

Synthesis, Spectroscopic, X-Ray Powder Diffraction and Molecular Docking Studies of Biologically Potent Organotin(IV) Complexes with N-Acetylated β -Amino Acids: An *In Vitro* and *In Vivo* Antidiabetic Activity

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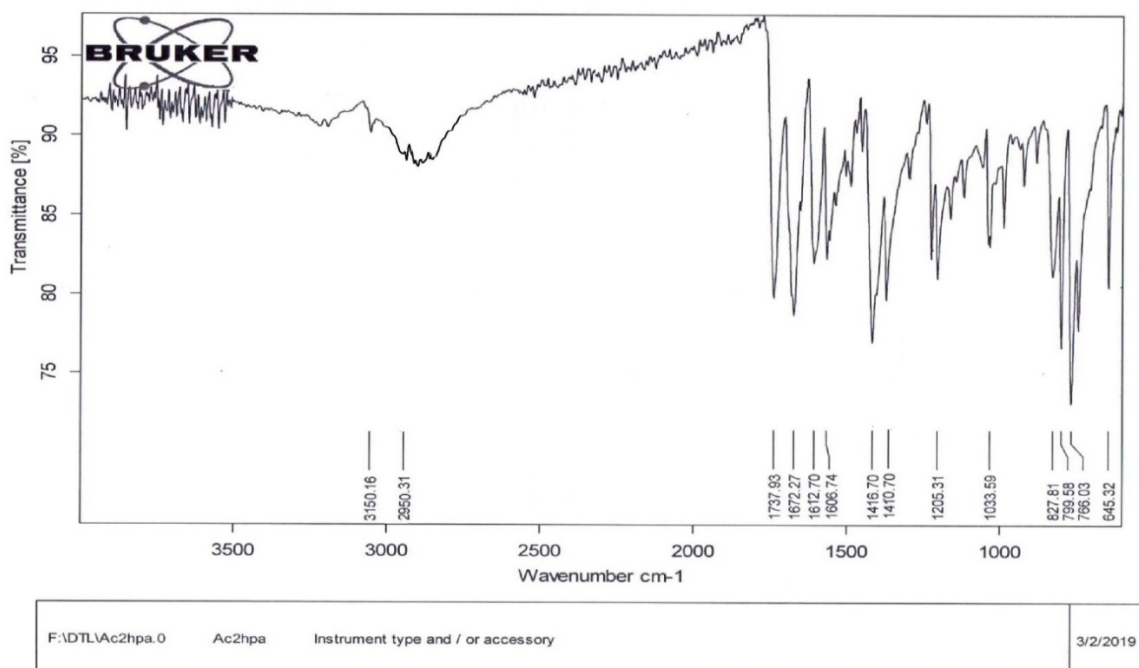
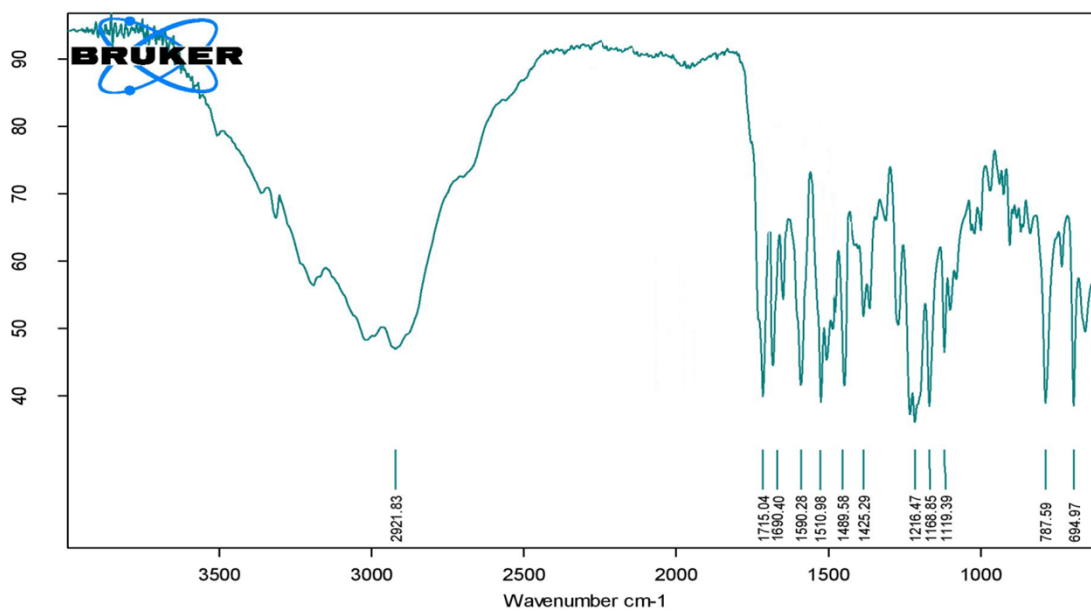
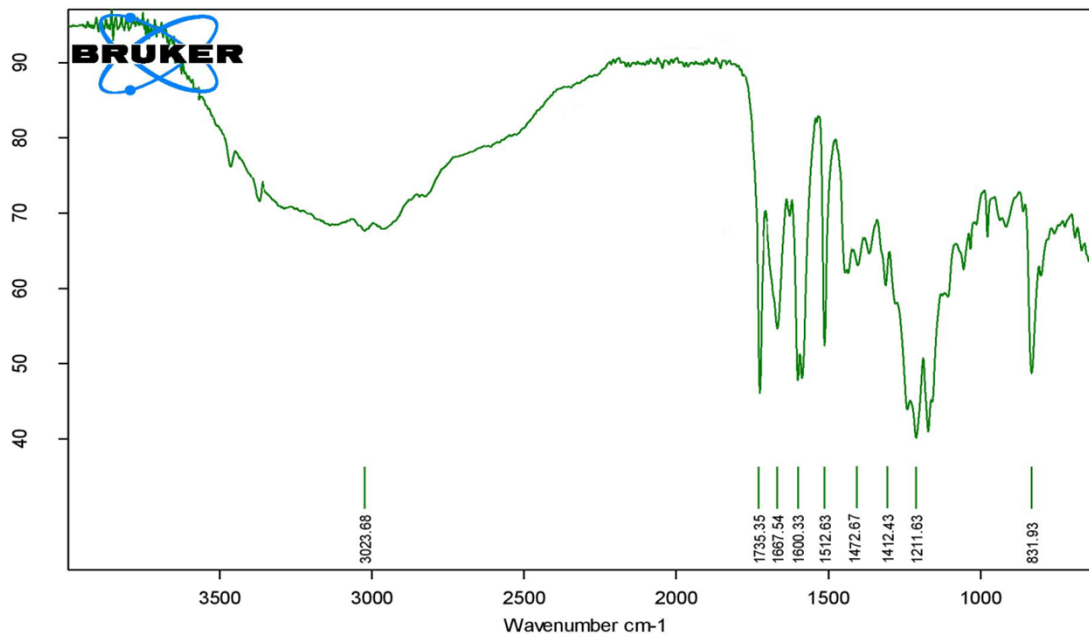


Fig. S1 FTIR spectrum of 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid **L₁**



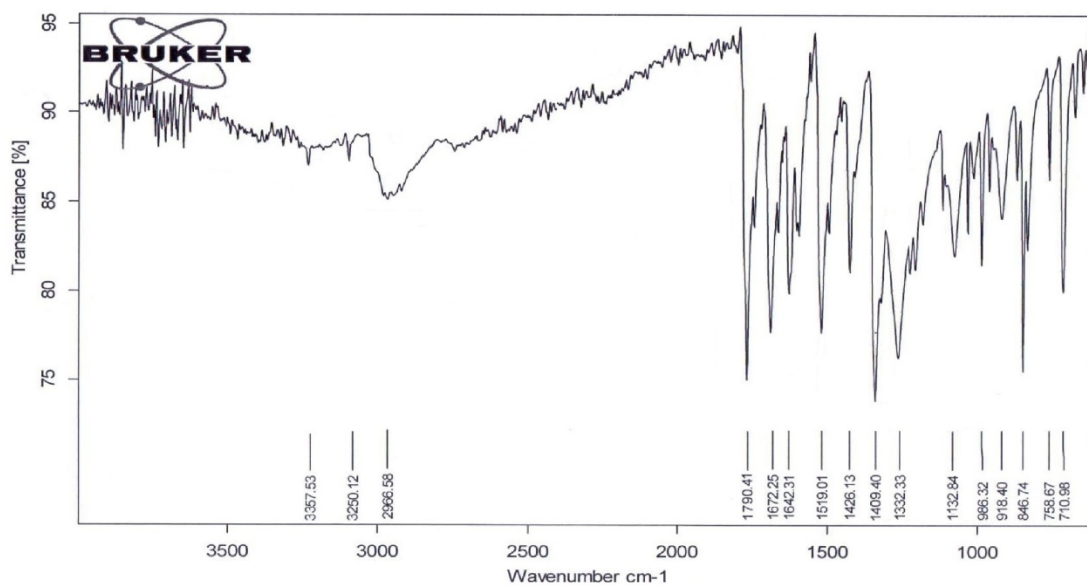
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Fig. S2 FTIR spectrum of the 3-Acetylamino-3(3-hydroxyphenyl) propanoic acid **L₂**



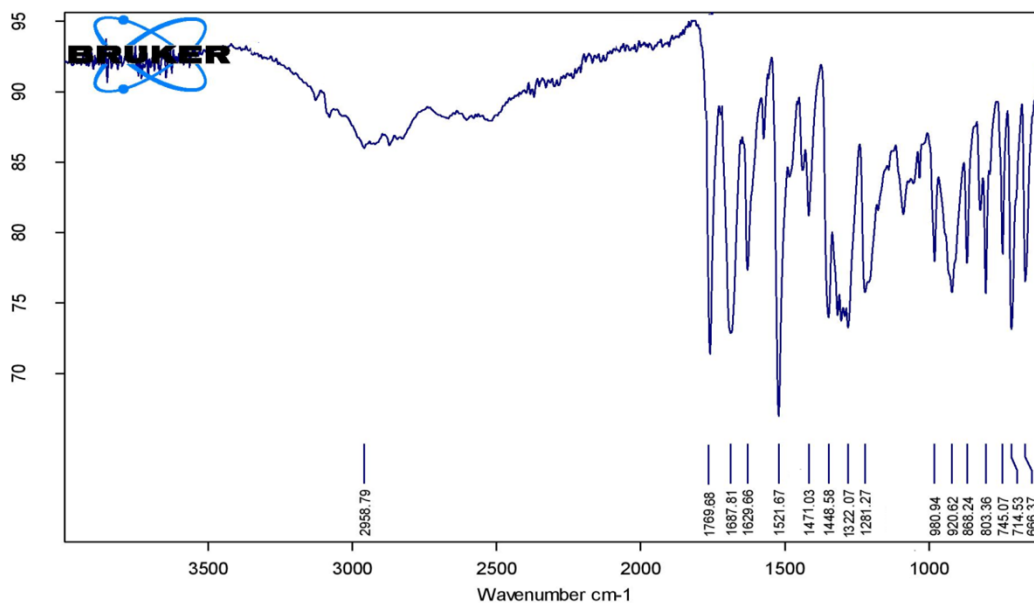
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Fig. S3 FTIR spectrum of 3-Acetylamino-3(4-hydroxyphenyl) propanoic acid **L₃**



F:\DTL\Ac2Npa.0	Ac2Npa	Instrument type and / or accessory	3/2/2019
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Fig. S4 FTIR spectrum of 3-Acetylamino-3(2-nitrophenyl) propanoic acid **L₄**



F:\DTL\Ac3npa.0	Ac3npa	Instrument type and / or accessory	3/2/2019
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Fig. S5 FTIR spectrum of the 3-Acetylamino-3(3-nitrophenyl) propanoic acid **L₅**

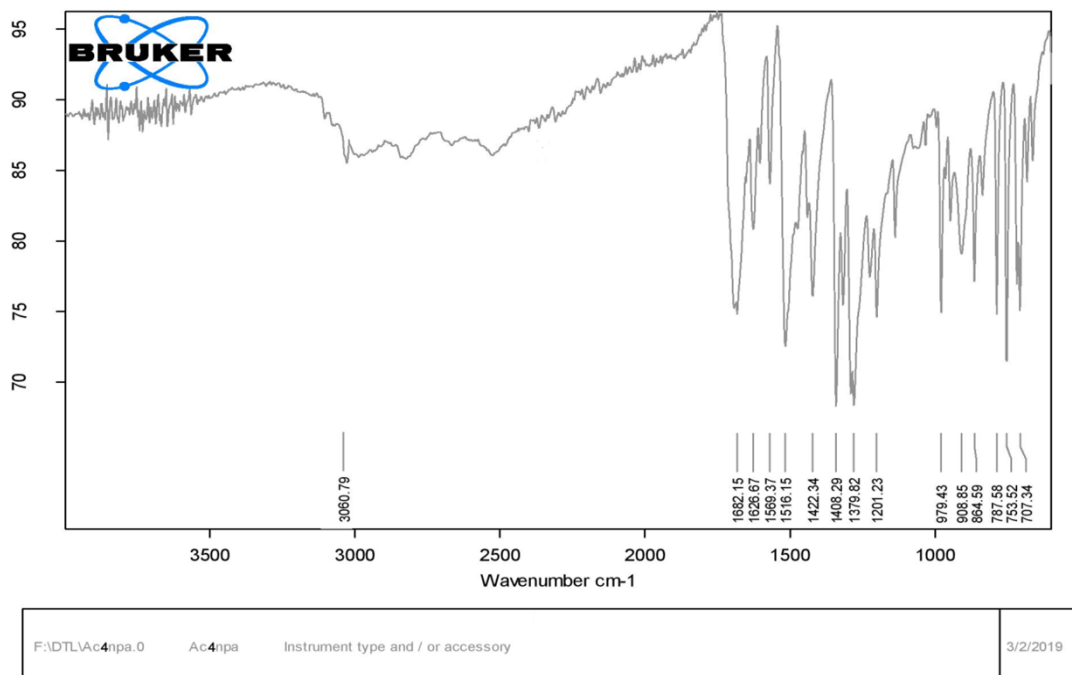


Fig. S6 FTIR spectrum of 3-Acetylamino-3(4-nitrophenyl) propanoic acid **L₆**

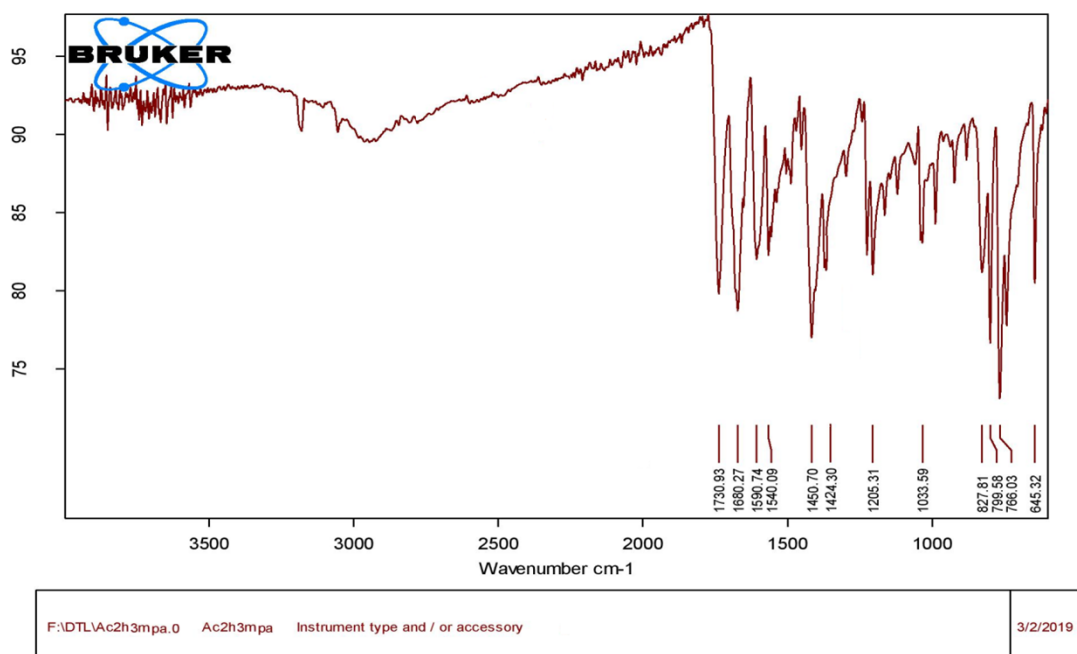
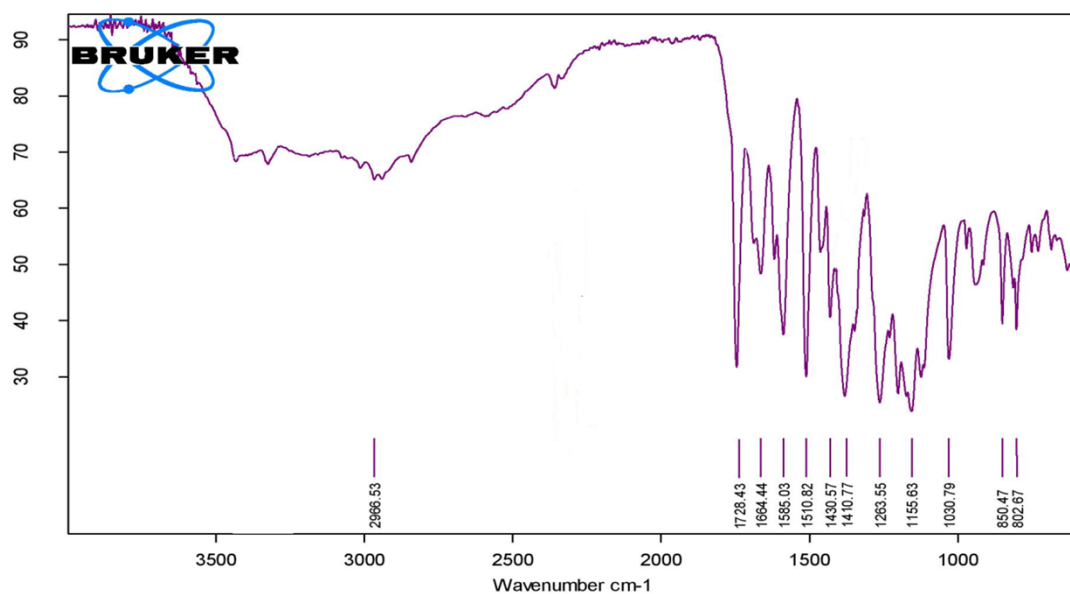
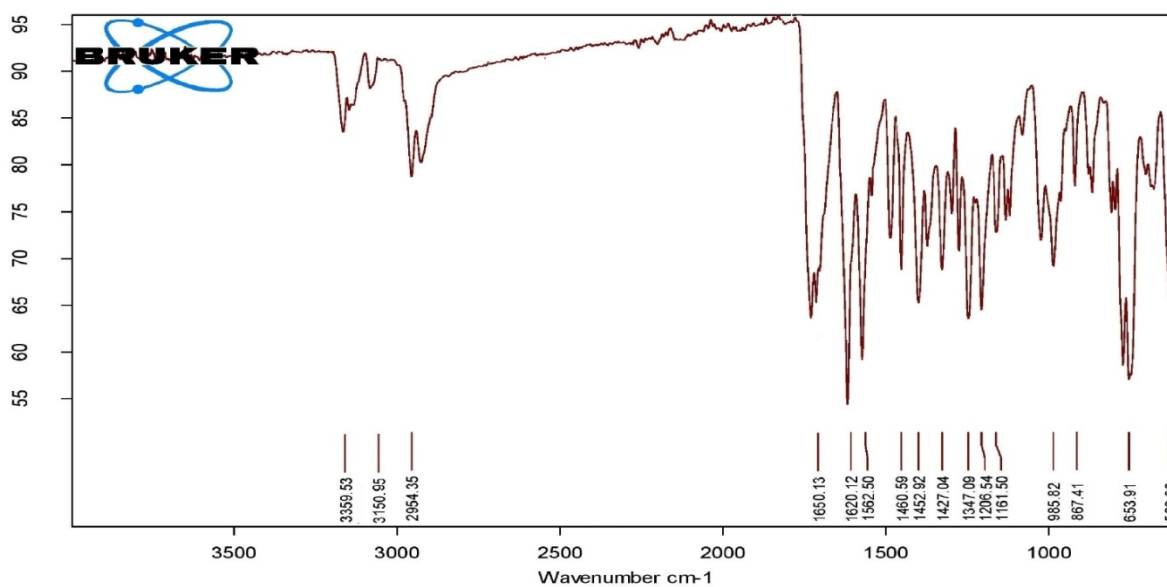


Fig. S7 FTIR spectrum of 3-Acetylamino-3(3-hydroxy-2-methoxyphenyl) propanoic acid **L₇**



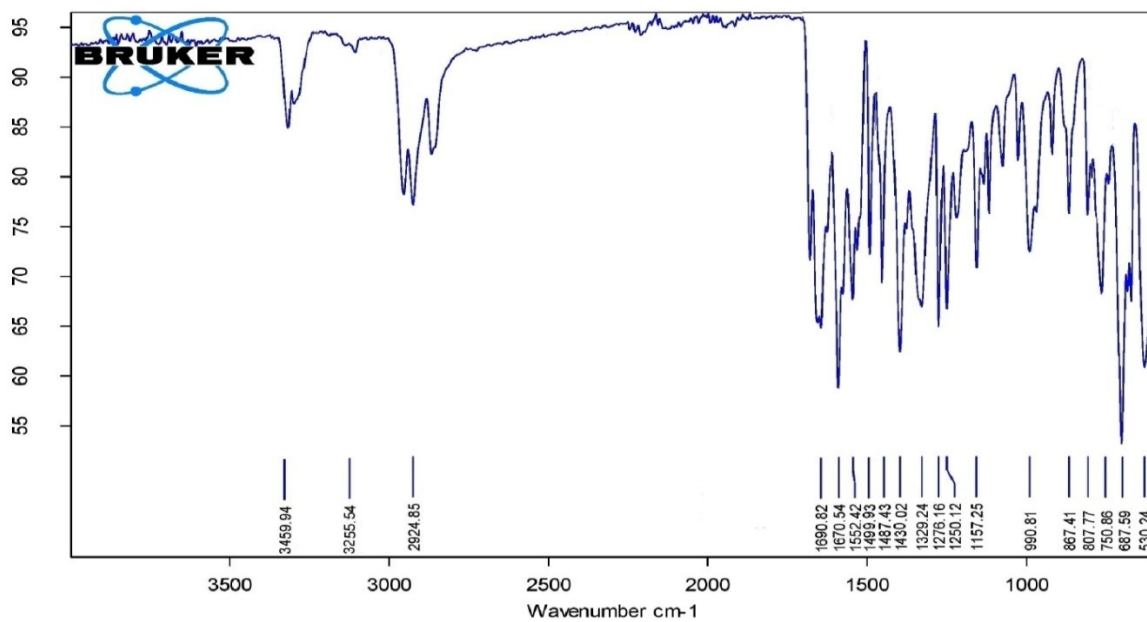
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Fig. S8 FTIR spectrum of 3-Acetylaminopropanoic acid **L**₈



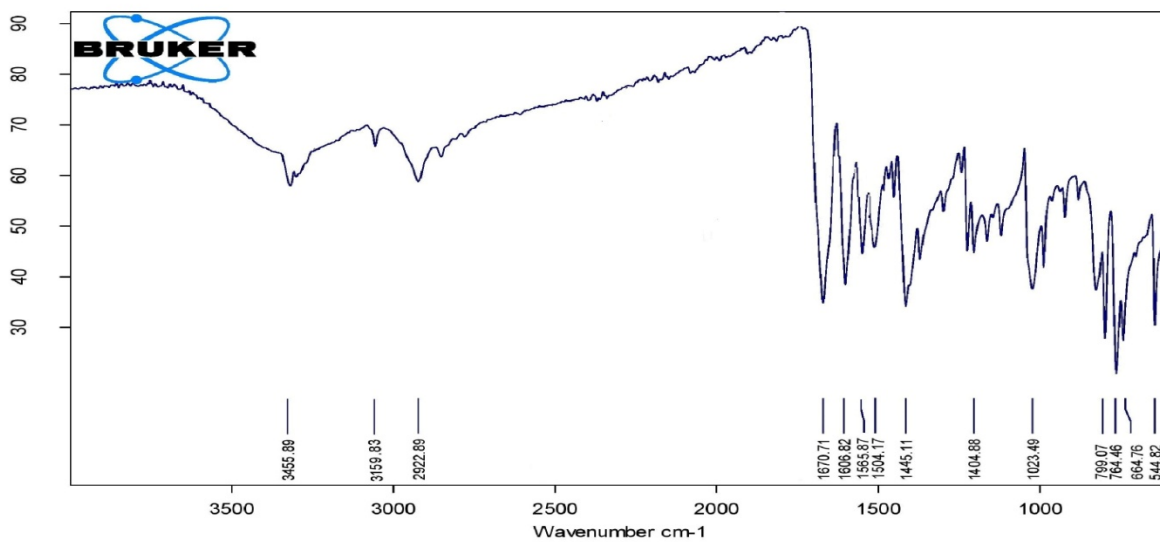
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Fig. S9 FTIR spectrum of the dibutyltin(IV) oxide monomer complex (**1**) with 3-Acetylaminopropanoic acid **L**₁



