ChemMedChem

Supporting Information

Structure-Activity-Relationship-Aided Design and Synthesis of xCT Antiporter Inhibitors

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Supporting Information

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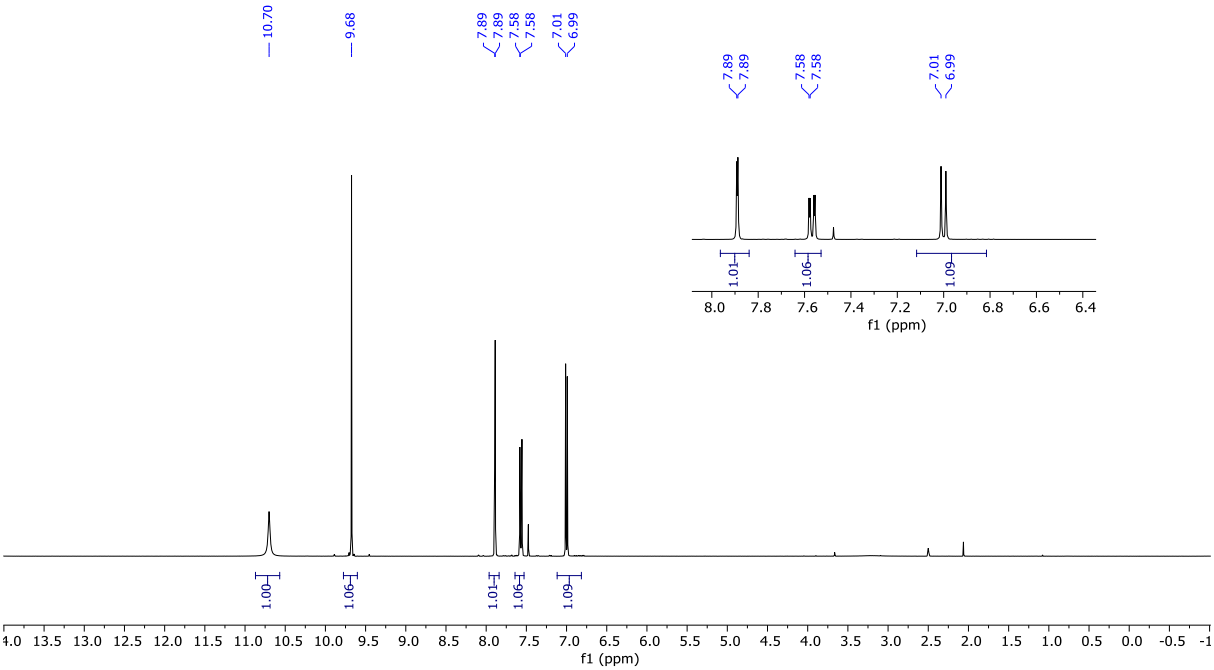
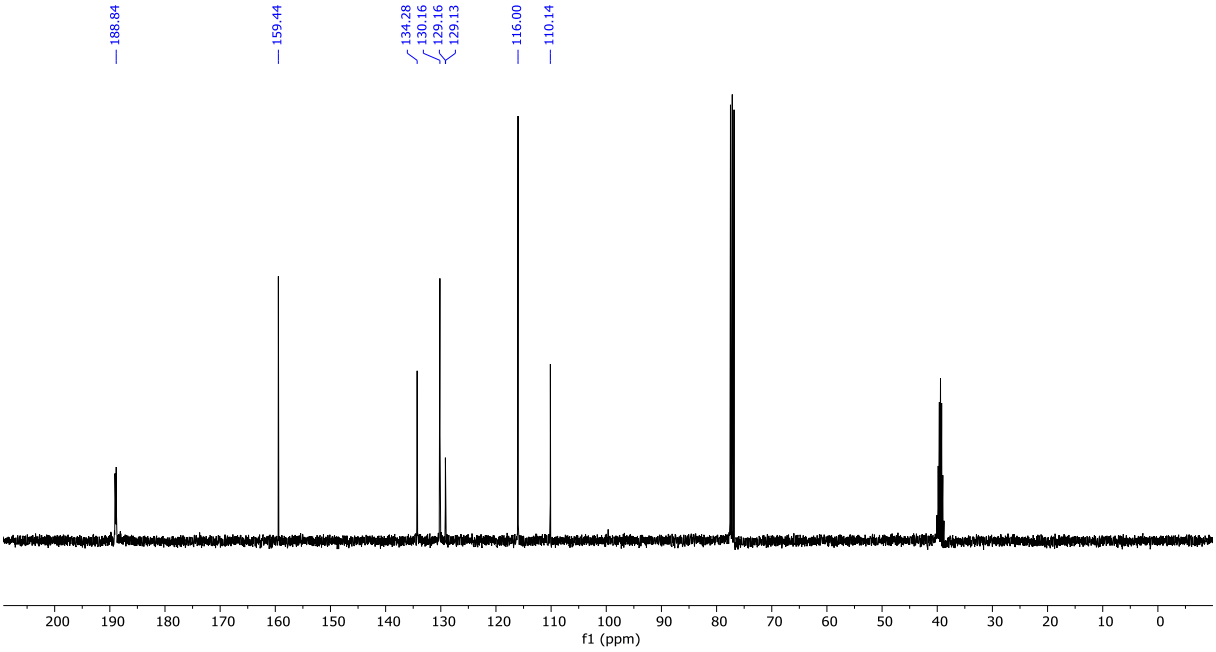
Compound 1

^{1}H NMR (400 MHz, DMSO) δ 10.70 (s, 1H), 9.68 (s, 1H), 7.89 (d, *J* = 2.0 Hz, 1H), 7.58 (dd, *J* = 8.3, 2.0 Hz, 1H), 7.00 (d, *J* = 8.3 Hz, 1H).

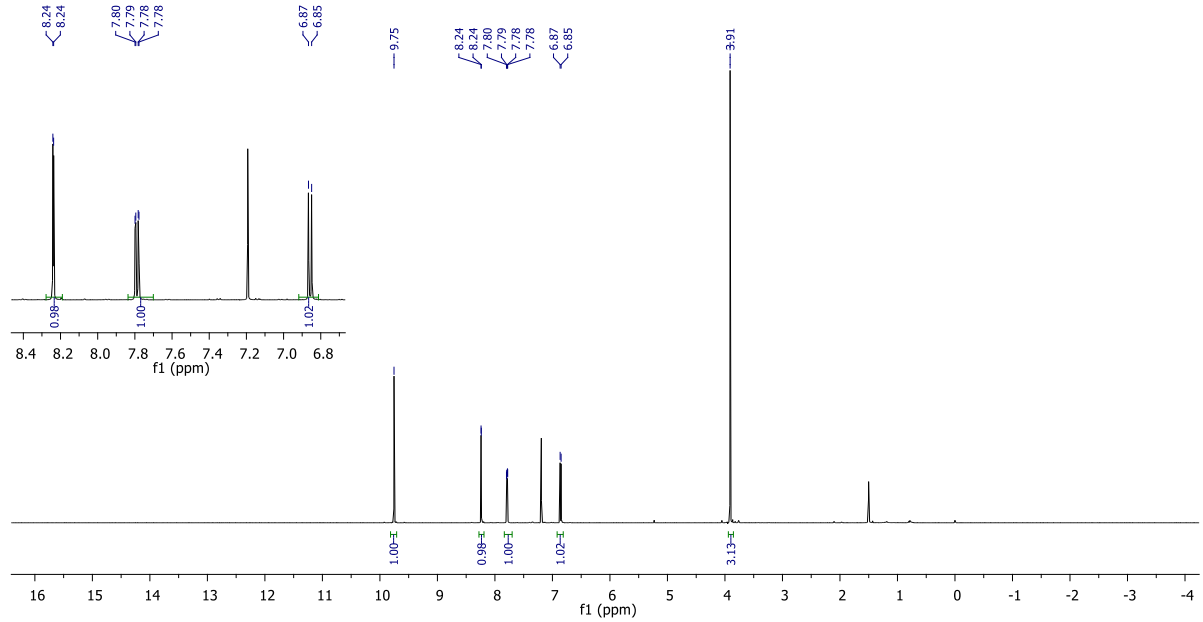


^{13}C NMR (101 MHz, $CDCl_3$) δ 188.84, 159.44, 134.28, 130.16, 129.16, 129.13, 116.00, 110.14.

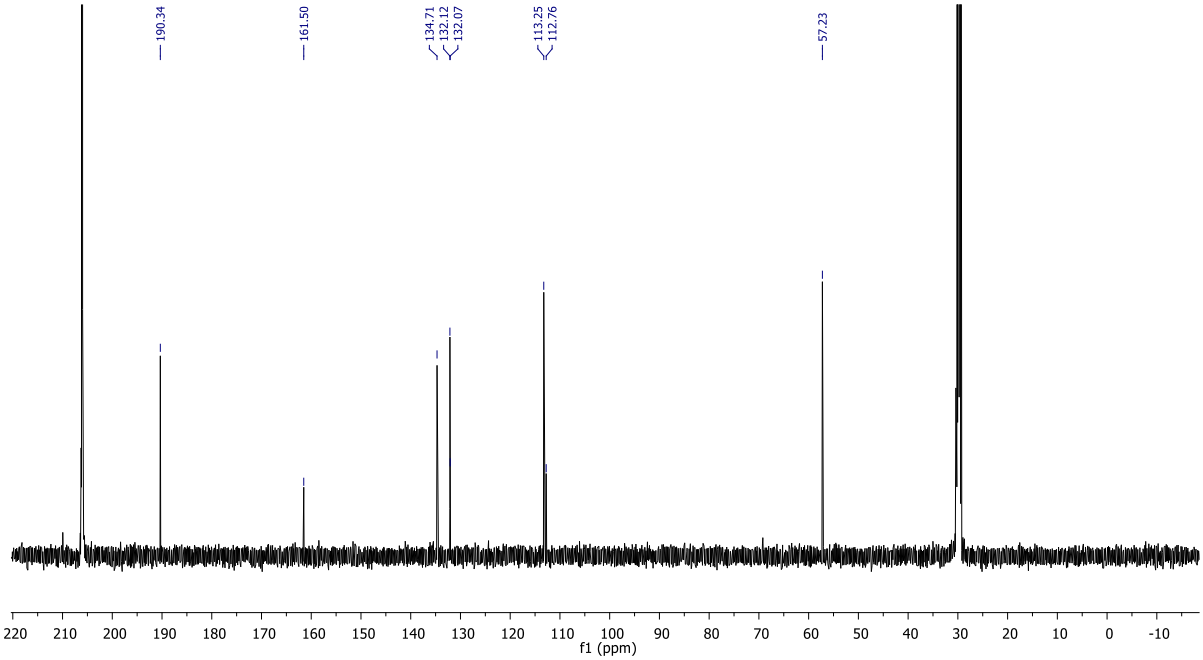


Compound 2a

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.75 (s, 1H), 8.24 (d, *J* = 2.0 Hz, 1H), 7.79 (dd, *J* = 8.5, 2.0 Hz, 1H), 6.86 (d, *J* = 8.5 Hz, 1H), 3.91 (s, 3H).

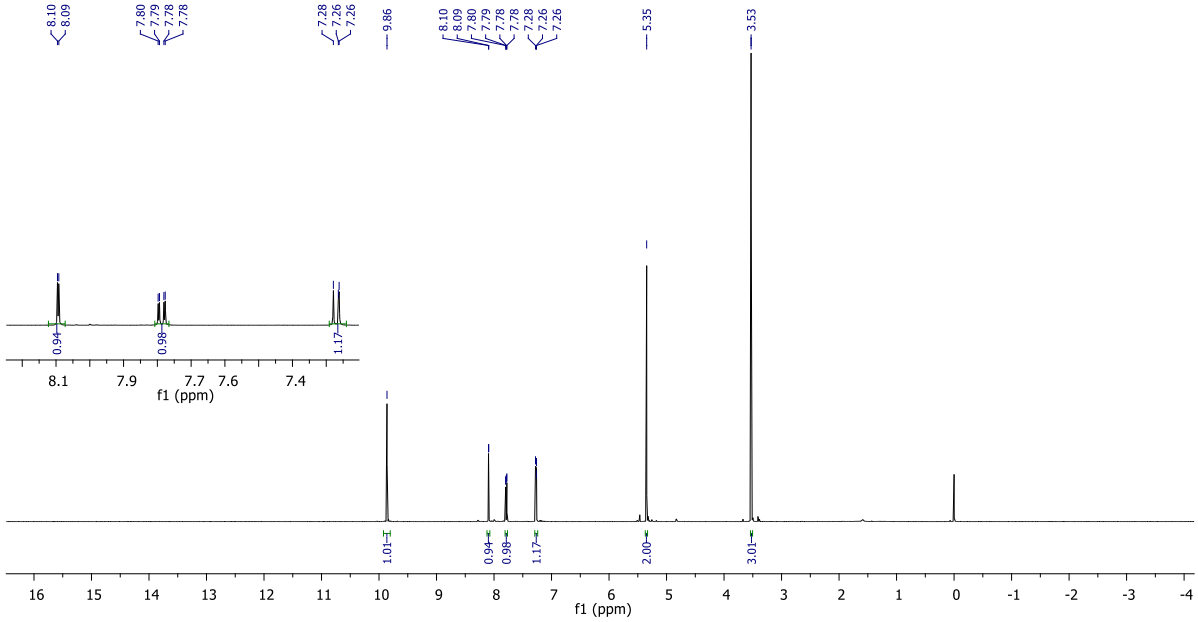


^{13}C NMR (126 MHz, Acetone) δ 190.34, 161.50, 134.71, 132.12, 132.07, 113.25, 112.76, 57.23.

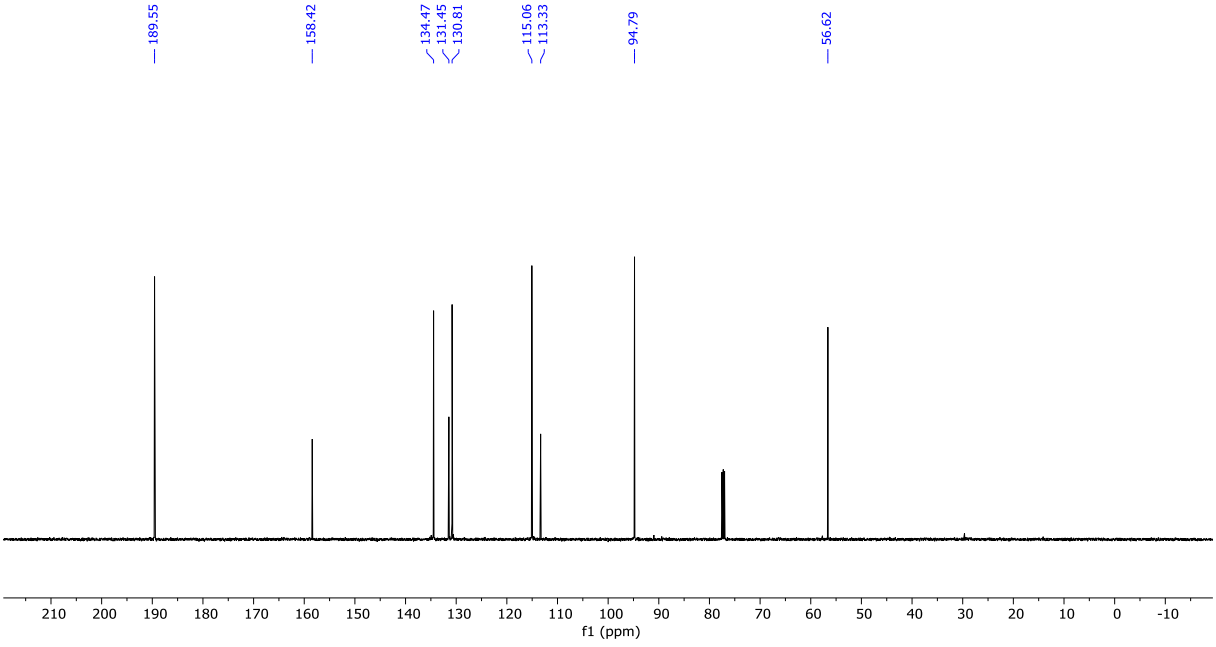


Compound 2b

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.86 (s, 1H), 8.09 (d, *J* = 2.0 Hz, 1H), 7.79 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.27 (d, *J* = 8.5 Hz, 1H), 5.35 (s, 2H), 3.53 (s, 3H).

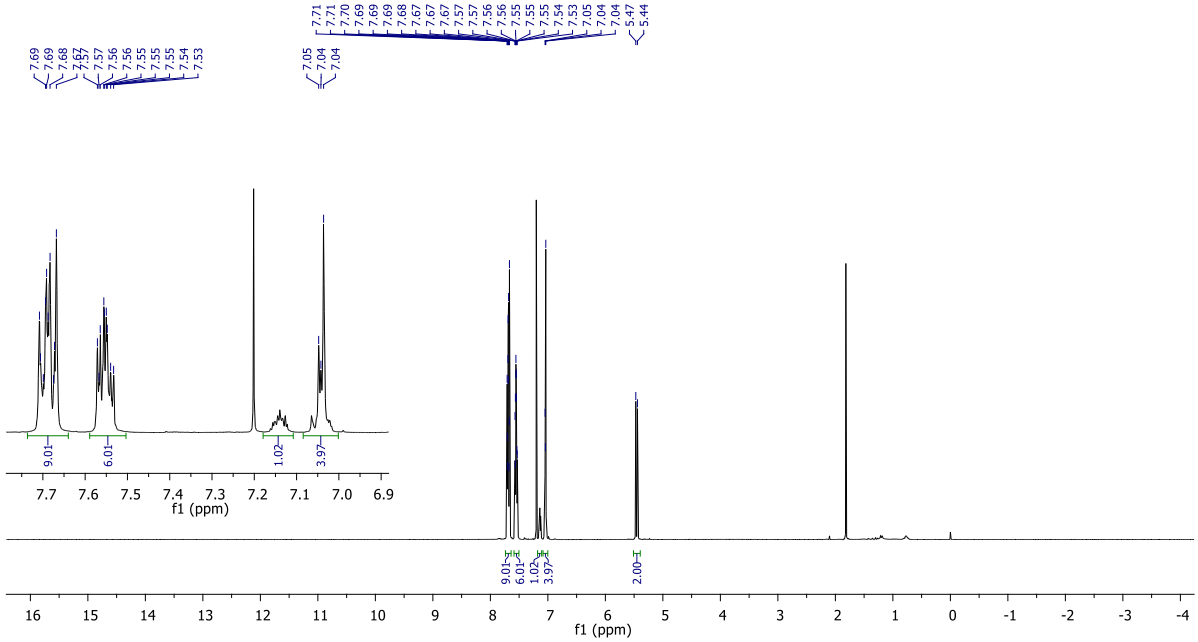


^{13}C NMR (126 MHz, $CDCl_3$) δ 189.55, 158.42, 134.47, 131.45, 130.81, 115.06, 113.33, 94.79, 56.62.



