Supplementary Information

Antischistosomal Activity of 1,4-Dihydropyridines

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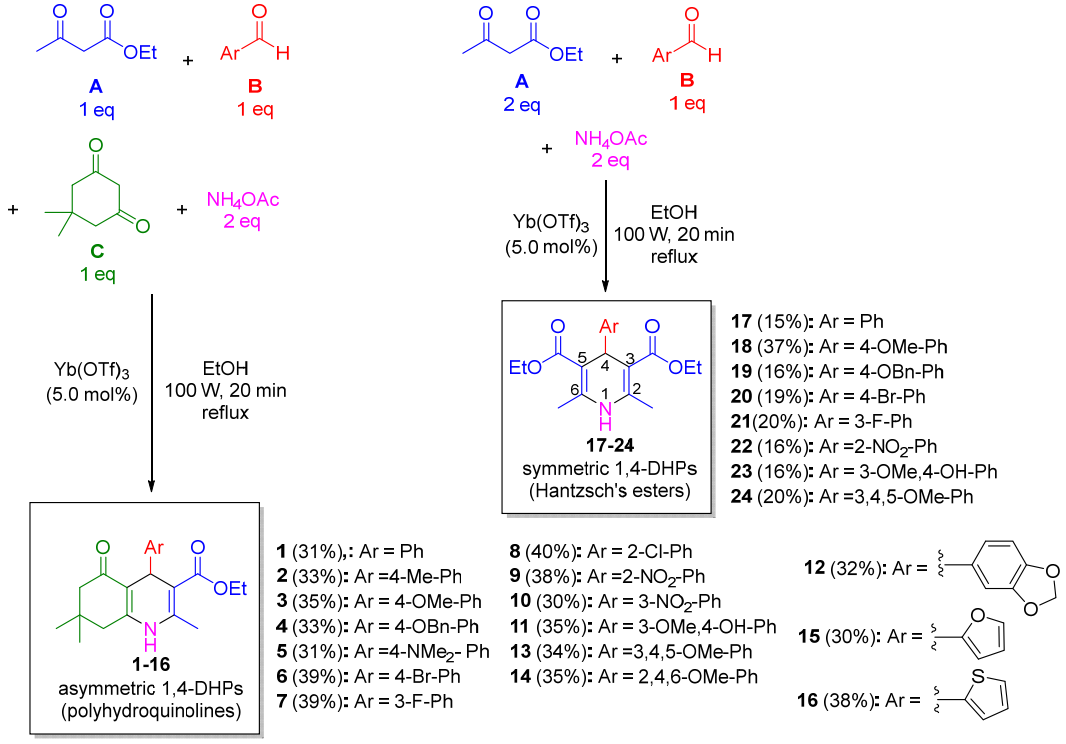
1. Experimental

The 1,4-DHPs **1-24** (Scheme 1) were synthesized according to the multicomponent one-pot methodology described in the literature [7,40]. In the general procedure to obtain compounds **1-16**, 2.0 mmol of dimedone (Aldrich), 2.0 mmol of ethyl acetoacetate (Aldrich), and 0.06 g (5.0 mol%) of ytterbium triflate (Aldrich), as the reaction catalyst, were diluted in ethanol (5.0 mL). Subsequently, 2.0 mmol of benzaldehyde (Aldrich) and 2.0 mmol of ammonium acetate (Scientific Exodus) were added. All the reagents were added at room temperature. The reaction mixture was taken to the microwave reactor CEM Focused Microwave™ Synthesis System, model Discover (CEM Corp, Matthews, NC), set in the Power Time, where it was maintained for 30 min at a fixed power of 100 W. After 30 min, the reaction mixture was filtered off under reduced pressure, and the resulting solid product was recrystallized from ethanol. Compounds **17-24** were obtained in the same conditions, except for the use of 4.0 mmol of ethyl acetoacetate (*i.e.*, 2.0 mmol of dimedone was replaced with 2.0 mmol ethyl acetoacetate).



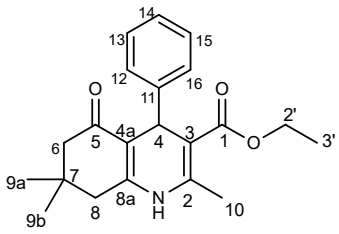
Scheme 1. Synthesis of compounds **1–24** through a microwave-assisted one-pot Hantzsch multicomponent reaction.

Compounds **1–24** were identified based on their NMR (^{1}H, ^{13}C, and DEPT 135) and mass spectra, and their minimal purity of 95% was checked using HPLC. Compounds **1-16** were isolated and tested as mixtures of enantiomers.

^{1}H and ^{13}CNMR, and DEPT 135 experiments were performed on a Bruker Avance DRX400 spectrometer (Karlsruhe, Germany, 400.13 MHz for 1H and 100.61 MHz for ^{13}C). A direct 5-mm probe head (BBO) was used for ^{13}C{^{1}H} NMR experiments and an inverse 5-mm probe head (BBI) was used for other experiments. Experiments were performed at 300 K and the concentrations for all samples were in the range of 10-15 mg mL^{-1}, in $CDCl_3$ using tetramethylsilane (TMS) as an internal reference.

Mass spectra were recorded on triple quadrupole MS equipment (QqQ) Xevo TQS (Waters, Milford, MA, USA) equipped with Z-spray operating in the positive ion mode and Acquiti-H class UPLC system. The sample was dissolved in methanol/water (9:1, v/v) at a concentration of 0.5 mg mL^{-1} and infused directly into the ESI source by using a Harvard Apparatus system (model 1746, Houston, MA, USA) at a flow rate of 5 µL min^{-1}. The capillary voltage was 3.20 kV, and the gas flow was 700 L/h (0.15 V). The desolvation temperature was set at 250°C.

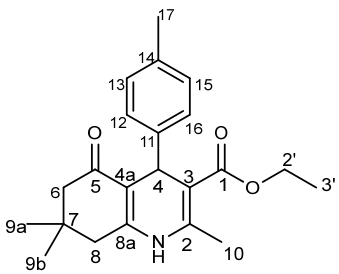
Compounds **1-16** were isolated as mixtures of enantiomers. All the tested compounds displayed purity higher than 95%, as confirmed by HPLC analyses. To this end, compounds **1-24** were dissolved in an acetonitrile:water 4:1 (v/v) solution to achieve a concentration of 0.5 mg mL^{-1}. These compounds were analyzed on a Shimadzu LC 6AD chromatograph fitted with a UV-vis SPD-20A operating at 270 nm and a DGU-20A5 degasser. A Phenomenex Luna C_{18} 100 Å (5 µm x 250 mm x 4.6 mm) column was used. The injection volume was 500 µL. A mixture of acetonitrile:water 4:1 (v/v) was used as the mobile phase at a flow rate of 1 mL min^{-1}. The total time of each analysis was 1 h.



1

(±)-ethyl 2,7,7-trimethyl-5-oxo-4-phenyl-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**1**). White powder, 31% yield. Purity (HPLC): > 95% (**Fig. S1**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S2**): δ 0.98 (3H, s, H9b), 1.11 (3H, *s*, H9a), 1.25 (3H, *t*, *J* = 7.0 Hz, H3′), 2.15-2.35 (4H, *m*, H6 and H8), 2.40 (3H, *s*, H10), 4.12 (2H, *q*, *J*= 6.8 Hz, H2′), 5.10 (1H, *s*, H4), 7.10 – 7.40 (5H, *m*, H12=16, H13=H15, and H14).^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S3** and **S4**): δ 14.0 (CH_3, C3′), 19.2 (CH_3, C10), 27.0 (CH_3, C9a), 29.2 (CH_3, C9b), 32.5 (C, C7), 36.5 (CH, C4), 41.0 (CH_2, C8), 50.8 (CH_2, C6), 59.7 (CH_2, C2′), 105.9 (C, C3), 111.9 (C, C4a), 125.8 (CH, C14), 127.8 (CH, C12=C16, C13=C15), 143.4 (C, C11), 146.9 (C, C8a), 148.4 (C, C2), 167.7 (C1′), 195.6 (C, C5). ESI(+)-MS (**Fig. S5**): *m*/*z* 378 (5%, $[M+K]^+$), *m*/*z* 362 (49%, $[M+Na]^+$), *m*/*z* 340 (100%, $[M+H]^+$), *m*/*z* 262 (15%, $[M+H-C_6H_6]^+$).

(±)-ethyl 2,7,7-trimethyl-5-oxo-4-(p-tolyl)-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (2). Yellowish powder, 33% yield. Purity (HPLC): > 95% (**Fig. S6**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S7**): δ 0.94 (3H, *s*, H9b), 1.07 (3H, *s*, H9a), 1.21 (3H, *t*, *J* = 7.1 Hz, H3′), 2.13-2.30 (4H, *m*, H6 and H8), 2.25 (3H, *s*, H17), 2.35 (3H, *s*, H10), 4.05 (2H, *q*, *J*= 7.1 Hz, H2′), 5.01 (1H, *s*, H4), 6.99 (2H, *d*, *J*=7.9 Hz, H13=H15), 7.18 (2H, *d*, *J*=7.9 Hz, H12=H16). ^{13}C (400 MHz, *CDCl*$_3$, **Fig. S8** and **S9**): δ 14.0 (CH_3, C3′), 19.3 (CH_3, C10), 20.9 (CH_3, C17), 27.1 (CH_3, C9a), 29.2 (CH_3, C9b), 32.6 (C, C7), 35.9 (CH, C4), 40.9 (CH_2, C8), 50.5 (CH_2, C6), 59.6 (CH_2, C2′), 106.1 (C, C3), 112.2 (C, C4a), 127.7 (CH, C13=C15), 128.4 (CH, C12=C16), 135.2 (C, C14), 143.0 (C, C11), 143.9 (C, C8a), 147.7 (C, C2), 167.3 (C, C1), 195.3 (C, C5). ESI(+)-MS (**Fig. S10**): *m*/*z* 392 (5%, $[M+K]^+$), *m*/*z* 376 (90%, $[M+Na]^+$), *m*/*z* 354 (100%, $[M+H]^+$), *m*/*z* 262 ($[M+H-C_7H_7]^+$).



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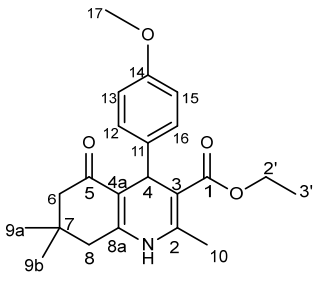
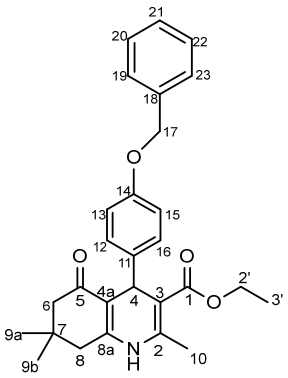


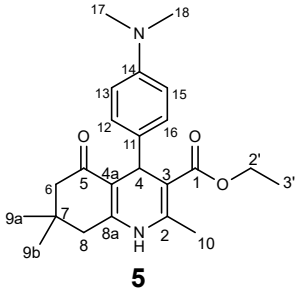
3

(±)-ethyl 4-(4-methoxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**3**). Yellowish powder, 35% yield. Purity (HPLC): > 95% (**Fig. S11**). NMR ^{1}H (400 MHz, *CDCl*$_3$, **Fig. S12**): δ 0.93 (3H, s, H9b), 1.07 (3H, *s*, H9a), 1.20 (3H, *t*, *J* = 7.1 Hz, H3′), 2.13-2.34 (4H, *m*, H6 and H8), 2.36 (3H, *s*, H10), 3.73 (3H, *s*, H17) 4.04 (2H, *q*, *J*= 7.1 Hz, H2′), 4.99 (1H, *s*, H4), 6.74 (2H, *d*, *J*=8.7 Hz, H13=H15), 7.21(2H, *d*, *J*=8.7 Hz, H12=H16).^{13}C (400 MHz, *CDCl*$_3$, **Fig. S13** and **S14**): δ 14.1 (CH_3, C3′), 19.2 (CH_3, C10), 27.1 (CH_3, C9a), 29.2 (C9b CH_3,), 32.4 (C, C7), 35.6 (CH, C4), 41.1 (CH_2, C8), 50.5 (CH_2, C6), 54.9 (CH_3, C17), 60.0 (CH_2, C2′), 106.3 (C, C3), 112.3 (C, C4a), 113.3 (CH, C13=C15), 129.1 (CH, C12=C16), 139.5 (C, C11) , 143.0 (C, C8a) , 147.4 (C, C2), 157.6 (C, C14), 167.4 (C, C1′), 197.6 (C, C5). ESI(+)-MS (**Fig. S15**): *m*/*z* 408 (5%, $[M+K]^+$), *m*/*z* 392 (100%, $[M+Na]^+$), *m*/*z* 370 (80%, $[M+H]^+$), *m*/*z* 262 (100%, $[M+H-C_7H_8O]^+$).



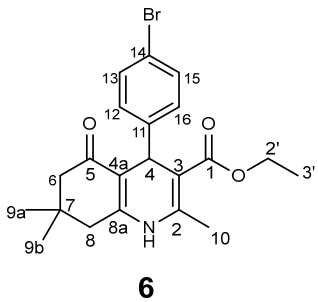
4

(±)-*ethyl 4-(4-(benzyloxy)phenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate* (**4**). Yellowish powder, 33% yield. Purity (HPLC): > 95% (**Fig. S16**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S17**): δ 0.94 (3H, *s*, H9b), 1.07 (3H, *s*, H9a), 1.20 (3H, *t*, *J* = 7.1 Hz, H3′), 2.13-2.30 (4H, *m*, H6 and H8), 2.37 (3H, *s*, H10), 4.05 (2H, *q*, *J*=7.1 Hz, H2′), 4.98 (2H, *s*, H17), 5.00 (1H, *s*, H4), 6.81 (2H, *d*, *J* = 8.5 Hz, H13=H15), 7.21 (2H, *d*, *J* = 8.5 Hz, H12=H16), 7.30-7.41 (5H, *m*, H19=H23, H20=H22, and H23).^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S18** and **S19**): δ 14.2 (CH_3, C3′), 19.7 (CH_3, C10), 27.4 (CH_3, C9a), 29.3 (CH_3, C9b), 32.8 (C, C7), 35.8 (CH, C4), 41.1 (CH_2, C8), 50.8 (CH_2, C6), 59.9 (CH_2, C2′), 70.0 (CH_2, C17), 106.4 (C, C3), 112.4 (C, C4a), 114.2 (CH, C13=C15), 128.6 (CH, C19=C23), 129.1 (CH, C21), 137.4 (CH, C20=C22), 140.0 (CH, C12=C16), 143.4 (C, C11=C18), 148.2 (C, C8a), 157.2 (C, C2), 167.7 (C, C1), 195.9 (C, C5). ESI(+)-MS (**Fig. S20**): *m*/*z* 484 (5%, $[M+K]^+$), *m*/*z* 468 (50%, $[M+Na]^+$), *m*/*z* 446 (40%, $[M+H]^+$), *m*/*z* 262 ($[M+H-C_{13}H_{12}O]^+$).



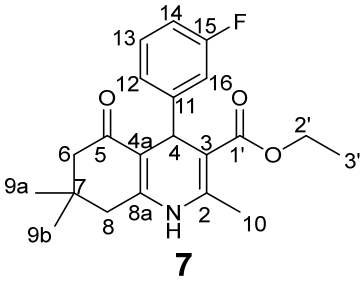
5

(±)-*ethyl 4-(4-(dimethylamino)phenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate* (**5**). Yellow powder, 31% yield. Purity (HPLC): > 95% (**Fig. S21**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S22**): δ 0.96 (3H, *s*, H9b), 1.07 (3H, *s*, H19a), 1.22 (3H, *t*, *J* = 7.0 Hz, H3′), 2.17-2.33 (4H, *m*, H6 and H8), 2.35 (3H, *s*, H10), 2.86 (6H, *s*, H17=H18), 4.04 (2H, *q*, *J*=7.0 Hz, H2′), 4.94 (1H, *s*, H4), 6.57 (2H, *d* , *J*= 8.8 Hz, H13=H15), 7.15 (2H, *d*, *J*= 8.8 Hz, H12=H16).^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S23** and **24**): δ 14.4 (CH_3, C3′), 19.4 (CH_3, C10), 27.4 (CH_3, C9a), 29.3 (CH_3, C9b), 32.7 (C, C7), 35.4 (CH, C4), 40.7 (CH_3, C17=C18), 40.9 (CH_2, C8), 50.9 (CH_2, C6), 59.9 (CH_2, C2′), 106.4 (C, C3),112.4 (C, C4a), 112.5 (CH, C12=C16), 128.9 (CH, C13=C15), 135.9 (C, C11), 143.4 (C, C14), 148.2 (C, C8a), 149.1 (C, C2), 167.9 (C, C1′), 196.1 (C, C5). ESI(+)-MS (**Fig. S25**): *m*/*z* 405 (35%, $[M+Na]^+$), *m*/*z* 383 (40%, $[M+H]^+$), *m*/*z* 262 (100%, $[M+H-C_6H_5NMe_2]^+$).



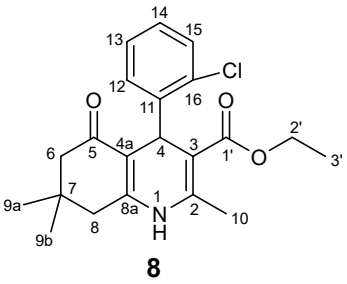
6

(±)-*ethyl 4-(4-bromophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate* (**6**). Yellowish powder, 39% yield. Purity (HPLC): > 95% (**Fig. S26**). NMR ^{1}H (400 MHz, *CDCl*$_3$, **Fig. S27**): δ 0.92 (3H, *s*, H9a), 1.06 (3H, *s*, H9b), 1.19 (3H, *t*, *J* = 7.1 Hz, H3′), 2.12-2.29 (4H, *m*, H6 and H8), 2.36 (3H, *s*, H10), 4.04 (2H, *q*, *J*=7.1 Hz, H2′), 5.00 (1H, *s*, H4), 7.17 (2H, *d* , *J*= 8.4 Hz, H12=H16), 7.30 (2H, *d*, *J*= 8.4 Hz, H13=H15).^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S28** and **29**): δ 14.7 (CH_3, C3′), 19.9 (CH_3, C10), 27.5 (CH_3, C9a), 29.9 (CH_3, C9b), 33.2 (C, C7), 36.7 (CH, C4) , 41.5 (CH_2, C8), 51.1 (CH_2, C6), 60.2 (CH_2, C2′), 106.1 (C, C3), 112.2 (C, C4a), 120.2 (C, C14), 130.3 (CH, C12=C16), 131.4 (CH, C13=C15), 144.1 (C, C11), 146.5 (C, C8a), 148.7 (C, C2), 167.6 (C, C1) ,195.9 (C, C5). ESI(+)-MS (**Fig. S30**): *m*/*z* 440/442 (30%, $[M+Na]^+$), *m*/*z* 418/420 (100%, $[M+H]^+$), *m*/*z* 262 (50%, $[M+H-C_6H_5Br]^+$).



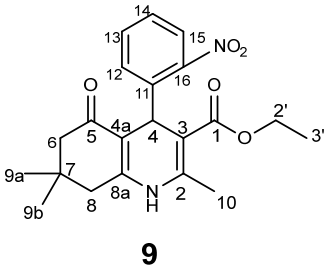
7

(±)-ethyl 4-(3-fluorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**7**). White powder, 39% yield. Purity (HPLC): > 95% (**Fig. S31**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S32**): δ 0.94 (3H, s, H9b), 1.08 (3H, *s*, H9a), 1.19 (3H, *t*, *J* = 7.1 Hz, H3′), 2.30-2.43 (4H, *m*, H6 and H8), 2.38 (3H, *s*, H10), 4.06 (2H, *q*, *J*=7.1 Hz, H2′), 5.06 (1H, *s*, H14), 6.79 (1H, *t*, *J*= 7.8 Hz, H13), 6.97 (1H, *d*, *J*= 9.9 Hz H12), 7.08-7.18 (2H, *m*, H14 and H16) .^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S33** and **S34**): δ 14.2 (CH_3, C3′), 19.7 (CH_3, C10), 27.0 (CH_3, C9a), 29.2 (CH_3, C9b), 32.8 (C, C7), 35.7 (CH, C4), 41.1 (CH_2, C8), 50.8 (CH_2, C6), 60.1 (CH_2, C2′), 105.7 (C, C3),111.6 (C, C4a), 112.5 (CH, C16), 114.4 (CH, C13), 122.2 (C, C11), 129.8 (CH, C14), 143.7 (CH, C12), 148.5 (C, C8a), 149.3 (C, C2), 163.9 (C, C15), 167.4 (C, C1′),195.7 (C, C5). ESI(+)-MS (**Fig. S35**): *m*/*z* 380 (45%, $[M+Na]^+$), *m*/*z* 358 (100%, $[M+H]^+$), *m*/*z* 262 (30%, $[M+H-C_6H_5F]^+$).



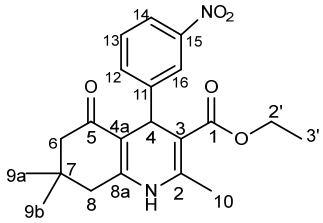
8

(±)-ethyl 4-(2-chlorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**8**). White powder, 40% yield. Purity (HPLC): > 95% (**Fig. S36**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S37**): δ 0.93 (3H, *s*, H9a), 1.08 (3H, *s*, H9b), 1.19 (3H, *t*, *J* = 7.1 Hz, H3′), 2.12-2.36 (4H, *m*, H6 and H8), 2.40 (3H, *s*, H10), 4.05 (2H, *q*, *J*= 7.1 Hz, H2′), 5.15 (1H, *s*, H4), 7.70 (1H, *d*, *J*= 7.7 Hz, H12), 7.91 (1H, *t*, *J* = 7.9 Hz, H13), 7.97 (1H, *d*, *J*=8.2 Hz, H15), 8.10 (1H, *t*, *J*= 1.9 Hz, H16).^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S38** and **S39**): δ 14.0 (CH_3, C3′), 19.4 (CH_3, C10), 26.9 (CH_3, C9a), 29.2 (CH_3, C9b), 32.6 (C, C7) , 36.8 (CH, C4), 40.91 (CH_2, C8), 50.4 (CH_2, C6), 59.9 (CH_2, C2′), 105.0 (C, C3), 111.2 (C, C4a), 121.1 (CH, C12), 122.6 (CH, C13), 128.4 (CH, C14), 134.7 (CH, C15), 144.03 (C, C16), 148.2 (C, C8a) , 148.9 (C, C11), 157 (C, C2), 166.7 (C, C1′), 195.2 (C, C5). ESI(+)-MS (**Fig. S40**): *m*/*z* 396 (100%, $[M+Na]^+$), *m*/*z* 374 (100%, $[M+H]^+$), *m*/*z* 262 (50%, $[M+H-C_6H_5Cl]^+$).



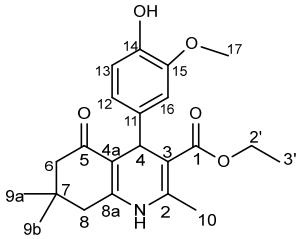
9

(±)-ethyl 2,7,7-trimethyl-4-(2-nitrophenyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**9**). Yellowish powder, 38% yield. Purity (HPLC): > 95% (**Fig. S41**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S42**): δ 0.93 (3H, *s*, H9b), 1.08 (3H, *s*, H9a), 1.18 (3H, *t*, *J* = 7.1 Hz, H3′), 2.11-2.35 (4H, *m*, H6 andH8), 2.39 (3H, *s*, H10), 4.03 (2H, *q*, *J*=7.1 Hz, H2′), 5.14 (1H, *s*, H4), 7.36 (1H, *t*, *J*= 7.9 Hz, H14), 7.70 (1H, *d*, *J*= 7.7 Hz, H12) 7.99 (1H, *d*, *J*= 8.2 Hz, H15), 8.10 (1H, *t*, *J*= 8.4 Hz, H=13).^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S43** and **S44**): δ 13.9 (CH_3, C3′), 19.4 (CH_3, C10), 26.8 (CH_3, C9a), 29.3 (CH_3, C9b), 32.9 (C, C7), 37.1 (CH, C4), 40.9 (CH_2, C8), 50.7 (CH_2, C6), 60.2 (CH_2, C2′), 104.8 (C, C3), 111.2 (C, C4a), 121.2 (CH, C15), 122.5 (CH, C14), 128.3 (CH, C12) , 134.7 (CH, C13), 144.1 (C, C11), 148.2 (C, C8a), 148.9 (C, C16), 166.5 (C, C1), 195.2 (C, C5). ESI(+)-MS (**Fig. S45**): *m*/*z* 407 (55%, $[M+Na]^+$), *m*/*z* 385 (100%, $[M+H]^+$).



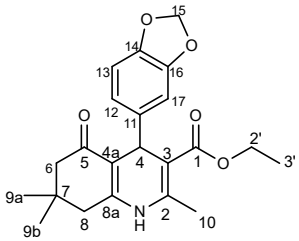
10

(±)-ethyl 2,7,7-trimethyl-4-(3-nitrophenyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**10**). White powder, 30% yield. Purity (HPLC): > 95% (**Fig. S46**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S47**): δ 0.93 (3H, *s*, H9b), 1.09 (3H, s, H9a), 1.19 (3H, *t*, *J* = 7.1 Hz, H3′), 2.12-2.36 (4H, *m*, H6 and H8),), 2.40 (3H, *s*, H10), 4.05 (2H, *q*, *J*=7.3 Hz, H2′), 5.15 (1H, s, H4), 7.41 (1H, *t* , *J*= 7.9 Hz, H14), 7.72 (1H, *d*, *J*= 7.7 Hz, H12) 7.97 (1H, *d*, *J*= 8.2 Hz, H15), 8.10 (1H, *t*, *J*=1.4 Hz, H13).^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S48** and **S49**): δ 14.2 (CH_3, C3′), 18.6 (CH_3, C10), 27.1 (CH_3, C9a), 29.6 (CH_3, C9b), 32.6 (C, C7), 35.4 (CH, C4), 41.6 (CH_2, C8), 51.0 (CH_2, C6), 59.5 (CH_2, C2′), 104.2 (C, C3), 110.6 (C, C4a), 121.2 (CH, C14), 122.5 (CH, C12), 128.3 (CH, C13) , 134.7 (CH, C16), 143.1 (C, C15), 147.9 (C, C11), 148.5 (C, C8a), 159.1 (C, C2), 168.4 (C, C1′), 195.7 (C, C5). ESI(+)-MS (**Fig. S50**): *m*/*z* 378 (5%, $[M+K]^+$), *m*/*z* 362 (70%, $[M+Na]^+$), *m*/*z* 340 (15%, $[M+H]^+$), *m*/*z* 262 (100%, $[M+H-C_6H_5NO_2]^+$).



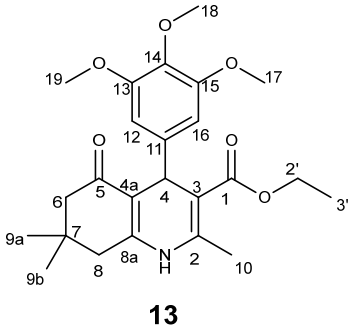
11

(±)-ethyl 4-(4-hydroxy-3-methoxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (11). Orangish powder, 35% yield. Purity (HPLC): > 95% (**Fig. S51**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S52**):): δ 0.94 (3H, *s*, H9b), 1.07 (3H, *s*, H9a), 1.21 (3H, *t*, *J* = 7.1 Hz, H3′), 2.14-2.34 (4H, *m*, H6 and H8), 2.36 (3H, *s*, H10), 3.84 (3H, *s*, H17), 4.08 (2H, *q*, *J*= 7.1 Hz, H2′), 4.96 (1H, *s*, H4), 6.69 (1H, *dd*, *J*=8.2 Hz, H12), 6.72 (1H, *d*, *J*=8.1 Hz, H13), 6.92 (1H, *d*, *J*=1.3 Hz, H16). ^{13}C NMR (400 MHz, *CDCl*$_3$, **Fig. S53** and **S54**): δ 14.4 (CH_3, C3′), 19.5 (CH_3, C10), 27.1 (CH_3, C9a), 29.6 (CH_3, C9b), 32.7 (C, C7), 36.0 (CH, C4), 41.3 (CH_2, C8), 50.8 (CH_2, C6), 55.9 (CH_2, C2′), 59.7 (CH_3, C17), 106.3 (C, C3), 111.3 (C, C4a), 112.3 (CH, C16) , 113.9 (CH, C13), 119.9 (CH, C12), 139.2 (C, C11), 143.3 (C, C14), 145.5 (C, C15), 146.9 (C, C8a), 147.8 (C, C2), 167.4 (C, C1), 195.6 (C, C5). ESI(+)-MS (**Fig. S55**): *m*/*z* 408 (40%, $[M+Na]^+$), *m*/*z* 386 (20%, $[M+H]^+$), *m*/*z* 262 (100%, $[M+H-C_7H_8O_2]^+$).



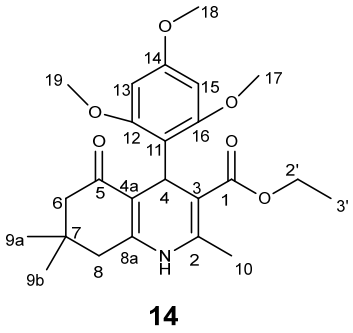
12

(±)-ethyl 4-(benzo[*d*][1,3]dioxol-5-yl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**12**). White powder, 32% yield. Purity (HPLC): > 95% (**Fig. S56**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S57**): δ 0.96 (3H, *s*, H9b), 1.07 (3H, *s*, H9a), 1.21 (3H, *t*, *J* = 7.1 Hz, H21), 2.14-2.30 (4H, *m*, H6 and H8), 2.35 (3H, s, H10), 4.07 (2H, *q*, *J*= 7.1, Hz, H2′), 4.97 (1H, s, H4), 5.86 (2H, *d J*=1.4 Hz, H15), 6.63 (1H, *d*, *J*=7.9 Hz, H13), 6.76-6.80 (2H, *m*, H12 and H17). ^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S58** and **S59**): δ 14.1 (CH_3, C3′), 19.2 (CH_3, C10), 27.10 (CH_3, C9a), 29.2 (CH_3, C9b), 32.5 (C, C7), 36.1 (CH, C4), 40.9 (CH_2, C8), 50.5 (CH_2, C6), 59.7 (CH_2, C2′), 100.4 (CH_2, C15), 106.1 (C, C3), 107.5 (CH, C13), 108.5 (CH, C17), 112.1 (C, C4a), 120.9 (CH, C12), 141.1 (C, C11), 142.9 (C, C14), 145.4 (C, C16), 146.9 (C, C8a), 147.6 (C, C2), 167.3 (C, C1), 195.4 (C, C5). ESI(+)-MS (**Fig. S60**): *m*/*z* 406 (100%, $[M+Na]^+$), *m*/*z* 384 (100%, $[M+H]^+$), *m*/*z* 262 (70%, $[M+H-C_7H_6O_2]^+$).



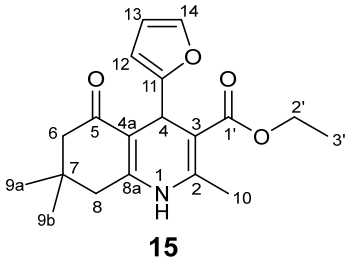
13

(±)-ethyl 2,7,7-trimethyl-5-oxo-4-(3,4,5-trimethoxyphenyl)-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**13**). White powder, 34% yield. Purity (HPLC): > 95% (**Fig. S61**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S62**): δ 0.97 (3H, *s*, H9b), 1.06 (3H, *s*, H9a), 1.23 (3H, *t*, *J* = 6.8 Hz, H3′), 2.21 (3H, *s*, H10), 2.34 (4H, *s*, H6-H8), 3.77 (9H, *s*, H17=H19 and H18), 4.09 (2H, *q*, *J*=6.8 Hz, H2′), 5.00 (1H, *s*, H4), 6.52 (2H, *s* , H12=H16).^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S63** and **S64**): δ 14.2 (CH_3, C3′), 19.7 (CH_3, C10), 27.1 (CH_3, C9a), 29.2 (CH_3, C9b), 32.9 (C, C7), 36.7 (CH, C4), 41.2 (CH_2, C8), 50.9 (CH_2, C6), 56.1 (CH_3, C19=C17), 59.9 (CH_2, C2′), 60.5 (CH_3, C18), 104.2 (C, C3), 105.1 (CH, C12=C16), 111.9 (C, C4a), 136.3 (C, C14) , 142.98 (C, C11), 143.4 (C, C13=C15), 148.4 (C, C8a), 152.7 (C, C2), 167.5 (C, C1), 195.8 (C, C5). ESI(+)-MS (**Fig. S65**): *m*/*z* 452 (55%, $[M+Na]^+$), *m*/*z* 430 (190%, $[M+H]^+$), *m*/*z* 262 (100%, $[M+H-C_9H_{12}O_3]^+$).



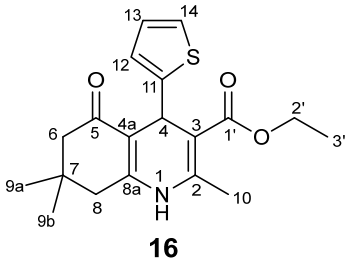
14

(±)-ethyl 2,7,7-trimethyl-5-oxo-4-(2,4,6-trimethoxyphenyl)-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**14**). White powder, 39% yield. Purity (HPLC): > 95% (**Fig. S66**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S67**): δ 0.90 (3H, s, H9b), 1.03 (3H, *s*, H9a), 1.24 (3H, *t*, *J* = 7.1 Hz, H3′), 2.01-2.19 (4H, *m*, H6 and H8), 2.25 (3H, *s*, H10), 3.74 (3H, *s*, H18), 3.79 (6H, *s*, H17=H19), 3.98 (2H, *q*, *J*= 7.1 Hz, H2′), 5.53 (1H, *s*, H4), 6.05 (2H, *s*, H13=H15).^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S68** and **S69**): δ 14.1 (CH_3, C3′), 18.6 (CH_3, C10), 26.9 (CH_3, C9a), 29.67 (CH_3, C9b), 32.6 (C, C7), 35.4 (CH, C4), 41.8 (CH_2, C8) 51.1 (CH_2, C6), 55.9 (CH_3, C17=C19), 58.6 (CH_3, C18), 59.6 (CH_2, C2′), 90.7 (C, C3), 104.4 (C, C11) , 110.8 (CH, C13=C15), 115.9 (C, C4a), 143.1 (C, C8a), 148.2 (C, C2), 148.6 (C, C12=C16), 159.3 (C, C14), 168.7 (C1′), 195.6 (C, C5). ESI(+)-MS (**Fig. S70**): *m*/*z* 468 (12%, $[M+K]^+$), *m*/*z* 452 (50%, $[M+Na]^+$), *m*/*z* 430 (25%, $[M+H]^+$), *m*/*z* 262 (100%, $[M+H-C_9H_{12}O_3]^+$).



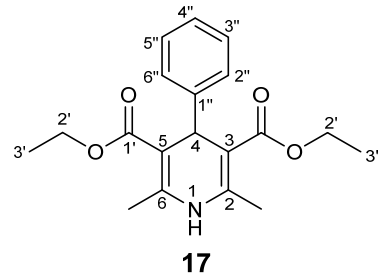
15

(±)-ethyl 4-(furan-2-yl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**15**). White powder, 30% yield. Purity (HPLC): > 95% (**Fig. S71**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S72**): δ 1.06 (3H, *s*, H9b), 1.08 (3H, *s*, H9a), 1.21 (3H, *t*, *J*=7.2 Hz, H3′), 2.19-2.34 (4H, *m*, H6-H8), 2.36 (3H, *s*, H10), 4.12 (2H, *q*, *J*= 7.1 Hz, H2′), 5.43 (1H, s, H4), 6.02 (1H, *d*, *J*= 3.2 Hz, H12), 6.21 (1H, *t*, *J*=6.9 Hz, H13), 7.18 (1H, *d*, *J*=3.1 Hz, H14).^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S73** and **S74**): δ 14.2 (CH_3, C3′), 19.4 (CH_3, C10), 27.5 (CH_3, C9a), 29.5 (CH_3, C9b), 32.8 (C, C7), 37.0 (CH, C4), 41.2 (CH_2, C8), 50.4 (CH_2, C6), 60.2 (CH_2, C2′), 106.3 (C, C3), 111.4 (C, C4a), 123.6 (CH, C12), 125.4 (CH, C14), 127.1 (CH, C13), 140.7 (C, C11), 148.4 (C, C8a), 157.4 (C, C2), 166.8 (C, C1′), 195.4 (C, C5). ESI(+)-MS (**Fig. S75**): *m*/*z* 368 (5%, $[M+K]^+$), *m*/*z* 352 (90%, $[M+Na]^+$), *m*/*z* 330 (12%, $[M+H]^+$), *m*/*z* 262 (100%, $[M+H-C_4H_4O]^+$).



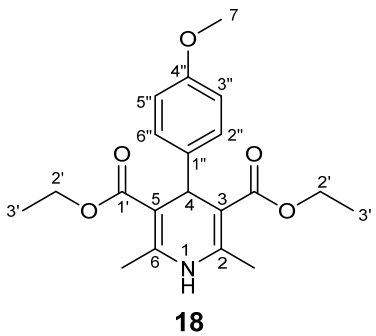
16

(±)-ethyl 2,7,7-trimethyl-5-oxo-4-(thiophen-2-yl)-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**16**). Beige powder, 38% yield. Purity (HPLC): > 95% (**Fig. S76**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S77**): δ 1.03 (3H, *s*, H9b), 1.10 (3H, *s*, H9a), 1.25 (3H, *t*, *J* = 7.1 Hz, H3′), 2.21-2.36 (4H, *m*, H6-H8), 2.38 (3H, *s*, H10), 4.14 (2H, *q*, *J*= 7.1 Hz, H2′), 5.41 (1H, *s*, H4), 6.81-6.84 (2H, *m*, H13 and H12), 7.03 (1H, *d*, *J*=4.9 Hz, H14).^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S78** and **S79**): δ 14.2 (CH_3, C3′), 19.4 (CH_3, C10), 27.2 (CH_3, C9a), 29.4 (CH_3, C9b), 32.7 (C, C7), 36.9 (CH, C4), 41.1 (CH_2, C8), 50.5 (CH_2, C6), 60.2 (CH_2, C2′), 106.3 (C, C3), 111.3 (C, C4a), 123.5 (CH, C12), 125.4 (CH, C14), 127.2 (CH, C13), 140.7 (C, C11), 148.4 (C, C8a), 157.6 (C, C2), 166.7 (C, C1), 195.3 (C, C5). ESI(+)-MS (**Fig. S80**): *m*/*z* 368 (65%, $[M+Na]^+$), *m*/*z* 346 (30%, $[M+H]^+$), *m*/*z* 262 (100%, $[M+H-C_4H_4S]^+$).



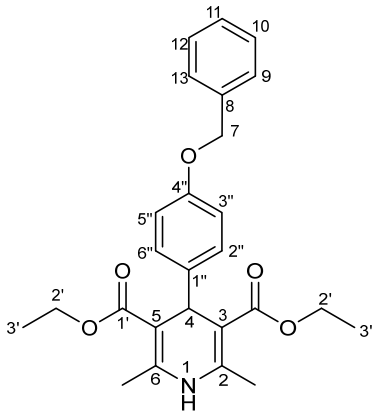
17

Diethyl 2,6-dimethyl-4-phenyl-1,4-dihydropyridine-3,5-dicarboxylate (**17**). Yellow powder, 15% yield. Purity (HPLC): > 95% (**Fig. S81**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S82**): 1.24 (6H, *t*, $J_{3',2'}$ = 7.1 Hz, H3′), 2.33 (6H, *s*, 2=6-CH_3), 4.08 (4H, *q*, $J_{2',3'}$ = 7.1 Hz, H2′), 4.98 (1H, *s*, H4), 7.15 – 7.32 (5H, *m*, H2″=H6″, H3″=H5″ and H4″). ^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S83** and **S84**): δ 14.1 (CH_3, C3′), 19.4 (CH_3, 2=6-CH_3), 39.4 (CH, C4), 59.5 (CH_2, C2′), 104.0 (C, C3=C5), 125.9 (CH, C4″), 127.6 (CH, C2″=C6″), 127.8 (CH, C3″=C5″), 143.6 (C, C1″), 147.6 (C, C2=C6), 167.7 (C, C1). ESI(+)-MS (**Fig. S85**): *m*/*z* 368 (8%, $[M+K]^+$), *m*/*z* 352 (100%, $[M+Na]^+$), *m*/*z* 330 (25%, $[M+H]^+$), *m*/*z* 284 (100%, $[M+H-C_2H_6O]^+$), *m*/*z* 252 (20%, $[M+H-C_6H_6]^+$).



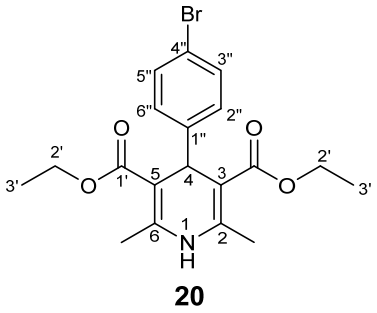
18

D*iethyl 4-(4-methoxyphenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate* (**18**). Yellow powder, 17% yield. Purity (HPLC): > 95% (**Fig. S86**). NMR ^{1}H (400 MHz, *CDCl*$_3$, **Fig. S87**): 1.22 (6H, *t*, $J_{3',2'}$ = 7.1 Hz, H3′), 2.32 (6H, *s*, 2=6-CH_3), 3.75 (3H, *s*, H7), 4.08 (4H, *q*, $J_{2',3'}$ = 5.2 Hz, H2′), 4.92 (1H, *s*, H4), 6.75 (2H, *d*, *J* = 7.7 Hz, H3″=H5″), 7.20 (2H, *d*, *J*=7.7 Hz, H2″=H6″).^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S88** and **S89**): δ 14.1 (CH_3, C3′), 19.4 (CH_3, 2=6-CH_3), 38.6 (CH, C4), 54.9 (CH_3, C7), 59.5 (CH_2, C2′), 104.2 (C, C3=C5), 113.0 (CH, C3″=C5″), 128.8 (CH, C2″=C6″), 140.1 (C, C1″), 143.3 (C, C2=C6), 157.7 (C, C4″), 167.5 (C, C1′). ESI(+)-MS (**Fig. S90**): *m*/*z* 398 (5%, $[M+K]^+$), *m*/*z* 382 (95%, $[M+Na]^+$), *m*/*z* 360 (12%, $[M+H]^+$), *m*/*z* 252 (100%, $[M+H-C_7H_8O]^+$).



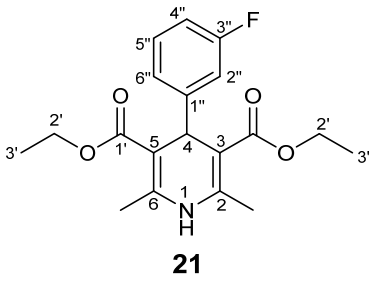
19

Diethyl 4-(4-(benzyloxy)phenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (**19**). Yellow powder, 16% yield. Purity (HPLC): > 95% (**Fig. S91**). NMR ^{1}H (400 MHz, *CDCl*$_3$, **Fig. S92**): 1.22 (6H, *t*, $J_{3',2'}$ = 7.1 Hz, H3′), 2.32 (6H, *s*, 2=6-CH$_3$), 4.09 (4H, *q*, $J_{2',3'}$ = 7.1 Hz, H2′), 4.93 (1H, *s*, H4), 5.00 (2H, *s* H7), 6.83 (2H, *d*, *J*= 8.7 Hz, H3″=H5″), 7.20 (2H, *d*, *J*= 8.7 Hz, H2″=H6″), 7.31-7.42 (5H, *m*, H8, H9=H13, and H10=H12). ^{13}C NMR (400 MHz, *CDCl*$_3$, **Fig. S93** and **S94**): δ 14.6 (CH$_3$, C3′), 19.4 (CH$_3$, 2=6-CH$_3$), 38.7 (CH, C4), 59.9 (CH$_2$, C2′), 70.2 (CH$_2$, C7), 104.6 (C, C3=C5), 114.2 (CH, C3″=C5″), 127.6 (CH, C9=C13), 127.9 (CH, C11), 128.7 (CH, C10=C12), 129.2 (CH, C2″=C6″), 137.6 (C, C8), 140.5 (C, C1″), 143.4 (C, C2=C6), 157.2 (C, C4″), 167.8 (C, C1′). ESI(+)-MS (**Fig. S95**): *m*/*z* 474 (13%, [M+K]$^+$), *m*/*z* 458 (100%, [M+Na]$^+$), *m*/*z* 436 (10%, [M+H]$^+$), *m*/*z* 252 (72%, [M+H-C$_{13}$H$_{12}$O]$^+$).



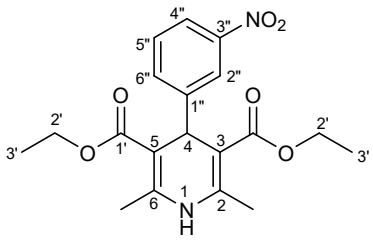
20

Diethyl 4-(4-bromophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (**20**). Yellow powder, 19% yield. Purity (HPLC): > 95% (**Fig. S96**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S97**): 1.21 (6H, *t*, $J_{3',2'}$ = 7.1 Hz, H3′), 1.60 (3H, *J*=7.1 Hz, H3′), 2.32 (6H, *s*, 2=6-CH$_3$), 4.08 (4H, *q*, $J_{2',3'}$ = 4.3 Hz, H2′), 4.93 (1H, *s*, H4), 7.16 (2H, *d*, *J*=8.4 Hz, H2″=H6″), 7.33 (2H, *d*, *J*=8.4 Hz, H3″=H5″) ^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S98** and **S99**): δ 14.9 (CH$_3$, C3′), 20.1 (CH$_3$, 2=6-CH$_3$), 39.6 (CH, C4), 60.2 (CH$_2$, C2′), 104.5 (C, C3=C5), 120.2 (C, C4″), 130.2 (CH, C2″=C6″), 131.2 (CH, C3″=C5″), 144.1 (C, C1″), 146.9 (C, C2=C6), 167.8 (C, C1′). ESI(+)-MS (**Fig. S100**): *m*/*z* 430/432 (100%, [M+Na]$^+$), *m*/*z* 408/410 (10%, [M+H]$^+$), *m*/*z* 362 (60%, [M+H-C$_2$H$_6$O]+), *m*/*z* 252(15%, [M+H-C$_6$H$_5$Br]$^+$).



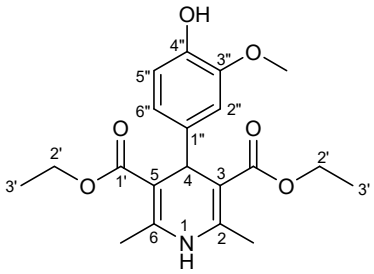
21

Diethyl 4-(3-fluorophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (**21**). Yellow powder, 20% yield. Purity (HPLC): > 95% (**Fig. S101**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S102**): 1.22 (6H, *t*, $J_{3',2'}$ = 7.1 Hz, H3′), 2.34 (6H, *s*, 2=6-CH$_3$), 4.09 (4H, *q*, $J_{2',3'}$ = 7.1 Hz, H2′), 4.99 (1H, *s*, H4), 6.81 (1H, *t*, *J*=7.2 Hz, H6″), 6.98 (1H, *d*, *J*= 8.2 Hz, H4″), 7.07 (1H, *d*, *J*= 6.9 Hz, H2″), 7.16 (1H, *dd*, *J*=7.4, and 8.2 Hz, H5″). ^{13}C NMR (400 MHz, *CDCl*$_3$, **Fig. S103** and **S104**): δ 14.3 (CH$_3$, C3′), 19.8 (CH$_3$, 2=6-CH$_3$), 39.7 (CH, C4), 59.9 (CH$_2$, C2′), 103.6 (C, C3=C5), 114.0 (CH, C4″), 115.1 (CH, C2″), 123.8 (CH, C6″), 129.3 (CH, C5″), 144.4 (C, C1″), 157.9 (C, C2=C6), 163.9 (C, C3′), 167.5 (C, C1′). ESI(+)-MS (**Fig. S105**): *m*/*z* 386 (20%, [M+K]$^+$), *m*/*z* 370 (100%, [M+Na]$^+$), *m*/*z* 348 (60%, [M+H]$^+$), *m*/*z* 302 (100%, [M+H-C$_2$H$_6$O]$^+$), *m*/*z* 274 (25%, [M+H-C$_2$H$_6$O-CO]$^+$), *m*/*z* 252 (20%, [M+H-C$_6$H$_5$F)]$^+$).



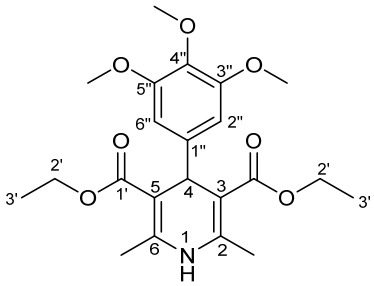
22

(±)-diethyl 2,6-dimethyl-4-(3″-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate (**22**). Yellow powder, 16% yield. Purity (HPLC): > 95% (**Fig. S106**). ^{1}H NMR (400 MHz, *CDCl*$_3$, **Fig. S107**): 1.22 (6H, *t*, $J_{3',2'}$ = 7.1 Hz, H3′), 2.36 (6H, *s*, 2=6-CH$_3$), 4.08 (4H, *q*, $J_{2',3'}$ = 7.1 Hz, H2′), 5.08 (1H, *s*, H4), 7.37 (1H, *t*, *J* = 7.9 Hz, H5″), 7.62 (1H, *d*, *J* = 7.7 Hz, H6″), 8.00 (1H, *d*, *J*= 8.2 Hz, H4″), 8.12 (1H, *t*, *J* = 1.8 Hz, H2″). ^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S108** and **S109**): *δ* 14.5 (CH$_3$, C3′), 19.7 (CH$_3$, 2=6-CH$_3$), 40.2 (CH, C4), 60.0 (CH$_2$, C2′), 103.4 (C, C3=C5), 121.3 (CH, C5″), 123.1 (CH, C6″), 128.7 (CH, C4″), 134.54 (CH, C2″), 144.6 (C, C3″), 148.3 (C, C1″), 149.8 (C, C2=C6), 167.1 (C, C1′). ESI(+)-MS (**Fig. S110**): *m*/*z* 413 (3%, [M+K]$^+$), *m*/*z* 397 (100%, [M+Na]$^+$), *m*/*z* 375 (10%, [M+H]$^+$), *m*/*z* 252 (50%, [M+H-C$_6$H$_5$NO$_2$]$^+$).



23

Diethyl 4-(4″-hydroxy-3″-methoxyphenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (**23**). Yellow powder, 16% yield. Purity (HPLC): > 95% (**Fig. S111**). NMR ^{1}H (400 MHz, *CDCl*$_3$, **Fig. S112**): 1.22 (6H, *t*, $J_{3',2'}$ = 7.1 Hz, H3′), 2.33 (6H, *s*, 2=6-CH$_3$), 3.84 (3H, *s*, 3-OCH$_3$), 4.11 (4H, *q*, $J_{2',3'}$ = 7.1 Hz, H2′), 4.92 (1H, *s*, H4), 6.75 (2H, *m*, H2= H6), 6.85 (1H, s, H2″).^{13}C (100 MHz, *CDCl*$_3$, **Fig. S113**and **S114**): *δ* 14.4 (CH$_3$, C3′), 19.8 (CH$_3$, 2=6-CH$_3$), 39.2 (CH, C4), 55.9 (CH$_3$, 3″-OCH$_3$), 59.7 (CH$_2$, C2′), 104.6 (C, C3=C5), 111.1 (CH, C5″), 113.9 (CH, C2″), 120.6 (CH, C6″), 140.2 (C, C1″), 143.6 (C, C4″), 144.0 (C3″), 145.9 (C, C2=C6), 167.8 (C1′). ESI(+)-MS (**Fig. S115**): *m*/*z* 414 (8%, [M+K]$^+$), *m*/*z* 398 (80%, [M+Na]$^+$), *m*/*z* 376 (15%, [M+H]$^+$), *m*/*z* 252 (100%, [M+H-C$_7$H$_8$O$_2$]$^+$)



24

Diethyl 2,6-dimethyl-4-(3″,4″,5″-trimethoxyphenyl)-1,4-dihydropyridine-3,5-dicarboxylate (**24**). Yellowish powder, 20% yield. Purity (HPLC): > 95% (**Fig. S116**). NMR ^{1}H (400 MHz, *CDCl*$_3$, **Fig. S117**): 1.25 (6H, *t*, $J_{3',2'}$ = 7.1 Hz, H3′), 2.34 (6H, s, 2=6-CH$_3$), 3.79 (9H, s, 3=5 and 4-OMe), 4.12 (4H, *q*, $J_{2',3'}$ = 7.1 Hz, H2′), 4.96 (1H, *s*, H7), 6.51 (2H, *s*, H2″=H6″).^{13}C NMR (100 MHz, *CDCl*$_3$, **Fig. S118** and **S119**): *δ* 14.2 (CH$_3$, C3′), 19.5 (CH$_3$, 2=6-CH$_3$), 39.4 (CH, C4), 55.7 (CH$_3$, 3″=5″-OCH$_3$), 59.6 (CH$_3$, 4″-OCH$_3$), 60.5 (CH$_2$, C2′), 103.9 (C, C3=C5), 104.8 (CH, C2″=C6″), 136.3 (C, C1″), 143.2 (C, C4″), 143.4 (C, C2=C6), 152.4 (C, C3″=C5″), 167.5 (C, C1′). ESI(+)-MS (**Fig. S120**): *m*/*z* 442 (100%, [M+Na]$^+$), *m*/*z* 420 (22%, [M+H]$^+$), *m*/*z* 252 (85%, [M+H-C$_9$H$_{12}$O$_3$]$^+$).

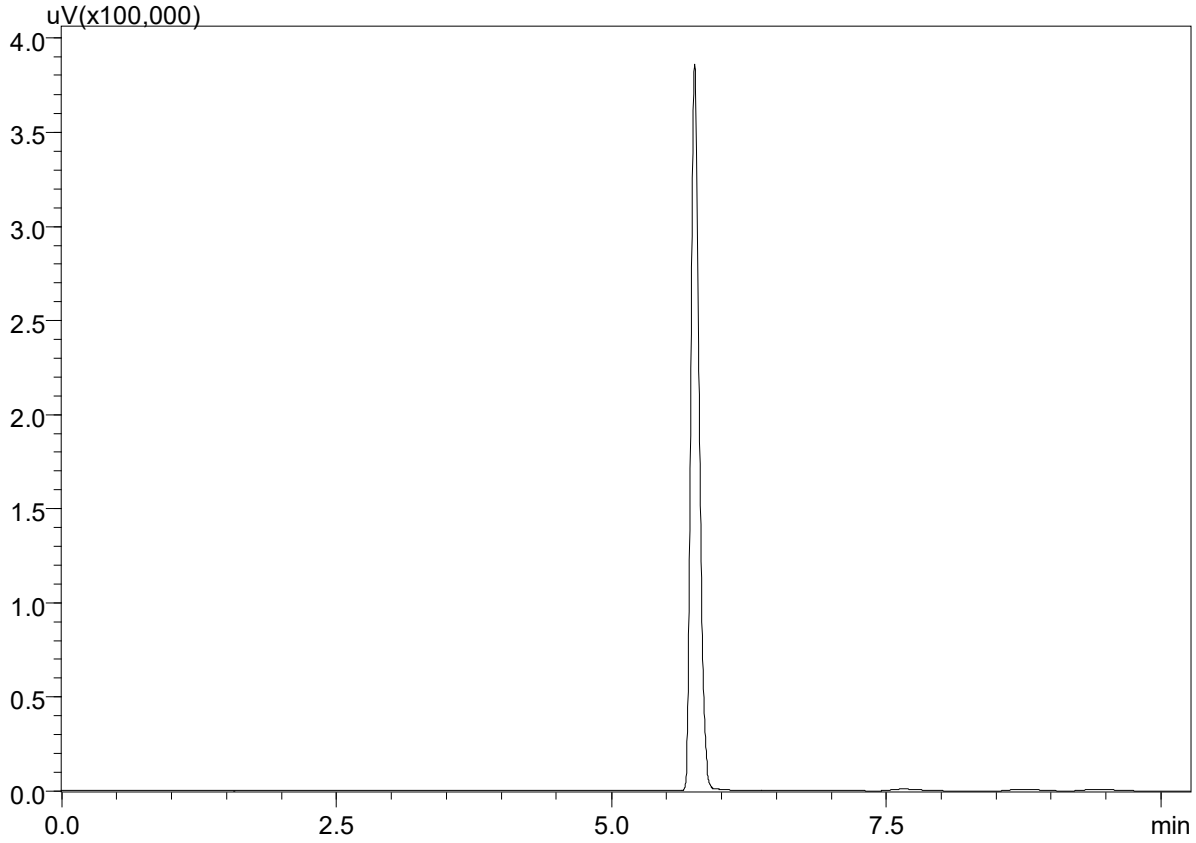


Figure S1: HPLC chromatogram of compound **1**.

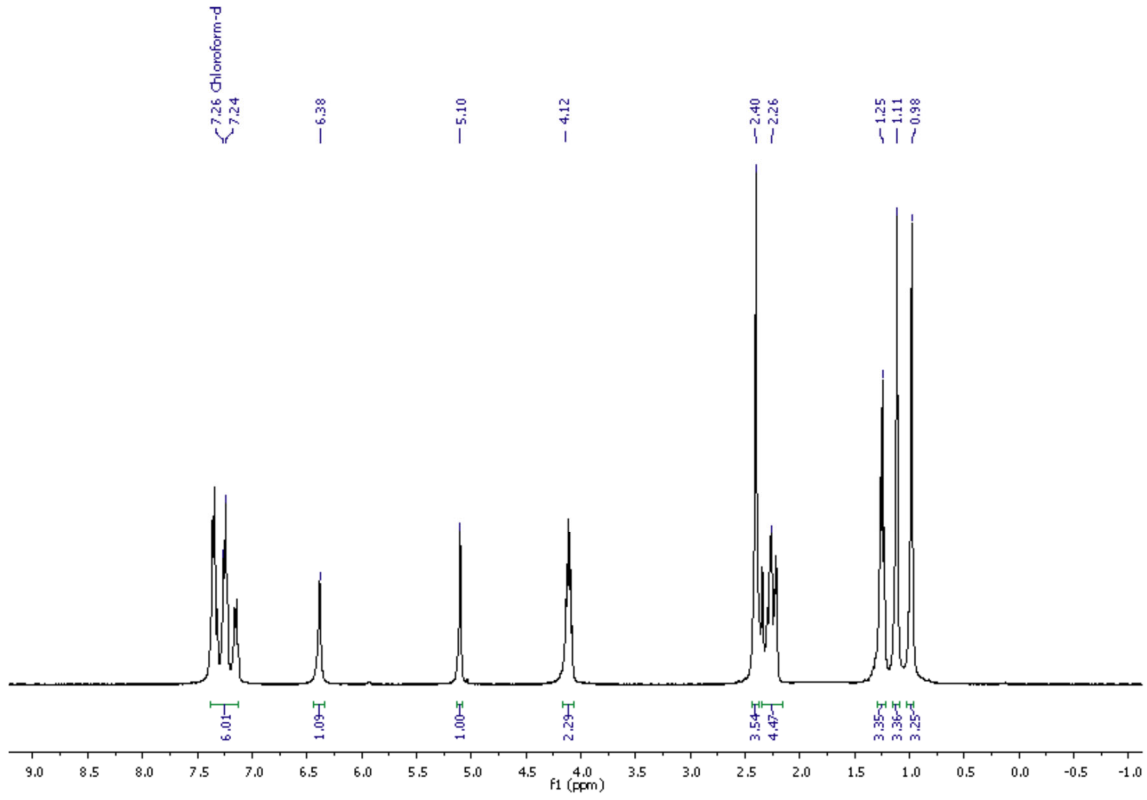


Figure S2.^{1}H NMR spectrum of compound **1** ($CDCl_3$, 400 MHz, TMS).

