.204)	2892.035(1190.876)
glucuronic acid	1283.441(842.594)	1067.326(518.171)	1246.574(910.65)	1032.86(424.542)
glutamic acid	8913.157(3993.644)	8273.382(4085.076)	8891.029(4135.891)	8300.256(4125.786)
glutamine	30937.275(21124.794)	32325.416(15805.25)	27801.838(15542.15)	32439.128(15970.123)
glutaric acid	568.461(206.452)	532.449(209.713)	574.647(209.789)	535.547(212.303)
glyceric acid	10747.598(4862.652)	9509.18(4092.259)	10877.706(4945.546)	9548.802(4138.782)
glycerol	94812.804(37180.866)	95386.449(35827.521)	94768.426(39627.514)	95732.535(36317.421)
glycerol-alpha-phosphate	970.676(374.848)	952.978(388.821)	983.456(371.538)	953.663(394.123)
glycine	68370.147(24574.146)	66183.809(20178.354)	65419.279(21264.336)	66699.453(20297.528)
glycolic acid	6131.461(2349.621)	6039.528(2582.552)	5853.515(2358.401)	6002.709(2618.469)
heptadecanoic acid	4659.657(1498.193)	4722.045(1568.799)	4730.838(1554.602)	4738.151(1582.092)
hydroxycarbamate NIST	9159.343(4227.978)	9278.079(4002.355)	9382.147(4686.494)	9319.419(4063.919)
indole-3-acetate	2888.461(1569.254)	2930.517(2502.67)	2886.25(1656.91)	2953.919(2541.819)
indole-3-lactate	1920.853(610.853)	2047.753(765.819)	1928.029(667.814)	2070.14(765.945)
indole-3-propionic acid	1758.569(1386.393)	2146.528(1481.229)	1827.75(1593.418)	2183.977(1491.28)
isoleucine	42005.147(16265.503)	42337.787(14176.603)	43098.574(18307.065)	42542.116(14223.111)
isopropylbenzene	16849.167(16235.754)	16249.494(18003.148)	18262.765(17708.733)	16298.965(18277.12)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
isothreonic acid	1867.461(718.975)	1810.944(701.346)	1772.471(715.529)	1826.884(701.858)
lactic acid	192717.833(119615.393)	173890.775(103094.546)	192678.868(114457.944)	171758.884(103576.056)
lauric acid	8363.078(12244.741)	10000.079(13605.883)	9314.75(14848.838)	9955.012(13819.512)
leucine	70058.255(22610.471)	77074.056(24098.618)	71820(24550.985)	77269.186(24091.818)
levoglucosan	1659.137(1216.05)	1870.697(1782.358)	1529.176(894.134)	1870.988(1812.067)
linoleic acid	1164.52(386.052)	1194.708(500.78)	1198.294(396.716)	1194.977(505.334)
lysine	15344.127(10811.81)	15204.719(7437.624)	14990.118(11169.501)	15319.256(7540.723)
lysine	18427.5(13565.891)	18658(9668.614)	17582.191(13501.045)	18648.163(9819.033)
lyxitol	3098.794(1031.473)	3248.989(1189.283)	3132.412(1034.536)	3225.488(1186.925)
maleic acid	878.186(349.551)	788.416(361.008)	851.632(350.688)	785.826(366.892)
maleimide	8053.353(10208.802)	6862.888(5737.055)	6768.412(3769.233)	6916.012(5828.894)
malic acid	1120.422(375.058)	1096.719(407.251)	1138.147(353.636)	1090.058(409.804)
maltose	1438.294(1117.335)	1611.483(3326.737)	1522.544(1310.21)	1619.837(3383.48)
mannitol	7384.294(34427.962)	2531.82(2424.356)	9382.632(42047.894)	2403.279(2037.218)
mannose	23546.755(8923.898)	30536.393(70206.191)	22654.794(9218.45)	30986.453(71369.263)
methionine	2349.51(1025.929)	2403.135(919.059)	2337.412(1031.868)	2422.814(918.995)
myo-inositol	21222.363(6524.406)	20873.449(7257.918)	20795.441(6090.007)	21064.256(7295.825)
myristic acid	2466.971(764.975)	2620.674(814.52)	2537.25(804.074)	2624.453(818.158)
N-acetylmethionine	2287.627(630.487)	2420.708(709.39)	2301.544(647.472)	2421.628(716.318)
N-acetylputrescine	2335.549(2188.271)	2392.753(2148.301)	2347.221(2525.656)	2411.477(2180.955)
nicotinic acid	22012.588(31343.256)	23151.326(37119.635)	20393.426(29744.69)	23701.186(37639.783)
ornithine	22444.167(16004.833)	23350.124(11618.996)	21495.647(14697.704)	23422.43(11691.106)
oxalic acid	38138.853(34967.284)	31155.685(23852.651)	38951.441(30778.027)	31253.128(23836.053)
oxoproline	148843.422(35478.319)	149227.169(31627.972)	148538.309(40405.122)	149327.919(31936.87)
palmitic acid	83826.745(26436.792)	87530.236(29254.435)	84827.985(28657.204)	87770.872(29640.081)
palmitoleic acid	620.618(273.823)	620.933(267.671)	593.971(269.69)	625.977(270.778)
pelargonic acid	29902.833(10040.315)	30430.506(13250.889)	30018.147(10233.407)	30625.291(13371.786)
pentadecanoic acid	10300.402(2114.862)	10098.079(2516.636)	10086.853(2173.19)	10036.256(2497.45)
phenylalanine	21140.618(6021.369)	22473.629(6495.431)	21719.412(6158.625)	22616.035(6532.526)
phosphate	62360.137(25668.008)	60891.899(24903.713)	61856.309(24654.349)	61628.128(24999.471)
phthalic acid	6103.99(2526.222)	6071.337(3064.102)	6055.574(2780.118)	6088.884(3112.388)
proline	10358.696(7248.838)	10114.865(6954.499)	9822.294(6694.674)	10273.558(7021.455)
pseudo uridine	2775.873(653.848)	2855.146(716.503)	2704.059(685.11)	2871.849(722.867)
pyrrole-2-carboxylic acid	6415.049(4040.235)	5793.022(3390.2)	6453.632(4334.966)	5733.477(3358.36)
pyruvic acid	11489.667(4788.685)	10820.404(3860.672)	10829.544(4837.382)	10764.674(3883.488)
quinic acid	1272.48(1447.647)	1600.753(1769.131)	1426.118(1615.364)	1578.547(1745.589)
ribonic acid	873.931(245.494)	868.337(240.982)	871.985(256.98)	866.93(244)
ribose	2038.549(602.463)	2037.371(644.28)	2063.721(569.019)	2019.605(644.323)
salicylic acid	4293.333(14512.238)	2853.427(9490.954)	4636.882(17195.631)	2906.756(9652.561)
serine	37492.01(17259.952)	38555.775(15218.55)	37454.265(17223.185)	38798.081(15359.179)
stearic acid	378059.412(154306.997)	405425.36(162088.008)	387684.956(176535.7)	405699.663(163820.179)
succinic acid	2428.686(828.589)	2106.888(729.61)	2470.044(851.573)	2121.686(737.847)
sucrose	671.637(698.395)	613.989(381.592)	661.397(755.413)	616.337(387.753)
tagatose	4063.725(4123.989)	3589.213(2553.245)	4486.853(4726.886)	3405.826(1874.604)
threitol	1452.196(807.611)	1395.584(582.087)	1448.044(828.449)	1399.756(591.753)
threonic acid	8560.99(4195.661)	7285.618(3051.907)	8697.882(4347.523)	7371.233(3044.807)
threonine	13282.686(4817.033)	14237.438(5929.372)	13059.941(5172.206)	14384.919(5972.952)
trans-4-hydroxyproline	1700(1224.851)	1418.764(658.035)	1583.5(1075.776)	1433.93(663.804)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
tryptophan	21152.706(10249.693)	21495.079(8899.268)	20456.412(10101.724)	21642.988(8927.827)
tyrosine	42719.343(12721.061)	44217.124(10941.659)	42160.985(11955.971)	44092.942(11061.251)
urea	785114.216(265741.232)	831665.056(279983.579)	773192.765(255076.842)	835214.047(283057.568)
uric acid	32108.833(16219.644)	33489.944(17068.328)	33592.912(17269.352)	33287.047(16813.956)
valine	79110.618(21747.997)	82792.506(32138.457)	81631.765(22525.532)	82766.407(32568.183)
Biogenic Amines (BA)				
(2R)-3-Hydroxyisovalerylcarnitine	1880.687(1046.064)	1825.6(555.898)	1964.082(1111.925)	1823.274(546.373)
(3-Carboxypropyl)trimethylammonium cation	16403.7(5302.415)	17555.878(5550.678)	17082.591(5521.617)	17650.284(5558.043)
(R)-Butyrylcarnitine	34078.718(15321.062)	37105.876(16533.628)	34942.84(16189.473)	37122.349(16792.039)
.beta.-Phenyl-.gamma.-aminobutyric acid	869.907(2440.04)	709.92(241.154)	1010.528(2952.619)	703.772(235.316)
.epsilon.-Caprolactam	87755.933(68018.05)	89742.427(68532.183)	97864.372(72253.16)	88548.606(69039.186)
1,2-Dimethylimidazole	1819.366(2845.633)	1694.49(1032.734)	1913.487(3270.852)	1665.473(999.874)
1-Acetyl-3-piperidinamine	1839.3(818.798)	1738.972(605.781)	1869.535(789.474)	1741.517(610.102)
1-Acetyl-4-piperidinamine	2047.585(2838.897)	1533.704(815.512)	2030.882(3074.765)	1526.143(826.822)
1-Methyladenosine A	4344.676(1038.43)	4455.103(1138.778)	4247.068(954.61)	4438.3(1139.104)
1-Methyl-L-histidine	22958.602(14651.539)	23284.637(14336.386)	21813.926(12773.707)	23553.407(14488.922)
1-Methylnicotinamide	14470.114(11101.857)	14251.823(7589.804)	14151.955(11178.5)	14172.234(7654.143)
1-Monostearin	2115.305(1451.321)	2830.121(4236.602)	2214.838(1447.189)	2838.533(4308.542)
1-Oleoyl-2-acetyl-sn-glycerol	9191.209(8932.606)	14964.193(39026.124)	9675.634(10096.748)	15001.706(39686.906)
1-Oleoyl-sn-glycero-3-phosphoethanolamine	6355.005(5324.408)	6525.509(3772.709)	6705.173(4473.497)	6383.607(3732.415)
1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	6410.996(4032.932)	6606.582(3360.162)	7007.096(4148.859)	6538.955(3387.552)
1-Phenylpyrrolidine	143.457(290.638)	117.902(39.385)	119.987(38.857)	117.753(40.034)
1-Stearoyl-2-arachidonoyl-sn-glycero-3-phospho-(1'-myo-inositol)	1329.25(881.122)	1346.97(825.295)	1450.035(901.658)	1341.422(838.428)
1-Stearoyl-2-arachidonoyl-sn-glycero-3-phosphoserine	1894.838(2682.073)	1778.287(2056.277)	2260.31(3019.281)	1784.815(2076.621)
1-Stearoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	6094.917(4604.091)	5803.43(2687.326)	6849.569(4993.056)	5777.603(2728.394)
2,2',2''-Nitrilotriethanol	4650.025(6102.206)	5725.159(8642.651)	5000.241(7220.226)	5778.639(8785.674)
2,2-Bishydroxymethyl]-2,2',2''-nitrilotriethanol	661.365(1011.212)	683.907(582.601)	740.988(1215.03)	687.713(591.539)
2,6-Diaminopimelic acid	658.783(580.92)	497.274(446.965)	597.387(510.284)	503.577(452.301)
2-Amino-1-phenylethanol	50064.106(14796.501)	51939.812(12195.207)	51385.965(15583.684)	51976.379(12402.231)
2-Hydroxyibuprofen	3646.161(11203.95)	2794.402(8390.204)	3815.493(12987.705)	2822.803(8533.437)
2-Indolinone	22360.698(11782.007)	25707.648(13967.826)	21831.879(11194.974)	25783.918(14012.867)
2-Methylbutyryl-L-carnitine	15742.272(6758.335)	19766.912(10894.625)	16474.913(7150.175)	19684.529(10960.024)
3-(1-Pyrazolyl)-alanine	358.412(1009.805)	338.461(595.673)	445.471(1212.875)	346.941(604.154)
3,4-Dimethoxybenzaldehyde	2111.85(1817.258)	2433.796(3874.558)	2365.347(1960.417)	2414.933(3935.923)
3,5-Dihydroxyphenylglycine	1521.258(1937.934)	1263.783(1225.374)	1207.551(1146.119)	1289.513(1238.172)
3-Amino-1-propanol	14759.177(17371.398)	11356.849(7175.122)	14919.726(18496.61)	11469.922(7268.15)
3-Aminoquinoline	2768.697(3284.974)	3229.232(3720.884)	2775.351(3446.016)	3309.084(3758.856)
3-Cysteinylacetaminophen	85.628(278.461)	31.56(22.915)	94.786(309.643)	31.33(22.996)
3-Dehydrocarnitine	2713.916(1241.044)	2870.766(1231.212)	2716.877(1166.048)	2807.342(1127.746)
3-Hydroxybutyrylcarnitine	3061.608(2849.628)	2805.221(2351.317)	3173.922(3045.39)	2827.079(2388.429)
3-Hydroxyyleylcarnitine	1499.787(2022.956)	1253.212(1804.396)	1701.127(2109.072)	1243.896(1798.729)
3-Hydroxypyridine	1971.739(3569.602)	3209.464(4987.632)	2499.475(4090.079)	3107.744(4861.246)
3-Methylglutaryl-L-carnitine	575.563(258.16)	1052.615(1965.769)	573.297(187.677)	1064.058(1998.76)
3-Methylxanthine	555.738(650.872)	522.536(446.424)	537.007(604.597)	513.71(445.158)
3-Pyridinemethanol	1549.304(1050.899)	1769.148(2316.24)	1653.049(1204.888)	1766.567(2354.01)
4,5,7-Trihydroxyisoflavone	507.397(2564.172)	124.958(731.854)	721.161(3093.783)	127.992(744.321)
4-Acetamidobutyric acid	3471.712(2342.69)	3727.521(2854.822)	3098.373(1702.956)	3756.798(2896.733)
4-Aminomethylcyclohexanecarboxylic acid;	1589.572(3239.52)	1326.667(747.566)	1479.649(2000.114)	1310.013(751.776)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
4-Fluoro-.alpha.-pyrrolidinobutiophenone	532.638(610.097)	458.298(230.627)	557.186(655.283)	458.501(234.515)
4'-Methyl-N-methylhexanophenone	2337.883(2599.719)	2483.552(2368.085)	2164.285(2224.075)	2511.922(2393.071)
4-Pyridoxic acid;	9506.692(32185.74)	3611.761(6927.589)	9769.983(37038.8)	3519.903(6939.346)
5'-S-Methyl-5'-thioadenosine	2295.417(2441.494)	2541.641(1775.543)	2262.935(1824.192)	2495.25(1746.721)
5'-S-Methylthioadenosine	2232.692(2448.886)	2396.981(1900.293)	2231.378(1881.53)	2343.903(1871.579)
6-Hydroxyflavone	1191.845(6678.29)	403.876(528.261)	1347.613(7984.023)	405.891(537.138)
6-Methoxynaphthaleneacetic acid	7862.951(2449.945)	9327.172(12784.412)	8028.875(2352.943)	9343.602(13002.803)
7.alpha.-Hydroxy-3-oxo-4-cholestenoic acid	7832.128(4085.847)	7971.016(3525.274)	7885.787(4371.77)	7902.631(3519.163)
7-Hydroxywarfarin	256.276(1326.793)	125.152(55.26)	316.493(1609.047)	124.8(55.977)
7-Methylguanosine	2894.162(982.806)	3126.746(1088.991)	2769.782(932.698)	3119.694(1106.789)
Acetazolamide	111.881(1032.576)	10.68(5.05)	9.858(5.071)	10.672(5.112)
Acetaminophen	8598.401(25412.26)	1888.819(3095.431)	11005.405(30203.075)	1911.304(3146.42)
Acetyl-DL-carnitine	4040.595(1781.273)	3886.498(1192.6)	4095.347(1885.905)	3904.943(1204.502)
Acyclovir	10042.642(38991.986)	102.244(109.125)	11367.848(39695.969)	103.086(110.886)
Adenosine	476.693(252.498)	554.001(724.574)	493.273(252.142)	559.269(736.49)
Ala-Ile	1117.937(531.714)	1022.708(379.234)	1120.486(516.01)	1031.695(382.119)
Albendazole	1404.595(9285.314)	342.564(133.753)	347.851(119.357)	336.326(123.991)
Albendazole sulfoxide	556.474(1732.254)	706.284(5840.411)	556.283(1593.204)	729.06(5940.08)
alpha-Methylhistidine;	18823.314(15559.922)	19428.048(15625.399)	16855.378(14043.866)	19790.576(15733.801)
Alprazolam	219.224(700.569)	79.36(42.975)	281.874(843.18)	79.176(43.537)
Aminodiphenylmethane	10035.44(39641.241)	4831.419(12787.502)	12822.363(47422.83)	4871.615(13000.8)
Androstan-3-ol-17-one 3-glucuronide	1018.393(816.112)	997.46(700.178)	1061.494(856.214)	987.382(709.035)
Arginine	66971.722(30497.565)	63686.741(31676.786)	63685.04(25678.028)	64501.784(31805.912)
Atenolol	2831.445(26482.196)	235.929(152.586)	232.143(116.582)	234.526(152.882)
Atorvastatin	310.188(170.392)	307.876(96.997)	321.126(194.431)	306.747(97.525)
Avobenzene	1620.013(901.713)	2204.034(6233.272)	1758.853(946.147)	2217.883(6339.81)
Benthiavalicarb-isopropyl	397.898(475.323)	338.666(425.872)	398.161(445.499)	335.46(432.386)
Benzophenone-3	79.42(118.399)	152.05(480.887)	72.709(70.367)	154.79(488.954)
Betaine	1396162.001(400978.201)	1465520.587(366608.787)	1391194.829(379473.219)	1467580.291(372092.124)
Betaine aldehyde cation	14682.235(107622.215)	56.189(19.083)	7983.037(65174.742)	55.811(19.183)
Betonicine	5018.889(9595.989)	5425.561(9356.727)	5418.853(11064.457)	5521.092(9493.804)
Biliverden	37882.387(29682.943)	38990.463(24851.237)	39249.673(27018.447)	39623.023(25017.01)
Borrelidin	1800.784(4109.912)	1698.556(4228.984)	1443.631(3762.587)	1739.927(4296.017)
Bradykinin	2350.694(4905.075)	2102.181(4523.581)	2167.847(4312.877)	2154.829(4592.393)
Caffeine	46358.68(97388.926)	86219.943(115602.167)	50554.399(106716.969)	83627.982(115088.639)
Carbamazepine	424.616(1432.071)	11883.366(108750.28)	403.365(1360.899)	12286.104(110608.577)
Carnitine	1001164.333(283021.215)	1045982.351(310270.412)	1025126.234(295143.84)	1042090.348(313096.555)
Choline cation	254611.526(57164.648)	282373.342(63913.774)	252335.789(56953.937)	281693.168(63982.361)
cis-10,11-Dihydroxy-10,11-dihydrocarbamazepine	525.109(153.075)	959.717(3818.829)	523.748(156.925)	972.976(3884.166)
Citrulline	19901.677(6196.281)	21504.169(6882.343)	19304.822(5922.577)	21774.49(6785.432)
Codeine-6-.beta.-D-glucuronide	774.993(5522.859)	232.532(91.583)	1031.562(6698.825)	231.962(93.078)
Coniferylaldehyde	765.911(462.54)	787.668(824.323)	784.989(491.256)	789.407(838.498)
Cotinine N-.beta.-D-glucuronide	76.449(283.47)	46.197(159.887)	101.112(341.741)	47.042(162.585)
Creatine	217981.51(118303.317)	203650.285(97913.88)	211908.405(121174.486)	205858.724(98348.005)
Creatinine	1006729.671(287698.034)	1029213.304(254200.686)	1033881.328(295858.663)	1022055.057(251490.929)
Cyclo(Leu-Pro)	2228.564(1706.261)	2027.347(1104.514)	2193.953(1508.134)	1964.97(1012.064)
D-.alpha.-Cyclohexylglycine	6326.782(6206.867)	8327.262(8211.34)	6294.91(5326.197)	8250.983(8285.554)
Decanoyl-L-carnitine	42146.5(48589.406)	42071.952(30458.853)	46740.83(55984.725)	42126.188(30821.977)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
D-erythro-Sphingosine-1-phosphate	7295.174(3378.972)	7543.128(3687.008)	7149.919(3292.013)	7567.496(3729.923)
Dexpanthenol	1546.048(2341.347)	2108.653(3911.294)	1667.173(2793.252)	2123.987(3977.94)
D-Fructose	34526.336(8214.427)	34866.41(9180.115)	33495.541(7851.696)	34735.272(9281.089)
Diazepam	370.721(2360.704)	46.476(76.296)	526.068(2856.845)	46.208(77.458)
Dinor-12-oxophytodienoic acid	525.23(862.885)	416.42(194.711)	557.78(959.241)	414.892(197.743)
Diphenhydramine	2585.349(6127.955)	3178.366(14715.458)	2824.194(7289.56)	3227.817(14967.412)
DL-Indole-3-lactic acid	37199.448(18913.594)	35604.136(12065.446)	38487.416(21614.263)	35443.174(12139.329)
D-Pyroglutamic acid	121612.569(22366.016)	123013.056(24064.978)	120213.273(22046.967)	123457.112(24079.229)
D-Turanose	525.908(351.452)	631.074(581.896)	511.203(333.272)	630.228(590.162)
Ergothioneine	767.24(1494.771)	719.663(431.749)	852.919(1799.119)	724.995(438.079)
Esomeprazole	2660.51(10721.074)	1307.945(4540.326)	2883.769(11843.121)	1322.815(4618.105)
Ethiolat	11862.296(20760.107)	9779.989(18228.881)	11778.576(20175.243)	9744.616(18528.037)
Ethylidethanolamine	734.979(766.768)	727.196(595.857)	697.378(488.565)	719.253(595.658)
Ethylenediaminetetraacetic acid	663091.766(891136.229)	496339.244(788805.165)	602816.808(882295.101)	507817.899(798840.96)
Ezetimibe	223.611(238.157)	234.24(306.197)	246.134(270.897)	234.272(311.216)
Fexofenadine	450.355(238.197)	841.091(3125.726)	440.082(123.375)	853.737(3178.997)
Gabapentin	62080.105(201779.015)	5287.117(32734.04)	42184.573(179451.146)	5380.885(33296.054)
Glaucine	860.63(2849.169)	574.959(169.559)	1020.539(3449.8)	572.998(170.928)
Glutamic acid	7933.975(3124.287)	7180.498(3426.266)	8006.862(3234.641)	7257.869(3456.197)
Glutamine	101505.785(19190.477)	102907.791(20574.24)	100918.678(18945.978)	103180.337(20602.324)
Glycocholic acid	4874.144(5532.195)	3707.728(3340.534)	4264.406(4640.264)	3686.655(3372.994)
Glycodeoxycholic acid	16574.334(17400.385)	14780.84(19064.118)	14727.616(15895.011)	14697.086(19278.505)
Gly-Pro-Arg	586.043(2198.483)	428.808(1170.147)	536.568(2176.596)	440.366(1188.677)
Guanidine	5493.87(8781.142)	4475.798(4190.121)	4774.838(3439.928)	4491.344(4261.485)
Guanine	6226.314(23441.739)	279.003(1082.414)	7109.677(24227.455)	284.1(1100.765)
Heptadecaphing-4-enine	5557.437(4651.009)	5538.189(4468.342)	6346.584(4544.059)	5406.862(4462.629)
Hexanoyl-L-carnitine	8996.499(13556.537)	8356.705(5002.169)	10094.335(16137.172)	8326.454(5023.511)
H-gamma-glutamyl-glutamine	2339.192(1792.988)	2006.339(1305.502)	2063.811(1241.507)	2042.336(1310.079)
Histidine	49555.943(23320.509)	53178.919(21745.875)	48156.01(21266.441)	53685.785(21575.736)
Homoarginine;	3381.815(2097.316)	3026.593(2160.863)	3192.592(2022.598)	3054.736(2192.018)
H-Pro-Hyp-OH	2228.15(1753.581)	1756.456(871.446)	2137.306(1824.059)	1786.547(866.895)
Hydroxybupropion	884.813(2016.341)	1883.832(8028.514)	599.334(949.899)	1142.921(3669.234)
Hypoxanthine	31281.328(19491.261)	30486.398(22288.554)	33840.545(21057.089)	30357.187(22599.14)
Ile-Glu-Arg	365.728(1522.667)	320.225(998.515)	363.02(1672.624)	328.745(1014.695)
Indole-3-propionic acid	1220.413(1004.075)	1438.512(994.93)	1286.035(1140.982)	1464.082(1001.703)
Irbesartan	34111.466(330125.328)	1632.597(1008.364)	49418.34(400452.975)	1628.175(1023.2)
Isoleucine	15404.33(5244.539)	15607.18(5393.939)	15857.795(5470.903)	15551.535(5413.814)
Isopentenyladenine	1014642.651(399845.125)	1046922.522(370983.691)	1040237.761(443711.938)	1051035.2(375459.37)
Isopropylamine	4749.851(1414.044)	5211.39(1333.561)	4703.129(1377.742)	5212.833(1349.979)
Kynurenine	2125.376(754.54)	2313.805(749.317)	2134.227(784.952)	2315.98(759.339)
Lamotrigine;	2244.641(22565.331)	18.464(16.389)	3293.018(27372.274)	18.308(16.126)
Lansoprazole	736.475(4048.63)	2665.031(13708.313)	874.922(4660.598)	2217.891(13107.924)
Lauric acid diethanolamide	413.111(567.669)	345.335(216.443)	384.371(227.102)	344.743(217.118)
Lauroyl-L-carnitine	5784.303(4911.391)	6763.368(3908.375)	6324.233(5264.912)	6730.446(3968.773)
L-Carnitine	16079.975(4595.436)	15890.768(4307.224)	15854.424(4409.427)	15894.437(4362.249)
L-Citrulline	20161.291(5985.134)	21758.529(6402.073)	19548.345(5692.582)	22022.422(6292.986)
L-Cysteine-glutathione disulfide	1116.696(1162.972)	1224.484(1444.167)	993.135(1007.08)	1252.166(1460.802)
L-Cystine	2137.312(1969.911)	2271.747(2210.344)	1920.176(1901.115)	2313.903(2235.856)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
Levocetirizine;	9007.024(38087.67)	5404.405(22513.101)	5961.791(22780.063)	5582.386(22881.407)
Linoleoylcarnitine	6028.057(4694.504)	6937.757(5240.418)	5446.701(3980.575)	6937.188(5311.453)
L-Leucine, methyl ester	936.172(1279.128)	734.385(675.979)	1016.061(1338.561)	744.236(684.933)
Losartan	1124.145(6579.061)	2289.546(19221.441)	1542.5(7964.007)	263.914(134.048)
L-Threonine	6399.383(2197.795)	6434.59(1928.87)	6121.688(1937.236)	6477.306(1940.987)
L-Tyrosine	3214.55(1382.508)	3345.219(1261.579)	3149.322(1298.755)	3360.462(1280.179)
Lysine	24048.561(14481.217)	23142.646(14133.037)	22328.548(12990.746)	23472.954(14233.908)
Matrine	2325.219(12579.91)	500.431(207.181)	1979.721(11338.092)	497.761(210.046)
Mefenorex	622.656(716.718)	3807.946(26441.59)	717.441(840.228)	3922.235(26891.457)
Meloxicam	28306.258(195269.072)	12851.881(121675.611)	40080.013(236137.948)	13294.223(123755.678)
Meprobamate	1573.996(3579.443)	932.297(1488.818)	1420.676(3236.736)	936.585(1514.249)
Metformin	7135.099(48045.124)	3475.203(23828.338)	9721.006(58168.254)	963.019(505.131)
Methacholine cation	56501.078(33409.327)	67485.057(42836.21)	60371.886(33845.977)	67825.387(43486.302)
Methionine	6161.544(1634.068)	6223.87(1770.355)	6127.603(1616.691)	6241.36(1792.871)
Methioninesulfoxide	753.827(372.4)	693.081(379.811)	736.68(312.772)	696.836(381.164)
Methylgallate	139.383(458.151)	67.958(251.269)	124.443(429.276)	62.674(248.786)
Metoprolol	897.413(4862.805)	234.563(653.184)	1030.256(5729.681)	236.384(664.401)
Metoprolol acid	7786.566(33910.371)	535.074(2767.371)	7101.932(33547.471)	544.392(2814.749)
Milnacipran	276.882(1331.735)	148.067(53.863)	344.499(1614.036)	147.503(54.686)
Modafinil	1075.48(6709.26)	71.168(24.162)	1446.432(8084.443)	71.001(24.362)
Modafinil acid	131.611(721.079)	24.78(13.35)	164.487(862.058)	24.762(13.498)
Montelukast-1,2-diol	75.941(301.129)	84.645(479.266)	94.825(363.323)	86.966(487.386)
Moxonidine	3500.133(2726.862)	3040.75(1987.891)	3269.679(2397.851)	3035.903(2015.855)
N-(3-(Aminomethyl)benzyl)acetamidine	20921.024(28034.826)	18034.449(15522.733)	21990.895(31106.262)	17947.809(15636.204)
N-.alpha.-Acetyl-L-arginine	3082.187(1181.981)	3213.461(1045.445)	2974.499(1008.387)	3239.071(1053.579)
N.alpha.-Methyl-L-lysine	29306.073(114182.748)	13134.602(36620.029)	38981.267(137655.472)	13367.14(37228.844)
N.epsilon.-Acetyl-L-lysine	2453.841(2107.986)	2280.92(1269.094)	2214.053(870.202)	2287.94(1287.955)
N.epsilon.-Methyl-L-lysine	8975.039(6927.428)	8793.019(6711.352)	8847.949(6185.507)	8950.23(6772.251)
N8-Acetylspermidine	3001.558(1211.178)	2900.086(896.957)	2933.751(1133.346)	2921.058(892.561)
N-Acetylaniline	707.391(950.515)	582.675(496.092)	687.736(1072.698)	585.421(501.727)
N-Acetyl-D-norleucine	3757.634(3749.095)	3860.092(3382.148)	3762.306(3311.768)	3925.62(3421.079)
N-Acetylhistidine	1008.892(648.298)	1039.722(610.487)	910.498(431.301)	1046.649(618.025)
N-Acetyl-L-carnosine	2954.051(1639.621)	2926.55(1628.741)	2790.698(1423.746)	2923.049(1604.241)
Naproxen	3476.065(13446.579)	4450.949(22153.769)	3552.838(13562.626)	2410.542(10255.922)
NEPSILON,NEPSILON,NEPSILON-TRIMETHYLLYSINE	13358.236(4821.32)	15219.514(11953.152)	12738.5(4616.782)	15324.205(12109.067)
N-Methylhistidine	35730.75(37645.645)	33537.29(29498.297)	34522.756(31691.234)	33848.774(29950.778)
N-Methylproline	11656.687(9296.226)	11510.001(9904.91)	11144.479(7784.066)	11702.239(10011.173)
Norleucine	15444.661(6060.568)	15678.34(4128.345)	16027.945(6891.363)	15607.118(4128.386)
Nudifloramide	64111.911(56284.553)	63703.328(37012.76)	65381.674(63955.93)	62610.205(35407.751)
Octanoylcarnitine	46353.596(55972.637)	47100.775(29066.033)	50793.521(65993.487)	46929.062(29425.169)
Oleoyl-L-carnitine	10823.414(8463.672)	11676.244(8434.192)	10434.869(7958.94)	11562.747(8454.363)
Omeprazole sulfone	4929.053(23929.418)	1843.877(13957.834)	4682.463(25395.639)	1902.955(14195.467)
Omeprazole sulfone N-oxide	1165.746(5101.882)	421.937(2441.309)	1203.344(5637.807)	433.673(2482.683)
Ondansetron	365.61(1271.909)	240.115(62.33)	240.038(61.294)	239.359(63.023)
Ornithine	3959.933(2287.816)	4022.624(2665.327)	3719.599(2105.118)	4077.565(2687.759)
p-Acetamidophenyl .beta.-D-glucuronide	766.028(3177.057)	171.088(73.211)	922.587(3756.171)	171.036(74.362)
Palmitamide	3270.611(17777.123)	1962.253(8761.313)	2255.543(11239.789)	1905.623(8878.473)
Pantoprazole	898.088(8152.763)	16270.845(118825.791)	1274.501(9889.644)	12249.767(113541.365)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
Pantothenic acid	10030.786(7968.504)	8465.694(5284.919)	9300.128(6599.677)	8462.982(5355.706)
Penciclovir	615.263(2184.586)	280.151(80.439)	333.415(306.869)	280.24(81.822)
Phenylacetylglutamine	31218.152(22442.043)	34681.21(38768.962)	29540.297(23675.457)	34874.898(39323.491)
Phenylacetyl-L-glutamine	14884.784(10785.176)	16607.075(17719.928)	14176.705(11371.852)	16687.101(17973.17)
Phenylalanine	55973.85(16422.42)	58120.533(13302.726)	57474.874(17249.079)	58127.78(13527.3)
Pipecolic acid	425.09(586.911)	426.157(508.716)	464.872(675.825)	429.944(516.87)
Piperine	5718.294(8337.056)	7720.583(10963.746)	4754.636(5578)	7636.219(11059.26)
Prazepam	288.862(1542.242)	137.608(93.414)	148.414(91.439)	137.501(94.513)
Proline	14486.098(6367.337)	14482.522(5997.29)	15009.419(6447.947)	14418.197(6063.209)
Propionylcarnitine	68344.79(23209.488)	71041.55(26326.498)	67631.021(23042.474)	71003.485(26698.093)
Pyrantel	372.256(111.716)	1129.226(7044.272)	383.177(96.807)	1153.099(7164.864)
Pyridoxal	1642.179(3991.664)	946.29(438.171)	1554.326(4323.843)	942.404(443.038)
Pyridoxine;	1022.88(4388.483)	435.057(382.972)	1120.681(5181.253)	436.614(389.41)
Quetiapine	369.86(1339.4)	222.872(66.167)	446.395(1621.698)	222.739(67.065)
Quetiapine sulfoxide	650.477(4802.113)	136.563(42.808)	895.536(5822.128)	136.001(43.418)
R(-)-O-Desmethylvenlafaxine	592.445(3164.213)	410.727(1880.497)	542.382(3282.244)	419.039(1912.463)
rac-4-Sulfoxypropranolol	202.948(514.821)	151.335(57.243)	232.419(621.83)	146.544(45.621)
Ranitidine	2507.731(13468.136)	205.008(53.061)	3294.597(16111.517)	204.252(53.547)
Ranitidine N-oxide	713.593(4219.564)	62.623(17.85)	961.933(5087.309)	62.584(18.092)
Ranitidine-S-oxide	213.634(515.841)	132.212(90.781)	246.652(618.406)	133.197(91.771)
Scopoletin	591.68(2509.742)	178.452(414.272)	434.817(2045.369)	176.338(420.311)
SDMA	9500.368(2703.971)	10370.308(2765.049)	9042.982(2572.939)	10476.979(2721.616)
Serotonin	18189.163(41222.489)	14668.474(23684.703)	22486.287(49447.018)	14792.877(24081.722)
Ser-Tyr-Lys	193.809(988.093)	91.613(175.965)	213.48(1141.475)	92.741(178.835)
Stachydrine	563959.448(691819.57)	612164.26(685817.817)	511672.999(618599.937)	621464.731(693246.546)
Sulfamethoxazole	41.919(48.984)	4622.278(43440.039)	45.834(55.18)	4780.702(44182.6)
Tapentadol-.beta.-D-glucuronide	221.214(1394.74)	127.85(761.689)	223.307(1554.834)	130.896(774.678)
Tauroursodeoxycholic acid	2706.846(6111.732)	1545.619(2380.983)	2178.484(4947.103)	1558.752(2419.545)
Telmisartan	4699.894(41335.897)	3856.6(30518.071)	6649.958(50137.588)	3969.104(31039.611)
Temazepam	279.199(1061.022)	153.782(115.023)	351.216(1283.164)	153.133(116.734)
Testosterone	3622.17(4140.278)	4445.438(4912.789)	3150.597(2338.175)	4523.775(4977.94)
Theanine;	1819.454(2742.739)	1366.781(1424.619)	1492.438(1917.573)	1396.886(1439.654)
Theobromine	43840.022(50239.28)	50274.237(39008.573)	45494.606(50281.908)	48151.022(37511.801)
threo-Dihydrobupropion	959.671(1263.114)	899.034(1318.122)	768.344(397.79)	838.135(1199.449)
Thr-Ile-Arg	334.018(1580.162)	174.397(391.703)	328.627(1774.274)	177.059(398.201)
Ticlopidine	228.217(1202.183)	52.712(180.862)	211.436(1291.966)	53.867(183.874)
Topiramate	883.512(3767.87)	360.884(470.487)	385.991(426.722)	361.833(478.507)
Toradol	356.538(2066.064)	150.603(104.488)	452.906(2504.906)	151.592(105.936)
trans-3'-Hydroxycotinine	2268.615(10601.908)	1686.299(5203.465)	3048.199(12814.502)	1720.57(5290.065)
Trazodone	2672.469(13819.619)	206.455(55.025)	1697.31(9177.841)	206.049(55.555)
Tri-2-ethylhexyl trimellitate	6954.814(58249.323)	2150.885(4550.116)	1351.522(2489.591)	2182.813(4622.634)
Trigonelline	62593.319(128404.523)	87574.388(113723.624)	74835.97(150041.321)	84879.579(111042.199)
Trileptal	378.242(124.735)	1737.665(13037.79)	385.504(132.649)	1782.652(13260.894)
Trimethoprim	234.855(71.982)	2512.23(21564.074)	238.109(68.142)	2590.361(21932.743)
Trimethylamine-N-oxide	22496.762(34083.237)	15784.326(13954.105)	23261.064(38326.745)	15894.929(14167.11)
Triptolide	572.071(359.723)	709.428(1341.517)	552.552(251.866)	716.691(1364.097)
Tryptophan	15719.222(4762.968)	15591.457(4927.165)	15909.637(4590.351)	15635.127(4890.189)
Tyrosine	6484.429(2346.848)	6649.41(2125.156)	6424.944(2350.708)	6679.864(2155)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
Urea	128763.489(48161.656)	135736.88(41188.088)	132639.649(47795.604)	135287.137(41375.423)
Urocanic acid;	20103.21(25401.881)	20113.659(16158.372)	20730.595(29343.465)	20194.811(16339.206)
Usnic acid	6421.074(38109.236)	5909.508(26905.817)	2675.635(1396.189)	3084.644(2776.796)
Complex Lipids (CL)				
AC (10:0)	14300.667(14495.722)	14592.903(12632.497)	14605.269(15294.075)	14549.52(12733.997)
AC (10:1)	7852.356(5661.808)	8700.584(5463.897)	7807.902(6119.907)	8702.836(5489.19)
AC (12:0)	6801.104(4854.843)	7472.708(4034.354)	7024.789(5213.572)	7500.509(4071.683)
AC (12:1)	5342.259(2975.805)	5782.079(2495.997)	5381.782(2875.004)	5793.067(2518.137)
AC (14:1)	7653.305(5643.002)	7865.258(4525.933)	7885.232(6002.322)	7914.837(4558.016)
AC (14:2)	4537.778(3261.62)	5105.633(2880.79)	4577.987(3375.946)	5138.183(2902.62)
AC (16:0)	10907.214(3516.947)	10958.197(3206.646)	11163.093(3655.045)	10942.32(3232.673)
AC (18:0)	4409.46(1523.433)	4658.607(1398.628)	4531.472(1619.583)	4656.223(1412.475)
AC (18:1)	15169.411(6563.264)	14716.482(4589.592)	15085.89(6843.601)	14640.462(4609.767)
AC (18:2)	9086.774(4258.756)	9507.785(3723.066)	8897.388(4404.011)	9460.75(3748.879)
AC (8:0)	5424.664(7636.621)	5324.659(5489.183)	5206.69(6508.227)	5274.749(5514.915)
CE (14:0)	483.105(328.13)	550.26(299.965)	518.33(358.842)	552.164(302.75)
CE (16:0)	6284.196(5322.107)	5971.764(4027.806)	6581.319(5737.272)	5931.384(4031.777)
CE (16:1)	44723.031(22333.233)	45240.669(19130.581)	46447.98(24469.213)	45051.908(19198.96)
CE (18:0)	3286.85(1793.581)	3220.682(1502.875)	3526.574(1877.186)	3200.334(1513.806)
CE (18:1)	32176.362(13035.556)	33019.476(10977.599)	32674.823(13317.324)	33024.184(11098.589)
CE (18:2)	360370.43(102450.354)	395504.729(97524.484)	360426.024(111369.215)	396258.771(98429.215)
CE (18:3)	13226.28(5296.356)	16158.621(6188.509)	13354.326(5702.323)	16259.704(6222.806)
CE (20:2)	7353.518(4456.574)	8560.232(3729.559)	7123.948(4300.333)	8629.842(3731.012)
CE (20:3)	65342.381(23690.393)	72249.761(24364.326)	65336.374(23908.2)	72329.291(24626.098)
CE (20:4)	760763.777(278873.716)	769431.808(251914.063)	776905.931(292801.179)	773402.023(253390.857)
CE (20:5)	17407.549(19917.453)	12423.777(8256.741)	17943.006(21644.577)	12547.557(8309.52)
CE (22:2)	686.936(506.637)	714.698(520.067)	770.278(535.802)	714.697(525.222)
CE (22:6)	132582.468(60465.938)	114384.853(39714.847)	130693.301(63530.758)	114958.904(39983.681)
Ceramide (d34:1) - ESI(+)	7991.308(2279.1)	7701.808(1766.753)	8163.665(2522.072)	7680.806(1778.694)
Ceramide (d36:1) - ESI(+)	5055.887(1639.5)	4781.199(1246.336)	5109.903(1645.787)	4787.826(1258.971)
Ceramide (d38:1) - ESI(+)	6696.998(1780.221)	6981.944(1458.36)	6733.486(1844.048)	6980.003(1432.779)
Ceramide (d40:1)	21686.844(5740.739)	23489.285(4735.334)	21904.442(6142.908)	23491.446(4760.333)
Ceramide (d41:1) - ESI (+)	6918.214(1876.08)	7517.217(1659.079)	7010.178(1921.702)	7513.459(1678.067)
Ceramide (d42:1) - ESI (+)	71508.239(18019.881)	78197.952(14457.978)	71968.394(19122.953)	78266.18(14617.875)
Ceramide (d42:2) A - ESI (+)	19273.129(4975.246)	18114.439(3325.542)	18973.318(5067.804)	18081.507(3355.413)
Ceramide (d42:2) B - ESI (+)	14981.161(4149.123)	17174.124(4245.274)	15181.345(4134.712)	17196.409(4290.779)
Ceramide (d32:1)	3595.683(1323.517)	3755.63(977.806)	3630.861(1393.167)	3750.835(988.134)
Ceramide (d33:1)	2916.634(935.773)	3016.705(807.728)	2879.441(921.486)	3015.656(806.98)
Ceramide (d34:0)	4886.997(2053.157)	4687(1716.579)	4742.189(2020.416)	4687.849(1736.201)
Ceramide (d34:1) - ESI(-)	18074.154(4880.408)	17694.653(3936.635)	17805.341(5062.865)	17578.908(3825.734)
Ceramide (d34:2)	3094.181(847.888)	3030.248(713.119)	3022.781(901.367)	3028.889(721.295)
Ceramide (d36:1) - ESI(-)	1637.345(721.82)	1539.002(608.946)	1614.569(707.754)	1523.585(587.181)
Ceramide (d38:1) - ESI(-)	11993.384(4407.452)	12156.053(3738.061)	11894.289(4485.06)	12116.782(3647.169)
Ceramide (d39:1)	6299.483(2739.989)	6979.275(2440.541)	6330.75(2703.721)	6939.846(2399.521)
Ceramide (d40:0)	1765.181(1227.484)	1564.678(901.085)	1693.591(1280.901)	1560.751(910.01)
Ceramide (d40:2)	6057.125(4179.286)	6235.898(4315.18)	6154.521(4337.808)	6241.05(4338.496)
Ceramide (d41:1) - ESI(-)	42041.811(15059.383)	46380.145(13427.707)	41883.777(14693.073)	46114.893(13216.731)
Ceramide (d42:0)	11948.609(7113.944)	11294.104(4976.297)	11573.042(7705.79)	11311.311(4978.851)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
Ceramide (d42:1) - ESI(-)	136674.648(44023.767)	149770.415(39576.94)	136190.726(44092.942)	149392.901(39527.405)
Ceramide (d42:2) A - ESI(-)	49252.166(17827.101)	47220.491(13180.04)	47781.287(19009.221)	46967.429(13005.976)
Ceramide (d42:2) B - ESI(-)	37317.754(16468.604)	35789.863(11255.565)	36310.405(16665.687)	35510.767(11062.936)
Ceramide (d43:1)	2528.23(1370.14)	2789.752(1196.521)	2528.074(1295.411)	2781.344(1188.393)
Ceramide (d44:1)	846.904(541.153)	822.512(399.283)	844.843(612.712)	824.67(403.621)
Cholesterol	266952.992(63543.111)	283483.733(67507.559)	270735.61(69029.172)	283563.583(68251.393)
DG (32:0)	2029.32(748.253)	1982.392(914.732)	2129.17(771.564)	1966.058(917.989)
DG (32:1)	5251.897(3457.449)	4947.61(2880.584)	5363.106(3601.043)	4879.383(2877.177)
DG (34:1)	1041.038(494.395)	999.382(487.017)	1067.266(507.496)	991.249(487.464)
DG (34:2)	32528.392(13807.47)	30539.842(13070.979)	32862.579(13681.52)	30129.214(12756.43)
DG (34:3)	5185.782(3045.124)	4572.847(2077.17)	5015.399(3044.733)	4519.506(2066.811)
DG (36:1)	6350.769(3167.505)	6121.406(3281.803)	6677.517(3265.854)	6040.81(3269.019)
DG (36:2)	55205.662(20357.43)	49677.788(17704.742)	54727.262(20725.423)	49332.853(17712.748)
DG (36:3)	70925.903(27194.121)	65340.022(22354.965)	69414.597(26559.636)	64824.688(22056.768)
DG (36:4) A	16838.454(8807.583)	16004.561(7408.839)	16138.078(8196.396)	15872.433(7304.423)
DG (36:4) B	4169.876(3637.695)	3516.148(2613.304)	4115.961(3435.276)	3573.376(2615.064)
DG (36:5)	2206.156(1211.632)	2086.253(902.788)	2190.083(1269.996)	2083.453(899.178)
DG (38:5)	10566.304(4064.74)	10089.518(3680.913)	11132.338(4362.87)	10071.225(3668.467)
DG (38:6)	6169.284(3104.712)	5407.065(2535.955)	6485.037(3285.409)	5393.998(2542.726)
FA (10:0) (capric acid)	1604.441(1050.232)	1407.005(1073.102)	1565.562(941.764)	1317.378(758.378)
FA (12:0) (lauric acid)	8080.776(5386.504)	8269.26(5625.99)	8644.72(6130.857)	7781.091(4038.99)
FA (14:0) (myristic acid)	46315.443(13985.33)	46285.78(10922.906)	48601.306(14763.115)	46064.933(10864.49)
FA (14:1) (physeteric acid)	5158.99(3232.701)	4681.581(1944.979)	5562.146(3597.282)	4714.16(1950.248)
FA (15:0) (pentadecylic acid)	10544.8(2976.688)	10266.457(2239.062)	10666.906(2745.41)	10279.316(2247.903)
FA (16:1) (palmitoleic acid)	87362.569(45359.632)	76933.028(35142.058)	88715.774(46306.12)	77631.404(35224.576)
FA (17:0) (margaric acid)	22117.789(4474.162)	21235.84(3887.35)	22367.807(4051.958)	21187.509(3901.147)
FA (18:1) (oleic acid)	1454192.087(480456.365)	1349284.059(394857.372)	1484484.426(491581.065)	1355919.32(392066.033)
FA (18:2) (linoleic acid)	573453.977(197151.585)	559405.212(162215.142)	588596.244(203846.628)	560450.802(160694.115)
FA (18:3) (linolenic acid)	52408.007(25261.774)	49568.813(16119.839)	53212.903(28367.993)	49968.942(15968.286)
FA (20:1) (eicosenoic acid)	18300.811(5932.05)	17239.139(4691.897)	18599.422(6446.265)	17284.272(4728.359)
FA (20:2) (eicosadienoic acid)	9414.386(2783.824)	9398.564(2656.075)	9545.485(2990.685)	9424.846(2651.935)
FA (20:3) (eicosatrienoic acid)	2064.852(782.798)	2106.53(696.017)	2055.843(802.71)	2122.482(695.112)
FA (20:3) (homo-gamma-linolenic acid)	9019.322(2564.168)	9232.52(2388.112)	9207.061(2815.945)	9251.423(2411.537)
FA (20:4) (arachidonic acid)	43084.156(11307.632)	45485.009(12124.954)	42956.129(11563.455)	45697.144(12175.132)
FA (20:5) (eicosapentaenoic acid)	7210.305(8172.735)	5310.154(4416.295)	7322.744(9333.703)	5362.462(4452.664)
FA (22:0) (behenic acid)	4796.588(1883.561)	4776.335(2235.782)	4695.661(1816.385)	4742.038(2208.438)
FA (22:6) (docosahexaenoic acid)	35785.158(23581.553)	31506.346(14537.092)	36117.296(25965.865)	31705.54(14638.937)
FA (24:0) (lignoceric acid)	9002.74(3316.901)	9144.823(3857.725)	8846.907(3295.393)	9154.153(3881.644)
FA (24:1) (nervonic acid)	3404.095(1062.601)	3216.118(871.277)	3325.956(1013.565)	3211.83(866.174)
Gal-Gal-Cer (d18:1/16:0)/Lactosylceramide (d18:1/16:0)	37250.999(11809.088)	37236.749(10987.775)	38126.573(12337.769)	37387.827(11064.047)
GlcCer (d38:1)	3730.008(1287.974)	3948.513(1065.45)	3692.222(1311.485)	3943.808(1066.52)
GlcCer (d40:1) - ESI(-)	22073.89(7846.193)	22731.523(6665.458)	21941.486(7818.015)	22781.953(6713.619)
GlcCer (d41:1)	12088.153(4455.943)	12743.895(4333.197)	11970.157(4433.761)	12764.296(4374.701)
GlcCer (d42:1) - ESI(-)	25575.096(9070.161)	26263.818(7929.532)	25292.022(8684.437)	26290.06(7978.255)
GlcCer (d42:2) - ESI(-)	19888.456(7749.181)	17973.465(6288.748)	19006.652(6801.252)	18012.501(6352.361)
GlcCer (d14:1(4E)/20:0(2OH))	6302.067(3492.07)	6460.128(3125.454)	6083.889(3036.22)	6470.613(3160.733)
GlcCer (d34:1)	7468.445(3751.415)	8251.003(4419.557)	7688.989(3880.188)	8293.003(4453.335)
GlcCer (d40:1) - ESI(+)	4100.143(1480.243)	4234.688(1219.049)	4209.927(1613.923)	4254.942(1225.185)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
GlcCer (d42:1) - ESI(+)	17983.989(6028.82)	18240.869(5395.163)	18380.701(6457.292)	18301.315(5441.569)
GlcCer (d42:2) - ESI(+)	13729.159(5608.295)	12051.673(4176.986)	13667.879(6015.572)	12118.9(4189.449)
Lactosylceramide (d18:1/24:1(15Z))	2755.733(1184.633)	2537.724(815.608)	2807.221(1233.763)	2555.792(813.809)
LPC (14:0) - ESI(-)	1816.114(1007.334)	2045.03(925.463)	1819.835(1054.556)	2025.459(893.736)
LPC (16:0) - ESI(-)	224092.722(72172.597)	240419.333(71704.173)	222259.354(76620.932)	239765.838(71679.031)
LPC (16:1) - ESI(-)	3256.883(1286.541)	3465.425(1194.712)	3186.752(1416.047)	3436.145(1176.568)
LPC (17:1)	2907.335(879.847)	2996.073(1096.874)	3045.115(902.533)	2990.696(1108.783)
LPC (18:0) A - ESI(-)	7418.389(3009.415)	8077.783(2590.056)	7345.942(3256.194)	8075.065(2619.873)
LPC (18:0) B - ESI(-)	99494.905(36134.374)	108242.985(32910.725)	98789.161(39113.631)	108552.619(33214.707)
LPC (18:1) - ESI(-)	47798.748(19375.801)	51591.653(19211.667)	46814.46(19406.559)	51560.576(19387.13)
LPC (18:2) - ESI(-)	60906.166(28020.858)	71522.652(31446.609)	59431.225(27583.488)	71157.294(31707.303)
LPC (20:0)	2602.173(1120.102)	2667.429(891.909)	2649.61(1193.281)	2693.924(883.003)
LPC (20:1) - ESI(-)	3013.633(1298.505)	2917.096(1050.301)	2986.298(1387.035)	2923.053(1061.524)
LPC (20:1) - ESI(+)	713.456(419.647)	654.494(268.413)	687.461(421.378)	657.034(270.807)
LPC (20:2) - ESI(-)	4059.133(1281.292)	4450.809(1469.606)	4092.816(1404.591)	4465.83(1480.733)
LPC (20:2) - ESI(+)	518.937(285.076)	598.846(314.265)	508.188(291.326)	606.59(313.175)
LPC (20:3) - ESI(-)	3582.326(1705.034)	4021.253(1564.565)	3554.185(1701.252)	3996.738(1552.401)
LPC (22:4)	1706.729(976.366)	1894.898(1004.387)	1846.79(1046.267)	1898.401(1012.839)
LPC (22:5) - ESI(-)	675.167(447.702)	664.823(383.062)	658.84(432.803)	667.096(386.874)
LPC (22:6)	18296.637(8748.95)	17120.89(7390.865)	18842.819(9702.32)	17162.43(7444.474)
LPC (o-16:0)	7726.959(3135.329)	8366.675(3289.673)	8201.817(3494.261)	8401.351(3319.459)
LPC (p-16:0)/LPC (o-16:1)	10752.235(4110.82)	11778.247(4172.532)	11259.487(4523.187)	11823.53(4198.094)
LPC (p-18:0)/LPC (o-18:1)	5609.615(1996.592)	5649.593(2083.157)	5692.896(2158.371)	5677.214(2098.323)
LPC (14:0) - ESI(+)	12225.274(5163.537)	14568.798(5062.405)	12517.868(5427.698)	14524.041(5082.835)
LPC (15:0)	12084.127(4819.914)	12943.535(4361.419)	12643.424(5011.723)	12914.073(4397.571)
LPC (16:0) - ESI(+)	1926106.937(412946.468)	2025455.264(509547.986)	1976669.593(444192.812)	2027571.315(515206.445)
LPC (16:1) - ESI(+)	18357.864(6537.325)	19256.04(6089.078)	18601.498(7542.127)	19201.023(6139.414)
LPC (18:0) - ESI(+)	597884.618(199525.827)	642665.246(221367.761)	615986.831(215521.358)	646231.415(221509.646)
LPC (18:1) - ESI(+)	267553.679(104625.2)	280752.212(113394.873)	271445.876(106754.861)	281850.679(114394.293)
LPC (18:2) - ESI(+)	453109.903(200728.084)	547483.468(267853.354)	458809.666(206629.29)	544878.381(267813.143)
LPC (18:3)	3781.745(1556.029)	4762.878(2448.244)	3797.375(1629.076)	4780.82(2472.778)
LPC (20:3) - ESI(+)	18658.988(7504.447)	20830.978(7040.033)	19454.931(8147.028)	20755.738(7092.886)
LPC (20:4)	92588.56(39171.901)	99801.287(39143.693)	97075.22(41447.985)	100006.125(39387.62)
LPC (20:5)	8554.056(10259.538)	6693.724(5097.151)	9211.575(11668.719)	6757.878(5138.079)
LPC (22:5) - ESI(+)	4133.499(2034.537)	4006.158(1626.825)	4363.375(2052.93)	4016.991(1636.58)
LPE (16:0)	3007.892(1492.945)	3345.916(1755.537)	3082.04(1618.03)	3326.568(1741.116)
LPE (18:2) - ESI(-)	4521.977(2417.216)	5517.915(3099.215)	4561.548(2543.135)	5398.702(3009.274)
LPE (20:4) - ESI(-)	3411.332(1579.491)	3835.167(1358.006)	3420.042(1601.323)	3805.198(1358.863)
LPE (22:6)	2511.314(1103.103)	2584.869(1142.272)	2485.081(1071.693)	2561.784(1140.98)
LPE (18:0)	2976.4(935.468)	3330.697(987.882)	3093.293(1012.022)	3316.427(994.418)
LPE (18:2) - ESI(+)	3940.782(1604.285)	4738.299(2407.019)	4018.716(1697.213)	4635.05(2259.741)
LPE (20:4) - ESI(+)	3205.181(1241.82)	3617.274(1320.76)	3270.867(1321.852)	3577.859(1287.694)
PC (16:0/9:0(CHO))	4327.064(2722.879)	4282.307(2603.353)	4589.78(2660.987)	4235.219(2523.464)
PC (32:0) - ESI(-)	14490.961(3964.7)	14558.291(3478.332)	14243.818(3899.426)	14492.211(3372.222)
PC (32:1) - ESI(-)	14447.376(7522.552)	14662.134(6394.392)	14331.384(7979.761)	14478.031(6097.206)
PC (32:2) - ESI(-)	13463.361(6508.264)	16204.369(5624.383)	13176.148(6724.934)	16078.818(5564.473)
PC (33:1) - ESI(-)	2353.684(1083.204)	2374.083(853.644)	2368.37(1072.803)	2357.216(835.239)
PC (33:2) - ESI(-)	3860.198(1605.855)	4336.55(1397.757)	3790.563(1586.109)	4295.957(1361.3)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
PC (34:0) - ESI(-)	8251.523(2184.754)	8469.609(1811.655)	8162.85(2256.349)	8443.034(1803.548)
PC (34:2) - ESI(-)	240630.097(60351.691)	258867.547(56457.148)	234017.313(61164.965)	257587.052(55868.894)
PC (34:3)	16244.273(6359.067)	18088.554(6094.852)	15419.188(6184.462)	17986.817(6025.427)
PC (34:4) - ESI(-)	3988.556(2296.794)	4598.624(1731.583)	3792.963(2208.225)	4571.552(1709.372)
PC (35:1) - ESI(-)	3093.959(1098.086)	3051.722(977.026)	3090.742(1032.773)	3045.792(940.977)
PC (35:2)	9207.837(2691.891)	9716.991(2633.897)	9074.31(2674.248)	9663.598(2629.522)
PC (35:4) - ESI(-)	2567.664(1136.268)	2622.666(936.586)	2574.127(1111.966)	2619.452(910.694)
PC (36:1) - ESI(-)	60700.134(17787.723)	61602.252(15986.223)	59845.797(18852.856)	61560.21(16024.035)
PC (36:3) A - ESI(-)	78001.315(26248.654)	80601.946(20165.252)	76641.547(27589.436)	80028.564(19163.692)
PC (36:3) B - ESI(-)	80122.729(25240.712)	84455.963(19138.885)	79288.754(26075.408)	83856.926(18245.131)
PC (36:4) A - ESI(-)	50001.555(19418.961)	58881.412(19057.435)	48211.317(20388.858)	58636.399(19196.913)
PC (36:4) B - ESI(-)	165608.498(45603.524)	172562.505(36378.869)	161093.155(45105.372)	172103.845(36230.461)
PC (36:5) A	2138.31(1339.816)	2567.216(1605.787)	1995.656(1373.916)	2570.171(1623.883)
PC (36:5) B	41857.83(35378.719)	33407.87(22725.882)	40052.72(36387.91)	33637.215(22867.504)
PC (37:2) - ESI(-)	1427.867(571.478)	1549.892(656.208)	1356.668(550.82)	1550.999(663.634)
PC (37:3)	19429.669(8642.077)	20766.774(7555.42)	19792.246(8796.838)	20590.196(7539.777)
PC (37:4) - ESI(-)	3610.43(1262.482)	3600.739(1164.94)	3532.53(1237.455)	3598.039(1176.602)
PC (38:2)	4724.469(1540.569)	4816.371(1178.537)	4591.821(1714.226)	4814.026(1183.586)
PC (38:3) - ESI(-)	29648.655(10260.002)	31432.948(7745.999)	29200.155(11217.103)	31334.232(7693.854)
PC (38:4) A - ESI(-)	57986.619(17566.019)	60883.346(16516.825)	56059.722(17810.736)	60997.571(16671.957)
PC (38:5) A - ESI(-)	19182.481(6029.043)	19166.914(4819.422)	18959.816(6263.795)	19173.336(4833.043)
PC (38:5) B - ESI(-)	12329.808(8869.88)	10448.295(4369.029)	12060.15(9605.348)	10497.711(4388.176)
PC (38:6) - ESI(-)	75564.438(34561.384)	68827.018(26086.774)	72807.158(34179.525)	68997.723(26204.556)
PC (39:6)	18191.534(9715.309)	16532.441(6454.175)	18918.135(10297.911)	16606.293(6492.648)
PC (40:4) - ESI(-)	3651.767(1838.864)	3888.447(1301.818)	3705.488(1955.064)	3873.374(1300.13)
PC (40:5) A - ESI(-)	4364.652(1888.948)	4187.943(1433.041)	4349.552(2003.557)	4197.426(1440.474)
PC (40:5) B - ESI(-)	1949.867(1019.491)	2160.184(912.295)	1979.401(1074.925)	2152.268(909.921)
PC (40:6) B	20657.541(8269.246)	18554.405(6543.511)	19980.918(8878.717)	18577.33(6547.096)
PC (40:7) - ESI(-)	2669.718(1393.762)	2433.114(925.635)	2555.608(1399.183)	2443.043(933.383)
PC (40:8) - ESI(-)	2630.788(1139.643)	2734.932(900.85)	2633.311(1250.357)	2743.855(903.745)
PC (42:5)	3139.766(1127.172)	3024.694(1140.962)	2966.434(1195.792)	3037.599(1149.787)
PC (42:6)	2237.693(1216.735)	2297.879(1311.502)	2279.388(1333.629)	2323.614(1315.028)
PC (o-32:0) - ESI(-)	2806.219(868.036)	2847.252(794.141)	2774.69(860.116)	2831.858(770.697)
PC (p-32:0)/PC (o-32:1) - ESI(-)	2338.644(927.886)	2365.854(804.708)	2303.7(928.299)	2361.585(783.92)
PC (p-32:0)/PC (o-32:1) - ESI(+)	29152.037(7872.188)	30771.998(7341.47)	29722.833(8485.24)	30799.486(7424.032)
PC (p-34:1)/PC (o-34:2) A	4520.84(2258.236)	5300.943(2014.065)	4404.968(2150.798)	5290.747(2023.083)
PC (p-34:1)/PC (o-34:2) B	2874.162(1241.363)	2975.868(1271.407)	2792.387(1096.742)	2982.974(1282.056)
PC (p-34:2)/PC (o-34:3) - ESI(-)	13080.94(4655.151)	15147.291(4618.811)	12669.044(4411.375)	15150.242(4671.192)
PC (p-36:1)/PC (o-36:2)	1579.393(1039.658)	1842.803(957.813)	1478.322(947.172)	1829.295(960.205)
PC (p-36:3)/PC (o-36:4) - ESI(-)	21432.678(7961.51)	23318.595(6892.306)	21046.155(8038.699)	23313.681(6922.909)
PC (p-36:3)/PC (o-36:4) - ESI(+)	227889.598(84207.01)	254677.838(68833.936)	234246.607(87202.856)	256174.875(68897.848)
PC (p-36:4)/PC (o-36:5) - ESI(-)	12136.93(5243.46)	13380.29(4590.962)	11751.521(5145.248)	13413.925(4630.98)
PC (p-38:3)/PC (o-38:4) - ESI(-)	7180.199(2581.694)	8011.26(2278.842)	7191.411(2419.954)	8002.046(2279.346)
PC (p-38:4)/PC (o-38:5) A	16408.903(5205.505)	17597.828(4431.343)	15768.113(4826.907)	17610.51(4453.417)
PC (p-38:4)/PC (o-38:5) B	2559.33(1097.47)	2769.763(1152.827)	2509.36(1016.701)	2776.522(1164.309)
PC (p-38:5)/PC (o-38:6)	1297.362(880.416)	1291.415(783.351)	1285.878(843.374)	1311.131(780.672)
PC (p-40:1)/PC (o-40:2)	1485.155(608.109)	1292.088(473.435)	1463.259(613.669)	1293.224(473.413)
PC (p-40:3)/PC (o-40:4)	1750.816(685.913)	1868.47(638.755)	1743.351(652.732)	1875.269(640.5)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
PC (p-40:4)/PC (o-40:5) - ESI(-)	1855.515(641.097)	1784.499(529.196)	1806.243(603.923)	1784.252(528.02)
PC (p-40:7)/PC (o-40:8)	12784.77(9315.863)	11294.973(6789.332)	11685.467(9260.77)	11384.19(6825.683)
PC (p-42:3)/PC (o-42:4)	4785.842(1784.509)	5178.399(1630.148)	5041.944(1885.999)	5200.635(1632.756)
PC (p-42:4)/PC (o-42:5) - ESI(-)	2268.307(909.076)	2270.498(870.57)	2184.702(855.245)	2261.696(864.096)
PC (p-42:5)/PC (o-42:6)	618.687(355.575)	610.366(274.685)	575.455(326.259)	615.095(273.578)
PC (p-44:4)/PC (o-44:5) - ESI(-)	2845.694(1045.311)	2893.365(908.463)	2733.951(944.072)	2883.804(896.937)
PC (p-44:5)/PC (o-44:6)	3310.494(1275.999)	3174.484(993.019)	3243.368(1220.927)	3191.614(997.8)
PC 34:4e	6443.081(2515.863)	7999.075(2933.128)	6404.258(2554.366)	8019.482(2940.252)
PC 38:7e	16964.282(13526.498)	15342.968(9446.371)	16856.913(13156.423)	15490.122(9504.09)
PC 40:5e	12165.024(3482.196)	12677.876(3009.874)	12025.323(3199.489)	12739.163(3013.606)
PC 40:6e	22316.948(7430.313)	21474.846(6189.986)	22197.188(7784.299)	21623.783(6175.042)
PC (28:0)	3246.565(4662.849)	3239.16(2348.658)	3558.295(5489.584)	3233.267(2374.737)
PC (30:0)	158777.616(83572.094)	179096.713(65617.314)	165216.361(93427.652)	179210.623(66049.201)
PC (31:0)	10922.351(4521.628)	11042.588(3052.892)	11358.688(4823.418)	11035.171(3032.178)
PC (31:1)	1677.788(1455.465)	1660.939(915.401)	1775.221(1628.096)	1645.448(908.327)
PC (32:0) - ESI(+)	256268.716(58170.605)	250135.791(53964.518)	259144.909(62925.656)	250462.669(54506.815)
PC (32:1) - ESI(+)	239846.485(124170.713)	249536.641(113064.066)	245455.432(139736.749)	248950.869(113280.227)
PC (32:2) - ESI(+)	56756.644(28246.729)	67703.831(25937.146)	55700.803(30016.44)	67635.726(26221.119)
PC (33:0)	10952.596(5641.864)	11592.978(3878.492)	11689.558(5842.141)	11572.727(3868.088)
PC (33:1) - ESI(+)	53543.632(20928.978)	53553.558(13337.174)	55279.073(22414.831)	53406.585(13204.347)
PC (33:2) - ESI(+)	78531.369(27527.116)	87270.676(25504.3)	78022.252(29190.385)	86943.817(25702.157)
PC (34:0) - ESI(+)	56673.124(14226.497)	56575.078(11243.201)	57988.448(15118.945)	56790.977(11270.355)
PC (34:1)	4013338.964(720952.007)	4067426.422(727466.087)	4062709.877(769160.87)	4072020.238(730603.307)
PC (34:2) - ESI(+)	8298954.78(1436737.757)	8880671.15(1333757.007)	8201779.521(1557049.345)	8871299.896(1346265.758)
PC (34:3) A	97711.278(31702.813)	106631.972(39043.209)	93915.056(33247.85)	106793.471(39461.44)
PC (34:3) B	108771.059(36242.03)	128990.918(46188.814)	106249.745(39129.52)	129387.848(46646.006)
PC (34:3) C	86598.612(39702.386)	108697.965(49708.994)	86591.607(42147.668)	109263.919(50139.319)
PC (34:4) - ESI(+)	17218.357(9083.701)	20014.966(7594.249)	17373.707(9531.92)	20065.065(7666.87)
PC (35:1) - ESI(+)	46139.315(13080.522)	45638.931(9232.36)	47505.991(12892.848)	45629.634(9303.389)
PC (35:2) A	109536.799(36351.893)	103212.896(30675.48)	107047.548(35343.348)	102815.658(30367.982)
PC (35:2) B	131176.614(32124.982)	137458.977(30973.043)	131382.573(33447.818)	137344.717(31226.014)
PC (35:3)	40372.126(10564.132)	44343.372(11336.707)	39709.617(11171.443)	44234.168(11390.527)
PC (35:4) - ESI(+)	22778.31(8961.192)	23974.006(6756.722)	23385.755(9416.11)	24010.791(6817.916)
PC (36:1) - ESI(+)	656088.196(185659.526)	660392.494(148989.452)	662290.869(195630.993)	663377.135(149374.666)
PC (36:2)	4529060.48(909760.507)	4996033.975(881985.183)	4402650.34(946009.211)	5002768.328(872906.035)
PC (36:3) A - ESI(+)	1277000.345(445850.9)	1366182.069(370360.325)	1221268.785(455608.087)	1369124.271(371511.618)
PC (36:3) B - ESI(+)	1639032.954(502617.113)	1716418.049(393778.108)	1637555.054(557291.285)	1714709.947(396710.519)
PC (36:4) A - ESI(+)	344228.244(141889.724)	433150.27(175314.159)	330340.32(148234.03)	432937.74(176243.894)
PC (36:4) B - ESI(+)	254789.338(417790.093)	206974.331(69274.833)	253436.033(397790.263)	206658.634(69438.458)
PC (36:4) C - ESI(+)	3945315.162(980469.466)	4037185.749(932394.375)	4000440.116(994299.382)	4055722.581(934890.426)
PC (36:5) C	63676.772(293144.05)	37777.207(75598.623)	81673.798(354897.755)	38098.298(76442.208)
PC (36:5) D	466335.725(583640.353)	328794.138(256617.495)	482947.978(643937.257)	332594.28(258248.921)
PC (36:5)A	10087.21(5302.765)	12082.737(6355.171)	9555.815(5406.625)	12156.017(6404.45)
PC (36:6)	7517.927(4687.721)	7514.303(3539.182)	7413.234(4814.471)	7549.236(3569.667)
PC (37:2) - ESI(+)	12948.098(3497.278)	14134.187(3647.086)	12778.893(3447.731)	14195.756(3645.96)
PC (37:4) - ESI(+)	51981.159(19322.358)	49132.105(16397.252)	52237.315(19599.551)	49370.279(16476.626)
PC (37:5)	36908.954(34432.55)	28967.669(14940.073)	38452.496(37877.76)	29236.369(15001.717)
PC (37:6)	9891.772(5465.158)	8696.041(4047.719)	9893.467(5484.538)	8736.468(4077.449)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
PC (38:3) - ESI(+)	545962.223(199887.214)	581406.422(170804.445)	541919.095(208893.159)	582742.133(172543.347)
PC (38:4) A - ESI(+)	129827.943(52570.47)	130649.431(33178.708)	128843.841(57666.719)	130983.455(33483.185)
PC (38:4) B - ESI(+)	138945.853(49865.612)	150899.97(43419.782)	145027.775(54570.879)	151336.198(43779.847)
PC (38:4) C - ESI(+)	2313829.998(565304.201)	2391882.015(574272.595)	2321739.659(589973.366)	2406694.888(570510.436)
PC (38:5) A	732724.247(176405.92)	721011.877(165292.616)	735715.185(170649.669)	725519.057(164432.584)
PC (38:5) B - ESI(+)	385628.57(330057.265)	324021.431(136699.566)	399379.583(365571.608)	326647.318(137120.575)
PC (38:6) A - ESI(+)	122703.865(38145.153)	135842.09(35120.916)	121779.409(39418.963)	136259.293(35324.013)
PC (38:6) B - ESI(+)	3683483.214(1066200.996)	3373471.275(825187.655)	3657273.591(1085634.511)	3389893.16(826762.373)
PC (38:7)	9067.129(4522.378)	8494.519(3671.831)	8767.372(4415.118)	8543.985(3698.92)
PC (39:4)	4951.364(1392.551)	4980.401(1209.519)	4979.359(1261.552)	5022.52(1190.291)
PC (40:4) - ESI(+)	40710.749(17107.156)	43768.486(14761.039)	43031.205(18895.324)	43907.06(14894.586)
PC (40:5) A - ESI(+)	160984.496(51414.716)	153215.298(48927.121)	163231.207(53799.49)	154338.924(48914.87)
PC (40:5) B - ESI(+)	39290.673(16831.51)	43514.802(16159.023)	40021.609(17513.652)	43527.988(16344.456)
PC (40:6) A	26324.155(8352.257)	26286.775(7120.512)	26474.383(8548.768)	26446.792(7116.955)
PC (40:6)B	523343.738(235330.416)	448154.607(162581.361)	511675.299(239359.315)	451652.474(162754.752)
PC (40:7) A - ESI(+)	14123.954(4521.843)	15295.102(4113.716)	14402.113(4851.312)	15322.173(4155.479)
PC (40:7) B - ESI(+)	294687.493(123648.862)	260986.662(85720.284)	280811.224(122348.869)	262880.664(85775.009)
PC (40:8) - ESI(+)	15239.14(4848.028)	15297.801(4079.753)	15498.392(5079.096)	15378.659(4090.812)
PC (42:10)	2726.931(1374.175)	2509.831(1360.724)	2763.544(1424.331)	2520.709(1364.459)
PC (o-32:0) - ESI(+)	33066.939(8835.009)	34463.696(8408.236)	33492.212(9809.329)	34464.353(8502.972)
PC (o-34:0)	4253.752(1544.24)	4625.498(1473.237)	4415.904(1695.302)	4629.054(1484.252)
PC (p-32:1)/PC (o-32:2)	7732.065(2525.44)	8442.017(2078.799)	7881.476(2808.747)	8457.282(2099.061)
PC (p-34:1)/PC (o-34:2)	90514.308(41518.544)	112732.145(42037.713)	91475.293(46037.028)	113376.226(42264.092)
PC (p-34:2)/PC (o-34:3) - ESI(+)	134516.098(48579.028)	167161.547(53529.226)	133658.768(49629.539)	167938.748(53754.934)
PC (p-36:1)/PC (o-36:2) B	4576.41(1860.937)	4990.913(1761.819)	4699.805(1853.413)	5003.991(1775.361)
PC (p-36:2)/PC (o-36:3)	18401.743(7473.236)	22260.671(8493.763)	18842.485(7779.36)	22351.138(8529.12)
PC (p-36:4)/PC (o-36:5) - ESI(+)	222255.821(73873.841)	244403.223(62140.636)	225724.835(75604.567)	245587.683(62296.124)
PC (p-36:5)/PC (o-36:6)	43163.98(47010.214)	35793.982(29043.548)	43410.782(44710.87)	36198.809(29253.43)
PC (p-38:3)/PC (o-38:4) A - ESI(+)	23415.263(7747.924)	26268.221(7020.386)	24191.48(8087.438)	26348.532(7078.493)
PC (p-38:3)/PC (o-38:4) B - ESI(+)	60681.832(24417.325)	68924.225(21887.47)	64483.935(25968.209)	69292.563(22001.673)
PC (p-38:4)/PC (o-38:5) A	244736.068(73932.864)	253186.358(52211.505)	242645.006(75267.53)	254571.544(51956.652)
PC (p-38:4)/PC (o-38:5) B	46348.51(17350.154)	52251.201(14810.562)	48112.295(17621.65)	52460.469(14869.201)
PC (p-38:5)/PC (o-38:6) A	47602.588(24906.045)	44907.468(17837.495)	46699.307(23405.806)	45238.272(17905.308)
PC (p-38:5)/PC (o-38:6) B	60693.148(18465.69)	63136.031(15203.868)	59728.294(17931.149)	63395.498(15228.685)
PC (p-38:6)/PC (o-38:7)	38202.501(19743.59)	36368.564(13760.086)	37586.507(18596.862)	36636.147(13802.699)
PC (p-40:4)/PC (o-40:5) - ESI(+)	17184.561(5389.491)	17672.249(4621.409)	17633.138(5716.339)	17791.313(4606.074)
PC (p-40:6)/PC (o-40:7) A	40200.774(19957.817)	35888.168(13738.726)	38247.611(19252.016)	36145.669(13781.758)
PC (p-40:6)/PC (o-40:7) B	13510.106(6889.457)	13100.064(5544.826)	13676.333(7015.166)	13204.922(5564.569)
PC (p-42:4)/PC (o-42:5) - ESI(+)	12900.718(4496.163)	12896.037(3917.285)	12934.468(4555.335)	12967.171(3931.021)
PC (p-42:5)/PC (o-42:6) A	10237.461(3726.694)	10713.657(3758.542)	10267.451(3866.404)	10795.536(3761.98)
PC (p-42:5)/PC (o-42:6) B	3974.188(1415.292)	3956.085(1237.45)	3945.197(1361.956)	3972.173(1245.398)
PC (p-44:4)/PC (o-44:5) - ESI(+)	14453.858(5455.893)	14223.731(4628.827)	14571.775(5549.4)	14252.115(4673.244)
PE (34:1)	1935.048(1193.975)	1997.27(1266.931)	1904.402(1183.166)	1990.722(1274.003)
PE (34:2) - ESI(-)	2982.653(1876.385)	3405.593(2151.45)	3017.52(1905.946)	3354.244(2128.94)
PE (36:1) - ESI(-)	418.862(181.396)	445.435(181.825)	421.311(174.493)	448.61(182.184)
PE (36:2)	7905.774(4135.38)	8803.532(4225.603)	7810.351(4304.96)	8670.866(4173.423)
PE (36:3)	2026.786(1248.378)	2279.738(1430.26)	2010.435(1307.713)	2242.802(1425.386)
PE (36:4) - ESI(-)	2941.499(1644.752)	3164.472(1950.982)	2992.312(1611.669)	3167.268(1969.338)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
PE (38:2)	629.602(222.186)	682.787(206.229)	629.87(231.692)	684.371(207.976)
PE (38:6) - ESI(-)	7437.759(5142.646)	7356.489(4624.489)	7280.063(4362.178)	7337.96(4644.972)
PE (p-34:1)/PE (o-34:2) - ESI(-)	2025.04(785.489)	2051.91(695.945)	1984.699(772.235)	2041.719(699.616)
PE (p-34:2)/PE (o-34:3)	3040.334(1576.283)	3609.46(1747.103)	2975.33(1597.431)	3620.102(1765.852)
PE (p-36:1)/PE (o-36:2) - ESI(-)	2760.373(1320.05)	3068.12(1351.566)	2780.87(1340.981)	3059.064(1365.731)
PE (p-36:2)/PE (o-36:3) - ESI(-)	5957.994(2773.012)	6972.062(2936.918)	5945.7(2826.471)	6966.226(2968.837)
PE (p-36:4)/PE (o-36:5) - ESI(-)	15261.909(9626.399)	15928.908(8581.977)	14636.588(9054.541)	15918.27(8632.217)
PE (p-36:5)/PE (o-36:6)	2102.097(2962.828)	1485.236(2041.939)	1988.288(2983.894)	1502.625(2061.638)
PE (p-38:3)/PE (o-38:4)	1340.345(687.934)	1513.805(782.147)	1359.457(685.127)	1510.431(785.885)
PE (p-38:5)/PE (o-38:6) - ESI(-)	11786.825(6628.023)	12149.489(5341.659)	11138.708(6249.873)	12145.504(5396.945)
PE (p-38:6)/PE (o-38:7)	7532.92(4292.66)	7188.888(3364.912)	6953.498(3689.32)	7182.481(3397.962)
PE (p-40:4)/PE (o-40:5)	3399.555(1897.801)	3410.027(1799.437)	3470.705(1947.091)	3406.803(1797.404)
PE (34:2) - ESI(+)	8757.929(6410.569)	9879.682(7371.827)	8750.926(6451.795)	9744.42(7401.492)
PE (36:1) - ESI(+)	3379.71(1611.842)	3316.561(1592.325)	3420.384(1649.593)	3271.575(1581.854)
PE (36:4) - ESI(+)	14739.008(7468.332)	15255.178(7705.241)	15153.184(7642.129)	15253.619(7780.05)
PE (38:4)	39570.697(19154.594)	40390.086(15772.1)	40941.692(20312.303)	40415.795(15919.094)
PE (38:6) - ESI(+)	20257.66(12022.688)	19884.696(11866.824)	19885.235(11213.456)	19983.065(11974.331)
PE (p-34:1)/PE (o-34:2) - ESI(+)	2742.254(1098.637)	2862.174(974.659)	2779.13(1152.772)	2867.889(984.373)
PE (p-36:1)/PE (o-36:2) - ESI(+)	2454.413(1024.933)	2762.367(992.448)	2525.096(1064.668)	2771.035(995.888)
PE (p-36:2)/PE (o-36:3) - ESI(+)	8991.903(3876.705)	11041.406(4021.531)	9186.075(4121.604)	11064.28(4038.724)
PE (p-36:4)/PE (o-36:5) - ESI(+)	29345.071(18055.185)	30532.635(14508.762)	30067.743(18241.048)	30699.183(14625.534)
PE (p-38:4)/PE (o-38:5)	42614.164(20321.576)	46103.9(17411.189)	44872.887(21563.563)	46295.619(17564.043)
PE (p-38:5)/PE (o-38:6) - ESI(+)	24747.834(11095.999)	26262.641(9101.812)	24924.424(11359.644)	26372.865(9176.145)
PE (p-40:4)/PE (o-40:5) A	2896.209(2724.733)	2989.973(2175.181)	3265.189(3067.35)	2999.456(2195.18)
PE (p-40:4)/PE (o-40:5) B	3708.007(1951.993)	3692.493(1528.458)	3894.973(2144.397)	3697.527(1544.524)
PE (p-40:5)/PE (o-40:6)	6740.897(2550.286)	6806.706(1987.436)	7168.298(2779.074)	6822.697(2006.254)
PG (34:0)/PG (17:0/17:0)	76853.368(21921.357)	85280.313(20224.124)	77047.644(24486.356)	85397.434(20410.267)
PI (38:4)/PI (18:0-20:4)	120817.481(39400.359)	124008.066(31642.823)	117906.601(39165.698)	124171.713(31804.055)
SM (d30:1) - ESI(-)	1704.845(1134.453)	1947.17(774.108)	1777.806(1209.982)	1946.128(781.97)
SM (d32:0) - ESI(-)	1032.341(809.55)	1064.49(657.551)	1052.653(876.669)	1068.301(658.928)
SM (d32:1) - ESI(-)	44492.705(15861.723)	49754.267(12913.605)	44905.165(15643.054)	49583.07(12911.672)
SM (d32:2) - ESI(-)	3030.003(1334.652)	3230.614(1251.27)	2989.558(1337.605)	3215.642(1261.181)
SM (d33:1) - ESI(-)	22975.489(8246.125)	25365.753(7028.514)	23436.193(7659.792)	25236.624(7029.047)
SM (d34:0) - ESI(-)	4927.976(1784.951)	5032.83(1672.907)	4838.108(1884.771)	5023.758(1690.769)
SM (d34:1) - ESI(-)	155715.48(39317.352)	163369.808(34296.98)	154490.25(40753.285)	162869.741(34351.86)
SM (d34:2) - ESI(-)	57475.881(14166.69)	60371.724(13403.338)	56155.122(14732.064)	60082.503(13418.706)
SM (d36:0) - ESI(-)	1066.803(653.242)	879.715(483.034)	1002.499(622.425)	882.868(486.728)
SM (d36:1) - ESI(-)	36132.26(10486.124)	36986.044(8862.176)	36042.616(11045.31)	36600.281(8385.189)
SM (d36:2) - ESI(-)	5807.249(1805.715)	5799.331(1630.41)	5816.71(1986.338)	5725.611(1571.265)
SM (d36:3) - ESI(-)	1713.798(653.047)	1804.421(563.54)	1683.146(688.603)	1796.262(567.166)
SM (d37:1)	2411.418(1019.95)	2404.494(818.507)	2448.956(995.601)	2381.08(789.395)
SM (d38:0)	696.441(811.576)	522.617(447.127)	658.1(856.002)	528.797(449.782)
SM (d38:2) - ESI(-)	4790.522(1380.077)	4974.002(1318.512)	4734.478(1521.276)	4944.864(1317.226)
SM (d39:1) - ESI(-)	12841.047(4278.992)	14353.601(3784.665)	12836.383(4287.686)	14266.495(3690.375)
SM (d39:2)	12449.201(3511.981)	12954.634(3279.589)	12344.23(3273.819)	12936.232(3308.728)
SM (d40:1) - ESI(-)	46897.381(13275.565)	50082.888(10695.858)	46268.966(13896.047)	49880.885(10511.163)
SM (d40:2) A - ESI(-)	12273.795(4442.543)	12319.223(4118.364)	12053.207(4935.659)	12228.38(4042.72)
SM (d40:2) B - ESI(-)	17613.206(5158.79)	18864.027(4350.959)	17514.243(5594.939)	18798.146(4345.106)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
SM (d40:3)	1079.194(398.684)	1151.905(387.017)	1035.02(427.889)	1147.152(390.039)
SM (d41:1) - ESI(-)	11075.677(11704.719)	13579.641(12424.293)	11680.563(11652.556)	13317.97(12444.504)
SM (d41:2) - ESI(-)	10157.654(3759.068)	10335.005(4166.592)	9996.252(3844.751)	10305.284(4191.64)
SM (d42:0) - ESI(+)	631.117(319.733)	572.32(282.695)	591.761(300.097)	578.069(283.225)
SM (d42:0) - ESI(-)	2435.513(802.742)	2325.825(740.385)	2419.733(779.856)	2327.178(747.955)
SM (d42:1) - ESI(-)	74113.422(22000.912)	76751.556(18783.673)	72052.032(22585.309)	76502.198(18837.417)
SM (d42:3) - ESI(-)	45369.2(13437.893)	44941.003(10551.682)	43401.392(13356.33)	44737.621(10584.166)
SM (d43:1) - ESI(-)	1610.475(804.178)	1785.517(763.855)	1553.823(723.228)	1779.224(769.915)
SM (d43:2) - ESI(-)	6637.877(3329.003)	6677.809(2804.014)	6466.335(3236.283)	6642.201(2791.712)
SM (d44:2)	3401.174(1320.178)	2954.684(961.942)	3336.859(1363.665)	2948.611(972.12)
SM (d41:3)	17542.807(4858.342)	18495.055(4033.934)	17704.279(4931.166)	18515.458(4062.311)
SM (d30:1) - ESI(+)	4627.855(3294.462)	5081.766(2205.718)	4775.897(3718.25)	5097.459(2227.118)
SM (d32:0) - ESI(+)	4527.417(2257.972)	4461.163(1515.584)	4607.612(2496.391)	4486.19(1523.778)
SM (d32:1) - ESI(+)	127487.665(50390.527)	141586.567(42157.93)	130331.981(48929.228)	141768.868(42598.043)
SM (d32:2) - ESI(+)	8419.355(3072.987)	8850.662(2752.191)	8297.594(2942.597)	8858.692(2771.314)
SM (d33:1) - ESI(+)	78897.543(30030.413)	81545.929(24155.104)	80879.826(28114.586)	81511.539(24404.167)
SM (d34:0) - ESI(+)	77128.042(21734.185)	77407.547(19252.704)	75967.563(22440.613)	77700.326(19302.556)
SM (d34:1) - ESI(+)	1815521.625(427328.564)	1839477.475(326129.156)	1829807.294(456742.429)	1839714.162(327659.875)
SM (d34:2) - ESI(+)	169414.754(41285.046)	172230.478(39764.32)	166715.327(39577.835)	171784.036(39237.286)
SM (d36:0) - ESI(+)	18743.046(8907.96)	15332.243(6070.249)	18501.059(8850.863)	15325.744(6136.489)
SM (d36:1) - ESI(+)	282139.394(75455.508)	277277.338(58280.773)	286608.787(80810.636)	276534.328(58672.045)
SM (d36:2) - ESI(+)	637435.743(182402.554)	634824.46(155709.619)	645217.266(198451.742)	631941.432(155065.972)
SM (d36:3) - ESI(+)	6491.66(2413.088)	6629.303(2061.528)	6504.584(2499.182)	6616.681(2057.058)
SM (d38:1)	224074.217(52840.443)	238184.289(46405.144)	224889.924(55064.028)	237892.274(46805.773)
SM (d38:2) - ESI(+)	102238.769(23254.677)	103697.728(23384.632)	101377.833(24030.293)	103522.414(23455.802)
SM (d39:1) - ESI(+)	55126.946(19385.078)	60979.282(17058.805)	55798.226(18703.686)	61069.426(17222.623)
SM (d40:0)	8519.977(3597.278)	7725.238(2745.348)	8245.94(3178.193)	7762.177(2765.776)
SM (d40:1) - ESI(+)	357194.17(87098.783)	373303.076(69403.177)	356136.642(95201.351)	373610.276(70067.044)
SM (d40:2) A - ESI(+)	192003.867(74381.653)	206939.521(72862.228)	192417.37(77642.359)	206037.77(73321.35)
SM (d40:2) B - ESI(+)	235158.05(59785.384)	255298.203(57750.75)	234598.41(62433.707)	255277.345(58240.397)
SM (d41:1) - ESI(+)	136526.853(38416.919)	143873.721(36214.448)	136536.489(37662.407)	143998.308(36485.875)
SM (d41:2) A - ESI(+)	41382.821(14921.589)	40584.006(12105.041)	41213.339(14198.137)	40572.482(12244.699)
SM (d41:2) B - ESI(+)	65492.772(20330.14)	72077.791(21032.207)	65452.643(18795.602)	72141.771(21186.803)
SM (d42:1) - ESI(+)	227228.943(65564.52)	235888.054(53178.336)	226271.686(69919.87)	236161.01(53650.016)
SM (d42:2)	552276.944(187216.547)	490026.241(121909.07)	533141.681(191035.12)	489051.667(121451.141)
SM (d42:3) - ESI(+)	360096.856(99212.364)	348735.256(79546.208)	351337.078(102485.414)	347985.851(79000.104)
SM (d43:1) - ESI(+)	6015.056(2273.428)	6198.991(2041.865)	6143.595(2380.371)	6211.676(2063.558)
SM (d43:2) - ESI(+)	14891.052(6807.646)	13945.815(5754.744)	14853.778(6738.376)	14011.678(5787.209)
TG (55:6)	10089.48(6268.964)	8140.342(3509.246)	10836.292(6923.778)	8162.42(3544.691)
TAG (58:7)/TAG (18:1/18:1/22:5)	17350.361(7968.934)	16648.95(5845.672)	18379.414(8761.489)	16682.467(5895.803)
TG (60:12)	6594.761(13689.356)	3710.704(4070.071)	7251.689(15923.376)	3747.563(4109.64)
TG (53:5)	10973.54(5251.608)	10286.984(3942.7)	10701.711(5371.822)	10283.557(3984.935)
TG (60:11)	8428.304(11674.572)	5497.847(3845.608)	9231.739(13322.028)	5529.571(3884.05)
TG (40:0)	6969.903(22773.737)	5975.792(11932.991)	8766.071(27447.345)	5516.076(11168.116)
TG (40:1)	1931.434(4239.428)	2087.013(3783.783)	2330.745(5058.917)	1968.038(3676.235)
TG (42:0)	9234.522(21761.184)	8844.978(15901.608)	11245.866(25798.217)	8330.903(15377.67)
TG (42:1)	6797.568(17520.658)	7739.975(16319.178)	8371.053(20878.024)	7245.426(15848.388)
TG (42:2)	2571.971(5933.309)	3829.423(10795.773)	3024.04(6989.384)	3574.733(10620.578)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
TG (42:3)	591.158(714.913)	671.443(879.22)	634.075(820.394)	653.157(872.519)
TG (44:0)	19087.048(32238.546)	17886.319(25507.344)	22032.526(36049.09)	17298.772(25360.152)
TG (44:1)	18788.092(29782.097)	19478.318(28152.179)	21422.802(33732.516)	18739.362(27855.392)
TG (44:2)	8060.679(14384.219)	10064.354(23367.775)	9291.989(16426.792)	9627.643(23332.334)
TG (46:0)	2913.683(2889.773)	3210.711(2865.495)	3263.752(3177.069)	3137.386(2856.567)
TG (46:1)	78988.174(99974.002)	74842.169(86950.751)	86568.493(106117.921)	73084.458(87126.607)
TG (46:2)	34399.438(37849.21)	37666.18(47712.032)	35611.907(37765.57)	36780.009(47775.698)
TG (46:3) A	601.482(563.369)	733.247(1466.526)	633.532(592.411)	723.044(1481.594)
TG (46:3) B	5520.005(7775.947)	5107.884(7131.762)	5695.095(8162.568)	5062.03(7173.612)
TG (46:4) A	1736.197(1706.675)	2452.533(7382.425)	1762.506(1820.052)	2419.562(7461.742)
TG (46:4) B	1520.942(1603.93)	2160.803(6838.834)	1542.796(1706.642)	2126.776(6910.973)
TG (46:5)	350.027(264.398)	426.476(1213.469)	333.912(252.928)	427.762(1227.467)
TG (48:0)	59633.947(40059.321)	72255.424(51804.827)	63645.305(44838.895)	70978.459(51616.694)
TG (48:1)	445353.036(404942.517)	421062.403(327886.505)	472991.329(429853.071)	415044.497(326050.448)
TG (48:2)	232753.491(212433.045)	215309.555(160839.721)	245026.006(228310.658)	212704.831(161577.038)
TG (48:3)	66257.783(45379.776)	68608.011(52545.382)	66098.171(46273.386)	67099.49(51897.774)
TG (48:4) A	14636.937(12229.537)	16489.544(19911.708)	13720.616(10557.492)	16069.028(19760.771)
TG (48:4) B	10569.309(10549.743)	12439.978(18504.13)	10642.263(9498.718)	12501.835(18692.523)
TG (48:5)	2394.932(2124.793)	2607.435(2613.644)	2220.184(1521.889)	2584.862(2630.897)
TG (48:6)	731.456(341.644)	1120.169(4094.332)	768.622(376.852)	1126.843(4141.361)
TG (49:0)	5475.884(3437.407)	5547.724(2851.467)	6051.479(3818.086)	5464.309(2799.55)
TG (49:1)	38039.35(31682.085)	32431.609(18199.476)	41285.123(34192.591)	31982.711(17744.358)
TG (49:2)	5347.71(2994.124)	4908.392(3180.31)	5728.394(3298.741)	4879.799(3157.426)
TG (49:3)	8782.798(5619.053)	8058.518(3765.588)	9036.136(6179.689)	7963.304(3692.852)
TG (50:0)	28294.36(17765.307)	35864.991(22391.136)	30391.144(18903.622)	35660.291(22608.173)
TG (50:1)	295740.881(378872.38)	268871.222(259991.973)	280015.863(359982.811)	270562.524(262438.083)
TG (50:2)	1473341.655(765417.549)	1337335.537(606243.723)	1496070.007(805949.723)	1325579.751(598746.002)
TG (50:3) A	599554.098(373888.427)	538070.653(271710.362)	600164.599(395106.976)	535146.928(273168.136)
TG (50:3) B	1463.989(2654.267)	1979.068(6822.777)	1763.535(3146.388)	2011.907(6898.091)
TG (50:4)	113705.603(61749.855)	111373.426(49803.428)	109116.643(60684.978)	110796.918(50230.457)
TG (50:5)	18164.523(11639.543)	17487.784(9234.201)	17215.323(11144.488)	17459.143(9338.397)
TG (50:6)	2907.741(1946.11)	2679.302(1733.966)	2888.373(1932.545)	2676.27(1749.673)
TG (51:2)	92658.55(49837.791)	81298.301(33345.525)	95995.942(52804.453)	80607.855(32858.485)
TG (51:3)	73828.122(33989.875)	68061.653(24068.889)	74772.231(36080.031)	67624.149(24009.33)
TG (51:4)	20600.271(10073.4)	19733.727(8062.558)	20408.26(10544.375)	19674.057(8144.825)
TG (51:5)	3397.515(1704.001)	3356.461(1275.262)	3369.705(1749.734)	3379.77(1279.789)
TG (52:1)	273344.812(258320.644)	254133.337(220416.288)	299612.616(284159.447)	249925.333(217933.538)
TG (52:2)	3924538.986(1182333.569)	3636556.102(1122279.122)	3897240.648(1199228.229)	3618259.341(1114269.185)
TG (52:3)	4416231.615(1252804.656)	4180937.847(1101985.633)	4352735.272(1257973.357)	4163977.057(1105637.788)
TG (52:4)	133068.448(44192.17)	130479.658(39344.454)	129212.885(42953.764)	130221.218(39754.166)
TG (52:5)	197791.574(102954.234)	174359.995(84000.915)	188522.527(102419.843)	174809.025(84916.187)
TG (52:6)	25178.432(15261.735)	23719.028(10920.524)	24829.566(14331.628)	23815.35(11027.619)
TG (53:0)	1583.982(681.915)	1815.471(661.05)	1653.076(772.232)	1812.115(664.526)
TG (53:1)	5936.774(4668.413)	5776.819(3671.696)	6579.165(5143.499)	5657.963(3538.034)
TG (53:2)	55792.745(24993.696)	51317.499(21651.56)	57210.703(25535.8)	50865.024(21381.082)
TG (53:3)	73056.718(28445.208)	67703.814(23631.61)	73975.978(29541.942)	67458.574(23817.209)
TG (53:4)	46389.39(19729.068)	43856.196(15698.609)	46487.513(21073.558)	43726.327(15855.445)
TG (54:1)	29942.881(33162.778)	29095.13(22321.153)	32980.657(38725.506)	28604.443(22047.713)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
TG (54:2)	321515.5(253928.808)	286249.499(201970.532)	342510.274(287785.315)	283770.114(202908.93)
TG (54:3)	1412729.685(654867.912)	1276837.39(524744.236)	1418543.926(711952.268)	1271328.969(528791.707)
TG (54:4)	1525311.494(686168.793)	1377217.291(578506.358)	1497286.416(718331.673)	1369710.413(579307.505)
TG (54:5) A	886580.788(456096.063)	802522.834(352287.756)	859118.306(461089.103)	799543.056(352238.975)
TG (54:5) B	262000.181(111804.806)	243734.88(92887.319)	276603.512(117509.484)	243850.79(93783.561)
TG (54:6) A	199405.641(130496.852)	176401.555(94248.554)	189949.756(133588.756)	176550.82(95020.055)
TG (54:6) B	1358.531(998.464)	1341.842(782.147)	1267.351(943.621)	1337.027(779.663)
TG (54:6) C	156170.234(80514.484)	137719.361(62448.4)	164443.237(85300.433)	138054.119(63101.913)
TG (54:7) A	49122.361(41128.683)	44915.907(27315.049)	46148.658(42649.079)	45158.064(27552.145)
TG (54:7) B	43061.59(27306.858)	34198.973(17471.92)	44910.216(29325.904)	34437.138(17594.818)
TG (54:8)	7077.455(4680.131)	6400.128(3571.251)	6692.688(4452.706)	6480.915(3565.906)
TG (54:9)	965.383(952.873)	800.15(740.888)	954.254(976.091)	812.865(744.458)
TG (55:1)	2381.308(1476.992)	2293.733(1193.428)	2558.87(1643.717)	2275.709(1190.663)
TG (55:2)	3209.3(1454.698)	3026.046(1288.231)	3381.591(1556.957)	2998.5(1282.234)
TG (56:1)	8425.454(9238.656)	8724.83(13724.801)	8763.968(8320.807)	8693.992(13861.114)
TG (56:10)	3107.113(3323.17)	2681.061(1812.641)	3124.173(3634.468)	2704.04(1827.021)
TG (56:2)	12956.986(10569.613)	12163.693(13180.75)	13287.1(10099.284)	12077.086(13305.387)
TG (56:3)	30313.86(19743.679)	27075.315(20697.58)	30931.238(20382.621)	26914.649(20902.266)
TG (56:4)	52216.171(23781.081)	49073.426(20687.965)	51533.089(23278.094)	48945.612(20887.754)
TG (56:5) A	53791.601(25940.471)	48027.297(18998.273)	56305.333(27049.785)	47916.754(19186.335)
TG (56:5) B	56496.764(28288.186)	50801.304(20794.293)	59319.214(30578.439)	50835.127(20990.189)
TG (56:5) C	113050.899(43777.393)	107344.31(43874.117)	119231.419(47437.588)	107123.484(44324.778)
TG (56:6)	257540.767(82209.876)	233475.447(74511.483)	266989.082(87830.794)	233954.485(75287.046)
TG (56:7) A	847.239(514.565)	783.159(401.886)	872.146(560.019)	784.776(405.716)
TG (56:7) B	187264.223(134086.996)	142003.825(96398.78)	195785.76(145844.838)	143108.577(97127.678)
TG (56:8) A	48927.531(26901.231)	42661.135(18087.989)	50526.41(29262.934)	42847.171(18199.922)
TG (56:8) B	88914.046(72816.031)	66492.66(53152.85)	90886.292(77615.502)	67041.347(53628.172)
TG (56:9)	16134.849(11093.145)	13921.157(6903.286)	16389.574(11696.97)	14029.73(6931.184)
TG (57:1)	1925.193(905.225)	1863.322(943.086)	2052.23(993.706)	1839.212(936.361)
TG (57:2)	2561.985(1153.018)	2479.474(1287.033)	2624.876(1205.603)	2467.196(1299.191)
TG (58:1)	6517.314(7345.499)	6747.301(10399.217)	6592.938(5718.528)	6753.942(10516.502)
TG (58:10)	19441.101(14120.814)	16598.368(8410.925)	19887.224(14764.054)	16693.484(8480.365)
TG (58:2)	10622.347(16674.782)	10834.266(23253.565)	10431.712(12802.421)	10856.796(23514.796)
TG (58:3)	6147.029(9675.465)	5932.174(10911.709)	6045.156(6379.053)	5963.783(11035.393)
TG (58:4)	3243.624(2529.139)	2899.892(2258.659)	3302.313(2621.221)	2902.309(2284.656)
TG (58:5)	3750.517(1804.936)	3824.305(1507.07)	3880.535(1953.617)	3827.191(1523.237)
TG (58:6)	14653.583(5134.288)	13533.44(3981.36)	15097.802(5479.822)	13527.491(4021.132)
TG (58:8)	61621.544(53618.106)	44303.591(28847.455)	64513.107(56652.202)	44689.771(29065.16)
TG (58:9)	45461.573(35467.981)	34450.345(20298.576)	47193.161(37869.486)	34669.934(20480.099)
TG (59:2)	1491.779(1048.687)	1415.968(980.975)	1568.91(1122.262)	1394.688(981.99)
TG (59:3)	1482.159(789.741)	1388.449(810.7)	1535.439(841.044)	1375.053(814.953)
TG (60:1)	2548.677(2775.351)	2609.795(3662.099)	2503.608(1975.486)	2618.535(3703.156)
TG (60:2)	5106.678(6459.935)	5391.177(12127.075)	5543.014(7335.457)	5404.857(12266.767)
TG (60:3)	3356.443(4588.274)	3498.227(6192.138)	3203.246(3043.682)	3529.114(6260.292)
TG (60:4)	1479.004(1459.393)	1489.448(1601.775)	1466.126(1074.068)	1490.622(1619.83)
TG (60:6)	1058.884(479.188)	956.092(409.713)	1097.963(497.494)	955.389(413.669)
TG (62:1)	1025.712(1380.888)	981.286(1057.831)	948.483(779.416)	979.935(1069.614)
TG (62:2)	1814.769(2212.815)	1781.426(2417.302)	1743.47(1504.294)	1779.345(2444.85)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
TG (62:3)	571.887(485.151)	559.893(537.266)	607.272(472.415)	563.684(542.663)
TG (62:4)	547.101(334.64)	613.733(374.856)	553.329(285.631)	614.578(379.088)
TG (64:2)	864.662(732.038)	883.063(767.604)	898.099(656.064)	876.015(775.005)
TG (64:3)	552.787(234.996)	552.569(261.395)	551.258(235.663)	551.657(261.368)
Oxylipins (OL)				
10-nitrolinoleic acid	0.186(0.36)	0.149(0.221)	0.164(0.299)	0.152(0.224)
10-nitrooleic acid	5.022(4.039)	4.734(2.95)	5.109(4.537)	4.796(2.976)
11(12)-epoxy-5,8,14,17- eicosatetraenoic acid	0.045(0.051)	0.046(0.062)	0.039(0.045)	0.047(0.063)
11,12-Dihydroxyicosa-5,8,14-trienoic acid	0.729(0.365)	0.798(0.415)	0.749(0.395)	0.797(0.415)
11,12-Epoxyeicosa-5,8,14-trienoic acid	0.298(0.235)	0.25(0.225)	0.305(0.239)	0.247(0.221)
11-Hydroxy-14,15-epoxyeicosatrienoic acid	0.137(0.271)	0.236(0.486)	0.154(0.311)	0.243(0.493)
11-Hydroxy-arachidonic acid	0.954(0.559)	0.918(0.459)	1.012(0.597)	0.932(0.458)
12(13)-epoxy-9,15-octadecadienoic acid	0.131(0.14)	0.155(0.255)	0.146(0.149)	0.155(0.258)
12,13-dihydroxyoctadec-9-enoic acid	3.714(2.623)	4.151(2.308)	3.81(2.822)	4.104(2.326)
12,13-dihydroxyoctadeca-9,15-dienoic acid	0.107(0.148)	0.111(0.152)	0.106(0.149)	0.114(0.154)
12,13-epoxy-9-octadecenoic acid	2.678(3.381)	3.027(3.742)	3.011(3.942)	2.93(3.764)
12-Hydroxy-5,8,10,14,17-eicosapentaenoic acid	1.953(2.755)	1.117(1.211)	2.101(3.071)	1.135(1.225)
12-Hydroxy-5,8,10,14-eicosatetraenoic acid	17.204(15.381)	15.752(12.397)	18.425(16.171)	15.915(12.52)
13-hydroxyoctadeca-9,11,15-trienoic acid	0.935(0.885)	0.869(0.593)	0.995(1.017)	0.848(0.589)
13-Hydroxyoctadecadienoic acid	19.586(7.961)	19.825(7.897)	19.316(8.205)	19.491(7.649)
13-ketooctadeca-9,11-dienoic acid	11.779(7.152)	12.915(7.243)	11.225(7.239)	12.965(7.347)
14(15)-epoxy-5,8,11,17-eicosatetraenoic acid	0.234(0.427)	0.211(0.435)	0.258(0.488)	0.218(0.441)
14,15-dihydroxyeicosa-5,8,11,17-tetraenoic acid	0.445(0.453)	0.503(0.551)	0.434(0.453)	0.512(0.558)
14,15-dihydroxyeicosa-5,8,11-trienoic acid	0.816(0.427)	0.868(0.394)	0.829(0.462)	0.865(0.395)
14-hydroxydocosa-4,7,10,12,16,19-hexaenoic acid	13.05(14.814)	10.01(9.899)	13.681(15.635)	10.17(9.989)
15(16)-epoxy-9,12-octadecadienoic acid	0.221(0.211)	0.382(0.521)	0.244(0.241)	0.389(0.529)
15,16-dihydroxyoctadeca-9,12-dienoic acid	11.678(8.843)	12.862(6.666)	11.356(9.682)	12.603(6.128)
15-Deoxy-delta-12,14-Prostaglandin J2	0.043(0.036)	0.05(0.053)	0.043(0.04)	0.05(0.054)
15-hydroxyeicosa-5,8,11,13,17-pentaenoic acid	0.387(0.417)	0.288(0.303)	0.416(0.473)	0.294(0.306)
15-hydroxyeicosa-5,8,11,13-tetraenoic acid	3.04(1.536)	2.905(1.282)	3.109(1.576)	2.925(1.285)
15-ketoeicosa-5,8,11,13-tetraenoic acid	0.159(0.211)	0.167(0.276)	0.151(0.228)	0.171(0.279)
15-Keto-prostaglandin E2	0.319(0.368)	0.405(0.635)	0.329(0.365)	0.408(0.645)
16(17)-epoxy-4,7,10,13,19-docosapentaenoic acid	0.189(0.199)	0.159(0.206)	0.195(0.213)	0.161(0.209)
17,18-dihydroxyeicosa-5,8,11,14-tetraenoic acid	6.057(5.778)	4.785(3.299)	5.77(4.594)	4.834(3.34)
17,18-Epoxy-5,8,11,14-eicosatetraenoic acid	0.09(0.188)	0.122(0.18)	0.084(0.183)	0.123(0.182)
17-hydroxy-4,7,10,13,15,19-docosahexaenoic acid	1.382(0.957)	1.263(1.094)	1.416(1.007)	1.291(1.102)
18-(3-ethyloxiran-2-yl)octadeca-4,7,10,13,16-pentaenoic acid	0.406(0.383)	0.403(0.512)	0.382(0.393)	0.408(0.519)
19,20-dihydroxydocosa-4,7,10,13,16-pentaenoic acid	1.929(1.019)	1.91(1)	1.897(1.084)	1.934(1.007)
20-Hydroxyarachidonic acid	4.005(8.301)	3.874(6.762)	3.017(6.041)	3.963(6.858)
4-hydroxydocosa-5,7,10,13,16,19-hexaenoic acid	0.763(0.83)	0.673(0.657)	0.854(0.96)	0.686(0.661)
5,15-dihydroxyeicosa-6,8,11,13-tetraenoic acid	0.038(0.055)	0.053(0.095)	0.04(0.058)	0.053(0.096)
5,6,15-trihydroxyeicosa-7,9,11,13-tetraenoic acid	0.157(0.194)	0.207(0.32)	0.163(0.194)	0.211(0.325)
5,6-dihydroxyeicosa-8,11,14-trienoic acid	0.665(0.513)	0.709(0.521)	0.711(0.529)	0.711(0.529)
5-Hydroxy-6,8,11,14,17-eicosapentaenoic acid	0.954(0.728)	0.874(0.675)	0.985(0.755)	0.886(0.682)
5-Hydroxy-6,8,11,14-eicosatetraenoic acid	3.249(2.155)	3.575(2.057)	3.219(2.294)	3.568(2.077)
5-ketoeicosa-6,8,11,14-tetraenoic acid	0.116(0.104)	0.137(0.127)	0.112(0.101)	0.137(0.129)
6-Ketoprostaglandin F1 alpha	0.111(0.191)	0.091(0.14)	0.109(0.209)	0.094(0.142)
6-trans-Leukotriene B4	0.046(0.066)	0.051(0.099)	0.041(0.057)	0.051(0.1)