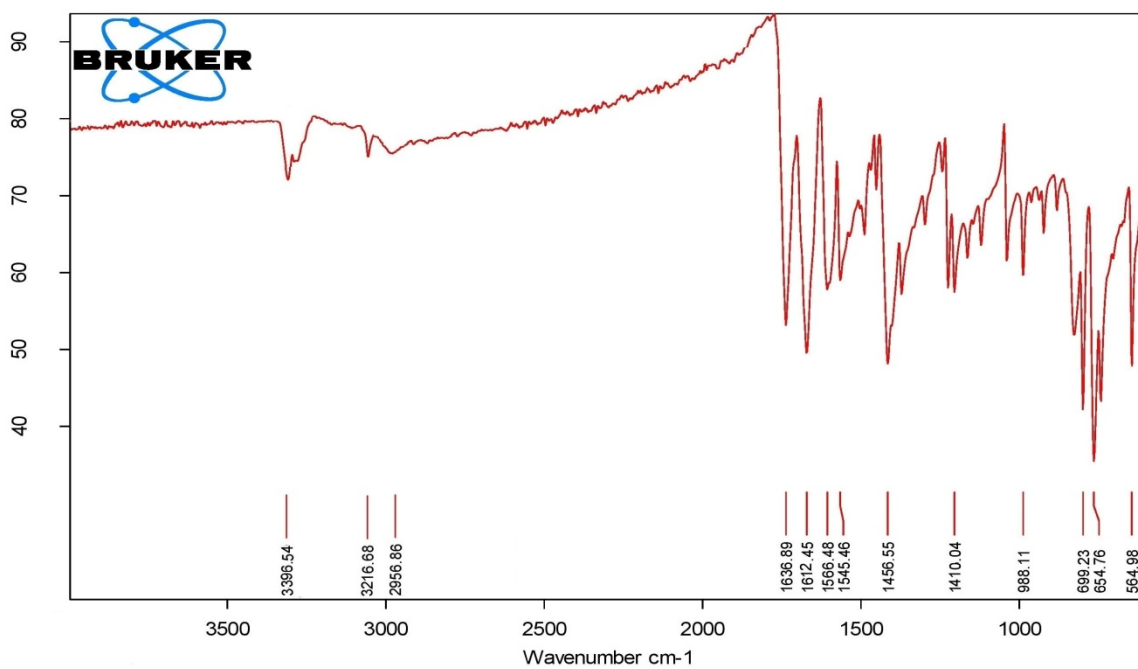
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Fig. S10 FTIR spectrum of the dibutyltin(IV) oxide dimer complex (**2**) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid **L**₁



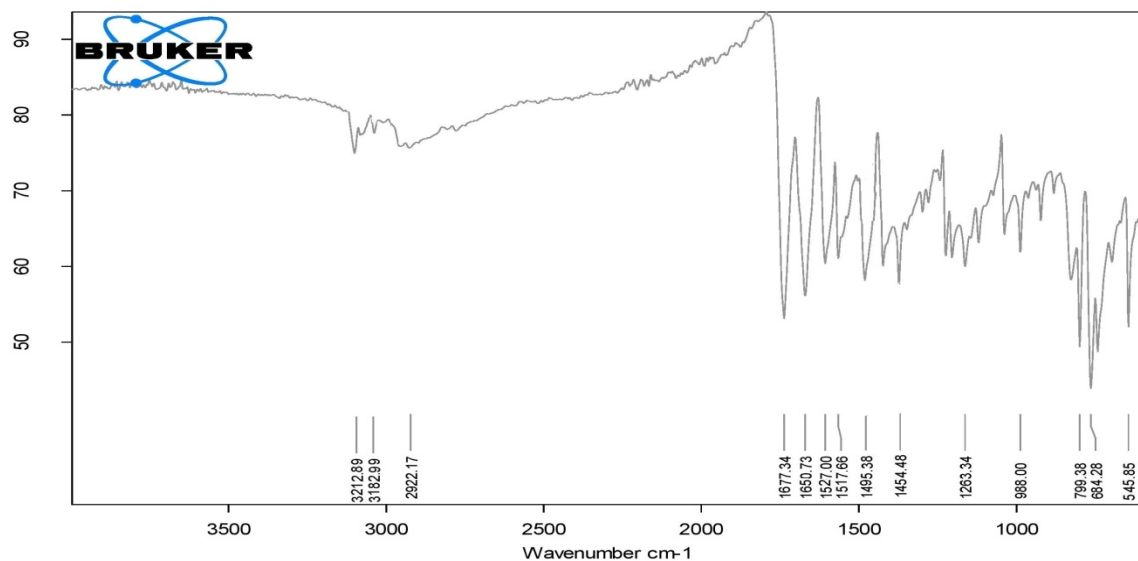
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Fig. S11 FTIR spectrum of the dibutyltin(IV) dichloride complex (**3**) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid **L**₁



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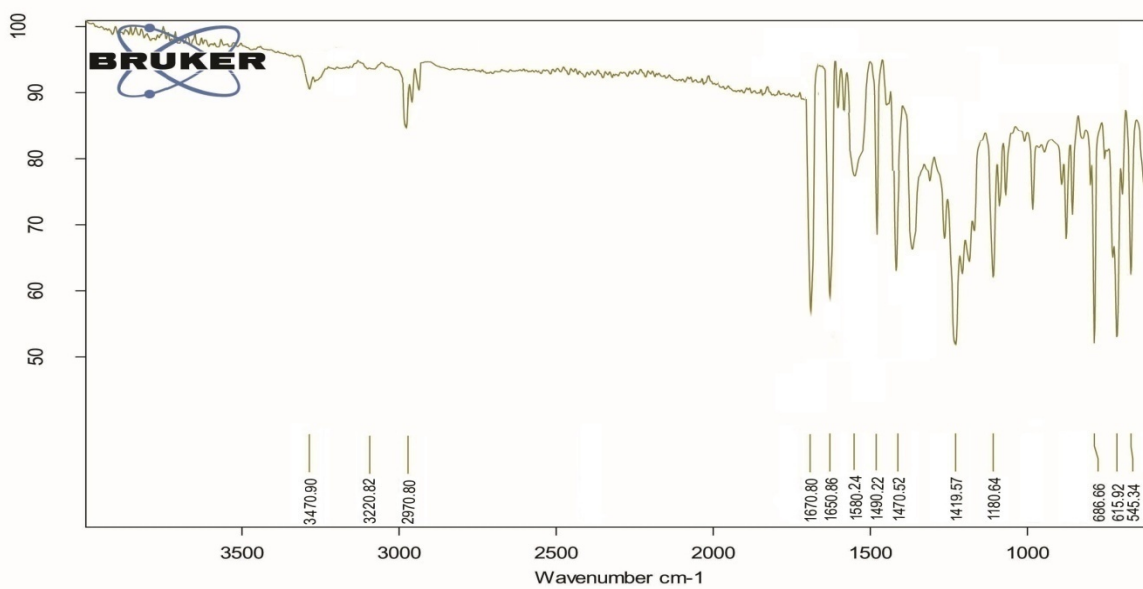
Fig. S12 FTIR spectrum of the tributyltin(IV) chloride complex (**4**) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid **L₁**



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Fig. S13 FTIR spectrum of the triphenyltin(IV) chloride complex (**5**) with 3-Acetylamino-3(2-

hydroxyphenyl) propanoic acid **L**₁



F:\DTL\Cyclohex3snclac2h.0 Cyclohex3snclac2h Instrument type and / or accessory 8/10/2019

Fig. S14 FTIR spectrum of the tricyclohexyltin(IV) chloride complex (**6**) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid **L**₁

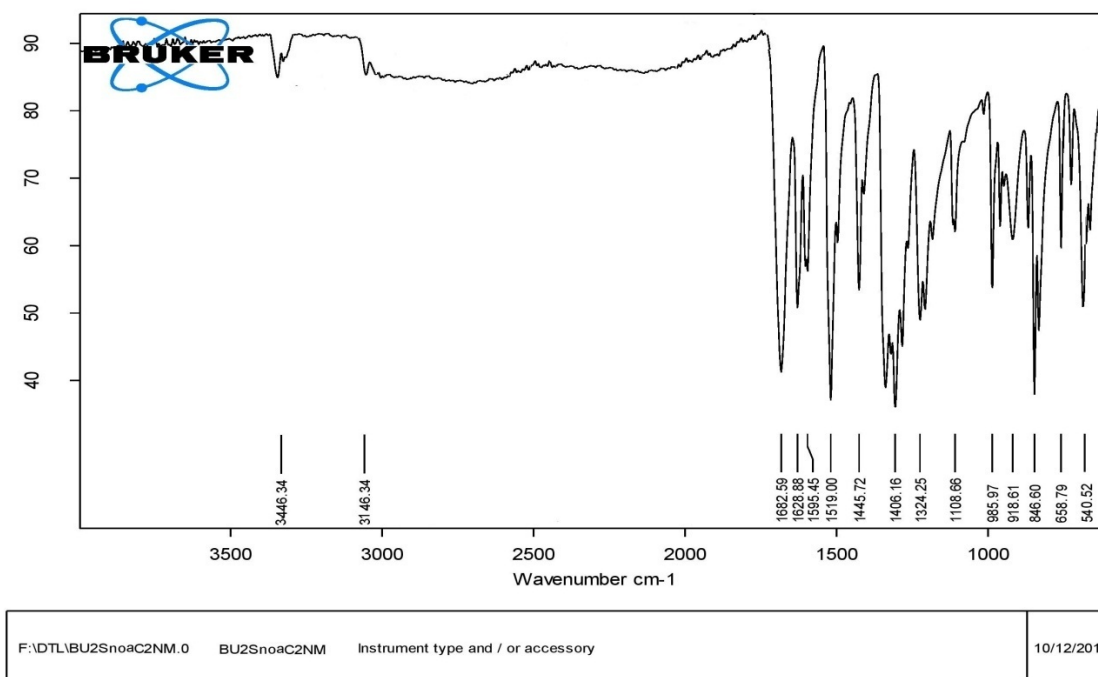


Fig. S15 FTIR spectrum of the dibutyltin(IV) oxide monomer complex (**7**) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid L_4

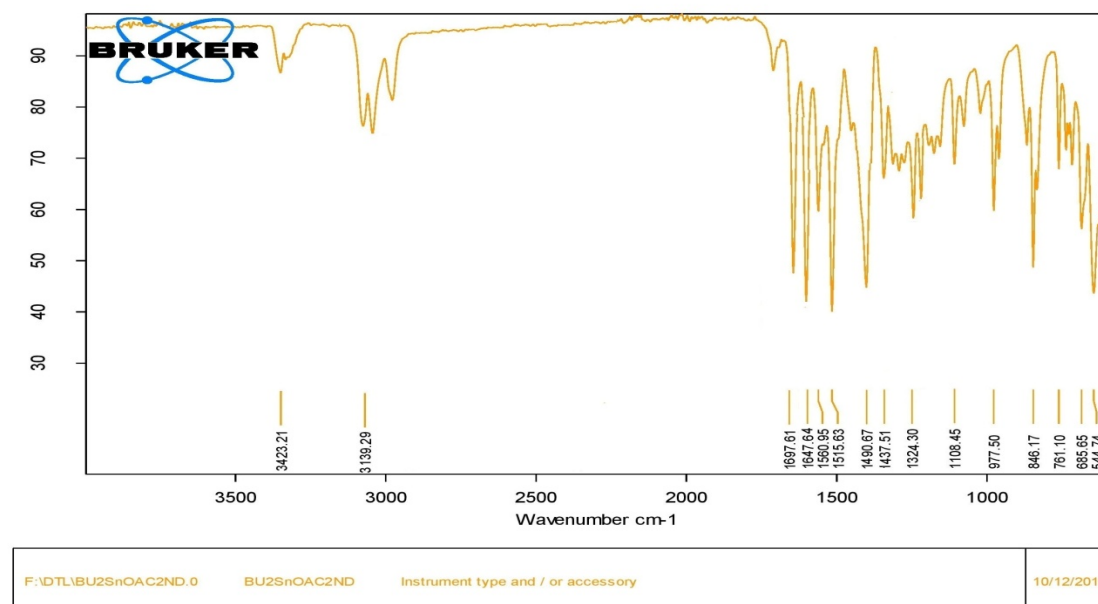


Fig. S16 FTIR spectrum of the dibutyltin(IV) oxide dimer complex (**8**) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid L_4

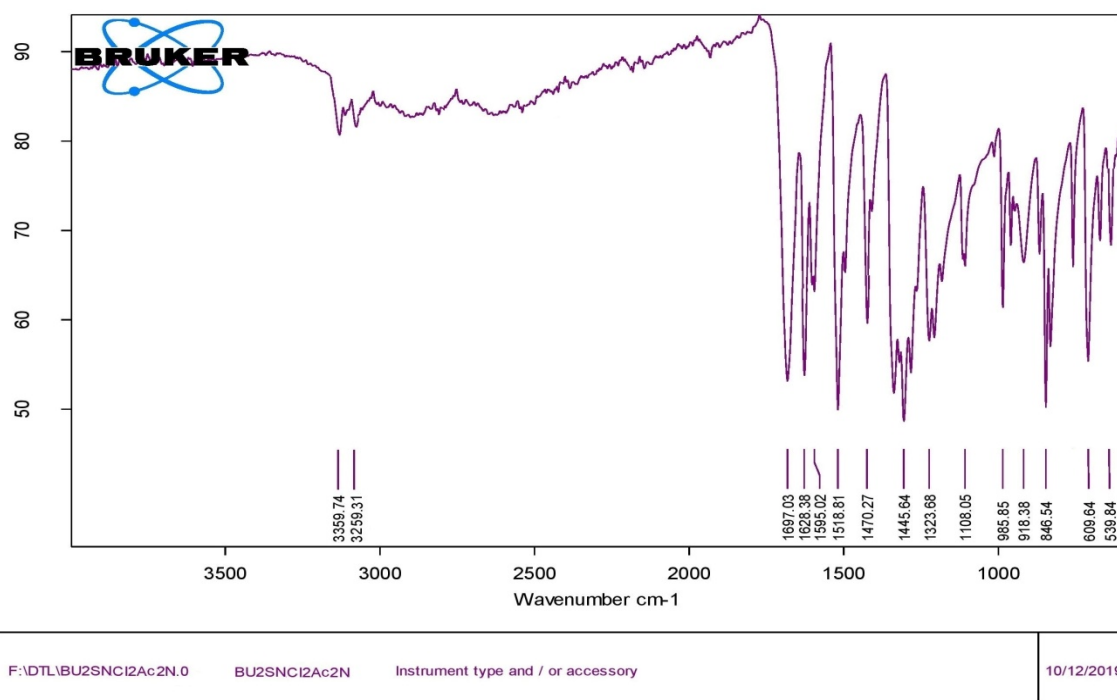


Fig. S17 FTIR spectrum of the dibutyltin(IV) dichloride complex (**9**) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid **L₄**

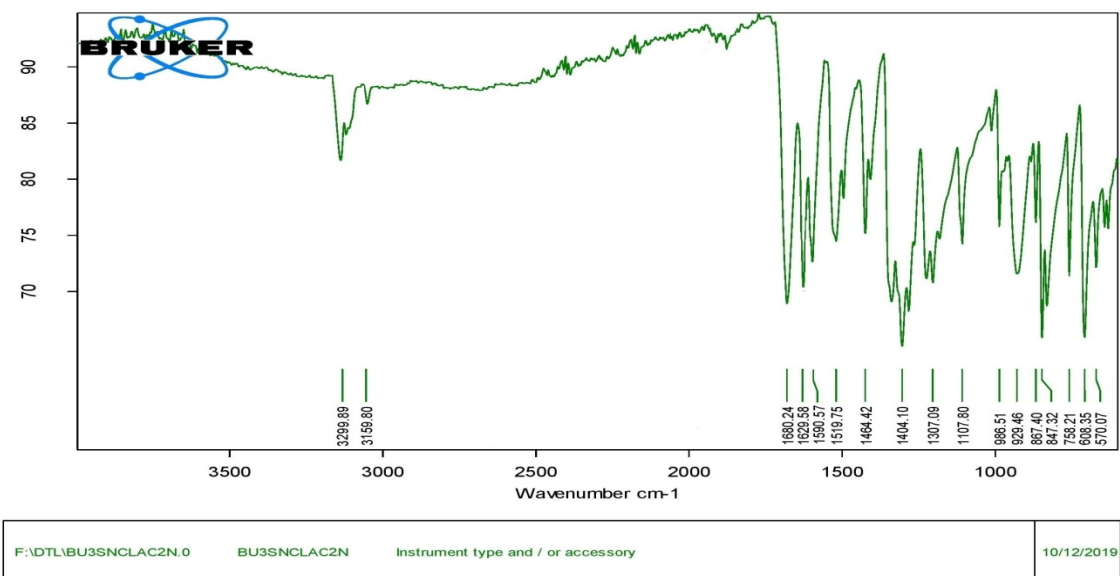


Fig. S18 FTIR spectrum of the tributyltin(IV) chloride complex (**10**) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid **L₄**

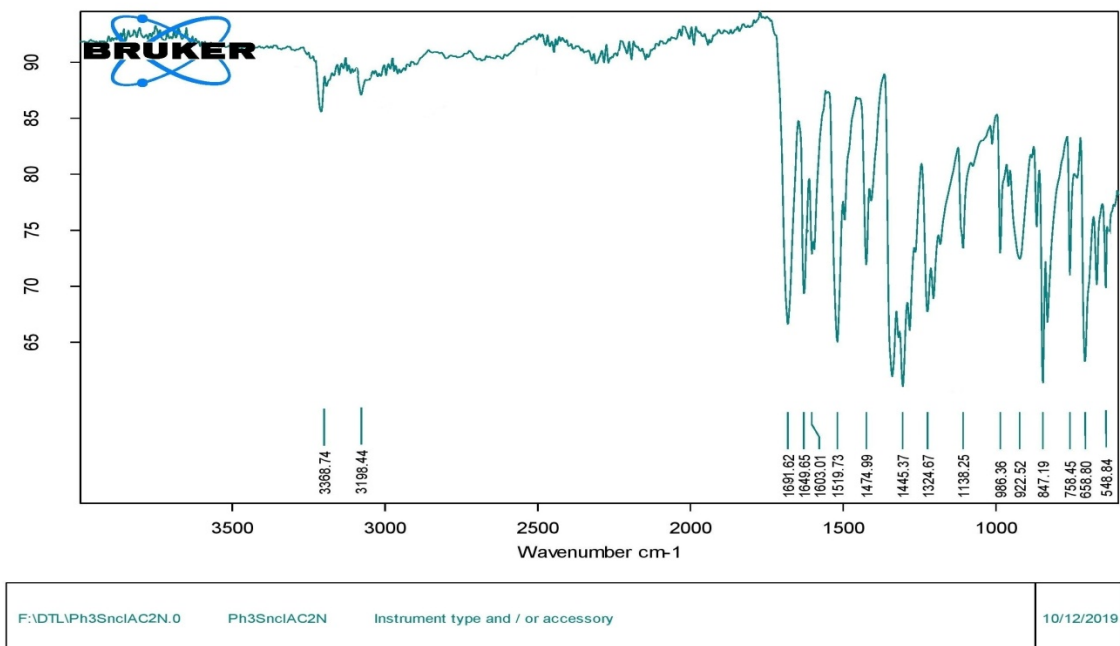


Fig. S19 FTIR spectrum of the triphenyltin(IV) chloride complex (**11**) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid **L₄**

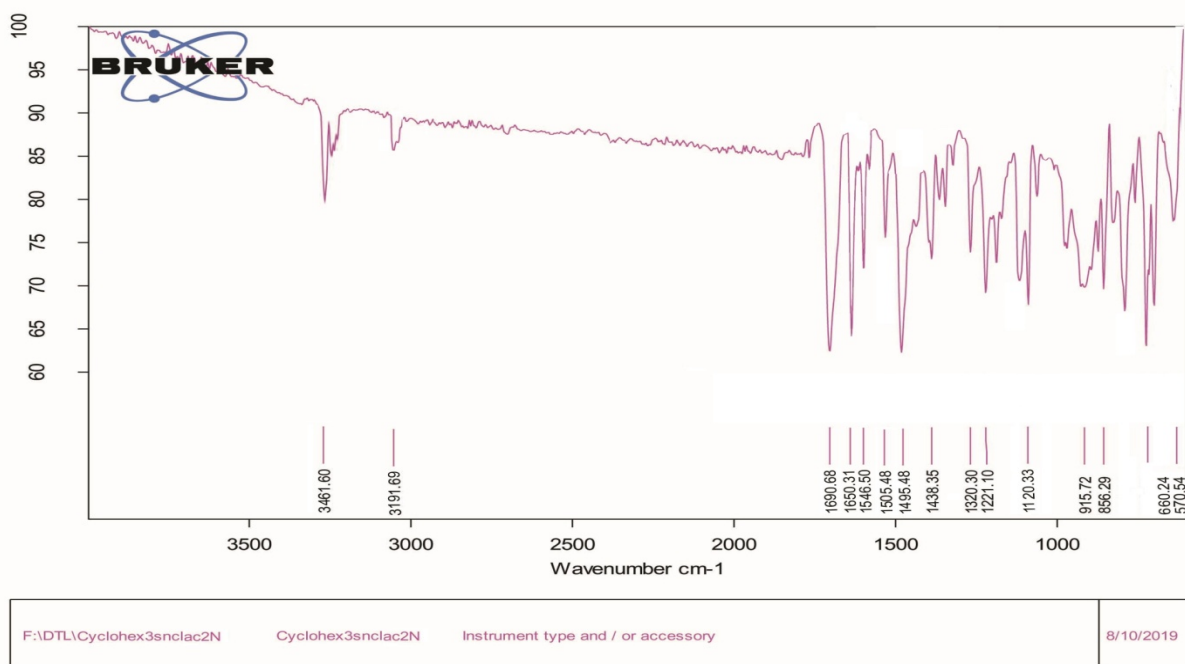


Fig. S20 FTIR spectrum of the tricyclohexyltin(IV) chloride complex (**12**) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid **L₄**

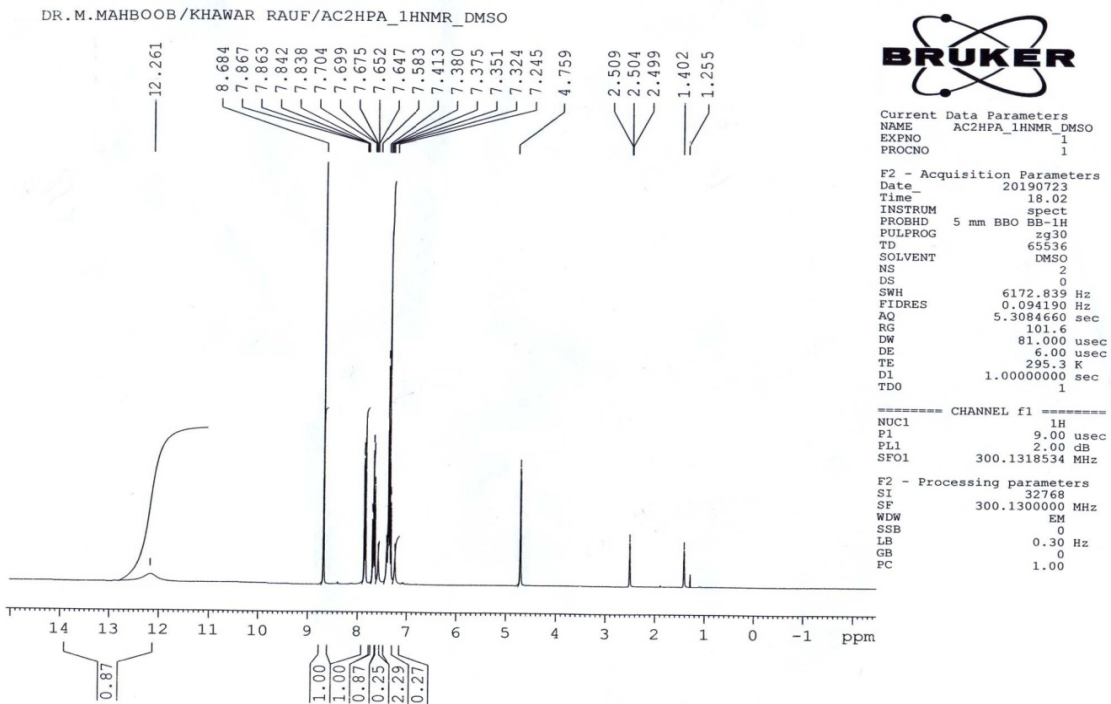


Fig. S21 ^1H NMR spectrum (400 MHz, DMSO) of 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid L_1