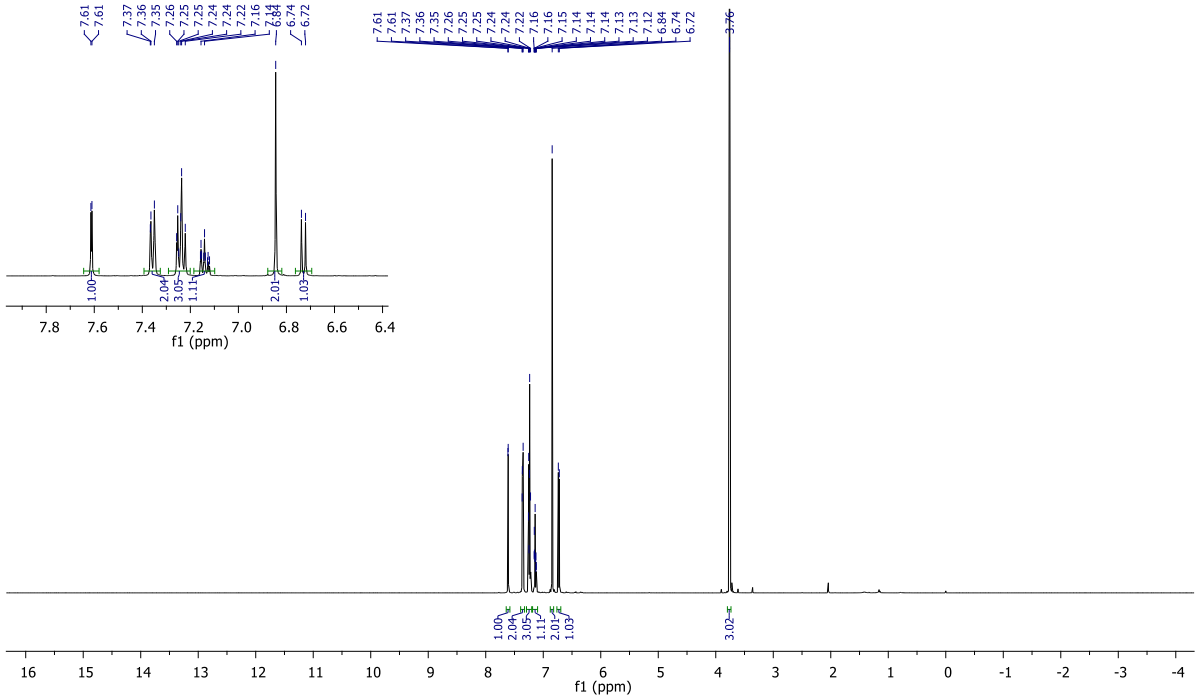
Compound 3

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 – 7.64 (m, 9H), 7.59 – 7.50 (m, 6H), 7.18 – 7.11 (m, 1H), 7.08 – 7.00 (m, 4H), 5.46 (d, *J* = 14.5 Hz, 2H).

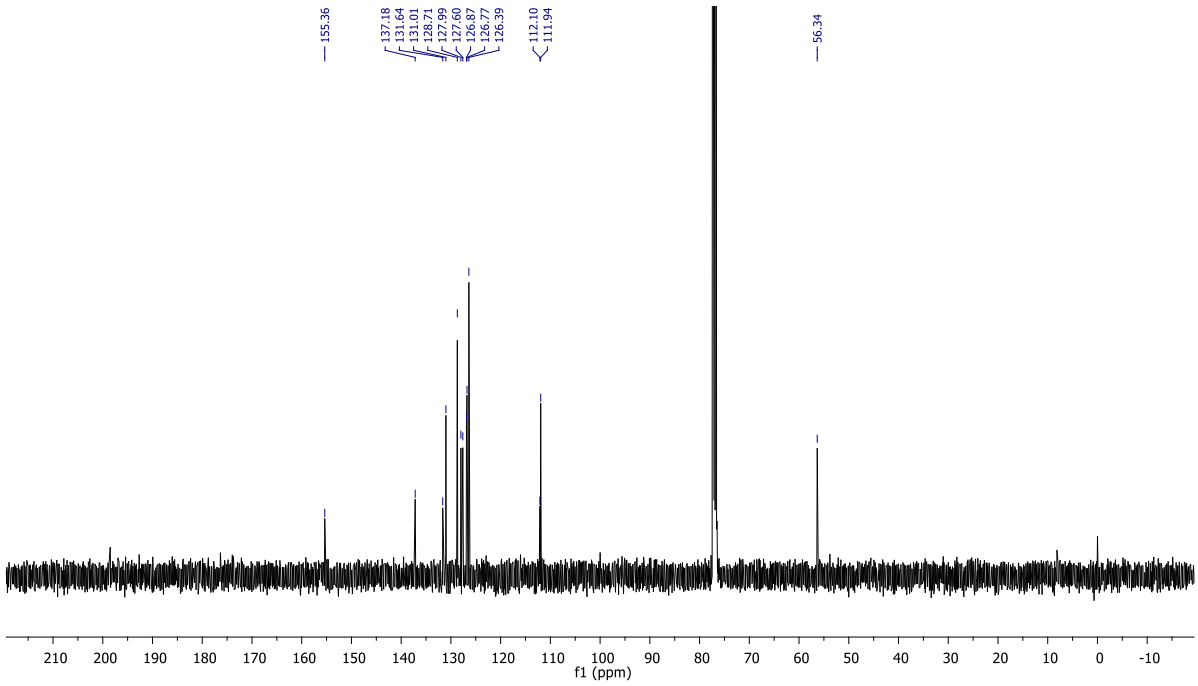


Compound 4

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 2.2 Hz, 1H), 7.39 – 7.33 (m, 2H), 7.24 (dt, *J* = 9.4, 5.0 Hz, 3H), 7.19 – 7.10 (m, 1H), 6.84 (s, 2H), 6.73 (d, *J* = 8.5 Hz, 1H), 3.76 (s, 3H).

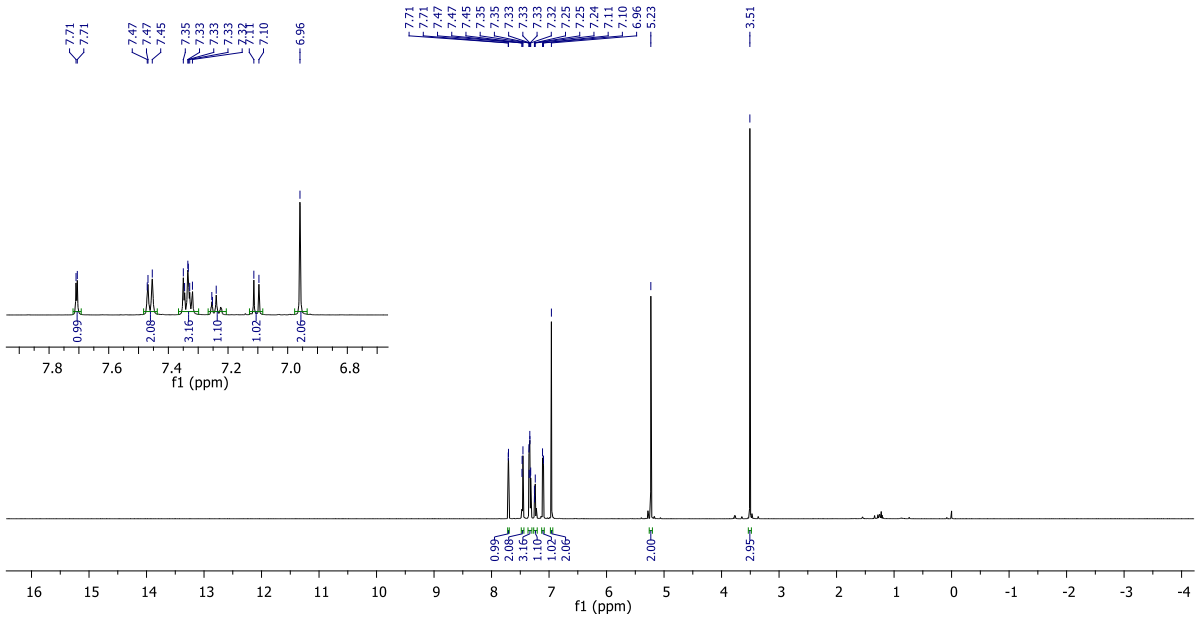


^{13}C NMR (126 MHz, $CDCl_3$) δ 155.36, 137.18, 131.64, 131.01, 128.71, 127.99, 127.60, 126.87, 126.77, 126.39, 112.10, 111.94, 56.34.

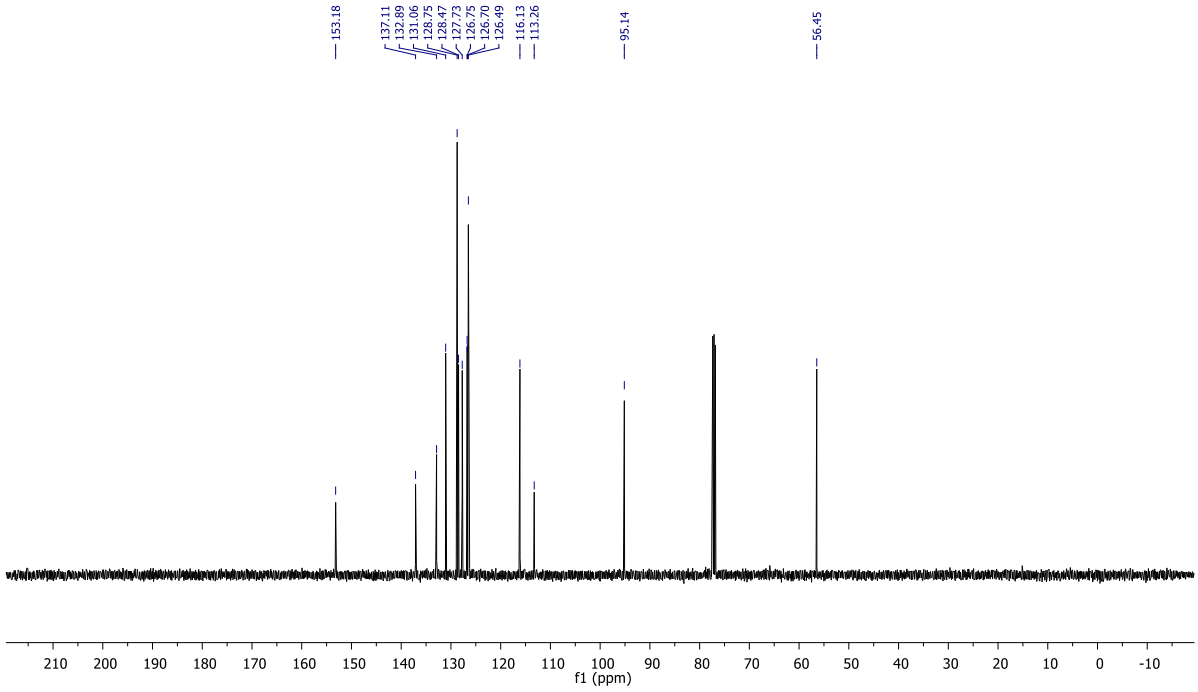


Compound 5

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 (d, *J* = 2.1 Hz, 1H), 7.48 – 7.44 (m, 2H), 7.37 – 7.30 (m, 3H), 7.27 – 7.21 (m, 1H), 7.10 (d, *J* = 8.5 Hz, 1H), 6.96 (s, 2H), 5.23 (s, 2H), 3.51 (s, 3H).

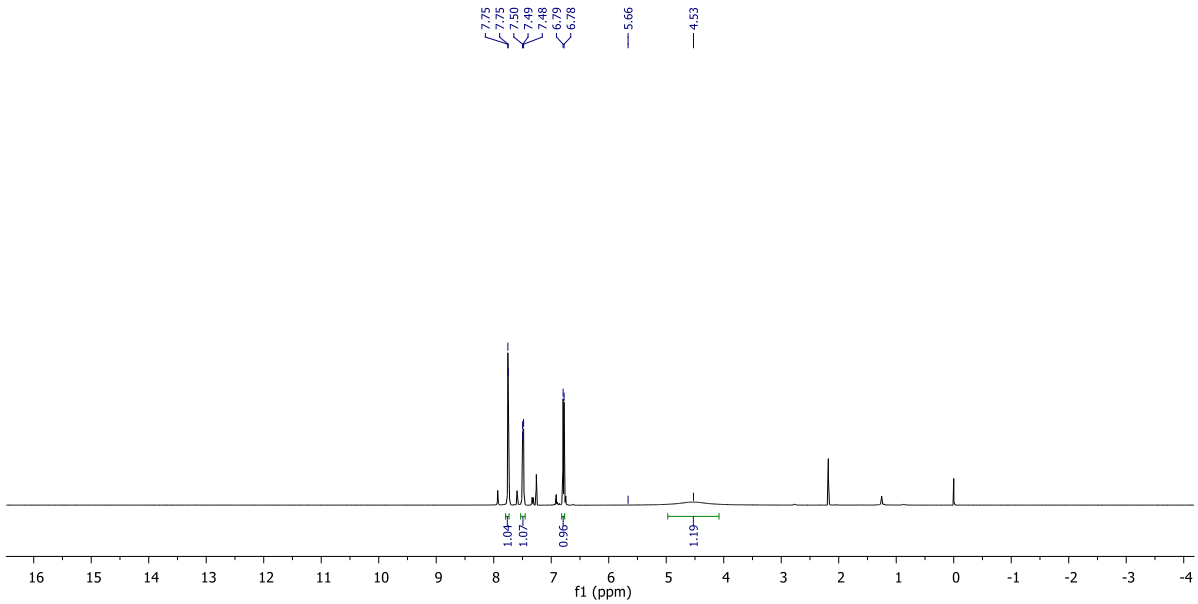


^{13}C NMR (126 MHz, $CDCl_3$) δ 153.18, 137.11, 132.89, 131.06, 128.75, 128.47, 127.73, 126.75, 126.70, 126.49, 116.13, 113.26, 95.14, 56.45.

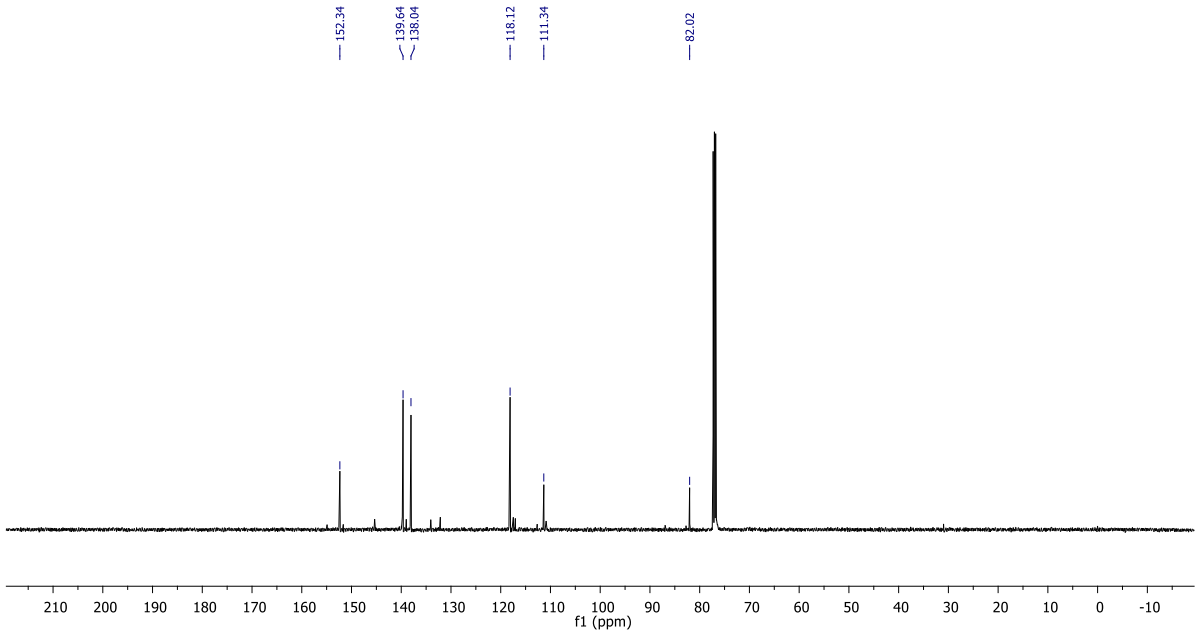


Compound 6

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (d, *J* = 1.7 Hz, 1H), 7.49 (dd, *J* = 8.6, 1.7 Hz, 1H), 6.78 (d, *J* = 8.6 Hz, 1H), 4.53 (s, 1H).

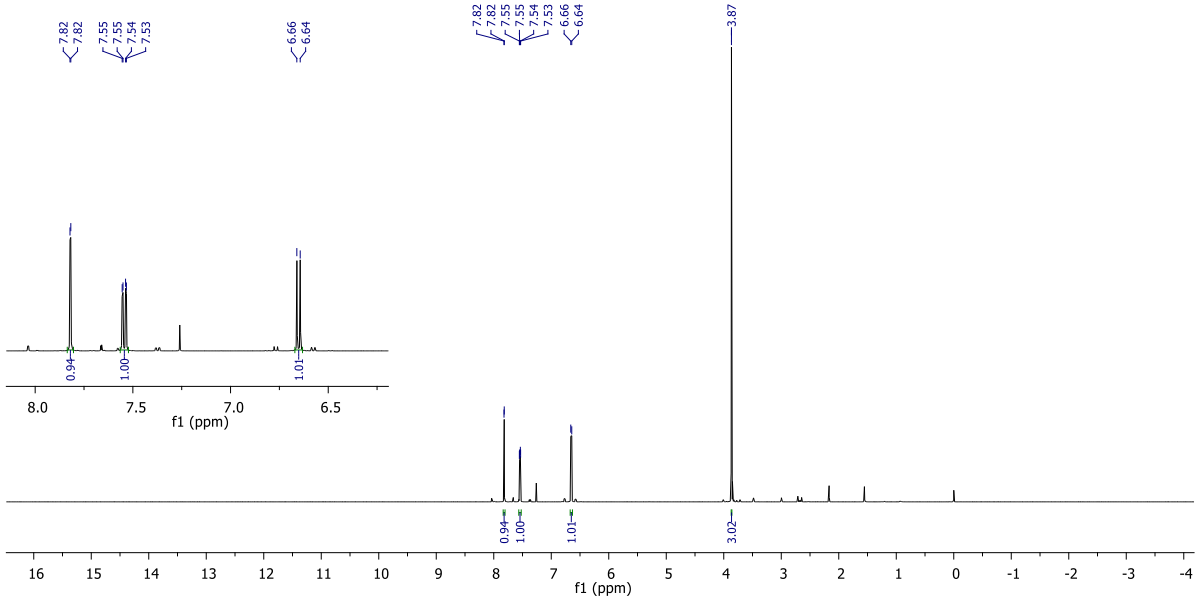


^{13}C NMR (126 MHz, $CDCl_3$) δ 152.34, 139.64, 138.04, 118.12, 111.34, 82.02.