Supplementary Table S1. Sample mean and standard deviations of metabolites in ME/CFS patients, controls, and their subgroups.

Metabolite	ME/CFS (n=106)	Control (n=91)	ME/CFS without sr-IBS (n=71)	Control without sr-IBS (n=88)
	mean (SD)	mean (SD)	mean (SD)	mean (SD)
8,15-dihydroxyeicosa-5,9,11,13-tetraenoic acid	0.121(0.272)	0.115(0.202)	0.12(0.307)	0.117(0.205)
8,9-dihydroxyeicosa-5,11,14-trienoic acid	0.391(0.311)	0.373(0.243)	0.397(0.313)	0.37(0.243)
8,9-Epoxyeicosa-5,11,14-trienoic acid	0.627(0.483)	0.848(0.762)	0.587(0.447)	0.871(0.764)
8-hydroxyeicosa-5,9,11,14-tetraenoic acid	0.707(0.521)	0.693(0.505)	0.713(0.509)	0.701(0.512)
9(10)-epoxy-12,15-octadecadienoic acid	1.238(2.543)	1.495(3.452)	1.369(3.033)	1.518(3.506)
9(10)-epoxy-12Z-octadecenoic acid	0.778(0.586)	0.789(0.455)	0.783(0.656)	0.775(0.453)
9,10-dihydroxyoctadec-12-enoic acid	3.994(2.996)	4.527(2.771)	3.997(3.128)	4.483(2.803)
9,10-dihydroxyoctadeca-12,15-dienoic acid	0.195(0.127)	0.233(0.156)	0.201(0.139)	0.234(0.156)
9,10-Epoxy stearic acid	2.482(2.294)	2.68(2.248)	2.594(2.481)	2.724(2.272)
9,11,15-trihydroxy-5,13,1Z-prostatrienoic acid	0.022(0.082)	0.033(0.09)	0.012(0.013)	0.034(0.092)
9,12,13-trihydroxyoctadec-10-enoic acid	6.746(3.013)	7.161(3.062)	6.405(3.09)	7.218(3.07)
9-Hydroxy-5,7,11,14,17-icosapentaenoic acid	0.259(0.225)	0.218(0.148)	0.258(0.231)	0.222(0.149)
9-hydroxyeicosa-5,7,11,14-tetraenoic acid	0.366(0.266)	0.386(0.267)	0.361(0.261)	0.388(0.268)
9-Hydroxylinoleic acid	9.759(4.207)	10.407(3.998)	9.531(4.066)	10.248(3.945)
9-hydroxyoctadeca-10,12,15-trienoic acid	0.602(0.484)	0.715(0.595)	0.662(0.51)	0.711(0.598)
9-ketooctadeca-10,12-dienoic acid	1.218(0.86)	1.249(0.847)	1.191(0.744)	1.227(0.844)
9-nitrooleic acid	0.611(0.737)	0.692(0.676)	0.607(0.817)	0.705(0.682)
9S,10R-dihydroxy-stearic acid	2.561(1.966)	2.883(2.166)	2.454(1.76)	2.913(2.186)
Leukotriene B4	0.079(0.051)	0.099(0.087)	0.072(0.045)	0.1(0.088)
Leukotriene B5	0.01(0.015)	0.012(0.018)	0.01(0.015)	0.012(0.018)
Prostaglandin D2	0.336(0.565)	0.54(0.959)	0.318(0.552)	0.525(0.939)
Prostaglandin E1	0.02(0.021)	0.019(0.026)	0.019(0.019)	0.019(0.026)
Prostaglandin E2	0.057(0.126)	0.052(0.08)	0.057(0.128)	0.054(0.081)
Prostaglandin E3	0.185(0.427)	0.14(0.232)	0.202(0.484)	0.143(0.235)
Prostaglandin F2a	0.83(0.921)	0.952(0.717)	0.637(0.59)	0.963(0.723)
Resolvin D1	0.147(0.362)	0.162(0.194)	0.105(0.101)	0.154(0.165)
Thromboxane B2	1.893(2.013)	2.178(4.62)	2.108(2.36)	2.226(4.69)
trans-12,13-epoxy-11-oxo-trans-9-octadecenoic acid	1.085(0.917)	1.082(0.66)	1.037(1.054)	1.088(0.664)

ME/CFS, myalgic encephalomyelitis/chronic fatigue syndrome; sr-IBS, self-reported physician diagnosed irritable bowel syndrome; SD, standard deviation