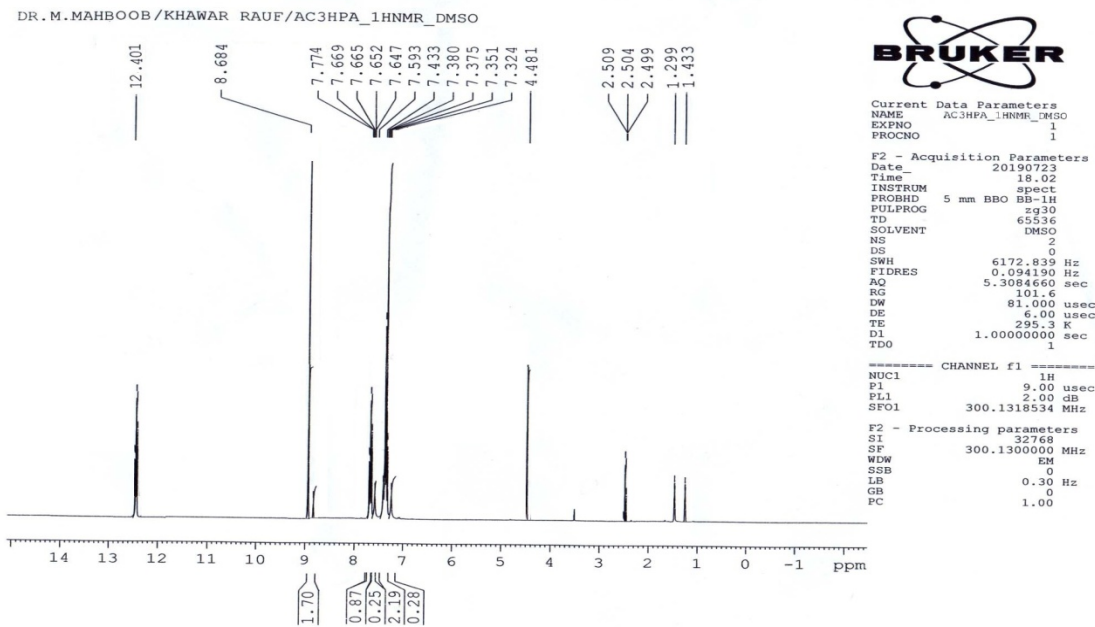


Fig. S22 ^1H NMR spectrum (400 MHz, DMSO) of 3-Acetylamino-3(3-hydroxyphenyl) propanoic acid L_2

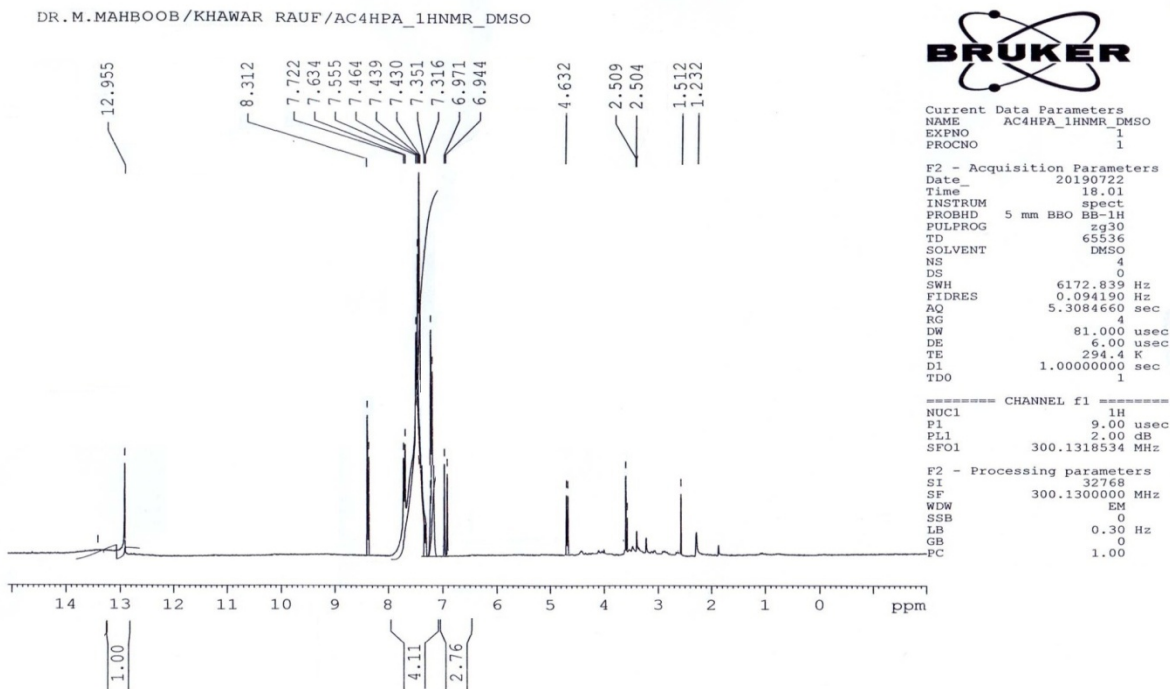


Fig. S23 ^1H NMR spectrum (400 MHz, DMSO) of 3-Acetylamino-3(4-hydroxyphenyl) propanoic acid **L₃**

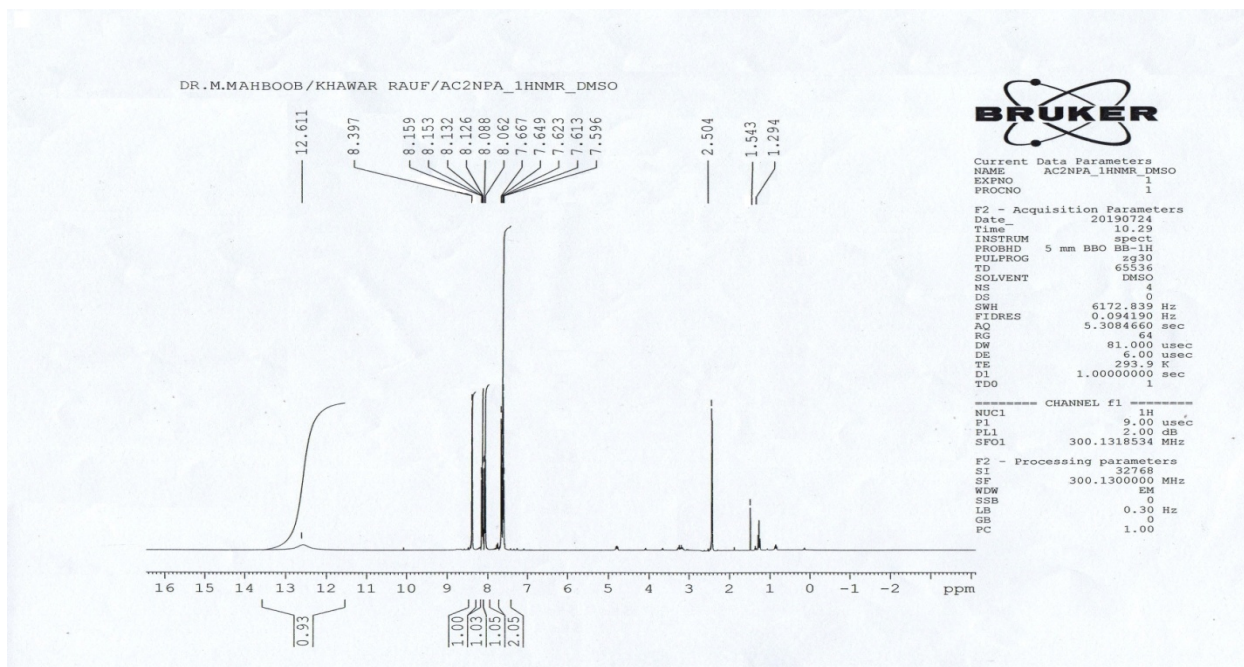


Fig. S24 ^1H NMR spectrum (400 MHz, DMSO) of 3-Acetylamino-3(2-nitrophenyl) propanoic acid

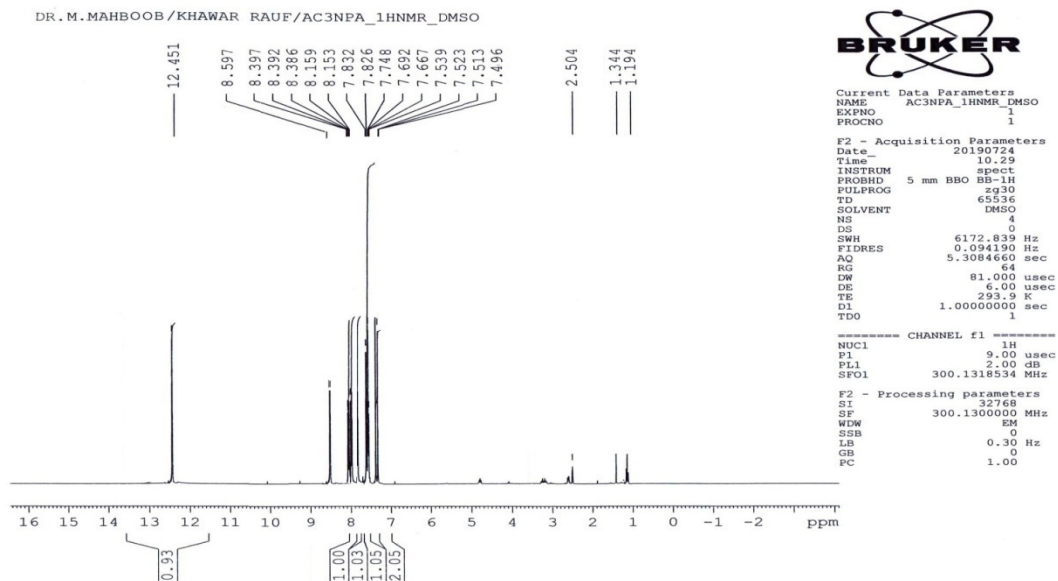


Fig. S25 ¹H NMR spectrum (400 MHz, DMSO) of 3-Acetylamino-3(3-nitrophenyl) propanoic acid

L₅

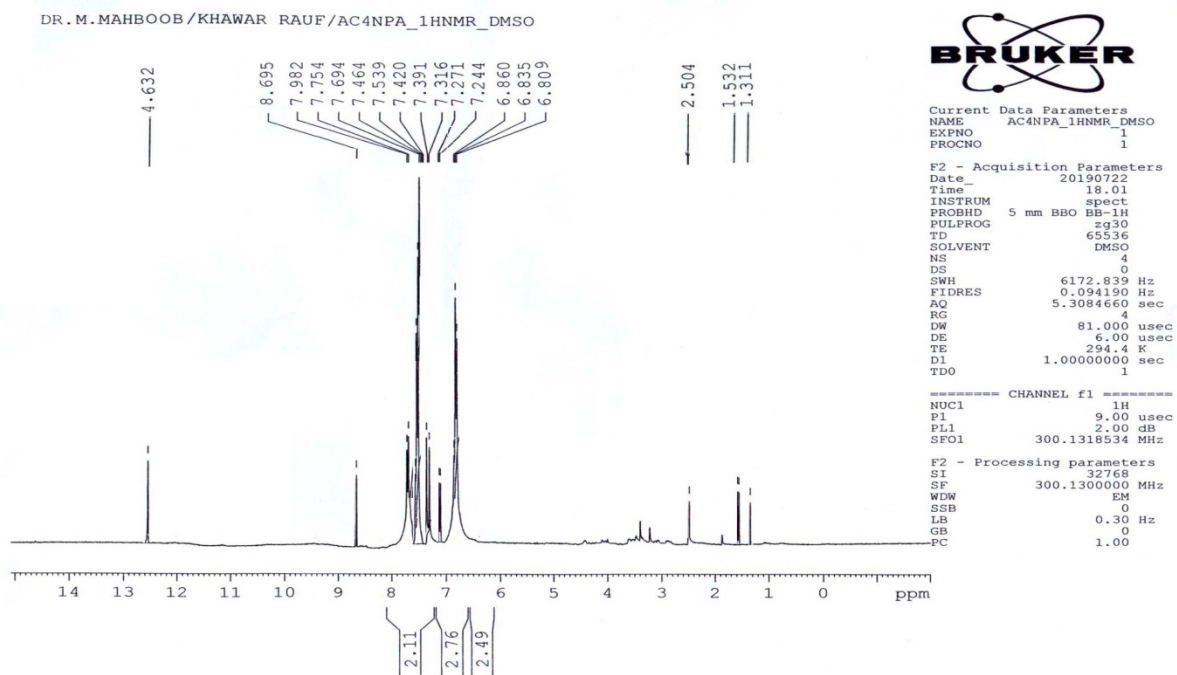


Fig. S26 ¹H NMR spectrum (400 MHz, DMSO) of 3-Acetylamino-3(4-nitrophenyl) propanoic acid

L₆

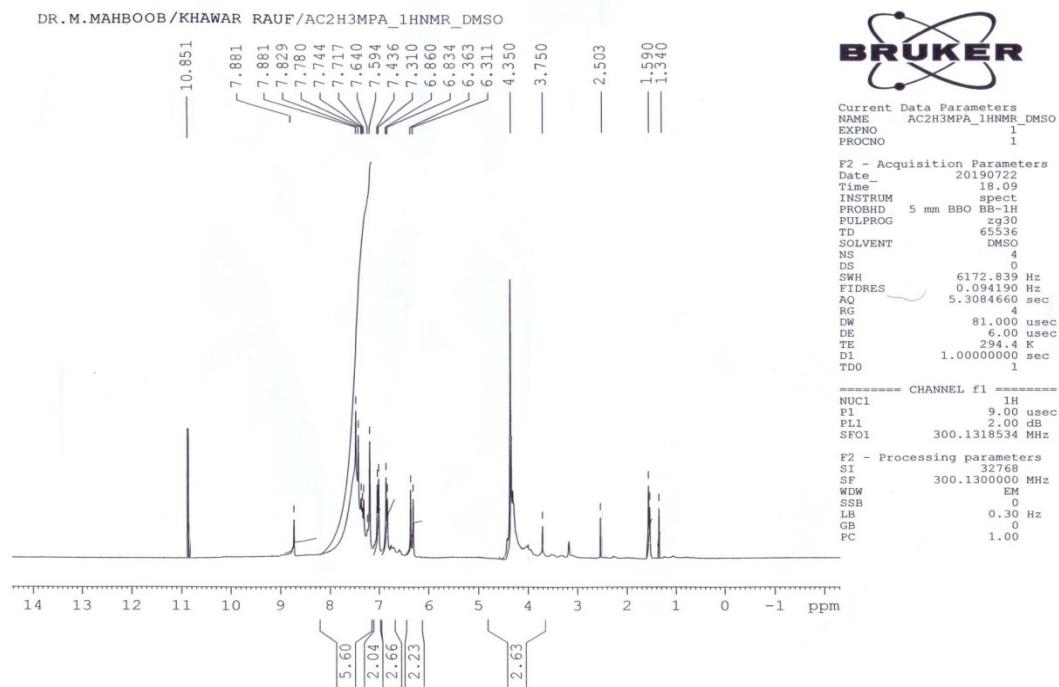


Fig. S27 ^1H NMR spectrum (400 MHz, DMSO) of 3-Acetylamino-3(2-hydroxy-3-methoxyphenyl) propanoic acid **L₇**

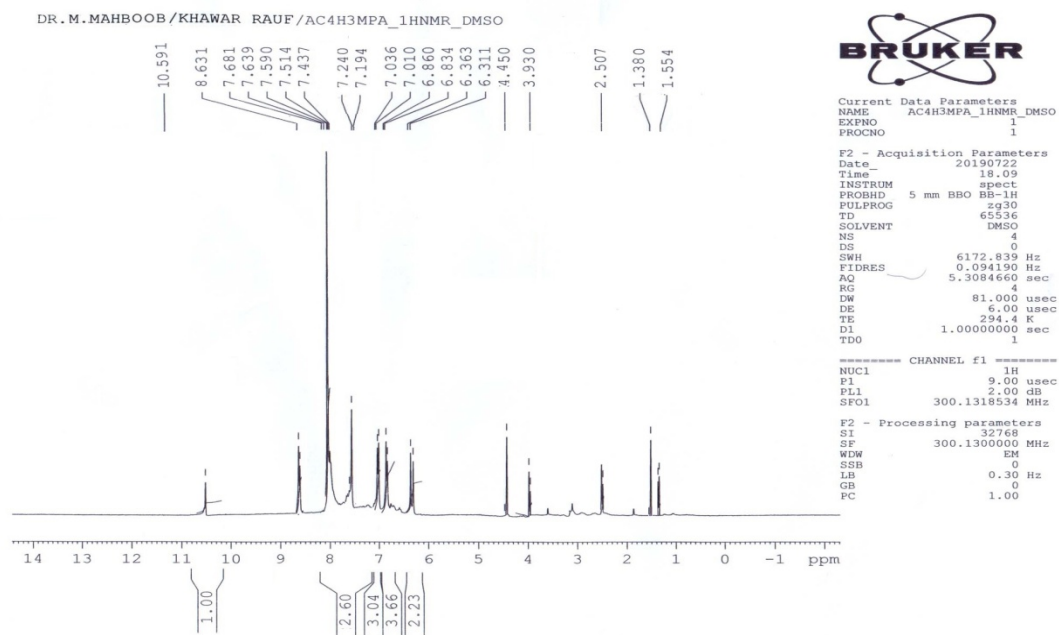


Fig. S28 ^1H NMR spectrum of 3-Acetylamino-3(4-hydroxy-3-methoxyphenyl) propanoic acid **L₈**

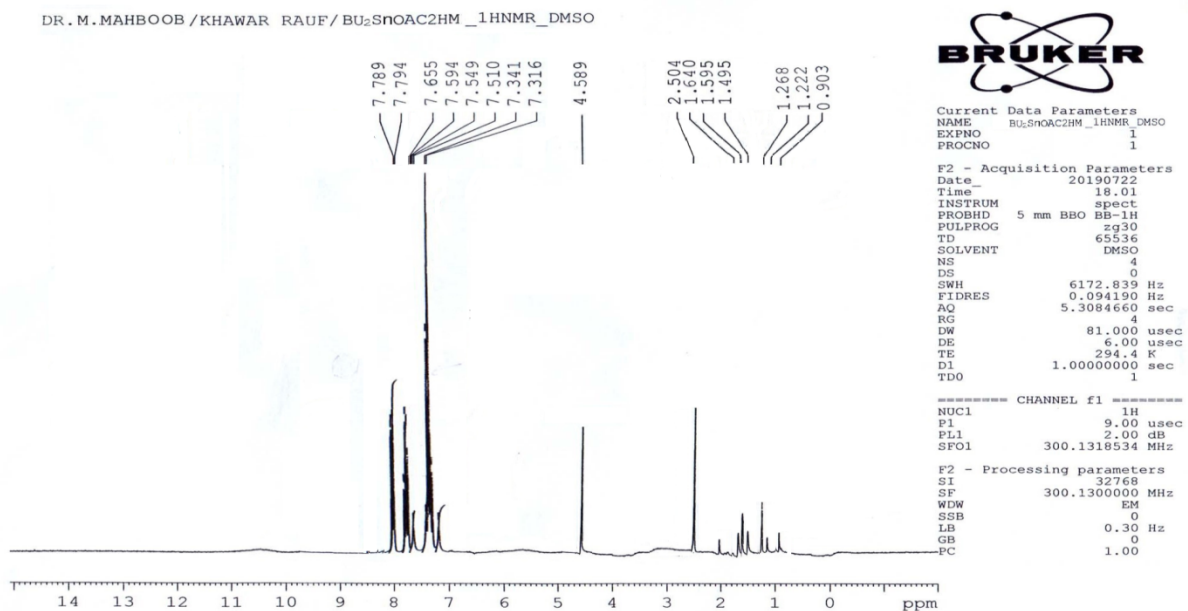


Fig. S29 ¹H NMR spectrum (400 MHz, DMSO) of the dibutyltin(IV) oxide monomer complex (1) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid L₁

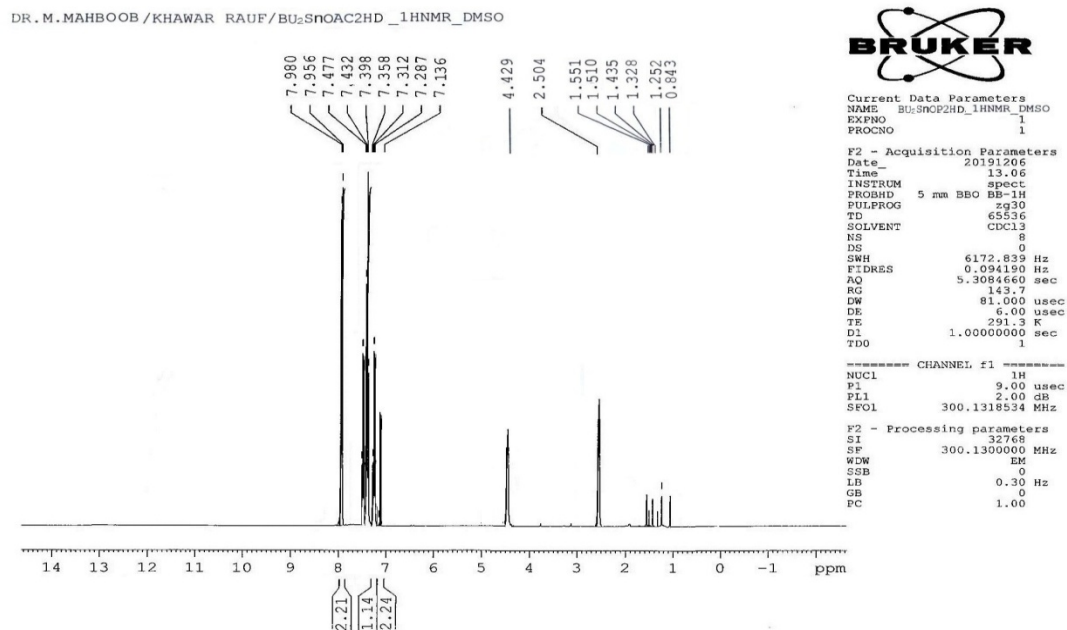


Fig. S30 ¹H NMR spectrum (400 MHz, DMSO) of the dibutyltin(IV) oxide dimer complex (2) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid L₁

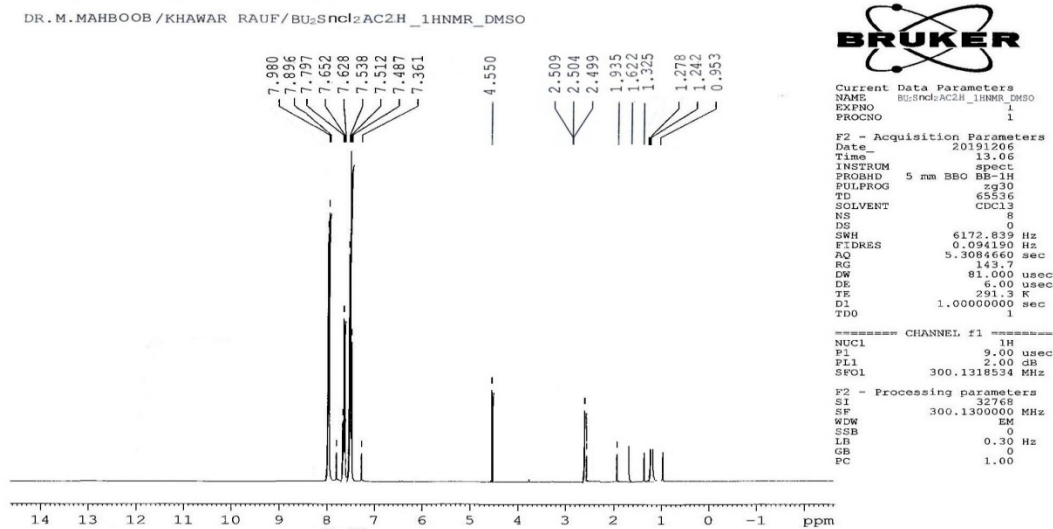


Fig. S31 ¹H NMR spectrum (400 MHz, DMSO) of the dibutyltin(IV) dichloride complex (**3**) with Acetylamino-3(2-hydroxyphenyl) propanoic acid **L**₁

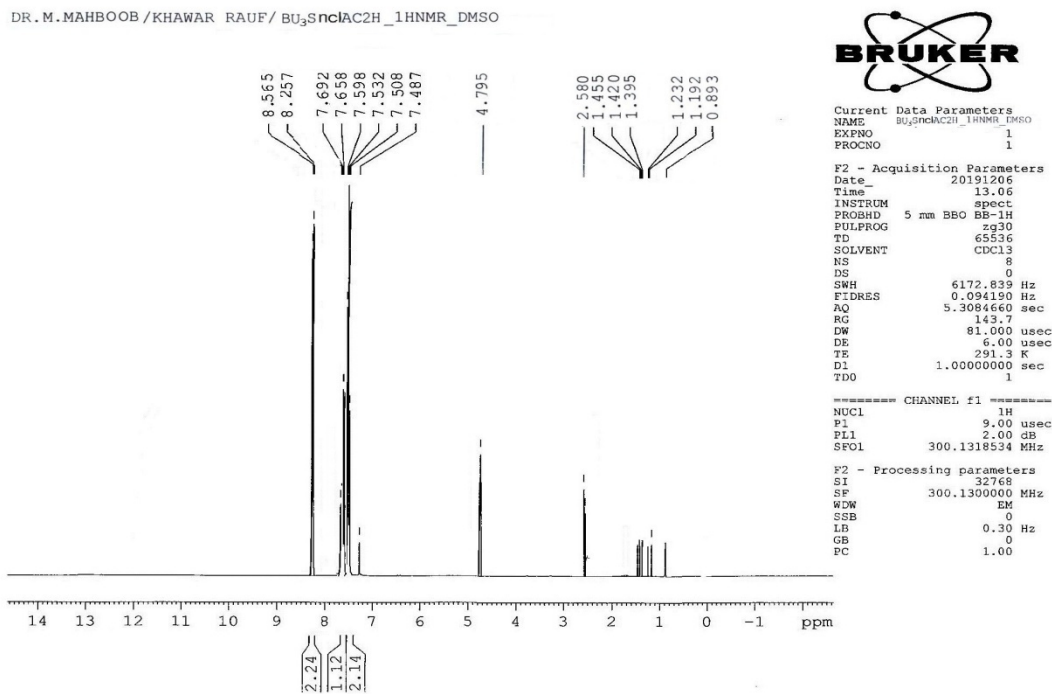


Fig. S32 ¹H NMR spectrum (400 MHz, DMSO) of the tributyltin(IV) chloride complex (**4**) with Acetylamino-3(2-hydroxyphenyl) propanoic acid **L**₁