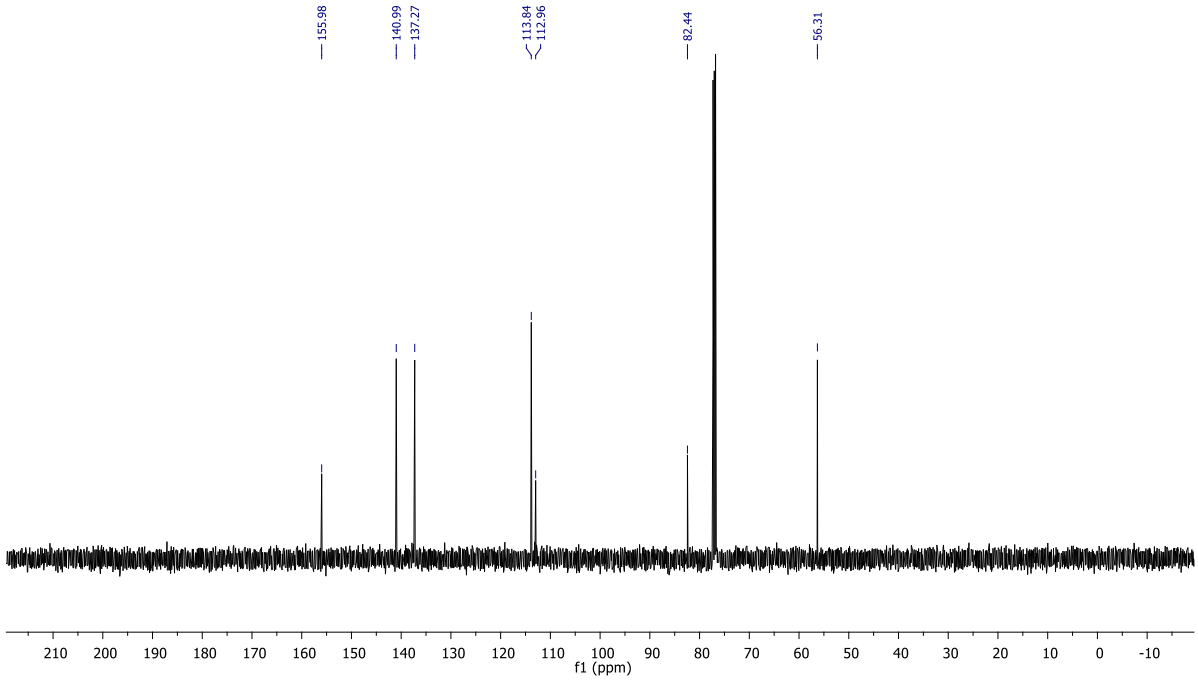


Compound 7a

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (d, *J* = 2.1 Hz, 1H), 7.54 (dd, *J* = 8.7, 2.1 Hz, 1H), 6.65 (d, *J* = 8.6 Hz, 1H), 3.87 (s, 3H).

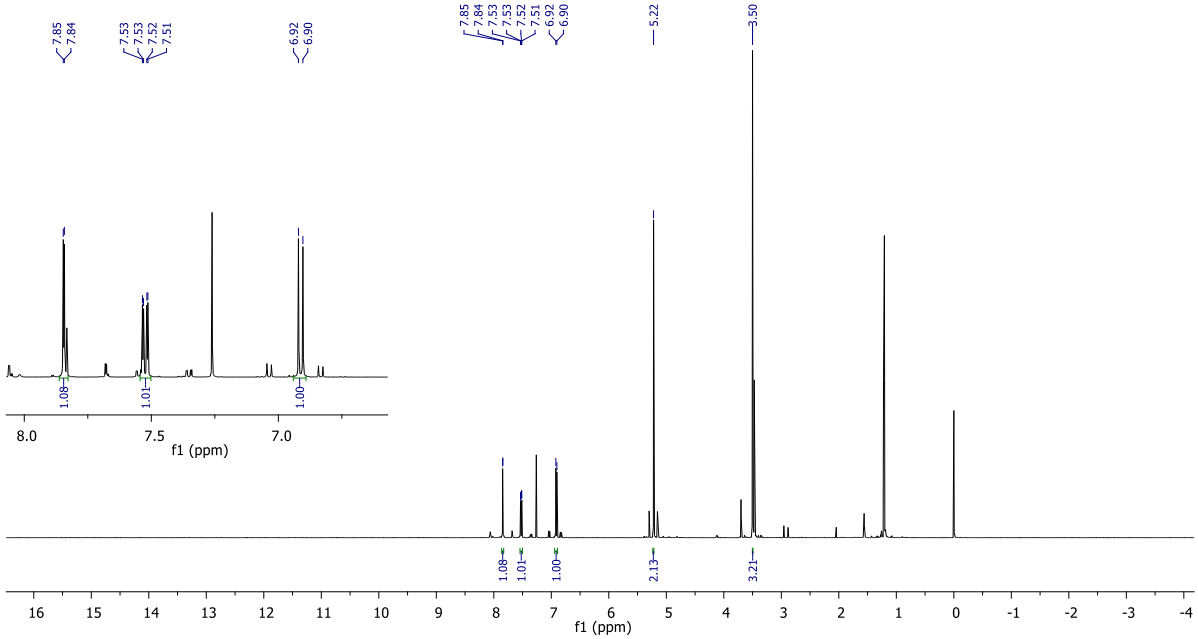


^{13}C NMR (126 MHz, $CDCl_3$) δ 155.98, 140.99, 137.27, 113.84, 112.96, 82.44, 56.31.

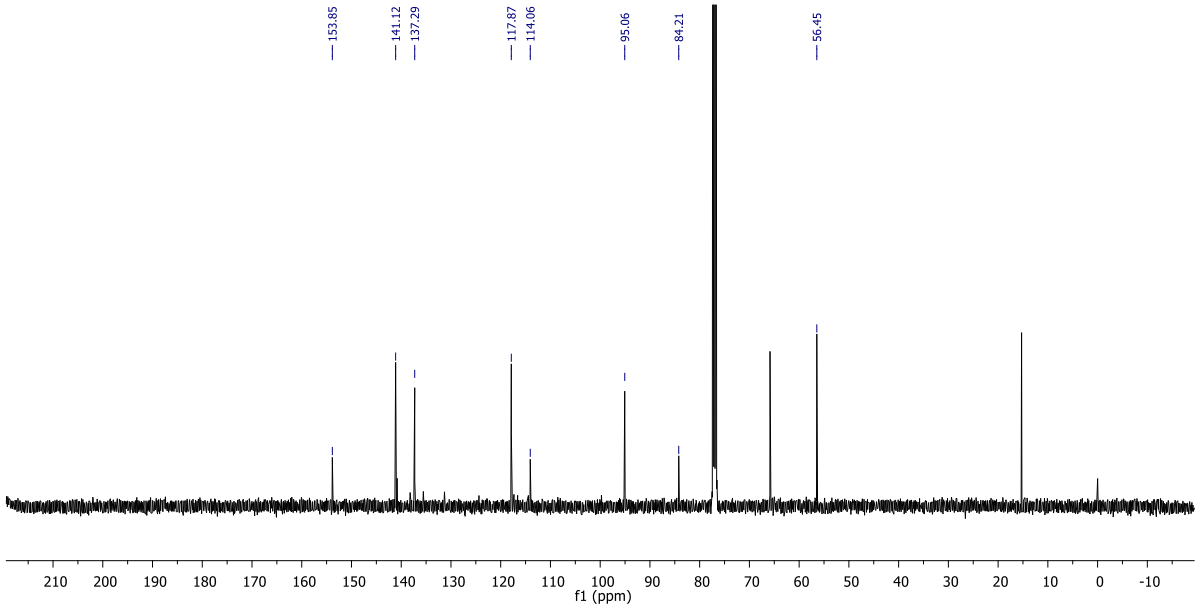


Compound 7b

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 2.1 Hz, 1H), 7.52 (dd, *J* = 8.7, 2.1 Hz, 1H), 6.91 (d, *J* = 8.7 Hz, 1H), 5.22 (s, 2H), 3.50 (s, 3H).

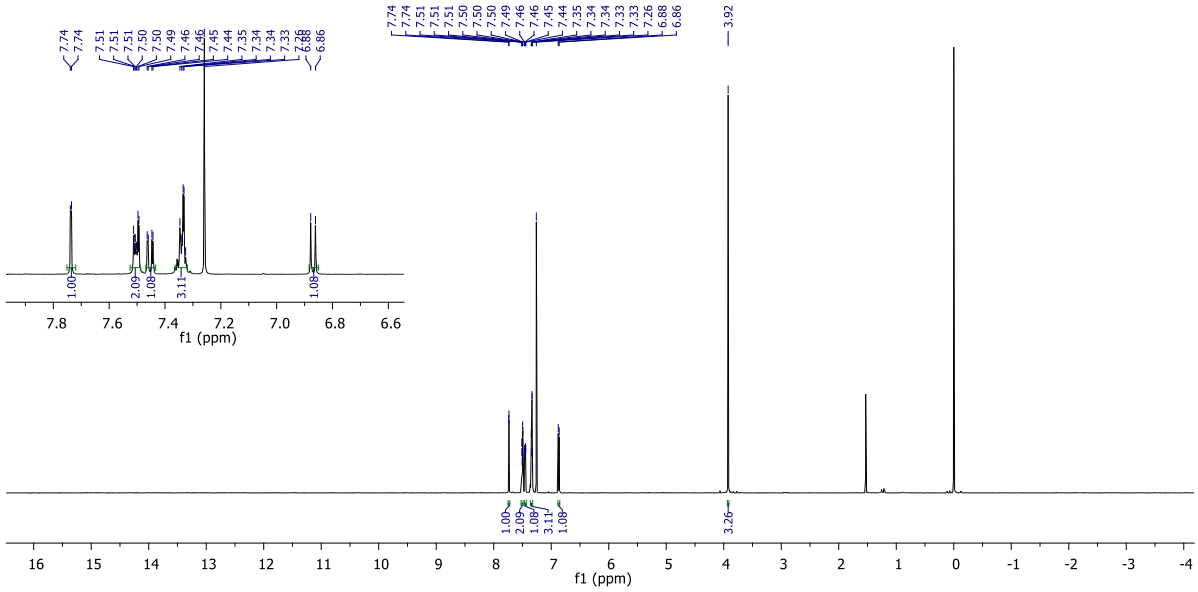


^{13}C NMR (126 MHz, $CDCl_3$) δ 153.85, 141.12, 137.29, 117.87, 114.06, 95.06, 84.21, 56.45.

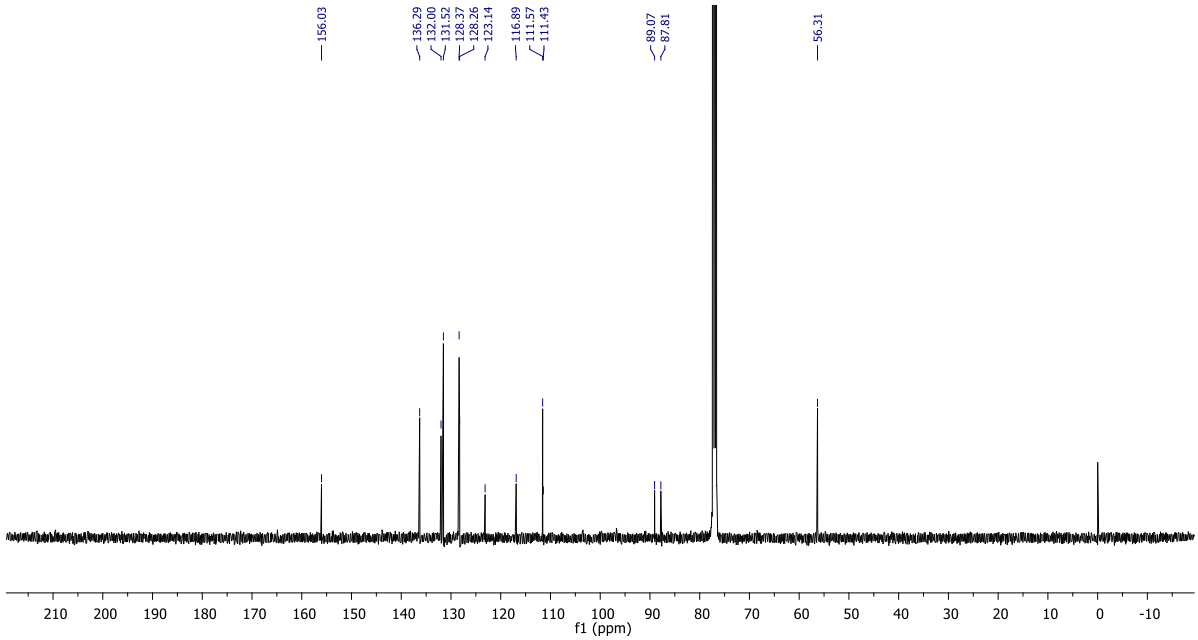


Compound 8

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 2.1 Hz, 1H), 7.52 – 7.49 (m, 2H), 7.45 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.36 – 7.32 (m, 3H), 6.87 (d, *J* = 8.5 Hz, 1H), 3.92 (s, 3H).

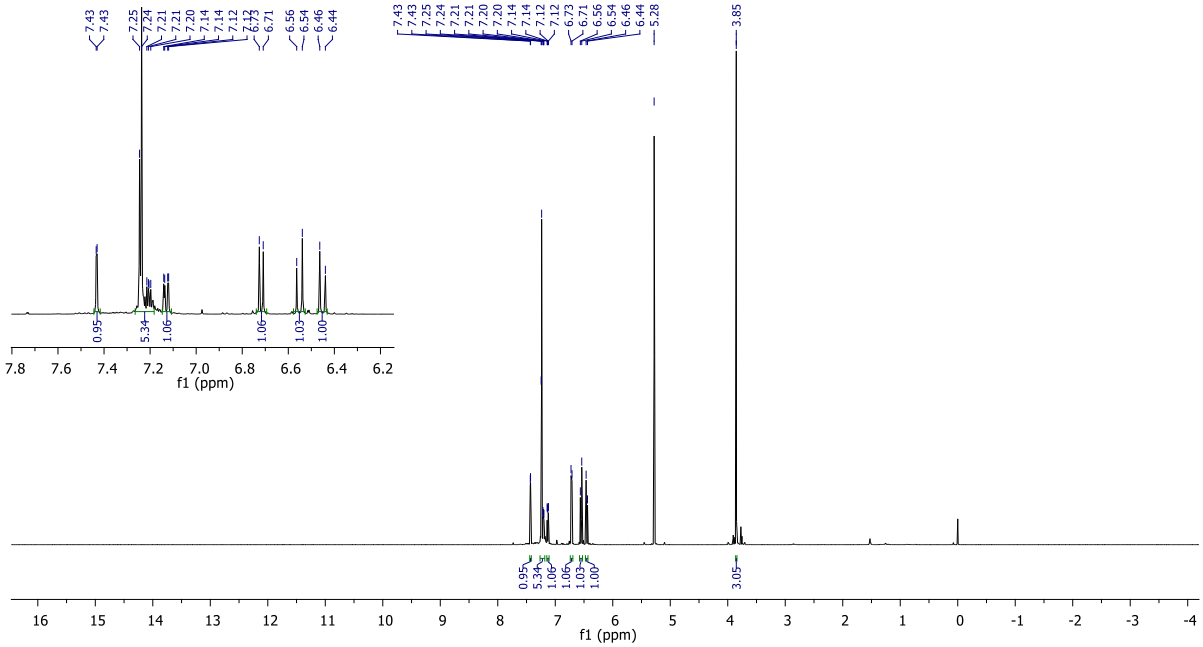


^{13}C NMR (126 MHz, $CDCl_3$) δ 156.03, 136.29, 132.00, 131.52, 128.37, 128.26, 123.14, 116.89, 111.57, 111.43, 89.07, 87.81, 56.31.

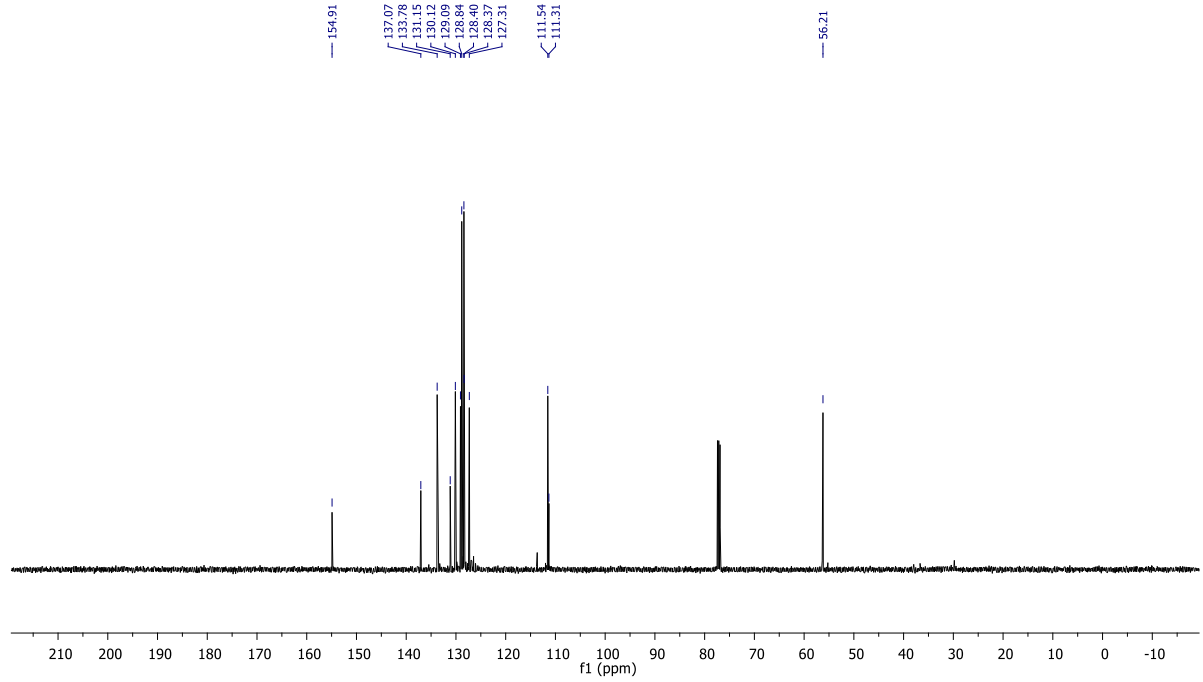


Compound 9

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 (d, *J* = 2.0 Hz, 1H), 7.26 – 7.18 (m, 5H), 7.13 (dd, *J* = 8.6, 2.1 Hz, 1H), 6.72 (d, *J* = 8.5 Hz, 1H), 6.55 (d, *J* = 12.2 Hz, 1H), 6.45 (d, *J* = 12.2 Hz, 1H), 3.85 (s, 3H).