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Primary Metabolites (PM)							
succinic acid	Lognormal	0.022	(0.006, 0.038)	0.009	0.177	1.216	(0.006, 0.038)
arachidic acid	Lognormal	0.024	(0.004, 0.044)	0.019	0.213	0.578	(0.005, 0.045)
leucine	Lognormal	-0.010	(-0.020, -0.001)	0.035	0.287	0.312	(-0.019, -0.001)
ornithine	Lognormal	-0.016	(-0.032, -0.001)	0.042	0.309	0.253	(-0.032, -0.002)
alpha-ketoglutarate	Lognormal	0.015	(0.000, 0.031)	0.056	0.361	0.211	(0.000, 0.032)
mannitol	Lognormal	0.029	(-0.002, 0.060)	0.067	0.396	0.187	(-0.003, 0.059)
maleic acid	Lognormal	0.026	(-0.002, 0.053)	0.075	0.409	0.169	(-0.002, 0.054)
aminomalonate	Lognormal	0.025	(-0.003, 0.053)	0.082	0.422	0.188	(-0.004, 0.052)
tyrosine	Lognormal	-0.008	(-0.016, 0.001)	0.088	0.430	0.153	(-0.016, 0.000)
glutaric acid	Lognormal	0.017	(-0.003, 0.037)	0.100	0.461	0.138	(-0.003, 0.036)
threonine	Lognormal	-0.010	(-0.023, 0.003)	0.146	0.551	0.093	(-0.023, 0.003)
indole-3-propionic acid	Lognormal	-0.018	(-0.043, 0.007)	0.171	0.582	0.081	(-0.042, 0.009)
benzoic acid	Lognormal	0.011	(-0.006, 0.028)	0.207	0.624	0.081	(-0.006, 0.028)
glycerol	Lognormal	0.007	(-0.004, 0.017)	0.209	0.628	0.060	(-0.004, 0.017)
glutamine	Lognormal	-0.012	(-0.033, 0.008)	0.235	0.667	0.066	(-0.033, 0.007)
lysine	Lognormal	-0.015	(-0.040, 0.011)	0.262	0.697	0.054	(-0.041, 0.010)
levoglucosan	Lognormal	-0.014	(-0.038, 0.010)	0.264	0.697	0.059	(-0.037, 0.012)
pelargonic acid	Lognormal	0.007	(-0.006, 0.020)	0.283	0.737	0.060	(-0.005, 0.020)
3-hydroxybutyric acid	Lognormal	0.015	(-0.014, 0.045)	0.312	0.743	0.051	(-0.013, 0.045)
threonic acid	Lognormal	0.010	(-0.009, 0.029)	0.316	0.743	0.051	(-0.009, 0.029)
urea	Lognormal	-0.005	(-0.014, 0.005)	0.320	0.743	0.056	(-0.014, 0.005)
glucuronic acid	Lognormal	0.010	(-0.010, 0.030)	0.325	0.746	0.055	(-0.009, 0.032)
oxoproline	Lognormal	-0.003	(-0.008, 0.003)	0.335	0.748	0.049	(-0.008, 0.003)
lysine	Lognormal	-0.009	(-0.027, 0.009)	0.341	0.754	0.049	(-0.027, 0.009)
2-deoxytetronic acid	Lognormal	0.010	(-0.011, 0.031)	0.341	0.754	0.054	(-0.011, 0.030)
pentadecanoic acid	Lognormal	0.005	(-0.005, 0.015)	0.346	0.756	0.049	(-0.005, 0.016)
phenylalanine	Lognormal	-0.005	(-0.015, 0.005)	0.350	0.760	0.049	(-0.015, 0.006)
2-hydroxybutanoic acid	Lognormal	0.008	(-0.009, 0.026)	0.354	0.760	0.048	(-0.009, 0.025)
beta-alanine	Lognormal	-0.010	(-0.033, 0.012)	0.363	0.764	0.048	(-0.033, 0.012)
2-ketoisocaproic acid	Lognormal	0.005	(-0.005, 0.015)	0.368	0.764	0.046	(-0.005, 0.014)
pyrrole-2-carboxylic acid	Lognormal	0.010	(-0.014, 0.034)	0.393	0.780	0.048	(-0.013, 0.034)
pseudo uridine	Lognormal	-0.005	(-0.015, 0.006)	0.395	0.781	0.050	(-0.015, 0.006)
malic acid	Lognormal	0.008	(-0.012, 0.028)	0.423	0.818	0.047	(-0.011, 0.029)
citrulline	Lognormal	-0.005	(-0.016, 0.007)	0.429	0.822	0.044	(-0.016, 0.007)
indole-3-lactate	Lognormal	-0.005	(-0.019, 0.009)	0.459	0.848	0.042	(-0.019, 0.010)
maleimide	Lognormal	0.007	(-0.011, 0.025)	0.463	0.848	0.041	(-0.011, 0.026)
1,2,4-benzenetriol	Lognormal	-0.013	(-0.047, 0.021)	0.463	0.848	0.047	(-0.046, 0.021)
tryptophan	Lognormal	-0.006	(-0.023, 0.011)	0.470	0.853	0.040	(-0.024, 0.010)
sucrose	Lognormal	0.012	(-0.021, 0.044)	0.479	0.856	0.045	(-0.019, 0.044)
fructose	Lognormal	-0.010	(-0.037, 0.017)	0.482	0.856	0.036	(-0.038, 0.017)
salicylic acid	Lognormal	0.010	(-0.019, 0.039)	0.487	0.856	0.042	(-0.017, 0.039)
erythritol	Lognormal	0.010	(-0.019, 0.039)	0.488	0.856	0.042	(-0.019, 0.039)
alanine	Lognormal	-0.007	(-0.026, 0.013)	0.498	0.862	0.043	(-0.027, 0.013)
quinic acid	Lognormal	-0.013	(-0.052, 0.025)	0.499	0.863	0.039	(-0.050, 0.026)
isoleucine	Lognormal	-0.003	(-0.014, 0.007)	0.505	0.867	0.037	(-0.013, 0.007)
glycerol-alpha-phosphate	Lognormal	0.009	(-0.017, 0.034)	0.512	0.877	0.041	(-0.016, 0.036)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
glucose-1-phosphate	Lognormal	0.005	(-0.010, 0.020)	0.525	0.883	0.038	(-0.010, 0.020)
lactic acid	Lognormal	-0.005	(-0.022, 0.011)	0.525	0.883	0.039	(-0.021, 0.012)
linoleic acid	Lognormal	0.007	(-0.015, 0.029)	0.555	0.891	0.040	(-0.016, 0.028)
gluconic acid	Lognormal	0.004	(-0.010, 0.019)	0.558	0.893	0.040	(-0.011, 0.019)
hydroxycarbamate NIST	Lognormal	-0.005	(-0.024, 0.013)	0.561	0.896	0.041	(-0.022, 0.013)
uric acid	Lognormal	-0.005	(-0.023, 0.013)	0.597	0.914	0.038	(-0.023, 0.013)
ribose	Lognormal	0.004	(-0.010, 0.017)	0.597	0.914	0.038	(-0.009, 0.018)
serine	Lognormal	-0.004	(-0.018, 0.011)	0.612	0.915	0.037	(-0.018, 0.011)
stearic acid	Lognormal	-0.002	(-0.009, 0.006)	0.612	0.915	0.034	(-0.009, 0.006)
lyxitol	Lognormal	-0.004	(-0.020, 0.012)	0.623	0.915	0.034	(-0.019, 0.012)
glyceric acid	Lognormal	0.005	(-0.015, 0.025)	0.625	0.915	0.036	(-0.016, 0.024)
phthalic acid	Lognormal	0.003	(-0.011, 0.017)	0.628	0.915	0.038	(-0.010, 0.018)
phosphate	Lognormal	-0.004	(-0.022, 0.013)	0.629	0.915	0.037	(-0.022, 0.013)
heptadecanoic acid	Lognormal	0.004	(-0.012, 0.019)	0.631	0.915	0.038	(-0.011, 0.020)
indole-3-acetate	Lognormal	0.005	(-0.015, 0.024)	0.640	0.920	0.037	(-0.013, 0.024)
conduritol-beta-exposide	Lognormal	0.007	(-0.022, 0.035)	0.649	0.925	0.038	(-0.023, 0.033)
4-hydroxybutyric acid	Lognormal	0.004	(-0.014, 0.023)	0.651	0.925	0.040	(-0.014, 0.022)
capric acid	Lognormal	-0.005	(-0.029, 0.018)	0.667	0.932	0.034	(-0.029, 0.020)
glutamic acid	Lognormal	0.003	(-0.013, 0.020)	0.683	0.932	0.033	(-0.013, 0.021)
2-hydroxyvaleric acid	Lognormal	0.004	(-0.014, 0.021)	0.691	0.932	0.036	(-0.015, 0.021)
methionine	Lognormal	-0.003	(-0.021, 0.014)	0.701	0.936	0.033	(-0.021, 0.014)
fumaric acid	Lognormal	-0.003	(-0.019, 0.013)	0.709	0.936	0.036	(-0.019, 0.014)
proline	Lognormal	-0.004	(-0.026, 0.018)	0.732	0.936	0.036	(-0.026, 0.019)
creatinine	Lognormal	0.003	(-0.018, 0.025)	0.747	0.936	0.033	(-0.019, 0.023)
N-acetylornithine	Lognormal	-0.002	(-0.013, 0.010)	0.761	0.939	0.030	(-0.013, 0.010)
threitol	Lognormal	0.003	(-0.014, 0.020)	0.764	0.941	0.037	(-0.014, 0.020)
adipic acid	Lognormal	-0.002	(-0.021, 0.016)	0.790	0.950	0.037	(-0.021, 0.015)
myo-inositol	Lognormal	-0.001	(-0.013, 0.010)	0.803	0.950	0.037	(-0.014, 0.011)
lauric acid	Lognormal	-0.003	(-0.024, 0.018)	0.805	0.950	0.031	(-0.023, 0.018)
isopropylbenzene	Lognormal	0.002	(-0.016, 0.020)	0.805	0.950	0.021	(-0.015, 0.021)
isothreonic acid	Lognormal	0.003	(-0.021, 0.028)	0.806	0.950	0.036	(-0.021, 0.028)
behenic acid	Lognormal	-0.002	(-0.016, 0.012)	0.812	0.950	0.035	(-0.016, 0.012)
ribonic acid	Lognormal	-0.002	(-0.019, 0.015)	0.822	0.950	0.033	(-0.020, 0.015)
citric acid	Lognormal	-0.002	(-0.018, 0.014)	0.822	0.950	0.029	(-0.017, 0.014)
2-aminobutyric acid	Lognormal	-0.001	(-0.014, 0.011)	0.835	0.950	0.033	(-0.014, 0.011)
pyruvic acid	Lognormal	-0.002	(-0.017, 0.013)	0.835	0.950	0.029	(-0.017, 0.013)
palmitoleic acid	Lognormal	-0.003	(-0.028, 0.023)	0.840	0.950	0.035	(-0.028, 0.023)
mannose	Lognormal	0.001	(-0.015, 0.017)	0.866	0.963	0.034	(-0.016, 0.017)
nicotinic acid	Lognormal	0.003	(-0.032, 0.037)	0.868	0.963	0.028	(-0.030, 0.038)
N-acetylputrescine	Lognormal	-0.001	(-0.019, 0.016)	0.883	0.966	0.032	(-0.020, 0.016)
myristic acid	Lognormal	0.001	(-0.013, 0.015)	0.887	0.968	0.037	(-0.012, 0.016)
palmitic acid	Lognormal	-0.001	(-0.008, 0.007)	0.896	0.972	0.028	(-0.008, 0.007)
1-methylgalactose NIST	Lognormal	0.002	(-0.030, 0.034)	0.897	0.973	0.033	(-0.030, 0.035)
caprylic acid	Lognormal	0.001	(-0.012, 0.013)	0.909	0.976	0.033	(-0.012, 0.013)
creatine	Lognormal	0.001	(-0.022, 0.024)	0.924	0.984	0.032	(-0.022, 0.022)
trans-4-hydroxyproline	Lognormal	-0.001	(-0.024, 0.021)	0.925	0.984	0.032	(-0.024, 0.020)
oxalic acid	Lognormal	-0.002	(-0.045, 0.041)	0.929	0.985	0.032	(-0.045, 0.040)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
valine	Lognormal	0.000	(-0.009, 0.009)	0.930	0.985	0.032	(-0.009, 0.008)
glucose	Lognormal	0.000	(-0.007, 0.007)	0.936	0.987	0.031	(-0.007, 0.007)
glycine	Lognormal	0.000	(-0.009, 0.009)	0.938	0.987	0.030	(-0.009, 0.009)
tagatose	Lognormal	0.000	(-0.017, 0.018)	0.963	0.990	0.029	(-0.018, 0.019)
glycolic acid	Lognormal	0.000	(-0.025, 0.026)	0.980	0.992	0.033	(-0.026, 0.025)
maltose	Lognormal	0.000	(-0.022, 0.022)	0.988	0.994	0.031	(-0.023, 0.022)
alloxanoic acid	Lognormal	0.000	(-0.030, 0.030)	0.997	0.997	0.031	(-0.030, 0.031)
Biogenic Amines (BA)							
Acetaminophen	Lognormal	0.068	(0.028, 0.108)	0.001	0.103	3.035	(0.026, 0.108)
2-Methylbutyryl-L-carnitine	Lognormal	-0.034	(-0.055, -0.012)	0.002	0.139	2.296	(-0.055, -0.012)
Acyclovir	Lognormal	0.112	(0.038, 0.185)	0.003	0.139	2.674	(0.040, 0.185)
Caffeine	Lognormal	-0.083	(-0.138, -0.028)	0.003	0.139	2.445	(-0.139, -0.030)
Guanine	Lognormal	0.091	(0.031, 0.152)	0.003	0.139	2.203	(0.031, 0.150)
Choline cation	Lognormal	-0.009	(-0.015, -0.003)	0.004	0.139	2.751	(-0.015, -0.003)
Theobromine	Lognormal	-0.063	(-0.108, -0.018)	0.007	0.173	1.573	(-0.107, -0.018)
Alprazolam	Lognormal	0.063	(0.016, 0.109)	0.009	0.178	0.963	(0.015, 0.109)
Piperine	Lognormal	-0.064	(-0.115, -0.014)	0.014	0.206	0.594	(-0.112, -0.010)
Albendazole sulfoxide	Lognormal	0.108	(0.021, 0.194)	0.015	0.208	0.673	(0.024, 0.194)
Isopropylamine	Lognormal	-0.014	(-0.024, -0.003)	0.017	0.208	0.649	(-0.024, -0.002)
3-Methylglutarylcarnitine	Lognormal	-0.032	(-0.059, -0.005)	0.019	0.214	0.502	(-0.057, -0.004)
Trigonelline	Lognormal	-0.044	(-0.081, -0.006)	0.023	0.225	0.552	(-0.079, -0.006)
Ranitidine N-oxide	Lognormal	0.055	(0.006, 0.104)	0.028	0.258	0.382	(0.008, 0.103)
7-Methylguanosine	Lognormal	-0.014	(-0.027, -0.002)	0.029	0.261	0.397	(-0.026, -0.002)
H-Pro-Hyp-OH	Lognormal	0.024	(0.002, 0.045)	0.031	0.268	0.362	(0.004, 0.045)
2,6-Diaminopimelic acid	Lognormal	0.042	(0.001, 0.084)	0.049	0.341	0.222	(-0.003, 0.081)
4,5,7-Trihydroxyisoflavone	Lognormal	0.082	(0.001, 0.164)	0.050	0.344	0.223	(-0.001, 0.164)
SDMA	Lognormal	-0.009	(-0.018, 0.000)	0.055	0.361	0.191	(-0.019, 0.000)
Methacholine cation	Lognormal	-0.018	(-0.037, 0.001)	0.058	0.367	0.213	(-0.037, 0.000)
D-Turanose	Lognormal	-0.026	(-0.054, 0.002)	0.067	0.396	0.182	(-0.052, 0.003)
H-gamma-glutamyl-glutamine	Lognormal	0.023	(-0.002, 0.047)	0.068	0.397	0.156	(0.000, 0.048)
Gabapentin	Lognormal	0.047	(-0.004, 0.099)	0.074	0.409	0.164	(-0.005, 0.097)
3-Cysteinyacetaminophen	Lognormal	0.081	(-0.008, 0.169)	0.075	0.409	0.157	(-0.014, 0.161)
Betaine	Lognormal	-0.006	(-0.012, 0.001)	0.077	0.416	0.166	(-0.012, 0.001)
Octanoylcarnitine	Lognormal	-0.017	(-0.035, 0.002)	0.077	0.416	0.134	(-0.036, 0.002)
3-Dehydrocarnitine	Lognormal	-0.013	(-0.028, 0.002)	0.084	0.430	0.129	(-0.027, 0.002)
Lamotrigine;	Lognormal	0.093	(-0.013, 0.199)	0.088	0.430	0.121	(-0.011, 0.201)
Ranitidine	Lognormal	0.035	(-0.005, 0.075)	0.088	0.430	0.140	(-0.004, 0.074)
Kynurenine	Lognormal	-0.012	(-0.026, 0.002)	0.090	0.432	0.144	(-0.026, 0.002)
Lauroyl-L-carnitine	Lognormal	-0.032	(-0.070, 0.006)	0.103	0.465	0.105	(-0.070, 0.009)
Tri-2-ethylhexyl trimellitate	Lognormal	-0.038	(-0.084, 0.008)	0.107	0.468	0.132	(-0.081, 0.008)
4-Acetamidobutyric acid	Lognormal	-0.017	(-0.037, 0.004)	0.107	0.468	0.112	(-0.038, 0.005)
Usnic acid	Lognormal	-0.036	(-0.080, 0.008)	0.108	0.471	0.125	(-0.081, 0.007)
cis-10,11-Dihydroxy-10,11-dihydrocarbamazepine	Lognormal	-0.016	(-0.036, 0.004)	0.112	0.481	0.119	(-0.036, 0.003)
Hydroxybupropion	Lognormal	-0.027	(-0.059, 0.006)	0.113	0.485	0.131	(-0.060, 0.005)
p-Acetamidophenyl .beta.-D-glucuronide	Lognormal	0.047	(-0.011, 0.105)	0.116	0.487	0.108	(-0.016, 0.101)
(R)-Butyrylcarnitine	Lognormal	-0.016	(-0.037, 0.005)	0.135	0.531	0.087	(-0.036, 0.005)
3-Hydroxypyridine	Lognormal	-0.049	(-0.113, 0.015)	0.137	0.532	0.083	(-0.113, 0.017)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
L-Citrulline	Lognormal	-0.007	(-0.016, 0.002)	0.140	0.537	0.088	(-0.017, 0.002)
N-Acetylhistidine	Lognormal	-0.015	(-0.036, 0.005)	0.150	0.554	0.091	(-0.037, 0.005)
L-Tyrosine	Lognormal	-0.013	(-0.031, 0.005)	0.157	0.566	0.091	(-0.030, 0.005)
Stachydrine	Lognormal	-0.025	(-0.062, 0.011)	0.169	0.582	0.087	(-0.063, 0.010)
NEPSILON,NEPSILON,NEPSILON-TRIMETHYLLYSINE	Lognormal	-0.008	(-0.020, 0.004)	0.171	0.582	0.080	(-0.021, 0.003)
Quetiapine	Lognormal	0.017	(-0.008, 0.042)	0.178	0.591	0.081	(-0.009, 0.040)
Linoleoylcarnitine	Lognormal	-0.022	(-0.055, 0.010)	0.179	0.591	0.078	(-0.056, 0.009)
Trazodone	Lognormal	0.027	(-0.013, 0.067)	0.189	0.599	0.078	(-0.010, 0.071)
Urea	Lognormal	-0.006	(-0.015, 0.003)	0.196	0.606	0.066	(-0.014, 0.004)
2-Indolinone	Lognormal	-0.012	(-0.031, 0.006)	0.199	0.609	0.074	(-0.031, 0.007)
N-alpha.-Acetyl-L-arginine	Lognormal	-0.009	(-0.023, 0.005)	0.211	0.628	0.077	(-0.023, 0.004)
Ergothioneine	Lognormal	-0.023	(-0.058, 0.013)	0.212	0.628	0.065	(-0.057, 0.012)
Acetazolamide	Lognormal	-0.033	(-0.085, 0.019)	0.213	0.629	0.067	(-0.086, 0.016)
4'-Methyl-N-methylhexanophenone	Lognormal	-0.034	(-0.087, 0.020)	0.219	0.636	0.072	(-0.086, 0.025)
Citrulline	Lognormal	-0.006	(-0.016, 0.004)	0.225	0.648	0.063	(-0.015, 0.004)
Thr-Ile-Arg	Lognormal	-0.029	(-0.076, 0.018)	0.226	0.648	0.073	(-0.076, 0.021)
L-Cystine	Lognormal	-0.013	(-0.035, 0.009)	0.235	0.667	0.046	(-0.035, 0.008)
Ala-Ile	Lognormal	0.011	(-0.008, 0.030)	0.238	0.671	0.064	(-0.007, 0.031)
7-Hydroxywarfarin	Lognormal	0.018	(-0.012, 0.048)	0.247	0.685	0.066	(-0.013, 0.048)
Prazepam	Lognormal	0.024	(-0.017, 0.065)	0.248	0.685	0.052	(-0.014, 0.070)
Fexofenadine	Lognormal	-0.015	(-0.039, 0.010)	0.248	0.685	0.067	(-0.041, 0.010)
Testosterone	Lognormal	-0.019	(-0.052, 0.013)	0.250	0.687	0.060	(-0.052, 0.014)
Pyrantel	Lognormal	-0.013	(-0.035, 0.009)	0.252	0.689	0.067	(-0.035, 0.011)
Glutamic acid	Lognormal	0.008	(-0.006, 0.023)	0.255	0.689	0.055	(-0.006, 0.023)
Methioninesulfoxide	Lognormal	0.011	(-0.008, 0.030)	0.257	0.692	0.057	(-0.007, 0.030)
Creatinine	Lognormal	-0.003	(-0.009, 0.002)	0.273	0.721	0.050	(-0.009, 0.002)
N.alpha.-Methyl-L-lysine	Lognormal	0.019	(-0.016, 0.054)	0.281	0.735	0.057	(-0.013, 0.055)
1-Methylnicotinamide	Lognormal	-0.011	(-0.030, 0.009)	0.284	0.737	0.061	(-0.030, 0.009)
Tyrosine	Lognormal	-0.007	(-0.021, 0.006)	0.286	0.737	0.059	(-0.020, 0.005)
Ethiolat	Lognormal	-0.018	(-0.051, 0.015)	0.288	0.737	0.061	(-0.052, 0.015)
Diazepam	Lognormal	0.032	(-0.027, 0.091)	0.291	0.739	0.057	(-0.028, 0.086)
L-Leucine, methyl ester	Lognormal	0.018	(-0.016, 0.052)	0.293	0.739	0.047	(-0.017, 0.051)
Guanidine	Lognormal	0.010	(-0.009, 0.029)	0.293	0.739	0.055	(-0.009, 0.028)
Ethylenediaminetetraacetic acid	Lognormal	0.041	(-0.036, 0.118)	0.294	0.739	0.053	(-0.035, 0.117)
Homoarginine;	Lognormal	0.010	(-0.008, 0.027)	0.295	0.739	0.045	(-0.007, 0.028)
Arginine	Lognormal	0.007	(-0.006, 0.019)	0.302	0.740	0.052	(-0.005, 0.020)
Bradykinin	Lognormal	0.059	(-0.053, 0.172)	0.303	0.740	0.052	(-0.053, 0.169)
Omeprazole sulfone N-oxide	Lognormal	0.033	(-0.030, 0.097)	0.306	0.743	0.058	(-0.024, 0.097)
3-Methylxanthine	Lognormal	-0.022	(-0.063, 0.020)	0.310	0.743	0.058	(-0.064, 0.019)
Hexanoyl-L-carnitine	Lognormal	-0.011	(-0.031, 0.010)	0.315	0.743	0.052	(-0.032, 0.010)
Propionylcarnitine	Lognormal	-0.004	(-0.013, 0.004)	0.316	0.743	0.044	(-0.013, 0.004)
Trimethylamine-N-oxide	Lognormal	0.013	(-0.012, 0.038)	0.318	0.743	0.050	(-0.011, 0.039)
Quetiapine sulfoxide	Lognormal	0.016	(-0.016, 0.048)	0.322	0.743	0.054	(-0.015, 0.048)
Indole-3-propionic acid	Lognormal	-0.014	(-0.043, 0.014)	0.327	0.747	0.052	(-0.042, 0.016)
3-Amino-1-propanol	Lognormal	0.009	(-0.009, 0.028)	0.331	0.747	0.048	(-0.010, 0.028)
Carnitine	Lognormal	-0.003	(-0.010, 0.003)	0.332	0.747	0.050	(-0.010, 0.003)
1-Acetyl-3-piperidinamine	Lognormal	0.008	(-0.009, 0.025)	0.333	0.747	0.054	(-0.008, 0.025)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
1-Monostearin	Lognormal	-0.017	(-0.050, 0.017)	0.335	0.748	0.049	(-0.051, 0.017)
(3-Carboxypropyl)trimethylammonium cation	Lognormal	-0.005	(-0.016, 0.006)	0.344	0.756	0.049	(-0.016, 0.006)
1-Oleoyl-2-acetyl-sn-glycerol	Lognormal	-0.017	(-0.053, 0.019)	0.345	0.756	0.052	(-0.054, 0.016)
6-Methoxynaphthaleneacetic acid	Lognormal	-0.006	(-0.018, 0.006)	0.347	0.756	0.052	(-0.018, 0.006)
N-Methylhistidine	Lognormal	-0.015	(-0.047, 0.017)	0.357	0.761	0.052	(-0.048, 0.016)
D-.alpha.-Cyclohexylglycine	Lognormal	-0.013	(-0.041, 0.015)	0.365	0.764	0.048	(-0.038, 0.018)
Histidine	Lognormal	-0.009	(-0.030, 0.011)	0.368	0.764	0.049	(-0.031, 0.009)
4-Pyridoxic acid;	Lognormal	0.020	(-0.024, 0.063)	0.376	0.768	0.050	(-0.022, 0.065)
1-Oleoyl-sn-glycero-3-phosphoethanolamine	Lognormal	-0.015	(-0.049, 0.019)	0.376	0.768	0.045	(-0.050, 0.017)
Oleoyl-L-carnitine	Lognormal	-0.016	(-0.051, 0.019)	0.377	0.768	0.048	(-0.049, 0.021)
Norleucine	Lognormal	-0.005	(-0.015, 0.006)	0.380	0.768	0.047	(-0.015, 0.006)
Lansoprazole	Lognormal	-0.042	(-0.137, 0.053)	0.384	0.771	0.045	(-0.143, 0.048)
.beta.-Phenyl-.gamma.-aminobutyric acid	Lognormal	-0.008	(-0.027, 0.010)	0.384	0.771	0.050	(-0.028, 0.011)
Topiramate	Lognormal	0.013	(-0.017, 0.043)	0.399	0.786	0.043	(-0.017, 0.041)
N-(3-(Aminomethyl)benzyl)acetamide	Lognormal	-0.014	(-0.045, 0.018)	0.401	0.789	0.037	(-0.044, 0.019)
Montelukast-1,2-diol	Lognormal	0.030	(-0.041, 0.100)	0.412	0.808	0.044	(-0.036, 0.102)
Omeprazole sulfone	Lognormal	0.026	(-0.037, 0.089)	0.414	0.810	0.046	(-0.042, 0.087)
Betonicine	Lognormal	-0.028	(-0.094, 0.039)	0.418	0.815	0.047	(-0.095, 0.040)
Phenylacetyl-L-glutamine	Lognormal	-0.014	(-0.046, 0.019)	0.422	0.818	0.039	(-0.043, 0.022)
Trimethoprim	Lognormal	-0.011	(-0.039, 0.016)	0.423	0.818	0.044	(-0.038, 0.018)
Ticlopidine	Lognormal	-0.033	(-0.115, 0.049)	0.430	0.822	0.042	(-0.121, 0.042)
alpha-Methylhistidine;	Lognormal	-0.018	(-0.064, 0.028)	0.435	0.828	0.046	(-0.066, 0.027)
N-Acetyl-L-carnosine	Lognormal	-0.007	(-0.026, 0.011)	0.439	0.829	0.039	(-0.025, 0.012)
Metoprolol acid	Lognormal	0.021	(-0.033, 0.074)	0.449	0.845	0.045	(-0.030, 0.076)
Phenylalanine	Lognormal	-0.003	(-0.010, 0.005)	0.455	0.848	0.040	(-0.009, 0.005)
L-Threonine	Lognormal	-0.004	(-0.015, 0.007)	0.456	0.848	0.041	(-0.015, 0.007)
Nudifloramide	Lognormal	-0.007	(-0.025, 0.011)	0.460	0.848	0.044	(-0.025, 0.012)
Dexpanthenol	Lognormal	-0.011	(-0.041, 0.019)	0.462	0.848	0.043	(-0.040, 0.019)
Aminodiphenylmethane	Lognormal	0.013	(-0.022, 0.047)	0.469	0.853	0.041	(-0.021, 0.046)
Coniferylaldehyde	Lognormal	0.008	(-0.014, 0.030)	0.475	0.856	0.042	(-0.014, 0.030)
1-Stearoyl-2-arachidonoyl-sn-glycero-3-phosphoserine	Lognormal	-0.029	(-0.109, 0.051)	0.483	0.856	0.035	(-0.111, 0.051)
3,4-Dimethoxybenzaldehyde	Lognormal	0.011	(-0.020, 0.041)	0.486	0.856	0.036	(-0.018, 0.041)
2-Amino-1-phenylethanol	Lognormal	-0.003	(-0.010, 0.005)	0.487	0.856	0.040	(-0.010, 0.005)
7.alpha.-Hydroxy-3-oxo-4-cholestenoic acid	Lognormal	-0.007	(-0.028, 0.013)	0.488	0.856	0.042	(-0.027, 0.012)
N.epsilon.-Methyl-L-lysine	Lognormal	0.010	(-0.019, 0.039)	0.490	0.856	0.043	(-0.019, 0.039)
N-Acetyl-D-norleucine	Lognormal	0.008	(-0.014, 0.030)	0.492	0.856	0.027	(-0.015, 0.029)
Benthiavalicarb-isopropyl	Lognormal	-0.012	(-0.049, 0.025)	0.514	0.879	0.040	(-0.050, 0.025)
Creatine	Lognormal	0.005	(-0.009, 0.019)	0.518	0.882	0.035	(-0.010, 0.019)
Albendazole	Lognormal	0.009	(-0.019, 0.037)	0.528	0.886	0.043	(-0.019, 0.036)
4-Aminomethylcyclohexanecarboxylic acid;	Lognormal	-0.009	(-0.037, 0.019)	0.529	0.886	0.038	(-0.036, 0.019)
Palmitamide	Lognormal	-0.012	(-0.050, 0.026)	0.533	0.890	0.044	(-0.052, 0.027)
Ranitidine-S-oxide	Lognormal	0.017	(-0.038, 0.072)	0.543	0.891	0.042	(-0.038, 0.070)
D-erythro-Sphingosine-1-phosphate	Lognormal	-0.007	(-0.030, 0.016)	0.548	0.891	0.035	(-0.031, 0.016)
Metoprolol	Lognormal	0.013	(-0.029, 0.054)	0.553	0.891	0.039	(-0.027, 0.058)
Tryptophan	Lognormal	0.003	(-0.007, 0.013)	0.564	0.899	0.037	(-0.007, 0.013)
1-Methyladenosine A	Lognormal	-0.003	(-0.012, 0.006)	0.572	0.901	0.038	(-0.011, 0.007)
rac-4-Sulfoxypropranolol	Lognormal	0.008	(-0.021, 0.037)	0.579	0.907	0.039	(-0.021, 0.036)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Modafinil acid	Lognormal	0.017	(-0.042, 0.075)	0.581	0.907	0.041	(-0.039, 0.077)
5'-S-Methyl-5'-thioadenosine	Lognormal	-0.020	(-0.092, 0.052)	0.583	0.907	0.032	(-0.093, 0.048)
Metformin	Lognormal	0.009	(-0.023, 0.041)	0.587	0.909	0.038	(-0.025, 0.041)
Pyridoxal	Lognormal	0.006	(-0.017, 0.030)	0.589	0.911	0.039	(-0.018, 0.029)
Serotonin	Lognormal	0.005	(-0.014, 0.024)	0.590	0.911	0.033	(-0.014, 0.025)
Theanine;	Lognormal	0.009	(-0.023, 0.040)	0.591	0.911	0.033	(-0.021, 0.043)
Irbesartan	Lognormal	0.006	(-0.016, 0.028)	0.594	0.913	0.038	(-0.015, 0.028)
1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	Lognormal	-0.009	(-0.044, 0.026)	0.615	0.915	0.035	(-0.045, 0.027)
3-Hydroxyoleylcarnitine	Lognormal	0.019	(-0.054, 0.092)	0.616	0.915	0.033	(-0.054, 0.091)
Telmisartan	Lognormal	0.007	(-0.021, 0.035)	0.617	0.915	0.034	(-0.020, 0.035)
Ile-Glu-Arg	Lognormal	-0.016	(-0.080, 0.047)	0.619	0.915	0.039	(-0.079, 0.048)
N8-Acetylspermidine	Lognormal	-0.003	(-0.017, 0.010)	0.619	0.915	0.032	(-0.017, 0.010)
Codeine-6-.beta.-D-glucuronide	Lognormal	0.007	(-0.021, 0.035)	0.621	0.915	0.039	(-0.020, 0.035)
Tauroursodeoxycholic acid	Lognormal	0.009	(-0.025, 0.042)	0.622	0.915	0.036	(-0.024, 0.043)
1,2-Dimethylimidazole	Lognormal	-0.005	(-0.025, 0.015)	0.630	0.915	0.041	(-0.025, 0.015)
Hypoxanthine	Lognormal	-0.004	(-0.020, 0.012)	0.636	0.920	0.031	(-0.021, 0.012)
DL-Indole-3-lactic acid	Lognormal	0.003	(-0.008, 0.013)	0.640	0.920	0.036	(-0.008, 0.013)
Sulfamethoxazole	Lognormal	-0.019	(-0.100, 0.061)	0.643	0.922	0.037	(-0.101, 0.061)
HeptadecaspHING-4-enine	Lognormal	0.025	(-0.084, 0.134)	0.652	0.925	0.031	(-0.084, 0.133)
Methylgallate	Lognormal	0.018	(-0.062, 0.098)	0.652	0.925	0.037	(-0.061, 0.099)
L-Cysteine-glutathione disulfide	Lognormal	-0.006	(-0.034, 0.022)	0.668	0.932	0.023	(-0.034, 0.023)
Atenolol	Lognormal	-0.009	(-0.050, 0.032)	0.670	0.932	0.035	(-0.048, 0.034)
6-Hydroxyflavone	Lognormal	0.008	(-0.030, 0.047)	0.672	0.932	0.034	(-0.029, 0.050)
Pyridoxine;	Lognormal	0.007	(-0.026, 0.040)	0.673	0.932	0.038	(-0.028, 0.040)
1-Stearoyl-2-arachidonoyl-sn-glycero-3-phospho-(1'-myo-inositol)	Lognormal	-0.019	(-0.106, 0.068)	0.675	0.932	0.034	(-0.105, 0.063)
Ethylidethanolamine	Lognormal	-0.006	(-0.032, 0.021)	0.679	0.932	0.033	(-0.031, 0.021)
Proline	Lognormal	-0.005	(-0.030, 0.020)	0.681	0.932	0.036	(-0.029, 0.022)
Glucine	Lognormal	0.004	(-0.016, 0.025)	0.683	0.932	0.035	(-0.016, 0.025)
Betaine aldehyde cation	Lognormal	0.010	(-0.041, 0.062)	0.689	0.932	0.032	(-0.038, 0.063)
(2R)-3-Hydroxyisovalerylcarnitine	Lognormal	-0.003	(-0.021, 0.014)	0.692	0.932	0.032	(-0.020, 0.014)
Milnacipran	Lognormal	0.007	(-0.029, 0.042)	0.700	0.936	0.033	(-0.028, 0.044)
Carbamazepine	Lognormal	-0.010	(-0.060, 0.041)	0.709	0.936	0.036	(-0.059, 0.042)
Biliverden	Lognormal	-0.004	(-0.023, 0.016)	0.709	0.936	0.035	(-0.022, 0.016)
trans-3'-Hydroxycotinine	Lognormal	0.006	(-0.025, 0.037)	0.721	0.936	0.033	(-0.026, 0.036)
Adenosine	Lognormal	-0.005	(-0.033, 0.023)	0.721	0.936	0.032	(-0.034, 0.022)
3-Hydroxybutyrylcarnitine	Lognormal	-0.005	(-0.033, 0.023)	0.724	0.936	0.034	(-0.032, 0.025)
1-Acetyl-4-piperidinamine	Lognormal	0.007	(-0.031, 0.045)	0.725	0.936	0.037	(-0.032, 0.045)
3-Pyridinemethanol	Lognormal	0.004	(-0.018, 0.026)	0.726	0.936	0.036	(-0.018, 0.026)
Avobenzone	Lognormal	-0.004	(-0.028, 0.020)	0.731	0.936	0.034	(-0.029, 0.019)
Lysine	Lognormal	0.002	(-0.010, 0.014)	0.733	0.936	0.025	(-0.010, 0.014)
Triptolide	Lognormal	-0.004	(-0.025, 0.018)	0.738	0.936	0.034	(-0.025, 0.017)
1-Methyl-L-histidine	Lognormal	-0.007	(-0.050, 0.036)	0.742	0.936	0.036	(-0.049, 0.040)
Androstan-3-ol-17-one 3-glucuronide	Lognormal	0.005	(-0.025, 0.035)	0.743	0.936	0.034	(-0.025, 0.033)
1-Stearoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	Lognormal	0.006	(-0.030, 0.042)	0.744	0.936	0.031	(-0.031, 0.040)
Cotinine N-.beta.-D-glucuronide	Lognormal	0.010	(-0.052, 0.073)	0.745	0.936	0.032	(-0.053, 0.072)
R-(-)-O-Desmethylvenlafaxine	Lognormal	-0.007	(-0.052, 0.037)	0.746	0.936	0.036	(-0.053, 0.036)
Meprobamate	Lognormal	0.005	(-0.026, 0.037)	0.750	0.936	0.035	(-0.024, 0.037)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Tapentadol-.beta.-D-glucuronide	Lognormal	-0.010	(-0.068, 0.049)	0.750	0.936	0.035	(-0.067, 0.050)
Acetyl-DL-carnitine	Lognormal	0.002	(-0.012, 0.017)	0.752	0.936	0.035	(-0.013, 0.017)
3-(1-Pyrazolyl)-alanine	Lognormal	0.010	(-0.054, 0.074)	0.754	0.936	0.035	(-0.051, 0.072)
Toradol	Lognormal	0.006	(-0.031, 0.043)	0.755	0.936	0.035	(-0.033, 0.042)
Pipecolic acid	Lognormal	-0.006	(-0.044, 0.032)	0.757	0.938	0.036	(-0.045, 0.031)
Esomeprazole	Lognormal	0.004	(-0.025, 0.034)	0.768	0.944	0.033	(-0.024, 0.035)
Meloxicam	Lognormal	0.016	(-0.092, 0.125)	0.769	0.944	0.036	(-0.100, 0.123)
3-Aminoquinoline	Lognormal	0.006	(-0.034, 0.046)	0.775	0.947	0.025	(-0.034, 0.048)
.epsilon.-Caprolactam	Lognormal	0.002	(-0.014, 0.019)	0.775	0.947	0.020	(-0.015, 0.019)
Scopoletin	Lognormal	-0.011	(-0.087, 0.065)	0.777	0.947	0.028	(-0.087, 0.064)
threo-Dihydrobupropion	Lognormal	-0.004	(-0.031, 0.023)	0.779	0.949	0.033	(-0.029, 0.023)
Benzophenone-3	Lognormal	-0.008	(-0.063, 0.047)	0.782	0.949	0.035	(-0.067, 0.045)
Pantothenic acid	Lognormal	0.003	(-0.019, 0.025)	0.786	0.950	0.033	(-0.018, 0.024)
5'-S-Methylthioadenosine	Lognormal	-0.011	(-0.089, 0.068)	0.787	0.950	0.031	(-0.088, 0.064)
Gly-Pro-Arg	Lognormal	-0.008	(-0.072, 0.055)	0.794	0.950	0.036	(-0.075, 0.052)
Lauric acid diethanolamide	Lognormal	0.006	(-0.037, 0.048)	0.797	0.950	0.030	(-0.036, 0.046)
Temazepam	Lognormal	0.005	(-0.033, 0.042)	0.803	0.950	0.032	(-0.033, 0.040)
Ser-Tyr-Lys	Lognormal	-0.007	(-0.065, 0.051)	0.809	0.950	0.035	(-0.065, 0.049)
Ondansetron	Lognormal	-0.003	(-0.024, 0.019)	0.816	0.950	0.034	(-0.025, 0.019)
Glycocholic acid	Lognormal	-0.004	(-0.040, 0.032)	0.817	0.950	0.034	(-0.041, 0.032)
N-Methylproline	Lognormal	-0.003	(-0.027, 0.021)	0.821	0.950	0.035	(-0.028, 0.021)
Borrelidin	Lognormal	-0.005	(-0.054, 0.043)	0.824	0.950	0.033	(-0.052, 0.044)
Isopentenyladenine	Lognormal	-0.001	(-0.010, 0.008)	0.826	0.950	0.033	(-0.010, 0.008)
Naproxen	Lognormal	0.005	(-0.037, 0.047)	0.827	0.950	0.035	(-0.038, 0.049)
Urocanic acid;	Lognormal	-0.002	(-0.020, 0.016)	0.828	0.950	0.031	(-0.020, 0.017)
N-Acetylalanine	Lognormal	0.006	(-0.052, 0.064)	0.834	0.950	0.033	(-0.048, 0.066)
Dinor-12-oxophytodienoic acid	Lognormal	-0.005	(-0.050, 0.041)	0.837	0.950	0.034	(-0.053, 0.040)
Modafinil	Lognormal	0.005	(-0.041, 0.050)	0.839	0.950	0.032	(-0.040, 0.050)
Penciclovir	Lognormal	0.002	(-0.025, 0.030)	0.862	0.963	0.028	(-0.026, 0.029)
2-Hydroxyibuprofen	Lognormal	-0.003	(-0.036, 0.030)	0.865	0.963	0.035	(-0.036, 0.030)
D-Pyroglutamic acid	Lognormal	0.000	(-0.006, 0.005)	0.867	0.963	0.031	(-0.005, 0.005)
Matrine	Lognormal	0.004	(-0.041, 0.049)	0.871	0.963	0.033	(-0.041, 0.049)
Losartan	Lognormal	0.003	(-0.035, 0.042)	0.874	0.963	0.036	(-0.036, 0.040)
Ornithine	Lognormal	-0.001	(-0.017, 0.015)	0.875	0.963	0.025	(-0.017, 0.014)
Mefenorex	Lognormal	-0.003	(-0.039, 0.033)	0.876	0.963	0.030	(-0.040, 0.032)
N.epsilon.-Acetyl-L-lysine	Lognormal	-0.001	(-0.016, 0.014)	0.882	0.965	0.032	(-0.016, 0.015)
Ezetimibe	Lognormal	0.003	(-0.033, 0.039)	0.886	0.968	0.032	(-0.033, 0.039)
Decanoyl-L-carnitine	Lognormal	-0.002	(-0.030, 0.027)	0.899	0.973	0.032	(-0.030, 0.026)
Glutamine	Lognormal	0.000	(-0.006, 0.005)	0.906	0.975	0.031	(-0.006, 0.005)
Trileptal	Lognormal	-0.001	(-0.024, 0.022)	0.906	0.975	0.032	(-0.026, 0.020)
Diphenhydramine	Lognormal	-0.001	(-0.023, 0.020)	0.910	0.976	0.031	(-0.021, 0.020)
Atorvastatin	Lognormal	-0.001	(-0.019, 0.017)	0.911	0.976	0.033	(-0.020, 0.017)
1-Phenylpyrrolidine	Lognormal	0.001	(-0.027, 0.030)	0.919	0.982	0.030	(-0.027, 0.030)
Isoleucine	Lognormal	-0.001	(-0.011, 0.010)	0.921	0.982	0.033	(-0.012, 0.010)
Pantoprazole	Lognormal	0.003	(-0.053, 0.059)	0.922	0.982	0.032	(-0.053, 0.062)
D-Fructose	Lognormal	0.000	(-0.007, 0.007)	0.926	0.984	0.029	(-0.007, 0.007)
L-Carnitine	Lognormal	0.000	(-0.011, 0.010)	0.941	0.987	0.032	(-0.010, 0.010)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Moxonidine	Lognormal	0.001	(-0.025, 0.026)	0.954	0.990	0.034	(-0.025, 0.027)
Phenylacetylglutamine	Lognormal	0.001	(-0.025, 0.026)	0.957	0.990	0.033	(-0.025, 0.027)
2,2-Bishydroxymethyl]-2,2',2''-nitrilotriethanol	Lognormal	-0.001	(-0.028, 0.026)	0.957	0.990	0.030	(-0.028, 0.026)
4-Fluoro-.alpha.-pyrrolidinobutiophenone	Lognormal	0.001	(-0.022, 0.023)	0.959	0.990	0.037	(-0.024, 0.024)
2,2',2''-Nitrilotriethanol	Lognormal	-0.001	(-0.025, 0.023)	0.961	0.990	0.032	(-0.025, 0.024)
3,5-Dihydroxyphenylglycine	Lognormal	-0.001	(-0.029, 0.028)	0.962	0.990	0.029	(-0.029, 0.028)
Methionine	Lognormal	0.000	(-0.009, 0.010)	0.971	0.990	0.034	(-0.010, 0.009)
Glycodeoxycholic acid	Lognormal	0.001	(-0.038, 0.039)	0.974	0.990	0.028	(-0.038, 0.039)
Levocetirizine;	Lognormal	0.001	(-0.070, 0.071)	0.984	0.993	0.035	(-0.070, 0.067)
Cyclo(Leu-Pro)	Lognormal	0.000	(-0.026, 0.025)	0.989	0.994	0.033	(-0.027, 0.025)
Complex Lipids (CL)							
PC (p-34:2)/PC (o-34:3) - ESI(+)	Lognormal	-0.018	(-0.027, -0.009)	0.000	0.062	44.620	(-0.027, -0.009)
PC (p-34:1)/PC (o-34:2)	Lognormal	-0.021	(-0.032, -0.010)	0.000	0.062	178.678	(-0.032, -0.011)
PE (p-36:2)/PE (o-36:3) - ESI(+)	Lognormal	-0.028	(-0.043, -0.013)	0.000	0.074	20.935	(-0.042, -0.013)
PC (36:2)	Lognormal	-0.007	(-0.011, -0.003)	0.000	0.074	11.241	(-0.011, -0.003)
PC (36:4) A - ESI(+)	Lognormal	-0.018	(-0.028, -0.008)	0.000	0.074	8.134	(-0.028, -0.007)
PC (p-36:1)/PC (o-36:2)	Lognormal	-0.055	(-0.086, -0.024)	0.001	0.074	11.555	(-0.087, -0.025)
PC (p-34:2)/PC (o-34:3) - ESI(-)	Lognormal	-0.020	(-0.032, -0.009)	0.001	0.074	12.281	(-0.031, -0.009)
PC (p-36:4)/PC (o-36:5) - ESI(-)	Lognormal	-0.021	(-0.034, -0.009)	0.001	0.103	7.046	(-0.033, -0.009)
PC (36:4) A - ESI(-)	Lognormal	-0.019	(-0.031, -0.008)	0.001	0.103	4.032	(-0.031, -0.008)
PC (p-34:1)/PC (o-34:2) A	Lognormal	-0.027	(-0.044, -0.011)	0.002	0.125	5.655	(-0.044, -0.011)
PE (p-34:2)/PE (o-34:3)	Lognormal	-0.037	(-0.060, -0.014)	0.002	0.126	5.662	(-0.060, -0.015)
PC (32:2) - ESI(-)	Lognormal	-0.027	(-0.043, -0.010)	0.002	0.135	7.389	(-0.044, -0.010)
LPC (18:2) - ESI(-)	Lognormal	-0.019	(-0.032, -0.007)	0.003	0.139	4.102	(-0.031, -0.006)
PC 34:4e	Lognormal	-0.022	(-0.036, -0.008)	0.003	0.139	4.327	(-0.035, -0.008)
PC (34:2) - ESI(+)	Lognormal	-0.005	(-0.008, -0.002)	0.003	0.139	2.039	(-0.008, -0.001)
SM (d39:1) - ESI(-)	Lognormal	-0.017	(-0.029, -0.006)	0.004	0.139	2.833	(-0.029, -0.006)
PE (p-36:2)/PE (o-36:3) - ESI(-)	Lognormal	-0.029	(-0.048, -0.010)	0.004	0.139	2.505	(-0.048, -0.010)
PC (p-36:3)/PC (o-36:4) - ESI(-)	Lognormal	-0.016	(-0.026, -0.005)	0.004	0.139	2.209	(-0.026, -0.006)
SM (d40:1) - ESI(-)	Lognormal	-0.012	(-0.020, -0.004)	0.004	0.143	2.357	(-0.020, -0.004)
PC (34:2) - ESI(-)	Lognormal	-0.009	(-0.016, -0.003)	0.005	0.171	1.878	(-0.016, -0.003)
PE (p-36:4)/PE (o-36:5) - ESI(-)	Lognormal	-0.023	(-0.039, -0.007)	0.005	0.171	1.112	(-0.038, -0.005)
LPC (18:3)	Lognormal	-0.025	(-0.043, -0.008)	0.006	0.172	1.596	(-0.044, -0.009)
SM (d32:1) - ESI(-)	Lognormal	-0.015	(-0.025, -0.004)	0.006	0.172	1.401	(-0.025, -0.004)
LPC (18:2) - ESI(+)	Lognormal	-0.015	(-0.025, -0.004)	0.007	0.173	1.455	(-0.024, -0.004)
Ceramide (d42:1) - ESI (+)	Lognormal	-0.009	(-0.015, -0.003)	0.007	0.173	1.584	(-0.016, -0.003)
LPE (20:4) - ESI(-)	Lognormal	-0.024	(-0.040, -0.007)	0.007	0.173	1.313	(-0.041, -0.007)
SM (d40:3)	Lognormal	-0.025	(-0.043, -0.007)	0.007	0.173	1.222	(-0.045, -0.008)
Ceramide (d41:1) - ESI(-)	Lognormal	-0.014	(-0.025, -0.004)	0.007	0.173	1.295	(-0.024, -0.003)
LPC (14:0) - ESI(+)	Lognormal	-0.021	(-0.036, -0.006)	0.008	0.177	1.300	(-0.036, -0.006)
PC (34:4) - ESI(-)	Lognormal	-0.033	(-0.056, -0.009)	0.008	0.177	0.952	(-0.054, -0.006)
PE (p-38:5)/PE (o-38:6) - ESI(-)	Lognormal	-0.021	(-0.036, -0.006)	0.008	0.177	1.045	(-0.036, -0.005)
PC (p-38:3)/PC (o-38:4) - ESI(-)	Lognormal	-0.016	(-0.028, -0.004)	0.008	0.177	1.287	(-0.028, -0.004)
LPE (18:2) - ESI(-)	Lognormal	-0.028	(-0.049, -0.007)	0.008	0.177	1.008	(-0.049, -0.008)
Ceramide (d42:1) - ESI(-)	Lognormal	-0.012	(-0.020, -0.003)	0.009	0.177	1.534	(-0.020, -0.003)
LPC (18:0) A - ESI(-)	Lognormal	-0.019	(-0.033, -0.005)	0.009	0.177	1.172	(-0.032, -0.005)
LPC (16:0) - ESI(-)	Lognormal	-0.010	(-0.018, -0.003)	0.010	0.185	0.725	(-0.018, -0.002)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
LPE (18:2) - ESI(+)	Lognormal	-0.022	(-0.039, -0.005)	0.010	0.185	1.241	(-0.039, -0.007)
LPC (20:3) - ESI(-)	Lognormal	-0.024	(-0.043, -0.006)	0.010	0.185	0.931	(-0.042, -0.006)
PC (34:3)	Lognormal	-0.016	(-0.029, -0.004)	0.010	0.187	0.795	(-0.029, -0.004)
CE (18:3)	Lognormal	-0.018	(-0.032, -0.004)	0.011	0.188	0.818	(-0.032, -0.004)
PC (p-38:4)/PC (o-38:5) A	Lognormal	-0.012	(-0.021, -0.003)	0.011	0.188	0.669	(-0.021, -0.002)
SM (d33:1) - ESI(-)	Lognormal	-0.015	(-0.026, -0.003)	0.012	0.188	1.010	(-0.026, -0.004)
SM (d36:3) - ESI(-)	Lognormal	-0.020	(-0.036, -0.005)	0.012	0.188	0.898	(-0.035, -0.005)
TG (56:6)	Lognormal	0.010	(0.002, 0.017)	0.012	0.188	0.715	(0.001, 0.017)
PC (p-36:2)/PC (o-36:3)	Lognormal	-0.016	(-0.028, -0.004)	0.012	0.188	1.014	(-0.028, -0.004)
SM (d43:1) - ESI(-)	Lognormal	-0.034	(-0.060, -0.008)	0.012	0.188	0.948	(-0.059, -0.008)
LPC (18:0) B - ESI(-)	Lognormal	-0.013	(-0.023, -0.003)	0.013	0.192	0.780	(-0.023, -0.003)
Ceramide (d42:2) B - ESI (+)	Lognormal	-0.011	(-0.020, -0.002)	0.013	0.192	0.654	(-0.020, -0.003)
TG (55:6)	Lognormal	0.020	(0.004, 0.036)	0.014	0.206	0.592	(0.004, 0.036)
SM (d40:2) B - ESI(-)	Lognormal	-0.012	(-0.021, -0.002)	0.015	0.208	0.846	(-0.021, -0.003)
TG (53:0)	Lognormal	-0.018	(-0.033, -0.004)	0.015	0.208	0.624	(-0.032, -0.003)
Ceramide (d39:1)	Lognormal	-0.021	(-0.037, -0.004)	0.016	0.208	0.560	(-0.037, -0.003)
PC (33:2) - ESI(-)	Lognormal	-0.020	(-0.036, -0.004)	0.016	0.208	0.580	(-0.037, -0.004)
CE (18:2)	Lognormal	-0.008	(-0.015, -0.002)	0.016	0.208	0.498	(-0.015, -0.001)
Ceramide (d40:1)	Lognormal	-0.010	(-0.018, -0.002)	0.016	0.208	0.689	(-0.018, -0.001)
PE (p-38:4)/PE (o-38:5)	Lognormal	-0.016	(-0.029, -0.003)	0.016	0.208	0.588	(-0.029, -0.003)
SM (d34:2) - ESI(-)	Lognormal	-0.009	(-0.016, -0.002)	0.017	0.208	0.649	(-0.015, -0.001)
PE (p-36:4)/PE (o-36:5) - ESI(+)	Lognormal	-0.017	(-0.031, -0.003)	0.017	0.208	0.522	(-0.031, -0.004)
PC (34:3) B	Lognormal	-0.011	(-0.020, -0.002)	0.018	0.213	0.579	(-0.021, -0.003)
PC (36:4) B - ESI(-)	Lognormal	-0.008	(-0.015, -0.001)	0.018	0.213	0.572	(-0.015, -0.001)
PC (36:5) A	Lognormal	-0.040	(-0.073, -0.007)	0.018	0.213	0.685	(-0.074, -0.009)
PC (38:4) A - ESI(-)	Lognormal	-0.010	(-0.019, -0.002)	0.019	0.213	0.478	(-0.019, -0.002)
TG (50:0)	Lognormal	-0.024	(-0.045, -0.004)	0.019	0.214	0.547	(-0.043, -0.003)
PE (p-36:1)/PE (o-36:2) - ESI(-)	Lognormal	-0.029	(-0.053, -0.005)	0.020	0.214	0.587	(-0.051, -0.003)
PC (34:3) C	Lognormal	-0.016	(-0.029, -0.003)	0.020	0.214	0.586	(-0.028, -0.003)
CE (20:2)	Lognormal	-0.023	(-0.043, -0.004)	0.020	0.214	0.490	(-0.043, -0.003)
FA (16:1) (palmitoleic acid)	Lognormal	0.016	(0.003, 0.030)	0.021	0.214	0.402	(0.002, 0.030)
SM (d42:1) - ESI(-)	Lognormal	-0.010	(-0.018, -0.002)	0.021	0.214	0.498	(-0.017, -0.001)
PC (p-36:3)/PC (o-36:4) - ESI(+)	Lognormal	-0.010	(-0.018, -0.002)	0.021	0.214	0.496	(-0.018, -0.002)
PC (32:2) - ESI(+)	Lognormal	-0.017	(-0.030, -0.003)	0.021	0.214	0.446	(-0.030, -0.003)
PE (p-38:5)/PE (o-38:6) - ESI(+)	Lognormal	-0.013	(-0.024, -0.002)	0.022	0.218	0.424	(-0.024, -0.001)
PC (p-36:4)/PC (o-36:5) - ESI(+)	Lognormal	-0.009	(-0.017, -0.001)	0.024	0.234	0.438	(-0.017, -0.001)
SM (d34:1) - ESI(-)	Lognormal	-0.007	(-0.014, -0.001)	0.024	0.239	0.407	(-0.014, -0.001)
TG (58:8)	Lognormal	0.020	(0.003, 0.038)	0.026	0.247	0.350	(0.002, 0.038)
PE (p-36:1)/PE (o-36:2) - ESI(+)	Lognormal	-0.020	(-0.037, -0.003)	0.026	0.247	0.437	(-0.037, -0.002)
PC (36:5)A	Lognormal	-0.020	(-0.037, -0.002)	0.027	0.256	0.349	(-0.038, -0.002)
LPE (18:0)	Lognormal	-0.014	(-0.026, -0.002)	0.028	0.258	0.347	(-0.026, -0.002)
TG (56:7) B	Lognormal	0.018	(0.002, 0.034)	0.029	0.261	0.401	(0.002, 0.033)
SM (d30:1) - ESI(-)	Lognormal	-0.029	(-0.056, -0.003)	0.029	0.261	0.377	(-0.055, -0.004)
PE (p-40:4)/PE (o-40:5) A	Lognormal	-0.024	(-0.045, -0.002)	0.031	0.268	0.236	(-0.046, -0.003)
PC (p-38:3)/PC (o-38:4) A - ESI(+)	Lognormal	-0.010	(-0.020, -0.001)	0.033	0.282	0.312	(-0.020, -0.001)
TG (58:9)	Lognormal	0.018	(0.002, 0.035)	0.033	0.282	0.310	(0.001, 0.034)
PC (40:8) - ESI(-)	Lognormal	-0.016	(-0.030, -0.001)	0.035	0.287	0.255	(-0.031, -0.001)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
PC (o-34:0)	Lognormal	-0.014	(-0.027, -0.001)	0.035	0.288	0.313	(-0.027, -0.001)
LPC (20:3) - ESI(+)	Lognormal	-0.013	(-0.025, -0.001)	0.036	0.288	0.266	(-0.025, 0.000)
PC (38:6) A - ESI(+)	Lognormal	-0.008	(-0.016, -0.001)	0.036	0.288	0.283	(-0.017, -0.001)
PC (38:3) - ESI(-)	Lognormal	-0.012	(-0.023, -0.001)	0.036	0.288	0.315	(-0.022, 0.000)
TG (54:7) B	Lognormal	0.016	(0.001, 0.032)	0.037	0.292	0.332	(0.000, 0.031)
LPC (14:0) - ESI(-)	Lognormal	-0.027	(-0.053, -0.002)	0.038	0.296	0.304	(-0.053, -0.002)
TG (62:4)	Lognormal	-0.028	(-0.055, -0.002)	0.039	0.298	0.303	(-0.054, 0.000)
LPC (16:1) - ESI(-)	Lognormal	-0.017	(-0.032, -0.001)	0.039	0.298	0.312	(-0.033, -0.001)
PC (p-38:4)/PC (o-38:5) B	Lognormal	-0.011	(-0.021, -0.001)	0.039	0.298	0.294	(-0.021, -0.001)
PC (34:0) - ESI(-)	Lognormal	-0.009	(-0.019, 0.000)	0.041	0.304	0.291	(-0.019, -0.001)
SM (d38:2) - ESI(-)	Lognormal	-0.011	(-0.022, 0.000)	0.042	0.309	0.283	(-0.023, -0.001)
PE (36:2)	Lognormal	-0.020	(-0.040, -0.001)	0.042	0.309	0.232	(-0.041, -0.001)
PI (38:4)/PI (18:0-20:4)	Lognormal	-0.008	(-0.016, 0.000)	0.044	0.319	0.285	(-0.016, 0.000)
PC (34:4) - ESI(+)	Lognormal	-0.017	(-0.033, 0.000)	0.046	0.327	0.282	(-0.033, 0.000)
PC (p-38:3)/PC (o-38:4) B - ESI(+)	Lognormal	-0.010	(-0.020, 0.000)	0.046	0.330	0.239	(-0.020, 0.000)
AC (10:1)	Lognormal	-0.020	(-0.039, 0.000)	0.048	0.336	0.266	(-0.039, 0.000)
TG (54:6) C	Lognormal	0.010	(0.000, 0.021)	0.051	0.348	0.186	(0.000, 0.021)
SM (d40:2) B - ESI(+)	Lognormal	-0.006	(-0.012, 0.000)	0.051	0.348	0.227	(-0.012, 0.000)
PE (p-34:1)/PE (o-34:2) - ESI(+)	Lognormal	-0.014	(-0.029, 0.000)	0.051	0.348	0.161	(-0.028, 0.001)
SM (d40:1) - ESI(+)	Lognormal	-0.006	(-0.011, 0.000)	0.053	0.351	0.231	(-0.011, 0.000)
PC (36:3) B - ESI(-)	Lognormal	-0.008	(-0.017, 0.000)	0.055	0.359	0.193	(-0.017, 0.000)
PC (36:3) A - ESI(+)	Lognormal	-0.007	(-0.013, 0.000)	0.057	0.365	0.211	(-0.013, 0.001)
PC (p-32:1)/PC (o-32:2)	Lognormal	-0.009	(-0.019, 0.000)	0.058	0.367	0.191	(-0.019, 0.000)
GlcCer (d42:2) - ESI(+)	Lognormal	0.012	(0.000, 0.024)	0.059	0.367	0.190	(-0.001, 0.024)
LPC (18:1) - ESI(-)	Lognormal	-0.011	(-0.022, 0.000)	0.059	0.367	0.211	(-0.021, 0.001)
TG (56:8) B	Lognormal	0.018	(-0.001, 0.036)	0.060	0.370	0.198	(0.000, 0.037)
PC (37:5)	Lognormal	0.016	(-0.001, 0.032)	0.061	0.374	0.213	(-0.001, 0.031)
PC (p-38:4)/PC (o-38:5) B	Lognormal	-0.017	(-0.034, 0.001)	0.062	0.376	0.185	(-0.034, 0.001)
SM (d38:1)	Lognormal	-0.006	(-0.011, 0.000)	0.063	0.376	0.147	(-0.012, 0.000)
SM (d36:1) - ESI(-)	Lognormal	-0.008	(-0.016, 0.001)	0.067	0.396	0.211	(-0.017, 0.000)
Ceramide (d43:1)	Lognormal	-0.033	(-0.068, 0.002)	0.069	0.399	0.182	(-0.069, 0.003)
DG (38:6)	Lognormal	0.015	(-0.001, 0.031)	0.070	0.404	0.169	(-0.001, 0.030)
PE (p-40:4)/PE (o-40:5) B	Lognormal	-0.013	(-0.026, 0.001)	0.071	0.404	0.126	(-0.026, 0.001)
TG (60:11)	Lognormal	0.025	(-0.002, 0.053)	0.071	0.406	0.159	(-0.004, 0.052)
TG (48:0)	Lognormal	-0.018	(-0.038, 0.002)	0.073	0.408	0.149	(-0.038, 0.002)
PE (p-34:1)/PE (o-34:2) - ESI(-)	Lognormal	-0.014	(-0.030, 0.001)	0.073	0.408	0.163	(-0.031, 0.001)
LPC (20:2) - ESI(+)	Lognormal	-0.028	(-0.058, 0.002)	0.073	0.408	0.159	(-0.057, 0.003)
GlcCer (d38:1)	Lognormal	-0.012	(-0.024, 0.001)	0.073	0.408	0.170	(-0.024, 0.001)
FA (18:1) (oleic acid)	Lognormal	0.007	(-0.001, 0.015)	0.078	0.416	0.155	(-0.001, 0.016)
PC (36:3) A - ESI(-)	Lognormal	-0.009	(-0.018, 0.001)	0.080	0.422	0.165	(-0.018, 0.001)
LPC (p-16:0)/LPC (o-16:1)	Lognormal	-0.011	(-0.023, 0.001)	0.080	0.422	0.159	(-0.023, 0.002)
LPC (20:2) - ESI(-)	Lognormal	-0.012	(-0.025, 0.001)	0.081	0.422	0.160	(-0.025, 0.000)
PE (p-38:3)/PE (o-38:4)	Lognormal	-0.022	(-0.048, 0.003)	0.082	0.422	0.156	(-0.048, 0.001)
Ceramide (d33:1)	Lognormal	-0.011	(-0.023, 0.001)	0.084	0.430	0.146	(-0.023, 0.002)
PC (40:5) B - ESI(-)	Lognormal	-0.020	(-0.042, 0.003)	0.085	0.430	0.145	(-0.042, 0.004)
PC (38:6) B - ESI(+)	Lognormal	0.005	(-0.001, 0.011)	0.086	0.430	0.121	(-0.001, 0.011)
PC (33:2) - ESI(+)	Lognormal	-0.008	(-0.017, 0.001)	0.087	0.430	0.121	(-0.017, 0.001)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
SM (d39:1) - ESI(+)	Lognormal	-0.008	(-0.018, 0.001)	0.089	0.430	0.121	(-0.018, 0.002)
Ceramide (d41:1) - ESI (+)	Lognormal	-0.008	(-0.018, 0.001)	0.089	0.430	0.103	(-0.018, 0.001)
FA (24:0) (lignoceric acid)	Lognormal	-0.010	(-0.021, 0.001)	0.091	0.434	0.132	(-0.021, 0.001)
PC (40:6)B	Lognormal	0.008	(-0.001, 0.017)	0.092	0.438	0.128	(-0.001, 0.017)
AC (18:0)	Lognormal	-0.010	(-0.022, 0.002)	0.097	0.457	0.131	(-0.023, 0.001)
LPE (16:0)	Lognormal	-0.018	(-0.039, 0.003)	0.098	0.460	0.130	(-0.038, 0.004)
AC (14:2)	Lognormal	-0.019	(-0.042, 0.004)	0.099	0.461	0.126	(-0.043, 0.004)
TG (46:0)	Lognormal	-0.028	(-0.061, 0.005)	0.100	0.461	0.131	(-0.060, 0.005)
PC (40:5) A - ESI(+)	Lognormal	0.007	(-0.001, 0.015)	0.101	0.461	0.142	(0.000, 0.015)
Ceramide (d38:1) - ESI(+)	Lognormal	-0.008	(-0.017, 0.001)	0.102	0.463	0.123	(-0.017, 0.002)
PE (36:3)	Lognormal	-0.024	(-0.052, 0.005)	0.103	0.465	0.113	(-0.052, 0.004)
PE (p-38:6)/PE (o-38:7)	Lognormal	-0.015	(-0.034, 0.003)	0.104	0.466	0.131	(-0.033, 0.004)
Ceramide (d38:1) - ESI(-)	Lognormal	-0.010	(-0.023, 0.002)	0.105	0.467	0.141	(-0.023, 0.002)
SM (d43:2) - ESI(-)	Lognormal	-0.018	(-0.040, 0.004)	0.106	0.468	0.120	(-0.039, 0.004)
Lactosylceramide (d18:1/24:1(15Z))	Lognormal	0.012	(-0.003, 0.027)	0.111	0.481	0.111	(-0.002, 0.028)
PC (37:2) - ESI(+)	Lognormal	-0.007	(-0.016, 0.002)	0.115	0.486	0.120	(-0.016, 0.001)
SM (d30:1) - ESI(+)	Lognormal	-0.016	(-0.037, 0.004)	0.115	0.486	0.119	(-0.037, 0.006)
PC (36:5) D	Lognormal	0.014	(-0.003, 0.032)	0.116	0.487	0.106	(-0.003, 0.032)
AC (18:2)	Lognormal	-0.011	(-0.025, 0.003)	0.117	0.489	0.112	(-0.026, 0.002)
PC (p-40:3)/PC (o-40:4)	Lognormal	-0.014	(-0.031, 0.003)	0.118	0.490	0.107	(-0.030, 0.005)
SM (d42:1) - ESI(+)	Lognormal	-0.005	(-0.012, 0.001)	0.119	0.490	0.108	(-0.012, 0.001)
PC (40:7) A - ESI(+)	Lognormal	-0.008	(-0.018, 0.002)	0.121	0.496	0.098	(-0.018, 0.002)
PC (37:6)	Lognormal	0.014	(-0.004, 0.031)	0.123	0.504	0.115	(-0.004, 0.030)
SM (d32:1) - ESI(+)	Lognormal	-0.008	(-0.018, 0.002)	0.127	0.516	0.109	(-0.018, 0.002)
TG (48:4) A	Lognormal	-0.021	(-0.047, 0.006)	0.128	0.519	0.104	(-0.047, 0.006)
Ceramide (d32:1)	Lognormal	-0.011	(-0.026, 0.003)	0.129	0.521	0.101	(-0.025, 0.005)
PC (40:4) - ESI(-)	Lognormal	-0.014	(-0.032, 0.004)	0.131	0.524	0.116	(-0.032, 0.004)
FA (20:5) (eicosapentaenoic acid)	Lognormal	0.019	(-0.005, 0.042)	0.131	0.526	0.105	(-0.004, 0.044)
AC (12:0)	Lognormal	-0.015	(-0.035, 0.005)	0.133	0.528	0.102	(-0.036, 0.004)
TG (56:5) B	Lognormal	0.009	(-0.003, 0.021)	0.133	0.528	0.106	(-0.003, 0.021)
TG (56:8) A	Lognormal	0.010	(-0.003, 0.023)	0.135	0.531	0.096	(-0.003, 0.023)
LPE (20:4) - ESI(+)	Lognormal	-0.012	(-0.028, 0.004)	0.136	0.531	0.110	(-0.029, 0.002)
CE (20:3)	Lognormal	-0.008	(-0.020, 0.003)	0.140	0.537	0.101	(-0.020, 0.003)
PC (30:0)	Lognormal	-0.010	(-0.023, 0.003)	0.140	0.537	0.111	(-0.024, 0.003)
PC (p-40:1)/PC (o-40:2)	Lognormal	0.013	(-0.005, 0.031)	0.144	0.547	0.096	(-0.004, 0.032)
PE (p-40:4)/PE (o-40:5)	Lognormal	-0.012	(-0.028, 0.004)	0.144	0.547	0.076	(-0.027, 0.005)
AC (12:1)	Lognormal	-0.014	(-0.033, 0.005)	0.145	0.547	0.105	(-0.033, 0.004)
PC (35:1) - ESI(+)	Lognormal	0.005	(-0.002, 0.012)	0.147	0.551	0.093	(-0.002, 0.012)
SM (d36:0) - ESI(+)	Lognormal	0.010	(-0.004, 0.025)	0.148	0.553	0.098	(-0.004, 0.025)
LPC (20:4)	Lognormal	-0.008	(-0.018, 0.003)	0.150	0.554	0.086	(-0.018, 0.002)
PC (38:2)	Lognormal	-0.009	(-0.021, 0.003)	0.150	0.554	0.105	(-0.020, 0.004)
PE (38:2)	Lognormal	-0.013	(-0.030, 0.005)	0.155	0.564	0.086	(-0.030, 0.005)
LPC (o-16:0)	Lognormal	-0.009	(-0.022, 0.003)	0.155	0.564	0.079	(-0.021, 0.004)
SM (d34:0) - ESI(-)	Lognormal	-0.010	(-0.023, 0.004)	0.156	0.564	0.102	(-0.024, 0.003)
TG (60:12)	Lognormal	0.026	(-0.010, 0.061)	0.159	0.573	0.086	(-0.010, 0.062)
FA (14:1) (physeteric acid)	Lognormal	0.013	(-0.005, 0.031)	0.161	0.577	0.079	(-0.005, 0.030)
TG (54:5) B	Lognormal	0.007	(-0.003, 0.016)	0.163	0.580	0.083	(-0.002, 0.016)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Cholesterol	Lognormal	-0.004	(-0.010, 0.002)	0.163	0.580	0.083	(-0.010, 0.002)
PC (40:7) B - ESI(+)	Lognormal	0.006	(-0.003, 0.015)	0.165	0.581	0.076	(-0.003, 0.015)
PE (34:2) - ESI(-)	Lognormal	-0.018	(-0.045, 0.008)	0.168	0.582	0.088	(-0.046, 0.008)
PC (35:3)	Lognormal	-0.005	(-0.013, 0.002)	0.168	0.582	0.079	(-0.013, 0.002)
PC (40:5) B - ESI(+)	Lognormal	-0.009	(-0.022, 0.004)	0.170	0.582	0.085	(-0.022, 0.004)
LPC (22:4)	Lognormal	-0.017	(-0.040, 0.007)	0.170	0.582	0.074	(-0.038, 0.008)
LPC (16:0) - ESI(+)	Lognormal	-0.003	(-0.008, 0.001)	0.171	0.582	0.078	(-0.008, 0.002)
LPE (22:6)	Lognormal	-0.012	(-0.030, 0.005)	0.172	0.582	0.071	(-0.031, 0.005)
PC (42:10)	Lognormal	0.014	(-0.006, 0.034)	0.172	0.582	0.078	(-0.007, 0.034)
PC (p-32:0)/PC (o-32:1) - ESI(-)	Lognormal	-0.011	(-0.026, 0.005)	0.173	0.585	0.084	(-0.025, 0.004)
AC (10:0)	Lognormal	-0.019	(-0.047, 0.008)	0.174	0.586	0.083	(-0.046, 0.009)
TG (56:5) A	Lognormal	0.009	(-0.004, 0.021)	0.179	0.591	0.086	(-0.004, 0.022)
TG (46:2)	Lognormal	-0.021	(-0.051, 0.009)	0.179	0.591	0.083	(-0.049, 0.011)
Ceramide (d42:2) B - ESI(-)	Lognormal	-0.012	(-0.029, 0.005)	0.179	0.591	0.088	(-0.029, 0.005)
SM (d44:2)	Lognormal	0.010	(-0.004, 0.024)	0.180	0.591	0.072	(-0.005, 0.023)
DG (38:5)	Lognormal	0.008	(-0.004, 0.019)	0.180	0.591	0.075	(-0.003, 0.019)
FA (22:0) (behenic acid)	Lognormal	-0.008	(-0.021, 0.004)	0.182	0.593	0.073	(-0.021, 0.004)
TG (58:6)	Lognormal	0.007	(-0.003, 0.018)	0.182	0.593	0.087	(-0.003, 0.018)
SM (d32:2) - ESI(-)	Lognormal	-0.013	(-0.033, 0.006)	0.184	0.596	0.086	(-0.033, 0.006)
TG (46:4) A	Lognormal	-0.024	(-0.060, 0.011)	0.185	0.596	0.085	(-0.060, 0.012)
TG (56:5) C	Lognormal	0.007	(-0.003, 0.018)	0.186	0.599	0.085	(-0.003, 0.018)
PE (34:1)	Lognormal	-0.019	(-0.048, 0.009)	0.189	0.599	0.076	(-0.048, 0.010)
Ceramide (d34:1) - ESI(-)	Lognormal	-0.005	(-0.013, 0.003)	0.189	0.599	0.076	(-0.013, 0.002)
LPC (18:0) - ESI(+)	Lognormal	-0.006	(-0.014, 0.003)	0.189	0.599	0.067	(-0.014, 0.003)
TG (44:0)	Lognormal	-0.022	(-0.055, 0.011)	0.190	0.599	0.074	(-0.055, 0.010)
PC (34:3) A	Lognormal	-0.006	(-0.015, 0.003)	0.191	0.599	0.074	(-0.016, 0.003)
SM (d42:3) - ESI(-)	Lognormal	-0.005	(-0.014, 0.003)	0.191	0.599	0.075	(-0.013, 0.003)
CE (20:5)	Lognormal	0.015	(-0.007, 0.036)	0.192	0.599	0.078	(-0.007, 0.036)
TG (42:0)	Lognormal	-0.023	(-0.058, 0.012)	0.193	0.599	0.075	(-0.059, 0.012)
PC (p-38:5)/PC (o-38:6) B	Lognormal	-0.006	(-0.014, 0.003)	0.193	0.599	0.076	(-0.014, 0.003)
TG (49:2)	Lognormal	0.013	(-0.007, 0.032)	0.196	0.606	0.085	(-0.006, 0.032)
PC (36:3) B - ESI(+)	Lognormal	-0.005	(-0.013, 0.003)	0.198	0.609	0.080	(-0.013, 0.003)
PC (38:5) B - ESI(+)	Lognormal	0.007	(-0.004, 0.018)	0.200	0.610	0.071	(-0.003, 0.018)
PC (p-38:4)/PC (o-38:5) A	Lognormal	-0.004	(-0.011, 0.002)	0.201	0.610	0.072	(-0.011, 0.002)
CE (14:0)	Lognormal	-0.022	(-0.056, 0.012)	0.203	0.616	0.080	(-0.059, 0.010)
PC (39:6)	Lognormal	0.010	(-0.005, 0.025)	0.206	0.622	0.063	(-0.006, 0.025)
PC (37:2) - ESI(-)	Lognormal	-0.013	(-0.034, 0.007)	0.210	0.628	0.063	(-0.033, 0.007)
PC (32:0) - ESI(-)	Lognormal	-0.005	(-0.014, 0.003)	0.214	0.631	0.072	(-0.014, 0.003)
TG (54:1)	Lognormal	-0.013	(-0.034, 0.008)	0.218	0.636	0.069	(-0.034, 0.009)
SM (d42:2)	Lognormal	0.004	(-0.003, 0.012)	0.218	0.636	0.065	(-0.003, 0.012)
SM (d36:2) - ESI(-)	Lognormal	-0.007	(-0.019, 0.004)	0.219	0.636	0.066	(-0.020, 0.004)
PE (38:4)	Lognormal	-0.007	(-0.017, 0.004)	0.222	0.642	0.055	(-0.018, 0.004)
TG (60:6)	Lognormal	0.013	(-0.008, 0.033)	0.226	0.648	0.075	(-0.008, 0.034)
PC (p-32:0)/PC (o-32:1) - ESI(+)	Lognormal	-0.005	(-0.012, 0.003)	0.234	0.667	0.059	(-0.012, 0.003)
GlcCer (d14:1(4E)/20:0(2OH))	Lognormal	-0.011	(-0.030, 0.007)	0.238	0.671	0.065	(-0.030, 0.007)
GlcCer (d41:1)	Lognormal	-0.007	(-0.020, 0.005)	0.247	0.685	0.067	(-0.019, 0.006)
PC (38:3) - ESI(+)	Lognormal	-0.005	(-0.013, 0.003)	0.247	0.685	0.062	(-0.013, 0.004)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
TG (40:1)	Lognormal	-0.023	(-0.061, 0.016)	0.247	0.685	0.061	(-0.061, 0.018)
PC (35:2)	Lognormal	-0.007	(-0.018, 0.005)	0.248	0.685	0.064	(-0.018, 0.005)
Ceramide (d44:1)	Lognormal	-0.014	(-0.039, 0.010)	0.251	0.688	0.055	(-0.038, 0.010)
PC (38:5) A	Lognormal	0.003	(-0.002, 0.009)	0.254	0.689	0.063	(-0.002, 0.009)
SM (d32:0) - ESI(-)	Lognormal	-0.031	(-0.085, 0.022)	0.254	0.689	0.063	(-0.085, 0.023)
TG (56:9)	Lognormal	0.011	(-0.008, 0.029)	0.257	0.692	0.061	(-0.008, 0.029)
TG (48:3)	Lognormal	-0.012	(-0.034, 0.009)	0.258	0.692	0.062	(-0.034, 0.007)
TG (54:6) B	Lognormal	-0.019	(-0.053, 0.014)	0.262	0.697	0.068	(-0.055, 0.012)
TG (48:5)	Lognormal	-0.018	(-0.048, 0.013)	0.264	0.697	0.063	(-0.046, 0.014)
SM (d41:2) B - ESI(+)	Lognormal	-0.005	(-0.013, 0.003)	0.264	0.697	0.052	(-0.013, 0.003)
TG (42:3)	Lognormal	-0.021	(-0.058, 0.016)	0.276	0.726	0.061	(-0.055, 0.019)
PC 40:5e	Lognormal	-0.005	(-0.014, 0.004)	0.279	0.730	0.056	(-0.014, 0.004)
TG (58:2)	Lognormal	-0.027	(-0.075, 0.022)	0.287	0.737	0.065	(-0.077, 0.023)
PC (p-44:4)/PC (o-44:5) - ESI(-)	Lognormal	-0.007	(-0.021, 0.006)	0.288	0.737	0.053	(-0.021, 0.006)
LPC (16:1) - ESI(+)	Lognormal	-0.006	(-0.016, 0.005)	0.288	0.737	0.060	(-0.016, 0.005)
PC (p-42:3)/PC (o-42:4)	Lognormal	-0.006	(-0.019, 0.006)	0.294	0.739	0.053	(-0.019, 0.005)
SM (d41:3)	Lognormal	-0.005	(-0.013, 0.004)	0.295	0.739	0.059	(-0.014, 0.003)
PC (38:7)	Lognormal	0.008	(-0.007, 0.023)	0.296	0.740	0.052	(-0.006, 0.023)
TG (48:4) B	Lognormal	-0.019	(-0.054, 0.016)	0.298	0.740	0.057	(-0.054, 0.015)
DG (36:4) B	Lognormal	0.019	(-0.016, 0.053)	0.299	0.740	0.054	(-0.015, 0.054)
Ceramide (d42:0)	Lognormal	-0.008	(-0.022, 0.007)	0.301	0.740	0.048	(-0.022, 0.006)
PE (p-40:5)/PE (o-40:6)	Lognormal	-0.005	(-0.014, 0.004)	0.303	0.740	0.044	(-0.014, 0.004)
PG (34:0)/PG (17:0/17:0)	Lognormal	-0.008	(-0.024, 0.008)	0.303	0.740	0.055	(-0.025, 0.007)
FA (18:2) (linoleic acid)	Lognormal	0.004	(-0.004, 0.012)	0.306	0.743	0.055	(-0.003, 0.012)
FA (20:1) (eicosenoic acid)	Lognormal	0.005	(-0.005, 0.015)	0.309	0.743	0.053	(-0.005, 0.015)
TG (42:1)	Lognormal	-0.033	(-0.098, 0.031)	0.314	0.743	0.052	(-0.098, 0.032)
DG (36:2)	Lognormal	0.005	(-0.005, 0.016)	0.314	0.743	0.051	(-0.005, 0.016)
TG (46:1)	Lognormal	-0.016	(-0.048, 0.015)	0.319	0.743	0.054	(-0.048, 0.016)
GlcCer (d40:1) - ESI(-)	Lognormal	-0.006	(-0.016, 0.005)	0.320	0.743	0.055	(-0.017, 0.005)
TG (50:4)	Lognormal	-0.007	(-0.022, 0.007)	0.322	0.743	0.049	(-0.021, 0.007)
PC (28:0)	Lognormal	-0.019	(-0.057, 0.019)	0.323	0.743	0.057	(-0.059, 0.016)
GlcCer (d42:2) - ESI(-)	Lognormal	0.006	(-0.006, 0.018)	0.323	0.743	0.050	(-0.006, 0.018)
TG (44:1)	Lognormal	-0.021	(-0.062, 0.021)	0.328	0.747	0.050	(-0.064, 0.020)
PC (36:1) - ESI(-)	Lognormal	-0.004	(-0.012, 0.004)	0.332	0.747	0.047	(-0.012, 0.004)
FA (18:3) (linolenic acid)	Lognormal	0.006	(-0.006, 0.018)	0.333	0.747	0.050	(-0.006, 0.018)
AC (8:0)	Lognormal	-0.014	(-0.042, 0.014)	0.333	0.747	0.054	(-0.042, 0.016)
TG (54:7) A	Lognormal	-0.010	(-0.031, 0.011)	0.338	0.751	0.050	(-0.033, 0.011)
Ceramide (d42:2) A - ESI(-)	Lognormal	-0.005	(-0.014, 0.005)	0.338	0.751	0.047	(-0.014, 0.005)
PC (p-36:1)/PC (o-36:2) B	Lognormal	-0.007	(-0.022, 0.008)	0.346	0.756	0.048	(-0.023, 0.007)
PE (36:4) - ESI(-)	Lognormal	-0.012	(-0.038, 0.013)	0.350	0.760	0.048	(-0.040, 0.012)
TG (40:0)	Lognormal	-0.014	(-0.044, 0.016)	0.352	0.760	0.043	(-0.044, 0.017)
TG (50:1)	Lognormal	-0.008	(-0.025, 0.009)	0.352	0.760	0.052	(-0.025, 0.008)
TG (46:3) A	Lognormal	-0.019	(-0.059, 0.021)	0.353	0.760	0.053	(-0.060, 0.022)
PC (p-42:5)/PC (o-42:6) A	Lognormal	-0.006	(-0.018, 0.006)	0.354	0.760	0.050	(-0.017, 0.007)
SM (d41:1) - ESI(+)	Lognormal	-0.003	(-0.011, 0.004)	0.356	0.761	0.045	(-0.011, 0.004)
PE (34:2) - ESI(+)	Lognormal	-0.031	(-0.098, 0.035)	0.361	0.764	0.052	(-0.101, 0.034)
PC (38:4) B - ESI(+)	Lognormal	-0.004	(-0.014, 0.005)	0.362	0.764	0.048	(-0.014, 0.005)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
PC (o-32:0) - ESI(-)	Lognormal	-0.006	(-0.018, 0.007)	0.364	0.764	0.047	(-0.018, 0.006)
TG (46:4) B	Lognormal	-0.020	(-0.062, 0.023)	0.365	0.764	0.047	(-0.060, 0.023)
TG (64:3)	Lognormal	-0.010	(-0.032, 0.012)	0.366	0.764	0.053	(-0.033, 0.011)
TG (42:2)	Lognormal	-0.037	(-0.117, 0.043)	0.370	0.767	0.048	(-0.117, 0.045)
LPC (20:5)	Lognormal	0.012	(-0.014, 0.038)	0.372	0.767	0.047	(-0.013, 0.038)
PE (36:1) - ESI(+)	Lognormal	-0.010	(-0.030, 0.011)	0.372	0.767	0.047	(-0.032, 0.011)
SM (d40:2) A - ESI(+)	Lognormal	-0.005	(-0.016, 0.006)	0.375	0.768	0.051	(-0.017, 0.005)
TG (51:2)	Lognormal	0.006	(-0.008, 0.020)	0.378	0.768	0.049	(-0.007, 0.020)
PC (35:2) A	Lognormal	0.004	(-0.005, 0.013)	0.379	0.768	0.047	(-0.005, 0.012)
TG (53:3)	Lognormal	0.005	(-0.006, 0.016)	0.381	0.768	0.049	(-0.006, 0.016)
SM (d40:2) A - ESI(-)	Lognormal	-0.008	(-0.025, 0.009)	0.382	0.768	0.054	(-0.024, 0.009)
TG (50:5)	Lognormal	-0.009	(-0.029, 0.011)	0.386	0.771	0.044	(-0.030, 0.011)
CE (22:6)	Lognormal	0.005	(-0.006, 0.016)	0.387	0.772	0.043	(-0.006, 0.017)
GlcCer (d42:1) - ESI(-)	Lognormal	-0.005	(-0.015, 0.006)	0.388	0.772	0.047	(-0.016, 0.005)
PC (o-32:0) - ESI(+)	Lognormal	-0.003	(-0.011, 0.004)	0.391	0.777	0.046	(-0.011, 0.004)
PC (37:4) - ESI(-)	Lognormal	-0.006	(-0.019, 0.008)	0.396	0.781	0.043	(-0.019, 0.007)
PC (36:5) C	Lognormal	0.008	(-0.011, 0.027)	0.424	0.818	0.043	(-0.010, 0.027)
TG (52:2)	Lognormal	0.003	(-0.004, 0.010)	0.425	0.818	0.044	(-0.004, 0.010)
AC (14:1)	Lognormal	-0.009	(-0.030, 0.012)	0.426	0.819	0.041	(-0.029, 0.013)
SM (d39:2)	Lognormal	-0.003	(-0.012, 0.005)	0.431	0.822	0.040	(-0.011, 0.005)
PC (32:1) - ESI(-)	Lognormal	-0.007	(-0.023, 0.010)	0.435	0.828	0.049	(-0.024, 0.009)
FA (20:3) (homo-gamma-linolenic acid)	Lognormal	0.004	(-0.005, 0.012)	0.437	0.829	0.039	(-0.005, 0.013)
PC (40:4) - ESI(+)	Lognormal	-0.005	(-0.016, 0.007)	0.439	0.829	0.041	(-0.016, 0.008)
TG (53:2)	Lognormal	0.005	(-0.008, 0.018)	0.455	0.848	0.045	(-0.009, 0.018)
PC (35:4) - ESI(-)	Lognormal	-0.007	(-0.024, 0.011)	0.456	0.848	0.039	(-0.024, 0.010)
Ceramide (d34:0)	Lognormal	-0.005	(-0.017, 0.008)	0.458	0.848	0.036	(-0.017, 0.008)
TG (58:10)	Lognormal	0.007	(-0.011, 0.025)	0.458	0.848	0.041	(-0.011, 0.025)
CE (22:2)	Lognormal	0.013	(-0.022, 0.048)	0.459	0.848	0.041	(-0.022, 0.047)
PC (34:1)	Lognormal	0.001	(-0.002, 0.005)	0.465	0.849	0.041	(-0.002, 0.005)
TG (58:4)	Lognormal	0.008	(-0.014, 0.030)	0.478	0.856	0.043	(-0.014, 0.031)
TG (52:4)	Lognormal	-0.003	(-0.012, 0.006)	0.479	0.856	0.040	(-0.012, 0.006)
LPC (15:0)	Lognormal	-0.005	(-0.018, 0.009)	0.481	0.856	0.041	(-0.018, 0.009)
SM (d37:1)	Lognormal	-0.007	(-0.027, 0.013)	0.481	0.856	0.043	(-0.027, 0.013)
PC (37:3)	Lognormal	-0.005	(-0.018, 0.008)	0.486	0.856	0.042	(-0.018, 0.008)
Ceramide (d42:2) A - ESI(+)	Lognormal	0.003	(-0.005, 0.010)	0.487	0.856	0.038	(-0.005, 0.010)
TG (48:1)	Lognormal	-0.007	(-0.027, 0.013)	0.489	0.856	0.039	(-0.028, 0.013)
PC (33:0)	Lognormal	-0.007	(-0.025, 0.012)	0.489	0.856	0.038	(-0.025, 0.012)
TG (56:3)	Lognormal	0.007	(-0.012, 0.025)	0.489	0.856	0.041	(-0.012, 0.025)
SM (d36:3) - ESI(+)	Lognormal	-0.004	(-0.016, 0.008)	0.493	0.857	0.037	(-0.016, 0.007)
TG (56:7) A	Lognormal	0.013	(-0.025, 0.052)	0.497	0.862	0.044	(-0.024, 0.050)
SM (d43:1) - ESI(+)	Lognormal	-0.005	(-0.019, 0.009)	0.502	0.865	0.041	(-0.019, 0.010)
DG (36:4) A	Lognormal	-0.006	(-0.022, 0.011)	0.504	0.867	0.042	(-0.022, 0.011)
FA (20:4) (arachidonic acid)	Lognormal	-0.002	(-0.009, 0.005)	0.515	0.879	0.037	(-0.009, 0.005)
TG (62:1)	Lognormal	-0.009	(-0.037, 0.019)	0.520	0.883	0.040	(-0.039, 0.018)
TG (48:2)	Lognormal	-0.007	(-0.028, 0.014)	0.522	0.883	0.040	(-0.029, 0.014)
TG (54:3)	Lognormal	0.003	(-0.007, 0.013)	0.522	0.883	0.040	(-0.007, 0.013)
PC (p-42:4)/PC (o-42:5) - ESI(-)	Lognormal	-0.006	(-0.023, 0.012)	0.523	0.883	0.039	(-0.023, 0.012)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
PC (35:4) - ESI(+)	Lognormal	-0.004	(-0.015, 0.007)	0.525	0.883	0.040	(-0.014, 0.008)
TG (56:1)	Lognormal	-0.008	(-0.033, 0.017)	0.533	0.890	0.038	(-0.033, 0.017)
PC (42:5)	Lognormal	0.004	(-0.009, 0.018)	0.535	0.891	0.038	(-0.009, 0.018)
PC (33:1) - ESI(+)	Lognormal	0.003	(-0.006, 0.012)	0.537	0.891	0.040	(-0.007, 0.012)
DG (32:0)	Lognormal	0.005	(-0.011, 0.021)	0.539	0.891	0.040	(-0.010, 0.021)
TG (59:2)	Lognormal	-0.007	(-0.031, 0.016)	0.540	0.891	0.040	(-0.031, 0.017)
Ceramide (d40:0)	Lognormal	-0.008	(-0.034, 0.018)	0.542	0.891	0.034	(-0.036, 0.016)
LPC (20:1) - ESI(+)	Lognormal	-0.008	(-0.035, 0.018)	0.543	0.891	0.040	(-0.035, 0.020)
LPC (18:1) - ESI(+)	Lognormal	-0.003	(-0.013, 0.007)	0.545	0.891	0.038	(-0.012, 0.008)
FA (15:0) (pentadecylic acid)	Lognormal	-0.003	(-0.012, 0.006)	0.546	0.891	0.038	(-0.012, 0.005)
SM (d34:1) - ESI(+)	Lognormal	-0.001	(-0.006, 0.003)	0.546	0.891	0.042	(-0.006, 0.003)
Ceramide (d36:1) - ESI(-)	Lognormal	-0.006	(-0.025, 0.013)	0.548	0.891	0.038	(-0.025, 0.013)
PC (p-34:1)/PC (o-34:2) B	Lognormal	-0.006	(-0.026, 0.014)	0.551	0.891	0.039	(-0.026, 0.013)
TG (49:0)	Lognormal	-0.006	(-0.027, 0.014)	0.553	0.891	0.039	(-0.026, 0.015)
PC (32:0) - ESI(+)	Lognormal	0.002	(-0.004, 0.007)	0.554	0.891	0.036	(-0.003, 0.007)
PC (p-40:6)/PC (o-40:7) A	Lognormal	0.004	(-0.009, 0.016)	0.554	0.891	0.032	(-0.009, 0.015)
LPC (20:1) - ESI(-)	Lognormal	-0.005	(-0.020, 0.011)	0.555	0.891	0.040	(-0.020, 0.011)
TG (53:1)	Lognormal	-0.008	(-0.036, 0.019)	0.565	0.899	0.036	(-0.036, 0.019)
SM (d41:2) - ESI(-)	Lognormal	-0.004	(-0.017, 0.010)	0.571	0.901	0.036	(-0.017, 0.010)
PC (p-42:5)/PC (o-42:6)	Lognormal	-0.008	(-0.035, 0.019)	0.572	0.901	0.038	(-0.036, 0.019)
PC (38:5) A - ESI(-)	Lognormal	-0.003	(-0.012, 0.007)	0.572	0.901	0.041	(-0.011, 0.007)
FA (20:2) (eicosadienoic acid)	Lognormal	0.003	(-0.008, 0.014)	0.572	0.901	0.036	(-0.007, 0.015)
PC (35:2) B	Lognormal	-0.002	(-0.008, 0.004)	0.579	0.907	0.034	(-0.008, 0.005)
SM (d43:2) - ESI(+)	Lognormal	0.004	(-0.011, 0.020)	0.583	0.907	0.039	(-0.012, 0.019)
PC (38:4) C - ESI(+)	Lognormal	-0.002	(-0.007, 0.004)	0.586	0.909	0.038	(-0.007, 0.004)
TG (46:3) B	Lognormal	-0.010	(-0.045, 0.026)	0.601	0.915	0.036	(-0.046, 0.025)
AC (16:0)	Lognormal	-0.003	(-0.013, 0.007)	0.602	0.915	0.039	(-0.013, 0.007)
GlcCer (d40:1) - ESI(+)	Lognormal	-0.003	(-0.016, 0.009)	0.605	0.915	0.034	(-0.016, 0.009)
SM (d32:2) - ESI(+)	Lognormal	-0.003	(-0.014, 0.008)	0.606	0.915	0.034	(-0.014, 0.008)
PC (39:4)	Lognormal	0.003	(-0.008, 0.013)	0.607	0.915	0.035	(-0.008, 0.013)
Ceramide (d34:1) - ESI(+)	Lognormal	0.002	(-0.006, 0.010)	0.611	0.915	0.037	(-0.006, 0.011)
PE (p-36:5)/PE (o-36:6)	Lognormal	-0.014	(-0.068, 0.040)	0.613	0.915	0.034	(-0.064, 0.044)
TG (58:5)	Lognormal	-0.004	(-0.022, 0.013)	0.617	0.915	0.036	(-0.022, 0.014)
TG (51:5)	Lognormal	-0.005	(-0.023, 0.014)	0.619	0.915	0.041	(-0.022, 0.013)
FA (17:0) (margaric acid)	Lognormal	0.002	(-0.005, 0.008)	0.623	0.915	0.037	(-0.005, 0.008)
SM (d34:2) - ESI(+)	Lognormal	-0.001	(-0.007, 0.004)	0.623	0.915	0.034	(-0.007, 0.004)
PC (p-44:4)/PC (o-44:5) - ESI(+)	Lognormal	0.003	(-0.009, 0.014)	0.626	0.915	0.035	(-0.009, 0.014)
FA (22:6) (docosahexaenoic acid)	Lognormal	0.003	(-0.011, 0.018)	0.629	0.915	0.035	(-0.009, 0.018)
TG (58:3)	Lognormal	0.007	(-0.020, 0.034)	0.630	0.915	0.038	(-0.021, 0.034)
PC (36:5) B	Lognormal	0.005	(-0.016, 0.027)	0.630	0.915	0.039	(-0.017, 0.027)
TG (60:1)	Lognormal	-0.007	(-0.035, 0.021)	0.634	0.918	0.038	(-0.034, 0.023)
AC (18:1)	Lognormal	-0.003	(-0.015, 0.009)	0.639	0.920	0.034	(-0.014, 0.009)
CE (18:0)	Lognormal	0.005	(-0.016, 0.025)	0.644	0.922	0.036	(-0.015, 0.026)
TG (54:2)	Lognormal	0.003	(-0.011, 0.017)	0.647	0.924	0.036	(-0.010, 0.018)
TG (52:1)	Lognormal	-0.004	(-0.023, 0.014)	0.647	0.924	0.035	(-0.023, 0.015)
PC (p-38:6)/PC (o-38:7)	Lognormal	-0.003	(-0.017, 0.010)	0.655	0.927	0.034	(-0.016, 0.012)
TG (50:2)	Lognormal	0.002	(-0.008, 0.013)	0.663	0.932	0.032	(-0.008, 0.013)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
TG (57:1)	Lognormal	-0.004	(-0.023, 0.014)	0.664	0.932	0.036	(-0.024, 0.013)
LPC (17:1)	Lognormal	0.003	(-0.011, 0.017)	0.664	0.932	0.036	(-0.010, 0.018)
PC (p-44:5)/PC (o-44:6)	Lognormal	0.003	(-0.011, 0.017)	0.666	0.932	0.036	(-0.010, 0.018)
SM (d34:0) - ESI(+)	Lognormal	-0.002	(-0.009, 0.006)	0.666	0.932	0.036	(-0.009, 0.005)
PC (38:5) B - ESI(-)	Lognormal	0.004	(-0.013, 0.020)	0.668	0.932	0.038	(-0.012, 0.020)
LPC (p-18:0)/LPC (o-18:1)	Lognormal	-0.003	(-0.017, 0.011)	0.677	0.932	0.037	(-0.017, 0.011)
PC (37:4) - ESI(+)	Lognormal	0.003	(-0.010, 0.015)	0.679	0.932	0.037	(-0.011, 0.014)
TG (54:8)	Lognormal	0.005	(-0.020, 0.031)	0.681	0.932	0.037	(-0.022, 0.029)
PC (40:6) B	Lognormal	0.003	(-0.010, 0.015)	0.685	0.932	0.034	(-0.009, 0.016)
TG (53:4)	Lognormal	0.002	(-0.010, 0.015)	0.686	0.932	0.038	(-0.010, 0.014)
LPC (20:0)	Lognormal	-0.003	(-0.019, 0.013)	0.686	0.932	0.035	(-0.019, 0.014)
TG (58:1)	Lognormal	-0.005	(-0.031, 0.021)	0.690	0.932	0.035	(-0.029, 0.023)
PE (36:4) - ESI(+)	Lognormal	-0.004	(-0.025, 0.017)	0.691	0.932	0.034	(-0.025, 0.017)
PC (p-40:7)/PC (o-40:8)	Lognormal	-0.008	(-0.046, 0.031)	0.693	0.932	0.033	(-0.049, 0.029)
Ceramide (d36:1) - ESI(+)	Lognormal	0.002	(-0.009, 0.014)	0.695	0.933	0.036	(-0.008, 0.014)
TG (54:4)	Lognormal	0.002	(-0.009, 0.013)	0.695	0.933	0.036	(-0.009, 0.012)
PC (31:1)	Lognormal	-0.007	(-0.041, 0.028)	0.698	0.935	0.037	(-0.040, 0.029)
PE (38:6) - ESI(-)	Lognormal	-0.005	(-0.031, 0.021)	0.704	0.936	0.035	(-0.029, 0.022)
LPC (22:5) - ESI(+)	Lognormal	0.004	(-0.015, 0.023)	0.707	0.936	0.034	(-0.014, 0.023)
PC (38:4) A - ESI(+)	Lognormal	-0.002	(-0.011, 0.007)	0.708	0.936	0.038	(-0.011, 0.008)
TG (52:5)	Lognormal	0.002	(-0.010, 0.015)	0.708	0.936	0.038	(-0.011, 0.015)
PC (34:0) - ESI(+)	Lognormal	-0.001	(-0.007, 0.004)	0.708	0.936	0.030	(-0.006, 0.005)
TG (51:3)	Lognormal	0.002	(-0.010, 0.014)	0.714	0.936	0.034	(-0.010, 0.015)
TG (59:3)	Lognormal	0.004	(-0.018, 0.026)	0.717	0.936	0.035	(-0.018, 0.024)
Gal-Gal-Cer (d18:1/16:0)/Lactosylceramide (d18:1/16:0)	Lognormal	0.002	(-0.007, 0.011)	0.717	0.936	0.031	(-0.007, 0.011)
PC 40:6e	Lognormal	0.002	(-0.008, 0.011)	0.720	0.936	0.035	(-0.008, 0.011)
TG (52:6)	Lognormal	-0.003	(-0.022, 0.015)	0.726	0.936	0.033	(-0.021, 0.016)
TG (48:6)	Lognormal	0.004	(-0.019, 0.028)	0.729	0.936	0.037	(-0.018, 0.028)
DG (34:1)	Lognormal	-0.004	(-0.028, 0.020)	0.731	0.936	0.033	(-0.027, 0.020)
FA (14:0) (myristic acid)	Lognormal	0.001	(-0.007, 0.010)	0.732	0.936	0.036	(-0.007, 0.010)
PE (36:1) - ESI(-)	Lognormal	-0.005	(-0.031, 0.022)	0.733	0.936	0.036	(-0.030, 0.023)
PC (36:1) - ESI(+)	Lognormal	0.001	(-0.005, 0.007)	0.733	0.936	0.036	(-0.005, 0.007)
TAG (58:7)/TAG (18:1/18:1/22:5)	Lognormal	0.002	(-0.011, 0.015)	0.734	0.936	0.035	(-0.012, 0.014)
TG (50:3) B	Lognormal	-0.013	(-0.088, 0.062)	0.735	0.936	0.035	(-0.084, 0.070)
TG (56:10)	Lognormal	0.005	(-0.026, 0.036)	0.739	0.936	0.032	(-0.027, 0.037)
SM (d41:2) A - ESI(+)	Lognormal	0.002	(-0.008, 0.012)	0.741	0.936	0.033	(-0.009, 0.012)
LPC (22:5) - ESI(-)	Lognormal	-0.005	(-0.038, 0.027)	0.741	0.936	0.031	(-0.037, 0.026)
TG (54:9)	Lognormal	0.009	(-0.047, 0.066)	0.742	0.936	0.033	(-0.049, 0.064)
FA (20:3) (eicosatrienoic acid)	Lognormal	0.002	(-0.012, 0.017)	0.747	0.936	0.037	(-0.013, 0.016)
SM (d42:0) - ESI(-)	Lognormal	-0.002	(-0.014, 0.010)	0.749	0.936	0.031	(-0.013, 0.011)
SM (d42:3) - ESI(+)	Lognormal	0.001	(-0.005, 0.008)	0.753	0.936	0.029	(-0.005, 0.008)
CE (20:4)	Lognormal	-0.001	(-0.011, 0.008)	0.759	0.939	0.033	(-0.011, 0.007)
PC 38:7e	Lognormal	-0.002	(-0.019, 0.014)	0.776	0.947	0.035	(-0.020, 0.014)
Ceramide (d40:2)	Lognormal	0.006	(-0.034, 0.046)	0.781	0.949	0.037	(-0.033, 0.046)
TG (51:4)	Lognormal	-0.002	(-0.017, 0.013)	0.786	0.950	0.035	(-0.017, 0.013)
PC (p-40:4)/PC (o-40:5) - ESI(+)	Lognormal	-0.001	(-0.010, 0.008)	0.789	0.950	0.034	(-0.010, 0.008)
TG (57:2)	Lognormal	-0.002	(-0.018, 0.014)	0.789	0.950	0.033	(-0.018, 0.015)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
DG (34:3)	Lognormal	0.002	(-0.016, 0.021)	0.794	0.950	0.030	(-0.015, 0.022)
TG (55:1)	Lognormal	-0.003	(-0.024, 0.018)	0.795	0.950	0.034	(-0.024, 0.018)
TG (62:2)	Lognormal	-0.004	(-0.035, 0.027)	0.797	0.950	0.034	(-0.034, 0.029)
SM (d38:0)	Lognormal	-0.008	(-0.068, 0.052)	0.799	0.950	0.034	(-0.069, 0.053)
PC (36:6)	Lognormal	-0.002	(-0.021, 0.016)	0.801	0.950	0.031	(-0.022, 0.015)
TG (54:6) A	Lognormal	-0.002	(-0.018, 0.014)	0.814	0.950	0.033	(-0.018, 0.015)
CE (18:1)	Lognormal	-0.001	(-0.014, 0.011)	0.814	0.950	0.036	(-0.014, 0.011)
Ceramide (d34:2)	Lognormal	-0.001	(-0.012, 0.009)	0.817	0.950	0.034	(-0.012, 0.010)
SM (d40:0)	Lognormal	0.001	(-0.011, 0.014)	0.821	0.950	0.034	(-0.011, 0.014)
PC (36:4) C - ESI(+)	Lognormal	-0.001	(-0.006, 0.005)	0.824	0.950	0.034	(-0.006, 0.005)
TG (50:6)	Lognormal	0.003	(-0.024, 0.030)	0.826	0.950	0.032	(-0.022, 0.030)
PC (40:8) - ESI(+)	Lognormal	-0.001	(-0.010, 0.008)	0.831	0.950	0.030	(-0.010, 0.008)
DG (32:1)	Lognormal	-0.002	(-0.025, 0.020)	0.832	0.950	0.033	(-0.025, 0.021)
SM (d33:1) - ESI(+)	Lognormal	-0.001	(-0.011, 0.009)	0.832	0.950	0.033	(-0.010, 0.009)
TG (64:2)	Lognormal	-0.003	(-0.034, 0.028)	0.833	0.950	0.034	(-0.035, 0.027)
PC (16:0/9:0(CHO))	Lognormal	-0.002	(-0.023, 0.018)	0.834	0.950	0.028	(-0.024, 0.016)
TG (46:5)	Lognormal	0.005	(-0.039, 0.048)	0.835	0.950	0.035	(-0.038, 0.048)
SM (d38:2) - ESI(+)	Lognormal	-0.001	(-0.007, 0.006)	0.837	0.950	0.032	(-0.007, 0.006)
DG (36:5)	Lognormal	-0.002	(-0.023, 0.018)	0.839	0.950	0.031	(-0.022, 0.019)
DG (34:2)	Lognormal	0.001	(-0.011, 0.013)	0.843	0.953	0.028	(-0.010, 0.013)
TG (55:2)	Lognormal	0.002	(-0.016, 0.019)	0.844	0.953	0.027	(-0.016, 0.019)
SM (d36:0) - ESI(-)	Lognormal	0.003	(-0.025, 0.030)	0.849	0.956	0.035	(-0.026, 0.030)
CE (16:0)	Lognormal	0.003	(-0.024, 0.029)	0.850	0.957	0.033	(-0.024, 0.030)
PC (35:1) - ESI(-)	Lognormal	0.001	(-0.013, 0.015)	0.858	0.963	0.032	(-0.013, 0.015)
TG (60:2)	Lognormal	-0.004	(-0.044, 0.037)	0.860	0.963	0.033	(-0.047, 0.036)
FA (24:1) (nervonic acid)	Lognormal	0.001	(-0.009, 0.010)	0.865	0.963	0.030	(-0.009, 0.010)
PC (p-40:6)/PC (o-40:7) B	Lognormal	-0.001	(-0.017, 0.014)	0.869	0.963	0.031	(-0.017, 0.014)
PC (40:7) - ESI(-)	Lognormal	-0.002	(-0.020, 0.017)	0.870	0.963	0.033	(-0.019, 0.017)
TG (62:3)	Lognormal	-0.003	(-0.038, 0.032)	0.871	0.963	0.029	(-0.037, 0.033)
LPC (22:6)	Lognormal	0.001	(-0.013, 0.015)	0.872	0.963	0.030	(-0.013, 0.016)
GlcCer (d42:1) - ESI(+)	Lognormal	0.001	(-0.009, 0.010)	0.875	0.963	0.029	(-0.009, 0.010)
DG (36:3)	Lognormal	0.001	(-0.010, 0.012)	0.877	0.963	0.031	(-0.010, 0.011)
PC (42:6)	Lognormal	0.002	(-0.023, 0.027)	0.877	0.963	0.033	(-0.022, 0.028)
PC (p-36:5)/PC (o-36:6)	Lognormal	0.002	(-0.019, 0.022)	0.878	0.963	0.035	(-0.019, 0.021)
TG (56:4)	Lognormal	0.001	(-0.012, 0.014)	0.879	0.964	0.035	(-0.012, 0.014)
TG (52:3)	Lognormal	0.000	(-0.006, 0.006)	0.892	0.972	0.033	(-0.006, 0.007)
FA (12:0) (lauric acid)	Lognormal	-0.001	(-0.017, 0.015)	0.893	0.972	0.031	(-0.018, 0.015)
PC (p-38:5)/PC (o-38:6) A	Lognormal	-0.001	(-0.015, 0.013)	0.901	0.975	0.032	(-0.015, 0.013)
CE (16:1)	Lognormal	0.001	(-0.013, 0.015)	0.903	0.975	0.031	(-0.013, 0.015)
SM (d41:1) - ESI(-)	Lognormal	0.006	(-0.090, 0.102)	0.904	0.975	0.035	(-0.092, 0.098)
PC (32:1) - ESI(+)	Lognormal	-0.001	(-0.012, 0.011)	0.911	0.976	0.032	(-0.011, 0.010)
SM (d36:2) - ESI(+)	Lognormal	0.000	(-0.007, 0.006)	0.921	0.982	0.033	(-0.007, 0.006)
PC (40:6) A	Lognormal	-0.001	(-0.012, 0.011)	0.929	0.985	0.034	(-0.012, 0.011)
TG (60:3)	Lognormal	0.001	(-0.029, 0.032)	0.934	0.987	0.035	(-0.031, 0.030)
GlcCer (d34:1)	Lognormal	-0.001	(-0.022, 0.020)	0.936	0.987	0.033	(-0.021, 0.020)
TG (44:2)	Lognormal	-0.003	(-0.077, 0.071)	0.937	0.987	0.036	(-0.079, 0.068)
DG (36:1)	Lognormal	0.001	(-0.016, 0.017)	0.942	0.987	0.032	(-0.015, 0.017)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
SM (d32:0) - ESI(+)	Lognormal	0.001	(-0.015, 0.016)	0.942	0.987	0.031	(-0.014, 0.018)
PC (33:1) - ESI(-)	Lognormal	-0.001	(-0.021, 0.020)	0.942	0.987	0.035	(-0.022, 0.022)
TG (50:3) A	Lognormal	0.000	(-0.013, 0.014)	0.945	0.988	0.033	(-0.013, 0.015)
PE (38:6) - ESI(+)	Lognormal	0.001	(-0.028, 0.030)	0.949	0.990	0.033	(-0.030, 0.029)
PC (p-40:4)/PC (o-40:5) - ESI(-)	Lognormal	0.000	(-0.013, 0.014)	0.958	0.990	0.033	(-0.013, 0.014)
TG (49:1)	Lognormal	0.001	(-0.021, 0.022)	0.962	0.990	0.033	(-0.020, 0.022)
PC (38:6) - ESI(-)	Lognormal	0.000	(-0.012, 0.012)	0.965	0.990	0.034	(-0.011, 0.012)
TG (56:2)	Lognormal	0.000	(-0.022, 0.021)	0.967	0.990	0.032	(-0.021, 0.021)
FA (10:0) (capric acid)	Lognormal	0.000	(-0.024, 0.025)	0.969	0.990	0.029	(-0.022, 0.027)
PC (31:0)	Lognormal	0.000	(-0.013, 0.012)	0.970	0.990	0.033	(-0.013, 0.013)
PC (p-38:5)/PC (o-38:6)	Lognormal	-0.001	(-0.038, 0.036)	0.972	0.990	0.036	(-0.036, 0.034)
SM (d42:0) - ESI(+)	Lognormal	0.000	(-0.026, 0.025)	0.973	0.990	0.032	(-0.026, 0.025)
PC (36:4) B - ESI(+)	Lognormal	0.000	(-0.012, 0.013)	0.974	0.990	0.032	(-0.012, 0.013)
PC (40:5) A - ESI(-)	Lognormal	0.000	(-0.015, 0.015)	0.975	0.990	0.031	(-0.016, 0.015)
TG (49:3)	Lognormal	0.000	(-0.021, 0.021)	0.977	0.992	0.030	(-0.021, 0.022)
PC (p-42:5)/PC (o-42:6) B	Lognormal	0.000	(-0.014, 0.014)	0.980	0.992	0.035	(-0.014, 0.014)
TG (60:4)	Lognormal	0.000	(-0.030, 0.031)	0.980	0.992	0.033	(-0.030, 0.032)
TG (53:5)	Lognormal	0.000	(-0.015, 0.015)	0.986	0.994	0.033	(-0.016, 0.014)
TG (54:5) A	Lognormal	0.000	(-0.012, 0.012)	0.990	0.994	0.031	(-0.012, 0.012)
PC (p-42:4)/PC (o-42:5) - ESI(+)	Lognormal	0.000	(-0.011, 0.011)	0.992	0.994	0.031	(-0.011, 0.011)
SM (d36:1) - ESI(+)	Lognormal	0.000	(-0.006, 0.006)	0.994	0.995	0.033	(-0.007, 0.006)
Oxylipins (OL)							
Resolvin D1	Gamma	-0.528	(-0.846, -0.210)	0.002	0.134	6.635	(-0.797, -0.224)
12-Hydroxy-5,8,10,14,17-eicosapentaenoic acid	Gamma	0.454	(0.092, 0.819)	0.011	0.188	3.134	(0.169, 0.724)
11,12-Epoxyeicosa-5,8,14-trienoic acid	Gamma	0.317	(0.056, 0.578)	0.018	0.213	0.442	(0.067, 0.588)
Prostaglandin F2a	Gamma	-0.293	(-0.560, -0.026)	0.026	0.247	0.239	(-0.577, 0.001)
9,11,15-trihydroxy-5,13,12-prostatrienoic acid	Gamma	-0.576	(-1.135, -0.019)	0.031	0.268	3.858	(-0.932, -0.211)
5-Hydroxy-6,8,11,14,17-eicosapentaenoic acid	Gamma	0.245	(0.010, 0.481)	0.034	0.285	0.311	(0.040, 0.468)
8,9-Epoxyeicosa-5,11,14-trienoic acid	Gamma	-0.260	(-0.520, 0.001)	0.040	0.302	0.165	(-0.529, -0.002)
16(17)-epoxy-4,7,10,13,19-docosapentaenoic acid	Gamma	0.343	(-0.022, 0.709)	0.052	0.348	0.257	(0.012, 0.714)
9-Hydroxy-5,7,11,14,17-icosapentaenoic acid	Gamma	0.242	(-0.015, 0.500)	0.053	0.351	0.180	(-0.002, 0.490)
15-hydroxyeicosa-5,8,11,13,17-pentaenoic acid	Gamma	0.323	(-0.020, 0.669)	0.057	0.365	0.228	(-0.014, 0.645)
17,18-Epoxy-5,8,11,14-eicosatetraenoic acid	Gamma	-0.420	(-0.849, 0.007)	0.060	0.368	0.576	(-0.785, -0.075)
Leukotriene B4	Gamma	-0.193	(-0.411, 0.026)	0.081	0.422	0.127	(-0.389, 0.005)
17,18-dihydroxyeicosa-5,8,11,14-tetraenoic acid	Lognormal	0.209	(-0.029, 0.447)	0.086	0.430	0.132	(-0.032, 0.439)
15,16-dihydroxyoctadeca-9,12-dienoic acid	Lognormal	-0.157	(-0.335, 0.022)	0.087	0.430	0.106	(-0.327, 0.033)
11-Hydroxy-14,15-epoxyeicosatrienoic acid	Gamma	-0.402	(-0.902, 0.104)	0.099	0.461	0.248	(-0.824, 0.010)
Prostaglandin D2	Gamma	-0.407	(-0.902, 0.091)	0.105	0.467	0.309	(-0.792, -0.008)
13-ketooctadeca-9,11-dienoic acid	Lognormal	-0.199	(-0.446, 0.047)	0.115	0.486	0.109	(-0.439, 0.057)
4-hydroxydocosa-5,7,10,13,16,19-hexaenoic acid	Gamma	0.221	(-0.075, 0.518)	0.137	0.532	0.089	(-0.054, 0.531)
15(16)-epoxy-9,12-octadecadienoic acid	Gamma	-0.264	(-0.655, 0.129)	0.155	0.564	0.124	(-0.612, 0.056)
9,10-dihydroxyoctadec-12-enoic acid	Lognormal	-0.134	(-0.322, 0.054)	0.164	0.581	0.069	(-0.319, 0.057)
9-Hydroxylinoleic acid	Lognormal	-0.078	(-0.202, 0.045)	0.215	0.634	0.064	(-0.206, 0.039)
15-Deoxy-delta-12,14-Prostaglandin J2	Gamma	-0.146	(-0.408, 0.116)	0.296	0.740	0.048	(-0.416, 0.119)
5-ketoeicosa-6,8,11,14-tetraenoic acid	Gamma	-0.151	(-0.447, 0.146)	0.303	0.740	0.050	(-0.471, 0.158)
14(15)-epoxy-5,8,11,17-eicosatetraenoic acid	Gamma	0.280	(-0.334, 0.895)	0.308	0.743	0.090	(-0.208, 0.775)
17-hydroxy-4,7,10,13,15,19-docosahexaenoic acid	Gamma	0.118	(-0.119, 0.357)	0.309	0.743	0.038	(-0.109, 0.376)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
15-Keto-prostaglandin E2	Gamma	-0.211	(-0.644, 0.224)	0.317	0.743	0.067	(-0.578, 0.151)
12,13-dihydroxyoctadec-9-enoic acid	Lognormal	-0.090	(-0.268, 0.087)	0.321	0.743	0.046	(-0.270, 0.083)
Prostaglandin E3	Gamma	0.280	(-0.378, 0.944)	0.330	0.747	0.095	(-0.259, 0.853)
10-nitrolinoleic acid	Gamma	0.190	(-0.251, 0.635)	0.362	0.764	0.060	(-0.168, 0.589)
8,9-dihydroxyeicosa-5,11,14-trienoic acid	Gamma	0.102	(-0.118, 0.322)	0.364	0.764	0.042	(-0.120, 0.338)
Prostaglandin E1	Gamma	0.162	(-0.203, 0.529)	0.366	0.764	0.050	(-0.166, 0.482)
9,10-dihydroxyoctadeca-12,15-dienoic acid	Gamma	-0.090	(-0.293, 0.114)	0.380	0.768	0.031	(-0.326, 0.130)
15-ketoeicosa-5,8,11,13-tetraenoic acid	Gamma	0.146	(-0.212, 0.505)	0.419	0.815	0.049	(-0.145, 0.435)
Leukotriene B5	Gamma	-0.198	(-0.691, 0.295)	0.443	0.834	0.066	(-0.614, 0.227)
12,13-epoxy-9-octadecenoic acid	Lognormal	-0.108	(-0.392, 0.176)	0.457	0.848	0.042	(-0.368, 0.199)
6-Ketoprostaglandin F1 alpha	Gamma	0.143	(-0.257, 0.544)	0.468	0.853	0.048	(-0.209, 0.484)
9,12,13-trihydroxyoctadec-10-enoic acid	Lognormal	-0.045	(-0.172, 0.083)	0.491	0.856	0.035	(-0.180, 0.068)
5-Hydroxy-6,8,11,14-eicosatetraenoic acid	Lognormal	-0.058	(-0.244, 0.127)	0.538	0.891	0.034	(-0.243, 0.138)
8-hydroxyeicosa-5,9,11,14-tetraenoic acid	Gamma	0.071	(-0.163, 0.306)	0.550	0.891	0.032	(-0.167, 0.331)
14,15-dihydroxyeicosa-5,8,11,17-tetraenoic acid	Gamma	-0.091	(-0.413, 0.232)	0.557	0.893	0.037	(-0.396, 0.245)
20-Hydroxyarachidonic acid	Lognormal	-0.100	(-0.448, 0.247)	0.572	0.901	0.031	(-0.486, 0.237)
12,13-dihydroxyoctadeca-9,15-dienoic acid	Gamma	-0.128	(-0.587, 0.336)	0.573	0.901	0.047	(-0.457, 0.207)
10-nitrooleic acid	Lognormal	0.063	(-0.160, 0.286)	0.581	0.907	0.034	(-0.151, 0.286)
12(13)-epoxy-9,15-octadecadienoic acid	Gamma	-0.101	(-0.485, 0.283)	0.594	0.913	0.039	(-0.397, 0.241)
9-hydroxyoctadeca-10,12,15-trienoic acid	Gamma	-0.067	(-0.315, 0.181)	0.598	0.915	0.028	(-0.302, 0.168)
8,15-dihydroxyeicosa-5,9,11,13-tetraenoic acid	Gamma	-0.125	(-0.625, 0.383)	0.631	0.915	0.053	(-0.544, 0.337)
9,10-Epoxy stearic acid	Lognormal	-0.071	(-0.368, 0.225)	0.638	0.920	0.036	(-0.358, 0.245)
19,20-dihydroxydocosa-4,7,10,13,16-pentaenoic acid	Lognormal	0.035	(-0.123, 0.193)	0.663	0.932	0.033	(-0.126, 0.179)
5,6-dihydroxyeicosa-8,11,14-trienoic acid	Gamma	0.047	(-0.172, 0.265)	0.671	0.932	0.025	(-0.168, 0.262)
18-(3-ethylloxiran-2-yl)octadeca-4,7,10,13,16-pentaenoic acid	Gamma	0.074	(-0.293, 0.441)	0.673	0.932	0.034	(-0.238, 0.384)
6-trans-Leukotriene B4	Gamma	-0.102	(-0.621, 0.426)	0.678	0.932	0.044	(-0.566, 0.303)
14,15-dihydroxyeicosa-5,8,11-trienoic acid	Gamma	-0.028	(-0.164, 0.108)	0.689	0.932	0.015	(-0.169, 0.110)
11,12-Dihydroxyeicosa-5,8,14-trienoic acid	Gamma	-0.027	(-0.173, 0.120)	0.723	0.936	0.016	(-0.167, 0.122)
11-Hydroxy-arachidonic acid	Gamma	0.031	(-0.144, 0.205)	0.725	0.936	0.021	(-0.151, 0.219)
5,6,15-trihydroxyeicosa-7,9,11,13-tetraenoic acid	Gamma	-0.055	(-0.385, 0.277)	0.745	0.936	0.031	(-0.388, 0.235)
Prostaglandin E2	Gamma	0.080	(-0.433, 0.596)	0.750	0.936	0.041	(-0.293, 0.422)
9S,10R-dihydroxy-stearic acid	Lognormal	-0.041	(-0.305, 0.223)	0.761	0.939	0.031	(-0.298, 0.227)
Thromboxane B2	Lognormal	0.036	(-0.205, 0.277)	0.771	0.945	0.034	(-0.194, 0.279)
9(10)-epoxy-12Z-octadecenoic acid	Gamma	-0.027	(-0.235, 0.181)	0.797	0.950	0.020	(-0.199, 0.150)
9-nitrooleic acid	Gamma	0.032	(-0.270, 0.337)	0.828	0.950	0.031	(-0.288, 0.326)
9-ketooctadeca-10,12-dienoic acid	Gamma	-0.024	(-0.240, 0.192)	0.830	0.950	0.026	(-0.271, 0.217)
13-Hydroxyoctadecadienoic acid	Lognormal	-0.012	(-0.128, 0.104)	0.835	0.950	0.031	(-0.120, 0.109)
trans-12,13-epoxy-11-oxo-trans-9-octadecenoic acid	Gamma	0.019	(-0.167, 0.205)	0.840	0.950	0.022	(-0.165, 0.226)
5,15-dihydroxyeicosa-6,8,11,13-tetraenoic acid	Gamma	0.029	(-0.423, 0.482)	0.894	0.972	0.039	(-0.393, 0.433)
9-hydroxyeicosa-5,7,11,14-tetraenoic acid	Gamma	-0.006	(-0.226, 0.215)	0.960	0.990	0.025	(-0.249, 0.230)
13-hydroxyoctadeca-9,11,15-trienoic acid	Gamma	0.006	(-0.232, 0.243)	0.960	0.990	0.025	(-0.229, 0.233)
11(12)-epoxy-5,8,14,17- eicosatetraenoic acid	Gamma	-0.009	(-0.419, 0.407)	0.965	0.990	0.040	(-0.385, 0.408)
12-Hydroxy-5,8,10,14-eicosatetraenoic acid	Lognormal	-0.004	(-0.215, 0.206)	0.967	0.990	0.025	(-0.211, 0.217)
14-hydroxydocosa-4,7,10,12,16,19-hexaenoic acid	Lognormal	-0.006	(-0.343, 0.332)	0.974	0.990	0.022	(-0.347, 0.318)
15-hydroxyeicosa-5,8,11,13-tetraenoic acid	Lognormal	-0.002	(-0.153, 0.150)	0.983	0.993	0.029	(-0.161, 0.141)
9(10)-epoxy-12,15-octadecadienoic acid	Gamma	-0.003	(-0.502, 0.499)	0.989	0.994	0.037	(-0.387, 0.361)

Supplementary Table S2. Regression and Bayesian estimates comparing all ME/CFS vs. all controls.

Metabolite	Regression Model	ME/CFS vs. Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI

ME/CFS, myalgic encephalomyelitis/chronic fatigue syndrome; CI, confidence interval; FDR, false discovery rate adjusted p-value; HD,; highest density credible intervals. Regression models were adjusted for age, sex, race/ethnicity, geographic/clinical site, season of sampling, body mass index, and self-reported irritable bowel syndrome. In PM, BA, and CL panels, estimated coefficients are interpreted as the differences in the mean values of log-log transformation of metabolite levels between cases and controls. In OL panel for lognormal regression, estimated coefficients are interpreted as the mean differences of log transformation of metabolite levels between two groups; for Gamma regression, estimated coefficients are interpreted as the log of fold change between two groups. Estimations in **bold** are significant. Criteria for significance: 1) FDR adjusted p-value from the regression model < 0.15, 2) BayesFactor >3, and 3) 95% highest density credible intervals not covering 0.

Supplementary Table S3. ChemRICH enrichment analysis comparing all ME/CFS vs. all controls

Cluster name	Cluster size	p-values	Key compound	Altered	Increased	Decreased	Altered Ratio
plasmalogens	24	4.7E-10	PE (p-36:2)/PE (o-36:3) - ESI(+)	16	0	12	0.7
unsaturated phosphatidylcholines	90	0.000000072	PC (36:2)	26	0	19	0.3
sphingomyelins	49	0.000047	SM (d39:1) - ESI(-)	18	0	14	0.4
HEPE	5	0.0001	12-Hydroxy-5,8,10,14,17-eicosapentaenoic acid	4	2	0	0.8
unsaturated phospholipid ethers	42	0.00016	PC (p-34:2)/PC (o-34:3) - ESI(+)	17	0	12	0.4
unsaturated ceramides	21	0.00017	Ceramide (d42:1) - ESI (+)	9	0	6	0.4
saturated lysophospholipids	10	0.00075	LPC (14:0) - ESI(+)	5	0	5	0.5
carnitines	27	0.00089	2-Methylbutyryl-L-carnitine	8	0	3	0.3
exposome_food	14	0.0041	Caffeine	7	1	5	0.5
unsaturated lysophosphatidylcholines	20	0.0044	LPC (18:2) - ESI(-)	9	0	5	0.4
unsaturated lysophosphoethanolamines	6	0.0051	LPE (18:2) - ESI(+)	3	0	3	0.5
saturated TGs	8	0.0052	TG (53:0)	3	0	2	0.4
unsaturated long chain TGs	41	0.011	TG (56:6)	10	7	1	0.2
dicarboxylic acids	9	0.013	succinic acid	5	2	0	0.6
prostaglandins	9	0.031	Prostaglandin F2a	2	0	2	0.2
EpODE	7	0.035	11,12-Epoxyeicosa-5,8,14-trienoic acid	3	1	1	0.4
unsaturated phosphatidylethanolamines	13	0.063	PE (36:2)	1	0	1	0.08
indoles	8	0.11	Kynurenine	1	0	0	0.1
amino acids, basic	8	0.13	Ornithine	2	0	0	0.2
OH-FA 22_6_1	3	0.13	Resolvin D1	1	0	1	0.3
cholesterol esters	13	0.16	CE (18:2)	3	0	3	0.2
saturated lysophosphoethanolamines	4	0.25	LPE (18:0)	1	0	1	0.2
unsaturated glucosylceramides	12	0.26	GlcCeramide (d42:2) - ESI(+)	2	0	0	0.2
amino acids	24	0.36	2,6-Diaminopimelic acid	1	1	0	0.04
amino acids, branched-chain	3	0.49	Leucine	1	0	1	0.3
unsaturated FFA	15	0.57	FA (16:1) (palmitoleic acid)	2	1	0	0.1
DiHETE	8	0.57	17,18-dihydroxyeicosa-5,8,11,14-tetraenoic acid	2	0	0	0.2
sugar alcohols	7	0.58	Mannitol	1	0	0	0.1
drugs	85	0.58	Acetaminophen	10	5	0	0.1
adenosine	4	0.59	7-Methylguanosine	1	0	1	0.2
dipeptides	16	0.65	H-Pro-Hyp-OH	2	1	0	0.1
saturated FFA	18	0.7	Arachidic acid	1	1	0	0.06
saturated phosphatidylcholines	9	0.73	PC (34:0) - ESI(-)	1	0	0	0.1
diglycerides	14	0.76	DG (38:6)	1	0	0	0.07
amino acids, aromatic	7	1	Tyrosine	0	0	0	0
amino acids, cyclic	6	1	Histidine	0	0	0	0
amino alcohols	3	1	3-Amino-1-propanol	0	0	0	0
benzene derivatives	6	1	Tri-2-ethylhexyl trimellitate	0	0	0	0
DiHETrE	5	1	19,20-dihydroxydocosa-4,7,10,13,16-pentaenoic acid	0	0	0	0
DiHODE	3	1	15,16-dihydroxyoctadeca-9,12-dienoic acid	0	0	0	0
DiHOME	4	1	9S,10R-dihydroxy-stearic acid	0	0	0	0

Supplementary Table S3. ChemRICH enrichment analysis comparing all ME/CFS vs. all controls

Cluster name	Cluster size	p-values	Key compound	Altered	Increased	Decreased	Altered Ratio
EpETrE	7	1	15(16)-epoxy-9,12-octadecadienoic acid	0	0	0	0
ethanolamines	3	1	Heptadecasphing-4-enine	0	0	0	0
guanidines	3	1	Guanidine	0	0	0	0
HETE	7	1	8-hydroxyeicosa-5,9,11,14-tetraenoic acid	0	0	0	0
hexoses	10	1	Levoglucosan	0	0	0	0
histidine	4	1	Ergothioneine	0	0	0	0
HODE	3	1	9-Hydroxylinoleic acid	0	0	0	0
hydroxybutyrates	7	1	Threonic acid	0	0	0	0
imidazoles	3	1	Creatinine	0	0	0	0
lipids	3	1	1-Monostearin	0	0	0	0
monounsaturated long chain TGs	16	1	TG (54:1)	0	0	0	0
monounsaturated TGs	18	1	TG (46:2)	0	0	0	0
nitroFA	3	1	10-nitrooleic acid	0	0	0	0
oxo-ODE	5	1	5-ketoeicosa-6,8,11,14-tetraenoic acid	0	0	0	0
pyridines	3	1	3-Hydroxypyridine	0	0	0	0
saturated ceramides	4	1	Ceramide (d42:0)	0	0	0	0
saturated sphingomyelins	10	1	SM (d36:0) - ESI(-)	0	0	0	0
sugar acids	3	1	Gluconic acid	0	0	0	0
unsaturated TGs	27	1	TG (48:4) A	0	0	0	0
xanthines	3	1	3-Methylxanthine	0	0	0	0

ME/CFS, myalgic encephalomyelitis/chronic fatigue syndrome.

Supplementary Table S4. Compound-level ChemRICH enrichment analysis comparing all ME/CFS vs. all controls.

Compound name	Effect size	p-values	Edirection
Plasmalogens			
PE (p-36:2)/PE (o-36:3) - ESI(+)	-0.028	0.00035	down
PE (p-34:2)/PE (o-34:3)	-0.036	0.0028	down
PE (p-36:2)/PE (o-36:3) - ESI(-)	-0.028	0.0056	down
PE (p-36:4)/PE (o-36:5) - ESI(-)	-0.022	0.0098	down
PE (p-38:5)/PE (o-38:6) - ESI(-)	-0.020	0.014	down
PE (p-38:4)/PE (o-38:5)	-0.015	0.022	down
PE (p-36:4)/PE (o-36:5) - ESI(+)	-0.016	0.023	down
PE (p-36:1)/PE (o-36:2) - ESI(+)	-0.020	0.026	down
PE (p-36:1)/PE (o-36:2) - ESI(-)	-0.028	0.027	down
PE (p-38:5)/PE (o-38:6) - ESI(+)	-0.013	0.029	down
PC (o-34:0)	-0.013	0.047	down
PE (p-40:4)/PE (o-40:5) A	-0.022	0.049	down
PE (p-34:1)/PE (o-34:2) - ESI(+)	-0.014	0.061	down
PE (p-40:4)/PE (o-40:5) B	-0.012	0.092	down
PE (p-34:1)/PE (o-34:2) - ESI(-)	-0.014	0.096	down
LPC (p-16:0)/LPC (o-16:1)	-0.010	0.097	down
PE (p-38:6)/PE (o-38:7)	-0.015	0.11	no change
PE (p-38:3) or PE (o-38:4)	-0.021	0.12	no change
PE (p-40:4)/PE (o-40:5)	-0.011	0.21	no change
PE(p-40:5)/PE(o-40:6)	-0.004	0.38	no change
PC (o-32:0) - ESI(-)	-0.005	0.45	no change
PC (o-32:0) - ESI(+)	-0.003	0.46	no change
PE (p-36:5)/PE (o-36:6)	-0.013	0.63	no change
LPC (p-18:0)/LPC (o-18:1)	-0.003	0.71	no change
Unsaturated Phosphatidylcholines			
PC (36:2)	-0.007	0.00028	down
PC (36:4) A - ESI(+)	-0.018	0.00039	down
PC (36:4) A - ESI(-)	-0.019	0.0014	down
PC (32:2) - ESI(-)	-0.027	0.002	down
PC (34:2) - ESI(+)	-0.005	0.0028	down
PC 34:4e	-0.021	0.0038	down
PC (34:2) - ESI(-)	-0.009	0.0065	down
PC (34:4) - ESI(-)	-0.032	0.0084	down
PC (34:3)	-0.016	0.013	down
PC (33:2) - ESI(-)	-0.019	0.019	down
PC(32:2)	-0.017	0.019	down
PC (34:3) B	-0.011	0.019	down
PC (36:5) A	-0.040	0.02	down
PC (34:3) C	-0.015	0.022	down
PC (36:5) A	-0.020	0.026	down
PC (36:4) B - ESI(-)	-0.008	0.03	down
PC (38:4) A - ESI(-)	-0.010	0.03	down
PC (40:8) - ESI(-)	-0.015	0.04	down
PC (38:6) A - ESI(+)	-0.008	0.041	down
PC (34:4) - ESI(+)	-0.016	0.05	down
PC (36:3) A - ESI(+)	-0.007	0.053	down
PC (38:3) - ESI(-)	-0.011	0.054	down
PC (37:5)	0.016	0.058	up
PC (40:5) A - ESI(+)	0.007	0.084	up
PC (33:2) - ESI(+)	-0.008	0.085	down

Supplementary Table S4. Compound-level ChemRICH enrichment analysis comparing all ME/CFS vs. all controls.