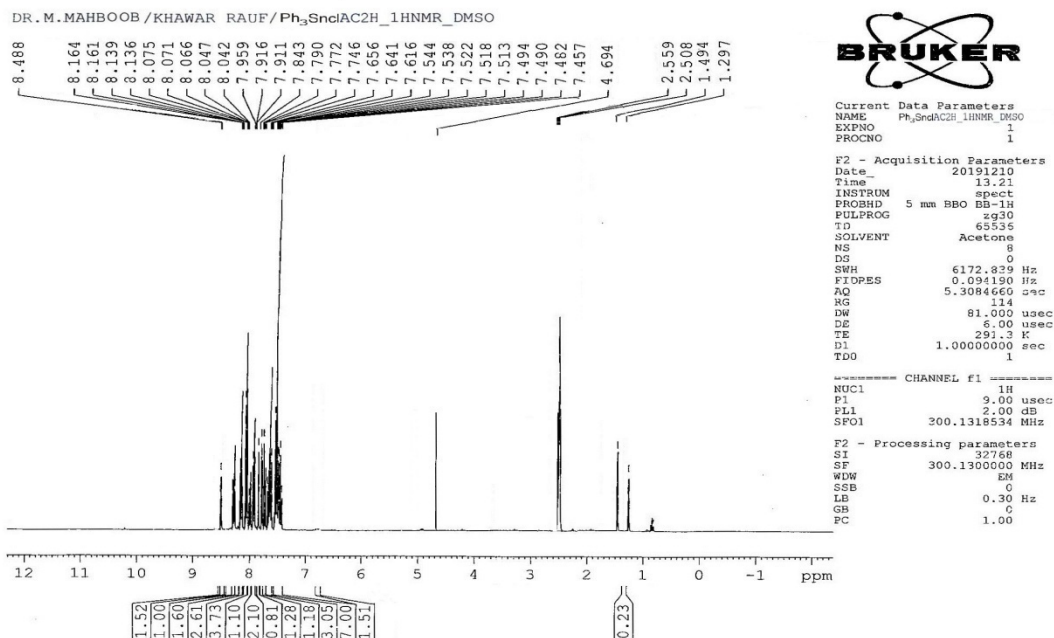


Fig. S33 ¹H NMR spectrum (400 MHz, DMSO) of the triphenyltin(IV) chloride complex (5) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid L₁

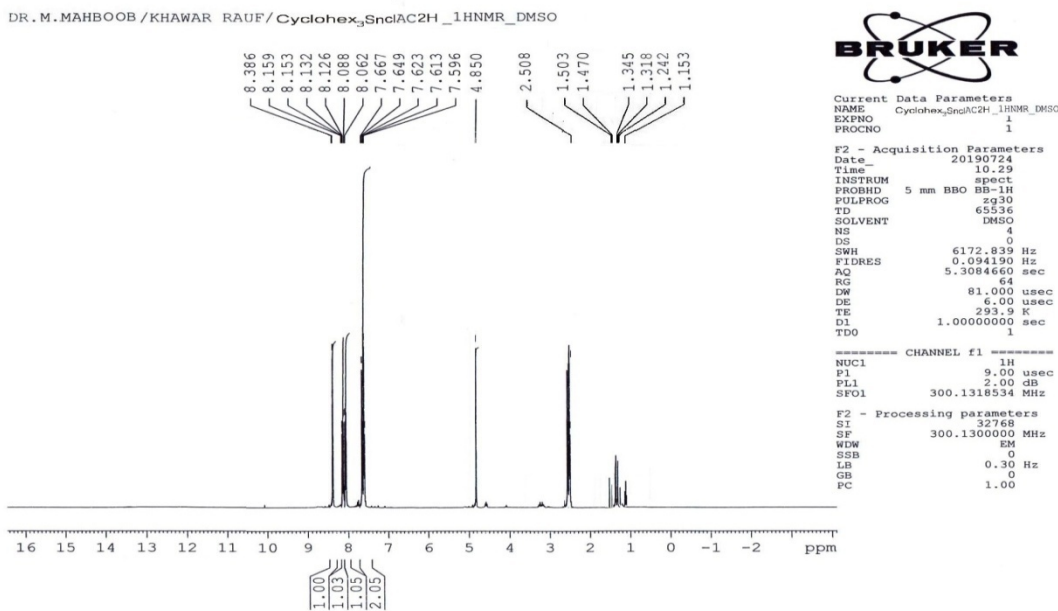


Fig. S34 ¹H NMR spectrum (400 MHz, DMSO) of the tricyclohexyltin(IV) chloride complex (6) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid L₁

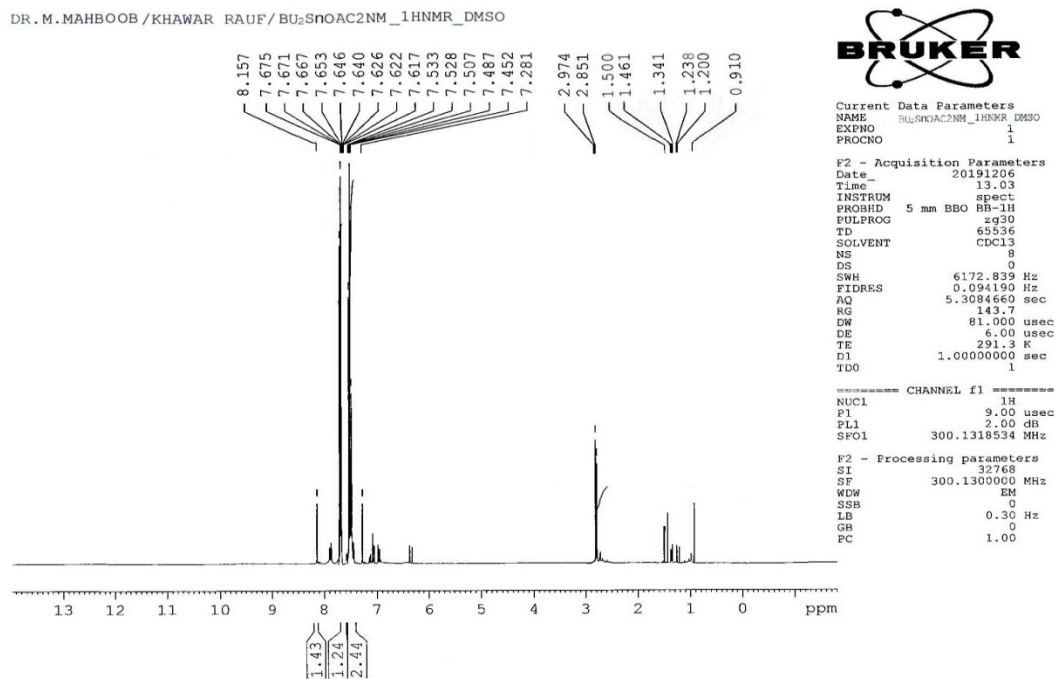


Fig. S35 ¹H NMR spectrum (400 MHz, DMSO) of the dibutyltin(IV) oxide monomer complex (7) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid L₄

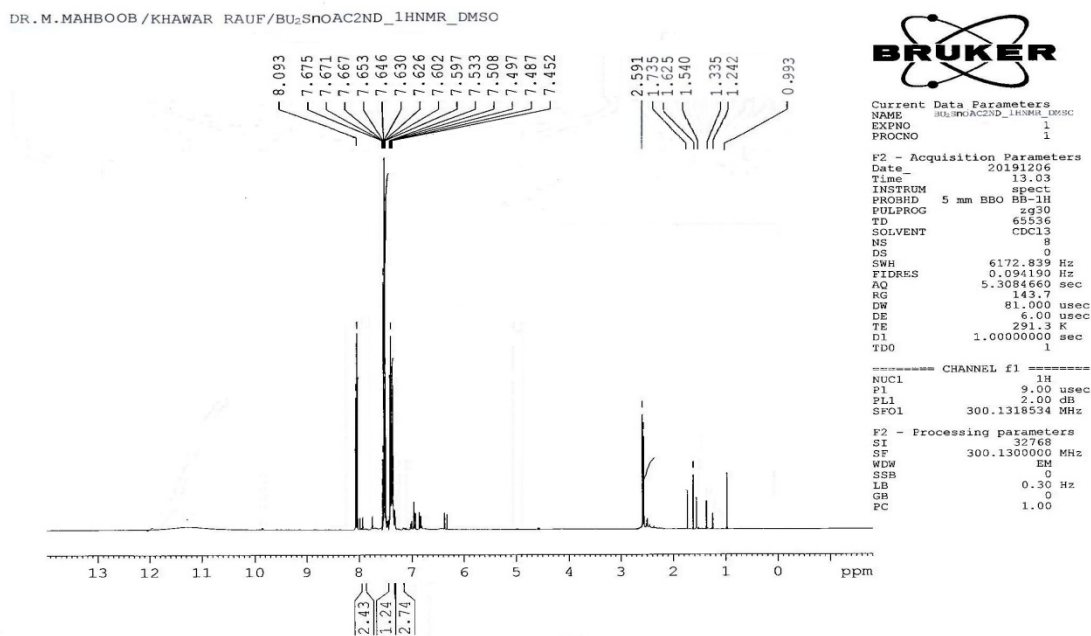


Fig. S36 ¹H NMR spectrum (400 MHz, DMSO) of the dibutyltin(IV) oxide dimer complex (8) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid L₄

DR. M. MAHBOOB / KHAWAR RAUF / BU₂SnCl₂AC2N_1HNMR_DMSO

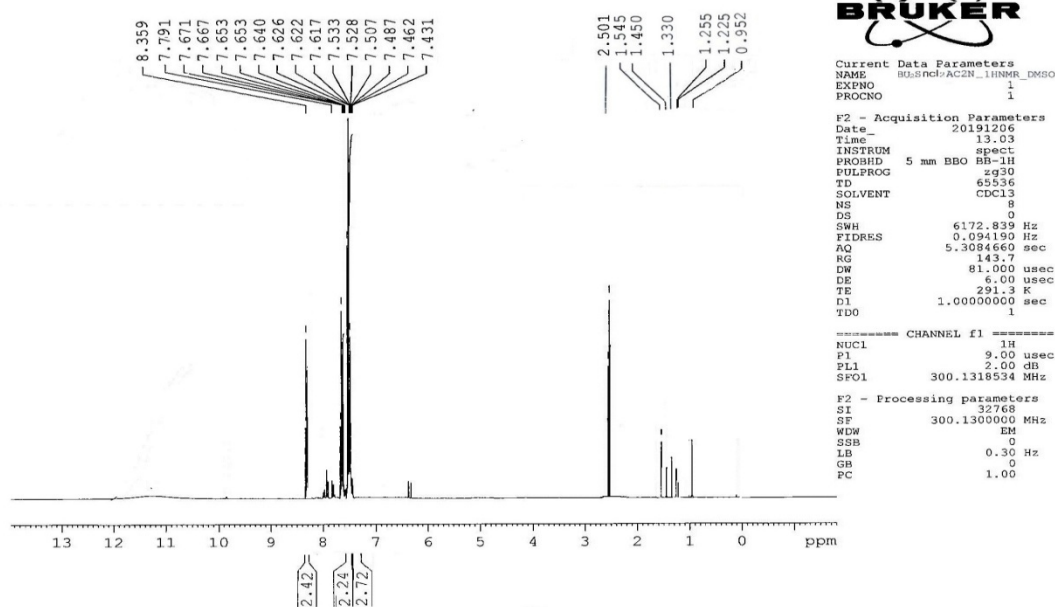


Fig. S37 ¹H NMR spectrum (400 MHz, DMSO) of the dibutyltin(IV) dichloride complex (9) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid L₄

DR. M. MAHBOOB / KHAWAR RAUF / BU₃SnClAC2N_1HNMR_DMSO

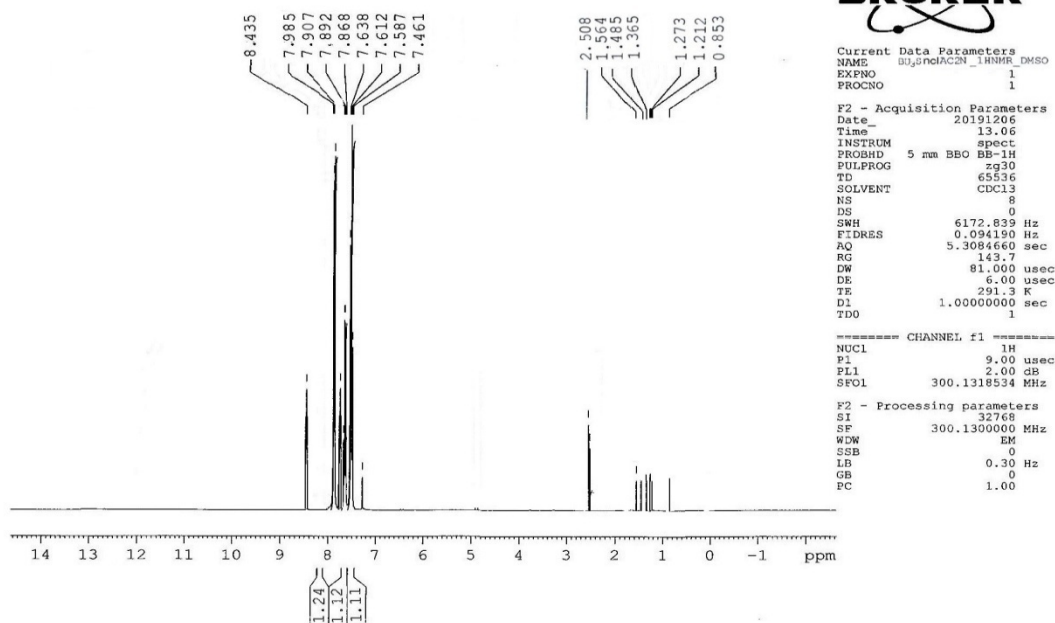


Fig. S38 ¹H NMR spectrum (400 MHz, DMSO) of the tributyltin(IV) chloride complex (10) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid L₄

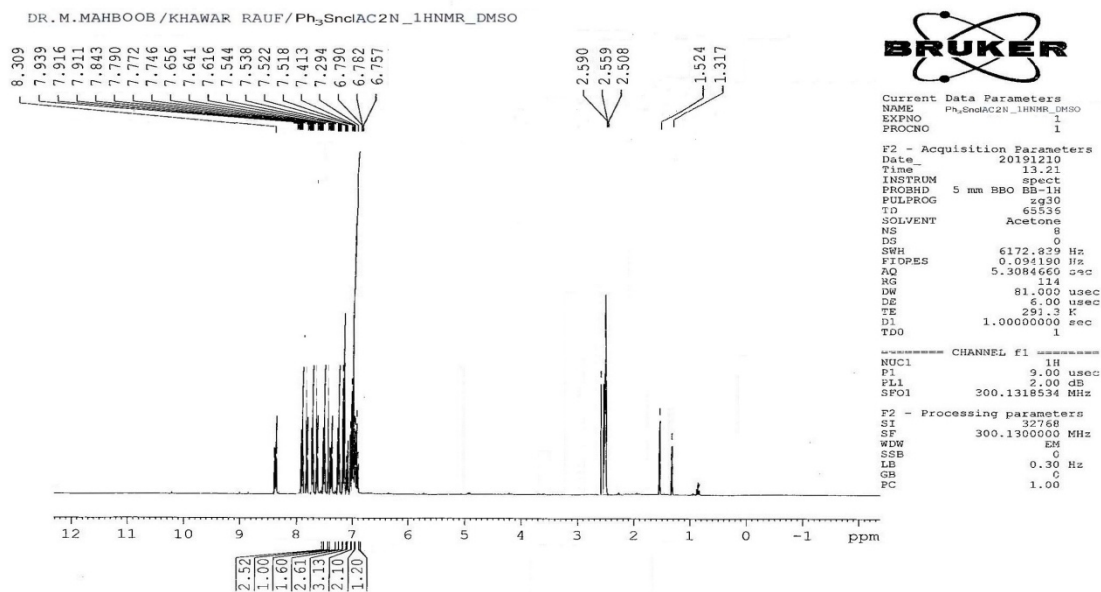


Fig. S39 ¹H NMR spectrum (400 MHz, DMSO) of the triphenyltin(IV) chloride complex (11) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid L₄

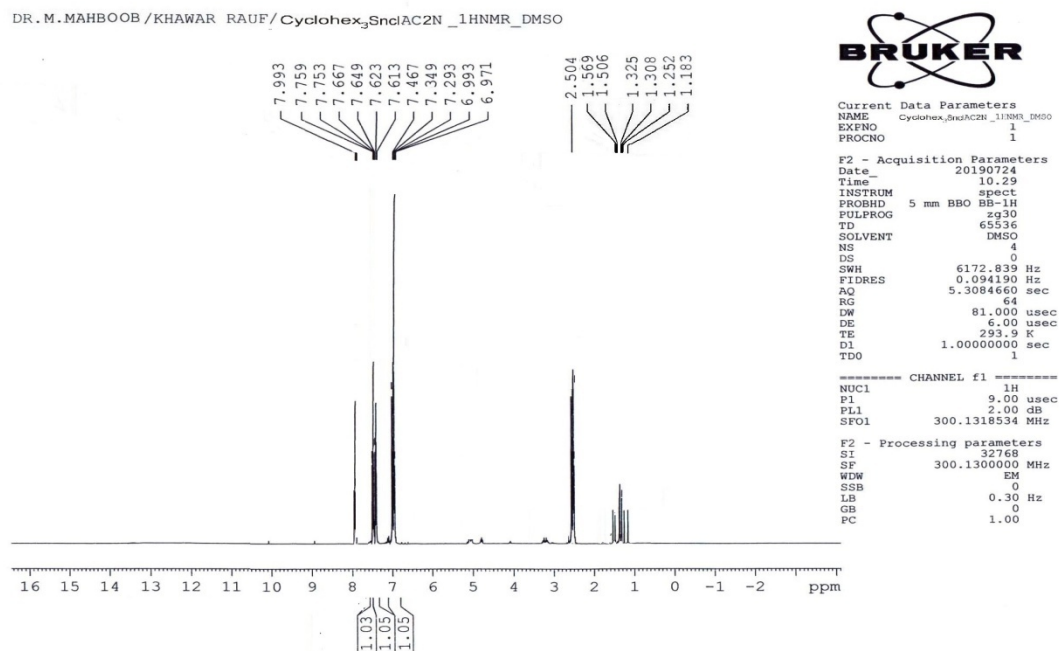


Fig. S40 ¹H NMR spectrum (400 MHz, DMSO) of the tricyclohexyltin(IV) chloride complex (12) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid L₄

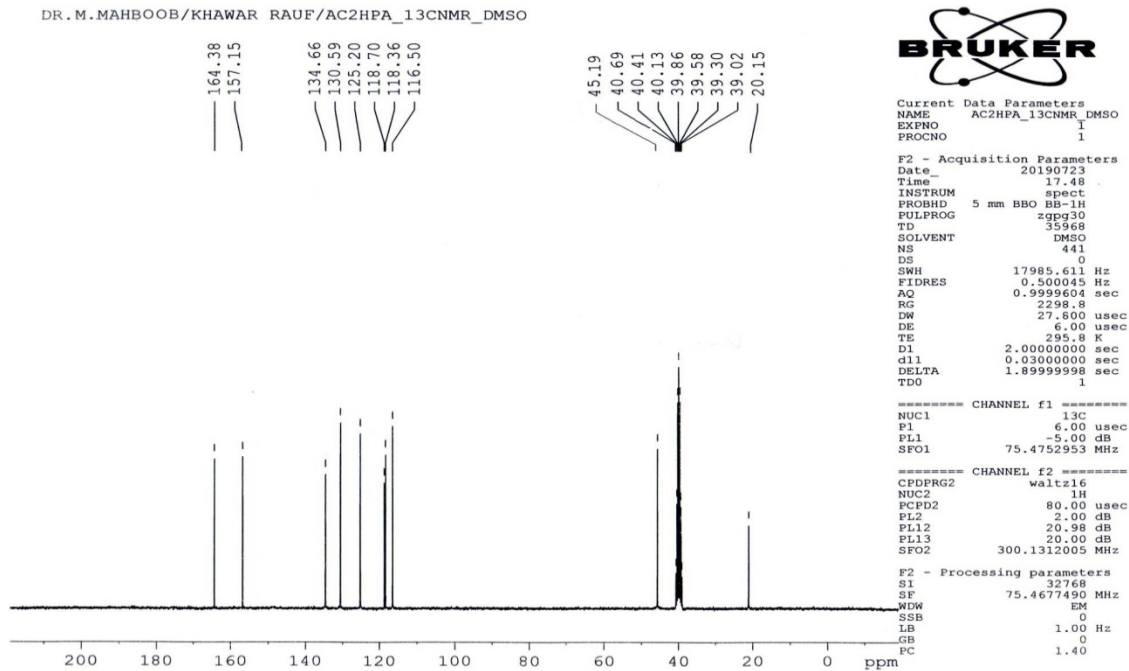


Fig. S41 ¹³C NMR spectrum (100 MHz, DMSO) of 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid L₁

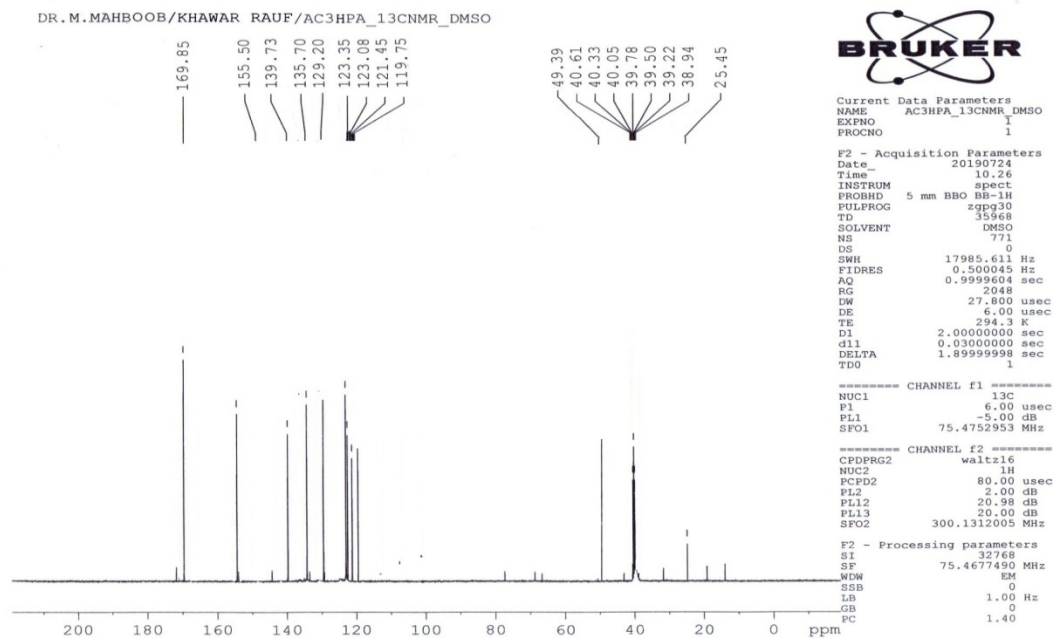


Fig. S42 ¹³C NMR spectrum (100 MHz, DMSO) of 3-Acetylamino-3(3-hydroxyphenyl) propanoic acid L₂