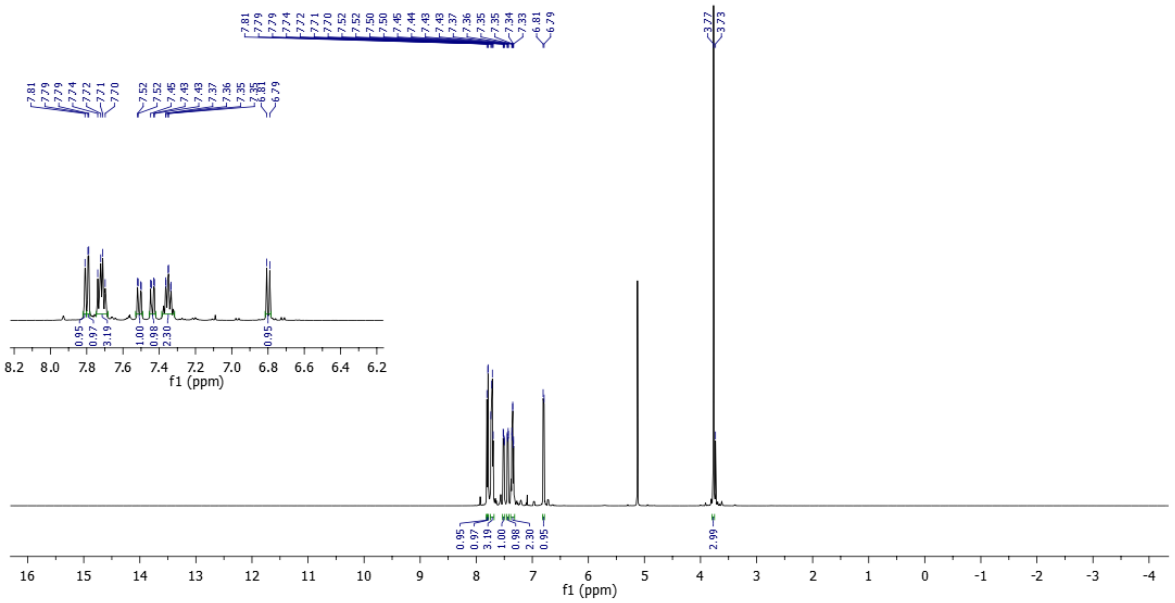


^{13}C NMR (126 MHz, $CDCl_3$) δ 154.91, 137.07, 133.78, 131.15, 130.12, 129.09, 128.84, 128.40, 128.37, 127.31, 111.54, 111.31, 56.21.

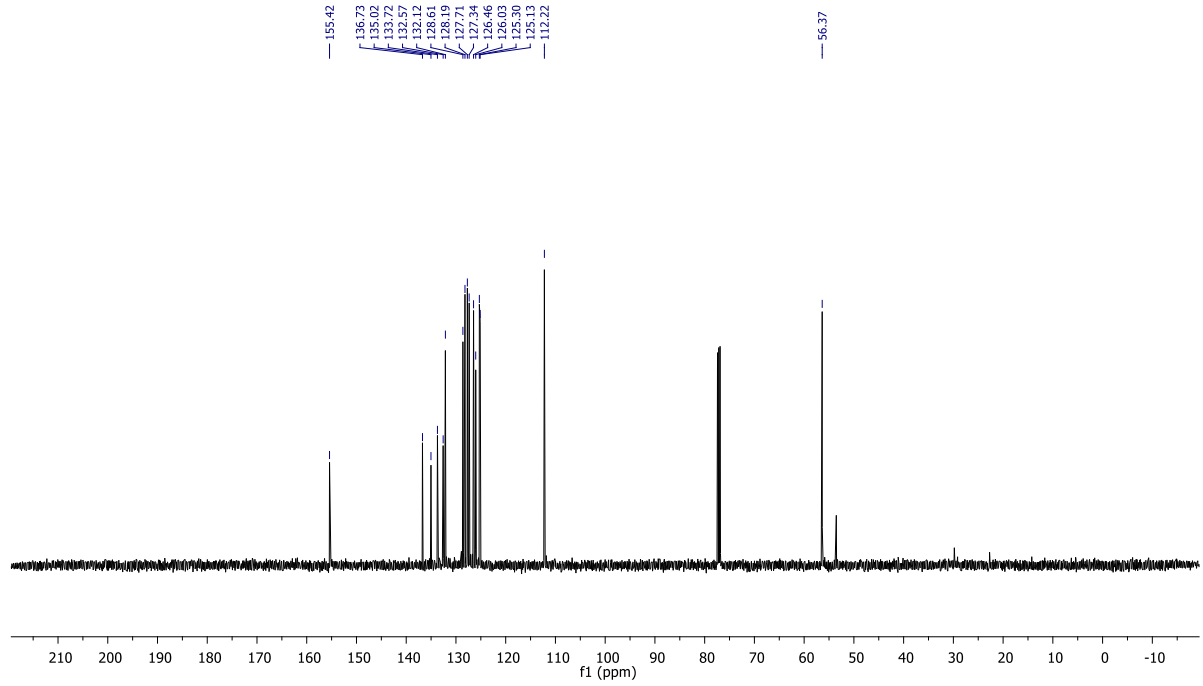


Compound 10

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.79 (d, *J* = 2.2 Hz, 1H), 7.72 (dd, *J* = 12.9, 7.6 Hz, 3H), 7.51 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.44 (dd, *J* = 8.5, 2.2 Hz, 1H), 7.39 – 7.32 (m, 2H), 6.80 (d, *J* = 8.5 Hz, 1H), 3.77 (s, 3H).

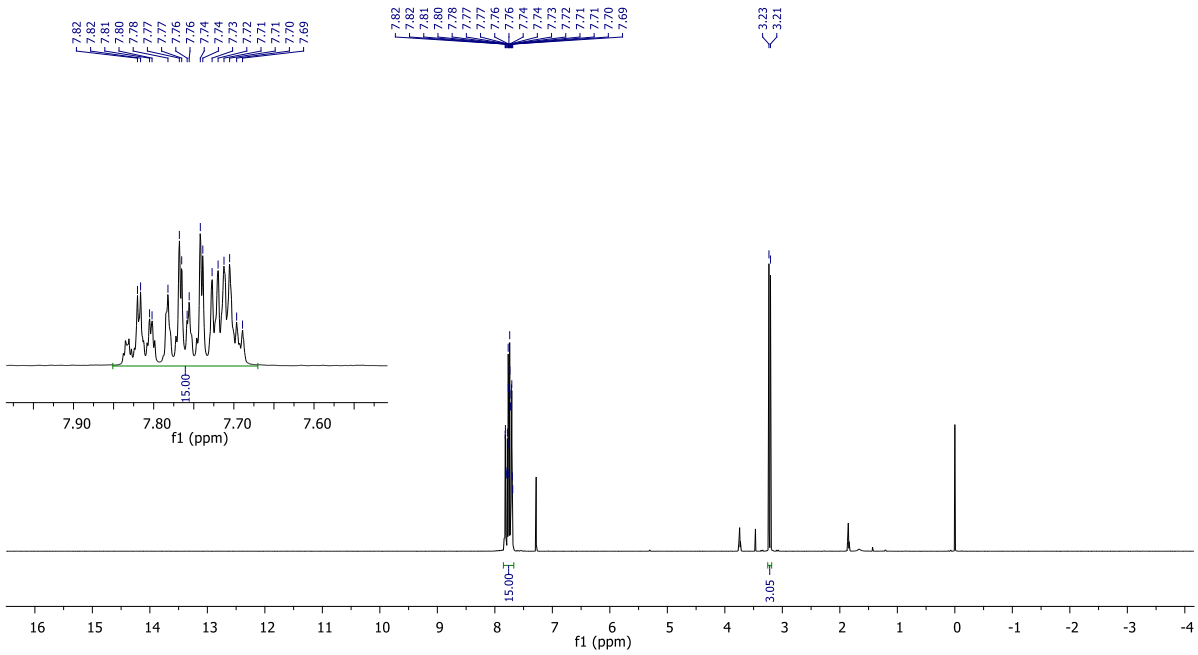


^{13}C NMR (126 MHz, $CDCl_3$) δ 155.42, 136.73, 135.02, 133.72, 132.57, 132.12, 128.61, 128.19, 127.71, 127.34, 126.46, 126.03, 125.30, 125.13, 112.22, 56.37 (one carbon peak is not visible)



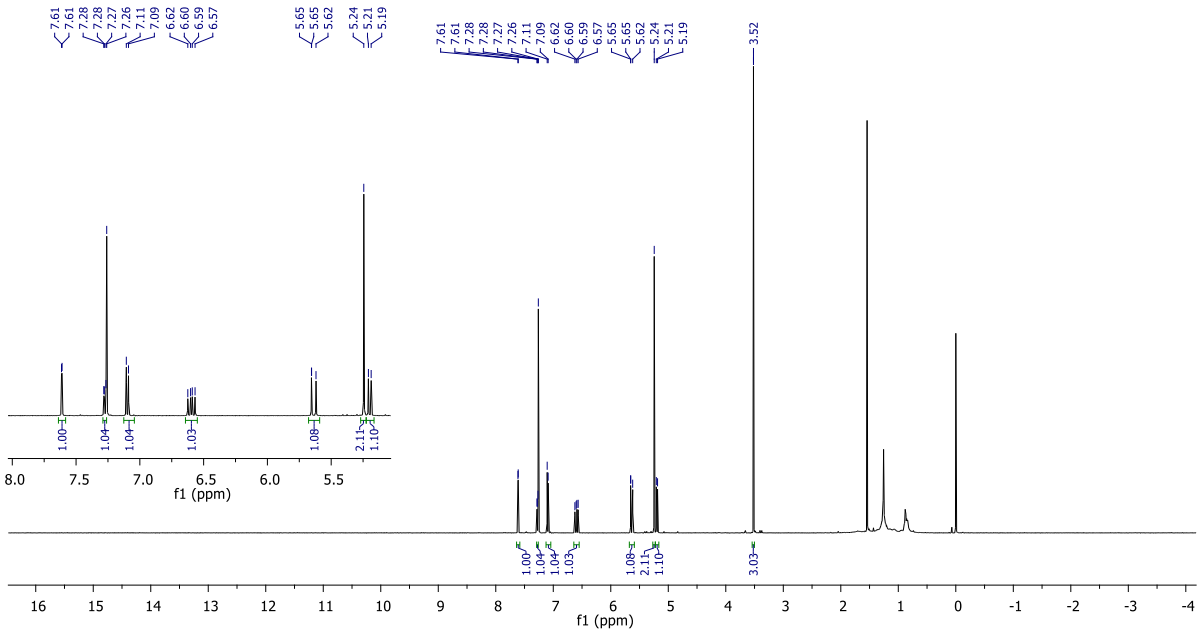
Compound 11

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 – 7.67 (m, 15H), 3.22 (d, *J* = 13.2 Hz, 3H).

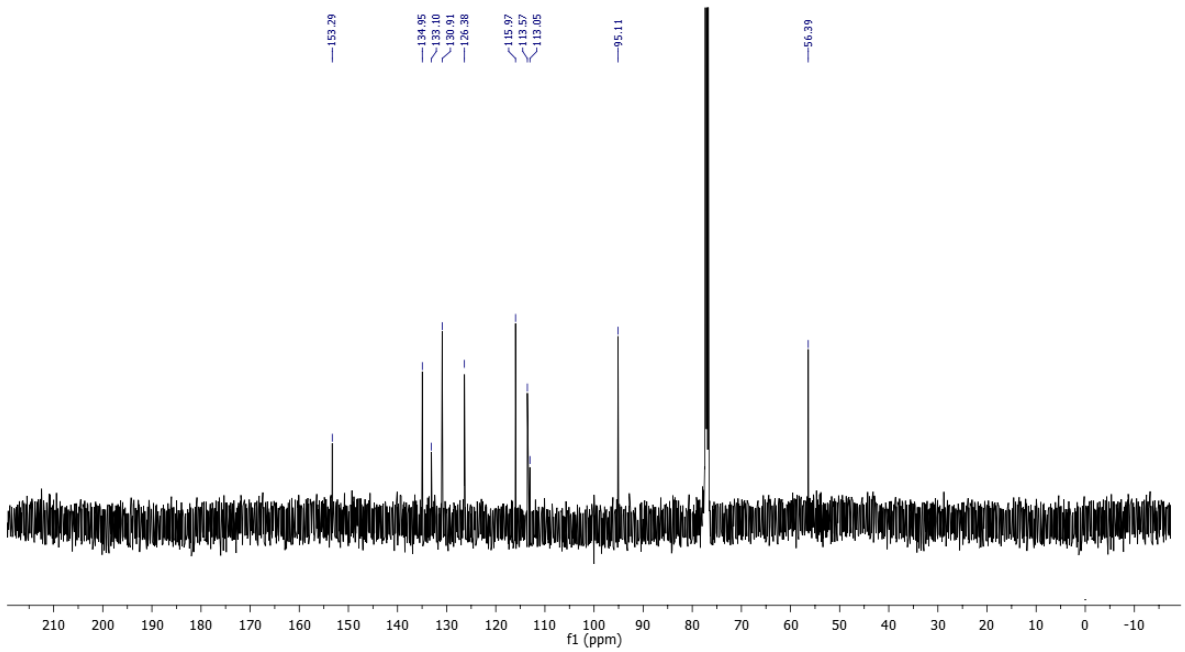


Compound 12

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 2.1 Hz, 1H), 7.27 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.10 (d, *J* = 8.5 Hz, 1H), 6.60 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.64 (d, *J* = 17.3 Hz, 1H), 5.24 (s, 2H), 5.20 (d, *J* = 10.7 Hz, 1H), 3.52 (s, 3H).

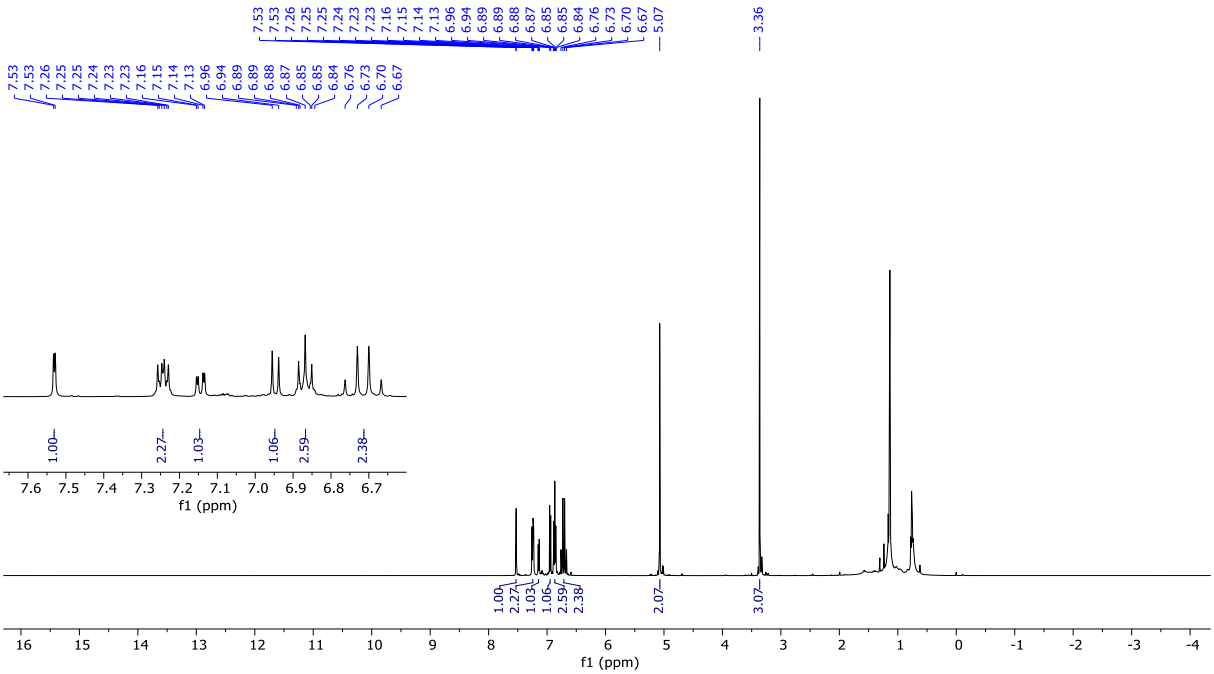


^{13}C NMR (126 MHz, $CDCl_3$) δ 153.29, 134.95, 133.10, 130.91, 126.38, 115.97, 113.57, 113.05, 95.11, 56.39.

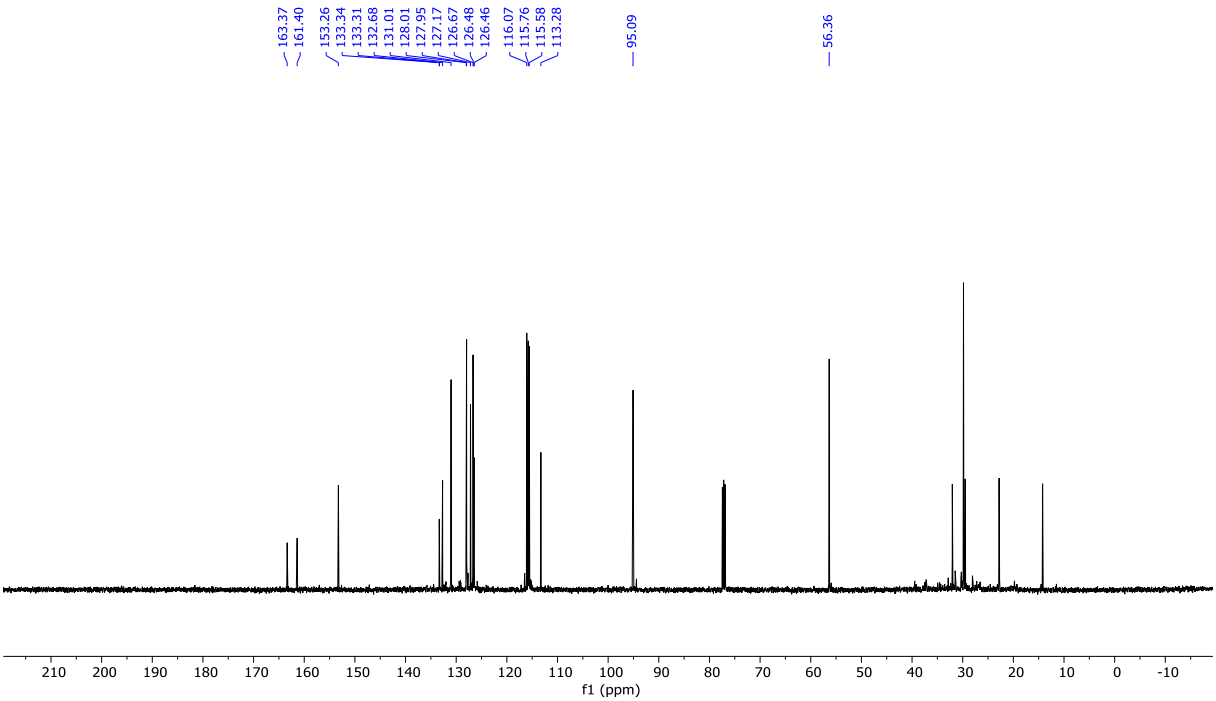


Compound 13

^{1}H NMR (500 MHz, $CDCl_3$) δ 3.36 (s, 3H), 5.07 (s, 2H), 6.65 – 6.77 (m, 2H), 6.82 – 6.91 (m, 3H), 6.95 (d, 1H), 7.14 (dd, 1H), 7.21 – 7.27 (m, 2H), 7.53 (d, 1H).

