

## Mass Spectrometry: From Proteomics to Metabolomics and Lipidomics

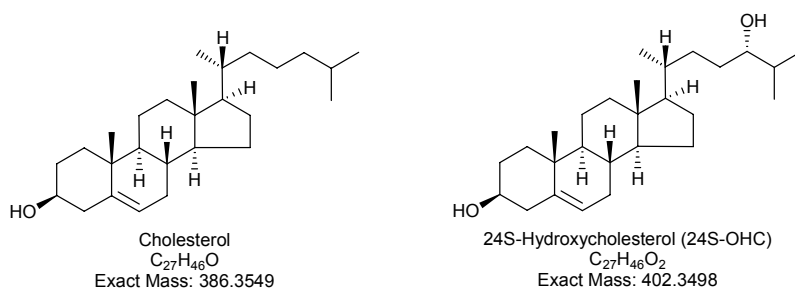
William J Griffiths and Yuqin Wang

Institute of Mass Spectrometry, School of Medicine, Swansea University, Singleton Park,  
Swansea SA2 8PP

### Supplementary Information

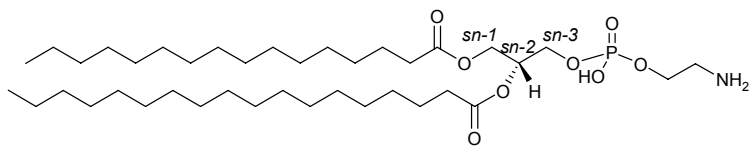
#### Lipid nomenclature used in this Tutorial Review

##### Sterols

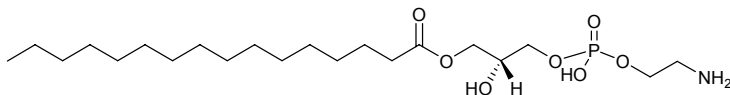


##### Glycerophospholipids

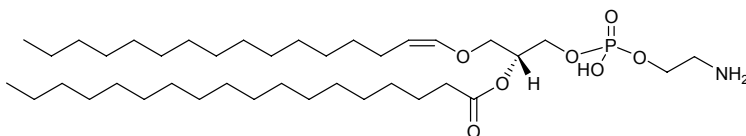
Phosphatidyl (Ptd) uniquely designates 1,2-diacyl species. The designations *sn-1*, *sn-2* and *sn-3* is used to designate the carbon atoms of the glycerol backbone, where *sn* refers to stereospecifically numbered.



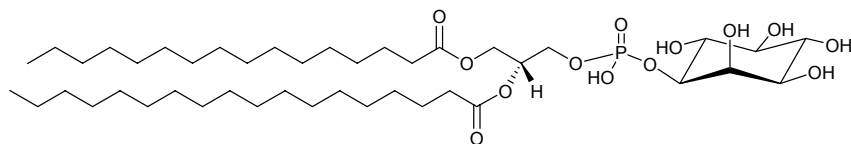
1-hexadecanoyl-2-octadecanoyl-sn-glycero-3-phosphoethanolamine PE(16:0/18:0) or PtdEtn (16:0/18:0)  
 $C_{39}H_{78}NO_8P$   
Exact Mass: 719.5465



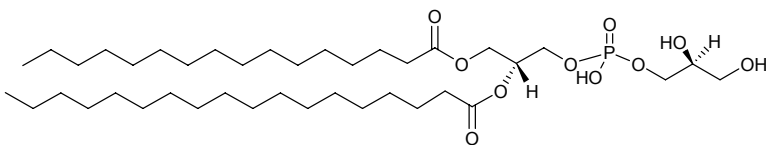
1-hexadecanoyl-sn-glycero-3-phosphoethanolamine PE(16:0/0:0) or LysoPEtn (16:0)  
 $C_{21}H_{44}NO_7P$   
Exact Mass: 453.2855



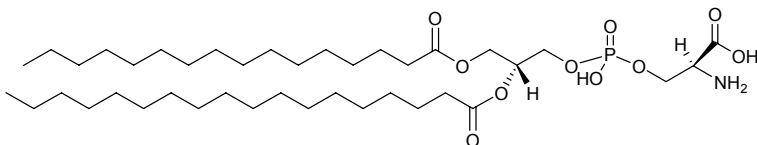
1-(1Z-hexadecenyl)-2-octadecanoyl-sn-glycero-3-phosphoethanolamine PE(O-16:1(1Z)/18:0) or  
PlsEtn (O-16:1/18:0)  
 $C_{39}H_{78}NO_7P$   
Exact Mass: 703.5516



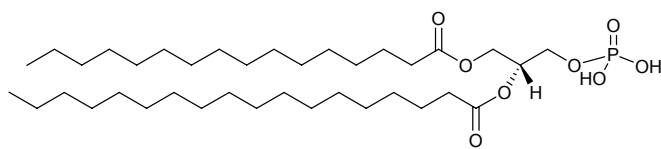
1-hexadecanoyl-2-octadecanoyl-sn-glycero-3-phospho-(1'-myo-inositol) PI(16:0/18:0) or PtdIns (16:0/18:0)  
 $C_{43}H_{83}O_{13}P$   
Exact Mass: 838.5571