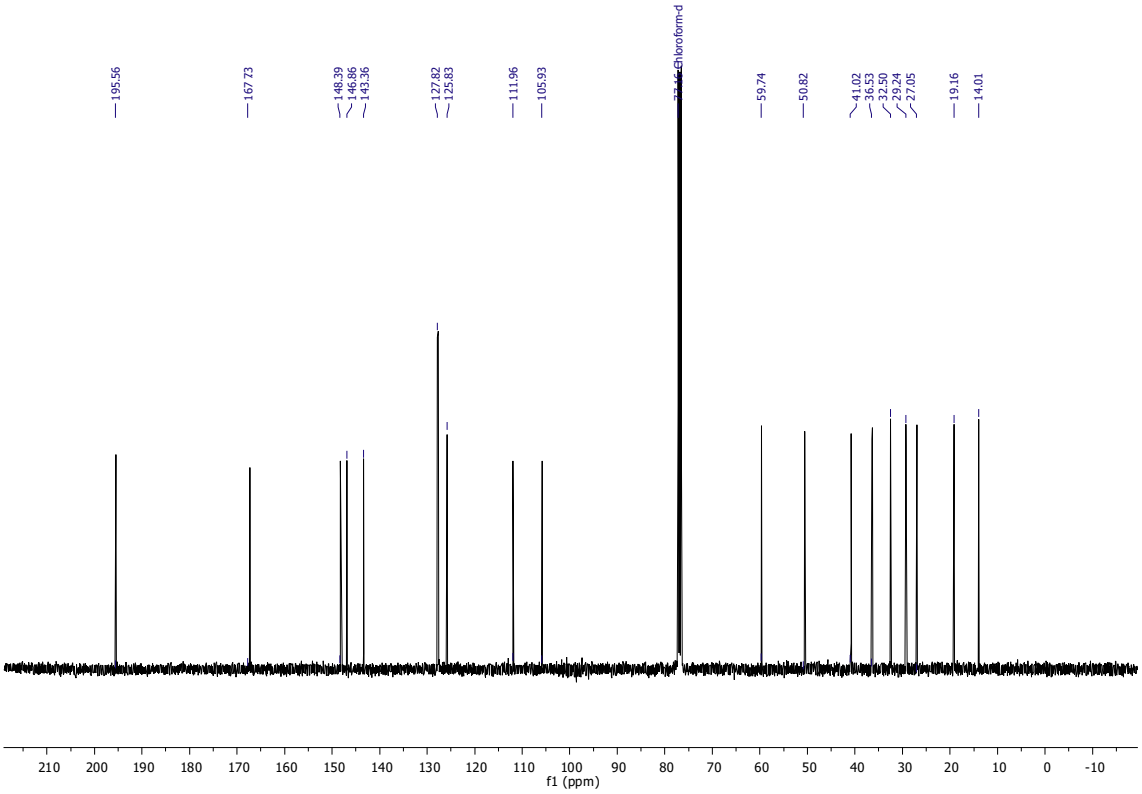


Figure S3.^{13}C NMR spectrum of compound **1** ($CDCl_3$, 100 MHz, TMS).

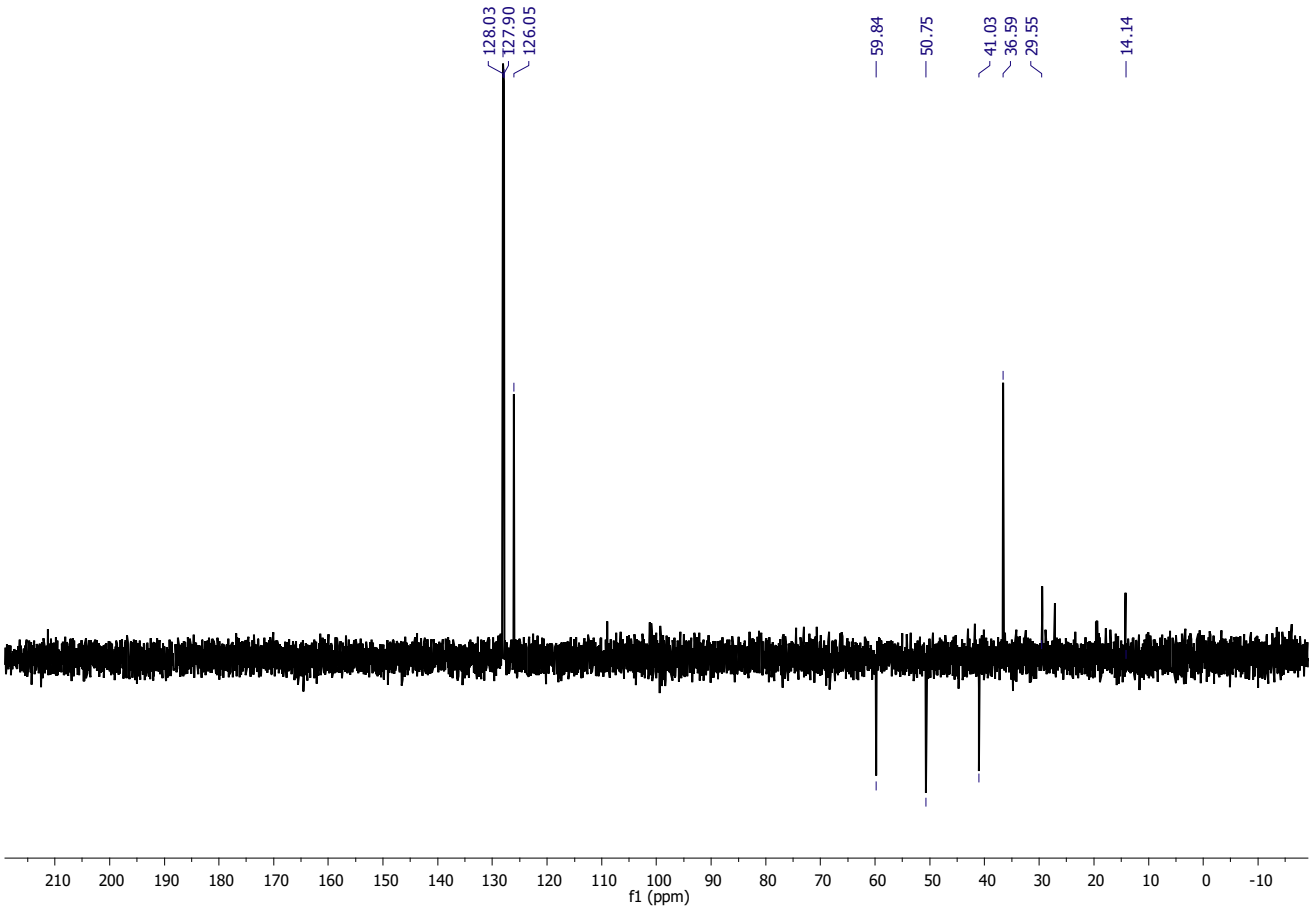


Figure S4. DEPT 135 spectrum of compound **1** ($CDCl_3$, 100 MHz, TMS).

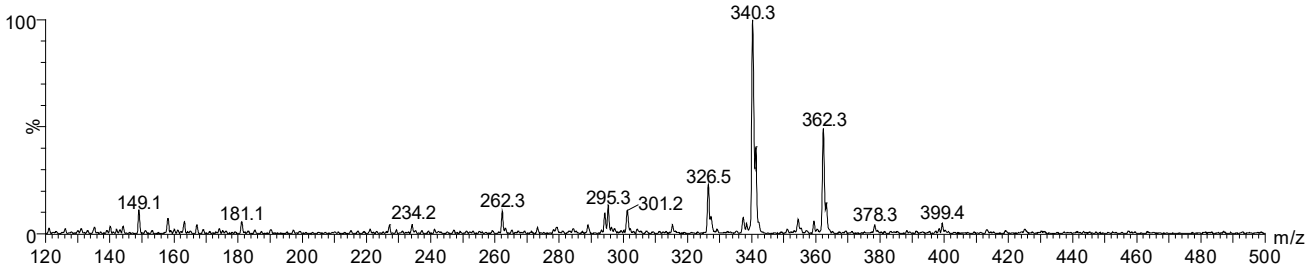


Figure S5. ESI (+) mass spectrum of compound **1**.

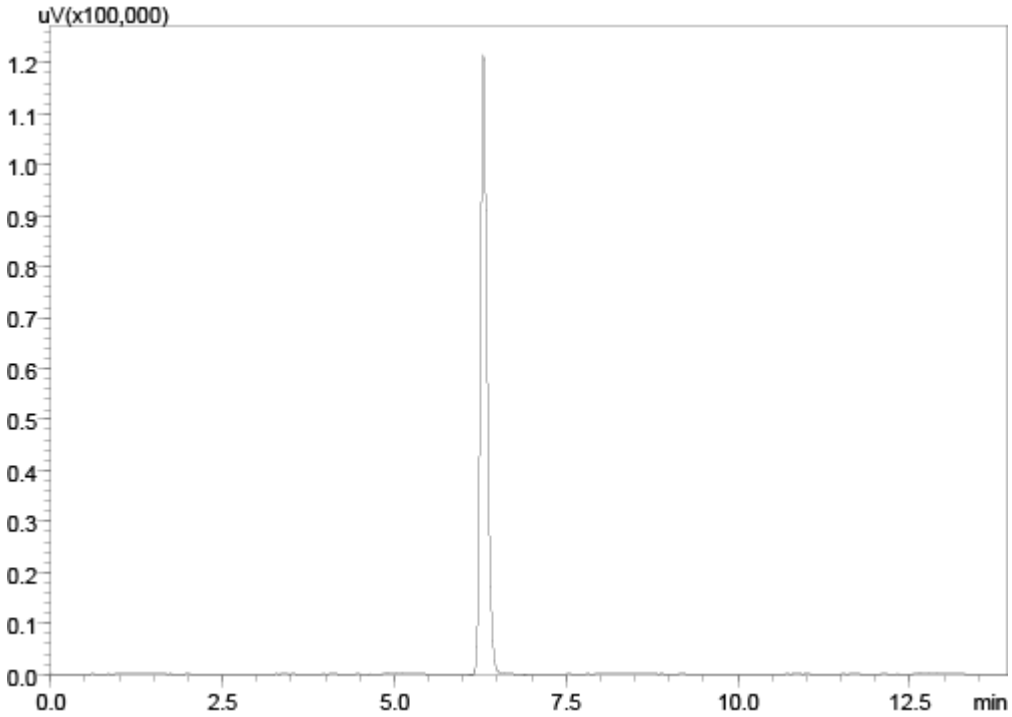


Figure S6: HPLC chromatogram of compound **2**.

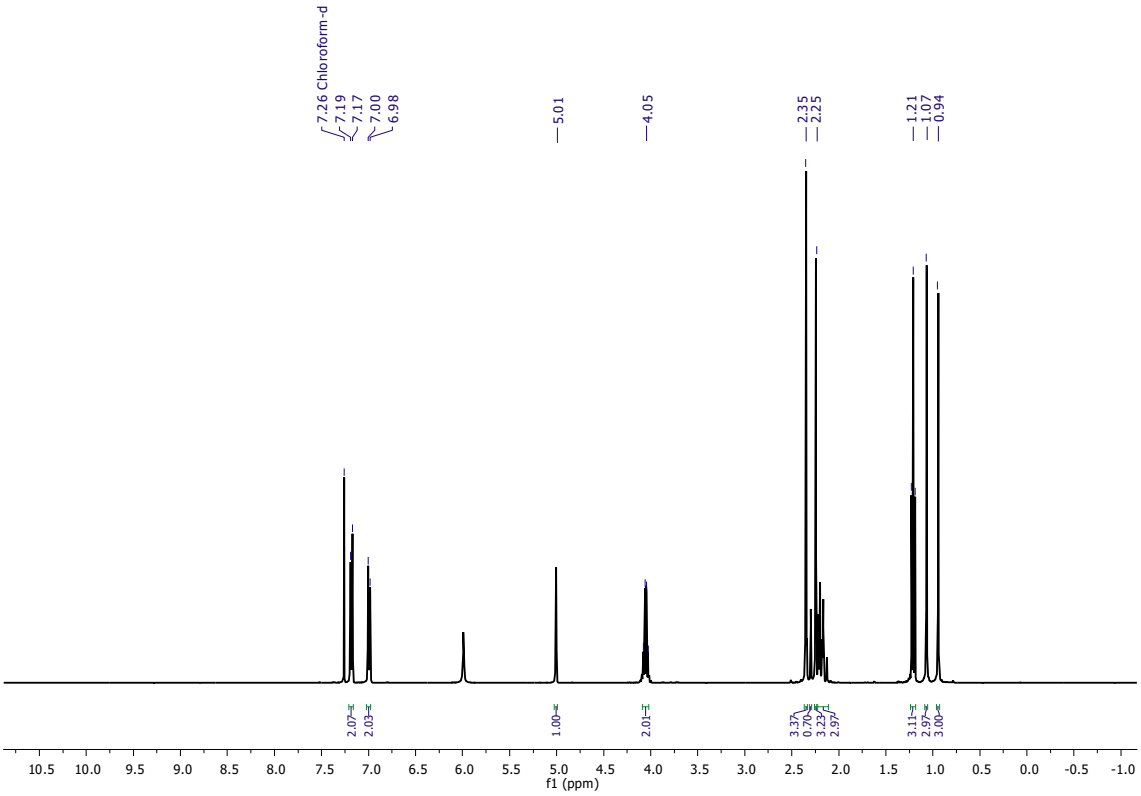


Figure S7.^{1}H NMR spectrum of compound **2** ($CDCl_3$, 400 MHz, TMS).

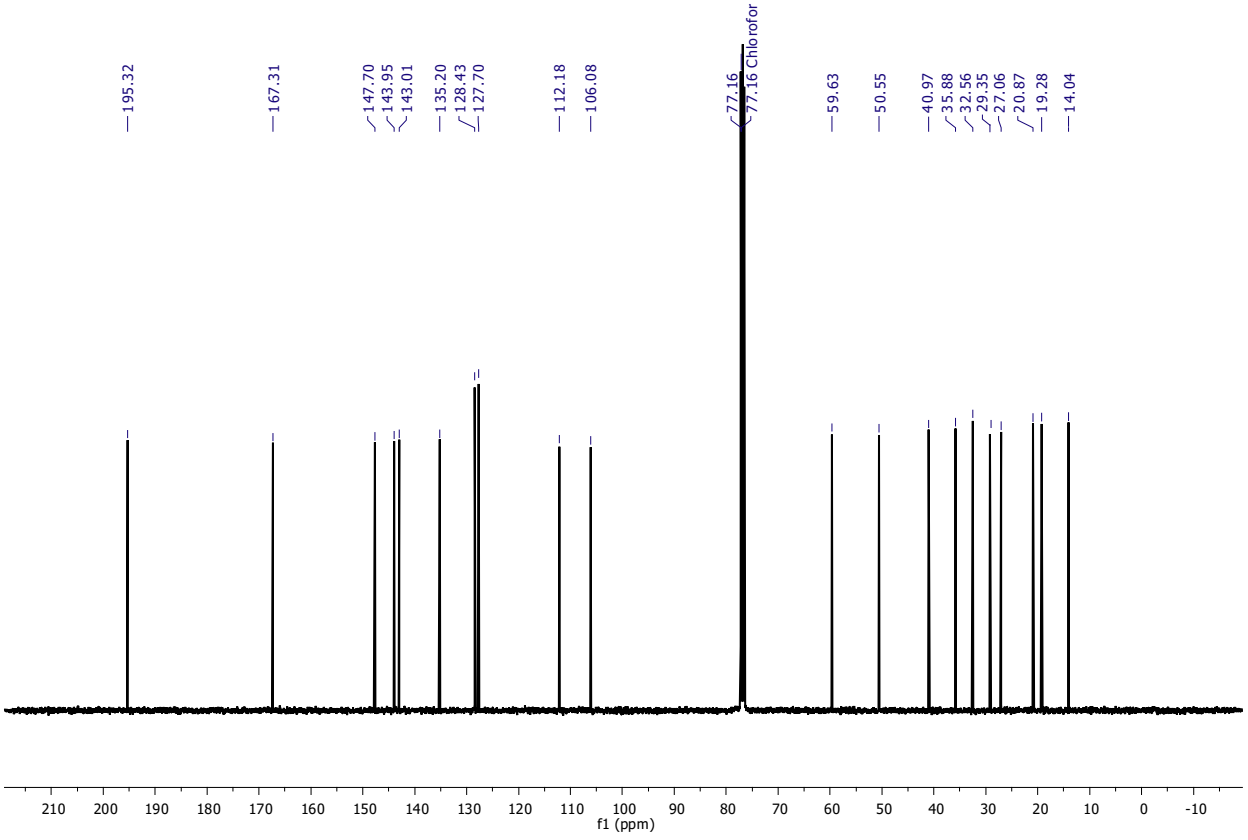


Figure S8.^{13}C NMR spectrum of compound **2** ($CDCl_3$, 100 MHz, TMS).

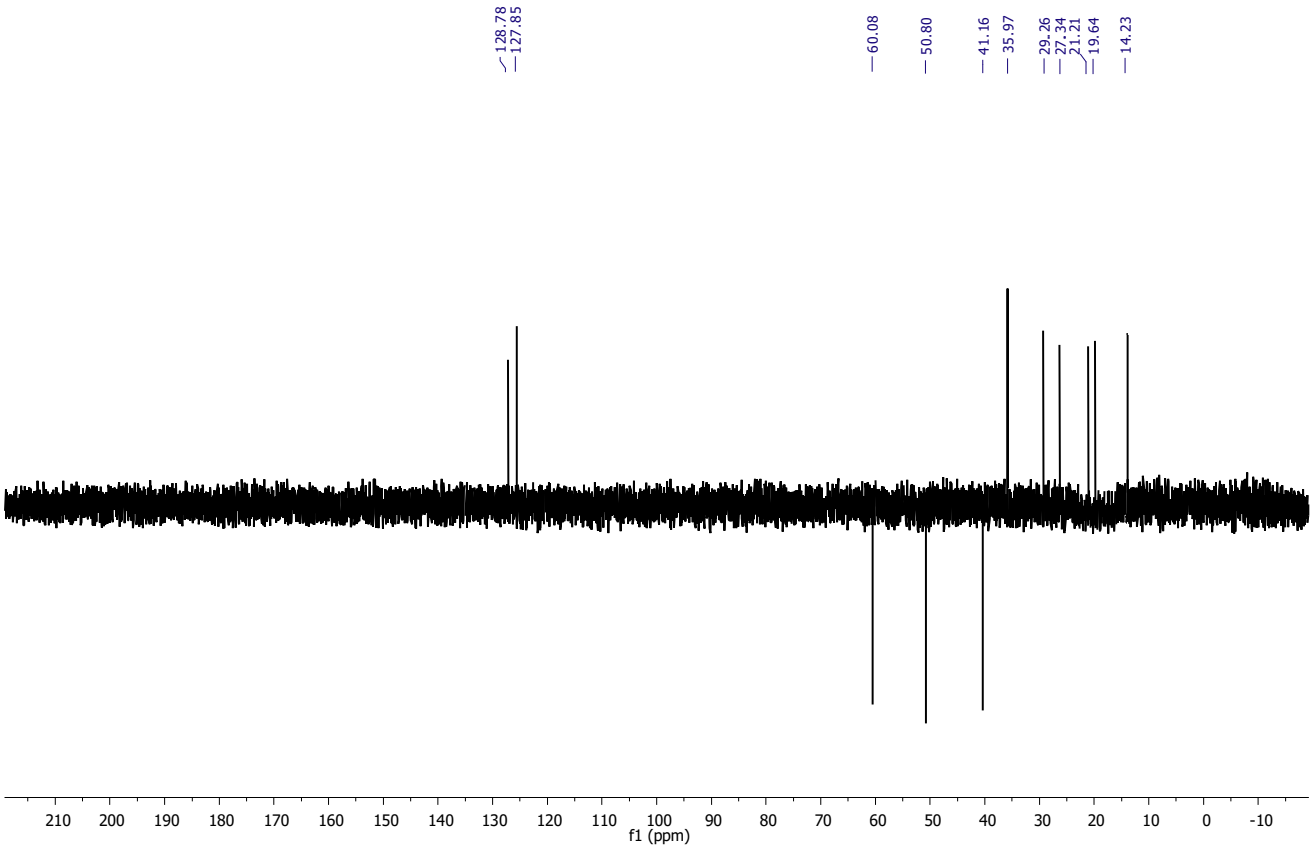


Figure S9.^{13}C NMR spectrum of compound **2** ($CDCl_3$, 100 MHz, TMS).

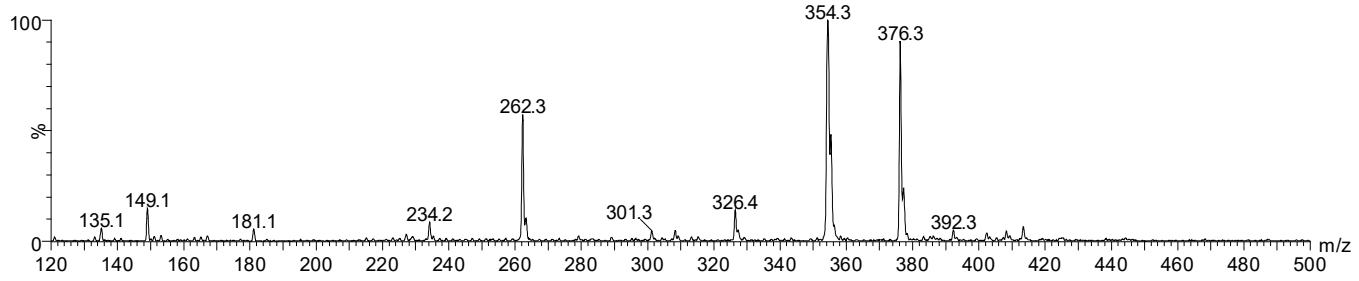


Figure S10. ESI (+) mass spectrum of compound **2**.

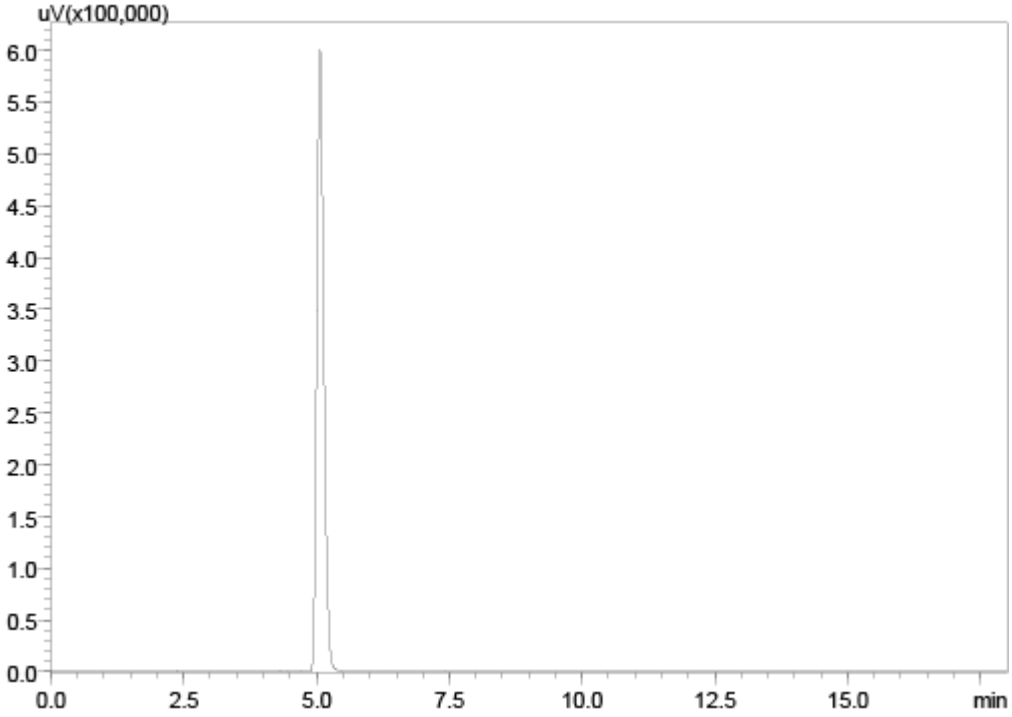


Figure S11: HPLC chromatogram of compound **3**.

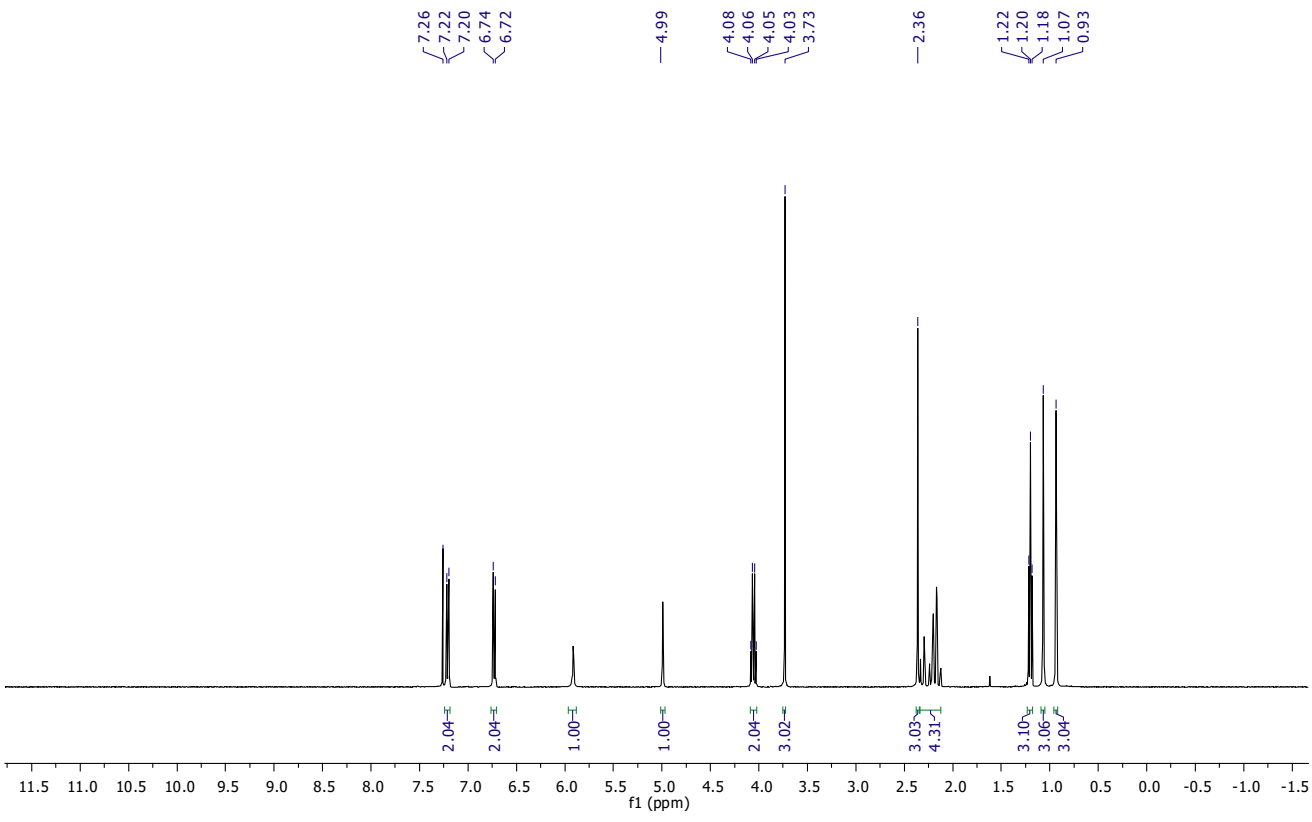


Figure S12.^{1}H NMR spectrum of compound **3** ($CDCl_3$, 400 MHz, TMS).

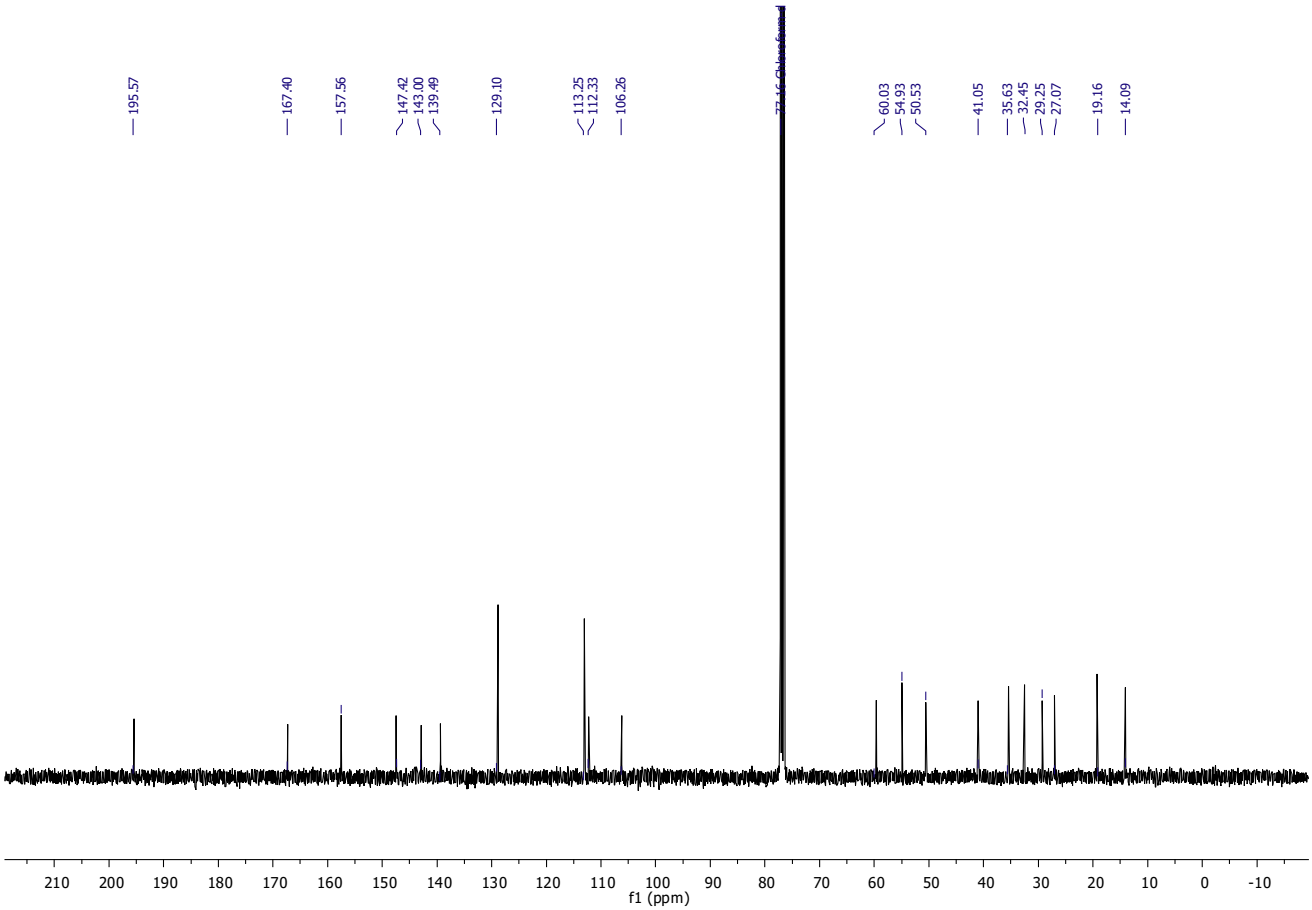


Figure S13.^{13}C NMR spectrum of compound **3** ($CDCl_3$, 100 MHz, TMS).

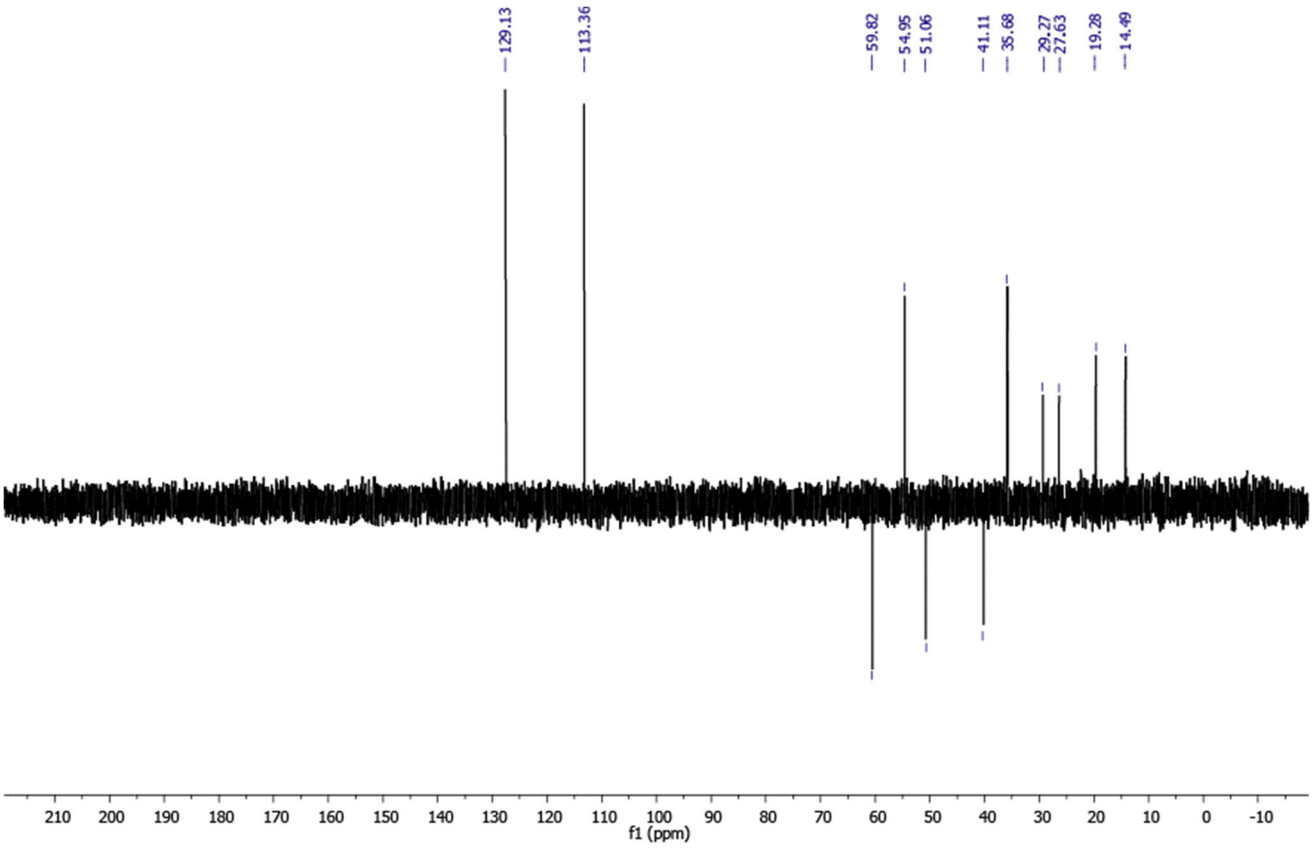


Figure S14. DEPT 135 spectrum of compound **3** ($CDCl_3$, 100 MHz, TMS).

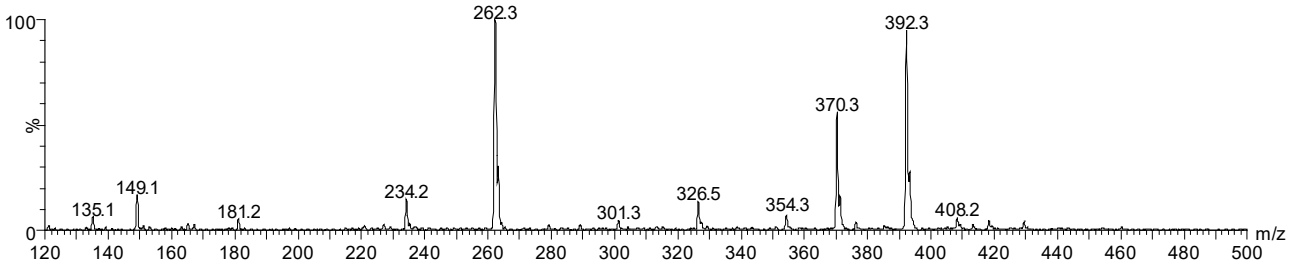


Figure S15. ESI (+) mass spectrum of compound **3**.

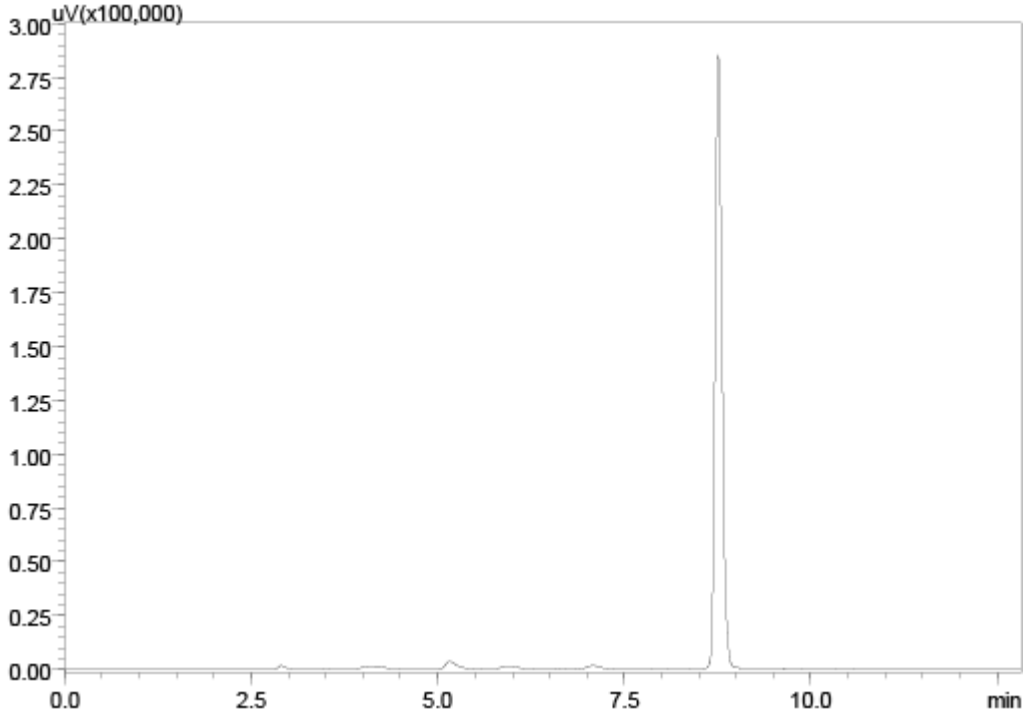


Figure S16: HPLC chromatogram of compound **4**.

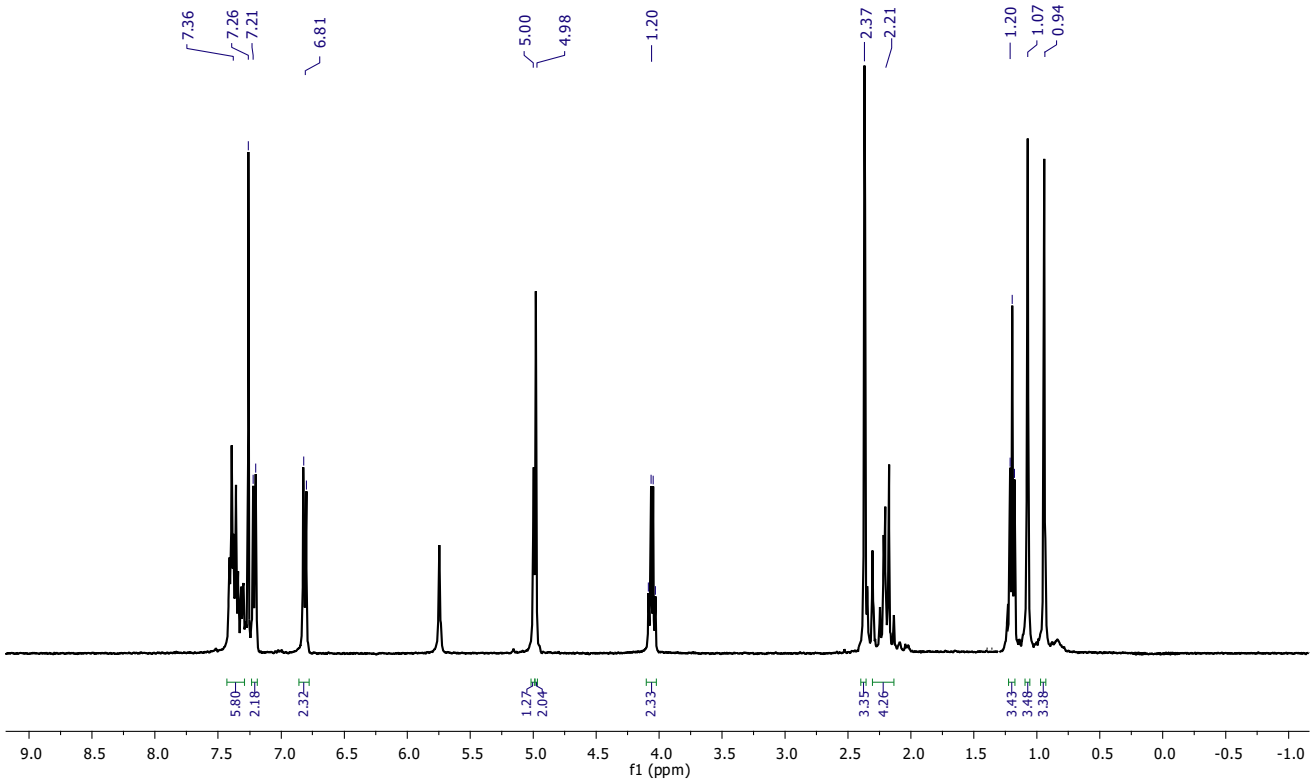


Figure S17.^{1}H NMR spectrum of compound **4** ($CDCl_3$, 400 MHz, TMS).

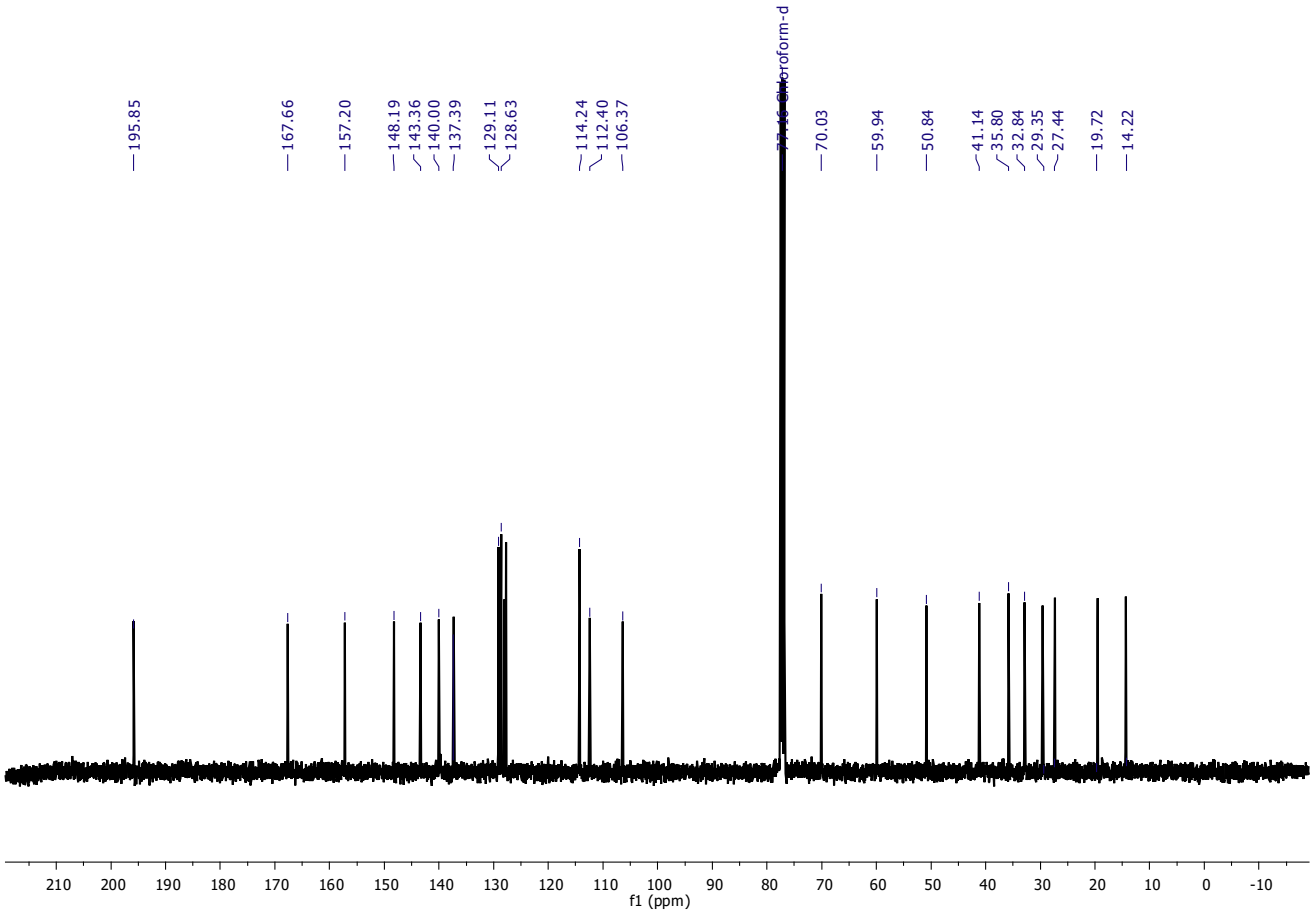


Figure S18.^{13}C NMR spectrum of compound **4** ($CDCl_3$, 100 MHz, TMS).

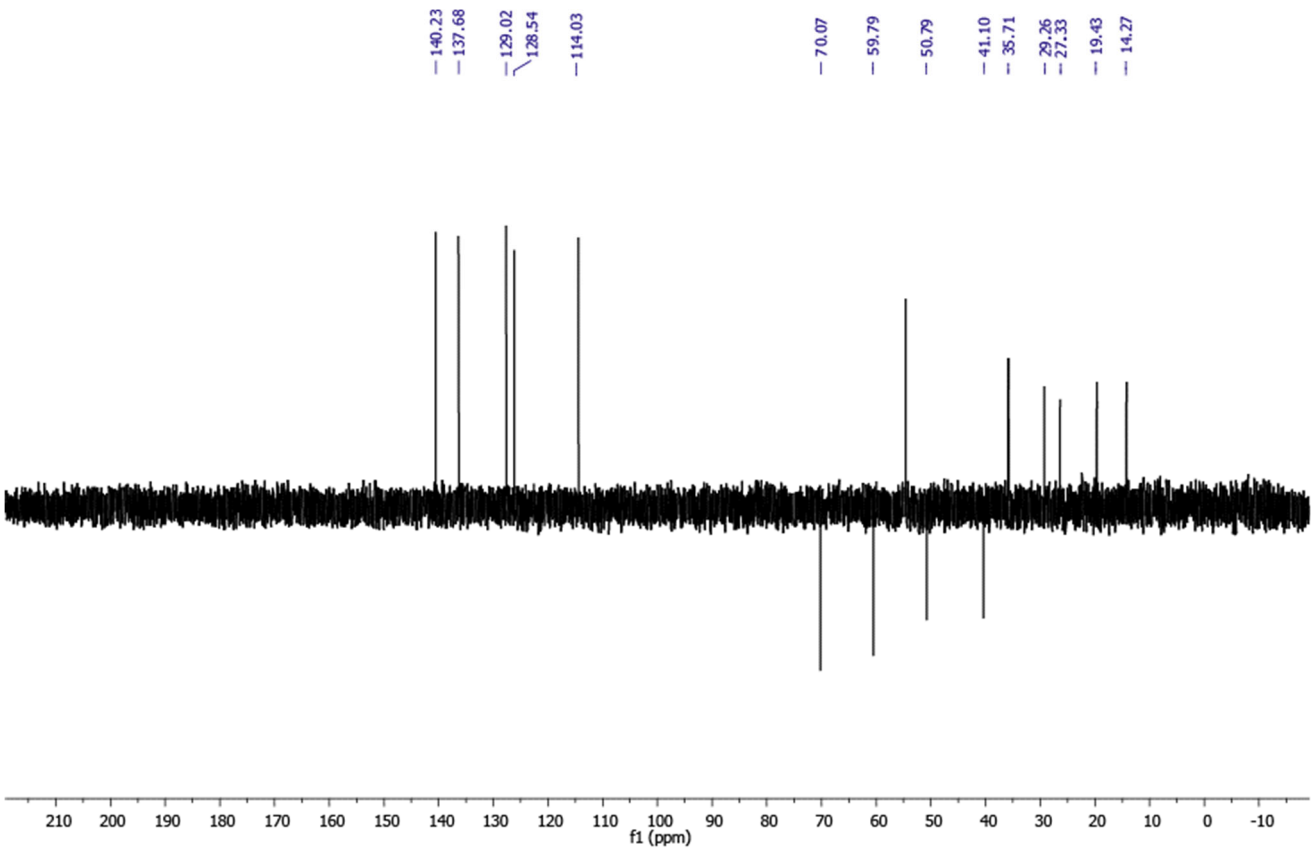


Figure S19. DEPT 135 spectrum of compound **4** ($CDCl_3$, 100 MHz, TMS).

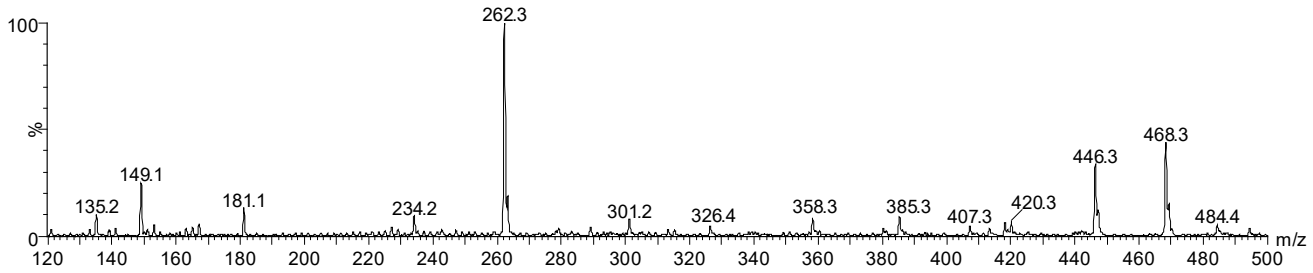


Figure S20. ESI (+) mass spectrum of compound **4**.

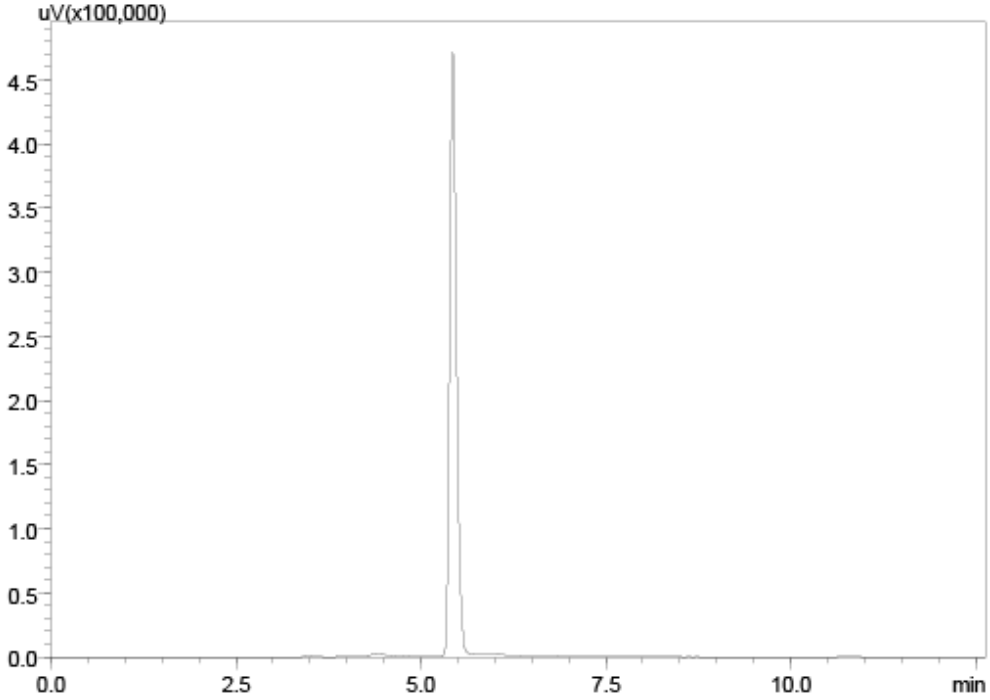


Figure S21: HPLC chromatogram of compound **5**.

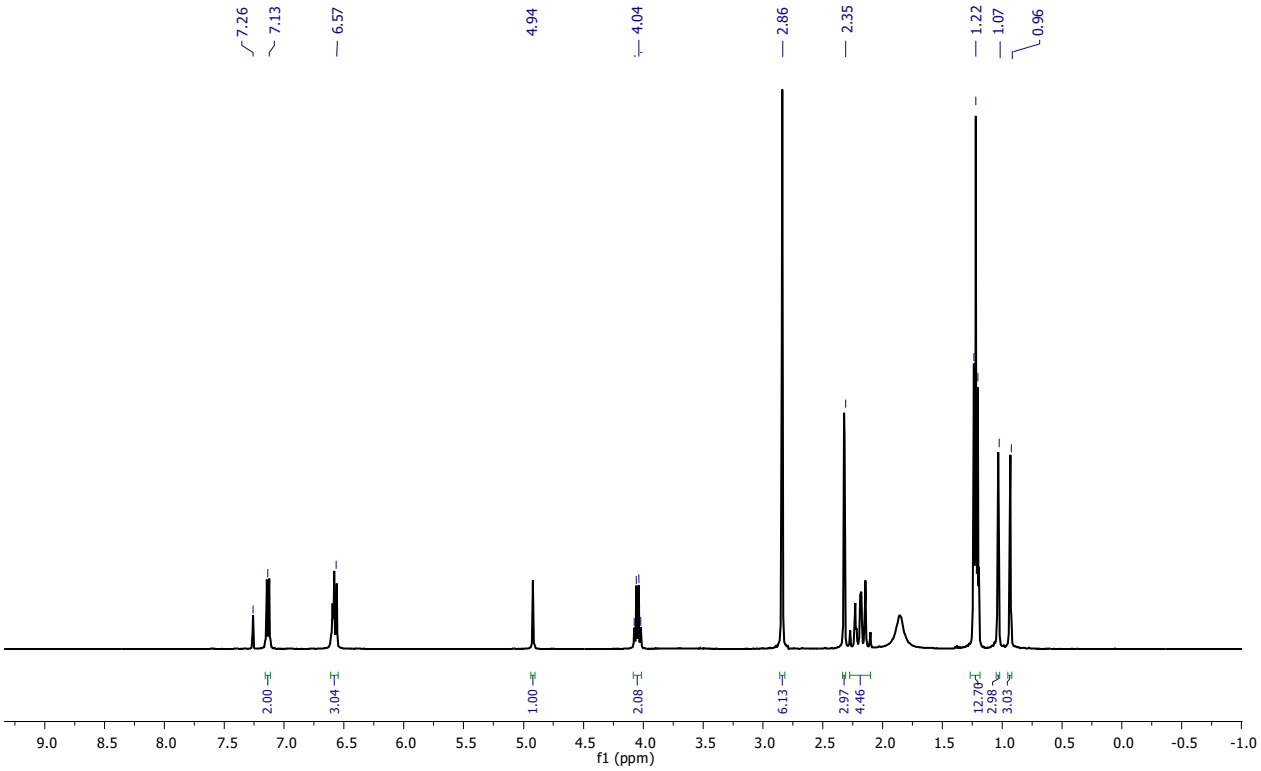


Figure S22.^{1}H NMR spectrum of compound **5** ($CDCl_3$, 400 MHz, TMS).

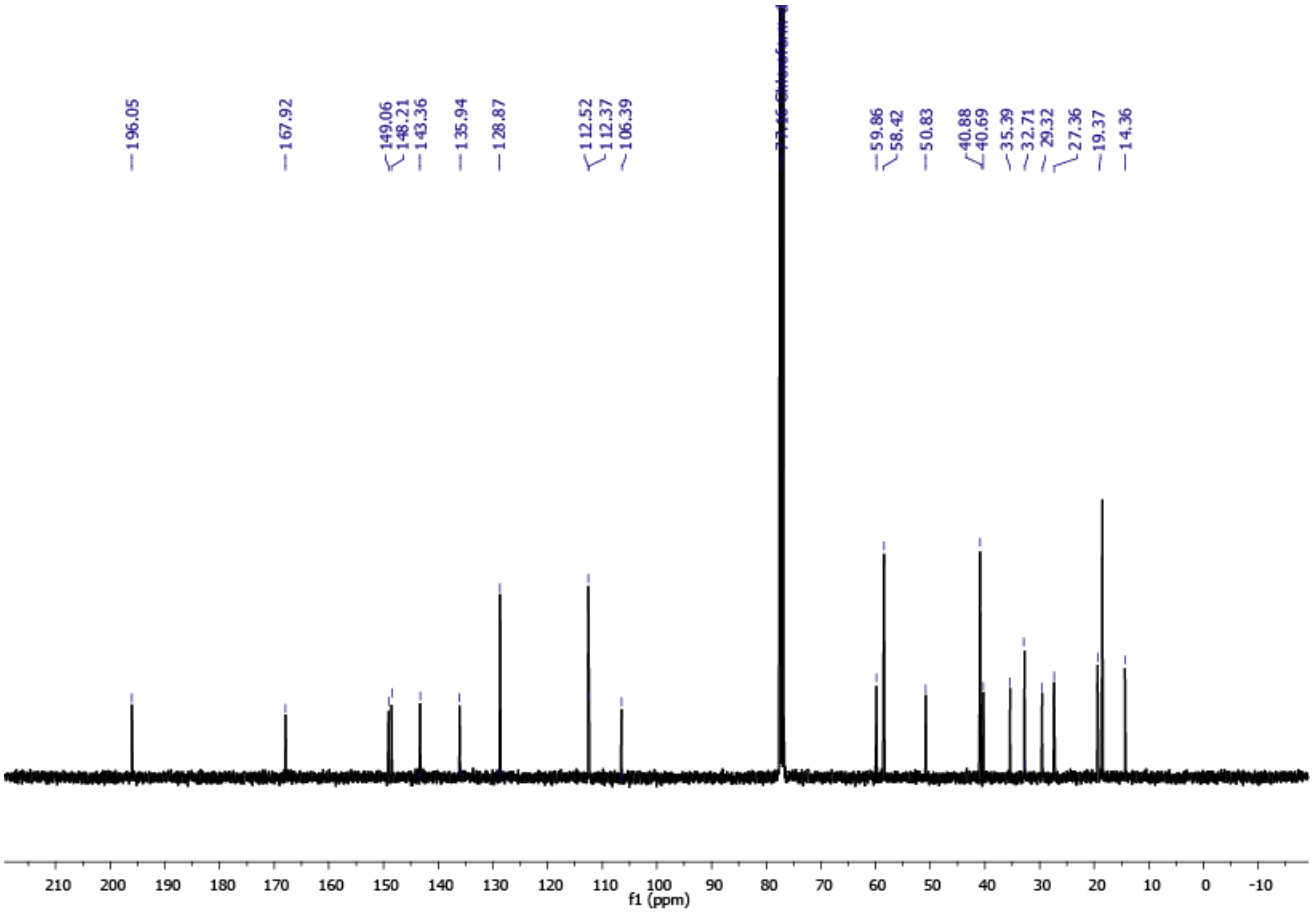


Figure S23.^{13}C NMR spectrum of compound **5** ($CDCl_3$, 100 MHz, TMS).

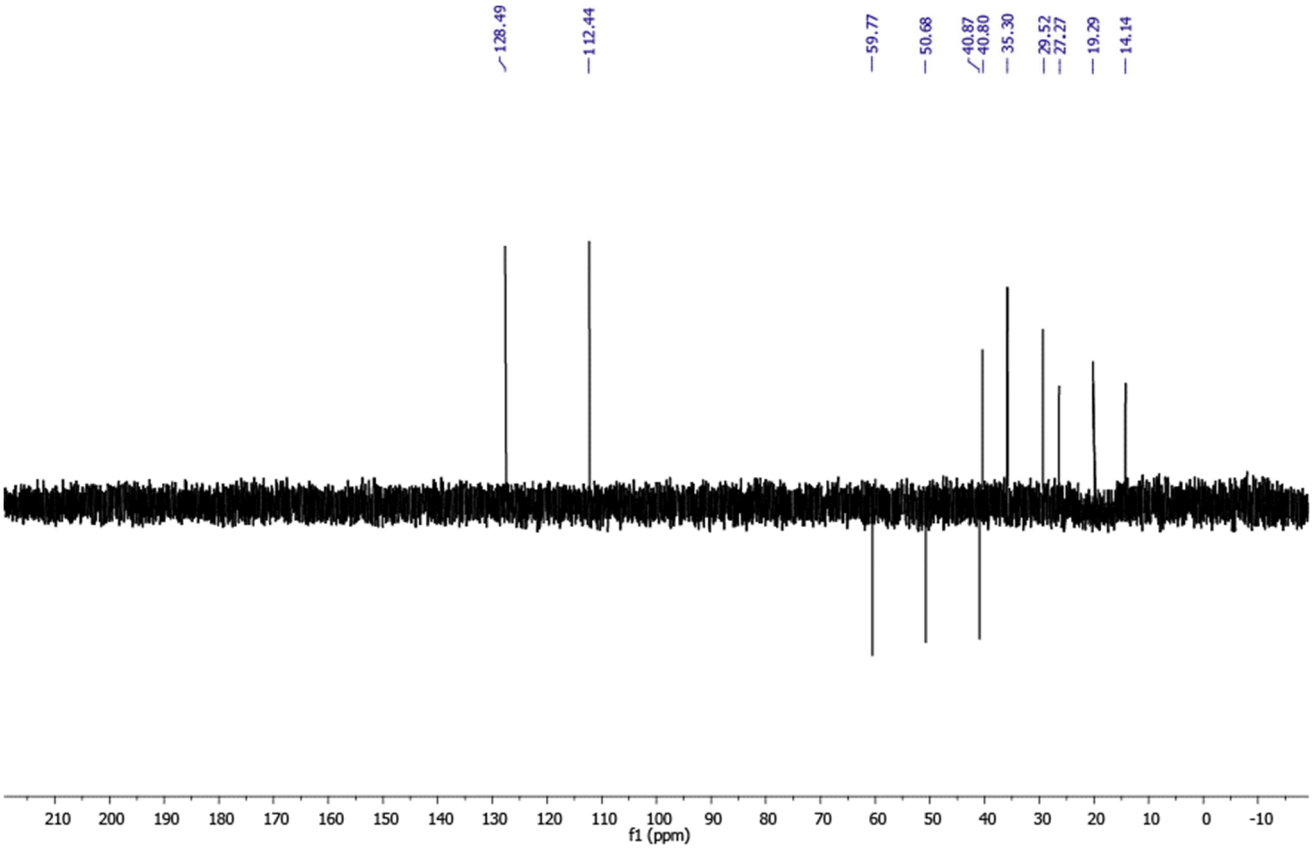


Figure S24. DEPT 135 spectrum of compound **5** ($CDCl_3$, 100 MHz, TMS).