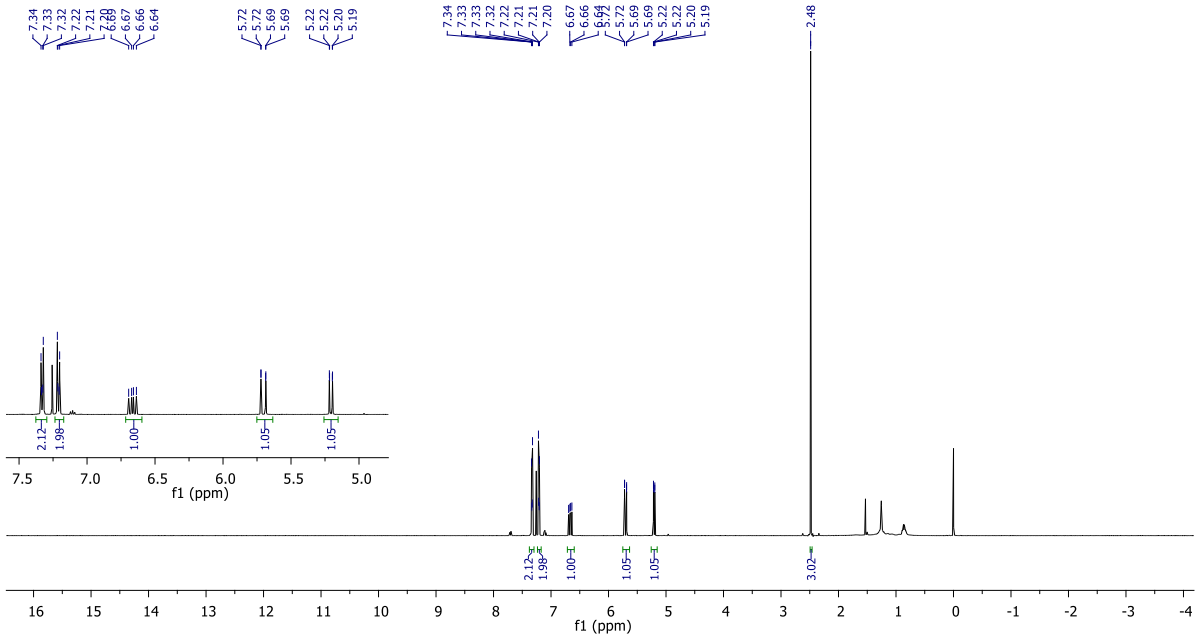


^{13}C NMR (126 MHz, $CDCl_3$) δ 162.38 (d, *J* = 247.1 Hz), 153.26, 133.32 (d, *J* = 3.4 Hz), 132.68, 131.01, 127.97 (d, *J* = 7.8 Hz), 127.17, 126.67, 126.47 (d, *J* = 2.3 Hz), 116.07, 115.67 (d, *J* = 21.8 Hz), 113.28, 95.09, 56.36.

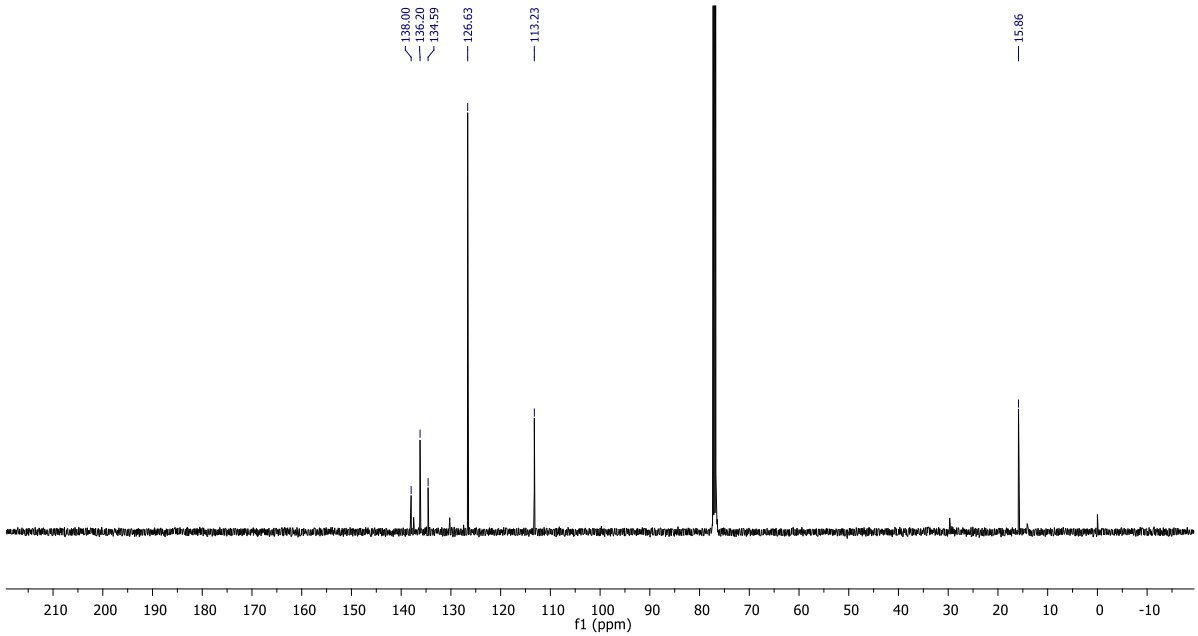


Compound 14

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.30 (m, 2H), 7.24 – 7.17 (m, 2H), 6.67 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.70 (dd, *J* = 17.6, 0.7 Hz, 1H), 5.21 (dd, *J* = 10.9, 0.7 Hz, 1H), 2.48 (s, 3H).

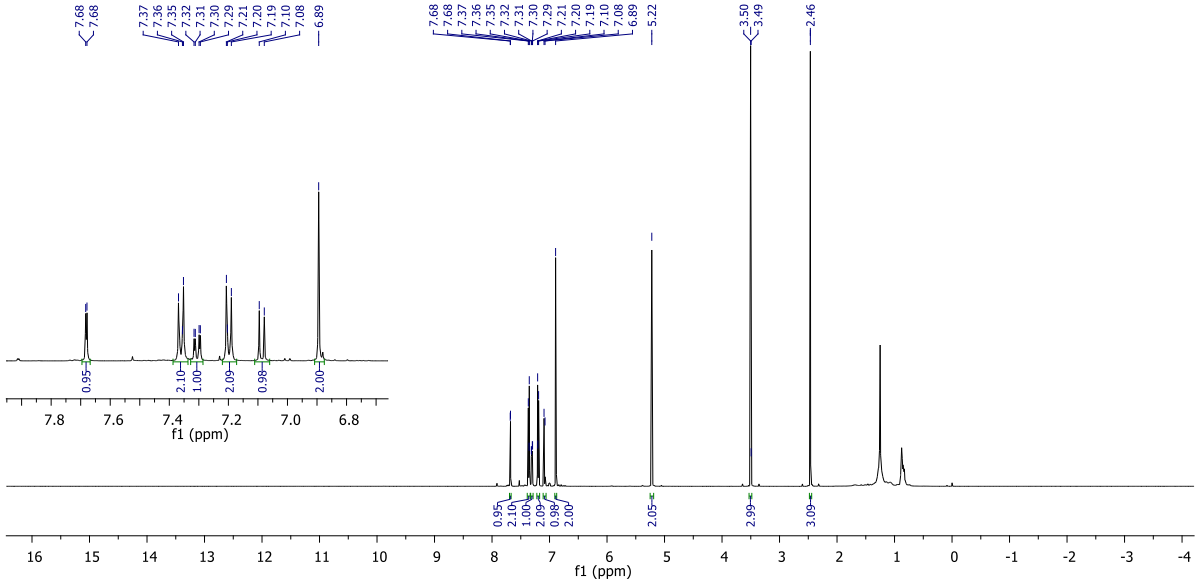


^{13}C NMR (126 MHz, $CDCl_3$) δ 138.00, 136.20, 134.59, 126.63 (4C), 113.23, 15.86.

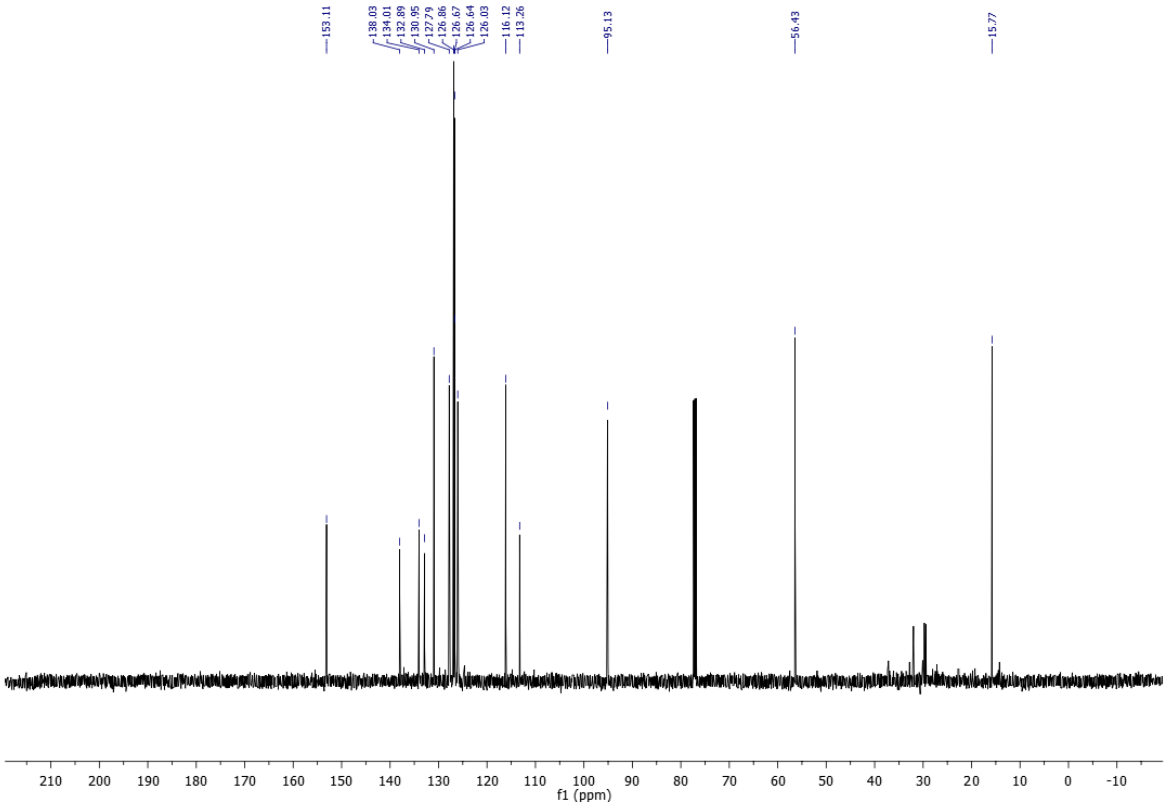


Compound 15

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 (d, *J* = 2.1 Hz, 1H), 7.39 – 7.34 (m, 2H), 7.31 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.22 – 7.17 (m, 2H), 7.09 (d, *J* = 8.5 Hz, 1H), 6.89 (s, 2H), 5.22 (s, 2H), 3.50 (s, 3H), 2.46 (s, 3H).

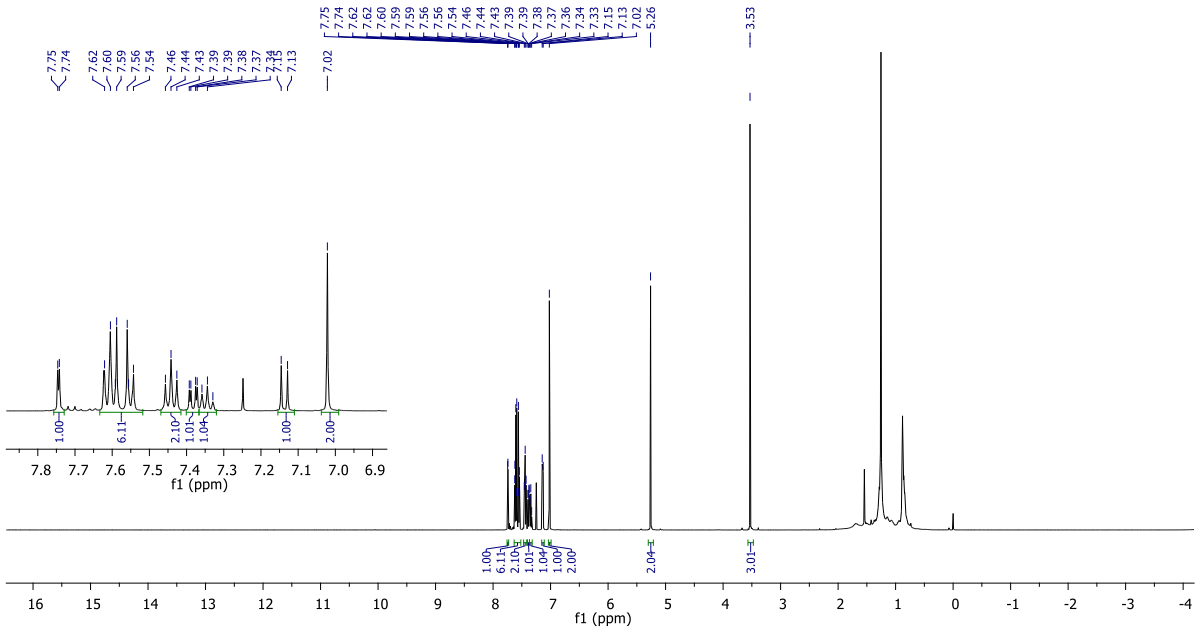


^{13}C NMR (126 MHz, $CDCl_3$) δ 153.11, 138.03, 134.01, 132.89, 130.95, 127.79, 126.86, 126.67, 126.64, 126.03, 116.12, 113.26, 95.13, 56.43, 15.77.

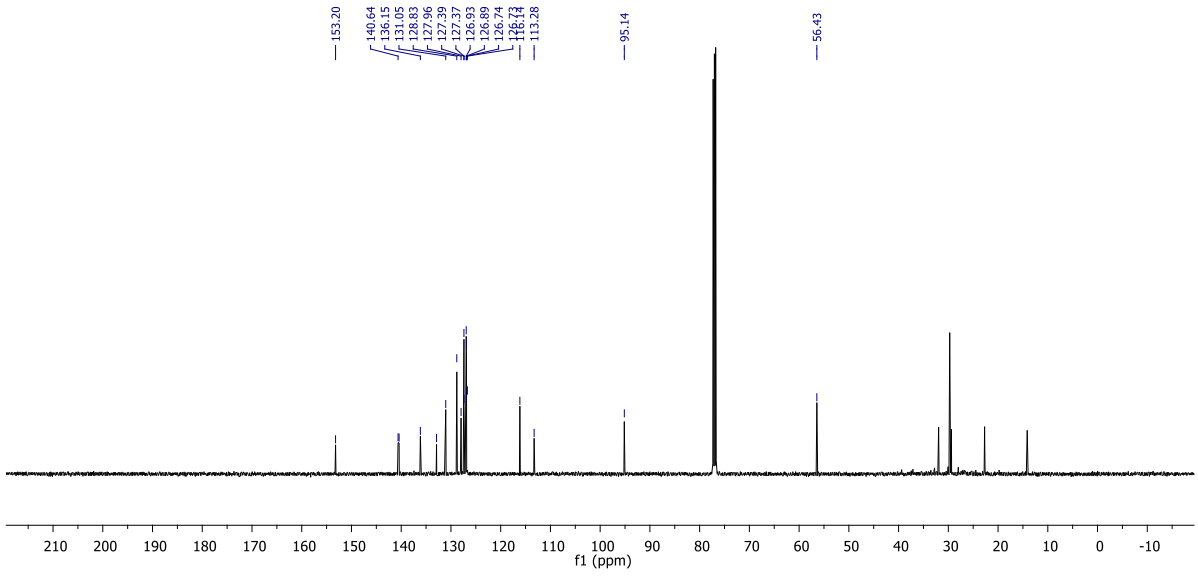


Compound 16

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 2.1 Hz, 1H), 7.63 – 7.52 (m, 6H), 7.44 (dd, *J* = 10.6, 4.8 Hz, 2H), 7.38 (dd, *J* = 8.5, 2.2 Hz, 1H), 7.37 – 7.32 (m, 1H), 7.14 (d, *J* = 8.5 Hz, 1H), 7.02 (s, 2H), 5.26 (s, 2H), 3.53 (s, 3H).

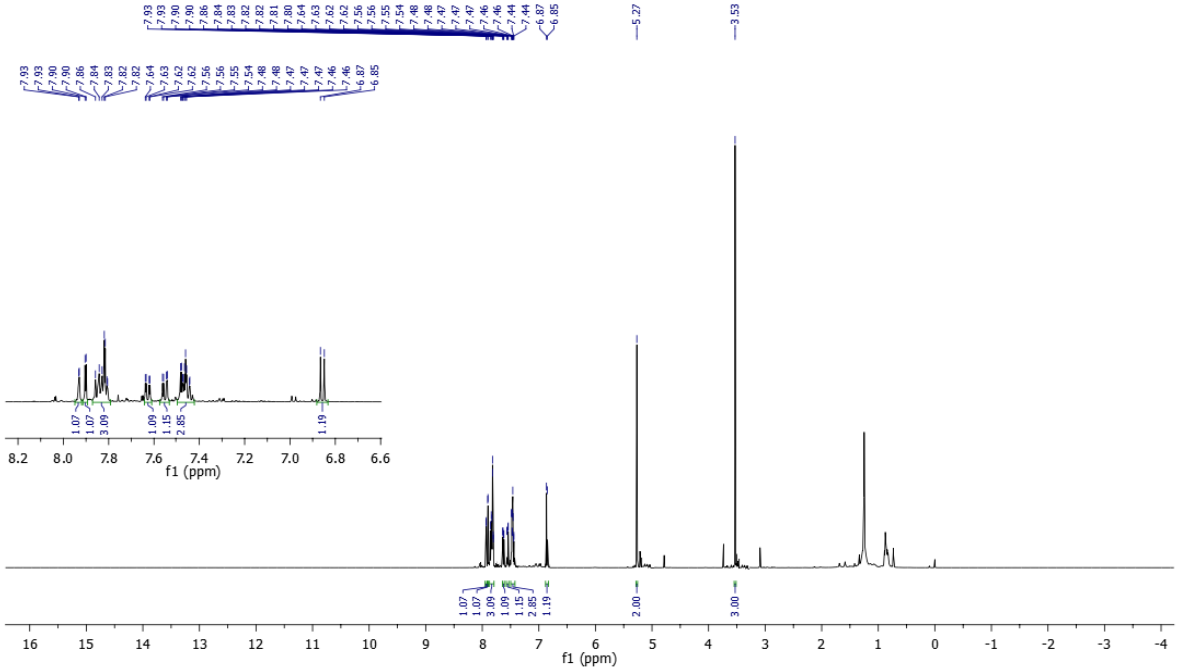


^{13}C NMR (126 MHz, $CDCl_3$) δ 153.20, 140.64, 140.42, 136.15, 132.89, 131.05, 128.83, 127.96, 127.39, 127.37, 126.93, 126.89, 126.74, 126.73, 116.14, 113.28, 95.14, 56.43.