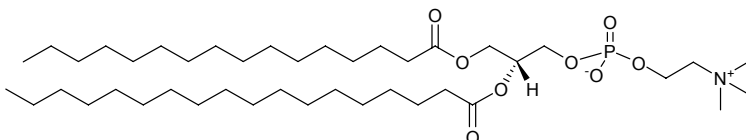
1-hexadecanoyl-2-octadecanoyl-sn-glycero-3-phospho-(1'-sn-glycerol) PG(16:0/18:0) or PtdGro (16:0/18:0)  
 $C_{40}H_{79}O_{10}P$   
Exact Mass: 750.5411



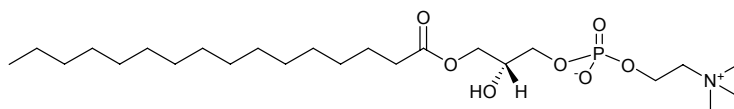
1-hexadecanoyl-2-octadecanoyl-sn-glycero-3-phosphoserine PS(16:0/18:0) or PtdSer (16:0/18:0)  
 $C_{40}H_{78}NO_{10}P$   
Exact Mass: 763.5363



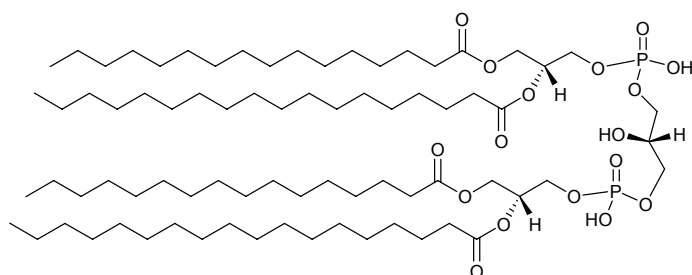
1-hexadecanoyl-2-octadecanoyl-sn-glycero-3-phosphate PA(16:0/18:0) or PtdH (16:0/18:0)  
 $C_{37}H_{73}O_8P$   
Exact Mass: 676.5043



1-hexadecanoyl-2-octadecanoyl-sn-glycero-3-phosphocholine PC(16:0/18:0) or PtdCho (16:0/18:0)  
 $C_{42}H_{84}NO_8P$   
Exact Mass: 761.5935

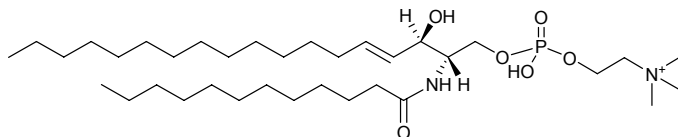


1-hexadecanoyl-sn-glycero-3-phosphocholine PC(16:0/0:0) LysoPCho (16:0)  
 $C_{24}H_{50}NO_7P$   
Exact Mass: 495.3325

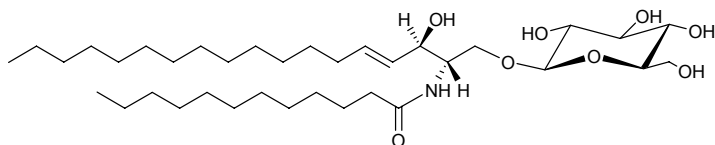


1',3'-Bis-[1-hexadecanoyl-2-octadecanoyl-sn-glycero-3-phospho]-sn-glycerol  
CL(1'-[16:0/18:0],3'-[16:0/18:0])  
 $C_{77}H_{150}O_{17}P_2$   
Exact Mass: 1409.0348

### Sphingolipids

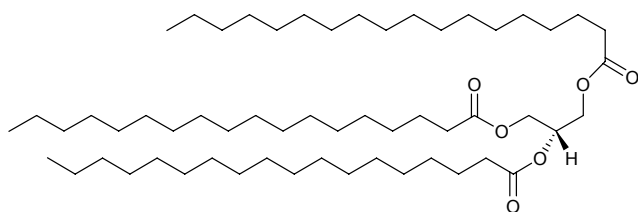


N-(dodecanoyl)-sphing-4-enine-1-phosphocholine SM(d18:1(4E)/12:0)  
 $C_{35}H_{72}N_2O_6P^+$   
Exact Mass: 647.5123



N-(dodecanoyl)-1-β-glucosyl-sphing-4-enine GlcCer(d18:1/12:0)  
 $C_{36}H_{69}NO_8$   
Exact Mass: 643.5023

### Glycerolipids



1,2,3-trioctadecanoyl-sn-glycerol TG(18:0/18:0/18:0) or TAG (18:0/18:0/18:0)  
 $C_{57}H_{110}O_6$   
Exact Mass: 890.8302