Compound name	Effect size	p-values	Edirection
PC (36:3) B - ESI(-)	-0.008	0.085	down
PC (36:3) A - ESI(-)	-0.008	0.1	down
PC (38:6) B - ESI(+)	0.005	0.1	up
PC (40:6) B	0.008	0.1	up
PC (36:5) D	0.014	0.11	no change
PC (37:2) - ESI(+)	-0.007	0.11	no change
PC (35:1) - ESI(+)	0.005	0.12	no change
PC (37:6)	0.013	0.12	no change
PC (40:5) B - ESI(-)	-0.018	0.13	no change
PC (40:7) A - ESI(+)	-0.008	0.15	no change
PC (38:2)	-0.009	0.17	no change
PC (35:3)	-0.005	0.17	no change
PC (42:10)	0.014	0.17	no change
PC (39:6)	0.010	0.19	no change
PC (36:3) B - ESI(+)	-0.005	0.19	no change
PC (38:5) B - ESI(+)	0.007	0.19	no change
PC (40:4) - ESI(-)	-0.012	0.2	no change
PC (34:3) A	-0.006	0.2	no change
PC (40:7) B - ESI(+)	0.006	0.21	no change
PC (37:2) - ESI(-)	-0.013	0.22	no change
PC (38:5) A	0.004	0.22	no change
PC (40:5) B - ESI(+)	-0.008	0.22	no change
PC (35:2)	-0.006	0.26	no change
PC (38:3) - ESI(+)	-0.005	0.27	no change
PC (38:7)	0.008	0.31	no change
PC 40:5e	-0.004	0.33	no change
PC (35:2) A	0.004	0.4	no change
PC (36:1) - ESI(-)	-0.004	0.41	no change
PC (36:5) C	0.008	0.42	no change
PC (34:1)	0.001	0.45	no change
PC (37:4) - ESI(-)	-0.005	0.46	no change
PC (38:4) B - ESI(+)	-0.004	0.46	no change
PC (33:1) - ESI(+)	0.003	0.48	no change
PC (32:1) - ESI(-)	-0.006	0.49	no change
PC (37:3)	-0.004	0.52	no change
PC (35:4) - ESI(-)	-0.005	0.54	no change
PC (42:5)	0.004	0.54	no change
PC (40:4) - ESI(+)	-0.004	0.54	no change
PC (35:2) B	-0.002	0.56	no change
PC (39:4)	0.003	0.57	no change
PC (35:4) - ESI(+)	-0.003	0.6	no change
PC (36:5) B	0.005	0.64	no change
PC (37:4) - ESI(+)	0.003	0.64	no change
PC (38:5) B - ESI(-)	0.004	0.65	no change
PC (38:4) C - ESI(+)	-0.001	0.65	no change
PC (p-42:5)/PC (o-42:6)	-0.006	0.66	no change
PC 40:6e	0.002	0.67	no change
PC (40:6) B	0.003	0.69	no change
PC (36:1) - ESI(+)	0.001	0.7	no change
PC (38:5) A - ESI(-)	-0.002	0.71	no change
PC (38:4) A - ESI(+)	-0.002	0.74	no change

Supplementary Table S4. Compound-level ChemRICH enrichment analysis comparing all ME/CFS vs. all controls.

Compound name	Effect size	p-values	Edirection
PC (35:1) - ESI(-)	0.002	0.76	no change
PC (31:1)	-0.005	0.76	no change
PC (36:6)	-0.003	0.77	no change
PC 38:7e	-0.002	0.78	no change
PC (42:6)	0.003	0.83	no change
PC (40:7) - ESI(-)	-0.002	0.86	no change
PC (40:8) - ESI(+)	-0.001	0.88	no change
PC (36:4) C - ESI(+)	0.000	0.89	no change
PC (40:5) A - ESI(-)	0.001	0.91	no change
PC (36:4) B - ESI(+)	0.001	0.93	no change
PC (32:1) - ESI(+)	0.000	0.95	no change
PC (38:6) - ESI(-)	0.000	0.98	no change
PC (33:1) - ESI(-)	0.000	0.99	no change
PC (40:6) A	0.000	1	no change
Sphingomyelins			
SM (d39:1) - ESI(-)	-0.017	0.0038	down
SM (d40:1) - ESI(-)	-0.012	0.0053	down
SM (d32:1) - ESI(-)	-0.015	0.0065	down
SM (d40:3)	-0.025	0.008	down
SM (d33:1) - ESI(-)	-0.014	0.016	down
SM (d43:1) - ESI(-)	-0.033	0.017	down
SM (d36:3) - ESI(-)	-0.019	0.018	down
SM (d40:2) B - ESI(-)	-0.011	0.019	down
SM (d42:1) - ESI(-)	-0.009	0.024	down
SM (d34:2) - ESI(-)	-0.008	0.026	down
SM (d30:1) - ESI(-)	-0.029	0.029	down
SM (d34:1) - ESI(-)	-0.007	0.037	down
SM (d40:1) - ESI(+)	-0.006	0.046	down
SM (d40:2) B - ESI(+)	-0.006	0.048	down
SM (d38:1)	-0.006	0.054	down
SM (d38:2) - ESI(-)	-0.011	0.055	down
SM (d39:1) - ESI(+)	-0.008	0.082	down
SM (d36:1) - ESI(-)	-0.007	0.091	down
SM (d42:1) - ESI(+)	-0.006	0.1	down
SM (d30:1) - ESI(+)	-0.016	0.11	no change
SM (d32:1) - ESI(-)	-0.008	0.13	no change
SM (d43:2) - ESI(-)	-0.017	0.13	no change
SM (d32:2) - ESI(-)	-0.013	0.18	no change
SM (d44:2)	0.009	0.21	no change
SM (d42:3) - ESI(-)	-0.005	0.22	no change
SM (d42:2)	0.004	0.23	no change
SM (d41:2) B - ESI(+)	-0.005	0.26	no change
SM (d36:2) - ESI(-)	-0.006	0.3	no change
SM (d41:1) - ESI(+)	-0.004	0.34	no change
SM (d40:2) A - ESI(-)	-0.008	0.35	no change
SM (d40:2) A - ESI(+)	-0.005	0.35	no change
SM (d41:3)	-0.004	0.37	no change
SM (d39:2)	-0.003	0.44	no change
SM (d37:1)	-0.007	0.5	no change
SM (d36:3) - ESI(+)	-0.004	0.53	no change
D-erythro-Sphingosine-1-phosphate	-0.007	0.54	no change

Supplementary Table S4. Compound-level ChemRICH enrichment analysis comparing all ME/CFS vs. all controls.

Compound name	Effect size	p-values	Edirection
SM (d43:1) - ESI(+)	-0.004	0.54	no change
SM (d43:2) - ESI(+)	0.005	0.56	no change
SM (d34:1) - ESI(-)	-0.001	0.58	no change
SM (d41:2) - ESI(-)	-0.004	0.59	no change
SM (d32:2) - ESI(+)	-0.003	0.64	no change
SM (d34:2) - ESI(-)	-0.001	0.65	no change
SM (d41:2) A - ESI(+)	0.002	0.72	no change
SM (d42:3) - ESI(+)	0.001	0.74	no change
SM (d38:2) - ESI(+)	-0.001	0.85	no change
SM (d41:1) - ESI(-)	0.007	0.88	no change
SM (d33:1) - ESI(+)	-0.001	0.89	no change
SM (d36:2) - ESI(-)	0.000	0.96	no change
SM (d36:1) - ESI(-)	0.000	0.99	no change
HEPE			
12-Hydroxy-5,8,10,14,17-eicosapentaenoic acid	0.440	0.015	up
5-Hydroxy-6,8,11,14,17-eicosapentaenoic acid	0.242	0.035	up
15-hydroxyeicosa-5,8,11,13,17-pentaenoic acid	0.321	0.058	up
9-Hydroxy-5,7,11,14,17-icosapentaenoic acid	0.222	0.069	up
4-hydroxydocosa-5,7,10,13,16,19-hexaenoic acid	0.213	0.16	no change
Unsaturated Phospholipid Ethers			
PC (p-34:2)/PC (o-34:3) - ESI(+)	-0.018	0.000084	down
PC (p-34:1)/PC (o-34:2)	-0.021	0.00015	down
PC (p-34:2)/PC (o-34:3) - ESI(-)	-0.020	0.00069	down
PC (p-36:1)/PC (o-36:2)	-0.054	0.00075	down
PC (p-36:4)/PC (o-36:5) - ESI(-)	-0.020	0.0017	down
PC (p-34:1)/PC (o-34:2) A	-0.026	0.0024	down
PC (p-36:3)/PC (o-36:4) - ESI(-)	-0.015	0.0081	down
PC(p-36:2)/PC(o-36:3)	-0.016	0.013	down
PC (p-38:3) or PC (o-38:4)	-0.015	0.014	down
PC (p-38:4) or PC (o-38:5) A	-0.011	0.019	down
PC(p-36:4)/PC(o-36:5)	-0.009	0.031	down
PC (p-36:3)/PC (o-36:4) - ESI(+)	-0.009	0.031	down
PC (p-38:4)/PC (o-38:5) B	-0.010	0.056	down
PC (p-32:1)/PC (o-32:2)	-0.009	0.06	down
PC (p-38:3)/PC (o-38:4) A - ESI(+)	-0.009	0.061	down
PC (p-38:3)/PC (o-38:4) B - ESI(+)	-0.010	0.069	down
PC (p-38:4)/PC (o-38:5) B	-0.016	0.082	down
PC (p-40:1)/PC (o-40:2)	0.014	0.13	no change
PC (p-40:3)/PC (o-40:4)	-0.012	0.16	no change
PC (p-38:4)/PC (o-38:5) A	-0.004	0.22	no change
PC (p-38:5)/PC (o-38:6) B	-0.005	0.22	no change
PC (p-32:0)/PC (o-32:1) - ESI(-)	-0.010	0.22	no change
PC (p-32:0)/PC (o-32:1) - ESI(+)	-0.004	0.26	no change
PC (p-44:4)/PC (o-44:5) - ESI(-)	-0.007	0.33	no change
PC (p-42:3)/PC (o-42:4)	-0.006	0.34	no change
PC (p-36:1)/PC (o-36:2) B	-0.007	0.38	no change
PC (p-42:5)/PC (o-42:6) A	-0.005	0.39	no change
PC (p-42:4)/PC (o-42:5) - ESI(-)	-0.005	0.57	no change
PC (p-40:6)/PC (o-40:7) A	0.003	0.58	no change
PC (p-34:1)/PC (o-34:2) B	-0.005	0.6	no change
PC (p-44:4)/PC (o-44:5) - ESI(+)	0.003	0.61	no change

Supplementary Table S4. Compound-level ChemRICH enrichment analysis comparing all ME/CFS vs. all controls.

Compound name	Effect size	p-values	Edirection
PC (p-38:6)/PC (o-38:7)	-0.003	0.65	no change
PC (p-44:5)/PC (o-44:6)	0.003	0.67	no change
PC (p-40:7)/PC (o-40:8)	-0.008	0.68	no change
PC (p-40:4)/PC (o-40:5) - ESI(+)	-0.001	0.87	no change
PC (p-40:4)/PC (o-40:5) - ESI(-)	0.001	0.87	no change
PC (p-36:5)/PC (o-36:6)	0.001	0.89	no change
PC (p-40:6)/PC (o-40:7) B	-0.001	0.89	no change
PC (p-38:5)/PC (o-38:6) A	-0.001	0.91	no change
PC (p-38:5)/PC (o-38:6)	-0.001	0.94	no change
PC (p-42:4)/PC (o-42:5) - ESI(+)	0.000	0.96	no change
PC (p-42:5)/PC (o-42:6) B	0.000	0.96	no change
Unsaturated Ceramides			
Ceramide (d42:1) - ESI (+)	-0.009	0.0056	down
Ceramide (d41:1) - ESI(-)	-0.014	0.01	down
Ceramide (d42:2) B - ESI (+)	-0.011	0.011	down
Ceramide (d42:1) - ESI(-)	-0.011	0.011	down
Ceramide (d40:1)	-0.010	0.014	down
Ceramide (d39:1)	-0.020	0.018	down
Ceramide (d43:1)	-0.032	0.078	down
Ceramide (d41:1) - ESI (+)	-0.008	0.089	down
Ceramide (d38:1) - ESI(+)	-0.008	0.096	down
Ceramide (d33:1)	-0.010	0.12	no change
Ceramide (d38:1) - ESI(-)	-0.010	0.12	no change
Ceramide (d32:1)	-0.011	0.13	no change
Ceramide (d42:2) B - ESI(-)	-0.011	0.2	no change
Ceramide (d34:1) - ESI(-)	-0.005	0.24	no change
Ceramide (d44:1)	-0.014	0.26	no change
Ceramide (d42:2) A - ESI(-)	-0.004	0.39	no change
Ceramide (d42:2) A - ESI (+)	0.003	0.49	no change
Ceramide (d34:1) - ESI(+)	0.002	0.59	no change
Ceramide (d36:1) - ESI(-)	-0.005	0.62	no change
Ceramide (d36:1) - ESI(+)	0.002	0.67	no change
Ceramide (d34:2)	-0.001	0.9	no change
Saturated Lysophospholipids			
LPC (14:0) - ESI(+)	-0.021	0.0081	down
LPC (18:0) A - ESI(-)	-0.018	0.014	down
LPC (16:0) - ESI(-)	-0.010	0.017	down
LPC (18:0) B - ESI(-)	-0.012	0.019	down
LPC (14:0) - ESI(-)	-0.026	0.046	down
LPC (16:0) - ESI(+)	-0.003	0.19	no change
LPC (o-16:0)	-0.008	0.2	no change
LPC (18:0) - ESI(+)	-0.006	0.2	no change
LPC (15:0)	-0.004	0.55	no change
LPC (20:0)	-0.004	0.65	no change
Carnitines			
2-Methylbutyryl-L-carnitine	-0.035	0.0023	down
3-Methylglutaryl-carnitine	-0.033	0.018	down
AC (10:1)	-0.020	0.042	down
Octanoylcarnitine	-0.017	0.07	down
AC (14:2)	-0.020	0.085	down
3-Dehydrocarnitine	-0.013	0.089	down

Supplementary Table S4. Compound-level ChemRICH enrichment analysis comparing all ME/CFS vs. all controls.

Compound name	Effect size	p-values	Edirection
AC (18:0)	-0.010	0.092	down
Lauroyl-L-carnitine	-0.033	0.092	down
AC (18:2)	-0.012	0.1	down
(R)-Butyrylcarnitine	-0.017	0.12	no change
AC (12:0)	-0.016	0.12	no change
AC (12:1)	-0.015	0.13	no change
AC (10:0)	-0.020	0.16	no change
Linoleoylcarnitine	-0.024	0.16	no change
Hexanoyl-L-carnitine	-0.011	0.28	no change
AC (8:0)	-0.014	0.32	no change
Propionylcarnitine	-0.004	0.32	no change
Oleoyl-L-carnitine	-0.017	0.35	no change
(3-Carboxypropyl)trimethylammonium cation	-0.005	0.37	no change
AC (14:1)	-0.010	0.38	no change
AC (16:0)	-0.003	0.58	no change
AC (18:1)	-0.003	0.58	no change
3-Hydroxyoleylcarnitine	0.018	0.63	no change
3-Hydroxybutyrylcarnitine	-0.006	0.66	no change
(2R)-3-Hydroxyisovaleroylcarnitine	-0.004	0.68	no change
Acetyl-DL-carnitine	0.002	0.82	no change
Decanoyl-L-carnitine	-0.003	0.85	no change
Food Exposome			
Caffeine	-0.084	0.0031	down
Choline	-0.009	0.0035	down
Theobromine	-0.064	0.0059	down
Piperine	-0.067	0.012	down
Trigonelline	-0.044	0.02	down
4,5,7-Trihydroxyisoflavone	0.083	0.047	up
Betaine	-0.006	0.075	down
Stachydrine	-0.025	0.17	no change
Coniferylaldehyde	0.008	0.51	no change
Theanine;	0.009	0.58	no change
Methylgallate	0.018	0.66	no change
6-Hydroxyflavone	0.008	0.68	no change
Betaine aldehyde cation	0.008	0.75	no change
Scopoletin	-0.012	0.76	no change
Unsaturated Lysophosphatidylcholines			
LPC (18:2) - ESI(-)	-0.019	0.004	down
LPC (18:3)	-0.025	0.006	down
LPC (18:2) - ESI(+)	-0.014	0.0067	down
LPC (20:3) - ESI(-)	-0.023	0.017	down
LPC (20:3) - ESI(+)	-0.012	0.045	down
LPC (16:1) - ESI(-)	-0.016	0.057	down
LPC (20:2) - ESI(-)	-0.027	0.077	down
LPC (20:2) - ESI(+)	-0.012	0.081	down
LPC (18:1) - ESI(-)	-0.010	0.082	down
LPC (20:4)	-0.007	0.19	no change
LPC (22:4)	-0.015	0.23	no change
LPC (16:1) - ESI(+)	-0.005	0.33	no change
LPC (20:5)	0.012	0.36	no change
LPC (20:1) - ESI(+)	-0.005	0.53	no change

Supplementary Table S4. Compound-level ChemRICH enrichment analysis comparing all ME/CFS vs. all controls.

Compound name	Effect size	p-values	Edirection
LPC (20:1) - ESI(-)	-0.008	0.55	no change
LPC (18:1) - ESI(+)	-0.003	0.55	no change
LPC (17:1)	0.004	0.61	no change
LPC (22:5) - ESI(+)	0.005	0.63	no change
LPC (22:5) - ESI(-)	-0.004	0.8	no change
LPC (22:6)	0.001	0.88	no change
Unsaturated Lysophosphoethanolamines			
LPE (18:2) - ESI(+)	-0.022	0.01	down
LPE (18:2) - ESI(-)	-0.027	0.011	down
LPE (20:4) - ESI(-)	-0.022	0.011	down
LPE (22:6)	-0.012	0.17	no change
LPE (20:4) - ESI(+)	-0.011	0.17	no change
1-Oleoyl-sn-glycero-3-phosphoethanolamine	-0.015	0.38	no change
Saturated Triglycerides			
TG (53:0)	-0.018	0.018	down
TG (50:0)	-0.024	0.021	down
TG (48:0)	-0.018	0.08	down
TG (46:0)	-0.027	0.11	no change
TG (42:0)	-0.022	0.2	no change
TG (44:0)	-0.021	0.21	no change
TG (40:0)	-0.014	0.37	no change
TG (49:0)	-0.005	0.6	no change
Unsaturated Long-chain Triglycerides			
TG (56:6)	0.010	0.01	up
TG (55:6)	0.021	0.012	up
TG (58:8)	0.019	0.032	up
TG (62:4)	-0.029	0.034	down
TG (56:7) B	0.018	0.034	up
TG (54:7) B	0.017	0.035	up
TG (58:9)	0.017	0.042	up
TG (54:6) C	0.011	0.043	up
TG (60:11)	0.025	0.072	up
TG (56:8) B	0.017	0.074	up
TG (56:5) B	0.009	0.12	no change
TG (56:8) A	0.010	0.13	no change
TG (54:5) B	0.007	0.14	no change
TG (56:5) A	0.009	0.17	no change
TG (58:6)	0.007	0.17	no change
TG (56:5) C	0.007	0.18	no change
TG (60:12)	0.025	0.18	no change
TG (60:6)	0.013	0.22	no change
TG (54:6) B	-0.021	0.24	no change
TG (56:9)	0.011	0.26	no change
TG (54:7) A	-0.010	0.33	no change
TG (64:3)	-0.010	0.37	no change
TG (58:10)	0.006	0.48	no change
TG (58:4)	0.008	0.48	no change
TG (56:7) A	0.014	0.49	no change
TG (56:3)	0.006	0.5	no change
TG (54:3)	0.003	0.52	no change
TG (58:5)	-0.005	0.61	no change

Supplementary Table S4. Compound-level ChemRICH enrichment analysis comparing all ME/CFS vs. all controls.

Compound name	Effect size	p-values	Edirection
TG (58:3)	0.006	0.64	no change
TG (54:8)	0.006	0.67	no change
TG (54:4)	0.002	0.71	no change
TG (59:3)	0.004	0.71	no change
TG (58:7)/TG (18:1/18:1/22:5)	0.002	0.72	no change
TG (56:10)	0.005	0.74	no change
TG (54:9)	0.009	0.75	no change
TG (54:6) A	-0.002	0.8	no change
TG (62:3)	-0.003	0.88	no change
TG (56:4)	0.001	0.91	no change
TG (60:3)	0.001	0.93	no change
TG (54:5) A	0.000	0.97	no change
TG (60:4)	0.000	0.99	no change
Dicarboxylic Acids			
succinic acid	0.022	0.007	up
alpha ketoglutarate	0.016	0.048	up
maleic acid	0.026	0.065	up
aminomalonnate	0.026	0.067	up
glutaric acid	0.017	0.088	up
malic acid	0.009	0.38	no change
fumaric acid	-0.003	0.74	no change
adipic acid	-0.002	0.79	no change
oxalic acid	-0.003	0.91	no change
Prostaglandins			
Prostaglandin F2a	-0.293	0.025	down
9,11,15-trihydroxy-5,13,12-prostatrienoic acid	-0.572	0.042	down
15-Deoxy-delta-12,14-Prostaglandin J2	-0.125	0.39	no change
Prostaglandin D2	-0.395	0.13	no change
15-Keto-prostaglandin E2	-0.156	0.45	no change
Prostaglandin E1	0.161	0.37	no change
Prostaglandin E2	0.066	0.82	no change
Prostaglandin E3	0.270	0.37	no change
6-Ketoprostaglandin F1 alpha	0.169	0.4	no change
EpODE			
11,12-Epoxyeicosa-5,8,14-trienoic acid	0.304	0.021	up
8,9-Epoxyeicosa-5,11,14-trienoic acid	-0.259	0.04	down
17,18-Epoxy-5,8,11,14-eicosatetraenoic acid	-0.424	0.055	down
11-Hydroxy-14,15-epoxyeicosatrienoic acid	-0.385	0.11	no change
14(15)-epoxy-5,8,11,17-eicosatetraenoic acid	0.278	0.31	no change
Thromboxane B2	0.069	0.75	no change
11(12)-epoxy-5,8,14,17- eicosatetraenoic acid	0.006	0.98	no change

ME/CFS, myalgic encephalomyelitis/chronic fatigue syndrome. Analytes in bold have p-values < 0.05.

Supplementary Table S5. ChemRICH enrichment analysis comparing female ME/CFS vs. female controls

Cluster name	Cluster size	p-values	Key compound	Altered	Increased	Decreased	Altered Ratio
plasmalogens	24	4.7E-10	PE (p-36:2)/PE (o-36:3) - ESI(+)	16	0	12	0.7
unsaturated phosphatidylcholines	90	0.000000072	PC (36:2)	26	0	19	0.3
HEPE	5	0.00000054	5-Hydroxy-6,8,11,14,17-eicosapentaenoic acid	5	4	0	1
sphingomyelins	49	0.000047	SM (d39:1) - ESI(-)	18	0	14	0.4
unsaturated phospholipid ethers	42	0.00016	PC (p-34:2)/PC (o-34:3) - ESI(+)	17	0	12	0.4
unsaturated ceramides	21	0.00017	Ceramide (d42:1) - ESI(+)	9	0	6	0.4
saturated lysophospholipids	10	0.00075	LPC (14:0) - ESI(+)	5	0	5	0.5
carnitines	27	0.00089	2-Methylbutyryl-L-carnitine	8	0	3	0.3
exposome food	14	0.0041	Caffeine	7	1	5	0.5
unsaturated lysophosphatidylcholines	20	0.0044	LPC (18:2) - ESI(-)	9	0	5	0.4
unsaturated lysophosphoethanolamines	6	0.0051	LPE (18:2) - ESI(+)	3	0	3	0.5
saturated TGs	8	0.0052	TG (53:0)	3	0	2	0.4
unsaturated long chain TGs	41	0.011	TG (56:6)	10	7	1	0.2
dicarboxylic acids	9	0.013	Succinic acid	5	2	0	0.6
EpODE	7	0.017	17,18-Epoxy-5,8,11,14-eicosatetraenoic acid	4	0	0	0.6
prostaglandins	9	0.031	Prostaglandin F2a	2	0	2	0.2
unsaturated phosphatidylethanolamines	13	0.063	PE (36:2)	1	0	1	0.08
indoles	8	0.11	Kynurenine	1	0	0	0.1
amino acids, basic	8	0.13	Ornithine	2	0	0	0.2
DiHOME	4	0.14	9,10-dihydroxyoctadec-12-enoic acid	1	0	0	0.2
DiHODE	3	0.16	15,16-dihydroxyoctadeca-9,12-dienoic acid	1	0	1	0.3
cholesterol esters	13	0.16	CE (18:2)	3	0	3	0.2
saturated lysophosphoethanolamines	4	0.25	LPE (18:0)	1	0	1	0.2
unsaturated glucosylceramides	12	0.26	GlcCer (d42:2) - ESI(+)	2	0	0	0.2
amino acids	24	0.36	2,6-Diaminopimelic acid	1	1	0	0.04
OH-FA_22_6_1	3	0.42	Resolvin D1	1	0	1	0.3
amino acids, branched-chain	3	0.49	Leucine	1	0	1	0.3
DiHETE	8	0.51	17,18-dihydroxyeicosa-5,8,11,14-tetraenoic acid	2	0	0	0.2
unsaturated FFA	15	0.57	FA (16:1) (palmitoleic acid)	2	1	0	0.1
sugar alcohols	7	0.58	Mannitol	1	0	0	0.1
drugs	85	0.58	Acetaminophen	10	5	0	0.1
adenosine	4	0.59	7-Methylguanosine	1	0	1	0.2
dipeptides	16	0.65	H-Pro-Hyp-OH	2	1	0	0.1
saturated FFA	18	0.7	Arachidic acid	1	1	0	0.06
saturated phosphatidylcholines	9	0.73	PC (34:0) - ESI(-)	1	0	0	0.1
diglycerides	14	0.76	DG (38:6)	1	0	0	0.07
HETE	7	0.93	8-hydroxyeicosa-5,9,11,14-tetraenoic acid	1	0	0	0.1
amino acids, aromatic	7	1	Tyrosine	0	0	0	0
amino acids, cyclic	6	1	Histidine	0	0	0	0
amino alcohols	3	1	3-Amino-1-propanol	0	0	0	0
benzene derivatives	6	1	Tri-2-ethylhexyl trimellitate	0	0	0	0
DiHETrE	5	1	8,9-dihydroxyeicosa-5,11,14-trienoic acid	0	0	0	0
EpETrE	7	1	15(16)-epoxy-9,12-octadecadienoic acid	0	0	0	0
ethanolamines	3	1	Heptadecaphing-4-enine	0	0	0	0
guanidines	3	1	Guanidine	0	0	0	0
hexoses	10	1	Levoglucosan	0	0	0	0
histidine	4	1	Ergothioneine	0	0	0	0
HODE	3	1	13-hydroxyoctadeca-9,11,15-trienoic acid	0	0	0	0
hydroxybutyrates	7	1	Threonic acid	0	0	0	0

Supplementary Table S5. ChemRICH enrichment analysis comparing female ME/CFS vs. female controls

Cluster name	Cluster size	p-values	Key compound	Altered	Increased	Decreased	Altered Ratio
imidazoles	3	1	Creatinine	0	0	0	0
lipids	3	1	1-Monostearin	0	0	0	0
monounsaturated long chain TGs	16	1	TG (54:1)	0	0	0	0
monounsaturated TGs	18	1	TG (46:2)	0	0	0	0
nitroFA	3	1	10-nitrooleic acid	0	0	0	0
oxo-ODE	5	1	15-ketoeicosa-5,8,11,13-tetraenoic acid	0	0	0	0
pyridines	3	1	3-Hydroxypyridine	0	0	0	0
saturated ceramides	4	1	Ceramide (d42:0)	0	0	0	0
saturated sphingomyelins	10	1	SM (d36:0) - ESI(-)	0	0	0	0
sugar acids	3	1	Gluconic acid	0	0	0	0
unsaturated TGs	27	1	TG (48:4) A	0	0	0	0
xanthines	3	1	3-Methylxanthine	0	0	0	0

ME/CFS, myalgic encephalomyelitis/chronic fatigue syndrome.