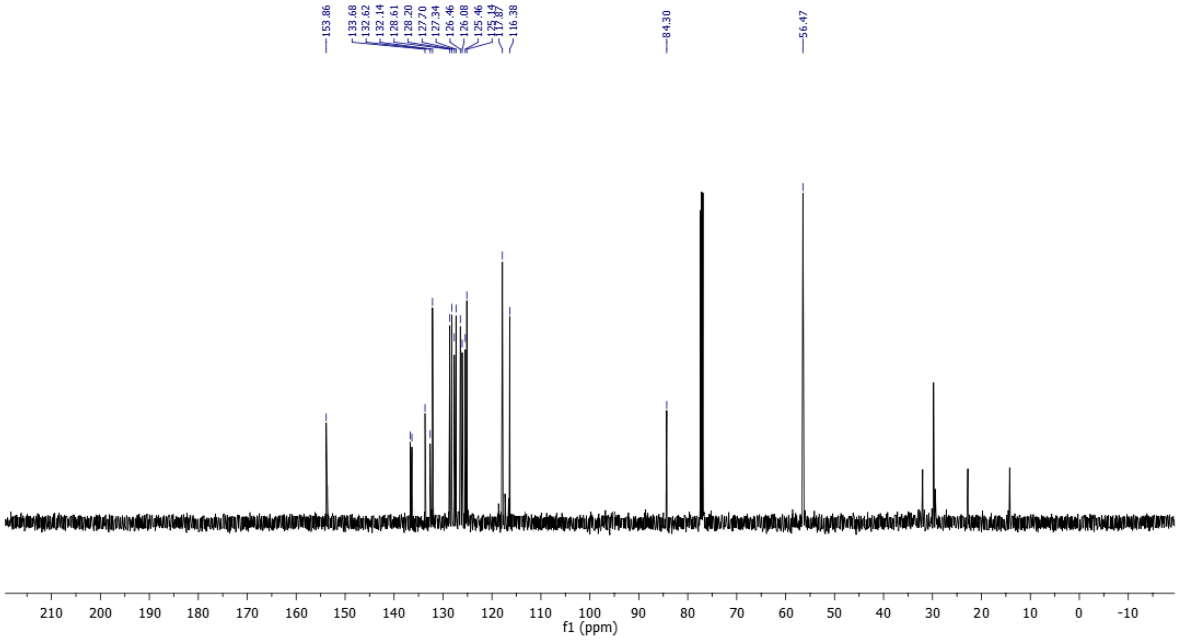


Compound 17

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 (d, *J* = 1.4 Hz, 1H), 7.90 (d, *J* = 2.3 Hz, 1H), 7.87 – 7.79 (m, 3H), 7.63 (dd, *J* = 8.5, 1.9 Hz, 1H), 7.55 (dd, *J* = 3.8, 1.9 Hz, 1H), 7.50 – 7.42 (m, 2H), 6.86 (d, *J* = 8.6 Hz, 1H), 5.27 (s, 2H), 3.53 (s, 3H).

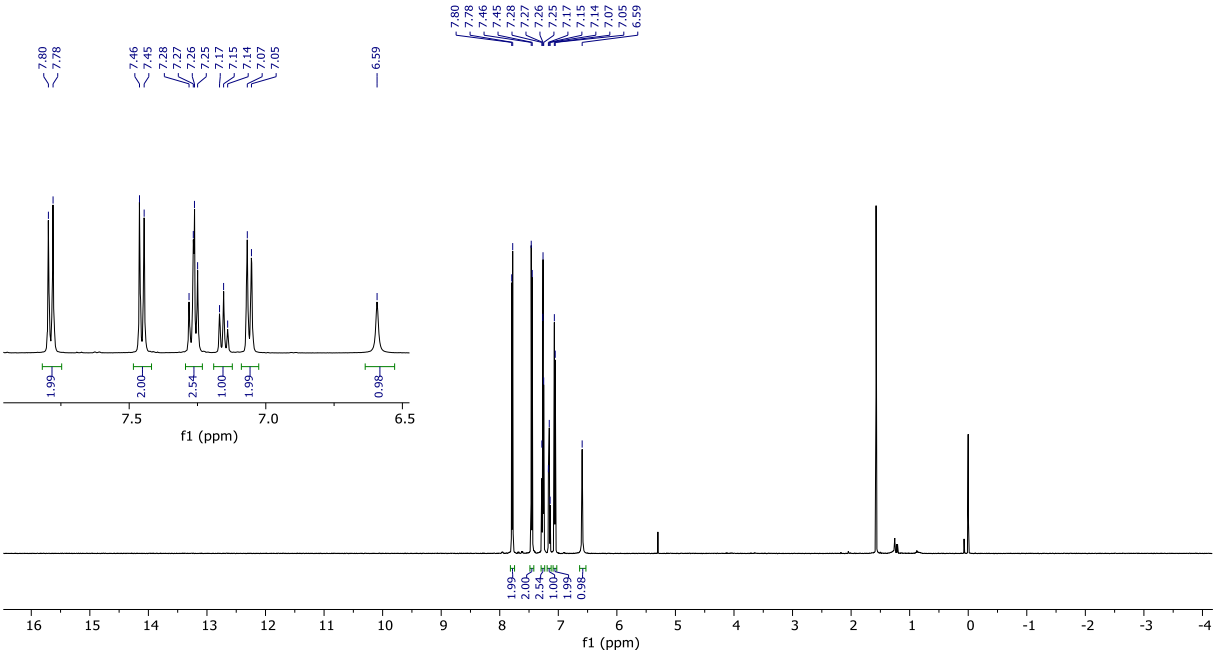


^{13}C NMR (126 MHz, $CDCl_3$) δ 153.86, 136.67, 136.36, 133.68, 132.62, 132.14, 128.61, 128.20, 127.70, 127.34, 126.46, 126.08, 125.46, 125.14, 117.87, 116.38, 84.30, 56.47.

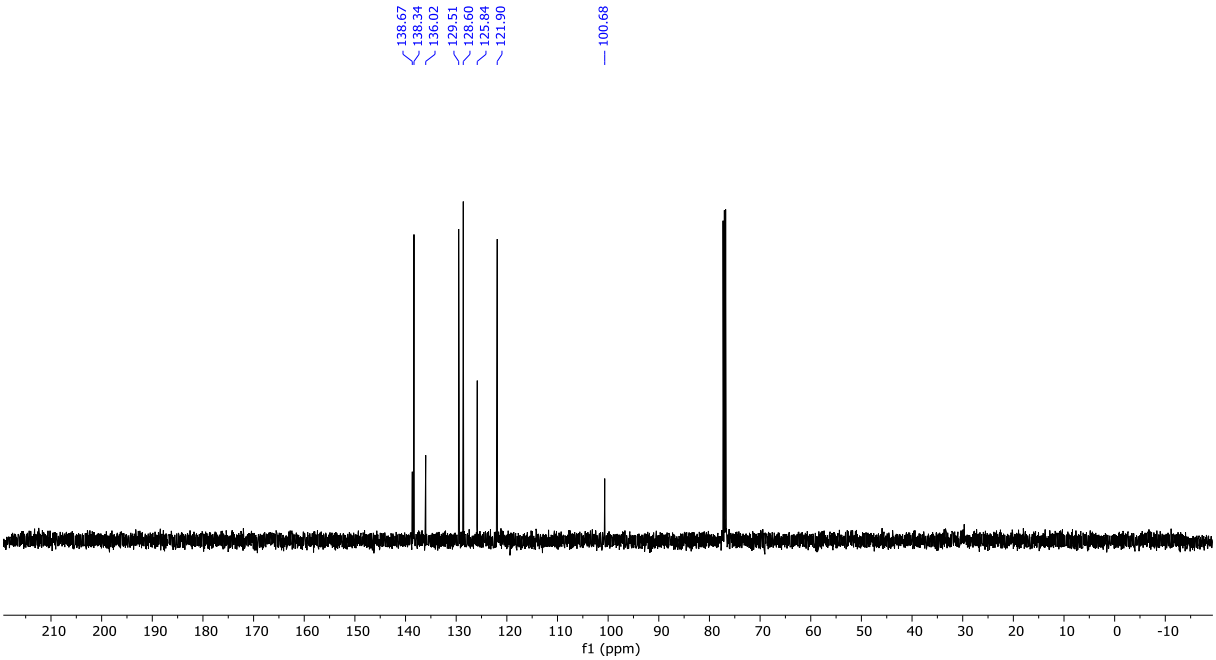


Compound 18

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.5 Hz, 2H), 7.45 (d, *J* = 8.5 Hz, 2H), 7.27 (t, *J* = 7.6 Hz, 2H), 7.15 (t, *J* = 7.6 Hz, 1H), 7.06 (d, *J* = 7.6 Hz, 2H), 6.59 (s, 1H).

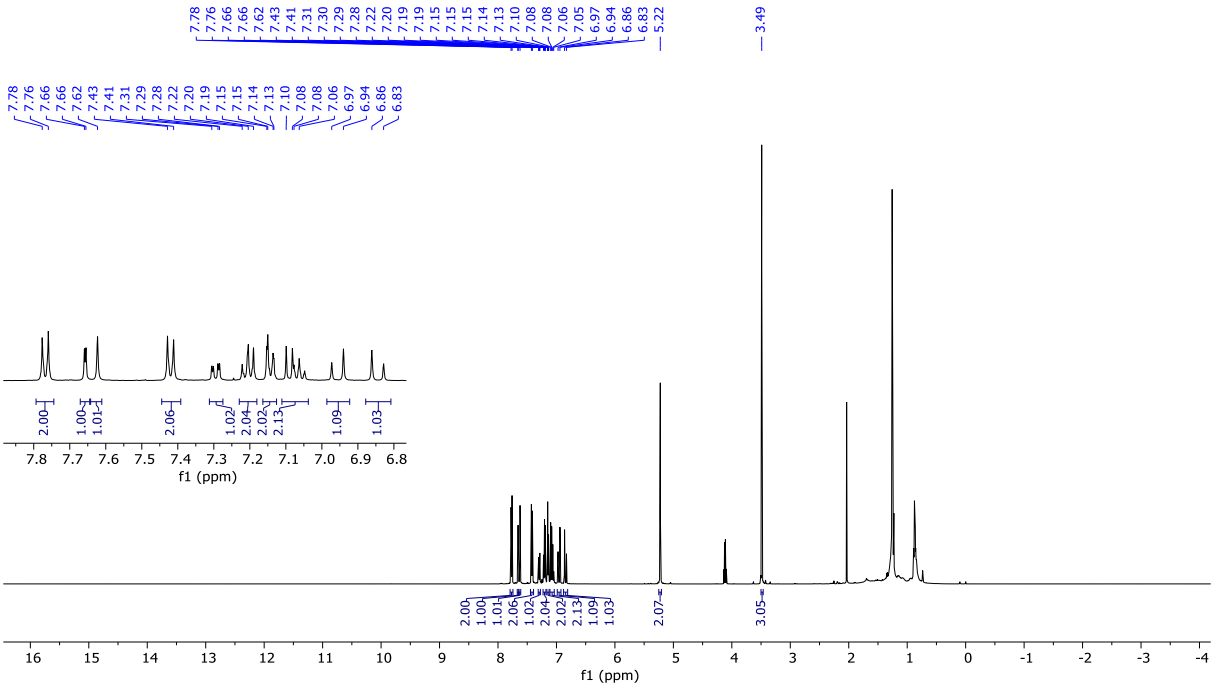


^{13}C NMR (126 MHz, $CDCl_3$) δ 138.67, 138.34, 136.02, 129.51, 128.60, 125.84, 121.90, 100.68.

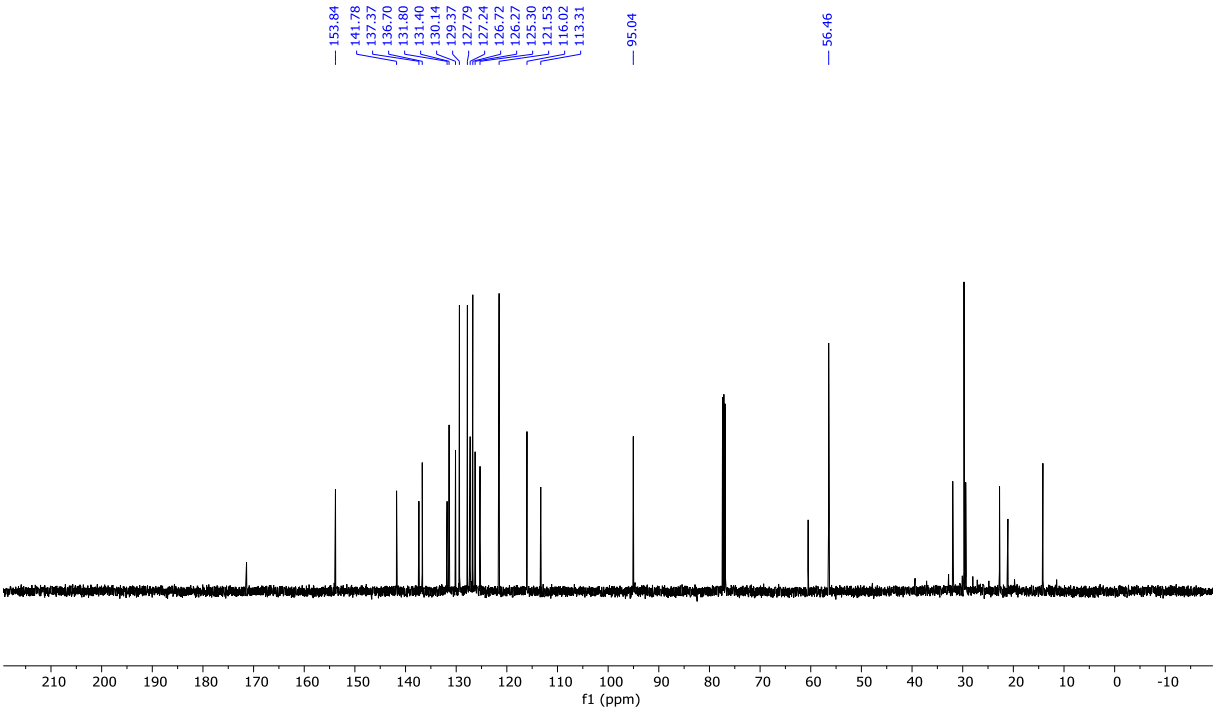


Compound 19

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.5 Hz, 2H), 7.66 (d, *J* = 2.1 Hz, 1H), 7.62 (s, 1H), 7.42 (d, *J* = 8.5 Hz, 2H), 7.29 (dd, *J* = 2.1, 8.6 Hz, 1H), 7.18 – 7.23 (m, 2H), 7.12 – 7.17 (m, 2H), 7.03 – 7.12 (m, 2H), 6.96 (d, *J* = 16.3 Hz, 1H), 6.84 (d, *J* = 16.3 Hz, 1H), 5.22 (s, 2H), 3.49 (s, 3H).

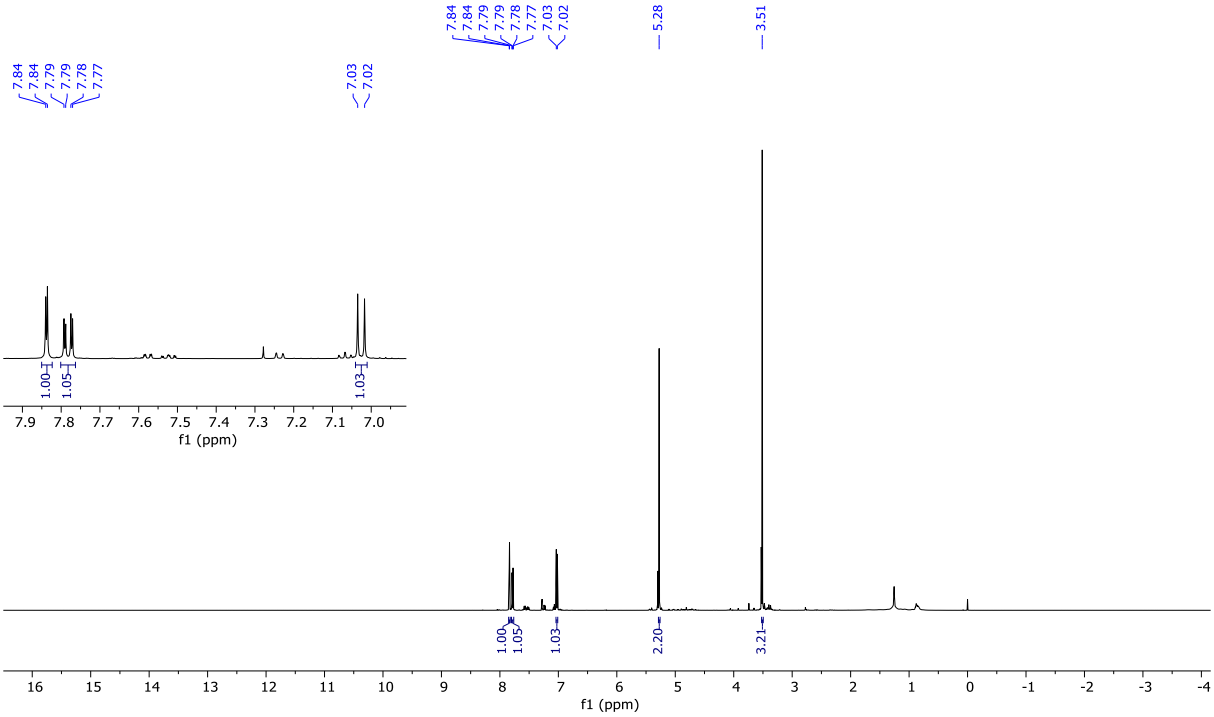


^{13}C NMR (126 MHz, $CDCl_3$, 27°C) δ 153.84, 141.78, 137.37, 136.70, 131.80, 131.40, 130.14, 129.37, 127.79, 127.24, 126.72, 126.27, 125.30, 121.53, 116.02, 113.31, 95.04, 56.46.

