

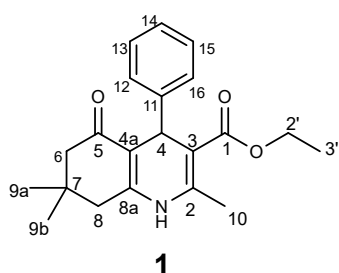
Supplementary Material

Anticancer Activity of 4-Aryl-1,4-Dihydropyridines

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Experimental: ^1H and ^{13}C NMR, 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 $^{13}\text{C}\{^1\text{H}\}$ 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 $\mu\text{L min}^{-1}$. 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.



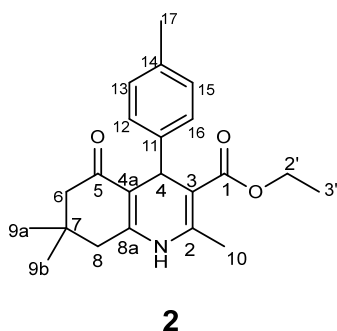
(±)-ethyl

2,7,7-trimethyl-5-oxo-4-phenyl-1,4,5,6,7,8-

hexahydroquinoline-3-carboxylate (1). White powder, 31% yield. ^1H

NMR (400 MHz, CDCl_3 , **Figure S1**): 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 , **Figure S2** and

S3): 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 (**Figure S4**): m/z 378 (5%, $[\text{M}+\text{K}]^+$), m/z 362 (49%, $[\text{M}+\text{Na}]^+$), m/z 340 (100%, $[\text{M}+\text{H}]^+$), m/z 262 (15%, $[\text{M}+\text{H}-\text{C}_6\text{H}_6]^+$).



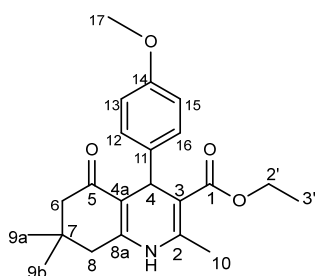
(±)-ethyl

2,7,7-trimethyl-5-oxo-4-(p-tolyl)-1,4,5,6,7,8-

hexahydroquinoline-3-carboxylate (2). Yellowish powder, 33% yield. ^1H

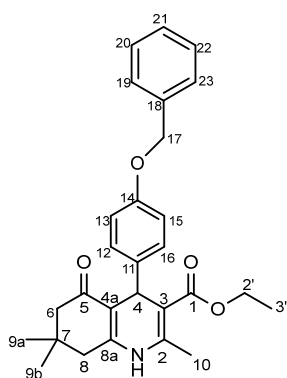
NMR (400 MHz, CDCl_3 , **Figure S5**): δ 0.94 (3H, s, H9b), 1.07 (3H, s, H9a), 1.21 (3H, t, $J = 7.1$ Hz, H3'), 2.13-2.30 (4H, m, H6 and H8), 2.25 (3H, s, H17), 2.35 (3H, s, H10), 4.05 (2H, q, $J = 7.1$ Hz, H2'), 5.01 (1H, s, H4), 6.99 (2H, d, $J = 7.9$ Hz, H13=H15), 7.18 (2H, d, $J = 7.9$ Hz, H12=H16). ^{13}C (400 MHz, CDCl_3 ,

Figure S6 and S7): δ 14.0 (CH₃, C3'), 19.3 (CH₃, C10), 20.9 (CH₃, C17), 27.1 (CH₃, C9a), 29.2 (CH₃, C9b), 32.6 (C, C7), 35.9 (CH, C4), 40.9 (CH₂, C8), 50.5 (CH₂, C6), 59.6 (CH₂, 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 (**Figure S8**): m/z 392 (5%, [M+K]⁺), m/z 376 (90%, [M+Na]⁺), m/z 354 (100%, [M+H]⁺), m/z 262 ([M+H-C₇H₇]⁺).



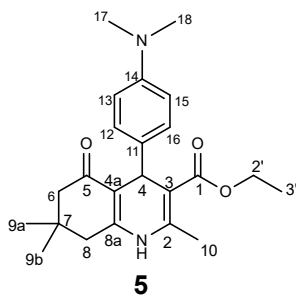
3

(±)-ethyl 4-(4-methoxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (3). Yellowish powder, 35% yield. NMR ¹H (400 MHz, CDCl₃, **Figure S9**): 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). ¹³C (400 MHz, CDCl₃, **Figure S10 and S11**): δ 14.1 (CH₃, C3'), 19.2 (CH₃, C10), 27.1 (CH₃, C9a), 29.2 (C9b CH₃), 32.4 (C, C7), 35.6 (CH, C4), 41.1 (CH₂, C8), 50.5 (CH₂, C6), 54.9 (CH₃, C17), 60.0 (CH₂, 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 (**Figure S12**): m/z 408 (5%, [M+K]⁺), m/z 392 (100%, [M+Na]⁺), m/z 370 (80%, [M+H]⁺), m/z 262 (100%, [M+H-C₇H₈O]⁺).

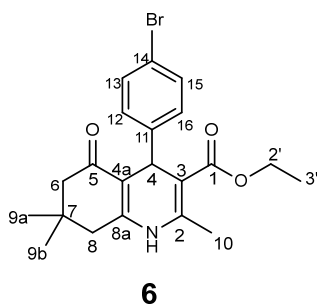


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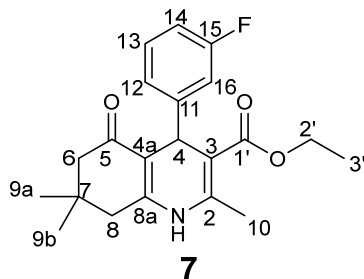
(±)-ethyl 4-(4(benzyloxy)phenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (4). Yellowish powder, 33% yield. ¹H NMR (400 MHz, CDCl₃, **Figure S13**): δ 0.94 (3H, s, H9b), 1.07 (3H, s, H9a), 1.20 (3H, *t*, *J* = 7.1 Hz, H3'), 2.13-2.30 (4H, *m*, H6 and H8), 2.37 (3H, s, H10), 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). ¹³C NMR (100 MHz, CDCl₃, **Figure S14 and S15**): δ 14.2 (CH₃, C3'), 19.7 (CH₃, C10), 27.4 (CH₃, C9a), 29.3 (CH₃, C9b), 32.8 (C, C7), 35.8 (CH, C4), 41.1 (CH₂, C8), 50.8 (CH₂, C6), 59.9 (CH₂, C2'), 70.0 (CH₂, 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 (**Figure S16**): m/z 484 (5%, [M+K]⁺), m/z 468 (50%, [M+Na]⁺), m/z 446 (40%, [M+H]⁺), m/z 262 ([M+H-C₁₃H₁₂O]⁺).



(±)-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. ^1H NMR (400 MHz, CDCl_3 , **Figure S17**): 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 , **Figure S18 and 19**): 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 (**Figure S20**): m/z 405 (35%, $[\text{M}+\text{Na}]^+$), m/z 383 (40%, $[\text{M}+\text{H}]^+$), m/z 262 (100%, $[\text{M}+\text{H}-\text{C}_6\text{H}_5\text{NMe}_2]^+$).

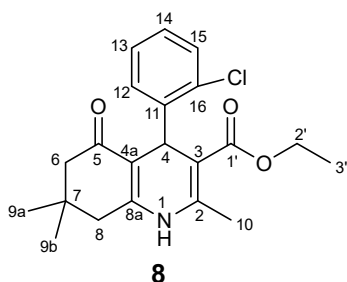


(±)-ethyl 4-(4-bromophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**6**). Yellowish powder, 39% yield. NMR ^1H (400 MHz, CDCl_3 , **Figure S21**): δ 0.92 (3H, s, H9a), 1.06 (3H, s, H9b), 1.19 (3H, t, $J = 7.1$ Hz, H3'), 2.12-2.29 (4H, m, H6 and H8), 2.36 (3H, s, H10), 4.04 (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 , **Figure S22 and 23**): 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 (**Figure S24**): m/z 440/442 (30%, $[\text{M}+\text{Na}]^+$), m/z 418/420 (100%, $[\text{M}+\text{H}]^+$), m/z 262 (50%, $[\text{M}+\text{H}-\text{C}_6\text{H}_5\text{Br}]^+$).



(±)-ethyl 4-(3-fluorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**7**). White powder, 39% yield. ^1H NMR (400 MHz, CDCl_3 , **Figure S25**): 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 , **Figure S26 and S27**): 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),

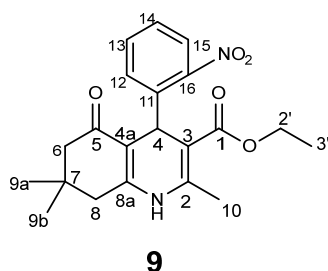
149.3 (C, C2), 163.9 (C, C15), 167.4 (C, C1'), 195.7 (C, C5). ESI(+)-MS (**Figure S28**): m/z 380 (45%, $[M+Na]^+$), m/z 358 (100%, $[M+H]^+$), m/z 262 (30%, $[M+H-C_6H_5F]^+$).



(±)-ethyl 4-(2-chlorophenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-

hexahydroquinoline-3-carboxylate (8). White powder, 40% yield. 1H NMR (400 MHz, $CDCl_3$, **Figure S29**): 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, $CDCl_3$, **Figure S30 and S31**): 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 (**Figure S32**): m/z 396 (100%, $[M+Na]^+$), m/z 374 (100%, $[M+H]^+$), m/z 262 (50%, $[M+H-C_6H_5Cl]^+$).

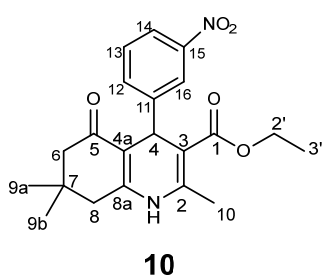


(±)-ethyl 2,7,7-trimethyl-4-(2-nitrophenyl)-5-oxo-1,4,5,6,7,8-

hexahydroquinoline-3-carboxylate (9). Yellowish powder, 38% yield.

1H NMR (400 MHz, $CDCl_3$, **Figure S33**): 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 and H8), 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, H13). ^{13}C NMR (100 MHz, $CDCl_3$, **Figure S34 and S35**): 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 (**Figure S36**): m/z 407 (55%, $[M+Na]^+$), m/z 385 (100%, $[M+H]^+$).



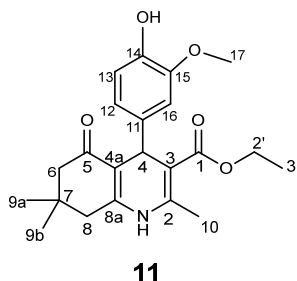
(±)-ethyl 2,7,7-trimethyl-4-(3-nitrophenyl)-5-oxo-1,4,5,6,7,8-

hexahydroquinoline-3-carboxylate (10). White powder, 30% yield.

1H NMR (400 MHz, $CDCl_3$, **Figure S37**): 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,

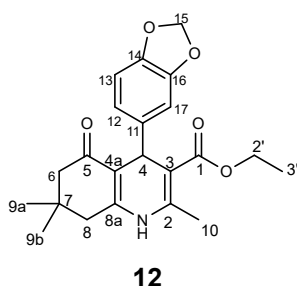
H14), 7.72 (1H, d, $J = 7.7$ Hz, H12), 7.97 (1H, d, $J = 8.2$ Hz, H15), 8.10 (1H, t, $J = 1.4$ Hz, H13). ^{13}C NMR

(100 MHz, $CDCl_3$, **Figure S38 and S29**): δ 14.2 (CH₃, C3'), 18.6 (CH₃, C10), 27.1 (CH₃, C9a), 29.6 (CH₃, C9b), 32.6 (C, C7), 35.4 (CH, C4), 41.6 (CH₂, C8), 51.0 (CH₂, C6), 59.5 (CH₂, 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 (**Figure S40**): m/z 378 (5%, [M+K]⁺), m/z 362 (70%, [M+Na]⁺), m/z 340 (15%, [M+H]⁺), m/z 262 (100%, [M+H-C₆H₅NO₂]⁺).



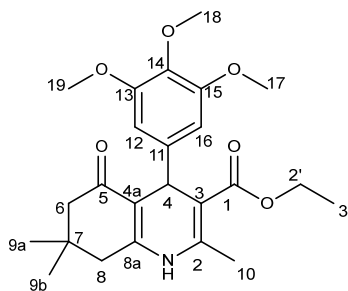
(±)-ethyl 4-(4-hydroxy-3-methoxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (11). Orangish powder, 35% yield. ¹H NMR (400 MHz, $CDCl_3$, **Figure S41**): δ 0.94 (3H, s, H9b), 1.07 (3H, s, H9a), 1.21 (3H, t, J = 7.1 Hz, H3'), 2.14-2.34 (4H, *m*, H6 and H8), 2.36 (3H, s, 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). ¹³C NMR (400 MHz, $CDCl_3$, **Figure S42 and S43**): δ 14.4 (CH₃, C3'), 19.5 (CH₃, C10), 27.1 (CH₃, C9a), 29.6 (CH₃, C9b), 32.7 (C, C7), 36.0 (CH, C4), 41.3 (CH₂, C8), 50.8 (CH₂, C6), 55.9 (CH₂, C2'), 59.7 (CH₃, 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 (**Figure S44**): m/z 408 (40%, [M+Na]⁺), m/z 386 (20%, [M+H]⁺), m/z 262 (100%, [M+H-C₇H₈O₂]⁺).



(±)-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. ¹H NMR (400 MHz, $CDCl_3$, **Figure S45**): 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

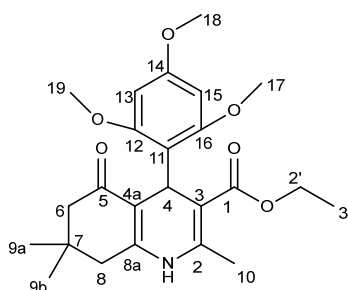
(1H, *d*, J = 7.9 Hz, H13), 6.76-6.80 (2H, *m*, H12 and H17). ¹³C NMR (100 MHz, $CDCl_3$, **Figure S46 and S47**): δ 14.1 (CH₃, C3'), 19.2 (CH₃, C10), 27.10 (CH₃, C9a), 29.2 (CH₃, C9b), 32.5 (C, C7), 36.1 (CH, C4), 40.9 (CH₂, C8), 50.5 (CH₂, C6), 59.7 (CH₂, C2'), 100.4 (CH₂, C15), 106.1 (C, C3), 107.5 (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 (**Figure S48**): m/z 406 (100%, [M+Na]⁺), m/z 384 (100%, [M+H]⁺), m/z 262 (70%, [M+H-C₇H₆O₂]⁺).



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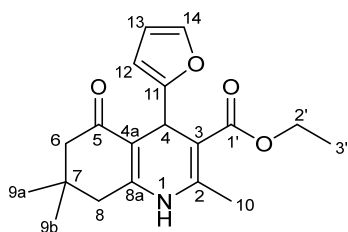
(±)-ethyl 2,7,7-trimethyl-5-oxo-4-(3,4,5-trimethoxyphenyl)-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**13**). White powder, 34% yield. ¹H NMR (400 MHz, CDCl₃, **Figure S49**): δ 0.97 (3H, s, H9b), 1.06 (3H, s, H9a), 1.23 (3H, t, *J* = 6.8 Hz, H3'), 2.21 (3H, s, H10), 2.34 (4H, s, H6-H8), 3.77 (9H, 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). ¹³C NMR (100 MHz, CDCl₃, **Figure S50** and

S51): δ 14.2 (CH₃, C3'), 19.7 (CH₃, C10), 27.1 (CH₃, C9a), 29.2 (CH₃, C9b), 32.9 (C, C7), 36.7 (CH, C4), 41.2 (CH₂, C8), 50.9 (CH₂, C6), 56.1 (CH₃, C19=C17), 59.9 (CH₂, C2'), 60.5 (CH₃, 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 (**Figure S52**): *m/z* 452 (55%, [M+Na]⁺), *m/z* 430 (190%, [M+H]⁺), *m/z* 262 (100%, [M+H-C₉H₁₂O₃]⁺).



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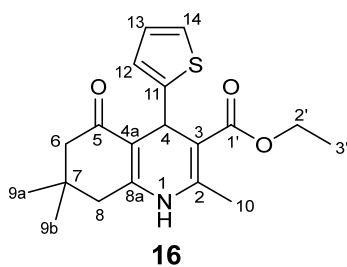
(±)-ethyl 2,7,7-trimethyl-5-oxo-4-(2,4,6-trimethoxyphenyl)-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**14**). White powder, 39% yield. ¹H NMR (400 MHz, CDCl₃, **Figure S53**): δ 0.90 (3H, s, H9b), 1.03 (3H, s, H9a), 1.24 (3H, t, *J* = 7.1 Hz, H3'), 2.01-2.19 (4H, m, H6 and H8), 2.25 (3H, s, H10), 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). ¹³C NMR (100 MHz, CDCl₃, **Figure S54** and **S55**): δ 14.1 (CH₃, C3'), 18.6 (CH₃, C10), 26.9 (CH₃, C9a), 29.67 (CH₃, C9b), 32.6 (C, C7), 35.4 (CH, C4), 41.8 (CH₂, C8), 51.1 (CH₂, C6), 55.9 (CH₃, C17=C19), 58.6 (CH₃, C18), 59.6 (CH₂, 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 (**Figure S56**): *m/z* 468 (12%, [M+K]⁺), *m/z* 452 (50%, [M+Na]⁺), *m/z* 430 (25%, [M+H]⁺), *m/z* 262 (100%, [M+H-C₉H₁₂O₃]⁺).



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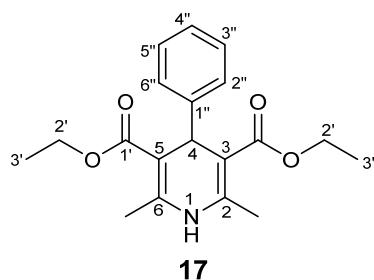
(±)-ethyl 4-(furan-2-yl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**15**). White powder, 30% yield. ¹H NMR (400 MHz, CDCl₃, **Figure S57**): δ 1.06 (3H, s, H9b), 1.08 (3H, s, H9a), 1.21 (3H, t, *J*=7.2 Hz, H3'), 2.19-2.34 (4H, m, H6-H8), 2.36 (3H, s, H10), 4.12 (2H, q, *J*=7.1 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). ¹³C NMR (100 MHz, CDCl₃, **Figure S58** and **S59**): δ 14.2 (CH₃, C3'), 19.4 (CH₃, C10), 27.5 (CH₃, C9a), 29.5 (CH₃, C9b), 32.8 (C, C7), 37.0 (CH, C4), 41.2 (CH₂, C8), 50.4 (CH₂, C6), 60.2 (CH₂, 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 (**Figure S60**): m/z 368 (5%, $[M+K]^+$), m/z 352 (90%, $[M+Na]^+$), m/z 330 (12%, $[M+H]^+$), m/z 262 (100%, $[M+H-C_4H_4O]^+$).

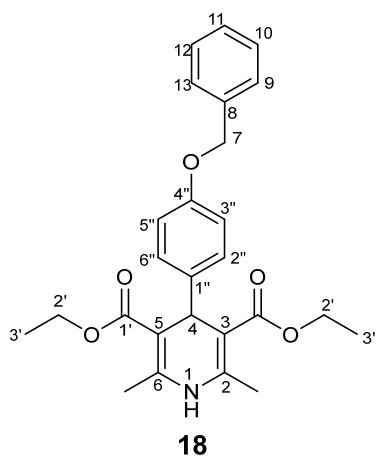


(±)-ethyl 2,7,7-trimethyl-5-oxo-4-(thiophen-2-yl)-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**16**). Beige powder, 38% yield. 1H NMR (400 MHz, $CDCl_3$, **Figure S61**): δ 1.03 (3H, *s*, H9b), 1.10 (3H, *s*, H9a), 1.25 (3H, *t*, $J = 7.1$ Hz, H3'), 2.21-2.36 (4H, *m*, H6-H8), 2.38 (3H, *s*, H10), 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, $CDCl_3$, **Figure S62 and S63**): δ 14.2 (CH₃, C3'), 19.4 (CH₃, C10), 27.2 (CH₃, C9a), 29.4 (CH₃, C9b), 32.7 (C, C7), 36.9 (CH, C4), 41.1 (CH₂, C8), 50.5 (CH₂, C6), 60.2 (CH₂, 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 (**Figure 64**):

m/z 368 (65%, $[M+Na]^+$), m/z 346 (30%, $[M+H]^+$), m/z 262 (100%, $[M+H-C_4H_4S]^+$).

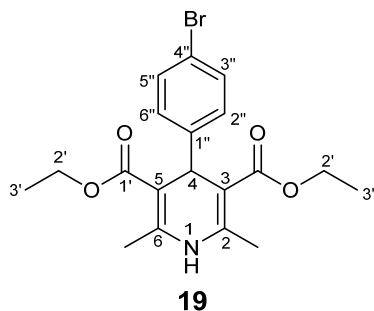


diethyl 2,6-dimethyl-4-phenyl-1,4-dihydropyridine-3,5-dicarboxylate (**17**). Yellow powder, 15% yield. 1H NMR (400 MHz, $CDCl_3$, **Figure S65**): 1.24 (6H, *t*, $J_{3',2'} = 7.1$ Hz, H3'), 2.33 (6H, *s*, 2=6-CH₃), 4.08 (4H, *q*, $J_{2',3'} = 7.1$ Hz, H2'), 4.98 (1H, *s*, H4), 7.15 – 7.32 (5H, *m*, H2''=H6'', H3''=H5'' and H4''). ^{13}C NMR (100 MHz, $CDCl_3$, **Figure S66 and S67**): δ 14.1 (CH₃, C3'), 19.4 (CH₃, 2=6-CH₃), 39.4 (CH, C4), 59.5 (CH₂, 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 (**Figure S68**): 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%, $[M+H-C_6H_6]^+$).



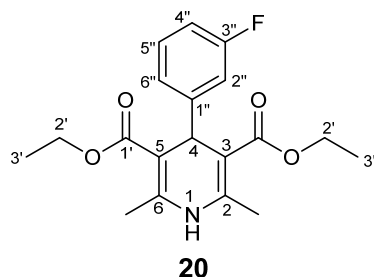
diethyl 4-(4-(benzyloxy)phenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (**18**). Yellow powder, 16% yield. NMR 1H (400 MHz, $CDCl_3$, **Figure S69**): 1.22 (6H, *t*, $J_{3',2'} = 7.1$ Hz, H3'), 2.32 (6H, *s*, 2=6-CH₃), 4.09 (4H, *q*, $J_{2',3'} = 7.1$ Hz, H2'), 4.93 (1H, *s*, H4), 5.00 (2H, *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, $CDCl_3$, **Figure S70 and S71**): δ 14.6 (CH₃, C3'), 19.4 (CH₃, 2=6-CH₃), 38.7 (CH, C4), 59.9 (CH₂, C2'), 70.2 (CH₂, 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 (**Figure S72**): m/z 474 (13%, [M+K]⁺), m/z 458 (100%, [M+Na]⁺), m/z 436 (10%, [M+H]⁺), m/z 252 (72%, [M+H-C₁₃H₁₂O]⁺).



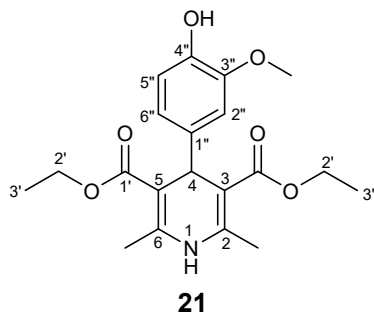
diethyl 4-(4-bromophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (19). Yellow powder, 19% yield. ¹H NMR (400 MHz, CDCl₃, **Figure S73**): 1.21 (6H, *t*, $J_{3',2'} = 7.1$ Hz, H3'), 1.60 (3H, *s*, $J = 7.1$ Hz, H3'), 2.32 (6H, *s*, 2=6-CH₃), 4.08 (4H, *q*, $J_{2',3'} = 4.3$ Hz, H2'), 4.93 (1H, *s*, H4), 7.16 (2H, *d*, $J = 8.4$ Hz, H2''=H6''), 7.33 (2H, *d*, $J = 8.4$ Hz, H3''=H5'')

¹³C NMR (100 MHz, CDCl₃, **Figure S74** and **S75**): δ 14.9 (CH₃, C3'), 20.1 (CH₃, 2=6-CH₃), 39.6 (CH, C4), 60.2 (CH₂, 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 (**Figure S76**): m/z 430/432 (100%, [M+Na]⁺), m/z 408/410 (10%, [M+H]⁺), m/z 362 (60%, [M+H-C₂H₆O]⁺), m/z 252 (15%, [M+H-C₆H₅Br]⁺).



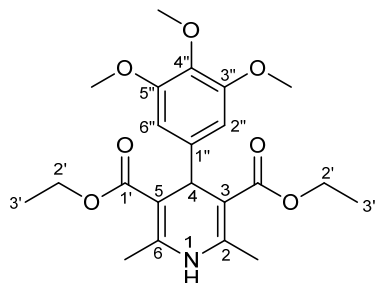
diethyl 4-(3-fluorophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (20). Yellow powder, 20% yield. ¹H NMR (400 MHz, CDCl₃, **Figure S81**): 1.22 (6H, *t*, $J_{3',2'} = 7.1$ Hz, H3'), 2.34 (6H, *s*, 2=6-CH₃), 4.09 (4H, *q*, $J_{2',3'} = 7.1$ Hz, H2'), 4.99 (1H, *s*, H4), 6.81 (1H, *t*, $J = 7.2$ 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''). ¹³C NMR (400 MHz, CDCl₃, **Figure S82** and **S83**): δ 14.3 (CH₃, C3'), 19.8 (CH₃, 2=6-CH₃), 39.7 (CH, C4), 59.9 (CH₂, 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 (**Figure S84**): m/z 386 (20%, [M+K]⁺), m/z 370 (100%, [M+Na]⁺), m/z 348 (60%, [M+H]⁺), m/z 302 (100%, [M+H-C₂H₆O]⁺), m/z 274 (25%, [M+H-C₂H₆O-CO]⁺), m/z 252 (20%, [M+H-C₆H₅F]⁺).

Figure S82 and **S83**): δ 14.3 (CH₃, C3'), 19.8 (CH₃, 2=6-CH₃), 39.7 (CH, C4), 59.9 (CH₂, 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 (**Figure S84**): m/z 386 (20%, [M+K]⁺), m/z 370 (100%, [M+Na]⁺), m/z 348 (60%, [M+H]⁺), m/z 302 (100%, [M+H-C₂H₆O]⁺), m/z 274 (25%, [M+H-C₂H₆O-CO]⁺), m/z 252 (20%, [M+H-C₆H₅F]⁺).



diethyl 4-(4''-hydroxy-3''-methoxyphenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (21). Yellow powder, 16% yield. NMR ¹H (400 MHz, CDCl₃, **Figure S81**): 1.22 (6H, *t*, $J_{3',2'} = 7.1$ Hz, H3'), 2.33 (6H, *s*, 2=6-CH₃), 3.84 (3H, *s*, 3-OCH₃), 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''). ¹³C (100 MHz, CDCl₃, **Figure S82** and **S83**): δ 14.4 (CH₃, C3'), 19.8 (CH₃,

2=6-CH₃), 39.2 (CH, C4), 55.9 (CH₃, 3''-OCH₃), 59.7 (CH₂, 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 (**Figure S84**): *m/z* 414 (8%, [M+K]⁺), *m/z* 398 (80%, [M+Na]⁺), *m/z* 376 (15%, [M+H]⁺), *m/z* 252 (100%, [M+H-C₇H₈O₂]⁺)



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diethyl 2,6-dimethyl-4-(3'',4'',5''-trimethoxyphenyl)-1,4-dihydropyridine-3,5-dicarboxylate (**22**). Yellowish powder, 20% yield. NMR ¹H (400 MHz, CDCl₃, **Figure S85**): 1.25 (6H, *t*, *J*_{3',2'} = 7.1 Hz, H3'), 2.34 (6H, *s*, 2=6-CH₃), 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''). ¹³C NMR (100 MHz, CDCl₃, **Figure S86 and S87**): δ 14.2 (CH₃, C3'), 19.5 (CH₃,

2=6-CH₃), 39.4 (CH, C4), 55.7 (CH₃, 3''=5''-OCH₃), 59.6 (CH₃, 4''-OCH₃), 60.5 (CH₂, 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 (**Figure S88**): *m/z* 442 (100%, [M+Na]⁺), *m/z* 420 (22%, [M+H]⁺), *m/z* 252 (85%, [M+H-C₉H₁₂O₃]⁺).

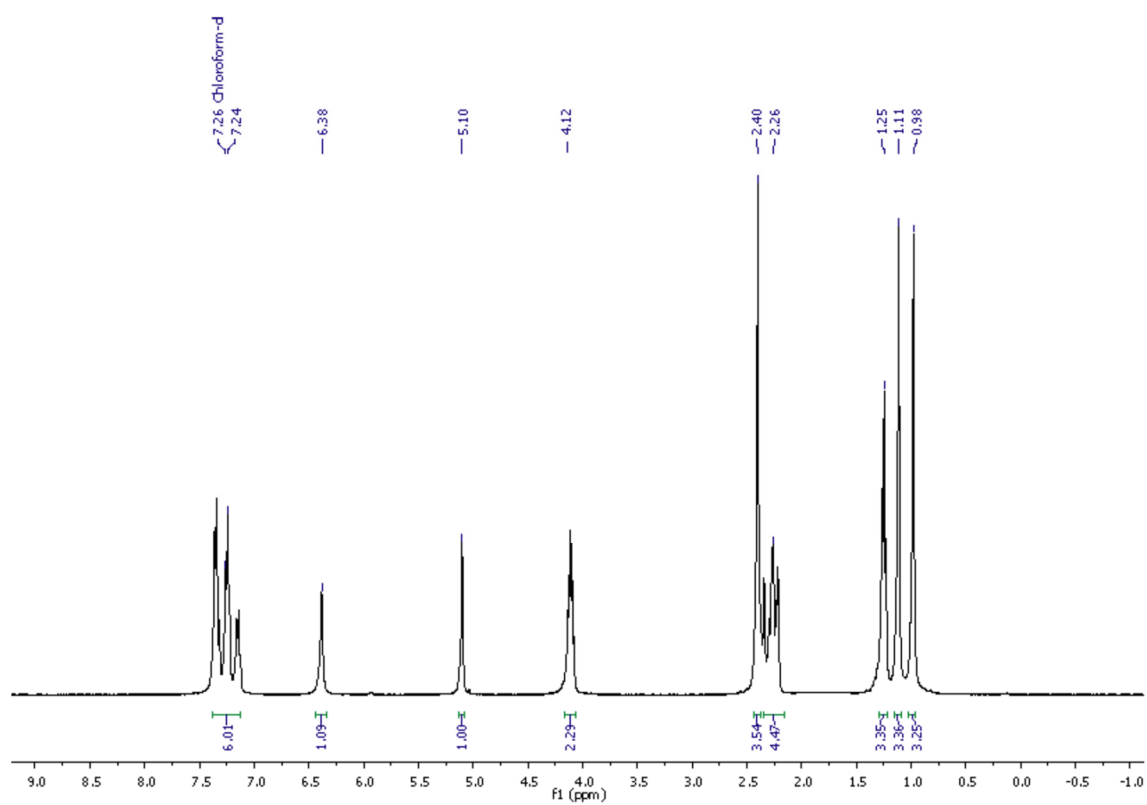


Figure S1. ¹H NMR spectrum of compound 1 (CDCl₃, 400 MHz, TMS).

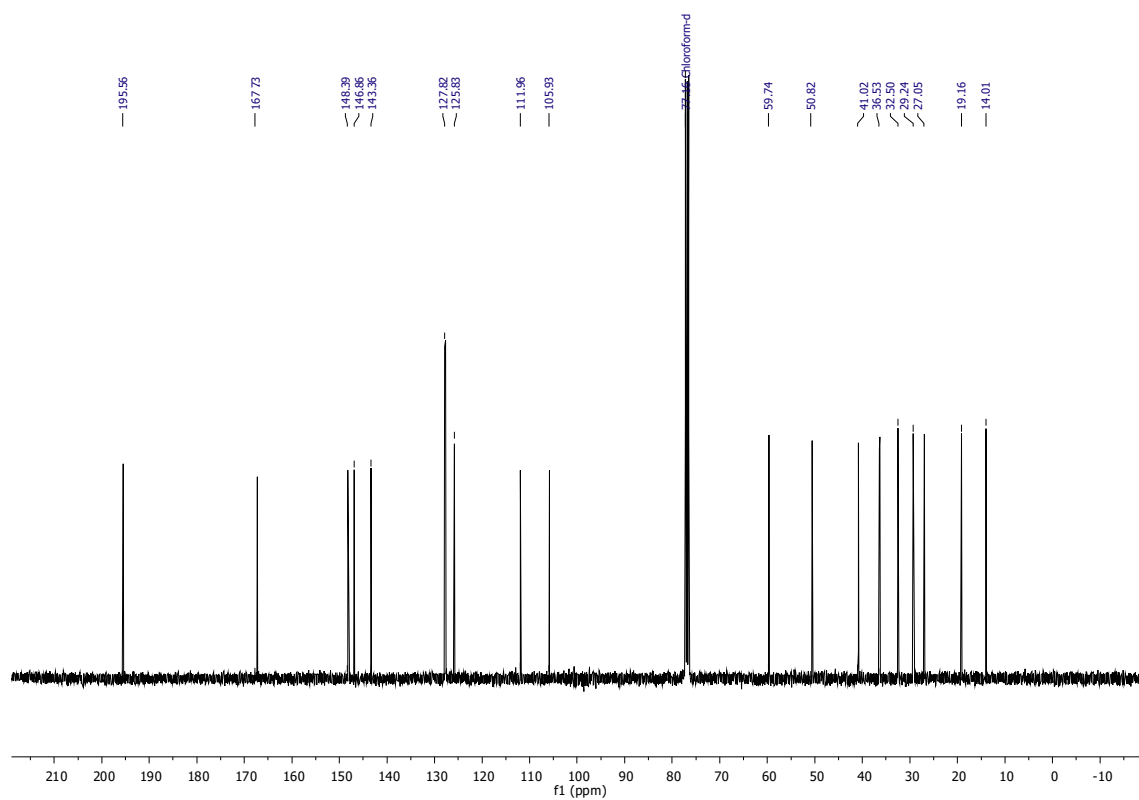


Figure S2. ¹³C NMR spectrum of compound 1 (CDCl₃, 100 MHz, TMS).

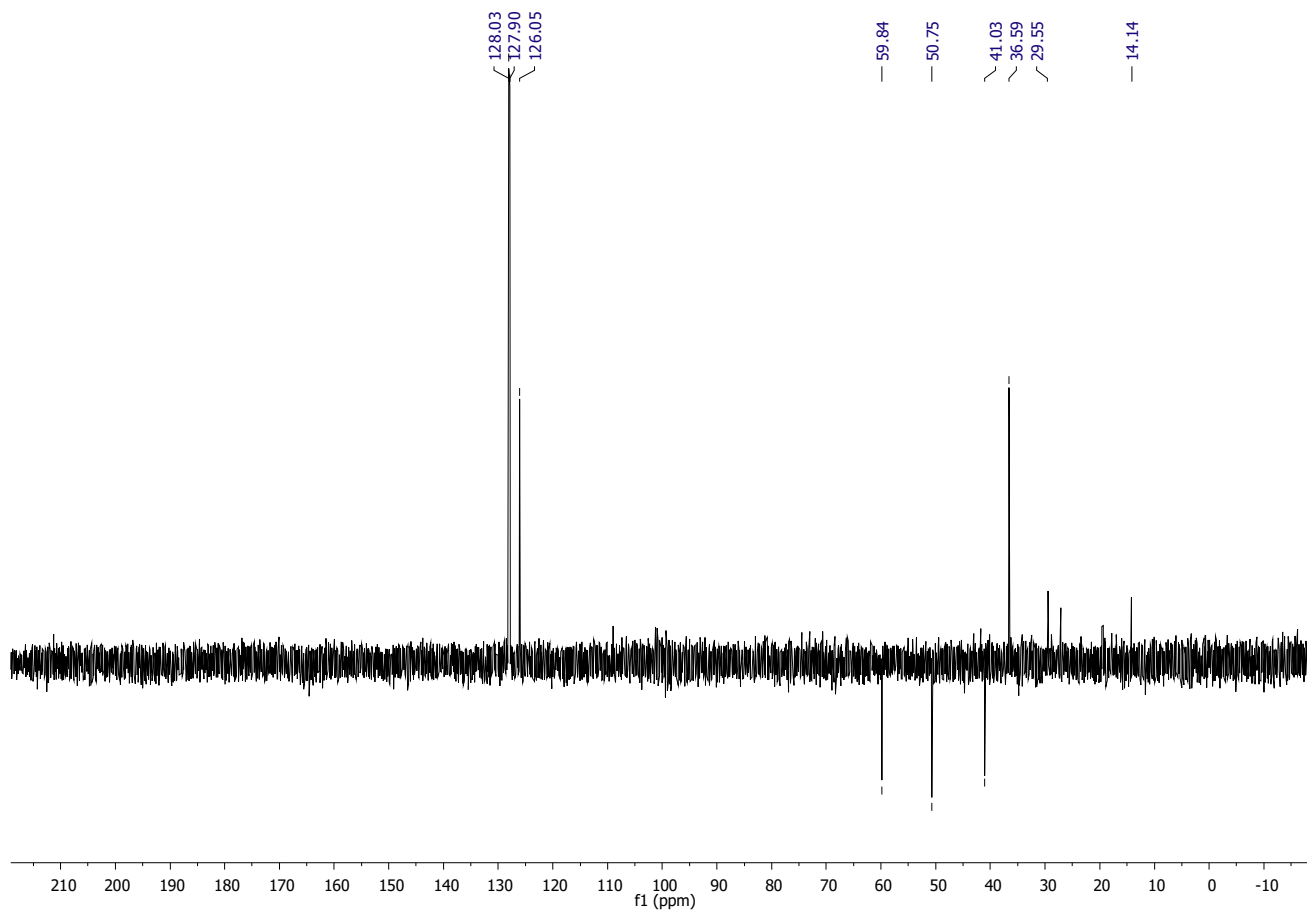


Figure S3. DEPT 135 spectrum of compound **1** (CDCl₃, 100 MHz, TMS).