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Primary Metabolites (PM)							
ornithine	Lognormal	-0.027	(-0.046, -0.008)	0.005	0.180	1.549	(-0.046, -0.008)
tyrosine	Lognormal	-0.012	(-0.022, -0.001)	0.032	0.315	0.463	(-0.022, -0.001)
threonine	Lognormal	-0.018	(-0.035, -0.001)	0.040	0.326	0.351	(-0.035, -0.001)
succinic acid	Lognormal	0.020	(0.000, 0.041)	0.050	0.373	0.302	(0.000, 0.041)
lysine	Lognormal	-0.021	(-0.043, 0.000)	0.057	0.383	0.263	(-0.043, 0.000)
phenylalanine	Lognormal	-0.012	(-0.025, 0.000)	0.060	0.390	0.259	(-0.025, 0.000)
fructose	Lognormal	-0.030	(-0.061, 0.001)	0.061	0.390	0.247	(-0.063, -0.001)
tagatose	Lognormal	-0.018	(-0.037, 0.001)	0.061	0.392	0.217	(-0.038, 0.000)
leucine	Lognormal	-0.011	(-0.023, 0.001)	0.063	0.399	0.254	(-0.024, 0.000)
glutamine	Lognormal	-0.024	(-0.051, 0.002)	0.072	0.419	0.209	(-0.051, 0.001)
methionine	Lognormal	-0.019	(-0.040, 0.002)	0.080	0.443	0.175	(-0.039, 0.002)
mannitol	Lognormal	0.034	(-0.004, 0.073)	0.085	0.444	0.198	(-0.003, 0.075)
pelargonic acid	Lognormal	0.014	(-0.002, 0.029)	0.089	0.451	0.163	(-0.002, 0.029)
arachidic acid	Lognormal	0.019	(-0.004, 0.042)	0.109	0.492	0.145	(-0.004, 0.042)
N-acetylputrescine	Lognormal	-0.014	(-0.034, 0.005)	0.146	0.535	0.107	(-0.033, 0.006)
creatinine	Lognormal	-0.018	(-0.042, 0.007)	0.159	0.559	0.099	(-0.042, 0.007)
urea	Lognormal	-0.007	(-0.018, 0.003)	0.177	0.591	0.105	(-0.017, 0.003)
citrulline	Lognormal	-0.010	(-0.025, 0.005)	0.190	0.601	0.088	(-0.024, 0.007)
erythritol	Lognormal	0.020	(-0.010, 0.051)	0.193	0.605	0.092	(-0.008, 0.052)
2-deoxytetronic acid	Lognormal	0.016	(-0.009, 0.040)	0.211	0.610	0.081	(-0.007, 0.042)
maleimide	Lognormal	0.014	(-0.008, 0.037)	0.214	0.610	0.081	(-0.008, 0.036)
2-hydroxybutanoic acid	Lognormal	0.013	(-0.009, 0.036)	0.236	0.633	0.075	(-0.009, 0.036)
oxoproline	Lognormal	-0.004	(-0.012, 0.003)	0.247	0.636	0.078	(-0.012, 0.004)
2-ketoisocaproic acid	Lognormal	0.008	(-0.005, 0.021)	0.247	0.636	0.073	(-0.005, 0.021)
glucose	Lognormal	-0.005	(-0.013, 0.003)	0.248	0.636	0.070	(-0.012, 0.004)
indole-3-propionic acid	Lognormal	-0.017	(-0.045, 0.012)	0.254	0.637	0.074	(-0.043, 0.013)
glutaric acid	Lognormal	0.014	(-0.011, 0.039)	0.273	0.650	0.074	(-0.012, 0.038)
alpha-ketoglutarate	Lognormal	0.010	(-0.008, 0.029)	0.286	0.657	0.068	(-0.009, 0.029)
tryptophan	Lognormal	-0.011	(-0.031, 0.010)	0.305	0.676	0.069	(-0.031, 0.011)
conduiritol-beta-exposide	Lognormal	0.018	(-0.016, 0.051)	0.308	0.676	0.070	(-0.015, 0.053)
sucrose	Lognormal	0.020	(-0.018, 0.057)	0.313	0.676	0.070	(-0.018, 0.058)
linoleic acid	Lognormal	0.013	(-0.013, 0.040)	0.329	0.685	0.062	(-0.012, 0.041)
alanine	Lognormal	-0.011	(-0.033, 0.012)	0.344	0.691	0.065	(-0.033, 0.012)
lysine	Lognormal	-0.013	(-0.041, 0.015)	0.364	0.704	0.061	(-0.043, 0.015)
isoleucine	Lognormal	-0.005	(-0.017, 0.006)	0.374	0.711	0.053	(-0.017, 0.006)
pseudo uridine	Lognormal	-0.006	(-0.019, 0.007)	0.393	0.728	0.055	(-0.019, 0.007)
hydroxycarbamate NIST	Lognormal	-0.008	(-0.031, 0.014)	0.461	0.775	0.052	(-0.032, 0.014)
levoglucosan	Lognormal	-0.011	(-0.040, 0.019)	0.480	0.789	0.053	(-0.039, 0.018)
mannose	Lognormal	-0.007	(-0.027, 0.013)	0.483	0.791	0.048	(-0.027, 0.013)
glycerol	Lognormal	0.004	(-0.008, 0.017)	0.499	0.806	0.041	(-0.008, 0.018)
indole-3-lactate	Lognormal	-0.006	(-0.023, 0.011)	0.512	0.810	0.050	(-0.023, 0.011)
serine	Lognormal	-0.006	(-0.024, 0.012)	0.518	0.811	0.051	(-0.024, 0.014)
beta-alanine	Lognormal	-0.008	(-0.034, 0.017)	0.521	0.813	0.049	(-0.035, 0.018)
quinic acid	Lognormal	-0.014	(-0.058, 0.030)	0.527	0.813	0.041	(-0.057, 0.029)
glycerol-alpha-phosphate	Lognormal	0.010	(-0.021, 0.041)	0.529	0.813	0.047	(-0.019, 0.042)
aminomalonnate	Lognormal	0.011	(-0.023, 0.045)	0.535	0.813	0.045	(-0.023, 0.043)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
heptadecanoic acid	Lognormal	0.006	(-0.014, 0.026)	0.542	0.821	0.045	(-0.015, 0.025)
phosphate	Lognormal	0.003	(-0.007, 0.014)	0.544	0.822	0.038	(-0.007, 0.014)
isothreonine acid	Lognormal	-0.009	(-0.037, 0.020)	0.551	0.829	0.049	(-0.036, 0.020)
citric acid	Lognormal	-0.006	(-0.027, 0.015)	0.560	0.836	0.038	(-0.028, 0.014)
behenic acid	Lognormal	-0.005	(-0.023, 0.013)	0.572	0.847	0.053	(-0.022, 0.014)
palmitic acid	Lognormal	0.003	(-0.007, 0.012)	0.576	0.847	0.045	(-0.007, 0.012)
ribose	Lognormal	-0.005	(-0.021, 0.012)	0.579	0.847	0.050	(-0.020, 0.013)
maltose	Lognormal	-0.007	(-0.033, 0.019)	0.593	0.858	0.045	(-0.033, 0.020)
pentadecanoic acid	Lognormal	-0.003	(-0.012, 0.007)	0.610	0.865	0.041	(-0.013, 0.007)
benzoic acid	Lognormal	0.006	(-0.016, 0.027)	0.611	0.865	0.047	(-0.018, 0.026)
3-hydroxybutyric acid	Lognormal	0.009	(-0.027, 0.046)	0.618	0.872	0.048	(-0.025, 0.049)
creatine	Lognormal	-0.007	(-0.037, 0.022)	0.626	0.873	0.046	(-0.037, 0.023)
fumaric acid	Lognormal	-0.005	(-0.027, 0.016)	0.631	0.874	0.045	(-0.028, 0.016)
myristic acid	Lognormal	0.004	(-0.013, 0.021)	0.637	0.878	0.046	(-0.012, 0.022)
glycolic acid	Lognormal	0.008	(-0.026, 0.043)	0.639	0.879	0.045	(-0.023, 0.045)
2-hydroxyvaleric acid	Lognormal	0.005	(-0.016, 0.026)	0.642	0.881	0.051	(-0.017, 0.025)
N-acetylorcarnitine	Lognormal	-0.003	(-0.018, 0.011)	0.648	0.887	0.038	(-0.018, 0.012)
malic acid	Lognormal	-0.005	(-0.025, 0.016)	0.660	0.895	0.043	(-0.025, 0.016)
alloxanoic acid	Lognormal	0.008	(-0.030, 0.046)	0.678	0.904	0.046	(-0.033, 0.045)
4-hydroxybutyric acid	Lognormal	0.005	(-0.019, 0.028)	0.689	0.906	0.048	(-0.019, 0.028)
threonine acid	Lognormal	0.005	(-0.020, 0.030)	0.701	0.908	0.041	(-0.021, 0.030)
gluconic acid	Lognormal	-0.003	(-0.020, 0.014)	0.707	0.913	0.040	(-0.020, 0.015)
isopropylbenzene	Lognormal	0.004	(-0.017, 0.025)	0.710	0.913	0.027	(-0.018, 0.025)
1,2,4-benzenetriol	Lognormal	-0.008	(-0.051, 0.035)	0.713	0.913	0.045	(-0.053, 0.033)
lauric acid	Lognormal	0.005	(-0.020, 0.029)	0.720	0.920	0.040	(-0.020, 0.029)
pyruvic acid	Lognormal	0.003	(-0.013, 0.018)	0.727	0.927	0.034	(-0.013, 0.018)
salicylic acid	Lognormal	0.006	(-0.029, 0.042)	0.731	0.927	0.043	(-0.028, 0.045)
pyrrole-2-carboxylic acid	Lognormal	0.005	(-0.022, 0.031)	0.734	0.928	0.041	(-0.024, 0.032)
stearic acid	Lognormal	0.002	(-0.008, 0.011)	0.734	0.928	0.038	(-0.008, 0.011)
lactic acid	Lognormal	-0.004	(-0.025, 0.017)	0.739	0.928	0.042	(-0.025, 0.017)
glucose-1-phosphate	Lognormal	0.003	(-0.016, 0.022)	0.749	0.928	0.040	(-0.015, 0.023)
palmitoleic acid	Lognormal	-0.005	(-0.038, 0.028)	0.755	0.931	0.042	(-0.039, 0.026)
lyxitol	Lognormal	-0.003	(-0.020, 0.015)	0.756	0.931	0.041	(-0.019, 0.015)
phthalic acid	Lognormal	0.003	(-0.015, 0.020)	0.764	0.931	0.040	(-0.013, 0.021)
glucuronic acid	Lognormal	-0.004	(-0.027, 0.020)	0.767	0.931	0.045	(-0.026, 0.021)
threitol	Lognormal	0.003	(-0.017, 0.023)	0.775	0.936	0.039	(-0.016, 0.023)
capric acid	Lognormal	-0.004	(-0.033, 0.025)	0.780	0.936	0.038	(-0.034, 0.024)
valine	Lognormal	0.002	(-0.010, 0.013)	0.782	0.936	0.038	(-0.009, 0.013)
glyceric acid	Lognormal	0.003	(-0.022, 0.029)	0.790	0.936	0.042	(-0.021, 0.029)
glutamic acid	Lognormal	-0.003	(-0.024, 0.019)	0.806	0.947	0.042	(-0.025, 0.019)
trans-4-hydroxyproline	Lognormal	-0.003	(-0.031, 0.024)	0.822	0.952	0.039	(-0.033, 0.024)
uric acid	Lognormal	-0.002	(-0.025, 0.020)	0.830	0.953	0.042	(-0.024, 0.021)
adipic acid	Lognormal	-0.002	(-0.025, 0.021)	0.850	0.964	0.043	(-0.025, 0.021)
1-methylgalactose NIST	Lognormal	-0.004	(-0.041, 0.034)	0.854	0.964	0.041	(-0.039, 0.034)
myo-inositol	Lognormal	0.001	(-0.011, 0.014)	0.864	0.966	0.041	(-0.012, 0.013)
maleic acid	Lognormal	0.002	(-0.026, 0.031)	0.866	0.966	0.036	(-0.026, 0.031)
indole-3-acetate	Lognormal	0.002	(-0.023, 0.026)	0.887	0.970	0.037	(-0.023, 0.026)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
proline	Lognormal	-0.002	(-0.028, 0.025)	0.900	0.973	0.041	(-0.028, 0.025)
2-aminobutyric acid	Lognormal	0.001	(-0.014, 0.016)	0.907	0.976	0.041	(-0.014, 0.016)
oxalic acid	Lognormal	0.002	(-0.054, 0.059)	0.933	0.990	0.041	(-0.057, 0.059)
caprylic acid	Lognormal	0.000	(-0.014, 0.013)	0.964	0.994	0.037	(-0.013, 0.013)
glycine	Lognormal	0.000	(-0.012, 0.012)	0.987	0.995	0.040	(-0.011, 0.013)
ribonic acid	Lognormal	0.000	(-0.020, 0.020)	0.993	0.997	0.039	(-0.020, 0.021)
nicotinic acid	Lognormal	0.000	(-0.041, 0.042)	0.995	0.997	0.032	(-0.043, 0.040)
Biogenic Amines (BA)							
Alprazolam	Lognormal	0.081	(0.030, 0.132)	0.002	0.121	3.486	(0.030, 0.130)
Acyclovir	Lognormal	0.152	(0.057, 0.247)	0.002	0.121	3.179	(0.056, 0.249)
Linoleoylcarnitine	Lognormal	-0.052	(-0.085, -0.018)	0.003	0.140	2.103	(-0.086, -0.018)
Guanine	Lognormal	0.117	(0.040, 0.194)	0.004	0.160	2.962	(0.042, 0.196)
Caffeine	Lognormal	-0.093	(-0.156, -0.030)	0.004	0.169	2.442	(-0.152, -0.028)
2-Methylbutyryl-L-carnitine	Lognormal	-0.039	(-0.068, -0.010)	0.009	0.206	1.009	(-0.067, -0.010)
Acetaminophen	Lognormal	0.064	(0.016, 0.113)	0.010	0.211	1.172	(0.019, 0.116)
Theobromine	Lognormal	-0.066	(-0.117, -0.015)	0.012	0.225	0.940	(-0.115, -0.012)
Tri-2-ethylhexyl trimellitate	Lognormal	-0.058	(-0.108, -0.008)	0.025	0.291	0.511	(-0.109, -0.009)
7-Methylguanosine	Lognormal	-0.017	(-0.032, -0.002)	0.026	0.300	0.456	(-0.032, -0.002)
Usnic acid	Lognormal	-0.056	(-0.105, -0.007)	0.028	0.312	0.440	(-0.105, -0.007)
Choline cation	Lognormal	-0.008	(-0.015, -0.001)	0.031	0.315	0.411	(-0.015, -0.001)
Piperine	Lognormal	-0.064	(-0.123, -0.005)	0.035	0.320	0.376	(-0.120, -0.002)
Trigonelline	Lognormal	-0.048	(-0.092, -0.004)	0.036	0.320	0.300	(-0.090, -0.001)
Oleoyl-L-carnitine	Lognormal	-0.041	(-0.079, -0.003)	0.036	0.320	0.363	(-0.080, -0.005)
Kynurenine	Lognormal	-0.018	(-0.034, -0.001)	0.038	0.322	0.346	(-0.034, -0.002)
Isopropylamine	Lognormal	-0.014	(-0.027, -0.001)	0.043	0.338	0.310	(-0.026, 0.000)
Octanoylcarnitine	Lognormal	-0.023	(-0.047, 0.000)	0.053	0.379	0.227	(-0.046, 0.001)
D-erythro-Sphingosine-1-phosphate	Lognormal	-0.024	(-0.048, 0.000)	0.054	0.379	0.251	(-0.048, 0.000)
1-Stearoyl-2-arachidonoyl-sn-glycero-3-phosphoserine	Lognormal	-0.081	(-0.168, 0.005)	0.067	0.413	0.184	(-0.173, 0.000)
Albendazole sulfoxide	Lognormal	0.100	(-0.007, 0.207)	0.068	0.414	0.236	(-0.002, 0.205)
Ranitidine N-oxide	Lognormal	0.052	(-0.004, 0.107)	0.070	0.416	0.204	(-0.002, 0.109)
H-Pro-Hyp-OH	Lognormal	0.025	(-0.002, 0.052)	0.074	0.428	0.202	(-0.002, 0.052)
4-Acetamidobutyric acid	Lognormal	-0.022	(-0.047, 0.002)	0.079	0.442	0.198	(-0.048, 0.003)
3-Methylglutarylcarnitine	Lognormal	-0.022	(-0.046, 0.003)	0.081	0.444	0.217	(-0.045, 0.002)
4,5,7-Trihydroxyisoflavone	Lognormal	0.087	(-0.010, 0.185)	0.081	0.444	0.191	(-0.005, 0.193)
7-Hydroxywarfarin	Lognormal	0.034	(-0.004, 0.072)	0.082	0.444	0.180	(-0.005, 0.073)
1-Monostearin	Lognormal	-0.032	(-0.068, 0.004)	0.084	0.444	0.172	(-0.068, 0.004)
SDMA	Lognormal	-0.010	(-0.021, 0.002)	0.093	0.457	0.161	(-0.021, 0.001)
Ergothioneine	Lognormal	-0.036	(-0.078, 0.006)	0.098	0.465	0.159	(-0.078, 0.006)
1-Oleoyl-2-acetyl-sn-glycerol	Lognormal	-0.034	(-0.075, 0.007)	0.110	0.493	0.126	(-0.079, 0.008)
L-Citrulline	Lognormal	-0.009	(-0.021, 0.002)	0.112	0.494	0.163	(-0.020, 0.002)
Pantoprazole	Lognormal	0.051	(-0.015, 0.116)	0.131	0.521	0.118	(-0.014, 0.114)
Phenylalanine	Lognormal	-0.007	(-0.016, 0.002)	0.133	0.521	0.113	(-0.016, 0.002)
D-Turanose	Lognormal	-0.023	(-0.053, 0.007)	0.134	0.521	0.114	(-0.052, 0.007)
Trazodone	Lognormal	0.042	(-0.013, 0.096)	0.138	0.529	0.120	(-0.012, 0.095)
2,6-Diaminopimelic acid	Lognormal	0.037	(-0.012, 0.086)	0.140	0.532	0.111	(-0.011, 0.085)
N-.alpha.-Acetyl-L-arginine	Lognormal	-0.012	(-0.028, 0.004)	0.141	0.533	0.119	(-0.029, 0.004)
2-Amino-1-phenylethanol	Lognormal	-0.007	(-0.016, 0.002)	0.143	0.535	0.117	(-0.016, 0.002)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Modafinil acid	Lognormal	0.051	(-0.017, 0.119)	0.143	0.535	0.125	(-0.018, 0.119)
Decanoyl-L-carnitine	Lognormal	-0.021	(-0.049, 0.007)	0.147	0.535	0.109	(-0.050, 0.010)
3-Amino-1-propanol	Lognormal	0.016	(-0.006, 0.039)	0.150	0.543	0.107	(-0.006, 0.040)
1-Oleoyl-sn-glycero-3-phosphoethanolamine	Lognormal	-0.027	(-0.063, 0.010)	0.155	0.555	0.114	(-0.063, 0.013)
H-gamma-glutamyl-glutamine	Lognormal	0.020	(-0.008, 0.049)	0.159	0.559	0.089	(-0.009, 0.049)
Lauroyl-L-carnitine	Lognormal	-0.032	(-0.076, 0.012)	0.160	0.561	0.092	(-0.076, 0.015)
L-Leucine, methyl ester	Lognormal	0.025	(-0.010, 0.060)	0.160	0.561	0.091	(-0.013, 0.059)
Glutamic acid	Lognormal	0.011	(-0.005, 0.028)	0.168	0.584	0.082	(-0.005, 0.027)
Citrulline	Lognormal	-0.008	(-0.021, 0.004)	0.176	0.591	0.100	(-0.022, 0.003)
Trimethylamine-N-oxide	Lognormal	0.019	(-0.009, 0.048)	0.176	0.591	0.085	(-0.010, 0.047)
3-Hydroxypyridine	Lognormal	-0.053	(-0.132, 0.025)	0.183	0.596	0.075	(-0.133, 0.022)
Losartan	Lognormal	-0.027	(-0.066, 0.013)	0.184	0.596	0.105	(-0.067, 0.014)
Lamotrigine;	Lognormal	0.091	(-0.044, 0.225)	0.189	0.601	0.093	(-0.045, 0.235)
Gabapentin	Lognormal	0.040	(-0.020, 0.101)	0.197	0.605	0.086	(-0.021, 0.097)
Pyridoxine;	Lognormal	0.027	(-0.014, 0.068)	0.202	0.610	0.076	(-0.016, 0.069)
N-Acetylhistidine	Lognormal	-0.017	(-0.043, 0.009)	0.203	0.610	0.090	(-0.043, 0.008)
Quetiapine	Lognormal	0.017	(-0.009, 0.044)	0.203	0.610	0.092	(-0.010, 0.042)
N-Methylhistidine	Lognormal	-0.024	(-0.062, 0.013)	0.206	0.610	0.087	(-0.060, 0.015)
.beta.-Phenyl-.gamma.-aminobutyric acid	Lognormal	-0.013	(-0.033, 0.007)	0.208	0.610	0.087	(-0.032, 0.008)
Testosterone	Lognormal	-0.025	(-0.063, 0.014)	0.210	0.610	0.077	(-0.062, 0.012)
Thr-Ile-Arg	Lognormal	-0.031	(-0.080, 0.017)	0.211	0.610	0.086	(-0.078, 0.018)
Dexpanthenol	Lognormal	-0.023	(-0.058, 0.013)	0.212	0.610	0.070	(-0.056, 0.015)
1-Stearoyl-2-arachidonoyl-sn-glycero-3-phospho-(1'-myo-inositol)	Lognormal	-0.058	(-0.150, 0.034)	0.220	0.621	0.091	(-0.144, 0.039)
Creatinine	Lognormal	-0.004	(-0.011, 0.003)	0.225	0.624	0.072	(-0.012, 0.003)
p-Acetamidophenyl .beta.-D-glucuronide	Lognormal	0.038	(-0.023, 0.098)	0.229	0.624	0.086	(-0.025, 0.096)
Ranitidine	Lognormal	0.028	(-0.017, 0.073)	0.230	0.624	0.084	(-0.019, 0.073)
(R)-Butyrylcarnitine	Lognormal	-0.017	(-0.045, 0.011)	0.231	0.624	0.078	(-0.046, 0.011)
Glycocholic acid	Lognormal	-0.023	(-0.062, 0.016)	0.245	0.636	0.068	(-0.061, 0.018)
N-Acetyl-D-norleucine	Lognormal	0.015	(-0.010, 0.040)	0.246	0.636	0.046	(-0.012, 0.038)
N.alpha.-Methyl-L-lysine	Lognormal	0.023	(-0.016, 0.062)	0.250	0.637	0.079	(-0.017, 0.062)
Betaine	Lognormal	-0.005	(-0.012, 0.003)	0.252	0.637	0.077	(-0.012, 0.003)
Norleucine	Lognormal	-0.006	(-0.017, 0.005)	0.252	0.637	0.071	(-0.018, 0.006)
Nudifloramide	Lognormal	-0.013	(-0.035, 0.009)	0.258	0.642	0.073	(-0.034, 0.010)
1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	Lognormal	-0.022	(-0.060, 0.016)	0.261	0.642	0.078	(-0.059, 0.016)
Fexofenadine	Lognormal	-0.018	(-0.049, 0.013)	0.263	0.642	0.073	(-0.048, 0.015)
Hexanoyl-L-carnitine	Lognormal	-0.015	(-0.042, 0.011)	0.263	0.642	0.069	(-0.042, 0.011)
cis-10,11-Dihydroxy-10,11-dihydrocarbamazepine	Lognormal	-0.015	(-0.042, 0.011)	0.264	0.642	0.073	(-0.042, 0.012)
Acetazolamide	Lognormal	-0.025	(-0.069, 0.019)	0.264	0.642	0.074	(-0.068, 0.017)
1-Acetyl-3-piperidinamine	Lognormal	0.011	(-0.009, 0.031)	0.271	0.649	0.072	(-0.009, 0.031)
Ala-Ile	Lognormal	0.013	(-0.010, 0.037)	0.272	0.650	0.070	(-0.010, 0.037)
Quetiapine sulfoxide	Lognormal	0.019	(-0.015, 0.052)	0.276	0.651	0.068	(-0.015, 0.052)
Tryptophan	Lognormal	0.007	(-0.006, 0.019)	0.283	0.657	0.067	(-0.005, 0.020)
Prazepam	Lognormal	0.028	(-0.023, 0.080)	0.285	0.657	0.064	(-0.021, 0.079)
Omeprazole sulfone N-oxide	Lognormal	0.042	(-0.035, 0.119)	0.287	0.657	0.067	(-0.037, 0.127)
Montelukast-1,2-diol	Lognormal	0.044	(-0.037, 0.125)	0.287	0.657	0.070	(-0.038, 0.129)
Diazepam	Lognormal	0.038	(-0.032, 0.108)	0.288	0.657	0.067	(-0.027, 0.114)
Irbesartan	Lognormal	0.017	(-0.014, 0.047)	0.289	0.657	0.067	(-0.014, 0.047)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Betonicine	Lognormal	-0.043	(-0.122, 0.037)	0.293	0.662	0.070	(-0.128, 0.035)
Adenosine	Lognormal	-0.017	(-0.048, 0.015)	0.306	0.676	0.064	(-0.049, 0.017)
Ethiolat	Lognormal	-0.021	(-0.062, 0.019)	0.309	0.676	0.065	(-0.059, 0.021)
Toradol	Lognormal	0.025	(-0.023, 0.072)	0.310	0.676	0.069	(-0.022, 0.071)
NEPSILON,NEPSILON,NEPSILON-TRIMETHYLLYSINE	Lognormal	-0.007	(-0.020, 0.006)	0.314	0.676	0.054	(-0.020, 0.007)
Histidine	Lognormal	-0.013	(-0.040, 0.013)	0.320	0.684	0.068	(-0.040, 0.014)
Codeine-6-.beta.-D-glucuronide	Lognormal	0.019	(-0.018, 0.056)	0.325	0.684	0.068	(-0.020, 0.056)
Ethylidethanolamine	Lognormal	-0.016	(-0.049, 0.016)	0.325	0.684	0.057	(-0.050, 0.015)
6-Hydroxyflavone	Lognormal	0.023	(-0.022, 0.068)	0.325	0.684	0.056	(-0.025, 0.065)
Omeprazole sulfone	Lognormal	0.037	(-0.039, 0.113)	0.340	0.691	0.064	(-0.039, 0.109)
L-Tyrosine	Lognormal	-0.011	(-0.034, 0.012)	0.342	0.691	0.063	(-0.034, 0.012)
Aminodiphenylmethane	Lognormal	0.020	(-0.021, 0.060)	0.345	0.691	0.065	(-0.021, 0.061)
1-Methylnicotinamide	Lognormal	-0.011	(-0.033, 0.011)	0.345	0.691	0.057	(-0.035, 0.011)
Phenylacetyl-L-glutamine	Lognormal	-0.020	(-0.062, 0.022)	0.354	0.701	0.054	(-0.061, 0.022)
Tauroursodeoxycholic acid	Lognormal	0.018	(-0.021, 0.057)	0.360	0.704	0.063	(-0.021, 0.060)
Tyrosine	Lognormal	-0.008	(-0.024, 0.009)	0.360	0.704	0.053	(-0.025, 0.008)
N-(3-(Aminomethyl)benzyl)acetamidine	Lognormal	-0.017	(-0.053, 0.019)	0.360	0.704	0.047	(-0.055, 0.021)
3-Dehydrocarnitine	Lognormal	-0.008	(-0.026, 0.009)	0.363	0.704	0.050	(-0.025, 0.010)
3-Hydroxyoleylcarnitine	Lognormal	0.039	(-0.045, 0.124)	0.363	0.704	0.060	(-0.042, 0.127)
Pyrantel	Lognormal	-0.014	(-0.043, 0.016)	0.369	0.709	0.062	(-0.042, 0.017)
Ile-Glu-Arg	Lognormal	-0.031	(-0.100, 0.038)	0.380	0.713	0.059	(-0.098, 0.042)
Moxonidine	Lognormal	-0.013	(-0.043, 0.016)	0.380	0.713	0.060	(-0.042, 0.016)
Ornithine	Lognormal	-0.008	(-0.027, 0.010)	0.380	0.713	0.045	(-0.028, 0.009)
L-Threonine	Lognormal	-0.006	(-0.020, 0.008)	0.385	0.721	0.061	(-0.019, 0.008)
3-Methylxanthine	Lognormal	-0.021	(-0.069, 0.027)	0.387	0.722	0.055	(-0.071, 0.027)
(3-Carboxypropyl)trimethylammonium cation	Lognormal	-0.005	(-0.017, 0.007)	0.401	0.733	0.052	(-0.017, 0.006)
Hydroxybupropion	Lognormal	-0.017	(-0.057, 0.023)	0.404	0.733	0.063	(-0.058, 0.022)
Glaucine	Lognormal	0.011	(-0.016, 0.038)	0.414	0.739	0.054	(-0.017, 0.035)
L-Cystine	Lognormal	-0.010	(-0.036, 0.015)	0.417	0.739	0.039	(-0.036, 0.015)
Methacholine cation	Lognormal	-0.009	(-0.032, 0.013)	0.421	0.739	0.051	(-0.032, 0.015)
Urea	Lognormal	-0.005	(-0.016, 0.006)	0.423	0.739	0.048	(-0.015, 0.006)
4-Fluoro-.alpha.-pyrrolidinobutiophenone	Lognormal	0.011	(-0.016, 0.038)	0.432	0.753	0.054	(-0.017, 0.039)
Benthiavalicarb-isopropyl	Lognormal	-0.017	(-0.062, 0.027)	0.444	0.763	0.052	(-0.064, 0.027)
Modafinil	Lognormal	0.021	(-0.033, 0.074)	0.447	0.765	0.054	(-0.032, 0.074)
Palmitamide	Lognormal	-0.018	(-0.066, 0.029)	0.452	0.768	0.058	(-0.068, 0.030)
alpha-Methylhistidine;	Lognormal	-0.020	(-0.073, 0.033)	0.455	0.771	0.052	(-0.075, 0.034)
Ranitidine-S-oxide	Lognormal	-0.023	(-0.084, 0.038)	0.459	0.775	0.049	(-0.086, 0.039)
Metoprolol acid	Lognormal	0.021	(-0.034, 0.075)	0.462	0.776	0.049	(-0.031, 0.076)
7.alpha.-Hydroxy-3-oxo-4-cholestenoic acid	Lognormal	-0.009	(-0.031, 0.014)	0.467	0.781	0.054	(-0.031, 0.015)
5'-S-Methyl-5'-thioadenosine	Lognormal	-0.031	(-0.113, 0.052)	0.470	0.781	0.045	(-0.119, 0.044)
Stachydrine	Lognormal	-0.016	(-0.059, 0.027)	0.470	0.781	0.051	(-0.061, 0.026)
Glycodeoxycholic acid	Lognormal	-0.016	(-0.058, 0.027)	0.474	0.784	0.047	(-0.056, 0.031)
Carnitine	Lognormal	-0.003	(-0.011, 0.005)	0.488	0.796	0.047	(-0.011, 0.005)
Topiramate	Lognormal	0.013	(-0.024, 0.051)	0.491	0.798	0.050	(-0.026, 0.051)
Meprobamate	Lognormal	0.012	(-0.022, 0.045)	0.504	0.806	0.052	(-0.023, 0.044)
DL-Indole-3-lactic acid	Lognormal	0.005	(-0.009, 0.018)	0.506	0.806	0.052	(-0.009, 0.018)
Ethylenediaminetetraacetic acid	Lognormal	0.031	(-0.060, 0.122)	0.507	0.806	0.047	(-0.064, 0.123)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Gly-Pro-Arg	Lognormal	-0.022	(-0.087, 0.043)	0.507	0.806	0.049	(-0.086, 0.041)
Pipecolic acid	Lognormal	-0.016	(-0.065, 0.032)	0.510	0.808	0.046	(-0.063, 0.031)
L-Cysteine-glutathione disulfide	Lognormal	-0.011	(-0.045, 0.022)	0.518	0.811	0.031	(-0.043, 0.024)
3-Cysteinyacetaminophen	Lognormal	0.034	(-0.069, 0.138)	0.518	0.811	0.046	(-0.067, 0.138)
Ezetimibe	Lognormal	0.015	(-0.030, 0.060)	0.523	0.813	0.048	(-0.032, 0.057)
1-Methyl-L-histidine	Lognormal	-0.016	(-0.063, 0.032)	0.525	0.813	0.046	(-0.063, 0.031)
Carbamazepine	Lognormal	-0.020	(-0.081, 0.041)	0.529	0.813	0.051	(-0.078, 0.044)
5'-S-Methylthioadenosine	Lognormal	-0.030	(-0.122, 0.063)	0.530	0.813	0.041	(-0.121, 0.067)
Dinor-12-oxophytodienoic acid	Lognormal	-0.016	(-0.067, 0.035)	0.532	0.813	0.047	(-0.070, 0.033)
Atorvastatin	Lognormal	0.007	(-0.016, 0.031)	0.536	0.814	0.052	(-0.016, 0.030)
N-Methylproline	Lognormal	-0.009	(-0.036, 0.019)	0.543	0.822	0.046	(-0.036, 0.019)
4'-Methyl-N-methylhexanophenone	Lognormal	-0.019	(-0.082, 0.044)	0.548	0.826	0.046	(-0.079, 0.046)
trans-3'-Hydroxycotinine	Lognormal	0.010	(-0.023, 0.043)	0.556	0.834	0.047	(-0.024, 0.042)
Guanidine	Lognormal	0.007	(-0.017, 0.031)	0.573	0.847	0.045	(-0.017, 0.030)
Telmisartan	Lognormal	0.009	(-0.026, 0.045)	0.597	0.859	0.040	(-0.027, 0.043)
Theanine;	Lognormal	0.010	(-0.028, 0.049)	0.601	0.861	0.038	(-0.028, 0.052)
Methylgallate	Lognormal	0.026	(-0.072, 0.124)	0.607	0.865	0.043	(-0.074, 0.123)
Avobenzon	Lognormal	0.007	(-0.020, 0.033)	0.613	0.867	0.047	(-0.019, 0.034)
3,4-Dimethoxybenzaldehyde	Lognormal	0.009	(-0.026, 0.044)	0.622	0.872	0.037	(-0.027, 0.043)
Trimethoprim	Lognormal	-0.009	(-0.046, 0.028)	0.624	0.872	0.045	(-0.045, 0.028)
Ticlopidine	Lognormal	-0.024	(-0.123, 0.074)	0.632	0.874	0.043	(-0.123, 0.075)
N.epsilon.-Acetyl-L-lysine	Lognormal	-0.005	(-0.024, 0.015)	0.634	0.876	0.046	(-0.024, 0.015)
2,2-Bishydroxymethyl]-2,2',2''-nitritotriethanol	Lognormal	-0.007	(-0.039, 0.024)	0.645	0.884	0.044	(-0.040, 0.025)
Betaine aldehyde cation	Lognormal	0.014	(-0.050, 0.078)	0.661	0.895	0.041	(-0.052, 0.075)
Pantothenic acid	Lognormal	-0.006	(-0.031, 0.020)	0.661	0.895	0.043	(-0.030, 0.021)
D-Pyroglutamic acid	Lognormal	-0.001	(-0.008, 0.005)	0.670	0.900	0.043	(-0.008, 0.005)
2-Indolinone	Lognormal	-0.005	(-0.028, 0.018)	0.682	0.905	0.043	(-0.028, 0.020)
Pyridoxal	Lognormal	0.006	(-0.024, 0.037)	0.685	0.906	0.041	(-0.022, 0.037)
(2R)-3-Hydroxyisovalerylcarnitine	Lognormal	-0.004	(-0.023, 0.015)	0.686	0.906	0.041	(-0.023, 0.015)
Arginine	Lognormal	0.003	(-0.013, 0.019)	0.689	0.906	0.039	(-0.014, 0.018)
Metoprolol	Lognormal	0.009	(-0.037, 0.056)	0.696	0.907	0.045	(-0.039, 0.056)
N-Acetyl-L-carnosine	Lognormal	-0.004	(-0.026, 0.018)	0.698	0.908	0.043	(-0.025, 0.018)
3-Hydroxybutyrylcarnitine	Lognormal	-0.006	(-0.040, 0.027)	0.710	0.913	0.043	(-0.038, 0.026)
4-Aminomethylcyclohexanecarboxylic acid;	Lognormal	-0.006	(-0.036, 0.025)	0.712	0.913	0.037	(-0.035, 0.026)
D-.alpha.-Cyclohexylglycine	Lognormal	-0.006	(-0.038, 0.026)	0.713	0.913	0.044	(-0.039, 0.027)
Urocanic acid;	Lognormal	-0.004	(-0.026, 0.018)	0.729	0.927	0.041	(-0.025, 0.019)
L-Carnitine	Lognormal	-0.002	(-0.015, 0.010)	0.742	0.928	0.042	(-0.014, 0.011)
Metformin	Lognormal	0.007	(-0.036, 0.051)	0.743	0.928	0.042	(-0.038, 0.049)
Cotinine N-.beta.-D-glucuronide	Lognormal	0.012	(-0.058, 0.081)	0.746	0.928	0.044	(-0.056, 0.083)
Glutamine	Lognormal	-0.001	(-0.008, 0.006)	0.750	0.928	0.040	(-0.008, 0.006)
Heptadecaphing-4-enine	Lognormal	0.021	(-0.107, 0.149)	0.750	0.928	0.039	(-0.106, 0.150)
Ser-Tyr-Lys	Lognormal	-0.010	(-0.072, 0.052)	0.759	0.931	0.042	(-0.075, 0.050)
3-Aminoquinoline	Lognormal	-0.007	(-0.054, 0.039)	0.762	0.931	0.031	(-0.056, 0.039)
Biliverden	Lognormal	-0.003	(-0.026, 0.019)	0.763	0.931	0.039	(-0.026, 0.018)
Borrelidin	Lognormal	0.008	(-0.048, 0.065)	0.769	0.931	0.041	(-0.047, 0.063)
Creatine	Lognormal	-0.003	(-0.019, 0.014)	0.769	0.931	0.045	(-0.019, 0.015)
Isopentenyladenine	Lognormal	-0.001	(-0.012, 0.009)	0.784	0.936	0.042	(-0.012, 0.008)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Indole-3-propionic acid	Lognormal	-0.004	(-0.036, 0.027)	0.786	0.936	0.040	(-0.035, 0.027)
D-Fructose	Lognormal	0.001	(-0.007, 0.009)	0.790	0.936	0.034	(-0.007, 0.008)
rac-4-Sulfoxypropranolol	Lognormal	0.004	(-0.028, 0.036)	0.799	0.945	0.040	(-0.025, 0.038)
3-Pyridinemethanol	Lognormal	0.004	(-0.024, 0.032)	0.800	0.945	0.042	(-0.025, 0.031)
Levocetirizine;	Lognormal	0.010	(-0.074, 0.095)	0.810	0.948	0.042	(-0.074, 0.097)
.epsilon.-Caprolactam	Lognormal	0.002	(-0.017, 0.021)	0.813	0.949	0.024	(-0.016, 0.021)
N-Acetylaniline	Lognormal	0.008	(-0.064, 0.080)	0.825	0.952	0.042	(-0.062, 0.081)
1,2-Dimethylimidazole	Lognormal	-0.003	(-0.029, 0.023)	0.827	0.952	0.041	(-0.028, 0.022)
R-(-)-O-Desmethylvenlafaxine	Lognormal	-0.006	(-0.060, 0.048)	0.833	0.955	0.041	(-0.059, 0.046)
Naproxen	Lognormal	-0.005	(-0.052, 0.042)	0.841	0.960	0.041	(-0.049, 0.043)
N8-Acetylspermidine	Lognormal	-0.002	(-0.017, 0.014)	0.843	0.960	0.035	(-0.016, 0.014)
1-Stearoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	Lognormal	-0.004	(-0.040, 0.033)	0.848	0.963	0.037	(-0.040, 0.034)
Propionylcarnitine	Lognormal	-0.001	(-0.011, 0.009)	0.851	0.964	0.035	(-0.011, 0.010)
Matrine	Lognormal	-0.005	(-0.057, 0.047)	0.856	0.964	0.039	(-0.058, 0.046)
Trileptal	Lognormal	-0.003	(-0.034, 0.028)	0.858	0.964	0.039	(-0.031, 0.030)
Androstan-3-ol-17-one 3-glucuronide	Lognormal	0.003	(-0.032, 0.038)	0.858	0.964	0.039	(-0.032, 0.039)
Serotonin	Lognormal	0.002	(-0.019, 0.023)	0.860	0.964	0.035	(-0.018, 0.022)
Lansoprazole	Lognormal	0.010	(-0.106, 0.126)	0.862	0.965	0.041	(-0.102, 0.131)
Atenolol	Lognormal	-0.003	(-0.044, 0.037)	0.870	0.966	0.040	(-0.043, 0.035)
1-Acetyl-4-piperidinamine	Lognormal	0.004	(-0.041, 0.049)	0.870	0.966	0.042	(-0.043, 0.047)
Homoarginine;	Lognormal	0.002	(-0.020, 0.023)	0.871	0.966	0.031	(-0.021, 0.023)
1-Phenylpyrrolidine	Lognormal	0.003	(-0.033, 0.039)	0.875	0.969	0.040	(-0.032, 0.038)
Acetyl-DL-carnitine	Lognormal	0.001	(-0.016, 0.019)	0.878	0.970	0.039	(-0.016, 0.019)
2-Hydroxyibuprofen	Lognormal	0.003	(-0.033, 0.038)	0.881	0.970	0.039	(-0.032, 0.039)
Milnacipran	Lognormal	0.003	(-0.039, 0.045)	0.882	0.970	0.039	(-0.039, 0.044)
Triptolide	Lognormal	0.002	(-0.025, 0.029)	0.887	0.970	0.036	(-0.025, 0.028)
2,2',2''-Nitrilotriethanol	Lognormal	0.002	(-0.029, 0.033)	0.889	0.971	0.039	(-0.032, 0.031)
Albendazole	Lognormal	0.003	(-0.035, 0.041)	0.893	0.973	0.040	(-0.037, 0.042)
Scopoletin	Lognormal	-0.006	(-0.096, 0.084)	0.894	0.973	0.031	(-0.095, 0.087)
Mefenorex	Lognormal	0.002	(-0.034, 0.039)	0.901	0.973	0.034	(-0.032, 0.041)
Diphenhydramine	Lognormal	-0.002	(-0.028, 0.025)	0.901	0.973	0.040	(-0.028, 0.023)
3-(1-Pyrazolyl)-alanine	Lognormal	0.005	(-0.071, 0.080)	0.905	0.975	0.038	(-0.075, 0.079)
Methionine	Lognormal	-0.001	(-0.012, 0.011)	0.919	0.982	0.038	(-0.013, 0.011)
Hypoxanthine	Lognormal	-0.001	(-0.020, 0.019)	0.935	0.990	0.034	(-0.021, 0.019)
Tapentadol-.beta.-D-glucuronide	Lognormal	0.002	(-0.056, 0.061)	0.943	0.994	0.041	(-0.059, 0.059)
Methioninesulfoxide	Lognormal	0.001	(-0.022, 0.024)	0.949	0.994	0.037	(-0.022, 0.024)
Ondansetron	Lognormal	0.001	(-0.027, 0.029)	0.952	0.994	0.037	(-0.029, 0.027)
threo-Dihydrobupropion	Lognormal	0.001	(-0.032, 0.034)	0.953	0.994	0.040	(-0.031, 0.035)
Isoleucine	Lognormal	0.000	(-0.012, 0.011)	0.954	0.994	0.038	(-0.012, 0.011)
Esomeprazole	Lognormal	0.001	(-0.038, 0.040)	0.955	0.994	0.042	(-0.041, 0.038)
Meloxicam	Lognormal	-0.003	(-0.123, 0.116)	0.957	0.994	0.042	(-0.123, 0.118)
3,5-Dihydroxyphenylglycine	Lognormal	0.001	(-0.034, 0.036)	0.959	0.994	0.036	(-0.036, 0.034)
Temazepam	Lognormal	0.001	(-0.042, 0.044)	0.960	0.994	0.039	(-0.040, 0.044)
Lauric acid diethanolamide	Lognormal	-0.001	(-0.048, 0.046)	0.961	0.994	0.041	(-0.049, 0.047)
4-Pyridoxic acid;	Lognormal	0.001	(-0.051, 0.053)	0.962	0.994	0.037	(-0.050, 0.053)
Phenylacetylglutamine	Lognormal	0.001	(-0.030, 0.031)	0.970	0.994	0.035	(-0.031, 0.031)
Penciclovir	Lognormal	-0.001	(-0.035, 0.034)	0.971	0.994	0.034	(-0.036, 0.032)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
6-Methoxynaphthaleneacetic acid	Lognormal	0.000	(-0.013, 0.012)	0.974	0.994	0.037	(-0.013, 0.012)
1-Methyladenosine A	Lognormal	0.000	(-0.011, 0.011)	0.977	0.995	0.038	(-0.011, 0.010)
Coniferylaldehyde	Lognormal	0.000	(-0.027, 0.027)	0.983	0.995	0.041	(-0.029, 0.026)
Bradykinin	Lognormal	0.001	(-0.113, 0.115)	0.984	0.995	0.038	(-0.113, 0.112)
Lysine	Lognormal	0.000	(-0.015, 0.016)	0.984	0.995	0.032	(-0.016, 0.016)
Benzophenone-3	Lognormal	0.001	(-0.071, 0.072)	0.987	0.995	0.040	(-0.069, 0.074)
Sulfamethoxazole	Lognormal	-0.001	(-0.102, 0.101)	0.990	0.997	0.040	(-0.111, 0.097)
Cyclo(Leu-Pro)	Lognormal	0.000	(-0.030, 0.029)	0.991	0.997	0.040	(-0.032, 0.027)
N.epsilon.-Methyl-L-lysine	Lognormal	0.000	(-0.034, 0.034)	0.993	0.997	0.036	(-0.034, 0.035)
Proline	Lognormal	0.000	(-0.034, 0.034)	1.000	1.000	0.039	(-0.035, 0.036)
Complex Lipids (CL)							
PC (p-34:2)/PC (o-34:3) - ESI(+)	Lognormal	-0.022	(-0.032, -0.011)	0.000	0.048	36.107	(-0.032, -0.012)
PE (p-36:2)/PE (o-36:3) - ESI(+)	Lognormal	-0.033	(-0.049, -0.017)	0.000	0.048	24.602	(-0.049, -0.016)
PC (p-34:1)/PC (o-34:2)	Lognormal	-0.025	(-0.038, -0.012)	0.000	0.054	26.013	(-0.038, -0.012)
PC (36:4) A - ESI(+)	Lognormal	-0.022	(-0.033, -0.010)	0.000	0.054	8.061	(-0.034, -0.010)
PC (36:2)	Lognormal	-0.009	(-0.013, -0.004)	0.000	0.054	14.972	(-0.013, -0.004)
PC 34:4e	Lognormal	-0.029	(-0.045, -0.014)	0.000	0.054	13.135	(-0.044, -0.012)
PC (36:4) A - ESI(-)	Lognormal	-0.025	(-0.038, -0.011)	0.000	0.054	11.432	(-0.037, -0.010)
PC (34:2) - ESI(+)	Lognormal	-0.006	(-0.010, -0.003)	0.000	0.054	6.913	(-0.010, -0.003)
PC (p-34:2)/PC (o-34:3) - ESI(-)	Lognormal	-0.025	(-0.038, -0.011)	0.001	0.054	7.542	(-0.038, -0.010)
PC (p-36:4)/PC (o-36:5) - ESI(-)	Lognormal	-0.025	(-0.040, -0.011)	0.001	0.064	7.044	(-0.040, -0.011)
PC (p-34:1)/PC (o-34:2) A	Lognormal	-0.035	(-0.055, -0.015)	0.001	0.064	6.285	(-0.057, -0.015)
PC (p-36:1)/PC (o-36:2)	Lognormal	-0.067	(-0.106, -0.029)	0.001	0.064	5.458	(-0.107, -0.030)
PE (p-34:2)/PE (o-34:3)	Lognormal	-0.042	(-0.066, -0.018)	0.001	0.064	6.155	(-0.067, -0.020)
SM (d40:3)	Lognormal	-0.035	(-0.055, -0.014)	0.001	0.064	6.392	(-0.055, -0.015)
PE (p-36:2)/PE (o-36:3) - ESI(-)	Lognormal	-0.032	(-0.052, -0.012)	0.002	0.125	2.051	(-0.052, -0.011)
PE (p-36:4)/PE (o-36:5) - ESI(-)	Lognormal	-0.026	(-0.044, -0.009)	0.003	0.157	2.676	(-0.044, -0.009)
CE (18:2)	Lognormal	-0.012	(-0.019, -0.004)	0.004	0.169	1.882	(-0.020, -0.003)
PC (36:5) A	Lognormal	-0.060	(-0.100, -0.019)	0.005	0.169	2.389	(-0.100, -0.017)
LPC (18:2) - ESI(-)	Lognormal	-0.022	(-0.036, -0.007)	0.005	0.169	2.295	(-0.037, -0.007)
PC (34:2) - ESI(-)	Lognormal	-0.011	(-0.018, -0.003)	0.005	0.169	3.075	(-0.017, -0.003)
PC (p-36:2)/PC (o-36:3)	Lognormal	-0.020	(-0.034, -0.006)	0.006	0.183	1.539	(-0.034, -0.006)
TG (56:6)	Lognormal	0.012	(0.004, 0.021)	0.006	0.183	2.004	(0.004, 0.021)
PC (p-36:3)/PC (o-36:4) - ESI(-)	Lognormal	-0.017	(-0.029, -0.005)	0.007	0.192	1.692	(-0.029, -0.004)
TG (55:6)	Lognormal	0.026	(0.008, 0.045)	0.007	0.192	1.601	(0.007, 0.044)
PC (36:5)A	Lognormal	-0.029	(-0.050, -0.008)	0.007	0.195	1.405	(-0.049, -0.008)
SM (d34:2) - ESI(-)	Lognormal	-0.011	(-0.018, -0.003)	0.008	0.202	1.323	(-0.019, -0.003)
SM (d34:1) - ESI(-)	Lognormal	-0.009	(-0.016, -0.003)	0.008	0.202	1.173	(-0.017, -0.003)
LPE (18:2) - ESI(-)	Lognormal	-0.032	(-0.055, -0.009)	0.008	0.202	1.353	(-0.057, -0.010)
TG (54:6) C	Lognormal	0.015	(0.004, 0.027)	0.009	0.202	1.126	(0.004, 0.027)
PC (34:3)	Lognormal	-0.019	(-0.033, -0.005)	0.009	0.202	1.163	(-0.033, -0.005)
PE (p-38:5)/PE (o-38:6) - ESI(-)	Lognormal	-0.023	(-0.040, -0.006)	0.009	0.202	1.093	(-0.041, -0.007)
LPE (18:2) - ESI(+)	Lognormal	-0.027	(-0.046, -0.007)	0.009	0.206	1.090	(-0.046, -0.005)
SM (d38:2) - ESI(-)	Lognormal	-0.016	(-0.028, -0.004)	0.010	0.211	1.159	(-0.028, -0.004)
LPC (18:2) - ESI(+)	Lognormal	-0.016	(-0.028, -0.004)	0.011	0.218	0.698	(-0.029, -0.003)
PE (p-36:1)/PE (o-36:2) - ESI(-)	Lognormal	-0.028	(-0.049, -0.007)	0.011	0.218	0.873	(-0.049, -0.007)
SM (d39:1) - ESI(-)	Lognormal	-0.016	(-0.029, -0.004)	0.011	0.218	1.051	(-0.028, -0.004)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
PC (32:2) - ESI(-)	Lognormal	-0.023	(-0.041, -0.006)	0.011	0.218	0.909	(-0.041, -0.005)
PC (p-38:4)/PC (o-38:5) A	Lognormal	-0.014	(-0.025, -0.003)	0.012	0.218	0.854	(-0.024, -0.003)
TG (54:7) B	Lognormal	0.022	(0.005, 0.040)	0.013	0.225	1.036	(0.006, 0.040)
PC (33:2) - ESI(+)	Lognormal	-0.013	(-0.024, -0.003)	0.013	0.225	0.837	(-0.024, -0.003)
AC (10:1)	Lognormal	-0.029	(-0.052, -0.006)	0.013	0.225	1.070	(-0.051, -0.007)
PC (34:3) B	Lognormal	-0.013	(-0.024, -0.003)	0.014	0.229	0.846	(-0.023, -0.003)
LPC (18:3)	Lognormal	-0.025	(-0.045, -0.005)	0.014	0.229	0.729	(-0.046, -0.006)
PE (p-38:4)/PE (o-38:5)	Lognormal	-0.015	(-0.027, -0.003)	0.015	0.239	0.663	(-0.027, -0.003)
CE (20:2)	Lognormal	-0.030	(-0.054, -0.006)	0.016	0.240	0.750	(-0.055, -0.007)
SM (d40:1) - ESI(-)	Lognormal	-0.011	(-0.020, -0.002)	0.016	0.242	0.682	(-0.020, -0.002)
PC (o-34:0)	Lognormal	-0.019	(-0.035, -0.004)	0.017	0.248	0.675	(-0.035, -0.004)
PC (35:2)	Lognormal	-0.015	(-0.027, -0.003)	0.017	0.249	0.672	(-0.027, -0.002)
Ceramide (d42:1) - ESI (+)	Lognormal	-0.008	(-0.015, -0.002)	0.019	0.256	0.671	(-0.016, -0.002)
FA (16:1) (palmitoleic acid)	Lognormal	0.018	(0.003, 0.033)	0.019	0.256	0.598	(0.003, 0.033)
PE (p-36:4)/PE (o-36:5) - ESI(+)	Lognormal	-0.017	(-0.032, -0.003)	0.019	0.256	0.515	(-0.031, -0.003)
PC (32:2) - ESI(+)	Lognormal	-0.018	(-0.033, -0.003)	0.020	0.266	0.646	(-0.033, -0.003)
TG (56:7) B	Lognormal	0.024	(0.004, 0.045)	0.021	0.274	0.582	(0.005, 0.046)
PC (p-38:3)/PC (o-38:4) - ESI(-)	Lognormal	-0.016	(-0.029, -0.003)	0.022	0.274	0.526	(-0.030, -0.003)
SM (d40:2) B - ESI(+)	Lognormal	-0.008	(-0.015, -0.001)	0.022	0.274	0.652	(-0.015, -0.002)
PE (p-40:4)/PE (o-40:5) A	Lognormal	-0.029	(-0.053, -0.004)	0.022	0.274	0.494	(-0.053, -0.004)
TG (54:5) B	Lognormal	0.013	(0.002, 0.023)	0.022	0.274	0.575	(0.002, 0.023)
SM (d40:2) B - ESI(-)	Lognormal	-0.012	(-0.023, -0.002)	0.022	0.274	0.661	(-0.023, -0.002)
TG (58:8)	Lognormal	0.024	(0.003, 0.046)	0.025	0.291	0.522	(0.003, 0.045)
PC (35:3)	Lognormal	-0.010	(-0.019, -0.001)	0.025	0.291	0.513	(-0.019, -0.001)
PC (p-36:4)/PC (o-36:5) - ESI(+)	Lognormal	-0.010	(-0.019, -0.001)	0.025	0.291	0.592	(-0.019, -0.002)
TG (56:5) B	Lognormal	0.016	(0.002, 0.029)	0.028	0.312	0.405	(0.002, 0.030)
TG (53:0)	Lognormal	-0.020	(-0.037, -0.002)	0.029	0.315	0.487	(-0.038, -0.002)
SM (d33:1) - ESI(-)	Lognormal	-0.015	(-0.028, -0.002)	0.029	0.315	0.371	(-0.029, -0.001)
PC (p-32:1)/PC (o-32:2)	Lognormal	-0.012	(-0.023, -0.001)	0.031	0.315	0.413	(-0.023, -0.001)
TG (62:4)	Lognormal	-0.034	(-0.064, -0.003)	0.031	0.315	0.492	(-0.063, -0.003)
PE (36:2)	Lognormal	-0.022	(-0.042, -0.002)	0.031	0.315	0.386	(-0.042, -0.002)
PE (p-36:1)/PE (o-36:2) - ESI(+)	Lognormal	-0.021	(-0.040, -0.002)	0.031	0.315	0.392	(-0.040, -0.002)
PE (p-34:1)/PE (o-34:2) - ESI(-)	Lognormal	-0.019	(-0.036, -0.002)	0.032	0.315	0.372	(-0.036, -0.002)
TG (50:0)	Lognormal	-0.026	(-0.050, -0.003)	0.032	0.315	0.405	(-0.048, -0.001)
SM (d32:1) - ESI(-)	Lognormal	-0.012	(-0.023, -0.001)	0.033	0.317	0.347	(-0.023, -0.001)
LPE (20:4) - ESI(-)	Lognormal	-0.021	(-0.040, -0.002)	0.033	0.317	0.414	(-0.040, -0.001)
PE (p-38:5)/PE (o-38:6) - ESI(+)	Lognormal	-0.013	(-0.025, -0.001)	0.033	0.317	0.381	(-0.025, -0.001)
SM (d42:3) - ESI(-)	Lognormal	-0.009	(-0.018, -0.001)	0.034	0.320	0.349	(-0.018, 0.000)
Ceramide (d41:1) - ESI(-)	Lognormal	-0.012	(-0.024, -0.001)	0.036	0.320	0.392	(-0.024, -0.001)
PC (p-32:0)/PC (o-32:1) - ESI(+)	Lognormal	-0.009	(-0.017, -0.001)	0.036	0.320	0.355	(-0.017, -0.001)
PC (36:4) B - ESI(-)	Lognormal	-0.008	(-0.015, -0.001)	0.037	0.322	0.357	(-0.015, 0.000)
DG (38:5)	Lognormal	0.015	(0.001, 0.028)	0.037	0.322	0.342	(0.001, 0.028)
DG (38:6)	Lognormal	0.020	(0.001, 0.038)	0.038	0.322	0.300	(0.001, 0.038)
Ceramide (d42:2) B - ESI (+)	Lognormal	-0.010	(-0.020, -0.001)	0.039	0.324	0.338	(-0.020, -0.001)
PC (34:3) C	Lognormal	-0.017	(-0.033, -0.001)	0.039	0.326	0.309	(-0.032, -0.002)
TG (58:9)	Lognormal	0.021	(0.001, 0.042)	0.042	0.337	0.285	(0.000, 0.042)
PE (p-34:1)/PE (o-34:2) - ESI(+)	Lognormal	-0.016	(-0.031, -0.001)	0.042	0.338	0.310	(-0.031, 0.000)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
SM (d42:1) - ESI(-)	Lognormal	-0.009	(-0.018, 0.000)	0.043	0.338	0.304	(-0.018, -0.001)
AC (18:2)	Lognormal	-0.018	(-0.034, -0.001)	0.043	0.338	0.292	(-0.034, -0.001)
Ceramide (d42:1) - ESI(-)	Lognormal	-0.010	(-0.019, 0.000)	0.048	0.365	0.294	(-0.020, -0.001)
Ceramide (d34:1) - ESI(-)	Lognormal	-0.008	(-0.017, 0.000)	0.048	0.365	0.255	(-0.018, 0.000)
PC (p-38:4)/PC (o-38:5) B	Lognormal	-0.012	(-0.023, 0.000)	0.048	0.365	0.300	(-0.024, -0.001)
CE (18:3)	Lognormal	-0.015	(-0.030, 0.000)	0.050	0.373	0.289	(-0.030, 0.000)
AC (14:2)	Lognormal	-0.027	(-0.054, 0.000)	0.050	0.373	0.294	(-0.056, -0.001)
PC (40:5) A - ESI(+)	Lognormal	0.010	(0.000, 0.019)	0.052	0.376	0.263	(0.000, 0.019)
PC (33:2) - ESI(-)	Lognormal	-0.018	(-0.037, 0.000)	0.052	0.376	0.258	(-0.035, 0.002)
PC (37:2) - ESI(+)	Lognormal	-0.010	(-0.021, 0.000)	0.052	0.376	0.286	(-0.020, 0.000)
LPC (14:0) - ESI(+)	Lognormal	-0.017	(-0.034, 0.000)	0.054	0.379	0.266	(-0.034, 0.001)
TG (54:6) B	Lognormal	-0.039	(-0.078, 0.000)	0.054	0.379	0.232	(-0.077, 0.003)
SM (d36:3) - ESI(-)	Lognormal	-0.018	(-0.037, 0.000)	0.056	0.380	0.234	(-0.038, 0.000)
FA (18:1) (oleic acid)	Lognormal	0.009	(0.000, 0.017)	0.056	0.380	0.229	(0.000, 0.017)
PC (p-36:3)/PC (o-36:4) - ESI(+)	Lognormal	-0.009	(-0.019, 0.000)	0.057	0.380	0.248	(-0.019, 0.000)
FA (14:1) (physeteric acid)	Lognormal	0.019	(0.000, 0.038)	0.058	0.383	0.238	(0.000, 0.038)
PC (34:0) - ESI(-)	Lognormal	-0.009	(-0.019, 0.000)	0.060	0.390	0.227	(-0.019, 0.001)
Ceramide (d40:1)	Lognormal	-0.008	(-0.016, 0.000)	0.064	0.399	0.230	(-0.016, 0.001)
SM (d36:0) - ESI(+)	Lognormal	0.015	(-0.001, 0.030)	0.064	0.399	0.238	(-0.001, 0.030)
LPC (16:0) - ESI(-)	Lognormal	-0.009	(-0.018, 0.000)	0.064	0.399	0.221	(-0.017, 0.001)
PE (p-40:5)/PE (o-40:6)	Lognormal	-0.010	(-0.021, 0.001)	0.066	0.407	0.213	(-0.022, 0.000)
LPC (18:0) A - ESI(-)	Lognormal	-0.015	(-0.032, 0.001)	0.069	0.414	0.220	(-0.031, 0.002)
PC (38:4) A - ESI(-)	Lognormal	-0.009	(-0.019, 0.001)	0.069	0.416	0.227	(-0.019, 0.001)
TG (54:7) A	Lognormal	-0.023	(-0.048, 0.002)	0.070	0.416	0.198	(-0.048, 0.001)
TG (56:8) B	Lognormal	0.022	(-0.002, 0.045)	0.072	0.419	0.190	(-0.001, 0.046)
PE (36:3)	Lognormal	-0.027	(-0.057, 0.002)	0.075	0.429	0.228	(-0.056, 0.003)
PC (37:4) - ESI(+)	Lognormal	0.011	(-0.001, 0.024)	0.076	0.430	0.209	(-0.001, 0.024)
PC (34:4) - ESI(-)	Lognormal	-0.024	(-0.051, 0.002)	0.077	0.434	0.191	(-0.052, 0.000)
SM (d36:1) - ESI(-)	Lognormal	-0.008	(-0.017, 0.001)	0.077	0.435	0.176	(-0.016, 0.001)
AC (12:1)	Lognormal	-0.020	(-0.043, 0.002)	0.080	0.443	0.205	(-0.042, 0.001)
Cholesterol	Lognormal	-0.006	(-0.014, 0.001)	0.082	0.444	0.195	(-0.014, 0.001)
PC (p-38:3)/PC (o-38:4) A - ESI(+)	Lognormal	-0.010	(-0.021, 0.001)	0.083	0.444	0.180	(-0.021, 0.001)
PC (p-38:3)/PC (o-38:4) B - ESI(+)	Lognormal	-0.010	(-0.022, 0.001)	0.086	0.444	0.158	(-0.021, 0.002)
AC (10:0)	Lognormal	-0.030	(-0.064, 0.004)	0.086	0.444	0.139	(-0.067, 0.004)
TG (60:11)	Lognormal	0.030	(-0.004, 0.065)	0.086	0.444	0.176	(-0.005, 0.064)
PC (p-38:4)/PC (o-38:5) B	Lognormal	-0.018	(-0.038, 0.003)	0.089	0.451	0.185	(-0.037, 0.003)
TG (52:4)	Lognormal	-0.009	(-0.020, 0.001)	0.092	0.457	0.177	(-0.019, 0.001)
LPC (18:0) B - ESI(-)	Lognormal	-0.010	(-0.022, 0.002)	0.092	0.457	0.133	(-0.022, 0.001)
SM (d41:2) B - ESI(+)	Lognormal	-0.008	(-0.017, 0.001)	0.092	0.457	0.151	(-0.017, 0.001)
TG (58:6)	Lognormal	0.011	(-0.002, 0.023)	0.093	0.457	0.176	(-0.001, 0.024)
PC (p-36:1)/PC (o-36:2) B	Lognormal	-0.014	(-0.031, 0.002)	0.093	0.457	0.158	(-0.031, 0.002)
PC (37:5)	Lognormal	0.017	(-0.003, 0.037)	0.094	0.457	0.154	(-0.004, 0.038)
PC (36:5) D	Lognormal	0.018	(-0.003, 0.040)	0.095	0.461	0.150	(-0.004, 0.039)
SM (d40:1) - ESI(+)	Lognormal	-0.005	(-0.011, 0.001)	0.096	0.464	0.165	(-0.011, 0.001)
PC (35:2) B	Lognormal	-0.006	(-0.013, 0.001)	0.097	0.465	0.177	(-0.014, 0.001)
PC (36:3) A - ESI(+)	Lognormal	-0.007	(-0.014, 0.001)	0.097	0.465	0.161	(-0.015, 0.001)
PC (p-32:0)/PC (o-32:1) - ESI(-)	Lognormal	-0.014	(-0.030, 0.002)	0.099	0.465	0.153	(-0.031, 0.002)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
SM (d43:1) - ESI(-)	Lognormal	-0.024	(-0.053, 0.004)	0.100	0.471	0.149	(-0.053, 0.006)
PC (40:6)B	Lognormal	0.010	(-0.002, 0.021)	0.103	0.480	0.153	(-0.002, 0.022)
TG (48:0)	Lognormal	-0.019	(-0.041, 0.004)	0.103	0.480	0.153	(-0.040, 0.005)
SM (d42:0) - ESI(+)	Lognormal	0.023	(-0.005, 0.051)	0.108	0.492	0.139	(-0.006, 0.051)
SM (d30:1) - ESI(-)	Lognormal	-0.023	(-0.051, 0.005)	0.109	0.492	0.154	(-0.050, 0.005)
PC (36:3) B - ESI(-)	Lognormal	-0.008	(-0.017, 0.002)	0.109	0.492	0.129	(-0.016, 0.002)
Ceramide (d32:1)	Lognormal	-0.012	(-0.027, 0.003)	0.109	0.492	0.141	(-0.026, 0.003)
PE (p-40:4)/PE (o-40:5) B	Lognormal	-0.013	(-0.028, 0.003)	0.110	0.493	0.106	(-0.027, 0.004)
DG (36:4) B	Lognormal	0.034	(-0.008, 0.076)	0.112	0.494	0.145	(-0.008, 0.077)
TG (48:4) A	Lognormal	-0.023	(-0.052, 0.005)	0.114	0.501	0.131	(-0.054, 0.005)
PC (34:3) A	Lognormal	-0.008	(-0.018, 0.002)	0.114	0.501	0.135	(-0.018, 0.002)
PC (35:1) - ESI(+)	Lognormal	0.007	(-0.002, 0.015)	0.115	0.501	0.130	(-0.002, 0.014)
LPC (p-16:0)/LPC (o-16:1)	Lognormal	-0.011	(-0.025, 0.003)	0.116	0.502	0.134	(-0.026, 0.002)
PC (p-38:5)/PC (o-38:6) B	Lognormal	-0.007	(-0.017, 0.002)	0.120	0.510	0.138	(-0.017, 0.002)
TG (49:2)	Lognormal	0.017	(-0.004, 0.039)	0.121	0.512	0.128	(-0.005, 0.038)
LPC (20:3) - ESI(-)	Lognormal	-0.017	(-0.038, 0.004)	0.121	0.512	0.127	(-0.039, 0.004)
Ceramide (d41:1) - ESI (+)	Lognormal	-0.008	(-0.018, 0.002)	0.122	0.512	0.135	(-0.018, 0.002)
AC (12:0)	Lognormal	-0.018	(-0.041, 0.005)	0.123	0.513	0.124	(-0.041, 0.005)
PC (36:3) A - ESI(-)	Lognormal	-0.008	(-0.019, 0.002)	0.124	0.515	0.119	(-0.018, 0.002)
FA (20:3) (homo-gamma-linolenic acid)	Lognormal	0.008	(-0.002, 0.018)	0.124	0.515	0.125	(-0.002, 0.017)
PC (42:10)	Lognormal	0.019	(-0.005, 0.043)	0.126	0.519	0.133	(-0.006, 0.042)
Lactosylceramide (d18:1/24:1(15Z))	Lognormal	0.013	(-0.004, 0.030)	0.127	0.520	0.125	(-0.004, 0.030)
TG (60:6)	Lognormal	0.019	(-0.005, 0.043)	0.129	0.521	0.110	(-0.006, 0.042)
PE (p-40:4)/PE (o-40:5)	Lognormal	-0.014	(-0.031, 0.004)	0.130	0.521	0.093	(-0.030, 0.004)
PC (38:5) A	Lognormal	0.005	(-0.001, 0.011)	0.130	0.521	0.125	(-0.001, 0.012)
PC (34:1)	Lognormal	0.003	(-0.001, 0.007)	0.130	0.521	0.109	(-0.001, 0.007)
TG (56:5) A	Lognormal	0.012	(-0.003, 0.027)	0.131	0.521	0.135	(-0.003, 0.027)
DG (36:4) A	Lognormal	-0.015	(-0.035, 0.004)	0.132	0.521	0.118	(-0.035, 0.004)
AC (8:0)	Lognormal	-0.026	(-0.060, 0.008)	0.133	0.521	0.123	(-0.059, 0.008)
Ceramide (d39:1)	Lognormal	-0.014	(-0.032, 0.004)	0.133	0.521	0.120	(-0.032, 0.004)
PC (38:6) A - ESI(+)	Lognormal	-0.007	(-0.016, 0.002)	0.134	0.521	0.117	(-0.016, 0.002)
PC (38:5) B - ESI(+)	Lognormal	0.010	(-0.003, 0.024)	0.135	0.523	0.120	(-0.002, 0.024)
SM (d40:0)	Lognormal	0.011	(-0.003, 0.025)	0.138	0.529	0.102	(-0.004, 0.025)
PC (o-32:0) - ESI(+)	Lognormal	-0.006	(-0.015, 0.002)	0.144	0.535	0.110	(-0.015, 0.002)
PE (p-38:3)/PE (o-38:4)	Lognormal	-0.022	(-0.052, 0.007)	0.145	0.535	0.119	(-0.053, 0.007)
TG (56:9)	Lognormal	0.016	(-0.005, 0.037)	0.145	0.535	0.116	(-0.006, 0.038)
TG (50:4)	Lognormal	-0.012	(-0.028, 0.004)	0.147	0.535	0.114	(-0.028, 0.004)
PC (p-34:1)/PC (o-34:2) B	Lognormal	-0.016	(-0.039, 0.006)	0.150	0.543	0.118	(-0.041, 0.005)
SM (d34:0) - ESI(-)	Lognormal	-0.011	(-0.027, 0.004)	0.154	0.551	0.096	(-0.025, 0.005)
PE (p-38:6)/PE (o-38:7)	Lognormal	-0.015	(-0.035, 0.006)	0.163	0.568	0.091	(-0.034, 0.007)
SM (d38:1)	Lognormal	-0.004	(-0.011, 0.002)	0.170	0.589	0.100	(-0.010, 0.002)
FA (24:0) (lignoceric acid)	Lognormal	-0.009	(-0.021, 0.004)	0.172	0.589	0.102	(-0.022, 0.003)
SM (d34:1) - ESI(+)	Lognormal	-0.004	(-0.009, 0.002)	0.173	0.591	0.094	(-0.008, 0.001)
CE (20:3)	Lognormal	-0.009	(-0.021, 0.004)	0.174	0.591	0.097	(-0.021, 0.004)
LPC (20:2) - ESI(+)	Lognormal	-0.025	(-0.061, 0.011)	0.175	0.591	0.106	(-0.061, 0.012)
PC (42:6)	Lognormal	0.018	(-0.008, 0.044)	0.177	0.591	0.099	(-0.009, 0.042)
DG (32:0)	Lognormal	0.012	(-0.005, 0.029)	0.179	0.593	0.094	(-0.007, 0.028)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
CE (20:5)	Lognormal	0.018	(-0.008, 0.045)	0.181	0.596	0.094	(-0.009, 0.045)
PC (o-32:0) - ESI(-)	Lognormal	-0.010	(-0.024, 0.004)	0.182	0.596	0.088	(-0.024, 0.005)
PC (32:0) - ESI(-)	Lognormal	-0.006	(-0.016, 0.003)	0.182	0.596	0.078	(-0.016, 0.003)
PC (40:8) - ESI(-)	Lognormal	-0.012	(-0.029, 0.005)	0.183	0.596	0.085	(-0.027, 0.006)
Ceramide (d38:1) - ESI(+)	Lognormal	-0.007	(-0.016, 0.003)	0.184	0.596	0.088	(-0.015, 0.004)
Ceramide (d43:1)	Lognormal	-0.019	(-0.046, 0.009)	0.189	0.601	0.092	(-0.049, 0.008)
SM (d42:1) - ESI(+)	Lognormal	-0.005	(-0.013, 0.003)	0.190	0.601	0.098	(-0.013, 0.003)
PC (37:2) - ESI(-)	Lognormal	-0.017	(-0.041, 0.008)	0.190	0.601	0.085	(-0.042, 0.008)
PC (38:3) - ESI(-)	Lognormal	-0.008	(-0.019, 0.004)	0.193	0.605	0.087	(-0.020, 0.004)
SM (d39:2)	Lognormal	-0.006	(-0.015, 0.003)	0.195	0.605	0.092	(-0.015, 0.003)
SM (d30:1) - ESI(+)	Lognormal	-0.014	(-0.035, 0.007)	0.195	0.605	0.102	(-0.036, 0.007)
LPC (o-16:0)	Lognormal	-0.010	(-0.025, 0.005)	0.196	0.605	0.088	(-0.025, 0.006)
LPC (20:2) - ESI(-)	Lognormal	-0.009	(-0.024, 0.005)	0.197	0.605	0.091	(-0.023, 0.006)
LPC (18:1) - ESI(-)	Lognormal	-0.009	(-0.022, 0.005)	0.197	0.605	0.085	(-0.022, 0.005)
LPC (20:3) - ESI(+)	Lognormal	-0.009	(-0.022, 0.004)	0.198	0.605	0.084	(-0.022, 0.004)
PC (38:6) B - ESI(+)	Lognormal	0.005	(-0.002, 0.012)	0.198	0.605	0.091	(-0.002, 0.012)
FA (20:3) (eicosatrienoic acid)	Lognormal	0.011	(-0.006, 0.029)	0.203	0.610	0.081	(-0.006, 0.029)
PC (p-44:4)/PC (o-44:5) - ESI(-)	Lognormal	-0.010	(-0.026, 0.005)	0.203	0.610	0.082	(-0.025, 0.005)
CE (14:0)	Lognormal	-0.025	(-0.064, 0.014)	0.205	0.610	0.091	(-0.063, 0.014)
TG (56:8) A	Lognormal	0.010	(-0.005, 0.024)	0.207	0.610	0.085	(-0.005, 0.025)
Ceramide (d33:1)	Lognormal	-0.009	(-0.024, 0.005)	0.208	0.610	0.085	(-0.023, 0.005)
TG (46:0)	Lognormal	-0.024	(-0.062, 0.014)	0.211	0.610	0.082	(-0.062, 0.015)
PE (38:6) - ESI(+)	Lognormal	0.021	(-0.012, 0.055)	0.213	0.610	0.083	(-0.010, 0.056)
SM (d34:2) - ESI(+)	Lognormal	-0.004	(-0.011, 0.002)	0.213	0.610	0.086	(-0.011, 0.003)
AC (18:0)	Lognormal	-0.009	(-0.023, 0.005)	0.214	0.610	0.083	(-0.023, 0.005)
TG (51:2)	Lognormal	0.010	(-0.006, 0.025)	0.217	0.615	0.085	(-0.006, 0.025)
LPC (14:0) - ESI(-)	Lognormal	-0.019	(-0.049, 0.011)	0.218	0.617	0.083	(-0.050, 0.011)
TG (54:6) A	Lognormal	-0.012	(-0.030, 0.007)	0.222	0.622	0.077	(-0.031, 0.006)
FA (22:0) (behenic acid)	Lognormal	-0.009	(-0.022, 0.005)	0.223	0.623	0.072	(-0.022, 0.005)
Ceramide (d42:2) B - ESI(-)	Lognormal	-0.014	(-0.035, 0.008)	0.224	0.624	0.086	(-0.037, 0.007)
SM (d39:1) - ESI(+)	Lognormal	-0.007	(-0.017, 0.004)	0.226	0.624	0.083	(-0.017, 0.004)
TG (50:5)	Lognormal	-0.014	(-0.037, 0.009)	0.226	0.624	0.090	(-0.036, 0.008)
TG (46:4) A	Lognormal	-0.025	(-0.066, 0.016)	0.230	0.624	0.075	(-0.068, 0.013)
GlcCer (d42:2) - ESI(+)	Lognormal	0.009	(-0.005, 0.023)	0.230	0.624	0.084	(-0.005, 0.024)
LPC (16:1) - ESI(-)	Lognormal	-0.011	(-0.029, 0.007)	0.231	0.624	0.079	(-0.030, 0.007)
PC (35:2) A	Lognormal	0.006	(-0.004, 0.016)	0.233	0.629	0.069	(-0.004, 0.016)
TG (51:4)	Lognormal	-0.010	(-0.025, 0.006)	0.236	0.633	0.077	(-0.026, 0.005)
PC (38:2)	Lognormal	-0.008	(-0.022, 0.005)	0.237	0.634	0.073	(-0.022, 0.004)
PC 40:5e	Lognormal	-0.006	(-0.017, 0.004)	0.239	0.636	0.076	(-0.016, 0.005)
PC (37:4) - ESI(-)	Lognormal	-0.010	(-0.025, 0.006)	0.240	0.636	0.080	(-0.026, 0.005)
SM (d36:3) - ESI(+)	Lognormal	-0.008	(-0.022, 0.006)	0.241	0.636	0.073	(-0.022, 0.005)
PE (34:2) - ESI(-)	Lognormal	-0.017	(-0.047, 0.012)	0.242	0.636	0.084	(-0.047, 0.011)
TG (48:5)	Lognormal	-0.021	(-0.055, 0.014)	0.243	0.636	0.071	(-0.055, 0.014)
GlcCer (d38:1)	Lognormal	-0.008	(-0.022, 0.006)	0.244	0.636	0.069	(-0.022, 0.005)
PC (p-42:4)/PC (o-42:5) - ESI(-)	Lognormal	-0.013	(-0.034, 0.009)	0.244	0.636	0.075	(-0.035, 0.009)
TG (54:9)	Lognormal	0.039	(-0.026, 0.104)	0.245	0.636	0.065	(-0.027, 0.101)
LPE (18:0)	Lognormal	-0.009	(-0.024, 0.006)	0.251	0.637	0.069	(-0.023, 0.007)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
TG (58:4)	Lognormal	0.015	(-0.010, 0.039)	0.252	0.637	0.085	(-0.012, 0.039)
PC (34:4) - ESI(+)	Lognormal	-0.010	(-0.028, 0.007)	0.254	0.637	0.071	(-0.027, 0.007)
TG (42:0)	Lognormal	-0.023	(-0.063, 0.017)	0.257	0.642	0.074	(-0.062, 0.015)
TG (53:2)	Lognormal	0.008	(-0.006, 0.022)	0.258	0.642	0.079	(-0.006, 0.022)
PC (p-38:4)/PC (o-38:5) A	Lognormal	-0.004	(-0.012, 0.003)	0.259	0.642	0.066	(-0.012, 0.003)
TG (46:3) A	Lognormal	-0.026	(-0.071, 0.019)	0.262	0.642	0.069	(-0.070, 0.017)
TG (56:5) C	Lognormal	0.007	(-0.006, 0.020)	0.265	0.642	0.068	(-0.005, 0.020)
PC (36:1) - ESI(+)	Lognormal	0.004	(-0.003, 0.011)	0.265	0.642	0.073	(-0.003, 0.010)
FA (20:1) (eicosenoic acid)	Lognormal	0.006	(-0.005, 0.017)	0.266	0.644	0.079	(-0.005, 0.017)
PC (37:6)	Lognormal	0.012	(-0.009, 0.033)	0.268	0.647	0.075	(-0.010, 0.032)
LPE (22:6)	Lognormal	-0.012	(-0.032, 0.009)	0.270	0.649	0.069	(-0.033, 0.009)
SM (d40:2) A - ESI(+)	Lognormal	-0.008	(-0.021, 0.006)	0.272	0.650	0.077	(-0.021, 0.006)
LPC (20:5)	Lognormal	0.018	(-0.014, 0.049)	0.274	0.651	0.071	(-0.011, 0.051)
SM (d36:2) - ESI(-)	Lognormal	-0.007	(-0.020, 0.006)	0.279	0.655	0.073	(-0.020, 0.007)
DG (36:5)	Lognormal	-0.014	(-0.038, 0.011)	0.279	0.655	0.071	(-0.037, 0.012)
PC (42:5)	Lognormal	0.009	(-0.007, 0.024)	0.282	0.657	0.074	(-0.007, 0.024)
SM (d44:2)	Lognormal	0.008	(-0.007, 0.024)	0.286	0.657	0.065	(-0.007, 0.023)
LPE (16:0)	Lognormal	-0.013	(-0.037, 0.011)	0.286	0.657	0.067	(-0.039, 0.011)
SM (d32:1) - ESI(+)	Lognormal	-0.006	(-0.017, 0.005)	0.287	0.657	0.065	(-0.018, 0.005)
SM (d41:3)	Lognormal	-0.005	(-0.015, 0.004)	0.289	0.657	0.069	(-0.015, 0.004)
TG (42:1)	Lognormal	-0.036	(-0.101, 0.030)	0.289	0.657	0.062	(-0.099, 0.030)
TG (60:12)	Lognormal	0.024	(-0.020, 0.068)	0.291	0.659	0.068	(-0.020, 0.070)
PC (p-40:3)/PC (o-40:4)	Lognormal	-0.011	(-0.031, 0.009)	0.297	0.668	0.063	(-0.030, 0.010)
PC (40:4) - ESI(-)	Lognormal	-0.011	(-0.032, 0.010)	0.298	0.668	0.062	(-0.033, 0.010)
FA (20:5) (eicosapentaenoic acid)	Lognormal	0.015	(-0.014, 0.044)	0.299	0.668	0.063	(-0.011, 0.048)
DG (36:2)	Lognormal	0.007	(-0.006, 0.020)	0.305	0.676	0.067	(-0.007, 0.019)
AC (14:1)	Lognormal	-0.013	(-0.038, 0.012)	0.309	0.676	0.063	(-0.039, 0.010)
SM (d40:2) A - ESI(-)	Lognormal	-0.009	(-0.027, 0.009)	0.312	0.676	0.067	(-0.027, 0.009)
DG (36:1)	Lognormal	0.009	(-0.009, 0.027)	0.312	0.676	0.064	(-0.009, 0.027)
LPC (17:1)	Lognormal	0.009	(-0.008, 0.025)	0.314	0.676	0.063	(-0.007, 0.026)
PG (34:0)/PG (17:0/17:0)	Lognormal	-0.011	(-0.032, 0.010)	0.314	0.676	0.061	(-0.032, 0.010)
SM (d43:2) - ESI(-)	Lognormal	-0.011	(-0.032, 0.010)	0.314	0.676	0.063	(-0.034, 0.010)
SM (d36:0) - ESI(-)	Lognormal	0.016	(-0.015, 0.048)	0.316	0.678	0.063	(-0.016, 0.048)
SM (d38:0)	Lognormal	0.036	(-0.035, 0.108)	0.321	0.684	0.065	(-0.034, 0.109)
TG (42:3)	Lognormal	-0.021	(-0.062, 0.020)	0.323	0.684	0.055	(-0.064, 0.019)
Ceramide (d44:1)	Lognormal	-0.014	(-0.040, 0.013)	0.325	0.684	0.068	(-0.039, 0.015)