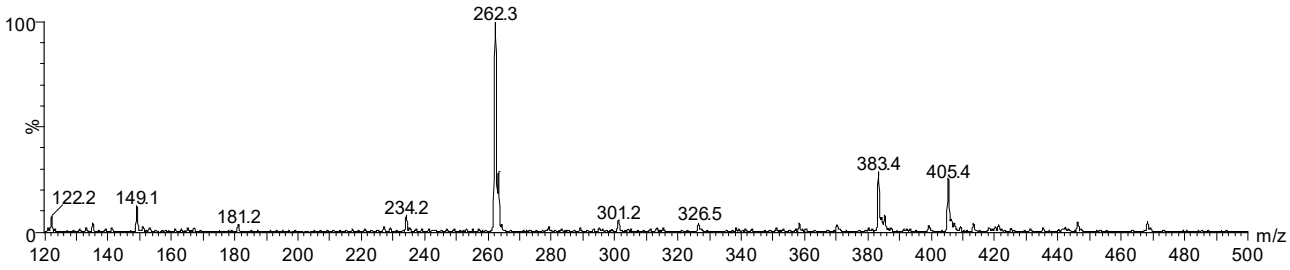


Figure S25. ESI (+) mass spectrum of compound **5**.

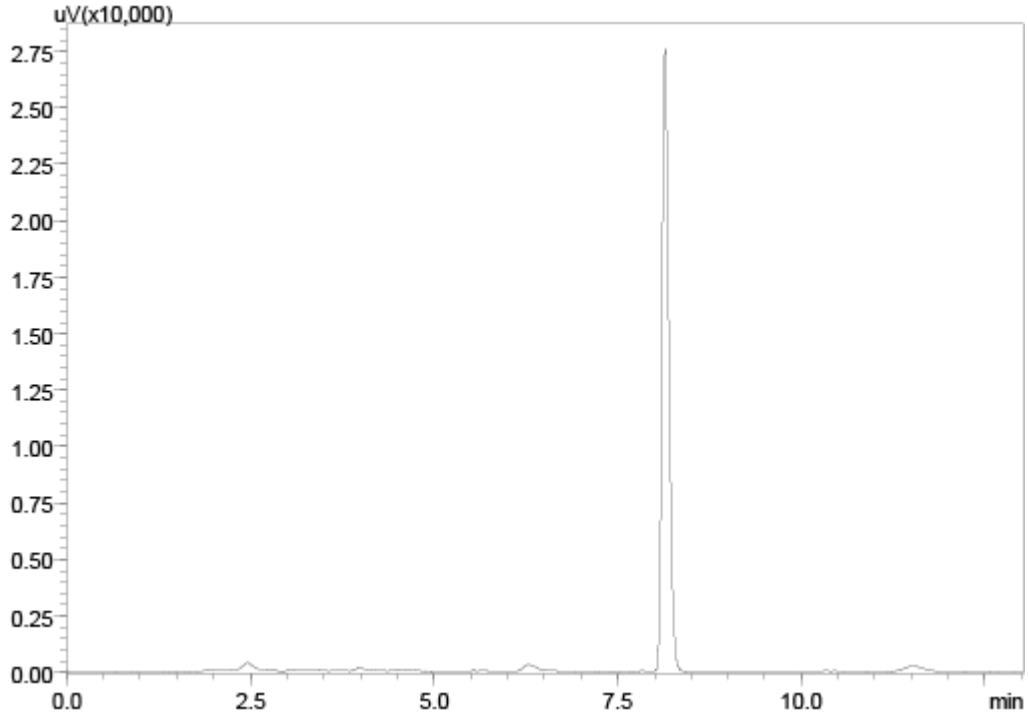


Figure S26: HPLC chromatogram of compound **6**.

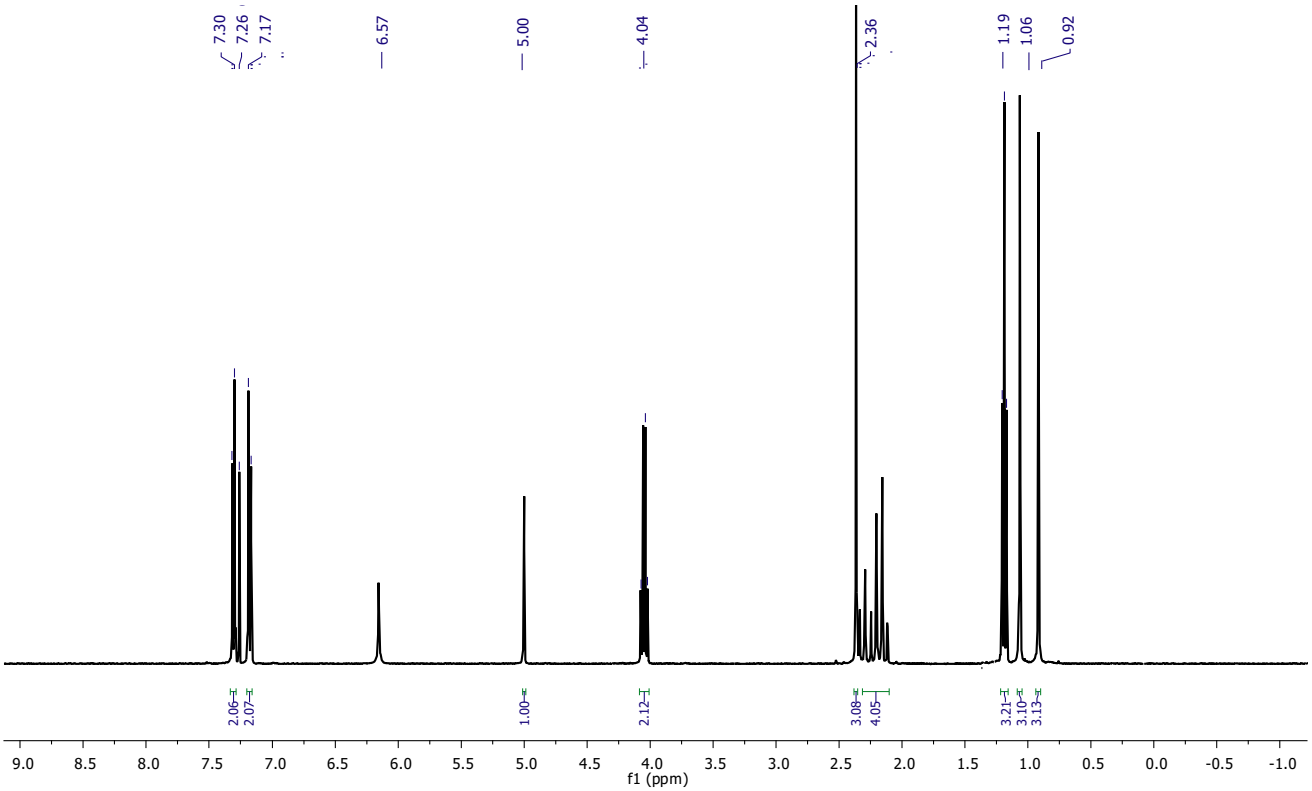


Figure S27.^{1}H NMR spectrum of compound **6** ($CDCl_3$, 400 MHz, TMS).

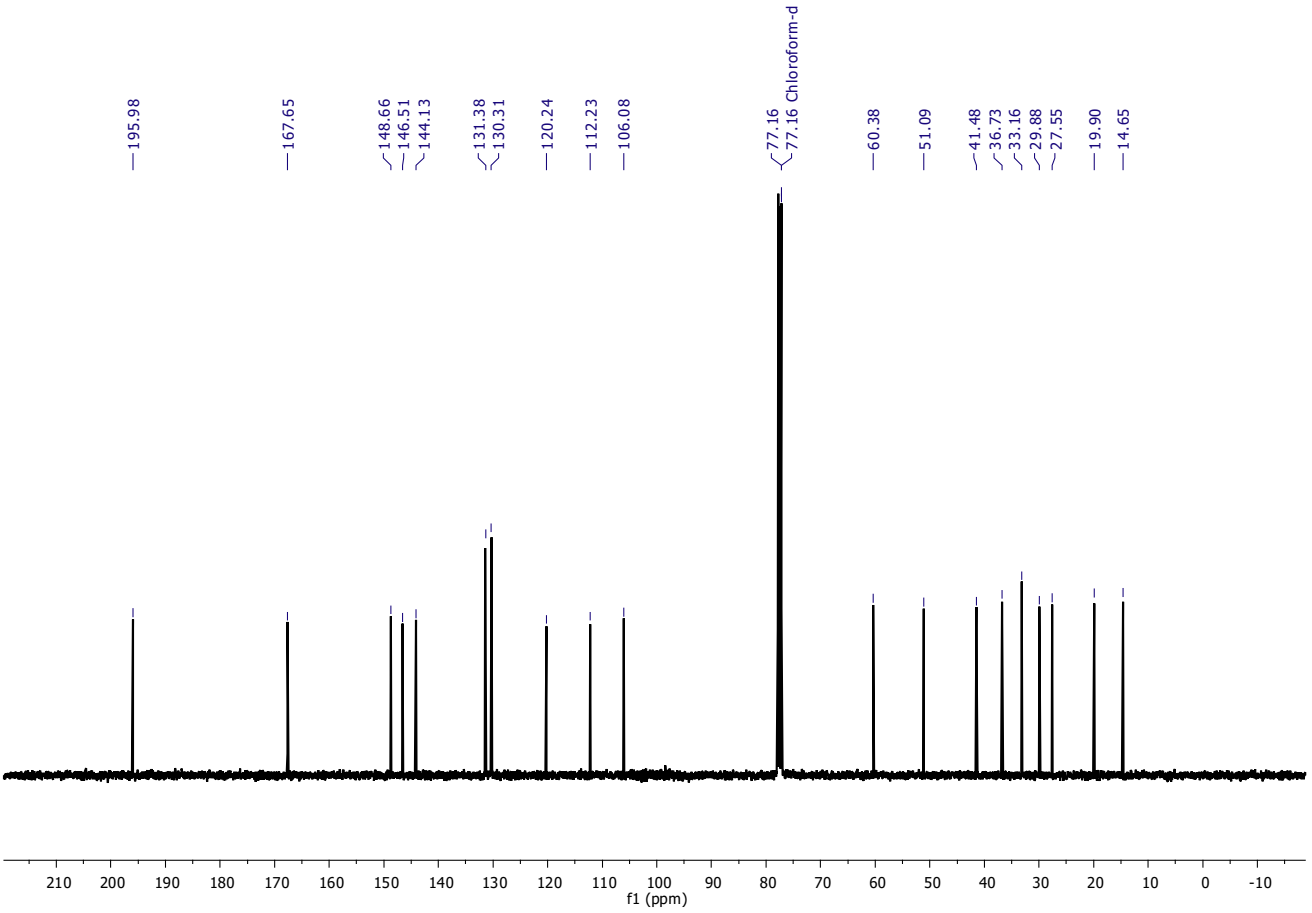


Figure S28.^{13}C NMR spectrum of compound **6** ($CDCl_3$, 100 MHz, TMS).

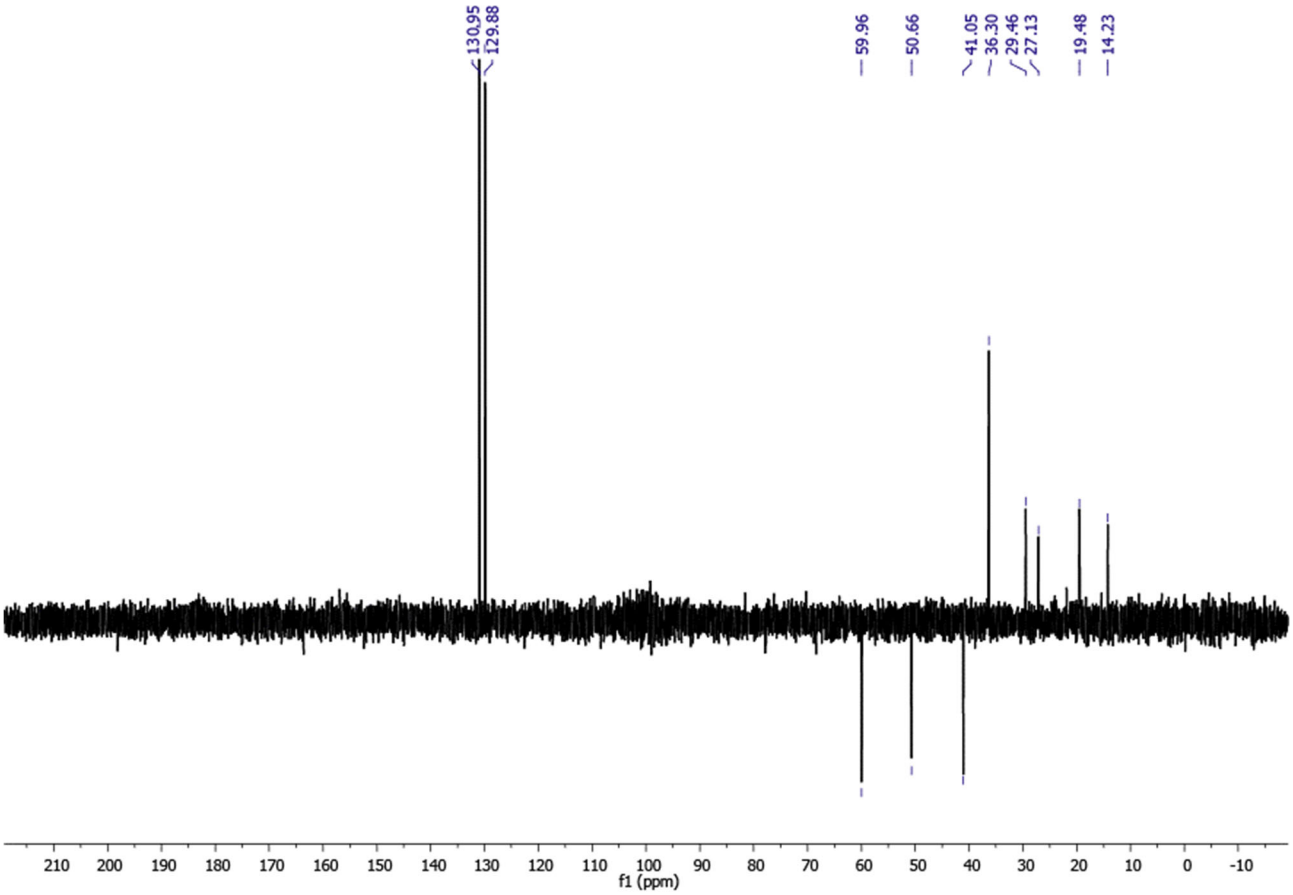


Figure S29. DEPT 135 spectrum of compound **6** ($CDCl_3$, 100 MHz, TMS).

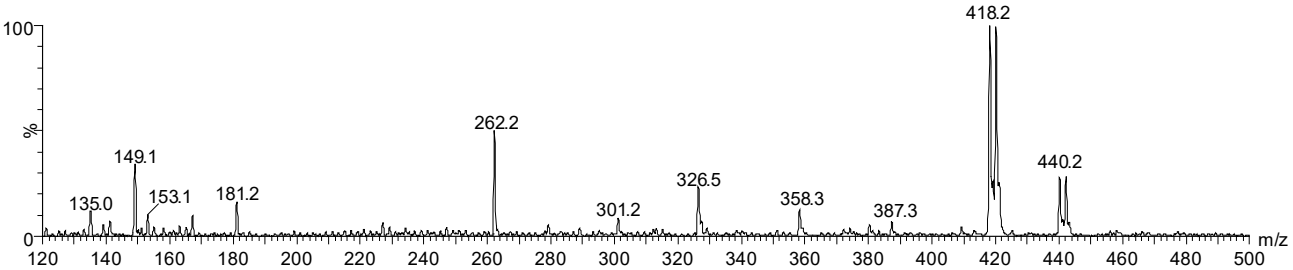


Figure S30. ESI (+) mass spectrum of compound **6**.

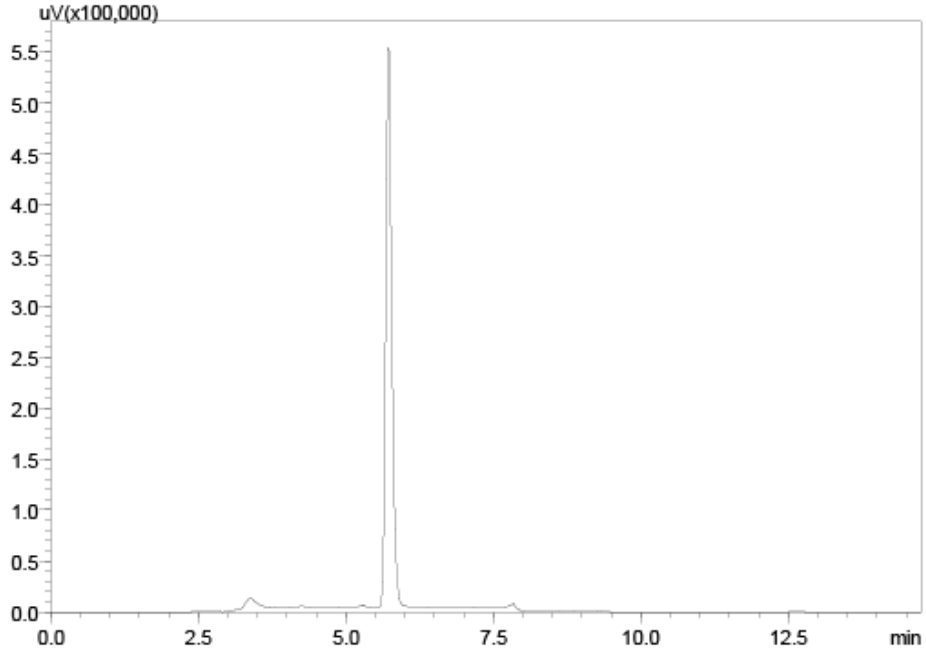


Figure S31: HPLC chromatogram of compound **7**.

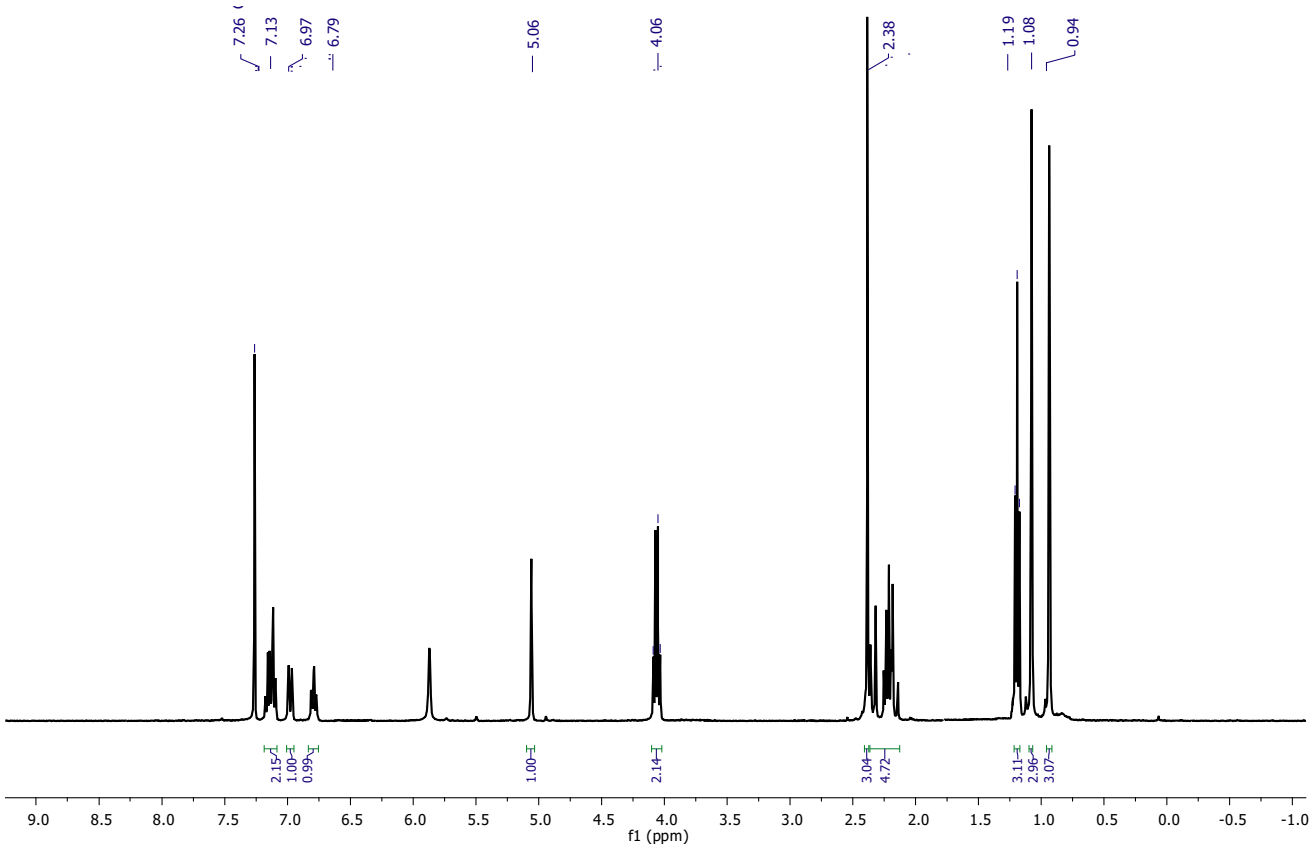


Figure S32.^{1}H NMR spectrum of compound **7** ($CDCl_3$, 400 MHz, TMS).

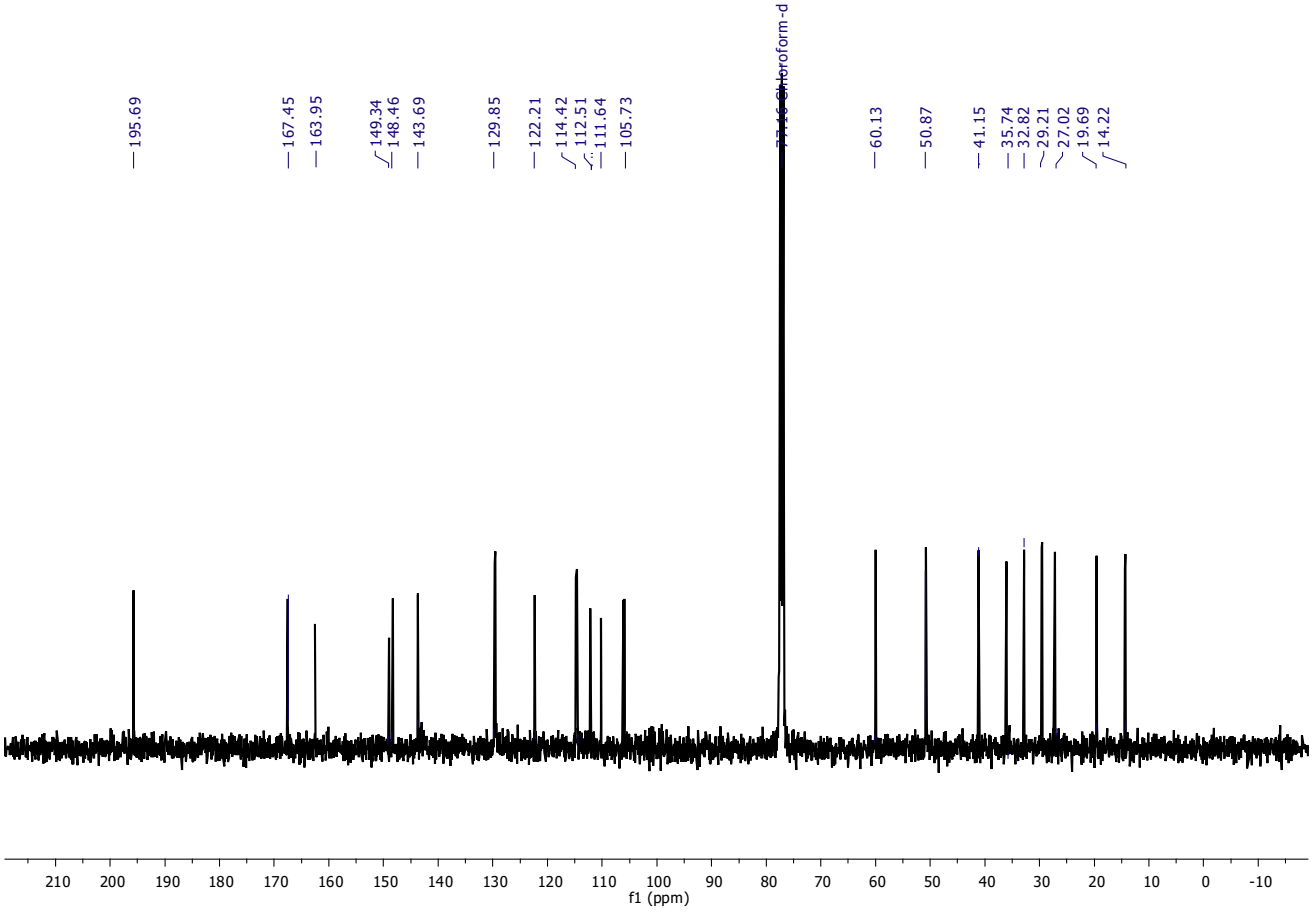


Figure S33.^{13}C NMR spectrum of compound **7** ($CDCl_3$, 100 MHz, TMS).

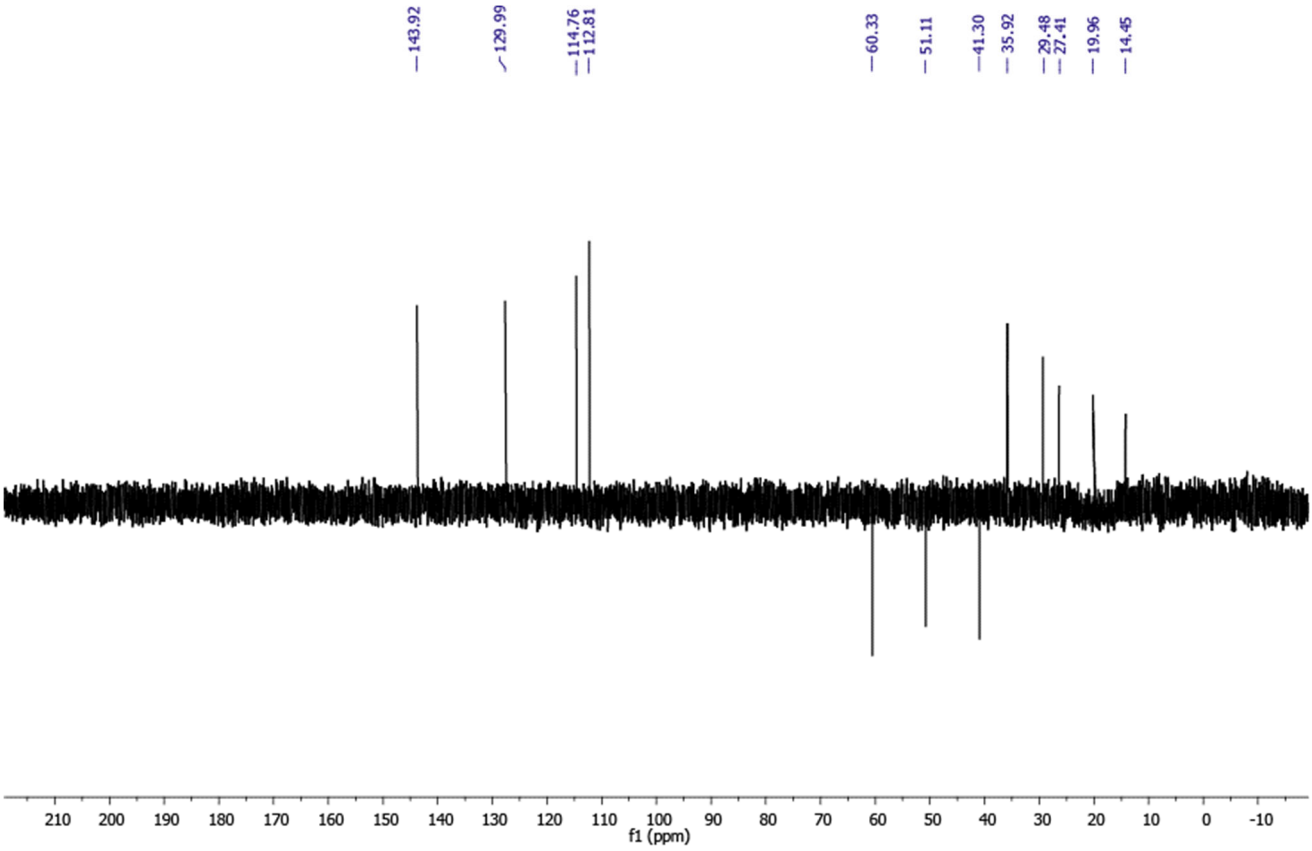


Figure S34. DEPT 135 spectrum of compound **7** ($CDCl_3$, 100 MHz, TMS).

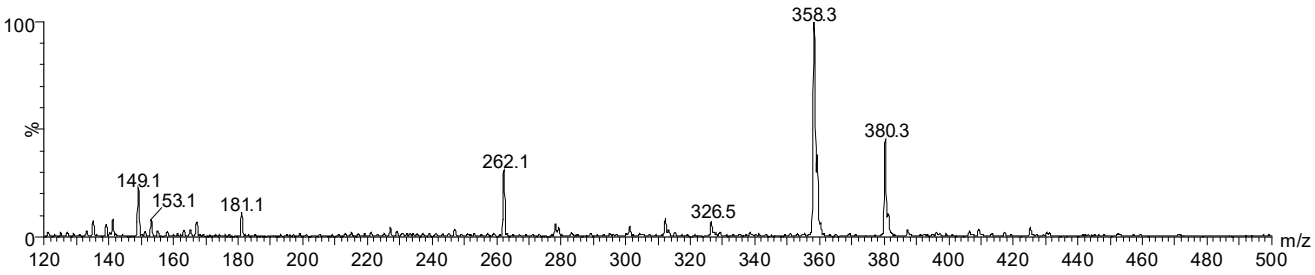


Figure S35. ESI (+) mass spectrum of compound **7**.

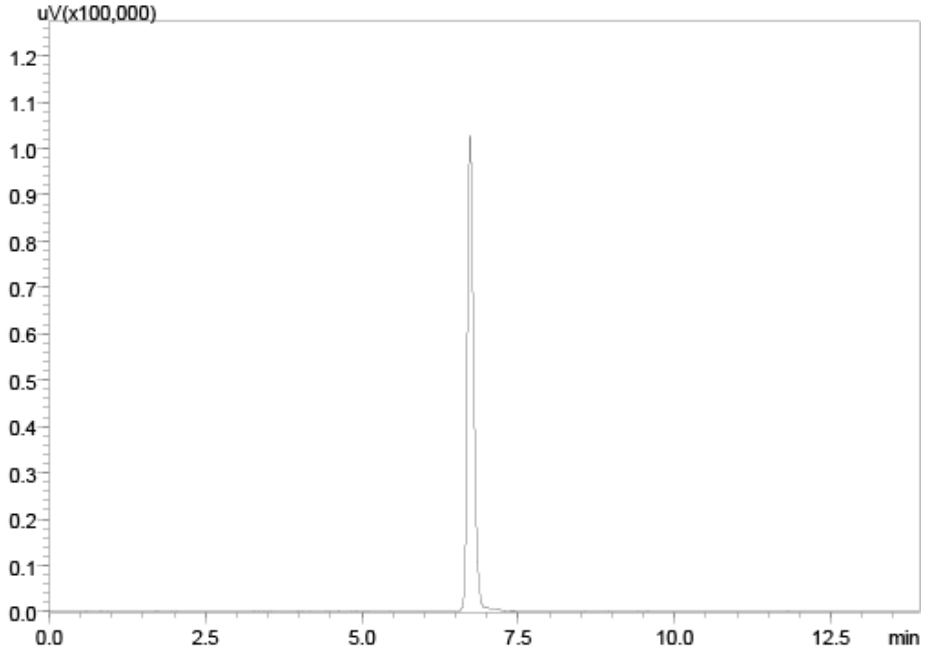


Figure S36: HPLC chromatogram of compound **8**.

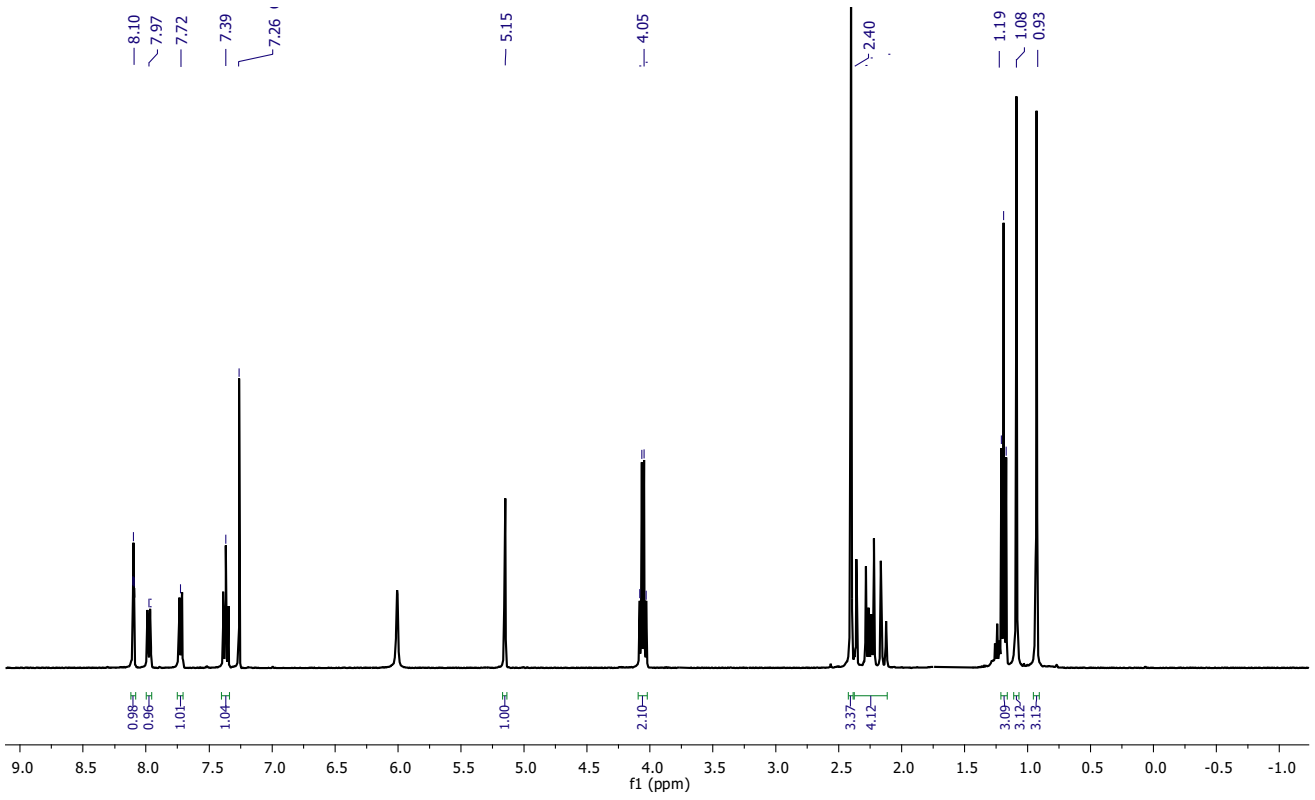


Figure S37.^{1}H NMR spectrum of compound **8** ($CDCl_3$, 400 MHz, TMS).

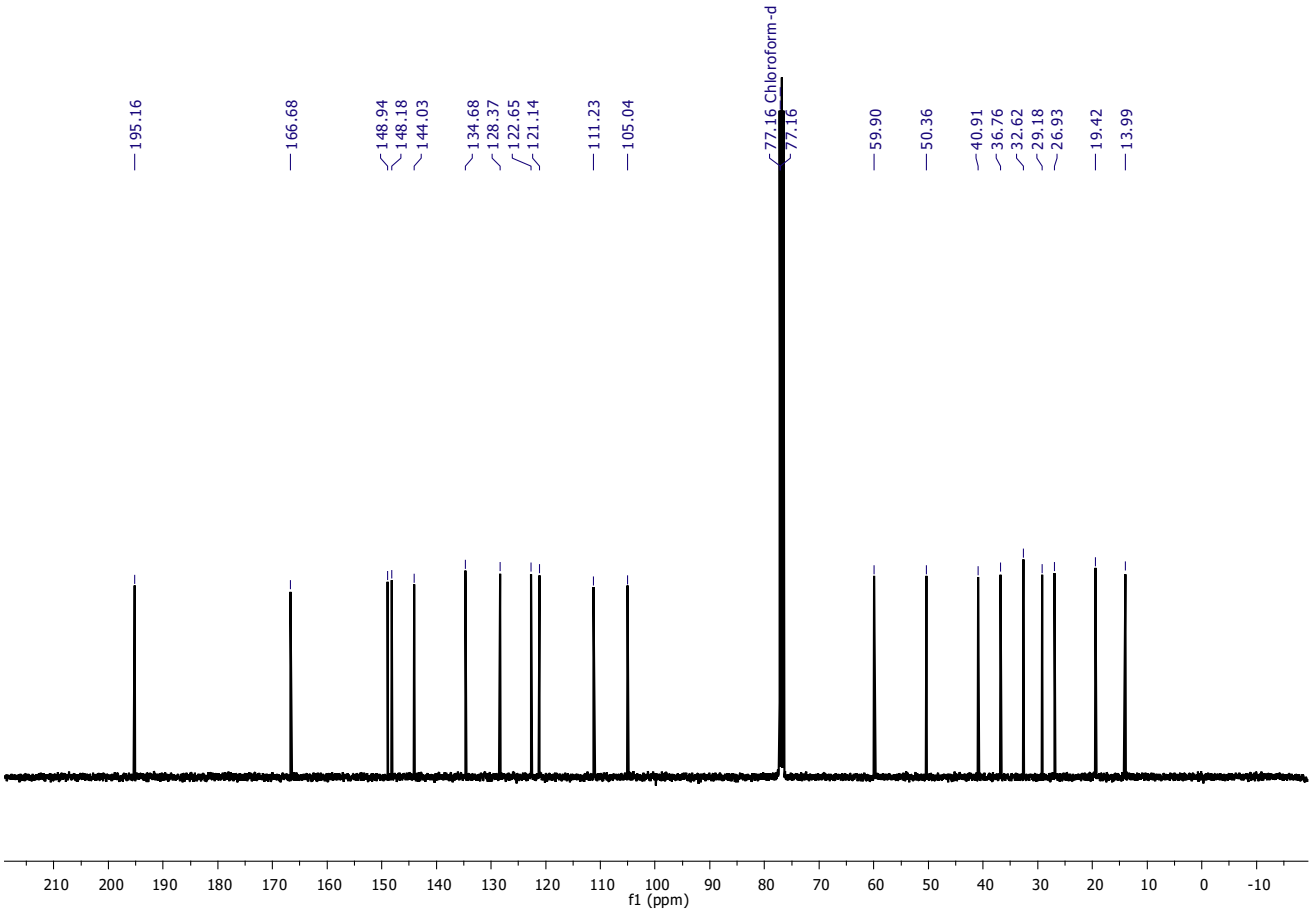


Figure S38.^{13}C NMR spectrum of compound **8** ($CDCl_3$, 100 MHz, TMS).

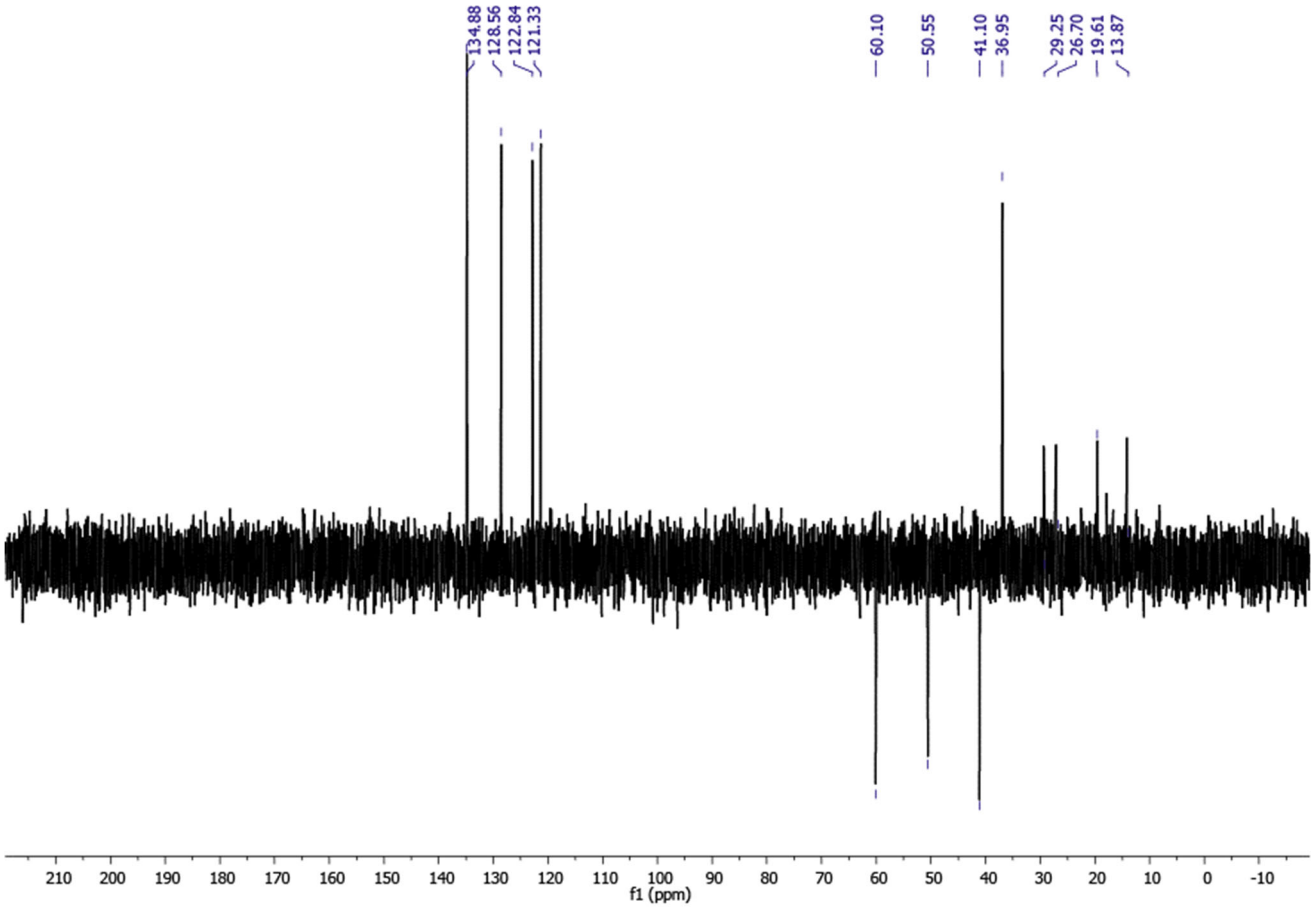


Figure S39. DEPT 135 spectrum of compound **8**($CDCl_3$, 100 MHz, TMS).

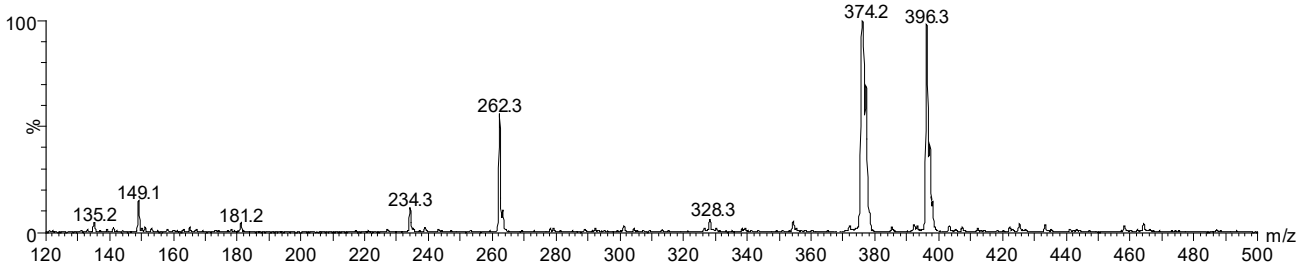


Figure S40. ESI (+) mass spectrum of compound **8**.

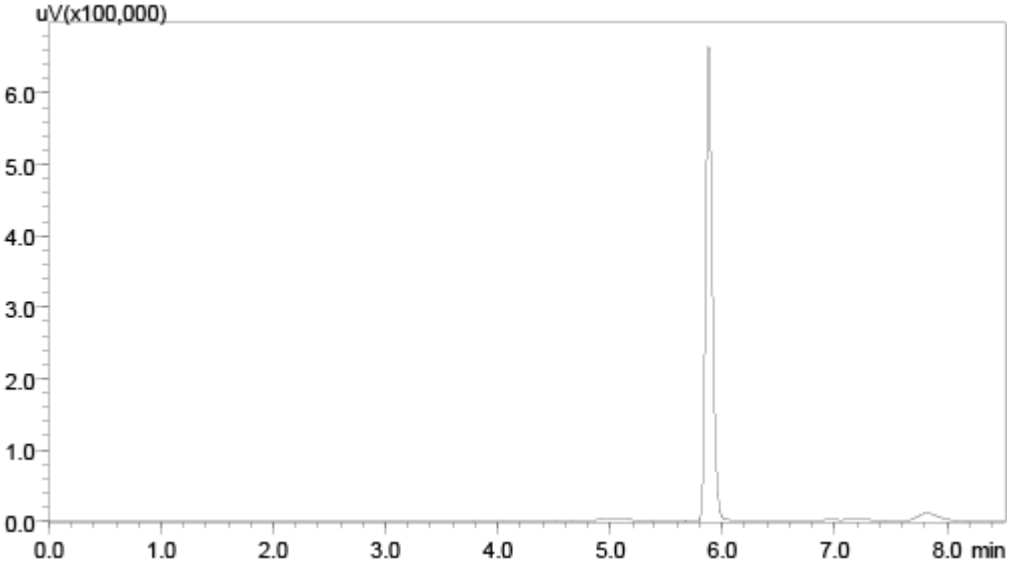


Figure S41: HPLC chromatogram of compound **9**.

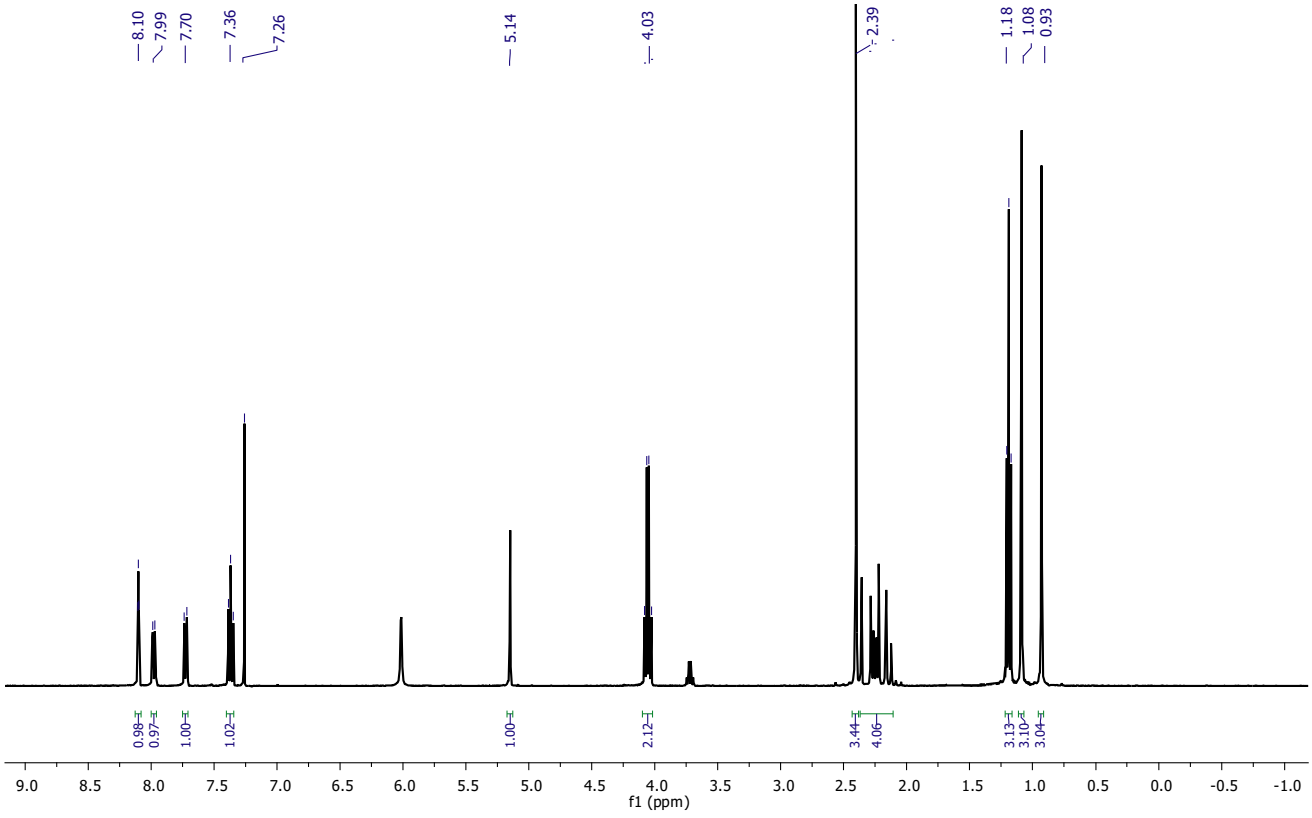


Figure S42.^{1}H NMR spectrum of compound **9** ($CDCl_3$, 400 MHz, TMS).

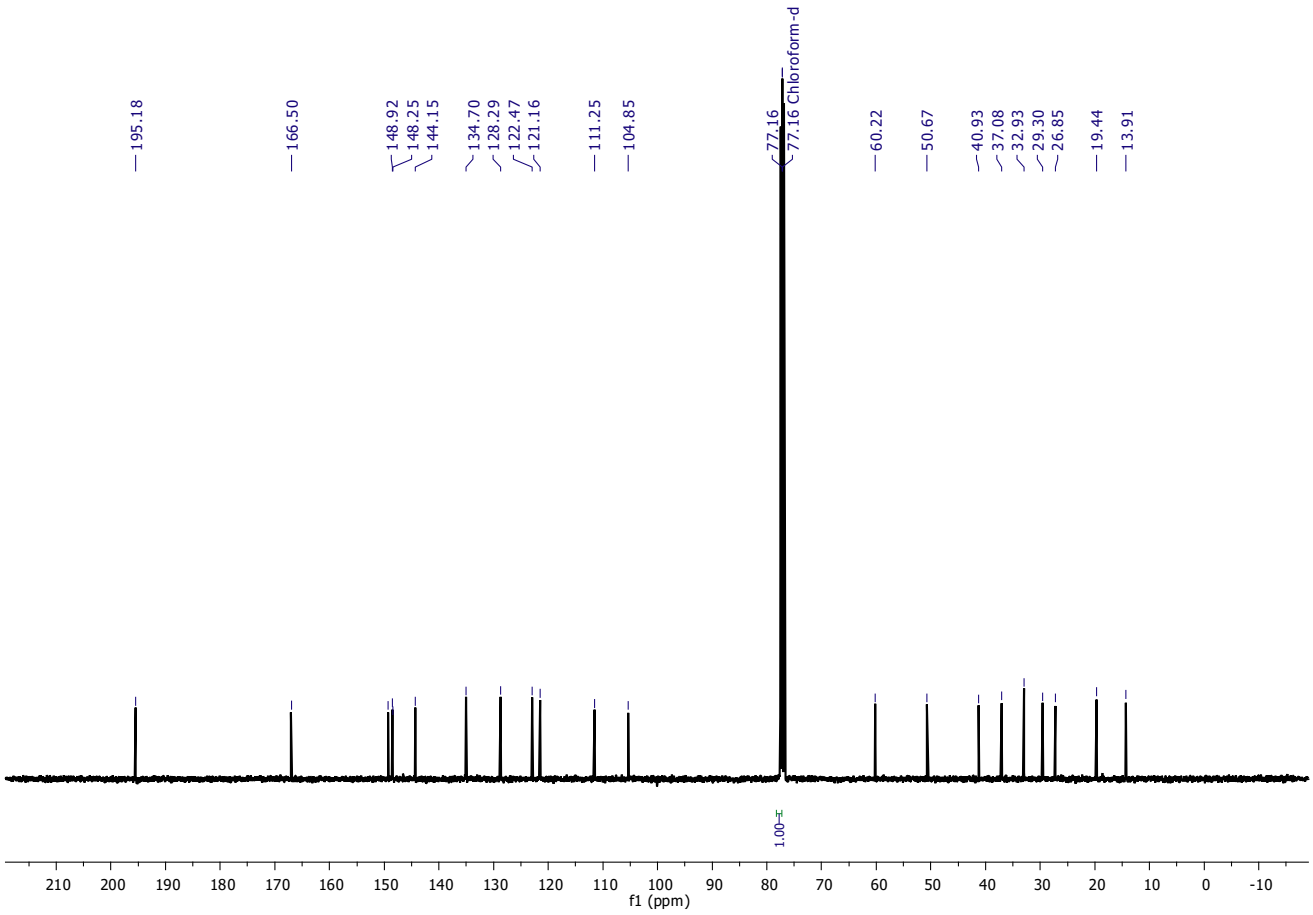


Figure S43.^{13}C NMR spectrum of compound **9** ($CDCl_3$, 100 MHz, TMS).

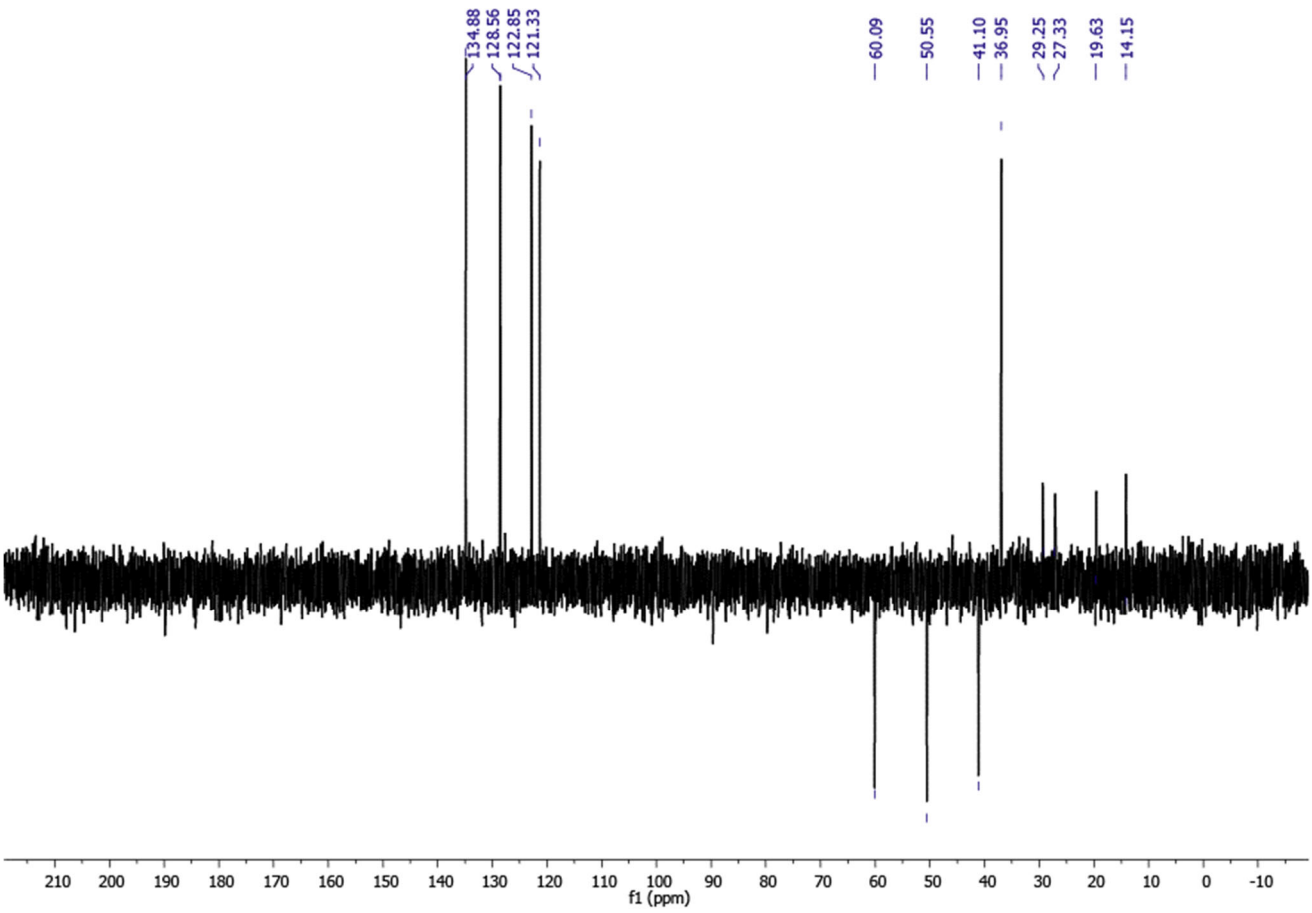


Figure S44. DEPT 135 spectrum of compound **9** ($CDCl_3$, 100 MHz, TMS).

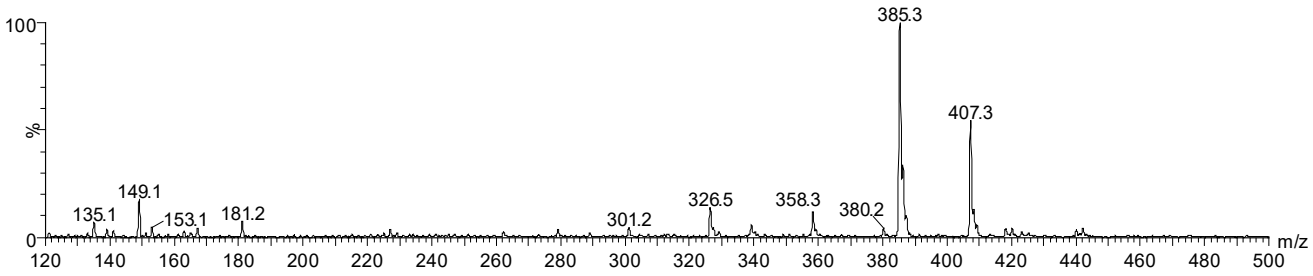


Figure S45. ESI (+) mass spectrum of compound **9**.

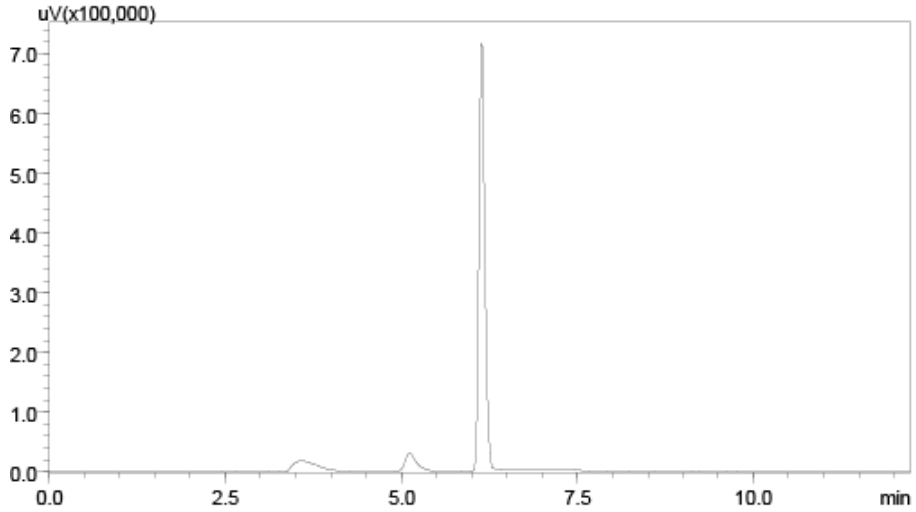


Figure S46: HPLC chromatogram of compound **10**.