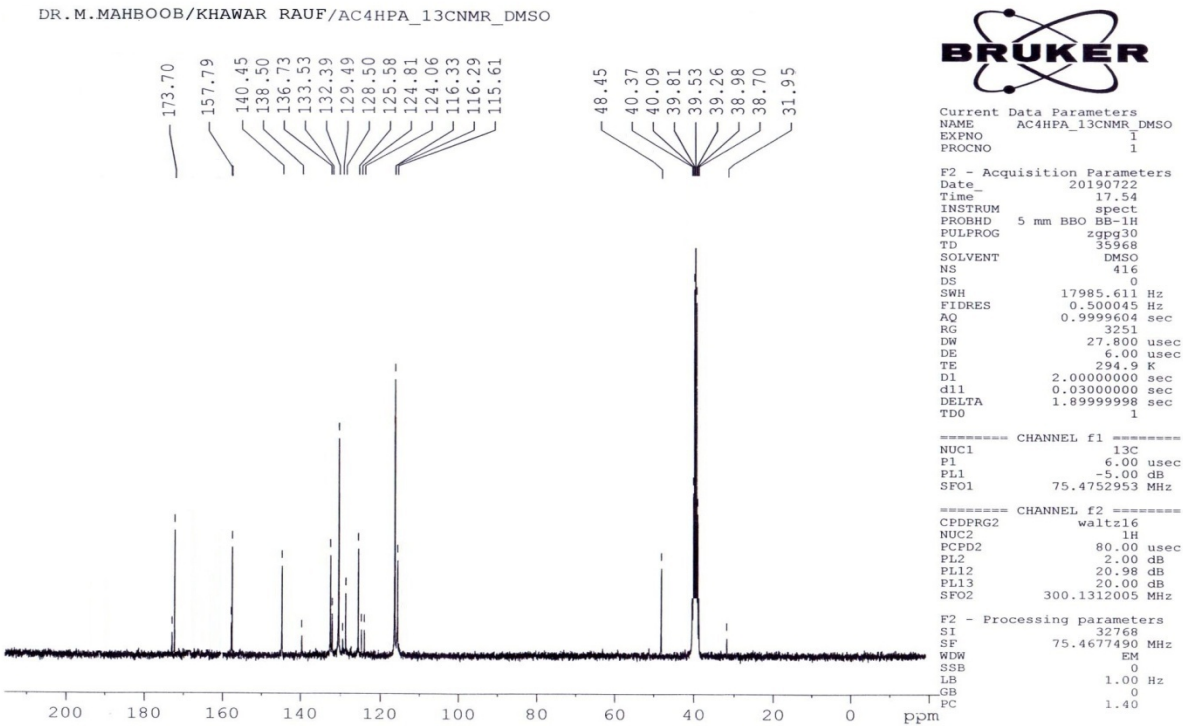


Fig. S43 ¹³C NMR spectrum (100 MHz, DMSO) of 3-Acetylamino-3(4-hydroxyphenyl) propanoic acid L₃

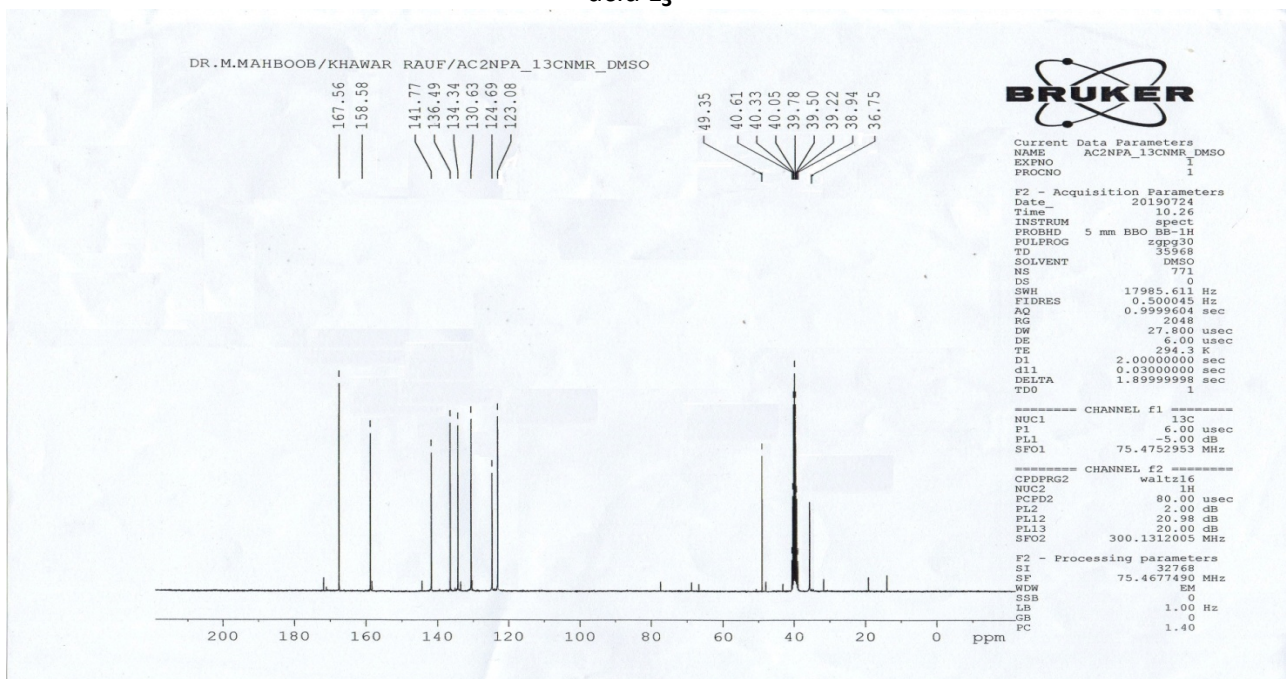
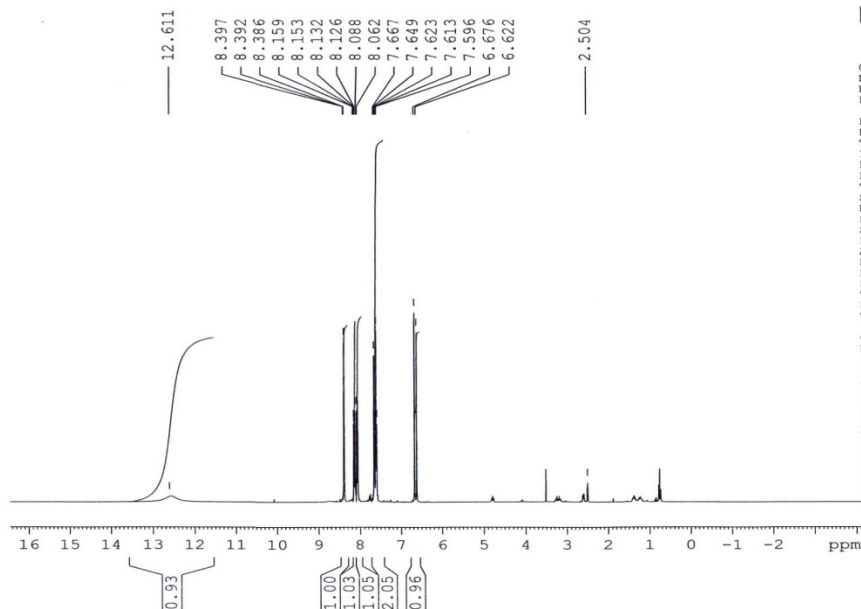


Fig. S44 ¹³C NMR spectrum (100 MHz, DMSO) of 3-Acetylamino-3(2-nitrophenyl) propanoic acid L₄

DR. AMIN BADSHAH/KHAWAR RAUF/AC3NPA_1HNMR_DMSO



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PROCNO 1

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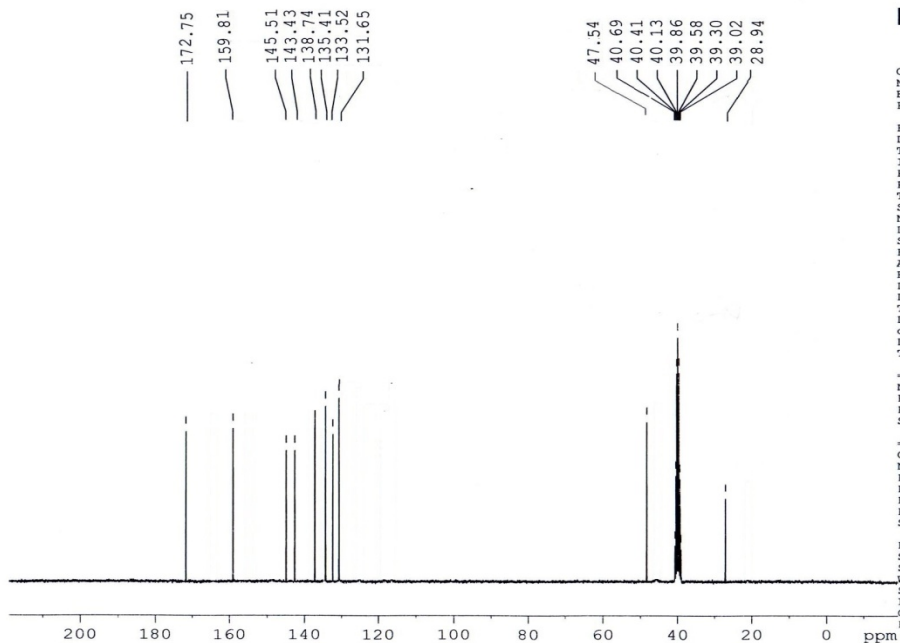
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LB 0.30 Hz
GB 0
PC 1.00

Fig. S45 ¹³C NMR spectrum (100 MHz, DMSO) of 3-Acetylamino-3(3-nitrophenyl) propanoic acid

L₅

DR. M. MAHBOOB/KHAWAR RAUF/AC4NPA_13CNMR_DMSO



Current Data Parameters
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EXPNO 1
PROCNO 1

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TDO 1

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PL13 20.00 dB
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Fig. S46 ¹³C NMR spectrum (100 MHz, DMSO) of 3-Acetylamino-3(4-hydroxyphenyl) propanoic acid L₆

L₆

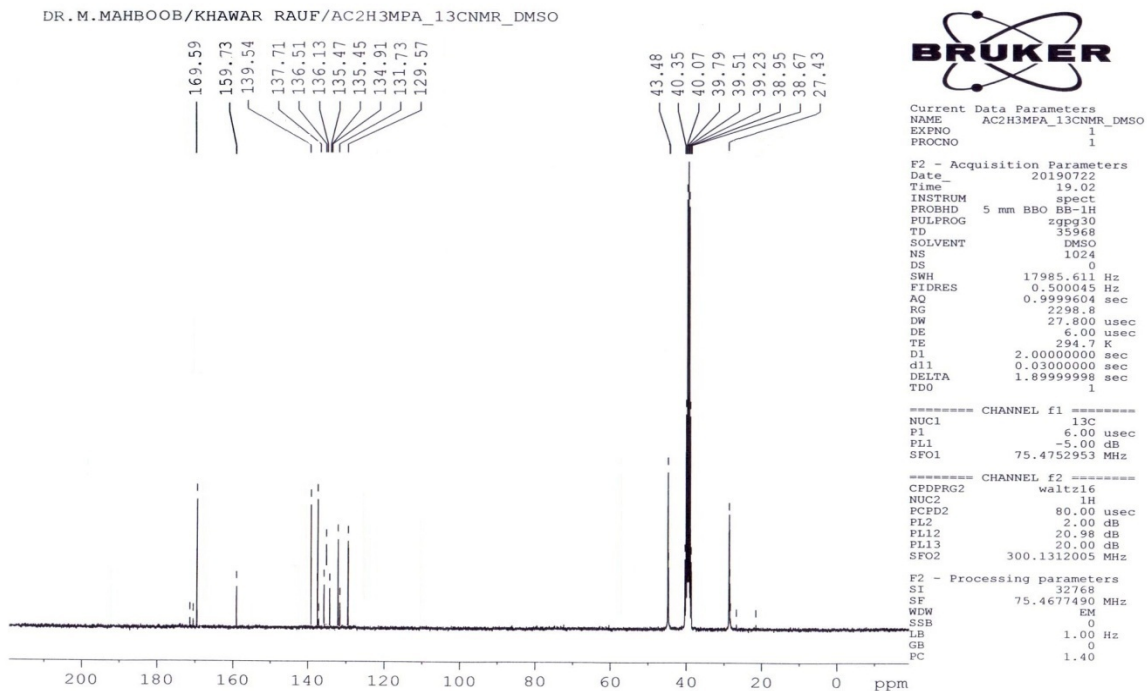


Fig. S47 ^{13}C NMR spectrum (100 MHz, DMSO) of 3-Acetylamino-3(2-hydroxy-3-methoxyphenyl) propanoic acid L_7

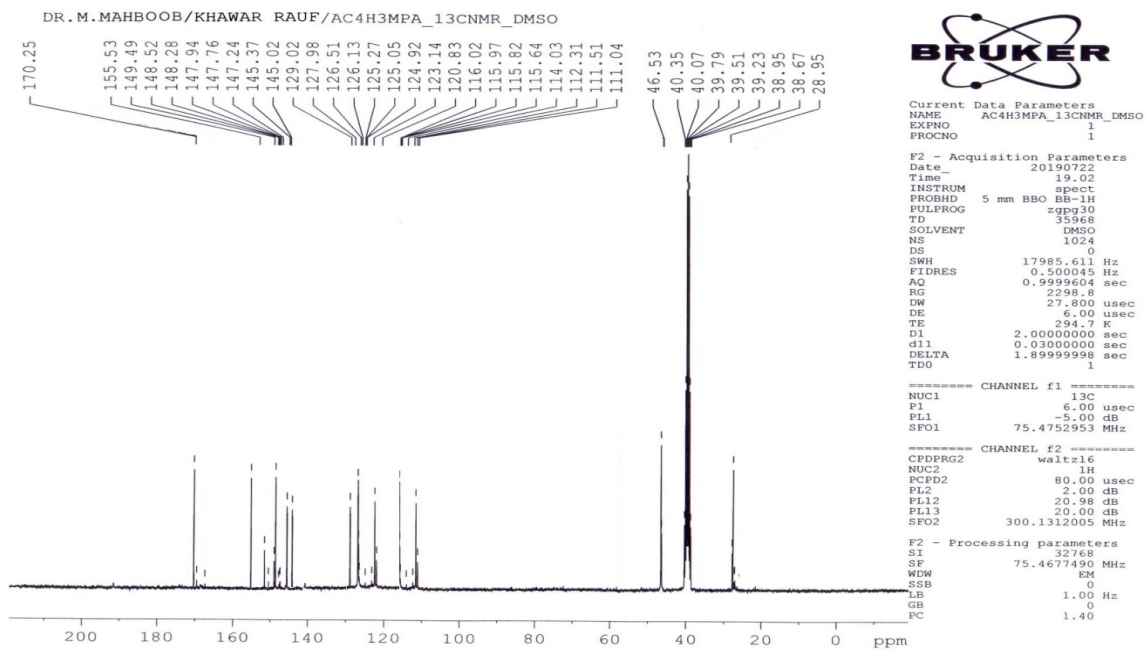


Fig. S48 ^{13}C NMR spectrum (100 MHz, DMSO) of 3-Acetylamino-3(4-hydroxy-3-methoxyphenyl) propanoic acid L_8

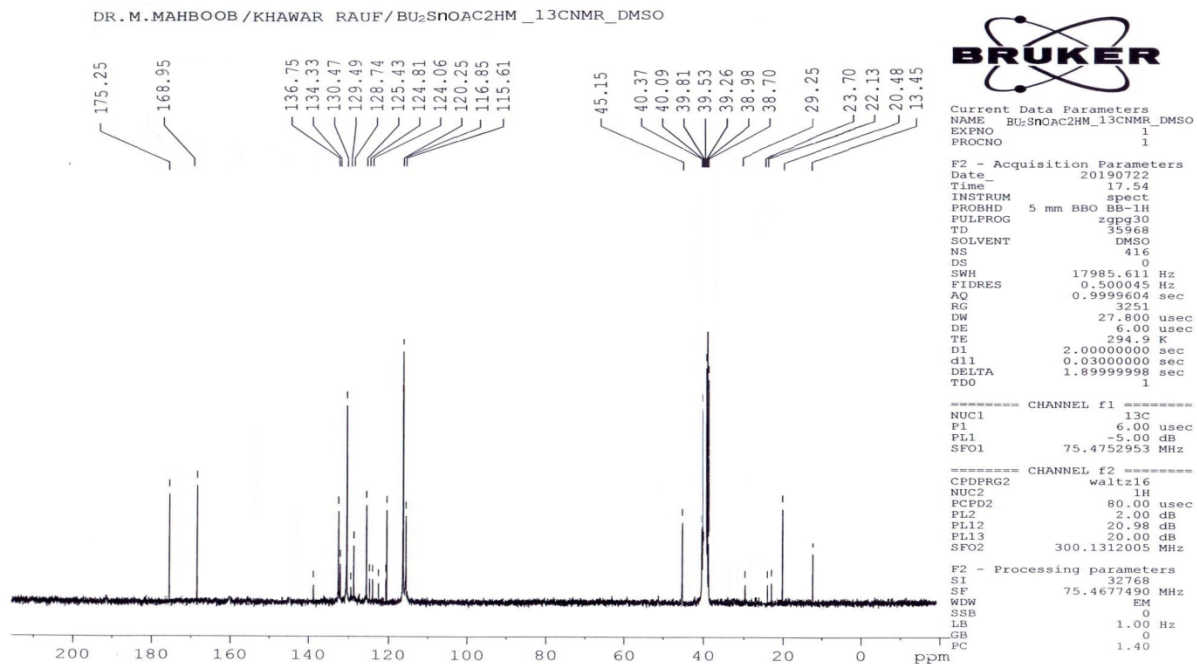


Fig. S49 ¹³C NMR spectrum (100 MHz, DMSO) of the dibutyltin(IV) oxide monomer complex (1) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid L₁

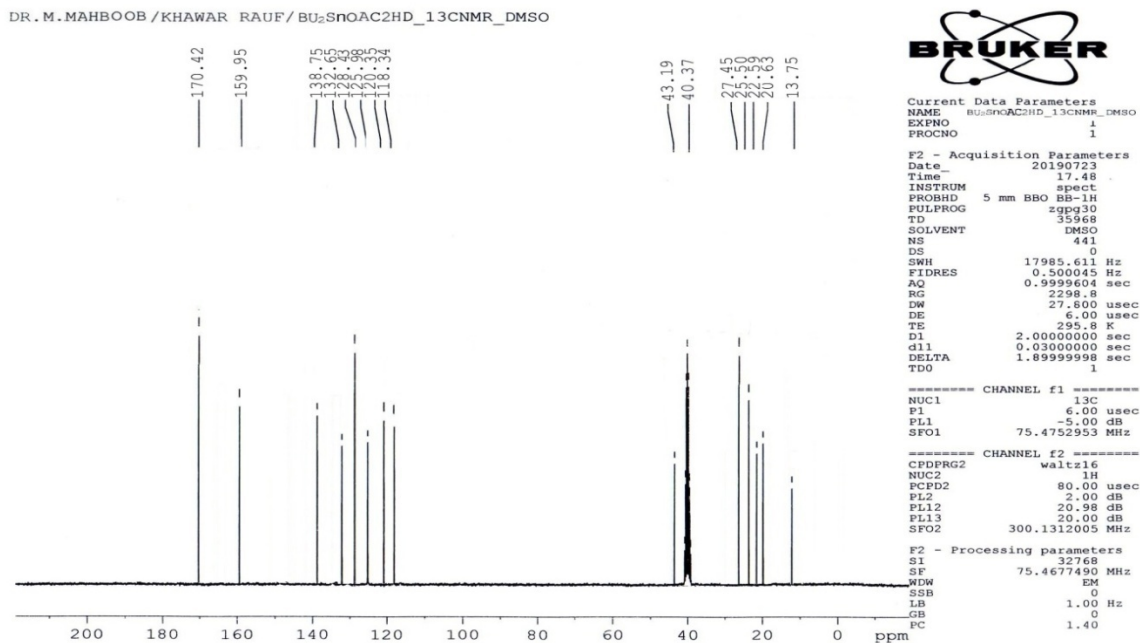


Fig. S50 ¹³C NMR spectrum (100 MHz, DMSO) of the dibutyltin(IV) oxide dimer complex (2) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid L₁

DR. M. MAHBOOB / KHAWAR RAUF / BU₂SnCl₂AC2H_13CNMR_DMSO

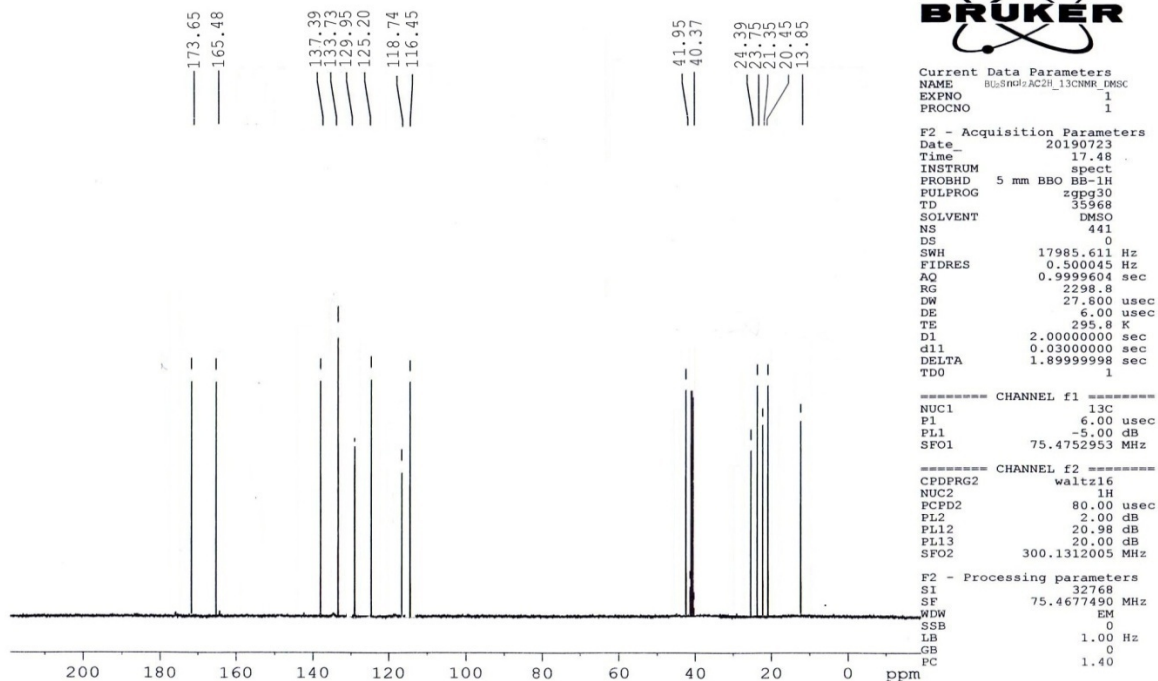


Fig. S51 ¹³C NMR spectrum (100 MHz, DMSO) of the dibutyltin(IV) dichloride complex (3) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid L₁

DR. M. MAHBOOB / KHAWAR RAUF / BU₃SnClAC2H_13CNMR_DMSO

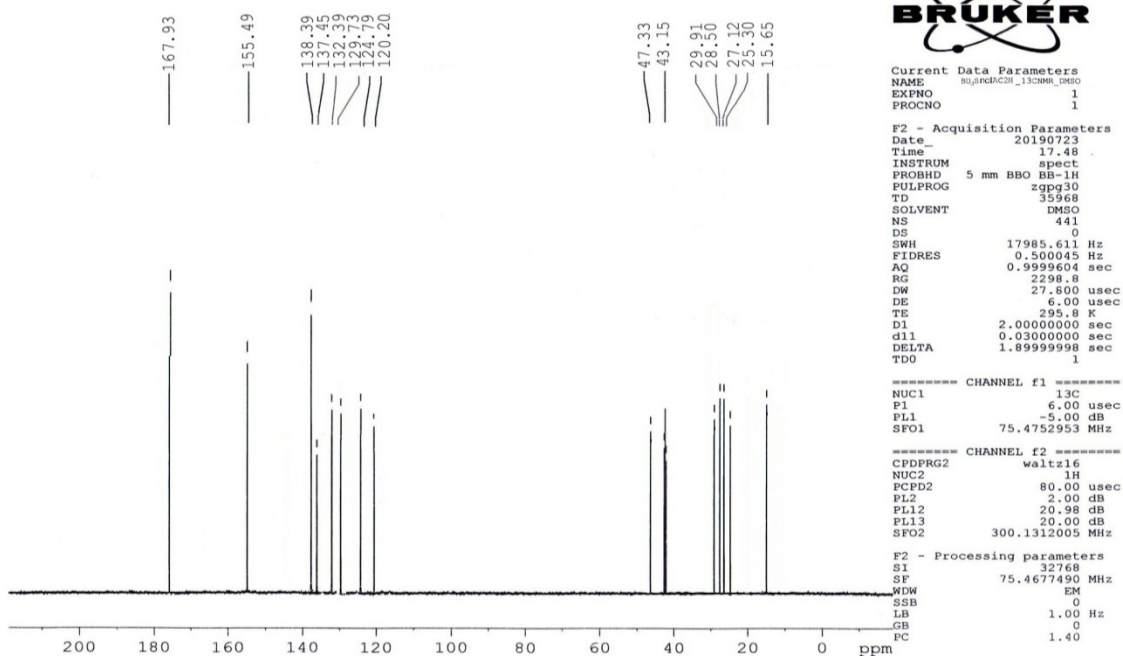


Fig. S52 ¹³C NMR spectrum (100 MHz, DMSO) of the tributyltin(IV) chloride complex (4) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid L₁