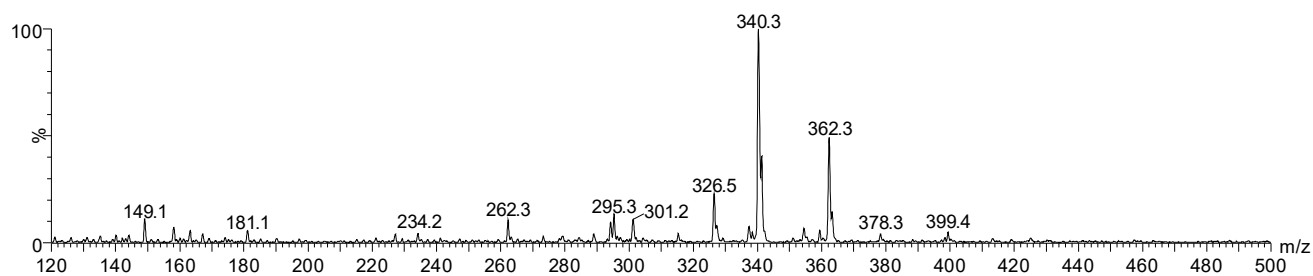


Figure S4. ESI (+) mass spectrum of compound **1**.

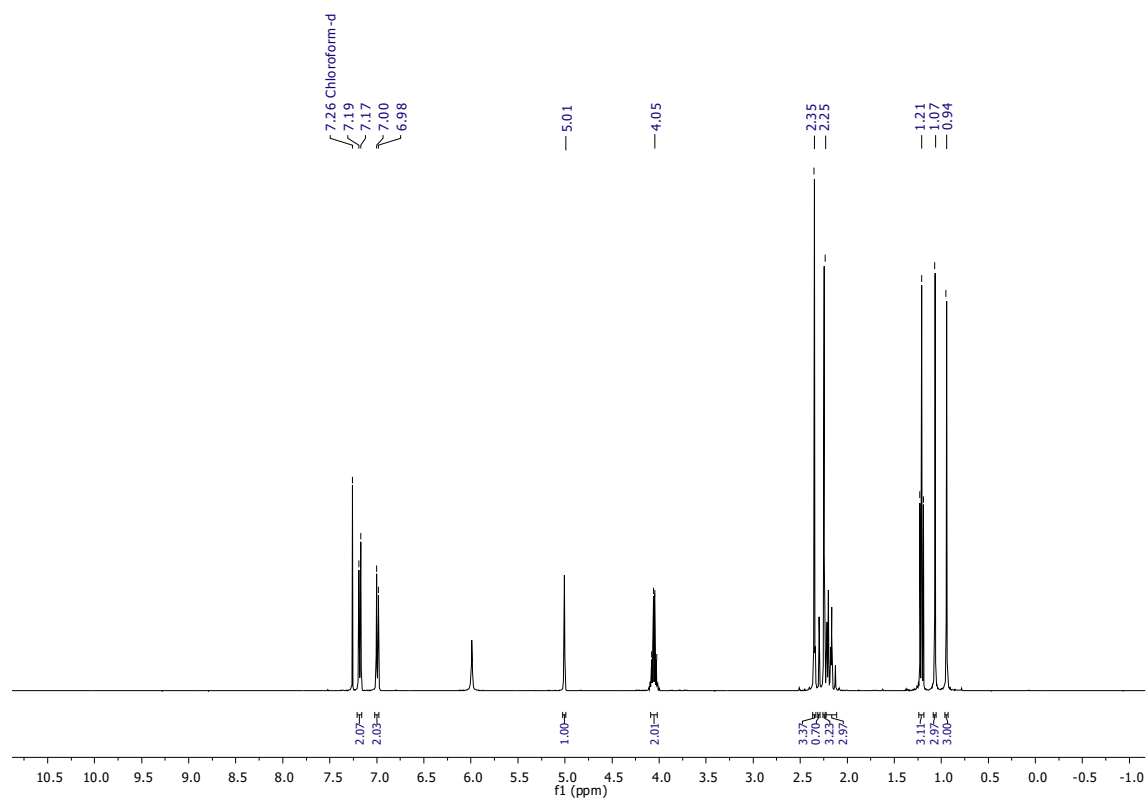


Figure S5. ¹H NMR spectrum of compound 2 (CDCl₃, 400 MHz, TMS).

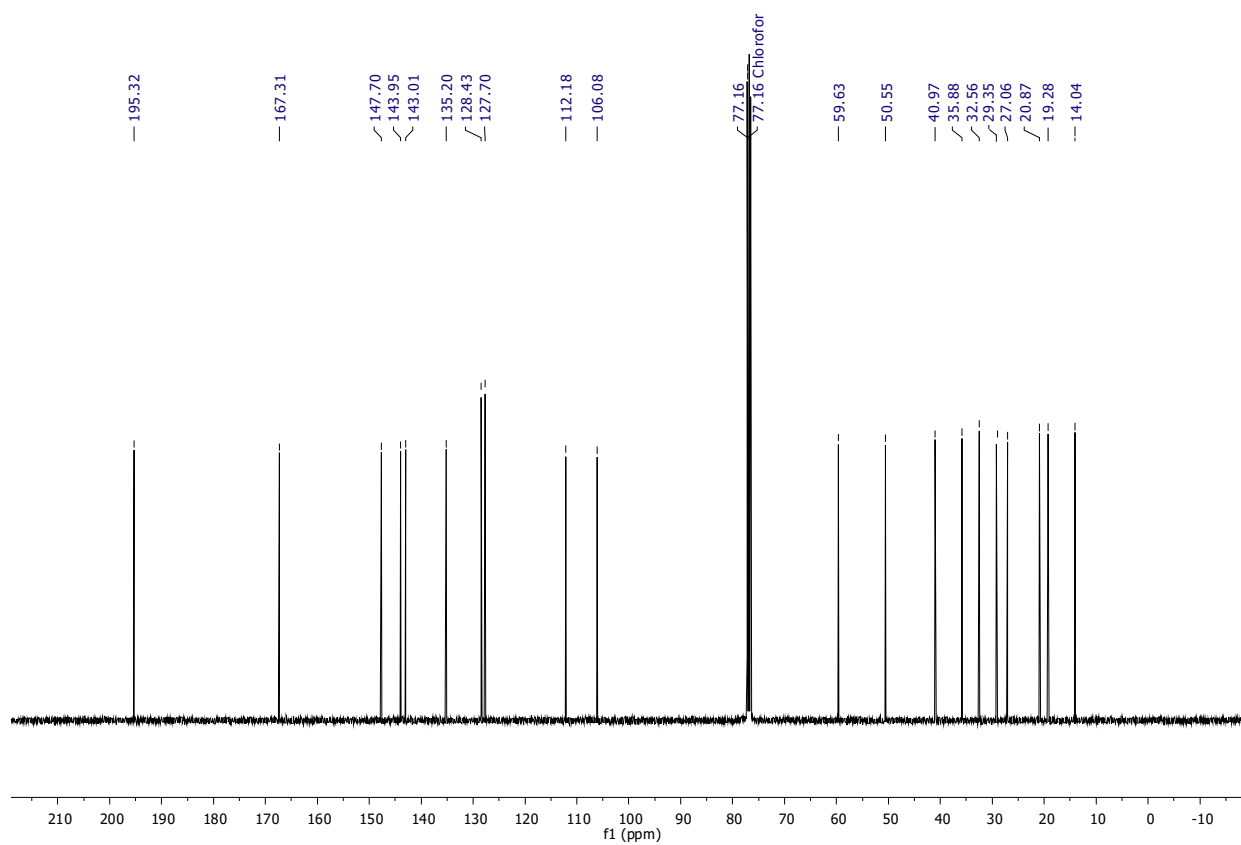


Figure S6. ¹³C NMR spectrum of compound 2 (CDCl₃, 100 MHz, TMS).

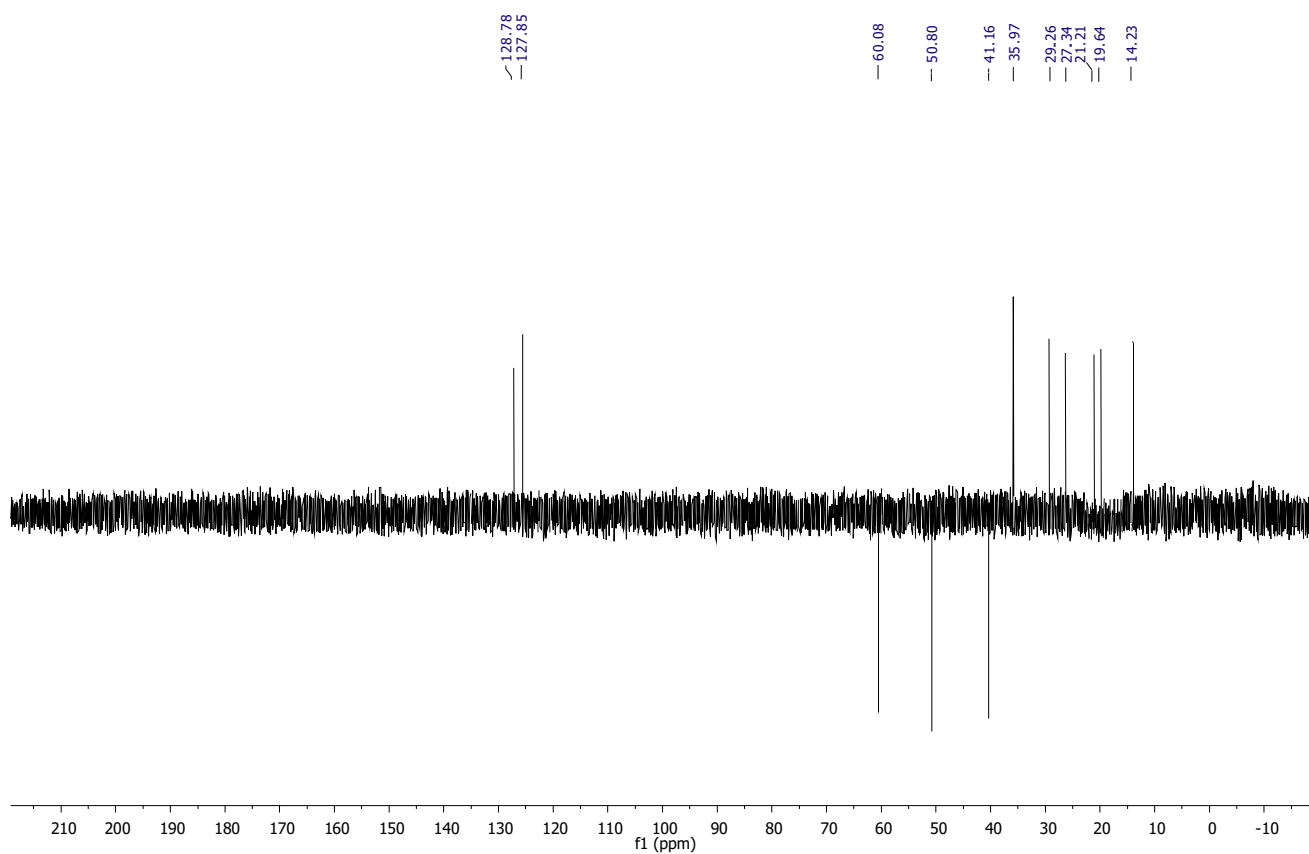


Figure S7. ¹³C NMR spectrum of compound 2 (CDCl₃, 100 MHz, TMS).

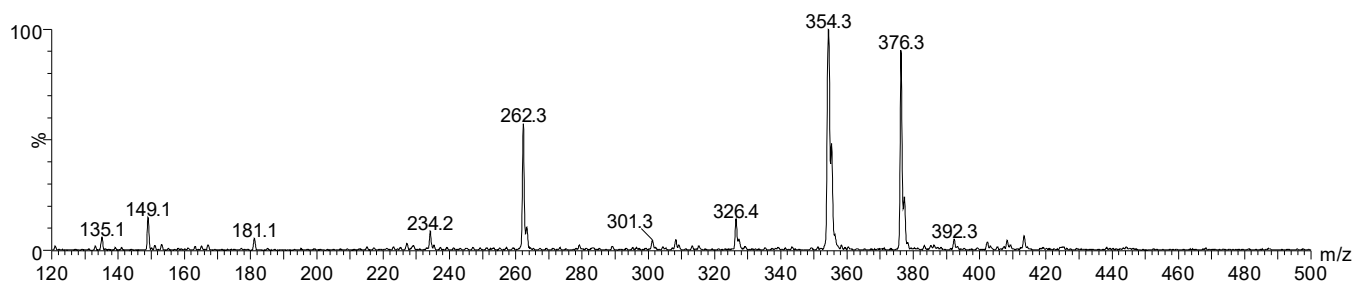


Figure S8. ESI (+) mass spectrum of compound 2.

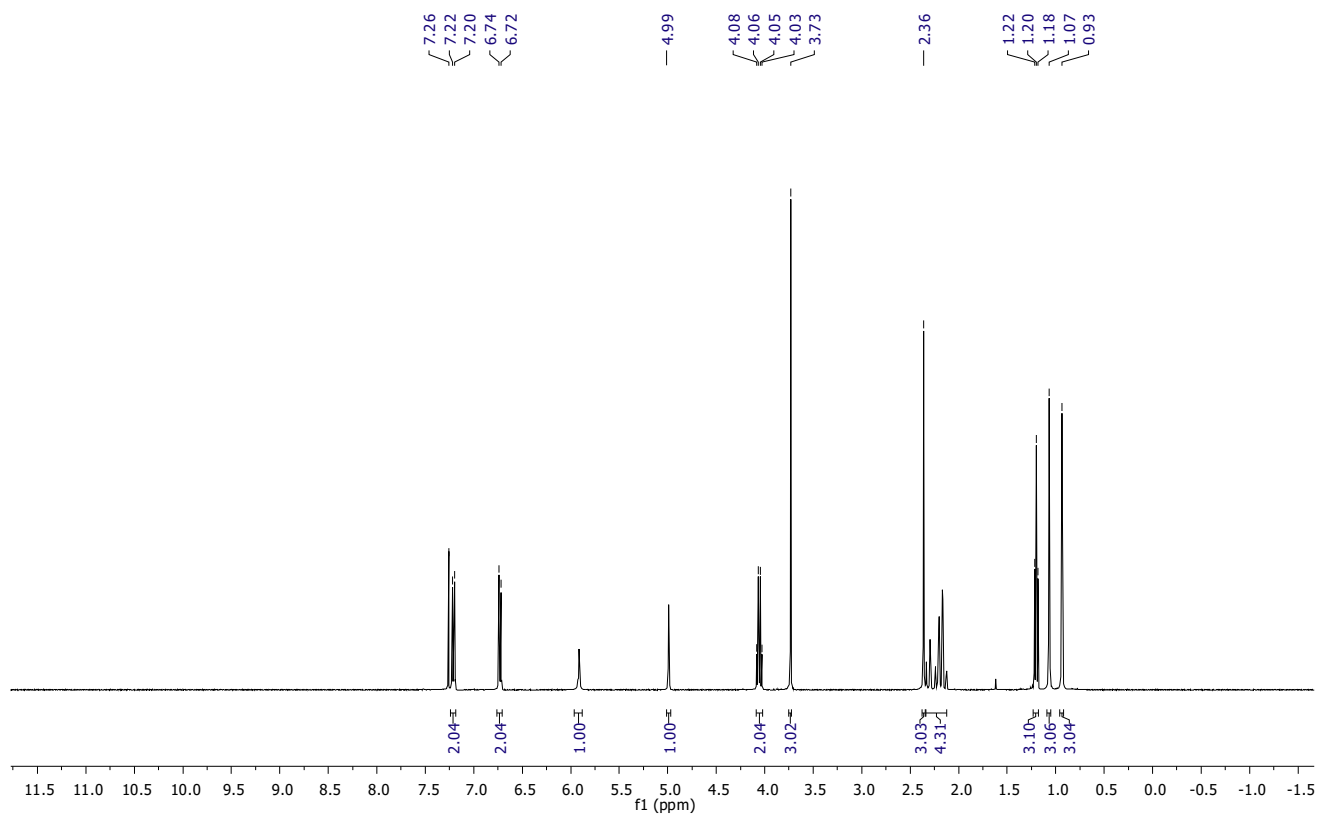


Figure S9. ¹H NMR spectrum of compound **3** (CDCl₃, 400 MHz, TMS).

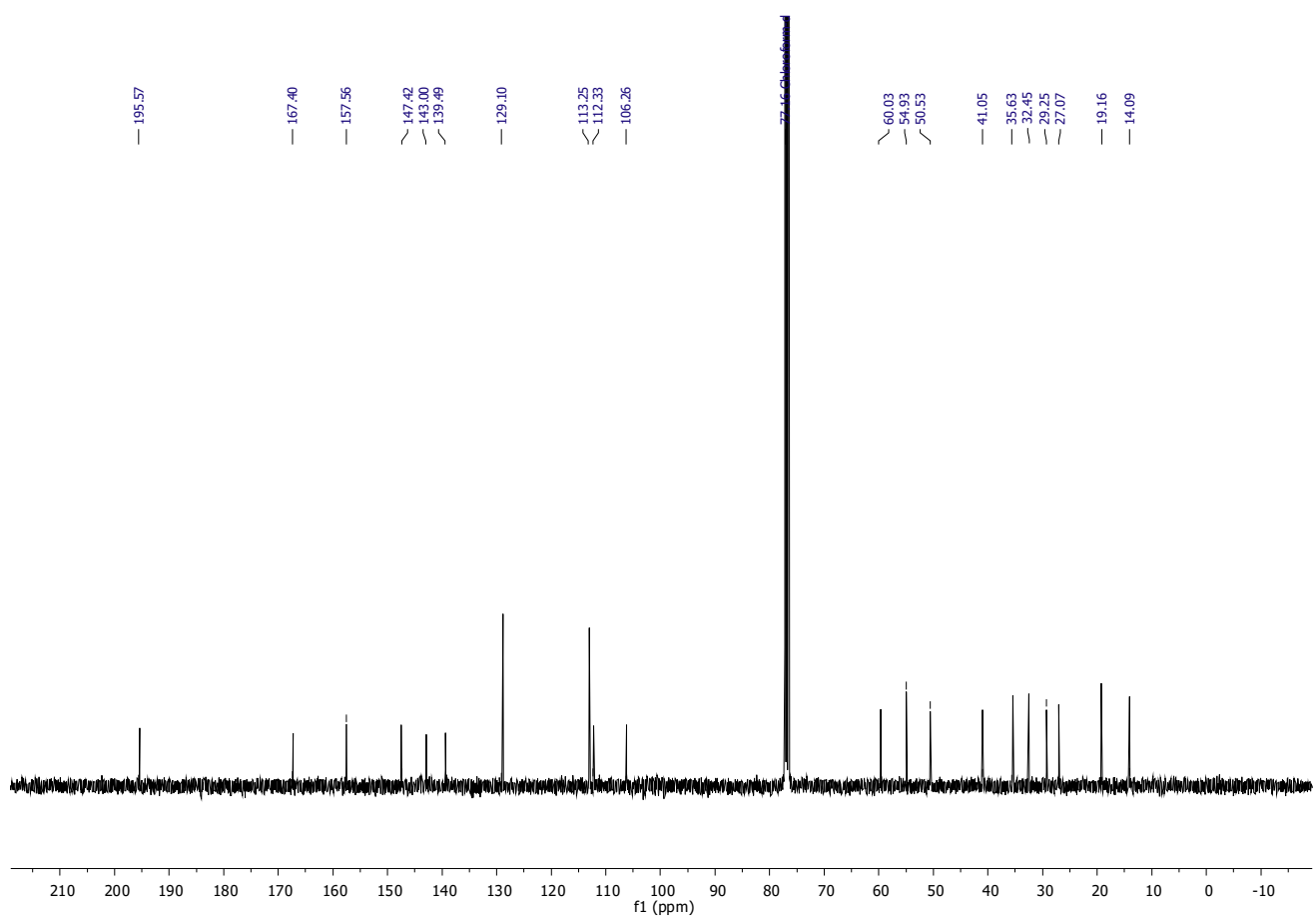


Figure S10. ¹³C NMR spectrum of compound **3** (CDCl₃, 100 MHz, TMS).

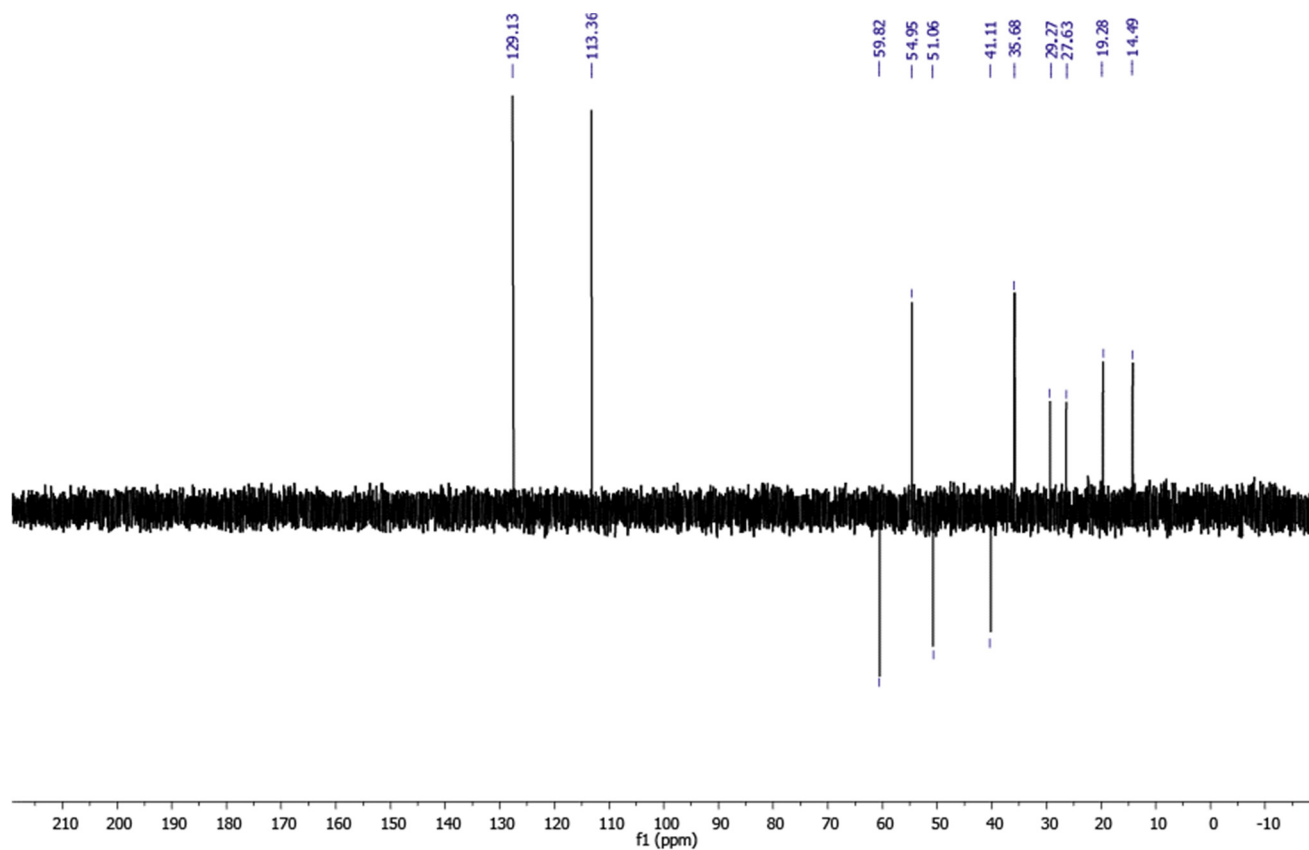


Figure S11. DEPT 135 spectrum of compound **3** (CDCl₃, 100 MHz, TMS).

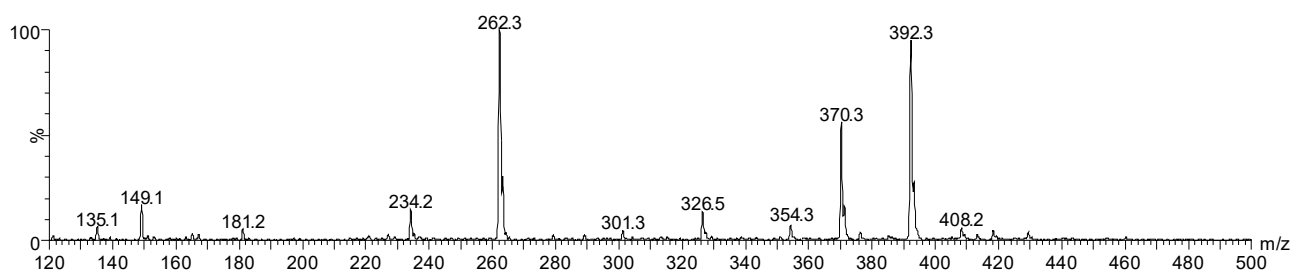


Figure S12. ESI (+) mass spectrum of compound **3**.

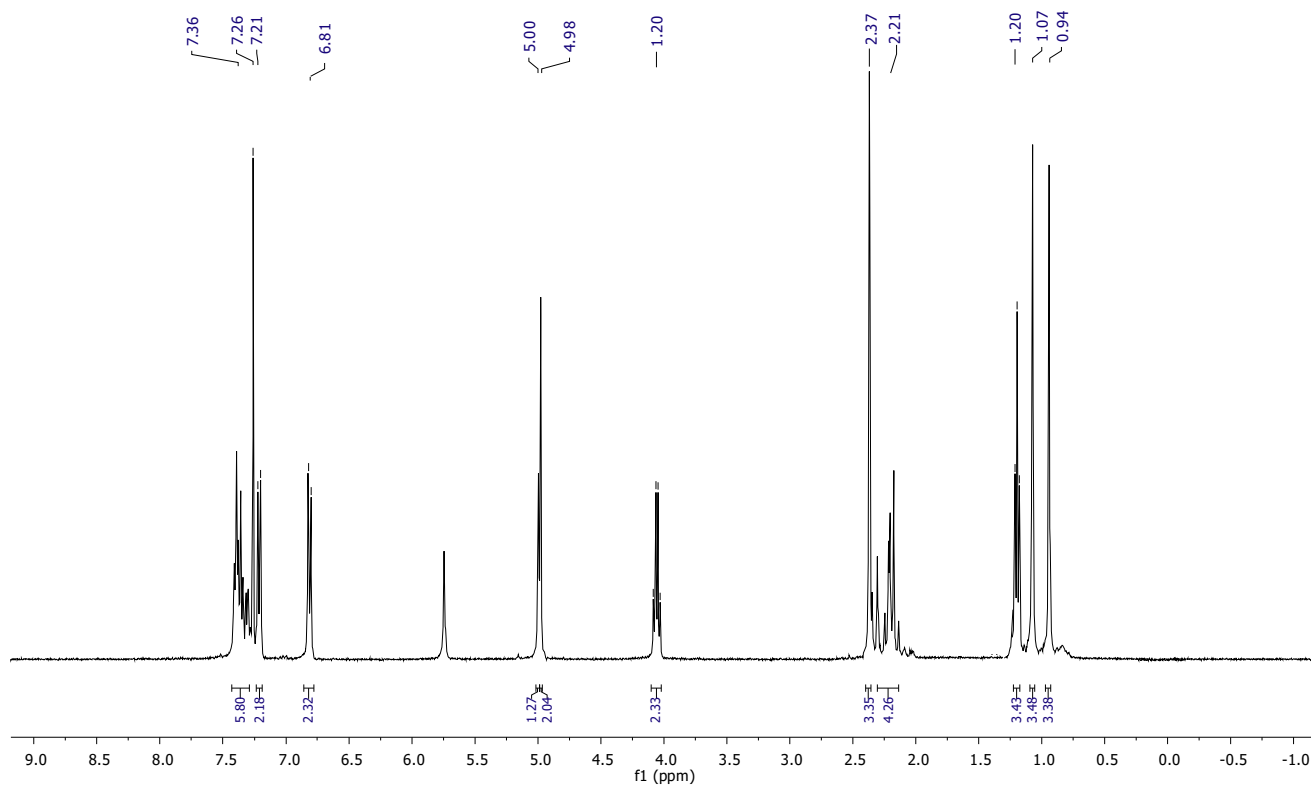


Figure S13. ¹H NMR spectrum of compound **4** (CDCl₃, 400 MHz, TMS).

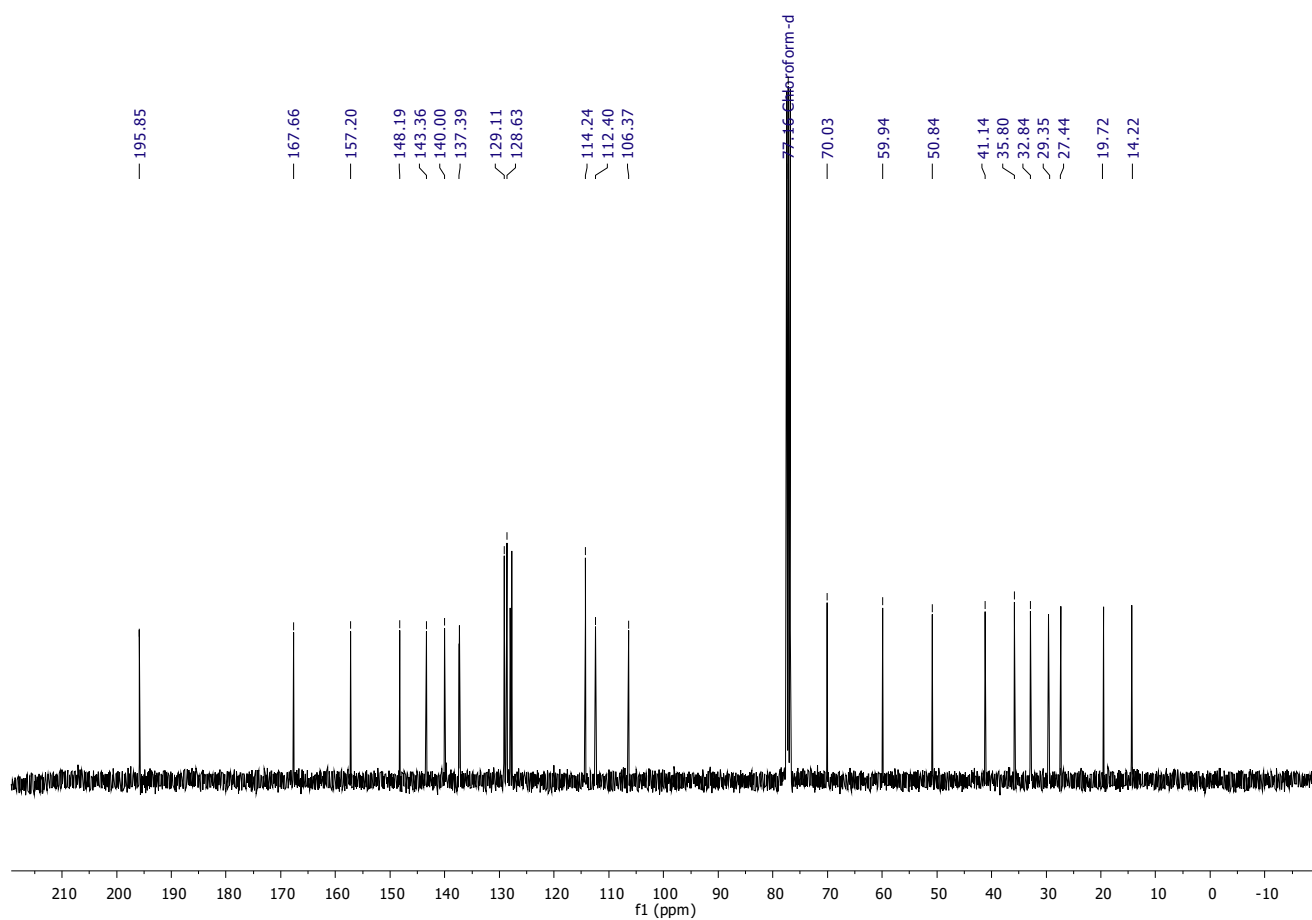


Figure S14. ¹³C NMR spectrum of compound **4** (CDCl₃, 100 MHz, TMS).

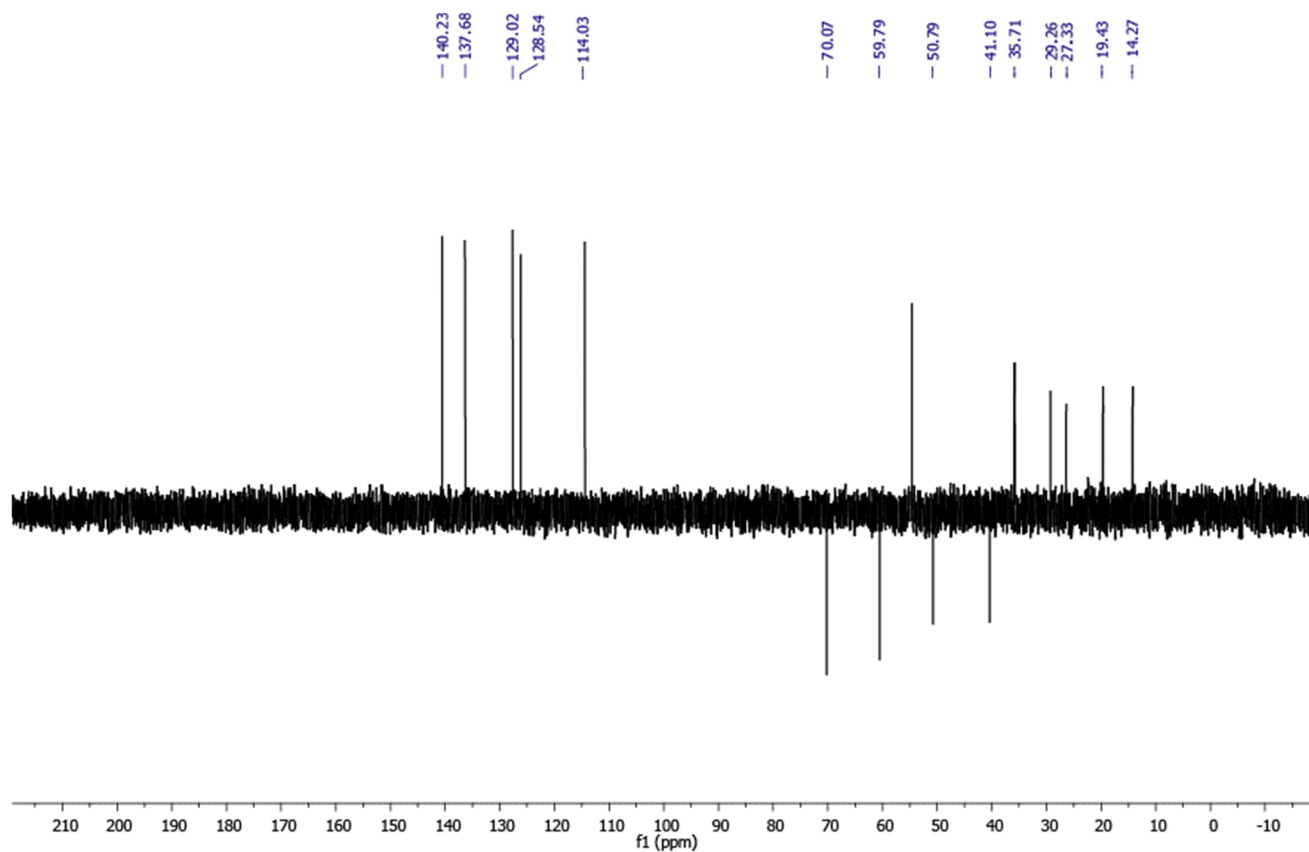


Figure S15. DEPT 135 spectrum of compound **4** (CDCl_3 , 100 MHz, TMS).