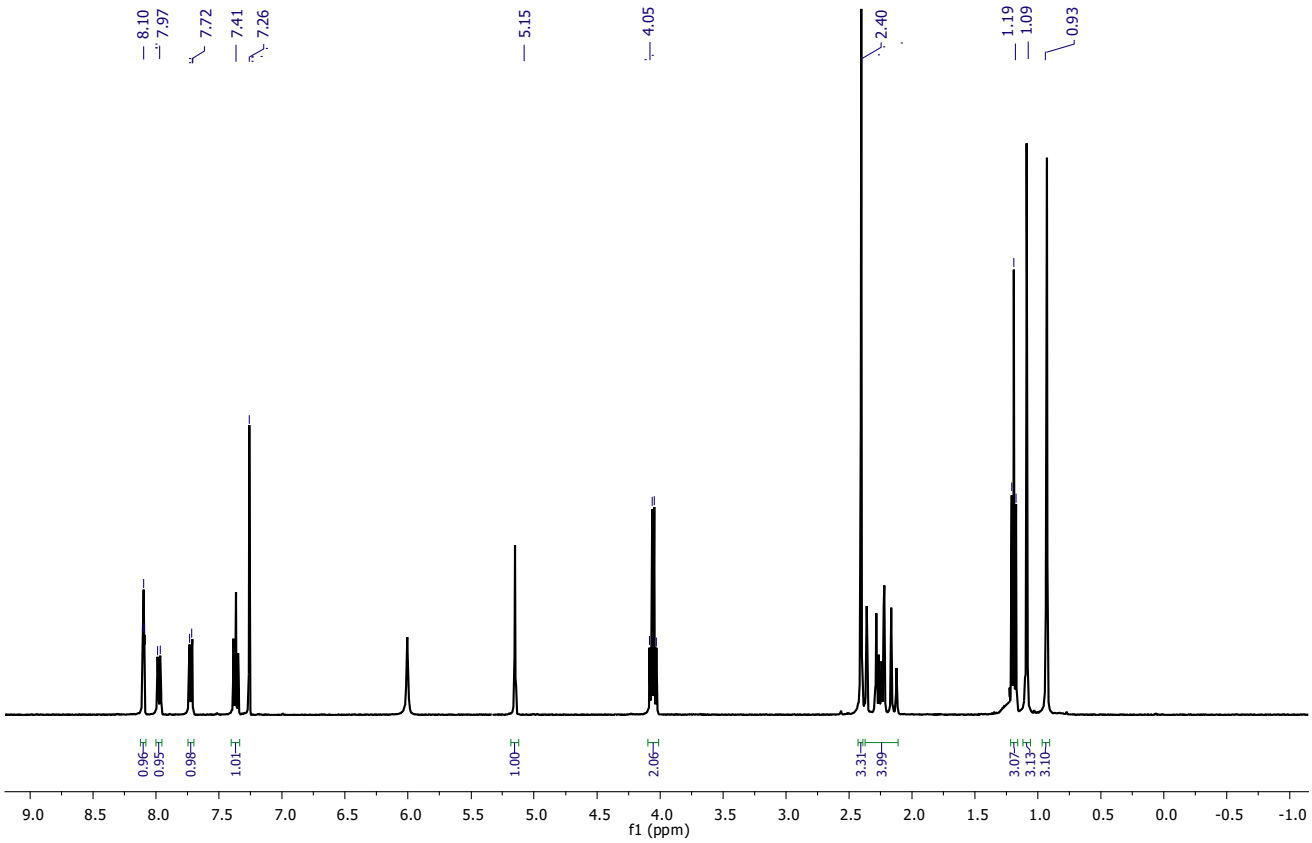


Figure S47.^{1}H NMR spectrum of compound **10** ($CDCl_3$, 400 MHz, TMS).

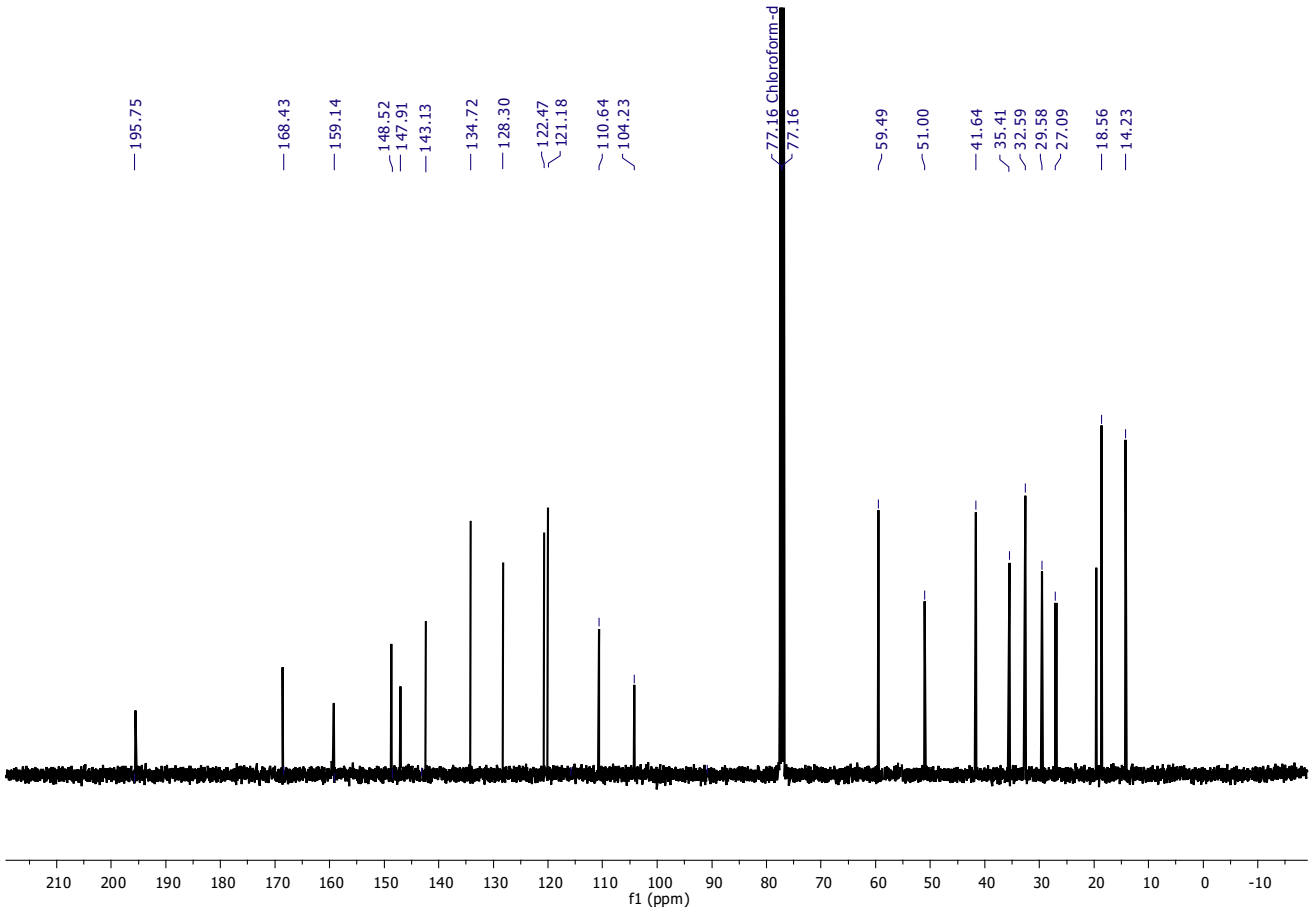


Figure S48.^{13}C NMR spectrum of compound **10** ($CDCl_3$, 100 MHz, TMS).

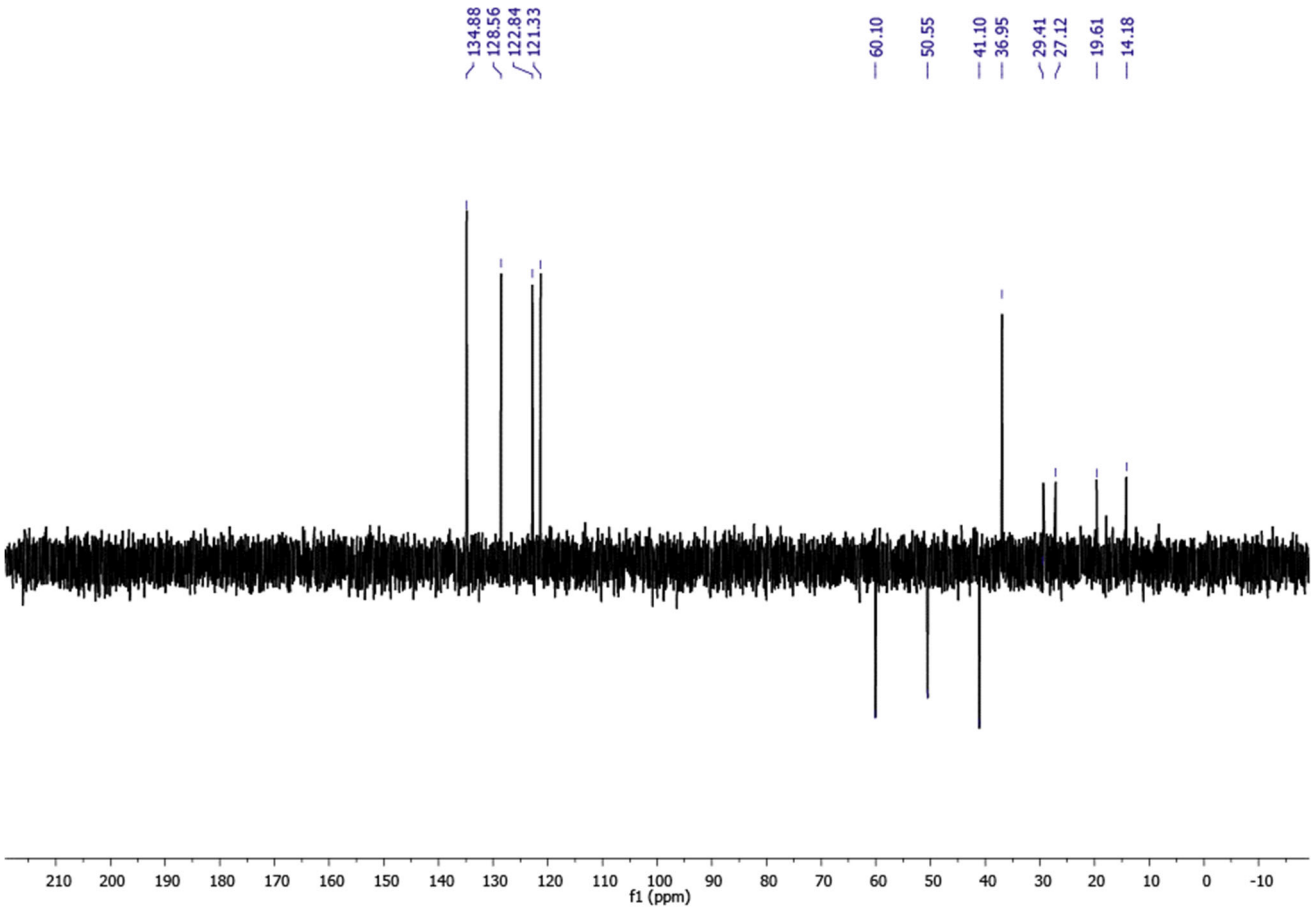


Figure S49. DEPT 135 spectrum of compound **10** ($CDCl_3$, 100 MHz, TMS).

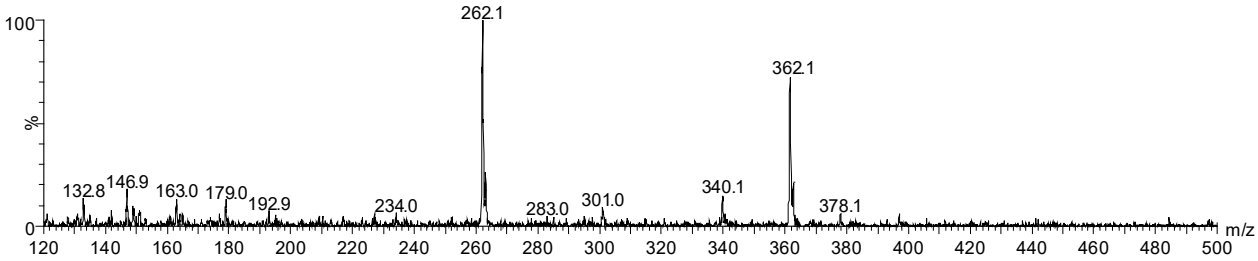


Figure S50. ESI (+) mass spectrum of compound **10.**

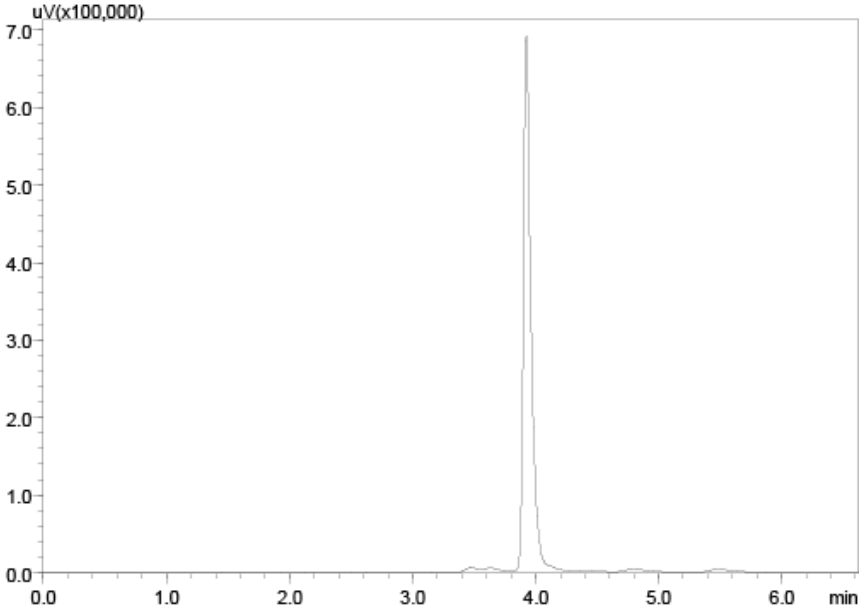


Figure S51: HPLC chromatogram of compound **11**.

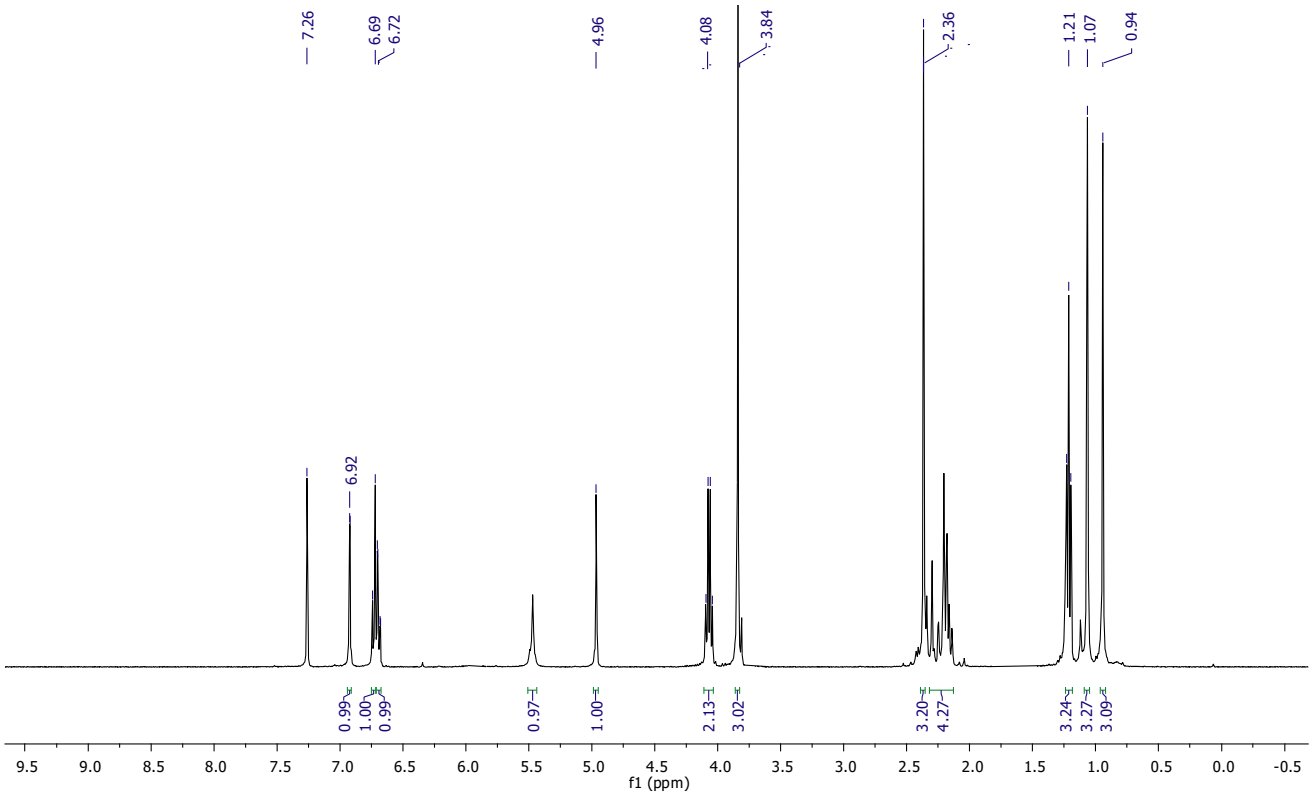


Figure S52.^{1}H NMR spectrum of compound **11** ($CDCl_3$, 400 MHz, TMS).

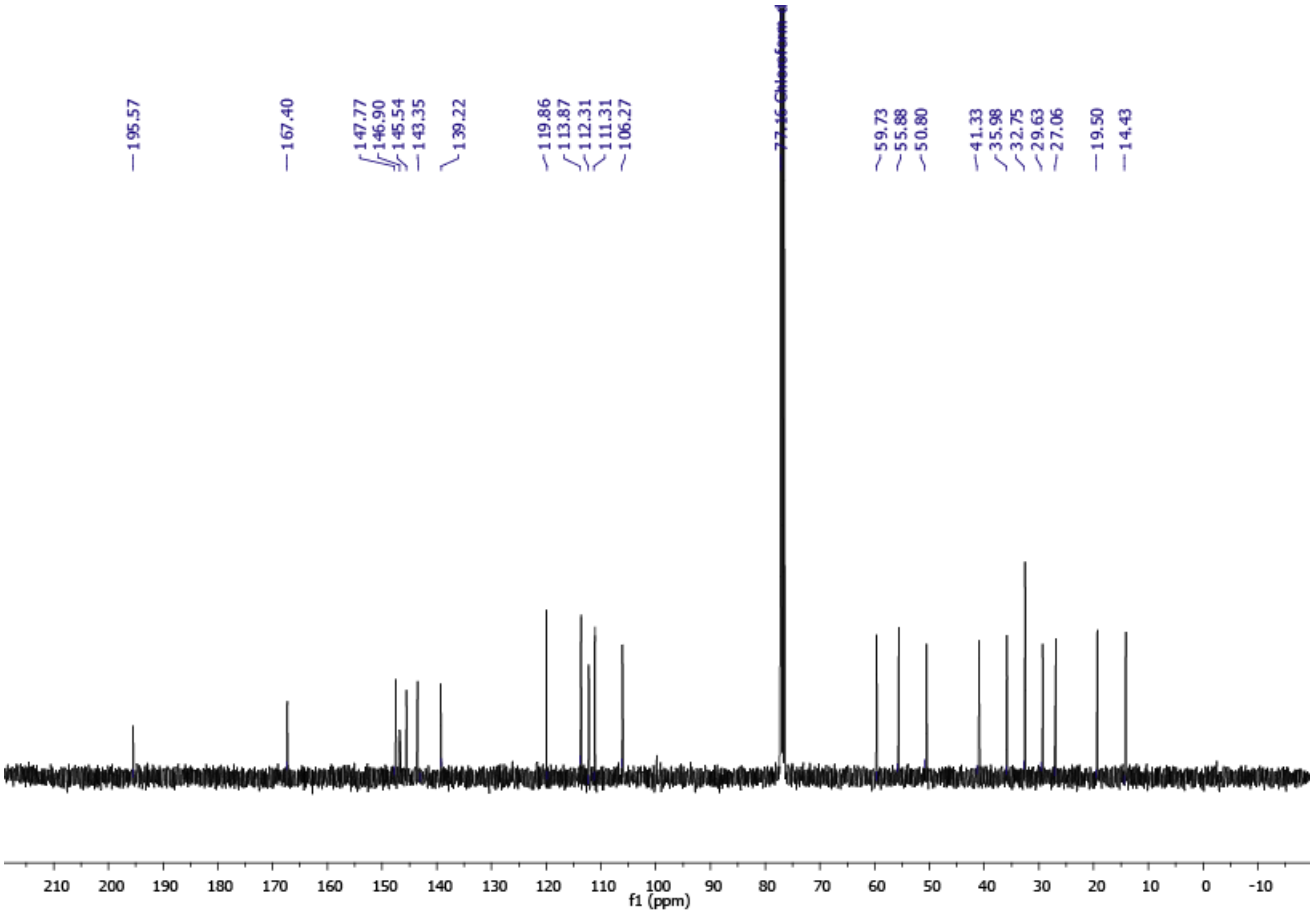


Figure S53.^{13}C NMR spectrum of compound **11** ($CDCl_3$, 100 MHz, TMS).

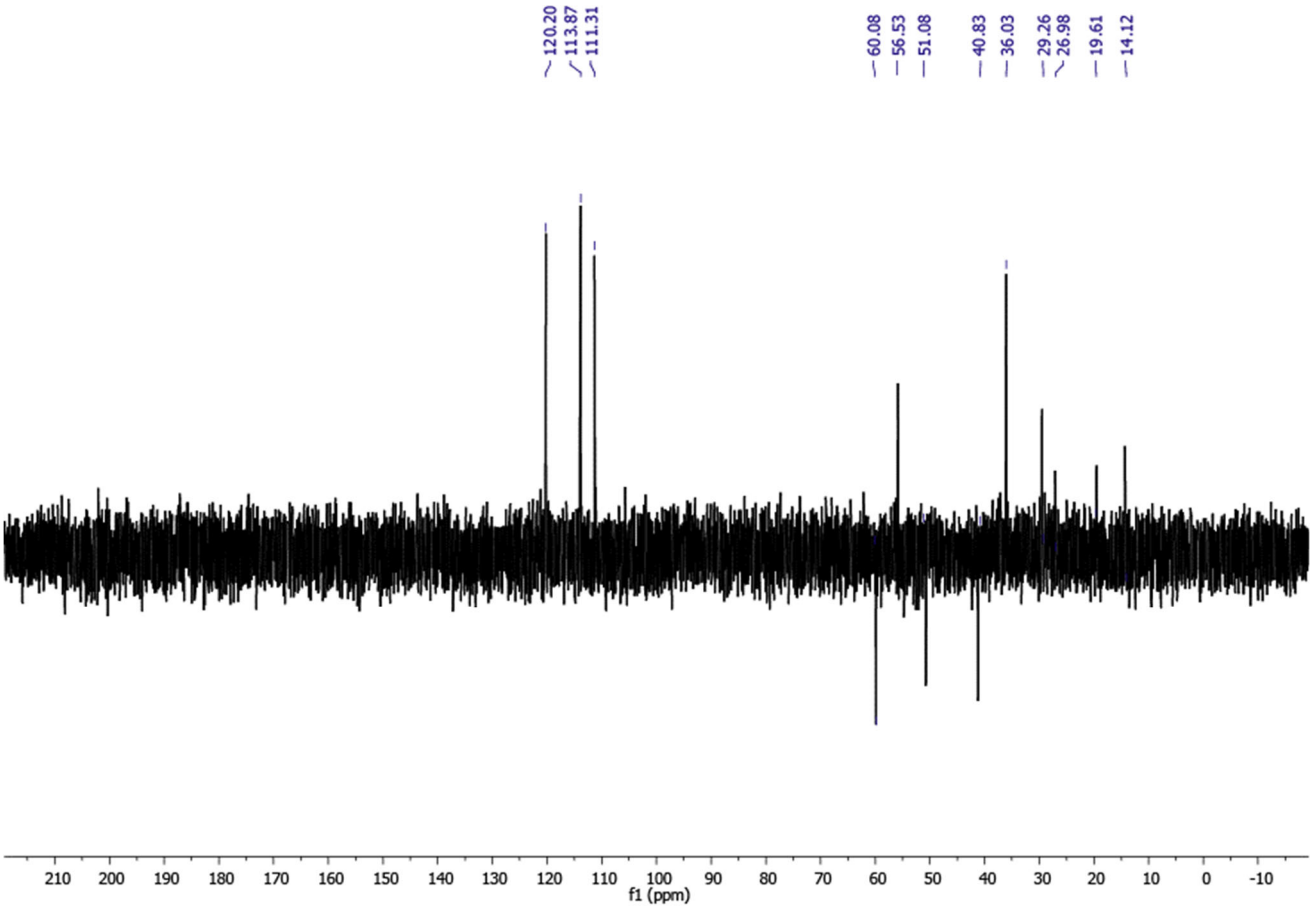


Figure S54. DEPT 135 spectrum of compound **11** ($CDCl_3$, 100 MHz, TMS).

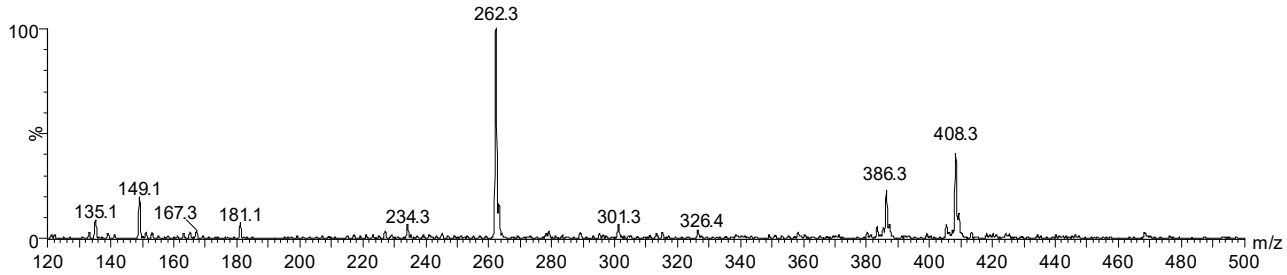


Figure S55. ESI (+) mass spectrum of compound **11.**

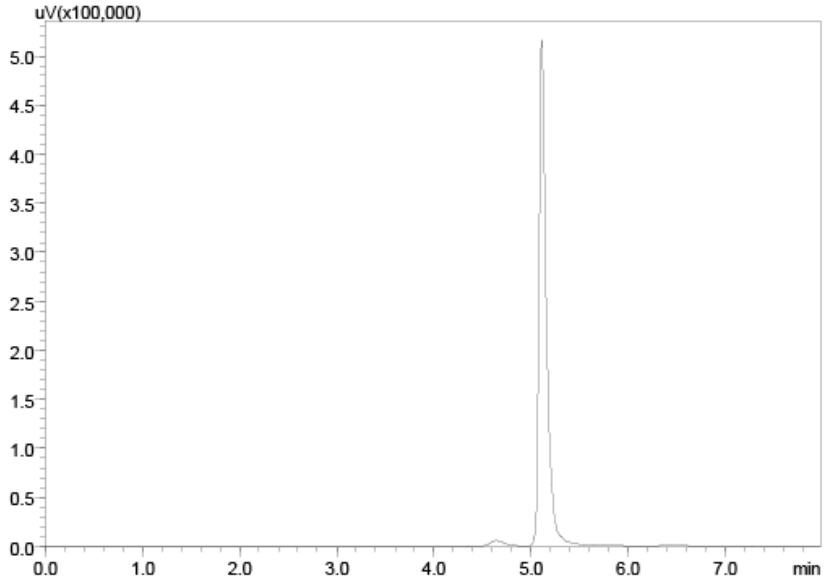


Figure S56: HPLC chromatogram of compound **12**.

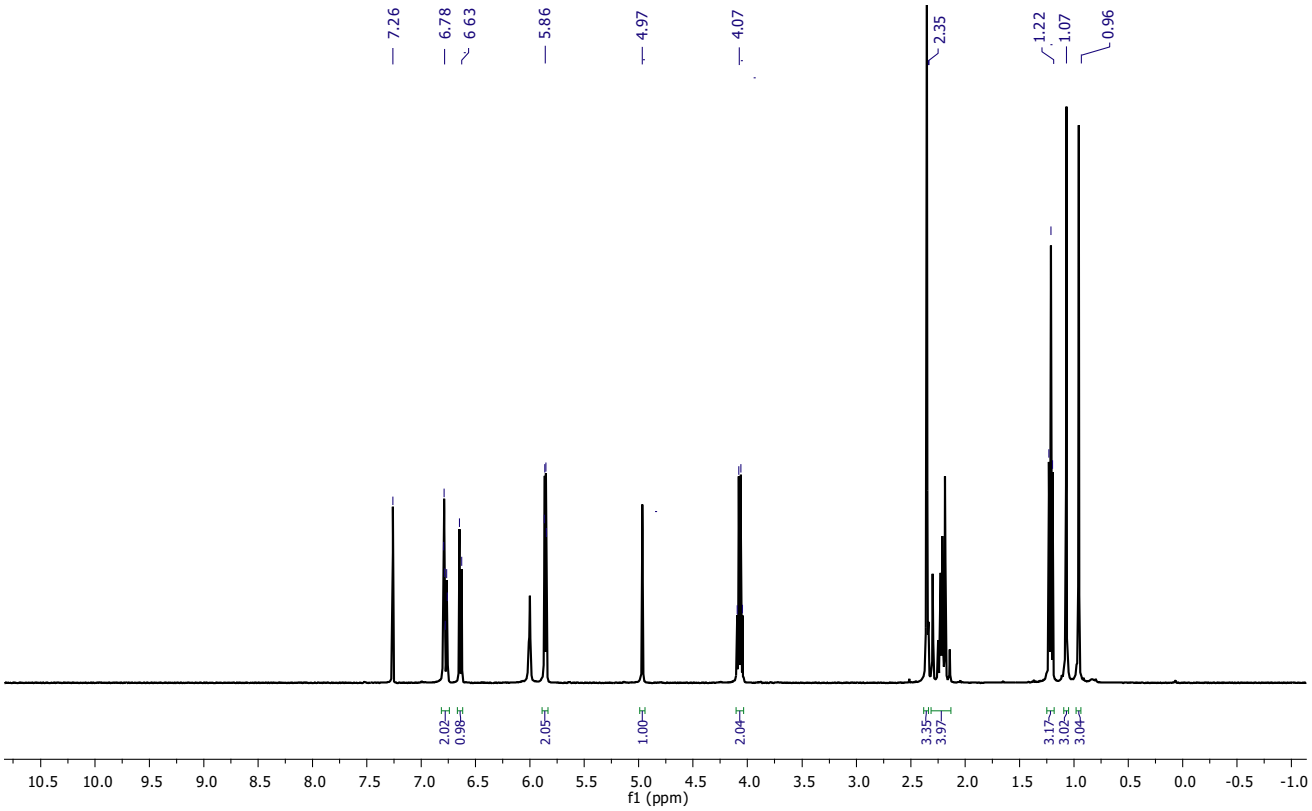


Figure S57.^{1}H NMR spectrum of compound **12** ($CDCl_3$, 400 MHz, TMS).

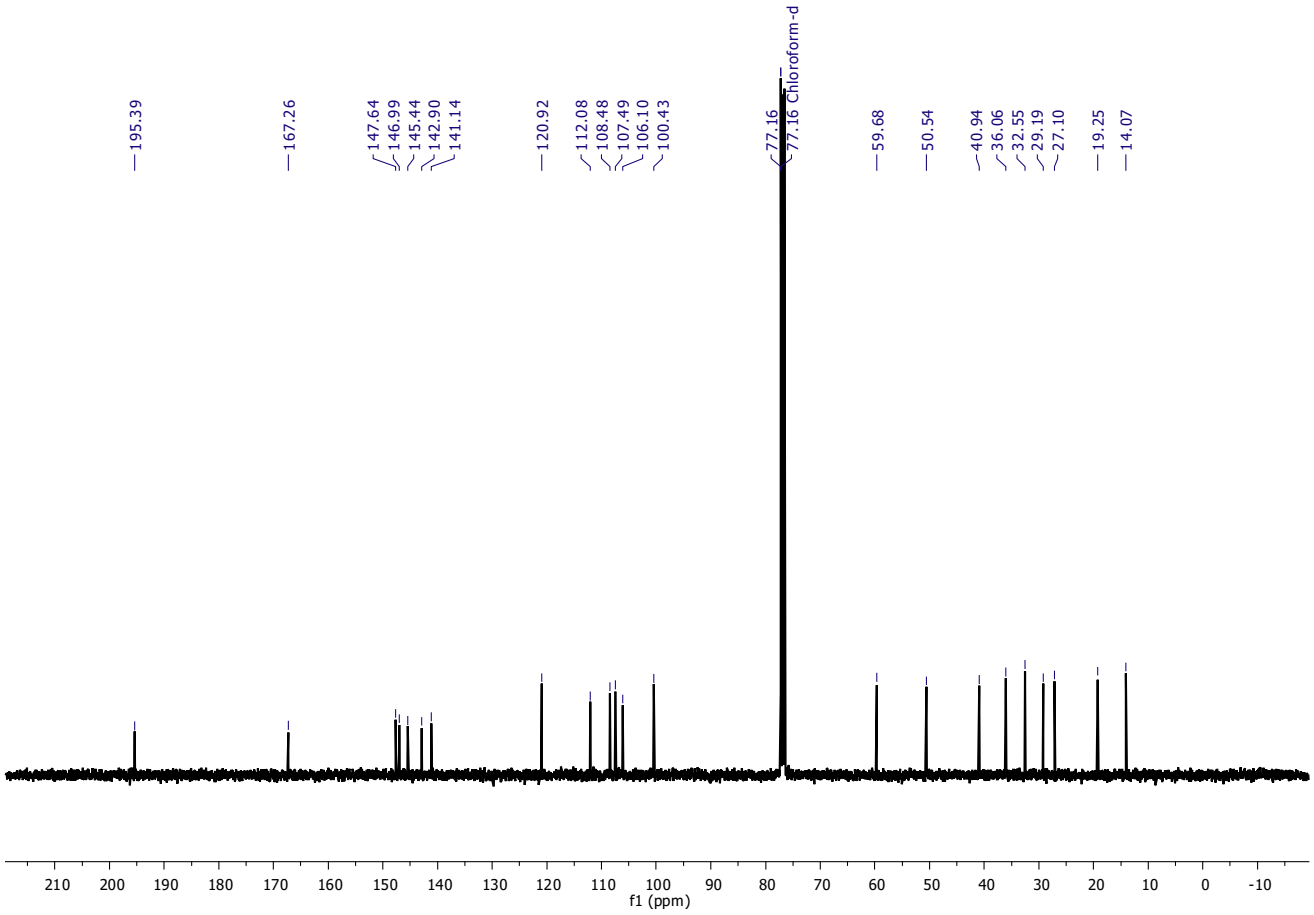


Figure S58.^{13}C NMR spectrum of compound **12** ($CDCl_3$, 100 MHz, TMS).

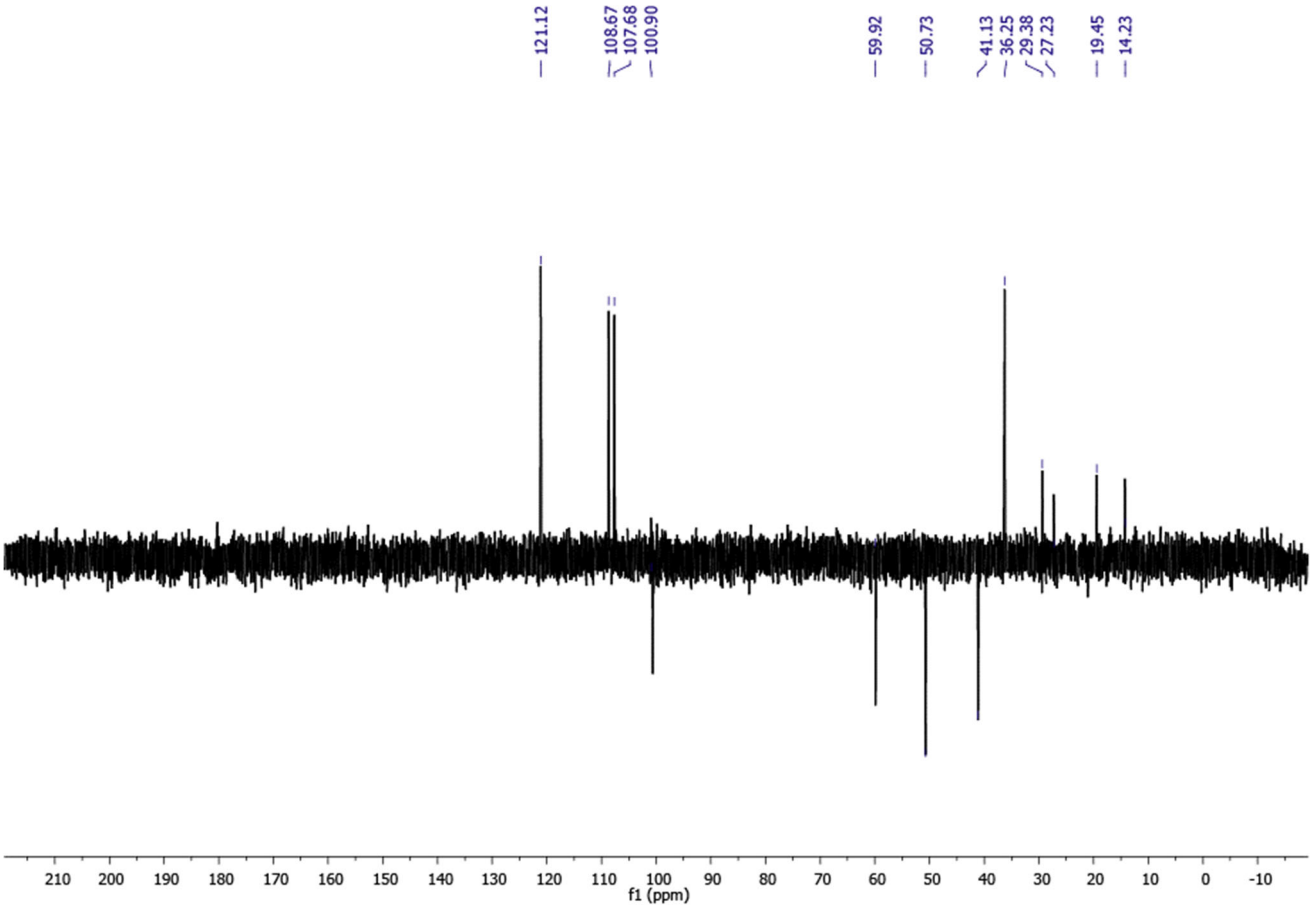


Figure S59. DEPT 135 spectrum of compound **12** ($CDCl_3$, 100 MHz, TMS).

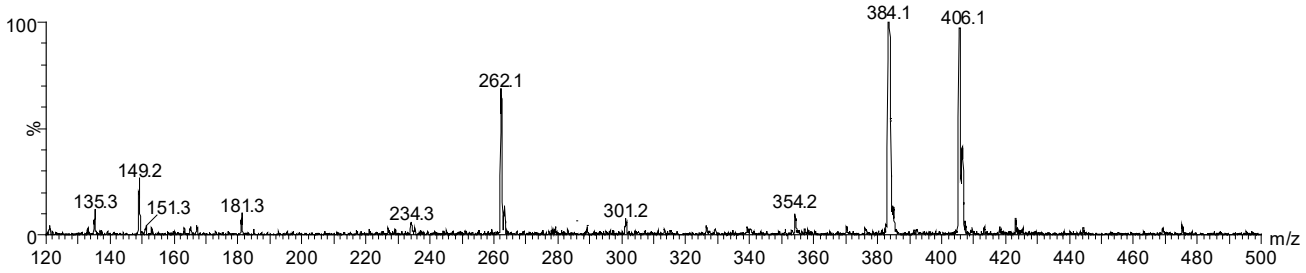


Figure S60. ESI (+) mass spectrum of compound **12.**

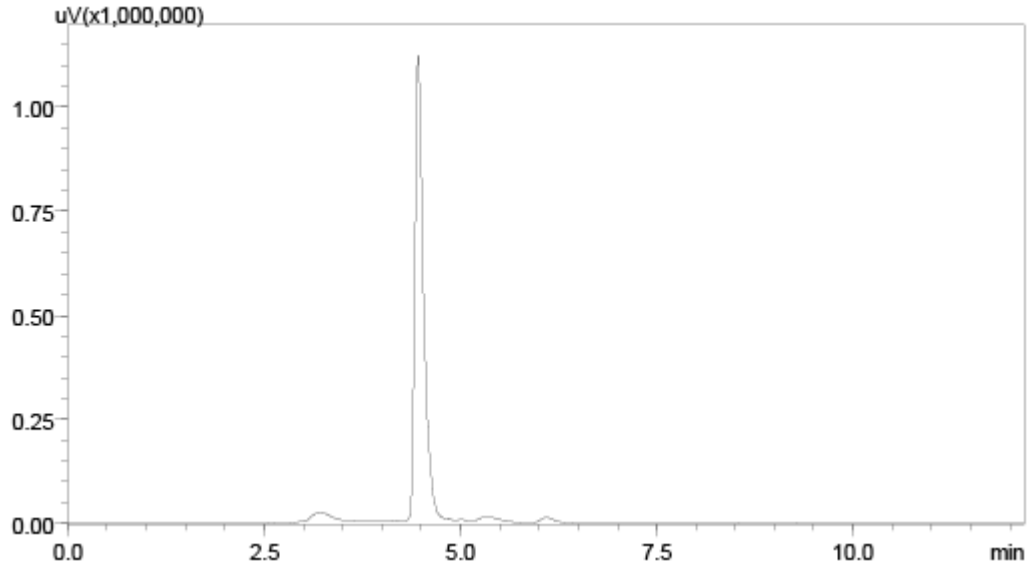


Figure S61: HPLC chromatogram of compound **13**.

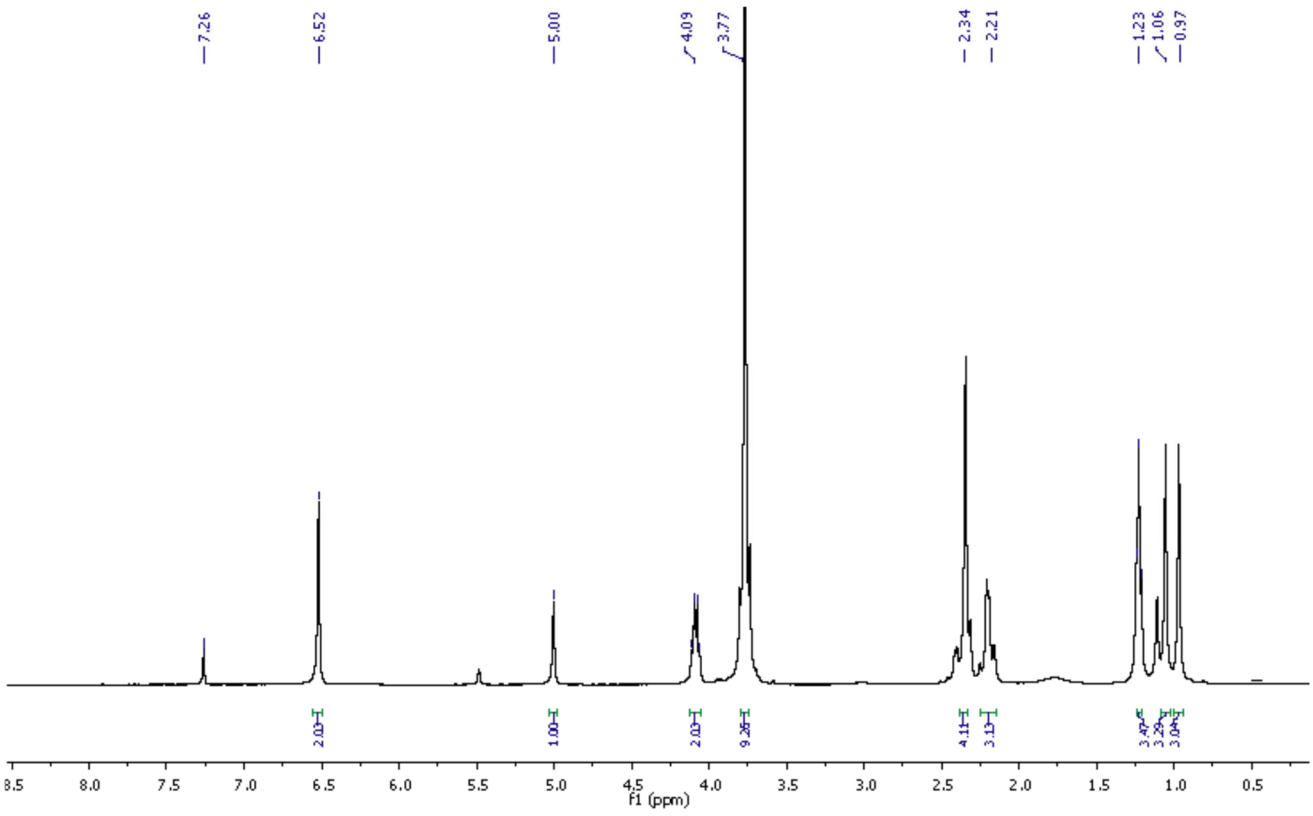


Figure S62.^{1}H NMR spectrum of compound **13** ($CDCl_3$, 400 MHz, TMS).

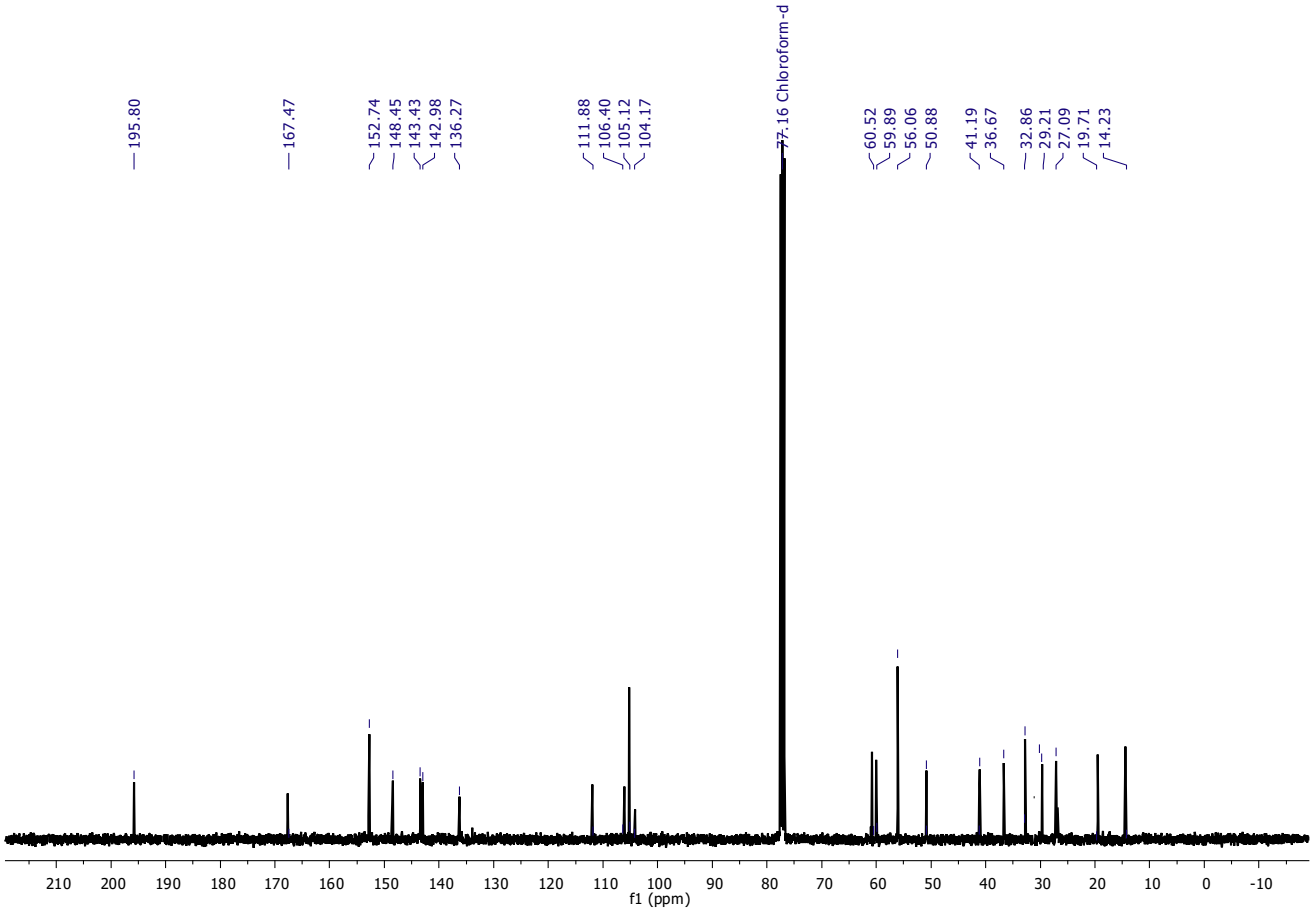


Figure S63.^{13}C NMR spectrum of compound **13** ($CDCl_3$, 100 MHz, TMS).

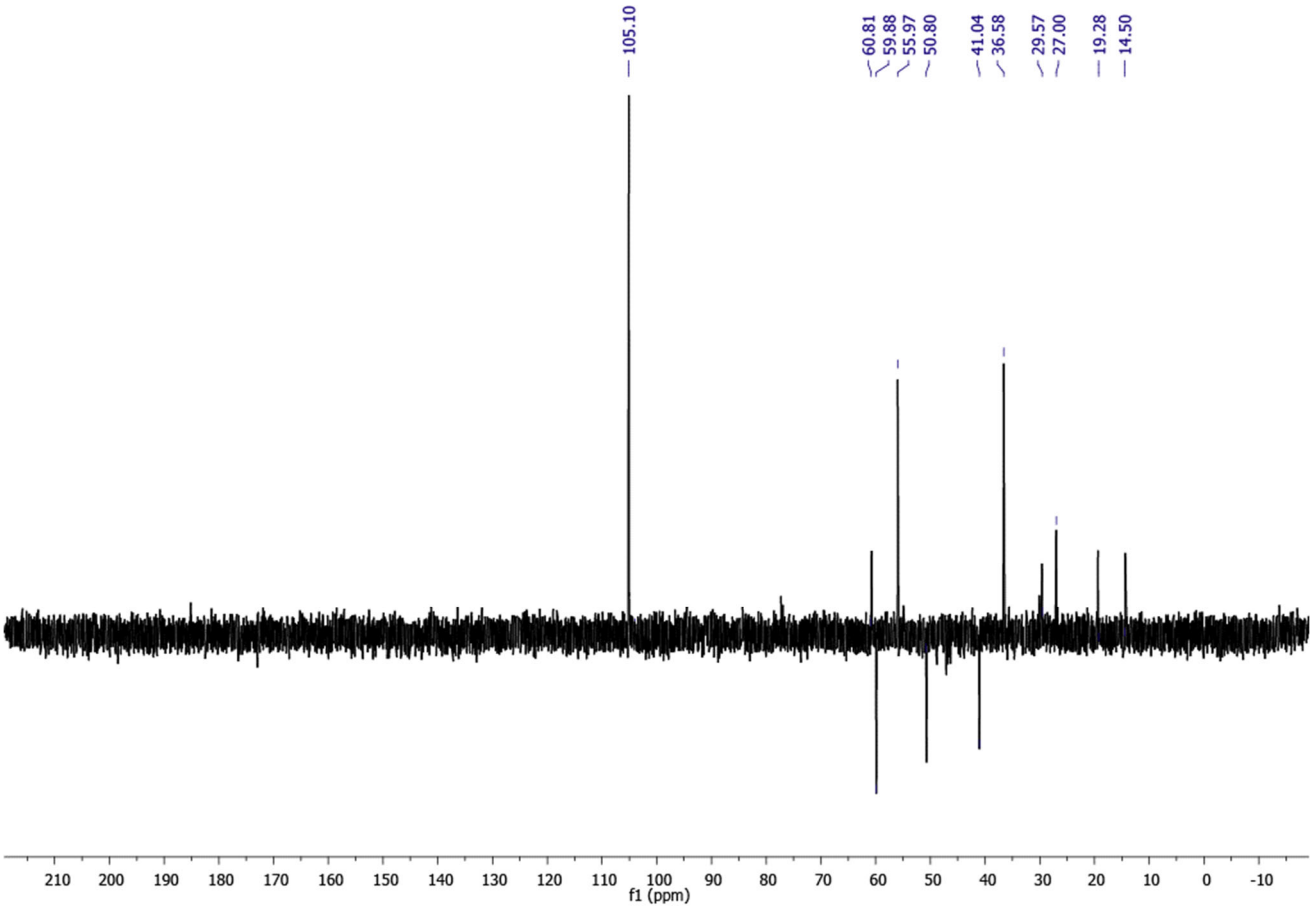


Figure S64. DEPT 135 spectrum of compound **13** ($CDCl_3$, 100 MHz, TMS).

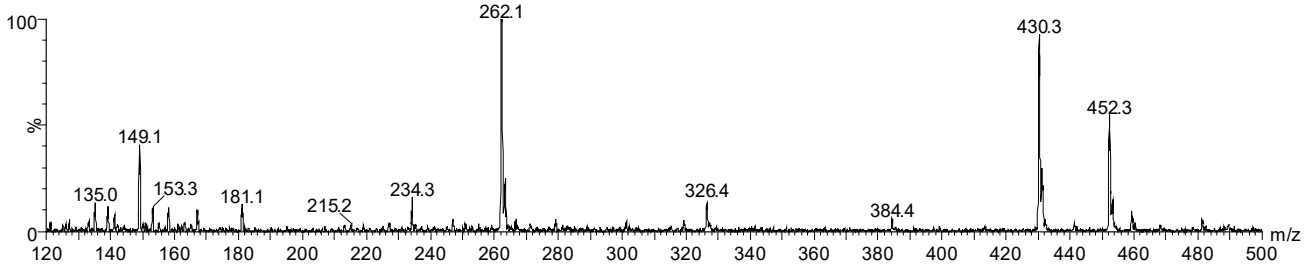


Figure S65. ESI (+) mass spectrum of compound **13.**

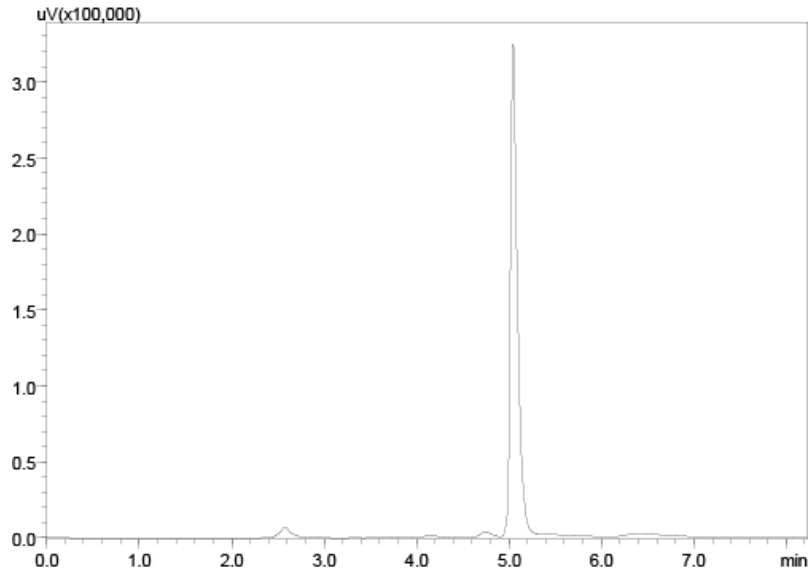


Figure S66: HPLC chromatogram of compound **14**.

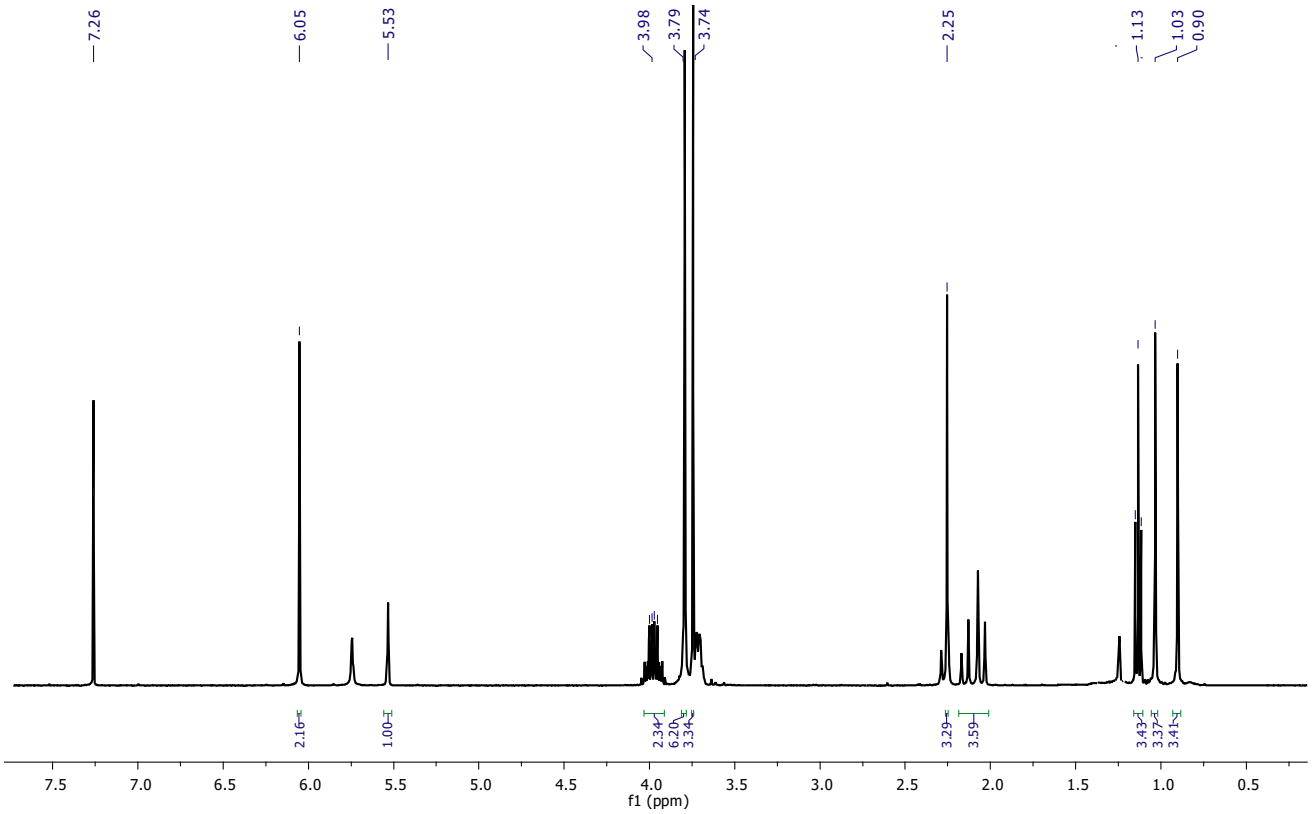


Figure S67.^{1}H NMR spectrum of compound **14** ($CDCl_3$, 400 MHz, TMS).