PC (36:3) B - ESI(+)	Lognormal	-0.003	(-0.010, 0.003)	0.326	0.684	0.062	(-0.011, 0.003)
TG (40:1)	Lognormal	-0.022	(-0.066, 0.022)	0.327	0.684	0.058	(-0.066, 0.023)
Ceramide (d38:1) - ESI(-)	Lognormal	-0.007	(-0.020, 0.007)	0.327	0.684	0.060	(-0.021, 0.006)
PC (33:1) - ESI(+)	Lognormal	0.006	(-0.006, 0.017)	0.333	0.690	0.061	(-0.005, 0.016)
TG (48:3)	Lognormal	-0.011	(-0.034, 0.011)	0.333	0.690	0.059	(-0.034, 0.011)
Ceramide (d42:2) A - ESI(-)	Lognormal	-0.005	(-0.015, 0.005)	0.333	0.690	0.063	(-0.015, 0.005)
SM (d32:2) - ESI(+)	Lognormal	-0.006	(-0.019, 0.006)	0.335	0.691	0.061	(-0.019, 0.006)
TG (44:0)	Lognormal	-0.018	(-0.054, 0.018)	0.336	0.691	0.057	(-0.056, 0.019)
TG (54:5) A	Lognormal	-0.007	(-0.021, 0.007)	0.337	0.691	0.058	(-0.020, 0.007)
TG (52:2)	Lognormal	0.004	(-0.004, 0.012)	0.337	0.691	0.062	(-0.004, 0.012)
PI (38:4)/PI (18:0-20:4)	Lognormal	-0.004	(-0.013, 0.004)	0.340	0.691	0.061	(-0.012, 0.004)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
PC (37:3)	Lognormal	-0.007	(-0.022, 0.008)	0.340	0.691	0.064	(-0.022, 0.007)
TG (56:3)	Lognormal	0.010	(-0.011, 0.031)	0.342	0.691	0.068	(-0.011, 0.031)
SM (d32:2) - ESI(-)	Lognormal	-0.010	(-0.029, 0.010)	0.343	0.691	0.059	(-0.028, 0.011)
TG (46:4) B	Lognormal	-0.024	(-0.074, 0.025)	0.343	0.691	0.060	(-0.078, 0.022)
TG (46:2)	Lognormal	-0.016	(-0.049, 0.017)	0.345	0.691	0.058	(-0.050, 0.016)
PC (p-40:1)/PC (o-40:2)	Lognormal	0.011	(-0.011, 0.033)	0.350	0.697	0.061	(-0.014, 0.031)
PE (34:1)	Lognormal	-0.015	(-0.046, 0.016)	0.354	0.701	0.061	(-0.049, 0.016)
SM (d41:1) - ESI(+)	Lognormal	-0.004	(-0.012, 0.004)	0.355	0.701	0.062	(-0.012, 0.005)
SM (d38:2) - ESI(+)	Lognormal	-0.003	(-0.010, 0.004)	0.355	0.701	0.059	(-0.011, 0.004)
LPC (15:0)	Lognormal	-0.007	(-0.021, 0.008)	0.361	0.704	0.052	(-0.021, 0.008)
PC (p-40:7)/PC (o-40:8)	Lognormal	-0.020	(-0.062, 0.022)	0.363	0.704	0.060	(-0.061, 0.023)
PC (p-42:3)/PC (o-42:4)	Lognormal	-0.007	(-0.021, 0.008)	0.363	0.704	0.053	(-0.021, 0.008)
PE (36:4) - ESI(+)	Lognormal	0.010	(-0.012, 0.033)	0.366	0.705	0.057	(-0.013, 0.033)
SM (d42:3) - ESI(+)	Lognormal	-0.003	(-0.010, 0.004)	0.366	0.705	0.061	(-0.011, 0.004)
GlcCer (d41:1)	Lognormal	-0.006	(-0.020, 0.007)	0.369	0.709	0.053	(-0.020, 0.008)
TG (58:3)	Lognormal	0.014	(-0.016, 0.043)	0.371	0.711	0.058	(-0.018, 0.041)
TG (48:4) B	Lognormal	-0.019	(-0.060, 0.022)	0.375	0.711	0.055	(-0.059, 0.022)
PC (39:6)	Lognormal	0.008	(-0.010, 0.026)	0.376	0.711	0.057	(-0.010, 0.026)
PE (p-36:5)/PE (o-36:6)	Lognormal	-0.030	(-0.096, 0.036)	0.376	0.711	0.055	(-0.098, 0.035)
PC (36:4) B - ESI(+)	Lognormal	0.007	(-0.008, 0.022)	0.377	0.711	0.058	(-0.008, 0.023)
TG (54:1)	Lognormal	-0.010	(-0.032, 0.012)	0.384	0.719	0.053	(-0.030, 0.014)
FA (18:2) (linoleic acid)	Lognormal	0.004	(-0.005, 0.012)	0.392	0.728	0.051	(-0.005, 0.012)
LPE (20:4) - ESI(+)	Lognormal	-0.008	(-0.026, 0.010)	0.393	0.728	0.058	(-0.025, 0.012)
PC (p-42:5)/PC (o-42:6) A	Lognormal	-0.006	(-0.020, 0.008)	0.398	0.733	0.051	(-0.020, 0.007)
LPC (16:1) - ESI(+)	Lognormal	-0.005	(-0.016, 0.007)	0.402	0.733	0.054	(-0.016, 0.007)
PC (40:7) B - ESI(+)	Lognormal	0.005	(-0.006, 0.015)	0.403	0.733	0.054	(-0.006, 0.015)
GlcCer (d40:1) - ESI(-)	Lognormal	-0.005	(-0.018, 0.007)	0.404	0.733	0.052	(-0.018, 0.007)
PE (38:2)	Lognormal	-0.008	(-0.028, 0.011)	0.405	0.733	0.052	(-0.028, 0.012)
PC (36:5) C	Lognormal	0.009	(-0.013, 0.031)	0.405	0.733	0.059	(-0.013, 0.032)
TG (55:2)	Lognormal	0.008	(-0.011, 0.028)	0.405	0.733	0.056	(-0.011, 0.027)
TG (51:5)	Lognormal	-0.008	(-0.027, 0.011)	0.409	0.737	0.057	(-0.026, 0.011)
GlcCer (d42:1) - ESI(-)	Lognormal	-0.005	(-0.017, 0.007)	0.410	0.737	0.052	(-0.017, 0.007)
TG (54:8)	Lognormal	0.013	(-0.017, 0.042)	0.410	0.737	0.053	(-0.017, 0.042)
PC (40:7) A - ESI(+)	Lognormal	-0.005	(-0.016, 0.006)	0.414	0.739	0.048	(-0.017, 0.007)
TG (50:1)	Lognormal	0.007	(-0.010, 0.025)	0.418	0.739	0.053	(-0.010, 0.026)
TG (54:2)	Lognormal	0.006	(-0.009, 0.021)	0.418	0.739	0.050	(-0.008, 0.021)
AC (18:1)	Lognormal	-0.006	(-0.019, 0.008)	0.419	0.739	0.050	(-0.018, 0.009)
TG (40:0)	Lognormal	-0.014	(-0.048, 0.020)	0.419	0.739	0.056	(-0.048, 0.022)
SM (d42:0) - ESI(-)	Lognormal	0.006	(-0.008, 0.020)	0.423	0.739	0.048	(-0.008, 0.021)
TG (58:10)	Lognormal	0.009	(-0.013, 0.031)	0.425	0.741	0.053	(-0.012, 0.031)
PC (39:4)	Lognormal	0.005	(-0.007, 0.017)	0.433	0.753	0.050	(-0.007, 0.017)
LPC (16:0) - ESI(+)	Lognormal	-0.002	(-0.008, 0.004)	0.437	0.757	0.050	(-0.008, 0.004)
TG (53:5)	Lognormal	-0.007	(-0.023, 0.010)	0.437	0.757	0.054	(-0.024, 0.011)
SM (d36:2) - ESI(+)	Lognormal	-0.003	(-0.010, 0.004)	0.438	0.757	0.056	(-0.010, 0.004)
Ceramide (d34:1) - ESI(+)	Lognormal	-0.004	(-0.014, 0.006)	0.445	0.763	0.048	(-0.014, 0.006)
Ceramide (d34:2)	Lognormal	-0.005	(-0.016, 0.007)	0.448	0.765	0.045	(-0.015, 0.008)
TG (56:10)	Lognormal	0.014	(-0.022, 0.051)	0.452	0.768	0.053	(-0.024, 0.050)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
PC (30:0)	Lognormal	-0.006	(-0.020, 0.009)	0.457	0.772	0.050	(-0.020, 0.009)
TG (59:3)	Lognormal	0.009	(-0.016, 0.034)	0.466	0.781	0.047	(-0.016, 0.035)
LPC (20:4)	Lognormal	-0.004	(-0.015, 0.007)	0.469	0.781	0.053	(-0.016, 0.007)
TAG (58:7)/TAG (18:1/18:1/22:5)	Lognormal	0.006	(-0.010, 0.022)	0.471	0.783	0.050	(-0.011, 0.021)
GlcCer (d14:1(4E)/20:0(2OH))	Lognormal	-0.008	(-0.030, 0.014)	0.473	0.783	0.051	(-0.030, 0.015)
TG (50:2)	Lognormal	0.005	(-0.008, 0.017)	0.475	0.784	0.049	(-0.008, 0.017)
TG (56:7) A	Lognormal	0.016	(-0.027, 0.059)	0.477	0.787	0.051	(-0.028, 0.059)
TG (60:4)	Lognormal	0.012	(-0.022, 0.046)	0.495	0.804	0.045	(-0.024, 0.045)
CE (18:1)	Lognormal	-0.005	(-0.019, 0.009)	0.497	0.806	0.050	(-0.019, 0.009)
TG (46:3) B	Lognormal	-0.013	(-0.052, 0.025)	0.499	0.806	0.051	(-0.052, 0.026)
GlcCer (d42:2) - ESI(-)	Lognormal	0.005	(-0.009, 0.018)	0.502	0.806	0.045	(-0.008, 0.018)
PE (36:1) - ESI(-)	Lognormal	0.010	(-0.019, 0.039)	0.504	0.806	0.049	(-0.019, 0.039)
LPC (18:0) - ESI(+)	Lognormal	-0.004	(-0.014, 0.007)	0.504	0.806	0.047	(-0.014, 0.007)
TG (64:2)	Lognormal	0.012	(-0.023, 0.047)	0.505	0.806	0.051	(-0.023, 0.048)
LPC (22:5) - ESI(+)	Lognormal	0.008	(-0.015, 0.030)	0.507	0.806	0.049	(-0.015, 0.030)
SM (d41:1) - ESI(-)	Lognormal	-0.035	(-0.141, 0.071)	0.515	0.811	0.052	(-0.136, 0.074)
TG (60:2)	Lognormal	0.015	(-0.031, 0.062)	0.516	0.811	0.046	(-0.032, 0.063)
PC (40:5) B - ESI(-)	Lognormal	-0.008	(-0.033, 0.017)	0.518	0.811	0.044	(-0.034, 0.018)
TG (56:2)	Lognormal	0.008	(-0.015, 0.030)	0.519	0.811	0.054	(-0.018, 0.030)
FA (20:2) (eicosadienoic acid)	Lognormal	0.004	(-0.008, 0.015)	0.523	0.813	0.050	(-0.009, 0.015)
AC (16:0)	Lognormal	-0.004	(-0.015, 0.008)	0.527	0.813	0.047	(-0.015, 0.007)
DG (32:1)	Lognormal	0.008	(-0.018, 0.034)	0.527	0.813	0.044	(-0.017, 0.035)
PC (p-40:6)/PC (o-40:7) B	Lognormal	-0.006	(-0.024, 0.012)	0.532	0.813	0.042	(-0.024, 0.012)
FA (14:0) (myristic acid)	Lognormal	0.003	(-0.006, 0.012)	0.533	0.813	0.046	(-0.006, 0.013)
TG (64:3)	Lognormal	-0.008	(-0.033, 0.017)	0.534	0.813	0.043	(-0.034, 0.016)
PC (p-38:5)/PC (o-38:6)	Lognormal	0.013	(-0.028, 0.053)	0.535	0.813	0.047	(-0.029, 0.052)
PC (32:0) - ESI(+)	Lognormal	0.002	(-0.004, 0.007)	0.551	0.829	0.044	(-0.004, 0.008)
TG (62:3)	Lognormal	0.013	(-0.030, 0.056)	0.558	0.836	0.049	(-0.029, 0.056)
PC (35:4) - ESI(-)	Lognormal	-0.006	(-0.025, 0.014)	0.559	0.836	0.042	(-0.026, 0.012)
TG (49:1)	Lognormal	0.007	(-0.017, 0.031)	0.563	0.838	0.047	(-0.018, 0.031)
PC (33:1) - ESI(-)	Lognormal	0.007	(-0.016, 0.030)	0.563	0.838	0.050	(-0.017, 0.029)
PC (36:1) - ESI(-)	Lognormal	-0.003	(-0.012, 0.007)	0.568	0.844	0.045	(-0.013, 0.006)
SM (d43:2) - ESI(+)	Lognormal	0.005	(-0.013, 0.023)	0.575	0.847	0.046	(-0.014, 0.023)
SM (d32:0) - ESI(+)	Lognormal	0.005	(-0.013, 0.023)	0.577	0.847	0.047	(-0.013, 0.023)
PC (p-38:6)/PC (o-38:7)	Lognormal	-0.005	(-0.020, 0.011)	0.578	0.847	0.044	(-0.020, 0.012)
PE (38:6) - ESI(-)	Lognormal	0.008	(-0.021, 0.037)	0.578	0.847	0.045	(-0.020, 0.036)
PC (32:1) - ESI(+)	Lognormal	0.004	(-0.009, 0.016)	0.578	0.847	0.044	(-0.009, 0.016)
PC (p-40:6)/PC (o-40:7) A	Lognormal	0.004	(-0.010, 0.018)	0.581	0.849	0.044	(-0.010, 0.019)
SM (d34:0) - ESI(+)	Lognormal	-0.002	(-0.011, 0.006)	0.586	0.853	0.044	(-0.011, 0.005)
PC (38:5) A - ESI(-)	Lognormal	-0.003	(-0.013, 0.007)	0.592	0.858	0.042	(-0.013, 0.008)
CE (16:1)	Lognormal	0.004	(-0.010, 0.018)	0.593	0.858	0.043	(-0.010, 0.017)
Ceramide (d40:0)	Lognormal	0.008	(-0.020, 0.036)	0.593	0.858	0.038	(-0.020, 0.035)
PC (p-42:5)/PC (o-42:6) B	Lognormal	-0.005	(-0.021, 0.012)	0.594	0.858	0.044	(-0.022, 0.013)
Ceramide (d42:0)	Lognormal	0.004	(-0.011, 0.020)	0.596	0.859	0.042	(-0.012, 0.020)
LPC (22:4)	Lognormal	-0.007	(-0.034, 0.019)	0.598	0.859	0.044	(-0.034, 0.019)
PC (35:1) - ESI(-)	Lognormal	0.004	(-0.012, 0.021)	0.599	0.859	0.039	(-0.012, 0.020)
TG (57:2)	Lognormal	0.005	(-0.013, 0.023)	0.608	0.865	0.047	(-0.013, 0.023)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
PC (40:6) B	Lognormal	0.004	(-0.011, 0.018)	0.609	0.865	0.042	(-0.010, 0.018)
PC (40:5) B - ESI(+)	Lognormal	-0.004	(-0.018, 0.011)	0.616	0.870	0.040	(-0.018, 0.011)
TG (42:2)	Lognormal	-0.024	(-0.118, 0.071)	0.621	0.872	0.044	(-0.115, 0.068)
CE (22:6)	Lognormal	0.003	(-0.010, 0.016)	0.622	0.872	0.041	(-0.009, 0.017)
TG (52:3)	Lognormal	-0.002	(-0.009, 0.005)	0.623	0.872	0.047	(-0.009, 0.005)
PC (38:7)	Lognormal	0.004	(-0.013, 0.022)	0.627	0.873	0.046	(-0.013, 0.021)
TG (60:3)	Lognormal	0.008	(-0.026, 0.043)	0.627	0.873	0.046	(-0.025, 0.044)
CE (22:2)	Lognormal	-0.010	(-0.052, 0.031)	0.629	0.873	0.043	(-0.055, 0.030)
FA (22:6) (docosahexaenoic acid)	Lognormal	0.004	(-0.013, 0.021)	0.629	0.873	0.043	(-0.014, 0.020)
PC (36:4) C - ESI(+)	Lognormal	0.001	(-0.004, 0.007)	0.639	0.879	0.042	(-0.004, 0.007)
DG (34:1)	Lognormal	-0.007	(-0.036, 0.023)	0.650	0.889	0.044	(-0.036, 0.023)
PE (36:1) - ESI(+)	Lognormal	-0.005	(-0.029, 0.018)	0.658	0.895	0.039	(-0.030, 0.017)
TG (53:1)	Lognormal	0.007	(-0.024, 0.037)	0.660	0.895	0.041	(-0.023, 0.039)
TG (46:1)	Lognormal	-0.008	(-0.043, 0.027)	0.661	0.895	0.039	(-0.045, 0.025)
PC (35:4) - ESI(+)	Lognormal	-0.003	(-0.015, 0.010)	0.664	0.897	0.040	(-0.016, 0.009)
SM (d42:2)	Lognormal	0.002	(-0.006, 0.010)	0.665	0.897	0.042	(-0.006, 0.010)
DG (36:3)	Lognormal	-0.003	(-0.016, 0.010)	0.671	0.900	0.043	(-0.016, 0.010)
SM (d37:1)	Lognormal	-0.004	(-0.023, 0.015)	0.672	0.900	0.044	(-0.023, 0.014)
LPC (20:1) - ESI(-)	Lognormal	-0.004	(-0.022, 0.014)	0.672	0.900	0.046	(-0.023, 0.015)
TG (53:3)	Lognormal	0.002	(-0.009, 0.014)	0.678	0.904	0.044	(-0.009, 0.014)
TG (52:5)	Lognormal	-0.003	(-0.017, 0.011)	0.681	0.905	0.041	(-0.016, 0.012)
TG (48:6)	Lognormal	0.006	(-0.023, 0.036)	0.681	0.905	0.045	(-0.023, 0.036)
TG (54:4)	Lognormal	-0.003	(-0.015, 0.010)	0.687	0.906	0.042	(-0.014, 0.010)
GlcCer (d34:1)	Lognormal	-0.005	(-0.032, 0.021)	0.688	0.906	0.043	(-0.033, 0.021)
SM (d41:2) - ESI(-)	Lognormal	-0.003	(-0.018, 0.012)	0.693	0.907	0.044	(-0.019, 0.011)
PC (p-40:4)/PC (o-40:5) - ESI(+)	Lognormal	-0.002	(-0.013, 0.009)	0.694	0.907	0.039	(-0.013, 0.008)
SM (d32:0) - ESI(-)	Lognormal	-0.013	(-0.076, 0.051)	0.696	0.907	0.044	(-0.075, 0.055)
LPC (22:6)	Lognormal	0.003	(-0.013, 0.020)	0.696	0.907	0.040	(-0.014, 0.020)
PC 38:7e	Lognormal	-0.004	(-0.024, 0.016)	0.699	0.908	0.040	(-0.024, 0.014)
LPC (20:1) - ESI(+)	Lognormal	-0.006	(-0.038, 0.026)	0.712	0.913	0.040	(-0.038, 0.027)
TG (50:6)	Lognormal	0.006	(-0.025, 0.037)	0.712	0.913	0.041	(-0.025, 0.036)
TG (55:1)	Lognormal	0.005	(-0.020, 0.029)	0.714	0.914	0.041	(-0.020, 0.030)
FA (15:0) (pentadecylic acid)	Lognormal	-0.002	(-0.012, 0.008)	0.728	0.927	0.038	(-0.012, 0.009)
TG (44:1)	Lognormal	-0.008	(-0.054, 0.038)	0.731	0.927	0.041	(-0.056, 0.041)
PC (28:0)	Lognormal	-0.008	(-0.052, 0.037)	0.733	0.928	0.042	(-0.050, 0.038)
TG (59:2)	Lognormal	-0.005	(-0.031, 0.022)	0.736	0.928	0.045	(-0.030, 0.023)
PC (38:3) - ESI(+)	Lognormal	-0.002	(-0.010, 0.007)	0.739	0.928	0.036	(-0.010, 0.007)
PC (p-42:4)/PC (o-42:5) - ESI(+)	Lognormal	-0.002	(-0.015, 0.011)	0.739	0.928	0.036	(-0.014, 0.011)
Ceramide (d36:1) - ESI(-)	Lognormal	-0.004	(-0.025, 0.018)	0.744	0.928	0.042	(-0.025, 0.018)
TG (62:1)	Lognormal	-0.005	(-0.037, 0.027)	0.745	0.928	0.042	(-0.038, 0.026)
PC (33:0)	Lognormal	-0.004	(-0.026, 0.018)	0.748	0.928	0.041	(-0.026, 0.018)
TG (52:6)	Lognormal	0.003	(-0.018, 0.025)	0.749	0.928	0.041	(-0.018, 0.024)
TG (46:5)	Lognormal	-0.008	(-0.057, 0.042)	0.762	0.931	0.043	(-0.060, 0.040)
FA (17:0) (margaric acid)	Lognormal	0.001	(-0.006, 0.009)	0.765	0.931	0.040	(-0.007, 0.008)
TG (58:1)	Lognormal	0.005	(-0.025, 0.034)	0.765	0.931	0.042	(-0.025, 0.034)
SM (d33:1) - ESI(+)	Lognormal	-0.002	(-0.013, 0.009)	0.767	0.931	0.044	(-0.013, 0.009)
PC (36:5) B	Lognormal	0.004	(-0.022, 0.030)	0.776	0.936	0.038	(-0.020, 0.030)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
TG (54:3)	Lognormal	0.002	(-0.010, 0.013)	0.778	0.936	0.042	(-0.009, 0.013)
FA (12:0) (lauric acid)	Lognormal	-0.003	(-0.022, 0.016)	0.779	0.936	0.041	(-0.022, 0.016)
CE (16:0)	Lognormal	-0.004	(-0.035, 0.026)	0.784	0.936	0.037	(-0.036, 0.025)
PE (38:4)	Lognormal	-0.002	(-0.013, 0.010)	0.785	0.936	0.034	(-0.014, 0.011)
TG (53:4)	Lognormal	-0.002	(-0.015, 0.011)	0.787	0.936	0.041	(-0.016, 0.011)
TG (60:1)	Lognormal	0.004	(-0.028, 0.037)	0.788	0.936	0.040	(-0.028, 0.036)
DG (34:3)	Lognormal	-0.003	(-0.026, 0.019)	0.789	0.936	0.037	(-0.026, 0.020)
PC (38:5) B - ESI(-)	Lognormal	0.003	(-0.017, 0.022)	0.792	0.937	0.041	(-0.018, 0.022)
FA (18:3) (linolenic acid)	Lognormal	0.002	(-0.011, 0.014)	0.801	0.945	0.042	(-0.012, 0.015)
GlcCer (d42:1) - ESI(+)	Lognormal	0.001	(-0.010, 0.013)	0.804	0.946	0.036	(-0.010, 0.012)
PC (31:1)	Lognormal	-0.005	(-0.043, 0.033)	0.807	0.947	0.040	(-0.042, 0.033)
PC (38:6) - ESI(-)	Lognormal	0.002	(-0.012, 0.015)	0.810	0.948	0.038	(-0.011, 0.015)
PC (p-44:4)/PC (o-44:5) - ESI(+)	Lognormal	-0.002	(-0.016, 0.012)	0.811	0.948	0.039	(-0.016, 0.013)
CE (18:0)	Lognormal	-0.003	(-0.028, 0.022)	0.811	0.948	0.036	(-0.028, 0.020)
PC (40:6) A	Lognormal	0.001	(-0.010, 0.013)	0.818	0.952	0.039	(-0.011, 0.013)
GlcCer (d40:1) - ESI(+)	Lognormal	-0.002	(-0.016, 0.013)	0.818	0.952	0.039	(-0.016, 0.012)
Ceramide (d34:0)	Lognormal	-0.002	(-0.015, 0.012)	0.820	0.952	0.031	(-0.014, 0.011)
TG (57:1)	Lognormal	0.002	(-0.019, 0.023)	0.823	0.952	0.038	(-0.019, 0.024)
PC (16:0/9:0(CHO))	Lognormal	-0.003	(-0.025, 0.020)	0.826	0.952	0.032	(-0.025, 0.021)
PC (38:4) A - ESI(+)	Lognormal	-0.001	(-0.012, 0.010)	0.826	0.952	0.041	(-0.012, 0.010)
TG (52:1)	Lognormal	0.002	(-0.018, 0.023)	0.827	0.952	0.037	(-0.018, 0.022)
TG (49:3)	Lognormal	0.003	(-0.021, 0.026)	0.830	0.953	0.042	(-0.021, 0.026)
Ceramide (d40:2)	Lognormal	0.005	(-0.043, 0.053)	0.830	0.953	0.043	(-0.041, 0.055)
PC (p-42:5)/PC (o-42:6)	Lognormal	-0.004	(-0.037, 0.030)	0.835	0.956	0.041	(-0.037, 0.030)
TG (56:1)	Lognormal	-0.003	(-0.031, 0.025)	0.839	0.959	0.039	(-0.031, 0.026)
CE (20:4)	Lognormal	0.001	(-0.009, 0.011)	0.843	0.960	0.041	(-0.008, 0.011)
TG (49:0)	Lognormal	-0.002	(-0.025, 0.021)	0.847	0.963	0.038	(-0.025, 0.023)
PC (40:5) A - ESI(-)	Lognormal	-0.002	(-0.019, 0.016)	0.852	0.964	0.040	(-0.019, 0.016)
SM (d36:1) - ESI(+)	Lognormal	-0.001	(-0.007, 0.006)	0.856	0.964	0.043	(-0.007, 0.006)
TG (58:5)	Lognormal	0.002	(-0.019, 0.022)	0.857	0.964	0.041	(-0.018, 0.023)
PC (38:4) C - ESI(+)	Lognormal	0.001	(-0.006, 0.007)	0.870	0.966	0.039	(-0.006, 0.007)
LPC (20:0)	Lognormal	-0.002	(-0.021, 0.018)	0.876	0.969	0.040	(-0.021, 0.018)
PC (40:7) - ESI(-)	Lognormal	-0.002	(-0.023, 0.020)	0.879	0.970	0.040	(-0.022, 0.021)
DG (34:2)	Lognormal	0.001	(-0.013, 0.015)	0.879	0.970	0.039	(-0.014, 0.015)
LPC (p-18:0)/LPC (o-18:1)	Lognormal	-0.001	(-0.018, 0.016)	0.882	0.970	0.038	(-0.018, 0.016)
TG (58:2)	Lognormal	0.003	(-0.039, 0.045)	0.886	0.970	0.040	(-0.038, 0.047)
PC (31:0)	Lognormal	0.001	(-0.014, 0.016)	0.894	0.973	0.036	(-0.015, 0.014)
PC (40:8) - ESI(+)	Lognormal	0.001	(-0.010, 0.011)	0.895	0.973	0.037	(-0.011, 0.010)
PC (p-38:5)/PC (o-38:6) A	Lognormal	-0.001	(-0.018, 0.015)	0.897	0.973	0.039	(-0.017, 0.015)
TG (62:2)	Lognormal	0.002	(-0.036, 0.040)	0.901	0.973	0.040	(-0.035, 0.040)
PE (34:2) - ESI(+)	Lognormal	-0.005	(-0.083, 0.074)	0.909	0.977	0.038	(-0.090, 0.068)
TG (50:3) A	Lognormal	0.001	(-0.014, 0.016)	0.910	0.977	0.037	(-0.015, 0.016)
TG (51:3)	Lognormal	0.001	(-0.012, 0.014)	0.915	0.981	0.039	(-0.012, 0.014)
PC (p-40:4)/PC (o-40:5) - ESI(-)	Lognormal	-0.001	(-0.017, 0.015)	0.916	0.981	0.040	(-0.017, 0.016)
PC (36:6)	Lognormal	0.001	(-0.020, 0.022)	0.919	0.982	0.039	(-0.019, 0.023)
FA (10:0) (capric acid)	Lognormal	0.001	(-0.028, 0.031)	0.920	0.982	0.037	(-0.026, 0.032)
Ceramide (d42:2) A - ESI (+)	Lognormal	0.000	(-0.009, 0.008)	0.925	0.986	0.034	(-0.008, 0.008)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Gal-Gal-Cer (d18:1/16:0)/Lactosylceramide (d18:1/16:0)	Lognormal	-0.001	(-0.012, 0.011)	0.927	0.986	0.036	(-0.011, 0.011)
PE (36:4) - ESI(-)	Lognormal	-0.001	(-0.030, 0.028)	0.927	0.986	0.034	(-0.031, 0.028)
LPC (18:1) - ESI(+)	Lognormal	-0.001	(-0.012, 0.011)	0.930	0.988	0.040	(-0.012, 0.011)
PC (p-36:5)/PC (o-36:6)	Lognormal	0.001	(-0.023, 0.025)	0.940	0.994	0.041	(-0.023, 0.026)
TG (56:4)	Lognormal	0.000	(-0.014, 0.015)	0.952	0.994	0.042	(-0.014, 0.015)
PC 40:6e	Lognormal	0.000	(-0.011, 0.011)	0.956	0.994	0.037	(-0.012, 0.010)
PC (p-44:5)/PC (o-44:6)	Lognormal	0.000	(-0.017, 0.016)	0.956	0.994	0.038	(-0.018, 0.016)
SM (d41:2) A - ESI(+)	Lognormal	0.000	(-0.012, 0.011)	0.956	0.994	0.041	(-0.012, 0.012)
TG (50:3) B	Lognormal	-0.002	(-0.099, 0.094)	0.963	0.994	0.036	(-0.101, 0.091)
TG (44:2)	Lognormal	-0.002	(-0.090, 0.086)	0.967	0.994	0.040	(-0.096, 0.082)
TG (48:1)	Lognormal	0.000	(-0.023, 0.022)	0.968	0.994	0.038	(-0.023, 0.021)
SM (d43:1) - ESI(+)	Lognormal	0.000	(-0.015, 0.015)	0.969	0.994	0.040	(-0.015, 0.015)
LPC (22:5) - ESI(-)	Lognormal	-0.001	(-0.040, 0.039)	0.970	0.994	0.040	(-0.040, 0.037)
TG (48:2)	Lognormal	0.000	(-0.024, 0.023)	0.971	0.994	0.038	(-0.026, 0.022)
FA (24:1) (nervonic acid)	Lognormal	0.000	(-0.011, 0.011)	0.972	0.994	0.037	(-0.010, 0.011)
FA (20:4) (arachidonic acid)	Lognormal	0.000	(-0.008, 0.009)	0.973	0.994	0.039	(-0.008, 0.009)
PC (40:4) - ESI(+)	Lognormal	0.000	(-0.014, 0.013)	0.976	0.995	0.039	(-0.015, 0.012)
PC (32:1) - ESI(-)	Lognormal	0.000	(-0.018, 0.018)	0.979	0.995	0.039	(-0.018, 0.017)
PC (38:4) B - ESI(+)	Lognormal	0.000	(-0.010, 0.010)	0.982	0.995	0.033	(-0.010, 0.010)
PC (34:0) - ESI(+)	Lognormal	0.000	(-0.006, 0.006)	0.985	0.995	0.034	(-0.006, 0.006)
Ceramide (d36:1) - ESI(+)	Lognormal	0.000	(-0.012, 0.012)	0.998	0.999	0.036	(-0.012, 0.013)
Oxylipins (OL)							
Resolvin D1	Gamma	-0.513	(-0.871, -0.156)	0.006	0.183	1.811	(-0.857, -0.173)
5-Hydroxy-6,8,11,14,17-eicosapentaenoic acid	Gamma	0.330	(0.072, 0.587)	0.013	0.225	0.520	(0.069, 0.597)
9-nitrooleic acid	Gamma	0.409	(0.089, 0.729)	0.013	0.225	0.588	(0.082, 0.778)
15,16-dihydroxyoctadeca-9,12-dienoic acid	Lognormal	-0.272	(-0.487, -0.057)	0.014	0.229	0.691	(-0.464, -0.041)
15-hydroxyeicosa-5,8,11,13,17-pentaenoic acid	Gamma	0.506	(0.101, 0.911)	0.016	0.239	0.788	(0.113, 0.947)
12-Hydroxy-5,8,10,14,17-eicosapentaenoic acid	Gamma	0.514	(0.080, 0.948)	0.022	0.274	2.049	(0.156, 0.855)
Prostaglandin F2a	Gamma	-0.338	(-0.647, -0.029)	0.034	0.320	0.228	(-0.688, -0.005)
Prostaglandin D2	Gamma	-0.619	(-1.188, -0.050)	0.035	0.320	1.241	(-1.107, -0.160)
4-hydroxydocosa-5,7,10,13,16,19-hexaenoic acid	Gamma	0.373	(0.021, 0.725)	0.040	0.326	0.245	(-0.001, 0.726)
9-Hydroxy-5,7,11,14,17-icosapentaenoic acid	Gamma	0.267	(-0.004, 0.538)	0.056	0.380	0.147	(-0.027, 0.566)
8,9-Epoxyeicosa-5,11,14-trienoic acid	Gamma	-0.292	(-0.590, 0.005)	0.056	0.380	0.129	(-0.632, 0.052)
9,10-dihydroxyoctadec-12-enoic acid	Lognormal	-0.228	(-0.461, 0.006)	0.058	0.383	0.245	(-0.458, 0.005)
11,12-Epoxyeicosa-5,8,14-trienoic acid	Gamma	0.298	(-0.024, 0.620)	0.072	0.419	0.148	(-0.034, 0.640)
11(12)-epoxy-5,8,14,17- eicosatetraenoic acid	Gamma	0.413	(-0.052, 0.878)	0.084	0.444	0.220	(-0.096, 0.893)
8-hydroxyeicosa-5,9,11,14-tetraenoic acid	Gamma	0.235	(-0.034, 0.504)	0.089	0.451	0.116	(-0.060, 0.550)
6-Ketoprostaglandin F1 alpha	Gamma	0.362	(-0.075, 0.799)	0.107	0.492	0.182	(-0.039, 0.786)
15-ketoeicosa-5,8,11,13-tetraenoic acid	Gamma	0.344	(-0.082, 0.770)	0.116	0.502	0.229	(-0.011, 0.688)
17,18-Epoxy-5,8,11,14-eicosatetraenoic acid	Gamma	-0.398	(-0.893, 0.098)	0.118	0.506	0.201	(-0.833, 0.038)
17,18-dihydroxyeicosa-5,8,11,14-tetraenoic acid	Lognormal	0.220	(-0.060, 0.501)	0.126	0.519	0.134	(-0.064, 0.489)
15-Deoxy-delta-12,14-Prostaglandin J2	Gamma	-0.232	(-0.539, 0.074)	0.140	0.532	0.096	(-0.547, 0.071)
15(16)-epoxy-9,12-octadecadienoic acid	Gamma	-0.315	(-0.739, 0.108)	0.146	0.535	0.107	(-0.706, 0.090)
9,11,15-trihydroxy-5,13,1Z-prostatrienoic acid	Gamma	-0.459	(-1.084, 0.166)	0.153	0.549	0.400	(-0.941, -0.071)
9,10-dihydroxyoctadeca-12,15-dienoic acid	Gamma	-0.178	(-0.423, 0.067)	0.157	0.556	0.060	(-0.460, 0.107)
9(10)-epoxy-12Z-octadecenoic acid	Gamma	-0.151	(-0.368, 0.065)	0.172	0.589	0.067	(-0.352, 0.050)
9(10)-epoxy-12,15-octadecadienoic acid	Gamma	0.393	(-0.177, 0.963)	0.179	0.593	0.198	(-0.095, 0.887)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Female ME/CFS vs. Female Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
10-nitrooleic acid	Lognormal	0.179	(-0.085, 0.442)	0.186	0.598	0.087	(-0.084, 0.456)
11-Hydroxy-arachidonic acid	Gamma	0.131	(-0.071, 0.333)	0.206	0.610	0.049	(-0.087, 0.356)
6-trans-Leukotriene B4	Gamma	-0.385	(-0.979, 0.210)	0.207	0.610	0.147	(-0.814, 0.142)
8,9-dihydroxyeicosa-5,11,14-trienoic acid	Gamma	0.159	(-0.095, 0.414)	0.221	0.621	0.056	(-0.087, 0.423)
13-hydroxyoctadeca-9,11,15-trienoic acid	Gamma	-0.149	(-0.395, 0.098)	0.240	0.636	0.049	(-0.418, 0.116)
12(13)-epoxy-9,15-octadecadienoic acid	Gamma	-0.256	(-0.694, 0.181)	0.253	0.637	0.092	(-0.622, 0.100)
Leukotriene B5	Gamma	-0.334	(-0.931, 0.263)	0.275	0.651	0.121	(-0.852, 0.152)
12,13-dihydroxyoctadec-9-enoic acid	Lognormal	-0.106	(-0.305, 0.093)	0.298	0.668	0.062	(-0.293, 0.093)
9-Hydroxylinoleic acid	Lognormal	-0.077	(-0.226, 0.072)	0.310	0.676	0.058	(-0.230, 0.071)
13-ketooctadeca-9,11-dienoic acid	Lognormal	-0.160	(-0.469, 0.148)	0.310	0.676	0.057	(-0.464, 0.149)
16(17)-epoxy-4,7,10,13,19-docosapentaenoic acid	Gamma	0.194	(-0.189, 0.577)	0.322	0.684	0.069	(-0.182, 0.560)
5,6-dihydroxyeicosa-8,11,14-trienoic acid	Gamma	0.122	(-0.132, 0.375)	0.348	0.694	0.043	(-0.131, 0.383)
17-hydroxy-4,7,10,13,15,19-docosahexaenoic acid	Gamma	0.116	(-0.139, 0.371)	0.375	0.711	0.043	(-0.193, 0.408)
9,12,13-trihydroxyoctadec-10-enoic acid	Lognormal	-0.064	(-0.211, 0.083)	0.394	0.728	0.046	(-0.208, 0.086)
10-nitrolinoleic acid	Gamma	0.199	(-0.265, 0.663)	0.402	0.733	0.069	(-0.258, 0.612)
Prostaglandin E2	Gamma	0.260	(-0.350, 0.871)	0.405	0.733	0.086	(-0.208, 0.727)
9-hydroxyeicosa-5,7,11,14-tetraenoic acid	Gamma	0.108	(-0.149, 0.365)	0.412	0.739	0.040	(-0.184, 0.391)
Prostaglandin E1	Gamma	0.178	(-0.250, 0.605)	0.417	0.739	0.054	(-0.175, 0.594)
8,15-dihydroxyeicosa-5,9,11,13-tetraenoic acid	Gamma	-0.253	(-0.866, 0.359)	0.419	0.739	0.077	(-0.782, 0.286)
9-hydroxyoctadeca-10,12,15-trienoic acid	Gamma	-0.127	(-0.436, 0.182)	0.422	0.739	0.043	(-0.425, 0.157)
14(15)-epoxy-5,8,11,17-eicosatetraenoic acid	Gamma	0.237	(-0.367, 0.841)	0.443	0.763	0.083	(-0.382, 0.869)
9,10-Epoxy stearic acid	Lognormal	0.132	(-0.205, 0.469)	0.445	0.763	0.049	(-0.205, 0.450)
5,6,15-trihydroxyeicosa-7,9,11,13-tetraenoic acid	Gamma	0.153	(-0.243, 0.548)	0.450	0.767	0.053	(-0.199, 0.538)
12,13-epoxy-9-octadecenoic acid	Lognormal	-0.118	(-0.430, 0.194)	0.460	0.775	0.052	(-0.410, 0.212)
Thromboxane B2	Lognormal	0.106	(-0.188, 0.399)	0.481	0.789	0.048	(-0.197, 0.382)
20-Hydroxyarachidonic acid	Lognormal	-0.155	(-0.587, 0.276)	0.482	0.789	0.039	(-0.588, 0.270)
Leukotriene B4	Gamma	-0.080	(-0.307, 0.147)	0.490	0.798	0.028	(-0.284, 0.151)
13-Hydroxyoctadecadienoic acid	Lognormal	-0.038	(-0.173, 0.097)	0.583	0.850	0.043	(-0.170, 0.105)
9S,10R-dihydroxy-stearic acid	Lognormal	-0.080	(-0.380, 0.221)	0.605	0.865	0.039	(-0.366, 0.220)
5-ketoeicosa-6,8,11,14-tetraenoic acid	Gamma	-0.088	(-0.424, 0.247)	0.607	0.865	0.043	(-0.460, 0.285)
Prostaglandin E3	Gamma	0.133	(-0.470, 0.735)	0.667	0.899	0.077	(-0.422, 0.914)
5,15-dihydroxyeicosa-6,8,11,13-tetraenoic acid	Gamma	-0.107	(-0.605, 0.392)	0.676	0.904	0.049	(-0.588, 0.364)
12,13-dihydroxyoctadeca-9,15-dienoic acid	Gamma	-0.112	(-0.662, 0.438)	0.690	0.906	0.048	(-0.504, 0.308)
14-hydroxydocosa-4,7,10,12,16,19-hexaenoic acid	Lognormal	0.079	(-0.309, 0.466)	0.691	0.906	0.032	(-0.293, 0.465)
trans-12,13-epoxy-11-oxo-trans-9-octadecenoic acid	Gamma	-0.031	(-0.217, 0.156)	0.748	0.928	0.025	(-0.251, 0.187)
14,15-dihydroxyeicosa-5,8,11,17-tetraenoic acid	Gamma	0.053	(-0.275, 0.380)	0.753	0.930	0.041	(-0.315, 0.424)
19,20-dihydroxydocosa-4,7,10,13,16-pentaenoic acid	Lognormal	0.028	(-0.150, 0.206)	0.760	0.931	0.038	(-0.146, 0.200)
5-Hydroxy-6,8,11,14-eicosatetraenoic acid	Lognormal	0.032	(-0.180, 0.244)	0.766	0.931	0.034	(-0.183, 0.242)
14,15-dihydroxyeicosa-5,8,11-trienoic acid	Gamma	-0.014	(-0.171, 0.144)	0.865	0.966	0.016	(-0.166, 0.139)
18-(3-ethyloxiran-2-yl)octadeca-4,7,10,13,16-pentaenoic acid	Gamma	-0.028	(-0.398, 0.343)	0.884	0.970	0.037	(-0.380, 0.314)
15-hydroxyeicosa-5,8,11,13-tetraenoic acid	Lognormal	0.011	(-0.162, 0.184)	0.902	0.973	0.035	(-0.167, 0.185)
12-Hydroxy-5,8,10,14-eicosatetraenoic acid	Lognormal	-0.008	(-0.244, 0.227)	0.945	0.994	0.027	(-0.240, 0.239)
11-Hydroxy-14,15-epoxyeicosatrienoic acid	Gamma	0.020	(-0.560, 0.600)	0.946	0.994	0.055	(-0.517, 0.562)
9-ketooctadeca-10,12-dienoic acid	Gamma	0.006	(-0.260, 0.273)	0.962	0.994	0.030	(-0.282, 0.324)
15-Keto-prostaglandin E2	Gamma	0.013	(-0.529, 0.554)	0.963	0.994	0.045	(-0.445, 0.476)
11,12-Dihydroxyeicosa-5,8,14-trienoic acid	Gamma	0.002	(-0.168, 0.172)	0.983	0.995	0.016	(-0.157, 0.169)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Primary Metabolites (PM)							
ornithine	Lognormal	0.002	(-0.027, 0.032)	0.884	0.975	0.058	(-0.028, 0.033)
tyrosine	Lognormal	0.005	(-0.011, 0.021)	0.528	0.899	0.072	(-0.010, 0.021)
threonine	Lognormal	0.005	(-0.017, 0.027)	0.672	0.928	0.069	(-0.016, 0.028)
succinic acid	Lognormal	0.016	(-0.014, 0.045)	0.306	0.864	0.122	(-0.015, 0.045)
lysine	Lognormal	0.020	(-0.017, 0.056)	0.302	0.864	0.104	(-0.019, 0.056)
phenylalanine	Lognormal	0.014	(-0.003, 0.032)	0.119	0.864	0.219	(-0.003, 0.033)
fructose	Lognormal	0.033	(-0.024, 0.090)	0.262	0.864	0.113	(-0.026, 0.092)
tagatose	Lognormal	0.038	(-0.001, 0.077)	0.065	0.864	0.305	(-0.004, 0.080)
leucine	Lognormal	-0.002	(-0.019, 0.015)	0.796	0.956	0.067	(-0.020, 0.016)
glutamine	Lognormal	0.016	(-0.016, 0.047)	0.343	0.864	0.101	(-0.019, 0.047)
methionine	Lognormal	0.032	(0.004, 0.060)	0.029	0.864	0.716	(0.005, 0.062)
mannitol	Lognormal	0.004	(-0.049, 0.057)	0.886	0.975	0.061	(-0.054, 0.057)
pelargonic acid	Lognormal	-0.014	(-0.034, 0.007)	0.205	0.864	0.143	(-0.036, 0.006)
arachidic acid	Lognormal	0.029	(-0.010, 0.068)	0.147	0.864	0.175	(-0.011, 0.069)
N-acetylputrescine	Lognormal	0.023	(-0.016, 0.062)	0.250	0.864	0.125	(-0.016, 0.067)
creatinine	Lognormal	0.057	(0.013, 0.102)	0.016	0.864	1.482	(0.012, 0.100)
urea	Lognormal	0.002	(-0.020, 0.024)	0.837	0.962	0.067	(-0.021, 0.024)
citrulline	Lognormal	0.006	(-0.011, 0.023)	0.472	0.884	0.072	(-0.011, 0.024)
erythritol	Lognormal	-0.035	(-0.103, 0.034)	0.327	0.864	0.105	(-0.106, 0.038)
2-deoxytetronic acid	Lognormal	0.010	(-0.037, 0.058)	0.672	0.928	0.073	(-0.036, 0.060)
maleimide	Lognormal	-0.021	(-0.054, 0.011)	0.207	0.864	0.136	(-0.053, 0.013)
2-hydroxybutanoic acid	Lognormal	0.010	(-0.021, 0.040)	0.538	0.902	0.081	(-0.021, 0.042)
oxoproline	Lognormal	-0.002	(-0.009, 0.005)	0.619	0.928	0.066	(-0.009, 0.006)
2-ketoisocaproic acid	Lognormal	-0.003	(-0.020, 0.014)	0.715	0.939	0.068	(-0.020, 0.014)
glucose	Lognormal	0.009	(-0.006, 0.024)	0.245	0.864	0.122	(-0.007, 0.023)
indole-3-propionic acid	Lognormal	-0.040	(-0.098, 0.018)	0.180	0.864	0.158	(-0.100, 0.016)
glutaric acid	Lognormal	0.007	(-0.026, 0.041)	0.670	0.928	0.069	(-0.028, 0.041)
alpha-ketoglutarate	Lognormal	0.026	(-0.007, 0.059)	0.128	0.864	0.247	(-0.007, 0.060)
tryptophan	Lognormal	0.001	(-0.029, 0.031)	0.943	0.994	0.067	(-0.028, 0.033)
conduiritol-beta-exposide	Lognormal	-0.028	(-0.085, 0.030)	0.353	0.869	0.109	(-0.088, 0.033)
sucrose	Lognormal	-0.024	(-0.087, 0.040)	0.468	0.884	0.082	(-0.089, 0.040)
linoleic acid	Lognormal	-0.008	(-0.052, 0.036)	0.726	0.945	0.072	(-0.055, 0.035)
alanine	Lognormal	0.006	(-0.037, 0.049)	0.793	0.956	0.066	(-0.037, 0.050)
lysine	Lognormal	-0.033	(-0.092, 0.026)	0.280	0.864	0.111	(-0.099, 0.026)
isoleucine	Lognormal	0.007	(-0.014, 0.028)	0.511	0.899	0.088	(-0.015, 0.028)
pseudo uridine	Lognormal	-0.008	(-0.027, 0.011)	0.428	0.873	0.096	(-0.027, 0.012)
hydroxycarbamate NIST	Lognormal	-0.016	(-0.047, 0.014)	0.302	0.864	0.111	(-0.050, 0.013)
levoglucosan	Lognormal	-0.045	(-0.091, 0.000)	0.057	0.864	0.415	(-0.091, 0.003)
mannose	Lognormal	0.027	(-0.002, 0.056)	0.077	0.864	0.454	(-0.003, 0.059)
glycerol	Lognormal	0.005	(-0.012, 0.022)	0.579	0.923	0.063	(-0.013, 0.023)
indole-3-lactate	Lognormal	-0.023	(-0.049, 0.003)	0.092	0.864	0.283	(-0.048, 0.004)
serine	Lognormal	0.006	(-0.019, 0.032)	0.628	0.928	0.084	(-0.020, 0.034)
beta-alanine	Lognormal	-0.022	(-0.073, 0.028)	0.394	0.873	0.095	(-0.078, 0.027)
quinic acid	Lognormal	-0.052	(-0.121, 0.018)	0.154	0.864	0.145	(-0.125, 0.020)
glycerol-alpha-phosphate	Lognormal	0.006	(-0.045, 0.058)	0.814	0.956	0.072	(-0.049, 0.060)
aminomalonnate	Lognormal	0.049	(-0.003, 0.102)	0.072	0.864	0.322	(-0.005, 0.100)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
heptadecanoic acid	Lognormal	-0.004	(-0.027, 0.020)	0.766	0.956	0.077	(-0.029, 0.020)
phosphate	Lognormal	-0.022	(-0.084, 0.040)	0.493	0.894	0.086	(-0.087, 0.043)
isothreonine acid	Lognormal	0.030	(-0.020, 0.081)	0.248	0.864	0.120	(-0.019, 0.084)
citric acid	Lognormal	0.003	(-0.016, 0.023)	0.732	0.949	0.059	(-0.018, 0.022)
behenic acid	Lognormal	-0.004	(-0.027, 0.018)	0.708	0.937	0.069	(-0.028, 0.018)
palmitic acid	Lognormal	-0.009	(-0.023, 0.004)	0.190	0.864	0.149	(-0.023, 0.004)
ribose	Lognormal	0.021	(-0.002, 0.044)	0.088	0.864	0.286	(-0.004, 0.043)
maltose	Lognormal	0.015	(-0.031, 0.060)	0.536	0.902	0.073	(-0.032, 0.062)
pentadecanoic acid	Lognormal	0.018	(-0.013, 0.048)	0.260	0.864	0.137	(-0.013, 0.049)
benzoic acid	Lognormal	0.022	(-0.011, 0.054)	0.195	0.864	0.162	(-0.011, 0.055)
3-hydroxybutyric acid	Lognormal	0.020	(-0.033, 0.073)	0.466	0.884	0.081	(-0.037, 0.072)
creatine	Lognormal	0.028	(-0.012, 0.068)	0.176	0.864	0.172	(-0.014, 0.071)
fumaric acid	Lognormal	-0.006	(-0.027, 0.015)	0.564	0.908	0.074	(-0.027, 0.016)
myristic acid	Lognormal	-0.008	(-0.034, 0.018)	0.540	0.902	0.087	(-0.033, 0.021)
glycolic acid	Lognormal	-0.012	(-0.035, 0.011)	0.314	0.864	0.099	(-0.035, 0.012)
2-hydroxyvaleric acid	Lognormal	-0.002	(-0.033, 0.028)	0.891	0.976	0.066	(-0.033, 0.031)
N-acetylorithine	Lognormal	-0.004	(-0.023, 0.015)	0.711	0.939	0.064	(-0.022, 0.017)
malic acid	Lognormal	0.024	(-0.029, 0.077)	0.382	0.873	0.097	(-0.030, 0.079)
alloxanoic acid	Lognormal	-0.024	(-0.070, 0.023)	0.319	0.864	0.091	(-0.069, 0.026)
4-hydroxybutyric acid	Lognormal	-0.013	(-0.043, 0.018)	0.419	0.873	0.093	(-0.045, 0.017)
threonine acid	Lognormal	0.017	(-0.011, 0.044)	0.235	0.864	0.126	(-0.010, 0.044)
gluconic acid	Lognormal	0.013	(-0.017, 0.043)	0.408	0.873	0.092	(-0.018, 0.043)
isopropylbenzene	Lognormal	0.001	(-0.032, 0.034)	0.962	0.996	0.040	(-0.033, 0.035)
1,2,4-benzenetriol	Lognormal	-0.050	(-0.103, 0.004)	0.075	0.864	0.292	(-0.106, 0.004)
lauric acid	Lognormal	-0.024	(-0.066, 0.019)	0.286	0.864	0.107	(-0.066, 0.021)
pyruvic acid	Lognormal	-0.016	(-0.055, 0.024)	0.450	0.884	0.093	(-0.057, 0.024)
salicylic acid	Lognormal	0.005	(-0.048, 0.059)	0.849	0.966	0.070	(-0.045, 0.062)
pyrrole-2-carboxylic acid	Lognormal	0.019	(-0.030, 0.068)	0.460	0.884	0.068	(-0.033, 0.065)
stearic acid	Lognormal	-0.010	(-0.024, 0.004)	0.160	0.864	0.168	(-0.025, 0.004)
lactic acid	Lognormal	-0.008	(-0.036, 0.020)	0.600	0.926	0.067	(-0.037, 0.021)
glucose-1-phosphate	Lognormal	0.000	(-0.023, 0.023)	0.987	0.996	0.059	(-0.024, 0.022)
palmitoleic acid	Lognormal	-0.003	(-0.041, 0.034)	0.863	0.968	0.074	(-0.043, 0.033)
lyxitol	Lognormal	-0.023	(-0.058, 0.012)	0.213	0.864	0.142	(-0.057, 0.014)
phthalic acid	Lognormal	-0.005	(-0.030, 0.019)	0.668	0.928	0.067	(-0.030, 0.019)
glucuronic acid	Lognormal	0.036	(-0.007, 0.078)	0.110	0.864	0.240	(-0.008, 0.079)
threitol	Lognormal	-0.023	(-0.055, 0.010)	0.177	0.864	0.170	(-0.056, 0.010)
capric acid	Lognormal	-0.024	(-0.070, 0.021)	0.302	0.864	0.106	(-0.068, 0.024)
valine	Lognormal	-0.002	(-0.019, 0.015)	0.842	0.962	0.068	(-0.019, 0.014)
glyceric acid	Lognormal	-0.001	(-0.030, 0.028)	0.938	0.993	0.059	(-0.030, 0.030)
glutamic acid	Lognormal	0.024	(-0.002, 0.051)	0.080	0.864	0.334	(-0.001, 0.052)
trans-4-hydroxyproline	Lognormal	-0.016	(-0.055, 0.024)	0.445	0.883	0.092	(-0.057, 0.024)
uric acid	Lognormal	-0.009	(-0.042, 0.024)	0.606	0.926	0.079	(-0.041, 0.027)
adipic acid	Lognormal	-0.019	(-0.051, 0.012)	0.243	0.864	0.133	(-0.050, 0.015)
1-methylgalactose NIST	Lognormal	0.012	(-0.057, 0.081)	0.743	0.949	0.071	(-0.059, 0.080)
myo-inositol	Lognormal	-0.015	(-0.044, 0.014)	0.311	0.864	0.115	(-0.044, 0.016)
maleic acid	Lognormal	0.075	(0.000, 0.150)	0.058	0.864	0.483	(0.002, 0.152)
indole-3-acetate	Lognormal	0.004	(-0.026, 0.034)	0.799	0.956	0.065	(-0.028, 0.035)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
proline	Lognormal	-0.008	(-0.051, 0.036)	0.736	0.949	0.066	(-0.052, 0.036)
2-aminobutyric acid	Lognormal	-0.002	(-0.027, 0.023)	0.854	0.966	0.064	(-0.028, 0.024)
oxalic acid	Lognormal	0.007	(-0.052, 0.067)	0.811	0.956	0.064	(-0.055, 0.066)
caprylic acid	Lognormal	-0.002	(-0.029, 0.026)	0.894	0.976	0.070	(-0.029, 0.026)
glycine	Lognormal	-0.001	(-0.015, 0.012)	0.865	0.968	0.063	(-0.013, 0.014)
ribonic acid	Lognormal	-0.008	(-0.042, 0.025)	0.627	0.928	0.085	(-0.044, 0.028)
nicotinic acid	Lognormal	0.017	(-0.055, 0.089)	0.648	0.928	0.070	(-0.052, 0.096)
Biogenic Amines (BA)							
Alprazolam	Lognormal	0.017	(-0.090, 0.123)	0.761	0.956	0.068	(-0.100, 0.118)
Acyclovir	Lognormal	0.013	(-0.093, 0.120)	0.806	0.956	0.066	(-0.093, 0.117)
Linoleoylcarnitine	Lognormal	0.046	(-0.037, 0.129)	0.284	0.864	0.118	(-0.039, 0.131)
Guanine	Lognormal	0.032	(-0.064, 0.127)	0.518	0.899	0.073	(-0.067, 0.127)
Caffeine	Lognormal	-0.106	(-0.210, -0.002)	0.052	0.864	0.381	(-0.211, -0.003)
2-Methylbutyryl-L-carnitine	Lognormal	-0.016	(-0.039, 0.007)	0.187	0.864	0.138	(-0.041, 0.006)
Acetaminophen	Lognormal	0.064	(-0.020, 0.148)	0.143	0.864	0.200	(-0.023, 0.153)
Theobromine	Lognormal	-0.086	(-0.174, 0.003)	0.065	0.864	0.339	(-0.173, 0.006)
Tri-2-ethylhexyl trimellitate	Lognormal	0.014	(-0.098, 0.126)	0.806	0.956	0.073	(-0.112, 0.127)
7-Methylguanosine	Lognormal	-0.015	(-0.042, 0.012)	0.294	0.864	0.109	(-0.041, 0.012)
Usnic acid	Lognormal	0.028	(-0.073, 0.129)	0.593	0.926	0.075	(-0.077, 0.128)
Choline cation	Lognormal	-0.009	(-0.021, 0.002)	0.116	0.864	0.183	(-0.021, 0.002)
Piperine	Lognormal	-0.090	(-0.190, 0.010)	0.086	0.864	0.239	(-0.182, 0.024)
Trigonelline	Lognormal	-0.069	(-0.136, -0.003)	0.048	0.864	0.370	(-0.137, 0.000)
Oleoyl-L-carnitine	Lognormal	0.049	(-0.034, 0.132)	0.256	0.864	0.134	(-0.035, 0.130)
Kynurenine	Lognormal	0.001	(-0.027, 0.029)	0.949	0.996	0.062	(-0.026, 0.032)
Isopropylamine	Lognormal	-0.017	(-0.038, 0.004)	0.124	0.864	0.196	(-0.037, 0.004)
Octanoylcarnitine	Lognormal	0.002	(-0.029, 0.033)	0.910	0.978	0.059	(-0.030, 0.033)
D-erythro-Sphingosine-1-phosphate	Lognormal	0.043	(-0.016, 0.102)	0.159	0.864	0.195	(-0.018, 0.101)
1-Stearoyl-2-arachidonoyl-sn-glycero-3-phosphoserine	Lognormal	0.110	(-0.086, 0.307)	0.278	0.864	0.097	(-0.093, 0.297)
Albendazole sulfoxide	Lognormal	0.099	(-0.058, 0.256)	0.224	0.864	0.136	(-0.066, 0.257)
Ranitidine N-oxide	Lognormal	0.072	(-0.037, 0.180)	0.203	0.864	0.148	(-0.033, 0.186)
H-Pro-Hyp-OH	Lognormal	0.018	(-0.019, 0.056)	0.343	0.864	0.101	(-0.021, 0.057)
4-Acetamidobutyric acid	Lognormal	-0.018	(-0.057, 0.022)	0.393	0.873	0.096	(-0.060, 0.021)
3-Methylglutarylcarnitine	Lognormal	-0.056	(-0.134, 0.021)	0.161	0.864	0.178	(-0.131, 0.026)
4,5,7-Trihydroxyisoflavone	Lognormal	0.067	(-0.094, 0.228)	0.420	0.873	0.091	(-0.101, 0.229)
7-Hydroxywarfarin	Lognormal	-0.015	(-0.069, 0.039)	0.582	0.924	0.074	(-0.071, 0.038)
1-Monostearin	Lognormal	0.044	(-0.038, 0.125)	0.299	0.864	0.112	(-0.041, 0.126)
SDMA	Lognormal	-0.004	(-0.022, 0.014)	0.661	0.928	0.063	(-0.023, 0.015)
Ergothioneine	Lognormal	-0.005	(-0.076, 0.066)	0.890	0.976	0.061	(-0.083, 0.062)
1-Oleoyl-2-acetyl-sn-glycerol	Lognormal	0.028	(-0.053, 0.110)	0.497	0.896	0.085	(-0.056, 0.116)
L-Citrulline	Lognormal	0.001	(-0.017, 0.019)	0.906	0.977	0.067	(-0.017, 0.020)
Pantoprazole	Lognormal	-0.088	(-0.200, 0.024)	0.130	0.864	0.208	(-0.194, 0.030)
Phenylalanine	Lognormal	0.009	(-0.004, 0.022)	0.164	0.864	0.164	(-0.003, 0.023)
D-Turanose	Lognormal	-0.028	(-0.093, 0.036)	0.399	0.873	0.092	(-0.092, 0.041)
Trazodone	Lognormal	-0.003	(-0.041, 0.035)	0.866	0.968	0.058	(-0.042, 0.035)
2,6-Diaminopimelic acid	Lognormal	0.058	(-0.030, 0.146)	0.207	0.864	0.146	(-0.032, 0.148)
N-.alpha.-Acetyl-L-arginine	Lognormal	-0.003	(-0.032, 0.026)	0.832	0.962	0.072	(-0.034, 0.026)
2-Amino-1-phenylethanol	Lognormal	0.009	(-0.004, 0.022)	0.179	0.864	0.146	(-0.005, 0.022)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Modafinil acid	Lognormal	-0.085	(-0.197, 0.028)	0.149	0.864	0.185	(-0.203, 0.024)
Decanoyl-L-carnitine	Lognormal	0.054	(-0.022, 0.130)	0.172	0.864	0.161	(-0.026, 0.135)
3-Amino-1-propanol	Lognormal	-0.021	(-0.057, 0.015)	0.254	0.864	0.125	(-0.060, 0.014)
1-Oleoyl-sn-glycero-3-phosphoethanolamine	Lognormal	0.002	(-0.082, 0.086)	0.965	0.996	0.064	(-0.088, 0.082)
H-gamma-glutamyl-glutamine	Lognormal	0.046	(-0.007, 0.098)	0.098	0.864	0.261	(-0.006, 0.101)
Lauroyl-L-carnitine	Lognormal	-0.030	(-0.114, 0.054)	0.494	0.896	0.077	(-0.107, 0.062)
L-Leucine, methyl ester	Lognormal	0.031	(-0.054, 0.115)	0.482	0.884	0.082	(-0.051, 0.123)
Glutamic acid	Lognormal	0.022	(-0.007, 0.050)	0.140	0.864	0.199	(-0.008, 0.049)
Citrulline	Lognormal	0.002	(-0.017, 0.022)	0.819	0.957	0.068	(-0.017, 0.023)
Trimethylamine-N-oxide	Lognormal	-0.020	(-0.076, 0.035)	0.480	0.884	0.078	(-0.073, 0.037)
3-Hydroxypyridine	Lognormal	-0.066	(-0.170, 0.038)	0.223	0.864	0.089	(-0.176, 0.041)
Losartan	Lognormal	0.076	(-0.024, 0.176)	0.143	0.864	0.239	(-0.021, 0.181)
Lamotrigine;	Lognormal	0.105	(-0.080, 0.289)	0.275	0.864	0.126	(-0.088, 0.296)
Gabapentin	Lognormal	0.044	(-0.063, 0.152)	0.425	0.873	0.097	(-0.063, 0.154)
Pyridoxine;	Lognormal	-0.036	(-0.090, 0.018)	0.203	0.864	0.134	(-0.089, 0.018)
N-Acetylhistidine	Lognormal	-0.006	(-0.043, 0.032)	0.771	0.956	0.060	(-0.044, 0.031)
Quetiapine	Lognormal	0.015	(-0.050, 0.080)	0.658	0.928	0.077	(-0.052, 0.081)
N-Methylhistidine	Lognormal	0.004	(-0.065, 0.073)	0.908	0.977	0.069	(-0.068, 0.074)
.beta.-Phenyl-.gamma.-aminobutyric acid	Lognormal	-0.010	(-0.055, 0.035)	0.661	0.928	0.068	(-0.054, 0.036)
Testosterone	Lognormal	-0.019	(-0.087, 0.049)	0.596	0.926	0.068	(-0.088, 0.050)
Thr-Ile-Arg	Lognormal	-0.010	(-0.120, 0.099)	0.854	0.966	0.067	(-0.122, 0.100)
Dexpanthenol	Lognormal	0.030	(-0.026, 0.086)	0.296	0.864	0.099	(-0.025, 0.086)
1-Stearoyl-2-arachidonoyl-sn-glycero-3-phospho-(1'-myo-inositol)	Lognormal	0.090	(-0.131, 0.312)	0.429	0.873	0.091	(-0.137, 0.320)
Creatinine	Lognormal	0.003	(-0.006, 0.011)	0.536	0.902	0.056	(-0.006, 0.012)
p-Acetamidophenyl .beta.-D-glucuronide	Lognormal	0.036	(-0.114, 0.185)	0.642	0.928	0.079	(-0.115, 0.200)
Ranitidine	Lognormal	0.064	(-0.027, 0.154)	0.176	0.864	0.167	(-0.030, 0.161)
(R)-Butyrylcarnitine	Lognormal	-0.009	(-0.029, 0.011)	0.393	0.873	0.080	(-0.030, 0.012)
Glycocholic acid	Lognormal	0.030	(-0.057, 0.117)	0.505	0.899	0.088	(-0.057, 0.119)
N-Acetyl-D-norleucine	Lognormal	-0.006	(-0.051, 0.039)	0.797	0.956	0.052	(-0.052, 0.043)
N.alpha.-Methyl-L-lysine	Lognormal	-0.014	(-0.084, 0.057)	0.706	0.937	0.067	(-0.087, 0.058)
Betaine	Lognormal	-0.008	(-0.018, 0.002)	0.146	0.864	0.217	(-0.018, 0.003)
Norleucine	Lognormal	0.000	(-0.026, 0.026)	0.980	0.996	0.068	(-0.026, 0.026)
Nudifloramide	Lognormal	0.007	(-0.027, 0.041)	0.688	0.930	0.067	(-0.027, 0.042)
1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	Lognormal	0.024	(-0.065, 0.112)	0.600	0.926	0.080	(-0.061, 0.117)
Fexofenadine	Lognormal	-0.001	(-0.044, 0.043)	0.979	0.996	0.065	(-0.046, 0.041)
Hexanoyl-L-carnitine	Lognormal	0.009	(-0.023, 0.041)	0.583	0.924	0.064	(-0.023, 0.043)
cis-10,11-Dihydroxy-10,11-dihydrocarbamazepine	Lognormal	-0.013	(-0.039, 0.012)	0.316	0.864	0.103	(-0.039, 0.013)
Acetazolamide	Lognormal	-0.025	(-0.188, 0.137)	0.763	0.956	0.066	(-0.185, 0.148)
1-Acetyl-3-piperidinamine	Lognormal	0.001	(-0.032, 0.034)	0.943	0.994	0.059	(-0.031, 0.035)
Ala-Ile	Lognormal	0.009	(-0.023, 0.040)	0.582	0.924	0.060	(-0.025, 0.041)
Quetiapine sulfoxide	Lognormal	0.007	(-0.081, 0.095)	0.877	0.972	0.072	(-0.084, 0.093)
Tryptophan	Lognormal	-0.005	(-0.024, 0.013)	0.575	0.920	0.079	(-0.024, 0.013)
Prazepam	Lognormal	0.019	(-0.054, 0.092)	0.613	0.928	0.072	(-0.053, 0.091)
Omeprazole sulfone N-oxide	Lognormal	-0.002	(-0.133, 0.130)	0.979	0.996	0.069	(-0.136, 0.135)
Montelukast-1,2-diol	Lognormal	-0.019	(-0.182, 0.143)	0.817	0.957	0.068	(-0.193, 0.142)
Diazepam	Lognormal	0.051	(-0.063, 0.165)	0.384	0.873	0.084	(-0.077, 0.164)
Irbesartan	Lognormal	-0.020	(-0.037, -0.002)	0.032	0.864	0.700	(-0.037, -0.001)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Betonicine	Lognormal	-0.058	(-0.186, 0.069)	0.376	0.873	0.095	(-0.184, 0.068)
Adenosine	Lognormal	0.043	(-0.018, 0.105)	0.175	0.864	0.144	(-0.020, 0.108)
Ethiolat	Lognormal	-0.009	(-0.074, 0.056)	0.790	0.956	0.068	(-0.077, 0.058)
Toradol	Lognormal	-0.038	(-0.097, 0.022)	0.223	0.864	0.142	(-0.099, 0.022)
NEPSILON,NEPSILON,NEPSILON-TRIMETHYLLYSINE	Lognormal	-0.002	(-0.030, 0.026)	0.870	0.968	0.063	(-0.031, 0.026)
Histidine	Lognormal	0.011	(-0.019, 0.041)	0.468	0.884	0.081	(-0.018, 0.042)
Codeine-6-.beta.-D-glucuronide	Lognormal	-0.011	(-0.049, 0.027)	0.559	0.905	0.071	(-0.052, 0.026)
Ethylidethanolamine	Lognormal	0.030	(-0.007, 0.068)	0.115	0.864	0.200	(-0.009, 0.067)
6-Hydroxyflavone	Lognormal	-0.033	(-0.113, 0.048)	0.432	0.876	0.091	(-0.118, 0.046)
Omeprazole sulfone	Lognormal	-0.001	(-0.133, 0.131)	0.985	0.996	0.072	(-0.138, 0.131)
L-Tyrosine	Lognormal	-0.016	(-0.043, 0.010)	0.236	0.864	0.132	(-0.042, 0.011)
Aminodiphenylmethane	Lognormal	-0.017	(-0.089, 0.056)	0.657	0.928	0.070	(-0.089, 0.059)
1-Methylnicotinamide	Lognormal	-0.015	(-0.056, 0.027)	0.495	0.896	0.086	(-0.056, 0.028)
Phenylacetyl-L-glutamine	Lognormal	0.019	(-0.034, 0.072)	0.484	0.884	0.077	(-0.034, 0.076)
Tauroursodeoxycholic acid	Lognormal	-0.011	(-0.085, 0.062)	0.762	0.956	0.063	(-0.088, 0.068)
Tyrosine	Lognormal	-0.007	(-0.030, 0.016)	0.558	0.905	0.077	(-0.031, 0.015)
N-(3-(Aminomethyl)benzyl)acetamidine	Lognormal	0.015	(-0.055, 0.084)	0.683	0.929	0.060	(-0.055, 0.086)
3-Dehydrocarnitine	Lognormal	-0.028	(-0.057, 0.001)	0.065	0.864	0.303	(-0.058, 0.005)
3-Hydroxyoleylcarnitine	Lognormal	-0.012	(-0.174, 0.150)	0.885	0.975	0.066	(-0.176, 0.153)
Pyrantel	Lognormal	-0.006	(-0.032, 0.021)	0.669	0.928	0.061	(-0.034, 0.020)
Ile-Glu-Arg	Lognormal	0.043	(-0.097, 0.184)	0.551	0.904	0.078	(-0.101, 0.180)
Moxonidine	Lognormal	0.053	(0.002, 0.105)	0.050	0.864	0.466	(-0.001, 0.103)
Ornithine	Lognormal	0.020	(-0.014, 0.053)	0.259	0.864	0.097	(-0.016, 0.053)
L-Threonine	Lognormal	0.002	(-0.018, 0.021)	0.854	0.966	0.063	(-0.018, 0.022)
3-Methylxanthine	Lognormal	-0.044	(-0.130, 0.042)	0.320	0.864	0.114	(-0.140, 0.040)
(3-Carboxypropyl)trimethylammonium cation	Lognormal	-0.006	(-0.034, 0.023)	0.691	0.930	0.073	(-0.035, 0.024)
Hydroxybupropion	Lognormal	-0.031	(-0.094, 0.032)	0.338	0.864	0.098	(-0.097, 0.027)
Glaucine	Lognormal	-0.007	(-0.035, 0.021)	0.617	0.928	0.069	(-0.035, 0.022)
L-Cystine	Lognormal	0.001	(-0.047, 0.048)	0.980	0.996	0.051	(-0.048, 0.047)
Methacholine cation	Lognormal	-0.032	(-0.067, 0.003)	0.076	0.864	0.327	(-0.069, 0.004)
Urea	Lognormal	-0.007	(-0.024, 0.009)	0.395	0.873	0.081	(-0.025, 0.010)
4-Fluoro-.alpha.-pyrrolidinobutiophenone	Lognormal	-0.010	(-0.055, 0.036)	0.674	0.928	0.077	(-0.057, 0.035)
Benthiavalicarb-isopropyl	Lognormal	-0.002	(-0.080, 0.076)	0.961	0.996	0.070	(-0.084, 0.077)
Modafinil	Lognormal	-0.043	(-0.127, 0.041)	0.318	0.864	0.101	(-0.118, 0.043)
Palmitamide	Lognormal	-0.002	(-0.069, 0.065)	0.955	0.996	0.068	(-0.070, 0.065)
alpha-Methylhistidine;	Lognormal	0.013	(-0.079, 0.105)	0.777	0.956	0.062	(-0.079, 0.109)
Ranitidine-S-oxide	Lognormal	0.079	(-0.039, 0.198)	0.198	0.864	0.144	(-0.049, 0.197)
Metoprolol acid	Lognormal	0.062	(-0.068, 0.192)	0.356	0.871	0.089	(-0.069, 0.195)
7.alpha.-Hydroxy-3-oxo-4-cholestenoic acid	Lognormal	-0.007	(-0.055, 0.042)	0.781	0.956	0.073	(-0.054, 0.045)
5'-S-Methyl-5'-thioadenosine	Lognormal	0.011	(-0.143, 0.166)	0.887	0.975	0.057	(-0.156, 0.159)
Stachydrine	Lognormal	-0.084	(-0.154, -0.014)	0.023	0.864	0.954	(-0.154, -0.016)
Glycodeoxycholic acid	Lognormal	0.027	(-0.061, 0.116)	0.548	0.904	0.074	(-0.060, 0.117)
Carnitine	Lognormal	-0.003	(-0.017, 0.010)	0.655	0.928	0.064	(-0.017, 0.011)
Topiramate	Lognormal	0.000	(-0.053, 0.052)	0.987	0.996	0.064	(-0.052, 0.054)
Meprobamate	Lognormal	0.000	(-0.075, 0.075)	0.999	1.000	0.068	(-0.074, 0.079)
DL-Indole-3-lactic acid	Lognormal	0.001	(-0.017, 0.019)	0.934	0.992	0.061	(-0.017, 0.019)
Ethylenediaminetetraacetic acid	Lognormal	0.068	(-0.084, 0.220)	0.384	0.873	0.100	(-0.093, 0.210)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Gly-Pro-Arg	Lognormal	0.048	(-0.104, 0.199)	0.542	0.902	0.079	(-0.107, 0.190)
Pipecolic acid	Lognormal	-0.004	(-0.059, 0.051)	0.887	0.975	0.052	(-0.062, 0.051)
L-Cysteine-glutathione disulfide	Lognormal	0.024	(-0.033, 0.081)	0.418	0.873	0.066	(-0.038, 0.083)
3-Cysteinyacetaminophen	Lognormal	0.216	(0.030, 0.401)	0.028	0.864	0.718	(0.033, 0.408)
Ezetimibe	Lognormal	-0.028	(-0.090, 0.034)	0.378	0.873	0.093	(-0.091, 0.038)
1-Methyl-L-histidine	Lognormal	0.032	(-0.066, 0.131)	0.526	0.899	0.086	(-0.065, 0.135)
Carbamazepine	Lognormal	0.048	(-0.035, 0.132)	0.265	0.864	0.114	(-0.037, 0.135)
5'-S-Methylthioadenosine	Lognormal	0.052	(-0.112, 0.215)	0.540	0.902	0.068	(-0.106, 0.218)
Dinor-12-oxophytodienoic acid	Lognormal	0.029	(-0.077, 0.135)	0.596	0.926	0.075	(-0.076, 0.134)
Atorvastatin	Lognormal	-0.016	(-0.047, 0.015)	0.315	0.864	0.097	(-0.048, 0.016)
N-Methylproline	Lognormal	-0.011	(-0.065, 0.043)	0.699	0.935	0.064	(-0.066, 0.042)
4'-Methyl-N-methylhexanophenone	Lognormal	-0.119	(-0.229, -0.009)	0.040	0.864	0.665	(-0.229, -0.014)
trans-3'-Hydroxycotinine	Lognormal	-0.013	(-0.080, 0.053)	0.699	0.935	0.057	(-0.084, 0.056)
Guanidine	Lognormal	0.009	(-0.022, 0.039)	0.572	0.917	0.076	(-0.022, 0.040)
Telmisartan	Lognormal	0.000	(-0.032, 0.033)	0.993	0.997	0.055	(-0.034, 0.032)
Theanine;	Lognormal	0.018	(-0.037, 0.073)	0.528	0.899	0.068	(-0.038, 0.072)
Methylgallate	Lognormal	-0.008	(-0.159, 0.143)	0.918	0.983	0.068	(-0.170, 0.141)
Avobenzon	Lognormal	-0.020	(-0.067, 0.028)	0.420	0.873	0.071	(-0.062, 0.033)
3,4-Dimethoxybenzaldehyde	Lognormal	0.014	(-0.049, 0.078)	0.661	0.928	0.064	(-0.053, 0.078)
Trimethoprim	Lognormal	-0.015	(-0.047, 0.017)	0.369	0.873	0.095	(-0.048, 0.019)
Ticlopidine	Lognormal	-0.073	(-0.235, 0.090)	0.386	0.873	0.091	(-0.232, 0.108)
N.epsilon.-Acetyl-L-lysine	Lognormal	0.008	(-0.016, 0.033)	0.506	0.899	0.086	(-0.017, 0.034)
2,2-Bishydroxymethyl]-2,2',2''-nitrioltriethanol	Lognormal	0.023	(-0.038, 0.083)	0.468	0.884	0.086	(-0.041, 0.084)
Betaine aldehyde cation	Lognormal	-0.007	(-0.087, 0.073)	0.868	0.968	0.048	(-0.090, 0.073)
Pantothenic acid	Lognormal	0.036	(-0.006, 0.079)	0.102	0.864	0.243	(-0.007, 0.081)
D-Pyroglutamic acid	Lognormal	0.007	(-0.001, 0.014)	0.085	0.864	0.274	(-0.001, 0.015)
2-Indolinone	Lognormal	-0.023	(-0.055, 0.009)	0.161	0.864	0.153	(-0.054, 0.010)
Pyridoxal	Lognormal	0.006	(-0.029, 0.042)	0.724	0.944	0.070	(-0.028, 0.044)
(2R)-3-Hydroxyisovaleroylcarnitine	Lognormal	0.001	(-0.036, 0.038)	0.958	0.996	0.054	(-0.036, 0.039)
Arginine	Lognormal	0.015	(-0.004, 0.035)	0.134	0.864	0.163	(-0.006, 0.034)
Metoprolol	Lognormal	0.046	(-0.049, 0.141)	0.350	0.864	0.102	(-0.049, 0.150)
N-Acetyl-L-carnosine	Lognormal	-0.001	(-0.038, 0.035)	0.942	0.994	0.063	(-0.042, 0.034)
3-Hydroxybutyrylcarnitine	Lognormal	0.011	(-0.043, 0.066)	0.692	0.930	0.075	(-0.043, 0.065)
4-Aminomethylcyclohexanecarboxylic acid;	Lognormal	0.012	(-0.051, 0.076)	0.703	0.937	0.067	(-0.050, 0.076)
D-.alpha.-Cyclohexylglycine	Lognormal	-0.029	(-0.089, 0.031)	0.350	0.864	0.092	(-0.091, 0.031)
Urocanic acid;	Lognormal	0.010	(-0.023, 0.043)	0.557	0.905	0.068	(-0.023, 0.044)
L-Carnitine	Lognormal	0.007	(-0.012, 0.026)	0.473	0.884	0.078	(-0.012, 0.027)
Metformin	Lognormal	0.005	(-0.031, 0.041)	0.778	0.956	0.055	(-0.029, 0.041)
Cotinine N-.beta.-D-glucuronide	Lognormal	-0.009	(-0.141, 0.123)	0.894	0.976	0.052	(-0.142, 0.125)
Glutamine	Lognormal	0.007	(-0.001, 0.016)	0.099	0.864	0.269	(-0.001, 0.016)
Heptadecasping-4-enine	Lognormal	0.059	(-0.168, 0.287)	0.613	0.928	0.065	(-0.180, 0.284)
Ser-Tyr-Lys	Lognormal	0.005	(-0.120, 0.129)	0.941	0.994	0.060	(-0.120, 0.130)
3-Aminoquinoline	Lognormal	0.030	(-0.060, 0.119)	0.518	0.899	0.071	(-0.070, 0.115)
Biliverden	Lognormal	0.009	(-0.031, 0.049)	0.661	0.928	0.069	(-0.031, 0.049)
Borrelidin	Lognormal	-0.027	(-0.127, 0.073)	0.606	0.926	0.076	(-0.132, 0.081)
Creatine	Lognormal	0.028	(0.001, 0.056)	0.050	0.864	0.447	(0.000, 0.057)
Isopentenyladenine	Lognormal	0.005	(-0.013, 0.022)	0.592	0.926	0.078	(-0.012, 0.023)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Indole-3-propionic acid	Lognormal	-0.048	(-0.114, 0.018)	0.163	0.864	0.175	(-0.118, 0.017)
D-Fructose	Lognormal	0.004	(-0.012, 0.019)	0.647	0.928	0.072	(-0.012, 0.019)
rac-4-Sulfoxypropranolol	Lognormal	0.020	(-0.049, 0.088)	0.577	0.921	0.079	(-0.047, 0.091)
3-Pyridinemethanol	Lognormal	-0.004	(-0.037, 0.030)	0.828	0.962	0.062	(-0.038, 0.029)
Levocetirizine;	Lognormal	0.002	(-0.140, 0.144)	0.981	0.996	0.071	(-0.150, 0.136)
.epsilon.-Caprolactam	Lognormal	0.009	(-0.030, 0.047)	0.653	0.928	0.055	(-0.030, 0.048)
N-Acetylalanine	Lognormal	0.016	(-0.093, 0.125)	0.780	0.956	0.075	(-0.095, 0.129)
1,2-Dimethylimidazole	Lognormal	-0.011	(-0.042, 0.019)	0.461	0.884	0.081	(-0.044, 0.016)
R-(-)-O-Desmethylvenlafaxine	Lognormal	0.000	(-0.089, 0.089)	1.000	1.000	0.065	(-0.088, 0.095)
Naproxen	Lognormal	0.027	(-0.074, 0.129)	0.601	0.926	0.082	(-0.076, 0.132)
N8-Acetylspermidine	Lognormal	-0.002	(-0.032, 0.028)	0.899	0.976	0.063	(-0.032, 0.029)
1-Stearoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	Lognormal	0.032	(-0.065, 0.130)	0.517	0.899	0.080	(-0.065, 0.133)
Propionylcarnitine	Lognormal	-0.008	(-0.025, 0.008)	0.339	0.864	0.088	(-0.026, 0.010)
Matrine	Lognormal	0.038	(-0.060, 0.137)	0.449	0.884	0.087	(-0.059, 0.139)
Trileptal	Lognormal	0.006	(-0.023, 0.035)	0.677	0.929	0.065	(-0.024, 0.038)
Androstan-3-ol-17-one 3-glucuronide	Lognormal	0.005	(-0.052, 0.062)	0.861	0.967	0.059	(-0.049, 0.066)
Serotonin	Lognormal	0.012	(-0.026, 0.050)	0.543	0.902	0.053	(-0.028, 0.049)
Lansoprazole	Lognormal	-0.165	(-0.330, 0.000)	0.056	0.864	0.390	(-0.332, 0.010)
Atenolol	Lognormal	0.018	(-0.087, 0.123)	0.739	0.949	0.067	(-0.096, 0.121)
1-Acetyl-4-piperidinamine	Lognormal	0.035	(-0.042, 0.113)	0.376	0.873	0.095	(-0.043, 0.116)