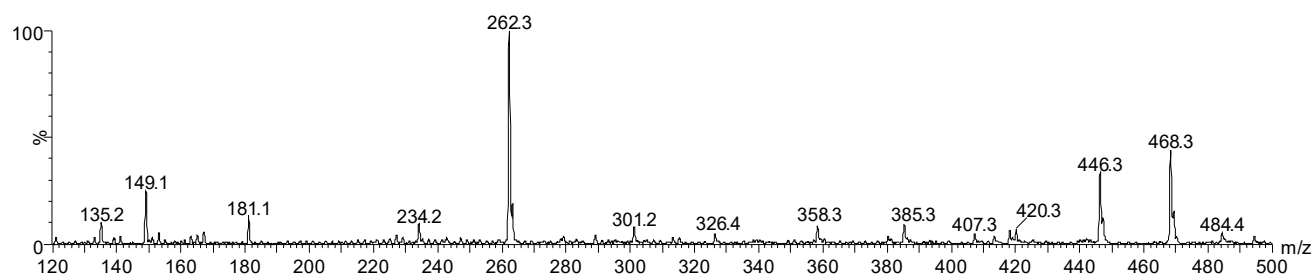


Figure S16. ESI (+) mass spectrum of compound **4**.

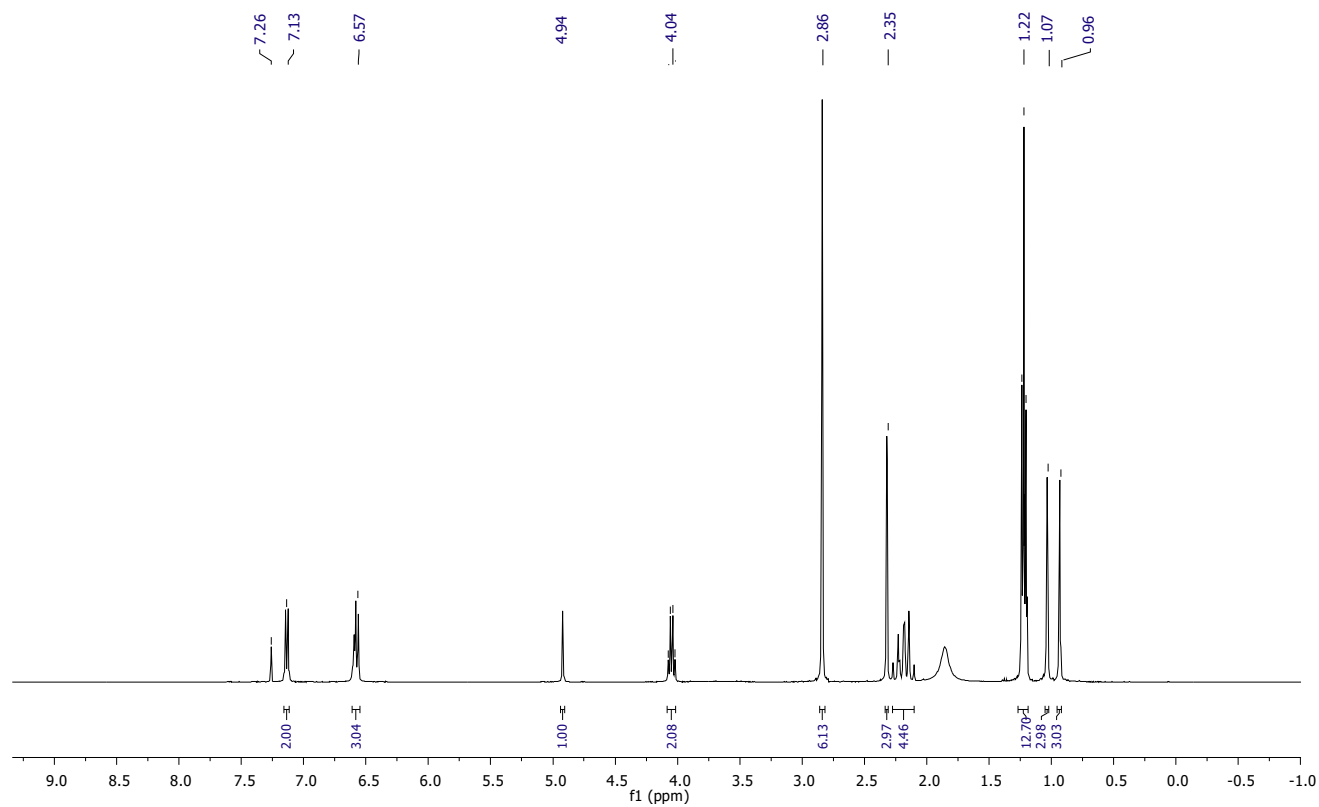


Figure S17. ¹H NMR spectrum of compound **5** (CDCl₃, 400 MHz, TMS).

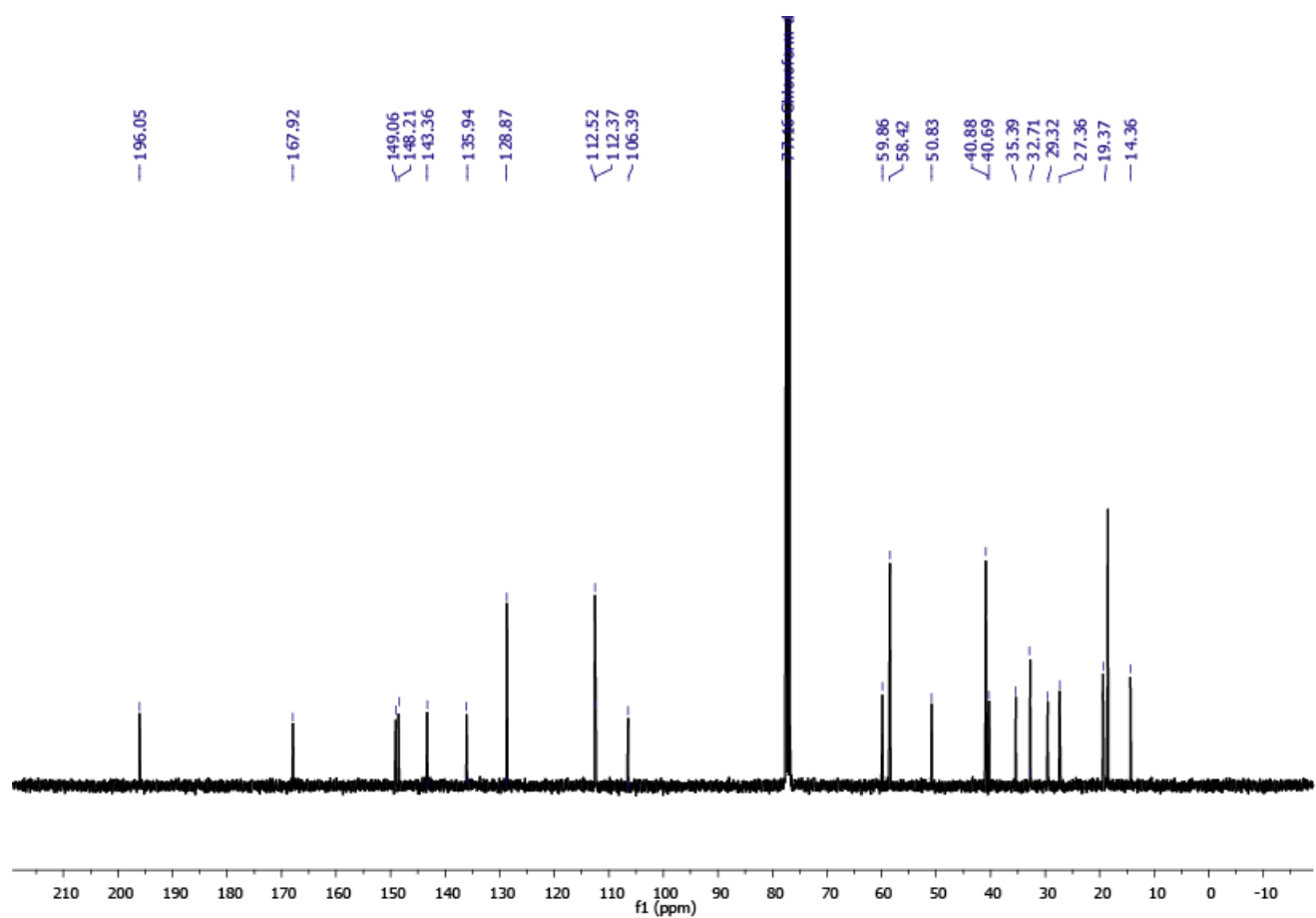


Figure S18. ¹³C NMR spectrum of compound **5** (CDCl₃, 100 MHz, TMS).

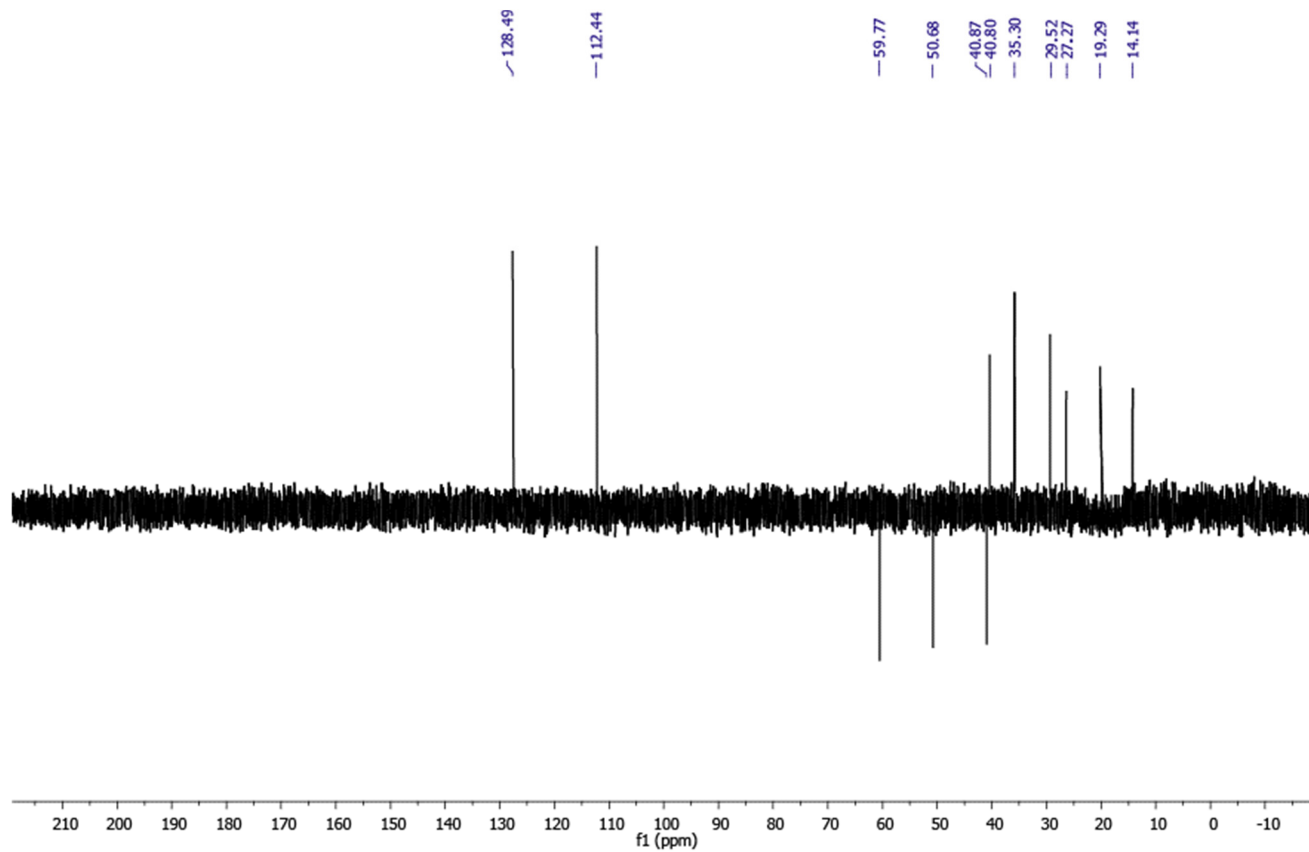


Figure S19. DEPT 135 spectrum of compound **5** (CDCl_3 , 100 MHz, TMS).

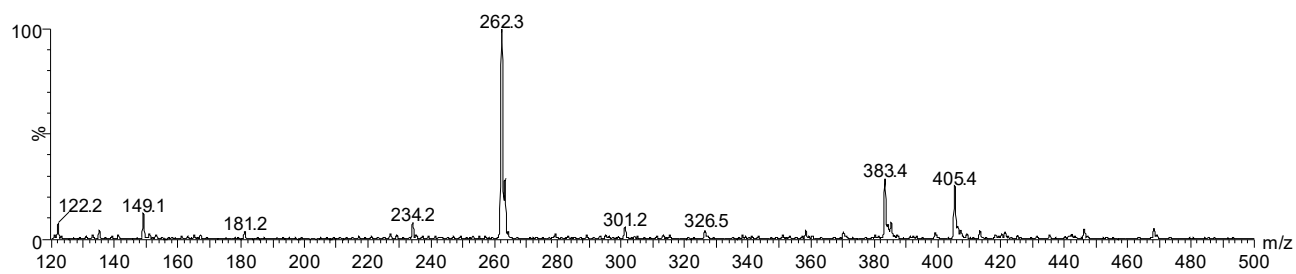


Figure S20. ESI (+) mass spectrum of compound **5**.

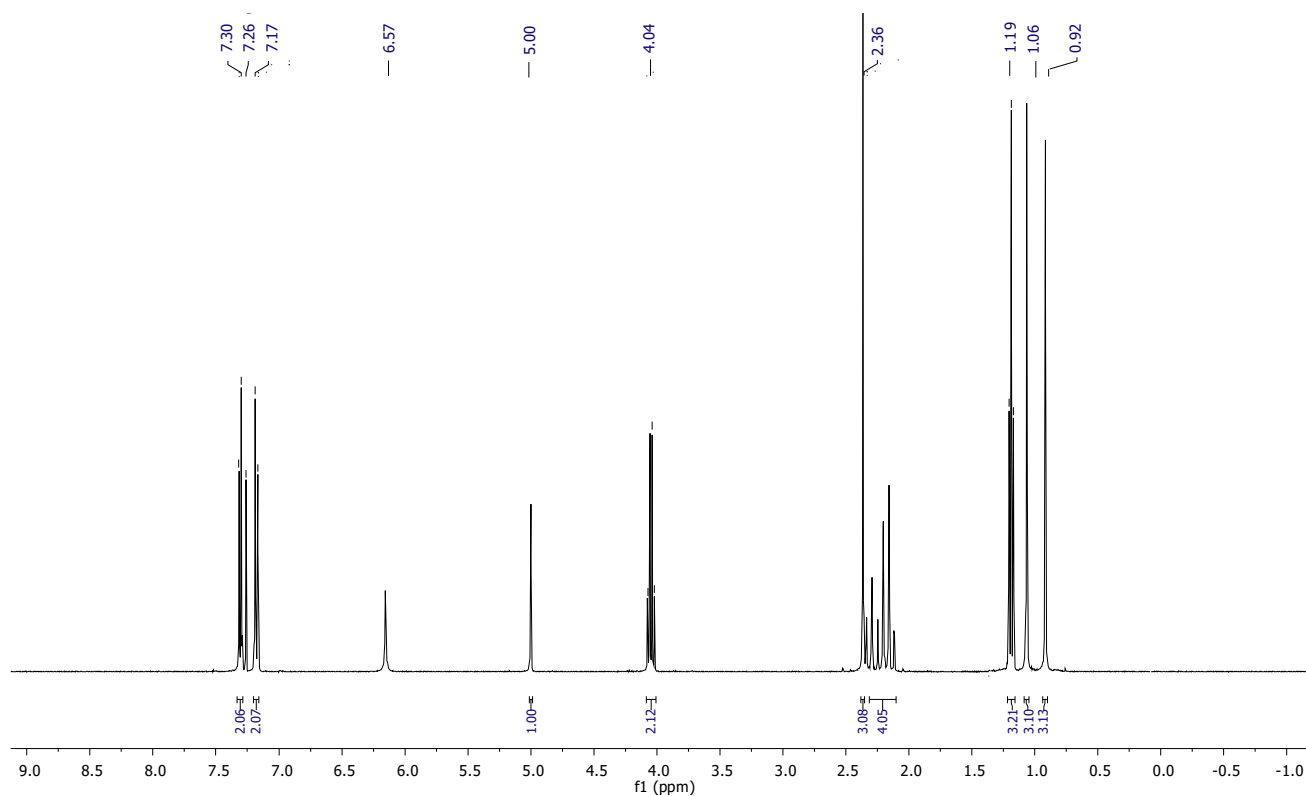


Figure S21. ¹H NMR spectrum of compound **6** (CDCl₃, 400 MHz, TMS).

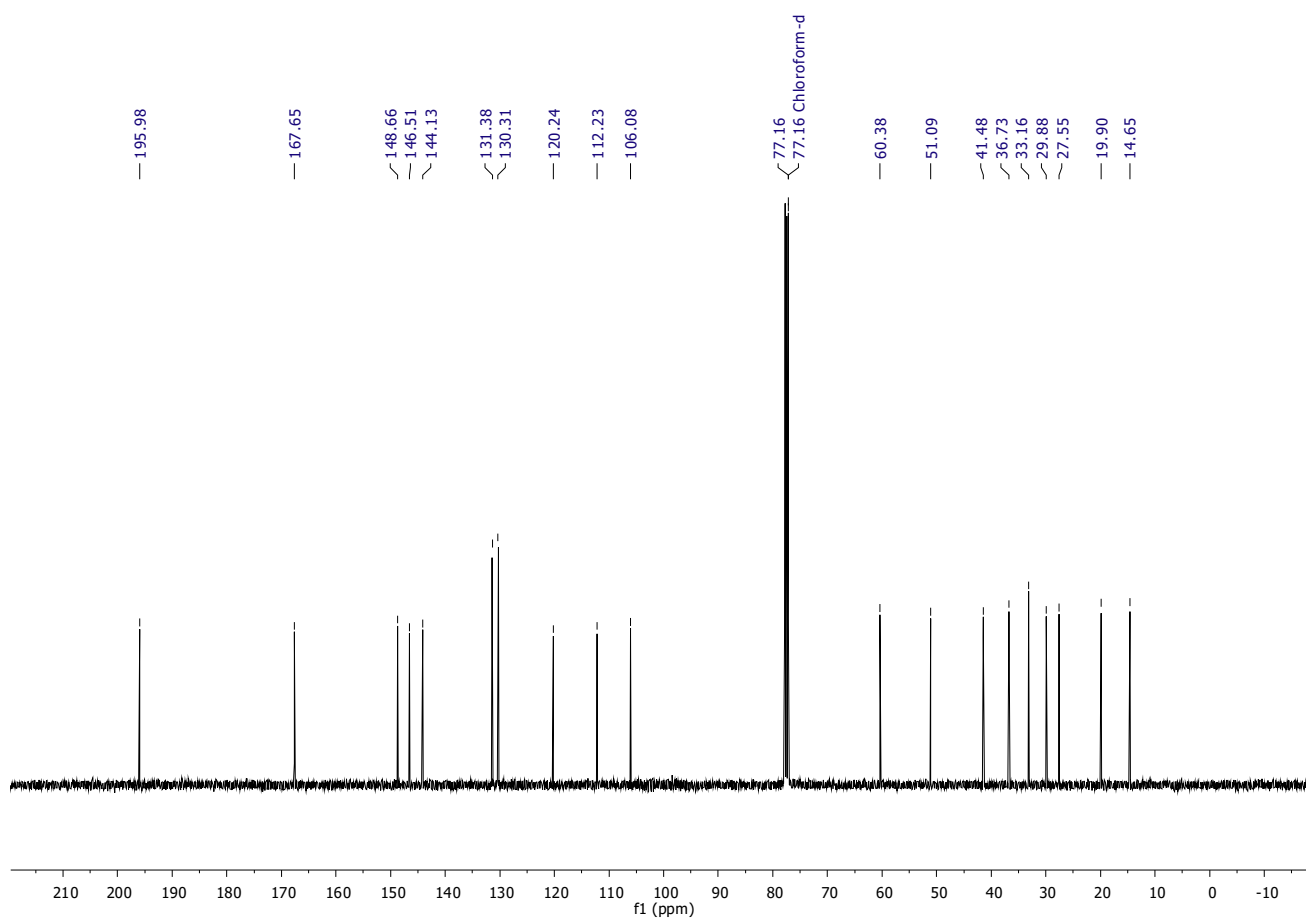


Figure S22. ¹³C NMR spectrum of compound **6** (CDCl₃, 100 MHz, TMS).

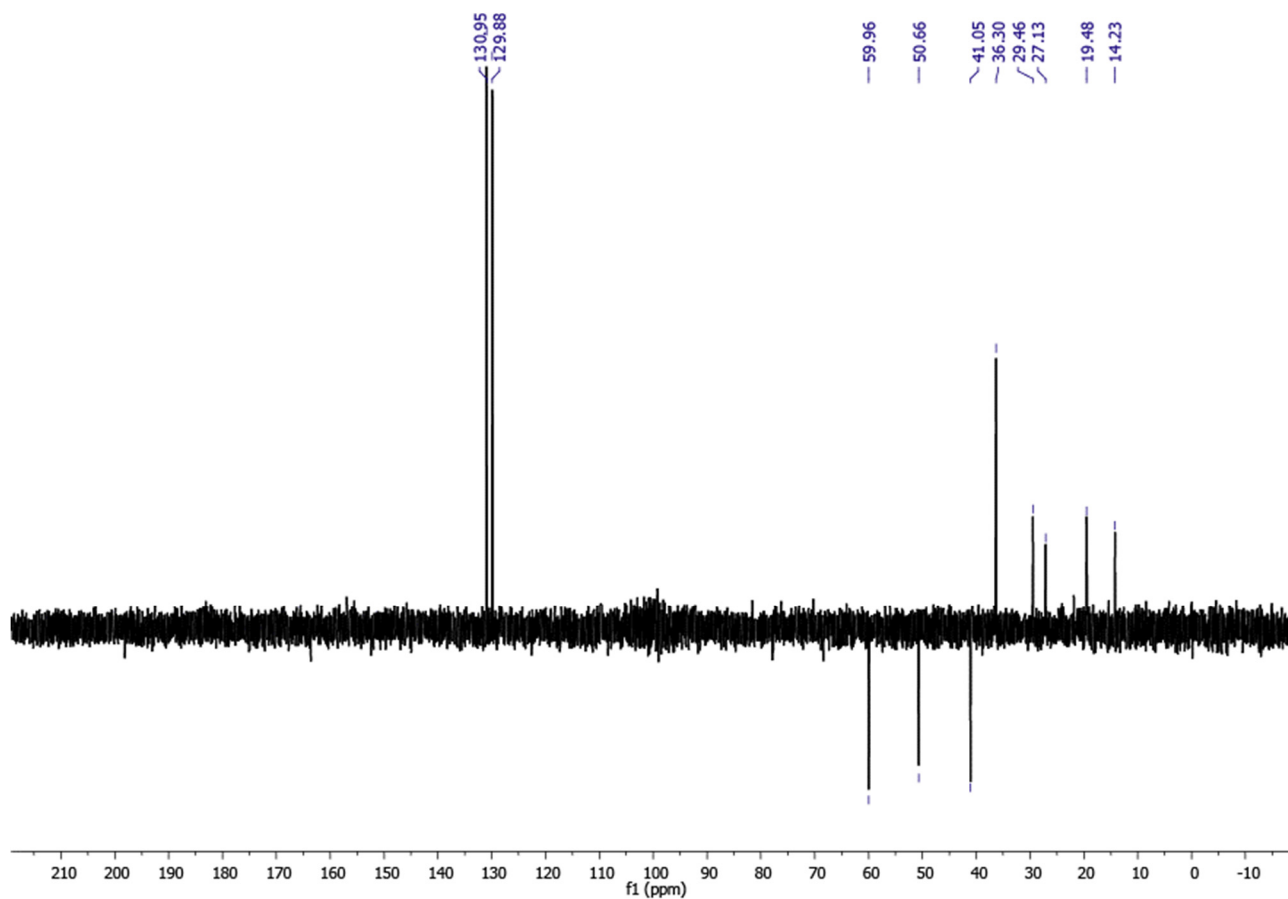


Figure S23. DEPT 135 spectrum of compound 6 (CDCl_3 , 100 MHz, TMS).

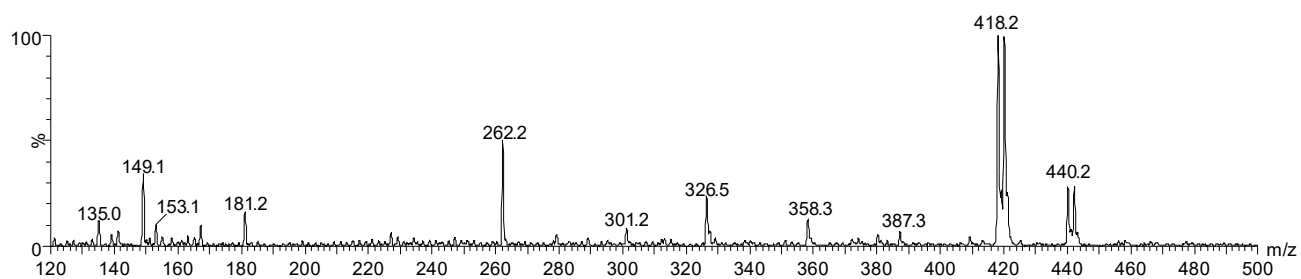


Figure S24. ESI (+) mass spectrum of compound 6.

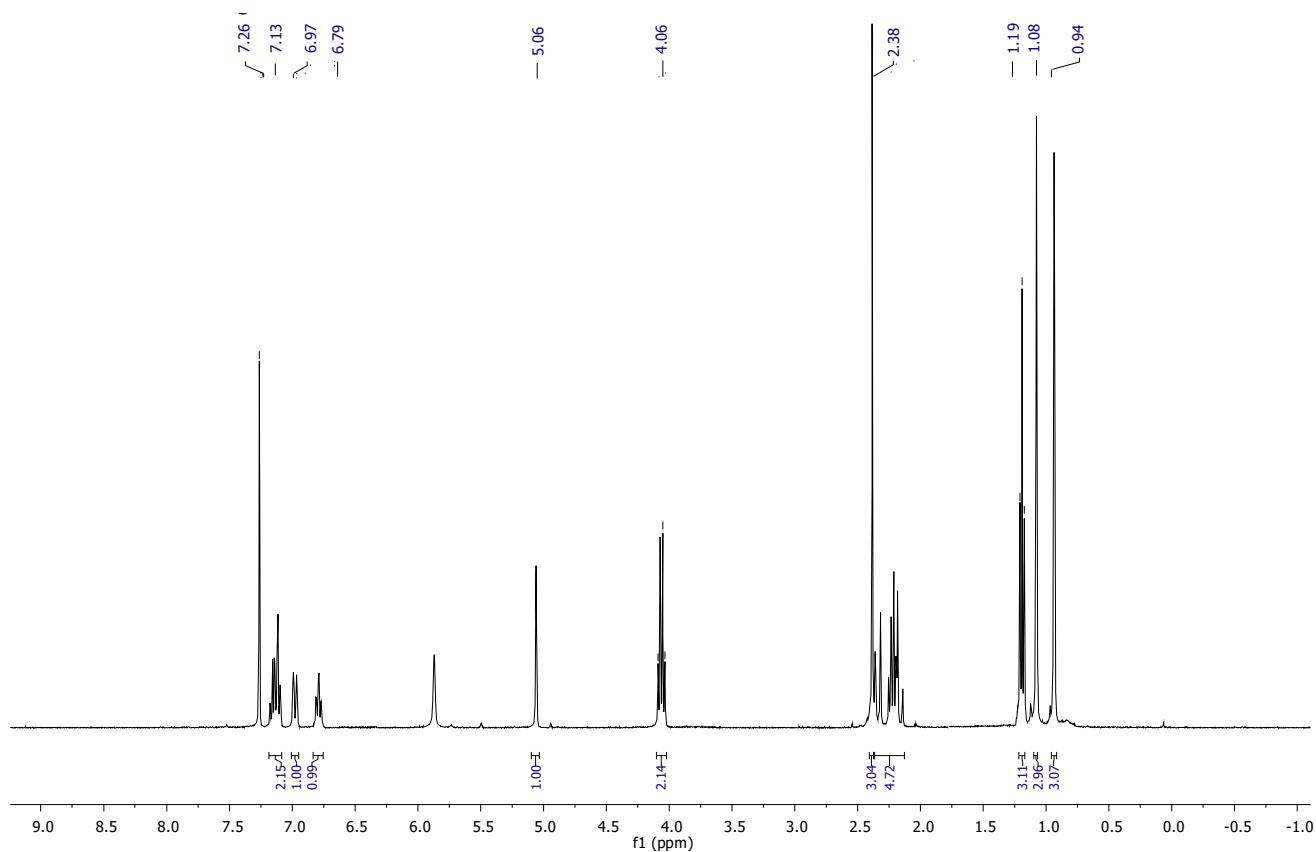


Figure S25. ¹H NMR spectrum of compound **7** (CDCl₃, 400 MHz, TMS).

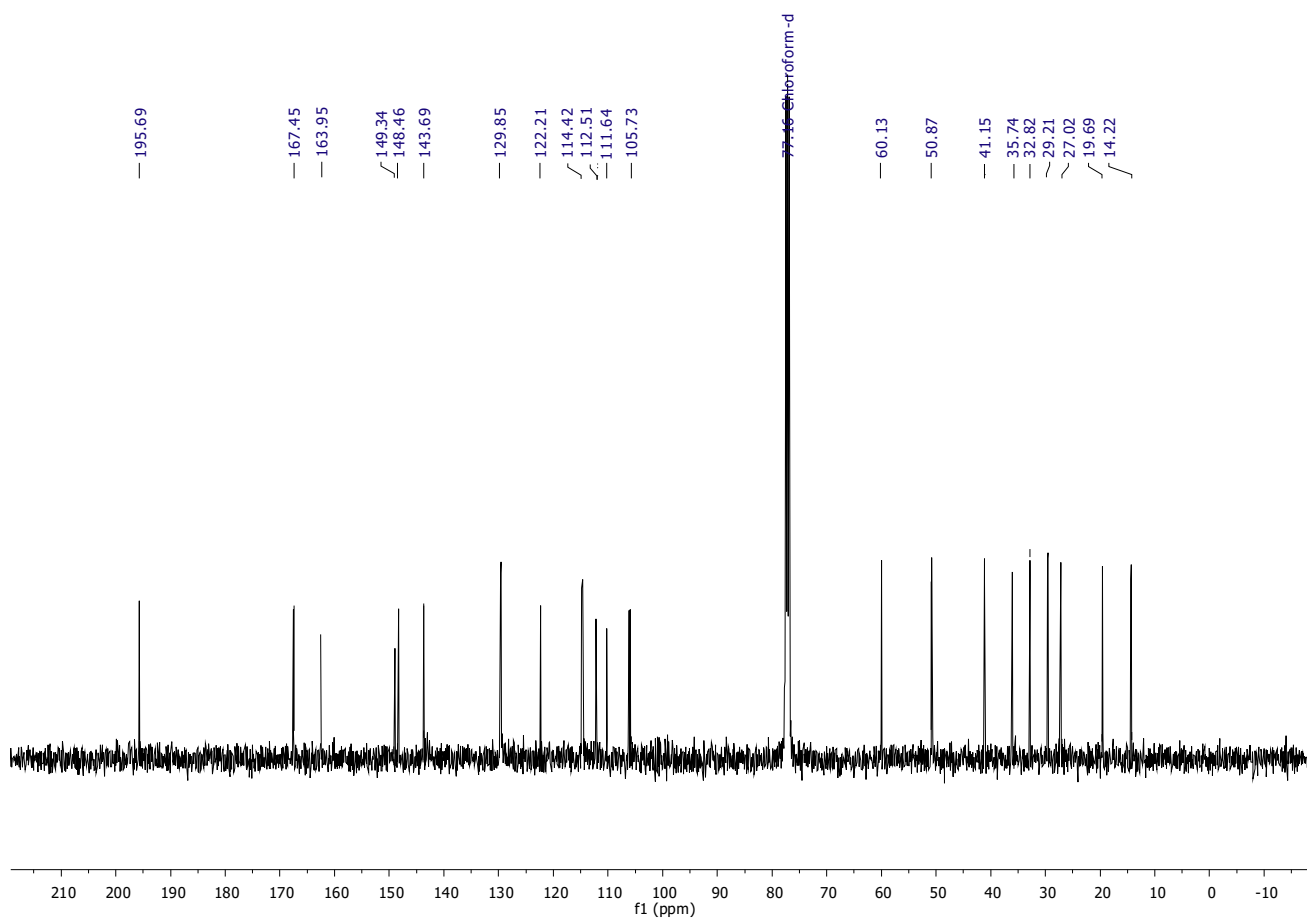


Figure S26. ¹³C NMR spectrum of compound **7** (CDCl₃, 100 MHz, TMS).

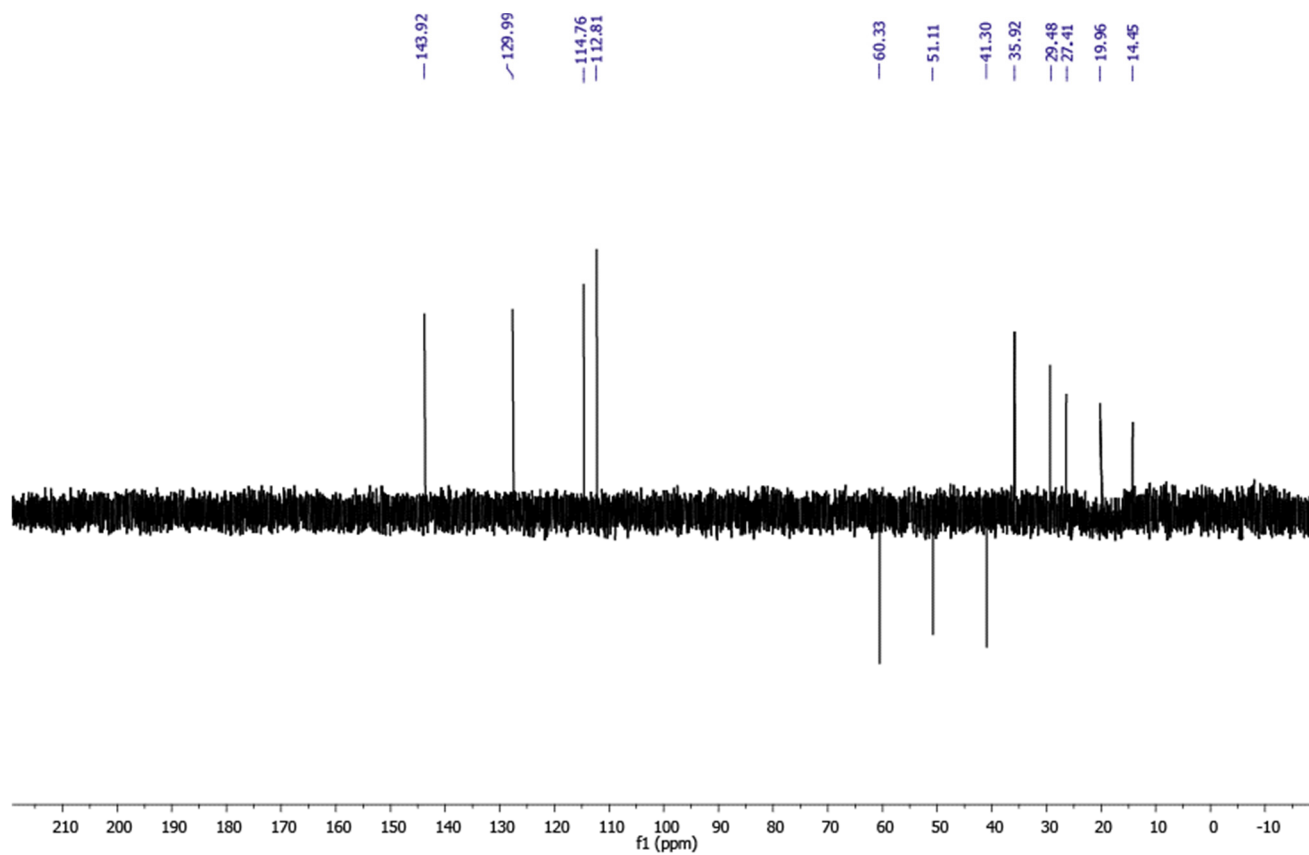


Figure S27. DEPT 135 spectrum of compound 7 (CDCl_3 , 100 MHz, TMS).