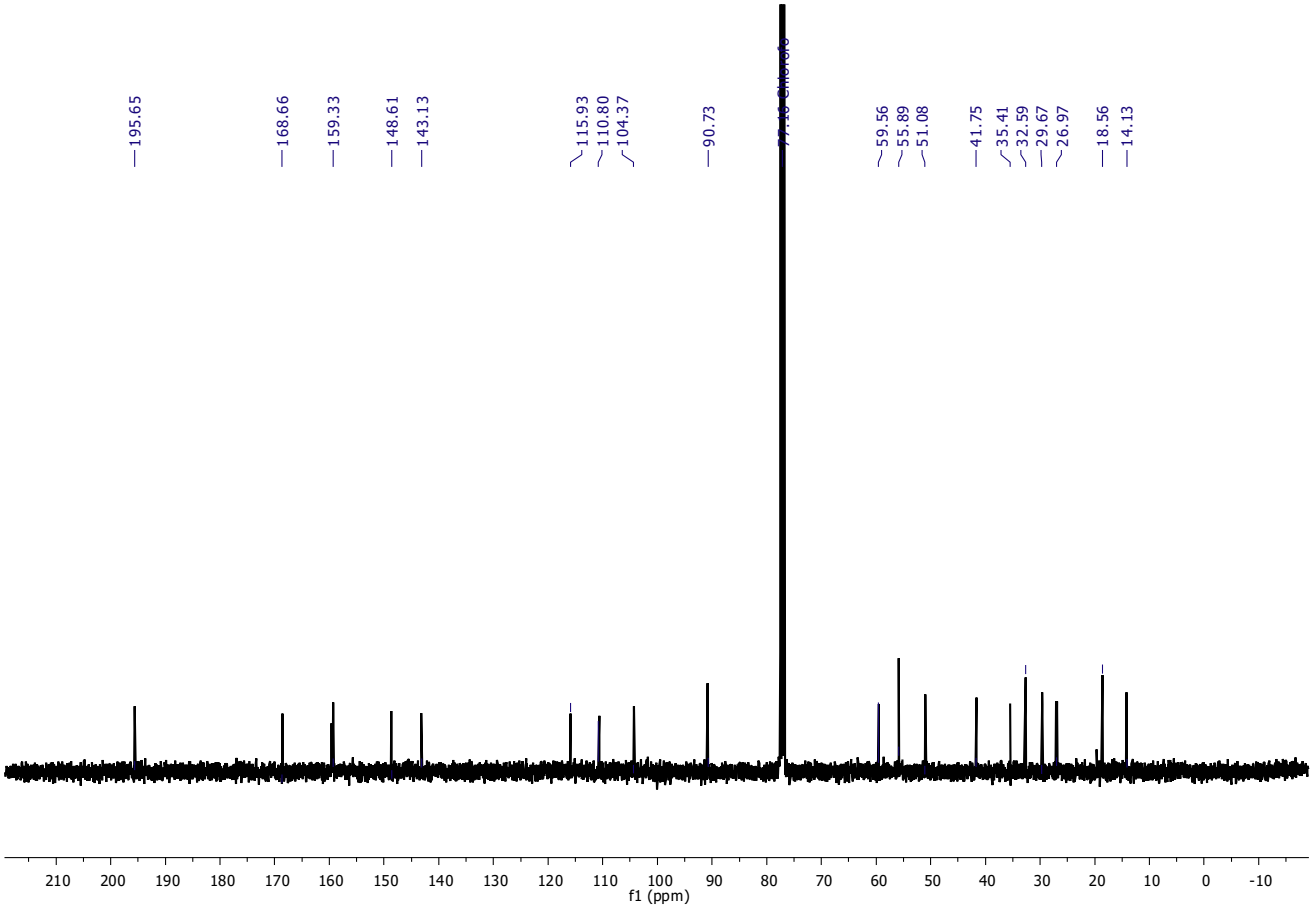


Figure S68.^{13}C NMR spectrum of compound **14** ($CDCl_3$, 100 MHz, TMS).

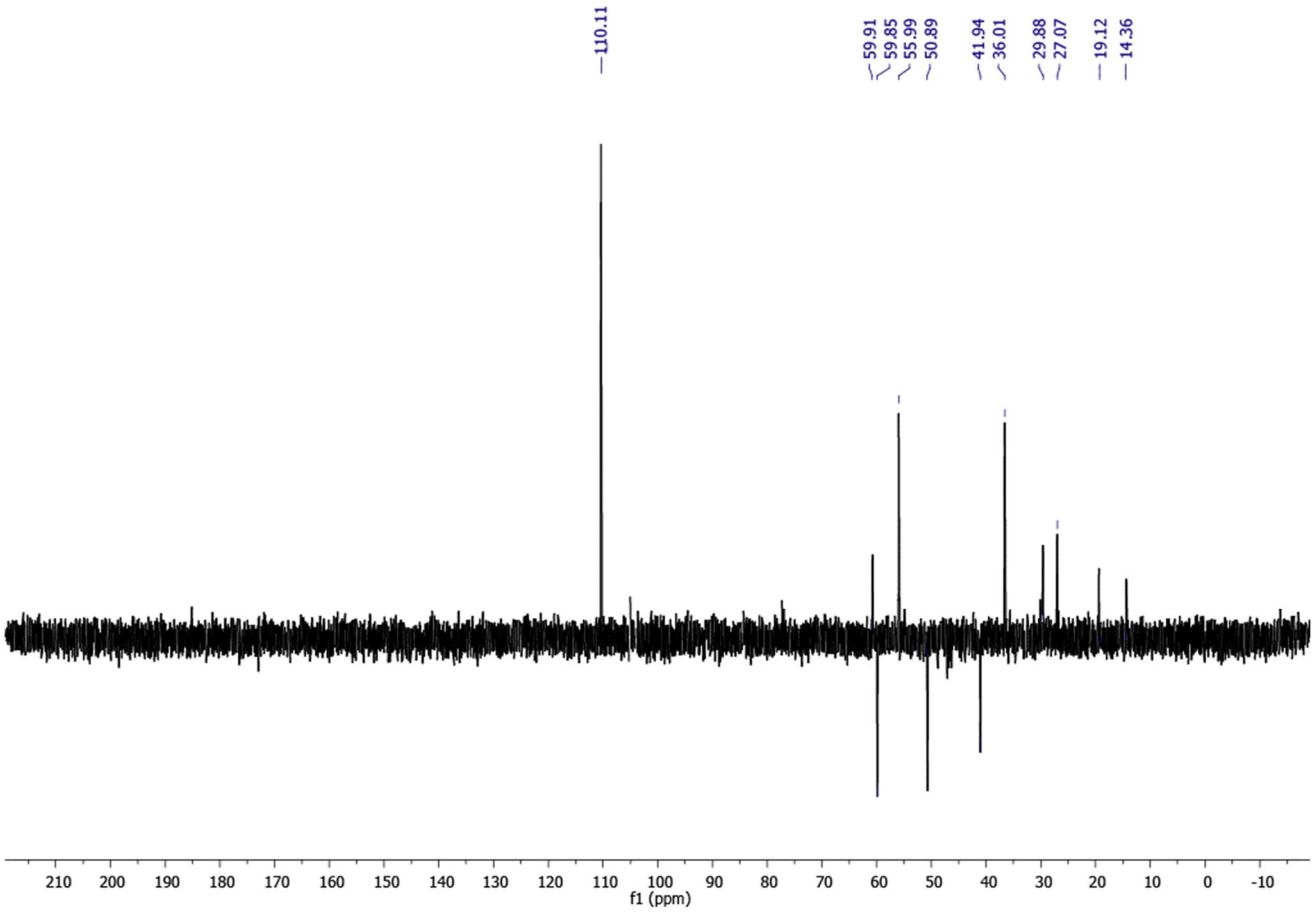


Figure S69. DEPT 135 spectrum of compound **14** ($CDCl_3$, 100 MHz, TMS).

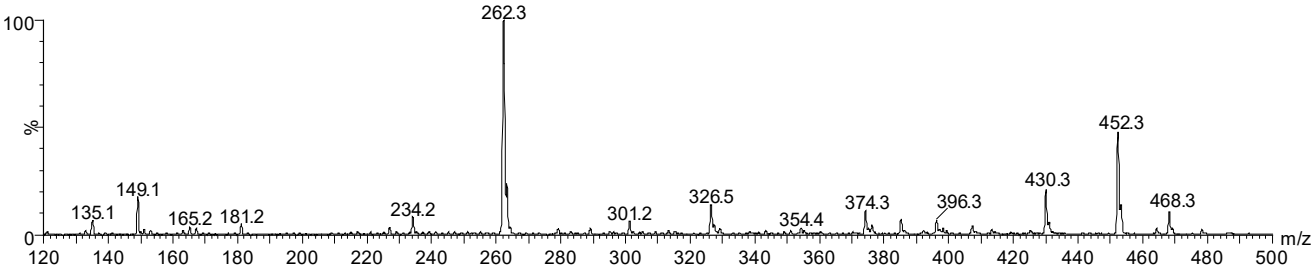


Figure S70. ESI (+) mass spectrum of compound **14.**

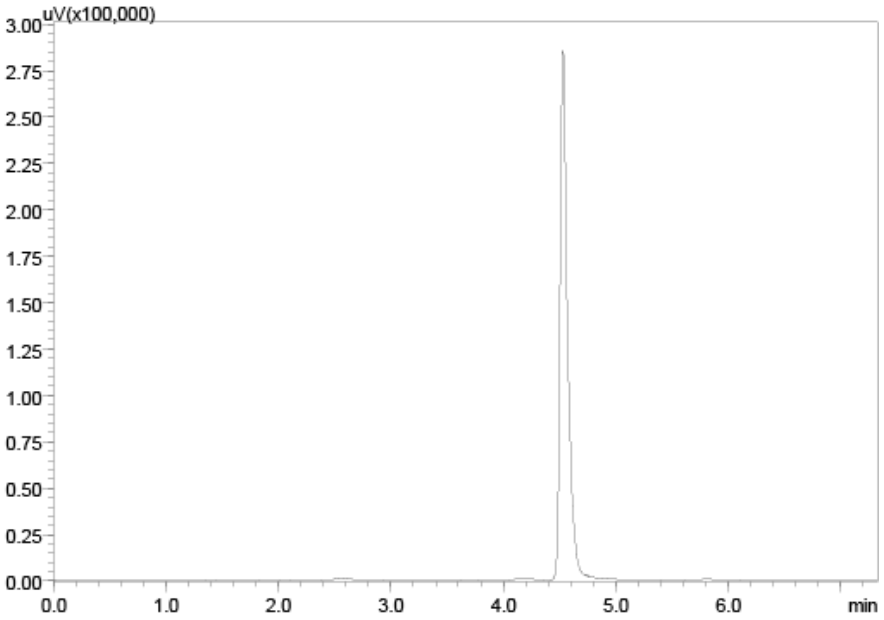


Figure S71: HPLC chromatogram of compound **15**.

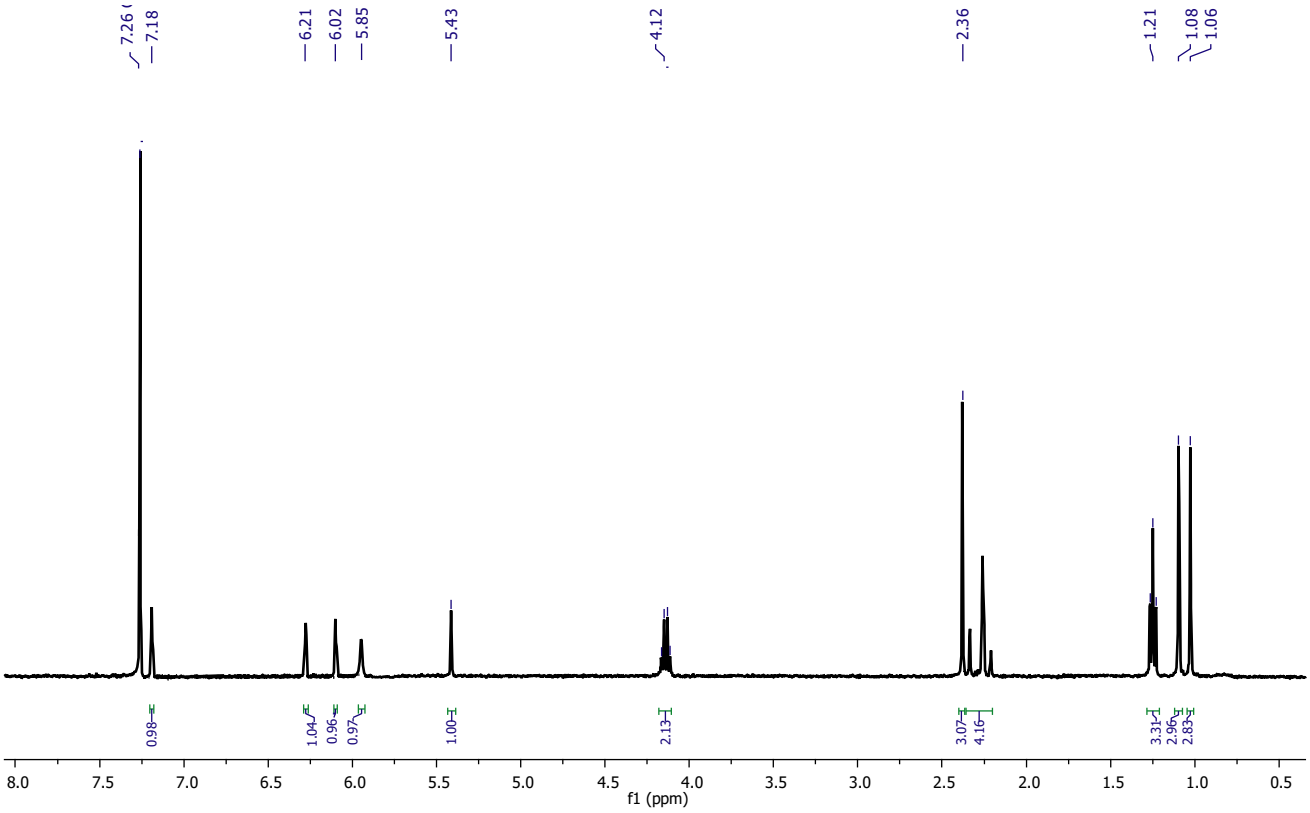


Figure S72.^{1}H NMR spectrum of compound **15** ($CDCl_3$, 400 MHz, TMS).

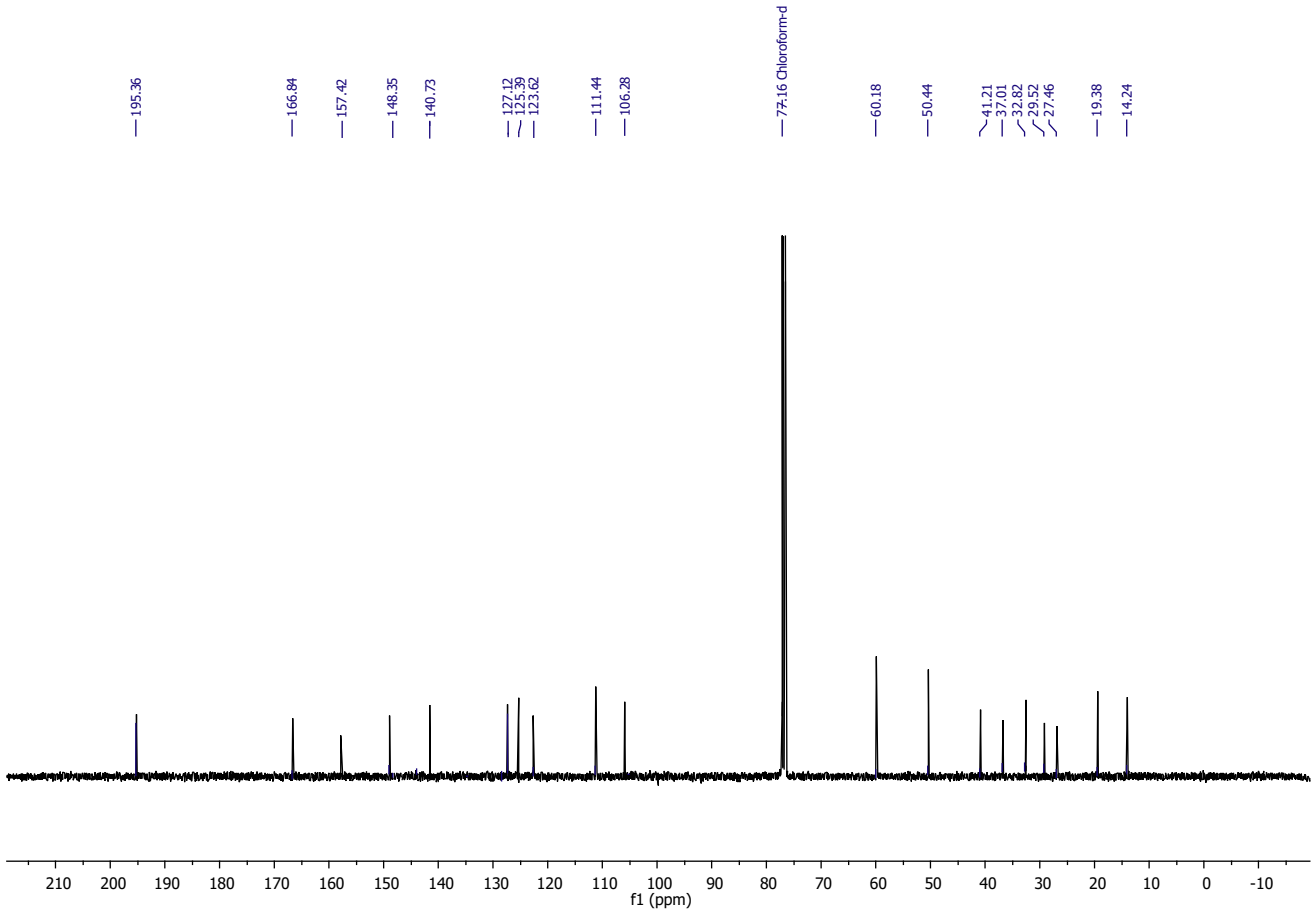


Figure S73.^{13}C NMR spectrum of compound **15**($CDCl_3$, 100 MHz, TMS).

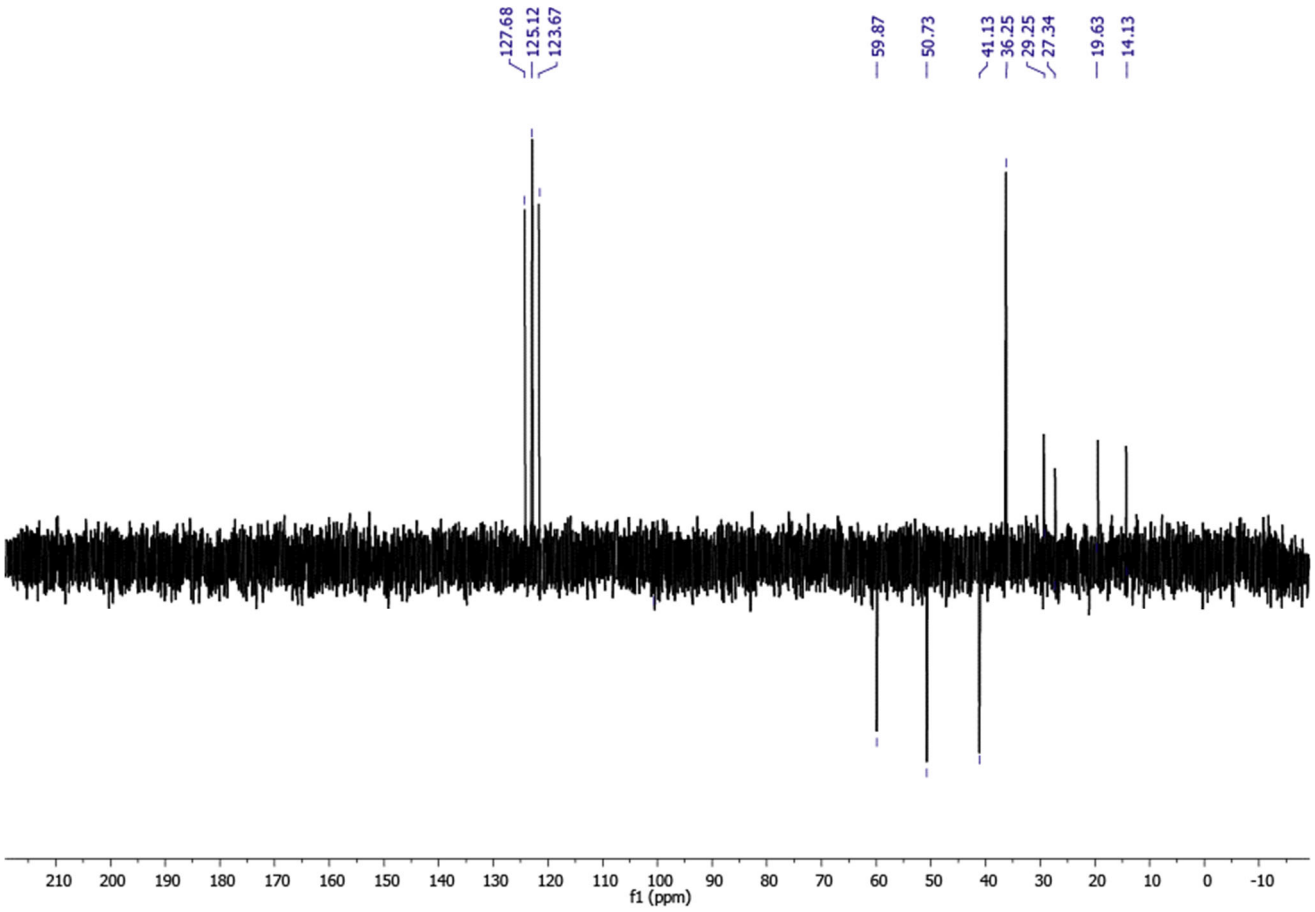


Figure S74. DEPT 135 spectrum of compound **15** ($CDCl_3$, 100 MHz, TMS).

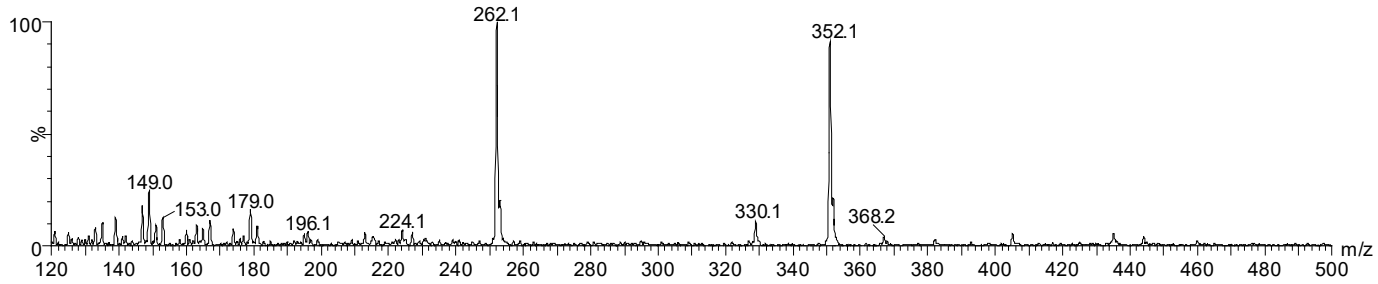


Figure S75. ESI (+) mass spectrum of compound **15.**

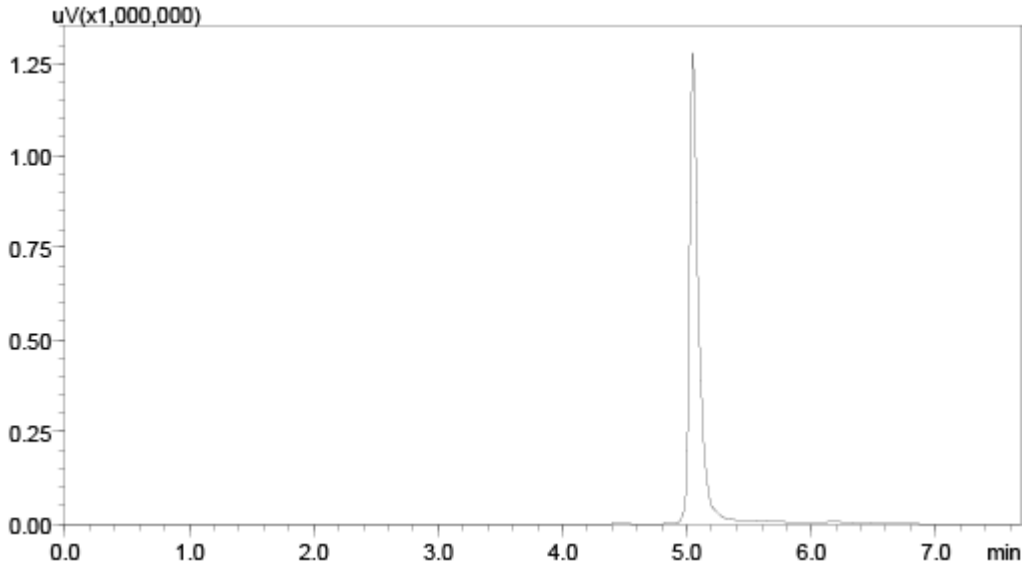


Figure S76: HPLC chromatogram of compound **16**.

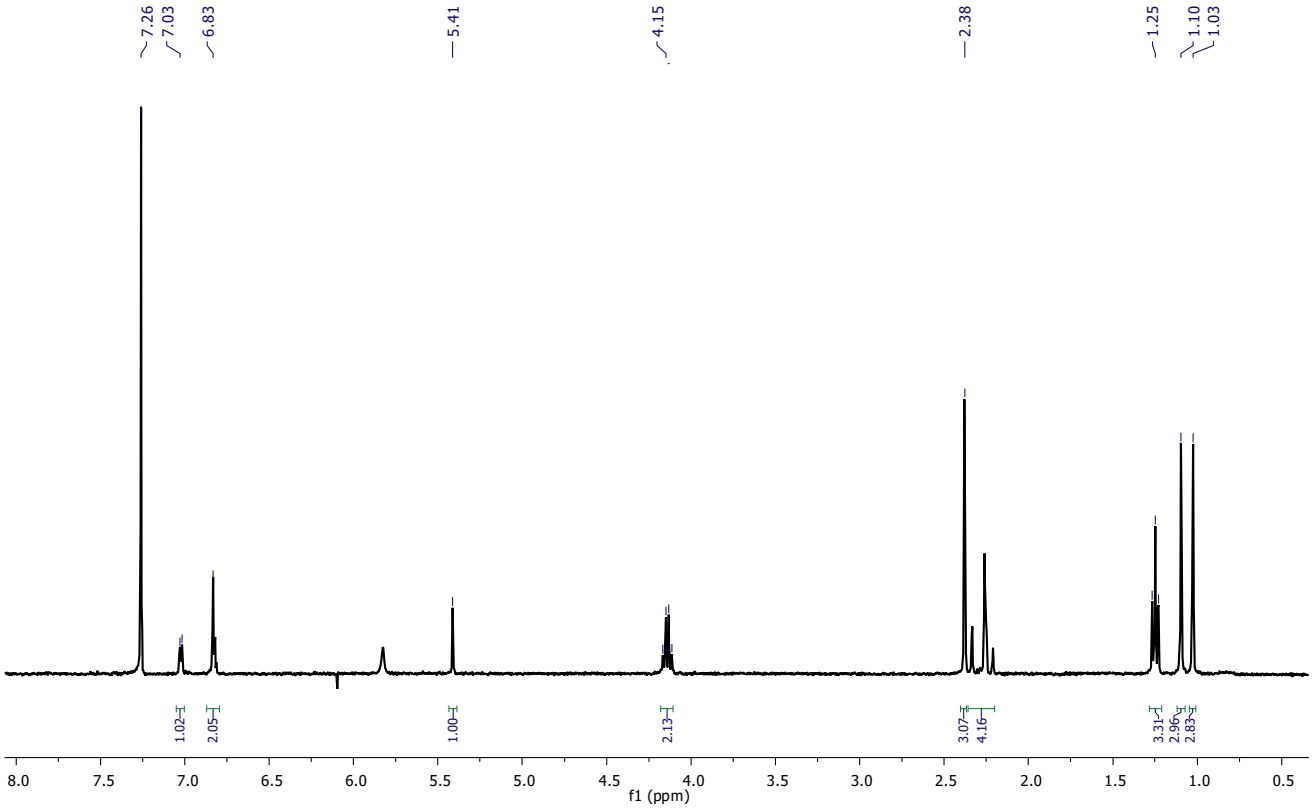


Figure S77.^{1}H NMR spectrum of compound **16** ($CDCl_3$, 400 MHz, TMS).

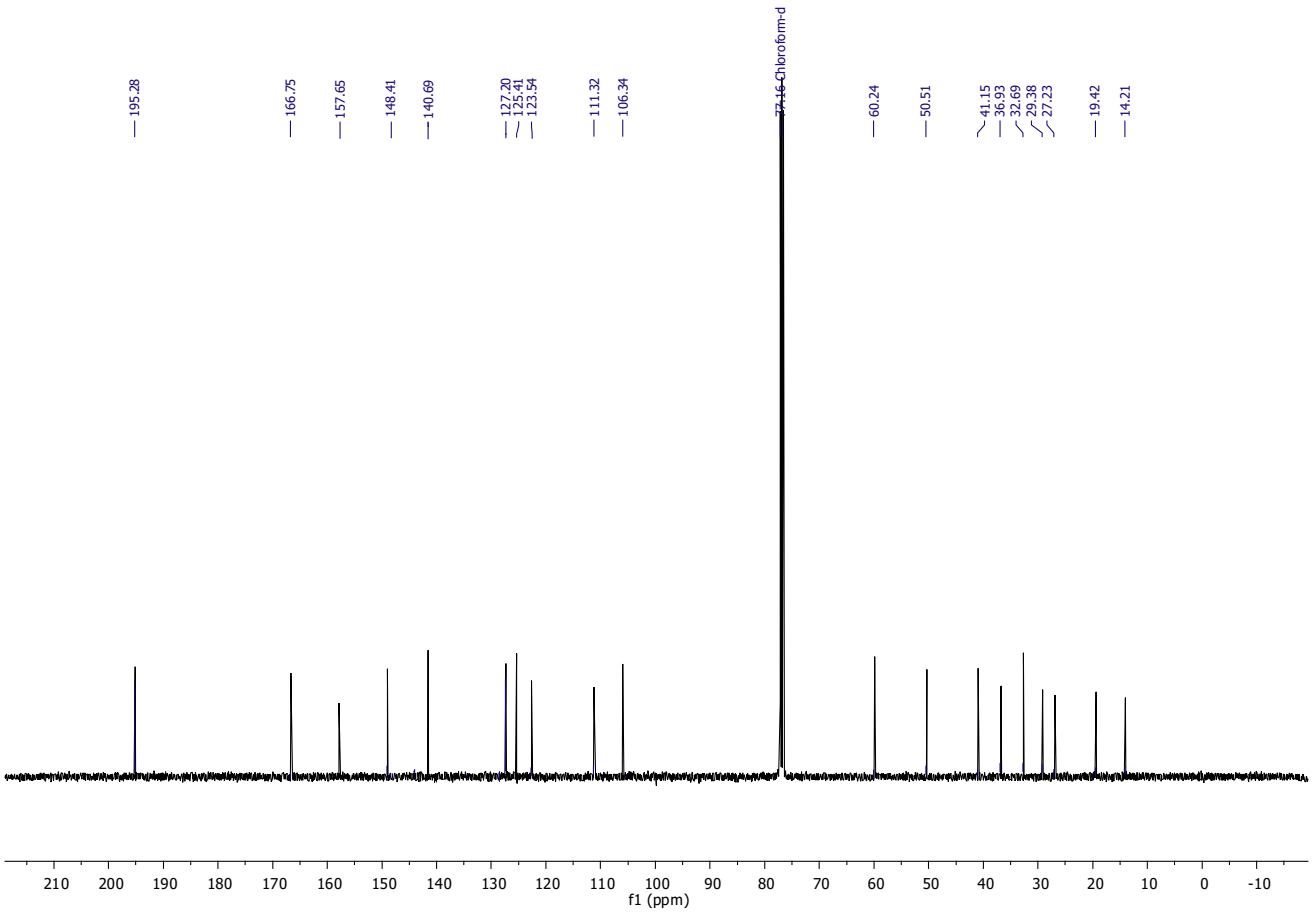


Figure S78.^{13}C NMR spectrum of compound **16** ($CDCl_3$, 100 MHz, TMS).

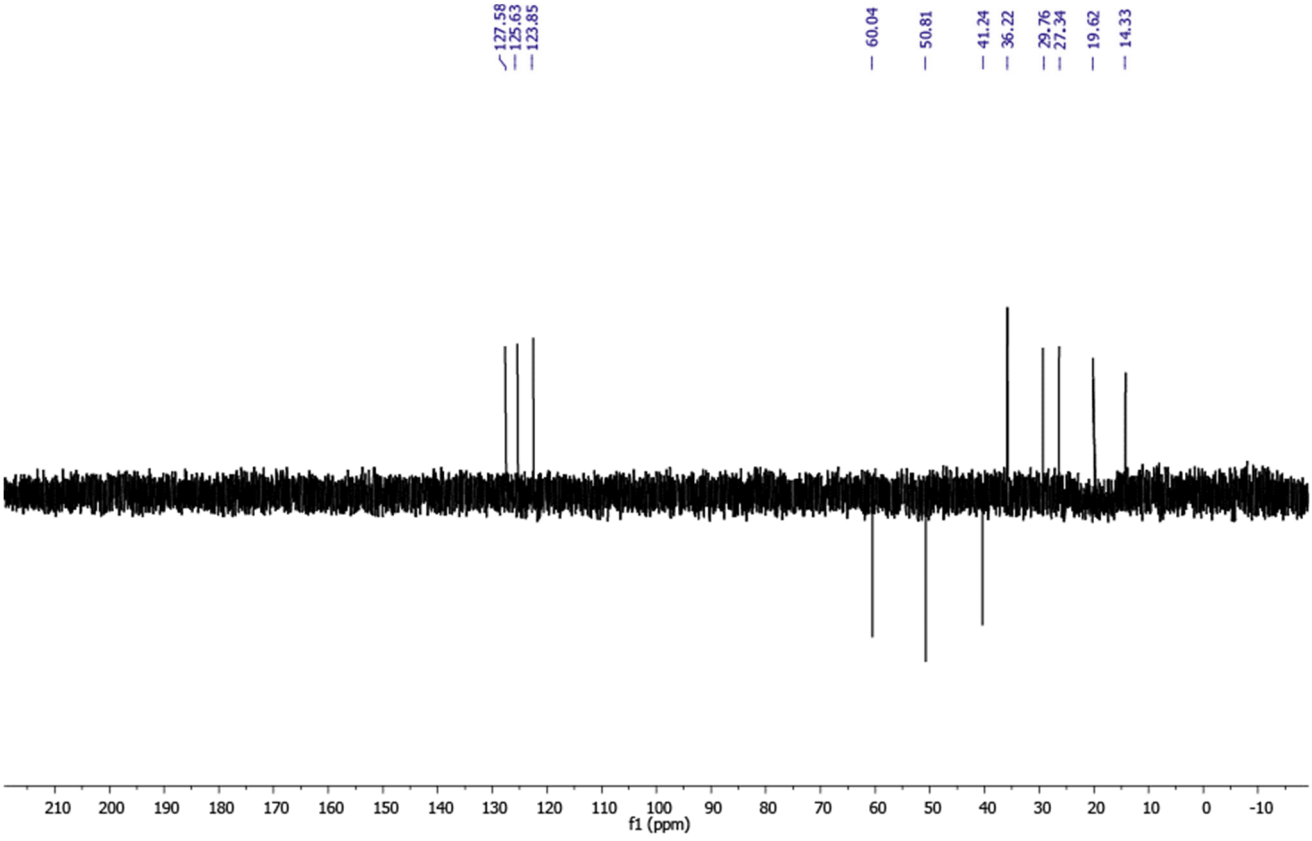


Figure S79. DEPT 135 spectrum of compound **16** ($CDCl_3$, 100 MHz, TMS).

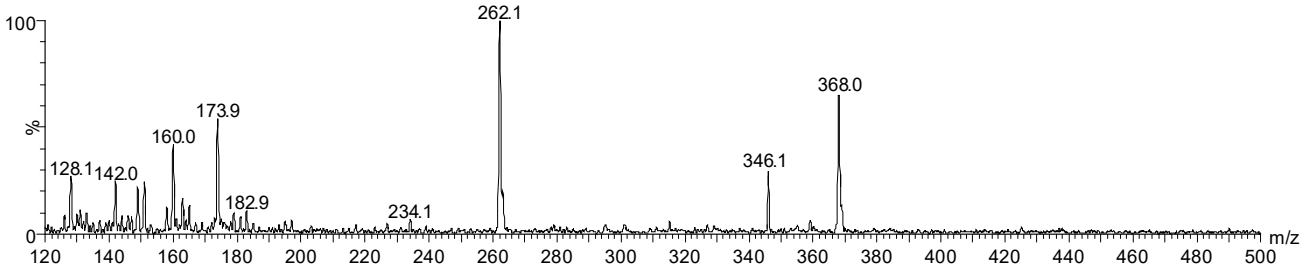


Figure S80. ESI (+) mass spectrum of compound **16.**

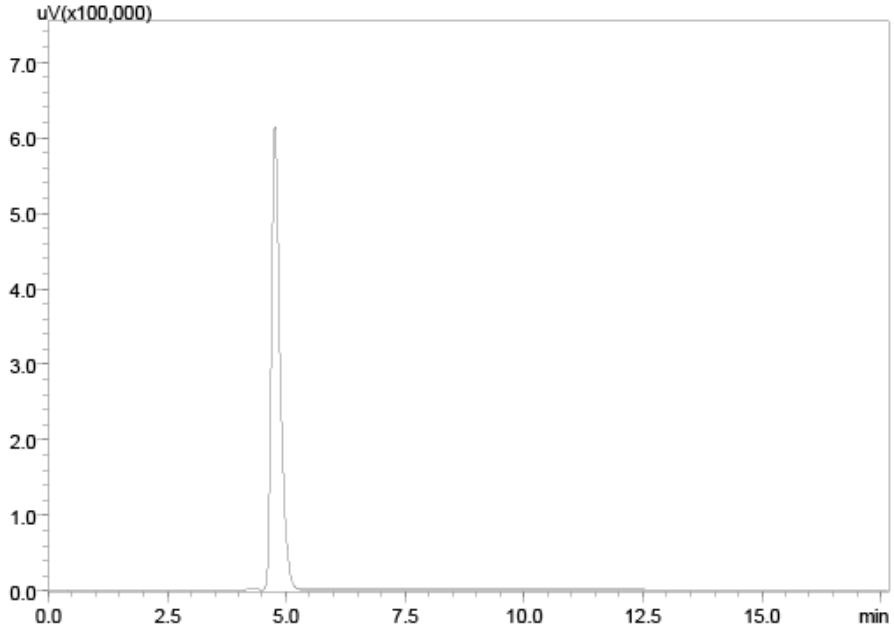


Figure S81: HPLC chromatogram of compound **17**

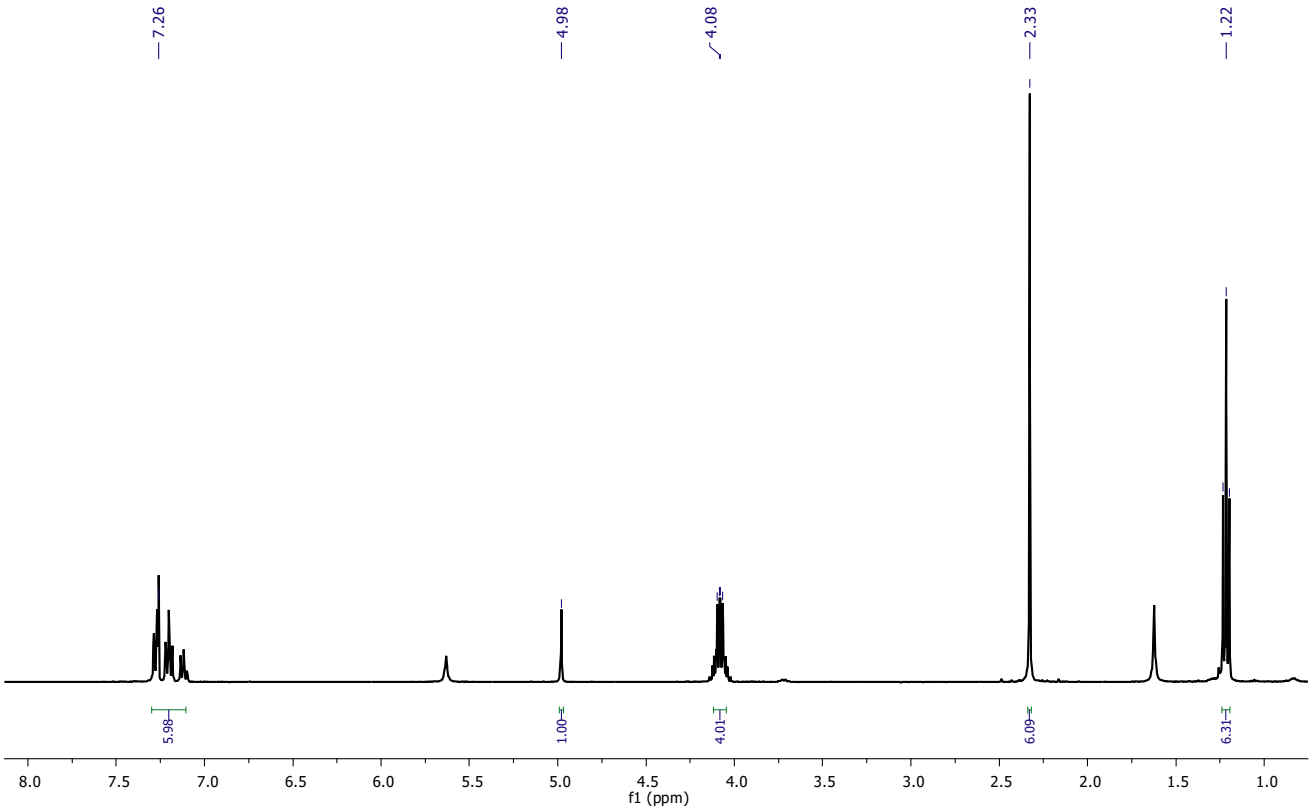


Figure S82.^{1}H NMR spectrum of compound **17** ($CDCl_3$, 400 MHz, TMS).

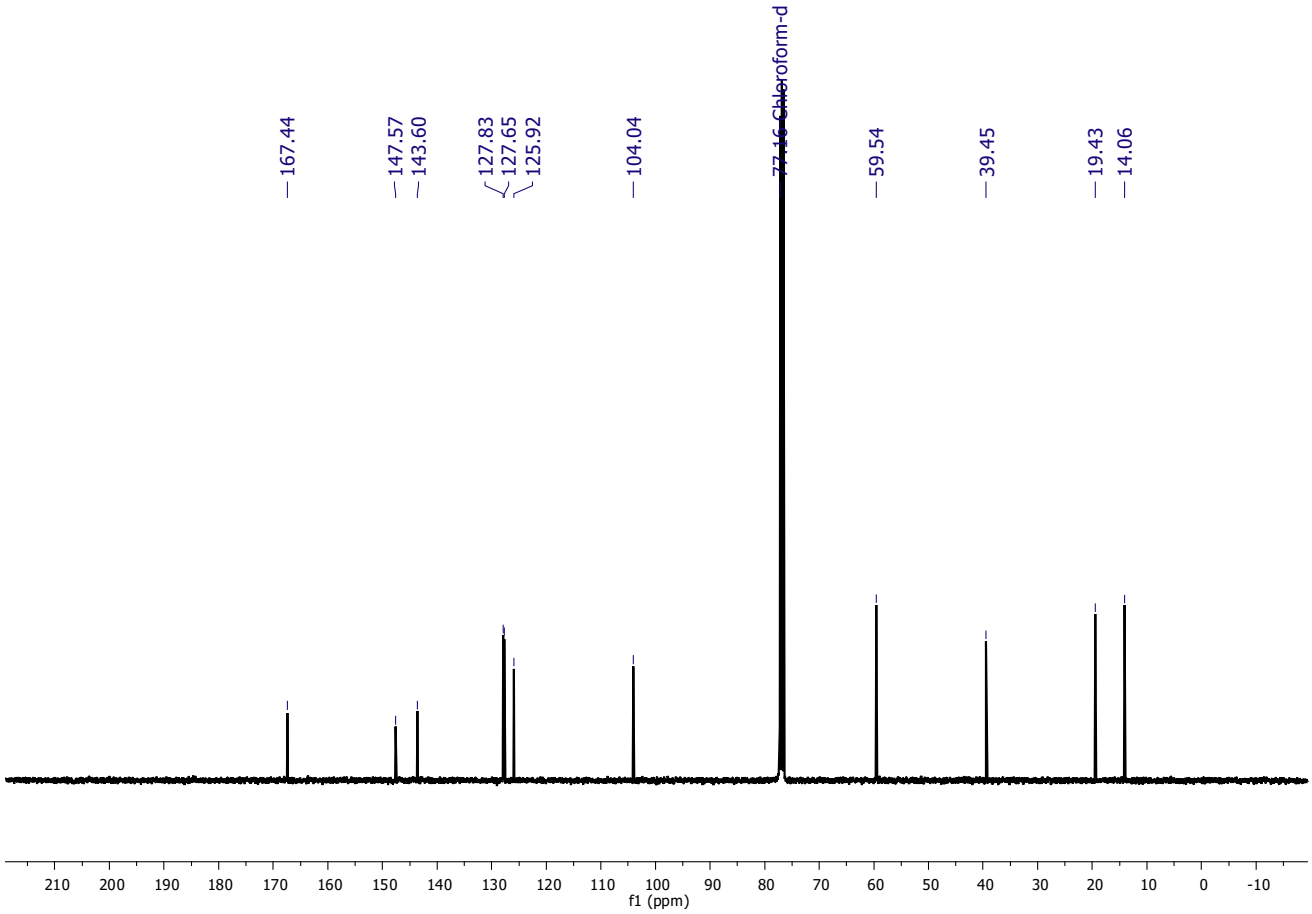


Figure S83.^{13}C NMR spectrum of compound **17** ($CDCl_3$, 100 MHz, TMS).

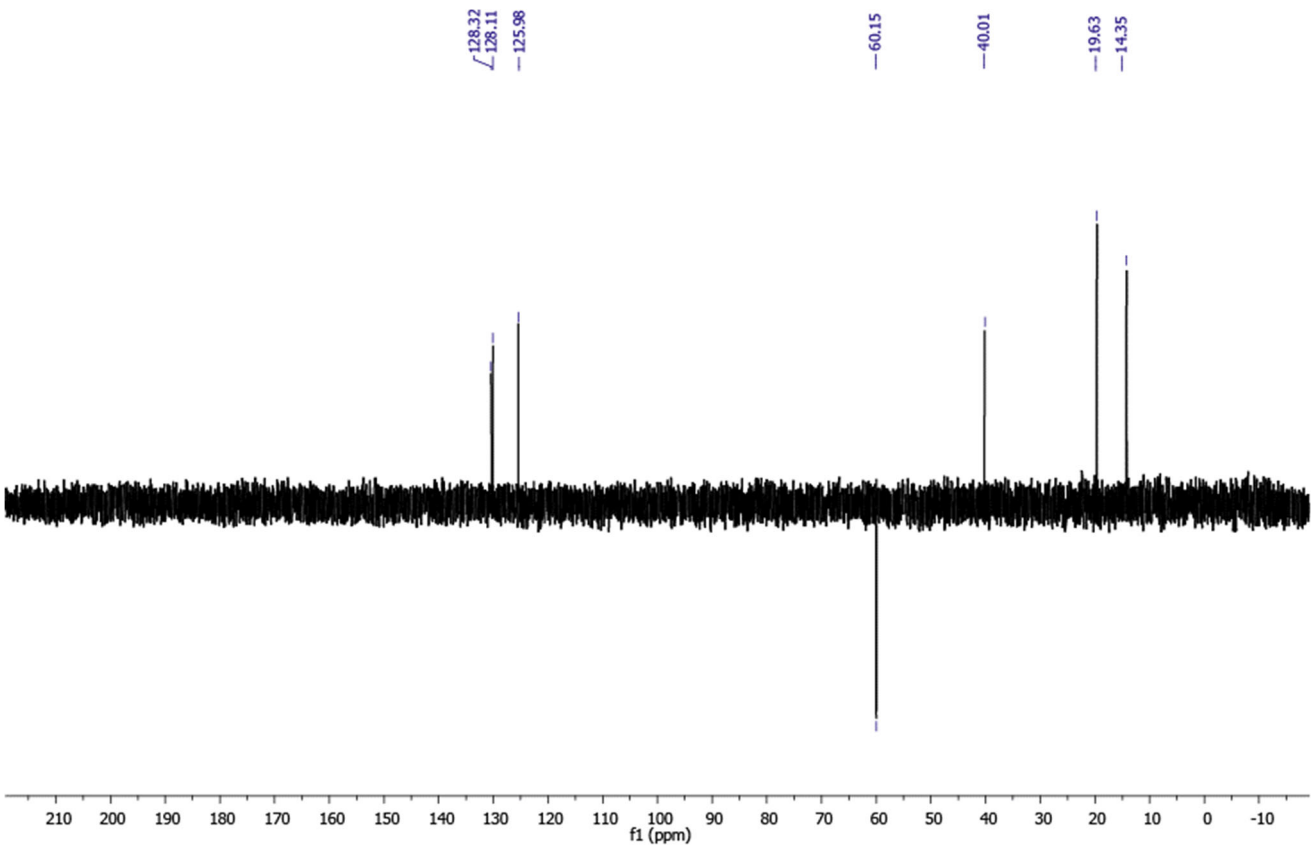


Figure S84. DEPT 135 spectrum of compound **17** ($CDCl_3$, 100 MHz, TMS).

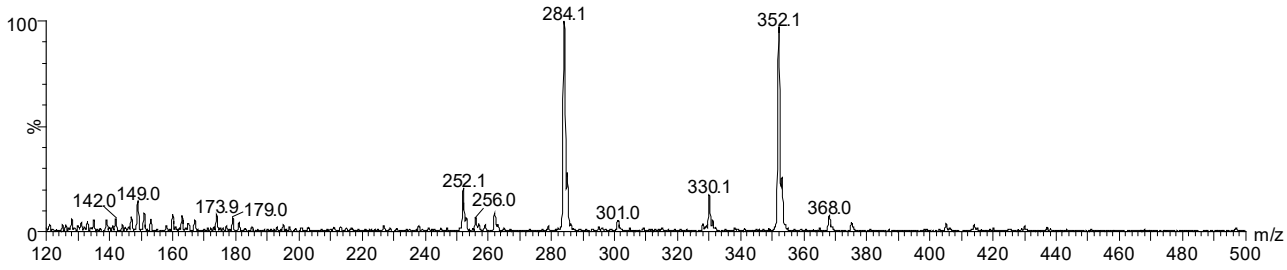


Figure S85. ESI (+) mass spectrum of compound **17.**

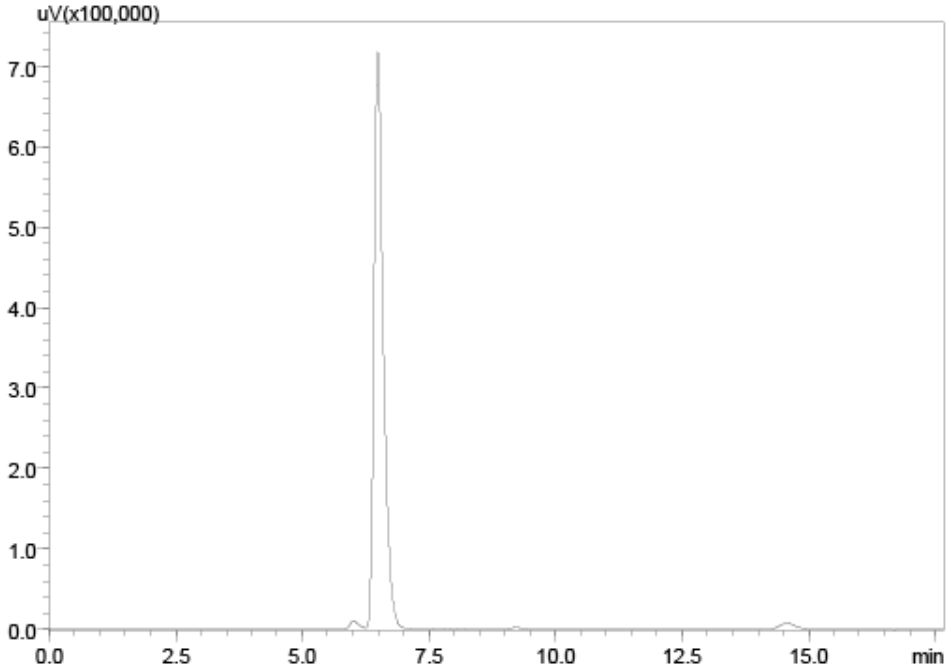


Figure S86: HPLC chromatogram of compound **18**.

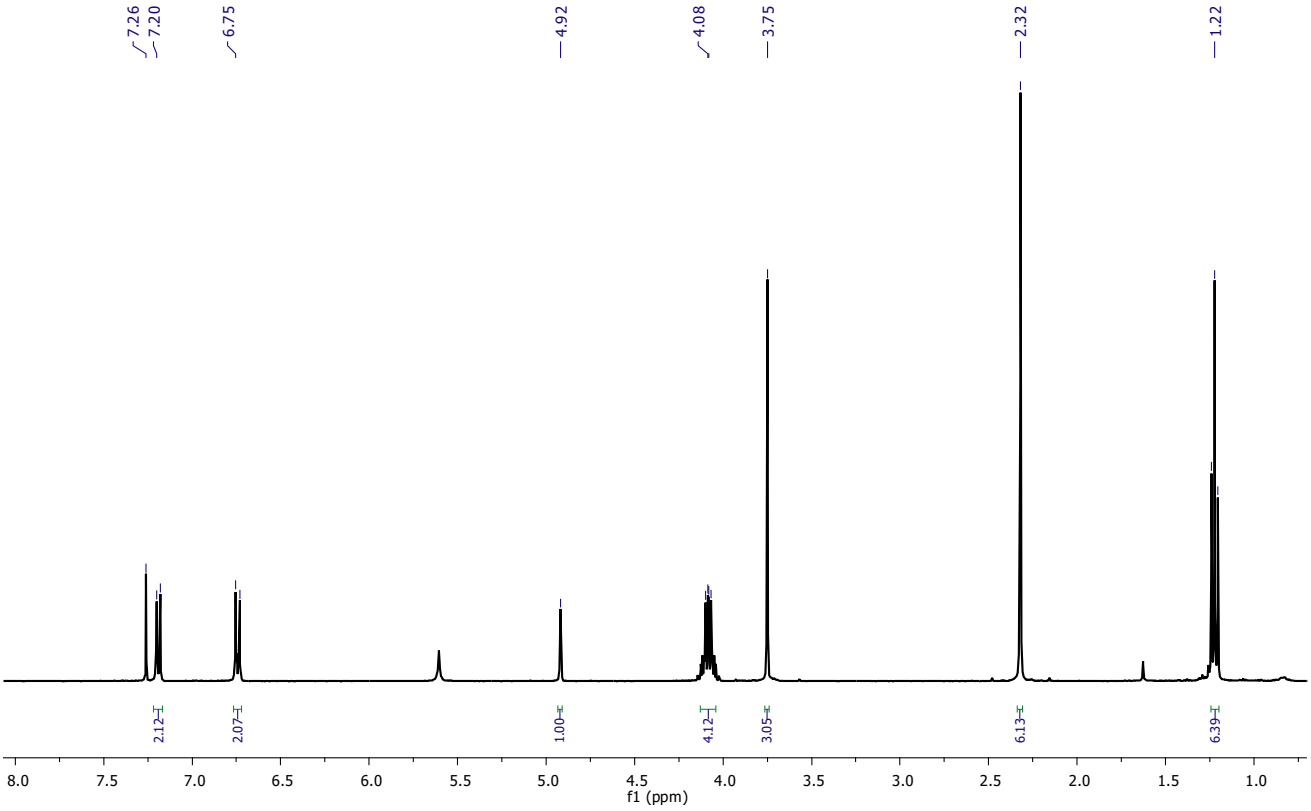


Figure S87.^{1}H NMR spectrum of compound **18** ($CDCl_3$, 400 MHz, TMS).

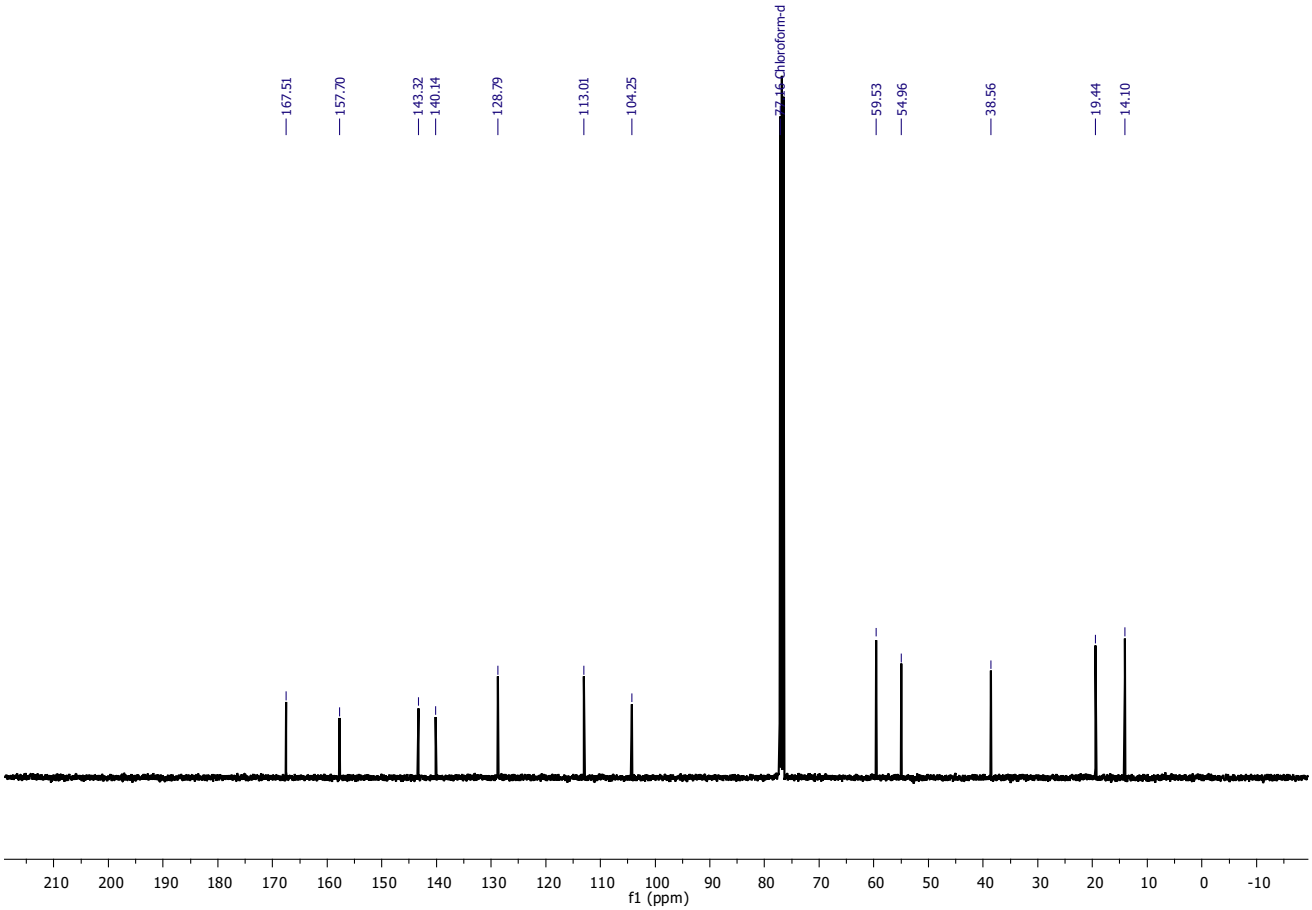


Figure S88.^{13}C NMR spectrum of compound **18** ($CDCl_3$, 100 MHz, TMS).

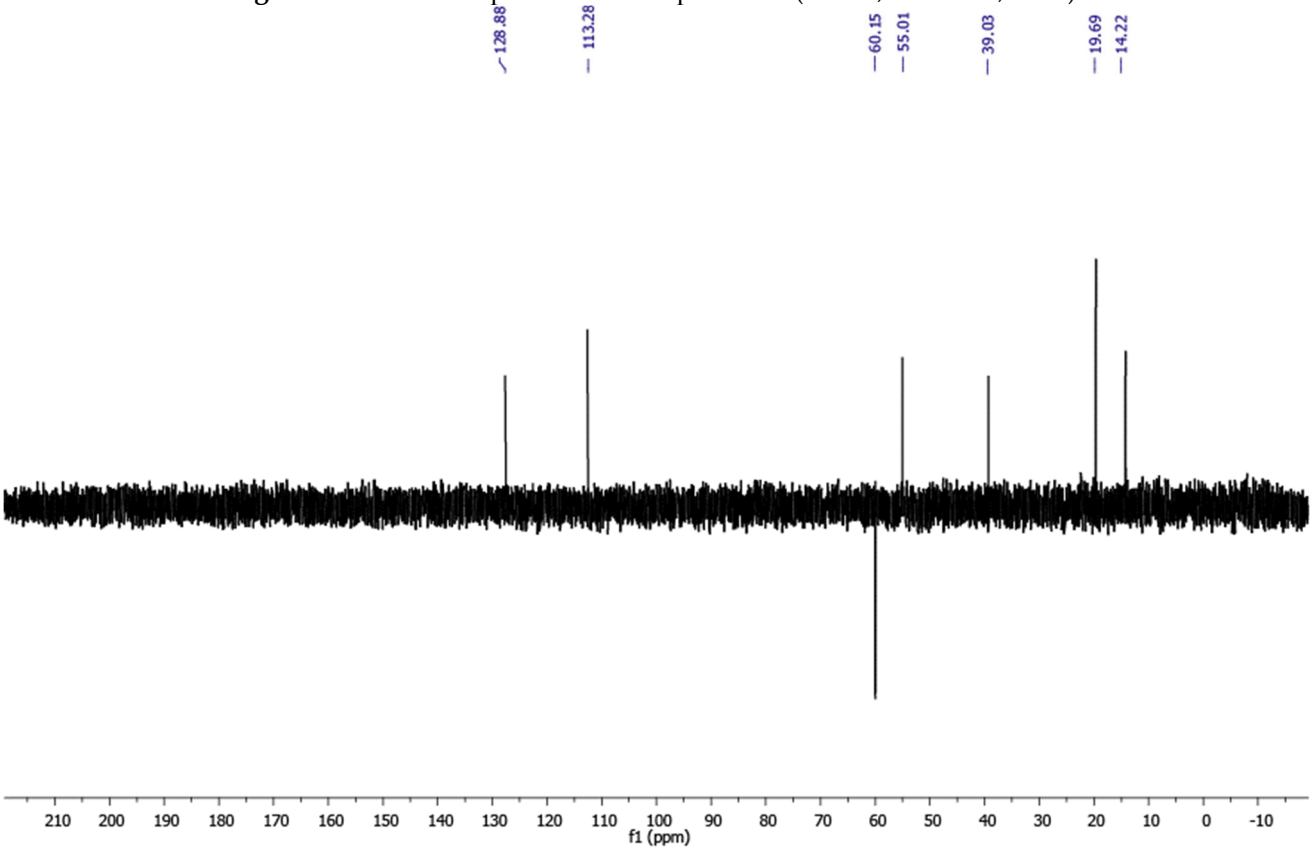


Figure S89. DEPT 135 spectrum of compound **18** ($CDCl_3$, 100 MHz, TMS).