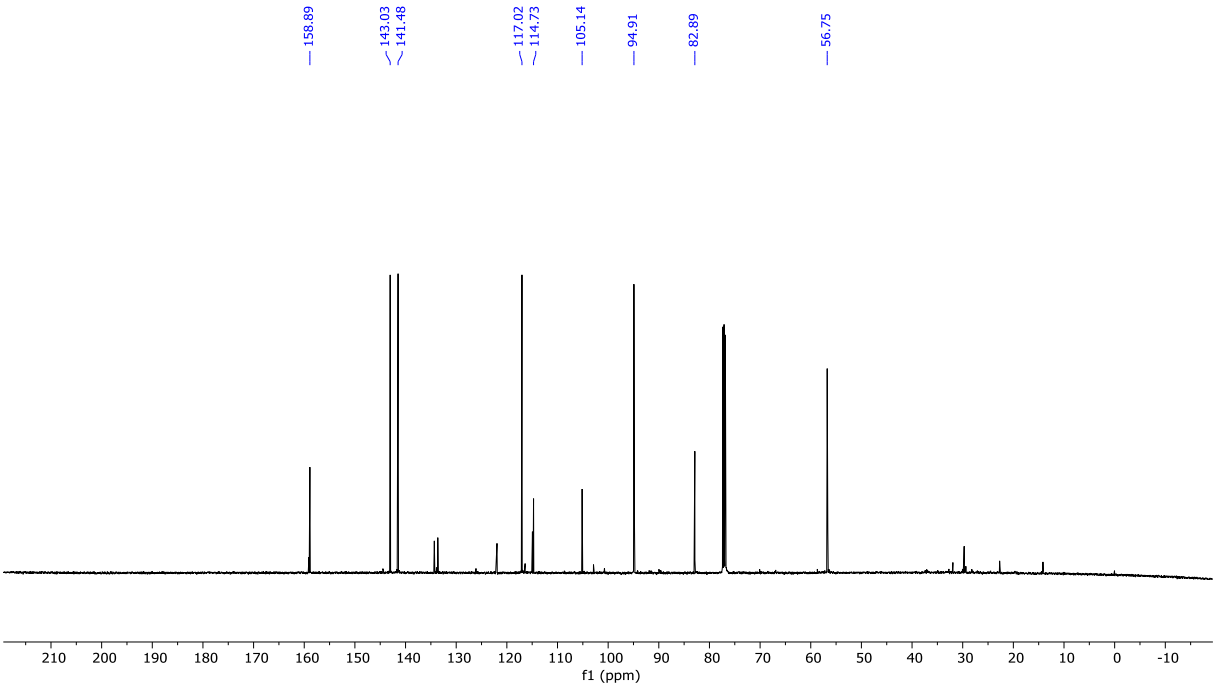


Compound 20

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 2.2 Hz, 1H), 7.78 (dd, *J* = 2.2, 8.9 Hz, 1H), 7.03 (d, *J* = 8.9 Hz, 1H), 5.28 (s, 2H), 3.51 (s, 3H).

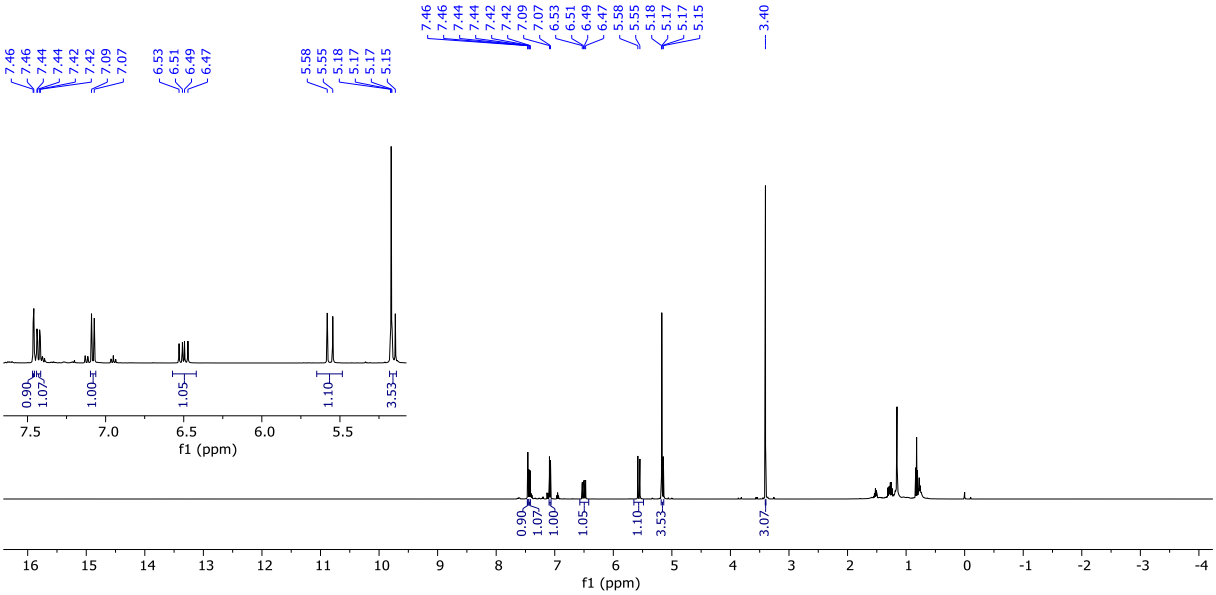


^{13}C NMR (126 MHz, $CDCl_3$) δ 158.89, 143.03, 141.48, 117.02, 114.73, 105.14, 94.91, 82.89, 56.75.

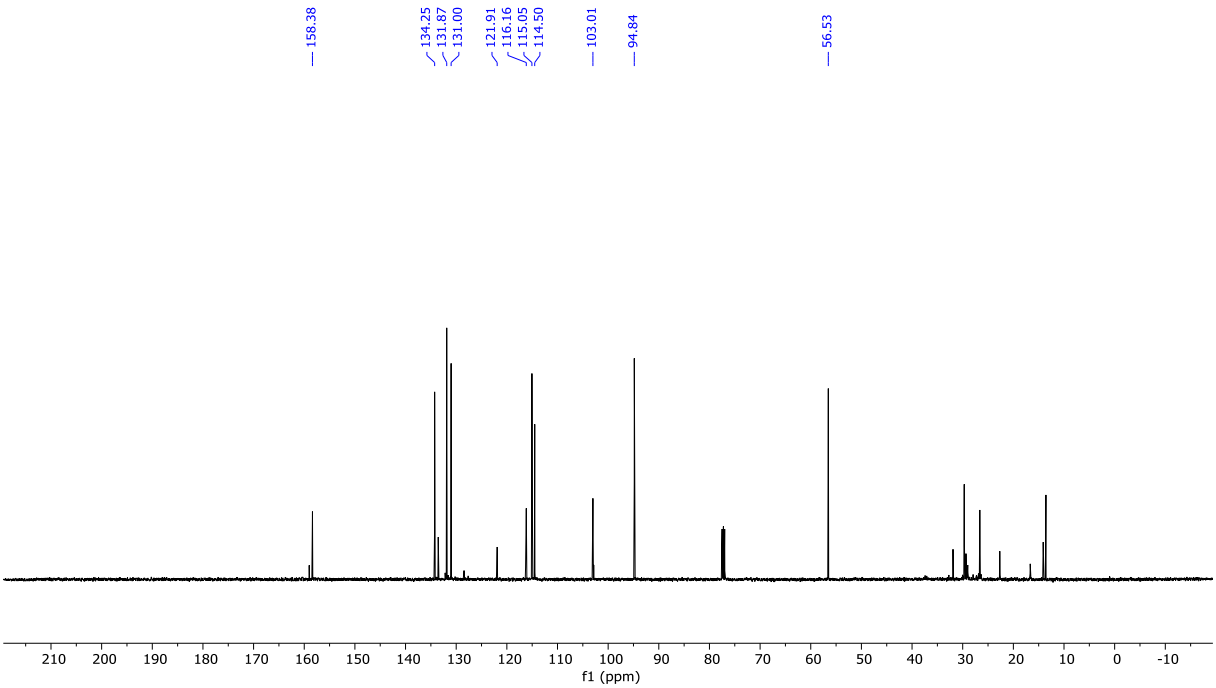


Compound 21

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 (d, *J* = 2.3 Hz, 1H), 7.43 (dd, *J* = 2.3, 8.8 Hz, 1H), 7.08 (d, *J* = 8.8 Hz, 1H), 6.50 (dd, *J* = 10.9, 17.6 Hz, 1H), 5.56 (d, *J* = 17.5 Hz, 1H), 5.14 – 5.18 (m, 4H), 3.40 (s, 3H).

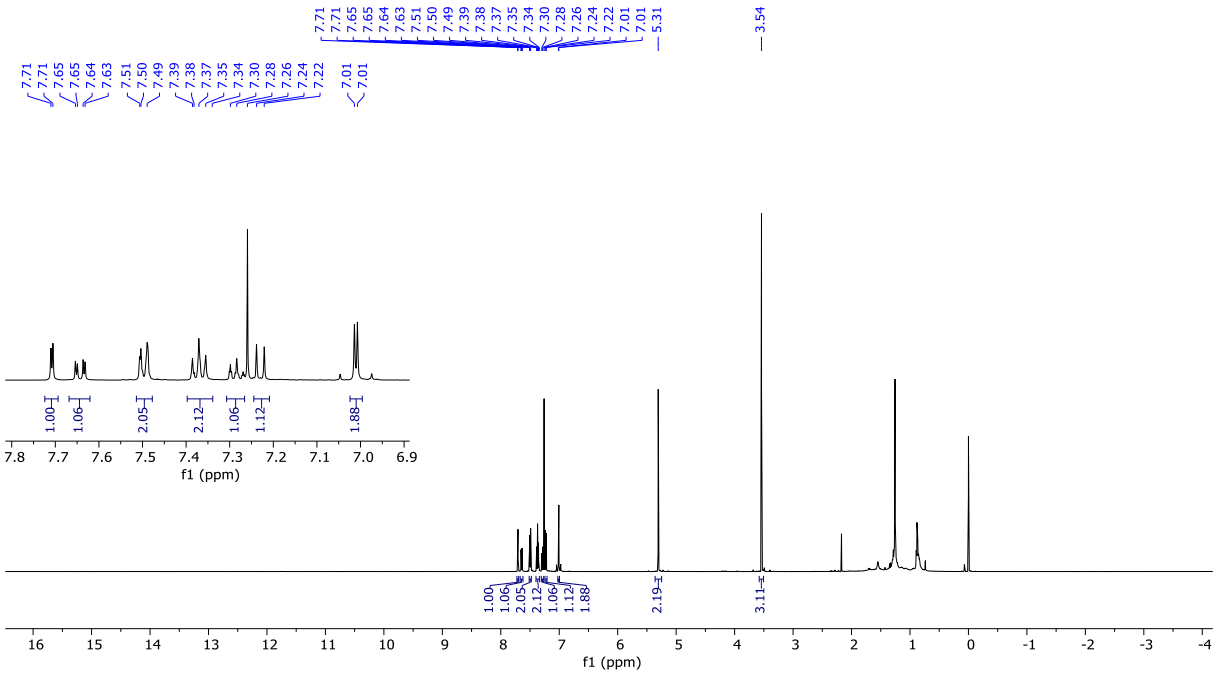


^{13}C NMR (126 MHz, $CDCl_3$) δ 158.38, 134.25, 131.87, 131.00, 121.91, 116.16, 115.05, 114.50, 103.01, 94.84, 56.53.

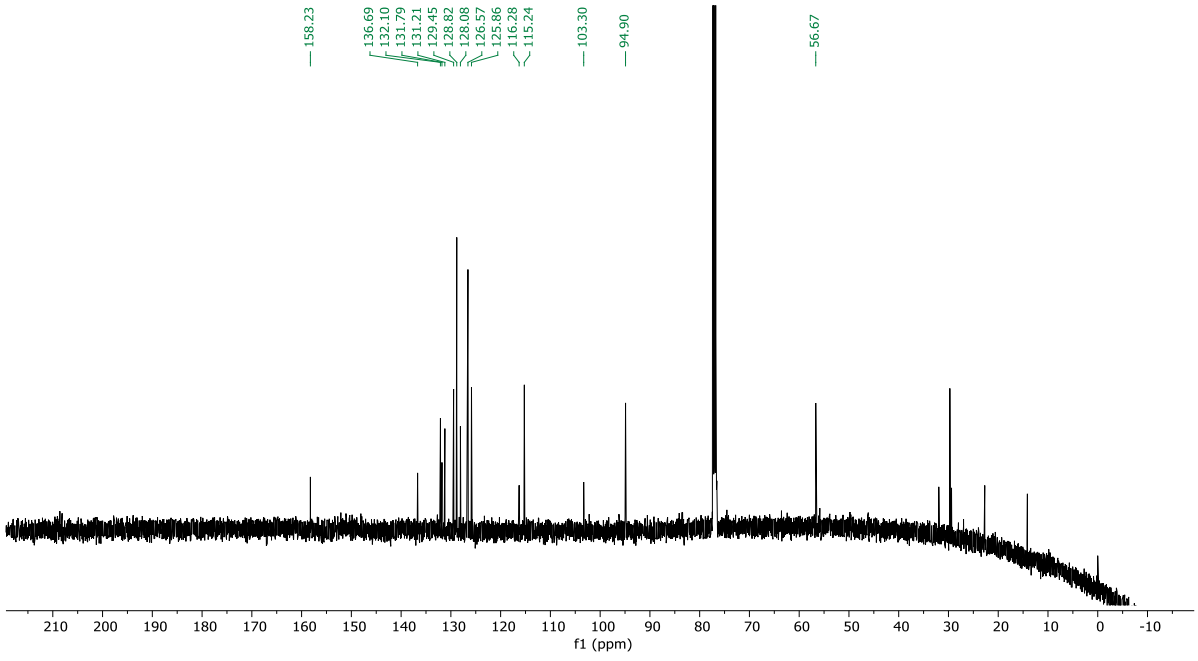


Compound 22

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 (d, *J* = 2.2 Hz, 1H), 7.64 (dd, *J* = 2.3, 8.8 Hz, 1H), 7.48 – 7.51 (m, 2H), 7.32 – 7.4 (m, 2H), 7.27 – 7.31 (m, 1H), 7.23 (d, *J* = 8.8 Hz, 1H), 7.01 (d, *J* = 3.5 Hz, 2H), 5.31 (s, 2H), 3.54 (s, 3H).



^{13}C NMR (126 MHz, $CDCl_3$) δ 158.23, 136.69, 132.10, 131.79, 131.21, 129.45, 128.82, 128.08, 126.57, 125.86, 116.28, 115.24, 103.30, 94.90, 56.67.



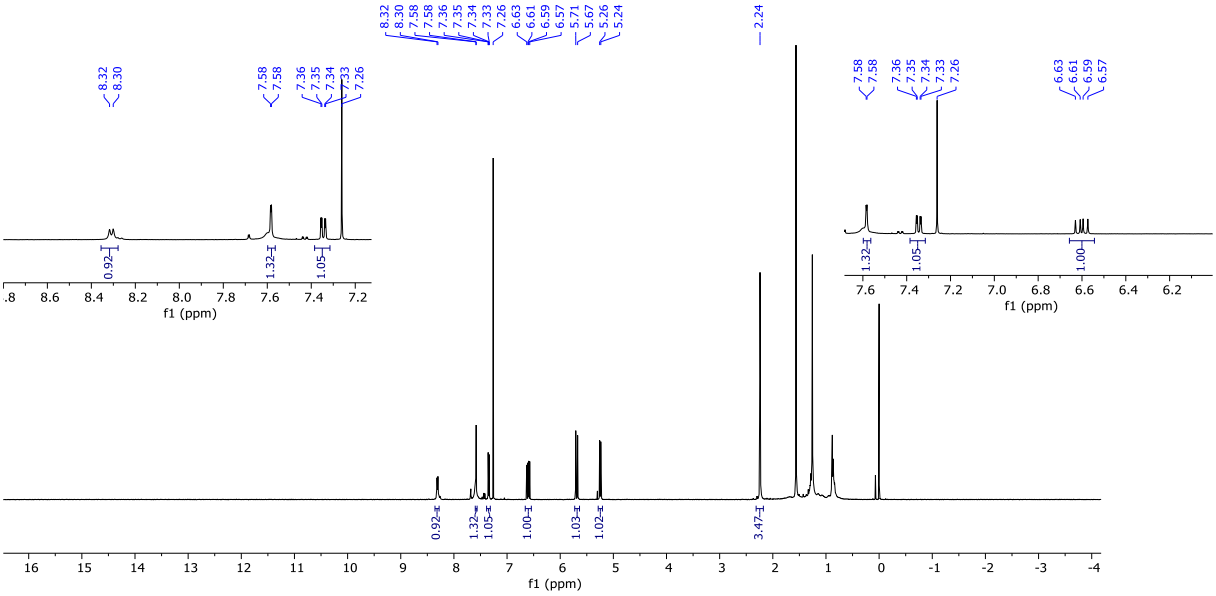
Compound 23

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.88 (s, 1H), 8.63 (d, *J* = 8.5 Hz, 1H), 8.09 (d, *J* = 1.9 Hz, 1H), 7.82 (dd, *J* = 1.8, 8.5 Hz, 1H), 2.77 (s, 1H), 2.30 (s, 3H).

Synthesis of Violaceic Acid and Related Compounds through Aryl Triazene
S. Ando, J. Burrows, K. Koide. *Organic Letters* **2017**, *19(5)*, 1116-1119

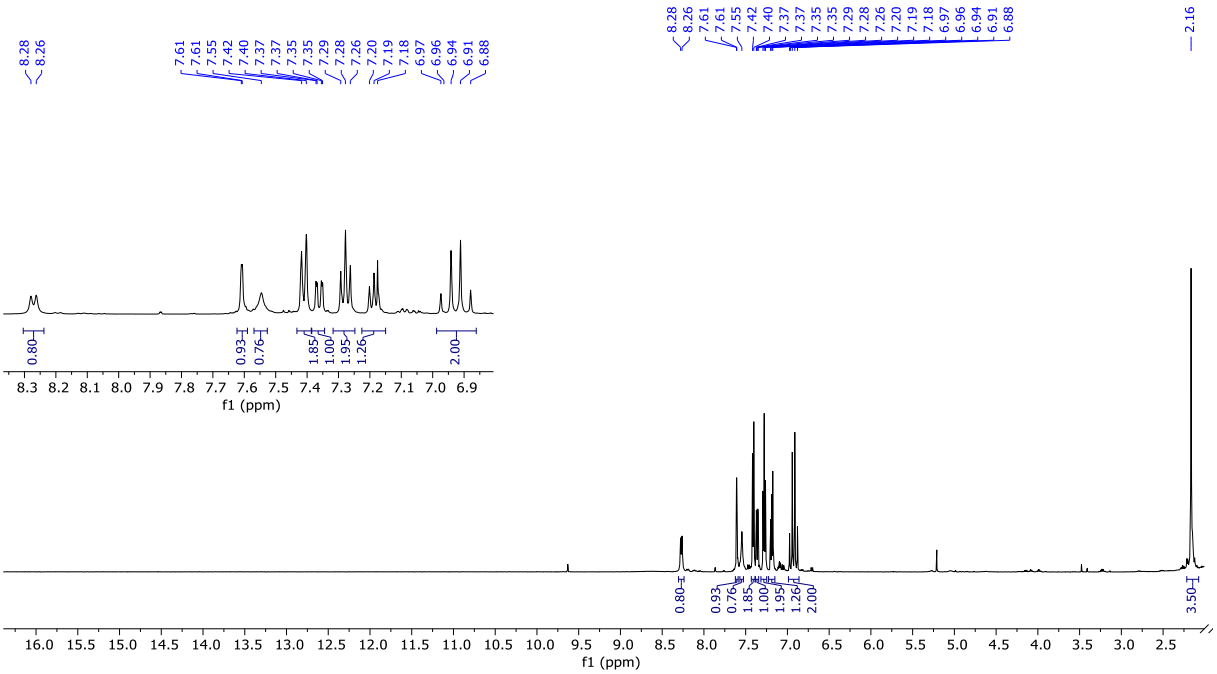
Compound 24

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.4 Hz, 1H), 7.58 (d, *J* = 1.8 Hz, 1H), 7.35 (dd, *J* = 1.9, 8.5 Hz, 1H), 6.60 (dd, *J* = 10.9, 17.6 Hz, 1H), 5.69 (d, *J* = 17.5 Hz, 1H), 5.25 (d, *J* = 10.9 Hz, 1H), 2.24 (s, 3H).