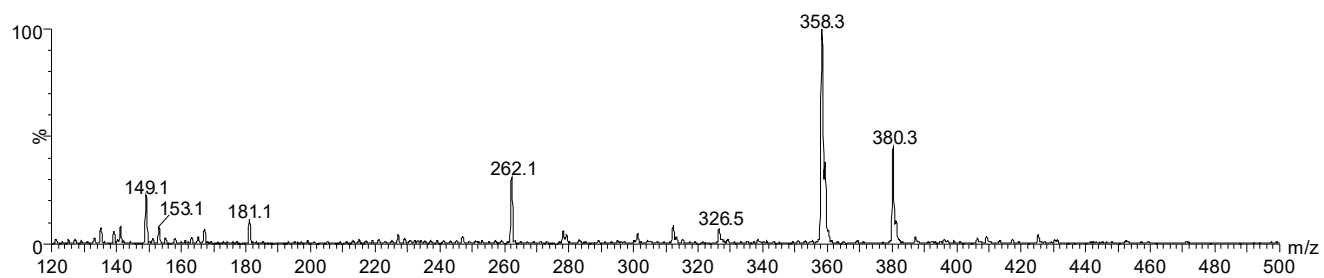


Figure S28. ESI (+) mass spectrum of compound 7.

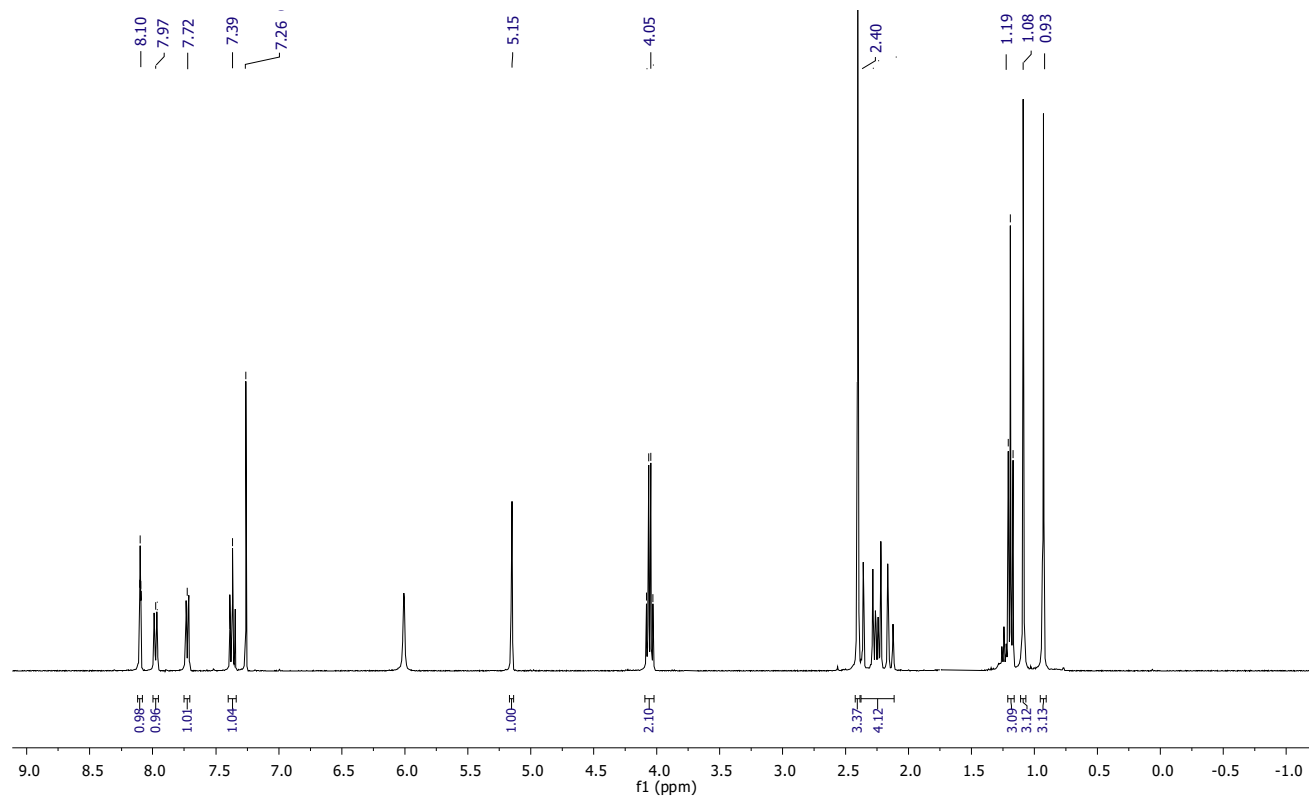


Figure S29. ¹H NMR spectrum of compound 8 (CDCl₃, 400 MHz, TMS).

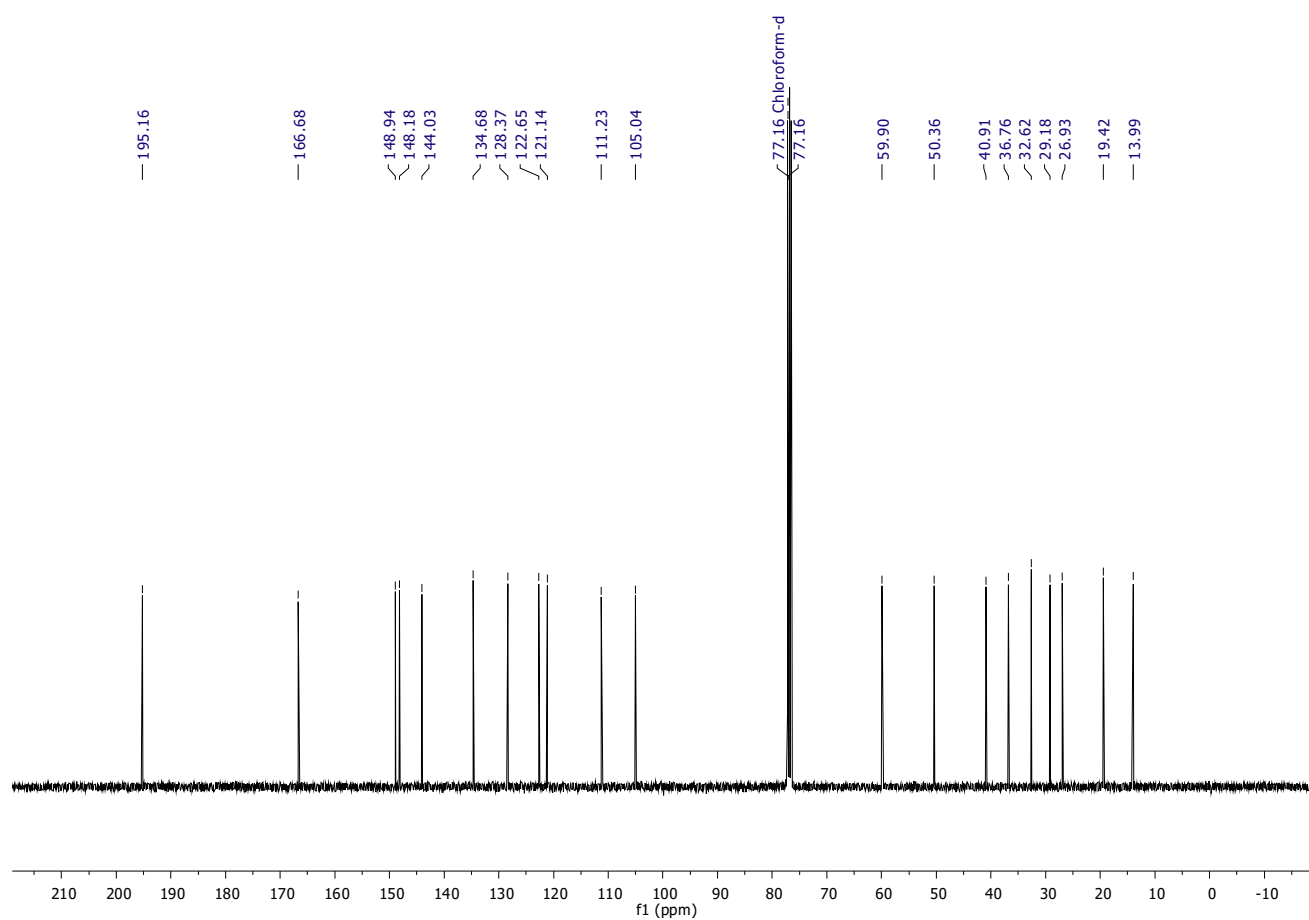


Figure S30. ¹³C NMR spectrum of compound 8 (CDCl₃, 100 MHz, TMS).

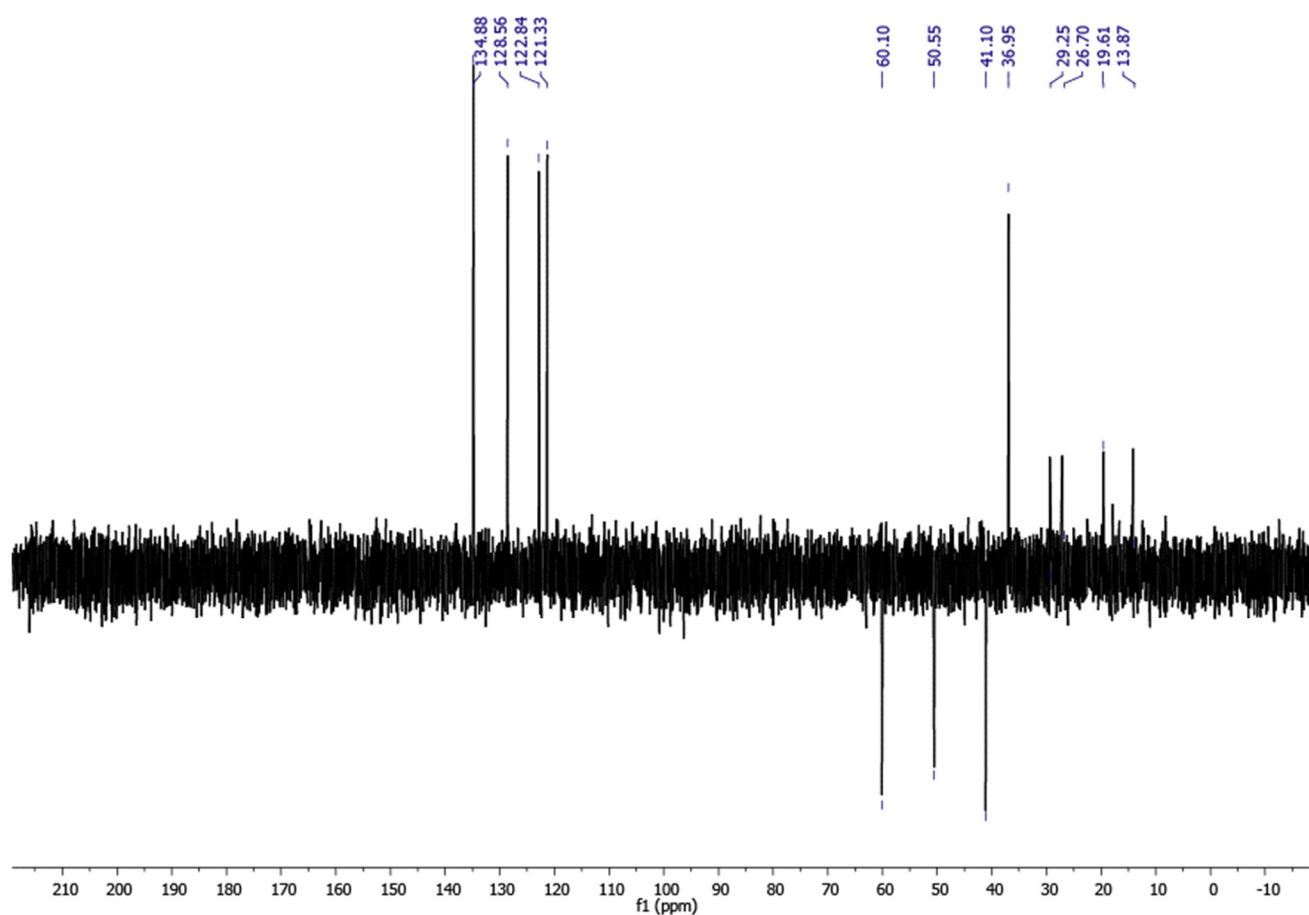


Figure S31. DEPT 135 spectrum of compound 8(CDCl₃, 100 MHz, TMS).

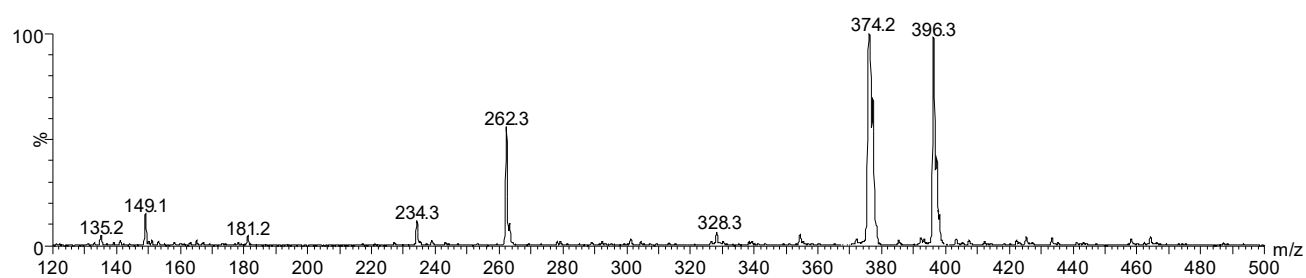


Figure S32. ESI (+) mass spectrum of compound 8.

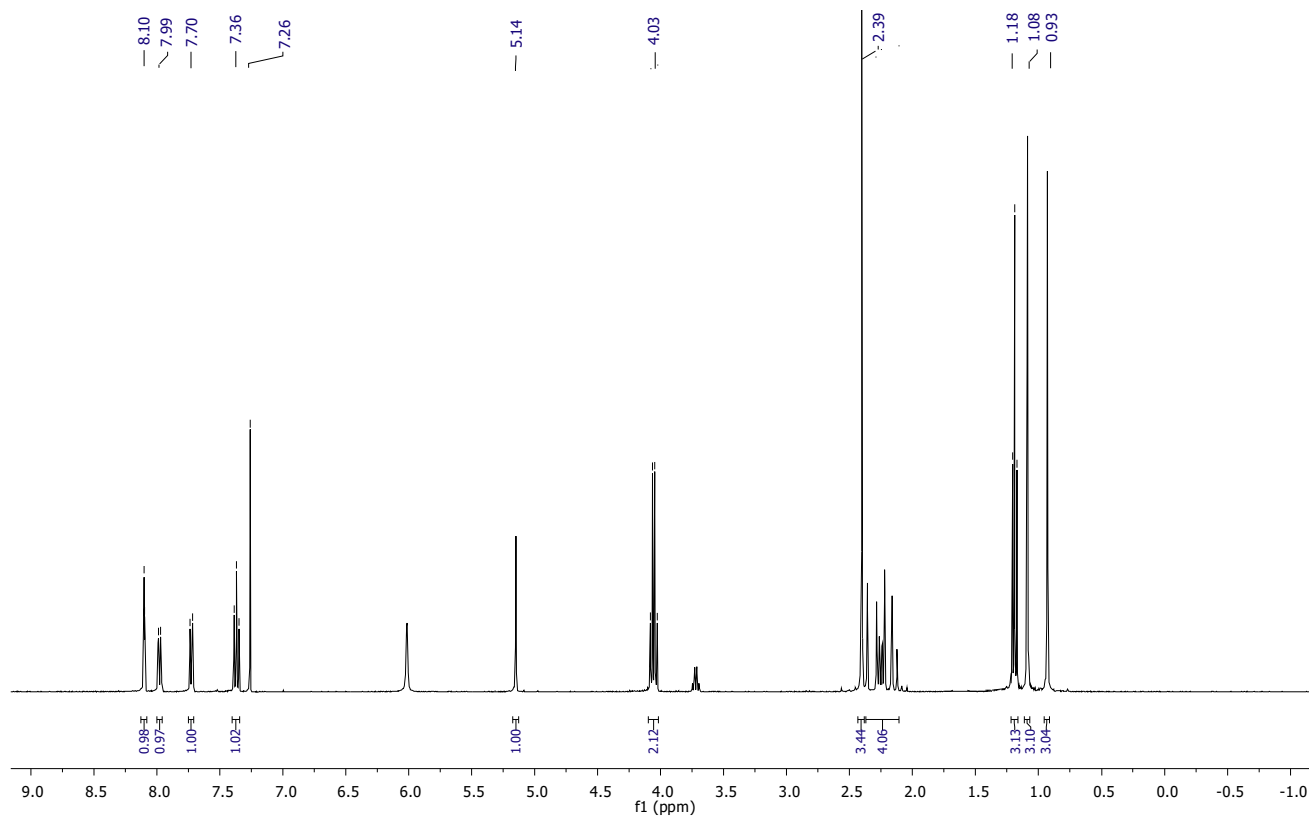


Figure S33. ¹H NMR spectrum of compound **9** (CDCl₃, 400 MHz, TMS).

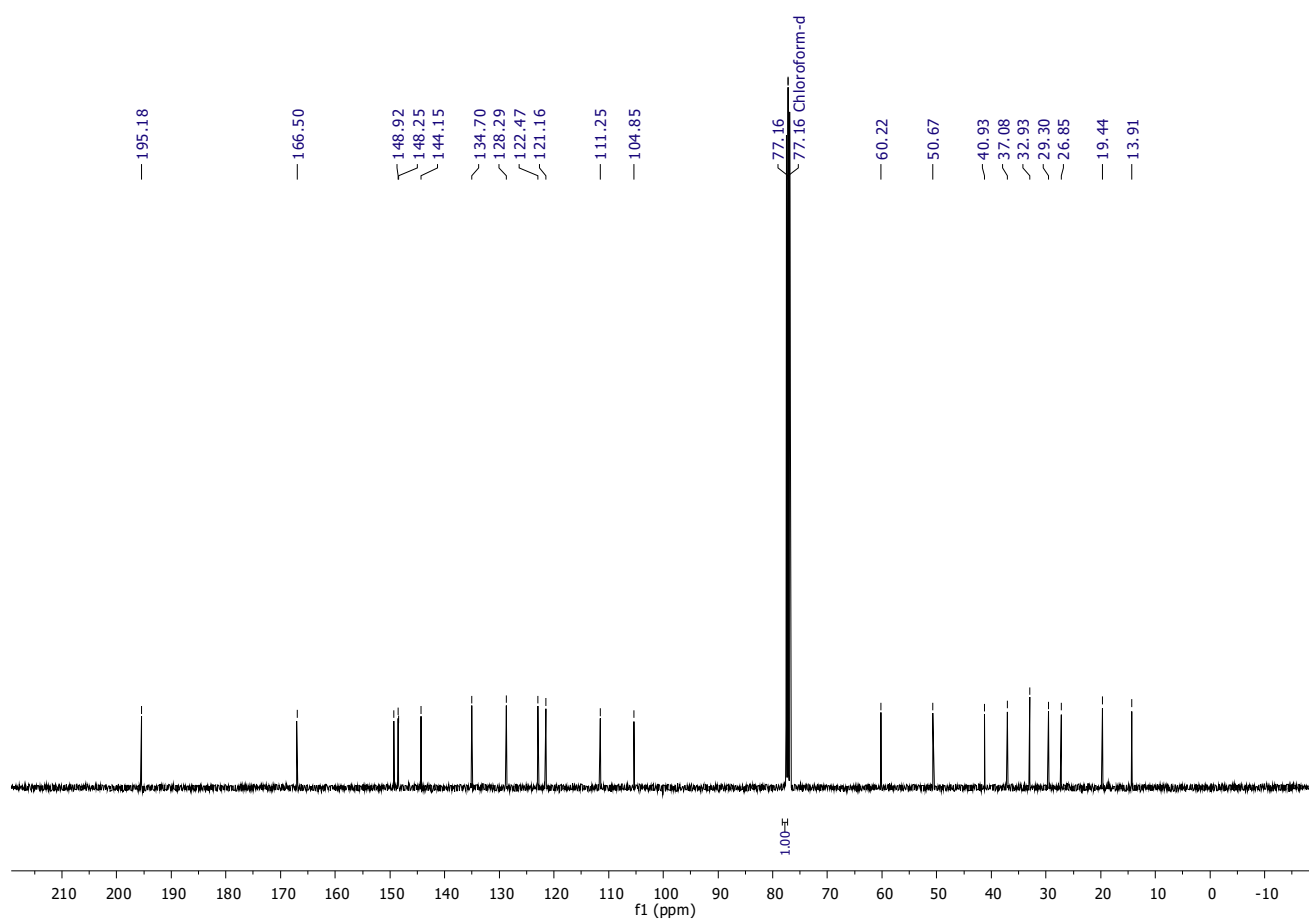


Figure S34. ¹³C NMR spectrum of compound **9** (CDCl₃, 100 MHz, TMS).

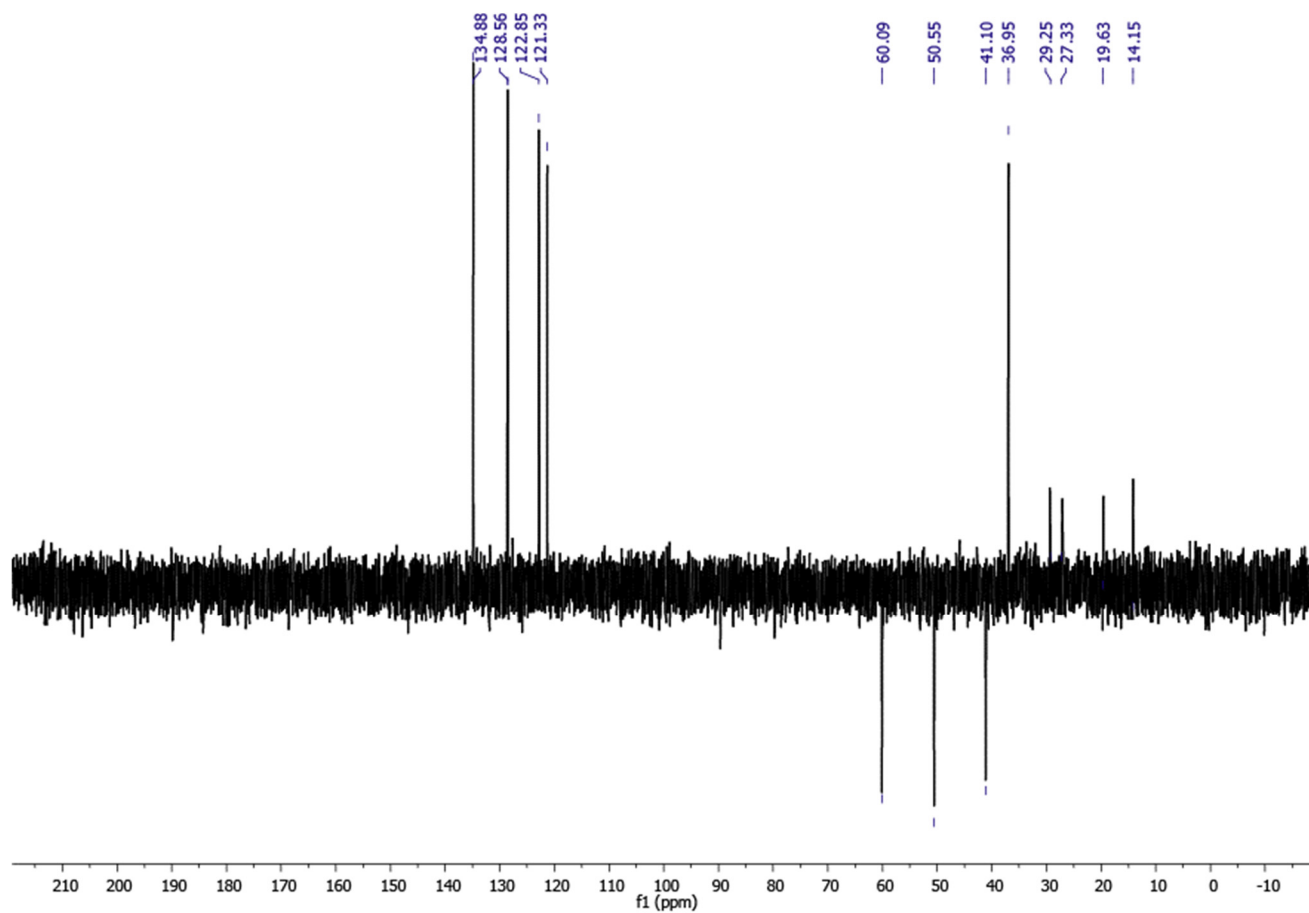


Figure S35. DEPT 135 spectrum of compound **9** (CDCl_3 , 100 MHz, TMS).

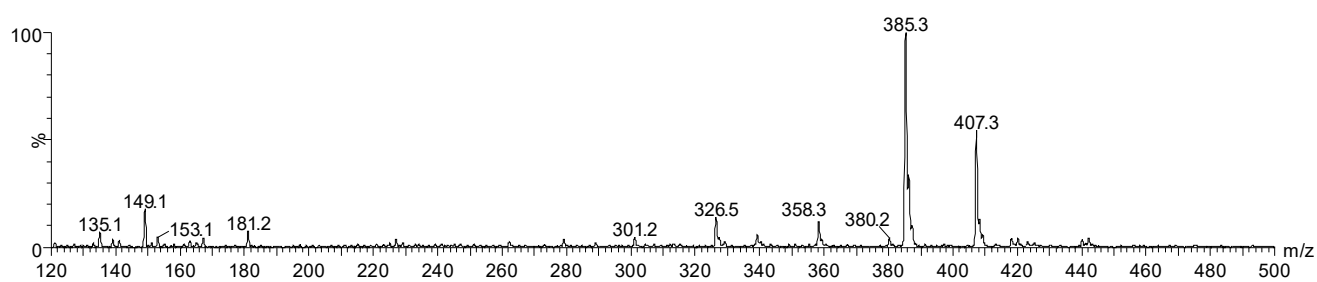


Figure S36. ESI (+) mass spectrum of compound **9**.

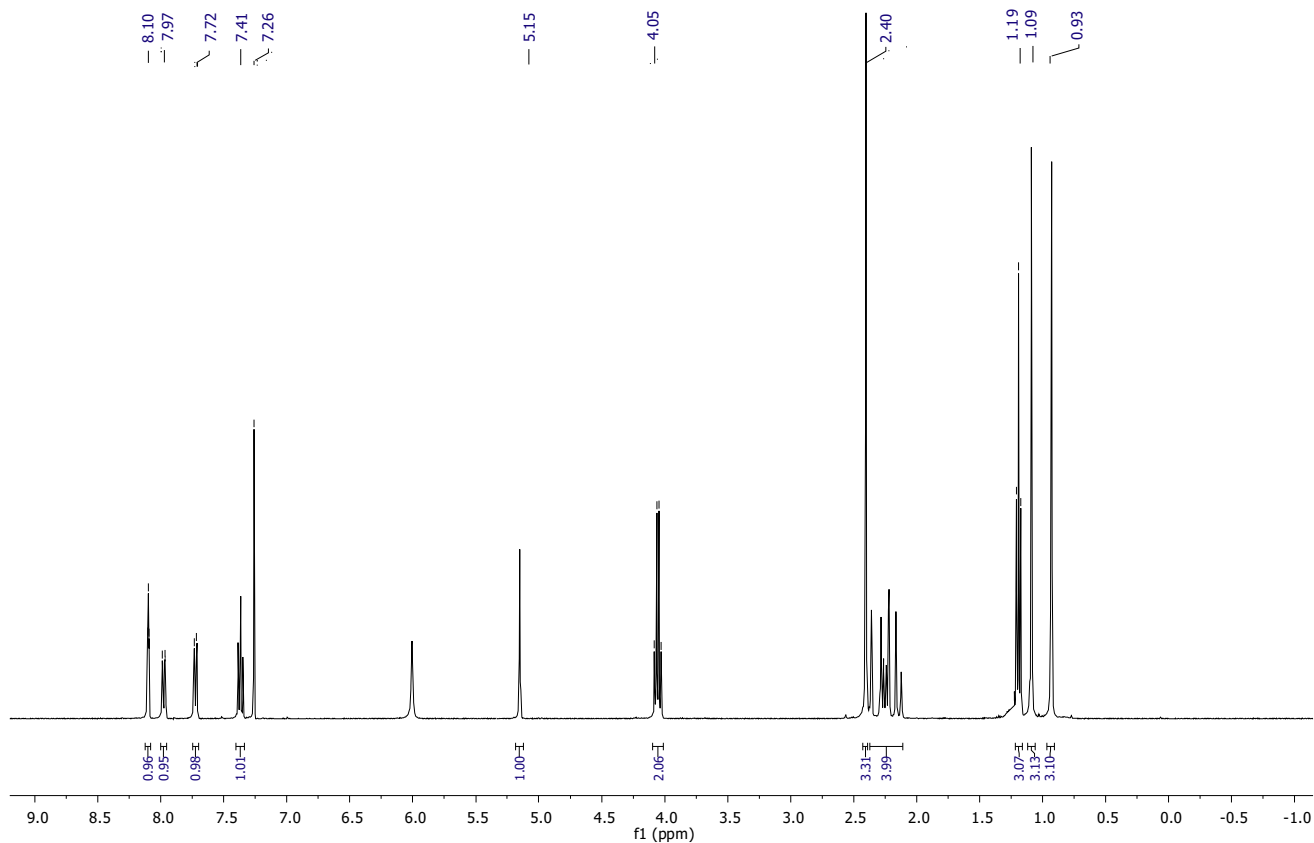


Figure S37. ¹H NMR spectrum of compound **10** (CDCl₃, 400 MHz, TMS).

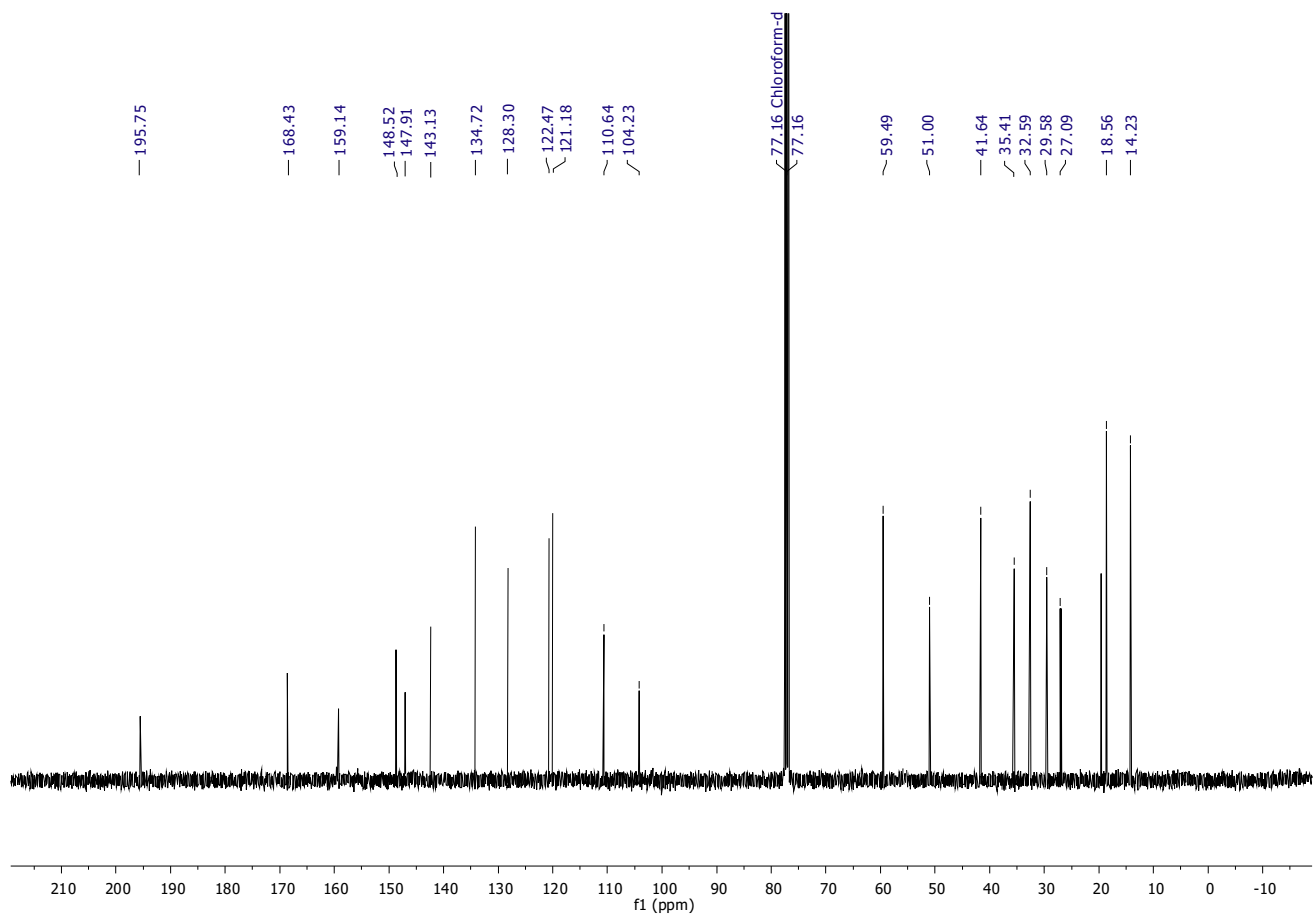


Figure S38. ¹³C NMR spectrum of compound **10** (CDCl₃, 100 MHz, TMS).

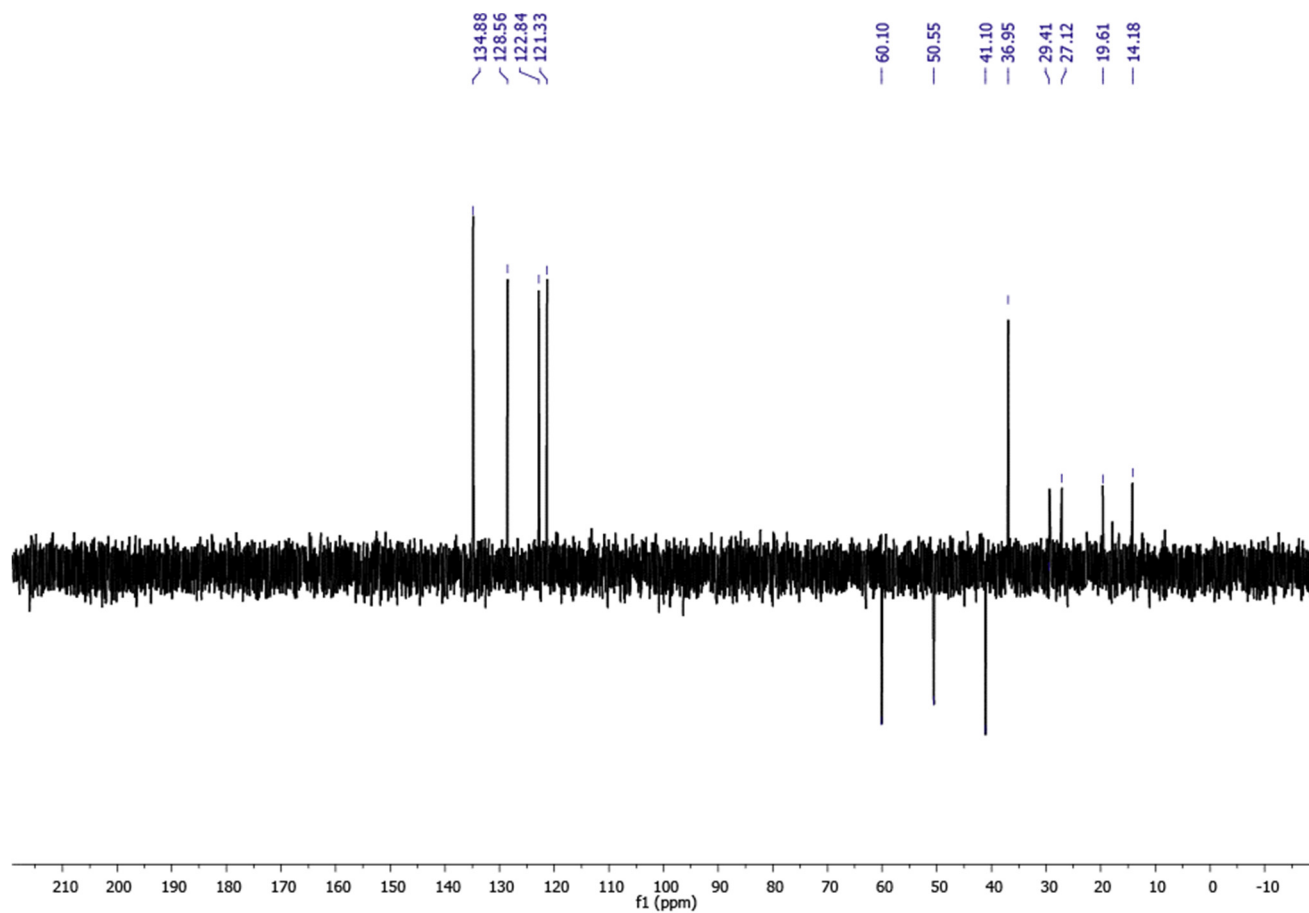


Figure S39. DEPT 135 spectrum of compound **10** (CDCl₃, 100 MHz, TMS).