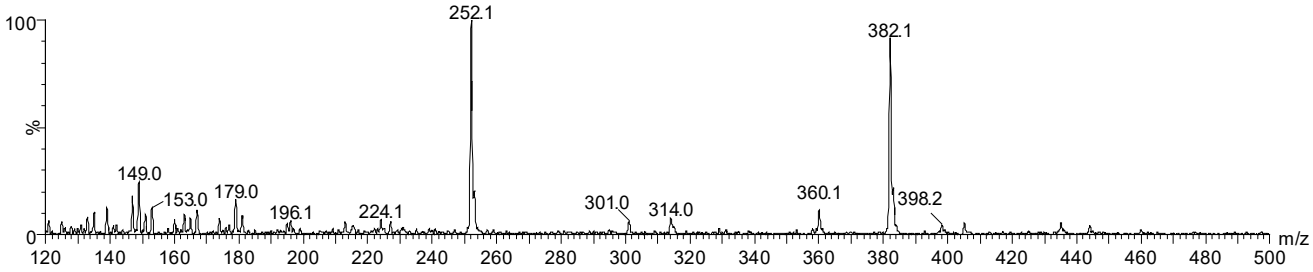


Figure S90. ESI (+) mass spectrum of compound **18.**

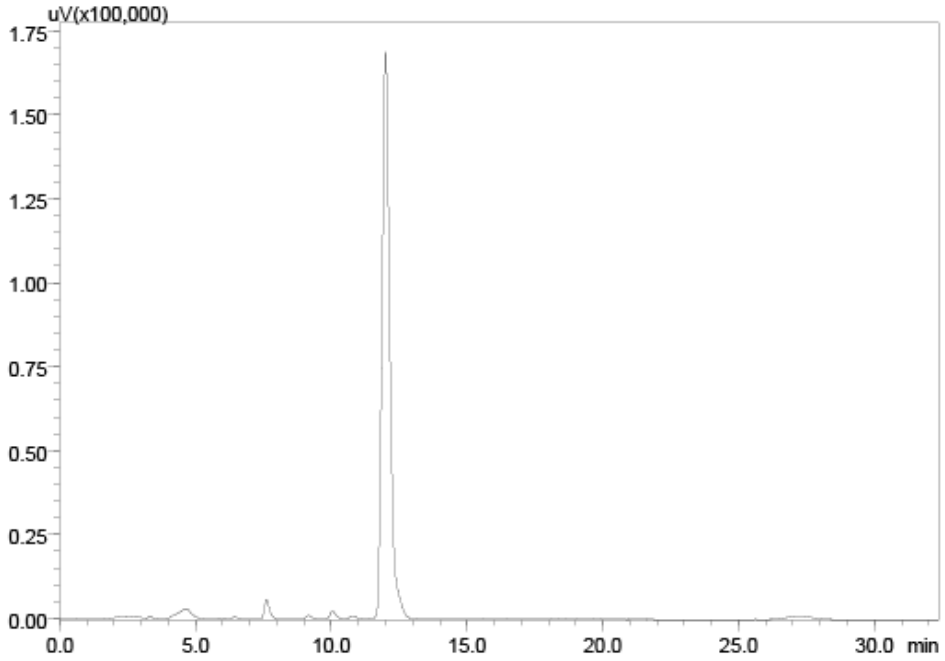


Figure S91: HPLC chromatogram of compound **19**.

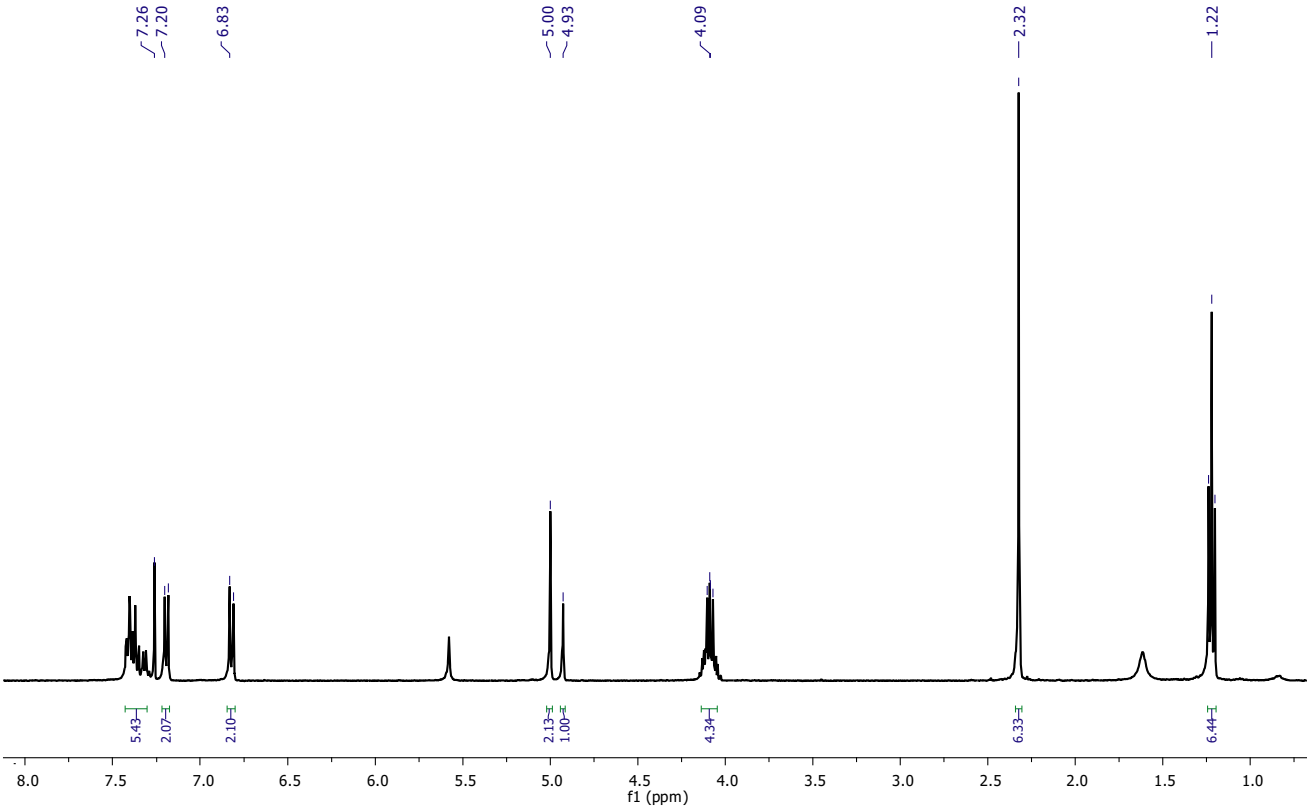


Figure S92.^{1}H NMR spectrum of compound **19** ($CDCl_3$, 400 MHz, TMS).

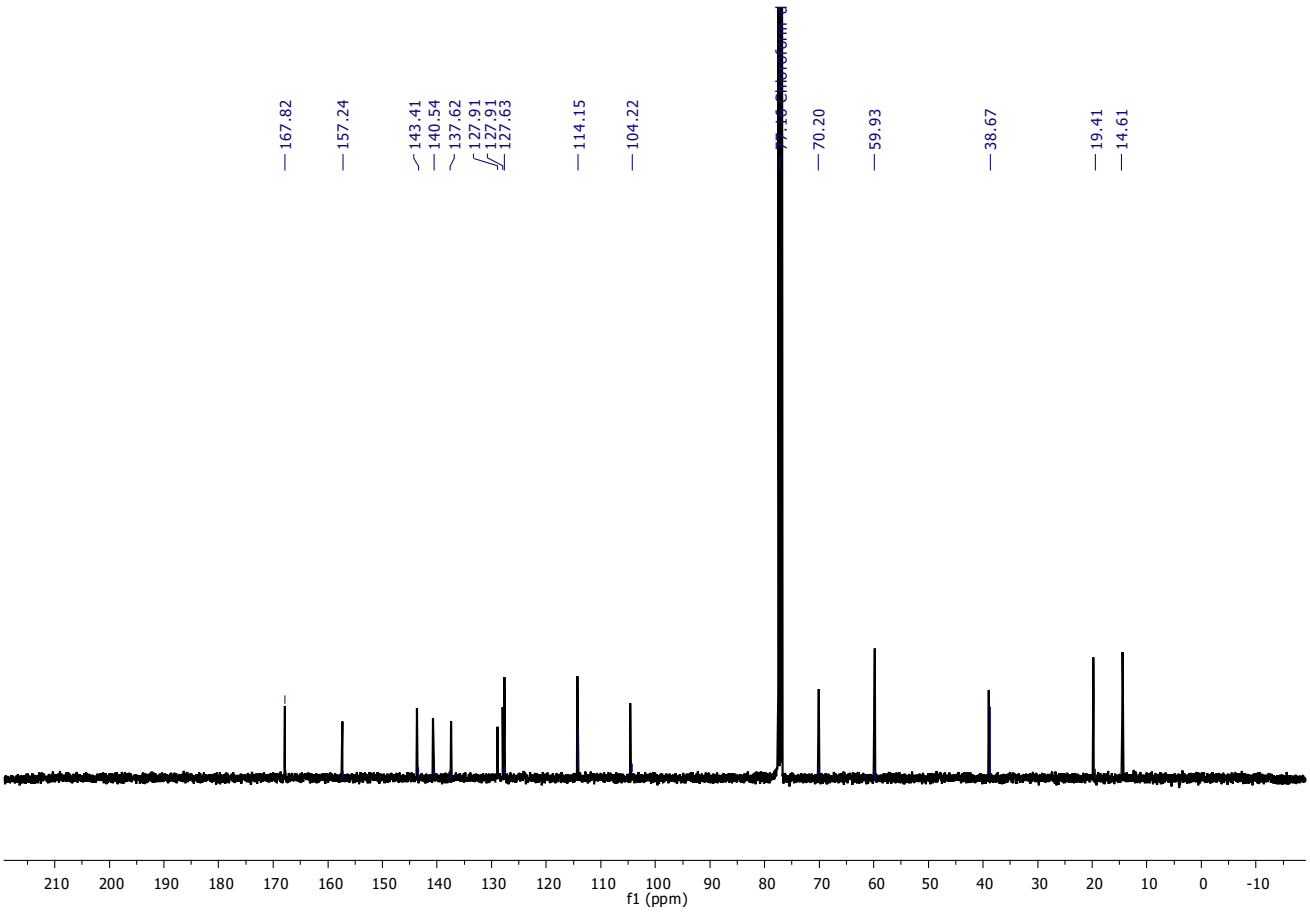


Figure S93.^{13}C NMR spectrum of compound **19** ($CDCl_3$, 100 MHz, TMS).

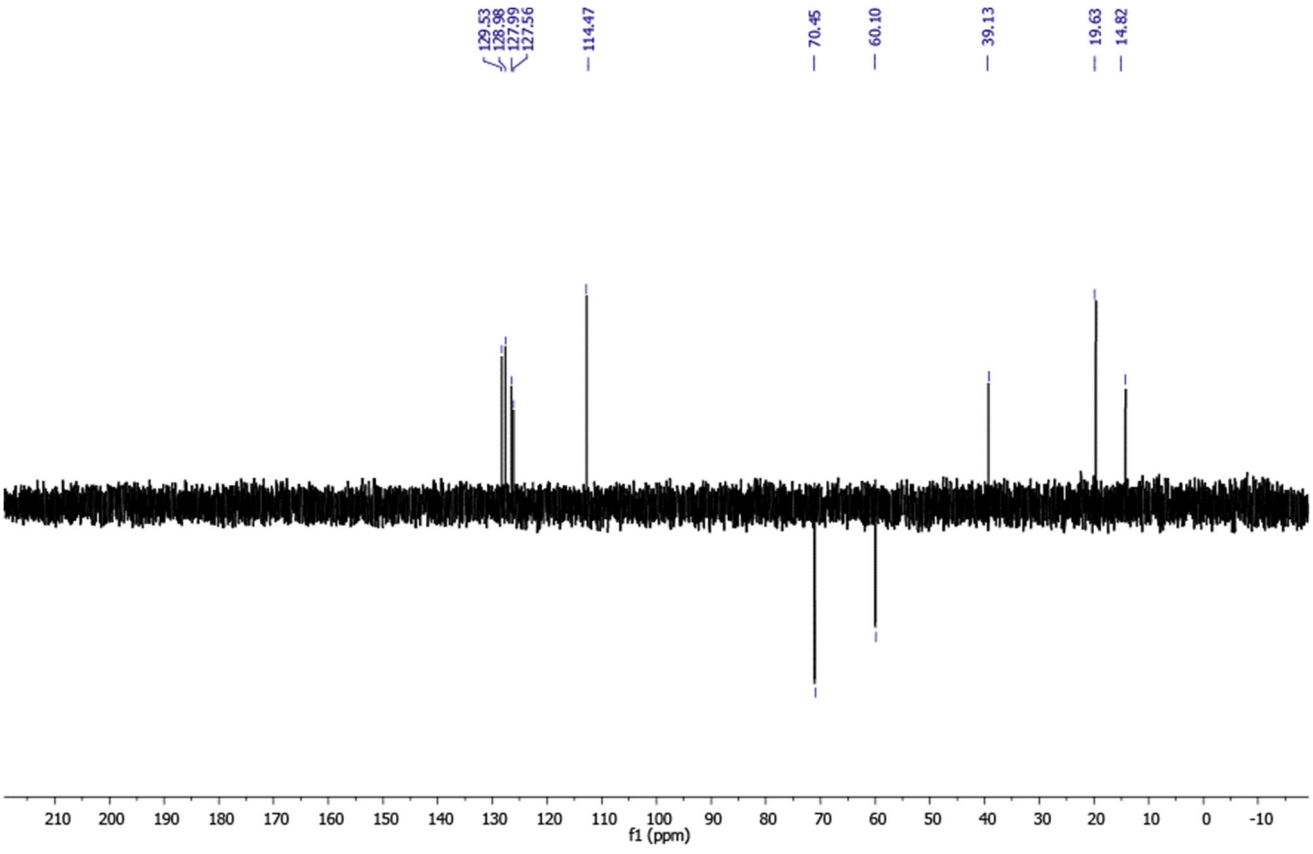


Figure S94. DEPT 135 spectrum of compound **19** ($CDCl_3$, 100 MHz, TMS).

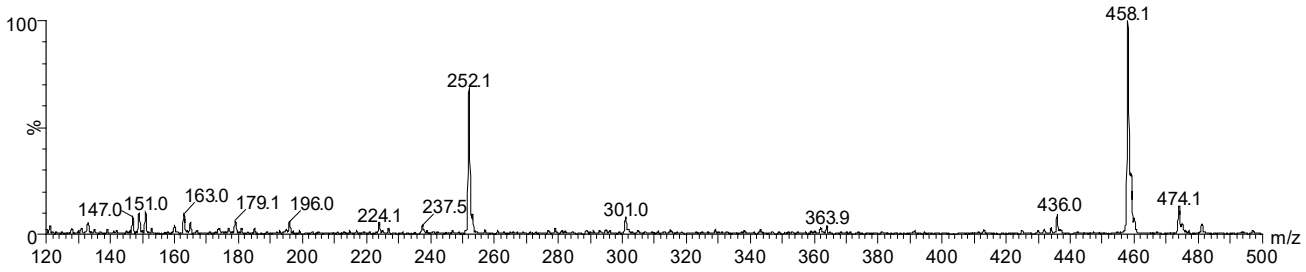


Figure S95. ESI (+) mass spectrum of compound **19.**

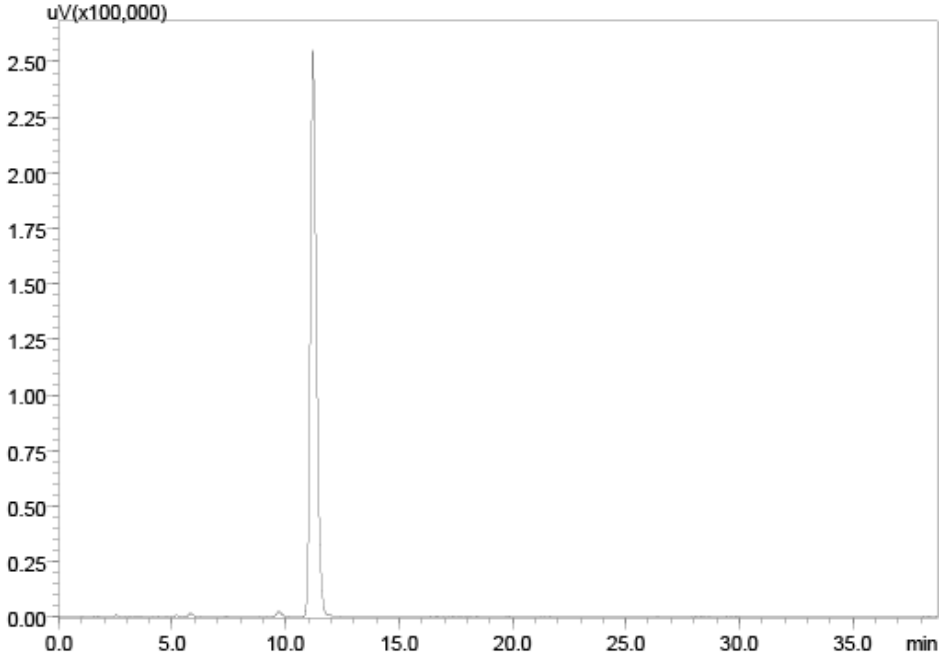


Figure S96: HPLC chromatogram of compound **20**.

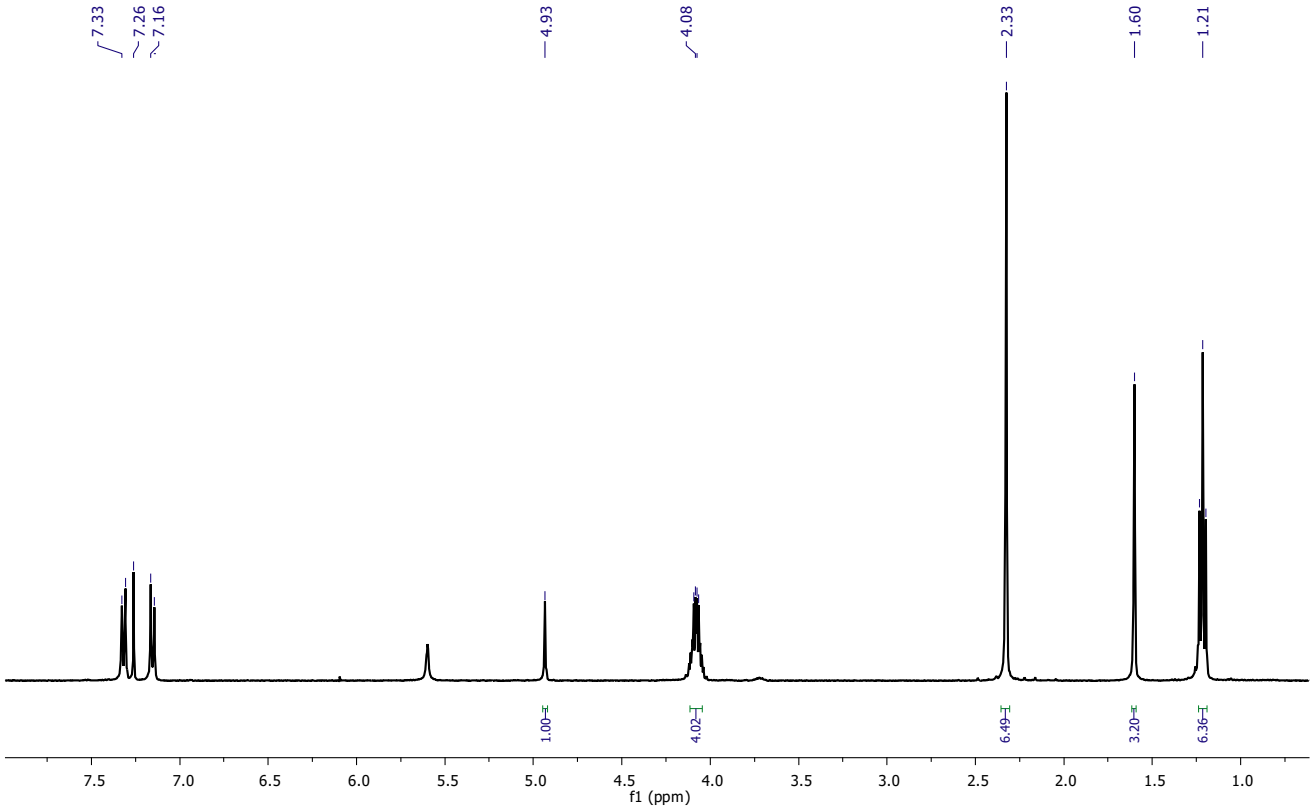


Figure S97.^{1}H NMR spectrum of compound **20** ($CDCl_3$, 400 MHz, TMS).

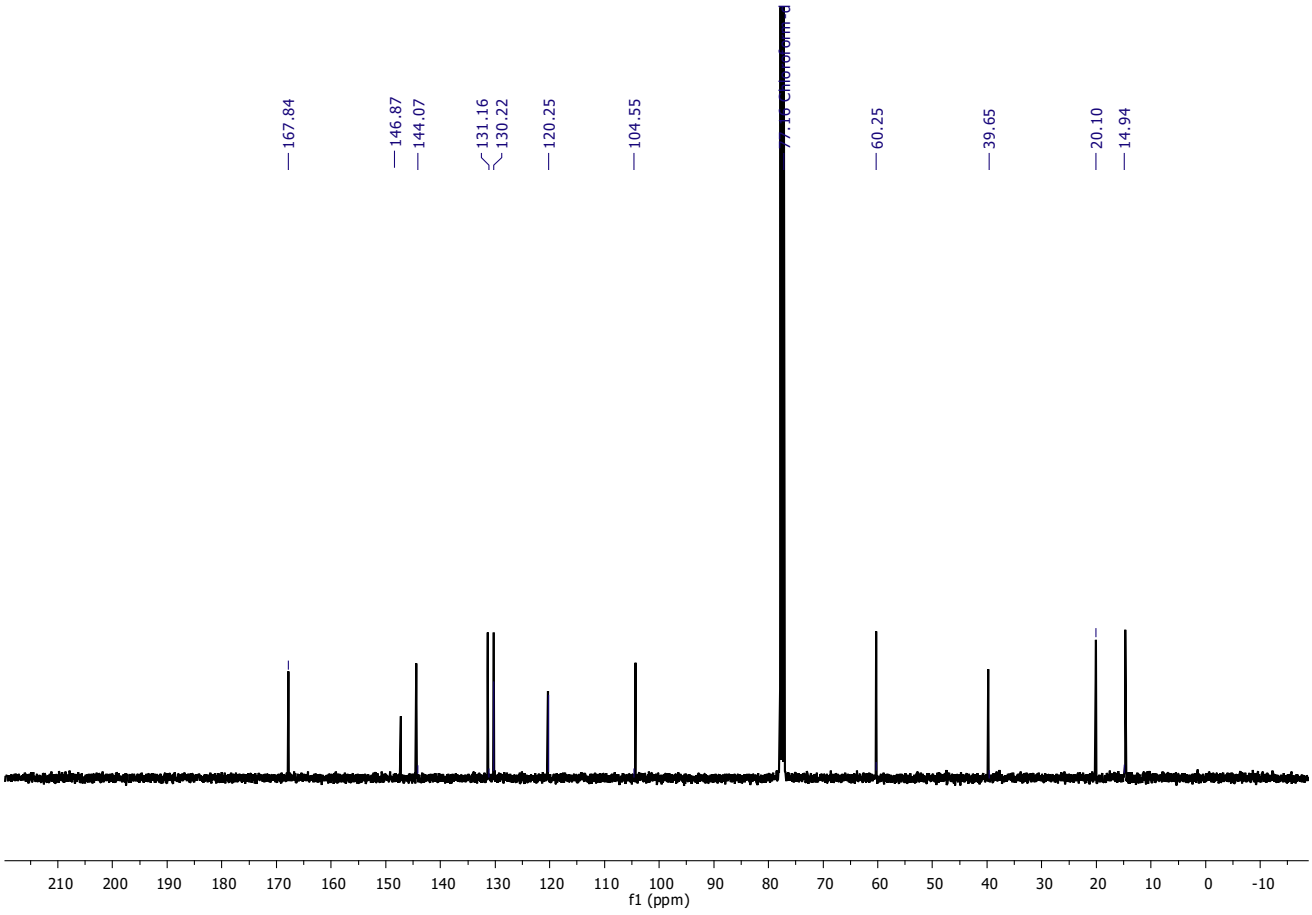


Figure S98.^{13}C NMR spectrum of compound **20** ($CDCl_3$, 100 MHz, TMS).

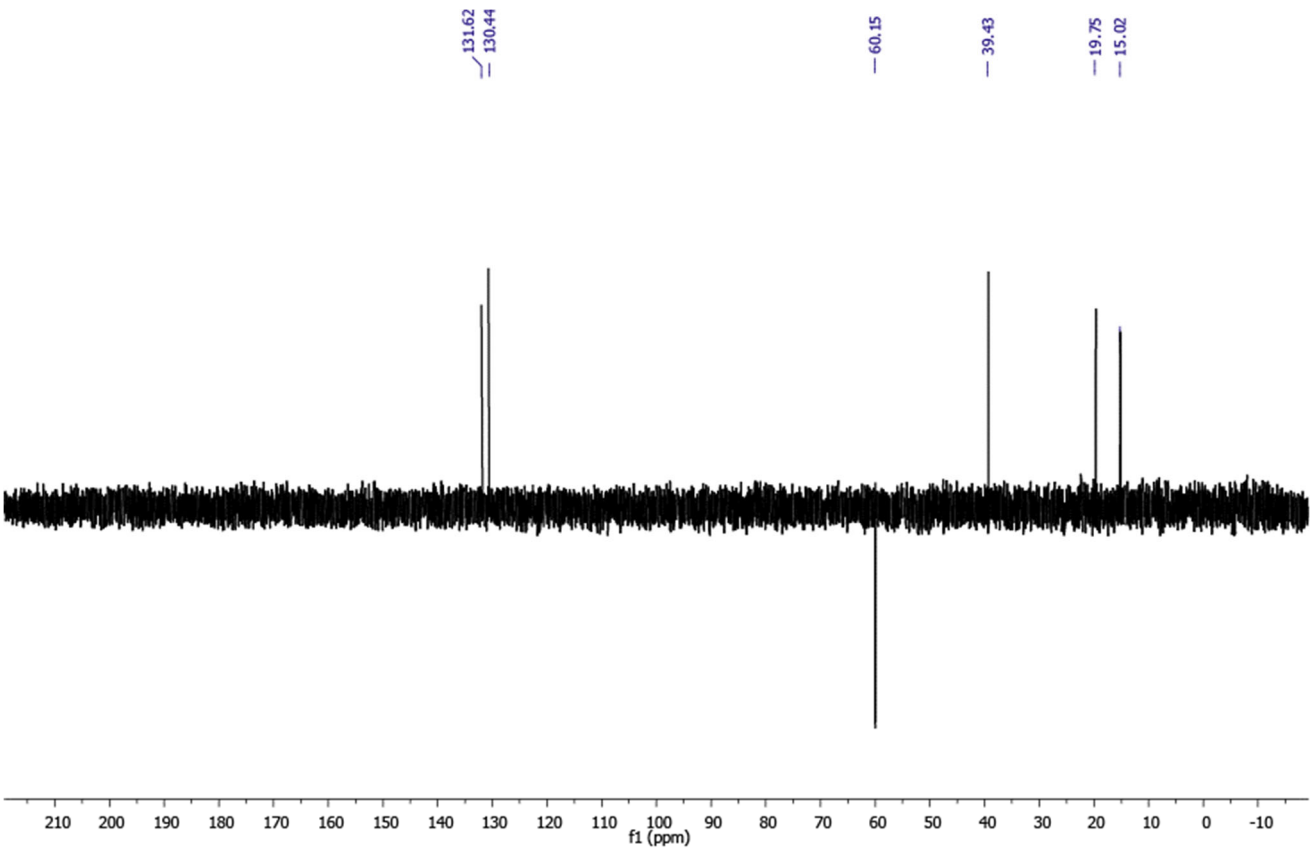


Figure S99. DEPT 135 spectrum of compound **20** ($CDCl_3$, 100 MHz, TMS).

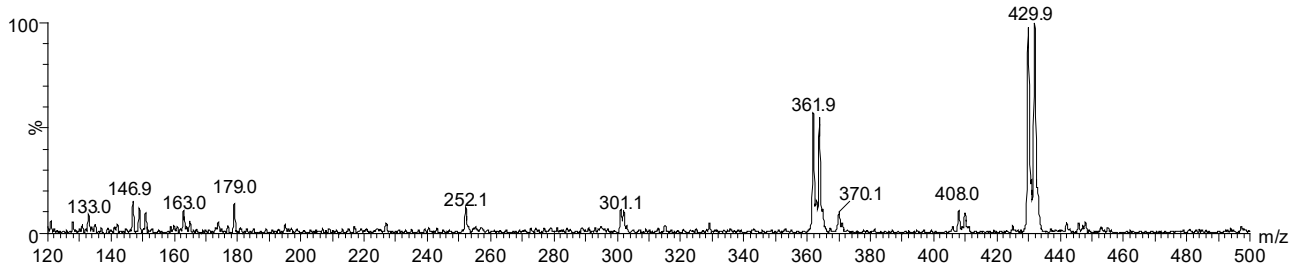


Figure S100. ESI (+) mass spectrum of compound **20.**

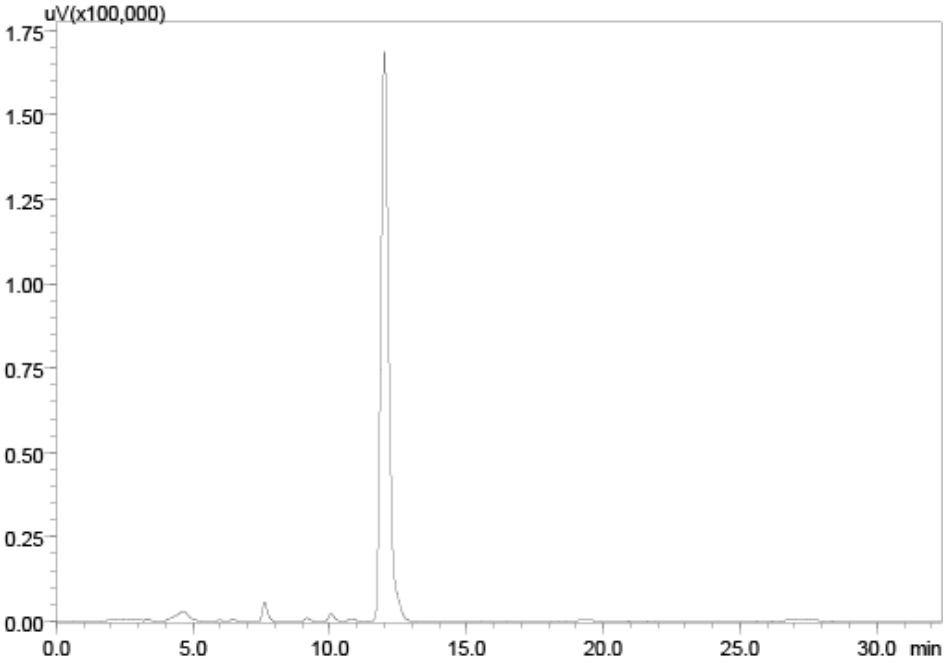


Figure S101: HPLC chromatogram of compound **21**.

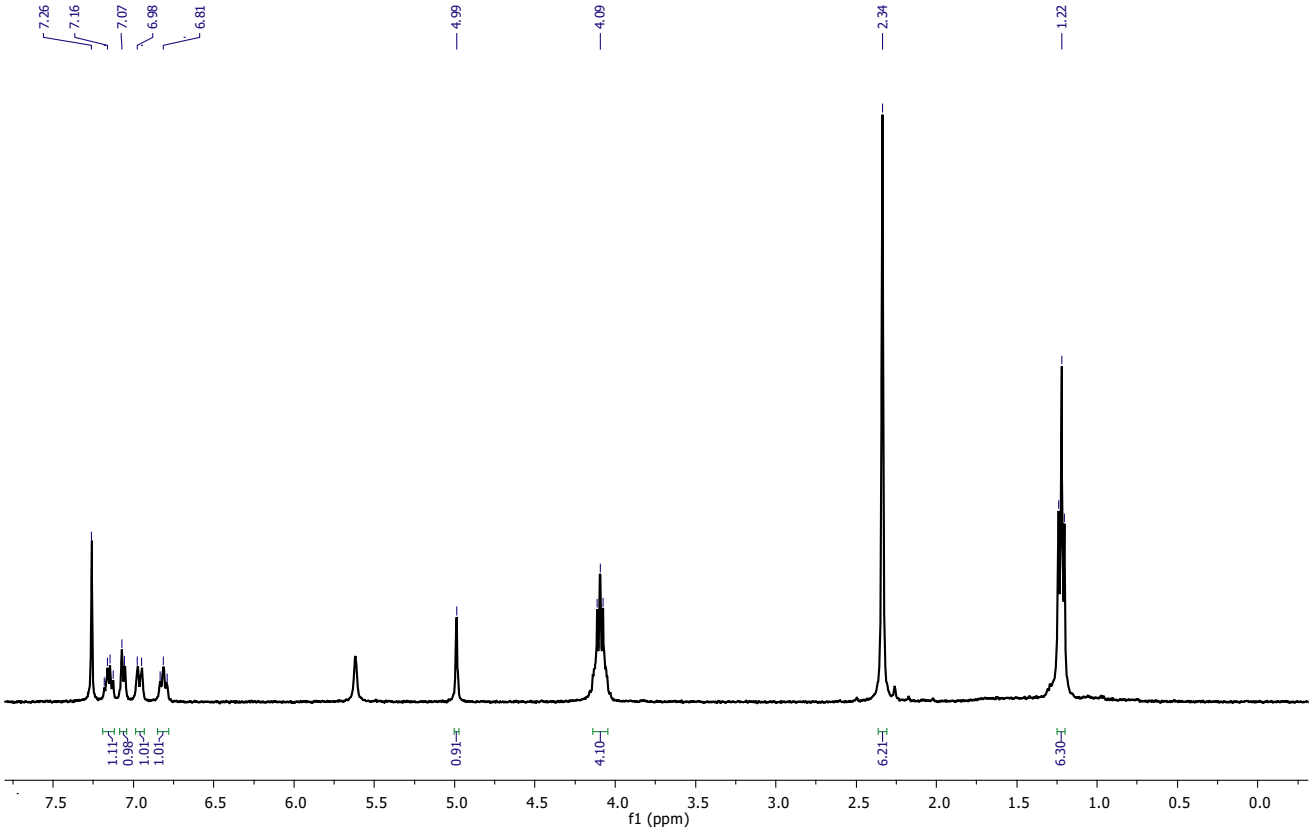


Figure S102.^{1}H NMR spectrum of compound **21** ($CDCl_3$, 400 MHz, TMS).

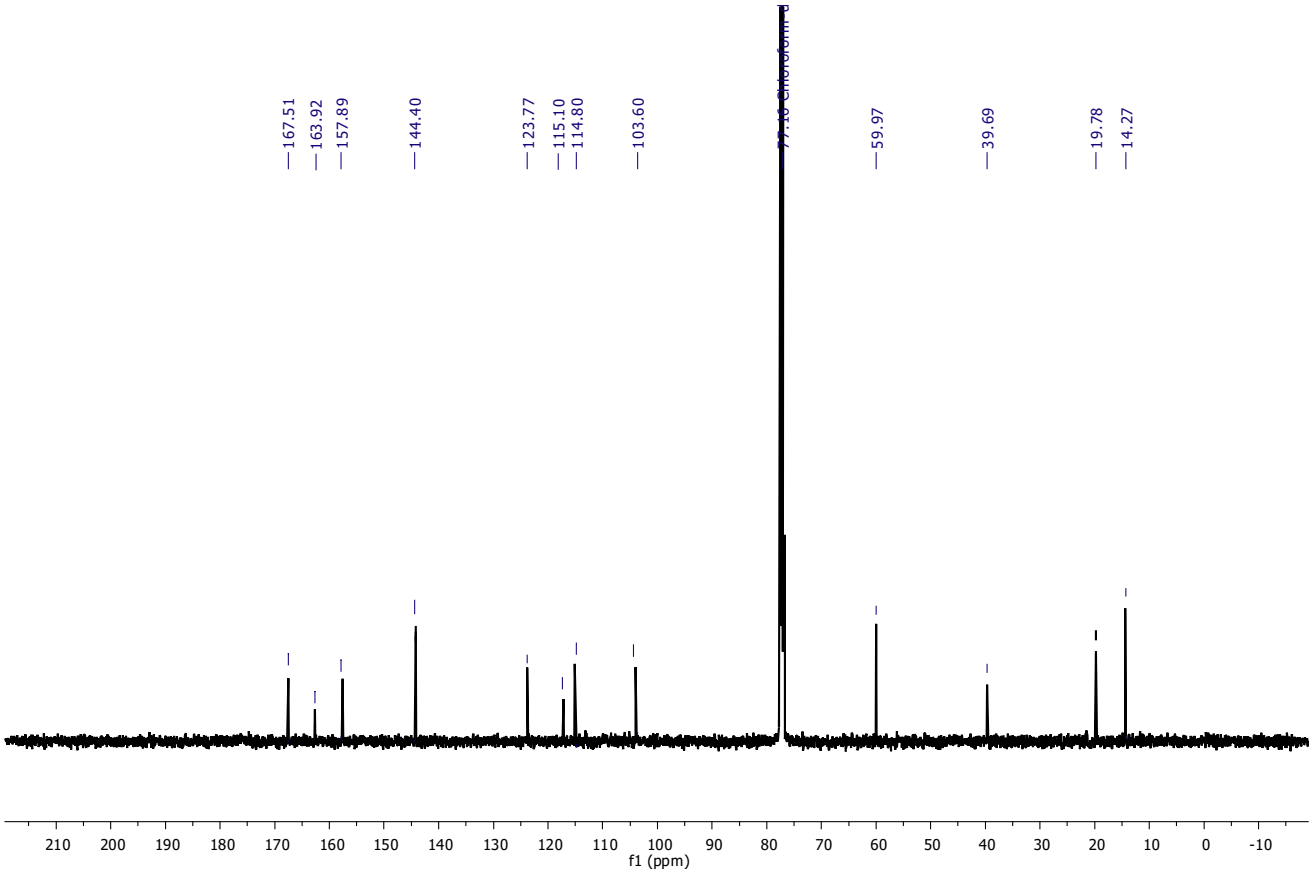


Figure S103.^{13}C NMR spectrum of compound **21** ($CDCl_3$, 100 MHz, TMS).

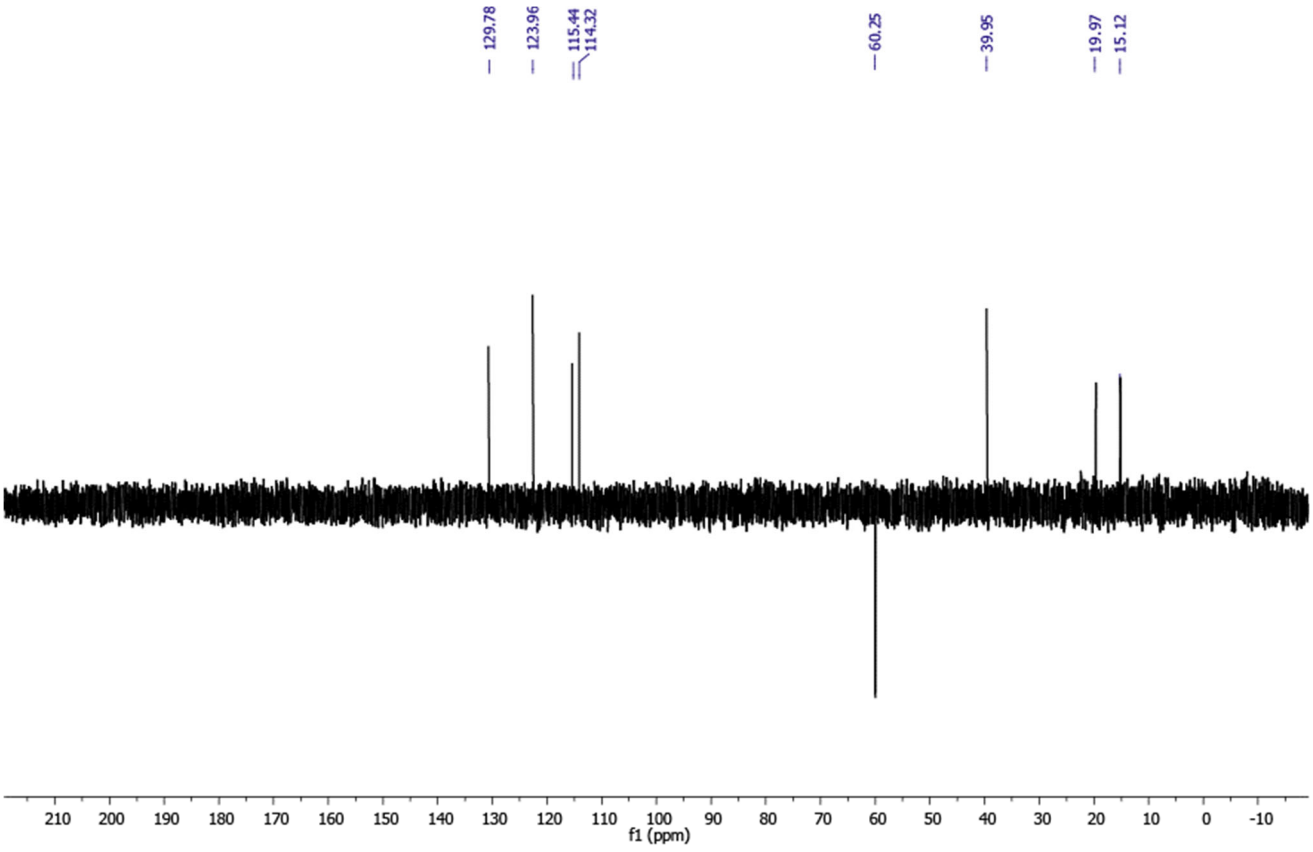


Figure S104. DEPT 135 spectrum of compound **21** ($CDCl_3$, 100 MHz, TMS).

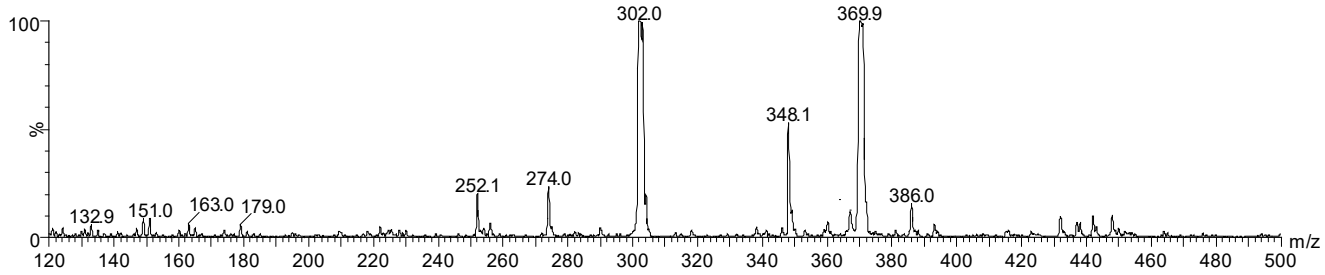


Figure S105. ESI (+) mass spectrum of compound **21.**

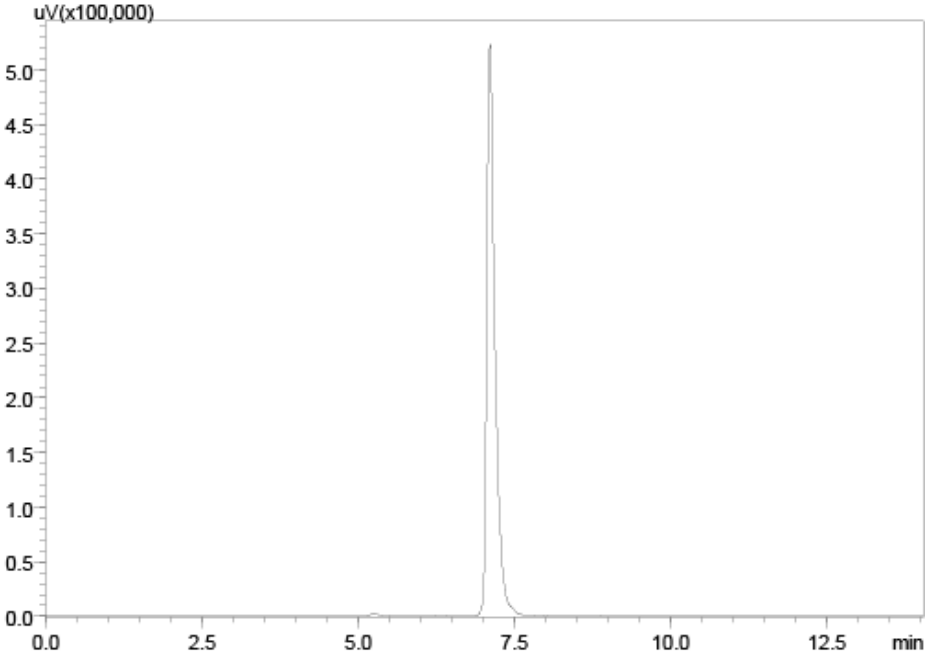


Figure S106: HPLC chromatogram of compound **22**.

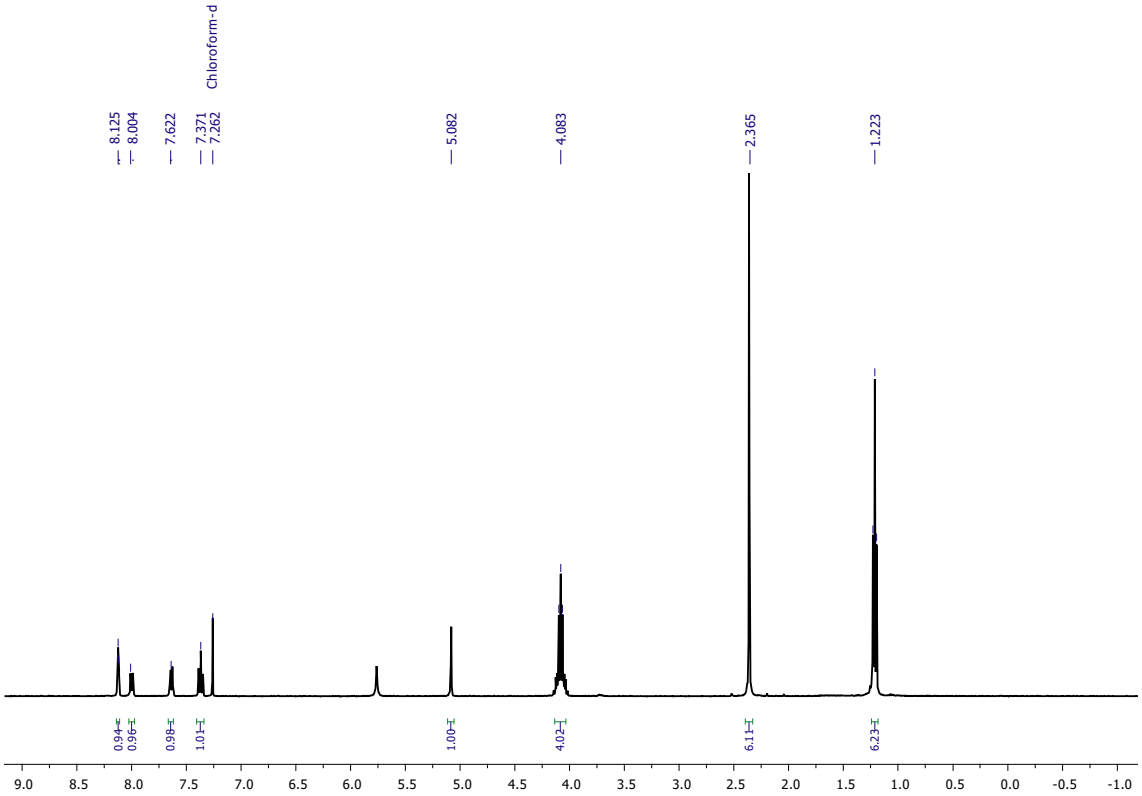


Figure S107.^{1}H NMR spectrum of compound **22** ($CDCl_3$, 400 MHz, TMS).

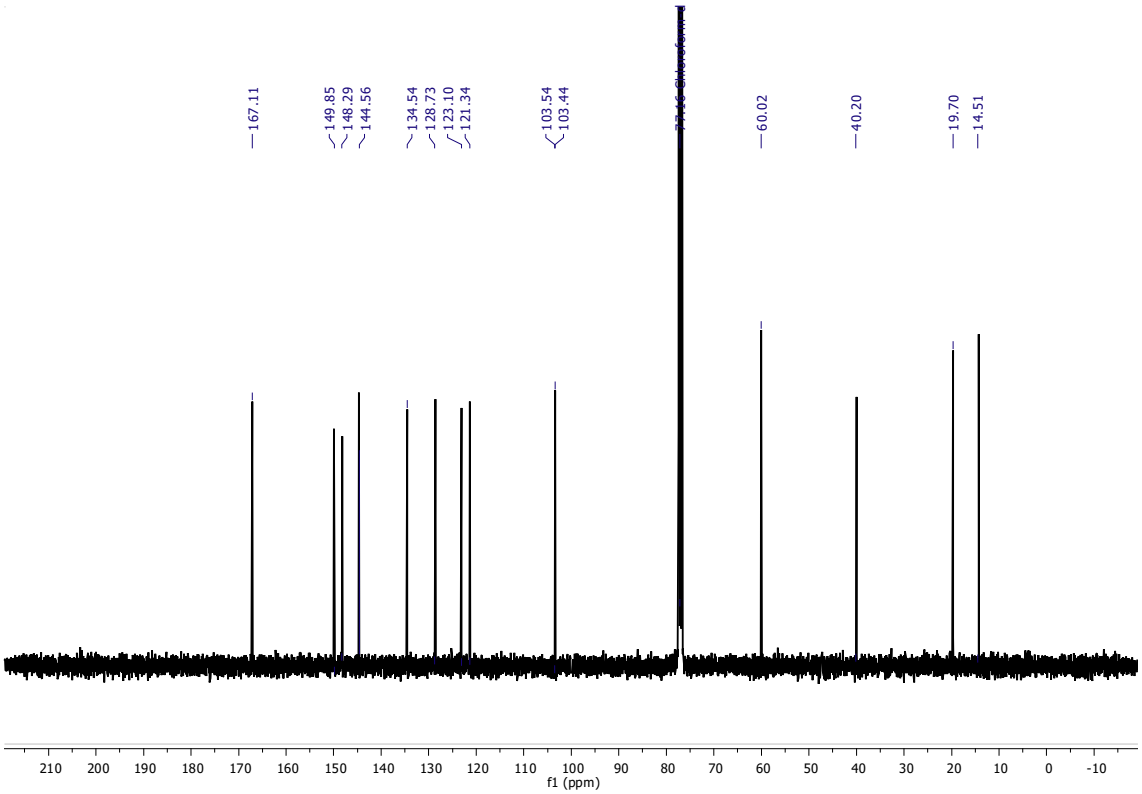


Figure S108.^{13}C NMR spectrum of compound **22** ($CDCl_3$, 100 MHz, TMS).

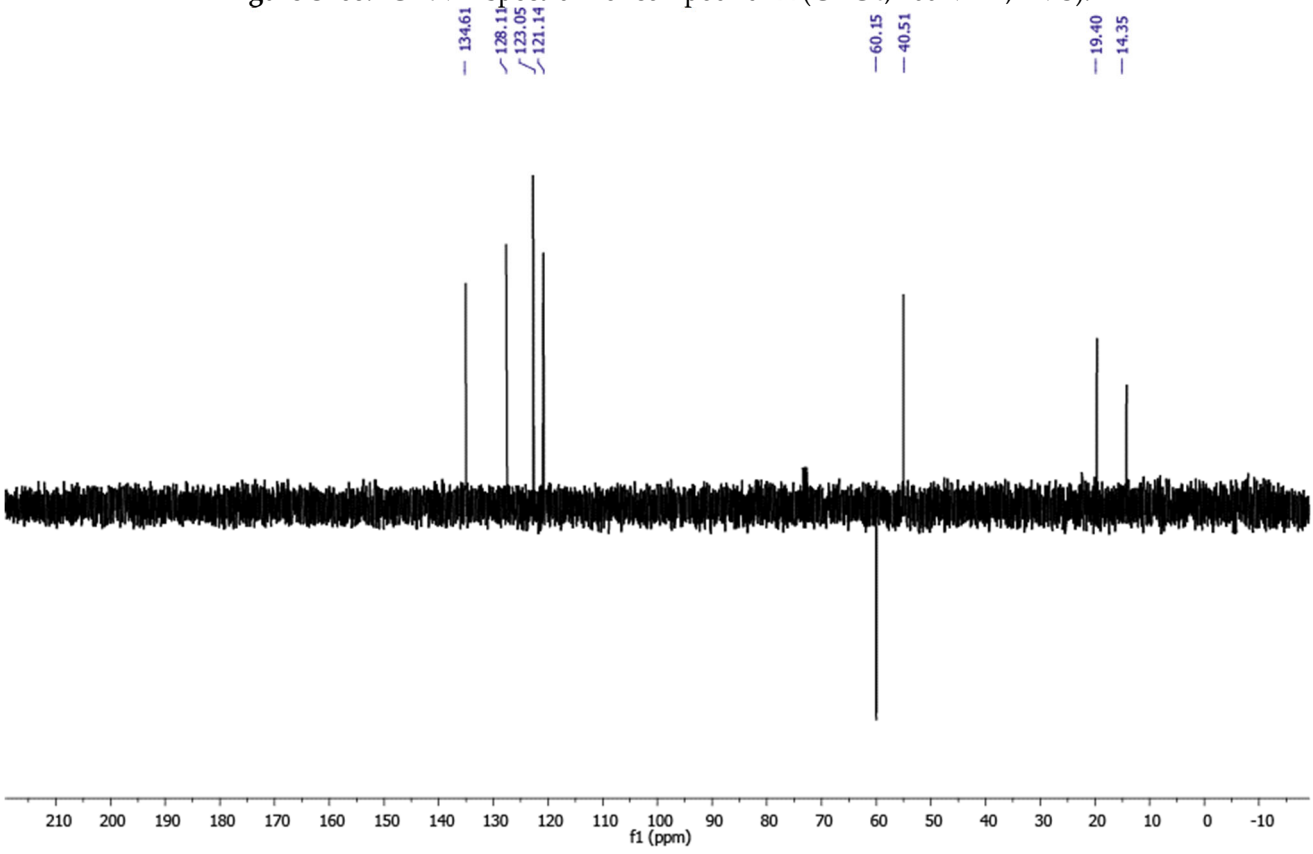


Figure S109. DEPT 135 spectrum of compound **22** ($CDCl_3$, 100 MHz, TMS).

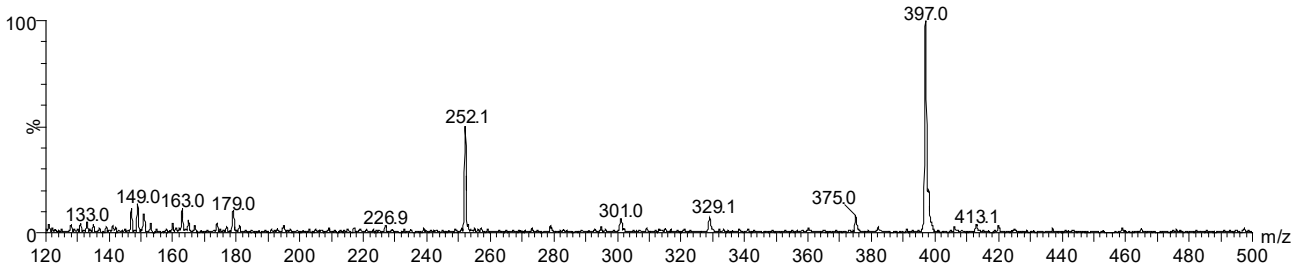


Figure S110. ESI (+) mass spectrum of compound **22.**

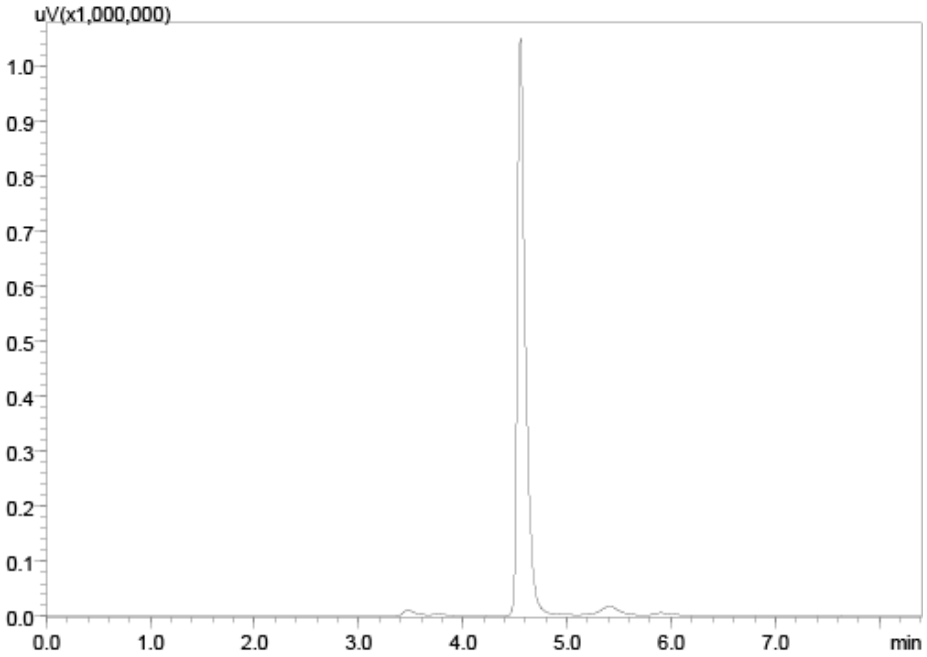
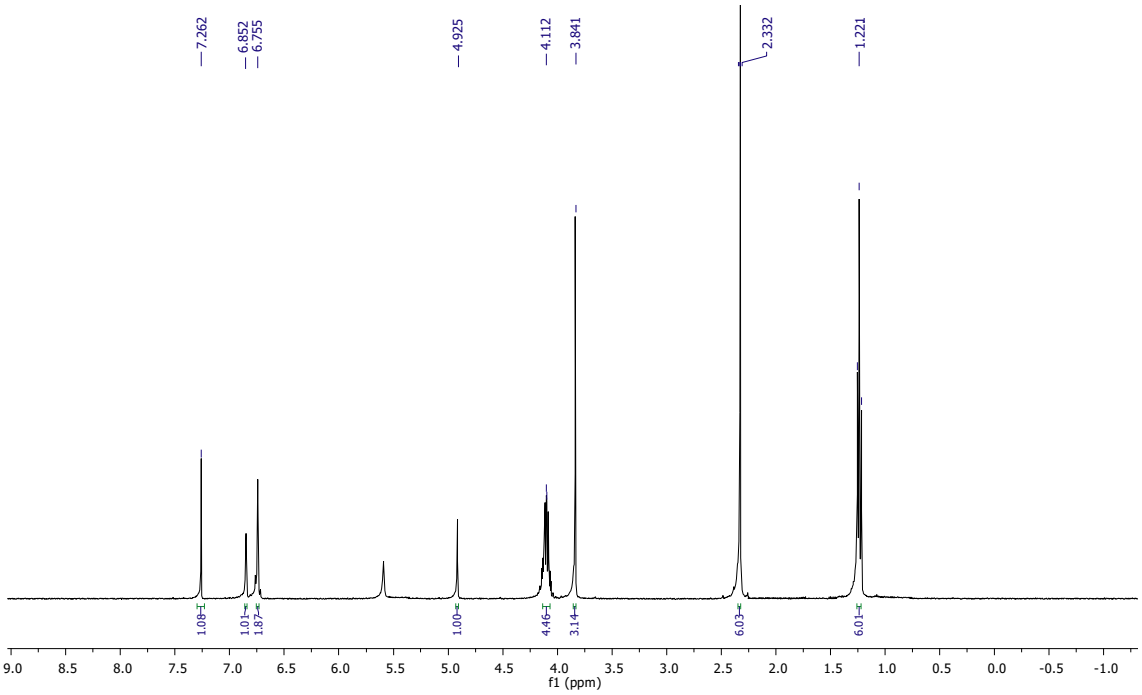


Figure S111: HPLC chromatogram of compound **23**.