Homoarginine;	Lognormal	0.037	(0.005, 0.069)	0.027	0.864	0.545	(0.003, 0.070)
1-Phenylpyrrolidine	Lognormal	0.003	(-0.047, 0.053)	0.909	0.977	0.062	(-0.047, 0.055)
Acetyl-DL-carnitine	Lognormal	0.007	(-0.021, 0.034)	0.624	0.928	0.068	(-0.022, 0.035)
2-Hydroxyibuprofen	Lognormal	-0.022	(-0.092, 0.047)	0.531	0.899	0.068	(-0.096, 0.048)
Milnacipran	Lognormal	0.031	(-0.042, 0.103)	0.413	0.873	0.081	(-0.047, 0.102)
Triptolide	Lognormal	-0.018	(-0.049, 0.013)	0.254	0.864	0.124	(-0.052, 0.012)
2,2',2''-Nitrilotriethanol	Lognormal	0.007	(-0.023, 0.036)	0.657	0.928	0.069	(-0.023, 0.038)
Albendazole	Lognormal	0.017	(-0.015, 0.048)	0.307	0.864	0.091	(-0.015, 0.050)
Scopoletin	Lognormal	-0.045	(-0.204, 0.115)	0.588	0.926	0.065	(-0.210, 0.109)
Mefenorex	Lognormal	0.010	(-0.084, 0.105)	0.835	0.962	0.061	(-0.088, 0.105)
Diphenhydramine	Lognormal	-0.003	(-0.036, 0.030)	0.859	0.967	0.054	(-0.036, 0.030)
3-(1-Pyrazolyl)-alanine	Lognormal	0.010	(-0.107, 0.126)	0.871	0.968	0.064	(-0.101, 0.136)
Methionine	Lognormal	0.008	(-0.010, 0.025)	0.389	0.873	0.094	(-0.010, 0.026)
Hypoxanthine	Lognormal	-0.002	(-0.033, 0.028)	0.887	0.975	0.047	(-0.033, 0.029)
Tapentadol-.beta.-D-glucuronide	Lognormal	-0.053	(-0.214, 0.108)	0.523	0.899	0.091	(-0.219, 0.120)
Methioninesulfoxide	Lognormal	0.038	(0.004, 0.072)	0.036	0.864	0.652	(0.001, 0.069)
Ondansetron	Lognormal	-0.005	(-0.028, 0.018)	0.668	0.928	0.061	(-0.028, 0.018)
threo-Dihydrobupropion	Lognormal	-0.011	(-0.061, 0.040)	0.681	0.929	0.065	(-0.060, 0.041)
Isoleucine	Lognormal	0.006	(-0.019, 0.030)	0.651	0.928	0.070	(-0.020, 0.030)
Esomeprazole	Lognormal	0.010	(-0.034, 0.055)	0.653	0.928	0.074	(-0.035, 0.058)
Meloxicam	Lognormal	0.078	(-0.181, 0.337)	0.560	0.905	0.082	(-0.189, 0.345)
3,5-Dihydroxyphenylglycine	Lognormal	0.007	(-0.044, 0.057)	0.798	0.956	0.062	(-0.041, 0.061)
Temazepam	Lognormal	0.026	(-0.052, 0.103)	0.521	0.899	0.083	(-0.059, 0.099)
Lauric acid diethanolamide	Lognormal	0.022	(-0.078, 0.122)	0.665	0.928	0.072	(-0.080, 0.126)
4-Pyridoxic acid;	Lognormal	0.050	(-0.035, 0.134)	0.260	0.864	0.124	(-0.037, 0.138)
Phenylacetylglutamine	Lognormal	0.016	(-0.034, 0.065)	0.539	0.902	0.071	(-0.039, 0.065)
Penciclovir	Lognormal	0.001	(-0.041, 0.043)	0.963	0.996	0.056	(-0.040, 0.045)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
6-Methoxynaphthaleneacetic acid	Lognormal	-0.018	(-0.050, 0.014)	0.280	0.864	0.119	(-0.051, 0.017)
1-Methyladenosine A	Lognormal	-0.003	(-0.019, 0.013)	0.695	0.932	0.064	(-0.020, 0.012)
Coniferylaldehyde	Lognormal	0.020	(-0.018, 0.058)	0.303	0.864	0.107	(-0.020, 0.060)
Bradykinin	Lognormal	0.258	(-0.018, 0.535)	0.075	0.864	0.301	(-0.004, 0.560)
Lysine	Lognormal	0.010	(-0.009, 0.029)	0.300	0.864	0.075	(-0.010, 0.029)
Benzophenone-3	Lognormal	-0.023	(-0.107, 0.061)	0.597	0.926	0.080	(-0.110, 0.058)
Sulfamethoxazole	Lognormal	-0.066	(-0.204, 0.071)	0.350	0.864	0.102	(-0.210, 0.067)
Cyclo(Leu-Pro)	Lognormal	-0.001	(-0.054, 0.052)	0.971	0.996	0.066	(-0.051, 0.055)
N.epsilon.-Methyl-L-lysine	Lognormal	0.030	(-0.029, 0.088)	0.328	0.864	0.102	(-0.032, 0.086)
Proline	Lognormal	-0.017	(-0.039, 0.006)	0.164	0.864	0.177	(-0.038, 0.009)
Complex Lipids (CL)							
PC (p-34:2)/PC (o-34:3) - ESI(+)	Lognormal	-0.010	(-0.031, 0.011)	0.343	0.864	0.106	(-0.031, 0.012)
PE (p-36:2)/PE (o-36:3) - ESI(+)	Lognormal	-0.020	(-0.059, 0.018)	0.310	0.864	0.117	(-0.062, 0.018)
PC (p-34:1)/PC (o-34:2)	Lognormal	-0.009	(-0.028, 0.010)	0.365	0.873	0.091	(-0.030, 0.011)
PC (36:4) A - ESI(+)	Lognormal	-0.015	(-0.034, 0.004)	0.128	0.864	0.174	(-0.033, 0.005)
PC (36:2)	Lognormal	-0.004	(-0.011, 0.003)	0.271	0.864	0.106	(-0.011, 0.004)
PC 34:4e	Lognormal	-0.007	(-0.040, 0.025)	0.666	0.928	0.073	(-0.039, 0.026)
PC (36:4) A - ESI(-)	Lognormal	-0.014	(-0.035, 0.006)	0.181	0.864	0.151	(-0.035, 0.007)
PC (34:2) - ESI(+)	Lognormal	0.000	(-0.006, 0.006)	0.900	0.976	0.061	(-0.006, 0.007)
PC (p-34:2)/PC (o-34:3) - ESI(-)	Lognormal	-0.016	(-0.038, 0.005)	0.144	0.864	0.169	(-0.037, 0.007)
PC (p-36:4)/PC (o-36:5) - ESI(-)	Lognormal	-0.019	(-0.046, 0.008)	0.176	0.864	0.169	(-0.046, 0.010)
PC (p-34:1)/PC (o-34:2) A	Lognormal	-0.013	(-0.042, 0.015)	0.363	0.873	0.107	(-0.043, 0.014)
PC (p-36:1)/PC (o-36:2)	Lognormal	-0.020	(-0.061, 0.021)	0.348	0.864	0.082	(-0.060, 0.025)
PE (p-34:2)/PE (o-34:3)	Lognormal	-0.032	(-0.090, 0.027)	0.291	0.864	0.119	(-0.091, 0.026)
SM (d40:3)	Lognormal	-0.002	(-0.040, 0.037)	0.933	0.992	0.060	(-0.042, 0.036)
PE (p-36:2)/PE (o-36:3) - ESI(-)	Lognormal	-0.028	(-0.077, 0.020)	0.259	0.864	0.138	(-0.078, 0.021)
PE (p-36:4)/PE (o-36:5) - ESI(-)	Lognormal	-0.021	(-0.060, 0.017)	0.282	0.864	0.118	(-0.062, 0.017)
CE (18:2)	Lognormal	0.003	(-0.010, 0.017)	0.637	0.928	0.065	(-0.010, 0.018)
PC (36:5) A	Lognormal	-0.020	(-0.075, 0.035)	0.480	0.884	0.076	(-0.078, 0.033)
LPC (18:2) - ESI(-)	Lognormal	-0.022	(-0.043, -0.001)	0.048	0.864	0.426	(-0.043, -0.001)
PC (34:2) - ESI(-)	Lognormal	-0.011	(-0.025, 0.004)	0.162	0.864	0.187	(-0.026, 0.005)
PC (p-36:2)/PC (o-36:3)	Lognormal	-0.007	(-0.033, 0.020)	0.636	0.928	0.076	(-0.033, 0.021)
TG (56:6)	Lognormal	0.004	(-0.011, 0.019)	0.615	0.928	0.073	(-0.013, 0.019)
PC (p-36:3)/PC (o-36:4) - ESI(-)	Lognormal	-0.016	(-0.037, 0.005)	0.145	0.864	0.204	(-0.038, 0.005)
TG (55:6)	Lognormal	-0.001	(-0.032, 0.029)	0.936	0.992	0.065	(-0.033, 0.030)
PC (36:5)A	Lognormal	-0.018	(-0.050, 0.013)	0.258	0.864	0.102	(-0.051, 0.014)
SM (d34:2) - ESI(-)	Lognormal	-0.006	(-0.023, 0.010)	0.460	0.884	0.092	(-0.024, 0.010)
SM (d34:1) - ESI(-)	Lognormal	-0.006	(-0.021, 0.009)	0.441	0.881	0.093	(-0.020, 0.009)
LPE (18:2) - ESI(-)	Lognormal	-0.033	(-0.074, 0.008)	0.119	0.864	0.194	(-0.073, 0.010)
TG (54:6) C	Lognormal	-0.006	(-0.031, 0.020)	0.672	0.928	0.069	(-0.032, 0.021)
PC (34:3)	Lognormal	-0.018	(-0.046, 0.009)	0.199	0.864	0.178	(-0.048, 0.010)
PE (p-38:5)/PE (o-38:6) - ESI(-)	Lognormal	-0.025	(-0.061, 0.011)	0.185	0.864	0.142	(-0.059, 0.015)
LPE (18:2) - ESI(+)	Lognormal	-0.022	(-0.053, 0.009)	0.176	0.864	0.164	(-0.054, 0.009)
SM (d38:2) - ESI(-)	Lognormal	-0.005	(-0.028, 0.018)	0.678	0.929	0.068	(-0.027, 0.019)
LPC (18:2) - ESI(+)	Lognormal	-0.016	(-0.037, 0.004)	0.123	0.864	0.176	(-0.039, 0.004)
PE (p-36:1)/PE (o-36:2) - ESI(-)	Lognormal	-0.035	(-0.113, 0.043)	0.390	0.873	0.112	(-0.116, 0.044)
SM (d39:1) - ESI(-)	Lognormal	-0.023	(-0.052, 0.006)	0.124	0.864	0.221	(-0.052, 0.007)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
PC (32:2) - ESI(-)	Lognormal	-0.041	(-0.084, 0.001)	0.065	0.864	0.438	(-0.085, 0.000)
PC (p-38:4)/PC (o-38:5) A	Lognormal	-0.012	(-0.030, 0.005)	0.174	0.864	0.173	(-0.030, 0.005)
TG (54:7) B	Lognormal	-0.012	(-0.045, 0.021)	0.471	0.884	0.091	(-0.046, 0.023)
PC (33:2) - ESI(+)	Lognormal	0.009	(-0.009, 0.026)	0.346	0.864	0.102	(-0.009, 0.027)
AC (10:1)	Lognormal	0.007	(-0.032, 0.047)	0.716	0.939	0.076	(-0.030, 0.049)
PC (34:3) B	Lognormal	-0.011	(-0.031, 0.010)	0.309	0.864	0.119	(-0.032, 0.011)
LPC (18:3)	Lognormal	-0.041	(-0.081, 0.000)	0.056	0.864	0.451	(-0.084, 0.000)
PE (p-38:4)/PE (o-38:5)	Lognormal	-0.016	(-0.055, 0.024)	0.441	0.881	0.085	(-0.057, 0.025)
CE (20:2)	Lognormal	-0.012	(-0.046, 0.023)	0.506	0.899	0.075	(-0.047, 0.025)
SM (d40:1) - ESI(-)	Lognormal	-0.016	(-0.036, 0.005)	0.136	0.864	0.205	(-0.036, 0.005)
PC (o-34:0)	Lognormal	0.004	(-0.021, 0.030)	0.748	0.951	0.062	(-0.021, 0.030)
PC (35:2)	Lognormal	0.003	(-0.019, 0.025)	0.788	0.956	0.061	(-0.019, 0.027)
Ceramide (d42:1) - ESI (+)	Lognormal	-0.007	(-0.022, 0.009)	0.418	0.873	0.098	(-0.022, 0.010)
FA (16:1) (palmitoleic acid)	Lognormal	0.020	(-0.010, 0.050)	0.200	0.864	0.133	(-0.010, 0.052)
PE (p-36:4)/PE (o-36:5) - ESI(+)	Lognormal	-0.011	(-0.047, 0.024)	0.531	0.899	0.071	(-0.048, 0.024)
PC (32:2) - ESI(+)	Lognormal	-0.016	(-0.049, 0.018)	0.364	0.873	0.106	(-0.048, 0.021)
TG (56:7) B	Lognormal	0.003	(-0.024, 0.030)	0.832	0.962	0.067	(-0.025, 0.030)
PC (p-38:3)/PC (o-38:4) - ESI(-)	Lognormal	-0.020	(-0.046, 0.006)	0.144	0.864	0.194	(-0.046, 0.006)
SM (d40:2) B - ESI(+)	Lognormal	0.002	(-0.011, 0.015)	0.778	0.956	0.068	(-0.011, 0.015)
PE (p-40:4)/PE (o-40:5) A	Lognormal	-0.005	(-0.054, 0.045)	0.856	0.966	0.044	(-0.053, 0.046)
TG (54:5) B	Lognormal	-0.009	(-0.028, 0.011)	0.395	0.873	0.094	(-0.028, 0.012)
SM (d40:2) B - ESI(-)	Lognormal	-0.010	(-0.031, 0.011)	0.347	0.864	0.108	(-0.031, 0.013)
TG (58:8)	Lognormal	0.006	(-0.029, 0.040)	0.745	0.949	0.064	(-0.030, 0.041)
PC (35:3)	Lognormal	0.002	(-0.012, 0.015)	0.803	0.956	0.054	(-0.013, 0.015)
PC (p-36:4)/PC (o-36:5) - ESI(+)	Lognormal	-0.005	(-0.024, 0.015)	0.657	0.928	0.082	(-0.024, 0.017)
TG (56:5) B	Lognormal	-0.004	(-0.028, 0.021)	0.765	0.956	0.071	(-0.030, 0.021)
TG (53:0)	Lognormal	-0.015	(-0.045, 0.016)	0.357	0.872	0.108	(-0.049, 0.015)
SM (d33:1) - ESI(-)	Lognormal	-0.015	(-0.040, 0.009)	0.216	0.864	0.159	(-0.040, 0.008)
PC (p-32:1)/PC (o-32:2)	Lognormal	-0.005	(-0.027, 0.016)	0.616	0.928	0.069	(-0.027, 0.016)
TG (62:4)	Lognormal	-0.011	(-0.067, 0.044)	0.691	0.930	0.074	(-0.066, 0.050)
PE (36:2)	Lognormal	-0.026	(-0.078, 0.027)	0.346	0.864	0.105	(-0.079, 0.029)
PE (p-36:1)/PE (o-36:2) - ESI(+)	Lognormal	-0.019	(-0.063, 0.024)	0.392	0.873	0.104	(-0.066, 0.024)
PE (p-34:1)/PE (o-34:2) - ESI(-)	Lognormal	-0.014	(-0.054, 0.025)	0.480	0.884	0.090	(-0.059, 0.022)
TG (50:0)	Lognormal	-0.007	(-0.049, 0.035)	0.741	0.949	0.068	(-0.050, 0.035)
SM (d32:1) - ESI(-)	Lognormal	-0.024	(-0.050, 0.002)	0.074	0.864	0.385	(-0.051, 0.003)
LPE (20:4) - ESI(-)	Lognormal	-0.039	(-0.076, -0.003)	0.042	0.864	0.715	(-0.076, -0.004)
PE (p-38:5)/PE (o-38:6) - ESI(+)	Lognormal	-0.010	(-0.038, 0.017)	0.464	0.884	0.077	(-0.038, 0.017)
SM (d42:3) - ESI(-)	Lognormal	-0.001	(-0.019, 0.018)	0.949	0.996	0.063	(-0.021, 0.017)
Ceramide (d41:1) - ESI(-)	Lognormal	-0.024	(-0.049, 0.002)	0.076	0.864	0.331	(-0.050, 0.002)
PC (p-32:0)/PC (o-32:1) - ESI(+)	Lognormal	0.010	(-0.009, 0.028)	0.304	0.864	0.117	(-0.010, 0.028)
PC (36:4) B - ESI(-)	Lognormal	-0.011	(-0.027, 0.005)	0.170	0.864	0.178	(-0.028, 0.004)
DG (38:5)	Lognormal	-0.010	(-0.031, 0.010)	0.330	0.864	0.103	(-0.032, 0.011)
DG (38:6)	Lognormal	0.000	(-0.032, 0.031)	0.987	0.996	0.061	(-0.031, 0.036)
Ceramide (d42:2) B - ESI (+)	Lognormal	-0.010	(-0.029, 0.009)	0.311	0.864	0.112	(-0.031, 0.008)
PC (34:3) C	Lognormal	-0.020	(-0.044, 0.004)	0.105	0.864	0.277	(-0.045, 0.003)
TG (58:9)	Lognormal	0.006	(-0.025, 0.036)	0.714	0.939	0.068	(-0.028, 0.035)
PE (p-34:1)/PE (o-34:2) - ESI(+)	Lognormal	-0.012	(-0.050, 0.025)	0.518	0.899	0.085	(-0.051, 0.029)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
SM (d42:1) - ESI(-)	Lognormal	-0.012	(-0.032, 0.008)	0.231	0.864	0.132	(-0.033, 0.007)
AC (18:2)	Lognormal	0.007	(-0.020, 0.033)	0.627	0.928	0.080	(-0.020, 0.035)
Ceramide (d42:1) - ESI(-)	Lognormal	-0.017	(-0.038, 0.004)	0.125	0.864	0.259	(-0.039, 0.005)
Ceramide (d34:1) - ESI(-)	Lognormal	0.002	(-0.018, 0.022)	0.830	0.962	0.071	(-0.019, 0.021)
PC (p-38:4)/PC (o-38:5) B	Lognormal	-0.007	(-0.030, 0.017)	0.584	0.924	0.082	(-0.032, 0.016)
CE (18:3)	Lognormal	-0.026	(-0.063, 0.011)	0.172	0.864	0.196	(-0.066, 0.010)
AC (14:2)	Lognormal	0.000	(-0.050, 0.049)	0.992	0.997	0.072	(-0.048, 0.051)
PC (40:5) A - ESI(+)	Lognormal	-0.002	(-0.018, 0.014)	0.792	0.956	0.069	(-0.017, 0.014)
PC (33:2) - ESI(-)	Lognormal	-0.028	(-0.065, 0.008)	0.132	0.864	0.222	(-0.067, 0.008)
PC (37:2) - ESI(+)	Lognormal	0.000	(-0.015, 0.016)	0.956	0.996	0.058	(-0.016, 0.016)
LPC (14:0) - ESI(+)	Lognormal	-0.036	(-0.070, -0.002)	0.046	0.864	0.578	(-0.072, -0.003)
TG (54:6) B	Lognormal	0.030	(-0.043, 0.103)	0.425	0.873	0.096	(-0.042, 0.105)
SM (d36:3) - ESI(-)	Lognormal	-0.036	(-0.063, -0.008)	0.015	0.864	1.197	(-0.064, -0.008)
FA (18:1) (oleic acid)	Lognormal	0.009	(-0.011, 0.028)	0.377	0.873	0.108	(-0.010, 0.030)
PC (p-36:3)/PC (o-36:4) - ESI(+)	Lognormal	-0.007	(-0.025, 0.010)	0.413	0.873	0.099	(-0.026, 0.010)
FA (14:1) (physeteric acid)	Lognormal	-0.008	(-0.053, 0.037)	0.739	0.949	0.070	(-0.056, 0.037)
PC (34:0) - ESI(-)	Lognormal	-0.010	(-0.033, 0.012)	0.381	0.873	0.097	(-0.034, 0.012)
Ceramide (d40:1)	Lognormal	-0.010	(-0.031, 0.011)	0.370	0.873	0.108	(-0.030, 0.012)
SM (d36:0) - ESI(+)	Lognormal	0.008	(-0.024, 0.040)	0.633	0.928	0.066	(-0.024, 0.041)
LPC (16:0) - ESI(-)	Lognormal	-0.021	(-0.038, -0.003)	0.025	0.864	0.751	(-0.038, -0.002)
PE (p-40:5)/PE (o-40:6)	Lognormal	0.006	(-0.013, 0.025)	0.529	0.899	0.056	(-0.014, 0.025)
LPC (18:0) A - ESI(-)	Lognormal	-0.035	(-0.062, -0.008)	0.014	0.864	1.869	(-0.062, -0.007)
PC (38:4) A - ESI(-)	Lognormal	-0.014	(-0.033, 0.004)	0.132	0.864	0.233	(-0.033, 0.005)
TG (54:7) A	Lognormal	0.013	(-0.030, 0.055)	0.570	0.915	0.078	(-0.031, 0.055)
TG (56:8) B	Lognormal	0.007	(-0.024, 0.038)	0.665	0.928	0.068	(-0.025, 0.038)
PE (36:3)	Lognormal	-0.030	(-0.103, 0.043)	0.427	0.873	0.094	(-0.106, 0.044)
PC (37:4) - ESI(+)	Lognormal	-0.018	(-0.051, 0.016)	0.316	0.864	0.112	(-0.053, 0.016)
PC (34:4) - ESI(-)	Lognormal	-0.061	(-0.117, -0.006)	0.036	0.864	0.735	(-0.117, -0.004)
SM (d36:1) - ESI(-)	Lognormal	-0.014	(-0.035, 0.008)	0.219	0.864	0.143	(-0.036, 0.007)
AC (12:1)	Lognormal	0.004	(-0.034, 0.041)	0.851	0.966	0.069	(-0.036, 0.043)
Cholesterol	Lognormal	0.005	(-0.004, 0.014)	0.269	0.864	0.101	(-0.004, 0.013)
PC (p-38:3)/PC (o-38:4) A - ESI(+)	Lognormal	-0.007	(-0.028, 0.013)	0.498	0.897	0.081	(-0.029, 0.013)
PC (p-38:3)/PC (o-38:4) B - ESI(+)	Lognormal	-0.006	(-0.028, 0.016)	0.620	0.928	0.074	(-0.027, 0.017)
AC (10:0)	Lognormal	0.008	(-0.043, 0.059)	0.752	0.952	0.069	(-0.047, 0.059)
TG (60:11)	Lognormal	0.007	(-0.040, 0.054)	0.778	0.956	0.068	(-0.042, 0.057)
PC (p-38:4)/PC (o-38:5) B	Lognormal	-0.026	(-0.063, 0.010)	0.170	0.864	0.179	(-0.064, 0.009)
TG (52:4)	Lognormal	0.014	(-0.005, 0.033)	0.167	0.864	0.191	(-0.006, 0.034)
LPC (18:0) B - ESI(-)	Lognormal	-0.025	(-0.044, -0.005)	0.017	0.864	1.323	(-0.044, -0.004)
SM (d41:2) B - ESI(+)	Lognormal	0.003	(-0.016, 0.022)	0.759	0.956	0.071	(-0.017, 0.021)
TG (58:6)	Lognormal	0.001	(-0.020, 0.023)	0.907	0.977	0.062	(-0.021, 0.023)
PC (p-36:1)/PC (o-36:2) B	Lognormal	0.007	(-0.025, 0.038)	0.674	0.928	0.072	(-0.025, 0.039)
PC (37:5)	Lognormal	0.001	(-0.027, 0.030)	0.930	0.991	0.065	(-0.027, 0.029)
PC (36:5) D	Lognormal	-0.011	(-0.042, 0.020)	0.484	0.884	0.086	(-0.042, 0.021)
SM (d40:1) - ESI(+)	Lognormal	-0.003	(-0.016, 0.010)	0.667	0.928	0.069	(-0.017, 0.010)
PC (35:2) B	Lognormal	0.008	(-0.005, 0.021)	0.217	0.864	0.126	(-0.005, 0.020)
PC (36:3) A - ESI(+)	Lognormal	-0.009	(-0.025, 0.006)	0.248	0.864	0.128	(-0.028, 0.005)
PC (p-32:0)/PC (o-32:1) - ESI(-)	Lognormal	-0.009	(-0.046, 0.029)	0.651	0.928	0.080	(-0.045, 0.032)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
SM (d43:1) - ESI(-)	Lognormal	-0.046	(-0.110, 0.019)	0.172	0.864	0.165	(-0.113, 0.015)
PC (40:6)B	Lognormal	0.006	(-0.011, 0.022)	0.525	0.899	0.082	(-0.011, 0.023)
TG (48:0)	Lognormal	-0.019	(-0.064, 0.027)	0.430	0.873	0.094	(-0.062, 0.030)
SM (d42:0) - ESI(+)	Lognormal	-0.068	(-0.126, -0.011)	0.025	0.864	0.799	(-0.128, -0.007)
SM (d30:1) - ESI(-)	Lognormal	-0.051	(-0.117, 0.015)	0.138	0.864	0.210	(-0.116, 0.019)
PC (36:3) B - ESI(-)	Lognormal	-0.013	(-0.032, 0.006)	0.201	0.864	0.167	(-0.032, 0.007)
Ceramide (d32:1)	Lognormal	-0.005	(-0.044, 0.035)	0.811	0.956	0.073	(-0.046, 0.034)
PE (p-40:4)/PE (o-40:5) B	Lognormal	-0.016	(-0.049, 0.017)	0.346	0.864	0.073	(-0.048, 0.017)
DG (36:4) B	Lognormal	-0.021	(-0.091, 0.048)	0.551	0.904	0.077	(-0.087, 0.054)
TG (48:4) A	Lognormal	-0.033	(-0.093, 0.027)	0.283	0.864	0.133	(-0.096, 0.029)
PC (34:3) A	Lognormal	-0.007	(-0.031, 0.017)	0.564	0.908	0.087	(-0.033, 0.017)
PC (35:1) - ESI(+)	Lognormal	0.002	(-0.014, 0.018)	0.814	0.956	0.073	(-0.014, 0.017)
LPC (p-16:0)/LPC (o-16:1)	Lognormal	-0.013	(-0.041, 0.015)	0.379	0.873	0.103	(-0.044, 0.015)
PC (p-38:5)/PC (o-38:6) B	Lognormal	0.000	(-0.022, 0.021)	0.969	0.996	0.071	(-0.024, 0.020)
TG (49:2)	Lognormal	-0.008	(-0.053, 0.036)	0.715	0.939	0.077	(-0.052, 0.038)
LPC (20:3) - ESI(-)	Lognormal	-0.046	(-0.080, -0.011)	0.013	0.864	1.640	(-0.082, -0.010)
Ceramide (d41:1) - ESI (+)	Lognormal	-0.011	(-0.036, 0.014)	0.385	0.873	0.100	(-0.036, 0.015)
AC (12:0)	Lognormal	-0.006	(-0.051, 0.040)	0.807	0.956	0.074	(-0.058, 0.038)
PC (36:3) A - ESI(-)	Lognormal	-0.011	(-0.032, 0.010)	0.310	0.864	0.119	(-0.031, 0.013)
FA (20:3) (homo-gamma-linolenic acid)	Lognormal	-0.005	(-0.026, 0.016)	0.634	0.928	0.070	(-0.026, 0.016)
PC (42:10)	Lognormal	-0.013	(-0.054, 0.028)	0.530	0.899	0.077	(-0.056, 0.029)
Lactosylceramide (d18:1/24:1(15Z))	Lognormal	0.011	(-0.025, 0.048)	0.553	0.904	0.078	(-0.025, 0.049)
TG (60:6)	Lognormal	-0.007	(-0.047, 0.033)	0.735	0.949	0.066	(-0.048, 0.033)
PE (p-40:4)/PE (o-40:5)	Lognormal	-0.016	(-0.055, 0.023)	0.437	0.881	0.070	(-0.053, 0.029)
PC (38:5) A	Lognormal	-0.003	(-0.016, 0.010)	0.648	0.928	0.076	(-0.017, 0.011)
PC (34:1)	Lognormal	-0.003	(-0.012, 0.006)	0.553	0.904	0.081	(-0.013, 0.006)
TG (56:5) A	Lognormal	0.001	(-0.026, 0.027)	0.953	0.996	0.077	(-0.026, 0.026)
DG (36:4) A	Lognormal	0.021	(-0.012, 0.054)	0.222	0.864	0.136	(-0.012, 0.053)
AC (8:0)	Lognormal	0.016	(-0.041, 0.072)	0.591	0.926	0.074	(-0.042, 0.071)
Ceramide (d39:1)	Lognormal	-0.038	(-0.080, 0.004)	0.082	0.864	0.296	(-0.078, 0.006)
PC (38:6) A - ESI(+)	Lognormal	-0.018	(-0.035, -0.001)	0.039	0.864	0.649	(-0.035, -0.001)
PC (38:5) B - ESI(+)	Lognormal	-0.006	(-0.024, 0.012)	0.509	0.899	0.085	(-0.023, 0.013)
SM (d40:0)	Lognormal	-0.013	(-0.037, 0.010)	0.275	0.864	0.107	(-0.037, 0.012)
PC (o-32:0) - ESI(+)	Lognormal	0.011	(-0.005, 0.027)	0.196	0.864	0.163	(-0.007, 0.027)
PE (p-38:3)/PE (o-38:4)	Lognormal	-0.038	(-0.088, 0.011)	0.139	0.864	0.226	(-0.091, 0.013)
TG (56:9)	Lognormal	-0.015	(-0.055, 0.025)	0.474	0.884	0.094	(-0.056, 0.025)
TG (50:4)	Lognormal	-0.002	(-0.037, 0.034)	0.930	0.991	0.077	(-0.039, 0.032)
PC (p-34:1)/PC (o-34:2) B	Lognormal	0.012	(-0.031, 0.054)	0.597	0.926	0.070	(-0.032, 0.055)
SM (d34:0) - ESI(-)	Lognormal	-0.010	(-0.039, 0.018)	0.475	0.884	0.086	(-0.040, 0.019)
PE (p-38:6)/PE (o-38:7)	Lognormal	-0.028	(-0.075, 0.019)	0.252	0.864	0.133	(-0.076, 0.019)
SM (d38:1)	Lognormal	-0.006	(-0.020, 0.008)	0.417	0.873	0.093	(-0.020, 0.008)
FA (24:0) (lignoceric acid)	Lognormal	-0.011	(-0.037, 0.016)	0.429	0.873	0.090	(-0.038, 0.017)
SM (d34:1) - ESI(+)	Lognormal	0.006	(-0.004, 0.017)	0.220	0.864	0.141	(-0.004, 0.017)
CE (20:3)	Lognormal	0.000	(-0.027, 0.026)	0.975	0.996	0.066	(-0.028, 0.027)
LPC (20:2) - ESI(+)	Lognormal	-0.039	(-0.097, 0.018)	0.188	0.864	0.162	(-0.093, 0.022)
PC (42:6)	Lognormal	-0.031	(-0.093, 0.032)	0.340	0.864	0.110	(-0.092, 0.035)
DG (32:0)	Lognormal	-0.005	(-0.040, 0.030)	0.773	0.956	0.066	(-0.039, 0.033)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
CE (20:5)	Lognormal	-0.006	(-0.046, 0.034)	0.765	0.956	0.068	(-0.050, 0.033)
PC (o-32:0) - ESI(-)	Lognormal	0.002	(-0.025, 0.028)	0.896	0.976	0.065	(-0.024, 0.029)
PC (32:0) - ESI(-)	Lognormal	-0.006	(-0.025, 0.013)	0.561	0.906	0.075	(-0.026, 0.014)
PC (40:8) - ESI(-)	Lognormal	-0.038	(-0.066, -0.010)	0.011	0.864	1.471	(-0.066, -0.008)
Ceramide (d38:1) - ESI(+)	Lognormal	-0.003	(-0.025, 0.019)	0.783	0.956	0.071	(-0.027, 0.019)
Ceramide (d43:1)	Lognormal	-0.066	(-0.183, 0.052)	0.281	0.864	0.134	(-0.186, 0.060)
SM (d42:1) - ESI(+)	Lognormal	-0.001	(-0.014, 0.012)	0.904	0.977	0.070	(-0.015, 0.013)
PC (37:2) - ESI(-)	Lognormal	-0.010	(-0.049, 0.028)	0.598	0.926	0.074	(-0.051, 0.028)
PC (38:3) - ESI(-)	Lognormal	-0.021	(-0.047, 0.005)	0.122	0.864	0.224	(-0.048, 0.005)
SM (d39:2)	Lognormal	0.003	(-0.017, 0.023)	0.772	0.956	0.065	(-0.017, 0.024)
SM (d30:1) - ESI(+)	Lognormal	-0.027	(-0.079, 0.025)	0.316	0.864	0.112	(-0.081, 0.028)
LPC (o-16:0)	Lognormal	-0.006	(-0.033, 0.020)	0.640	0.928	0.070	(-0.033, 0.023)
LPC (20:2) - ESI(-)	Lognormal	-0.022	(-0.053, 0.010)	0.185	0.864	0.154	(-0.053, 0.011)
LPC (18:1) - ESI(-)	Lognormal	-0.028	(-0.048, -0.008)	0.011	0.864	1.679	(-0.048, -0.006)
LPC (20:3) - ESI(+)	Lognormal	-0.023	(-0.048, 0.002)	0.085	0.864	0.293	(-0.049, 0.003)
PC (38:6) B - ESI(+)	Lognormal	0.007	(-0.003, 0.018)	0.195	0.864	0.149	(-0.004, 0.018)
FA (20:3) (eicosatrienoic acid)	Lognormal	-0.018	(-0.050, 0.015)	0.293	0.864	0.126	(-0.052, 0.014)
PC (p-44:4)/PC (o-44:5) - ESI(-)	Lognormal	-0.006	(-0.032, 0.020)	0.643	0.928	0.072	(-0.031, 0.020)
CE (14:0)	Lognormal	0.002	(-0.072, 0.075)	0.968	0.996	0.060	(-0.072, 0.082)
TG (56:8) A	Lognormal	0.005	(-0.024, 0.035)	0.721	0.943	0.075	(-0.025, 0.036)
Ceramide (d33:1)	Lognormal	-0.012	(-0.040, 0.016)	0.394	0.873	0.106	(-0.041, 0.015)
TG (46:0)	Lognormal	-0.042	(-0.114, 0.030)	0.258	0.864	0.129	(-0.117, 0.029)
PE (38:6) - ESI(+)	Lognormal	-0.049	(-0.113, 0.014)	0.134	0.864	0.191	(-0.113, 0.015)
SM (d34:2) - ESI(+)	Lognormal	0.008	(-0.005, 0.020)	0.232	0.864	0.131	(-0.004, 0.021)
AC (18:0)	Lognormal	-0.009	(-0.035, 0.018)	0.519	0.899	0.101	(-0.036, 0.019)
TG (51:2)	Lognormal	-0.003	(-0.036, 0.031)	0.865	0.968	0.069	(-0.035, 0.033)
LPC (14:0) - ESI(-)	Lognormal	-0.058	(-0.110, -0.005)	0.038	0.864	0.720	(-0.110, -0.005)
TG (54:6) A	Lognormal	0.018	(-0.017, 0.053)	0.311	0.864	0.125	(-0.019, 0.053)
FA (22:0) (behenic acid)	Lognormal	-0.006	(-0.037, 0.025)	0.685	0.929	0.071	(-0.038, 0.026)
Ceramide (d42:2) B - ESI(-)	Lognormal	-0.007	(-0.035, 0.020)	0.615	0.928	0.079	(-0.036, 0.020)
SM (d39:1) - ESI(+)	Lognormal	-0.012	(-0.035, 0.010)	0.279	0.864	0.114	(-0.034, 0.011)
TG (50:5)	Lognormal	-0.009	(-0.058, 0.040)	0.708	0.937	0.079	(-0.060, 0.039)
TG (46:4) A	Lognormal	-0.045	(-0.125, 0.035)	0.280	0.864	0.139	(-0.128, 0.030)
GlcCer (d42:2) - ESI(+)	Lognormal	0.022	(-0.006, 0.050)	0.130	0.864	0.232	(-0.006, 0.050)
LPC (16:1) - ESI(-)	Lognormal	-0.043	(-0.076, -0.010)	0.015	0.864	1.339	(-0.075, -0.006)
PC (35:2) A	Lognormal	-0.004	(-0.021, 0.013)	0.651	0.928	0.072	(-0.021, 0.014)
TG (51:4)	Lognormal	0.016	(-0.021, 0.052)	0.408	0.873	0.101	(-0.021, 0.052)
PC (38:2)	Lognormal	-0.012	(-0.038, 0.014)	0.370	0.873	0.098	(-0.037, 0.017)
PC 40:5e	Lognormal	0.001	(-0.017, 0.020)	0.881	0.975	0.073	(-0.018, 0.021)
PC (37:4) - ESI(-)	Lognormal	0.000	(-0.026, 0.027)	0.979	0.996	0.065	(-0.026, 0.028)
SM (d36:3) - ESI(+)	Lognormal	0.004	(-0.019, 0.027)	0.719	0.942	0.066	(-0.019, 0.028)
PE (34:2) - ESI(-)	Lognormal	-0.037	(-0.096, 0.022)	0.223	0.864	0.139	(-0.103, 0.020)
TG (48:5)	Lognormal	-0.035	(-0.104, 0.033)	0.321	0.864	0.119	(-0.109, 0.032)
GlcCer (d38:1)	Lognormal	-0.027	(-0.052, -0.003)	0.035	0.864	0.650	(-0.054, -0.004)
PC (p-42:4)/PC (o-42:5) - ESI(-)	Lognormal	0.007	(-0.024, 0.038)	0.658	0.928	0.073	(-0.024, 0.040)
TG (54:9)	Lognormal	-0.093	(-0.213, 0.026)	0.133	0.864	0.203	(-0.210, 0.025)
LPE (18:0)	Lognormal	-0.028	(-0.049, -0.006)	0.017	0.864	1.366	(-0.047, -0.004)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
TG (58:4)	Lognormal	-0.012	(-0.065, 0.040)	0.653	0.928	0.085	(-0.066, 0.041)
PC (34:4) - ESI(+)	Lognormal	-0.035	(-0.077, 0.006)	0.103	0.864	0.272	(-0.078, 0.005)
TG (42:0)	Lognormal	-0.037	(-0.112, 0.038)	0.343	0.864	0.103	(-0.110, 0.044)
TG (53:2)	Lognormal	-0.003	(-0.035, 0.029)	0.869	0.968	0.071	(-0.034, 0.031)
PC (p-38:4)/PC (o-38:5) A	Lognormal	-0.002	(-0.017, 0.014)	0.849	0.966	0.081	(-0.018, 0.014)
TG (46:3) A	Lognormal	-0.026	(-0.120, 0.068)	0.596	0.926	0.088	(-0.124, 0.065)
TG (56:5) C	Lognormal	0.009	(-0.011, 0.028)	0.405	0.873	0.093	(-0.013, 0.028)
PC (36:1) - ESI(+)	Lognormal	-0.009	(-0.020, 0.001)	0.084	0.864	0.261	(-0.019, 0.002)
FA (20:1) (eicosenoic acid)	Lognormal	0.011	(-0.012, 0.034)	0.340	0.864	0.098	(-0.011, 0.034)
PC (37:6)	Lognormal	0.017	(-0.017, 0.051)	0.323	0.864	0.124	(-0.016, 0.054)
LPE (22:6)	Lognormal	-0.027	(-0.061, 0.007)	0.131	0.864	0.220	(-0.061, 0.010)
SM (d40:2) A - ESI(+)	Lognormal	0.003	(-0.018, 0.024)	0.765	0.956	0.072	(-0.017, 0.025)
LPC (20:5)	Lognormal	-0.024	(-0.069, 0.021)	0.296	0.864	0.132	(-0.074, 0.021)
SM (d36:2) - ESI(-)	Lognormal	-0.014	(-0.041, 0.012)	0.292	0.864	0.124	(-0.043, 0.011)
DG (36:5)	Lognormal	0.026	(-0.014, 0.067)	0.214	0.864	0.152	(-0.012, 0.065)
PC (42:5)	Lognormal	0.001	(-0.031, 0.032)	0.961	0.996	0.073	(-0.030, 0.034)
SM (d44:2)	Lognormal	0.014	(-0.015, 0.044)	0.346	0.864	0.082	(-0.016, 0.046)
LPE (16:0)	Lognormal	-0.045	(-0.090, -0.001)	0.054	0.864	0.421	(-0.095, -0.001)
SM (d32:1) - ESI(+)	Lognormal	-0.013	(-0.037, 0.011)	0.288	0.864	0.121	(-0.039, 0.012)
SM (d41:3)	Lognormal	0.000	(-0.022, 0.021)	0.979	0.996	0.070	(-0.021, 0.023)
TG (42:1)	Lognormal	-0.061	(-0.230, 0.108)	0.483	0.884	0.088	(-0.242, 0.101)
TG (60:12)	Lognormal	0.026	(-0.034, 0.085)	0.400	0.873	0.081	(-0.039, 0.086)
PC (p-40:3)/PC (o-40:4)	Lognormal	-0.024	(-0.057, 0.009)	0.168	0.864	0.179	(-0.060, 0.010)
PC (40:4) - ESI(-)	Lognormal	-0.019	(-0.056, 0.018)	0.317	0.864	0.109	(-0.057, 0.018)
FA (20:5) (eicosapentaenoic acid)	Lognormal	0.018	(-0.026, 0.063)	0.419	0.873	0.105	(-0.027, 0.066)
DG (36:2)	Lognormal	0.003	(-0.018, 0.024)	0.789	0.956	0.069	(-0.018, 0.025)
AC (14:1)	Lognormal	0.005	(-0.040, 0.051)	0.819	0.957	0.073	(-0.041, 0.052)
SM (d40:2) A - ESI(-)	Lognormal	-0.017	(-0.062, 0.028)	0.460	0.884	0.089	(-0.062, 0.026)
DG (36:1)	Lognormal	-0.024	(-0.064, 0.015)	0.230	0.864	0.138	(-0.066, 0.015)
LPC (17:1)	Lognormal	-0.018	(-0.047, 0.010)	0.214	0.864	0.162	(-0.047, 0.014)
PG (34:0)/PG (17:0/17:0)	Lognormal	-0.001	(-0.013, 0.012)	0.900	0.976	0.061	(-0.013, 0.013)
SM (d43:2) - ESI(-)	Lognormal	-0.029	(-0.091, 0.034)	0.373	0.873	0.098	(-0.096, 0.034)
SM (d36:0) - ESI(-)	Lognormal	-0.042	(-0.104, 0.020)	0.196	0.864	0.159	(-0.111, 0.018)
SM (d38:0)	Lognormal	-0.149	(-0.266, -0.032)	0.017	0.864	1.419	(-0.263, -0.030)
TG (42:3)	Lognormal	-0.032	(-0.120, 0.056)	0.477	0.884	0.087	(-0.121, 0.057)
Ceramide (d44:1)	Lognormal	-0.023	(-0.083, 0.038)	0.468	0.884	0.093	(-0.081, 0.041)
PC (36:3) B - ESI(+)	Lognormal	-0.006	(-0.031, 0.020)	0.668	0.928	0.081	(-0.033, 0.019)
TG (40:1)	Lognormal	-0.041	(-0.122, 0.040)	0.327	0.864	0.111	(-0.126, 0.049)
Ceramide (d38:1) - ESI(-)	Lognormal	-0.018	(-0.050, 0.013)	0.263	0.864	0.115	(-0.050, 0.014)
PC (33:1) - ESI(+)	Lognormal	-0.002	(-0.023, 0.018)	0.842	0.962	0.071	(-0.023, 0.019)
TG (48:3)	Lognormal	-0.028	(-0.080, 0.024)	0.296	0.864	0.124	(-0.086, 0.021)
Ceramide (d42:2) A - ESI(-)	Lognormal	-0.010	(-0.033, 0.013)	0.414	0.873	0.084	(-0.033, 0.014)
SM (d32:2) - ESI(+)	Lognormal	0.004	(-0.021, 0.029)	0.741	0.949	0.063	(-0.020, 0.030)
TG (44:0)	Lognormal	-0.046	(-0.118, 0.026)	0.223	0.864	0.147	(-0.120, 0.030)
TG (54:5) A	Lognormal	0.017	(-0.009, 0.043)	0.216	0.864	0.147	(-0.012, 0.042)
TG (52:2)	Lognormal	-0.002	(-0.017, 0.012)	0.743	0.949	0.070	(-0.016, 0.014)
PI (38:4)/PI (18:0-20:4)	Lognormal	-0.021	(-0.042, 0.000)	0.054	0.864	0.447	(-0.043, 0.000)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
PC (37:3)	Lognormal	0.007	(-0.023, 0.038)	0.649	0.928	0.078	(-0.024, 0.039)
TG (56:3)	Lognormal	0.000	(-0.044, 0.043)	0.987	0.996	0.074	(-0.043, 0.046)
SM (d32:2) - ESI(-)	Lognormal	-0.027	(-0.078, 0.024)	0.307	0.864	0.119	(-0.078, 0.024)
TG (46:4) B	Lognormal	-0.036	(-0.125, 0.054)	0.439	0.881	0.107	(-0.123, 0.058)
TG (46:2)	Lognormal	-0.048	(-0.118, 0.022)	0.189	0.864	0.189	(-0.119, 0.021)
PC (p-40:1)/PC (o-40:2)	Lognormal	0.018	(-0.015, 0.051)	0.285	0.864	0.103	(-0.016, 0.051)
PE (34:1)	Lognormal	-0.049	(-0.114, 0.016)	0.146	0.864	0.174	(-0.115, 0.020)
SM (d41:1) - ESI(+)	Lognormal	0.000	(-0.018, 0.017)	0.969	0.996	0.064	(-0.017, 0.017)
SM (d38:2) - ESI(+)	Lognormal	0.009	(-0.006, 0.024)	0.243	0.864	0.148	(-0.006, 0.024)
LPC (15:0)	Lognormal	0.001	(-0.033, 0.035)	0.955	0.996	0.072	(-0.034, 0.036)
PC (p-40:7)/PC (o-40:8)	Lognormal	-0.002	(-0.092, 0.089)	0.973	0.996	0.065	(-0.093, 0.092)
PC (p-42:3)/PC (o-42:4)	Lognormal	0.000	(-0.023, 0.023)	0.989	0.997	0.061	(-0.022, 0.024)
PE (36:4) - ESI(+)	Lognormal	-0.040	(-0.090, 0.011)	0.134	0.864	0.204	(-0.094, 0.010)
SM (d42:3) - ESI(+)	Lognormal	0.013	(-0.003, 0.029)	0.130	0.864	0.231	(-0.004, 0.029)
GlcCer (d41:1)	Lognormal	-0.021	(-0.048, 0.006)	0.139	0.864	0.198	(-0.048, 0.007)
TG (58:3)	Lognormal	-0.007	(-0.073, 0.059)	0.837	0.962	0.070	(-0.077, 0.058)
TG (48:4) B	Lognormal	-0.046	(-0.117, 0.025)	0.211	0.864	0.153	(-0.119, 0.027)
PC (39:6)	Lognormal	0.017	(-0.012, 0.046)	0.268	0.864	0.130	(-0.013, 0.047)
PE (p-36:5)/PE (o-36:6)	Lognormal	-0.001	(-0.109, 0.108)	0.992	0.997	0.062	(-0.107, 0.119)
PC (36:4) B - ESI(+)	Lognormal	-0.022	(-0.046, 0.003)	0.098	0.864	0.253	(-0.046, 0.006)
TG (54:1)	Lognormal	-0.024	(-0.080, 0.032)	0.402	0.873	0.097	(-0.081, 0.032)
FA (18:2) (linoleic acid)	Lognormal	0.011	(-0.009, 0.031)	0.289	0.864	0.121	(-0.010, 0.032)
LPE (20:4) - ESI(+)	Lognormal	-0.023	(-0.055, 0.009)	0.164	0.864	0.165	(-0.055, 0.011)
PC (p-42:5)/PC (o-42:6) A	Lognormal	0.000	(-0.029, 0.028)	0.974	0.996	0.071	(-0.030, 0.029)
LPC (16:1) - ESI(+)	Lognormal	-0.008	(-0.032, 0.016)	0.528	0.899	0.084	(-0.032, 0.017)
PC (40:7) B - ESI(+)	Lognormal	0.008	(-0.012, 0.028)	0.452	0.884	0.086	(-0.012, 0.028)
GlcCer (d40:1) - ESI(-)	Lognormal	-0.012	(-0.034, 0.010)	0.284	0.864	0.113	(-0.034, 0.011)
PE (38:2)	Lognormal	-0.032	(-0.070, 0.006)	0.104	0.864	0.275	(-0.069, 0.007)
PC (36:5) C	Lognormal	0.009	(-0.035, 0.052)	0.702	0.937	0.077	(-0.039, 0.052)
TG (55:2)	Lognormal	-0.013	(-0.055, 0.029)	0.549	0.904	0.083	(-0.053, 0.032)
TG (51:5)	Lognormal	-0.007	(-0.056, 0.042)	0.791	0.956	0.071	(-0.055, 0.047)
GlcCer (d42:1) - ESI(-)	Lognormal	-0.010	(-0.032, 0.012)	0.362	0.873	0.100	(-0.032, 0.014)
TG (54:8)	Lognormal	-0.024	(-0.078, 0.031)	0.405	0.873	0.104	(-0.080, 0.034)
PC (40:7) A - ESI(+)	Lognormal	-0.018	(-0.039, 0.003)	0.095	0.864	0.245	(-0.040, 0.003)
TG (50:1)	Lognormal	-0.053	(-0.094, -0.012)	0.015	0.864	1.192	(-0.096, -0.011)
TG (54:2)	Lognormal	-0.005	(-0.042, 0.032)	0.794	0.956	0.070	(-0.040, 0.033)
AC (18:1)	Lognormal	0.008	(-0.016, 0.033)	0.508	0.899	0.083	(-0.017, 0.032)
TG (40:0)	Lognormal	-0.023	(-0.091, 0.045)	0.509	0.899	0.085	(-0.097, 0.043)
SM (d42:0) - ESI(-)	Lognormal	-0.012	(-0.033, 0.008)	0.231	0.864	0.109	(-0.033, 0.009)
TG (58:10)	Lognormal	-0.008	(-0.043, 0.026)	0.638	0.928	0.075	(-0.042, 0.028)
PC (39:4)	Lognormal	0.003	(-0.021, 0.026)	0.825	0.962	0.067	(-0.021, 0.027)
LPC (16:0) - ESI(+)	Lognormal	-0.006	(-0.017, 0.004)	0.221	0.864	0.152	(-0.017, 0.004)
TG (53:5)	Lognormal	0.012	(-0.024, 0.047)	0.520	0.899	0.080	(-0.026, 0.048)
SM (d36:2) - ESI(+)	Lognormal	0.009	(-0.007, 0.025)	0.273	0.864	0.121	(-0.008, 0.025)
Ceramide (d34:1) - ESI(+)	Lognormal	0.027	(0.012, 0.042)	0.001	0.452	9.566	(0.012, 0.042)
Ceramide (d34:2)	Lognormal	0.008	(-0.018, 0.033)	0.548	0.904	0.083	(-0.019, 0.034)
TG (56:10)	Lognormal	-0.041	(-0.103, 0.021)	0.202	0.864	0.157	(-0.103, 0.025)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
PC (30:0)	Lognormal	-0.023	(-0.053, 0.008)	0.155	0.864	0.186	(-0.054, 0.008)
TG (59:3)	Lognormal	-0.019	(-0.069, 0.032)	0.472	0.884	0.092	(-0.072, 0.031)
LPC (20:4)	Lognormal	-0.018	(-0.045, 0.008)	0.173	0.864	0.167	(-0.046, 0.007)
TAG (58:7)/TAG (18:1/18:1/22:5)	Lognormal	-0.006	(-0.030, 0.017)	0.605	0.926	0.085	(-0.031, 0.018)
GlcCer (d14:1(4E)/20:0(2OH))	Lognormal	-0.029	(-0.066, 0.008)	0.132	0.864	0.201	(-0.066, 0.007)
TG (50:2)	Lognormal	-0.004	(-0.028, 0.020)	0.749	0.951	0.071	(-0.029, 0.021)
TG (56:7) A	Lognormal	0.009	(-0.068, 0.086)	0.813	0.956	0.063	(-0.065, 0.090)
TG (60:4)	Lognormal	-0.028	(-0.100, 0.045)	0.458	0.884	0.091	(-0.107, 0.046)
CE (18:1)	Lognormal	0.008	(-0.020, 0.035)	0.587	0.926	0.069	(-0.019, 0.037)
TG (46:3) B	Lognormal	-0.011	(-0.097, 0.074)	0.793	0.956	0.073	(-0.093, 0.083)
GlcCer (d42:2) - ESI(-)	Lognormal	0.001	(-0.026, 0.028)	0.920	0.983	0.061	(-0.027, 0.029)
PE (36:1) - ESI(-)	Lognormal	-0.062	(-0.123, -0.001)	0.053	0.864	0.447	(-0.127, -0.001)
LPC (18:0) - ESI(+)	Lognormal	-0.013	(-0.029, 0.002)	0.106	0.864	0.273	(-0.028, 0.004)
TG (64:2)	Lognormal	-0.047	(-0.116, 0.021)	0.184	0.864	0.178	(-0.115, 0.022)
LPC (22:5) - ESI(+)	Lognormal	-0.018	(-0.051, 0.016)	0.305	0.864	0.109	(-0.050, 0.017)
SM (d41:1) - ESI(-)	Lognormal	0.117	(-0.110, 0.343)	0.320	0.864	0.125	(-0.121, 0.349)
TG (60:2)	Lognormal	-0.063	(-0.154, 0.029)	0.186	0.864	0.198	(-0.150, 0.031)
PC (40:5) B - ESI(-)	Lognormal	-0.049	(-0.102, 0.004)	0.075	0.864	0.375	(-0.101, 0.005)
TG (56:2)	Lognormal	-0.020	(-0.075, 0.035)	0.478	0.884	0.095	(-0.075, 0.039)
FA (20:2) (eicosadienoic acid)	Lognormal	0.010	(-0.017, 0.036)	0.483	0.884	0.095	(-0.017, 0.037)
AC (16:0)	Lognormal	0.005	(-0.018, 0.028)	0.677	0.929	0.084	(-0.019, 0.028)
DG (32:1)	Lognormal	-0.034	(-0.081, 0.013)	0.167	0.864	0.170	(-0.082, 0.015)
PC (p-40:6)/PC (o-40:7) B	Lognormal	0.008	(-0.025, 0.040)	0.642	0.928	0.077	(-0.027, 0.038)
FA (14:0) (myristic acid)	Lognormal	0.001	(-0.018, 0.020)	0.950	0.996	0.072	(-0.019, 0.019)
TG (64:3)	Lognormal	-0.006	(-0.055, 0.042)	0.805	0.956	0.070	(-0.054, 0.044)
PC (p-38:5)/PC (o-38:6)	Lognormal	-0.055	(-0.142, 0.031)	0.216	0.864	0.169	(-0.149, 0.031)
PC (32:0) - ESI(+)	Lognormal	0.004	(-0.008, 0.017)	0.511	0.899	0.079	(-0.008, 0.017)
TG (62:3)	Lognormal	-0.050	(-0.113, 0.012)	0.124	0.864	0.237	(-0.112, 0.017)
PC (35:4) - ESI(-)	Lognormal	-0.012	(-0.050, 0.025)	0.522	0.899	0.085	(-0.050, 0.027)
TG (49:1)	Lognormal	-0.019	(-0.070, 0.032)	0.472	0.884	0.085	(-0.072, 0.032)
PC (33:1) - ESI(-)	Lognormal	-0.024	(-0.074, 0.025)	0.342	0.864	0.111	(-0.075, 0.028)
PC (36:1) - ESI(-)	Lognormal	-0.013	(-0.030, 0.004)	0.153	0.864	0.208	(-0.031, 0.005)
SM (d43:2) - ESI(+)	Lognormal	0.007	(-0.028, 0.042)	0.689	0.930	0.079	(-0.028, 0.043)
SM (d32:0) - ESI(+)	Lognormal	-0.012	(-0.045, 0.020)	0.466	0.884	0.084	(-0.048, 0.019)
PC (p-38:6)/PC (o-38:7)	Lognormal	-0.001	(-0.030, 0.029)	0.958	0.996	0.068	(-0.029, 0.030)
PE (38:6) - ESI(-)	Lognormal	-0.053	(-0.110, 0.005)	0.079	0.864	0.309	(-0.116, 0.005)
PC (32:1) - ESI(+)	Lognormal	-0.012	(-0.040, 0.016)	0.416	0.873	0.100	(-0.042, 0.017)
PC (p-40:6)/PC (o-40:7) A	Lognormal	0.002	(-0.025, 0.029)	0.896	0.976	0.070	(-0.024, 0.033)
SM (d34:0) - ESI(+)	Lognormal	0.002	(-0.016, 0.020)	0.811	0.956	0.066	(-0.016, 0.021)
PC (38:5) A - ESI(-)	Lognormal	-0.010	(-0.031, 0.011)	0.356	0.871	0.101	(-0.031, 0.012)
CE (16:1)	Lognormal	-0.003	(-0.041, 0.034)	0.859	0.967	0.070	(-0.042, 0.037)
Ceramide (d40:0)	Lognormal	-0.052	(-0.117, 0.012)	0.120	0.864	0.231	(-0.119, 0.015)
PC (p-42:5)/PC (o-42:6) B	Lognormal	0.016	(-0.012, 0.044)	0.260	0.864	0.121	(-0.013, 0.045)
Ceramide (d42:0)	Lognormal	-0.042	(-0.078, -0.005)	0.033	0.864	0.768	(-0.079, -0.005)
LPC (22:4)	Lognormal	-0.033	(-0.088, 0.021)	0.241	0.864	0.112	(-0.092, 0.019)
PC (35:1) - ESI(-)	Lognormal	-0.015	(-0.043, 0.013)	0.303	0.864	0.107	(-0.044, 0.014)
TG (57:2)	Lognormal	-0.023	(-0.062, 0.016)	0.263	0.864	0.131	(-0.065, 0.016)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
PC (40:6) B	Lognormal	-0.005	(-0.032, 0.022)	0.704	0.937	0.074	(-0.034, 0.023)
PC (40:5) B - ESI(+)	Lognormal	-0.012	(-0.042, 0.017)	0.422	0.873	0.091	(-0.043, 0.017)
TG (42:2)	Lognormal	-0.086	(-0.241, 0.069)	0.282	0.864	0.121	(-0.241, 0.070)
CE (22:6)	Lognormal	0.012	(-0.011, 0.035)	0.323	0.864	0.107	(-0.010, 0.035)
TG (52:3)	Lognormal	0.007	(-0.006, 0.021)	0.268	0.864	0.130	(-0.005, 0.021)
PC (38:7)	Lognormal	0.012	(-0.018, 0.043)	0.422	0.873	0.099	(-0.020, 0.045)
TG (60:3)	Lognormal	-0.010	(-0.085, 0.065)	0.803	0.956	0.076	(-0.090, 0.067)
CE (22:2)	Lognormal	0.098	(0.035, 0.161)	0.004	0.864	3.006	(0.032, 0.164)
FA (22:6) (docosahexaenoic acid)	Lognormal	-0.003	(-0.031, 0.025)	0.815	0.956	0.067	(-0.033, 0.026)
PC (36:4) C - ESI(+)	Lognormal	-0.004	(-0.016, 0.009)	0.545	0.903	0.087	(-0.017, 0.009)
DG (34:1)	Lognormal	-0.004	(-0.046, 0.038)	0.845	0.963	0.063	(-0.045, 0.042)
PE (36:1) - ESI(+)	Lognormal	-0.028	(-0.074, 0.018)	0.234	0.864	0.144	(-0.073, 0.019)
TG (53:1)	Lognormal	-0.046	(-0.114, 0.022)	0.196	0.864	0.168	(-0.118, 0.025)
TG (46:1)	Lognormal	-0.052	(-0.122, 0.017)	0.146	0.864	0.192	(-0.127, 0.017)
PC (35:4) - ESI(+)	Lognormal	-0.002	(-0.029, 0.024)	0.856	0.966	0.075	(-0.030, 0.023)
SM (d42:2)	Lognormal	0.013	(-0.004, 0.029)	0.138	0.864	0.205	(-0.004, 0.030)
DG (36:3)	Lognormal	0.011	(-0.009, 0.032)	0.280	0.864	0.131	(-0.010, 0.031)
SM (d37:1)	Lognormal	-0.024	(-0.082, 0.033)	0.406	0.873	0.089	(-0.082, 0.030)
LPC (20:1) - ESI(-)	Lognormal	-0.012	(-0.045, 0.020)	0.460	0.884	0.091	(-0.044, 0.022)
TG (53:3)	Lognormal	0.012	(-0.016, 0.039)	0.419	0.873	0.098	(-0.015, 0.040)
TG (52:5)	Lognormal	0.011	(-0.019, 0.040)	0.486	0.884	0.083	(-0.018, 0.042)
TG (48:6)	Lognormal	-0.020	(-0.058, 0.019)	0.321	0.864	0.124	(-0.060, 0.018)
TG (54:4)	Lognormal	0.015	(-0.009, 0.039)	0.233	0.864	0.143	(-0.009, 0.039)
GlcCer (d34:1)	Lognormal	0.018	(-0.012, 0.047)	0.252	0.864	0.123	(-0.013, 0.048)
SM (d41:2) - ESI(-)	Lognormal	-0.015	(-0.045, 0.015)	0.328	0.864	0.116	(-0.044, 0.017)
PC (p-40:4)/PC (o-40:5) - ESI(+)	Lognormal	0.003	(-0.015, 0.022)	0.745	0.949	0.072	(-0.016, 0.022)
SM (d32:0) - ESI(-)	Lognormal	-0.067	(-0.180, 0.046)	0.255	0.864	0.137	(-0.181, 0.048)
LPC (22:6)	Lognormal	-0.009	(-0.037, 0.019)	0.526	0.899	0.083	(-0.037, 0.018)
PC 38:7e	Lognormal	-0.005	(-0.041, 0.031)	0.799	0.956	0.072	(-0.041, 0.034)
LPC (20:1) - ESI(+)	Lognormal	-0.025	(-0.074, 0.025)	0.335	0.864	0.094	(-0.074, 0.026)
TG (50:6)	Lognormal	-0.034	(-0.088, 0.019)	0.218	0.864	0.151	(-0.090, 0.021)
TG (55:1)	Lognormal	-0.023	(-0.069, 0.024)	0.345	0.864	0.104	(-0.071, 0.025)
FA (15:0) (pentadecylic acid)	Lognormal	-0.004	(-0.025, 0.016)	0.684	0.929	0.080	(-0.026, 0.016)
TG (44:1)	Lognormal	-0.074	(-0.162, 0.013)	0.105	0.864	0.275	(-0.170, 0.014)
PC (28:0)	Lognormal	-0.064	(-0.138, 0.011)	0.101	0.864	0.249	(-0.139, 0.015)
TG (59:2)	Lognormal	-0.013	(-0.070, 0.044)	0.653	0.928	0.081	(-0.070, 0.047)
PC (38:3) - ESI(+)	Lognormal	-0.009	(-0.027, 0.010)	0.363	0.873	0.094	(-0.027, 0.010)
PC (p-42:4)/PC (o-42:5) - ESI(+)	Lognormal	0.009	(-0.013, 0.032)	0.429	0.873	0.091	(-0.013, 0.033)
Ceramide (d36:1) - ESI(-)	Lognormal	-0.010	(-0.054, 0.034)	0.659	0.928	0.073	(-0.054, 0.035)
TG (62:1)	Lognormal	-0.010	(-0.073, 0.052)	0.752	0.952	0.071	(-0.075, 0.054)
PC (33:0)	Lognormal	-0.004	(-0.045, 0.037)	0.842	0.962	0.071	(-0.043, 0.040)
TG (52:6)	Lognormal	-0.030	(-0.072, 0.012)	0.172	0.864	0.178	(-0.073, 0.012)
TG (46:5)	Lognormal	0.008	(-0.086, 0.102)	0.868	0.968	0.069	(-0.087, 0.107)
FA (17:0) (margaric acid)	Lognormal	0.003	(-0.008, 0.015)	0.585	0.925	0.074	(-0.008, 0.015)
TG (58:1)	Lognormal	-0.034	(-0.094, 0.026)	0.273	0.864	0.137	(-0.099, 0.027)
SM (d33:1) - ESI(+)	Lognormal	0.002	(-0.019, 0.024)	0.826	0.962	0.070	(-0.019, 0.025)
PC (36:5) B	Lognormal	-0.006	(-0.049, 0.037)	0.797	0.956	0.066	(-0.052, 0.038)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
TG (54:3)	Lognormal	0.006	(-0.018, 0.031)	0.603	0.926	0.088	(-0.019, 0.029)
FA (12:0) (lauric acid)	Lognormal	-0.001	(-0.035, 0.032)	0.932	0.992	0.074	(-0.036, 0.034)
CE (16:0)	Lognormal	0.029	(-0.021, 0.079)	0.268	0.864	0.103	(-0.025, 0.078)
PE (38:4)	Lognormal	-0.017	(-0.041, 0.008)	0.195	0.864	0.118	(-0.041, 0.008)
TG (53:4)	Lognormal	0.012	(-0.018, 0.042)	0.443	0.881	0.089	(-0.018, 0.044)
TG (60:1)	Lognormal	-0.030	(-0.091, 0.031)	0.342	0.864	0.109	(-0.092, 0.033)
DG (34:3)	Lognormal	0.016	(-0.022, 0.054)	0.413	0.873	0.084	(-0.023, 0.055)
PC (38:5) B - ESI(-)	Lognormal	-0.004	(-0.038, 0.031)	0.840	0.962	0.071	(-0.039, 0.034)
FA (18:3) (linolenic acid)	Lognormal	0.020	(-0.010, 0.050)	0.195	0.864	0.161	(-0.011, 0.050)
GlcCer (d42:1) - ESI(+)	Lognormal	0.001	(-0.018, 0.020)	0.919	0.983	0.060	(-0.019, 0.021)
PC (31:1)	Lognormal	-0.002	(-0.087, 0.083)	0.963	0.996	0.072	(-0.082, 0.088)
PC (38:6) - ESI(-)	Lognormal	-0.011	(-0.036, 0.015)	0.405	0.873	0.090	(-0.035, 0.017)
PC (p-44:4)/PC (o-44:5) - ESI(+)	Lognormal	0.019	(-0.005, 0.042)	0.129	0.864	0.231	(-0.004, 0.044)
CE (18:0)	Lognormal	0.042	(0.010, 0.074)	0.014	0.864	1.498	(0.010, 0.076)
PC (40:6) A	Lognormal	-0.006	(-0.036, 0.024)	0.707	0.937	0.070	(-0.037, 0.026)
GlcCer (d40:1) - ESI(+)	Lognormal	-0.006	(-0.034, 0.022)	0.674	0.928	0.077	(-0.036, 0.021)
Ceramide (d34:0)	Lognormal	-0.016	(-0.046, 0.014)	0.308	0.864	0.091	(-0.050, 0.012)
TG (57:1)	Lognormal	-0.026	(-0.070, 0.018)	0.248	0.864	0.131	(-0.070, 0.018)
PC (16:0/9:0(CHO))	Lognormal	-0.005	(-0.053, 0.043)	0.840	0.962	0.057	(-0.056, 0.042)
PC (38:4) A - ESI(+)	Lognormal	-0.002	(-0.020, 0.015)	0.786	0.956	0.070	(-0.021, 0.016)
TG (52:1)	Lognormal	-0.023	(-0.069, 0.024)	0.343	0.864	0.106	(-0.070, 0.023)
TG (49:3)	Lognormal	-0.008	(-0.058, 0.043)	0.771	0.956	0.071	(-0.060, 0.044)
Ceramide (d40:2)	Lognormal	-0.011	(-0.090, 0.068)	0.787	0.956	0.071	(-0.092, 0.070)
PC (p-42:5)/PC (o-42:6)	Lognormal	-0.023	(-0.076, 0.030)	0.399	0.873	0.110	(-0.076, 0.033)
TG (56:1)	Lognormal	-0.020	(-0.081, 0.040)	0.511	0.899	0.082	(-0.077, 0.046)
CE (20:4)	Lognormal	-0.004	(-0.028, 0.020)	0.766	0.956	0.079	(-0.028, 0.022)
TG (49:0)	Lognormal	-0.014	(-0.060, 0.032)	0.556	0.905	0.091	(-0.060, 0.034)
PC (40:5) A - ESI(-)	Lognormal	-0.002	(-0.035, 0.031)	0.902	0.976	0.068	(-0.038, 0.031)
SM (d36:1) - ESI(+)	Lognormal	0.006	(-0.011, 0.023)	0.526	0.899	0.083	(-0.011, 0.023)
TG (58:5)	Lognormal	-0.020	(-0.058, 0.019)	0.321	0.864	0.123	(-0.057, 0.020)
PC (38:4) C - ESI(+)	Lognormal	-0.004	(-0.017, 0.009)	0.508	0.899	0.087	(-0.017, 0.010)
LPC (20:0)	Lognormal	-0.013	(-0.046, 0.020)	0.442	0.881	0.084	(-0.047, 0.022)
PC (40:7) - ESI(-)	Lognormal	-0.012	(-0.050, 0.025)	0.525	0.899	0.079	(-0.049, 0.026)
DG (34:2)	Lognormal	0.003	(-0.020, 0.026)	0.797	0.956	0.062	(-0.022, 0.026)
LPC (p-18:0)/LPC (o-18:1)	Lognormal	-0.006	(-0.032, 0.020)	0.637	0.928	0.082	(-0.031, 0.021)
TG (58:2)	Lognormal	-0.132	(-0.277, 0.013)	0.083	0.864	0.342	(-0.285, 0.021)
PC (31:0)	Lognormal	0.001	(-0.025, 0.027)	0.917	0.983	0.073	(-0.024, 0.028)
PC (40:8) - ESI(+)	Lognormal	-0.011	(-0.029, 0.008)	0.262	0.864	0.109	(-0.030, 0.009)
PC (p-38:5)/PC (o-38:6) A	Lognormal	0.000	(-0.027, 0.026)	0.973	0.996	0.065	(-0.028, 0.026)
TG (62:2)	Lognormal	-0.024	(-0.081, 0.033)	0.417	0.873	0.102	(-0.086, 0.032)
PE (34:2) - ESI(+)	Lognormal	-0.119	(-0.260, 0.022)	0.107	0.864	0.292	(-0.268, 0.020)
TG (50:3) A	Lognormal	-0.004	(-0.037, 0.028)	0.801	0.956	0.076	(-0.036, 0.029)
TG (51:3)	Lognormal	0.008	(-0.024, 0.039)	0.639	0.928	0.078	(-0.025, 0.039)
PC (p-40:4)/PC (o-40:5) - ESI(-)	Lognormal	0.001	(-0.022, 0.025)	0.908	0.977	0.065	(-0.022, 0.026)
PC (36:6)	Lognormal	-0.015	(-0.056, 0.026)	0.481	0.884	0.093	(-0.058, 0.026)
FA (10:0) (capric acid)	Lognormal	-0.005	(-0.052, 0.041)	0.824	0.962	0.056	(-0.054, 0.042)
Ceramide (d42:2) A - ESI (+)	Lognormal	0.012	(-0.006, 0.030)	0.198	0.864	0.165	(-0.007, 0.030)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Gal-Gal-Cer (d18:1/16:0)/Lactosylceramide (d18:1/16:0)	Lognormal	0.012	(-0.002, 0.026)	0.101	0.864	0.277	(-0.002, 0.026)
PE (36:4) - ESI(-)	Lognormal	-0.047	(-0.103, 0.010)	0.112	0.864	0.234	(-0.106, 0.008)
LPC (18:1) - ESI(+)	Lognormal	-0.016	(-0.038, 0.005)	0.148	0.864	0.203	(-0.038, 0.005)
PC (p-36:5)/PC (o-36:6)	Lognormal	-0.008	(-0.049, 0.034)	0.711	0.939	0.069	(-0.051, 0.033)
TG (56:4)	Lognormal	0.006	(-0.022, 0.034)	0.681	0.929	0.084	(-0.023, 0.036)
PC 40:6e	Lognormal	0.007	(-0.013, 0.027)	0.503	0.899	0.085	(-0.013, 0.027)
PC (p-44:5)/PC (o-44:6)	Lognormal	0.016	(-0.013, 0.044)	0.299	0.864	0.107	(-0.014, 0.046)
SM (d41:2) A - ESI(+)	Lognormal	0.007	(-0.016, 0.031)	0.543	0.902	0.083	(-0.015, 0.032)
TG (50:3) B	Lognormal	-0.047	(-0.150, 0.057)	0.381	0.873	0.116	(-0.150, 0.067)
TG (44:2)	Lognormal	-0.027	(-0.177, 0.123)	0.724	0.944	0.077	(-0.187, 0.123)
TG (48:1)	Lognormal	-0.030	(-0.075, 0.016)	0.206	0.864	0.172	(-0.074, 0.018)
SM (d43:1) - ESI(+)	Lognormal	-0.001	(-0.035, 0.033)	0.958	0.996	0.061	(-0.036, 0.033)
LPC (22:5) - ESI(-)	Lognormal	-0.038	(-0.096, 0.020)	0.203	0.864	0.158	(-0.099, 0.019)
TG (48:2)	Lognormal	-0.034	(-0.084, 0.017)	0.197	0.864	0.166	(-0.083, 0.017)
FA (24:1) (nervonic acid)	Lognormal	-0.002	(-0.022, 0.018)	0.841	0.962	0.052	(-0.024, 0.018)
FA (20:4) (arachidonic acid)	Lognormal	-0.010	(-0.023, 0.004)	0.176	0.864	0.140	(-0.023, 0.004)
PC (40:4) - ESI(+)	Lognormal	-0.009	(-0.033, 0.015)	0.452	0.884	0.087	(-0.032, 0.017)
PC (32:1) - ESI(-)	Lognormal	-0.029	(-0.070, 0.013)	0.185	0.864	0.176	(-0.071, 0.013)
PC (38:4) B - ESI(+)	Lognormal	-0.010	(-0.033, 0.013)	0.407	0.873	0.091	(-0.034, 0.014)
PC (34:0) - ESI(+)	Lognormal	-0.002	(-0.014, 0.010)	0.736	0.949	0.058	(-0.015, 0.010)
Ceramide (d36:1) - ESI(+)	Lognormal	0.020	(-0.007, 0.046)	0.163	0.864	0.176	(-0.009, 0.046)
Oxylipins (OL)							
Resolvin D1	Gamma	-0.282	(-0.991, 0.426)	0.439	0.881	0.099	(-1.004, 0.410)
5-Hydroxy-6,8,11,14,17-eicosapentaenoic acid	Gamma	0.055	(-0.345, 0.455)	0.788	0.956	0.043	(-0.386, 0.454)
9-nitrooleic acid	Gamma	-0.634	(-1.110, -0.158)	0.013	0.864	0.503	(-1.279, -0.003)
15,16-dihydroxyoctadeca-9,12-dienoic acid	Lognormal	0.072	(-0.280, 0.425)	0.690	0.930	0.059	(-0.277, 0.445)
15-hydroxyeicosa-5,8,11,13,17-pentaenoic acid	Gamma	-0.180	(-0.668, 0.308)	0.474	0.884	0.070	(-0.747, 0.395)
12-Hydroxy-5,8,10,14,17-eicosapentaenoic acid	Gamma	0.205	(-0.315, 0.725)	0.444	0.882	0.071	(-0.349, 0.790)
Prostaglandin F2a	Gamma	-0.150	(-0.625, 0.326)	0.540	0.902	0.067	(-0.729, 0.514)
Prostaglandin D2	Gamma	0.617	(-0.488, 1.722)	0.280	0.864	0.121	(-0.708, 1.337)
4-hydroxydocosa-5,7,10,13,16,19-hexaenoic acid	Gamma	-0.065	(-0.654, 0.523)	0.829	0.962	0.054	(-0.677, 0.511)
9-Hydroxy-5,7,11,14,17-icosapentaenoic acid	Gamma	0.189	(-0.285, 0.664)	0.438	0.881	0.067	(-0.364, 0.689)
8,9-Epoxyeicosa-5,11,14-trienoic acid	Gamma	-0.037	(-0.486, 0.412)	0.873	0.969	0.054	(-0.543, 0.484)
9,10-dihydroxyoctadec-12-enoic acid	Lognormal	0.060	(-0.279, 0.398)	0.732	0.949	0.060	(-0.302, 0.392)
11,12-Epoxyeicosa-5,8,14-trienoic acid	Gamma	0.426	(-0.006, 0.859)	0.061	0.864	0.228	(-0.035, 0.906)
11(12)-epoxy-5,8,14,17- eicosatetraenoic acid	Gamma	-1.314	(-1.984, -0.645)	0.000	0.374	5.610	(-2.063, -0.433)
8-hydroxyeicosa-5,9,11,14-tetraenoic acid	Gamma	-0.330	(-0.848, 0.188)	0.219	0.864	0.114	(-0.950, 0.267)
6-Ketoprostaglandin F1 alpha	Gamma	-0.620	(-1.324, 0.084)	0.092	0.864	0.326	(-1.336, 0.037)
15-ketoeicosa-5,8,11,13-tetraenoic acid	Gamma	-0.217	(-0.800, 0.366)	0.470	0.884	0.080	(-0.779, 0.402)
17,18-Epoxy-5,8,11,14-eicosatetraenoic acid	Gamma	-0.820	(-1.753, 0.113)	0.093	0.864	0.394	(-1.788, 0.186)
17,18-dihydroxyeicosa-5,8,11,14-tetraenoic acid	Lognormal	0.108	(-0.398, 0.613)	0.679	0.929	0.064	(-0.381, 0.661)
15-Deoxy-delta-12,14-Prostaglandin J2	Gamma	-0.091	(-0.626, 0.445)	0.742	0.949	0.075	(-0.784, 0.559)
15(16)-epoxy-9,12-octadecadienoic acid	Gamma	-0.043	(-0.655, 0.570)	0.892	0.976	0.059	(-0.660, 0.592)
9,11,15-trihydroxy-5,13,1Z-prostatrienoic acid	Gamma	-0.734	(-1.454, -0.014)	0.053	0.864	0.650	(-1.489, 0.011)
9,10-dihydroxyoctadeca-12,15-dienoic acid	Gamma	0.307	(0.011, 0.645)	0.054	0.864	1.568	(-0.009, 0.549)
9(10)-epoxy-12Z-octadecenoic acid	Gamma	0.214	(-0.237, 0.665)	0.358	0.872	0.067	(-0.204, 0.639)
9(10)-epoxy-12,15-octadecadienoic acid	Gamma	-0.277	(-0.847, 0.294)	0.347	0.864	0.099	(-1.019, 0.338)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
10-nitrooleic acid	Lognormal	-0.127	(-0.610, 0.356)	0.610	0.928	0.073	(-0.658, 0.357)
11-Hydroxy-arachidonic acid	Gamma	-0.095	(-0.449, 0.259)	0.602	0.926	0.047	(-0.481, 0.322)
6-trans-Leukotriene B4	Gamma	0.781	(0.124, 1.438)	0.025	0.864	0.581	(-0.017, 1.491)
8,9-dihydroxyeicosa-5,11,14-trienoic acid	Gamma	-0.006	(-0.492, 0.480)	0.981	0.996	0.058	(-0.593, 0.572)
13-hydroxyoctadeca-9,11,15-trienoic acid	Gamma	0.230	(-0.238, 0.699)	0.340	0.864	0.072	(-0.204, 0.730)
12(13)-epoxy-9,15-octadecadienoic acid	Gamma	0.500	(-0.032, 1.031)	0.073	0.864	0.177	(-0.226, 1.167)
Leukotriene B5	Gamma	0.384	(-0.498, 1.265)	0.399	0.873	0.144	(-0.857, 1.507)
12,13-dihydroxyoctadec-9-enoic acid	Lognormal	-0.178	(-0.573, 0.217)	0.382	0.873	0.084	(-0.598, 0.227)
9-Hydroxylinoleic acid	Lognormal	0.000	(-0.241, 0.241)	0.998	1.000	0.059	(-0.242, 0.255)
13-ketooctadeca-9,11-dienoic acid	Lognormal	-0.252	(-0.698, 0.195)	0.276	0.864	0.106	(-0.716, 0.199)
16(17)-epoxy-4,7,10,13,19-docosapentaenoic acid	Gamma	0.271	(-0.365, 0.906)	0.409	0.873	0.096	(-0.510, 1.015)
5,6-dihydroxyeicosa-8,11,14-trienoic acid	Gamma	0.001	(-0.445, 0.448)	0.995	0.998	0.051	(-0.503, 0.503)
17-hydroxy-4,7,10,13,15,19-docosahexaenoic acid	Gamma	0.217	(-0.247, 0.680)	0.365	0.873	0.071	(-0.310, 0.716)
9,12,13-trihydroxyoctadec-10-enoic acid	Lognormal	0.070	(-0.198, 0.338)	0.613	0.928	0.061	(-0.189, 0.339)
10-nitrolinoleic acid	Gamma	0.386	(-0.311, 1.083)	0.284	0.864	0.119	(-0.445, 1.141)
Prostaglandin E2	Gamma	-0.221	(-0.798, 0.357)	0.458	0.884	0.082	(-0.815, 0.386)
9-hydroxyeicosa-5,7,11,14-tetraenoic acid	Gamma	-0.232	(-0.656, 0.192)	0.290	0.864	0.082	(-0.691, 0.264)
Prostaglandin E1	Gamma	0.309	(-0.320, 0.939)	0.341	0.864	0.099	(-0.335, 0.935)
8,15-dihydroxyeicosa-5,9,11,13-tetraenoic acid	Gamma	-0.350	(-1.137, 0.437)	0.388	0.873	0.123	(-1.374, 0.779)
9-hydroxyoctadeca-10,12,15-trienoic acid	Gamma	0.091	(-0.289, 0.471)	0.643	0.928	0.048	(-0.347, 0.551)
14(15)-epoxy-5,8,11,17-eicosatetraenoic acid	Gamma	0.809	(-0.142, 1.760)	0.103	0.864	0.435	(-0.145, 1.677)
9,10-Epoxy stearic acid	Lognormal	-0.591	(-1.261, 0.078)	0.091	0.864	0.269	(-1.271, 0.138)
5,6,15-trihydroxyeicosa-7,9,11,13-tetraenoic acid	Gamma	-0.583	(-1.229, 0.063)	0.085	0.864	0.365	(-1.263, 0.038)
12,13-epoxy-9-octadecenoic acid	Lognormal	-0.291	(-0.946, 0.363)	0.388	0.873	0.093	(-0.986, 0.373)
Thromboxane B2	Lognormal	0.031	(-0.432, 0.494)	0.897	0.976	0.063	(-0.441, 0.513)
20-Hydroxyarachidonic acid	Lognormal	0.208	(-0.372, 0.788)	0.486	0.884	0.070	(-0.352, 0.823)
Leukotriene B4	Gamma	-0.324	(-0.760, 0.111)	0.152	0.864	0.120	(-0.787, 0.147)
13-Hydroxyoctadecadienoic acid	Lognormal	0.011	(-0.251, 0.273)	0.935	0.992	0.068	(-0.253, 0.279)
9S,10R-dihydroxy-stearic acid	Lognormal	0.064	(-0.467, 0.594)	0.815	0.956	0.068	(-0.475, 0.619)
5-ketoeicosa-6,8,11,14-tetraenoic acid	Gamma	-0.282	(-0.848, 0.284)	0.335	0.864	0.107	(-0.975, 0.426)
Prostaglandin E3	Gamma	0.969	(0.038, 1.901)	0.048	0.864	0.431	(-0.267, 2.086)
5,15-dihydroxyeicosa-6,8,11,13-tetraenoic acid	Gamma	0.444	(-0.426, 1.314)	0.323	0.864	0.138	(-0.464, 1.207)
12,13-dihydroxyoctadeca-9,15-dienoic acid	Gamma	-0.100	(-0.765, 0.566)	0.771	0.956	0.073	(-0.765, 0.580)
14-hydroxydocosa-4,7,10,12,16,19-hexaenoic acid	Lognormal	-0.129	(-0.919, 0.662)	0.751	0.952	0.054	(-0.947, 0.690)
trans-12,13-epoxy-11-oxo-trans-9-octadecenoic acid	Gamma	0.112	(-0.336, 0.560)	0.628	0.928	0.053	(-0.390, 0.593)
14,15-dihydroxyeicosa-5,8,11,17-tetraenoic acid	Gamma	-0.563	(-1.200, 0.075)	0.091	0.864	0.267	(-1.276, 0.116)
19,20-dihydroxydocosa-4,7,10,13,16-pentaenoic acid	Lognormal	0.105	(-0.241, 0.452)	0.555	0.905	0.062	(-0.259, 0.435)
5-Hydroxy-6,8,11,14-eicosatetraenoic acid	Lognormal	-0.179	(-0.596, 0.238)	0.405	0.873	0.074	(-0.580, 0.229)
14,15-dihydroxyeicosa-5,8,11-trienoic acid	Gamma	0.031	(-0.256, 0.330)	0.839	0.962	0.067	(-0.295, 0.359)
18-(3-ethyloxiran-2-yl)octadeca-4,7,10,13,16-pentaenoic acid	Gamma	0.354	(-0.262, 0.969)	0.267	0.864	0.112	(-0.291, 1.021)
15-hydroxyeicosa-5,8,11,13-tetraenoic acid	Lognormal	0.071	(-0.267, 0.409)	0.682	0.929	0.061	(-0.283, 0.397)
12-Hydroxy-5,8,10,14-eicosatetraenoic acid	Lognormal	0.087	(-0.400, 0.574)	0.728	0.947	0.052	(-0.414, 0.575)
11-Hydroxy-14,15-epoxyeicosatrienoic acid	Gamma	-0.642	(-1.380, 0.096)	0.096	0.864	0.337	(-1.450, 0.103)
9-ketooctadeca-10,12-dienoic acid	Gamma	-0.187	(-0.539, 0.162)	0.278	0.864	0.092	(-0.720, 0.184)
15-Keto-prostaglandin E2	Gamma	-0.673	(-1.265, -0.081)	0.032	0.864	0.515	(-1.369, 0.054)
11,12-Dihydroxyeicosa-5,8,14-trienoic acid	Gamma	-0.038	(-0.345, 0.268)	0.807	0.956	0.040	(-0.417, 0.352)