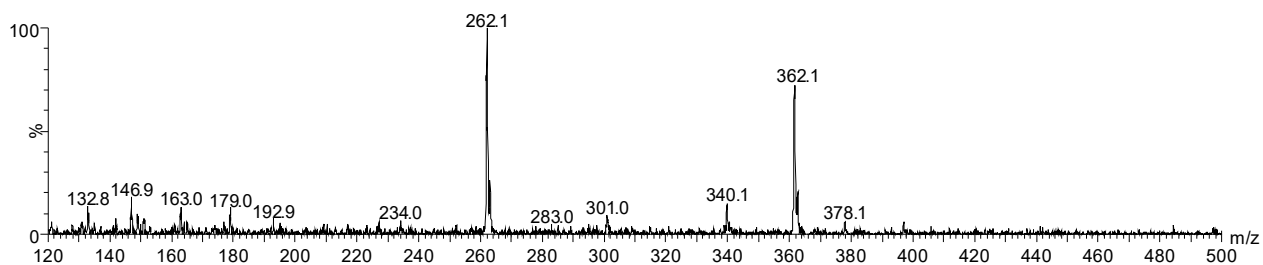


Figure S40. ESI (+) mass spectrum of compound **10**.

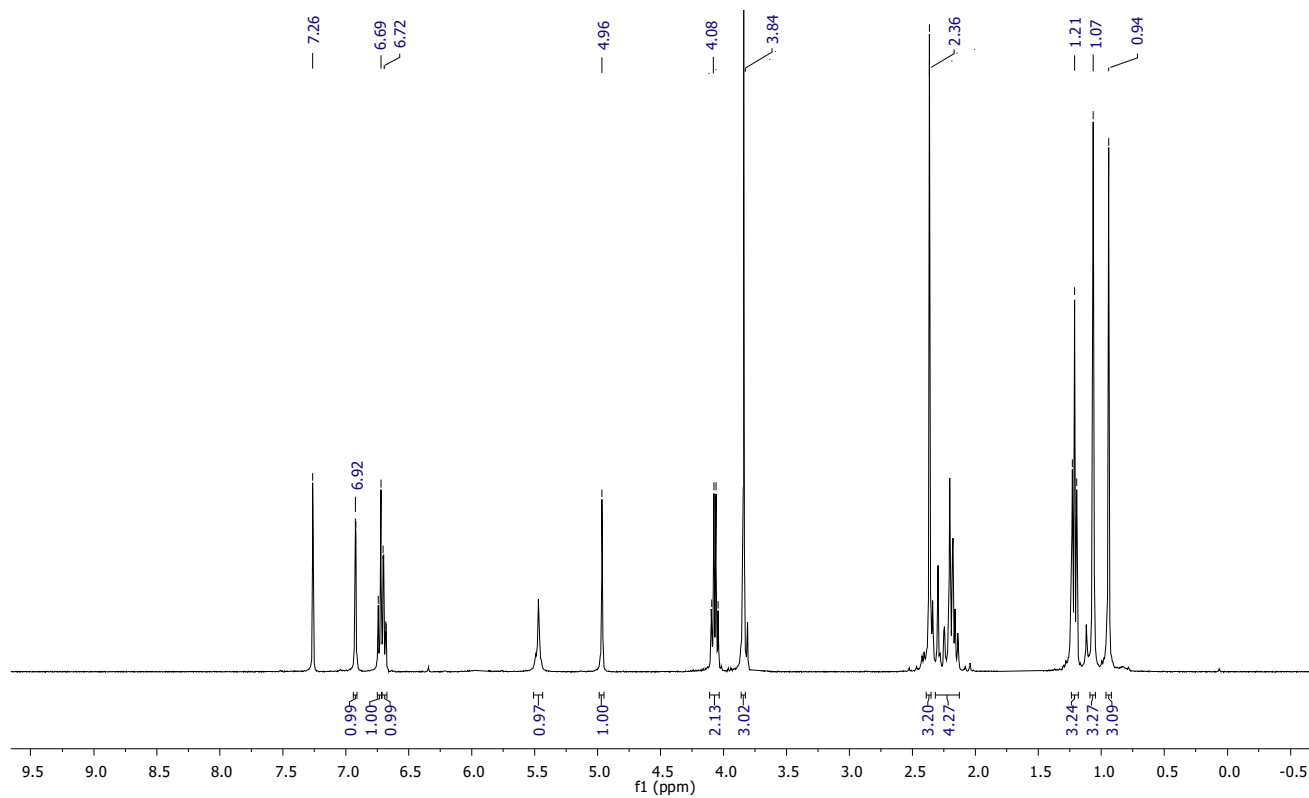


Figure S41. ¹H NMR spectrum of compound **11** (CDCl₃, 400 MHz, TMS).

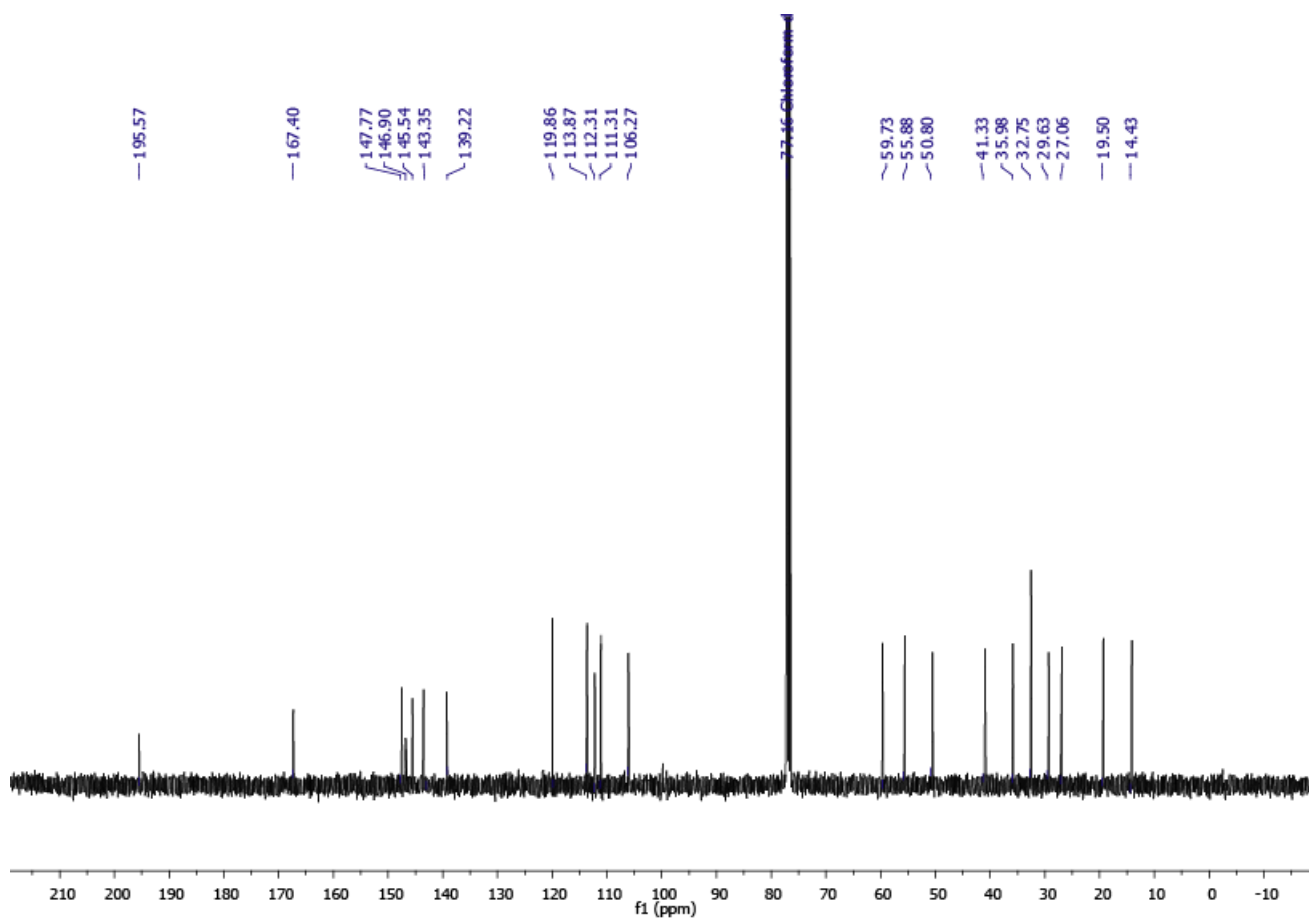


Figure S42. ¹³C NMR spectrum of compound **11** (CDCl₃, 100 MHz, TMS).

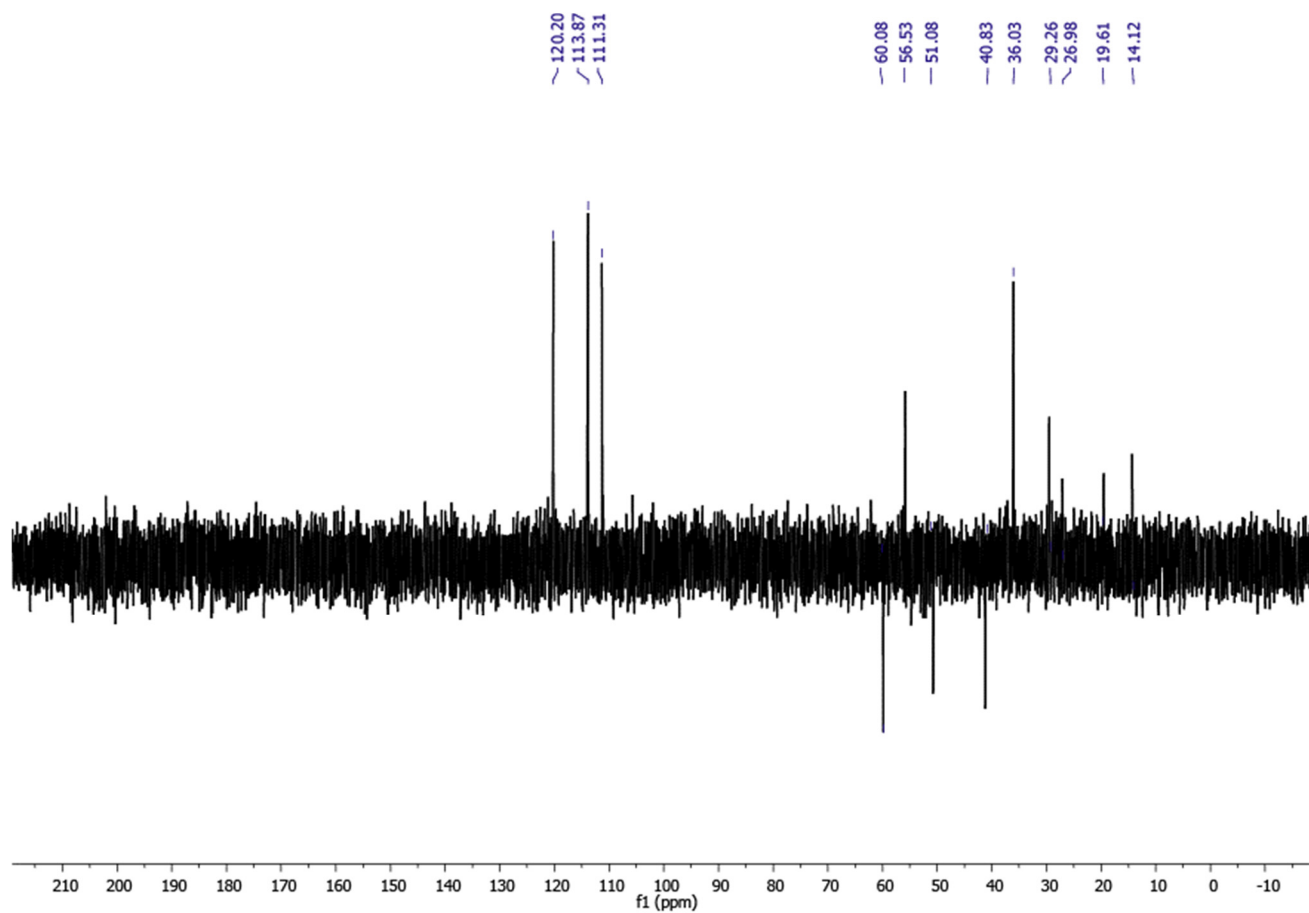


Figure S43. DEPT 135 spectrum of compound **11** (CDCl₃, 100 MHz, TMS).

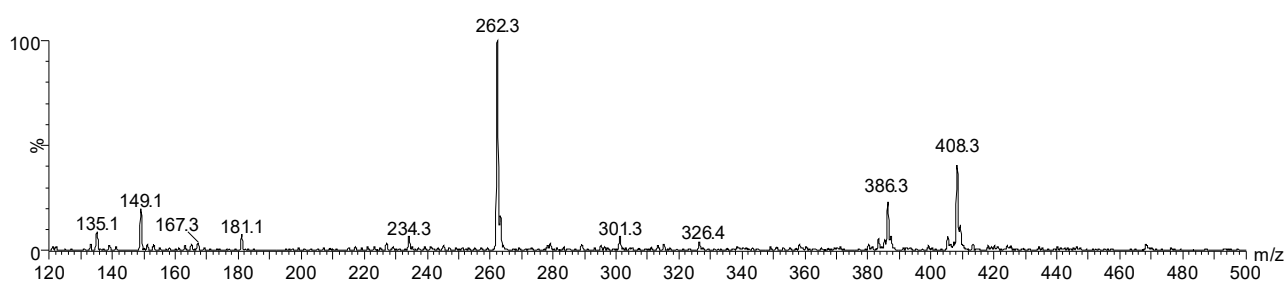


Figure S44. ESI (+) mass spectrum of compound **11**.

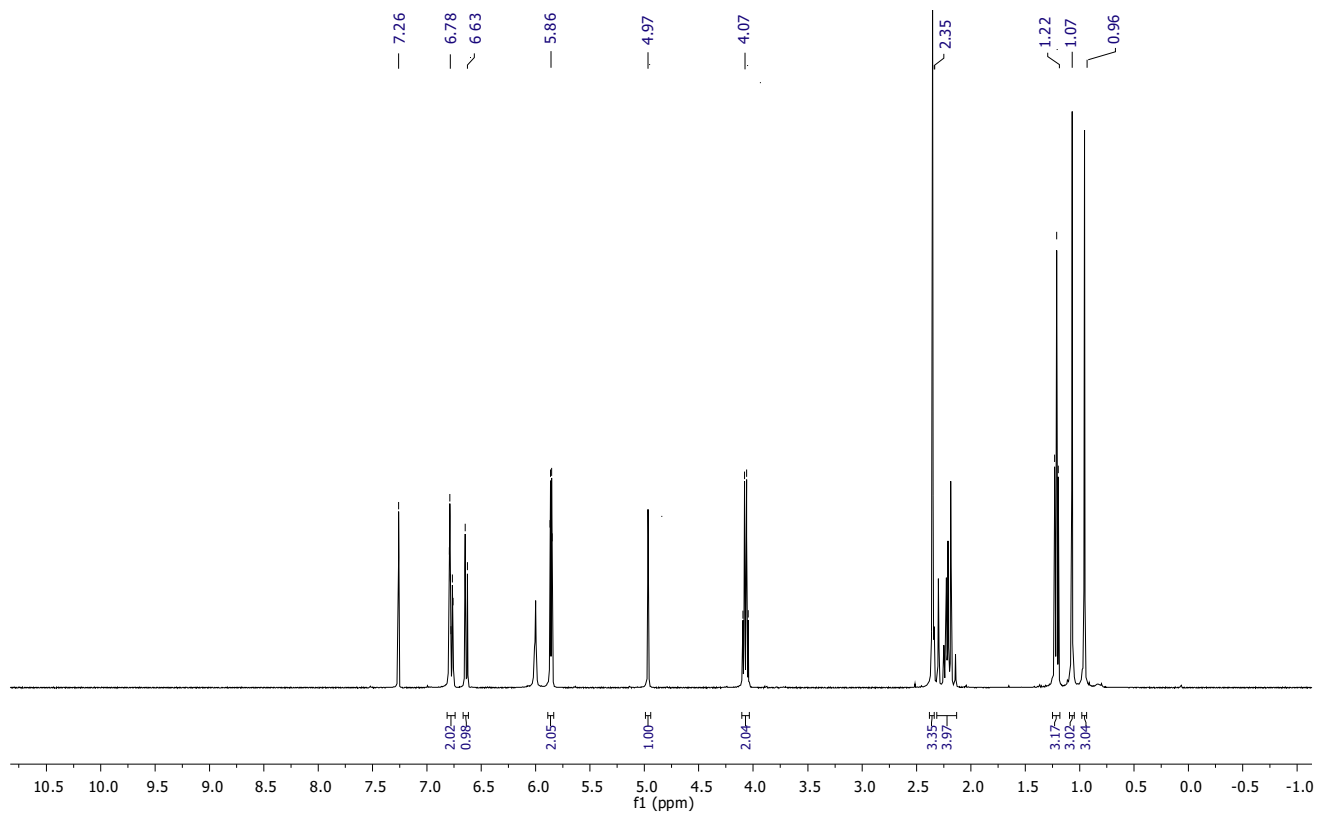


Figure S45. ¹H NMR spectrum of compound **12** (CDCl₃, 400 MHz, TMS).

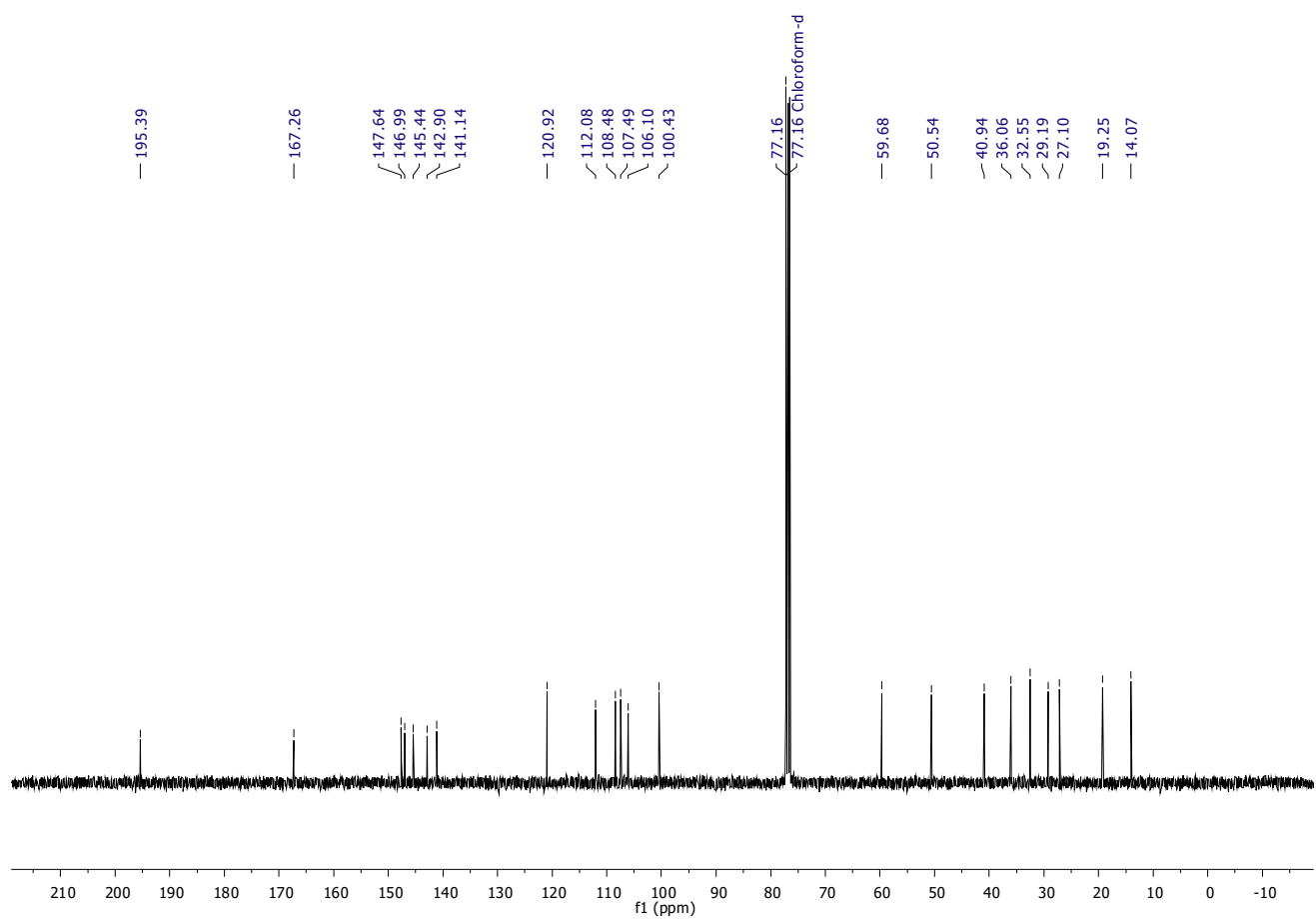


Figure S46. ¹³C NMR spectrum of compound **12** (CDCl₃, 100 MHz, TMS).

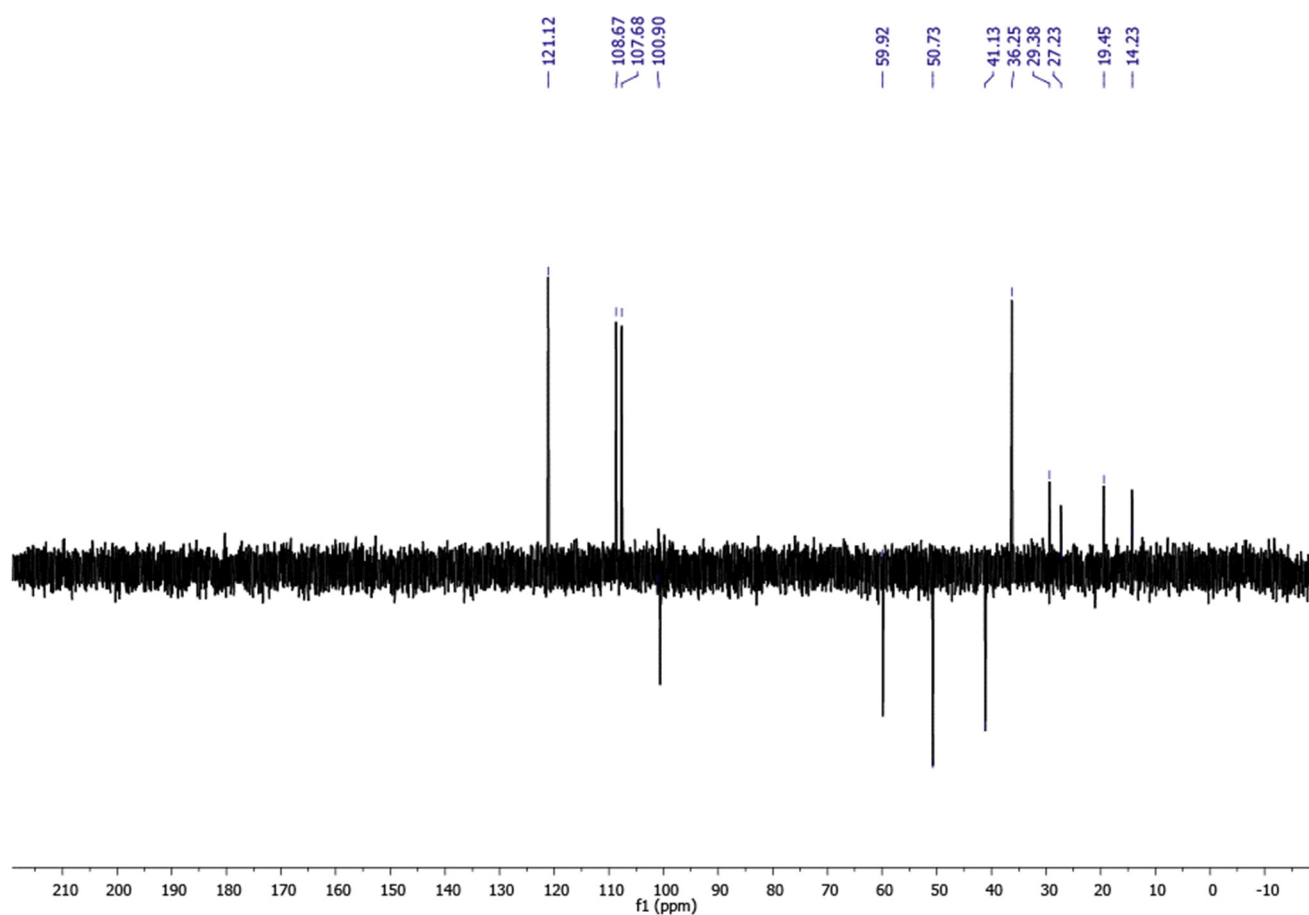


Figure S47. DEPT 135 spectrum of compound **12** (CDCl_3 , 100 MHz, TMS).

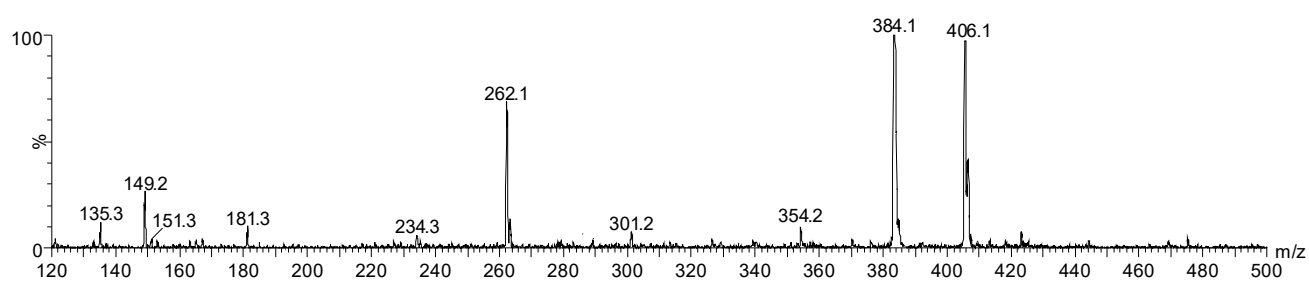


Figure S48. ESI (+) mass spectrum of compound **12**.

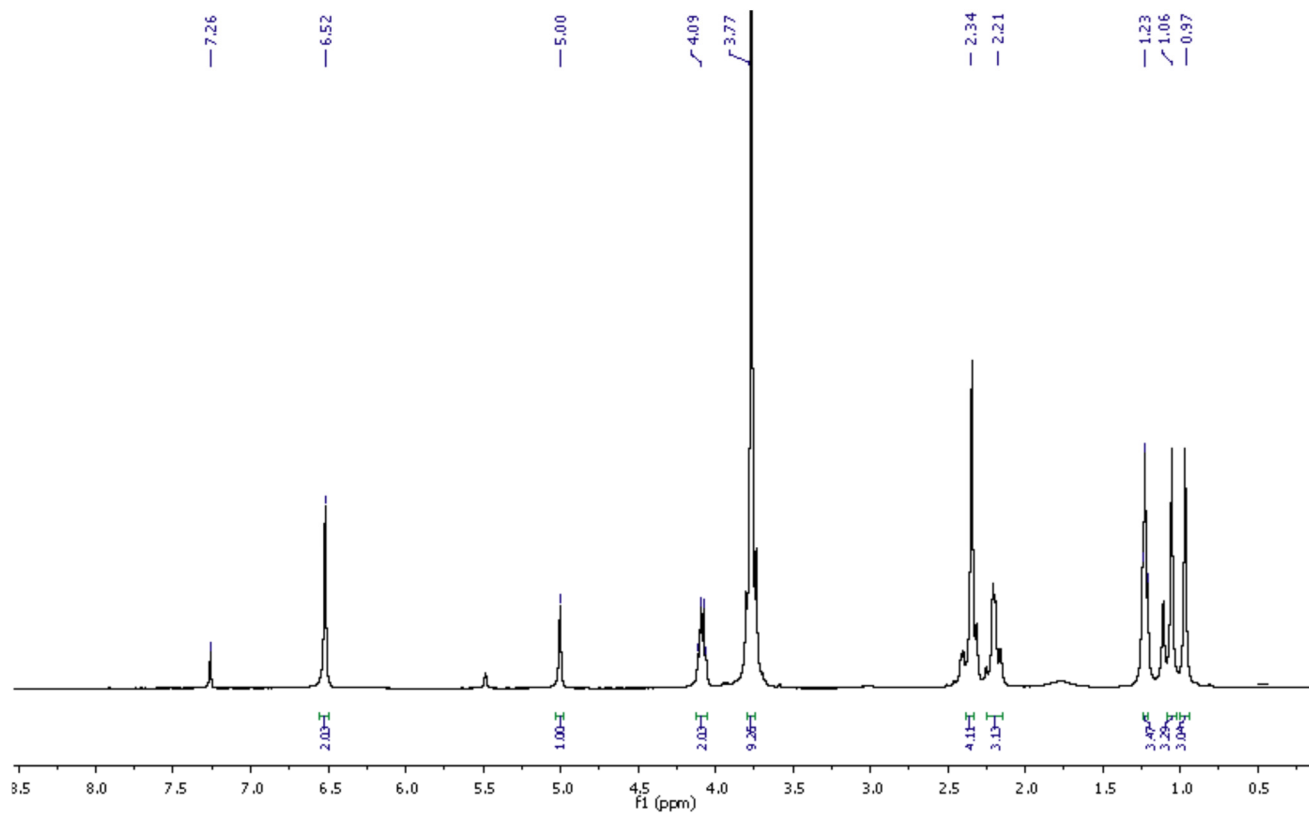


Figure S49. ¹H NMR spectrum of compound **13** (CDCl₃, 400 MHz, TMS).

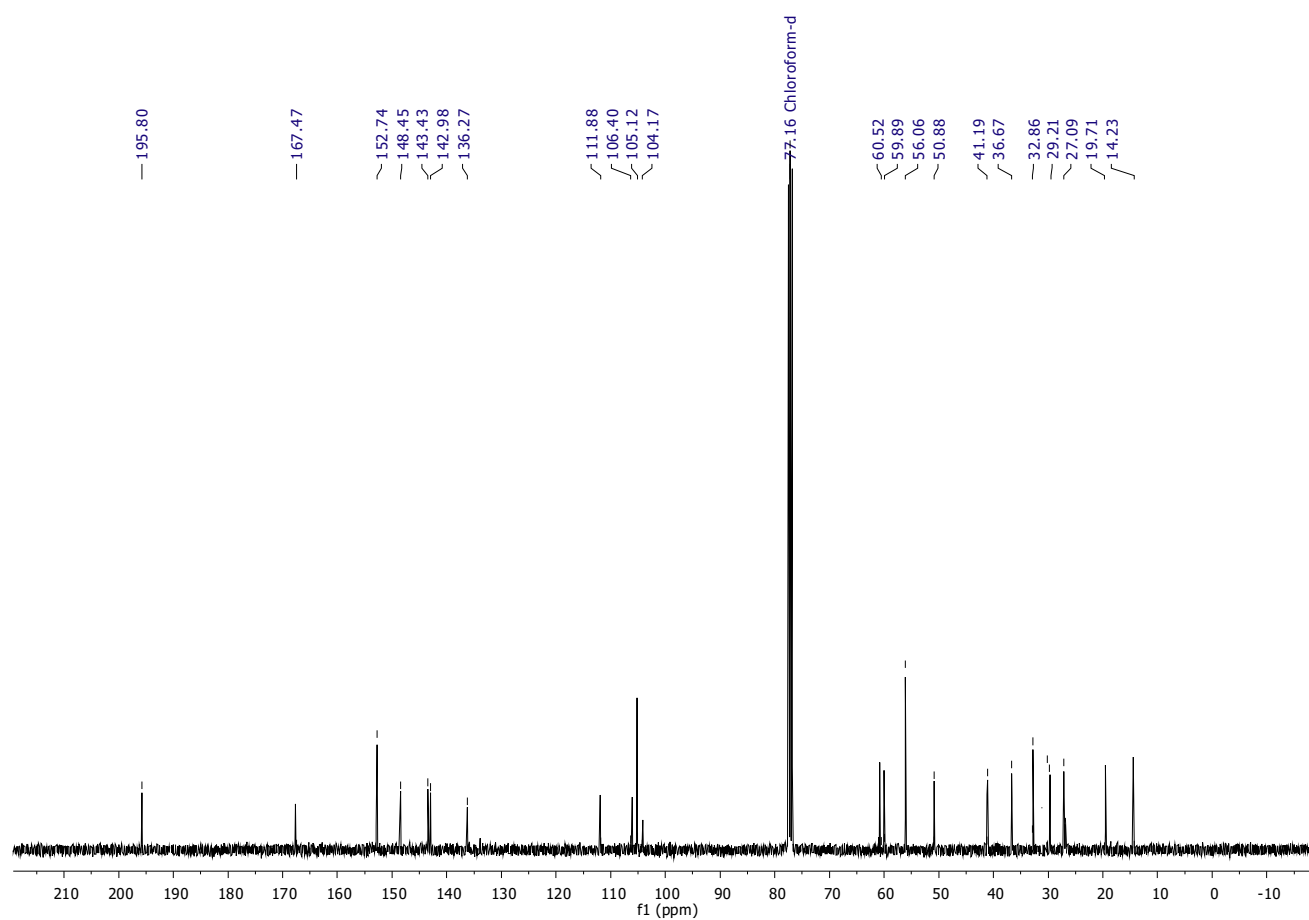


Figure S50. ¹³C NMR spectrum of compound **13** (CDCl₃, 100 MHz, TMS).

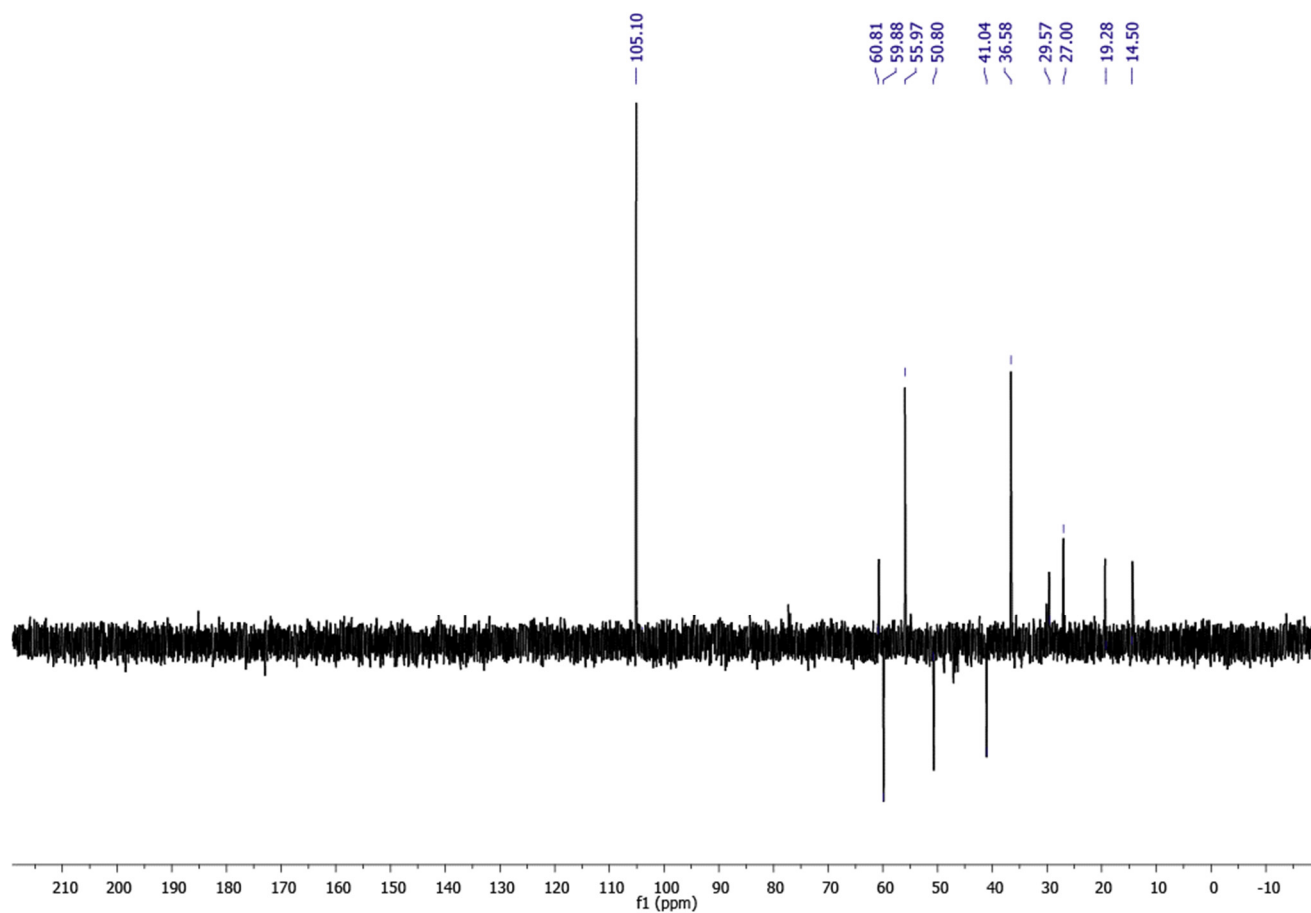


Figure S51. DEPT 135 spectrum of compound **13** (CDCl₃, 100 MHz, TMS).