Figur112.^{1}H NMR spectrum of compound **23** ($CDCl_3$, 400 MHz, TMS).

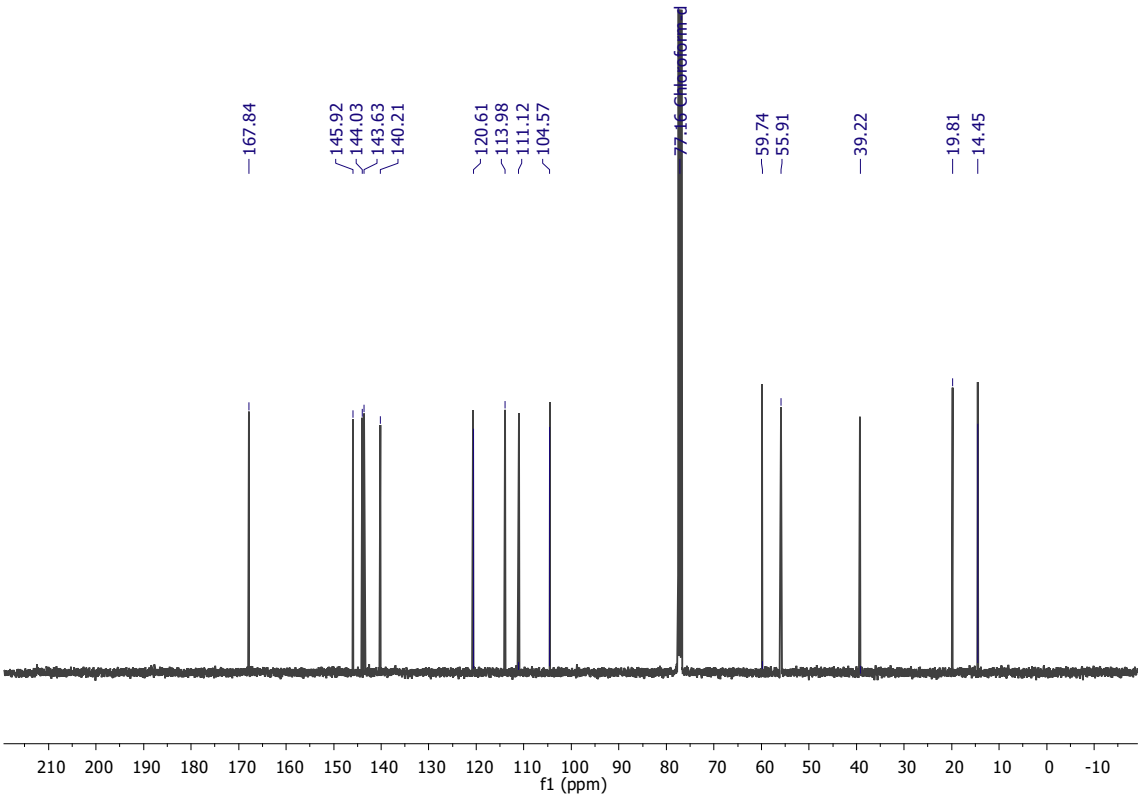


Figure S113.^{13}C NMR spectrum of compound **23** ($CDCl_3$, 100 MHz, TMS).

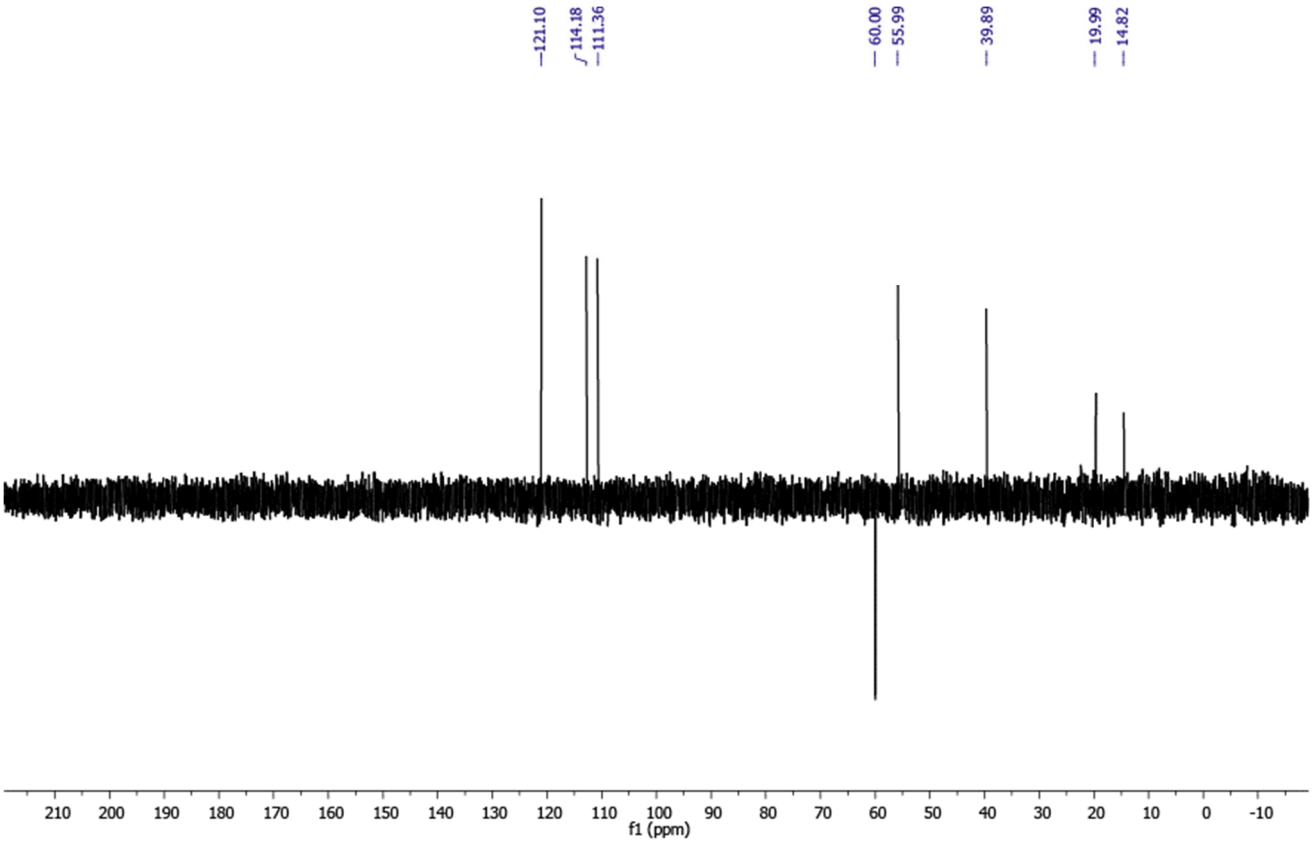


Figure S114. DEPT 135 spectrum of compound **23** ($CDCl_3$, 100 MHz, TMS).

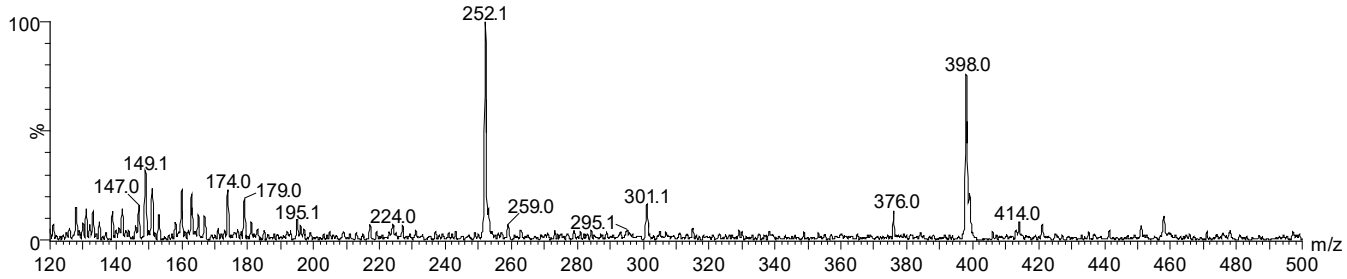


Figure S115. ESI (+) mass spectrum of compound **23.**

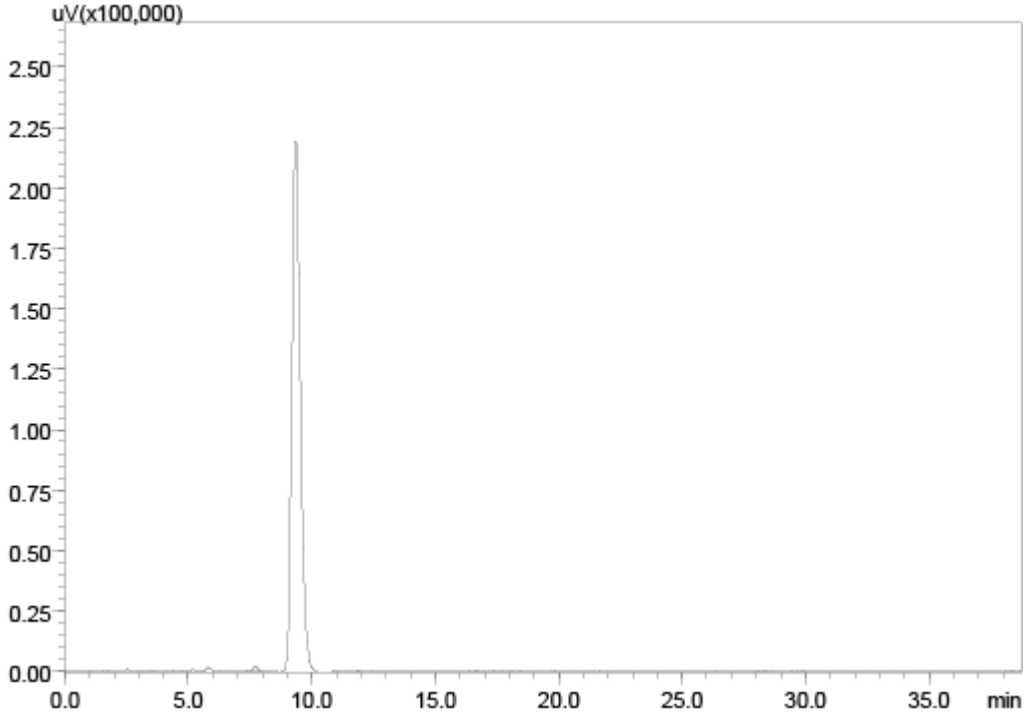


Figure S116: HPLC chromatogram of compound **24**.

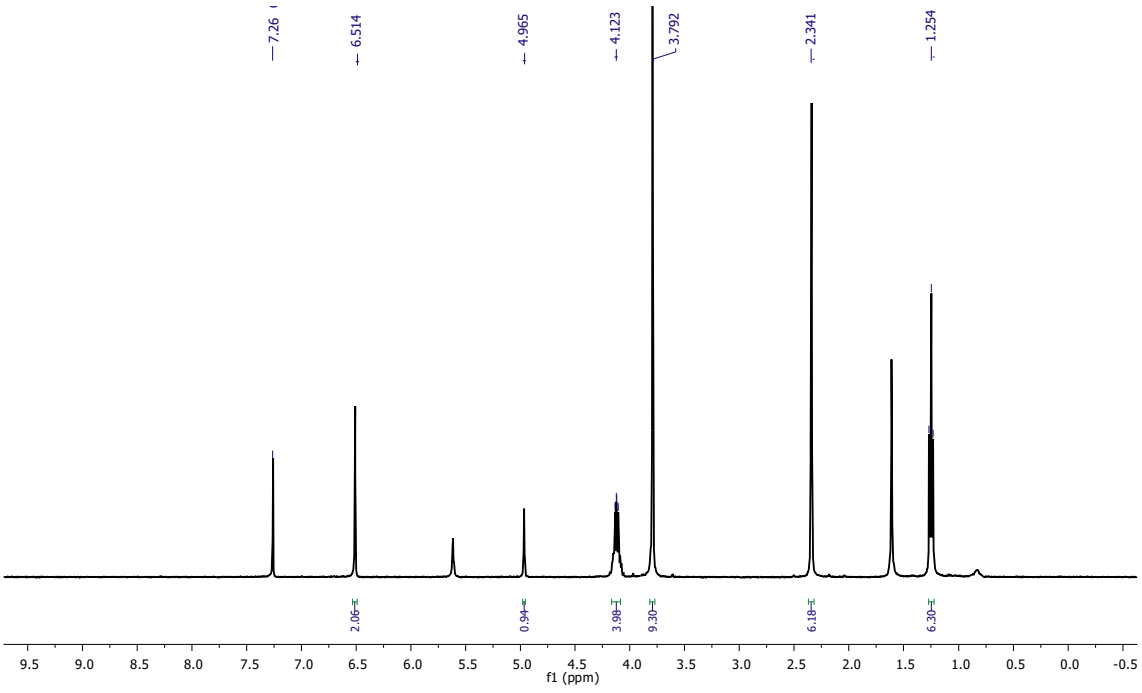


Figure S117.^{1}H NMR spectrum of compound **24** ($CDCl_3$, 400 MHz, TMS).

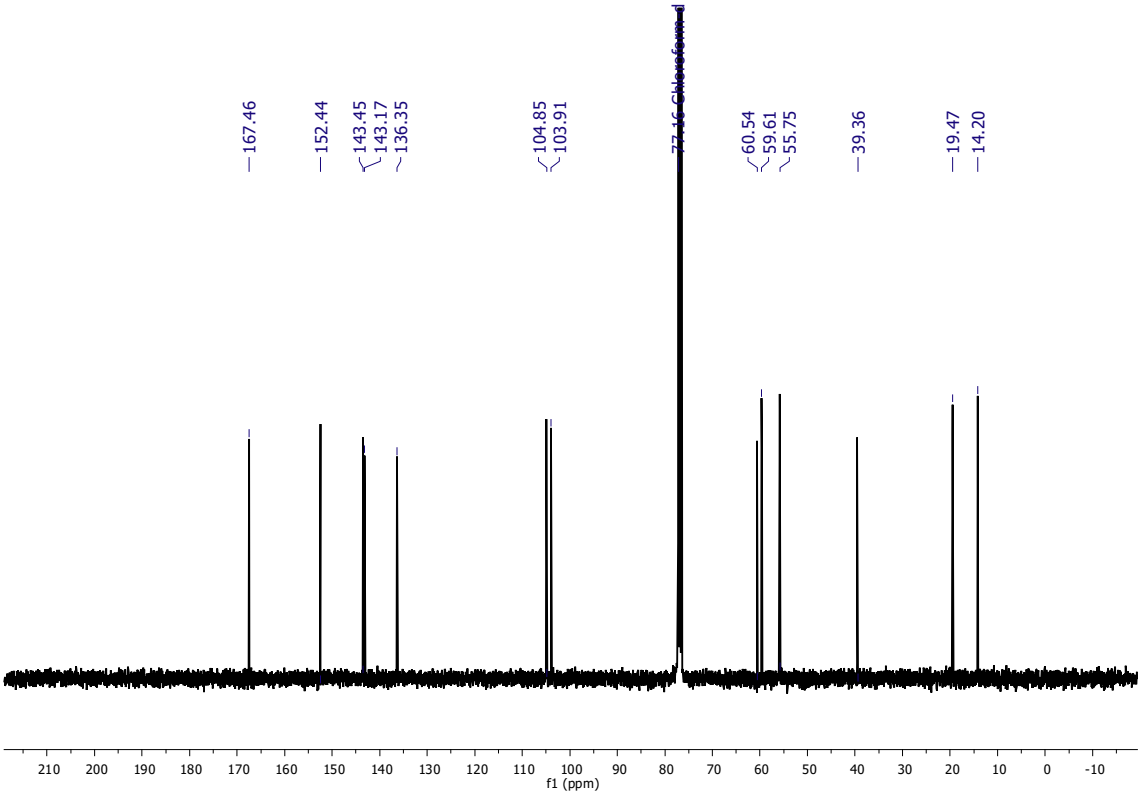


Figure S118.^{13}C NMR spectrum of compound **24** ($CDCl_3$, 100 MHz, TMS).

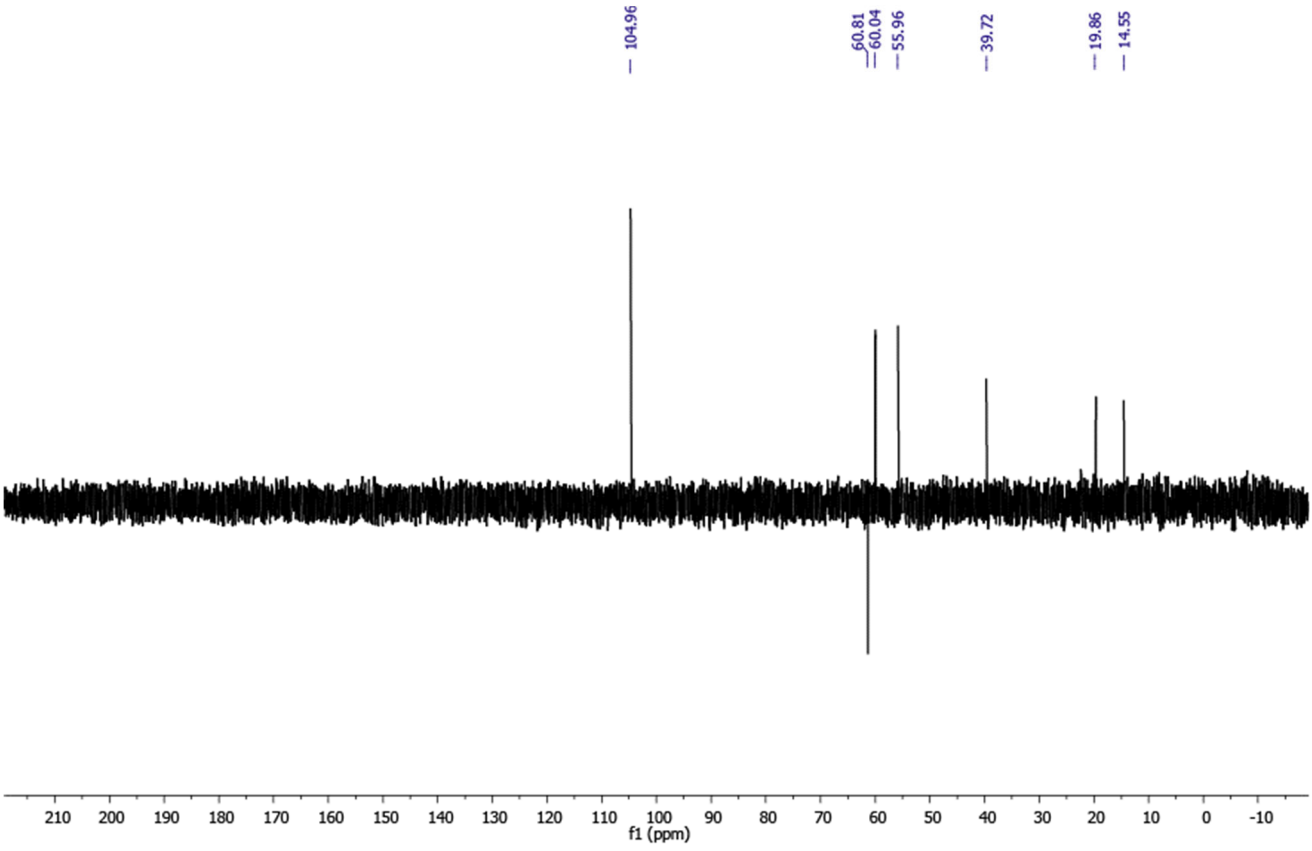


Figure S119. DEPT 135 spectrum of compound **24** ($CDCl_3$, 100 MHz, TMS).

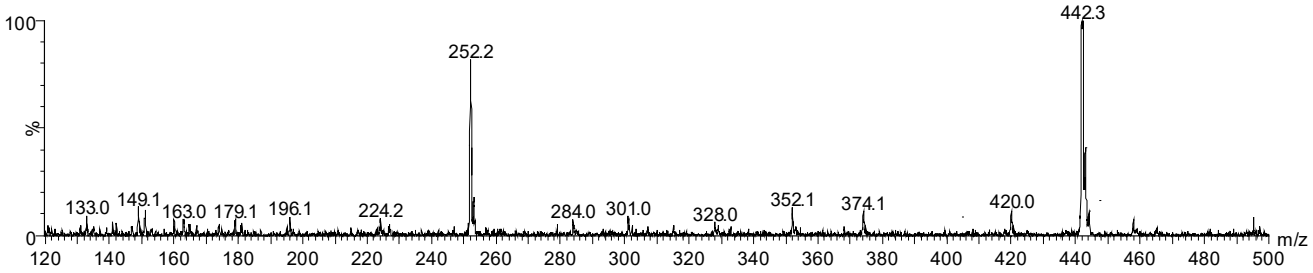


Figure S120. ESI (+) mass spectrum of compound **24.**

Table SI 1. Score values of ORO and QLA tested in four score functions (ChemPLP, GoldScore, ChemScore and ASP) in *Sm*DHODH (PDB ID 6UY4) redocking experiments.

Entry	Score function			
	ChemPLP	GoldScore	ChemScore	ASP
ORO	58.90	46.37	31.43	34.36
QLA	74.62	52.40	34.95	38.80

2D diagrams of ligand-protein interactions

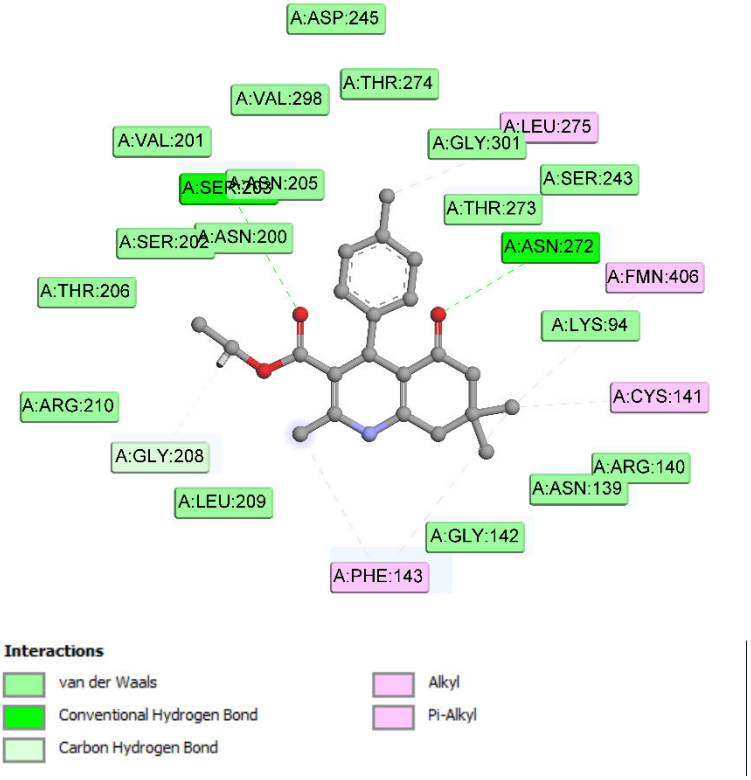


Figure SI 1 – Intermolecular interactions between compound **2** and residues from ORO active site of *Sm*DHODH (PDB ID 6UY4).

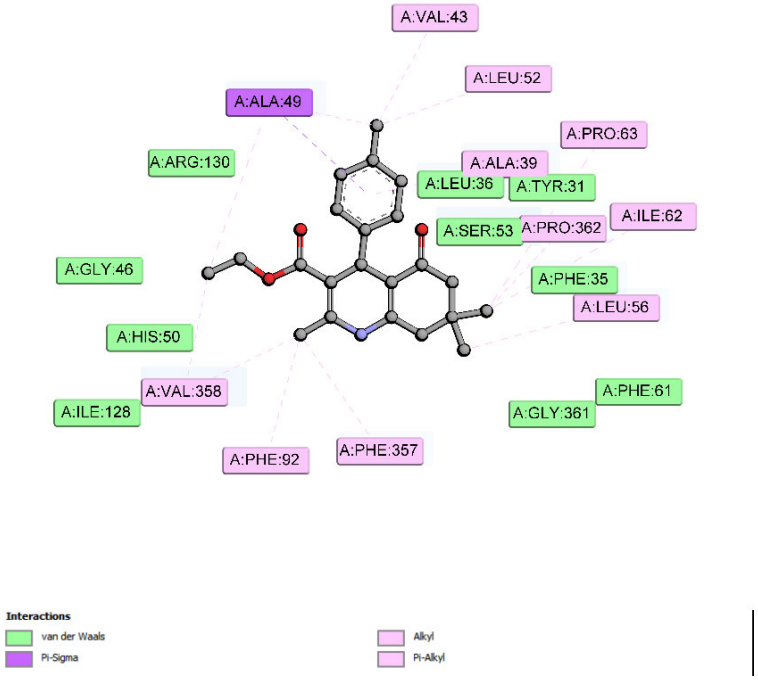


Figure SI 2 – Intermolecular interactions between compound **2** and residues from QLA active site of *Sm*DHODH (PDB ID 6UY4).

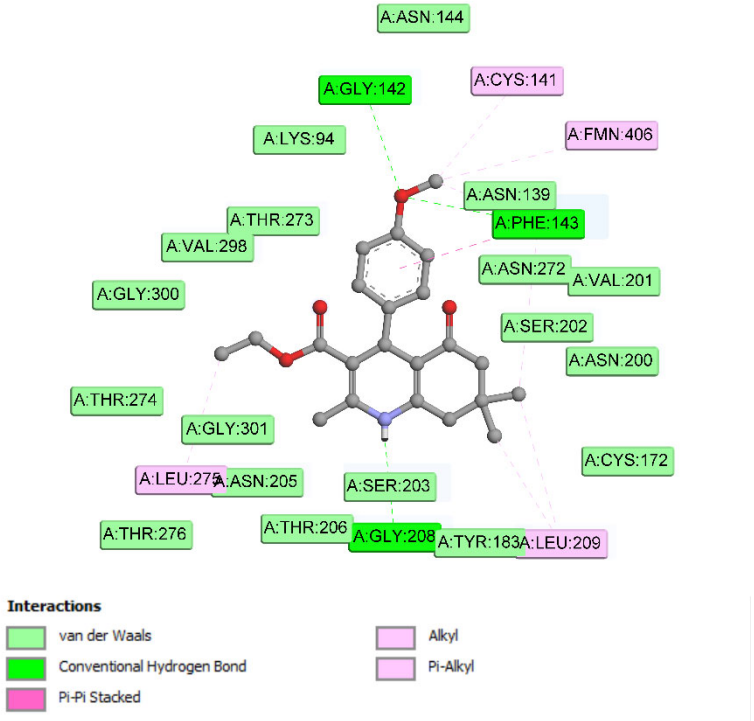


Figure SI 3 – Intermolecular interactions between compound **3** and residues from ORO active site of *Sm*DHODH (PDB ID 6UY4).

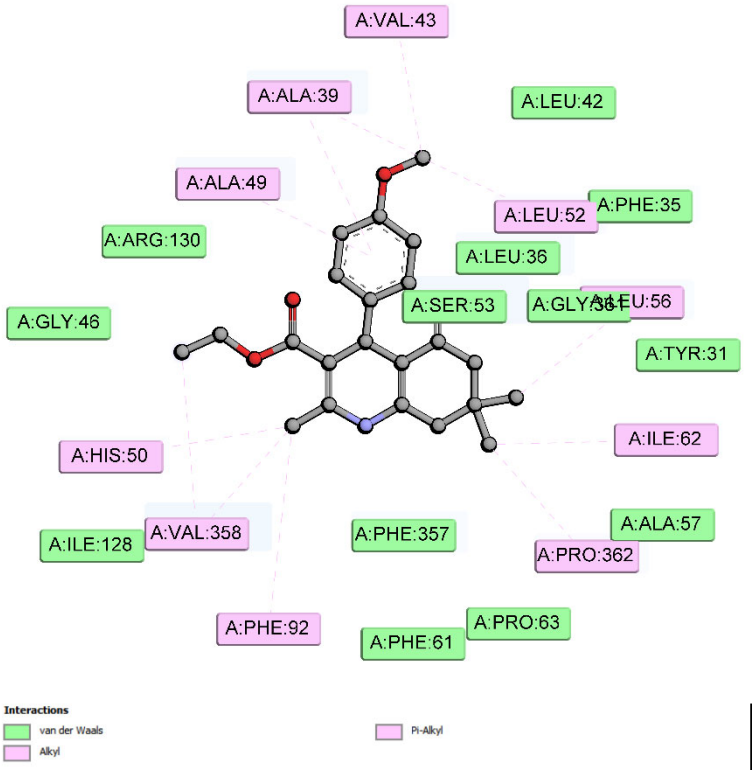


Figure SI 4 – Intermolecular interactions between compound **3** and residues from QLA active site of *Sm*DHODH (PDB ID 6UY4).

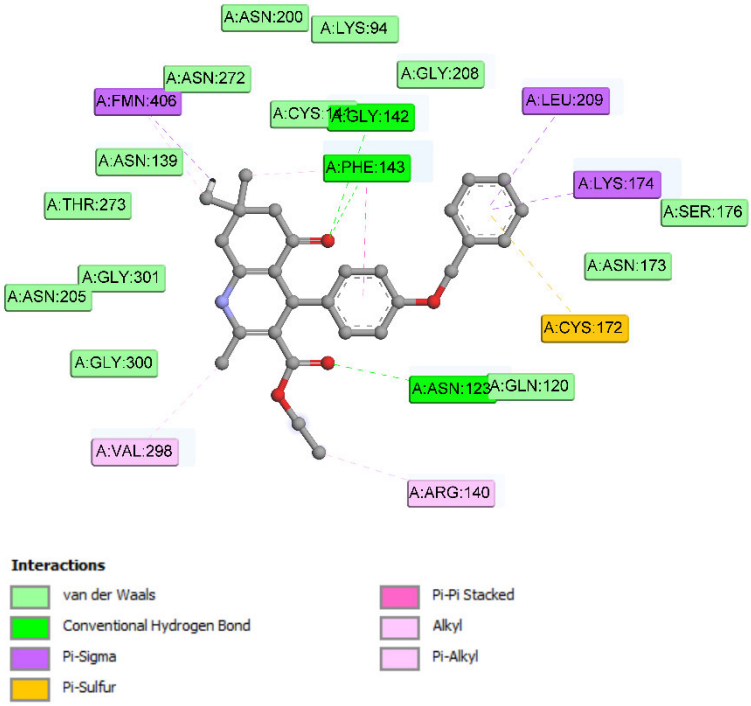


Figure SI 5 – Intermolecular interactions between compound **4** and residues from ORO active site of *Sm*DHODH (PDB ID 6UY4).

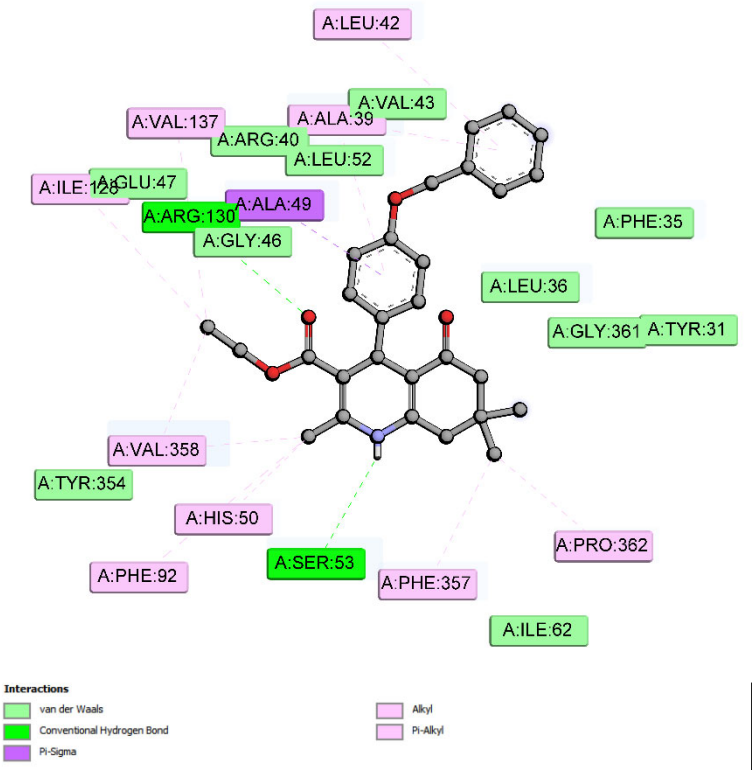


Figure SI 6 – Intermolecular interactions between compound **4** and residues from QLA active site of *Sm*DHODH (PDB ID 6UY4).

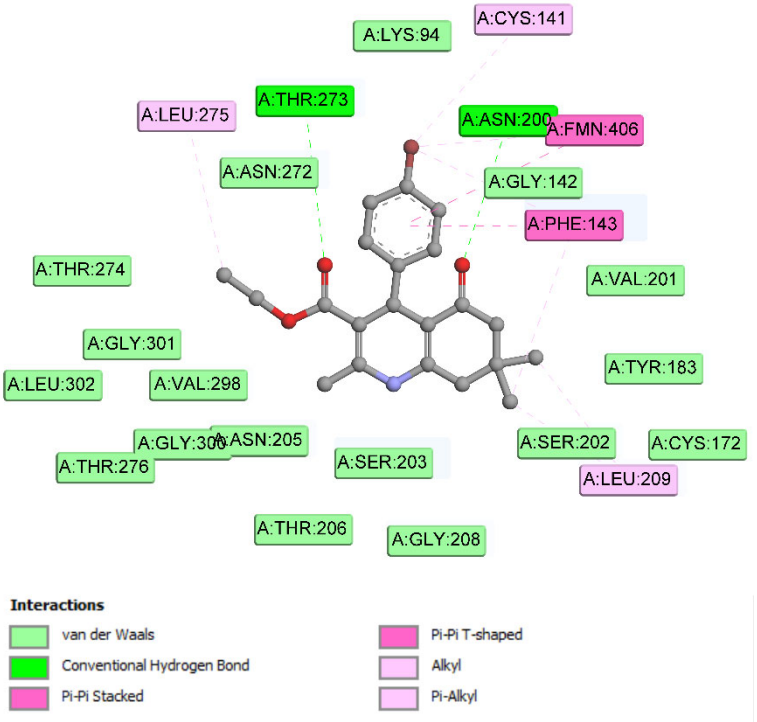


Figure SI 7 – Intermolecular interactions between compound **6** and residues from ORO active site of *Sm*DHODH (PDB ID 6UY4).

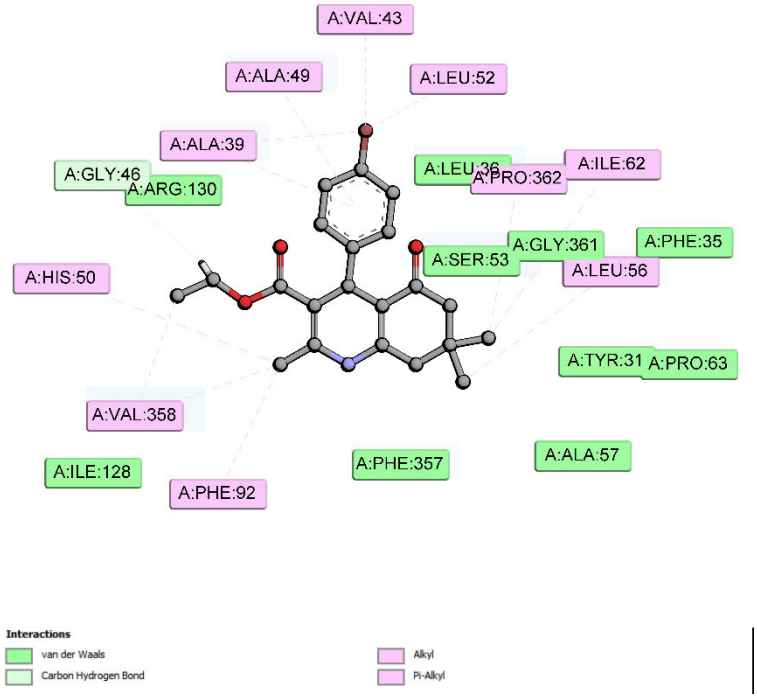


Figure SI 8 – Intermolecular interactions between compound **6** and residues from QLA active site of *Sm*DHODH (PDB ID 6UY4).

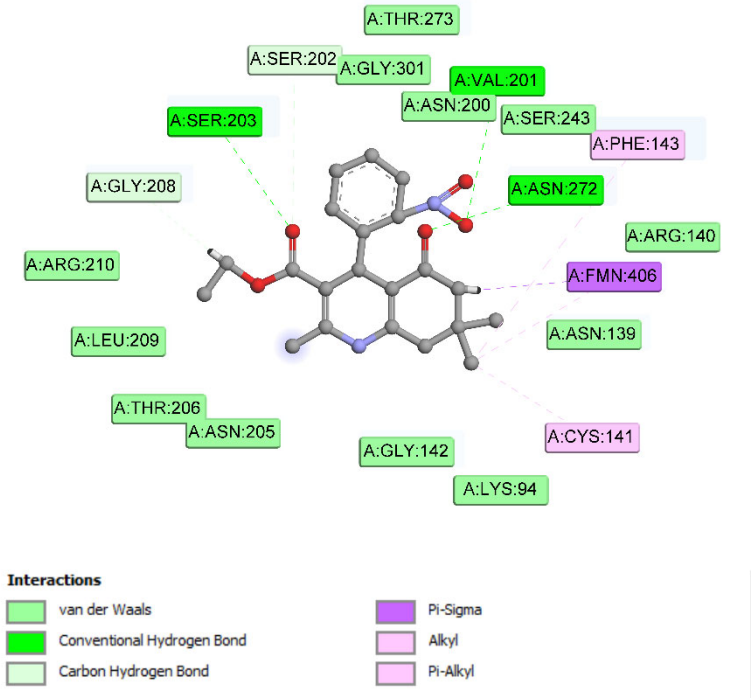


Figure SI 9 – Intermolecular interactions between compound **9** and residues from ORO active site of *Sm*DHODH (PDB ID 6UY4).

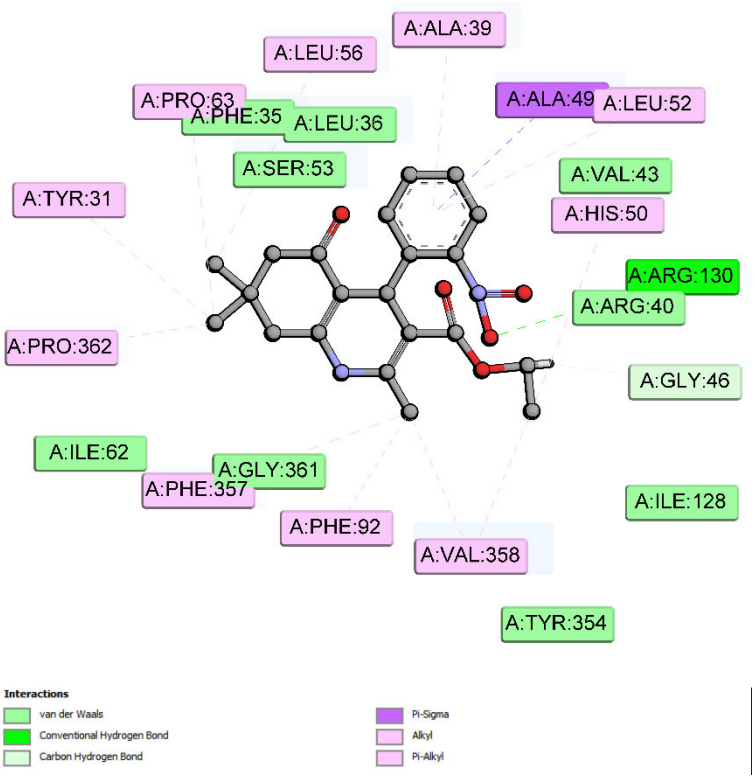


Figure SI 10 – Intermolecular interactions between compound **9** and residues from QLA active site of *Sm*DHODH (PDB ID 6UY4).

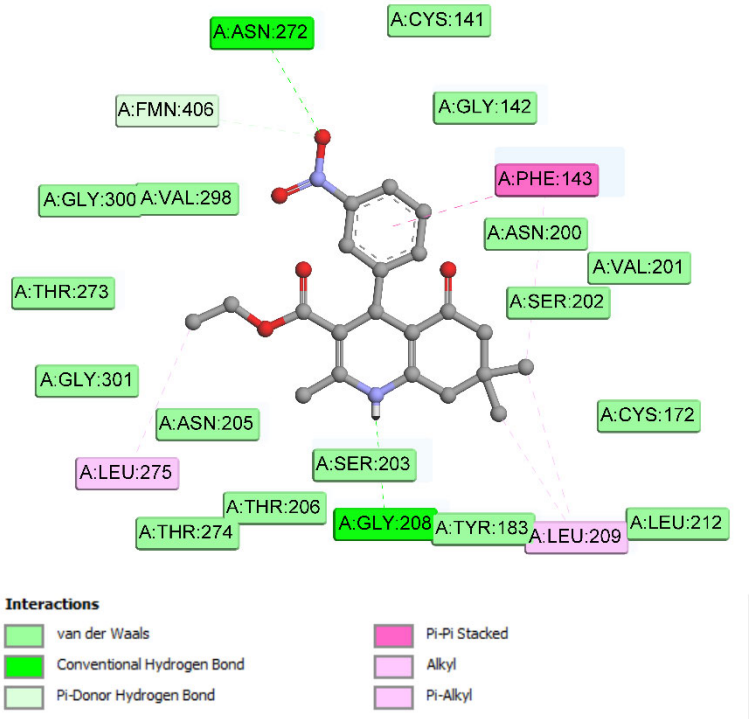


Figure SI 11 – Intermolecular interactions between compound **10** and residues from ORO active site of *Sm*DHODH (PDB ID 6UY4).

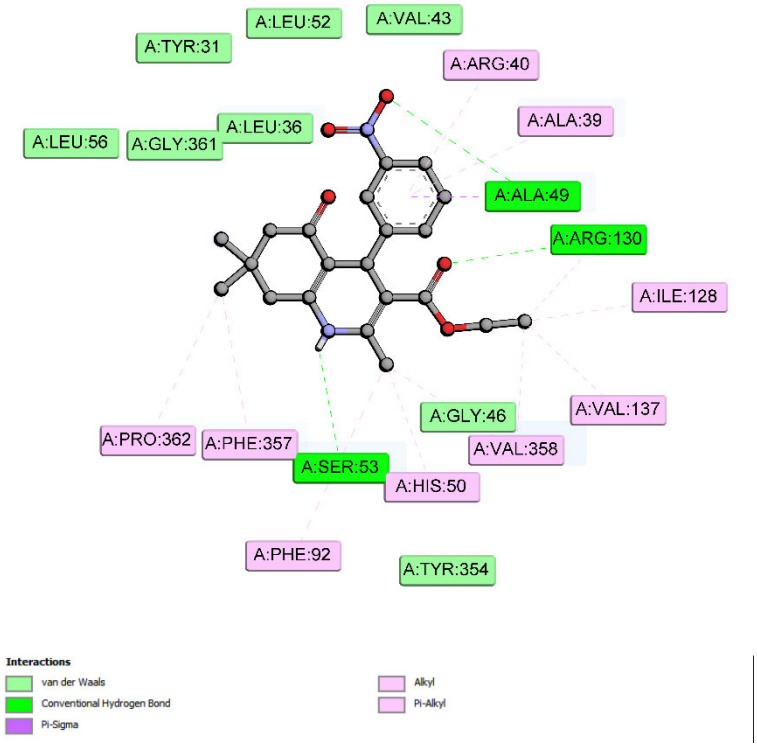


Figure SI 12 – Intermolecular interactions between compound **10** and residues from QLA active site of *Sm*DHODH (PDB ID 6UY4).

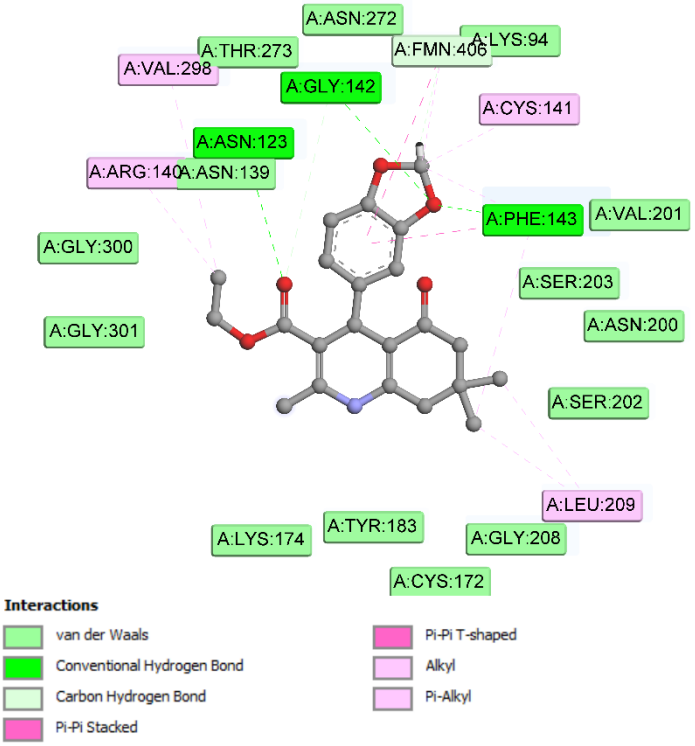


Figure SI 13 – Intermolecular interactions between compound **12** and residues from ORO active site of *Sm*DHODH (PDB ID 6UY4).

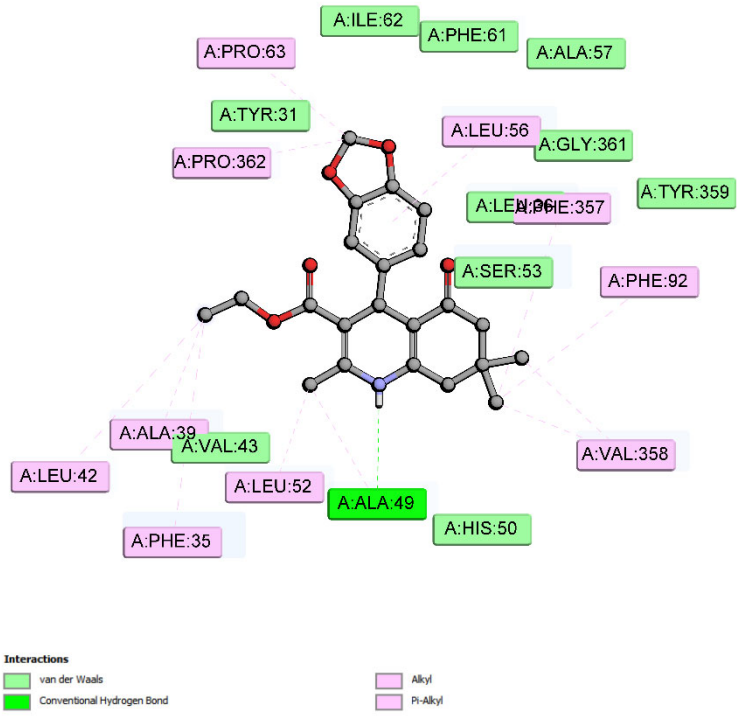


Figure SI 14 – Intermolecular interactions between compound **12** and residues from QLA active site of *Sm*DHODH (PDB ID 6UY4).

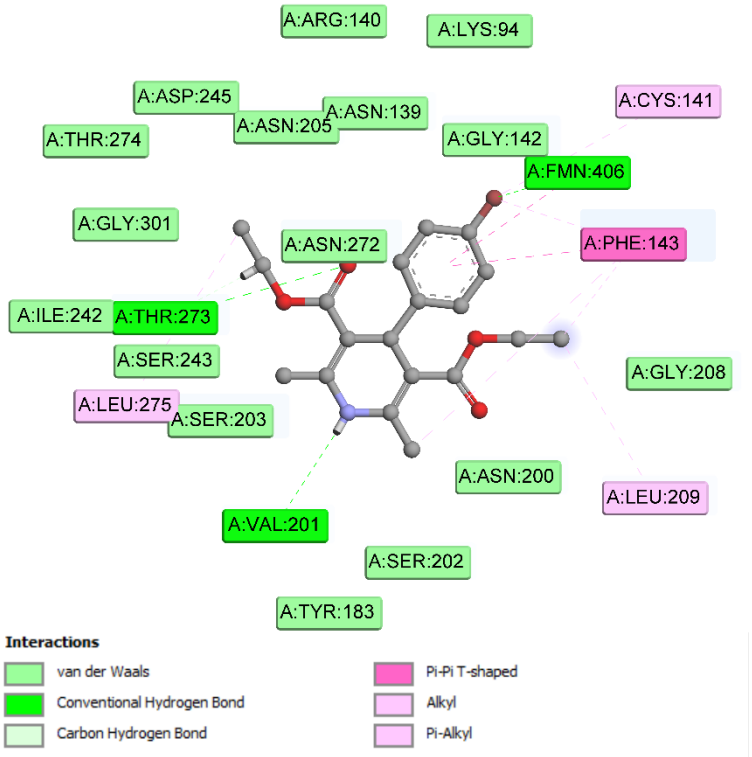


Figure SI 15 – Intermolecular interactions between compound **20** and residues from ORO active site of *Sm*DHODH (PDB ID 6UY4).

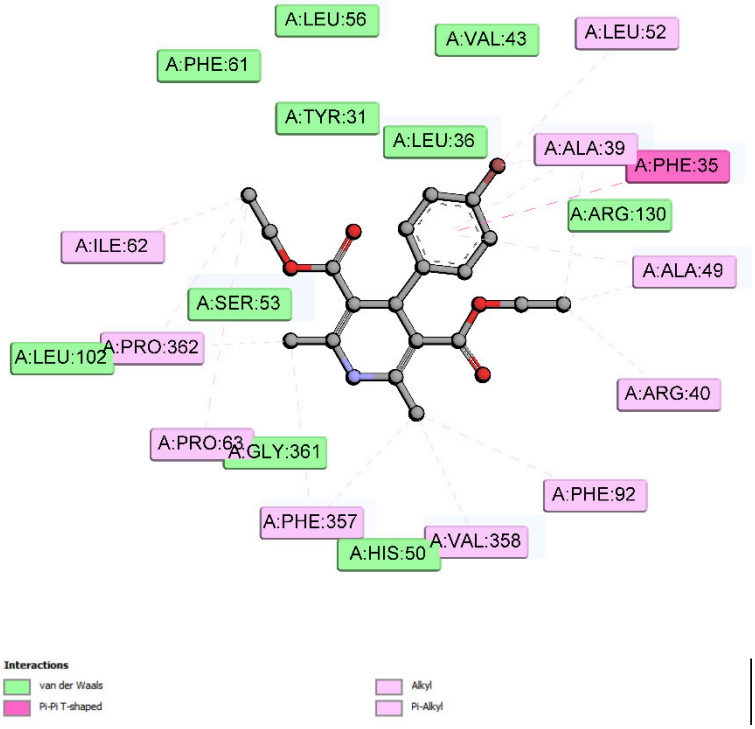


Figure SI 16 – Intermolecular interactions between compound **20** and residues from QLA active site of *Sm*DHODH (PDB ID 6UY4).

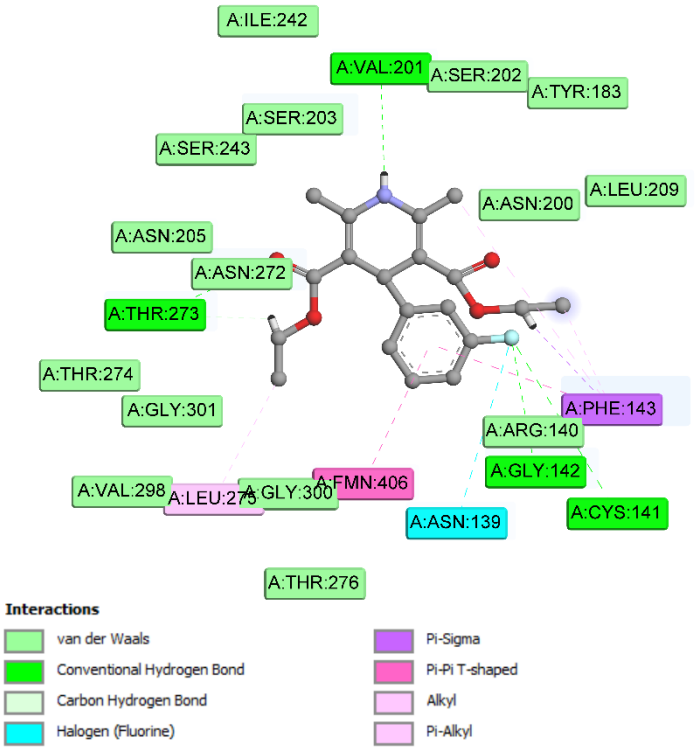


Figure SI 17 – Intermolecular interactions between compound **21** and residues from ORO active site of *Sm*DHODH (PDB ID 6UY4).

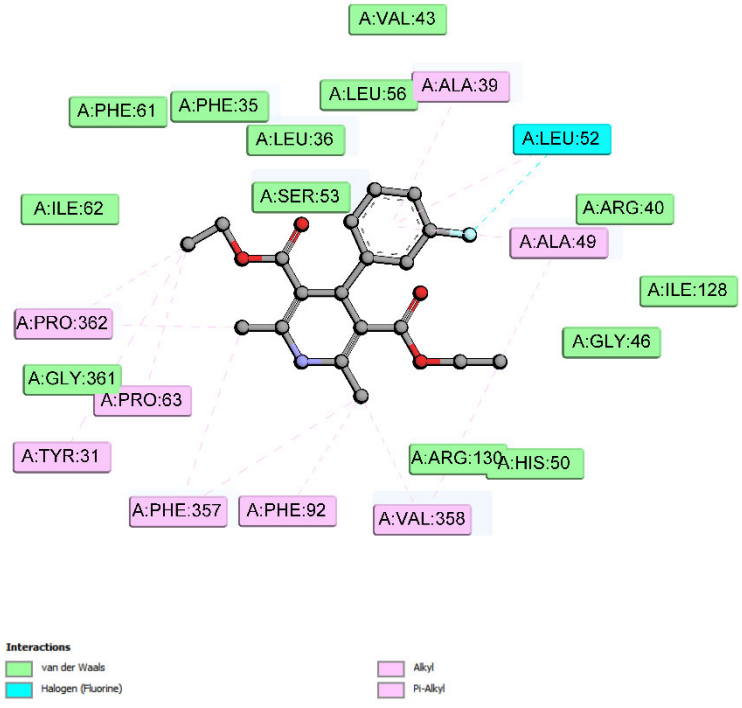


Figure SI 18 – Intermolecular interactions between compound **21** and residues from QLA active site of *Sm*DHODH (PDB ID 6UY4).

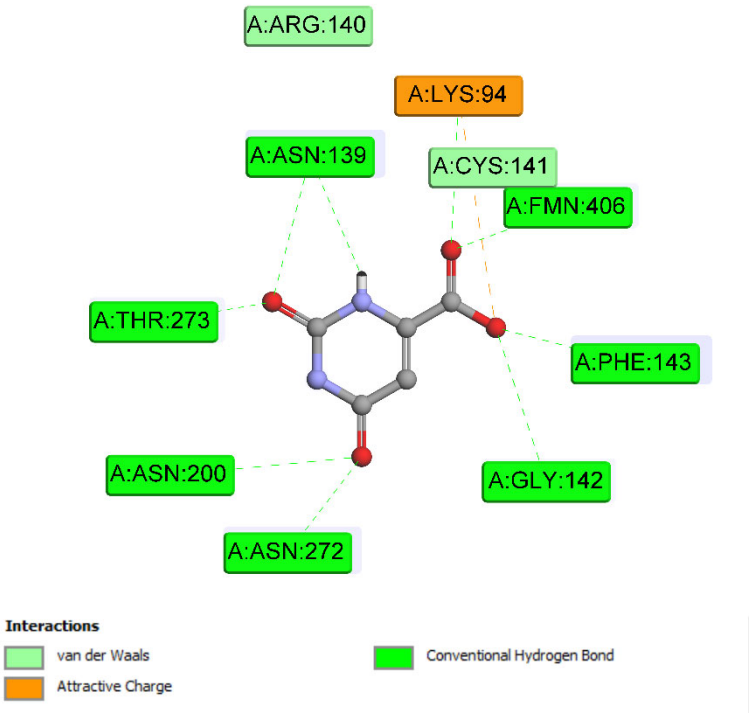


Figure SI 19 – Intermolecular interactions between compound **ORO** and residues from ORO active site of *Sm*DHODH (PDB ID 6UY4).

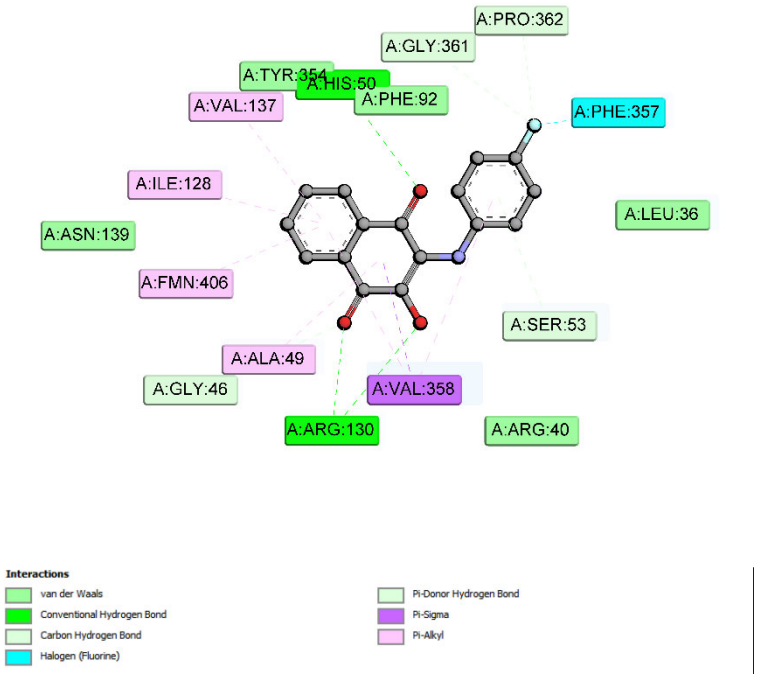


Figure SI 20 – Intermolecular interactions between compound **QLA** and residues from QLA active site of *Sm*DHODH (PDB ID 6UY4).