DR. M. MAHBOOB / KHAWAR RA'JF / Ph₃SnClAC2H_13CNMR_DMSO

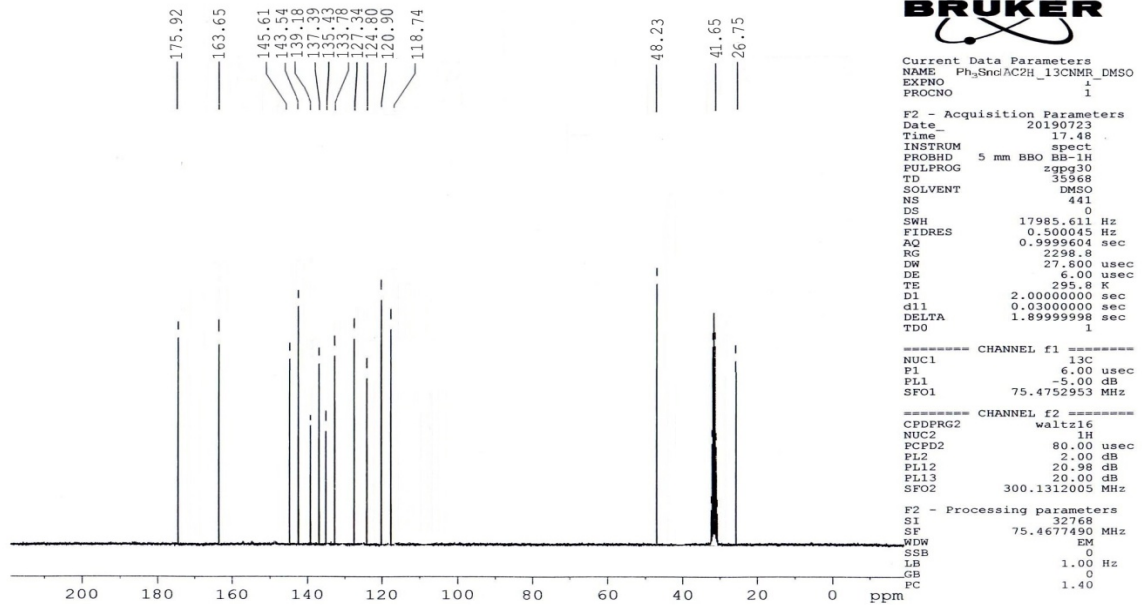


Fig. S53 ¹³C NMR spectrum (100 MHz, DMSO) of the triphenyltin(IV) chloride complex (5) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid L₁

DR. M. MAHBOOB / KHAWAR RAUF / Cyclohex₃SnClAC2H_13CNMR_DMSO

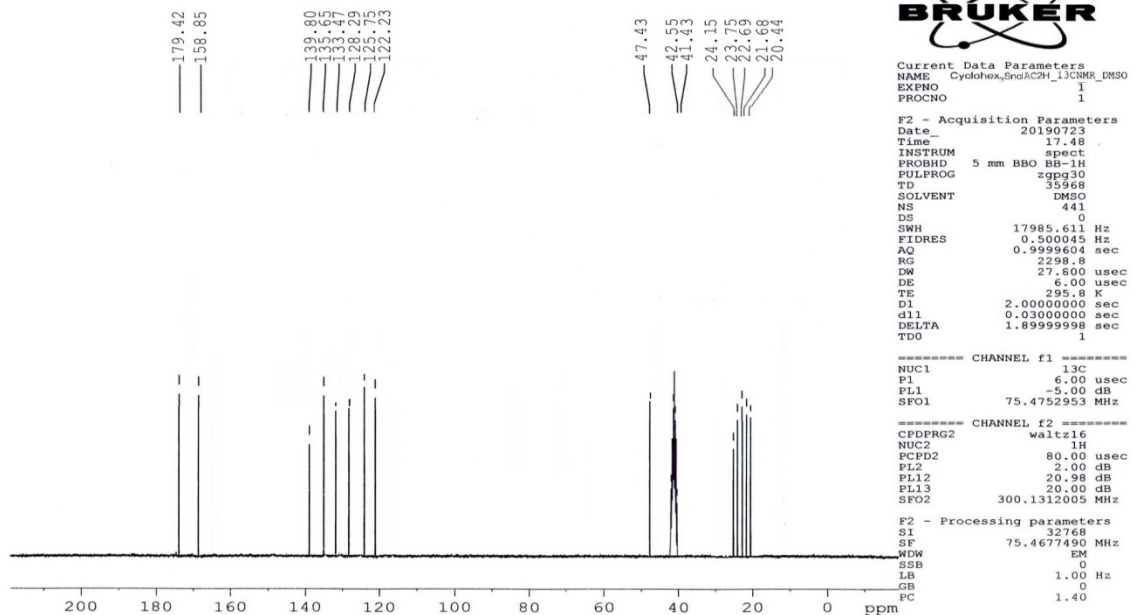


Fig. S54 ¹³C NMR spectrum (100 MHz, DMSO) of the tricyclohexyltin(IV) chloride complex (6) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid L₁

DR. M. MAHBOOB / KHAWAR RAUF / BU₂SnOAC2NM_13CNMR_DMSO

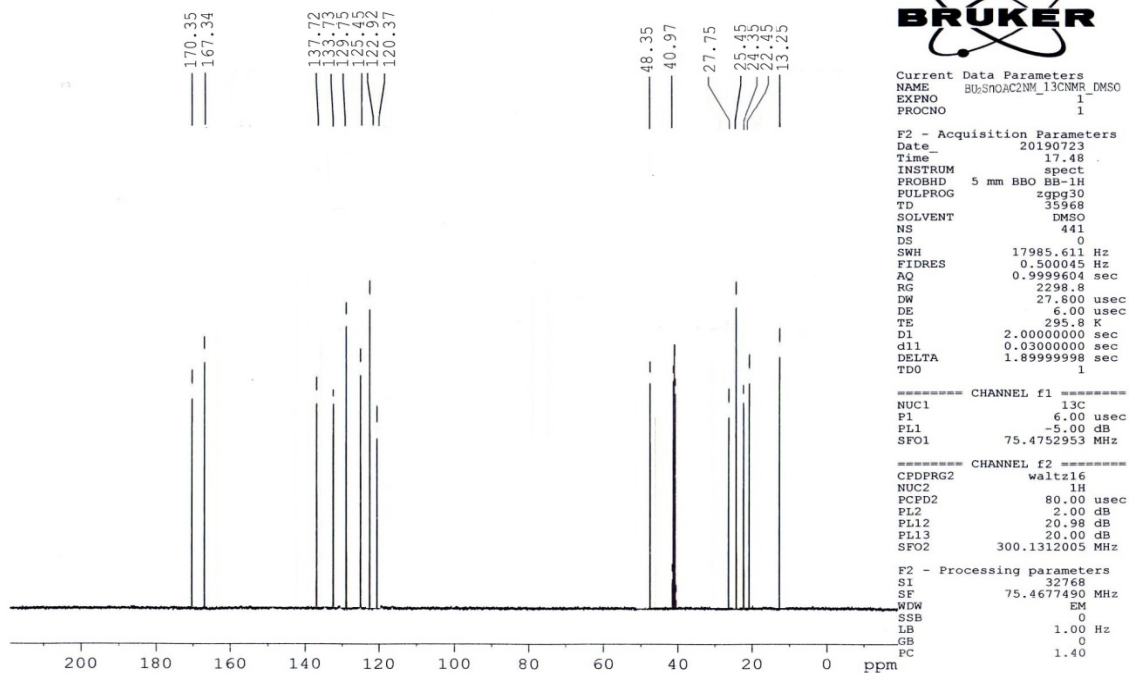


Fig. S55 ¹³C NMR spectrum (100 MHz, DMSO) of the dibutyltin(IV) oxide monomer complex (7) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid L₄

DR. M. MAHBOOB / KHAWAR RAUF / BU₂SnOAC2ND_13CNMR_DMSO

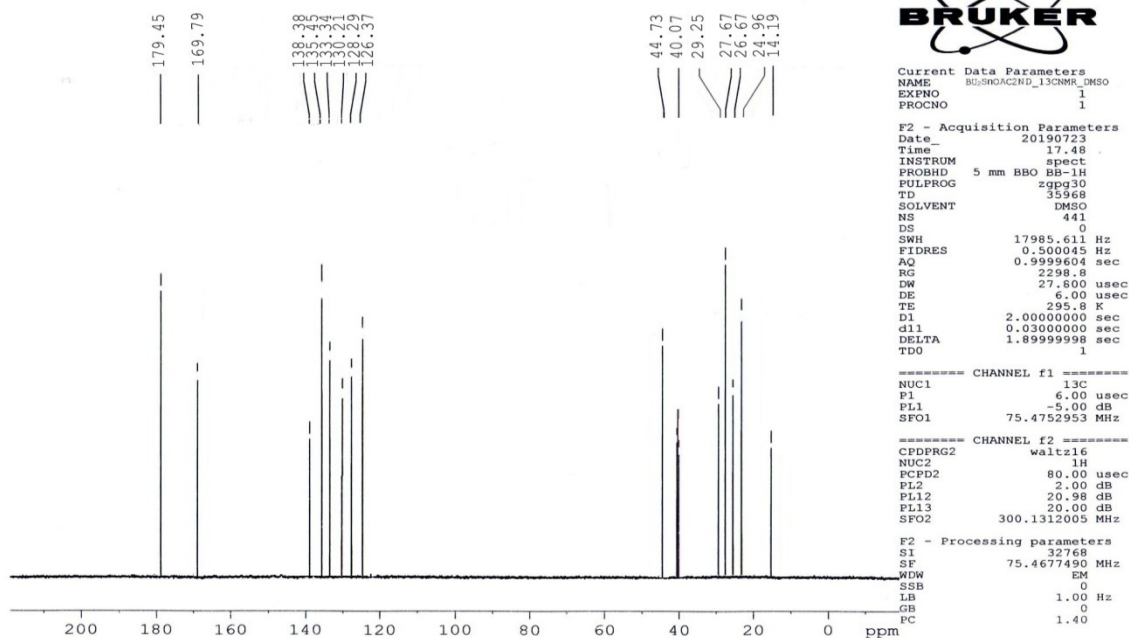


Fig. S56 ¹³C NMR spectrum (100 MHz, DMSO) of the dibutyltin(IV) oxide dimer complex (8) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid L₄

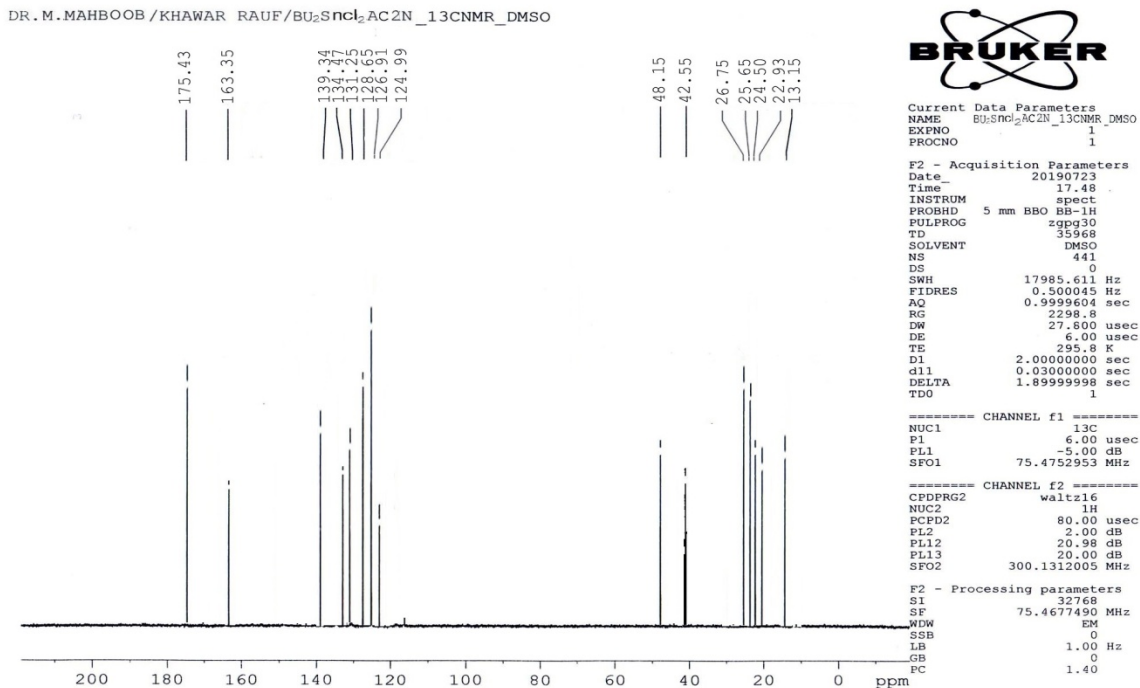


Fig. S57 ¹³C NMR spectrum (100 MHz, DMSO) of the dibutyltin(IV) dichloride complex (**9**) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid **L₄**

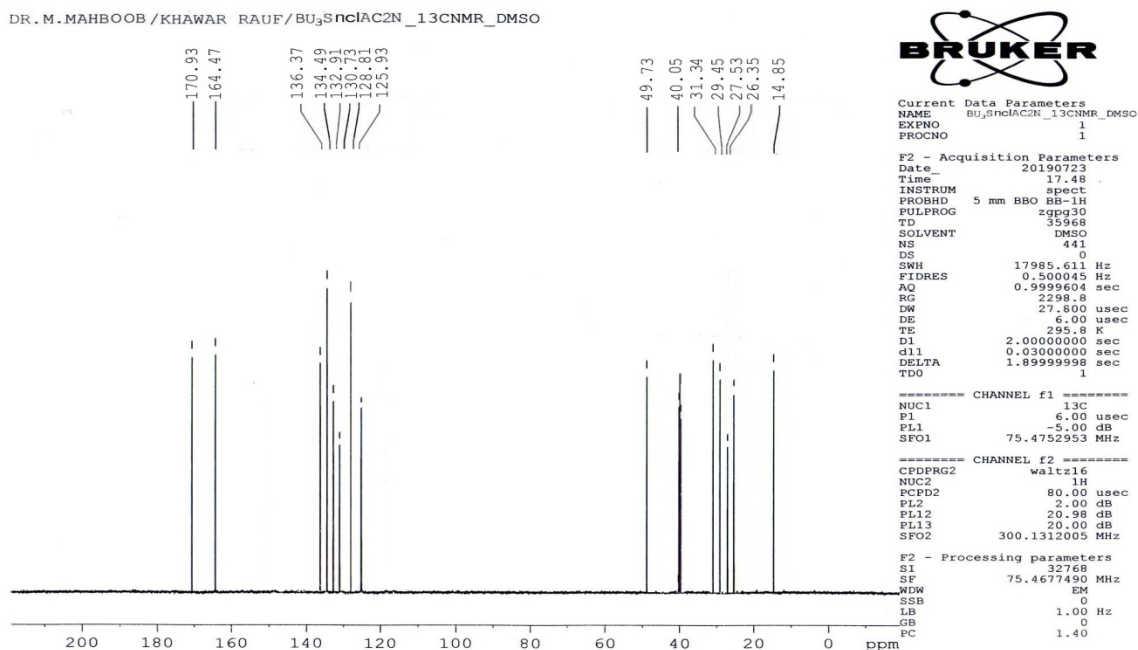


Fig. S58 ¹³C NMR spectrum (100 MHz, DMSO) of the tributyltin(IV) chloride complex (**10**) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid **L₄**

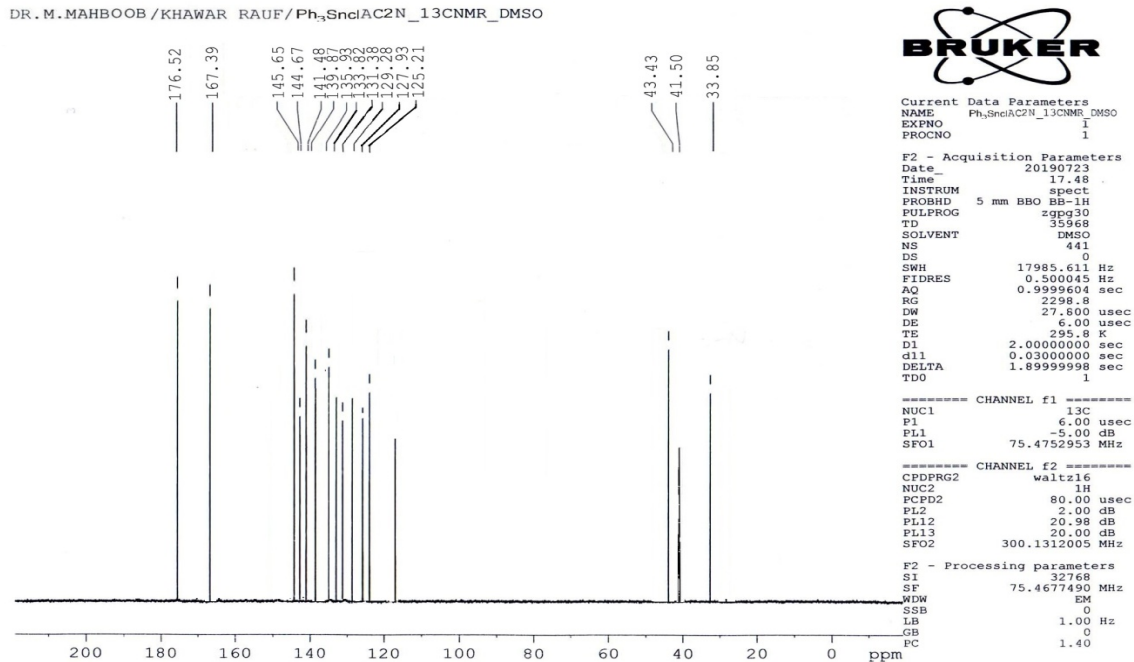


Fig. S59 ¹³C NMR spectrum (100 MHz, DMSO) of the triphenyltin(IV) chloride complex (**11**) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid **L₄**

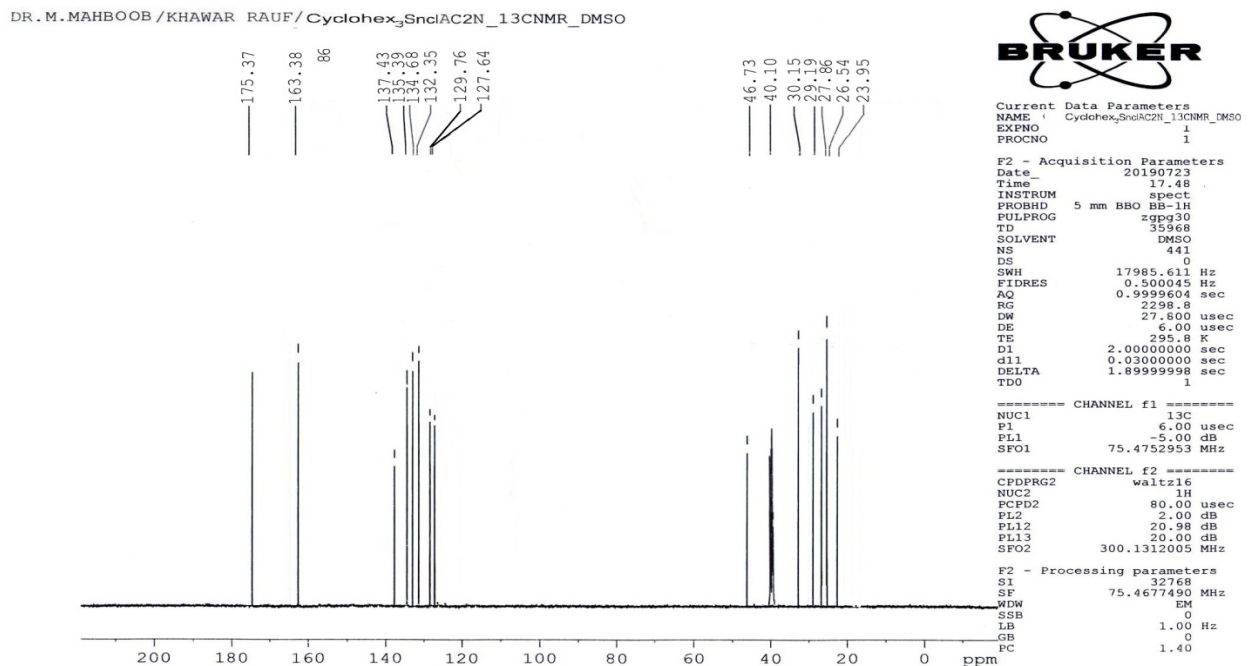
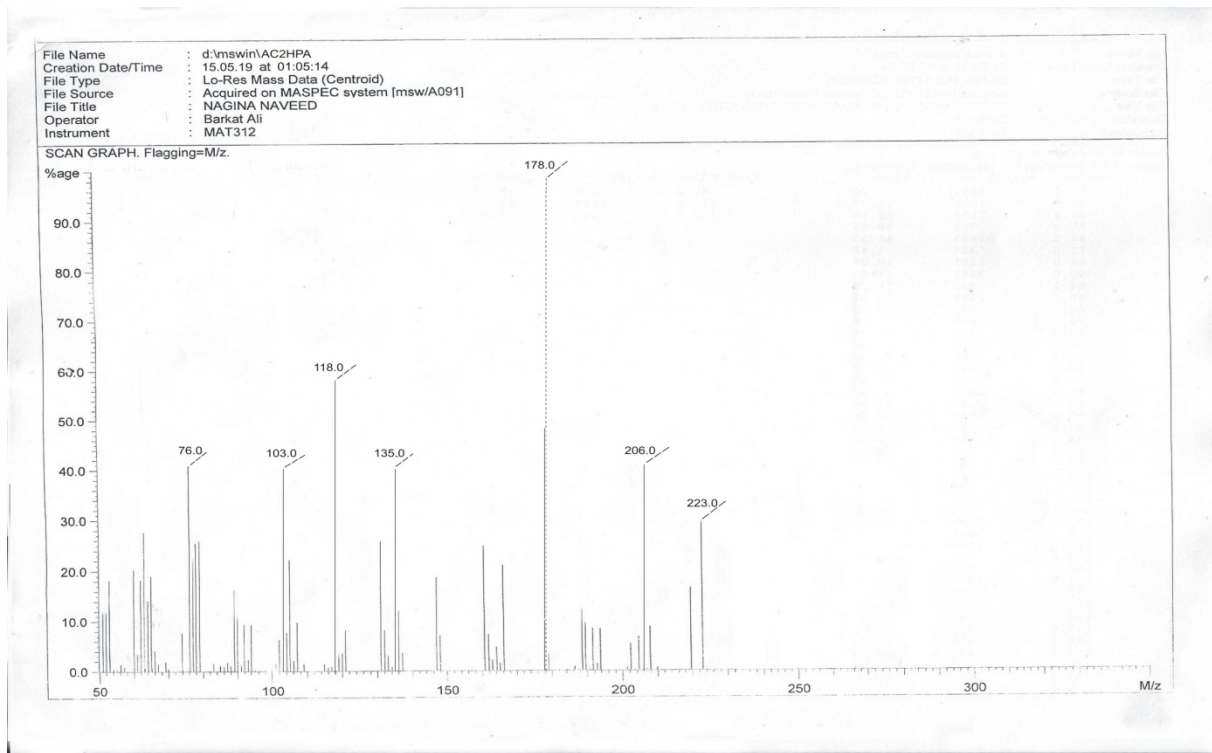


Fig. S60 ¹³C NMR spectrum (100 MHz, DMSO) of the tricyclohexyltin(IV) chloride complex (**12**) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid **L₄**



g. S61 EI Mass spectrum of 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid **L₁**

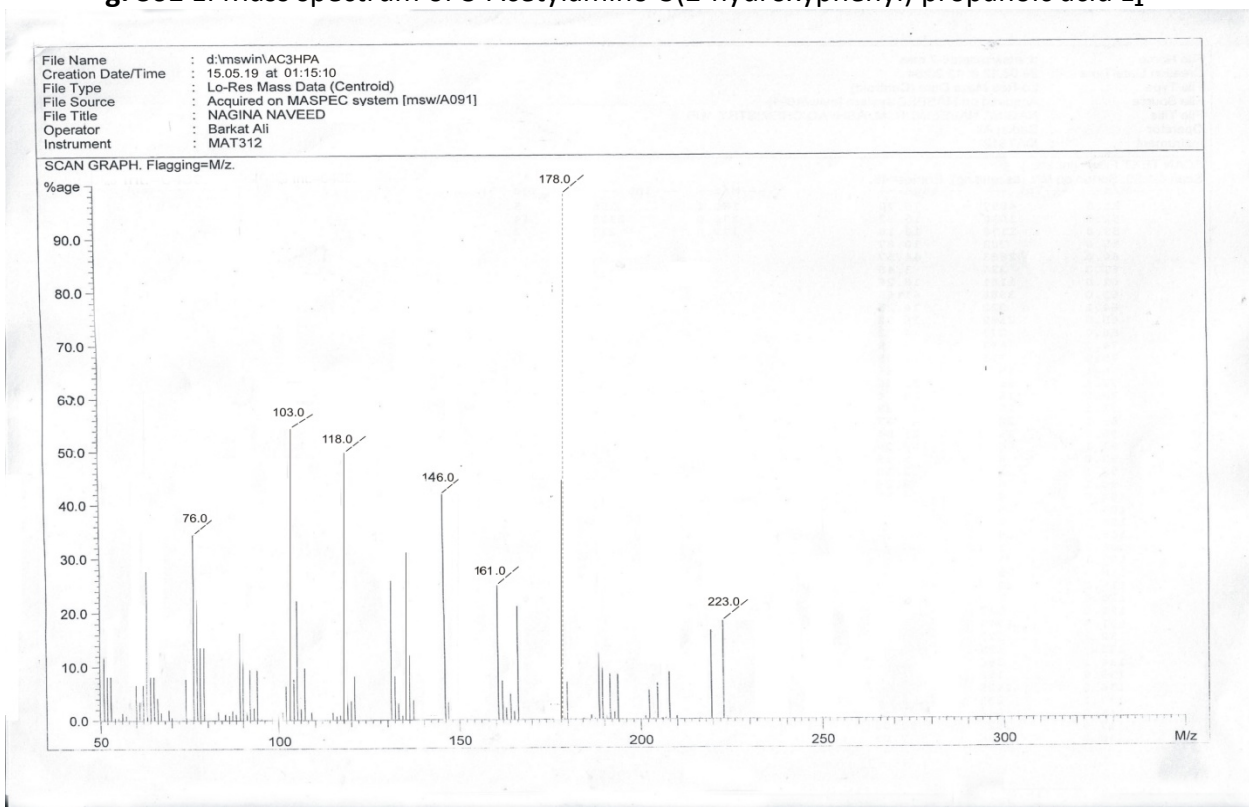


Fig. S62 EI Mass spectrum of 3-Acetylamino-3(3-hydroxyphenyl) propanoic acid **L₂**