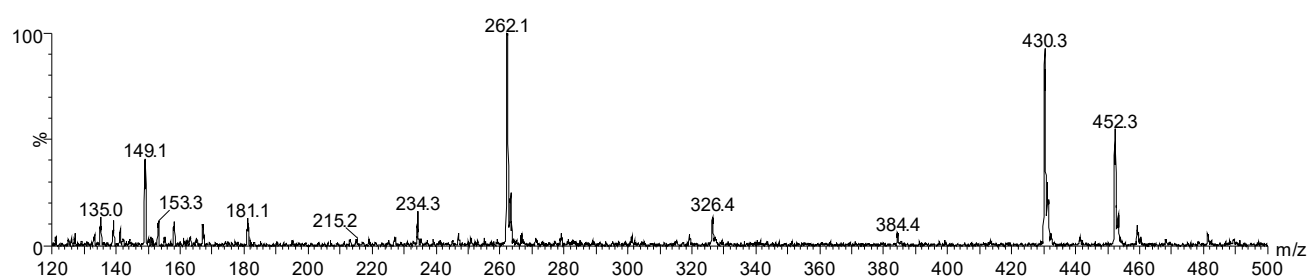


Figure S52. ESI (+) mass spectrum of compound **13**.

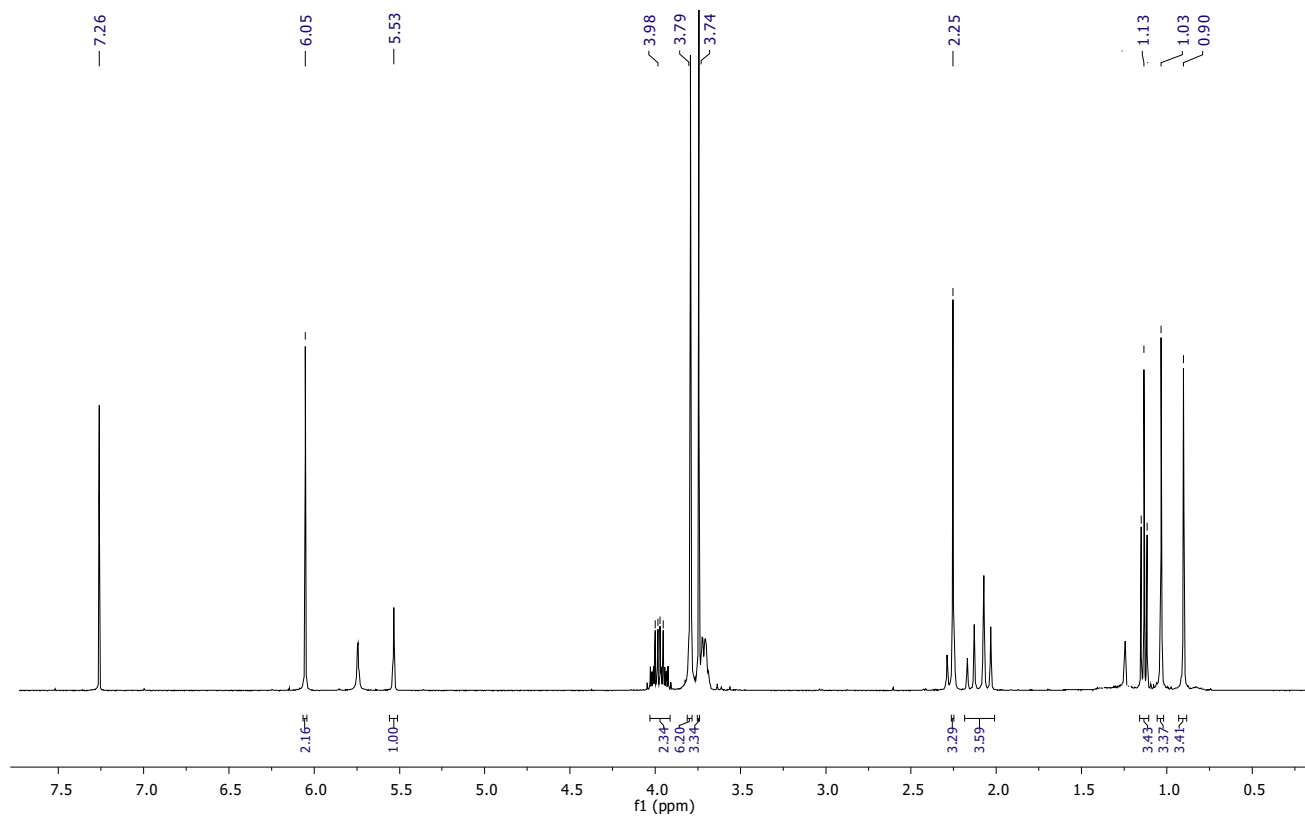


Figure S53. ^1H NMR spectrum of compound **14** (CDCl_3 , 400 MHz, TMS).

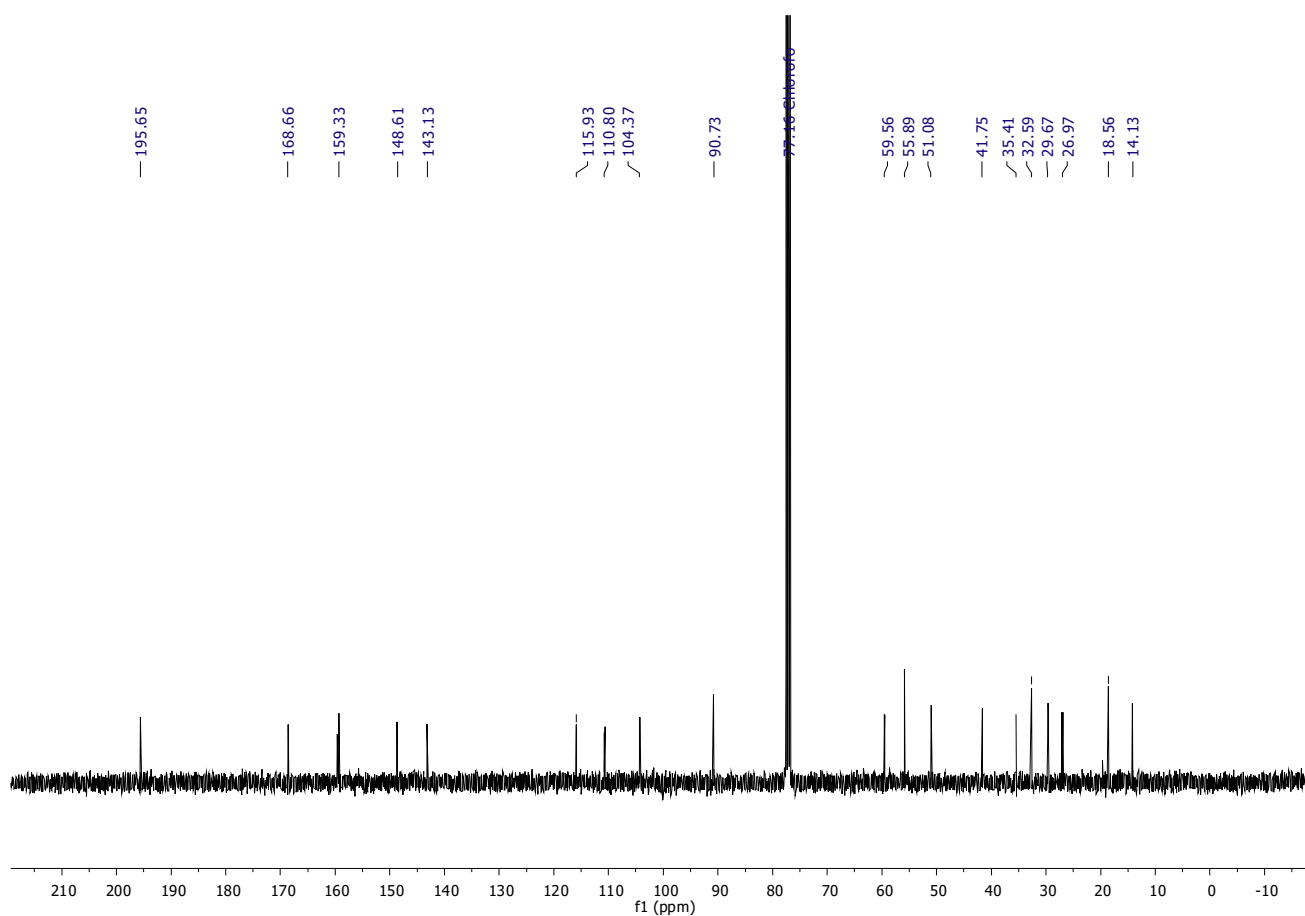


Figure S54. ^{13}C NMR spectrum of compound **14** (CDCl_3 , 100 MHz, TMS).

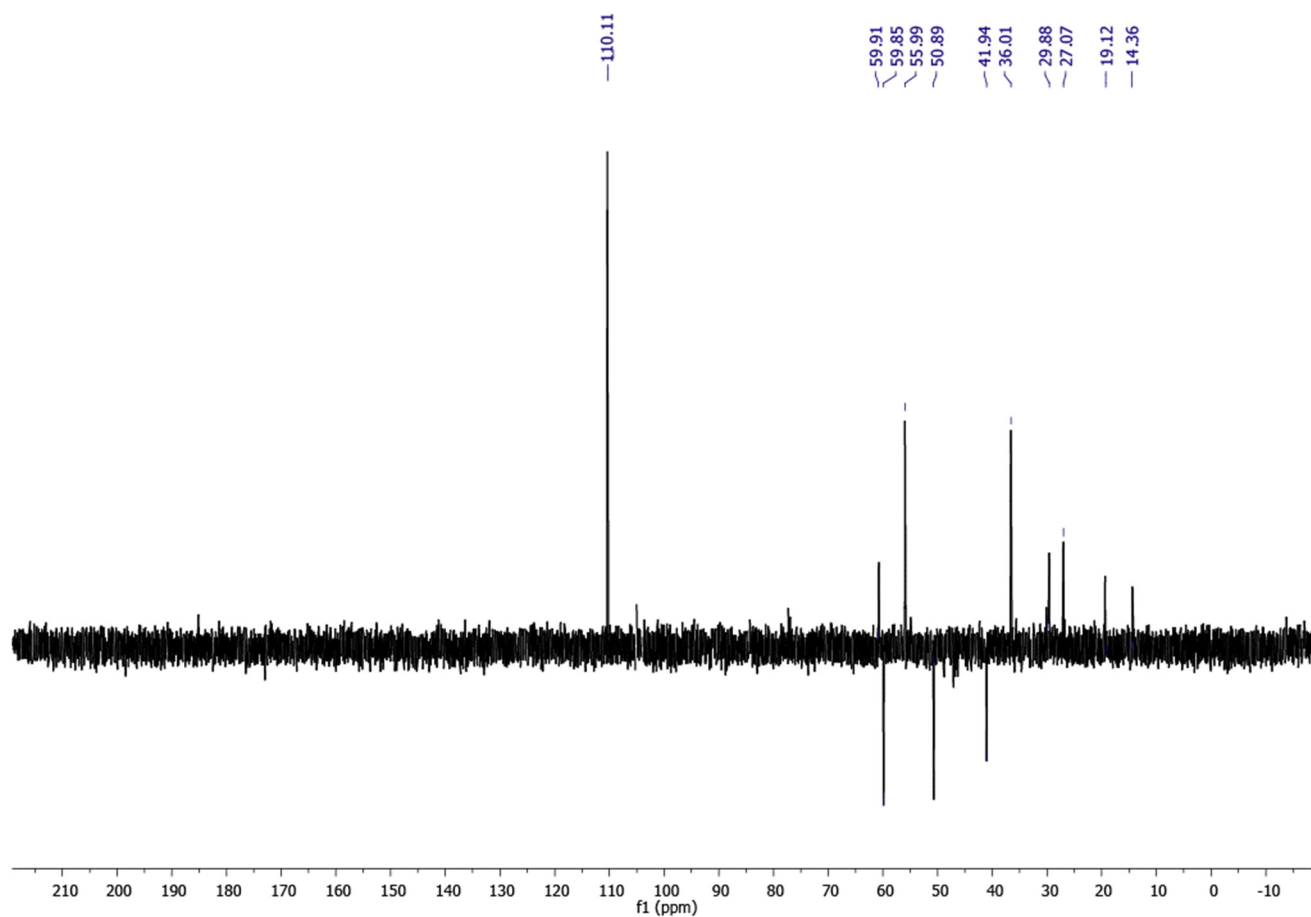


Figure S55. DEPT 135 spectrum of compound **14** (CDCl₃, 100 MHz, TMS).

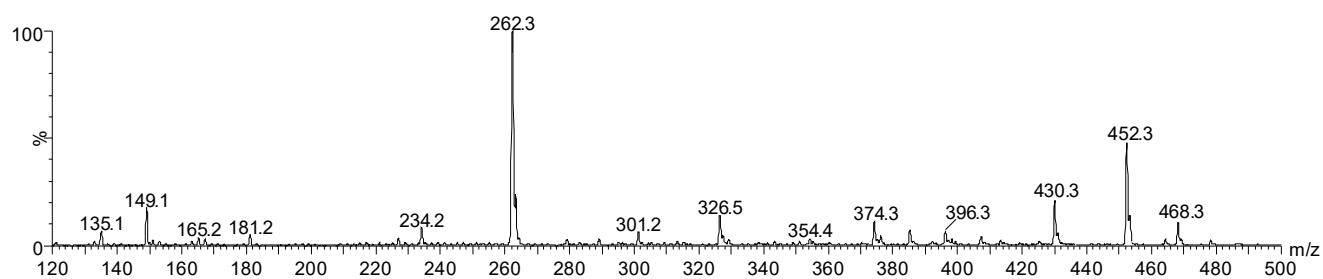


Figure S56. ESI (+) mass spectrum of compound **14**.

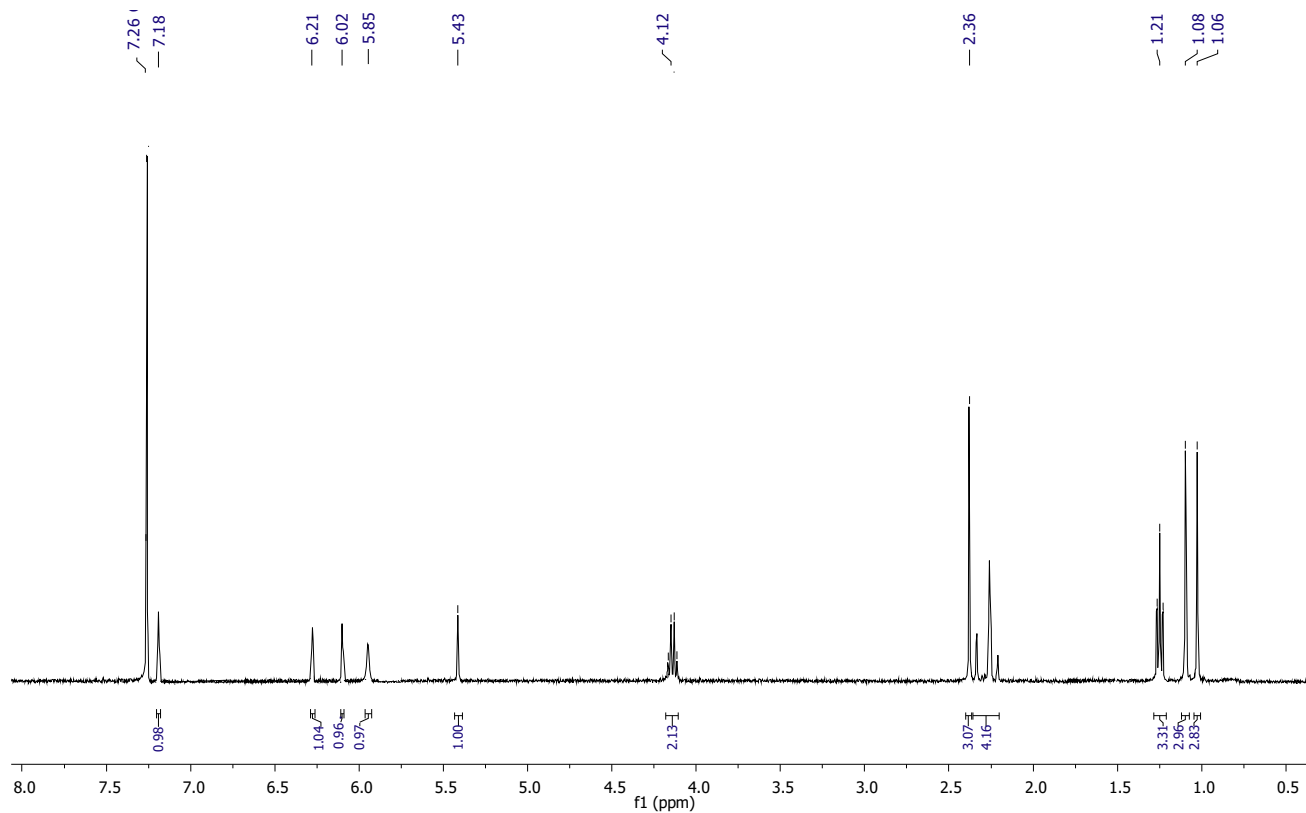


Figure S57. ¹H NMR spectrum of compound **15** (CDCl₃, 400 MHz, TMS).

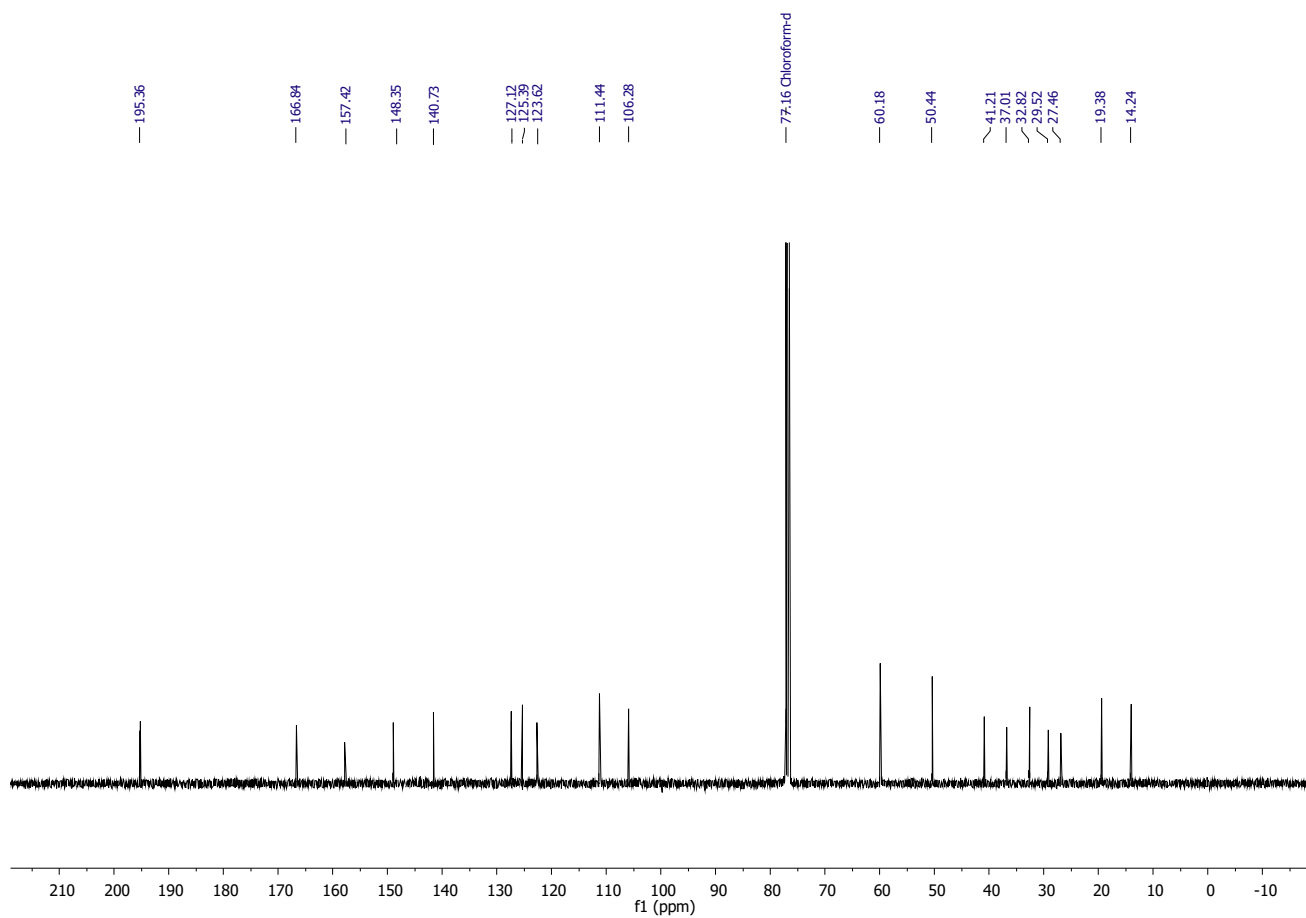


Figure S58. ¹³C NMR spectrum of compound **15** (CDCl₃, 100 MHz, TMS).

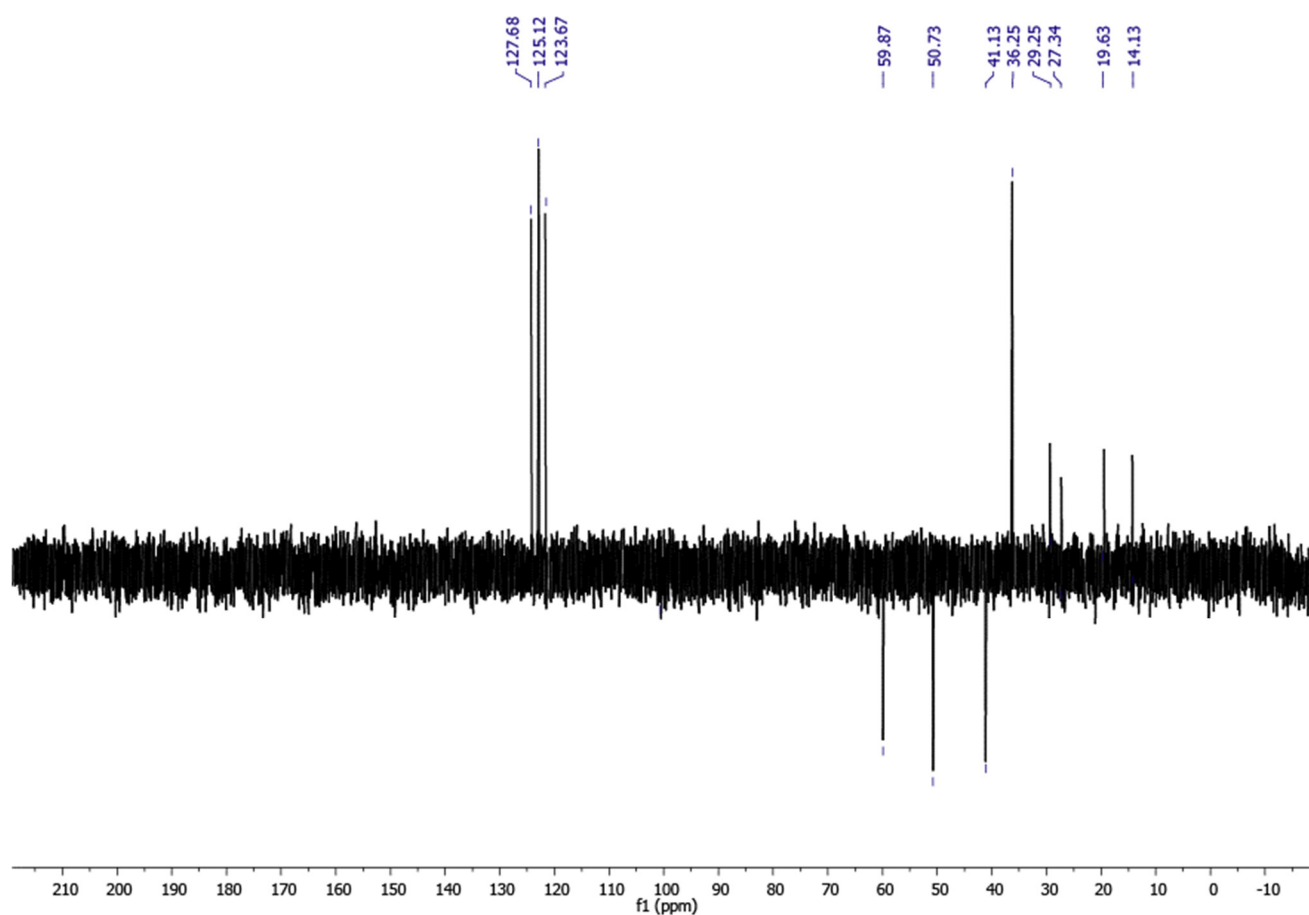


Figure S59. DEPT 135 spectrum of compound **15** (CDCl_3 , 100 MHz, TMS).

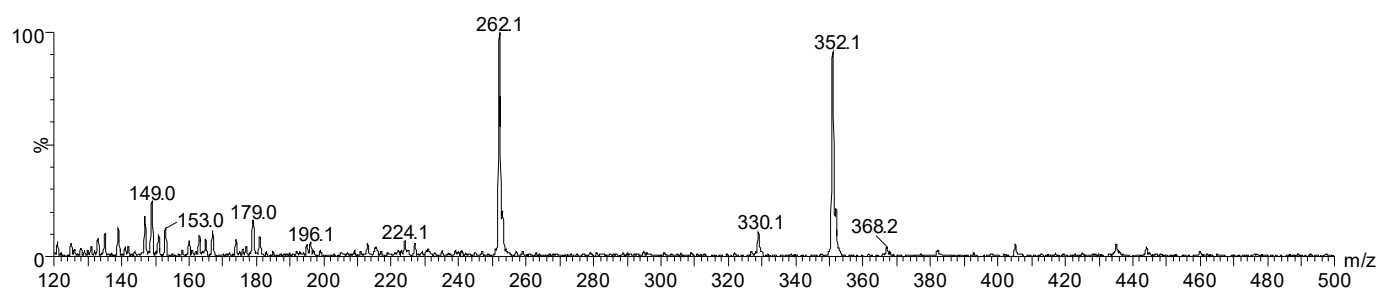


Figure S60. ESI (+) mass spectrum of compound **15**.

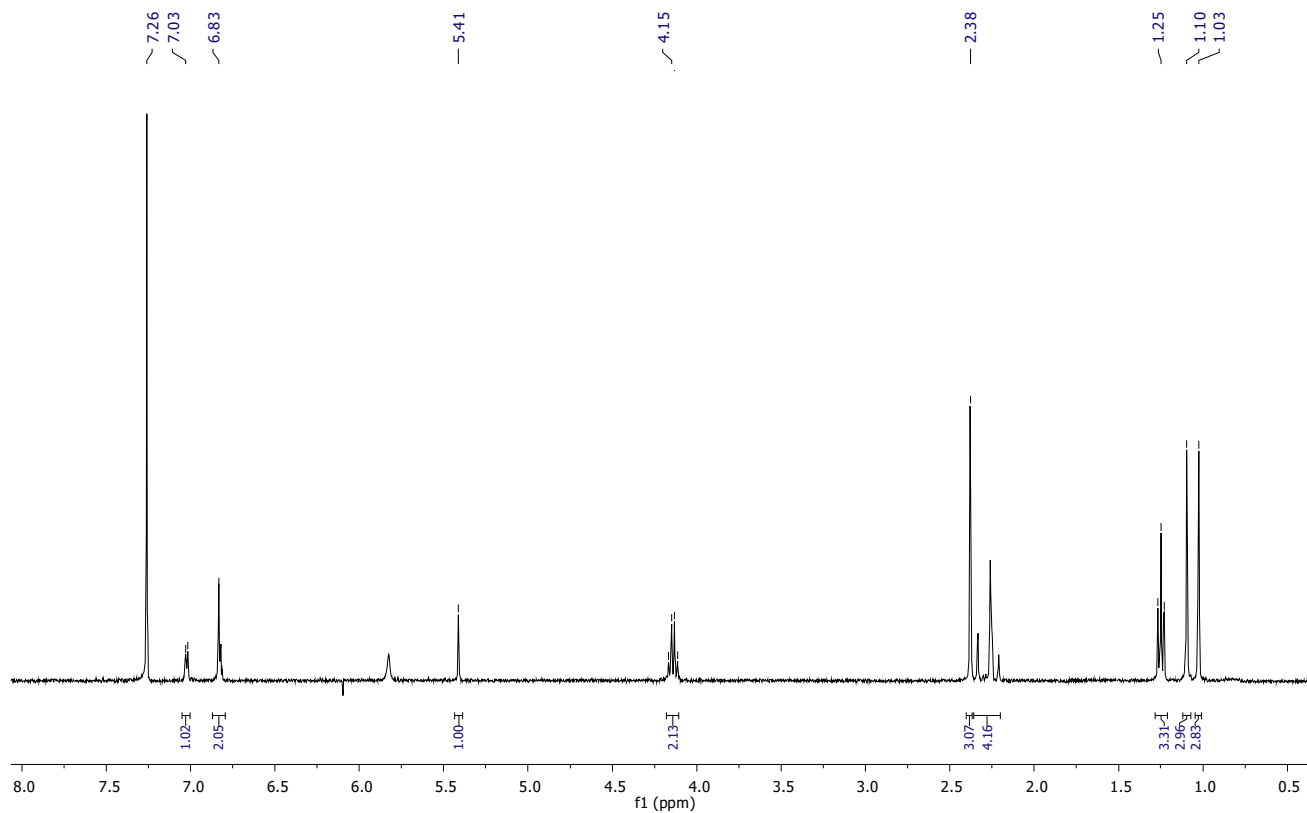


Figure S61. ¹H NMR spectrum of compound **16** (CDCl₃, 400 MHz, TMS).

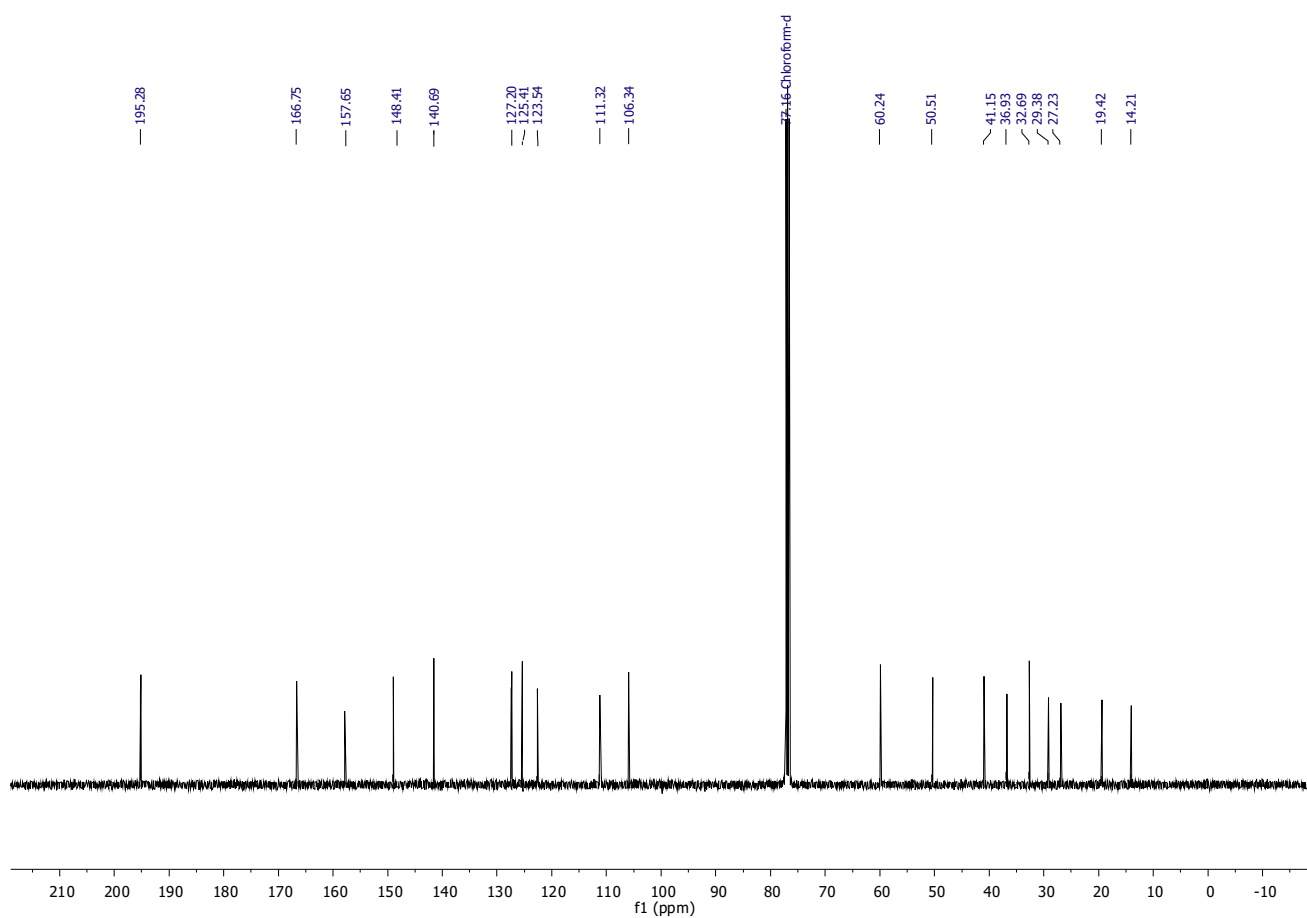


Figure S62. ¹³C NMR spectrum of compound **16** (CDCl₃, 100 MHz, TMS).