Ligands coordinates after docking (best conformations)

ORO active site

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5	C	12.3733	15.1526	52.4240	C.2	1 <1>	0.0650
6	C	13.4235	16.2196	52.7943	C.3	1 <1>	0.0471
7	C	13.8611	18.4284	54.1124	C.2	1 <1>	0.1621
8	C	13.3149	19.5918	54.8925	C.3	1 <1>	0.0157
9	C	12.4430	19.0620	56.0409	C.3	1 <1>	-0.0228
10	C	11.2895	18.2247	55.4163	C.3	1 <1>	-0.0086
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7 C 12.9131 15.5489 50.7103 C.2 1 <1> 0.1621
8 C 12.4630 15.4105 49.2825 C.3 1 <1> 0.0157
9 C 11.1106 14.6829 49.2500 C.3 1 <1> -0.0228
10 C 11.3054 13.2852 49.9063 C.3 1 <1> -0.0086
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7	C	12.0500	18.2083	56.3119	C.2	1 <1> 0.1621
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16	O	9.5994	13.4979	57.4864	O.2	1 <1> -0.2452
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36	H	13.3659	19.5153	57.3570	H	1 <1> 0.0350
37	H	12.7532	20.1931	55.8080	H	1 <1> 0.0350
38	H	15.2658	17.7605	57.4452	H	1 <1> 0.0331
39	H	15.6452	16.9461	55.8976	H	1 <1> 0.0331
40	H	15.7379	20.0706	56.6845	H	1 <1> 0.0235
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44	H	13.3156	17.5143	54.0891	H	1 <1> 0.0235
45	H	13.7592	19.1823	53.5853	H	1 <1> 0.0235
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     7 C          13.2246  16.1310  50.4027 C.2          1 <1>          0.1621
     8 C          12.5593  15.7908  49.0980 C.3          1 <1>          0.0157
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   15 C         15.4585  14.2460  54.7776 C.2      1 <1>           0.3375
   16 O         16.1055  15.2700  54.9166 O.2      1 <1>          -0.2452
   17 C         12.3823  16.2591  54.0515 C.ar     1 <1>          -0.0566
   18 C         11.8021  17.2892  54.7975 C.ar     1 <1>          -0.0475
   19 C         12.4712  18.5052  54.9565 C.ar     1 <1>           0.0179
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   21 C         14.3109  17.6626  53.6280 C.ar     1 <1>          -0.0566
   22 C         14.0435  11.6951  54.1575 C.3      1 <1>          -0.0260
   23 Br        11.6753  19.9087  55.9781 Br       1 <1>          -0.0503
   24 O         15.6068  13.3283  55.7740 O.3      1 <1>          -0.4616
   25 C         17.9014  13.3290  56.3327 C.3      1 <1>          -0.0306
   26 C         16.4698  13.3291  56.8466 C.3      1 <1>           0.0900
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   28 H         15.2662  15.6354  52.1989 H        1 <1>           0.0450
   29 H         13.2864  15.2176  48.4808 H        1 <1>           0.0350
   30 H         12.2905  16.7142  48.5385 H        1 <1>           0.0350
   31 H         12.4267  12.9469  49.3767 H        1 <1>           0.0331
   32 H         10.9817  13.0226  50.4296 H        1 <1>           0.0331
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   36 H          9.4277  14.9630  50.4414 H        1 <1>           0.0235
   37 H         10.7220  15.9018  51.2452 H        1 <1>           0.0235
   38 H          9.9514  16.5417  49.7521 H        1 <1>           0.0235
   39 H         11.8471  15.3258  53.9678 H        1 <1>           0.0621
   40 H         10.8333  17.1389  55.2564 H        1 <1>           0.0629
   41 H         14.2519  19.6280  54.4979 H        1 <1>           0.0629
   42 H         15.2863  17.8252  53.1865 H        1 <1>           0.0621
   43 H         13.4685  10.8410  53.7431 H        1 <1>           0.0290
   44 H         15.1107  11.3904  54.1974 H        1 <1>           0.0290
   45 H         13.6487  11.8691  55.1793 H        1 <1>           0.0290
   46 H         18.6083  13.3330  57.1893 H        1 <1>           0.0262
   47 H         18.0863  12.4224  55.7178 H        1 <1>           0.0262
   48 H         18.0837  14.2324  55.7125 H        1 <1>           0.0262
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Compound **9**
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USER_CHARGES

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2 C 11.8604 16.9794 54.4295 C.2 1 <1> 0.0158

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 3 N       11.0898  15.8045  54.3165 N.pl3       1 <1>          -0.3205
 4 C       11.2680  14.8395  53.2872 C.2         1 <1>           0.0157
 5 C       12.2656  14.9779  52.3383 C.2         1 <1>           0.0651
 6 C       13.2108  16.2193  52.4441 C.3         1 <1>           0.0493
 7 C       13.5851  18.5322  53.6607 C.2         1 <1>           0.1621
 8 C       13.0587  19.6046  54.5742 C.3         1 <1>           0.0157
 9 C       12.6338  18.9630  55.9004 C.3         1 <1>          -0.0228
10 C       11.5248  17.9237  55.5810 C.3         1 <1>          -0.0086
11 O       14.6246  18.7311  53.0563 O.2         1 <1>          -0.2923
12 C       12.0715  20.0373  56.8510 C.3         1 <1>          -0.0591
13 C       13.8413  18.2830  56.5958 C.3         1 <1>          -0.0591
14 C       14.6603  15.7926  52.7441 C.ar        1 <1>          -0.0050
15 C       12.4063  13.9138  51.2285 C.2         1 <1>           0.3375
16 O       13.2336  14.0883  50.3516 O.2         1 <1>          -0.2452
17 C       15.7863  15.8471  51.8352 C.ar        1 <1>           0.1302
18 C       17.0452  15.4075  52.3110 C.ar        1 <1>          -0.0312
19 C       17.2213  14.9535  53.6131 C.ar        1 <1>          -0.0596
20 C       16.1502  14.9285  54.4904 C.ar        1 <1>          -0.0613
21 C       14.8937  15.3450  54.0667 C.ar        1 <1>          -0.0555
22 C       10.2754  13.6903  53.3203 C.3         1 <1>          -0.0260
23 O       11.7410  12.7329  51.1107 O.3         1 <1>          -0.4616
24 C       12.8003  10.7094  51.6818 C.3         1 <1>          -0.0306
25 C       12.0997  11.5172  50.6001 C.3         1 <1>           0.0900
26 N       15.7288  16.3339  50.4765 N.pl3       1 <1>           0.0567
27 O       14.6754  16.6183  49.9895 O.2         1 <1>          -0.1261
28 O       16.7963  16.4374  49.7201 O.2         1 <1>          -0.1261
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31 H       12.1586  20.0549  54.0994 H           1 <1>           0.0350
32 H       13.8122  20.4119  54.7112 H           1 <1>           0.0350
33 H       10.5699  18.4223  55.3043 H           1 <1>           0.0331
34 H       11.3317  17.3381  56.5068 H           1 <1>           0.0331
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36 H       11.7378  19.5787  57.8070 H           1 <1>           0.0235
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43 H       16.2922  14.5840  55.5065 H           1 <1>           0.0618
44 H       14.0862  15.3098  54.7872 H           1 <1>           0.0621
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47 H       10.7982  12.7269  53.4938 H           1 <1>           0.0290
48 H       13.1228   9.7302  51.2687 H           1 <1>           0.0262
49 H       13.6965  11.2558  52.0474 H           1 <1>           0.0262
50 H       12.1106  10.5325  52.5340 H           1 <1>           0.0262
51 H       11.2034  10.9553  50.2728 H           1 <1>           0.0695
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Compound 10
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     4 C         12.6566  11.9550  53.0169 C.2         1 <1>          0.0157
     5 C         13.4613  12.9835  53.4723 C.2         1 <1>          0.0650
     6 C         13.4916  14.2988  52.6480 C.3         1 <1>          0.0472
     7 C         12.8694  15.4124  50.3596 C.2         1 <1>          0.1621
     8 C         12.3259  15.2726  48.9645 C.3         1 <1>          0.0157
     9 C         10.9544  14.5859  49.0277 C.3         1 <1>          -0.0228
    10 C         11.1547  13.1901  49.6838 C.3         1 <1>          -0.0086
    11 O         13.4019  16.4594  50.6917 O.2         1 <1>          -0.2923
    12 C         10.3895  14.4066  47.6056 C.3         1 <1>          -0.0591
    13 C          9.9511  15.4387  49.8457 C.3         1 <1>          -0.0591
    14 C         12.8699  15.4459  53.4341 C.ar        1 <1>          -0.0330
    15 C         14.2914  12.8002  54.7581 C.2         1 <1>          0.3375
    16 O         13.7988  12.1860  55.6878 O.2         1 <1>          -0.2452
    17 C         13.5319  16.6804  53.5684 C.ar        1 <1>          -0.0274
    18 C         12.9460  17.7491  54.2716 C.ar        1 <1>          0.1265
    19 C         11.6696  17.5698  54.8353 C.ar        1 <1>          -0.0315
    20 C         10.9965  16.3557  54.6921 C.ar        1 <1>          -0.0593
    21 C         11.5870  15.3029  53.9931 C.ar        1 <1>          -0.0575
    22 C         12.5145  10.6161  53.7169 C.3         1 <1>          -0.0260
    23 O         15.5791  13.1858  54.9853 O.3         1 <1>          -0.4616
    24 C         17.7965  13.6084  55.6588 C.3         1 <1>          -0.0306
    25 C         16.4575  12.9819  56.0177 C.3         1 <1>          0.0900
    26 N         13.6363  18.9918  54.4045 N.pl3        1 <1>          0.0564
    27 O         13.3499  19.7552  55.2777 O.2         1 <1>          -0.1261
    28 O         14.6007  19.3132  53.5683 O.2         1 <1>          -0.1261
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    30 H         14.5389  14.4991  52.3586 H           1 <1>          0.0450
    31 H         13.0158  14.6150  48.3901 H           1 <1>          0.0350
    32 H         12.2914  16.2599  48.4527 H           1 <1>          0.0350
    33 H         11.6786  12.4902  48.9965 H           1 <1>          0.0331
    34 H         10.1485  12.7605  49.8846 H           1 <1>          0.0331
    35 H         11.0800  13.8000  46.9809 H           1 <1>          0.0235
    36 H          9.4058  13.8900  47.6370 H           1 <1>          0.0235
    37 H         10.2523  15.3927  47.1116 H           1 <1>          0.0235
    38 H          8.9571  14.9430  49.8791 H           1 <1>          0.0235
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     39 H         10.2828  15.5853  50.8949 H         1 <1>          0.0235
     40 H          9.8243  16.4403  49.3813 H         1 <1>          0.0235
     41 H         14.5080  16.8066  53.1164 H         1 <1>          0.0643
     42 H         11.1883  18.3708  55.3816 H         1 <1>          0.0640
     43 H         10.0114  16.2311  55.1226 H         1 <1>          0.0618
     44 H         11.0439  14.3719  53.8887 H         1 <1>          0.0621
     45 H         11.8394   9.9300  53.1642 H         1 <1>          0.0290
     46 H         13.5007  10.1099  53.7834 H         1 <1>          0.0290
     47 H         12.0658  10.7485  54.7234 H         1 <1>          0.0290
     48 H         18.5267  13.4271  56.4758 H         1 <1>          0.0262
     49 H         18.1902  13.1611  54.7208 H         1 <1>          0.0262
     50 H         17.6794  14.7039  55.5171 H         1 <1>          0.0262
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Compound **12**

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     3 N           9.1297  14.0877  53.5123 N.pl3        1 <1>         -0.3205
     4 C           9.4333  14.0045  54.9029 C.2          1 <1>          0.0157
     5 C          10.6628  14.3836  55.3626 C.2          1 <1>          0.0650
     6 C          11.7159  14.9229  54.3857 C.3          1 <1>          0.0473
     7 C          12.2593  15.4172  51.8897 C.2          1 <1>          0.1621
     8 C          11.7567  15.7024  50.5017 C.3          1 <1>          0.0157
     9 C           9.6467  14.4821  51.0743 C.3          1 <1>         -0.0086
    10 O          13.4430  15.5658  52.1534 O.2          1 <1>         -0.2923
    11 C          12.0878  16.3391  54.7879 C.ar         1 <1>         -0.0315
    12 C          11.0616  14.3117  56.8157 C.2          1 <1>          0.3375
    13 O          10.1894  14.3238  57.6737 O.2          1 <1>         -0.2452
    14 C          11.1173  17.2041  55.3498 C.ar         1 <1>         -0.0121
    15 C          11.5158  18.4886  55.7068 C.ar         1 <1>          0.1665
    16 C          12.7810  18.9233  55.5318 C.ar         1 <1>          0.1662
    17 C          13.7716  18.1165  54.9818 C.ar         1 <1>         -0.0159
    18 C          13.4167  16.8085  54.6065 C.ar         1 <1>         -0.0540
    19 C           8.3448  13.4752  55.8079 C.3          1 <1>         -0.0260
    20 O          10.7859  19.4654  56.2511 O.3          1 <1>         -0.4526
    21 C          11.6224  20.5643  56.4295 C.3          1 <1>          0.2332
    22 O          12.8774  20.1839  55.9614 O.3          1 <1>         -0.4526
    23 C          10.8262  14.5618  50.0603 C.3          1 <1>         -0.0228
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      26 O        12.3632  14.2036  57.1913 O.3     1 <1>       -0.4616
      27 C        12.0771  12.7147  59.0673 C.3     1 <1>       -0.0306
      28 C        12.8181  13.9062  58.4637 C.3     1 <1>        0.0900
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      30 H        12.6031  14.2556  54.4594 H       1 <1>        0.0450
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      32 H        11.1598  16.6409  50.5395 H       1 <1>        0.0350
      33 H         8.9449  15.3347  50.9435 H       1 <1>        0.0331
      34 H         9.0739  13.5523  50.8632 H       1 <1>        0.0331
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      36 H        14.7813  18.4825  54.8489 H       1 <1>        0.0655
      37 H        14.1724  16.1622  54.1782 H       1 <1>        0.0622
      38 H         7.4307  13.2168  55.2340 H       1 <1>        0.0290
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      50 H        10.9879  12.9267  59.1064 H       1 <1>        0.0262
      51 H        12.2465  11.7932  58.4745 H       1 <1>        0.0262
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Compound **20**
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USER_CHARGES

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2 C 15.7811 15.6162 51.1329 C.2 1 <1> 0.0157
3 N 14.8420 15.7444 50.0712 N.pl3 1 <1> -0.3207
4 C 13.4376 15.6307 50.2452 C.2 1 <1> 0.0157
5 C 12.9215 15.4360 51.4871 C.2 1 <1> 0.0651

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 6 C        13.8471  15.3533  52.7042 C.3     1 <1>       0.0506
 7 C        16.3622  15.2645  53.5588 C.2     1 <1>       0.3375
 8 C        17.2442  15.7023  50.7460 C.3     1 <1>      -0.0260
 9 O        17.4103  15.8841  53.4931 O.2     1 <1>      -0.2452
10 C        13.5063  16.5268  53.6198 C.ar    1 <1>      -0.0350
11 C        11.4443  15.2922  51.7559 C.2     1 <1>       0.3375
12 O        10.6520  15.0410  50.8598 O.2     1 <1>      -0.2452
13 C        12.8437  16.3420  54.8490 C.ar    1 <1>      -0.0566
14 C        12.5354  17.4357  55.6629 C.ar    1 <1>      -0.0475
15 C        12.8810  18.7287  55.2636 C.ar    1 <1>       0.0179
16 C        13.5316  18.9296  54.0445 C.ar    1 <1>      -0.0475
17 C        13.8398  17.8395  53.2267 C.ar    1 <1>      -0.0566
18 C        12.5797  15.7332  49.0033 C.3     1 <1>      -0.0260
19 Br       12.4561  20.2197  56.3784 Br      1 <1>      -0.0503
20 O        16.2245  14.4751  54.6610 O.3     1 <1>      -0.4616
21 C        18.1785  13.2265  55.1097 C.3     1 <1>      -0.0306
22 C        17.1338  14.1881  55.6549 C.3     1 <1>       0.0900
23 O        10.9916  15.4193  53.0316 O.3     1 <1>      -0.4616
24 C         8.9532  14.1497  52.9592 C.3     1 <1>      -0.0306
25 C         9.6654  15.4190  53.4215 C.3     1 <1>       0.0900
26 H        15.2010  15.9015  49.1177 H       1 <1>       0.1516
27 H        13.6055  14.3768  53.1556 H       1 <1>       0.0451
28 H        17.7250  16.5834  51.2177 H       1 <1>       0.0290
29 H        17.7706  14.7683  51.0358 H       1 <1>       0.0290
30 H        17.3704  15.8290  49.6507 H       1 <1>       0.0290
31 H        12.5427  15.3609  55.1809 H       1 <1>       0.0621
32 H        12.0229  17.2767  56.6029 H       1 <1>       0.0629
33 H        13.7976  19.9300  53.7282 H       1 <1>       0.0629
34 H        14.3419  18.0179  52.2839 H       1 <1>       0.0621
35 H        13.1965  15.8884  48.0937 H       1 <1>       0.0290
36 H        12.0055  14.7944  48.8556 H       1 <1>       0.0290
37 H        11.8904  16.5996  49.0842 H       1 <1>       0.0290
38 H        18.9167  12.9841  55.9033 H       1 <1>       0.0262
39 H        17.6921  12.2866  54.7723 H       1 <1>       0.0262
40 H        18.7117  13.6885  54.2514 H       1 <1>       0.0262
41 H        17.6678  15.0879  55.9769 H       1 <1>       0.0695
42 H        16.6178  13.7050  56.5129 H       1 <1>       0.0695
43 H         7.8834  14.1962  53.2527 H       1 <1>       0.0262
44 H         9.0192  14.0611  51.8538 H       1 <1>       0.0262
45 H         9.4052  13.2484  53.4217 H       1 <1>       0.0262
46 H         9.5888  15.5343  54.5247 H       1 <1>       0.0695
47 H         9.1630  16.2874  52.9457 H       1 <1>       0.0695
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Compound **21**
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 3 N        14.7937  15.7612  50.0869 N.pl3      1 <1>         -0.3207
 4 C        13.4062  15.6809  50.3771 C.2        1 <1>          0.0157
 5 C        12.9893  15.5347  51.6622 C.2        1 <1>          0.0652
 6 C        14.0090  15.4702  52.8028 C.3        1 <1>          0.0507
 7 C        16.5831  15.3575  53.4539 C.2        1 <1>          0.3375
 8 C        17.2417  15.6921  50.5671 C.3        1 <1>         -0.0260
 9 O        17.6095  16.0007  53.3137 O.2        1 <1>         -0.2452
10 C        13.7646  16.6768  53.7060 C.ar       1 <1>         -0.0324
11 C        11.5364  15.4292  52.0536 C.2        1 <1>          0.3375
12 O        10.6837  15.0651  51.2571 O.2        1 <1>         -0.2452
13 C        13.2454  16.5368  55.0081 C.ar       1 <1>         -0.0224
14 C        13.0225  17.6602  55.8104 C.ar       1 <1>          0.1237
15 C        13.3124  18.9369  55.3256 C.ar       1 <1>         -0.0264
16 C        13.8203  19.0939  54.0353 C.ar       1 <1>         -0.0588
17 C        14.0427  17.9748  53.2289 C.ar       1 <1>         -0.0575
18 C        12.4523  15.7627  49.2056 C.3        1 <1>         -0.0260
19 F        12.5183  17.5099  57.0599 F          1 <1>         -0.2055
20 O        11.1754  15.7220  53.3312 O.3        1 <1>         -0.4616
21 C         8.9337  14.8607  53.4035 C.3        1 <1>         -0.0306
22 C         9.8914  15.9940  53.7652 C.3        1 <1>          0.0900
23 O        16.5470  14.5573  54.5565 O.3        1 <1>         -0.4616
24 C        17.0277  13.2491  56.4633 C.3        1 <1>         -0.0306
25 C        17.5777  13.9267  55.2174 C.3        1 <1>          0.0900
26 H        15.0768  15.8819  49.1030 H          1 <1>          0.1516
27 H        13.7881  14.5128  53.3027 H          1 <1>          0.0451
28 H        17.7742  16.5776  50.9703 H          1 <1>          0.0290
29 H        17.7735  14.7573  50.8434 H          1 <1>          0.0290
30 H        17.2808  15.7829  49.4617 H          1 <1>          0.0290
31 H        12.9911  15.5673  55.4069 H          1 <1>          0.0649
32 H        13.1389  19.8057  55.9473 H          1 <1>          0.0646
33 H        14.0407  20.0841  53.6582 H          1 <1>          0.0619
34 H        14.4347  18.1188  52.2298 H          1 <1>          0.0621
35 H        12.9959  15.8777  48.2449 H          1 <1>          0.0290
36 H        11.8517  14.8314  49.1349 H          1 <1>          0.0290
37 H        11.7870  16.6448  49.3140 H          1 <1>          0.0290
38 H         7.9057  15.1248  53.7296 H          1 <1>          0.0262
39 H         8.9327  14.7038  52.3037 H          1 <1>          0.0262
40 H         9.2284  13.9153  53.9033 H          1 <1>          0.0262
41 H         9.8868  16.1789  54.8615 H          1 <1>          0.0695
42 H         9.5403  16.9160  53.2557 H          1 <1>          0.0695
43 H        17.8504  12.7393  57.0080 H          1 <1>          0.0262
44 H        16.5657  14.0037  57.1349 H          1 <1>          0.0262
45 H        16.2616  12.4956  56.1814 H          1 <1>          0.0262
46 H        18.0244  13.1410  54.5994 H          1 <1>          0.0695
47 H        18.3428  14.6720  55.5256 H          1 <1>          0.0695
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Compound **ORO**

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GASTEIGER
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2	C2	15.1684	19.0383	56.0343	C.ar	1 <1>	0.3273
3	O2	16.1884	18.8099	56.6980	O.2	1 <1>	-0.2467
4	N3	15.2971	19.0004	54.6954	N.am	1 <1>	-0.2751
5	C4	14.2816	19.2750	53.8624	C.ar	1 <1>	0.2547
6	O4	14.4025	19.2539	52.6529	O.2	1 <1>	-0.2677
7	C5	13.0952	19.6859	54.4171	C.ar	1 <1>	0.0334
8	C6	12.9367	19.7198	55.7900	C.ar	1 <1>	0.1375
9	C7	11.6583	20.2736	56.3202	C.2	1 <1>	0.4027
10	O71	10.7672	19.4398	56.3158	O.co2	1 <1>	-0.2389
11	O72	11.5619	21.4201	56.6956	O.co2	1 <1>	-0.2389
12	HN1	13.8714	19.5269	57.5586	H	1 <1>	0.1706
13	HN3	16.1663	18.6944	54.2953	H	1 <1>	0.1734
14	H5	12.2819	19.9392	53.7930	H	1 <1>	0.0695

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QLA active site

Compound **2**

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USER_CHARGES


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     3 N         17.6213  34.2307  64.1023 N.pl3       1 <1>         -0.3205
     4 C         17.7104  32.9118  64.6338 C.2         1 <1>          0.0157
     5 C         17.9113  32.7077  65.9776 C.2         1 <1>          0.0650
     6 C         17.9912  33.9301  66.9146 C.3         1 <1>          0.0471
     7 C         18.1451  36.5320  67.0339 C.2         1 <1>          0.1621
     8 C         18.3460  37.8435  66.3267 C.3         1 <1>          0.0157
     9 C         17.3546  37.9411  65.1574 C.3         1 <1>         -0.0228
    10 C         17.6306  36.7476  64.1977 C.3         1 <1>         -0.0086
    11 O         18.1396  36.4996  68.2547 O.2         1 <1>         -0.2923
    12 C         17.5654  39.2656  64.3994 C.3         1 <1>         -0.0591
    13 C         15.8936  37.9029  65.6735 C.3         1 <1>         -0.0591
    14 C         16.8197  33.8753  67.8884 C.ar        1 <1>         -0.0352
    15 C         17.9994  31.2950  66.5466 C.2         1 <1>          0.3375
    16 O         18.7314  31.0920  67.5004 O.2         1 <1>         -0.2452
    17 C         15.6814  34.6854  67.7213 C.ar        1 <1>         -0.0574
    18 C         14.6157  34.6115  68.6228 C.ar        1 <1>         -0.0586
    19 C         14.6644  33.7238  69.7071 C.ar        1 <1>         -0.0504
    20 C         15.7892  32.9065  69.8755 C.ar        1 <1>         -0.0586
    21 C         16.8542  32.9783  68.9746 C.ar        1 <1>         -0.0574
    22 C         17.6002  31.7808  63.6314 C.3         1 <1>         -0.0260
    23 C         13.5271  33.6349  70.6810 C.3         1 <1>         -0.0397
    24 O         17.2996  30.2093  66.1129 O.3         1 <1>         -0.4616
    25 C         16.1437  28.1648  65.8648 C.3         1 <1>         -0.0306
    26 C         16.8406  29.1210  66.8206 C.3         1 <1>          0.0900
    27 H         17.4709  34.3538  63.0896 H           1 <1>          0.1516
    28 H         18.9690  33.9227  67.4256 H           1 <1>          0.0450
    29 H         19.3766  37.8533  65.9072 H           1 <1>          0.0350
    30 H         18.2596  38.6941  67.0388 H           1 <1>          0.0350
    31 H         18.5834  36.8869  63.6413 H           1 <1>          0.0331
    32 H         16.8128  36.7182  63.4445 H           1 <1>          0.0331
    33 H         18.6048  39.3366  64.0120 H           1 <1>          0.0235
    34 H         16.8680  39.3392  63.5371 H           1 <1>          0.0235
    35 H         17.3868  40.1336  65.0704 H           1 <1>          0.0235
    36 H         15.1801  37.9860  64.8256 H           1 <1>          0.0235
    37 H         15.6626  36.9583  66.2089 H           1 <1>          0.0235
    38 H         15.7056  38.7486  66.3697 H           1 <1>          0.0235
    39 H         15.5972  35.3648  66.8871 H           1 <1>          0.0621
    40 H         13.7508  35.2449  68.4697 H           1 <1>          0.0620
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     41 H        15.8406  32.2117  70.7048 H        1 <1>          0.0620
     42 H        17.7113  32.3337  69.1251 H        1 <1>          0.0621
     43 H        17.4925  32.1642  62.5954 H        1 <1>          0.0290
     44 H        18.5167  31.1543  63.6614 H        1 <1>          0.0290
     45 H        16.6996  31.1649  63.8300 H        1 <1>          0.0290
     46 H        12.7083  34.3382  70.4184 H        1 <1>          0.0278
     47 H        13.1166  32.6032  70.6821 H        1 <1>          0.0278
     48 H        13.8892  33.8831  71.7009 H        1 <1>          0.0278
     49 H        15.7711  27.2802  66.4233 H        1 <1>          0.0262
     50 H        15.2832  28.6714  65.3777 H        1 <1>          0.0262
     51 H        16.8543  27.8225  65.0826 H        1 <1>          0.0262
     52 H        17.6940  28.5906  67.2964 H        1 <1>          0.0695
     53 H        16.0999  29.4200  67.5689 H        1 <1>          0.0695
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Compound **3**

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USER_CHARGES


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     2 C         17.3668  34.6661  64.3925 C.2          1 <1>          0.0158
     3 N         17.0533  33.4019  63.8380 N.pl3        1 <1>         -0.3205
     4 C         17.1691  32.1812  64.5635 C.2          1 <1>          0.0157
     5 C         17.5915  32.1781  65.8708 C.2          1 <1>          0.0650
     6 C         17.8934  33.5237  66.5613 C.3          1 <1>          0.0471
     7 C         18.1932  36.0917  66.2108 C.2          1 <1>          0.1621
     8 C         18.3323  37.2547  65.2682 C.3          1 <1>          0.0157
     9 C         17.1582  37.2423  64.2778 C.3          1 <1>         -0.0228
    10 C         17.2029  35.8937  63.5024 C.3          1 <1>         -0.0086
    11 O         18.3992  36.2540  67.4037 O.2          1 <1>         -0.2923
    12 C         17.2991  38.4092  63.2819 C.3          1 <1>         -0.0591
    13 C         15.8096  37.4004  65.0252 C.3          1 <1>         -0.0591
    14 C         16.9084  33.7144  67.7091 C.ar         1 <1>         -0.0350
    15 C         17.7086  30.8710  66.6488 C.2          1 <1>          0.3375
    16 O         18.4814  30.8167  67.5904 O.2          1 <1>         -0.2452
    17 C         15.9069  34.7005  67.6670 C.ar         1 <1>         -0.0542
    18 C         15.0105  34.8504  68.7286 C.ar         1 <1>         -0.0197
    19 C         15.0878  34.0211  69.8521 C.ar         1 <1>          0.1201
    20 C         16.0811  33.0246  69.8979 C.ar         1 <1>         -0.0197
    21 C         16.9768  32.8730  68.8367 C.ar         1 <1>         -0.0542
    22 C         16.8305  30.9173  63.7992 C.3          1 <1>         -0.0260
    23 O         16.9940  29.7336  66.4203 O.3          1 <1>         -0.4616
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  24 C        16.4725  27.4347  66.2771 C.3     1 <1>       -0.0306
  25 C        16.9108  28.5834  67.1724 C.3     1 <1>        0.0900
  26 O        14.1916  34.2103  70.8550 O.3     1 <1>       -0.4951
  27 C        14.4093  33.9460  72.1913 C.3     1 <1>        0.0788
  28 H        16.7344  33.3741  62.8578 H       1 <1>        0.1516
  29 H        18.9437  33.5221  66.8987 H       1 <1>        0.0450
  30 H        19.2732  37.1176  64.6900 H       1 <1>        0.0350
  31 H        18.4140  38.2116  65.8300 H       1 <1>        0.0350
  32 H        18.0495  35.8685  62.7818 H       1 <1>        0.0331
  33 H        16.2657  35.8088  62.9097 H       1 <1>        0.0331
  34 H        18.2571  38.3366  62.7231 H       1 <1>        0.0235
  35 H        16.4665  38.3991  62.5456 H       1 <1>        0.0235
  36 H        17.2836  39.3839  63.8159 H       1 <1>        0.0235
  37 H        14.9641  37.4031  64.3041 H       1 <1>        0.0235
  38 H        15.6291  36.5736  65.7436 H       1 <1>        0.0235
  39 H        15.7883  38.3578  65.5890 H       1 <1>        0.0235
  40 H        15.7962  35.3480  66.8108 H       1 <1>        0.0622
  41 H        14.2457  35.6153  68.6746 H       1 <1>        0.0654
  42 H        16.1699  32.3606  70.7471 H       1 <1>        0.0654
  43 H        17.7301  32.0971  68.8947 H       1 <1>        0.0622
  44 H        16.5624  31.1385  62.7453 H       1 <1>        0.0290
  45 H        17.7064  30.2348  63.7842 H       1 <1>        0.0290
  46 H        15.9494  30.4121  64.2446 H       1 <1>        0.0290
  47 H        16.4046  26.4993  66.8719 H       1 <1>        0.0262
  48 H        15.4768  27.6532  65.8354 H       1 <1>        0.0262
  49 H        17.2088  27.2872  65.4586 H       1 <1>        0.0262
  50 H        17.9061  28.3394  67.6036 H       1 <1>        0.0695
  51 H        16.1566  28.6798  67.9599 H       1 <1>        0.0695
  52 H        13.4948  34.2017  72.7648 H       1 <1>        0.0660
  53 H        14.6296  32.8672  72.3384 H       1 <1>        0.0660
  54 H        15.2506  34.5632  72.5726 H       1 <1>        0.0660
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Compound **4**

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SMALL
USER_CHARGES


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     2 C          17.5112  32.5733  64.5868 C.2         1 <1>          0.0158
     3 N          16.7482  31.4891  64.0912 N.pl3       1 <1>          -0.3205
     4 C          16.5814  30.2638  64.7989 C.2         1 <1>          0.0157
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5	C	17.1614	30.0786	66.0309	C.2	1 <1> 0.0650
6	C	17.9604	31.2382	66.6609	C.3	1 <1> 0.0471
7	C	18.9862	33.6032	66.2553	C.2	1 <1> 0.1621
8	C	19.3431	34.7043	65.2958	C.3	1 <1> 0.0157
9	C	18.0948	35.0920	64.4891	C.3	1 <1> -0.0228
10	C	17.6105	33.8266	63.7233	C.3	1 <1> -0.0086
11	O	19.3999	33.6469	67.4036	O.2	1 <1> -0.2923
12	C	18.4468	36.1985	63.4765	C.3	1 <1> -0.0591
13	C	16.9812	35.6257	65.4257	C.3	1 <1> -0.0591
14	C	17.2596	31.6755	67.9424	C.ar	1 <1> -0.0350
15	C	16.9740	28.7689	66.7915	C.2	1 <1> 0.3375
16	O	17.1966	28.7506	67.9900	O.2	1 <1> -0.2452
17	C	17.6455	31.1789	69.2005	C.ar	1 <1> -0.0542
18	C	16.9945	31.5986	70.3635	C.ar	1 <1> -0.0196
19	C	15.9414	32.5303	70.2943	C.ar	1 <1> 0.1210
20	C	15.5624	33.0340	69.0463	C.ar	1 <1> -0.0196
21	C	16.2141	32.6172	67.8834	C.ar	1 <1> -0.0542
22	C	15.7634	29.1975	64.0987	C.3	1 <1> -0.0260
23	O	15.2762	32.9680	71.3944	O.3	1 <1> -0.4874
24	C	14.2327	33.8744	71.4021	C.3	1 <1> 0.1146
25	C	14.5036	35.0287	72.3350	C.ar	1 <1> -0.0104
26	C	15.4646	35.9838	71.9629	C.ar	1 <1> -0.0554
27	C	15.7472	37.0688	72.7982	C.ar	1 <1> -0.0614
28	C	15.0737	37.2110	74.0134	C.ar	1 <1> -0.0617
29	C	14.1160	36.2684	74.3953	C.ar	1 <1> -0.0614
30	C	13.8291	35.1813	73.5634	C.ar	1 <1> -0.0554
31	O	16.5418	27.5882	66.2665	O.3	1 <1> -0.4616
32	C	16.9973	25.4281	65.4289	C.3	1 <1> -0.0306
33	C	16.8133	26.2981	66.6629	C.3	1 <1> 0.0900
34	H	16.3020	31.5996	63.1682	H	1 <1> 0.1516
35	H	18.9960	30.9007	66.8378	H	1 <1> 0.0450
36	H	20.1036	34.3087	64.5863	H	1 <1> 0.0350
37	H	19.7951	35.5668	65.8338	H	1 <1> 0.0350
38	H	18.2969	33.5722	62.8863	H	1 <1> 0.0331
39	H	16.6188	34.0569	63.2753	H	1 <1> 0.0331
40	H	19.2462	35.8583	62.7833	H	1 <1> 0.0235
41	H	17.5564	36.4736	62.8708	H	1 <1> 0.0235
42	H	18.8091	37.1089	64.0015	H	1 <1> 0.0235
43	H	16.0848	35.9163	64.8367	H	1 <1> 0.0235
44	H	16.6576	34.8659	66.1675	H	1 <1> 0.0235
45	H	17.3368	36.5202	65.9810	H	1 <1> 0.0235
46	H	18.4623	30.4803	69.2979	H	1 <1> 0.0622
47	H	17.3224	31.1941	71.3116	H	1 <1> 0.0654
48	H	14.7576	33.7553	68.9765	H	1 <1> 0.0654
49	H	15.9000	33.0273	66.9315	H	1 <1> 0.0622
50	H	15.4319	29.5330	63.0939	H	1 <1> 0.0290
51	H	16.3730	28.2799	63.9590	H	1 <1> 0.0290
52	H	14.8405	28.9704	64.6703	H	1 <1> 0.0290
53	H	14.0864	34.2777	70.3761	H	1 <1> 0.0748
54	H	13.3030	33.3618	71.7333	H	1 <1> 0.0748
55	H	15.9956	35.8872	71.0235	H	1 <1> 0.0621

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     58 H        13.5951  36.3800  75.3375 H     1 <1>       0.0618
     59 H        13.0828  34.4668  73.8854 H     1 <1>       0.0621
     60 H        17.2198  24.3839  65.7347 H     1 <1>       0.0262
     61 H        16.0704  25.4337  64.8164 H     1 <1>       0.0262
     62 H        17.8408  25.8104  64.8153 H     1 <1>       0.0262
     63 H        17.7503  26.2744  67.2607 H     1 <1>       0.0695
     64 H        15.9791  25.8740  67.2291 H     1 <1>       0.0695
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Compound **6**

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USER_CHARGES


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     2 C         17.3357  34.5638  64.3820 C.2          1 <1>          0.0158
     3 N         16.9857  33.3075  63.8315 N.pl3        1 <1>         -0.3205
     4 C         17.0974  32.0824  64.5502 C.2          1 <1>          0.0157
     5 C         17.5519  32.0669  65.8466 C.2          1 <1>          0.0650
     6 C         17.8954  33.4045  66.5332 C.3          1 <1>          0.0471
     7 C         18.2327  35.9679  66.1835 C.2          1 <1>          0.1621
     8 C         18.3689  37.1317  65.2415 C.3          1 <1>          0.0157
     9 C         17.1703  37.1438  64.2809 C.3          1 <1>         -0.0228
    10 C         17.1716  35.7974  63.5003 C.3          1 <1>         -0.0086
    11 O         18.4714  36.1221  67.3713 O.2          1 <1>         -0.2923
    12 C         17.3069  38.3117  63.2855 C.3          1 <1>         -0.0591
    13 C         15.8439  37.3229  65.0624 C.3          1 <1>         -0.0591
    14 C         16.9432  33.6090  67.7060 C.ar         1 <1>         -0.0351
    15 C         17.6643  30.7551  66.6173 C.2          1 <1>          0.3375
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   16 O        18.3919  30.7103  67.5947 O.2     1 <1>       -0.2452
   17 C        15.9685  34.6250  67.6987 C.ar    1 <1>       -0.0566
   18 C        15.1016  34.7864  68.7834 C.ar    1 <1>       -0.0475
   19 C        15.1912  33.9355  69.8878 C.ar    1 <1>        0.0179
   20 C        16.1459  32.9165  69.9051 C.ar    1 <1>       -0.0475
   21 C        17.0136  32.7507  68.8227 C.ar    1 <1>       -0.0566
   22 C        16.7168  30.8277  63.7905 C.3     1 <1>       -0.0260
   23 Br       14.0035  34.1589  71.3664 Br      1 <1>       -0.0503
   24 O        16.9912  29.6024  66.3437 O.3     1 <1>       -0.4616
   25 C        16.4673  27.3041  66.1996 C.3     1 <1>       -0.0306
   26 C        16.8564  28.4630  67.1046 C.3     1 <1>        0.0900
   27 H        16.6422  33.2889  62.8594 H       1 <1>        0.1516
   28 H        18.9536  33.3826  66.8443 H       1 <1>        0.0450
   29 H        19.2924  36.9801  64.6394 H       1 <1>        0.0350
   30 H        18.4815  38.0850  65.8042 H       1 <1>        0.0350
   31 H        17.9994  35.7599  62.7586 H       1 <1>        0.0331
   32 H        16.2185  35.7314  62.9308 H       1 <1>        0.0331
   33 H        18.2492  38.2242  62.7026 H       1 <1>        0.0235
   34 H        16.4560  38.3191  62.5704 H       1 <1>        0.0235
   35 H        17.3221  39.2846  63.8229 H       1 <1>        0.0235
   36 H        14.9808  37.3432  64.3627 H       1 <1>        0.0235
   37 H        15.6667  36.4968  65.7825 H       1 <1>        0.0235
   38 H        15.8537  38.2785  65.6297 H       1 <1>        0.0235
   39 H        15.8566  35.2862  66.8532 H       1 <1>        0.0621
   40 H        14.3563  35.5711  68.7620 H       1 <1>        0.0629
   41 H        16.2161  32.2510  70.7560 H       1 <1>        0.0629
   42 H        17.7448  31.9526  68.8550 H       1 <1>        0.0621
   43 H        16.4268  31.0576  62.7442 H       1 <1>        0.0290
   44 H        17.5795  30.1294  63.7515 H       1 <1>        0.0290
   45 H        15.8379  30.3368  64.2560 H       1 <1>        0.0290
   46 H        16.3584  26.3772  66.8015 H       1 <1>        0.0262
   47 H        15.5014  27.5211  65.6953 H       1 <1>        0.0262
   48 H        17.2513  27.1422  65.4294 H       1 <1>        0.0262
   49 H        17.8223  28.2205  67.5989 H       1 <1>        0.0695
   50 H        16.0562  28.5732  67.8433 H       1 <1>        0.0695
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Compound **9**

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USER_CHARGES


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     3 N          17.7312  34.0555  64.5511 N.pl3        1 <1>          -0.3205
     4 C          17.6369  32.6964  64.9589 C.2          1 <1>          0.0157
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   5 C        17.6474  32.3462  66.2976 C.2      1 <1>       0.0651
   6 C        17.7427  33.4945  67.3550 C.3      1 <1>       0.0493
   7 C        18.1833  36.0768  67.6827 C.2      1 <1>       0.1621
   8 C        18.6121  37.3929  67.0947 C.3      1 <1>       0.0157
   9 C        17.7587  37.6845  65.8546 C.3      1 <1>      -0.0228
  10 C        17.9969  36.5301  64.8433 C.3      1 <1>      -0.0086
  11 O        18.0127  35.9972  68.8868 O.2      1 <1>      -0.2923
  12 C        18.1895  39.0202  65.2189 C.3      1 <1>      -0.0591
  13 C        16.2577  37.7865  66.2296 C.3      1 <1>      -0.0591
  14 C        16.4632  33.5738  68.2091 C.ar     1 <1>      -0.0050
  15 C        17.5630  30.8553  66.6898 C.2      1 <1>       0.3375
  16 O        18.0999  30.4897  67.7202 O.2      1 <1>      -0.2452
  17 C        16.2024  32.8709  69.4480 C.ar     1 <1>       0.1302
  18 C        14.9554  33.0857  70.0832 C.ar     1 <1>      -0.0312
  19 C        14.0051  33.9561  69.5617 C.ar     1 <1>      -0.0596
  20 C        14.2666  34.6496  68.3920 C.ar     1 <1>      -0.0613
  21 C        15.4748  34.4668  67.7299 C.ar     1 <1>      -0.0555
  22 C        17.5464  31.6992  63.8168 C.3      1 <1>      -0.0260
  23 O        16.9044  29.8551  66.0441 O.3      1 <1>      -0.4616
  24 C        15.8488  27.9044  65.2547 C.3      1 <1>      -0.0306
  25 C        16.6401  28.5566  66.3781 C.3      1 <1>       0.0900
  26 N        17.1281  31.9740  70.1000 N.pl3    1 <1>       0.0567
  27 O        18.2828  31.9832  69.7933 O.2      1 <1>      -0.1261
  28 O        16.7447  31.0989  70.9998 O.2      1 <1>      -0.1261
  29 H        17.7081  34.2793  63.5445 H        1 <1>       0.1516
  30 H        18.6623  33.3032  67.9139 H        1 <1>       0.0451
  31 H        19.6740  37.3015  66.7748 H        1 <1>       0.0350
  32 H        18.5533  38.2033  67.8550 H        1 <1>       0.0350
  33 H        19.0096  36.5929  64.3879 H        1 <1>       0.0331
  34 H        17.2596  36.6442  64.0182 H        1 <1>       0.0331
  35 H        19.2633  38.9935  64.9339 H        1 <1>       0.0235
  36 H        17.5930  39.2293  64.3044 H        1 <1>       0.0235
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  40 H        16.0965  38.6021  66.9672 H        1 <1>       0.0235
  41 H        14.7092  32.5802  71.0081 H        1 <1>       0.0640
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  44 H        15.6365  35.0312  66.8201 H        1 <1>       0.0621
  45 H        17.5846  32.1977  62.8260 H        1 <1>       0.0290
  46 H        18.4045  30.9950  63.8519 H        1 <1>       0.0290
  47 H        16.5799  31.1547  63.8490 H        1 <1>       0.0290
  48 H        15.6026  26.8567  65.5290 H        1 <1>       0.0262
  49 H        14.9021  28.4602  65.0808 H        1 <1>       0.0262
  50 H        16.4454  27.9021  64.3181 H        1 <1>       0.0262
  51 H        17.5831  27.9919  66.5118 H        1 <1>       0.0695
  52 H        15.9947  28.5473  67.2605 H        1 <1>       0.0695
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Compound **10**
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USER_CHARGES

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3 N 16.4906 31.5394 64.2132 N.pl3 1 <1> -0.3205
4 C 16.3363 30.2548 64.8096 C.2 1 <1> 0.0157
5 C 17.0222 29.9138 65.9609 C.2 1 <1> 0.0650
6 C 17.9406 30.9887 66.6024 C.3 1 <1> 0.0472
7 C 19.1291 33.2940 66.2322 C.2 1 <1> 0.1621
8 C 19.4628 34.4388 65.3161 C.3 1 <1> 0.0157
9 C 18.1654 34.9852 64.7040 C.3 1 <1> -0.0228
10 C 17.4906 33.8268 63.9155 C.3 1 <1> -0.0086
11 O 19.6849 33.2139 67.3160 O.2 1 <1> -0.2923
12 C 18.4854 36.1427 63.7390 C.3 1 <1> -0.0591
13 C 17.2202 35.5208 65.8098 C.3 1 <1> -0.0591
14 C 17.3982 31.4274 67.9565 C.ar 1 <1> -0.0330
15 C 16.8620 28.5041 66.5636 C.2 1 <1> 0.3375
16 O 17.0460 28.3564 67.7588 O.2 1 <1> -0.2452
17 C 16.4369 32.4499 68.0601 C.ar 1 <1> -0.0274
18 C 15.9158 32.8369 69.3084 C.ar 1 <1> 0.1265
19 C 16.3644 32.1727 70.4647 C.ar 1 <1> -0.0315
20 C 17.3037 31.1448 70.3713 C.ar 1 <1> -0.0593
21 C 17.8137 30.7695 69.1284 C.ar 1 <1> -0.0575
22 C 15.3960 29.3181 64.0737 C.3 1 <1> -0.0260
23 O 16.4594 27.3647 65.9326 O.3 1 <1> -0.4616
24 C 17.8882 25.5111 66.2003 C.3 1 <1> -0.0306
25 C 16.4640 26.0394 66.2830 C.3 1 <1> 0.0900
26 N 14.9470 33.8821 69.3947 N.pl3 1 <1> 0.0564
27 O 14.4944 34.2048 70.4523 O.2 1 <1> -0.1261
28 O 14.5405 34.5075 68.3102 O.2 1 <1> -0.1261
29 H 15.9543 31.7656 63.3619 H 1 <1> 0.1516
30 H 18.9624 30.5736 66.6670 H 1 <1> 0.0450
31 H 20.0964 34.0458 64.4899 H 1 <1> 0.0350
32 H 20.0483 35.2176 65.8535 H 1 <1> 0.0350
33 H 18.0487 33.5921 62.9827 H 1 <1> 0.0331
34 H 16.4754 34.1665 63.6134 H 1 <1> 0.0331
35 H 19.1645 35.8031 62.9276 H 1 <1> 0.0235
36 H 17.5548 36.5324 63.2723 H 1 <1> 0.0235
37 H 18.9826 36.9770 64.2795 H 1 <1> 0.0235
38 H 16.2876 35.9253 65.3610 H 1 <1> 0.0235
39 H 16.9245 34.7287 66.5290 H 1 <1> 0.0235
40 H 17.7136 36.3371 66.3801 H 1 <1> 0.0235

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     41 H        16.0917  32.9415  67.1589 H     1 <1>       0.0643
     42 H        15.9840  32.4435  71.4413 H     1 <1>       0.0640
     43 H        17.6359  30.6348  71.2663 H     1 <1>       0.0618
     44 H        18.5367  29.9649  69.0788 H     1 <1>       0.0621
     45 H        14.9749  29.7881  63.1607 H     1 <1>       0.0290
     46 H        15.9398  28.4080  63.7435 H     1 <1>       0.0290
     47 H        14.5292  29.0539  64.7146 H     1 <1>       0.0290
     48 H        17.9029  24.4303  66.4558 H     1 <1>       0.0262
     49 H        18.2865  25.6413  65.1711 H     1 <1>       0.0262
     50 H        18.5403  26.0585  66.9137 H     1 <1>       0.0262
     51 H        16.1152  25.8993  67.3236 H     1 <1>       0.0695
     52 H        15.8813  25.4753  65.5451 H     1 <1>       0.0695
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Compound **12**

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SMALL
USER_CHARGES


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     2 C         16.2760  33.4088  66.7675 C.2          1 <1>          0.0158
     3 N         15.2173  33.4060  67.7126 N.pl3        1 <1>          -0.3205
     4 C         15.0760  34.4012  68.7237 C.2          1 <1>          0.0157
     5 C         15.9554  35.4448  68.7897 C.2          1 <1>          0.0650
     6 C         17.0870  35.5626  67.7601 C.3          1 <1>          0.0473
     7 C         18.2454  34.4354  65.7212 C.2          1 <1>          0.1621
     8 C         18.1521  33.4875  64.5578 C.3          1 <1>          0.0157
     9 C         16.3589  32.2440  65.7857 C.3          1 <1>          -0.0086
    10 O         19.2043  35.1857  65.8226 O.2          1 <1>          -0.2923
    11 C         16.9344  36.8689  67.0013 C.ar         1 <1>          -0.0315
    12 C         15.8783  36.5274  69.8373 C.2          1 <1>          0.3375
    13 O         15.8647  37.6985  69.4834 O.2          1 <1>          -0.2452
    14 C         17.8990  37.8966  67.1399 C.ar         1 <1>          -0.0121
    15 C         17.7124  39.0695  66.4149 C.ar         1 <1>          0.1665
    16 C         16.6528  39.2495  65.5993 C.ar         1 <1>          0.1662
    17 C         15.6753  38.2747  65.4295 C.ar         1 <1>          -0.0159
    18 C         15.8215  37.0704  66.1410 C.ar         1 <1>          -0.0540
    19 C         13.9323  34.2276  69.6962 C.3          1 <1>          -0.0260
    20 O         18.4830  40.1597  66.3828 O.3          1 <1>          -0.4526
    21 C         17.8884  41.0679  65.5107 C.3          1 <1>          0.2332
    22 O         16.7310  40.4571  65.0350 O.3          1 <1>          -0.4526
    23 C         17.7360  32.1005  65.0724 C.3          1 <1>          -0.0228
    24 C         17.5986  31.1219  63.8901 C.3          1 <1>          -0.0591
    25 C         18.8012  31.5386  66.0469 C.3          1 <1>          -0.0591
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```
   26 O        15.7934  36.2311  71.1610 O.3     1 <1>       -0.4616
   27 C        15.6833  36.4923  73.5564 C.3     1 <1>       -0.0306
   28 C        15.5233  37.1300  72.1776 C.3     1 <1>        0.0900
   29 H        14.5460  32.6238  67.6824 H       1 <1>        0.1516
   30 H        18.0456  35.5544  68.3248 H       1 <1>        0.0450
   31 H        19.1063  33.4672  63.9861 H       1 <1>        0.0350
   32 H        17.3534  33.8580  63.8772 H       1 <1>        0.0350
   33 H        15.5400  32.4059  65.0511 H       1 <1>        0.0331
   34 H        16.1423  31.2878  66.3109 H       1 <1>        0.0331
   35 H        18.7604  37.7803  67.7855 H       1 <1>        0.0658
   36 H        14.8321  38.4369  64.7709 H       1 <1>        0.0655
   37 H        15.0735  36.2968  66.0223 H       1 <1>        0.0622
   38 H        13.3458  33.3123  69.4728 H       1 <1>        0.0290
   39 H        14.3219  34.1246  70.7309 H       1 <1>        0.0290
   40 H        13.2347  35.0882  69.6260 H       1 <1>        0.0290
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   42 H        17.6312  42.0033  66.0512 H       1 <1>        0.1166
   43 H        17.2790  30.1187  64.2461 H       1 <1>        0.0235
   44 H        18.5676  31.0131  63.3565 H       1 <1>        0.0235
   45 H        16.8429  31.4883  63.1618 H       1 <1>        0.0235
   46 H        19.7851  31.4506  65.5375 H       1 <1>        0.0235
   47 H        18.9315  32.1837  66.9406 H       1 <1>        0.0235
   48 H        18.5052  30.5294  66.4060 H       1 <1>        0.0235
   49 H        15.4197  37.2351  74.3386 H       1 <1>        0.0262
   50 H        15.0062  35.6173  73.6496 H       1 <1>        0.0262
   51 H        16.7279  36.1629  73.7285 H       1 <1>        0.0262
   52 H        16.1790  38.0227  72.0812 H       1 <1>        0.0695
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Compound **20**

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SMALL
USER_CHARGES


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     2 C         17.6559  35.3844  64.2253 C.2         1 <1>          0.0157
     3 N         17.2762  34.0795  63.8028 N.pl3       1 <1>         -0.3207
     4 C         17.4216  32.9188  64.6073 C.2         1 <1>          0.0157
     5 C         17.9021  33.0271  65.8738 C.2         1 <1>          0.0651
     6 C         18.2743  34.3985  66.4443 C.3         1 <1>          0.0506
     7 C         18.5737  36.9900  65.9358 C.2         1 <1>          0.3375
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 8 C        17.4872  36.4933  63.2056 C.3        1 <1>        -0.0260
 9 O        19.3680  37.0992  66.8546 O.2        1 <1>        -0.2452
10 C        17.3492  34.6688  67.6286 C.ar       1 <1>        -0.0350
11 C        18.0990  31.8437  66.7880 C.2        1 <1>         0.3375
12 O        17.6002  30.7551  66.5425 O.2        1 <1>        -0.2452
13 C        16.1872  33.9049  67.8531 C.ar       1 <1>        -0.0566
14 C        15.3530  34.1808  68.9401 C.ar       1 <1>        -0.0475
15 C        15.6631  35.2222  69.8177 C.ar       1 <1>         0.0179
16 C        16.8074  35.9936  69.6050 C.ar       1 <1>        -0.0475
17 C        17.6430  35.7228  68.5184 C.ar       1 <1>        -0.0566
18 C        17.0247  31.5972  63.9870 C.3        1 <1>        -0.0260
19 Br       14.5192  35.5961  71.3004 Br         1 <1>        -0.0503
20 O        18.1009  38.1665  65.4365 O.3        1 <1>        -0.4616
21 C        17.5541  40.4196  64.9859 C.3        1 <1>        -0.0306
22 C        18.4359  39.4601  65.7702 C.3        1 <1>         0.0900
23 O        18.8728  31.9891  67.8963 O.3        1 <1>        -0.4616
24 C        17.9023  31.0949  69.9040 C.3        1 <1>        -0.0306
25 C        19.0441  31.0448  68.8912 C.3        1 <1>         0.0900
26 H        16.8997  33.9647  62.8500 H          1 <1>         0.1516
27 H        19.3288  34.2836  66.7452 H          1 <1>         0.0451
28 H        16.7447  37.2395  63.5547 H          1 <1>         0.0290
29 H        18.4655  36.9796  63.0060 H          1 <1>         0.0290
30 H        17.1057  36.1046  62.2387 H          1 <1>         0.0290
31 H        15.9043  33.1065  67.1854 H          1 <1>         0.0621
32 H        14.4621  33.5864  69.0964 H          1 <1>         0.0629
33 H        17.0499  36.8047  70.2795 H          1 <1>         0.0629
34 H        18.5237  36.3352  68.3701 H          1 <1>         0.0621
35 H        16.6615  31.7284  62.9464 H          1 <1>         0.0290
36 H        17.8994  30.9146  63.9469 H          1 <1>         0.0290
37 H        16.1989  31.1344  64.5669 H          1 <1>         0.0290
38 H        17.8168  41.4675  65.2436 H          1 <1>         0.0262
39 H        17.7033  40.2696  63.8954 H          1 <1>         0.0262
40 H        16.4852  40.2453  65.2340 H          1 <1>         0.0262
41 H        18.2535  39.6567  66.8315 H          1 <1>         0.0695
42 H        19.4981  39.6564  65.5075 H          1 <1>         0.0695
43 H        18.0875  30.3536  70.7095 H          1 <1>         0.0262
44 H        17.8421  32.1084  70.3551 H          1 <1>         0.0262
45 H        16.9321  30.8553  69.4227 H          1 <1>         0.0262
46 H        19.1323  30.0295  68.4468 H          1 <1>         0.0695
47 H        19.9892  31.2726  69.4276 H          1 <1>         0.0695
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Compound **21**

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USER_CHARGES


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     2 C          17.7986  35.0395  64.7247 C.2          1 <1>            0.0157
     3 N          17.6045  33.7703  64.1110 N.pl3        1 <1>           -0.3207
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   4 C        17.6219  32.5417  64.8222 C.2     1 <1>       0.0157
   5 C        17.7829  32.5412  66.1716 C.2     1 <1>       0.0652
   6 C        17.9318  33.8616  66.9325 C.3     1 <1>       0.0507
   7 C        18.1943  36.4991  66.7392 C.2     1 <1>       0.3375
   8 C        17.8122  36.2371  63.7956 C.3     1 <1>      -0.0260
   9 O        18.2395  36.5575  67.9562 O.2     1 <1>      -0.2452
  10 C        16.7404  33.9826  67.8797 C.ar    1 <1>      -0.0324
  11 C        17.8250  31.2808  66.9991 C.2     1 <1>       0.3375
  12 O        18.4315  31.2309  68.0592 O.2     1 <1>      -0.2452
  13 C        15.7014  34.9063  67.6522 C.ar    1 <1>      -0.0224
  14 C        14.6266  35.0023  68.5416 C.ar    1 <1>       0.1237
  15 C        14.5738  34.1810  69.6692 C.ar    1 <1>      -0.0264
  16 C        15.5985  33.2657  69.9136 C.ar    1 <1>      -0.0588
  17 C        16.6757  33.1674  69.0292 C.ar    1 <1>      -0.0575
  18 C        17.4583  31.2748  64.0114 C.3     1 <1>      -0.0260
  19 F        13.6362  35.8992  68.3115 F       1 <1>      -0.2055
  20 O        17.1491  30.1842  66.5641 O.3     1 <1>      -0.4616
  21 C        16.3985  27.9098  66.3745 C.3     1 <1>      -0.0306
  22 C        16.9996  28.9993  67.2601 C.3     1 <1>       0.0900
  23 O        18.2993  37.6968  66.0975 O.3     1 <1>      -0.4616
  24 C        18.2624  39.9721  65.4649 C.3     1 <1>      -0.0306
  25 C        18.2723  38.9738  66.6126 C.3     1 <1>       0.0900
  26 H        17.4706  33.7371  63.0894 H       1 <1>       0.1516
  27 H        18.8904  33.7540  67.4662 H       1 <1>       0.0451
  28 H        16.9669  36.9192  64.0203 H       1 <1>       0.0290
  29 H        18.7805  36.7742  63.8803 H       1 <1>       0.0290
  30 H        17.6923  35.9328  62.7351 H       1 <1>       0.0290
  31 H        15.7203  35.5702  66.8022 H       1 <1>       0.0649
  32 H        13.7417  34.2567  70.3573 H       1 <1>       0.0646
  33 H        15.5595  32.6323  70.7902 H       1 <1>       0.0619
  34 H        17.4618  32.4527  69.2387 H       1 <1>       0.0621
  35 H        17.3441  31.4954  62.9297 H       1 <1>       0.0290
  36 H        18.3553  30.6299  64.1232 H       1 <1>       0.0290
  37 H        16.5468  30.7289  64.3332 H       1 <1>       0.0290
  38 H        16.2548  26.9841  66.9704 H       1 <1>       0.0262
  39 H        15.4133  28.2421  65.9835 H       1 <1>       0.0262
  40 H        17.0667  27.6771  65.5202 H       1 <1>       0.0262
  41 H        17.9767  28.6726  67.6781 H       1 <1>       0.0695
  42 H        16.3022  29.1783  68.1054 H       1 <1>       0.0695
  43 H        18.2444  41.0071  65.8672 H       1 <1>       0.0262
  44 H        19.1729  39.8450  64.8415 H       1 <1>       0.0262
  45 H        17.3632  39.8166  64.8313 H       1 <1>       0.0262
  46 H        17.3610  39.1488  67.1937 H       1 <1>       0.0695
  47 H        19.1781  39.1521  67.2320 H       1 <1>       0.0695
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48 25 47 1

Compound **QLA**
@<TRIPOS>MOLECULE
*****|dQLA_minim|mol2|1|dock30
31 33 1
SMALL
USER_CHARGES

@<TRIPOS>ATOM

1	C	16.1184	25.0828	63.4861	C.ar	1 <1>	-0.0610
2	C	15.6680	26.0256	62.5611	C.ar	1 <1>	-0.0610
3	C	15.5869	27.3738	62.9181	C.ar	1 <1>	-0.0502
4	C	15.9583	27.7904	64.2099	C.ar	1 <1>	0.0346
5	C	16.4122	26.8400	65.1416	C.ar	1 <1>	0.0363
6	C	16.4891	25.4847	64.7715	C.ar	1 <1>	-0.0501
7	C	15.8805	29.2178	64.6058	C.2	1 <1>	0.2114
8	C	16.2992	29.6574	65.9708	C.2	1 <1>	0.1251
9	C	16.7086	28.7258	66.8766	C.2	1 <1>	0.1896
10	C	16.7947	27.2853	66.5013	C.2	1 <1>	0.2298
11	O	17.1728	26.4672	67.3273	O.2	1 <1>	-0.2833
12	O	15.4867	30.0487	63.7999	O.2	1 <1>	-0.2852
13	O	16.9929	29.0853	68.1498	O.3	1 <1>	-0.5019
14	N	16.1826	31.0563	66.2857	N.pl3	1 <1>	-0.3085
15	C	16.9647	32.1359	65.7618	C.ar	1 <1>	0.0316
16	C	17.7597	31.9041	64.6247	C.ar	1 <1>	-0.0378
17	C	18.5589	32.9193	64.0910	C.ar	1 <1>	-0.0247
18	C	18.5879	34.1776	64.6946	C.ar	1 <1>	0.1235
19	C	17.8241	34.4186	65.8382	C.ar	1 <1>	-0.0247
20	C	17.0218	33.4064	66.3743	C.ar	1 <1>	-0.0378
21	F	19.3662	35.1605	64.1785	F	1 <1>	-0.2055
22	H	16.1798	24.0389	63.2071	H	1 <1>	0.0618
23	H	15.3811	25.7116	61.5659	H	1 <1>	0.0618
24	H	15.2349	28.0884	62.1846	H	1 <1>	0.0625
25	H	16.8345	24.7368	65.4742	H	1 <1>	0.0625
26	H	17.5131	29.8699	68.3717	H	1 <1>	0.2924
27	H	15.3985	31.3269	66.8988	H	1 <1>	0.1524
28	H	17.7534	30.9336	64.1442	H	1 <1>	0.0637
29	H	19.1579	32.7275	63.2100	H	1 <1>	0.0647
30	H	17.8586	35.3892	66.3162	H	1 <1>	0.0647
31	H	16.4690	33.6221	67.2773	H	1 <1>	0.0637

@<TRIPOS>BOND

1	1	2	ar
2	1	6	ar
3	1	22	1
4	2	3	ar
5	2	23	1
6	3	4	ar
7	3	24	1
8	4	5	ar
9	4	7	1
10	5	6	ar
11	5	10	1
12	6	25	1
13	7	8	1
14	7	12	2
15	8	9	2
16	8	14	1
17	9	10	1
18	9	13	1

19 10 11 2
20 13 26 1
21 14 15 1
22 14 27 1
23 15 16 ar
24 15 20 ar
25 16 17 ar
26 16 28 1
27 17 18 ar
28 17 29 1
29 18 19 ar
30 18 21 1
31 19 20 ar
32 19 30 1
33 20 31 1