Supplementary Table S6. Regression and Bayesian estimates comparing sex-stratified ME/CFS vs. controls.

Metabolite	Regression Model	Male ME/CFS vs. Male Controls					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI

ME/CFS, myalgic encephalomyelitis/chronic fatigue syndrome; CI, confidence interval; FDR, false discovery rate adjusted p-value; HDI, highest density credible intervals. Regression models were adjusted for age, race/ethnicity, geographic/clinical site, season of sampling, body mass index, and self-reported irritable bowel syndrome. In PM, BA, and CL panels, estimated coefficients are interpreted as the differences in the mean values of log-log transformation of metabolite levels between cases and controls. In OL panel for lognormal regression, estimated coefficients are interpreted as the mean differences of log transformation of metabolite levels between two groups; for Gamma regression, estimated coefficients are interpreted as the log of fold change between two groups. Estimations in **bold** are significant. Criteria for significance: 1) FDR adjusted p-value from the regression model < 0.15, 2) BayesFactor > 3, and 3) 95% highest density credible intervals not covering 0.

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Primary Metabolites (PM)							
mannitol	Lognormal	0.039	(0.006, 0.072)	0.021	0.327	0.495	(0.005, 0.072)
succinic acid	Lognormal	0.020	(0.002, 0.038)	0.027	0.352	0.403	(0.001, 0.038)
arachidic acid	Lognormal	0.023	(0.002, 0.044)	0.034	0.362	0.353	(0.004, 0.046)
ornithine	Lognormal	-0.016	(-0.032, 0.000)	0.046	0.383	0.247	(-0.032, -0.001)
leucine	Lognormal	-0.010	(-0.021, 0.000)	0.050	0.397	0.242	(-0.020, 0.000)
maleic acid	Lognormal	0.031	(0.000, 0.062)	0.054	0.402	0.235	(-0.002, 0.061)
threonine	Lognormal	-0.013	(-0.028, 0.002)	0.098	0.522	0.146	(-0.027, 0.003)
glucuronic acid	Lognormal	0.017	(-0.004, 0.039)	0.109	0.553	0.141	(-0.003, 0.039)
2-hydroxybutanoic acid	Lognormal	0.014	(-0.004, 0.032)	0.118	0.560	0.115	(-0.005, 0.032)
alpha-ketoglutarate	Lognormal	0.013	(-0.003, 0.029)	0.119	0.560	0.106	(-0.003, 0.030)
tyrosine	Lognormal	-0.007	(-0.015, 0.002)	0.148	0.628	0.099	(-0.016, 0.002)
pentadecanoic acid	Lognormal	0.009	(-0.003, 0.020)	0.151	0.635	0.089	(-0.003, 0.020)
glutaric acid	Lognormal	0.015	(-0.006, 0.037)	0.160	0.648	0.097	(-0.006, 0.037)
3-hydroxybutyric acid	Lognormal	0.023	(-0.009, 0.055)	0.167	0.658	0.082	(-0.010, 0.054)
indole-3-propionic acid	Lognormal	-0.019	(-0.046, 0.008)	0.170	0.659	0.088	(-0.047, 0.007)
levoglucosan	Lognormal	-0.017	(-0.043, 0.008)	0.191	0.678	0.087	(-0.043, 0.007)
ribose	Lognormal	0.009	(-0.005, 0.023)	0.215	0.698	0.085	(-0.006, 0.023)
1,2,4-benzenetriol	Lognormal	-0.021	(-0.055, 0.014)	0.245	0.724	0.071	(-0.056, 0.013)
2-ketoisocaproic acid	Lognormal	0.007	(-0.005, 0.018)	0.250	0.724	0.059	(-0.005, 0.018)
urea	Lognormal	-0.006	(-0.016, 0.004)	0.255	0.724	0.067	(-0.015, 0.004)
aminomalonate	Lognormal	0.017	(-0.012, 0.045)	0.263	0.726	0.068	(-0.014, 0.045)
indole-3-lactate	Lognormal	-0.008	(-0.023, 0.007)	0.285	0.741	0.061	(-0.022, 0.008)
glutamine	Lognormal	-0.011	(-0.032, 0.010)	0.310	0.757	0.054	(-0.033, 0.010)
pyrrole-2-carboxylic acid	Lognormal	0.013	(-0.012, 0.039)	0.314	0.757	0.059	(-0.011, 0.039)
glucose-1-phosphate	Lognormal	0.008	(-0.008, 0.025)	0.314	0.757	0.057	(-0.007, 0.026)
oxoproline	Lognormal	-0.003	(-0.010, 0.003)	0.321	0.758	0.059	(-0.009, 0.003)
citrulline	Lognormal	-0.006	(-0.018, 0.006)	0.324	0.760	0.054	(-0.018, 0.006)
erythritol	Lognormal	0.016	(-0.016, 0.047)	0.327	0.761	0.059	(-0.015, 0.050)
pseudo uridine	Lognormal	-0.006	(-0.017, 0.006)	0.328	0.763	0.056	(-0.017, 0.006)
glycerol	Lognormal	0.006	(-0.006, 0.017)	0.332	0.764	0.048	(-0.006, 0.017)
benzoic acid	Lognormal	0.009	(-0.010, 0.028)	0.345	0.772	0.058	(-0.010, 0.028)
malic acid	Lognormal	0.010	(-0.011, 0.032)	0.352	0.784	0.052	(-0.012, 0.030)
beta-alanine	Lognormal	-0.011	(-0.036, 0.013)	0.364	0.805	0.055	(-0.037, 0.011)
2-deoxytetronic acid	Lognormal	0.010	(-0.012, 0.032)	0.384	0.825	0.052	(-0.012, 0.033)
proline	Lognormal	-0.009	(-0.032, 0.013)	0.407	0.834	0.048	(-0.031, 0.013)
phenylalanine	Lognormal	-0.005	(-0.015, 0.006)	0.414	0.834	0.044	(-0.015, 0.006)
pelargonic acid	Lognormal	0.006	(-0.008, 0.020)	0.421	0.834	0.047	(-0.008, 0.019)
isoleucine	Lognormal	-0.004	(-0.016, 0.007)	0.428	0.838	0.048	(-0.015, 0.007)
tagatose	Lognormal	0.007	(-0.011, 0.026)	0.437	0.846	0.042	(-0.012, 0.026)
4-hydroxybutyric acid	Lognormal	0.008	(-0.012, 0.027)	0.439	0.848	0.049	(-0.012, 0.027)
2-hydroxyvaleric acid	Lognormal	0.007	(-0.011, 0.025)	0.456	0.855	0.045	(-0.012, 0.026)
glycine	Lognormal	-0.003	(-0.013, 0.006)	0.488	0.879	0.042	(-0.013, 0.006)
lysine	Lognormal	-0.010	(-0.038, 0.018)	0.491	0.879	0.040	(-0.036, 0.019)
sucrose	Lognormal	0.012	(-0.022, 0.046)	0.501	0.890	0.046	(-0.023, 0.048)
glycerol-alpha-phosphate	Lognormal	0.009	(-0.018, 0.036)	0.519	0.896	0.044	(-0.020, 0.035)
myo-inositol	Lognormal	-0.004	(-0.017, 0.008)	0.520	0.896	0.044	(-0.016, 0.008)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
phosphate	Lognormal	-0.007	(-0.027, 0.014)	0.521	0.896	0.040	(-0.028, 0.014)
lactic acid	Lognormal	-0.005	(-0.022, 0.011)	0.530	0.896	0.040	(-0.021, 0.012)
indole-3-acetate	Lognormal	0.006	(-0.014, 0.027)	0.542	0.898	0.042	(-0.014, 0.026)
lysine	Lognormal	-0.005	(-0.023, 0.013)	0.563	0.909	0.037	(-0.024, 0.011)
glucose	Lognormal	0.002	(-0.005, 0.010)	0.568	0.914	0.038	(-0.006, 0.010)
tryptophan	Lognormal	-0.005	(-0.022, 0.012)	0.571	0.914	0.036	(-0.022, 0.011)
palmitoleic acid	Lognormal	-0.008	(-0.034, 0.019)	0.573	0.914	0.042	(-0.035, 0.018)
stearic acid	Lognormal	-0.002	(-0.011, 0.006)	0.578	0.916	0.038	(-0.010, 0.006)
alanine	Lognormal	-0.006	(-0.029, 0.016)	0.584	0.919	0.043	(-0.031, 0.015)
hydroxycarbamate NIST	Lognormal	-0.005	(-0.025, 0.014)	0.590	0.924	0.039	(-0.026, 0.014)
methionine	Lognormal	-0.005	(-0.022, 0.013)	0.611	0.933	0.039	(-0.024, 0.013)
heptadecanoic acid	Lognormal	0.004	(-0.013, 0.021)	0.614	0.933	0.037	(-0.012, 0.020)
lyxitol	Lognormal	-0.004	(-0.020, 0.012)	0.619	0.934	0.041	(-0.019, 0.011)
linoleic acid	Lognormal	0.006	(-0.018, 0.029)	0.634	0.938	0.040	(-0.019, 0.028)
trans-4-hydroxyproline	Lognormal	-0.005	(-0.028, 0.018)	0.653	0.938	0.036	(-0.027, 0.018)
maleimide	Lognormal	0.004	(-0.015, 0.024)	0.663	0.938	0.035	(-0.016, 0.022)
glyceric acid	Lognormal	0.004	(-0.015, 0.024)	0.667	0.938	0.036	(-0.016, 0.024)
quinic acid	Lognormal	-0.009	(-0.050, 0.032)	0.672	0.938	0.038	(-0.050, 0.031)
ribonic acid	Lognormal	-0.004	(-0.023, 0.015)	0.689	0.942	0.037	(-0.024, 0.015)
mannose	Lognormal	-0.004	(-0.021, 0.014)	0.695	0.945	0.038	(-0.020, 0.015)
adipic acid	Lognormal	-0.004	(-0.023, 0.015)	0.701	0.945	0.036	(-0.023, 0.015)
threonic acid	Lognormal	0.004	(-0.017, 0.025)	0.701	0.945	0.039	(-0.018, 0.025)
fructose	Lognormal	-0.005	(-0.034, 0.023)	0.709	0.946	0.035	(-0.033, 0.021)
glutamic acid	Lognormal	0.003	(-0.015, 0.022)	0.725	0.948	0.034	(-0.015, 0.022)
serine	Lognormal	-0.003	(-0.017, 0.012)	0.727	0.948	0.037	(-0.017, 0.012)
gluconic acid	Lognormal	0.003	(-0.013, 0.018)	0.747	0.955	0.037	(-0.014, 0.017)
condurotol-beta-expoxide	Lognormal	0.005	(-0.026, 0.036)	0.755	0.955	0.038	(-0.028, 0.034)
myristic acid	Lognormal	0.002	(-0.012, 0.017)	0.759	0.955	0.039	(-0.013, 0.017)
behenic acid	Lognormal	-0.002	(-0.019, 0.014)	0.768	0.955	0.037	(-0.019, 0.013)
phthalic acid	Lognormal	0.002	(-0.013, 0.018)	0.769	0.955	0.037	(-0.013, 0.016)
nicotinic acid	Lognormal	-0.005	(-0.042, 0.033)	0.798	0.960	0.032	(-0.042, 0.034)
maltose	Lognormal	0.002	(-0.022, 0.027)	0.847	0.981	0.033	(-0.022, 0.028)
isopropylbenzene	Lognormal	0.002	(-0.017, 0.021)	0.850	0.981	0.023	(-0.017, 0.020)
citric acid	Lognormal	0.001	(-0.014, 0.017)	0.858	0.981	0.031	(-0.014, 0.017)
isothreonic acid	Lognormal	-0.002	(-0.030, 0.025)	0.859	0.981	0.035	(-0.031, 0.023)
uric acid	Lognormal	-0.002	(-0.020, 0.017)	0.860	0.981	0.035	(-0.021, 0.017)
palmitic acid	Lognormal	-0.001	(-0.009, 0.008)	0.872	0.984	0.034	(-0.009, 0.008)
2-aminobutyric acid	Lognormal	-0.001	(-0.015, 0.013)	0.880	0.984	0.036	(-0.015, 0.013)
glycolic acid	Lognormal	0.002	(-0.027, 0.031)	0.887	0.984	0.035	(-0.025, 0.033)
salicylic acid	Lognormal	0.002	(-0.028, 0.032)	0.893	0.984	0.035	(-0.027, 0.032)
capric acid	Lognormal	0.002	(-0.023, 0.026)	0.904	0.984	0.034	(-0.022, 0.027)
caprylic acid	Lognormal	0.001	(-0.013, 0.015)	0.907	0.984	0.034	(-0.012, 0.015)
N-acetylputrescine	Lognormal	-0.001	(-0.020, 0.018)	0.914	0.988	0.035	(-0.020, 0.019)
creatinine	Lognormal	0.001	(-0.022, 0.025)	0.918	0.989	0.033	(-0.022, 0.025)
lauric acid	Lognormal	0.001	(-0.022, 0.024)	0.932	0.990	0.032	(-0.022, 0.023)
threitol	Lognormal	0.001	(-0.017, 0.018)	0.945	0.994	0.031	(-0.016, 0.019)
fumaric acid	Lognormal	0.000	(-0.019, 0.018)	0.962	0.998	0.034	(-0.019, 0.017)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
valine	Lognormal	0.000	(-0.010, 0.010)	0.973	0.998	0.035	(-0.010, 0.010)
creatine	Lognormal	0.000	(-0.025, 0.025)	0.978	0.998	0.035	(-0.025, 0.025)
1-methylgalactose NIST	Lognormal	0.000	(-0.035, 0.034)	0.979	0.998	0.033	(-0.035, 0.034)
alloxanoic acid	Lognormal	0.000	(-0.031, 0.030)	0.980	0.998	0.032	(-0.032, 0.030)
pyruvic acid	Lognormal	0.000	(-0.017, 0.016)	0.983	0.998	0.031	(-0.017, 0.016)
oxalic acid	Lognormal	0.000	(-0.041, 0.040)	0.986	0.998	0.036	(-0.039, 0.042)
N-acetylornithine	Lognormal	0.000	(-0.013, 0.012)	0.988	0.998	0.034	(-0.012, 0.012)
Biogenic Amines (BA)							
Acetaminophen	Lognormal	0.066	(0.023, 0.109)	0.003	0.291	2.586	(0.024, 0.109)
Acyclovir	Lognormal	0.104	(0.031, 0.177)	0.006	0.310	1.688	(0.034, 0.180)
Guanine	Lognormal	0.087	(0.026, 0.148)	0.006	0.310	1.280	(0.022, 0.147)
2-Methylbutyryl-L-carnitine	Lognormal	-0.035	(-0.059, -0.010)	0.006	0.310	1.361	(-0.060, -0.011)
Alprazolam	Lognormal	0.068	(0.018, 0.119)	0.008	0.310	0.850	(0.015, 0.118)
SDMA	Lognormal	-0.013	(-0.022, -0.003)	0.011	0.310	0.900	(-0.022, -0.003)
Choline cation	Lognormal	-0.008	(-0.014, -0.002)	0.015	0.310	0.591	(-0.014, -0.001)
L-Citrulline	Lognormal	-0.012	(-0.021, -0.002)	0.017	0.310	0.620	(-0.022, -0.002)
Ranitidine N-oxide	Lognormal	0.061	(0.011, 0.111)	0.019	0.325	0.680	(0.011, 0.110)
Albendazole sulfoxide	Lognormal	0.105	(0.014, 0.195)	0.024	0.339	0.458	(0.015, 0.197)
Caffeine	Lognormal	-0.064	(-0.120, -0.008)	0.026	0.351	0.416	(-0.119, -0.008)
Citrulline	Lognormal	-0.011	(-0.021, -0.001)	0.032	0.352	0.398	(-0.021, 0.000)
Piperine	Lognormal	-0.053	(-0.102, -0.005)	0.033	0.362	0.383	(-0.103, -0.006)
Gabapentin	Lognormal	0.048	(0.003, 0.093)	0.037	0.369	0.322	(0.004, 0.093)
4-Acetamidobutyric acid	Lognormal	-0.021	(-0.041, -0.001)	0.040	0.373	0.339	(-0.040, -0.001)
3-Methylglutaryl-carnitine	Lognormal	-0.031	(-0.060, -0.002)	0.040	0.373	0.349	(-0.059, -0.002)
Methacholine cation	Lognormal	-0.017	(-0.034, -0.001)	0.041	0.374	0.276	(-0.033, -0.001)
3-Cysteinylacetaminophen	Lognormal	0.094	(0.004, 0.184)	0.042	0.376	0.314	(0.006, 0.186)
Theobromine	Lognormal	-0.044	(-0.087, -0.002)	0.042	0.376	0.247	(-0.088, -0.001)
D-Turanose	Lognormal	-0.029	(-0.057, -0.001)	0.044	0.381	0.288	(-0.058, -0.001)
N-Acetylhistidine	Lognormal	-0.021	(-0.041, 0.000)	0.049	0.395	0.211	(-0.041, 0.000)
Metformin	Lognormal	0.030	(0.000, 0.060)	0.053	0.402	0.229	(0.001, 0.061)
Isopropylamine	Lognormal	-0.011	(-0.023, 0.000)	0.055	0.402	0.232	(-0.023, 0.000)
L-Cystine	Lognormal	-0.022	(-0.045, 0.000)	0.056	0.402	0.160	(-0.044, 0.000)
Ranitidine	Lognormal	0.041	(-0.001, 0.082)	0.057	0.405	0.205	(-0.002, 0.083)
Betaine	Lognormal	-0.006	(-0.012, 0.000)	0.066	0.426	0.191	(-0.012, 0.000)
4,5,7-Trihydroxyisoflavone	Lognormal	0.082	(-0.008, 0.172)	0.077	0.473	0.164	(-0.006, 0.175)
p-Acetamidophenyl .beta.-D-glucuronide	Lognormal	0.054	(-0.006, 0.115)	0.078	0.475	0.161	(-0.008, 0.113)
Quetiapine	Lognormal	0.024	(-0.003, 0.050)	0.079	0.478	0.165	(-0.001, 0.050)
rac-4-Sulfoxypropranolol	Lognormal	0.026	(-0.003, 0.054)	0.080	0.479	0.178	(-0.001, 0.056)
7-Methylguanosine	Lognormal	-0.012	(-0.026, 0.001)	0.082	0.479	0.165	(-0.027, 0.001)
Stachydrine	Lognormal	-0.032	(-0.068, 0.005)	0.094	0.516	0.138	(-0.068, 0.007)
Trazodone	Lognormal	0.031	(-0.005, 0.067)	0.096	0.520	0.141	(-0.005, 0.066)
Trigonelline	Lognormal	-0.033	(-0.073, 0.006)	0.098	0.522	0.122	(-0.074, 0.006)
NEPSILON,NEPSILON,NEPSILON-TRIMETHYLLYSINE	Lognormal	-0.011	(-0.024, 0.002)	0.101	0.533	0.114	(-0.023, 0.003)
(R)-Butyrylcarnitine	Lognormal	-0.016	(-0.035, 0.003)	0.111	0.557	0.115	(-0.034, 0.004)
Lamotrigine;	Lognormal	0.085	(-0.020, 0.190)	0.114	0.557	0.124	(-0.016, 0.190)
Tri-2-ethylhexyl trimellitate	Lognormal	-0.035	(-0.080, 0.010)	0.126	0.579	0.095	(-0.079, 0.010)
N-.alpha.-Acetyl-L-arginine	Lognormal	-0.011	(-0.025, 0.003)	0.134	0.605	0.113	(-0.024, 0.004)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
cis-10,11-Dihydroxy-10,11-dihydrocarbamazepine	Lognormal	-0.017	(-0.038, 0.005)	0.139	0.612	0.122	(-0.039, 0.006)
3,4-Dimethoxybenzaldehyde	Lognormal	0.023	(-0.007, 0.053)	0.141	0.612	0.081	(-0.007, 0.052)
2,6-Diaminopimelic acid	Lognormal	0.031	(-0.011, 0.074)	0.151	0.635	0.097	(-0.015, 0.074)
Guanidine	Lognormal	0.013	(-0.005, 0.032)	0.154	0.641	0.086	(-0.005, 0.032)
4'-Methyl-N-methylhexanophenone	Lognormal	-0.038	(-0.091, 0.014)	0.157	0.646	0.102	(-0.090, 0.014)
Quetiapine sulfoxide	Lognormal	0.024	(-0.009, 0.058)	0.161	0.648	0.088	(-0.010, 0.058)
Kynurenine	Lognormal	-0.011	(-0.025, 0.004)	0.163	0.650	0.073	(-0.025, 0.004)
Metoprolol acid	Lognormal	0.036	(-0.015, 0.087)	0.169	0.659	0.079	(-0.014, 0.090)
3-Dehydrocarnitine	Lognormal	-0.010	(-0.025, 0.004)	0.171	0.659	0.075	(-0.024, 0.005)
L-Tyrosine	Lognormal	-0.013	(-0.031, 0.006)	0.177	0.664	0.083	(-0.031, 0.006)
Ergothioneine	Lognormal	-0.027	(-0.066, 0.012)	0.180	0.665	0.080	(-0.063, 0.014)
Pantoprazole	Lognormal	0.037	(-0.017, 0.092)	0.182	0.667	0.088	(-0.017, 0.095)
Losartan	Lognormal	0.024	(-0.012, 0.061)	0.193	0.678	0.075	(-0.011, 0.063)
7-Hydroxywarfarin	Lognormal	0.021	(-0.011, 0.054)	0.200	0.687	0.076	(-0.013, 0.052)
H-Pro-Hyp-OH	Lognormal	0.014	(-0.008, 0.036)	0.203	0.687	0.078	(-0.008, 0.036)
Octanoylcarnitine	Lognormal	-0.012	(-0.031, 0.007)	0.205	0.691	0.059	(-0.032, 0.005)
Naproxen	Lognormal	0.026	(-0.014, 0.067)	0.208	0.692	0.071	(-0.017, 0.065)
1-Stearoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	Lognormal	0.022	(-0.013, 0.056)	0.217	0.698	0.072	(-0.008, 0.059)
Bradykinin	Lognormal	0.076	(-0.044, 0.196)	0.217	0.698	0.072	(-0.040, 0.198)
Ticlopidine	Lognormal	-0.051	(-0.132, 0.030)	0.218	0.698	0.071	(-0.127, 0.036)
2-Indolinone	Lognormal	-0.013	(-0.033, 0.007)	0.220	0.701	0.075	(-0.033, 0.007)
Coniferylaldehyde	Lognormal	0.014	(-0.008, 0.036)	0.226	0.715	0.067	(-0.007, 0.036)
Topiramate	Lognormal	0.016	(-0.010, 0.041)	0.229	0.716	0.066	(-0.008, 0.042)
alpha-Methylhistidine;	Lognormal	-0.029	(-0.077, 0.018)	0.229	0.716	0.072	(-0.080, 0.016)
Omeprazole sulfone N-oxide	Lognormal	0.039	(-0.025, 0.103)	0.229	0.716	0.075	(-0.022, 0.107)
Histidine	Lognormal	-0.012	(-0.031, 0.008)	0.232	0.716	0.080	(-0.031, 0.006)
Propionylcarnitine	Lognormal	-0.006	(-0.015, 0.004)	0.232	0.716	0.061	(-0.015, 0.004)
Betaine aldehyde cation	Lognormal	0.028	(-0.018, 0.075)	0.239	0.724	0.059	(-0.021, 0.073)
Prazepam	Lognormal	0.022	(-0.015, 0.059)	0.251	0.724	0.055	(-0.017, 0.058)
Methylgallate	Lognormal	0.045	(-0.032, 0.122)	0.251	0.724	0.073	(-0.027, 0.129)
Albendazole	Lognormal	0.011	(-0.008, 0.031)	0.252	0.724	0.061	(-0.008, 0.031)
Heptadecasping-4-enine	Lognormal	0.063	(-0.045, 0.171)	0.254	0.724	0.058	(-0.045, 0.171)
1-Acetyl-3-piperidinamine	Lognormal	0.009	(-0.007, 0.026)	0.261	0.726	0.060	(-0.007, 0.026)
Indole-3-propionic acid	Lognormal	-0.018	(-0.050, 0.014)	0.263	0.726	0.064	(-0.048, 0.014)
Acetazolamide	Lognormal	-0.028	(-0.078, 0.021)	0.264	0.726	0.066	(-0.075, 0.024)
Phenylacetyl-L-glutamine	Lognormal	-0.021	(-0.058, 0.016)	0.267	0.729	0.061	(-0.057, 0.016)
Tyrosine	Lognormal	-0.008	(-0.022, 0.006)	0.270	0.731	0.066	(-0.022, 0.006)
Omeprazole sulfone	Lognormal	0.034	(-0.026, 0.094)	0.271	0.731	0.066	(-0.023, 0.098)
N.alpha.-Methyl-L-lysine	Lognormal	0.021	(-0.016, 0.059)	0.271	0.731	0.064	(-0.017, 0.059)
.epsilon.-Caprolactam	Lognormal	0.009	(-0.008, 0.027)	0.284	0.739	0.038	(-0.008, 0.026)
Hydroxybupropion	Lognormal	-0.015	(-0.043, 0.013)	0.296	0.752	0.060	(-0.045, 0.013)
Diazepam	Lognormal	0.034	(-0.030, 0.099)	0.300	0.753	0.054	(-0.032, 0.097)
Milnacipran	Lognormal	0.019	(-0.017, 0.055)	0.301	0.753	0.057	(-0.019, 0.054)
DL-Indole-3-lactic acid	Lognormal	0.006	(-0.005, 0.017)	0.301	0.753	0.058	(-0.005, 0.017)
Metoprolol	Lognormal	0.021	(-0.019, 0.062)	0.302	0.753	0.056	(-0.020, 0.061)
3,5-Dihydroxyphenylglycine	Lognormal	-0.015	(-0.043, 0.013)	0.307	0.757	0.049	(-0.043, 0.014)
Testosterone	Lognormal	-0.017	(-0.051, 0.016)	0.311	0.757	0.055	(-0.050, 0.017)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
N-Acetyl-L-carnosine	Lognormal	-0.010	(-0.030, 0.010)	0.311	0.757	0.048	(-0.030, 0.010)
L-Cysteine-glutathione disulfide	Lognormal	-0.015	(-0.043, 0.014)	0.314	0.757	0.039	(-0.043, 0.013)
Betonicine	Lognormal	-0.034	(-0.102, 0.033)	0.319	0.757	0.054	(-0.105, 0.031)
Cyclo(Leu-Pro)	Lognormal	0.012	(-0.012, 0.036)	0.321	0.758	0.049	(-0.011, 0.037)
3-Hydroxypyridine	Lognormal	-0.034	(-0.102, 0.034)	0.331	0.764	0.046	(-0.106, 0.032)
Ornithine	Lognormal	-0.008	(-0.025, 0.008)	0.334	0.764	0.042	(-0.025, 0.008)
Homoarginine;	Lognormal	0.009	(-0.010, 0.028)	0.339	0.765	0.045	(-0.009, 0.028)
N-Methylhistidine	Lognormal	-0.016	(-0.049, 0.017)	0.352	0.784	0.053	(-0.050, 0.018)
H-gamma-glutamyl-glutamine	Lognormal	0.011	(-0.013, 0.036)	0.372	0.819	0.039	(-0.014, 0.036)
Serotonin	Lognormal	0.009	(-0.011, 0.030)	0.378	0.820	0.041	(-0.010, 0.030)
L-Threonine	Lognormal	-0.005	(-0.017, 0.006)	0.389	0.825	0.055	(-0.016, 0.007)
Trimethylamine-N-oxide	Lognormal	0.012	(-0.015, 0.038)	0.389	0.825	0.047	(-0.014, 0.038)
Matrine	Lognormal	0.020	(-0.025, 0.064)	0.390	0.825	0.050	(-0.030, 0.060)
(3-Carboxypropyl)trimethylammonium cation	Lognormal	-0.005	(-0.017, 0.007)	0.392	0.827	0.047	(-0.017, 0.006)
Glaucine	Lognormal	0.009	(-0.012, 0.031)	0.396	0.832	0.050	(-0.014, 0.031)
Androstan-3-ol-17-one 3-glucuronide	Lognormal	0.013	(-0.018, 0.044)	0.400	0.832	0.045	(-0.017, 0.044)
Ala-Ile	Lognormal	0.008	(-0.011, 0.027)	0.405	0.834	0.045	(-0.012, 0.027)
Lauroyl-L-carnitine	Lognormal	-0.015	(-0.051, 0.021)	0.407	0.834	0.052	(-0.050, 0.023)
N8-Acetylspermidine	Lognormal	-0.006	(-0.019, 0.008)	0.410	0.834	0.046	(-0.019, 0.008)
Urea	Lognormal	-0.004	(-0.013, 0.005)	0.412	0.834	0.042	(-0.013, 0.006)
3-Hydroxyoleylcarnitine	Lognormal	0.032	(-0.045, 0.108)	0.419	0.834	0.046	(-0.046, 0.109)
Codeine-6-.beta.-D-glucuronide	Lognormal	0.012	(-0.017, 0.042)	0.422	0.834	0.052	(-0.017, 0.041)
Fexofenadine	Lognormal	-0.010	(-0.035, 0.015)	0.429	0.838	0.047	(-0.035, 0.016)
3-Pyridinemethanol	Lognormal	0.010	(-0.014, 0.034)	0.431	0.838	0.049	(-0.015, 0.034)
4-Pyridoxic acid;	Lognormal	0.017	(-0.027, 0.062)	0.444	0.854	0.048	(-0.030, 0.060)
N-Methylproline	Lognormal	-0.010	(-0.035, 0.015)	0.449	0.854	0.048	(-0.034, 0.016)
Tryptophan	Lognormal	0.004	(-0.006, 0.014)	0.456	0.855	0.039	(-0.007, 0.014)
D-Fructose	Lognormal	0.003	(-0.004, 0.010)	0.459	0.855	0.037	(-0.005, 0.010)
Pyrantel	Lognormal	-0.009	(-0.033, 0.015)	0.459	0.855	0.043	(-0.031, 0.015)
Aminodiphenylmethane	Lognormal	0.014	(-0.023, 0.052)	0.461	0.856	0.043	(-0.021, 0.051)
Linoleoylcarnitine	Lognormal	-0.012	(-0.046, 0.021)	0.470	0.863	0.042	(-0.045, 0.021)
Hexanoyl-L-carnitine	Lognormal	-0.008	(-0.030, 0.014)	0.475	0.863	0.041	(-0.030, 0.014)
Penciclovir	Lognormal	0.007	(-0.013, 0.028)	0.482	0.873	0.038	(-0.013, 0.028)
1-Methyl-L-histidine	Lognormal	-0.015	(-0.056, 0.027)	0.490	0.879	0.045	(-0.056, 0.029)
Trimethoprim	Lognormal	-0.011	(-0.041, 0.020)	0.492	0.879	0.048	(-0.043, 0.020)
Meprobamate	Lognormal	0.011	(-0.020, 0.041)	0.501	0.890	0.045	(-0.020, 0.041)
6-Methoxynaphthaleneacetic acid	Lognormal	-0.004	(-0.017, 0.008)	0.507	0.894	0.044	(-0.018, 0.009)
L-Leucine, methyl ester	Lognormal	0.012	(-0.023, 0.046)	0.508	0.894	0.042	(-0.021, 0.048)
Esomeprazole	Lognormal	0.010	(-0.020, 0.041)	0.517	0.896	0.039	(-0.022, 0.038)
Temazepam	Lognormal	0.013	(-0.028, 0.054)	0.521	0.896	0.041	(-0.026, 0.058)
3-Amino-1-propanol	Lognormal	0.006	(-0.013, 0.026)	0.523	0.896	0.045	(-0.013, 0.026)
Methioninesulfoxide	Lognormal	0.006	(-0.013, 0.025)	0.528	0.896	0.041	(-0.013, 0.025)
Thr-Ile-Arg	Lognormal	-0.015	(-0.061, 0.031)	0.529	0.896	0.044	(-0.064, 0.031)
Modafinil acid	Lognormal	0.018	(-0.039, 0.075)	0.534	0.896	0.041	(-0.037, 0.075)
Borrelidin	Lognormal	-0.015	(-0.063, 0.033)	0.537	0.896	0.043	(-0.061, 0.035)
Irbesartan	Lognormal	0.008	(-0.017, 0.032)	0.540	0.898	0.043	(-0.015, 0.032)
Proline	Lognormal	0.004	(-0.009, 0.018)	0.542	0.898	0.041	(-0.010, 0.017)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
4-Fluoro-.alpha.-pyrrolidinobutiophenone	Lognormal	0.007	(-0.016, 0.030)	0.558	0.908	0.041	(-0.015, 0.030)
Glutamic acid	Lognormal	0.005	(-0.011, 0.020)	0.560	0.909	0.035	(-0.010, 0.019)
Carnitine	Lognormal	-0.002	(-0.009, 0.005)	0.563	0.909	0.036	(-0.009, 0.005)
N.epsilon.-Methyl-L-lysine	Lognormal	0.009	(-0.022, 0.039)	0.565	0.911	0.040	(-0.022, 0.039)
Lauric acid diethanolamide	Lognormal	0.012	(-0.030, 0.055)	0.572	0.914	0.041	(-0.034, 0.052)
1-Phenylpyrrolidine	Lognormal	0.007	(-0.018, 0.033)	0.573	0.914	0.039	(-0.019, 0.032)
Ezetimibe	Lognormal	0.011	(-0.027, 0.048)	0.583	0.919	0.040	(-0.031, 0.048)
Ethylenediaminetetraacetic acid	Lognormal	0.022	(-0.058, 0.102)	0.594	0.928	0.037	(-0.055, 0.107)
Dinor-12-oxophytodienoic acid	Lognormal	0.012	(-0.034, 0.057)	0.609	0.933	0.042	(-0.036, 0.055)
Montelukast-1,2-diol	Lognormal	0.019	(-0.057, 0.095)	0.622	0.934	0.037	(-0.055, 0.096)
1-Methylnicotinamide	Lognormal	-0.005	(-0.024, 0.015)	0.624	0.934	0.039	(-0.024, 0.015)
Ethiolat	Lognormal	-0.008	(-0.042, 0.025)	0.624	0.934	0.039	(-0.041, 0.025)
trans-3'-Hydroxycotinine	Lognormal	0.008	(-0.027, 0.043)	0.642	0.938	0.037	(-0.027, 0.043)
Usnic acid	Lognormal	-0.009	(-0.049, 0.030)	0.644	0.938	0.041	(-0.051, 0.030)
1-Methyladenosine A	Lognormal	-0.002	(-0.012, 0.007)	0.644	0.938	0.035	(-0.012, 0.008)
Telmisartan	Lognormal	0.007	(-0.023, 0.038)	0.645	0.938	0.033	(-0.022, 0.039)
Ser-Tyr-Lys	Lognormal	0.014	(-0.044, 0.071)	0.646	0.938	0.037	(-0.047, 0.072)
5'-S-Methylthioadenosine	Lognormal	0.018	(-0.058, 0.094)	0.649	0.938	0.032	(-0.056, 0.093)
Decanoyl-L-carnitine	Lognormal	0.007	(-0.023, 0.037)	0.653	0.938	0.038	(-0.025, 0.038)
Biliverden	Lognormal	-0.004	(-0.024, 0.015)	0.657	0.938	0.038	(-0.023, 0.016)
threo-Dihydrobupropion	Lognormal	0.005	(-0.018, 0.029)	0.658	0.938	0.035	(-0.018, 0.029)
N-(3-(Aminomethyl)benzyl)acetamidine	Lognormal	-0.008	(-0.043, 0.027)	0.660	0.938	0.031	(-0.044, 0.025)
1-Monostearin	Lognormal	-0.008	(-0.043, 0.028)	0.664	0.938	0.037	(-0.042, 0.028)
Nudifloramide	Lognormal	-0.004	(-0.020, 0.013)	0.665	0.938	0.039	(-0.022, 0.013)
Arginine	Lognormal	0.003	(-0.010, 0.016)	0.669	0.938	0.032	(-0.010, 0.016)
D-.alpha.-Cyclohexylglycine	Lognormal	-0.006	(-0.034, 0.022)	0.676	0.938	0.036	(-0.032, 0.023)
N-Acetyl-D-norleucine	Lognormal	0.005	(-0.018, 0.028)	0.677	0.938	0.022	(-0.019, 0.026)
Meloxicam	Lognormal	0.024	(-0.089, 0.136)	0.682	0.939	0.040	(-0.091, 0.142)
Carbamazepine	Lognormal	-0.011	(-0.064, 0.042)	0.684	0.939	0.037	(-0.066, 0.044)
Acetyl-DL-carnitine	Lognormal	0.003	(-0.012, 0.018)	0.689	0.942	0.038	(-0.012, 0.019)
Cotinine N-.beta.-D-glucuronide	Lognormal	0.014	(-0.054, 0.082)	0.689	0.942	0.035	(-0.058, 0.082)
Ranitidine-S-oxide	Lognormal	0.012	(-0.047, 0.071)	0.693	0.945	0.035	(-0.047, 0.072)
2,2-Bishydroxymethyl]-2,2',2''-nitrioltriethanol	Lognormal	0.006	(-0.023, 0.035)	0.694	0.945	0.037	(-0.023, 0.034)
D-Pyroglutamic acid	Lognormal	-0.001	(-0.007, 0.004)	0.701	0.945	0.038	(-0.007, 0.004)
Dexpanthenol	Lognormal	-0.006	(-0.038, 0.025)	0.701	0.945	0.036	(-0.038, 0.026)
Lysine	Lognormal	-0.002	(-0.013, 0.009)	0.704	0.946	0.025	(-0.014, 0.009)
Tapentadol-.beta.-D-glucuronide	Lognormal	-0.012	(-0.072, 0.049)	0.707	0.946	0.039	(-0.074, 0.048)
(2R)-3-Hydroxyisovalerylcarnitine	Lognormal	-0.003	(-0.019, 0.013)	0.715	0.948	0.035	(-0.019, 0.014)
1,2-Dimethylimidazole	Lognormal	0.004	(-0.016, 0.023)	0.718	0.948	0.035	(-0.016, 0.024)
N.epsilon.-Acetyl-L-lysine	Lognormal	-0.003	(-0.017, 0.012)	0.719	0.948	0.037	(-0.018, 0.012)
D-erythro-Sphingosine-1-phosphate	Lognormal	-0.004	(-0.028, 0.019)	0.727	0.948	0.037	(-0.028, 0.018)
6-Hydroxyflavone	Lognormal	0.007	(-0.033, 0.047)	0.727	0.948	0.034	(-0.035, 0.045)
Toradol	Lognormal	0.007	(-0.033, 0.047)	0.729	0.948	0.035	(-0.031, 0.046)
.beta.-Phenyl-.gamma.-aminobutyric acid	Lognormal	-0.003	(-0.023, 0.016)	0.731	0.948	0.033	(-0.023, 0.017)
Sulfamethoxazole	Lognormal	-0.015	(-0.103, 0.072)	0.731	0.948	0.035	(-0.101, 0.073)
Levocetirizine;	Lognormal	0.012	(-0.059, 0.084)	0.736	0.952	0.039	(-0.058, 0.085)
Norleucine	Lognormal	-0.002	(-0.013, 0.009)	0.741	0.954	0.037	(-0.013, 0.010)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
3-Methylxanthine	Lognormal	-0.007	(-0.048, 0.035)	0.754	0.955	0.034	(-0.051, 0.034)
Atenolol	Lognormal	0.006	(-0.030, 0.041)	0.756	0.955	0.036	(-0.028, 0.042)
Phenylacetylglutamine	Lognormal	-0.004	(-0.033, 0.024)	0.766	0.955	0.033	(-0.034, 0.023)
1-Acetyl-4-piperidinamine	Lognormal	0.006	(-0.033, 0.044)	0.769	0.955	0.035	(-0.034, 0.044)
Urocanic acid;	Lognormal	-0.003	(-0.021, 0.016)	0.770	0.955	0.035	(-0.021, 0.016)
Phenylalanine	Lognormal	-0.001	(-0.009, 0.007)	0.771	0.955	0.032	(-0.010, 0.006)
Modafinil	Lognormal	0.007	(-0.038, 0.051)	0.773	0.955	0.036	(-0.041, 0.049)
4-Aminomethylcyclohexanecarboxylic acid;	Lognormal	0.004	(-0.023, 0.031)	0.779	0.958	0.031	(-0.024, 0.032)
Theanine;	Lognormal	-0.004	(-0.036, 0.027)	0.783	0.958	0.032	(-0.034, 0.029)
Triptolide	Lognormal	-0.003	(-0.024, 0.018)	0.783	0.958	0.036	(-0.024, 0.019)
3-(1-Pyrazolyl)-alanine	Lognormal	0.010	(-0.059, 0.078)	0.784	0.958	0.035	(-0.054, 0.076)
Pyridoxal	Lognormal	0.003	(-0.019, 0.025)	0.790	0.958	0.035	(-0.019, 0.025)
Glycodeoxycholic acid	Lognormal	0.005	(-0.034, 0.044)	0.790	0.958	0.034	(-0.036, 0.042)
2-Amino-1-phenylethanol	Lognormal	-0.001	(-0.009, 0.007)	0.791	0.958	0.035	(-0.009, 0.008)
Creatinine	Lognormal	-0.001	(-0.007, 0.005)	0.792	0.958	0.031	(-0.007, 0.005)
3-Hydroxybutyrylcarnitine	Lognormal	-0.004	(-0.033, 0.026)	0.798	0.960	0.036	(-0.033, 0.024)
1-Oleoyl-2-acetyl-sn-glycerol	Lognormal	-0.005	(-0.041, 0.032)	0.801	0.961	0.036	(-0.041, 0.032)
Glutamine	Lognormal	-0.001	(-0.006, 0.005)	0.801	0.961	0.034	(-0.007, 0.005)
7.alpha.-Hydroxy-3-oxo-4-cholestenoic acid	Lognormal	-0.003	(-0.023, 0.018)	0.806	0.963	0.033	(-0.024, 0.017)
Ondansetron	Lognormal	0.002	(-0.014, 0.018)	0.811	0.963	0.031	(-0.015, 0.018)
Pyridoxine;	Lognormal	0.004	(-0.029, 0.037)	0.811	0.963	0.036	(-0.030, 0.036)
Isoleucine	Lognormal	0.001	(-0.010, 0.012)	0.818	0.968	0.034	(-0.009, 0.012)
L-Carnitine	Lognormal	-0.001	(-0.012, 0.010)	0.824	0.972	0.034	(-0.012, 0.010)
Pantothenic acid	Lognormal	0.002	(-0.020, 0.024)	0.830	0.976	0.038	(-0.018, 0.026)
Atorvastatin	Lognormal	0.002	(-0.017, 0.021)	0.860	0.981	0.035	(-0.018, 0.021)
R-(-)-O-Desmethylvenlafaxine	Lognormal	-0.004	(-0.048, 0.040)	0.861	0.981	0.036	(-0.049, 0.038)
Diphenhydramine	Lognormal	-0.002	(-0.024, 0.020)	0.862	0.981	0.034	(-0.025, 0.019)
Trileptal	Lognormal	0.002	(-0.023, 0.028)	0.862	0.981	0.036	(-0.025, 0.027)
Avobenzon	Lognormal	0.002	(-0.022, 0.026)	0.862	0.981	0.032	(-0.022, 0.026)
Gly-Pro-Arg	Lognormal	0.006	(-0.059, 0.070)	0.862	0.981	0.038	(-0.057, 0.067)
Oleoyl-L-carnitine	Lognormal	-0.003	(-0.038, 0.032)	0.862	0.981	0.036	(-0.038, 0.032)
Tauroursodeoxycholic acid	Lognormal	0.003	(-0.030, 0.036)	0.865	0.981	0.034	(-0.031, 0.036)
2,2',2''-Nitrilotriethanol	Lognormal	0.002	(-0.024, 0.028)	0.870	0.984	0.036	(-0.023, 0.029)
Methionine	Lognormal	0.001	(-0.009, 0.011)	0.872	0.984	0.034	(-0.010, 0.011)
2-Hydroxyibuprofen	Lognormal	-0.003	(-0.036, 0.030)	0.878	0.984	0.037	(-0.037, 0.029)
1-Stearoyl-2-arachidonoyl-sn-glycero-3-phospho-(1'-myo-inositol)	Lognormal	0.007	(-0.082, 0.095)	0.882	0.984	0.035	(-0.081, 0.098)
Palmitamide	Lognormal	0.003	(-0.034, 0.040)	0.884	0.984	0.037	(-0.033, 0.040)
Lansoprazole	Lognormal	-0.007	(-0.104, 0.090)	0.886	0.984	0.035	(-0.109, 0.089)
1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	Lognormal	0.003	(-0.035, 0.040)	0.889	0.984	0.029	(-0.034, 0.039)
1-Oleoyl-sn-glycero-3-phosphoethanolamine	Lognormal	-0.002	(-0.039, 0.034)	0.894	0.984	0.032	(-0.038, 0.034)
Isopentenyladenine	Lognormal	-0.001	(-0.010, 0.009)	0.894	0.984	0.035	(-0.010, 0.009)
1-Stearoyl-2-arachidonoyl-sn-glycero-3-phosphoserine	Lognormal	-0.005	(-0.087, 0.077)	0.900	0.984	0.028	(-0.084, 0.082)
Creatine	Lognormal	0.001	(-0.014, 0.016)	0.905	0.984	0.036	(-0.013, 0.017)
3-Aminoquinoline	Lognormal	0.002	(-0.040, 0.045)	0.910	0.985	0.027	(-0.040, 0.043)
5'-S-Methyl-5'-thioadenosine	Lognormal	0.003	(-0.063, 0.069)	0.925	0.990	0.028	(-0.060, 0.073)
Hypoxanthine	Lognormal	0.001	(-0.016, 0.018)	0.932	0.990	0.032	(-0.017, 0.017)
Glycocholic acid	Lognormal	0.001	(-0.034, 0.037)	0.935	0.991	0.032	(-0.033, 0.037)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Ile-Glu-Arg	Lognormal	-0.002	(-0.068, 0.063)	0.941	0.991	0.035	(-0.066, 0.064)
Moxonidine	Lognormal	0.001	(-0.025, 0.027)	0.952	0.997	0.035	(-0.026, 0.027)
N-Acetylalanine	Lognormal	0.002	(-0.060, 0.064)	0.956	0.998	0.033	(-0.057, 0.062)
Adenosine	Lognormal	0.001	(-0.028, 0.030)	0.965	0.998	0.035	(-0.029, 0.031)
Pipecolic acid	Lognormal	0.001	(-0.040, 0.041)	0.968	0.998	0.032	(-0.044, 0.041)
Scopoletin	Lognormal	0.001	(-0.074, 0.076)	0.972	0.998	0.025	(-0.073, 0.078)
Benthiavalicarb-isopropyl	Lognormal	0.000	(-0.036, 0.035)	0.982	0.998	0.033	(-0.036, 0.034)
Mefenorex	Lognormal	0.000	(-0.039, 0.038)	0.983	0.998	0.029	(-0.039, 0.039)
Ethylidethanolamine	Lognormal	0.000	(-0.027, 0.027)	0.991	0.998	0.035	(-0.028, 0.026)
Benzophenone-3	Lognormal	0.000	(-0.059, 0.059)	0.999	0.999	0.032	(-0.057, 0.059)
Complex Lipids (CL)							
PC (p-34:2)/PC (o-34:3) - ESI(+)	Lognormal	-0.019	(-0.028, -0.010)	0.000	0.076	16.961	(-0.029, -0.010)
PC (36:2)	Lognormal	-0.008	(-0.012, -0.004)	0.000	0.076	8.626	(-0.012, -0.004)
PC (p-34:1)/PC (o-34:2)	Lognormal	-0.022	(-0.033, -0.010)	0.000	0.076	30.007	(-0.034, -0.010)
PE (p-36:2)/PE (o-36:3) - ESI(+)	Lognormal	-0.029	(-0.045, -0.013)	0.000	0.081	6.915	(-0.044, -0.013)
PC (p-36:4)/PC (o-36:5) - ESI(-)	Lognormal	-0.020	(-0.032, -0.008)	0.001	0.218	6.200	(-0.031, -0.008)
PC (p-36:1)/PC (o-36:2)	Lognormal	-0.052	(-0.084, -0.020)	0.002	0.218	4.636	(-0.085, -0.022)
PC (36:4) A - ESI(+)	Lognormal	-0.017	(-0.028, -0.007)	0.002	0.218	3.025	(-0.027, -0.007)
PC (p-34:2)/PC (o-34:3) - ESI(-)	Lognormal	-0.019	(-0.030, -0.007)	0.002	0.248	3.502	(-0.031, -0.007)
PC 34:4e	Lognormal	-0.023	(-0.037, -0.008)	0.003	0.248	3.559	(-0.037, -0.009)
PE (p-34:2)/PE (o-34:3)	Lognormal	-0.036	(-0.060, -0.012)	0.004	0.310	2.620	(-0.060, -0.013)
PC (36:4) A - ESI(-)	Lognormal	-0.018	(-0.030, -0.006)	0.005	0.310	2.130	(-0.030, -0.006)
PC (p-34:1)/PC (o-34:2) A	Lognormal	-0.025	(-0.042, -0.008)	0.005	0.310	1.458	(-0.042, -0.008)
PC (32:2) - ESI(-)	Lognormal	-0.024	(-0.040, -0.007)	0.006	0.310	1.525	(-0.041, -0.007)
PC (34:4) - ESI(-)	Lognormal	-0.030	(-0.053, -0.008)	0.009	0.310	1.080	(-0.055, -0.008)
TG (62:4)	Lognormal	-0.035	(-0.061, -0.009)	0.010	0.310	0.863	(-0.061, -0.007)
PE (p-36:4)/PE (o-36:5) - ESI(+)	Lognormal	-0.018	(-0.031, -0.004)	0.010	0.310	0.778	(-0.031, -0.005)
LPC (18:3)	Lognormal	-0.024	(-0.043, -0.006)	0.010	0.310	0.976	(-0.042, -0.006)
SM (d43:1) - ESI(-)	Lognormal	-0.032	(-0.056, -0.008)	0.011	0.310	0.889	(-0.058, -0.008)
LPC (14:0) - ESI(+)	Lognormal	-0.021	(-0.036, -0.005)	0.011	0.310	0.909	(-0.036, -0.005)
PE (p-36:4)/PE (o-36:5) - ESI(-)	Lognormal	-0.020	(-0.035, -0.005)	0.012	0.310	0.614	(-0.035, -0.004)
PE (p-36:2)/PE (o-36:3) - ESI(-)	Lognormal	-0.026	(-0.046, -0.006)	0.012	0.310	0.805	(-0.046, -0.005)
PC (p-36:2)/PC (o-36:3)	Lognormal	-0.016	(-0.029, -0.004)	0.012	0.310	0.903	(-0.029, -0.004)
PC (p-36:3)/PC (o-36:4) - ESI(-)	Lognormal	-0.013	(-0.024, -0.003)	0.012	0.310	0.736	(-0.023, -0.002)
LPC (18:0) B - ESI(-)	Lognormal	-0.014	(-0.025, -0.003)	0.013	0.310	0.830	(-0.025, -0.003)
LPC (18:0) A - ESI(-)	Lognormal	-0.019	(-0.034, -0.004)	0.013	0.310	0.880	(-0.035, -0.005)
SM (d40:3)	Lognormal	-0.026	(-0.046, -0.006)	0.013	0.310	1.103	(-0.045, -0.007)
SM (d39:1) - ESI(-)	Lognormal	-0.015	(-0.027, -0.003)	0.013	0.310	0.723	(-0.027, -0.003)
PC (p-36:4)/PC (o-36:5) - ESI(+)	Lognormal	-0.010	(-0.018, -0.002)	0.014	0.310	0.750	(-0.018, -0.002)
PE (p-38:5)/PE (o-38:6) - ESI(-)	Lognormal	-0.019	(-0.034, -0.004)	0.014	0.310	0.951	(-0.034, -0.005)
PC (p-36:3)/PC (o-36:4) - ESI(+)	Lognormal	-0.011	(-0.019, -0.002)	0.015	0.310	0.697	(-0.019, -0.002)
SM (d40:1) - ESI(-)	Lognormal	-0.011	(-0.020, -0.002)	0.015	0.310	0.745	(-0.019, -0.002)
Ceramide (d42:1) - ESI (+)	Lognormal	-0.009	(-0.016, -0.002)	0.015	0.310	0.947	(-0.015, -0.002)
LPC (18:2) - ESI(-)	Lognormal	-0.017	(-0.030, -0.003)	0.016	0.310	0.720	(-0.030, -0.003)
SM (d32:1) - ESI(-)	Lognormal	-0.013	(-0.024, -0.003)	0.016	0.310	0.795	(-0.023, -0.002)
PE (p-38:5)/PE (o-38:6) - ESI(+)	Lognormal	-0.014	(-0.026, -0.003)	0.016	0.310	0.660	(-0.026, -0.003)
CE (18:3)	Lognormal	-0.018	(-0.033, -0.003)	0.017	0.310	0.690	(-0.032, -0.003)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
Ceramide (d42:2) B - ESI (+)	Lognormal	-0.011	(-0.020, -0.002)	0.018	0.311	0.514	(-0.020, -0.002)
PC (p-38:4)/PC (o-38:5) A	Lognormal	-0.011	(-0.021, -0.002)	0.019	0.327	0.453	(-0.021, -0.002)
Ceramide (d42:1) - ESI(-)	Lognormal	-0.011	(-0.019, -0.002)	0.020	0.327	0.496	(-0.019, -0.002)
PE (p-38:4)/PE (o-38:5)	Lognormal	-0.016	(-0.030, -0.003)	0.020	0.327	0.567	(-0.029, -0.003)
LPC (16:0) - ESI(-)	Lognormal	-0.010	(-0.018, -0.002)	0.021	0.327	0.530	(-0.018, -0.002)
Ceramide (d41:1) - ESI(-)	Lognormal	-0.013	(-0.023, -0.002)	0.021	0.327	0.480	(-0.024, -0.002)
PC (34:2) - ESI(+)	Lognormal	-0.004	(-0.007, -0.001)	0.021	0.327	0.553	(-0.007, -0.001)
LPC (18:2) - ESI(+)	Lognormal	-0.013	(-0.024, -0.002)	0.022	0.327	0.460	(-0.024, -0.002)
PC (34:2) - ESI(-)	Lognormal	-0.008	(-0.015, -0.001)	0.022	0.327	0.578	(-0.015, -0.001)
PE (p-36:1)/PE (o-36:2) - ESI(+)	Lognormal	-0.020	(-0.038, -0.003)	0.023	0.336	0.558	(-0.038, -0.003)
CE (20:2)	Lognormal	-0.022	(-0.042, -0.003)	0.024	0.339	0.437	(-0.043, -0.004)
LPC (20:2) - ESI(+)	Lognormal	-0.037	(-0.069, -0.005)	0.026	0.351	0.455	(-0.067, -0.004)
PC (34:3)	Lognormal	-0.014	(-0.027, -0.002)	0.026	0.351	0.383	(-0.028, -0.002)
PC (p-38:4)/PC (o-38:5) B	Lognormal	-0.012	(-0.022, -0.001)	0.028	0.352	0.413	(-0.022, -0.001)
Ceramide (d40:1)	Lognormal	-0.010	(-0.018, -0.001)	0.028	0.352	0.391	(-0.018, -0.001)
TG (50:0)	Lognormal	-0.024	(-0.046, -0.003)	0.029	0.352	0.431	(-0.045, -0.003)
LPE (20:4) - ESI(-)	Lognormal	-0.019	(-0.036, -0.002)	0.030	0.352	0.323	(-0.037, -0.002)
TG (53:0)	Lognormal	-0.018	(-0.033, -0.002)	0.030	0.352	0.403	(-0.033, -0.002)
LPC (20:3) - ESI(-)	Lognormal	-0.021	(-0.041, -0.002)	0.030	0.352	0.362	(-0.041, -0.002)
PC (p-38:3)/PC (o-38:4) - ESI(-)	Lognormal	-0.013	(-0.025, -0.001)	0.030	0.352	0.353	(-0.025, -0.002)
TG (56:6)	Lognormal	0.009	(0.001, 0.017)	0.030	0.352	0.364	(0.001, 0.018)
SM (d36:3) - ESI(-)	Lognormal	-0.019	(-0.035, -0.002)	0.031	0.352	0.355	(-0.036, -0.001)
PC (38:4) A - ESI(-)	Lognormal	-0.010	(-0.019, -0.001)	0.032	0.352	0.376	(-0.018, -0.001)
Ceramide (d39:1)	Lognormal	-0.019	(-0.035, -0.002)	0.032	0.352	0.394	(-0.035, -0.002)
PC (36:5) A	Lognormal	-0.037	(-0.072, -0.003)	0.034	0.362	0.322	(-0.071, -0.001)
CE (18:2)	Lognormal	-0.008	(-0.015, -0.001)	0.034	0.362	0.331	(-0.015, 0.000)
PC (32:2) - ESI(+)	Lognormal	-0.016	(-0.031, -0.001)	0.035	0.368	0.321	(-0.031, -0.001)
PC (34:3) B	Lognormal	-0.011	(-0.020, -0.001)	0.036	0.369	0.316	(-0.020, -0.001)
PC (34:3) C	Lognormal	-0.015	(-0.029, -0.001)	0.037	0.369	0.386	(-0.029, -0.001)
PC (36:5)A	Lognormal	-0.020	(-0.038, -0.001)	0.038	0.373	0.310	(-0.038, -0.001)
TG (55:6)	Lognormal	0.018	(0.001, 0.035)	0.039	0.373	0.259	(-0.001, 0.035)
SM (d30:1) - ESI(-)	Lognormal	-0.028	(-0.055, -0.002)	0.039	0.373	0.285	(-0.056, -0.002)
PC (p-38:3)/PC (o-38:4) A - ESI(+)	Lognormal	-0.010	(-0.020, -0.001)	0.039	0.373	0.269	(-0.020, -0.001)
SM (d33:1) - ESI(-)	Lognormal	-0.011	(-0.022, -0.001)	0.040	0.373	0.322	(-0.023, -0.001)
LPE (18:2) - ESI(-)	Lognormal	-0.022	(-0.044, -0.001)	0.044	0.381	0.298	(-0.045, -0.002)
Ceramide (d43:1)	Lognormal	-0.029	(-0.057, -0.001)	0.044	0.381	0.241	(-0.056, 0.001)
SM (d40:2) B - ESI(-)	Lognormal	-0.010	(-0.020, 0.000)	0.045	0.382	0.318	(-0.020, -0.001)
PC (33:2) - ESI(-)	Lognormal	-0.016	(-0.032, 0.000)	0.045	0.382	0.253	(-0.032, 0.000)
PI (38:4)/PI (18:0-20:4)	Lognormal	-0.009	(-0.018, 0.000)	0.046	0.383	0.302	(-0.018, 0.000)
SM (d42:1) - ESI(-)	Lognormal	-0.009	(-0.017, 0.000)	0.049	0.395	0.253	(-0.017, 0.000)
LPE (18:0)	Lognormal	-0.013	(-0.027, 0.000)	0.049	0.395	0.278	(-0.026, 0.000)
PC (37:2) - ESI(+)	Lognormal	-0.009	(-0.018, 0.000)	0.050	0.397	0.250	(-0.019, -0.001)
LPC (14:0) - ESI(-)	Lognormal	-0.026	(-0.052, 0.000)	0.052	0.402	0.211	(-0.050, 0.001)
SM (d34:2) - ESI(-)	Lognormal	-0.008	(-0.015, 0.000)	0.052	0.402	0.269	(-0.015, 0.000)
TG (58:8)	Lognormal	0.018	(0.000, 0.036)	0.053	0.402	0.236	(0.001, 0.036)
TG (58:9)	Lognormal	0.017	(0.000, 0.034)	0.054	0.402	0.203	(0.000, 0.034)
PC (36:3) A - ESI(+)	Lognormal	-0.007	(-0.014, 0.000)	0.055	0.402	0.218	(-0.014, 0.000)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
PC (38:6) A - ESI(+)	Lognormal	-0.008	(-0.016, 0.000)	0.056	0.402	0.223	(-0.016, 0.000)
PE (p-34:1)/PE (o-34:2) - ESI(+)	Lognormal	-0.015	(-0.029, 0.000)	0.057	0.405	0.205	(-0.030, 0.001)
PE (p-36:1)/PE (o-36:2) - ESI(-)	Lognormal	-0.026	(-0.052, 0.001)	0.058	0.405	0.219	(-0.051, 0.000)
SM (d40:1) - ESI(+)	Lognormal	-0.006	(-0.012, 0.000)	0.059	0.405	0.249	(-0.011, 0.000)
PC (p-38:3)/PC (o-38:4) B - ESI(+)	Lognormal	-0.010	(-0.021, 0.000)	0.059	0.405	0.197	(-0.021, 0.000)
TG (56:7) B	Lognormal	0.016	(-0.001, 0.033)	0.059	0.405	0.210	(-0.001, 0.033)
PC (o-34:0)	Lognormal	-0.014	(-0.028, 0.000)	0.059	0.405	0.235	(-0.028, -0.001)
AC (10:1)	Lognormal	-0.020	(-0.040, 0.001)	0.060	0.407	0.237	(-0.041, -0.001)
LPE (18:2) - ESI(+)	Lognormal	-0.017	(-0.034, 0.001)	0.061	0.408	0.233	(-0.035, -0.001)
PC (36:4) B - ESI(-)	Lognormal	-0.006	(-0.013, 0.000)	0.062	0.414	0.213	(-0.014, 0.000)
SM (d40:2) B - ESI(+)	Lognormal	-0.006	(-0.013, 0.000)	0.064	0.424	0.188	(-0.012, 0.001)
PC (34:4) - ESI(+)	Lognormal	-0.016	(-0.033, 0.001)	0.065	0.424	0.197	(-0.033, 0.001)
FA (16:1) (palmitoleic acid)	Lognormal	0.014	(-0.001, 0.028)	0.066	0.426	0.187	(-0.001, 0.027)
PC (40:8) - ESI(-)	Lognormal	-0.014	(-0.030, 0.001)	0.070	0.447	0.171	(-0.030, 0.001)
TG (60:11)	Lognormal	0.026	(-0.002, 0.055)	0.071	0.449	0.159	(-0.004, 0.055)
PC (38:3) - ESI(-)	Lognormal	-0.011	(-0.023, 0.001)	0.073	0.460	0.185	(-0.022, 0.001)
LPC (p-16:0)/LPC (o-16:1)	Lognormal	-0.012	(-0.025, 0.001)	0.075	0.471	0.173	(-0.025, 0.001)
SM (d39:1) - ESI(+)	Lognormal	-0.009	(-0.019, 0.001)	0.076	0.472	0.163	(-0.019, 0.001)
LPC (16:1) - ESI(-)	Lognormal	-0.016	(-0.033, 0.002)	0.077	0.473	0.175	(-0.033, 0.001)
TG (54:7) B	Lognormal	0.015	(-0.002, 0.031)	0.081	0.479	0.176	(-0.001, 0.030)
PE (p-40:4)/PE (o-40:5) A	Lognormal	-0.019	(-0.040, 0.002)	0.082	0.479	0.111	(-0.041, 0.003)
PC (p-32:1)/PC (o-32:2)	Lognormal	-0.009	(-0.020, 0.001)	0.083	0.480	0.152	(-0.020, 0.001)
SM (d30:1) - ESI(+)	Lognormal	-0.019	(-0.040, 0.002)	0.084	0.486	0.157	(-0.040, 0.002)
PE (36:2)	Lognormal	-0.018	(-0.039, 0.002)	0.085	0.488	0.163	(-0.038, 0.002)
PC (37:5)	Lognormal	0.014	(-0.002, 0.030)	0.087	0.494	0.165	(-0.001, 0.031)
GlcCer (d42:2) - ESI(+)	Lognormal	0.011	(-0.002, 0.024)	0.087	0.494	0.143	(-0.001, 0.024)
PE (p-40:4)/PE (o-40:5) B	Lognormal	-0.011	(-0.024, 0.002)	0.092	0.515	0.115	(-0.025, 0.001)
LPC (18:0) - ESI(+)	Lognormal	-0.008	(-0.017, 0.001)	0.093	0.516	0.162	(-0.017, 0.001)
DG (38:6)	Lognormal	0.014	(-0.002, 0.031)	0.094	0.516	0.138	(-0.001, 0.031)
SM (d34:1) - ESI(-)	Lognormal	-0.006	(-0.012, 0.001)	0.095	0.516	0.128	(-0.012, 0.001)
PC (p-38:4)/PC (o-38:5) B	Lognormal	-0.015	(-0.032, 0.002)	0.095	0.516	0.148	(-0.032, 0.002)
TG (54:6) C	Lognormal	0.009	(-0.002, 0.021)	0.098	0.522	0.124	(-0.002, 0.020)
LPC (20:2) - ESI(-)	Lognormal	-0.012	(-0.026, 0.002)	0.102	0.537	0.123	(-0.027, 0.002)
LPC (20:3) - ESI(+)	Lognormal	-0.011	(-0.023, 0.002)	0.103	0.537	0.117	(-0.024, 0.002)
SM (d42:1) - ESI(+)	Lognormal	-0.006	(-0.013, 0.001)	0.104	0.542	0.138	(-0.013, 0.001)
PC (35:1) - ESI(+)	Lognormal	0.006	(-0.001, 0.013)	0.107	0.546	0.129	(-0.001, 0.013)
FA (24:0) (lignoceric acid)	Lognormal	-0.009	(-0.021, 0.002)	0.107	0.546	0.126	(-0.021, 0.002)
LPC (18:1) - ESI(-)	Lognormal	-0.010	(-0.022, 0.002)	0.111	0.557	0.123	(-0.022, 0.002)
PC (p-38:4)/PC (o-38:5) A	Lognormal	-0.006	(-0.013, 0.001)	0.112	0.557	0.120	(-0.013, 0.001)
SM (d32:1) - ESI(+)	Lognormal	-0.008	(-0.019, 0.002)	0.113	0.557	0.134	(-0.019, 0.001)
Ceramide (d33:1)	Lognormal	-0.010	(-0.023, 0.002)	0.114	0.557	0.121	(-0.023, 0.002)
SM (d38:2) - ESI(-)	Lognormal	-0.010	(-0.022, 0.002)	0.116	0.560	0.115	(-0.022, 0.002)
TG (56:8) B	Lognormal	0.015	(-0.004, 0.035)	0.116	0.560	0.109	(-0.004, 0.035)
PC (34:0) - ESI(-)	Lognormal	-0.008	(-0.017, 0.002)	0.119	0.560	0.126	(-0.017, 0.002)
PC (p-38:5)/PC (o-38:6) B	Lognormal	-0.007	(-0.015, 0.002)	0.119	0.560	0.114	(-0.015, 0.002)
Ceramide (d38:1) - ESI(+)	Lognormal	-0.007	(-0.016, 0.002)	0.120	0.560	0.108	(-0.016, 0.002)
PC (p-40:1)/PC (o-40:2)	Lognormal	0.015	(-0.004, 0.033)	0.120	0.560	0.101	(-0.004, 0.033)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
PC (p-40:3)/PC (o-40:4)	Lognormal	-0.013	(-0.030, 0.003)	0.121	0.560	0.126	(-0.031, 0.002)
SM (d38:1)	Lognormal	-0.005	(-0.011, 0.001)	0.123	0.568	0.124	(-0.012, 0.001)
Ceramide (d41:1) - ESI(+)	Lognormal	-0.008	(-0.018, 0.002)	0.130	0.594	0.105	(-0.018, 0.002)
TG (48:4) A	Lognormal	-0.020	(-0.046, 0.006)	0.133	0.605	0.100	(-0.046, 0.006)
PC 40:5e	Lognormal	-0.007	(-0.016, 0.002)	0.134	0.605	0.100	(-0.016, 0.002)
SM (d36:0) - ESI(+)	Lognormal	0.012	(-0.004, 0.027)	0.138	0.612	0.109	(-0.004, 0.027)
AC (14:2)	Lognormal	-0.018	(-0.041, 0.006)	0.139	0.612	0.106	(-0.040, 0.006)
PC (33:2) - ESI(+)	Lognormal	-0.007	(-0.016, 0.002)	0.140	0.612	0.084	(-0.016, 0.002)
PC (38:6) B - ESI(+)	Lognormal	0.004	(-0.001, 0.010)	0.140	0.612	0.100	(-0.002, 0.010)
PC (36:5) D	Lognormal	0.013	(-0.004, 0.031)	0.143	0.619	0.089	(-0.004, 0.031)
LPE (16:0)	Lognormal	-0.016	(-0.038, 0.006)	0.145	0.622	0.102	(-0.038, 0.005)
TG (48:0)	Lognormal	-0.016	(-0.037, 0.005)	0.148	0.628	0.096	(-0.037, 0.004)
SM (d44:2)	Lognormal	0.011	(-0.004, 0.026)	0.151	0.635	0.091	(-0.005, 0.025)
TG (56:5) A	Lognormal	0.010	(-0.004, 0.023)	0.154	0.641	0.094	(-0.003, 0.023)
SM (d43:2) - ESI(-)	Lognormal	-0.016	(-0.038, 0.006)	0.157	0.646	0.094	(-0.038, 0.006)
PC (36:3) B - ESI(-)	Lognormal	-0.006	(-0.015, 0.002)	0.159	0.648	0.091	(-0.015, 0.002)
TG (56:5) B	Lognormal	0.009	(-0.003, 0.021)	0.160	0.648	0.091	(-0.003, 0.021)
PC (37:6)	Lognormal	0.012	(-0.005, 0.029)	0.162	0.650	0.089	(-0.004, 0.029)
Ceramide (d42:2) B - ESI(-)	Lognormal	-0.010	(-0.024, 0.004)	0.164	0.652	0.093	(-0.024, 0.004)
FA (20:5) (eicosapentaenoic acid)	Lognormal	0.018	(-0.007, 0.043)	0.168	0.659	0.082	(-0.006, 0.043)
PC (40:5) B - ESI(-)	Lognormal	-0.016	(-0.038, 0.007)	0.169	0.659	0.081	(-0.038, 0.007)
PC (36:3) A - ESI(-)	Lognormal	-0.007	(-0.017, 0.003)	0.171	0.659	0.097	(-0.017, 0.003)
PE (p-34:1)/PE (o-34:2) - ESI(-)	Lognormal	-0.012	(-0.028, 0.005)	0.173	0.661	0.089	(-0.028, 0.006)
Ceramide (d38:1) - ESI(-)	Lognormal	-0.009	(-0.022, 0.004)	0.176	0.664	0.088	(-0.021, 0.005)
LPC (o-16:0)	Lognormal	-0.010	(-0.024, 0.004)	0.176	0.664	0.080	(-0.023, 0.005)
TG (46:0)	Lognormal	-0.024	(-0.059, 0.011)	0.178	0.664	0.083	(-0.061, 0.008)
PE (p-38:6)/PE (o-38:7)	Lognormal	-0.013	(-0.031, 0.006)	0.179	0.664	0.083	(-0.030, 0.006)
FA (18:1) (oleic acid)	Lognormal	0.006	(-0.003, 0.015)	0.180	0.665	0.092	(-0.003, 0.014)
TG (60:6)	Lognormal	0.015	(-0.007, 0.036)	0.185	0.675	0.080	(-0.009, 0.035)
TG (58:6)	Lognormal	0.008	(-0.004, 0.019)	0.187	0.678	0.073	(-0.004, 0.019)
TG (49:2)	Lognormal	0.014	(-0.007, 0.035)	0.188	0.678	0.085	(-0.006, 0.035)
PC (40:7) A - ESI(+)	Lognormal	-0.007	(-0.018, 0.003)	0.189	0.678	0.081	(-0.018, 0.004)
SM (d42:2)	Lognormal	0.005	(-0.002, 0.012)	0.189	0.678	0.070	(-0.002, 0.012)
PE (36:3)	Lognormal	-0.020	(-0.049, 0.010)	0.190	0.678	0.089	(-0.049, 0.011)
PC (40:5) B - ESI(+)	Lognormal	-0.009	(-0.023, 0.004)	0.192	0.678	0.079	(-0.023, 0.005)
PC (38:3) - ESI(+)	Lognormal	-0.006	(-0.015, 0.003)	0.193	0.678	0.080	(-0.015, 0.003)
GlcCer (d14:1(4E)/20:0(2OH))	Lognormal	-0.013	(-0.032, 0.006)	0.193	0.678	0.078	(-0.033, 0.005)
PE (38:2)	Lognormal	-0.012	(-0.031, 0.006)	0.194	0.678	0.081	(-0.031, 0.006)
PC (42:10)	Lognormal	0.013	(-0.007, 0.033)	0.196	0.682	0.069	(-0.006, 0.032)
TG (46:2)	Lognormal	-0.020	(-0.051, 0.010)	0.197	0.684	0.082	(-0.051, 0.012)
LPC (20:4)	Lognormal	-0.007	(-0.018, 0.004)	0.200	0.687	0.073	(-0.019, 0.004)
LPC (22:4)	Lognormal	-0.016	(-0.041, 0.009)	0.201	0.687	0.079	(-0.042, 0.008)
PC (p-42:5)/PC (o-42:6) A	Lognormal	-0.008	(-0.021, 0.004)	0.202	0.687	0.078	(-0.021, 0.005)
PC (30:0)	Lognormal	-0.009	(-0.023, 0.005)	0.202	0.687	0.069	(-0.024, 0.004)
AC (12:0)	Lognormal	-0.013	(-0.033, 0.007)	0.206	0.691	0.080	(-0.034, 0.006)
PC (37:2) - ESI(-)	Lognormal	-0.014	(-0.036, 0.008)	0.207	0.692	0.083	(-0.037, 0.008)
FA (14:1) (physeteric acid)	Lognormal	0.012	(-0.007, 0.030)	0.208	0.692	0.074	(-0.006, 0.031)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
TG (56:8) A	Lognormal	0.009	(-0.005, 0.023)	0.210	0.696	0.071	(-0.006, 0.022)
CE (20:3)	Lognormal	-0.007	(-0.019, 0.004)	0.211	0.696	0.074	(-0.019, 0.005)
PE (p-38:3)/PE (o-38:4)	Lognormal	-0.016	(-0.041, 0.009)	0.212	0.698	0.072	(-0.042, 0.008)
Ceramide (d44:1)	Lognormal	-0.017	(-0.043, 0.010)	0.215	0.698	0.070	(-0.042, 0.011)
TG (60:12)	Lognormal	0.024	(-0.014, 0.061)	0.215	0.698	0.068	(-0.013, 0.059)
SM (d41:2) B - ESI(+)	Lognormal	-0.005	(-0.014, 0.003)	0.217	0.698	0.074	(-0.014, 0.003)
TG (56:5) C	Lognormal	0.007	(-0.004, 0.019)	0.219	0.698	0.074	(-0.004, 0.020)
LPC (16:0) - ESI(+)	Lognormal	-0.003	(-0.009, 0.002)	0.224	0.710	0.071	(-0.009, 0.002)
PE (p-40:4)/PE (o-40:5)	Lognormal	-0.010	(-0.026, 0.006)	0.230	0.716	0.052	(-0.027, 0.005)
Ceramide (d32:1)	Lognormal	-0.009	(-0.025, 0.006)	0.232	0.716	0.067	(-0.024, 0.006)
AC (12:1)	Lognormal	-0.012	(-0.031, 0.008)	0.237	0.724	0.068	(-0.032, 0.007)
CE (20:5)	Lognormal	0.013	(-0.009, 0.035)	0.238	0.724	0.060	(-0.008, 0.035)
TG (58:2)	Lognormal	-0.030	(-0.080, 0.020)	0.243	0.724	0.075	(-0.079, 0.021)
TG (54:5) B	Lognormal	0.006	(-0.004, 0.016)	0.243	0.724	0.065	(-0.005, 0.015)
PE (34:1)	Lognormal	-0.018	(-0.049, 0.013)	0.247	0.724	0.063	(-0.048, 0.014)
PC (38:2)	Lognormal	-0.008	(-0.021, 0.005)	0.248	0.724	0.069	(-0.021, 0.005)
PC (40:5) A - ESI(+)	Lognormal	0.005	(-0.003, 0.013)	0.249	0.724	0.073	(-0.004, 0.014)
Lactosylceramide (d18:1/24:1(15Z))	Lognormal	0.009	(-0.006, 0.025)	0.250	0.724	0.059	(-0.006, 0.025)
GlcCer (d38:1)	Lognormal	-0.008	(-0.021, 0.005)	0.251	0.724	0.069	(-0.021, 0.005)
PC (38:5) B - ESI(+)	Lognormal	0.006	(-0.004, 0.017)	0.252	0.724	0.063	(-0.005, 0.017)
SM (d41:3)	Lognormal	-0.005	(-0.014, 0.004)	0.254	0.724	0.068	(-0.014, 0.004)
TG (46:4) A	Lognormal	-0.022	(-0.058, 0.015)	0.255	0.724	0.065	(-0.057, 0.017)
TG (54:6) B	Lognormal	-0.020	(-0.054, 0.014)	0.255	0.724	0.070	(-0.053, 0.015)
TG (54:7) A	Lognormal	-0.012	(-0.034, 0.009)	0.261	0.726	0.063	(-0.034, 0.009)
PC (40:6)B	Lognormal	0.005	(-0.004, 0.015)	0.261	0.726	0.061	(-0.004, 0.014)
AC (10:0)	Lognormal	-0.017	(-0.047, 0.013)	0.262	0.726	0.067	(-0.048, 0.013)
SM (d32:2) - ESI(-)	Lognormal	-0.012	(-0.033, 0.009)	0.262	0.726	0.070	(-0.033, 0.009)
TG (48:5)	Lognormal	-0.017	(-0.047, 0.013)	0.264	0.726	0.063	(-0.047, 0.012)
PE (38:4)	Lognormal	-0.006	(-0.017, 0.005)	0.264	0.726	0.047	(-0.017, 0.005)
AC (18:0)	Lognormal	-0.007	(-0.020, 0.005)	0.265	0.726	0.055	(-0.019, 0.005)
DG (38:5)	Lognormal	0.007	(-0.005, 0.019)	0.271	0.731	0.055	(-0.005, 0.019)
PC (35:3)	Lognormal	-0.004	(-0.012, 0.003)	0.272	0.731	0.060	(-0.012, 0.003)
TG (44:0)	Lognormal	-0.019	(-0.054, 0.015)	0.273	0.731	0.062	(-0.055, 0.013)
LPE (20:4) - ESI(+)	Lognormal	-0.009	(-0.024, 0.007)	0.273	0.731	0.057	(-0.025, 0.006)
PC (p-44:4)/PC (o-44:5) - ESI(-)	Lognormal	-0.008	(-0.022, 0.006)	0.276	0.731	0.060	(-0.023, 0.006)
FA (17:0) (margaric acid)	Lognormal	0.003	(-0.003, 0.009)	0.276	0.731	0.059	(-0.003, 0.010)
PC (p-42:3)/PC (o-42:4)	Lognormal	-0.007	(-0.020, 0.006)	0.276	0.731	0.055	(-0.019, 0.006)
TG (48:3)	Lognormal	-0.012	(-0.033, 0.010)	0.278	0.733	0.061	(-0.034, 0.009)
PC (p-42:5)/PC (o-42:6)	Lognormal	-0.015	(-0.043, 0.012)	0.279	0.733	0.066	(-0.042, 0.014)
PC (40:4) - ESI(-)	Lognormal	-0.010	(-0.029, 0.008)	0.279	0.733	0.063	(-0.030, 0.007)
TG (48:4) B	Lognormal	-0.021	(-0.058, 0.017)	0.280	0.733	0.068	(-0.062, 0.016)
AC (18:2)	Lognormal	-0.008	(-0.023, 0.007)	0.282	0.737	0.059	(-0.022, 0.006)
FA (22:0) (behenic acid)	Lognormal	-0.007	(-0.019, 0.006)	0.289	0.748	0.051	(-0.020, 0.006)
PC (34:1)	Lognormal	0.002	(-0.002, 0.006)	0.291	0.750	0.057	(-0.002, 0.006)
CE (14:0)	Lognormal	-0.019	(-0.055, 0.016)	0.291	0.750	0.057	(-0.055, 0.018)
SM (d41:1) - ESI(+)	Lognormal	-0.004	(-0.012, 0.003)	0.294	0.752	0.060	(-0.012, 0.003)
GlcCer (d42:2) - ESI(-)	Lognormal	0.007	(-0.006, 0.019)	0.296	0.752	0.053	(-0.005, 0.019)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
SM (d32:0) - ESI(-)	Lognormal	-0.031	(-0.089, 0.027)	0.296	0.752	0.066	(-0.090, 0.027)
PC (36:3) B - ESI(+)	Lognormal	-0.005	(-0.014, 0.004)	0.296	0.752	0.059	(-0.013, 0.004)
TG (54:1)	Lognormal	-0.012	(-0.035, 0.011)	0.301	0.753	0.054	(-0.035, 0.010)
PC (34:3) A	Lognormal	-0.005	(-0.015, 0.005)	0.302	0.753	0.055	(-0.015, 0.005)
TG (42:0)	Lognormal	-0.019	(-0.056, 0.017)	0.305	0.757	0.060	(-0.054, 0.019)
SM (d42:3) - ESI(-)	Lognormal	-0.005	(-0.013, 0.004)	0.306	0.757	0.054	(-0.013, 0.004)
PE (34:2) - ESI(-)	Lognormal	-0.014	(-0.042, 0.013)	0.306	0.757	0.060	(-0.041, 0.013)
TG (50:4)	Lognormal	-0.008	(-0.022, 0.007)	0.310	0.757	0.060	(-0.023, 0.006)
PC (39:6)	Lognormal	0.008	(-0.007, 0.023)	0.311	0.757	0.050	(-0.008, 0.023)
FA (20:1) (eicosenoic acid)	Lognormal	0.006	(-0.005, 0.016)	0.314	0.757	0.056	(-0.005, 0.017)
FA (20:3) (homo-gamma-linolenic acid)	Lognormal	0.005	(-0.005, 0.014)	0.317	0.757	0.051	(-0.005, 0.014)
DG (36:2)	Lognormal	0.006	(-0.005, 0.016)	0.318	0.757	0.051	(-0.006, 0.016)
PC (p-32:0)/PC (o-32:1) - ESI(-)	Lognormal	-0.008	(-0.023, 0.007)	0.323	0.760	0.055	(-0.024, 0.008)
CE (22:2)	Lognormal	0.018	(-0.018, 0.054)	0.325	0.760	0.058	(-0.019, 0.053)
Ceramide (d42:0)	Lognormal	-0.008	(-0.023, 0.008)	0.325	0.760	0.049	(-0.024, 0.006)
TG (50:5)	Lognormal	-0.010	(-0.031, 0.010)	0.331	0.764	0.053	(-0.032, 0.010)
Cholesterol	Lognormal	-0.003	(-0.009, 0.003)	0.333	0.764	0.051	(-0.009, 0.003)
Ceramide (d34:1) - ESI(+)	Lognormal	0.004	(-0.004, 0.013)	0.334	0.764	0.054	(-0.004, 0.013)
FA (10:0) (capric acid)	Lognormal	0.012	(-0.013, 0.037)	0.335	0.764	0.051	(-0.012, 0.038)
SM (d34:0) - ESI(-)	Lognormal	-0.007	(-0.022, 0.007)	0.336	0.764	0.054	(-0.023, 0.007)
SM (d36:1) - ESI(-)	Lognormal	-0.004	(-0.014, 0.005)	0.336	0.764	0.057	(-0.013, 0.004)
TG (42:2)	Lognormal	-0.041	(-0.125, 0.043)	0.338	0.764	0.049	(-0.128, 0.043)
TG (51:5)	Lognormal	-0.009	(-0.028, 0.010)	0.338	0.764	0.051	(-0.027, 0.010)
DG (32:0)	Lognormal	0.008	(-0.009, 0.025)	0.340	0.765	0.056	(-0.009, 0.026)
PC (40:7) B - ESI(+)	Lognormal	0.004	(-0.005, 0.014)	0.343	0.769	0.051	(-0.005, 0.013)
FA (12:0) (lauric acid)	Lognormal	0.008	(-0.009, 0.024)	0.361	0.802	0.051	(-0.009, 0.023)
PC (28:0)	Lognormal	-0.018	(-0.058, 0.021)	0.364	0.805	0.051	(-0.059, 0.021)
PC (38:5) A	Lognormal	0.003	(-0.003, 0.008)	0.376	0.820	0.052	(-0.003, 0.009)
TG (46:1)	Lognormal	-0.015	(-0.048, 0.018)	0.376	0.820	0.047	(-0.047, 0.016)
TG (42:1)	Lognormal	-0.031	(-0.098, 0.037)	0.376	0.820	0.049	(-0.098, 0.038)
TG (44:1)	Lognormal	-0.020	(-0.063, 0.024)	0.379	0.820	0.052	(-0.066, 0.024)
Ceramide (d42:2) A - ESI (+)	Lognormal	0.004	(-0.004, 0.012)	0.379	0.820	0.046	(-0.005, 0.011)
TG (46:3) A	Lognormal	-0.019	(-0.061, 0.023)	0.380	0.820	0.049	(-0.058, 0.025)
SM (d43:1) - ESI(+)	Lognormal	-0.007	(-0.022, 0.009)	0.381	0.820	0.053	(-0.022, 0.009)
LPC (16:1) - ESI(+)	Lognormal	-0.005	(-0.016, 0.006)	0.381	0.820	0.052	(-0.017, 0.006)
PC (p-36:1)/PC (o-36:2) B	Lognormal	-0.006	(-0.021, 0.008)	0.389	0.825	0.048	(-0.022, 0.008)
TG (50:1)	Lognormal	-0.008	(-0.025, 0.010)	0.390	0.825	0.049	(-0.026, 0.009)
TG (42:3)	Lognormal	-0.017	(-0.056, 0.022)	0.390	0.825	0.050	(-0.055, 0.024)
TG (52:2)	Lognormal	0.003	(-0.004, 0.010)	0.393	0.827	0.045	(-0.004, 0.010)
LPE (22:6)	Lognormal	-0.008	(-0.025, 0.010)	0.397	0.832	0.049	(-0.025, 0.011)
FA (14:0) (myristic acid)	Lognormal	0.004	(-0.005, 0.012)	0.398	0.832	0.048	(-0.005, 0.012)
SM (d40:2) A - ESI(+)	Lognormal	-0.005	(-0.017, 0.007)	0.400	0.832	0.048	(-0.017, 0.007)
PC (38:4) C - ESI(+)	Lognormal	-0.002	(-0.008, 0.003)	0.403	0.834	0.048	(-0.009, 0.003)
AC (8:0)	Lognormal	-0.013	(-0.043, 0.017)	0.404	0.834	0.048	(-0.044, 0.015)
SM (d39:2)	Lognormal	-0.004	(-0.013, 0.005)	0.407	0.834	0.040	(-0.012, 0.005)
PC (p-32:0)/PC (o-32:1) - ESI(+)	Lognormal	-0.003	(-0.011, 0.005)	0.410	0.834	0.043	(-0.011, 0.004)
PC (38:4) B - ESI(+)	Lognormal	-0.004	(-0.014, 0.006)	0.413	0.834	0.045	(-0.014, 0.006)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
PC (p-38:6)/PC (o-38:7)	Lognormal	-0.005	(-0.019, 0.008)	0.414	0.834	0.043	(-0.019, 0.008)
PE (p-40:5)/PE (o-40:6)	Lognormal	-0.004	(-0.014, 0.006)	0.415	0.834	0.037	(-0.014, 0.005)
TG (40:1)	Lognormal	-0.017	(-0.057, 0.024)	0.418	0.834	0.049	(-0.057, 0.025)
LPC (20:5)	Lognormal	0.011	(-0.016, 0.039)	0.420	0.834	0.047	(-0.017, 0.039)
PC (33:1) - ESI(+)	Lognormal	0.004	(-0.006, 0.014)	0.420	0.834	0.046	(-0.005, 0.015)
TG (51:2)	Lognormal	0.006	(-0.008, 0.020)	0.425	0.837	0.051	(-0.009, 0.020)
PE (36:4) - ESI(-)	Lognormal	-0.011	(-0.038, 0.016)	0.425	0.837	0.045	(-0.038, 0.017)
PC (36:5) C	Lognormal	0.009	(-0.013, 0.030)	0.427	0.838	0.042	(-0.012, 0.030)
TG (64:3)	Lognormal	-0.009	(-0.031, 0.013)	0.428	0.838	0.044	(-0.029, 0.015)
GlcCer (d41:1)	Lognormal	-0.005	(-0.018, 0.008)	0.431	0.838	0.047	(-0.018, 0.007)
TG (56:9)	Lognormal	0.008	(-0.012, 0.027)	0.432	0.838	0.048	(-0.011, 0.028)
SM (d40:2) A - ESI(-)	Lognormal	-0.008	(-0.027, 0.012)	0.448	0.854	0.045	(-0.027, 0.013)
PC (32:0) - ESI(+)	Lognormal	0.002	(-0.003, 0.008)	0.448	0.854	0.041	(-0.003, 0.008)
LPC (20:0)	Lognormal	-0.007	(-0.023, 0.010)	0.448	0.854	0.045	(-0.023, 0.011)
SM (d32:2) - ESI(+)	Lognormal	-0.004	(-0.016, 0.007)	0.455	0.855	0.040	(-0.016, 0.008)
PC (35:2) A	Lognormal	0.003	(-0.005, 0.012)	0.456	0.855	0.046	(-0.005, 0.012)
TG (52:6)	Lognormal	-0.007	(-0.026, 0.011)	0.456	0.855	0.047	(-0.026, 0.012)
LPC (20:1) - ESI(-)	Lognormal	-0.006	(-0.023, 0.010)	0.456	0.855	0.045	(-0.022, 0.011)
PC (40:4) - ESI(+)	Lognormal	-0.005	(-0.017, 0.007)	0.458	0.855	0.045	(-0.017, 0.008)
PC (38:7)	Lognormal	0.006	(-0.010, 0.022)	0.459	0.855	0.042	(-0.010, 0.022)
CE (18:0)	Lognormal	0.008	(-0.013, 0.029)	0.465	0.861	0.047	(-0.013, 0.028)
PG (34:0)/PG (17:0/17:0)	Lognormal	-0.007	(-0.025, 0.011)	0.466	0.861	0.042	(-0.025, 0.012)
TG (46:4) B	Lognormal	-0.016	(-0.060, 0.027)	0.469	0.863	0.045	(-0.060, 0.027)
PC (32:0) - ESI(-)	Lognormal	-0.003	(-0.012, 0.006)	0.473	0.863	0.043	(-0.011, 0.006)
TG (62:1)	Lognormal	-0.010	(-0.038, 0.018)	0.474	0.863	0.045	(-0.039, 0.017)
PC (35:2)	Lognormal	-0.004	(-0.016, 0.007)	0.475	0.863	0.047	(-0.016, 0.007)
Ceramide (d34:1) - ESI(-)	Lognormal	-0.003	(-0.012, 0.005)	0.475	0.863	0.043	(-0.013, 0.004)
LPC (20:1) - ESI(+)	Lognormal	-0.010	(-0.039, 0.018)	0.475	0.863	0.046	(-0.039, 0.018)
LPC (p-18:0)/LPC (o-18:1)	Lognormal	-0.005	(-0.020, 0.010)	0.475	0.863	0.045	(-0.020, 0.010)
TG (52:4)	Lognormal	-0.003	(-0.013, 0.006)	0.490	0.879	0.045	(-0.013, 0.006)
AC (14:1)	Lognormal	-0.008	(-0.030, 0.014)	0.490	0.879	0.043	(-0.030, 0.014)
TG (53:3)	Lognormal	0.004	(-0.007, 0.015)	0.497	0.887	0.044	(-0.007, 0.015)
TG (53:2)	Lognormal	0.005	(-0.009, 0.018)	0.504	0.892	0.043	(-0.010, 0.018)
PC (33:0)	Lognormal	-0.006	(-0.024, 0.012)	0.509	0.894	0.043	(-0.023, 0.012)
Ceramide (d42:2) A - ESI(-)	Lognormal	-0.003	(-0.013, 0.007)	0.514	0.896	0.039	(-0.014, 0.007)
FA (18:2) (linoleic acid)	Lognormal	0.003	(-0.006, 0.011)	0.514	0.896	0.038	(-0.006, 0.012)
DG (36:4) A	Lognormal	-0.006	(-0.022, 0.011)	0.516	0.896	0.040	(-0.022, 0.011)
GlcCer (d40:1) - ESI(-)	Lognormal	-0.004	(-0.015, 0.008)	0.518	0.896	0.041	(-0.015, 0.008)
PE (34:2) - ESI(+)	Lognormal	-0.022	(-0.088, 0.044)	0.522	0.896	0.040	(-0.091, 0.044)
TG (60:1)	Lognormal	-0.009	(-0.038, 0.019)	0.523	0.896	0.044	(-0.039, 0.019)
LPC (15:0)	Lognormal	-0.004	(-0.018, 0.009)	0.528	0.896	0.042	(-0.018, 0.009)
SM (d36:3) - ESI(+)	Lognormal	-0.004	(-0.016, 0.008)	0.528	0.896	0.039	(-0.016, 0.008)
CE (22:6)	Lognormal	0.004	(-0.008, 0.015)	0.529	0.896	0.040	(-0.008, 0.015)
TG (56:3)	Lognormal	0.006	(-0.013, 0.026)	0.530	0.896	0.041	(-0.014, 0.026)
FA (20:4) (arachidonic acid)	Lognormal	-0.002	(-0.009, 0.005)	0.533	0.896	0.038	(-0.009, 0.005)
PC (p-40:7)/PC (o-40:8)	Lognormal	-0.013	(-0.054, 0.028)	0.533	0.896	0.039	(-0.053, 0.029)
FA (22:6) (docosahexaenoic acid)	Lognormal	0.005	(-0.010, 0.019)	0.535	0.896	0.041	(-0.010, 0.019)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
TG (40:0)	Lognormal	-0.010	(-0.042, 0.022)	0.536	0.896	0.041	(-0.042, 0.021)
Ceramide (d36:1) - ESI(+)	Lognormal	0.004	(-0.008, 0.015)	0.537	0.896	0.039	(-0.008, 0.015)
PC (36:1) - ESI(-)	Lognormal	-0.003	(-0.012, 0.006)	0.541	0.898	0.042	(-0.012, 0.005)
TG (56:1)	Lognormal	-0.008	(-0.034, 0.018)	0.545	0.899	0.042	(-0.034, 0.018)
TG (48:2)	Lognormal	-0.007	(-0.029, 0.015)	0.545	0.899	0.039	(-0.031, 0.015)
LPC (18:1) - ESI(+)	Lognormal	-0.003	(-0.014, 0.008)	0.550	0.905	0.044	(-0.014, 0.008)
Ceramide (d34:0)	Lognormal	-0.004	(-0.017, 0.009)	0.551	0.905	0.034	(-0.017, 0.008)
PE (36:1) - ESI(+)	Lognormal	-0.007	(-0.029, 0.015)	0.553	0.907	0.039	(-0.029, 0.015)
PC (o-32:0) - ESI(+)	Lognormal	-0.002	(-0.010, 0.006)	0.557	0.908	0.038	(-0.011, 0.005)
PC (37:4) - ESI(-)	Lognormal	-0.004	(-0.018, 0.010)	0.558	0.908	0.042	(-0.018, 0.010)
TG (48:1)	Lognormal	-0.006	(-0.027, 0.015)	0.558	0.908	0.039	(-0.028, 0.014)
TG (58:10)	Lognormal	0.006	(-0.013, 0.024)	0.563	0.909	0.042	(-0.012, 0.026)
PC (35:4) - ESI(+)	Lognormal	-0.003	(-0.014, 0.008)	0.575	0.914	0.038	(-0.014, 0.007)
TG (53:1)	Lognormal	-0.008	(-0.037, 0.021)	0.578	0.916	0.040	(-0.037, 0.020)
PC (p-42:4)/PC (o-42:5) - ESI(-)	Lognormal	-0.005	(-0.024, 0.013)	0.581	0.917	0.038	(-0.024, 0.013)
PC 38:7e	Lognormal	-0.005	(-0.021, 0.012)	0.585	0.920	0.037	(-0.022, 0.011)
FA (20:2) (eicosadienoic acid)	Lognormal	0.003	(-0.009, 0.015)	0.596	0.930	0.042	(-0.009, 0.015)
TG (54:3)	Lognormal	0.003	(-0.008, 0.013)	0.598	0.931	0.042	(-0.008, 0.014)
LPC (17:1)	Lognormal	0.004	(-0.011, 0.019)	0.599	0.931	0.039	(-0.010, 0.020)
PC (35:2) B	Lognormal	-0.002	(-0.008, 0.005)	0.600	0.931	0.035	(-0.009, 0.005)
DG (36:4) B	Lognormal	0.010	(-0.027, 0.047)	0.600	0.931	0.040	(-0.026, 0.048)
TG (58:4)	Lognormal	0.006	(-0.017, 0.030)	0.605	0.933	0.041	(-0.018, 0.031)
TG (59:3)	Lognormal	0.006	(-0.017, 0.029)	0.605	0.933	0.037	(-0.017, 0.029)
GlcCer (d42:1) - ESI(-)	Lognormal	-0.003	(-0.014, 0.008)	0.609	0.933	0.036	(-0.013, 0.008)
CE (16:0)	Lognormal	0.007	(-0.020, 0.034)	0.613	0.933	0.034	(-0.019, 0.034)
SM (d34:2) - ESI(+)	Lognormal	-0.002	(-0.008, 0.005)	0.613	0.933	0.036	(-0.008, 0.005)
TG (56:7) A	Lognormal	0.011	(-0.031, 0.052)	0.619	0.934	0.041	(-0.034, 0.049)
PC (p-40:4)/PC (o-40:5) - ESI(+)	Lognormal	-0.002	(-0.012, 0.007)	0.619	0.934	0.037	(-0.012, 0.007)
SM (d34:0) - ESI(+)	Lognormal	-0.002	(-0.010, 0.006)	0.620	0.934	0.035	(-0.010, 0.006)
PC (35:4) - ESI(-)	Lognormal	-0.004	(-0.020, 0.012)	0.624	0.934	0.039	(-0.020, 0.012)
PC (34:0) - ESI(+)	Lognormal	-0.001	(-0.007, 0.004)	0.625	0.934	0.032	(-0.007, 0.004)
TG (48:6)	Lognormal	0.006	(-0.019, 0.032)	0.631	0.938	0.039	(-0.020, 0.031)
PC (p-44:4)/PC (o-44:5) - ESI(+)	Lognormal	0.003	(-0.009, 0.015)	0.636	0.938	0.039	(-0.009, 0.015)
PC (p-40:6)/PC (o-40:7) B	Lognormal	-0.004	(-0.019, 0.011)	0.637	0.938	0.036	(-0.019, 0.012)
SM (d34:1) - ESI(+)	Lognormal	-0.001	(-0.006, 0.004)	0.638	0.938	0.034	(-0.006, 0.004)
PC (35:1) - ESI(-)	Lognormal	0.003	(-0.011, 0.018)	0.639	0.938	0.037	(-0.010, 0.018)
GlcCer (d40:1) - ESI(+)	Lognormal	-0.003	(-0.016, 0.010)	0.641	0.938	0.036	(-0.017, 0.009)
Ceramide (d40:2)	Lognormal	0.010	(-0.032, 0.052)	0.646	0.938	0.038	(-0.030, 0.051)
TG (54:2)	Lognormal	0.004	(-0.011, 0.019)	0.647	0.938	0.040	(-0.011, 0.019)
DG (34:2)	Lognormal	0.003	(-0.009, 0.014)	0.648	0.938	0.033	(-0.009, 0.014)
SM (d42:0) - ESI(+)	Lognormal	-0.006	(-0.034, 0.021)	0.648	0.938	0.037	(-0.033, 0.022)
PC (33:1) - ESI(-)	Lognormal	0.005	(-0.016, 0.025)	0.650	0.938	0.037	(-0.015, 0.027)
TG (58:1)	Lognormal	-0.006	(-0.032, 0.020)	0.651	0.938	0.035	(-0.030, 0.021)
PC (36:5) B	Lognormal	0.005	(-0.017, 0.028)	0.651	0.938	0.038	(-0.016, 0.027)
FA (18:3) (linolenic acid)	Lognormal	0.003	(-0.010, 0.016)	0.662	0.938	0.040	(-0.011, 0.015)
PC (16:0/9:0(CHO))	Lognormal	0.005	(-0.016, 0.026)	0.662	0.938	0.031	(-0.015, 0.026)
PC (38:4) A - ESI(+)	Lognormal	-0.002	(-0.012, 0.008)	0.662	0.938	0.038	(-0.012, 0.008)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
FA (24:1) (nervonic acid)	Lognormal	0.002	(-0.008, 0.012)	0.664	0.938	0.034	(-0.008, 0.012)
TG (50:2)	Lognormal	0.003	(-0.009, 0.014)	0.667	0.938	0.036	(-0.008, 0.014)
SM (d38:0)	Lognormal	-0.014	(-0.077, 0.049)	0.668	0.938	0.036	(-0.077, 0.048)
SM (d41:1) - ESI(-)	Lognormal	0.023	(-0.082, 0.127)	0.669	0.938	0.039	(-0.081, 0.129)
TG (58:5)	Lognormal	-0.004	(-0.022, 0.014)	0.670	0.938	0.036	(-0.021, 0.014)
PC (38:5) B - ESI(-)	Lognormal	0.004	(-0.013, 0.021)	0.671	0.938	0.038	(-0.013, 0.021)
TG (49:0)	Lognormal	-0.005	(-0.026, 0.017)	0.675	0.938	0.037	(-0.025, 0.017)
SM (d36:2) - ESI(-)	Lognormal	-0.003	(-0.015, 0.010)	0.676	0.938	0.038	(-0.015, 0.010)
TG (46:3) B	Lognormal	-0.008	(-0.044, 0.029)	0.677	0.938	0.037	(-0.042, 0.030)
PE (p-36:5)/PE (o-36:6)	Lognormal	-0.011	(-0.065, 0.042)	0.678	0.938	0.037	(-0.063, 0.043)
PC (36:6)	Lognormal	-0.004	(-0.022, 0.014)	0.680	0.939	0.034	(-0.021, 0.015)
PC (p-38:5)/PC (o-38:6) A	Lognormal	-0.003	(-0.016, 0.011)	0.682	0.939	0.035	(-0.016, 0.011)
PC (40:8) - ESI(+)	Lognormal	-0.002	(-0.011, 0.007)	0.684	0.939	0.033	(-0.011, 0.007)
PC (40:6) B	Lognormal	0.003	(-0.011, 0.016)	0.700	0.945	0.040	(-0.011, 0.016)
TG (51:4)	Lognormal	-0.003	(-0.018, 0.012)	0.701	0.945	0.036	(-0.019, 0.013)
FA (15:0) (pentadecylic acid)	Lognormal	-0.002	(-0.010, 0.007)	0.705	0.946	0.033	(-0.010, 0.007)
SM (d36:1) - ESI(+)	Lognormal	0.001	(-0.006, 0.008)	0.706	0.946	0.038	(-0.005, 0.009)
TG (54:6) A	Lognormal	-0.003	(-0.020, 0.014)	0.715	0.948	0.036	(-0.019, 0.014)
Ceramide (d40:0)	Lognormal	-0.005	(-0.034, 0.023)	0.718	0.948	0.030	(-0.034, 0.023)
TG (58:3)	Lognormal	0.005	(-0.023, 0.033)	0.722	0.948	0.036	(-0.023, 0.033)
PC (37:4) - ESI(+)	Lognormal	0.002	(-0.010, 0.015)	0.722	0.948	0.035	(-0.010, 0.014)
PC (38:5) A - ESI(-)	Lognormal	-0.002	(-0.011, 0.008)	0.725	0.948	0.037	(-0.011, 0.008)
PC (32:1) - ESI(-)	Lognormal	-0.003	(-0.020, 0.014)	0.728	0.948	0.035	(-0.020, 0.015)
Gal-Gal-Cer (d18:1/16:0)/Lactosylceramide (d18:1/16:0)	Lognormal	0.002	(-0.007, 0.011)	0.728	0.948	0.033	(-0.007, 0.011)
SM (d43:2) - ESI(+)	Lognormal	0.003	(-0.014, 0.019)	0.729	0.948	0.037	(-0.014, 0.020)
LPC (22:5) - ESI(+)	Lognormal	0.003	(-0.016, 0.023)	0.730	0.948	0.038	(-0.016, 0.023)
CE (16:1)	Lognormal	0.003	(-0.012, 0.017)	0.739	0.954	0.033	(-0.011, 0.017)
TG (62:2)	Lognormal	-0.005	(-0.035, 0.025)	0.742	0.955	0.035	(-0.036, 0.025)
SM (d42:3) - ESI(+)	Lognormal	0.001	(-0.006, 0.008)	0.745	0.955	0.036	(-0.006, 0.008)
TG (62:3)	Lognormal	-0.006	(-0.042, 0.030)	0.747	0.955	0.035	(-0.043, 0.031)
TG (51:3)	Lognormal	0.002	(-0.010, 0.015)	0.751	0.955	0.032	(-0.011, 0.015)
TG (52:1)	Lognormal	-0.003	(-0.023, 0.017)	0.753	0.955	0.036	(-0.025, 0.015)
DG (36:1)	Lognormal	0.003	(-0.014, 0.020)	0.755	0.955	0.036	(-0.014, 0.019)
PE (36:4) - ESI(+)	Lognormal	-0.004	(-0.026, 0.019)	0.756	0.955	0.033	(-0.026, 0.018)
SM (d42:0) - ESI(-)	Lognormal	-0.002	(-0.015, 0.011)	0.756	0.955	0.033	(-0.015, 0.011)
SM (d41:2) A - ESI(+)	Lognormal	0.002	(-0.009, 0.012)	0.759	0.955	0.031	(-0.008, 0.013)
PC (37:3)	Lognormal	-0.002	(-0.016, 0.011)	0.759	0.955	0.037	(-0.016, 0.012)
SM (d37:1)	Lognormal	-0.003	(-0.022, 0.016)	0.759	0.955	0.037	(-0.022, 0.016)
DG (34:1)	Lognormal	-0.004	(-0.029, 0.021)	0.767	0.955	0.032	(-0.030, 0.021)
TG (54:4)	Lognormal	0.002	(-0.010, 0.013)	0.769	0.955	0.033	(-0.009, 0.014)
TG (54:8)	Lognormal	-0.004	(-0.029, 0.021)	0.771	0.955	0.039	(-0.028, 0.021)
PC (p-42:4)/PC (o-42:5) - ESI(+)	Lognormal	-0.002	(-0.013, 0.010)	0.772	0.955	0.032	(-0.012, 0.010)
SM (d33:1) - ESI(+)	Lognormal	-0.001	(-0.011, 0.008)	0.773	0.955	0.036	(-0.011, 0.009)
PC (p-38:5)/PC (o-38:6)	Lognormal	-0.005	(-0.043, 0.032)	0.778	0.958	0.039	(-0.041, 0.033)
PC (42:5)	Lognormal	0.002	(-0.013, 0.017)	0.780	0.958	0.035	(-0.013, 0.018)
CE (20:4)	Lognormal	-0.001	(-0.011, 0.008)	0.785	0.958	0.038	(-0.011, 0.008)
TG (59:2)	Lognormal	-0.003	(-0.028, 0.021)	0.785	0.958	0.033	(-0.030, 0.019)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
SM (d36:2) - ESI(+)	Lognormal	0.001	(-0.006, 0.008)	0.791	0.958	0.034	(-0.006, 0.008)
DG (34:3)	Lognormal	0.003	(-0.016, 0.022)	0.795	0.959	0.031	(-0.016, 0.022)
PC (o-32:0) - ESI(-)	Lognormal	-0.002	(-0.014, 0.011)	0.795	0.959	0.035	(-0.015, 0.011)
LPC (22:5) - ESI(-)	Lognormal	-0.004	(-0.039, 0.030)	0.802	0.961	0.031	(-0.036, 0.032)
GlcCer (d42:1) - ESI(+)	Lognormal	0.001	(-0.009, 0.011)	0.804	0.963	0.032	(-0.008, 0.012)
DG (36:5)	Lognormal	-0.003	(-0.023, 0.018)	0.806	0.963	0.033	(-0.024, 0.019)
TG (52:5)	Lognormal	0.002	(-0.011, 0.014)	0.812	0.963	0.034	(-0.011, 0.014)
TG (53:4)	Lognormal	0.002	(-0.011, 0.014)	0.815	0.967	0.034	(-0.013, 0.014)
TG (50:3) B	Lognormal	-0.009	(-0.088, 0.069)	0.819	0.968	0.038	(-0.088, 0.067)
PC (40:6) A	Lognormal	-0.001	(-0.013, 0.010)	0.823	0.972	0.035	(-0.013, 0.009)
TG (57:2)	Lognormal	-0.002	(-0.019, 0.015)	0.828	0.975	0.033	(-0.019, 0.014)
TG (60:2)	Lognormal	-0.004	(-0.046, 0.037)	0.834	0.979	0.033	(-0.044, 0.036)
PC (40:7) - ESI(-)	Lognormal	-0.002	(-0.021, 0.017)	0.835	0.979	0.038	(-0.021, 0.018)
SM (d41:2) - ESI(-)	Lognormal	-0.002	(-0.016, 0.013)	0.838	0.981	0.034	(-0.016, 0.013)
PE (36:1) - ESI(-)	Lognormal	-0.003	(-0.027, 0.022)	0.843	0.981	0.033	(-0.027, 0.024)
TG (46:5)	Lognormal	0.005	(-0.041, 0.051)	0.843	0.981	0.038	(-0.039, 0.050)
PC (p-34:1)/PC (o-34:2) B	Lognormal	-0.002	(-0.021, 0.018)	0.846	0.981	0.033	(-0.022, 0.017)
TG (53:5)	Lognormal	-0.002	(-0.017, 0.014)	0.849	0.981	0.035	(-0.017, 0.015)
PC (p-44:5)/PC (o-44:6)	Lognormal	0.001	(-0.013, 0.016)	0.849	0.981	0.033	(-0.013, 0.015)
DG (36:3)	Lognormal	0.001	(-0.010, 0.012)	0.852	0.981	0.031	(-0.010, 0.011)
PC (42:6)	Lognormal	-0.003	(-0.030, 0.024)	0.853	0.981	0.032	(-0.028, 0.025)
TG (56:10)	Lognormal	0.003	(-0.029, 0.035)	0.854	0.981	0.033	(-0.027, 0.037)
Ceramide (d34:2)	Lognormal	-0.001	(-0.013, 0.010)	0.854	0.981	0.035	(-0.013, 0.010)
PE (38:6) - ESI(-)	Lognormal	-0.002	(-0.029, 0.024)	0.861	0.981	0.035	(-0.028, 0.025)
TG (52:3)	Lognormal	0.001	(-0.006, 0.007)	0.864	0.981	0.034	(-0.006, 0.007)
TAG (58:7)/TAG (18:1/18:1/22:5)	Lognormal	0.001	(-0.013, 0.015)	0.881	0.984	0.038	(-0.013, 0.014)
PE (38:6) - ESI(+)	Lognormal	-0.002	(-0.034, 0.030)	0.882	0.984	0.033	(-0.034, 0.031)
PC (38:6) - ESI(-)	Lognormal	0.001	(-0.011, 0.013)	0.884	0.984	0.034	(-0.011, 0.013)
PC (36:4) C - ESI(+)	Lognormal	0.000	(-0.006, 0.005)	0.884	0.984	0.036	(-0.006, 0.005)
TG (55:2)	Lognormal	0.001	(-0.017, 0.020)	0.889	0.984	0.036	(-0.017, 0.020)
Ceramide (d36:1) - ESI(-)	Lognormal	-0.001	(-0.021, 0.018)	0.890	0.984	0.034	(-0.021, 0.018)
PC (36:4) B - ESI(+)	Lognormal	0.001	(-0.012, 0.014)	0.892	0.984	0.033	(-0.012, 0.014)
SM (d36:0) - ESI(-)	Lognormal	0.002	(-0.028, 0.032)	0.893	0.984	0.035	(-0.028, 0.032)
TG (54:5) A	Lognormal	-0.001	(-0.013, 0.012)	0.896	0.984	0.033	(-0.013, 0.012)
PC (p-40:4)/PC (o-40:5) - ESI(-)	Lognormal	0.001	(-0.013, 0.014)	0.901	0.984	0.034	(-0.014, 0.014)
GlcCer (d34:1)	Lognormal	0.001	(-0.020, 0.023)	0.902	0.984	0.038	(-0.021, 0.023)
TG (60:3)	Lognormal	-0.002	(-0.033, 0.029)	0.905	0.984	0.035	(-0.033, 0.031)
TG (60:4)	Lognormal	-0.002	(-0.034, 0.030)	0.905	0.984	0.036	(-0.035, 0.029)
PC (p-40:6)/PC (o-40:7) A	Lognormal	0.001	(-0.012, 0.013)	0.914	0.988	0.034	(-0.011, 0.013)
TG (56:4)	Lognormal	0.001	(-0.013, 0.014)	0.923	0.990	0.035	(-0.012, 0.015)
TG (49:1)	Lognormal	0.001	(-0.021, 0.023)	0.926	0.990	0.032	(-0.021, 0.024)
CE (18:1)	Lognormal	-0.001	(-0.013, 0.012)	0.927	0.990	0.033	(-0.012, 0.013)
LPC (22:6)	Lognormal	0.001	(-0.014, 0.015)	0.929	0.990	0.033	(-0.014, 0.016)
FA (20:3) (eicosatrienoic acid)	Lognormal	0.001	(-0.015, 0.016)	0.929	0.990	0.033	(-0.014, 0.016)
SM (d32:0) - ESI(+)	Lognormal	-0.001	(-0.017, 0.016)	0.930	0.990	0.032	(-0.017, 0.016)
AC (18:1)	Lognormal	0.001	(-0.011, 0.012)	0.931	0.990	0.034	(-0.012, 0.013)
PC (36:1) - ESI(+)	Lognormal	0.000	(-0.006, 0.006)	0.932	0.990	0.032	(-0.006, 0.006)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
PC (39:4)	Lognormal	0.000	(-0.011, 0.010)	0.937	0.991	0.033	(-0.012, 0.010)
PC (40:5) A - ESI(-)	Lognormal	-0.001	(-0.017, 0.016)	0.938	0.991	0.035	(-0.017, 0.015)
PC (31:0)	Lognormal	0.000	(-0.012, 0.013)	0.946	0.994	0.035	(-0.012, 0.013)
PC (32:1) - ESI(+)	Lognormal	0.000	(-0.012, 0.013)	0.947	0.994	0.035	(-0.012, 0.012)
SM (d40:0)	Lognormal	0.000	(-0.013, 0.013)	0.957	0.998	0.033	(-0.014, 0.012)
PC (p-42:5)/PC (o-42:6) B	Lognormal	0.000	(-0.015, 0.014)	0.961	0.998	0.035	(-0.016, 0.014)
TG (64:2)	Lognormal	-0.001	(-0.031, 0.030)	0.964	0.998	0.036	(-0.027, 0.032)
PC 40:6e	Lognormal	0.000	(-0.010, 0.010)	0.968	0.998	0.032	(-0.010, 0.010)
TG (50:3) A	Lognormal	0.000	(-0.014, 0.014)	0.976	0.998	0.031	(-0.014, 0.015)
TG (49:3)	Lognormal	0.000	(-0.022, 0.022)	0.977	0.998	0.033	(-0.023, 0.021)
TG (55:1)	Lognormal	0.000	(-0.022, 0.022)	0.978	0.998	0.035	(-0.022, 0.022)
AC (16:0)	Lognormal	0.000	(-0.010, 0.011)	0.978	0.998	0.032	(-0.010, 0.011)
DG (32:1)	Lognormal	0.000	(-0.023, 0.023)	0.981	0.998	0.030	(-0.024, 0.022)
TG (57:1)	Lognormal	0.000	(-0.020, 0.019)	0.983	0.998	0.033	(-0.019, 0.019)
TG (44:2)	Lognormal	0.001	(-0.078, 0.079)	0.987	0.998	0.035	(-0.080, 0.079)
TG (54:9)	Lognormal	0.000	(-0.060, 0.059)	0.988	0.998	0.033	(-0.061, 0.059)
PC (p-36:5)/PC (o-36:6)	Lognormal	0.000	(-0.020, 0.020)	0.989	0.998	0.034	(-0.021, 0.020)
TG (56:2)	Lognormal	0.000	(-0.022, 0.022)	0.992	0.998	0.035	(-0.024, 0.023)
TG (50:6)	Lognormal	0.000	(-0.027, 0.028)	0.996	0.998	0.034	(-0.028, 0.027)
PC (31:1)	Lognormal	0.000	(-0.036, 0.036)	0.996	0.998	0.034	(-0.036, 0.037)
SM (d38:2) - ESI(+)	Lognormal	0.000	(-0.007, 0.007)	0.997	0.998	0.033	(-0.007, 0.007)
Oxylipins (OL)							
11,12-Epoxyeicosa-5,8,14-trienoic acid	Gamma	0.383	(0.102, 0.666)	0.007	0.310	1.128	(0.108, 0.672)
8,9-Epoxyeicosa-5,11,14-trienoic acid	Gamma	-0.351	(-0.614, -0.086)	0.008	0.310	0.680	(-0.631, -0.086)
Prostaglandin F2a	Gamma	-0.348	(-0.637, -0.058)	0.016	0.310	0.294	(-0.670, -0.013)
Resolvin D1	Gamma	-0.379	(-0.683, -0.073)	0.016	0.310	0.597	(-0.674, -0.055)
12-Hydroxy-5,8,10,14,17-eicosapentaenoic acid	Gamma	0.451	(0.077, 0.828)	0.017	0.310	3.271	(0.158, 0.720)
9,11,15-trihydroxy-5,13,17-prostatrienoic acid	Gamma	-0.520	(-0.990, -0.049)	0.022	0.327	2.494	(-0.880, -0.175)
Leukotriene B4	Gamma	-0.246	(-0.473, -0.018)	0.037	0.369	0.332	(-0.437, -0.028)
11-Hydroxy-14,15-epoxyeicosatrienoic acid	Gamma	-0.525	(-1.040, -0.005)	0.041	0.375	0.705	(-0.971, -0.107)
5-Hydroxy-6,8,11,14,17-eicosapentaenoic acid	Gamma	0.236	(-0.009, 0.483)	0.052	0.402	0.189	(0.010, 0.468)
17,18-Epoxy-5,8,11,14-eicosatetraenoic acid	Gamma	-0.428	(-0.874, 0.022)	0.064	0.424	0.460	(-0.810, -0.045)
16(17)-epoxy-4,7,10,13,19-docosapentaenoic acid	Gamma	0.324	(-0.067, 0.717)	0.082	0.479	0.166	(-0.053, 0.691)
9-Hydroxy-5,7,11,14,17-icosapentaenoic acid	Gamma	0.205	(-0.051, 0.462)	0.105	0.542	0.092	(-0.043, 0.464)
8,9-dihydroxyeicosa-5,11,14-trienoic acid	Gamma	0.181	(-0.046, 0.410)	0.114	0.557	0.073	(-0.061, 0.416)
17,18-dihydroxyeicosa-5,8,11,14-tetraenoic acid	Lognormal	0.194	(-0.060, 0.448)	0.137	0.612	0.100	(-0.050, 0.453)
15-hydroxyeicosa-5,8,11,13,17-pentaenoic acid	Gamma	0.268	(-0.097, 0.637)	0.145	0.622	0.112	(-0.060, 0.626)
13-ketooctadeca-9,11-dienoic acid	Lognormal	-0.196	(-0.471, 0.079)	0.165	0.653	0.079	(-0.476, 0.077)
5-ketoeicosa-6,8,11,14-tetraenoic acid	Gamma	-0.198	(-0.499, 0.105)	0.177	0.664	0.067	(-0.535, 0.150)
Prostaglandin D2	Gamma	-0.350	(-0.884, 0.197)	0.177	0.664	0.145	(-0.784, 0.097)
4-hydroxydocosa-5,7,10,13,16,19-hexaenoic acid	Gamma	0.187	(-0.125, 0.501)	0.236	0.724	0.065	(-0.126, 0.519)
15,16-dihydroxyoctadeca-9,12-dienoic acid	Lognormal	-0.110	(-0.294, 0.074)	0.244	0.724	0.056	(-0.297, 0.077)
15(16)-epoxy-9,12-octadecadienoic acid	Gamma	-0.242	(-0.687, 0.210)	0.248	0.724	0.080	(-0.602, 0.135)
9,10-dihydroxyoctadec-12-enoic acid	Lognormal	-0.116	(-0.316, 0.083)	0.255	0.724	0.050	(-0.313, 0.084)
9,12,13-trihydroxyoctadec-10-enoic acid	Lognormal	-0.071	(-0.210, 0.068)	0.318	0.757	0.047	(-0.218, 0.073)
15-Deoxy-delta-12,14-Prostaglandin J2	Gamma	-0.158	(-0.454, 0.140)	0.319	0.757	0.052	(-0.454, 0.138)
9-Hydroxylinoleic acid	Lognormal	-0.057	(-0.188, 0.073)	0.389	0.825	0.043	(-0.182, 0.079)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI
5,6-dihydroxyeicosa-8,11,14-trienoic acid	Gamma	0.094	(-0.135, 0.324)	0.412	0.834	0.033	(-0.137, 0.326)
15-Keto-prostaglandin E2	Gamma	-0.191	(-0.680, 0.306)	0.415	0.834	0.064	(-0.596, 0.226)
14,15-dihydroxyeicosa-5,8,11,17-tetraenoic acid	Gamma	-0.138	(-0.483, 0.212)	0.420	0.834	0.046	(-0.472, 0.202)
11(12)-epoxy-5,8,14,17- eicosatetraenoic acid	Gamma	-0.162	(-0.591, 0.273)	0.447	0.854	0.057	(-0.573, 0.259)
12,13-dihydroxyoctadeca-9,15-dienoic acid	Gamma	-0.186	(-0.659, 0.295)	0.448	0.854	0.059	(-0.568, 0.149)
Prostaglandin E1	Gamma	0.126	(-0.239, 0.494)	0.484	0.875	0.044	(-0.188, 0.447)
14(15)-epoxy-5,8,11,17-eicosatetraenoic acid	Gamma	0.200	(-0.465, 0.874)	0.504	0.892	0.081	(-0.368, 0.711)
12,13-dihydroxyoctadec-9-enoic acid	Lognormal	-0.061	(-0.251, 0.129)	0.529	0.896	0.038	(-0.258, 0.130)
17-hydroxy-4,7,10,13,15,19-docosahexaenoic acid	Gamma	0.075	(-0.177, 0.328)	0.551	0.905	0.033	(-0.178, 0.358)
10-nitrolinoleic acid	Gamma	0.120	(-0.319, 0.564)	0.571	0.914	0.045	(-0.253, 0.499)
Leukotriene B5	Gamma	-0.150	(-0.680, 0.385)	0.577	0.916	0.057	(-0.645, 0.303)
20-Hydroxyarachidonic acid	Lognormal	-0.096	(-0.447, 0.254)	0.590	0.924	0.029	(-0.436, 0.269)
5,6,15-trihydroxyeicosa-7,9,11,13-tetraenoic acid	Gamma	-0.090	(-0.424, 0.249)	0.609	0.933	0.037	(-0.397, 0.240)
8-hydroxyeicosa-5,9,11,14-tetraenoic acid	Gamma	0.064	(-0.183, 0.312)	0.613	0.933	0.030	(-0.205, 0.329)
9,10-Epoxy stearic acid	Lognormal	-0.083	(-0.405, 0.239)	0.614	0.933	0.037	(-0.399, 0.229)
8,15-dihydroxyeicosa-5,9,11,13-tetraenoic acid	Gamma	-0.140	(-0.660, 0.393)	0.616	0.934	0.058	(-0.614, 0.324)
9,10-dihydroxyoctadeca-12,15-dienoic acid	Gamma	-0.051	(-0.273, 0.173)	0.647	0.938	0.026	(-0.294, 0.186)
15-ketoeicosa-5,8,11,13-tetraenoic acid	Gamma	0.085	(-0.307, 0.480)	0.669	0.938	0.036	(-0.224, 0.398)
5-Hydroxy-6,8,11,14-eicosatetraenoic acid	Lognormal	-0.039	(-0.241, 0.163)	0.707	0.946	0.031	(-0.238, 0.157)
9S,10R-dihydroxy-stearic acid	Lognormal	-0.049	(-0.326, 0.228)	0.731	0.948	0.036	(-0.323, 0.235)
10-nitrooleic acid	Lognormal	0.042	(-0.202, 0.285)	0.736	0.952	0.033	(-0.209, 0.283)
9-nitrooleic acid	Gamma	-0.049	(-0.364, 0.270)	0.760	0.955	0.031	(-0.350, 0.269)
9-hydroxyoctadeca-10,12,15-trienoic acid	Gamma	-0.039	(-0.301, 0.224)	0.763	0.955	0.025	(-0.297, 0.216)
18-(3-ethyloxiran-2-yl)octadeca-4,7,10,13,16-pentaenoic acid	Gamma	0.049	(-0.332, 0.433)	0.786	0.958	0.035	(-0.247, 0.406)
19,20-dihydroxydocosa-4,7,10,13,16-pentaenoic acid	Lognormal	0.024	(-0.149, 0.196)	0.788	0.958	0.031	(-0.156, 0.188)
12(13)-epoxy-9,15-octadecadienoic acid	Gamma	-0.049	(-0.477, 0.384)	0.811	0.963	0.038	(-0.411, 0.289)
9(10)-epoxy-12Z-octadecenoic acid	Gamma	0.020	(-0.210, 0.251)	0.864	0.981	0.020	(-0.173, 0.218)
Prostaglandin E3	Gamma	0.046	(-0.612, 0.715)	0.872	0.984	0.062	(-0.556, 0.566)
14,15-dihydroxyeicosa-5,8,11-trienoic acid	Gamma	-0.011	(-0.158, 0.136)	0.882	0.984	0.016	(-0.153, 0.159)
14-hydroxydocosa-4,7,10,12,16,19-hexaenoic acid	Lognormal	0.022	(-0.307, 0.350)	0.897	0.984	0.022	(-0.306, 0.338)
11,12-Dihydroxyicosa-5,8,14-trienoic acid	Gamma	-0.010	(-0.171, 0.151)	0.902	0.984	0.016	(-0.167, 0.151)
5,15-dihydroxyeicosa-6,8,11,13-tetraenoic acid	Gamma	0.028	(-0.467, 0.531)	0.907	0.984	0.049	(-0.420, 0.508)
9-ketooctadeca-10,12-dienoic acid	Gamma	-0.013	(-0.235, 0.210)	0.908	0.984	0.030	(-0.247, 0.266)
12,13-epoxy-9-octadecenoic acid	Lognormal	-0.017	(-0.323, 0.290)	0.916	0.988	0.034	(-0.338, 0.269)
9-hydroxyeicosa-5,7,11,14-tetraenoic acid	Gamma	-0.012	(-0.242, 0.220)	0.918	0.989	0.027	(-0.267, 0.242)
13-Hydroxyoctadecadienoic acid	Lognormal	-0.005	(-0.127, 0.118)	0.938	0.991	0.030	(-0.128, 0.118)
Thromboxane B2	Lognormal	-0.010	(-0.275, 0.254)	0.939	0.991	0.036	(-0.288, 0.246)
12-Hydroxy-5,8,10,14-eicosatetraenoic acid	Lognormal	0.009	(-0.212, 0.229)	0.940	0.991	0.025	(-0.229, 0.218)
15-hydroxyeicosa-5,8,11,13-tetraenoic acid	Lognormal	-0.005	(-0.166, 0.155)	0.948	0.994	0.029	(-0.172, 0.159)
13-hydroxyoctadeca-9,11,15-trienoic acid	Gamma	0.007	(-0.239, 0.254)	0.957	0.998	0.025	(-0.240, 0.246)
trans-12,13-epoxy-11-oxo-trans-9-octadecenoic acid	Gamma	-0.005	(-0.209, 0.200)	0.960	0.998	0.020	(-0.219, 0.197)
6-Ketoprostaglandin F1 alpha	Gamma	0.009	(-0.398, 0.420)	0.963	0.998	0.038	(-0.342, 0.389)
6-trans-Leukotriene B4	Gamma	-0.004	(-0.491, 0.490)	0.987	0.998	0.038	(-0.426, 0.452)
9(10)-epoxy-12,15-octadecadienoic acid	Gamma	0.003	(-0.537, 0.549)	0.990	0.998	0.041	(-0.389, 0.422)
11-Hydroxy-arachidonic acid	Gamma	0.001	(-0.178, 0.180)	0.994	0.998	0.019	(-0.188, 0.190)
Prostaglandin E2	Gamma	0.002	(-0.528, 0.537)	0.995	0.998	0.039	(-0.380, 0.381)

Supplementary Table S7. Regression and Bayesian estimates comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Metabolite	Regression Model	ME/CFS without sr-IBS vs. Controls without sr-IBS					
		Estimated Coefficient	95% CI	p-value	FDR	BayesFactor	95% HDI

ME/CFS, myalgic encephalomyelitis/chronic fatigue syndrome; sr-IBS, self-reported physician diagnosed irritable bowel syndrome; CI, confidence interval; FDR, false discovery rate adjusted p-value; HDI, highest density credible intervals. Regression models were adjusted for age, sex, race/ethnicity, geographic/clinical site, season of sampling, and body mass index. In PM, BA, and CL panels, estimated coefficients are interpreted as the differences in the mean values of log-log transformation of metabolite levels between cases and controls. In OL panel for lognormal regression, estimated coefficients are interpreted as the mean differences of log transformation of metabolite levels between two groups; for Gamma regression, estimated coefficients are interpreted as the log of fold change between two groups. Estimations in **bold** are significant. Criteria for significance: 1) FDR adjusted p-value from the regression model < 0.15, 2) BayesFactor > 3, and 3) 95% highest density credible intervals not covering 0.

Supplementary Table S8. ChemRICH enrichment analysis comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Cluster name	Cluster size	p-values	Key compound	Altered	Increased	Decreased	Altered Ratio
plasmalogens	24	0.000000058	PE (p-36:2)/PE (o-36:3) - ESI(+)	15	0	9	0.6
unsaturated phospholipid ethers	42	0.000003	PC (p-34:2)/PC (o-34:3) - ESI(+)	17	0	14	0.4
sphingomyelins	49	0.000019	SM (d43:1) - ESI(-)	19	0	11	0.4
unsaturated phosphatidylcholines	90	0.000041	PC (36:2)	24	0	16	0.3
exposome food	14	0.00015	Choline	8	0	4	0.6
unsaturated ceramides	21	0.0002	Ceramide (d42:1) - ESI (+)	7	0	7	0.3
saturated lysophospholipids	10	0.00056	LPC (14:0) - ESI(+)	6	0	4	0.6
HEPE	5	0.00074	12-Hydroxy-5,8,10,14,17-eicosapentaenoic acid	2	1	0	0.4
unsaturated lysophosphatidylcholines	20	0.0055	LPC (18:3)	6	0	5	0.3
unsaturated long chain TGs	41	0.012	TG (62:4)	9	2	1	0.2
EpODE	7	0.017	11,12-Epoxyeicosa-5,8,14-trienoic acid	4	1	2	0.6
carnitines	27	0.028	2-Methylbutyryl-L-carnitine	3	0	2	0.1
saturated TGs	8	0.029	TG (50:0)	2	0	2	0.2
saturated lysophosphoethanolamines	4	0.069	LPE (18:0)	1	0	1	0.2
unsaturated lysophosphoethanolamines	6	0.071	LPE (20:4) - ESI(-)	3	0	2	0.5
drugs	85	0.074	Acetaminophen	15	7	2	0.2
amino acids	24	0.088	L-Citrulline	4	0	2	0.2
unsaturated FFA	15	0.094	FA (16:1) (palmitoleic acid)	1	0	0	0.07
dicarboxylic acids	9	0.14	Succinic acid	2	1	0	0.2
cholesterol esters	13	0.27	CE (18:3)	3	0	3	0.2
dipeptides	16	0.41	N-Acetylhistidine	1	0	1	0.06
prostaglandins	9	0.43	Prostaglandin F2a	2	0	2	0.2
OH-FA 22_6_1	3	0.45	Resolvin D1	1	0	1	0.3
amino acids, basic	8	0.46	SDMA	2	0	2	0.2
unsaturated phosphatidylethanolamines	13	0.48	PE (36:2)	1	0	0	0.08
amino acids, branched-chain	3	0.53	Leucine	1	0	1	0.3
unsaturated glucosylceramides	12	0.65	GlcCer (d42:2) - ESI(+)	1	0	0	0.08
DiHETE	8	0.69	Leukotriene B4	1	0	1	0.1
adenosine	4	0.73	7-Methylguanosine	1	0	0	0.2
sugar alcohols	7	0.76	Mannitol	1	1	0	0.1
saturated FFA	18	0.76	Arachidic acid	1	1	0	0.06
diglycerides	14	0.81	DG (38:6)	1	0	0	0.07
amino acids, aromatic	7	1	Tyrosine	0	0	0	0
amino acids, cyclic	6	1	Histidine	0	0	0	0
amino alcohols	3	1	3-Amino-1-propanol	0	0	0	0
benzene derivatives	6	1	Tri-2-ethylhexyl trimellitate	0	0	0	0
DiHETrE	5	1	8,9-dihydroxyeicosa-5,11,14-trienoic acid	0	0	0	0
DiHODE	3	1	15,16-dihydroxyoctadeca-9,12-dienoic acid	0	0	0	0
DiHOME	4	1	9,10-dihydroxyoctadec-12-enoic acid	0	0	0	0
EpETrE	7	1	15(16)-epoxy-9,12-octadecadienoic acid	0	0	0	0
ethanolamines	3	1	Heptadecaphing-4-enine	0	0	0	0
guanidines	3	1	Guanidine	0	0	0	0
HETE	7	1	20-Hydroxyarachidonic acid	0	0	0	0
hexoses	10	1	Levoglucofan	0	0	0	0
histidine	4	1	Ergothioneine	0	0	0	0
HODE	3	1	9-Hydroxylinoleic acid	0	0	0	0
hydroxybutyrates	7	1	2-hydroxybutanoic acid	0	0	0	0
imidazoles	3	1	1,2-Dimethylimidazole	0	0	0	0
indoles	8	1	Kynurenine	0	0	0	0

Supplementary Table S8. ChemRICH enrichment analysis comparing ME/CFS without sr-IBS vs. controls without sr-IBS.

Cluster name	Cluster size	p-values	Key compound	Altered	Increased	Decreased	Altered Ratio
lipids	3	1	Dinor-12-oxophytodienoic acid	0	0	0	0
monounsaturated long chain TGs	16	1	TG (58:2)	0	0	0	0
monounsaturated TGs	18	1	TG (49:2)	0	0	0	0
nitroFA	3	1	10-nitrolinoleic acid	0	0	0	0
oxo-ODE	5	1	13-ketooctadeca-9,11-dienoic acid	0	0	0	0
pyridines	3	1	3-Hydroxypyridine	0	0	0	0
saturated ceramides	4	1	Ceramide (d42:0)	0	0	0	0
saturated phosphatidylcholines	9	1	PC (34:0) - ESI(-)	0	0	0	0
saturated sphingomyelins	10	1	SM (d32:0) - ESI(-)	0	0	0	0
sugar acids	3	1	Glyceric acid	0	0	0	0
unsaturated TGs	27	1	TG (48:4) A	0	0	0	0
xanthines	3	1	3-Methylxanthine	0	0	0	0

ME/CFS, myalgic encephalomyelitis/chronic fatigue syndrome; sr-IBS, self-reported physician diagnosed irritable bowel syndrome.

Supplementary Table S9. AUROC values and associated 95% CIs predicting ME/CFS and ME/CFS subgroups.

Predictive Modeling		All Metabolites		Metabolites with BF>1		Metabolites with BF>3	
		AUROC	95% CI	AUROC	95% CI	AUROC	95% CI
ME/CFS vs. Controls	Lasso	0.636	(0.450, 0.822)	0.656	(0.477, 0.834)	0.608	(0.424, 0.793)
	Adaptive Lasso	0.644	(0.462, 0.827)	0.575	(0.388, 0.762)	0.575	(0.388, 0.762)
	Random Forests	0.589	(0.402, 0.776)	0.656	(0.478, 0.833)	0.631	(0.447, 0.814)
	XGBoost	0.589	(0.402, 0.776)	0.567	(0.377, 0.756)	0.592	(0.406, 0.777)
	Model Average	0.589	(0.402, 0.776)	0.656	(0.478, 0.833)	0.633	(0.451, 0.816)
Female ME/CFS vs. Female Controls	Lasso	0.709	(0.480, 0.938)	0.794	(0.612, 0.976)	0.745	(0.538, 0.953)
	Adaptive Lasso	0.703	(0.474, 0.932)	0.721	(0.489, 0.953)	0.727	(0.496, 0.959)
	Random Forests	0.691	(0.471, 0.911)	0.673	(0.447, 0.898)	0.764	(0.553, 0.975)
	XGBoost	0.655	(0.425, 0.884)	0.624	(0.387, 0.862)	0.776	(0.571, 0.980)
	Model Average	0.679	(0.455, 0.902)	0.770	(0.570, 0.969)	0.739	(0.527, 0.952)
ME/CFS without sr-IBS vs. Controls without sr-IBS	Lasso	0.500	(0.500, 0.500)	0.810	(0.654, 0.966)	0.873	(0.747, 0.999)
	Adaptive Lasso	0.552	(0.332, 0.772)	0.679	(0.453, 0.905)	0.588	(0.365, 0.812)
	Random Forests	0.638	(0.432, 0.844)	0.862	(0.733, 0.991)	0.810	(0.641, 0.979)
	XGBoost	0.588	(0.373, 0.804)	0.738	(0.544, 0.931)	0.756	(0.572, 0.939)
	Model Average	0.638	(0.432, 0.844)	0.864	(0.736, 0.993)	0.837	(0.675, 0.999)

ME/CFS, myalgic encephalomyelitis/chronic fatigue syndrome; sr-IBS, self-reported physician diagnosed irritable bowel syndrome; BF, BayesFactor; AUROC, area under the receiver operating characteristic; CI, confidence interval. The predictive models were first trained in the 80% randomly-selected training set and were validated in the remaining 20% test set.