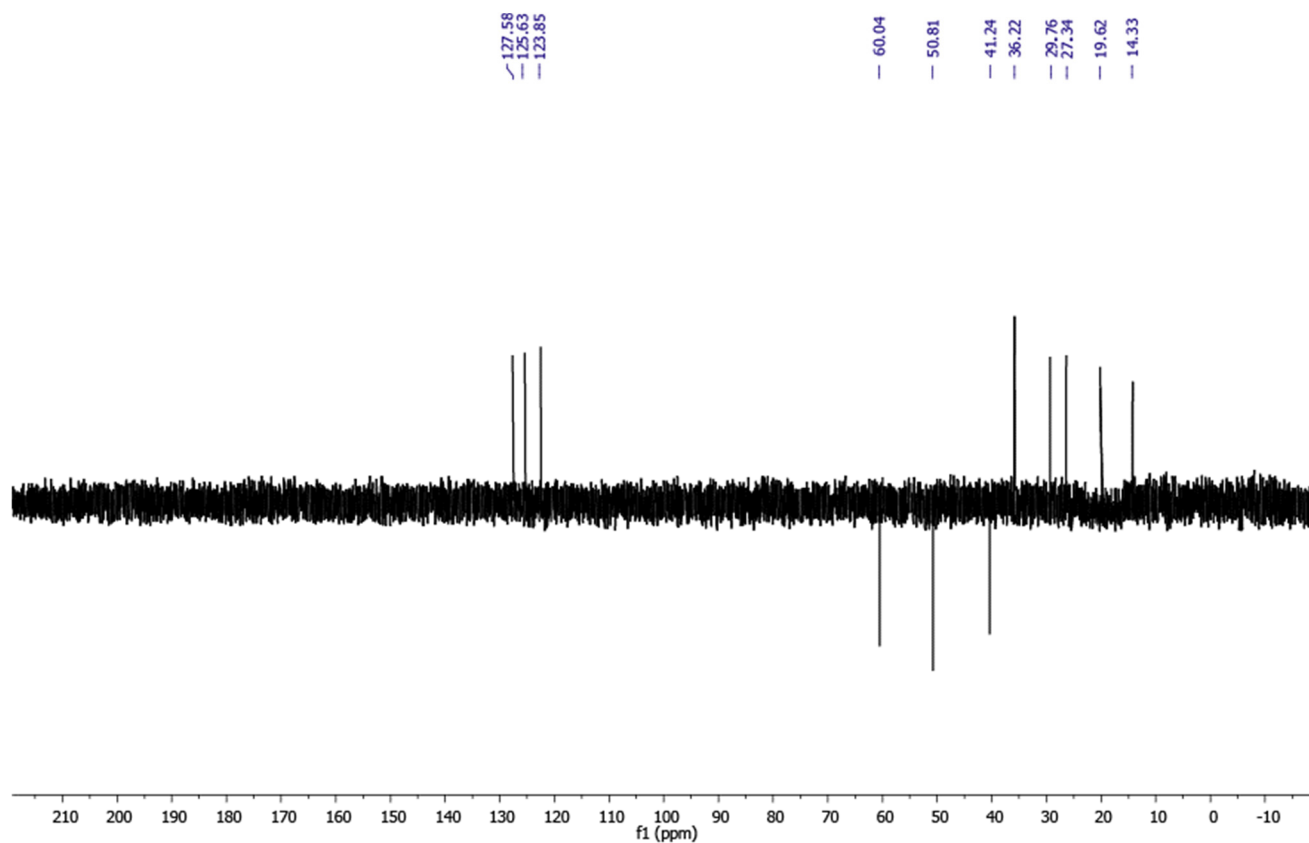


Figure S63. DEPT 135 spectrum of compound **16** (CDCl_3 , 100 MHz, TMS).

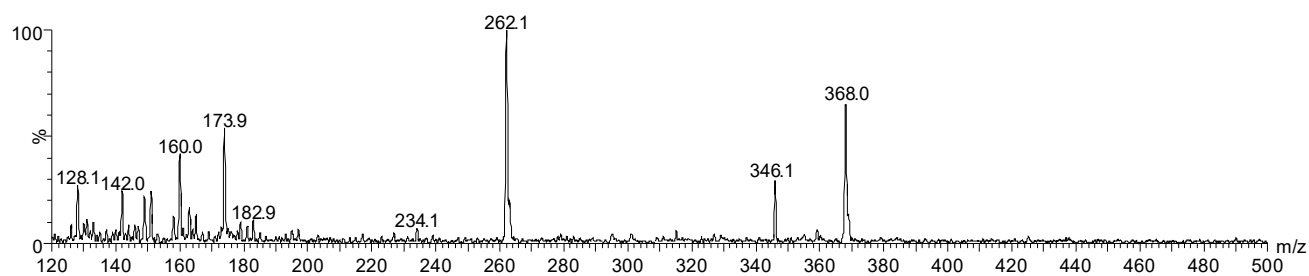


Figure S64. ESI (+) mass spectrum of compound **16**.

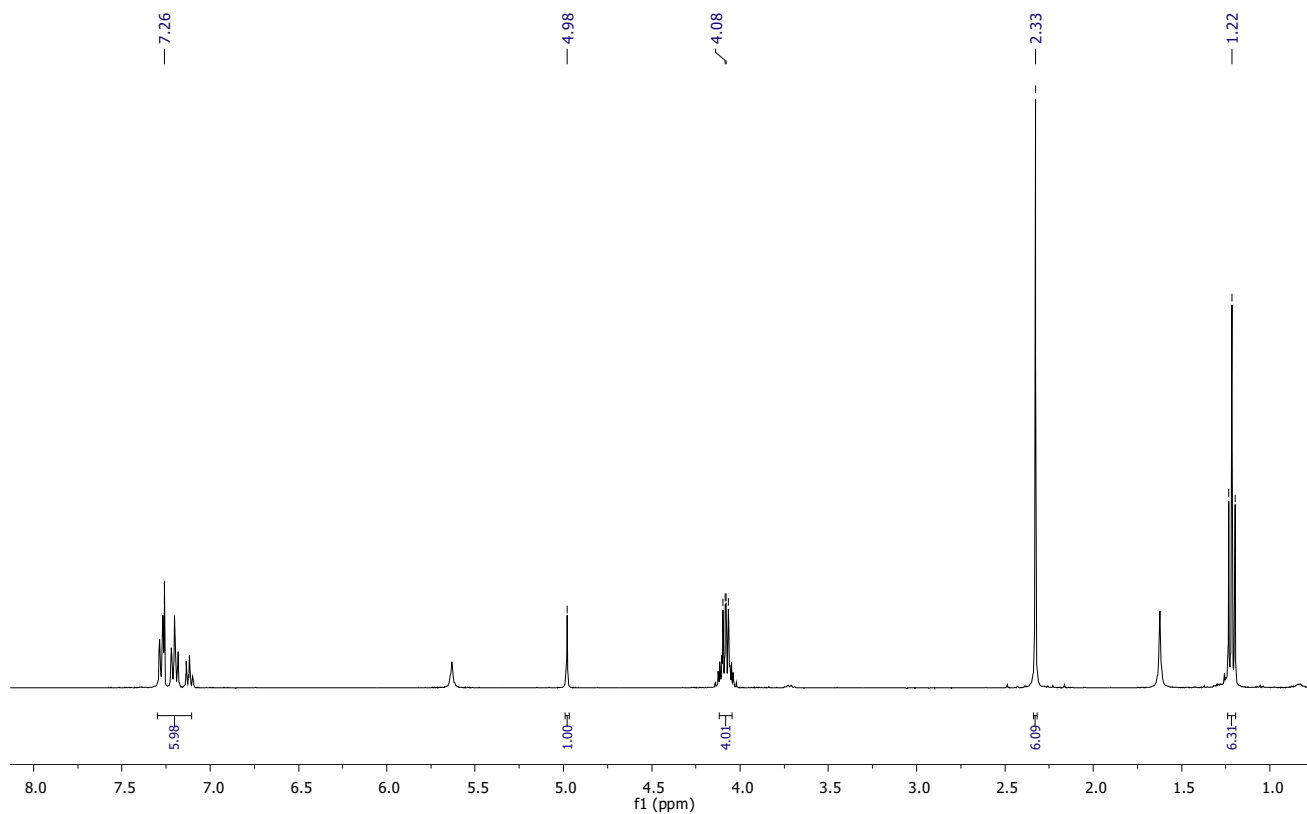


Figure S65. ¹H NMR spectrum of compound **17** (CDCl₃, 400 MHz, TMS).

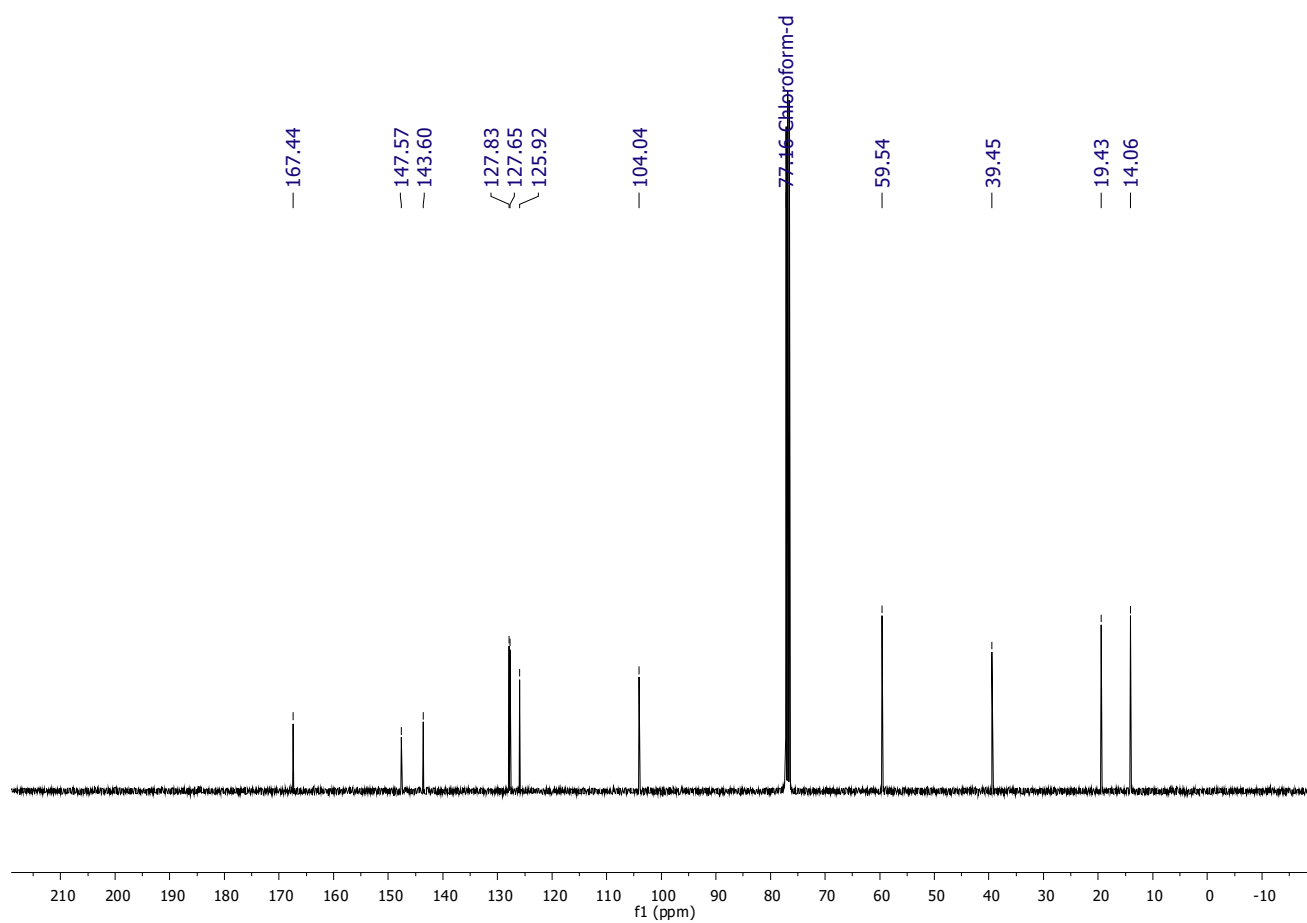


Figure S66. ¹³C NMR spectrum of compound **17** (CDCl₃, 100 MHz, TMS).

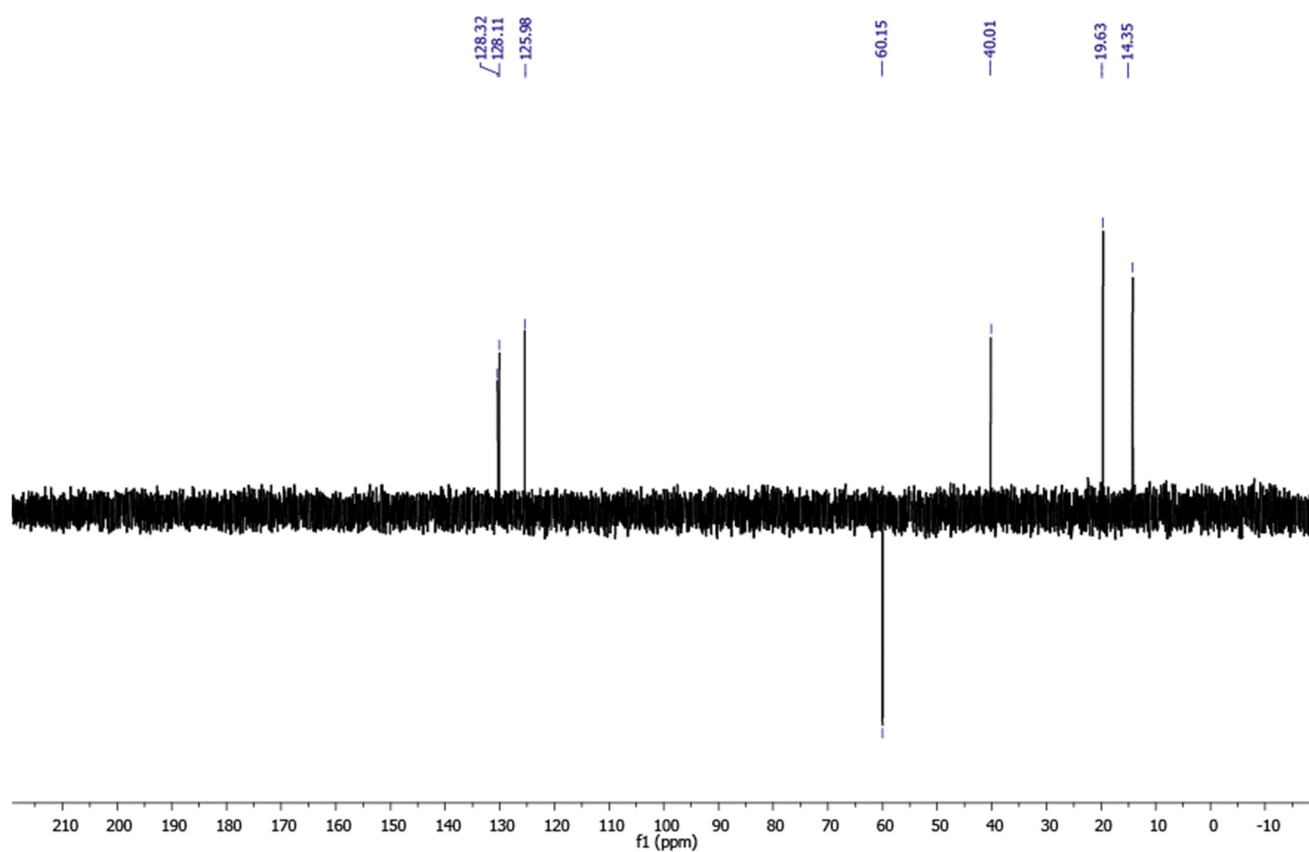


Figure S67. DEPT 135 spectrum of compound **17** (CDCl_3 , 100 MHz, TMS).

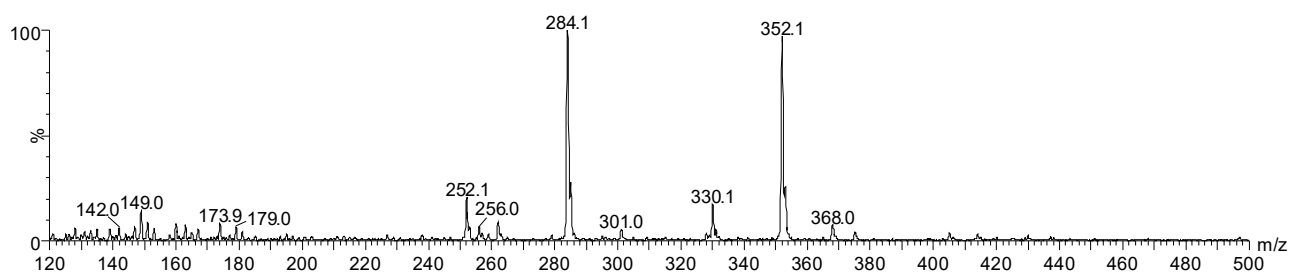


Figure S68. ESI (+) mass spectrum of compound **17**.

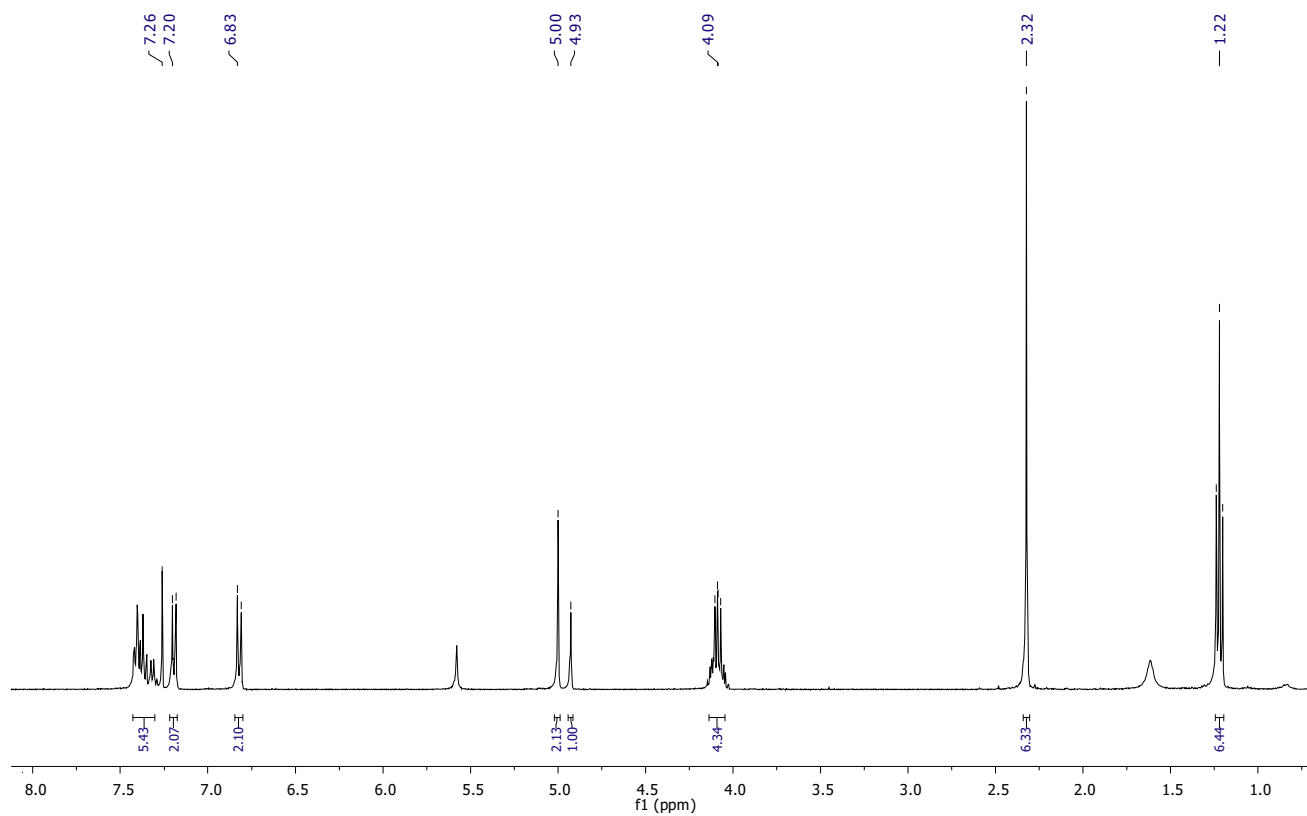


Figure S69. ¹H NMR spectrum of compound **18** (CDCl₃, 400 MHz, TMS).

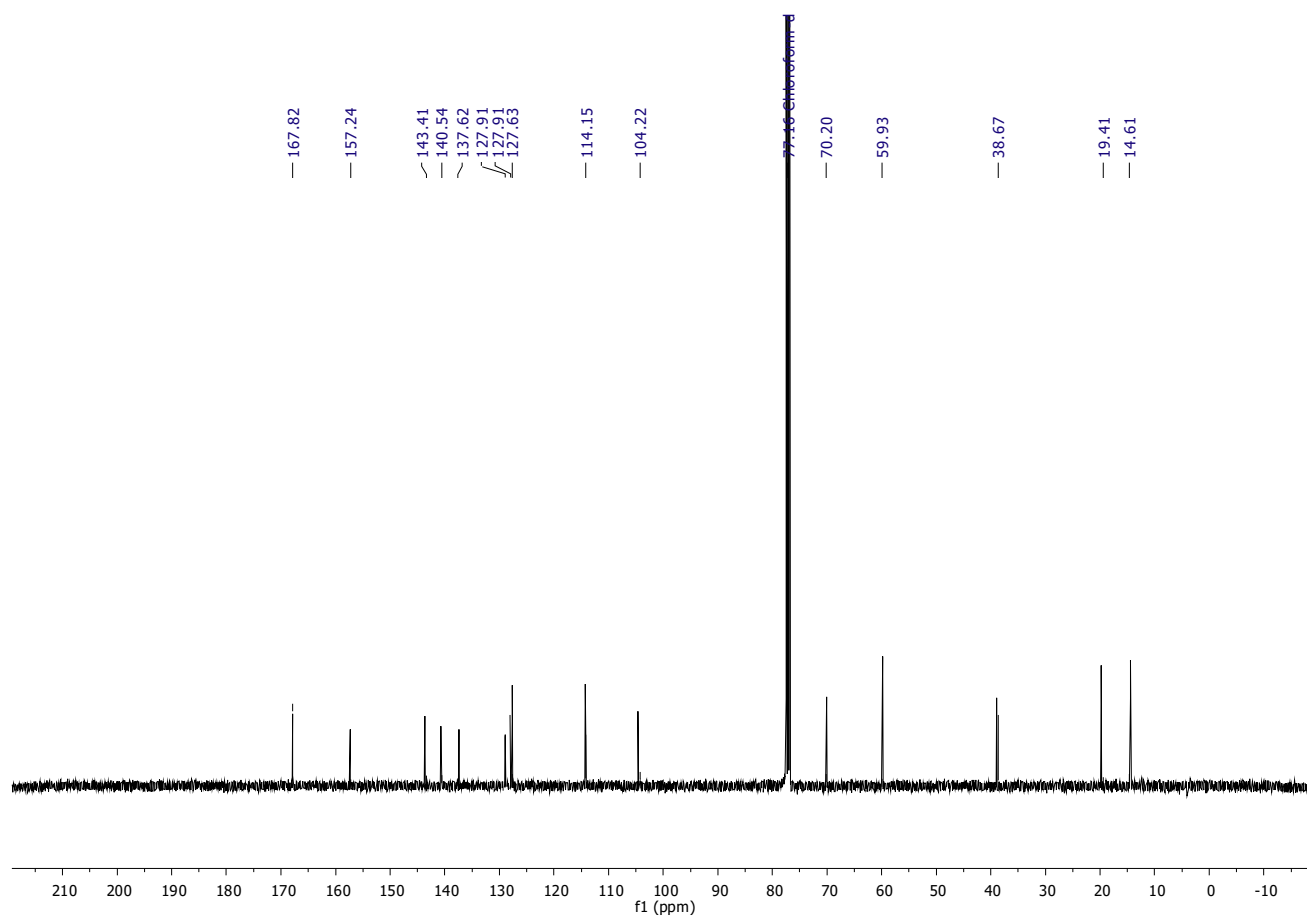


Figure S70. ¹³C NMR spectrum of compound **18** (CDCl₃, 100 MHz, TMS).

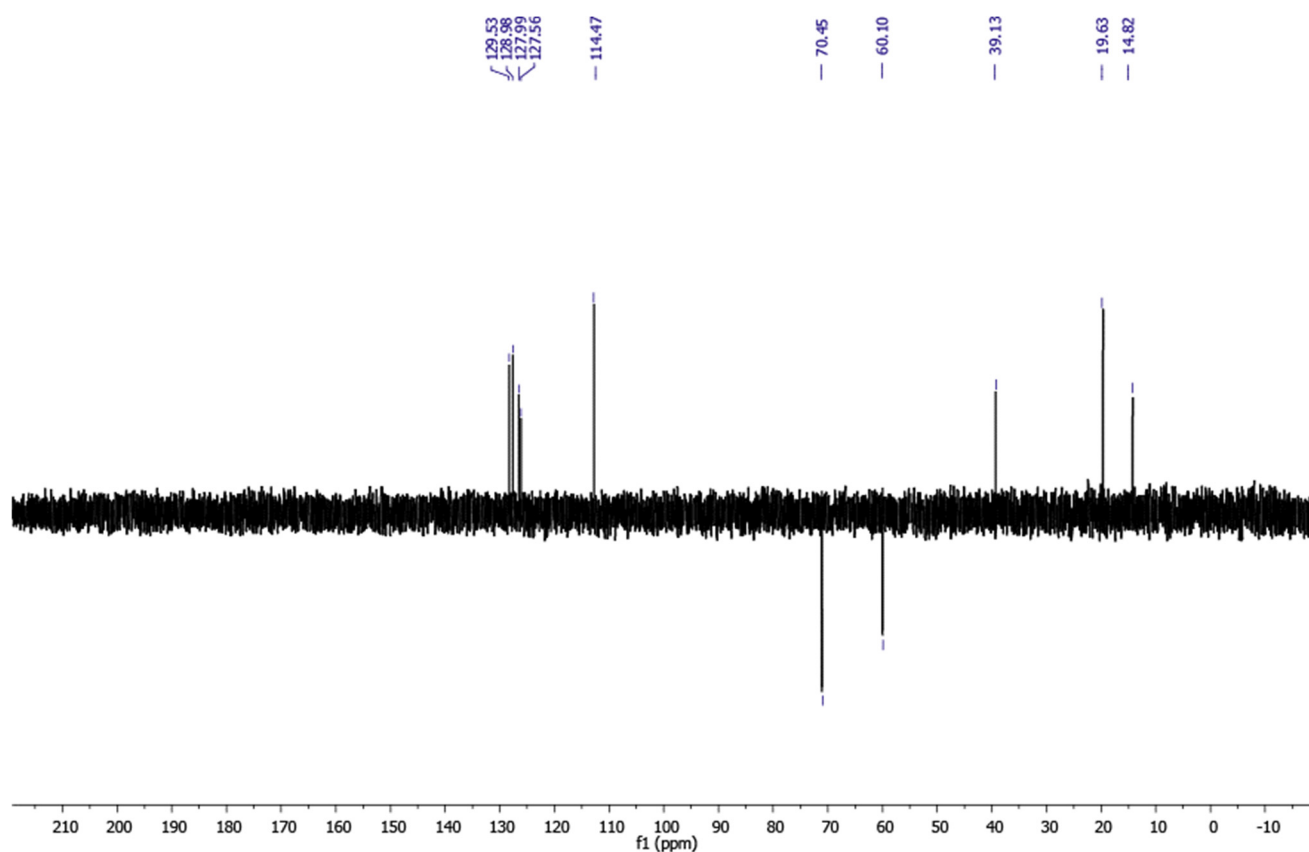


Figure S71. DEPT 135 spectrum of compound **18** (CDCl₃, 100 MHz, TMS).

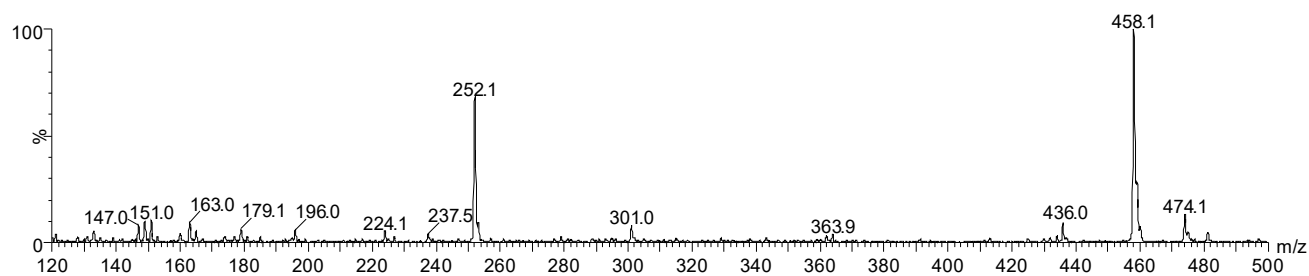


Figure S72. ESI (+) mass spectrum of compound **18**.

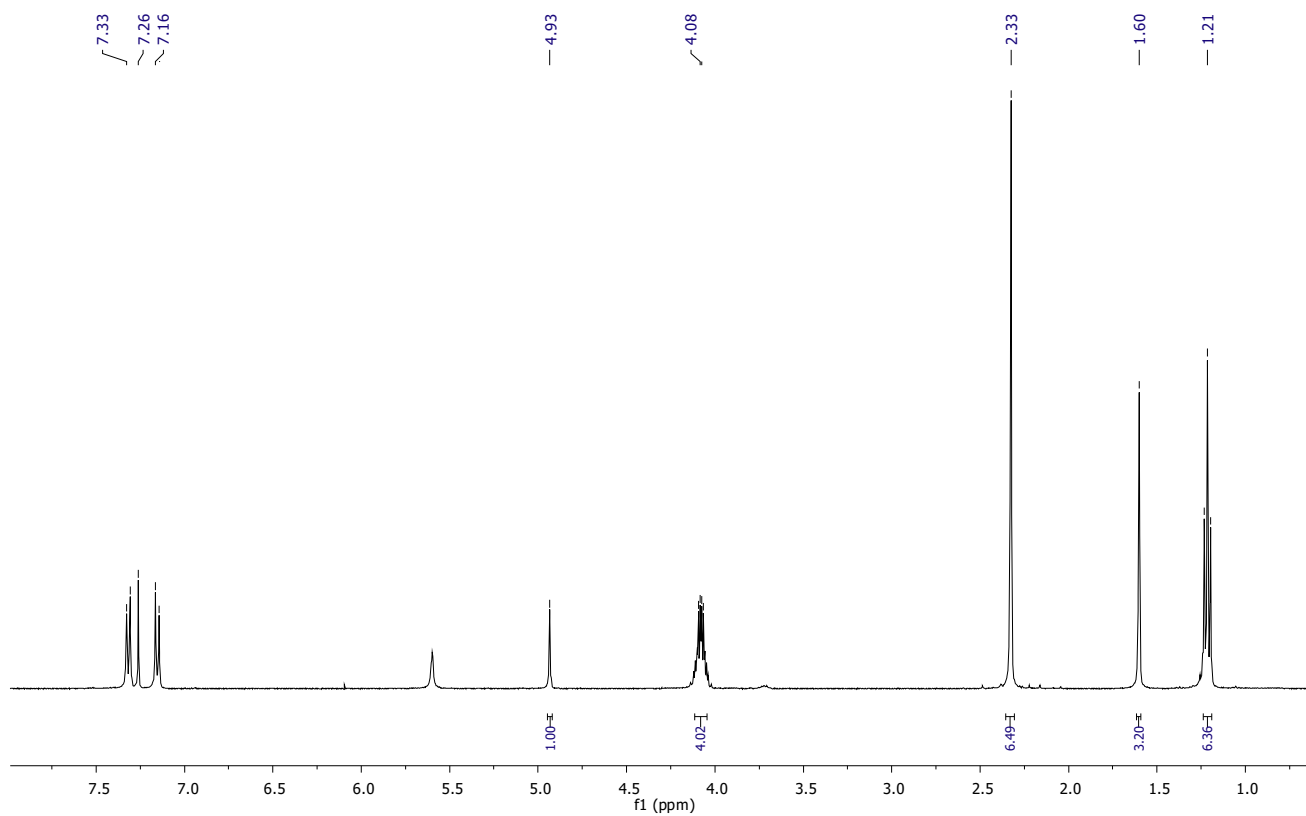


Figure S73. ¹H NMR spectrum of compound **19** (CDCl₃, 400 MHz, TMS).

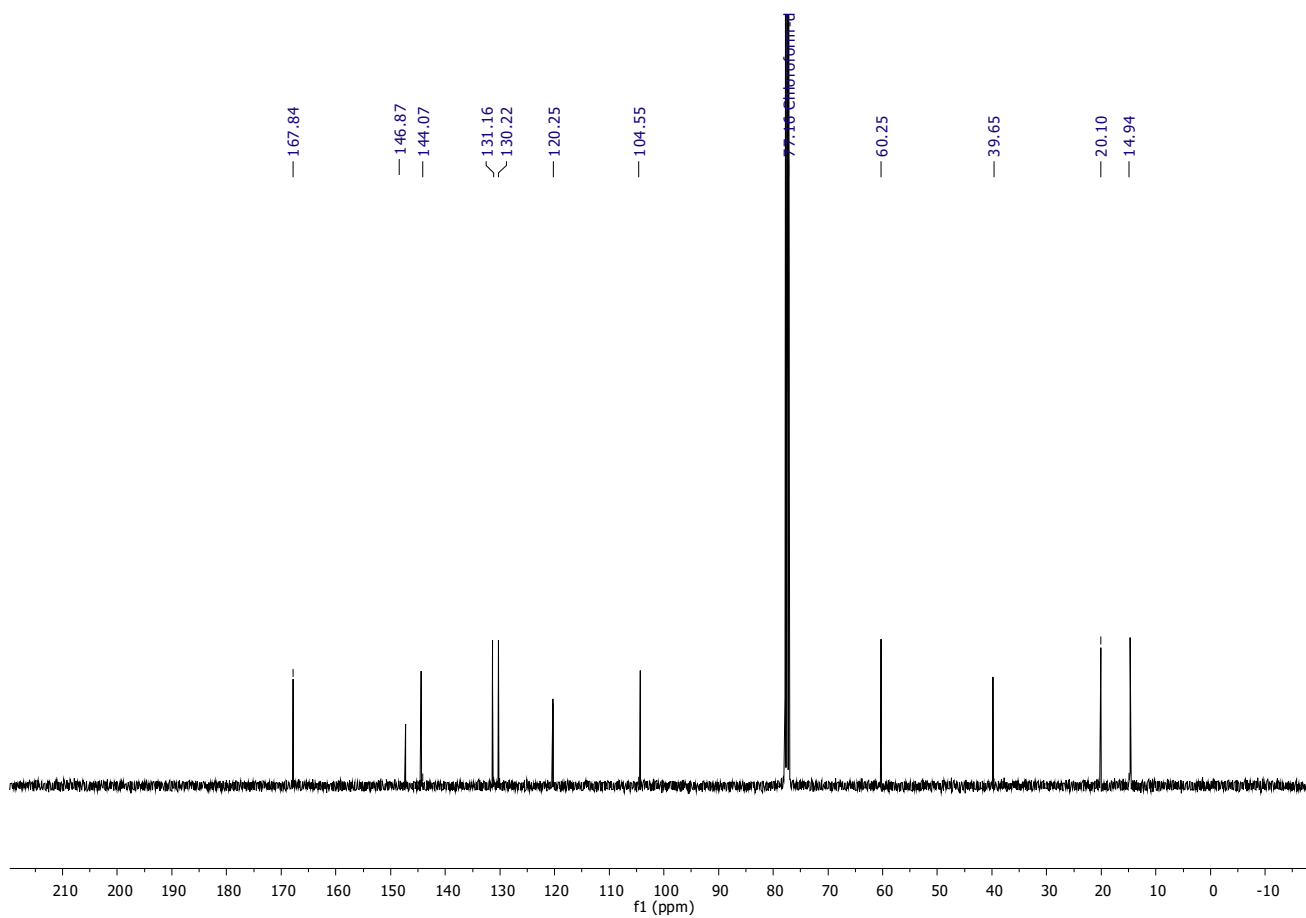


Figure S74. ¹³C NMR spectrum of compound **19** (CDCl₃, 100 MHz, TMS).