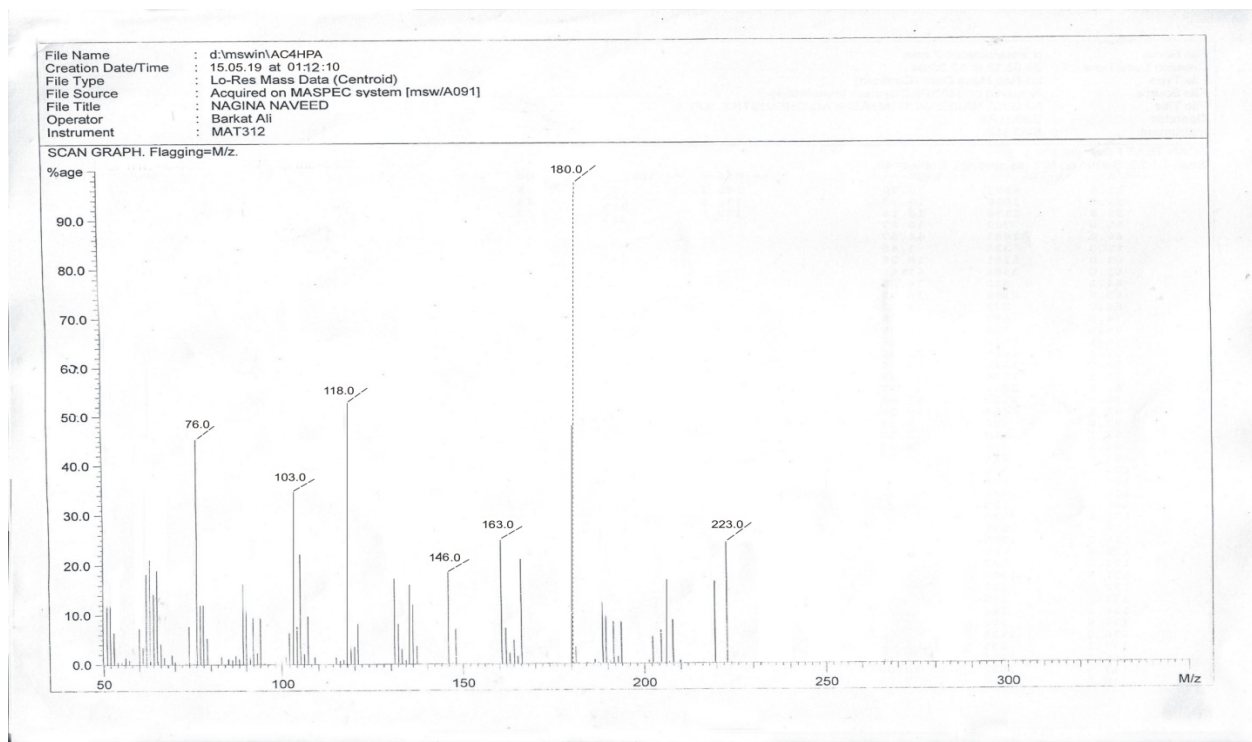


Fig. S63 EI Mass spectrum of 3-Acetylamino-3(4-hydroxyphenyl) propanoic acid **L₃**

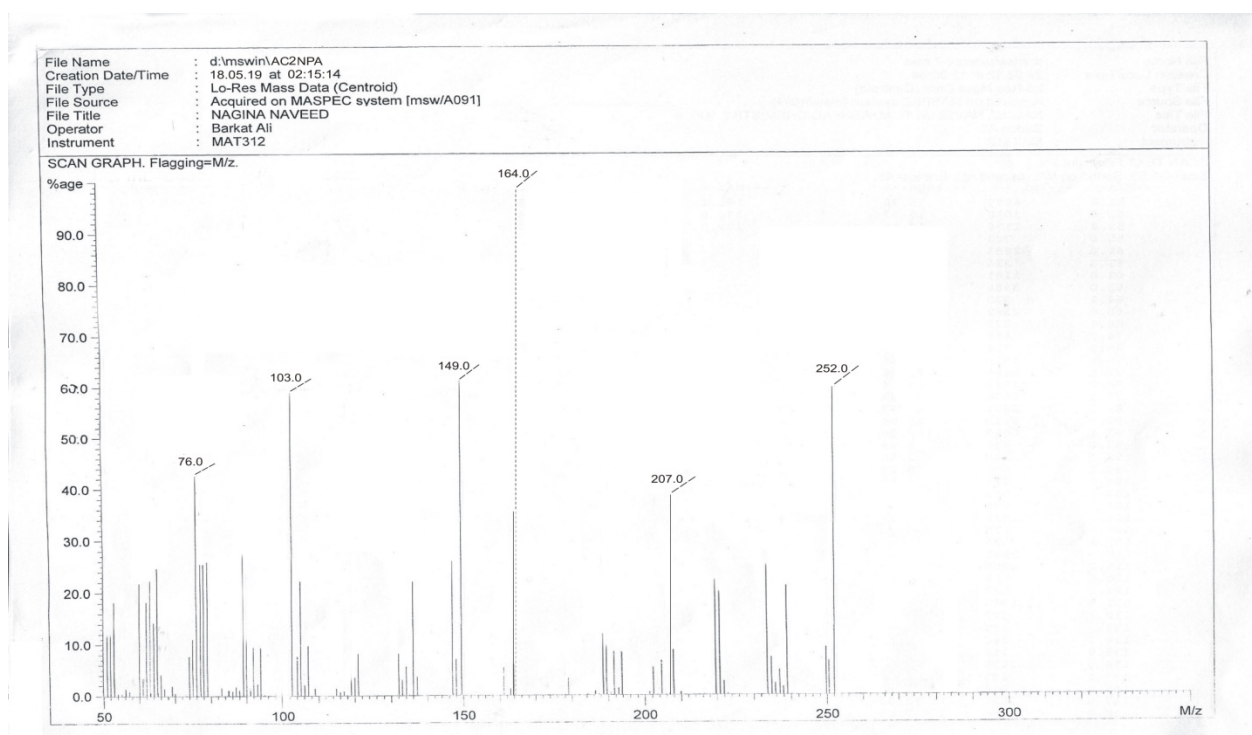


Fig. S64 EI Mass spectrum of 3-Acetylamino-3(2-nitrophenyl) propanoic acid **L₄**

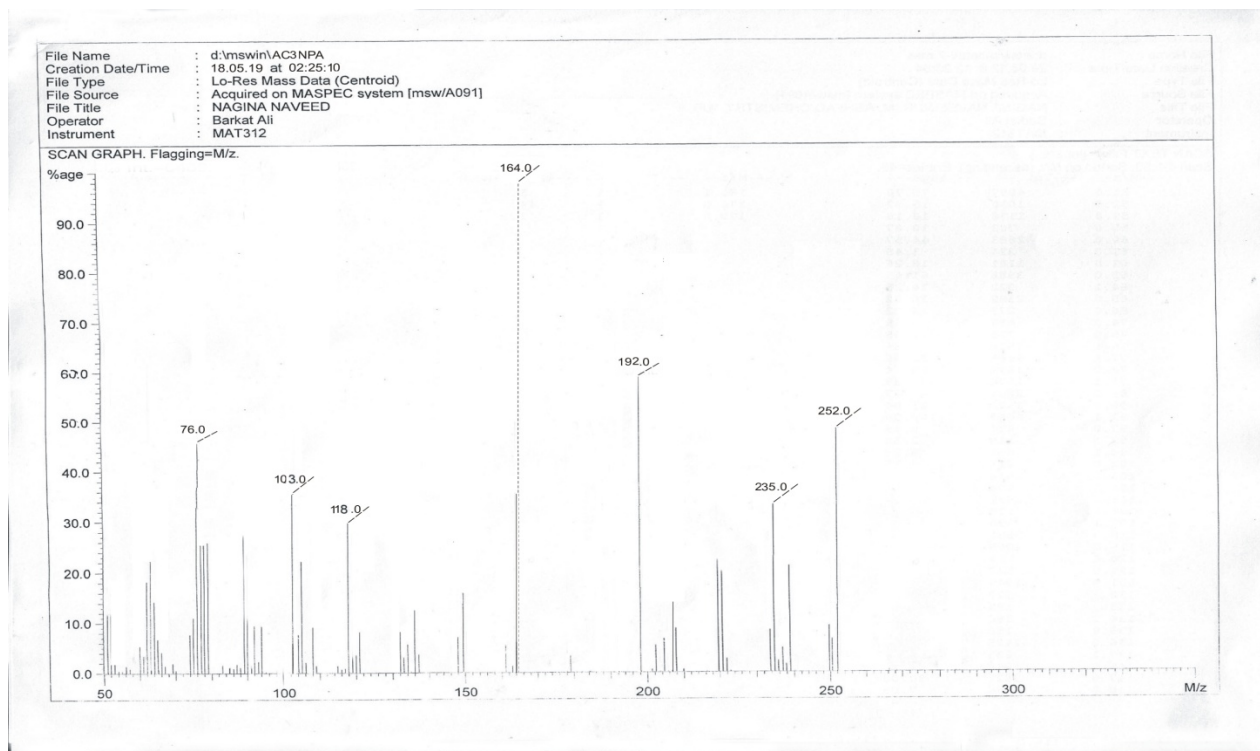


Fig. S65 EI Mass spectrum of 3-Acetylamino-3(3-nitrophenyl) propanoic acid **L₅**

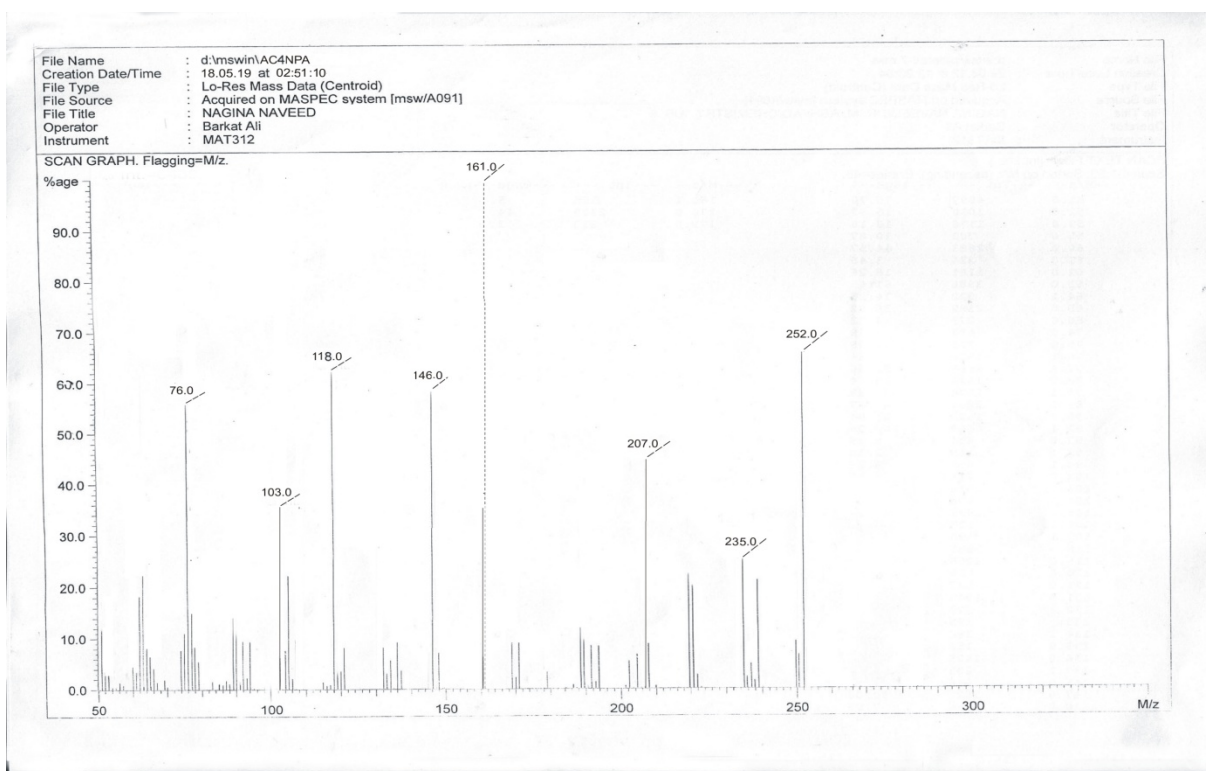


Fig. S66 EI Mass spectrum of 3-Acetylamino-3(4-hydroxyphenyl) propanoic acid **L₆**

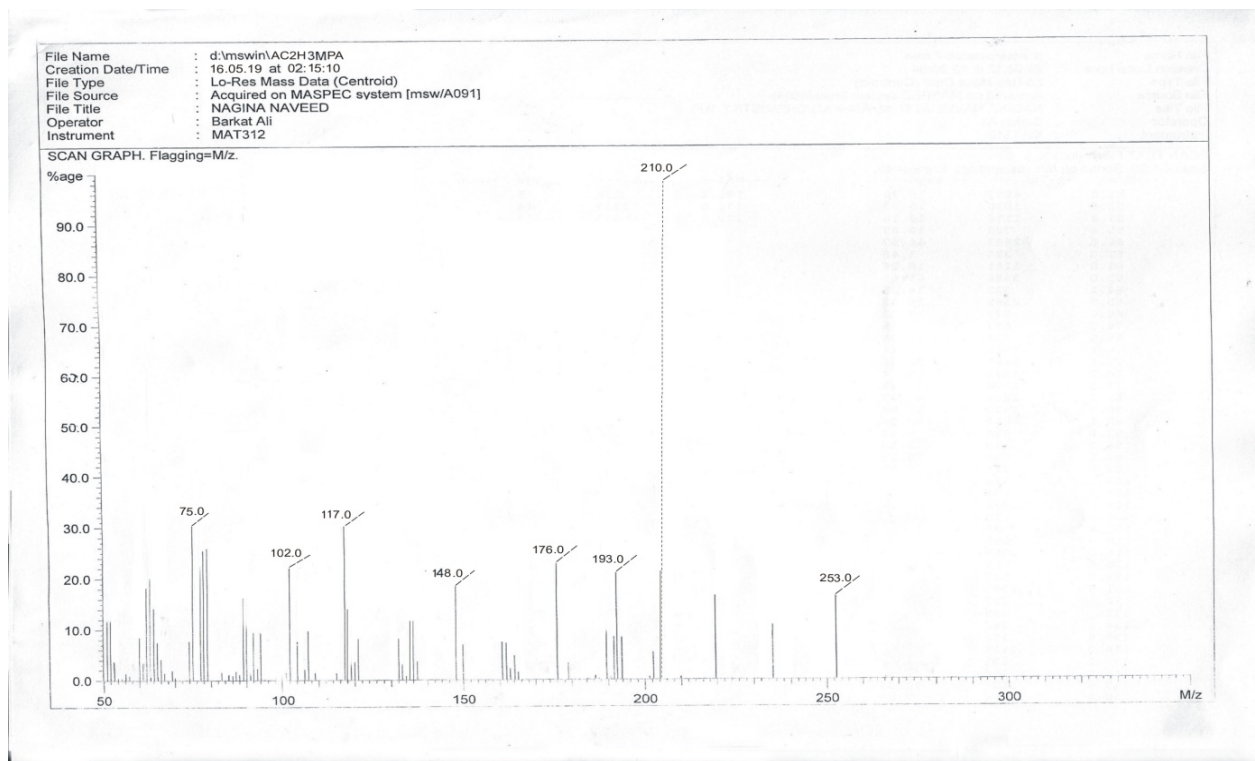


Fig. S67 EI Mass spectrum of 3-Acetylamino-3(2-hydroxy-3-methoxyphenyl) propanoic acid **L₇**

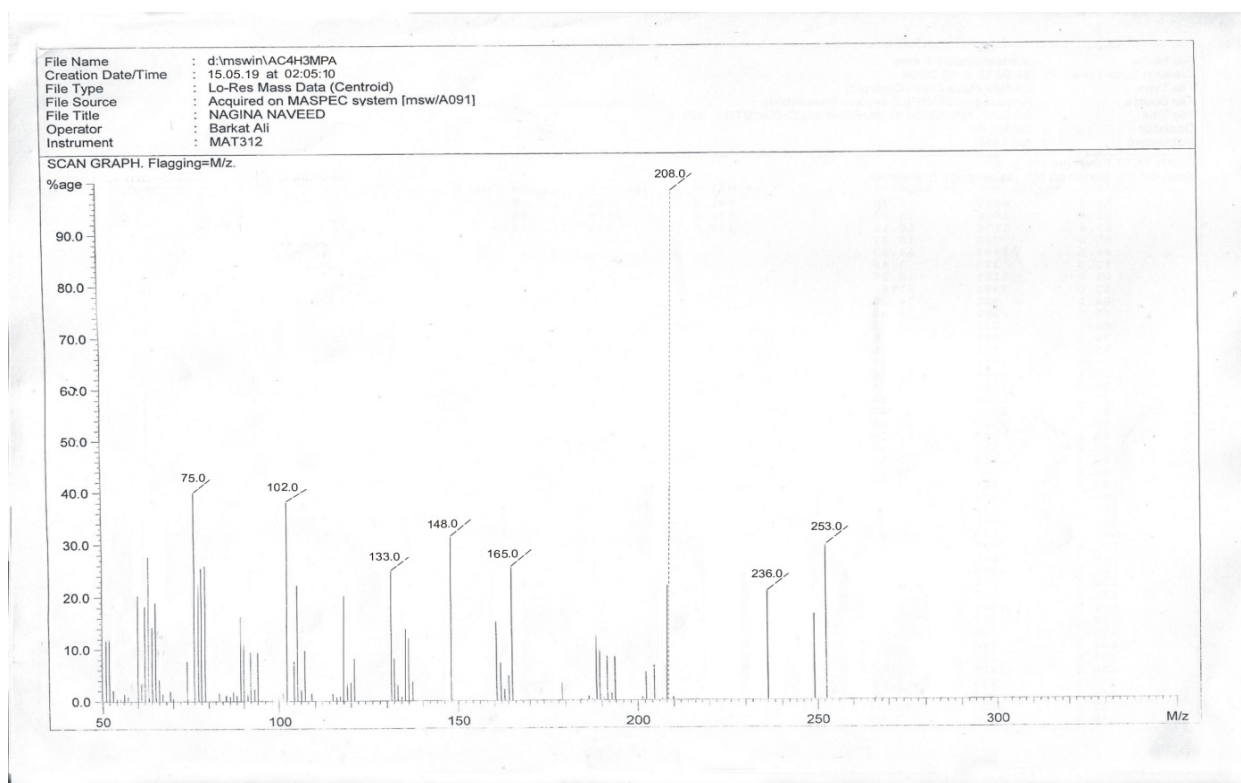


Fig. S68 EI Mass spectrum of 3-Acetylamino-3(4-hydroxy-3-methoxyphenyl) propanoic acid **L₈**

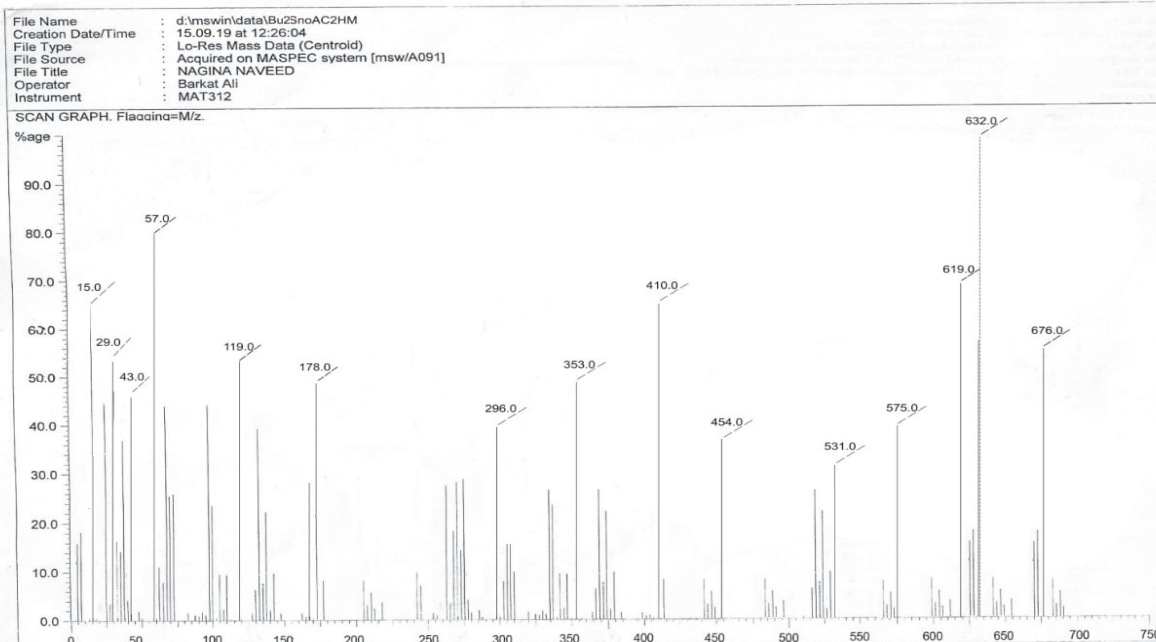


Fig. S69 EI Mass spectrum of dibutyltin(IV) oxide monomer complex (1) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid L_1

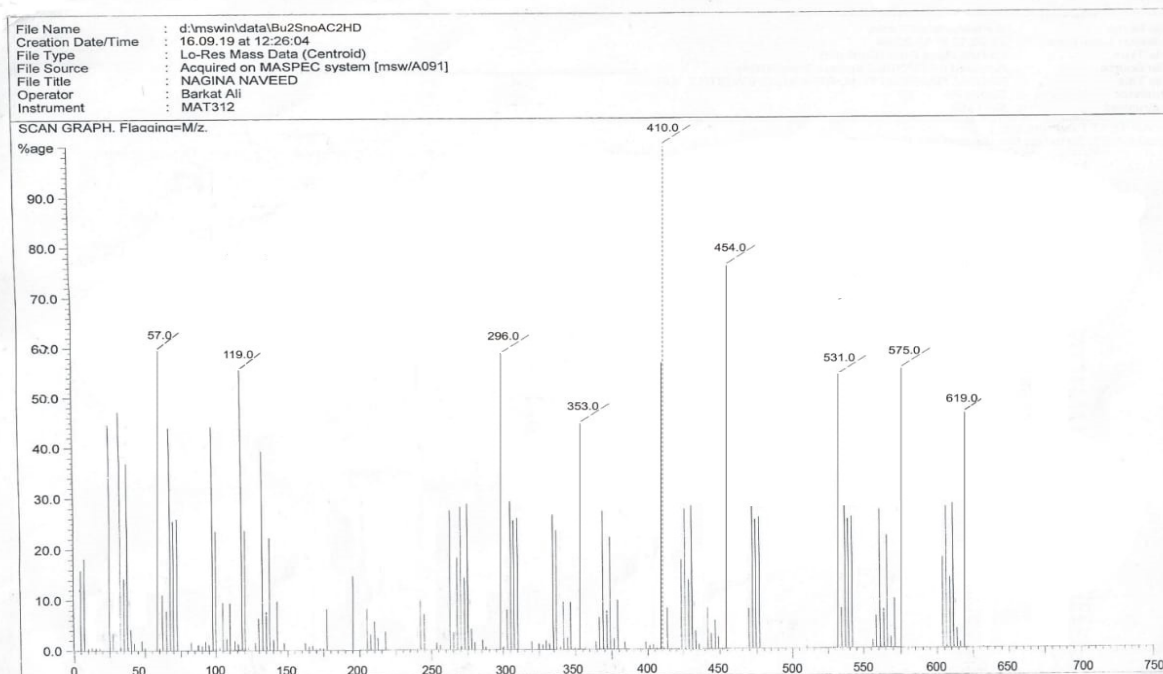


Fig. S70 EI Mass spectrum of dibutyltin(IV) oxide dimer complex (2) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid L_1

File Name : d:\mswin\data\Bu2Sncl2AC2H
Creation Date/Time : 16.09.19 at 10:22:04
File Type : Lo-Res Mass Data (Centroid)
File Source : Acquired on MASPEC system [msw/A091]
File Title : NAGINA NAVEED
Operator : Barkat Ali
Instrument : MAT312

SCAN GRAPH. Flaccino=M/z.