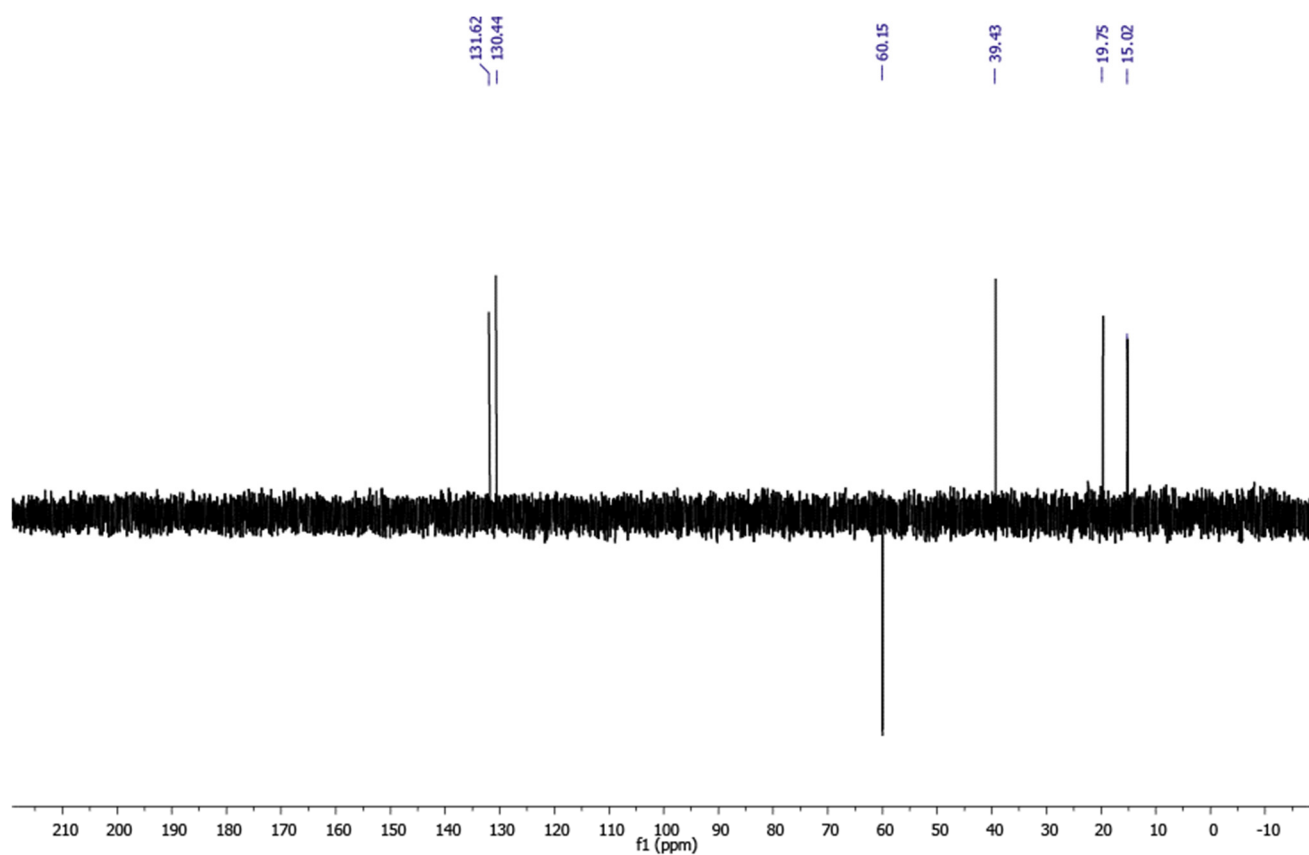


Figure S75. DEPT 135 spectrum of compound **19** (CDCl₃, 100 MHz, TMS).

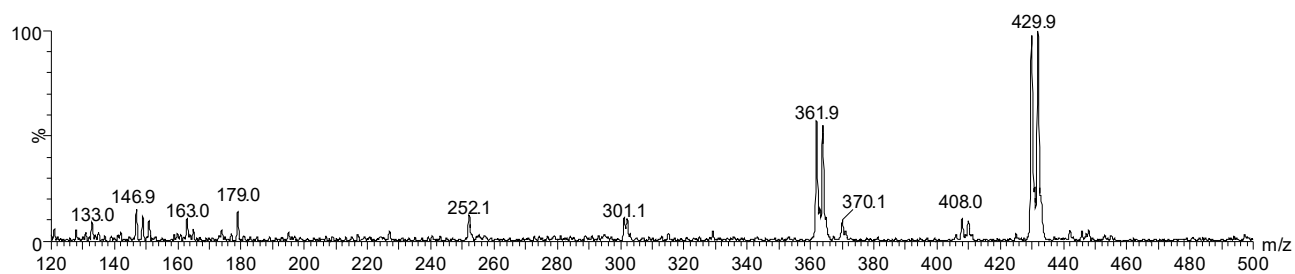


Figure S76. ESI (+) mass spectrum of compound **19**.

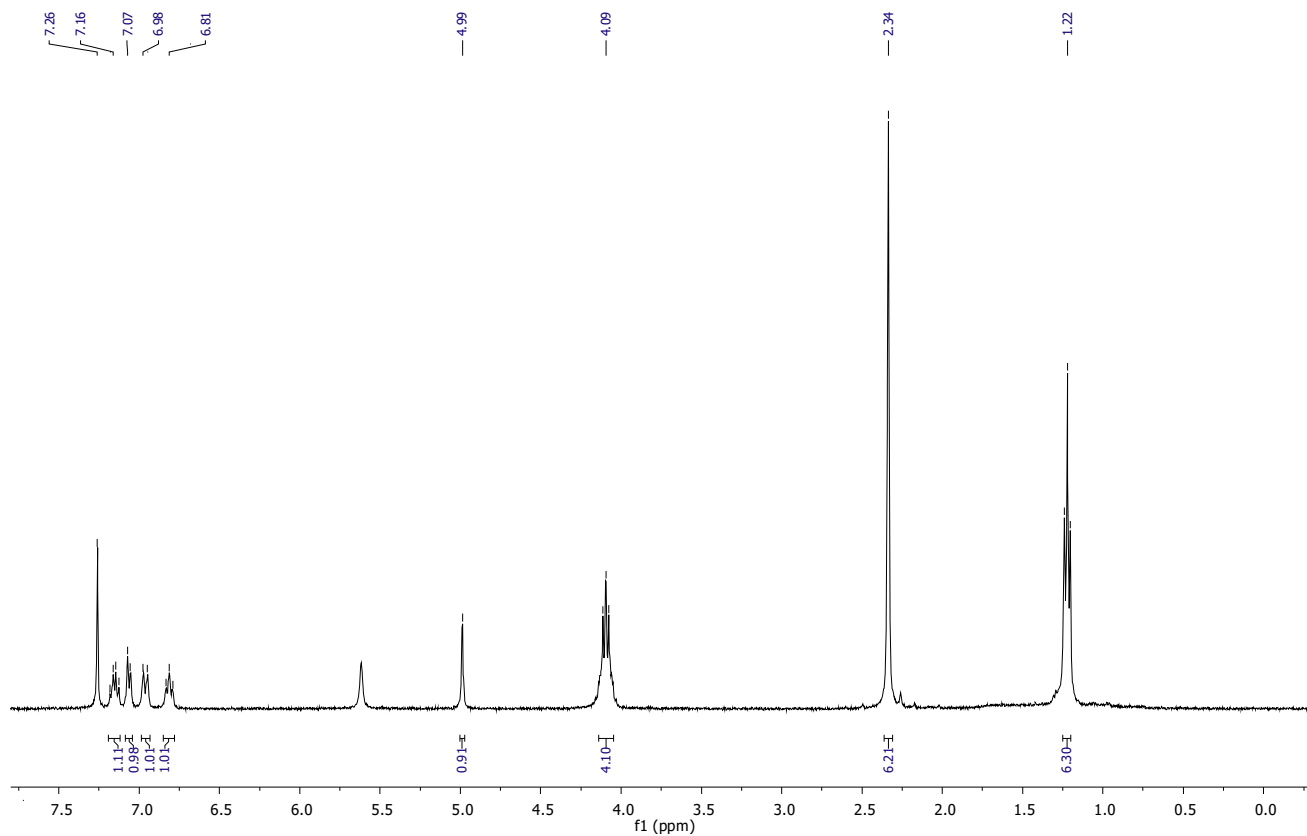


Figure S77. ^1H NMR spectrum of compound **20** (CDCl_3 , 400 MHz, TMS).

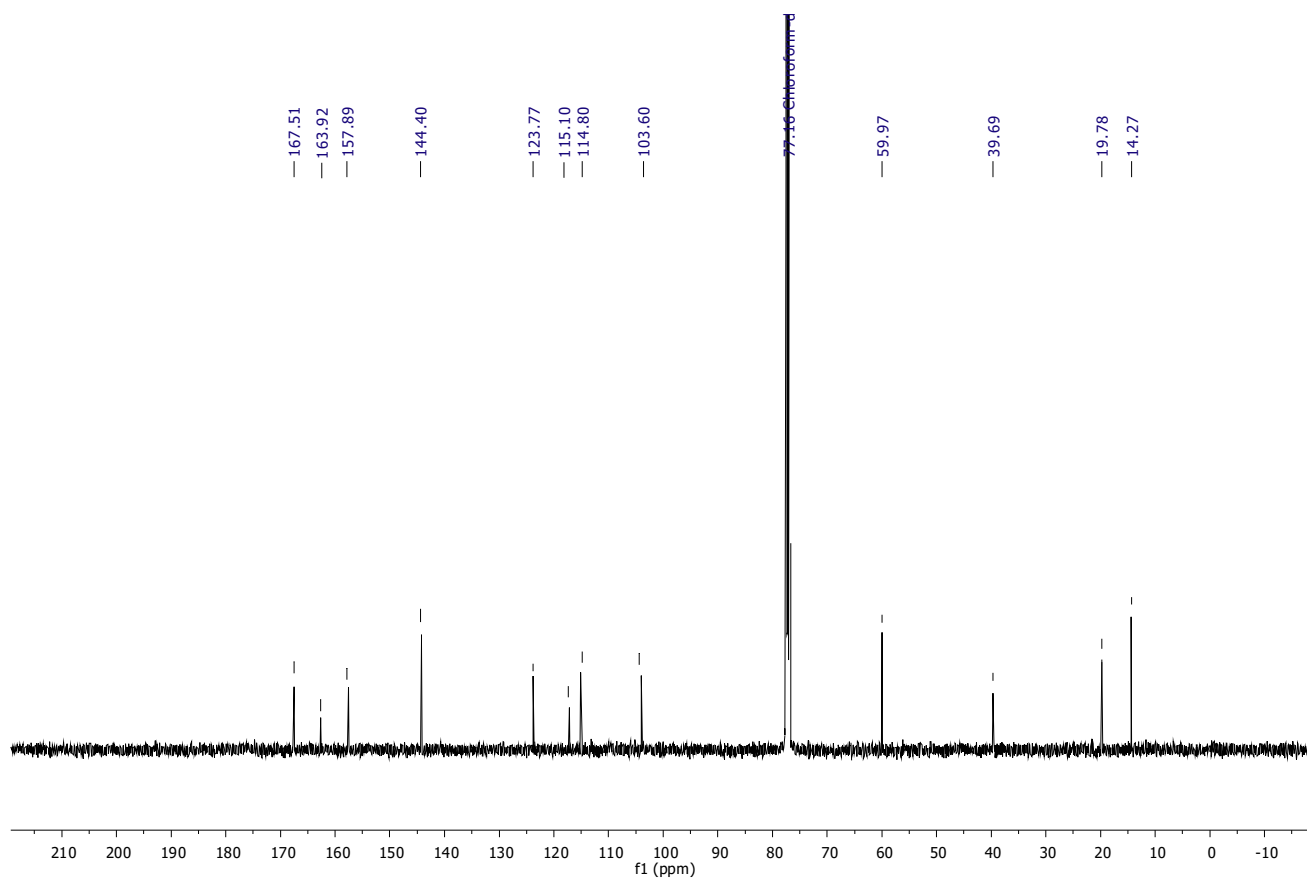


Figure S78. ^{13}C NMR spectrum of compound **20** (CDCl_3 , 100 MHz, TMS).

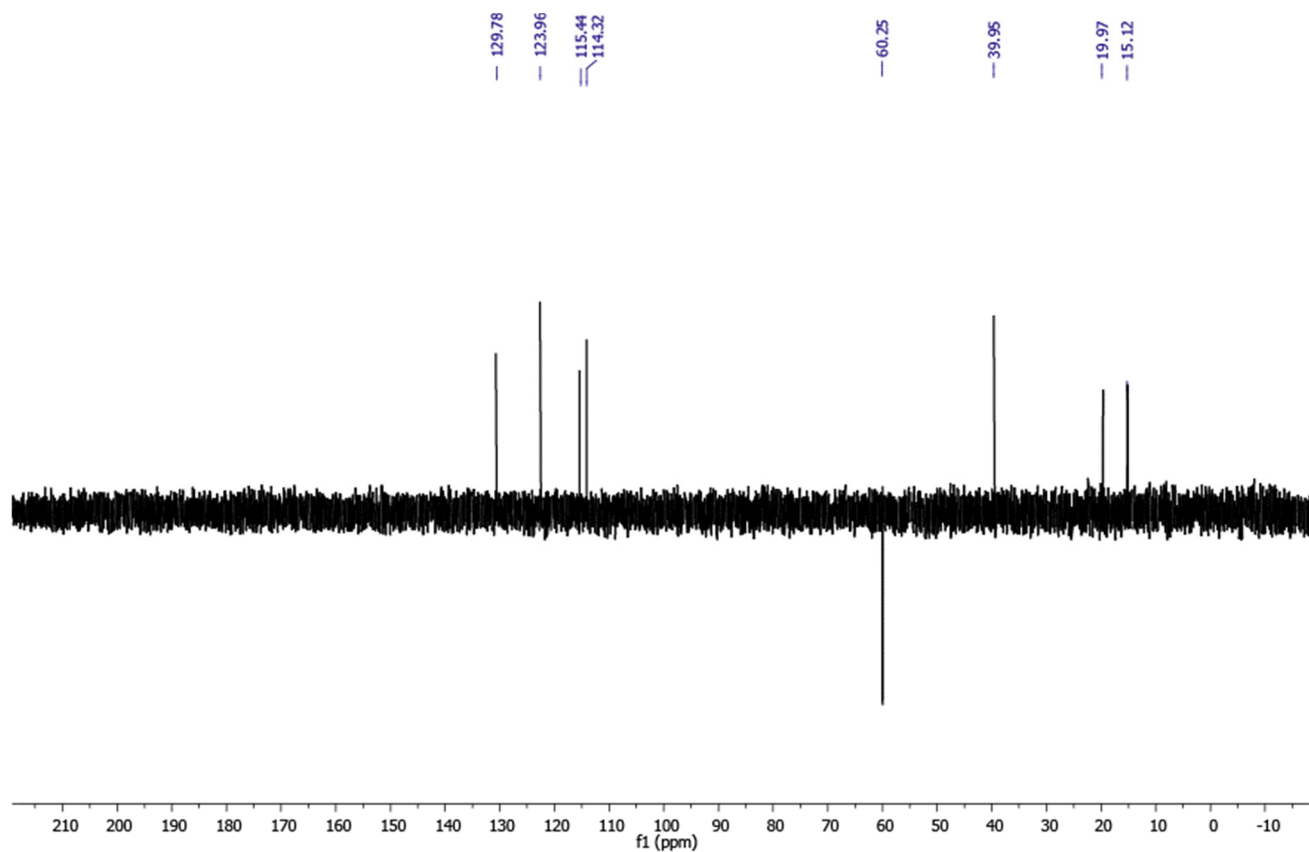


Figure S79. DEPT 135 spectrum of compound **20** (CDCl_3 , 100 MHz, TMS).

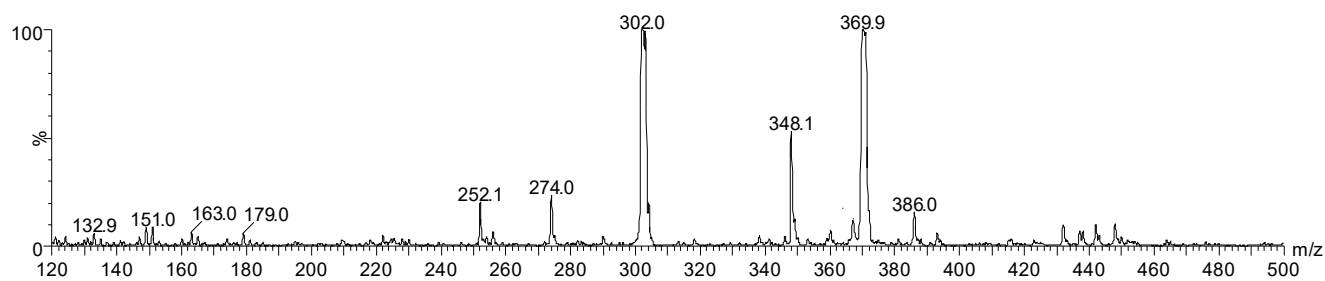


Figure S80. ESI (+) mass spectrum of compound **20**.

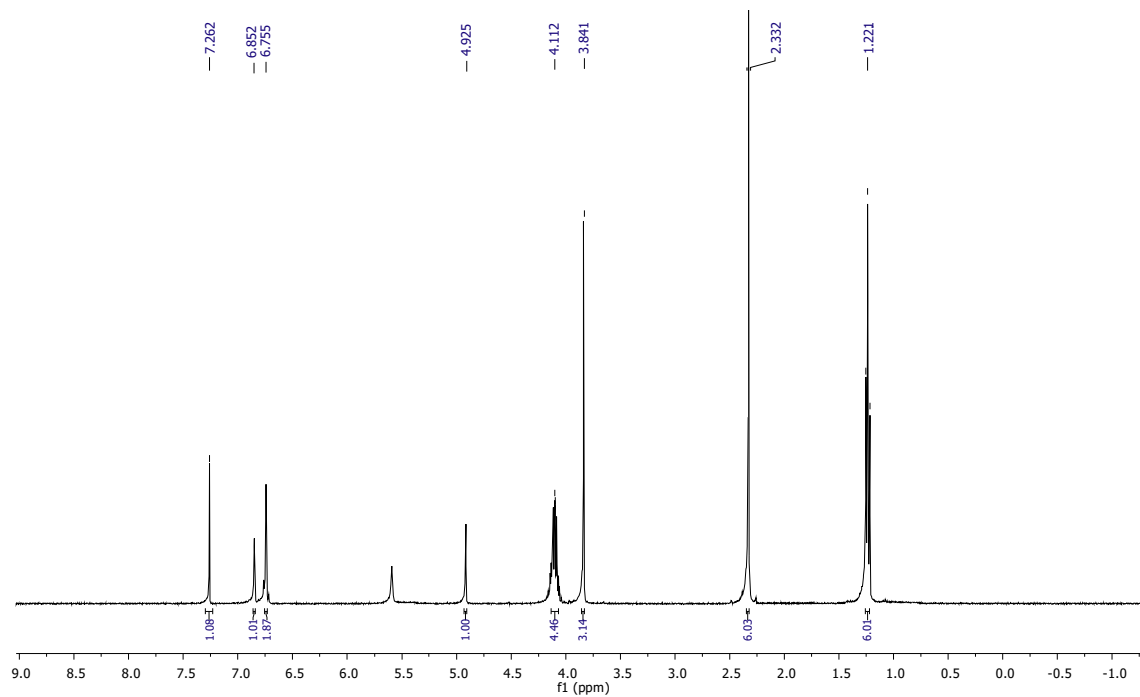


Figure S81. ¹H NMR spectrum of compound **21** (CDCl₃, 400 MHz, TMS).

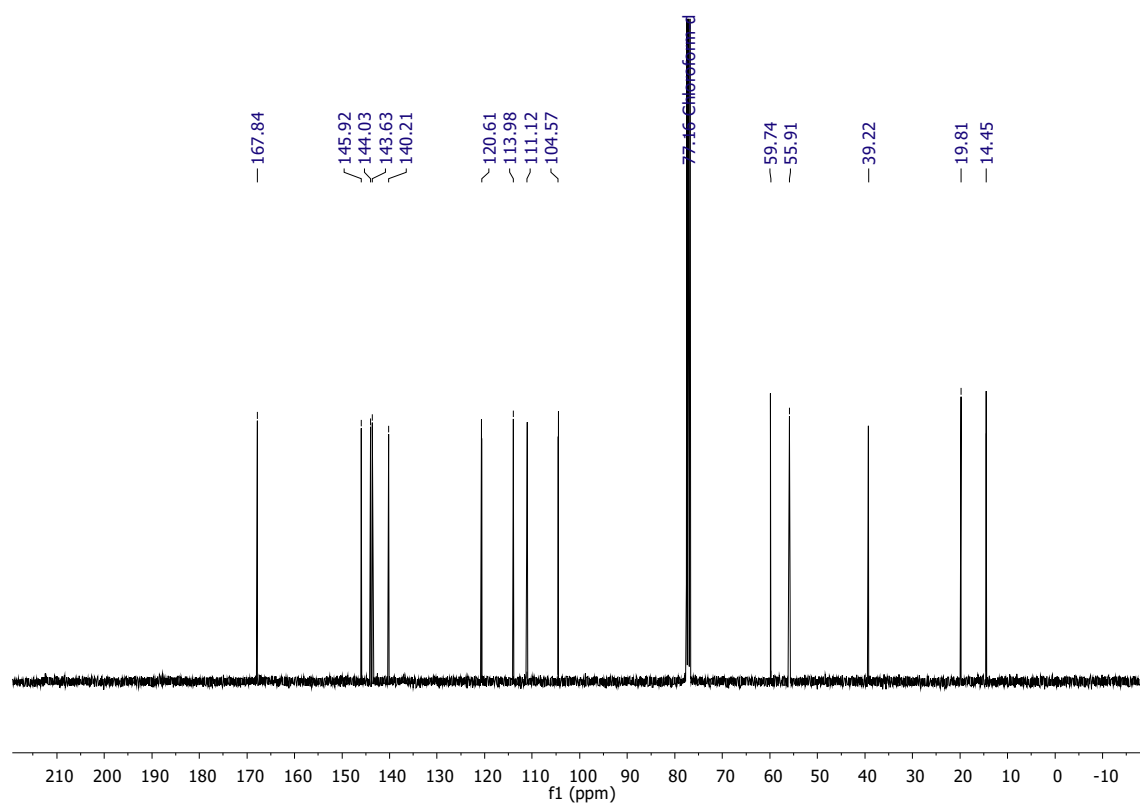


Figure S82. ¹³C NMR spectrum of compound **21** (CDCl₃, 100 MHz, TMS).

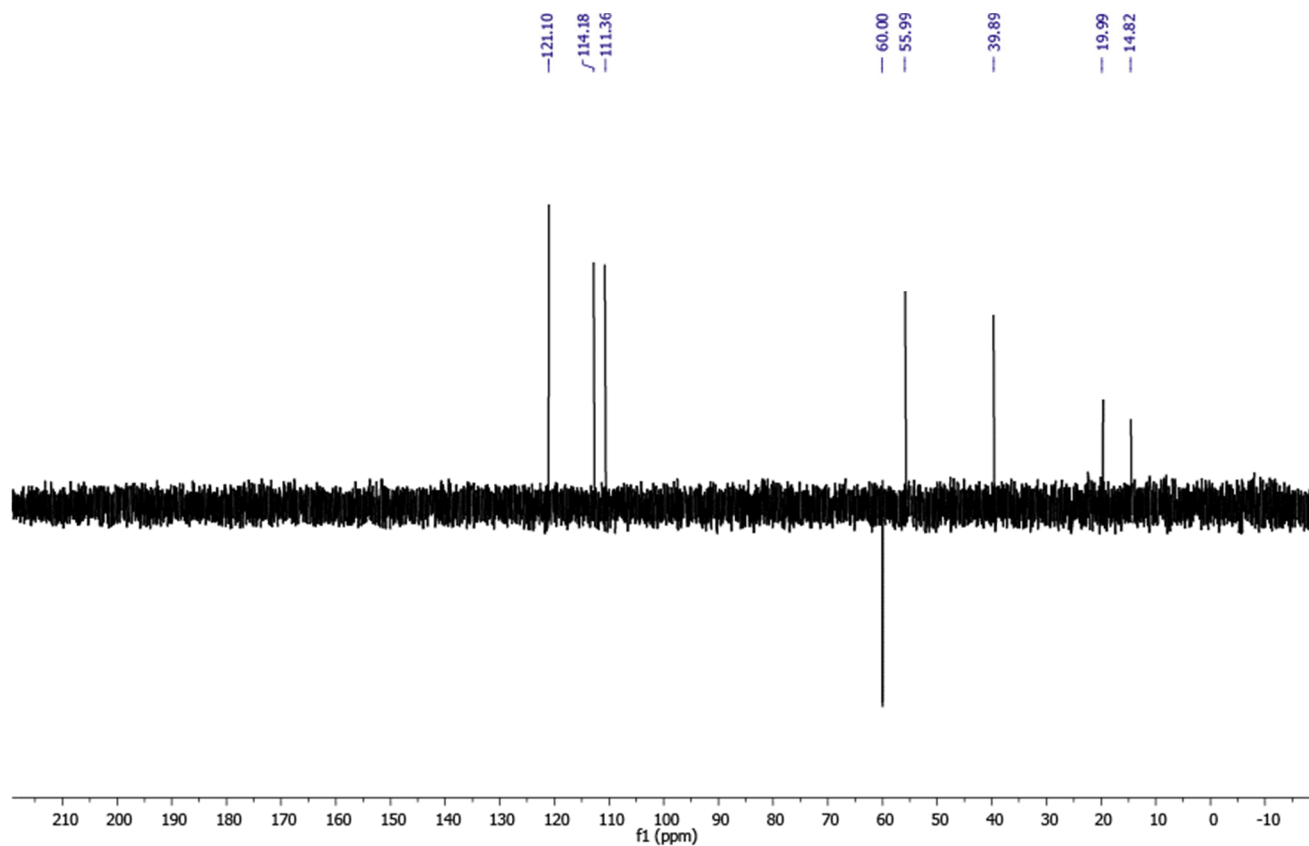


Figure S83. DEPT 135 spectrum of compound **21** (CDCl₃, 100 MHz, TMS).

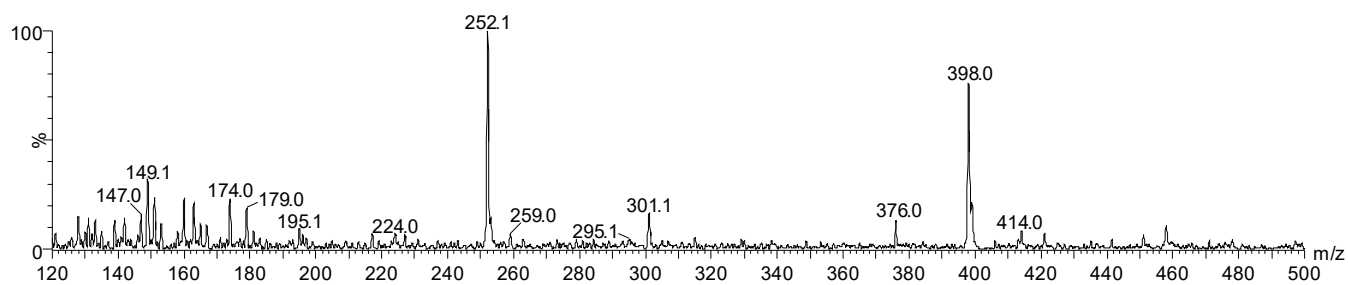


Figure S84. ESI (+) mass spectrum of compound **21**.

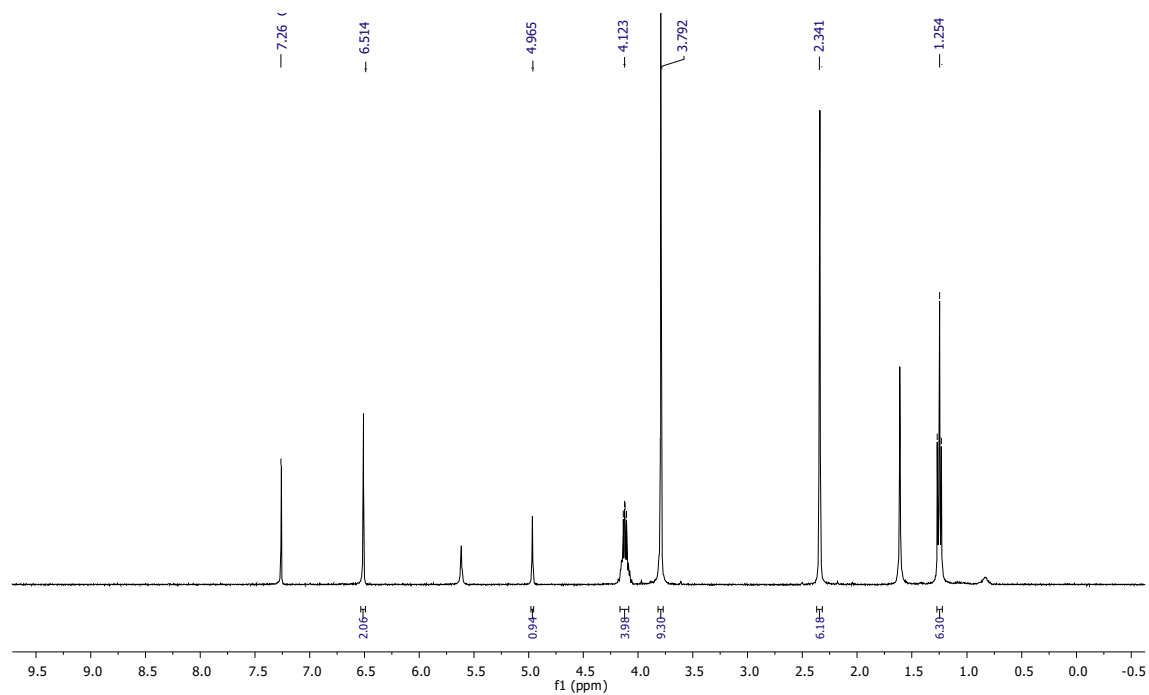


Figure S85. ¹H NMR spectrum of compound **22** (CDCl₃, 400 MHz, TMS).

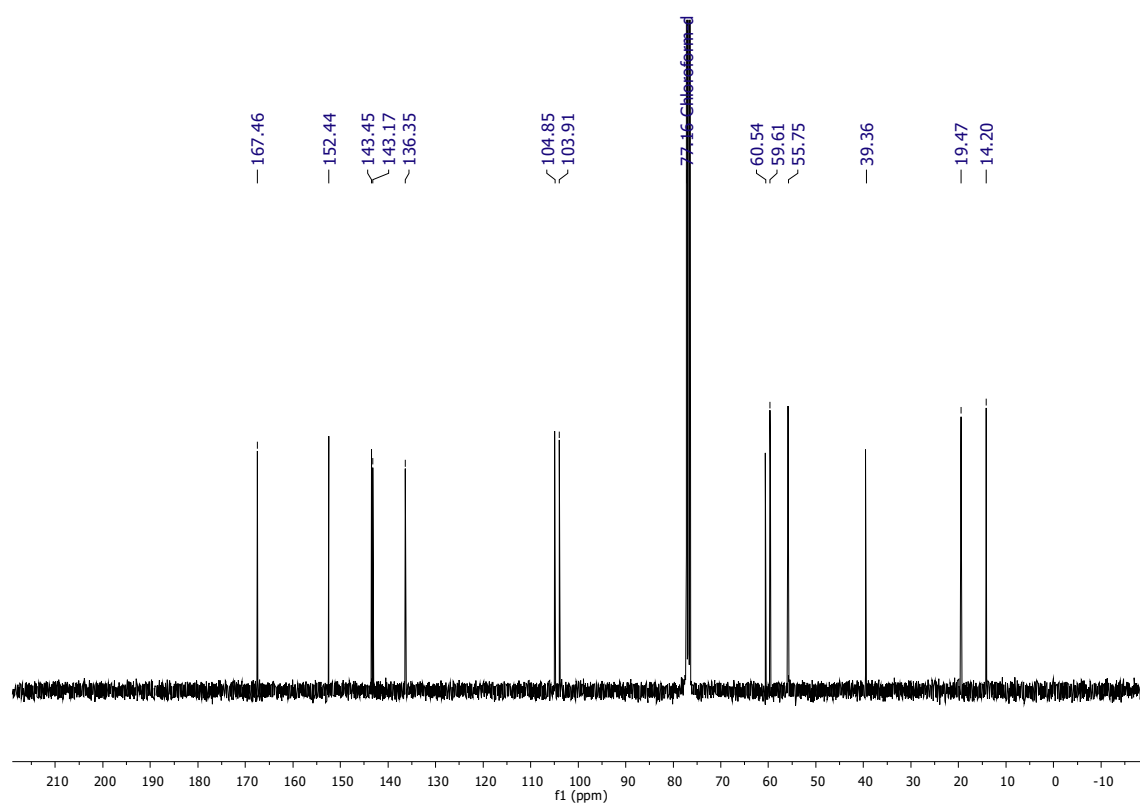


Figure S86. ¹³C NMR spectrum of compound **22** (CDCl₃, 100 MHz, TMS).

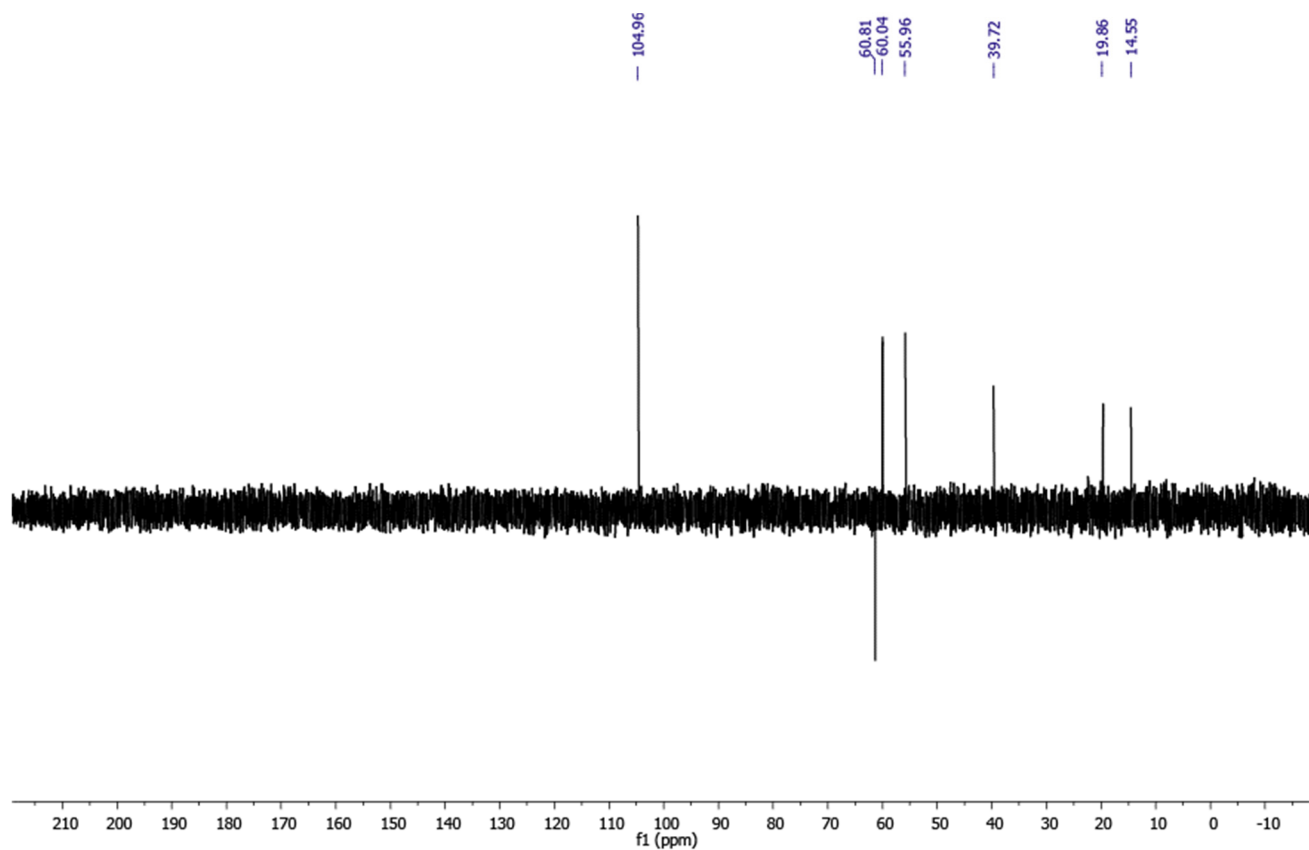


Figure S87. DEPT 135 spectrum of compound **22** (CDCl₃, 100 MHz, TMS).

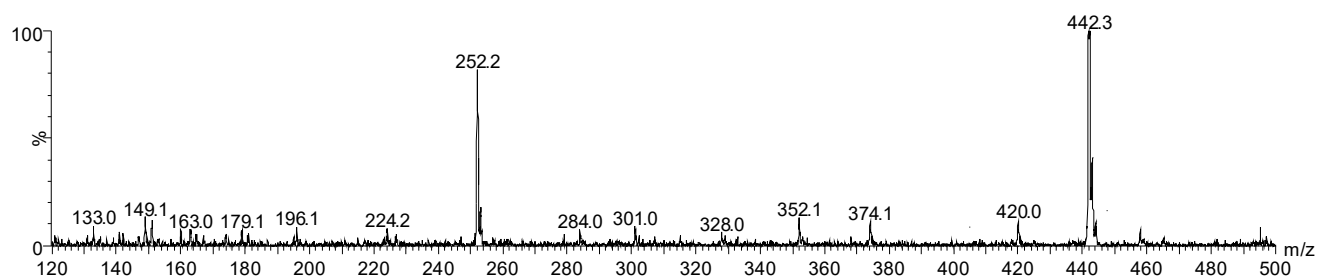


Figure S88. ESI (+) mass spectrum of compound **22**.