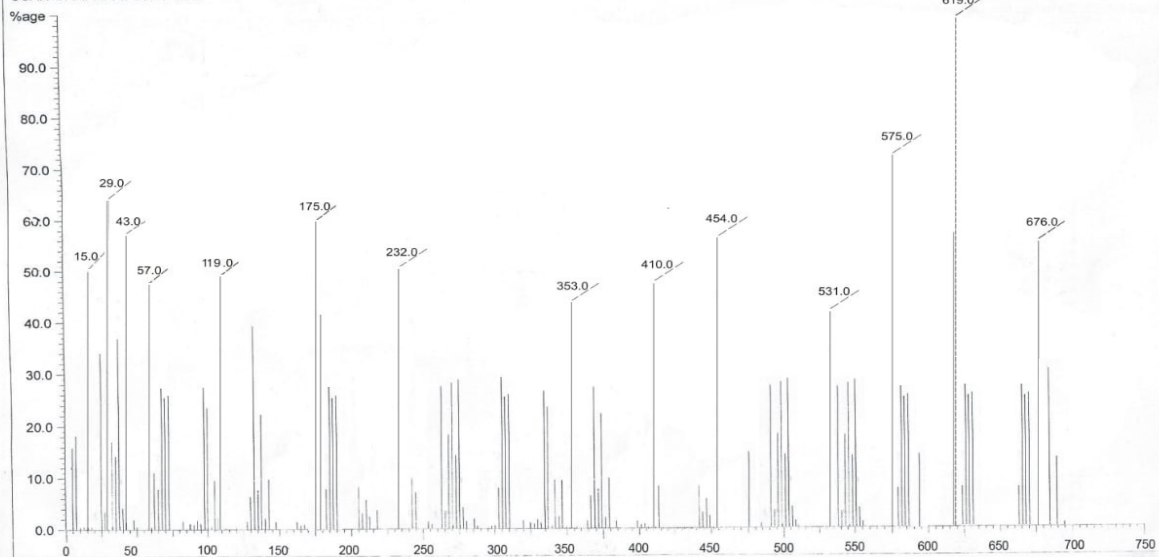


Fig. S71 EI Mass spectrum of dibutyltin(IV) dichloride complex (**3**) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid **L₁**

File Name : d:\mswin\data\Bu3SnclAC2H
Creation Date/Time : 16.09.19 at 01:54:09
File Type : Lo-Res Mass Data (Centroid)
File Source : Acquired on MASPEC system [msw/A091]
File Title : NAGINA NAVEED
Operator : Barkat Ali
Instrument : MAT312

SCAN GRAPH. Flaccino=M/z.

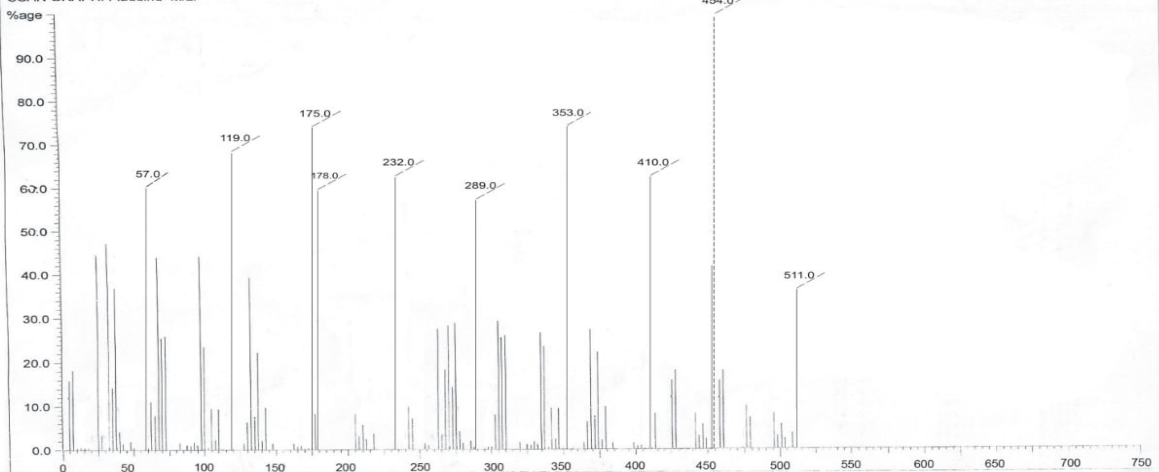


Fig. S72 EI Mass spectrum of tributyltin(IV) chloride complex (**4**) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid **L₁**

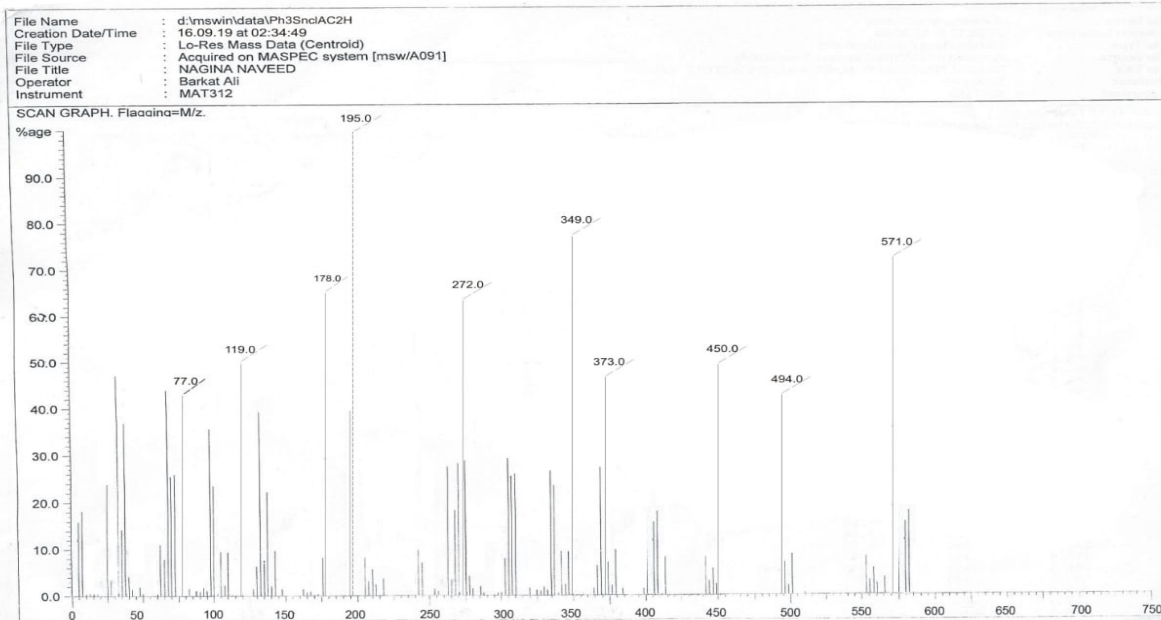


Fig. S73 EI Mass spectrum of triphenyltin(IV) chloride complex (5) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid L_1

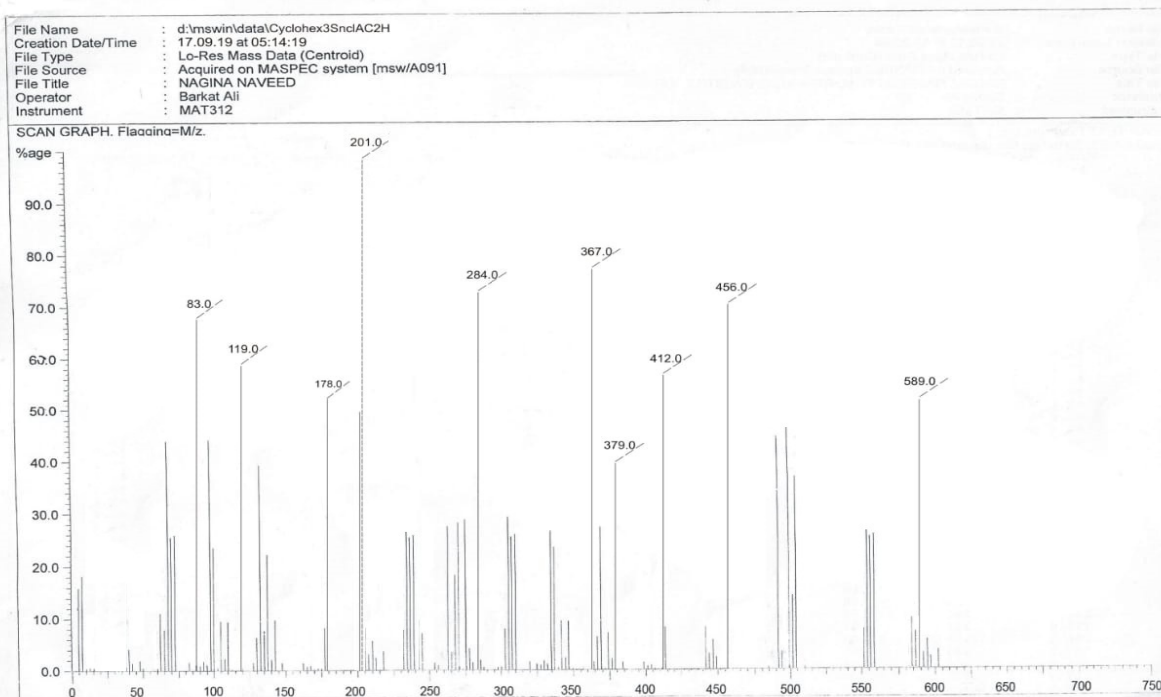


Fig. S74 EI Mass spectrum of tricyclohexyltin(IV) chloride complex (6) with 3-Acetylamino-3(2-hydroxyphenyl) propanoic acid L_1

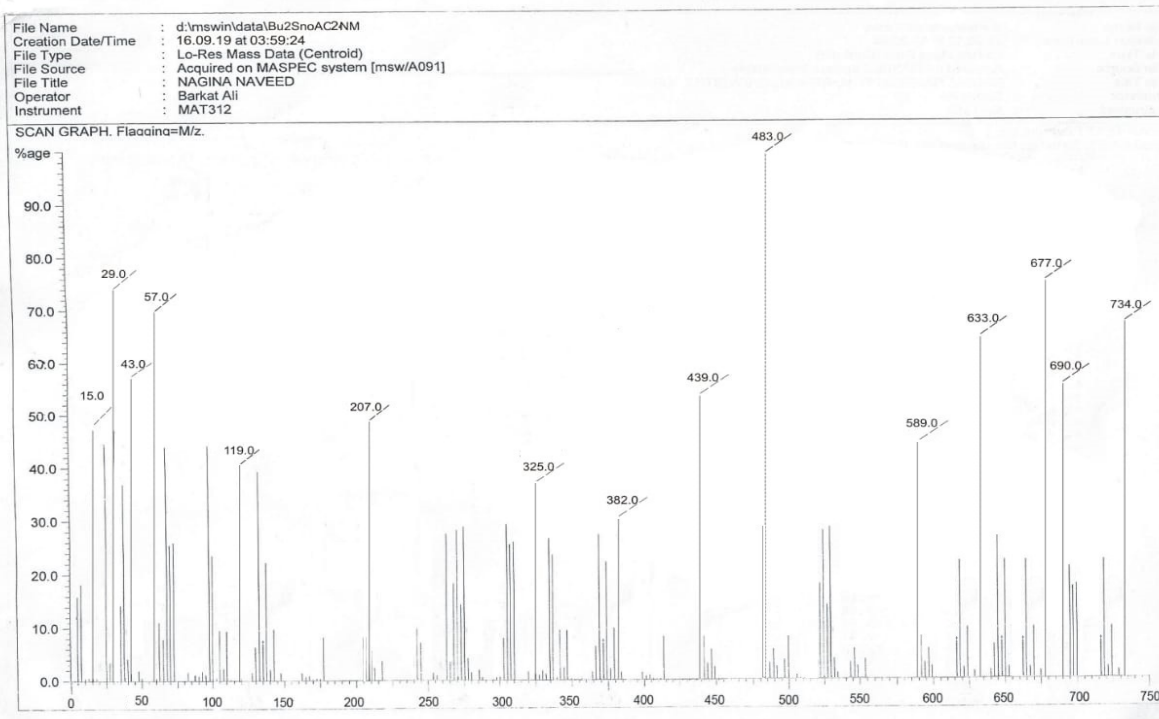
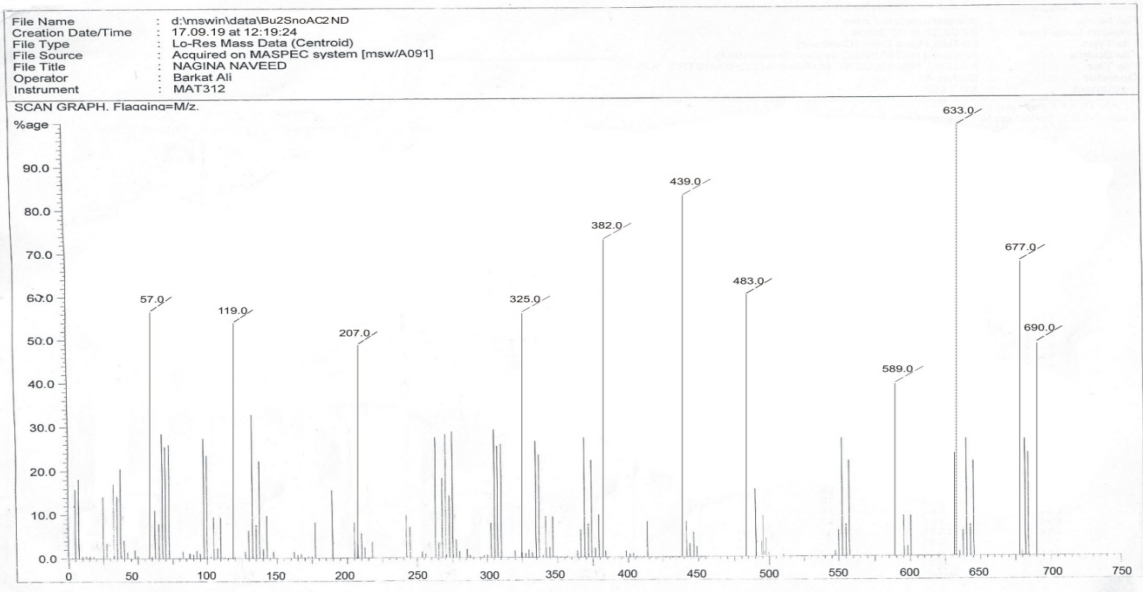
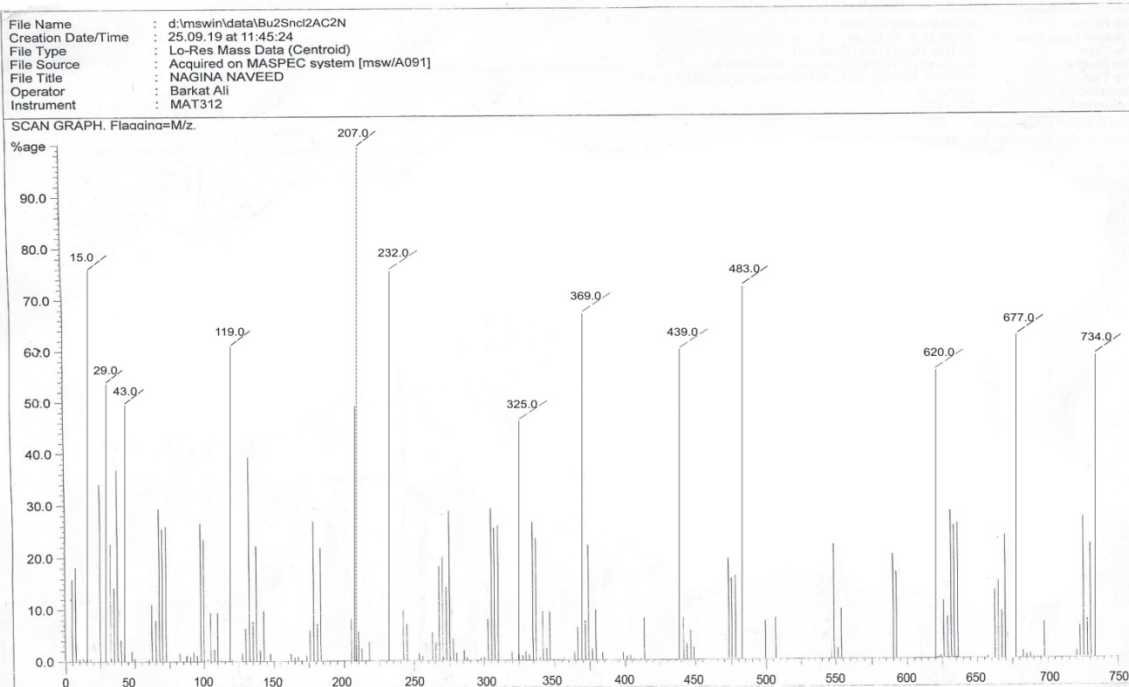


Fig. S75 EI Mass spectrum of dibutyltin(IV) oxide monomer complex (**7**) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid L_4



Fi

g. S76 EI Mass spectrum of dibutyltin(IV) oxide dimer complex (**8**) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid L_4



Fi

g. S77 EI Mass spectrum of dibutyltin(IV) dichloride complex (**9**) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid **L₄**

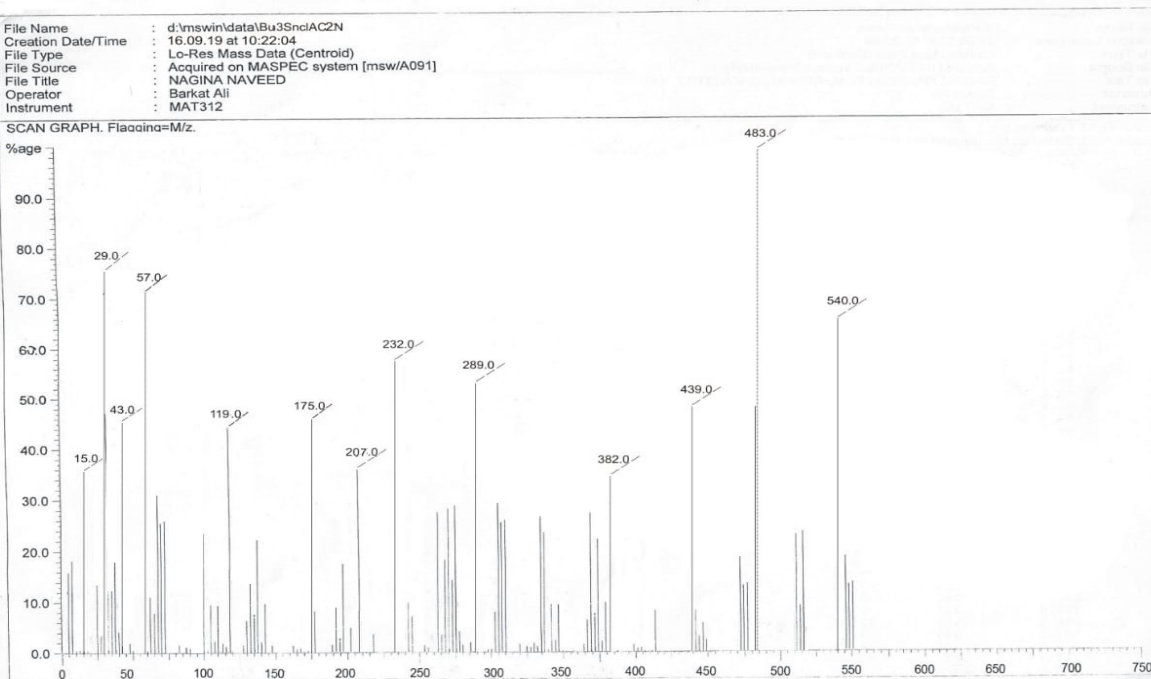


Fig. S78 EI Mass spectrum of tributyltin(IV) chloride complex (**10**) with 3-Acetylamino-3(2-

nitrophenyl) propanoic acid **L₄**

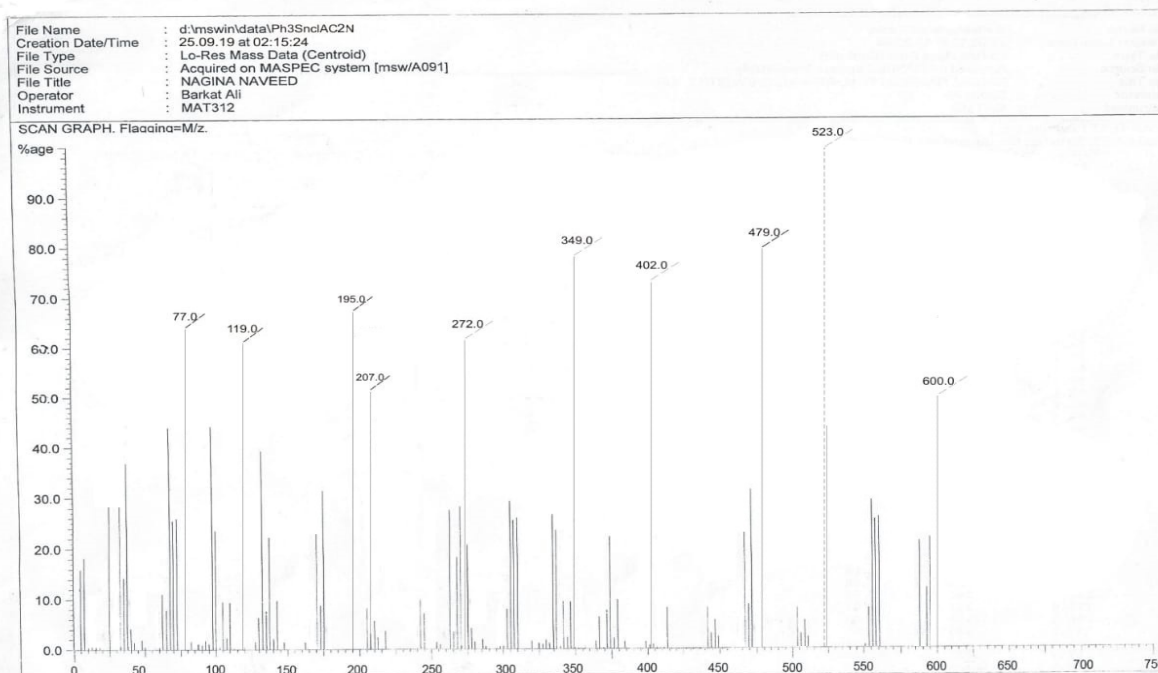


Fig. S79 EI Mass spectrum of triphenyltin(IV) chloride complex (**11**) with 3-Acetylamino-3(2-nitrophenyl) propanoic acid **L₄**

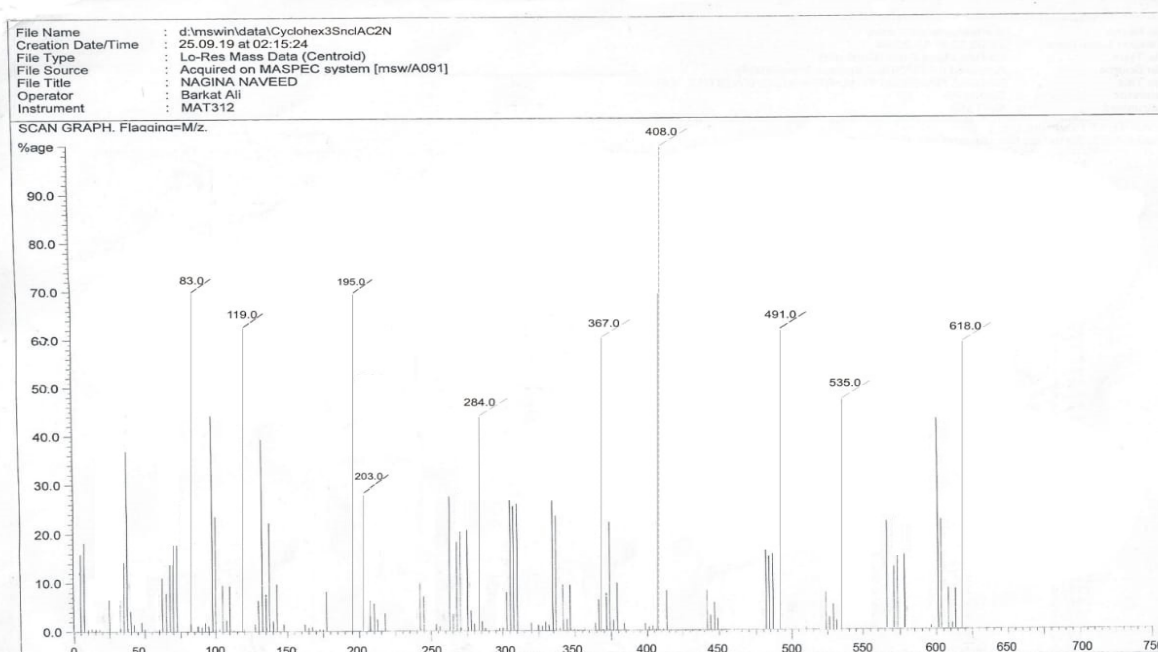


Fig. S80 EI Mass spectrum of tricyclohexyltin(IV) chloride complex (**12**) with 3-Acetylamino-3(2-

nitrophenyl) propanoic acid L₄