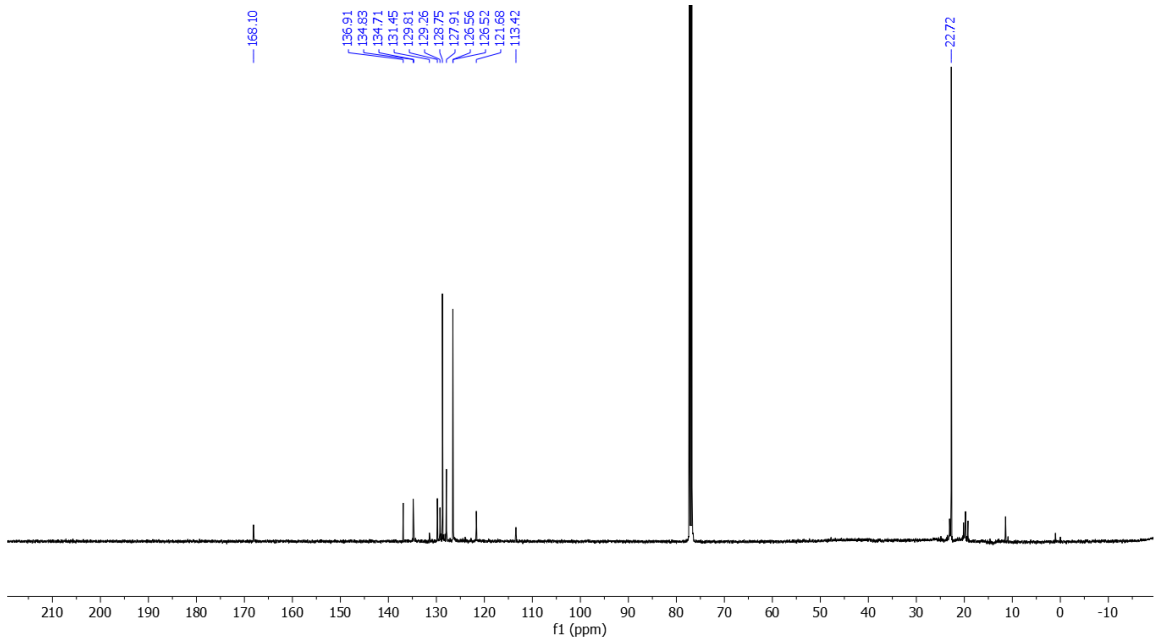


Compound 25

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.5 Hz, 1H), 7.59 – 7.63 (m, 1H), 7.55 (s, 1H), 7.41 (d, *J* = 7.4 Hz, 2H), 7.36 (dd, *J* = 1.8, 8.6 Hz, 1H), 7.28 (t, *J* = 7.6 Hz, 2H), 7.15 – 7.23 (m, 1H), 6.86 – 6.99 (m, 2H), 2.16 (s, 3H).

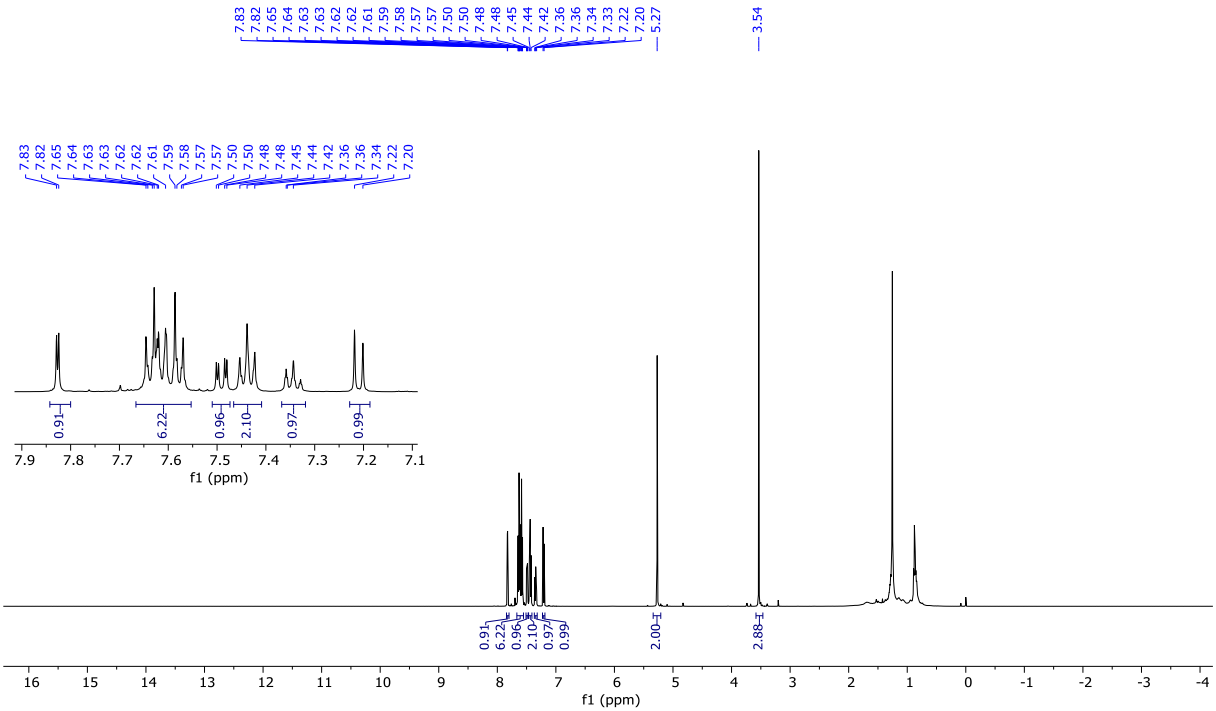


^{13}C NMR (126 MHz, $CDCl_3$, 27°C) δ 168.10, 136.91, 134.83, 134.71, 131.45, 129.81, 129.26, 128.75, 127.91, 126.56, 126.52, 121.68, 113.42, 22.72

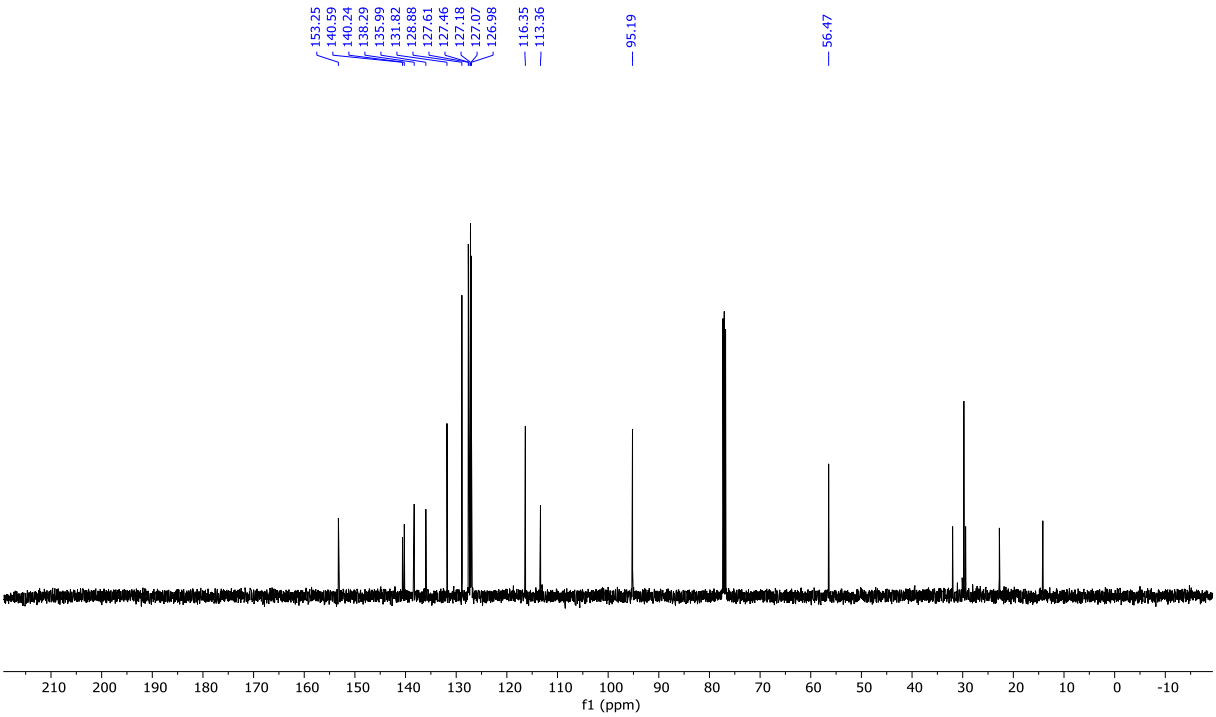


Compound 26

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 2.2 Hz, 1H), 7.55 – 7.67 (m, 6H), 7.49 (dd, *J* = 2.3, 8.5 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.31 – 7.38 (m, 1H), 7.21 (d, *J* = 8.6 Hz, 1H), 5.27 (s, 2H), 3.54 (s, 3H).

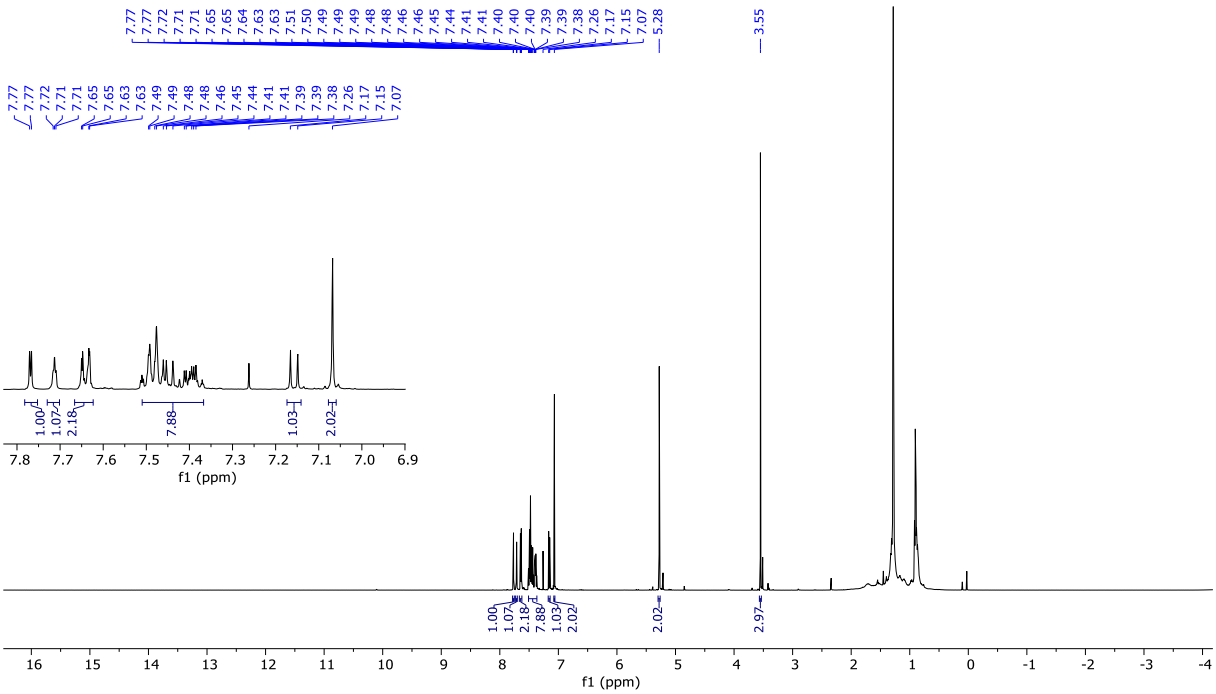


^{13}C NMR (126 MHz, $CDCl_3$, 27°C) δ 153.25, 140.59, 140.24, 138.29, 135.99, 131.82, 128.88, 127.61, 127.46, 127.18, 127.07, 126.98, 116.35, 113.36, 95.19, 56.47.

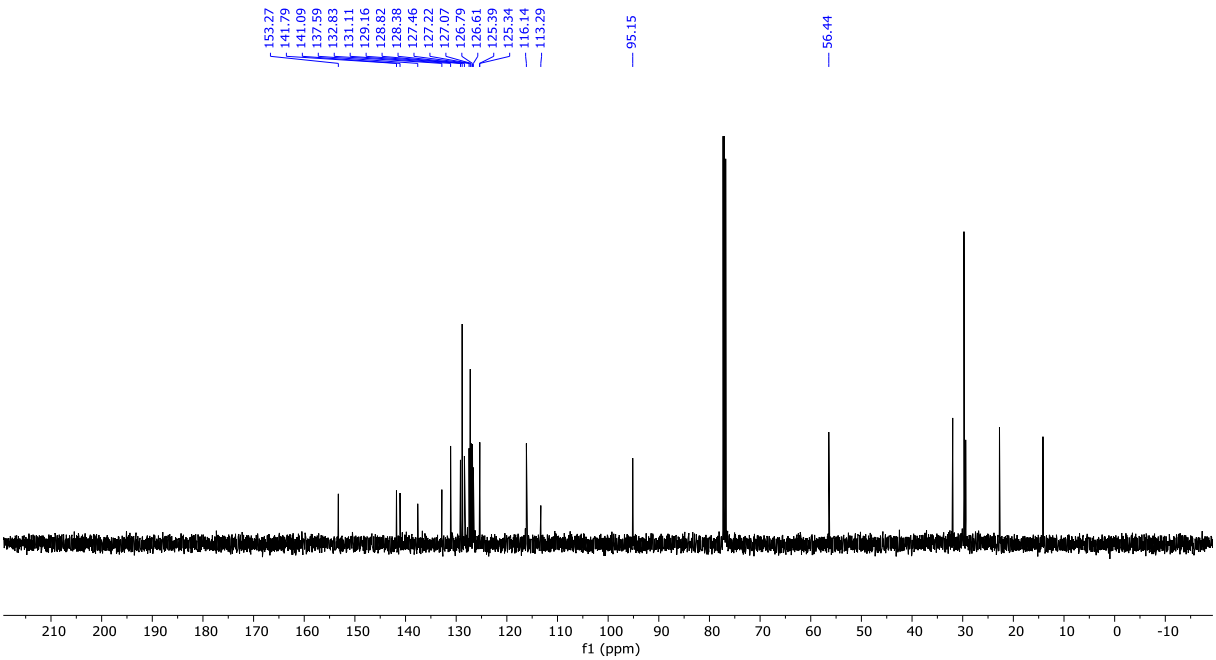


Compound 27

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 2.2 Hz, 1H), 7.71 (t, *J* = 1.6 Hz, 1H), 7.61 – 7.67 (m, 2H), 7.37 – 7.51 (m, 7H), 7.16 (d, *J* = 8.5 Hz, 1H), 7.07 (s, 2H), 5.28 (s, 2H), 3.55 (s, 3H).

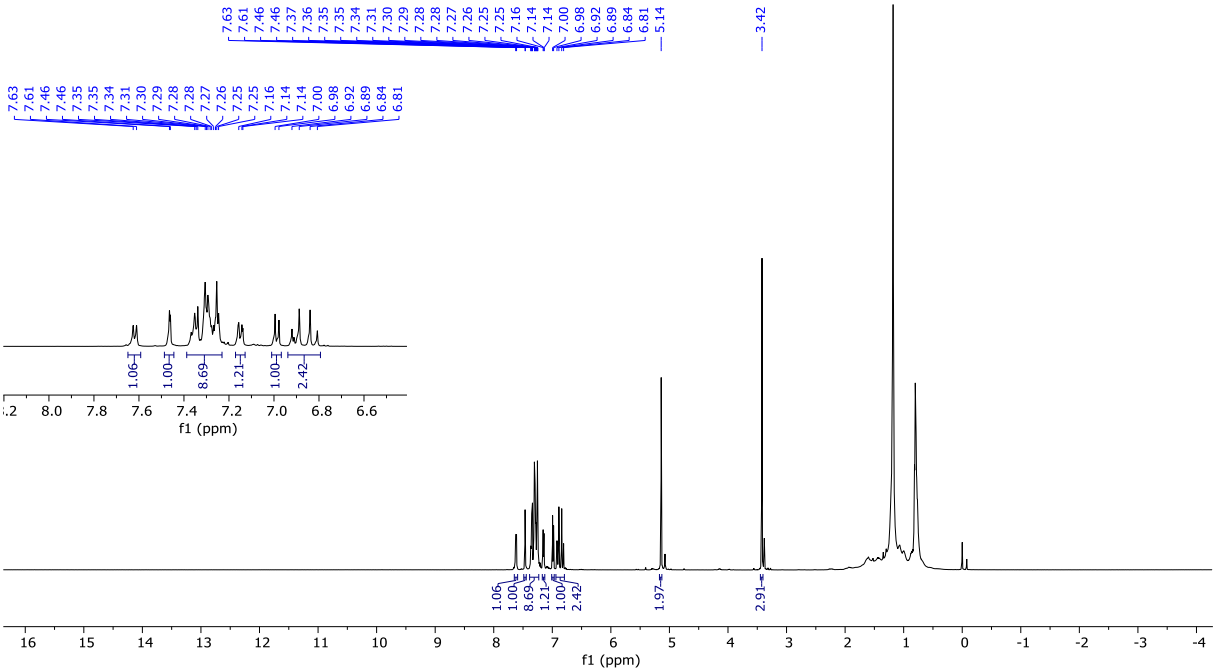


^{13}C NMR (126 MHz, $CDCl_3$, 27°C) δ 153.27, 141.79, 141.09, 137.59, 132.83, 131.11, 129.16, 128.82, 128.38, 127.46, 127.22, 127.07, 126.79, 126.61, 125.39, 125.34, 116.14, 113.29, 95.15, 56.44.

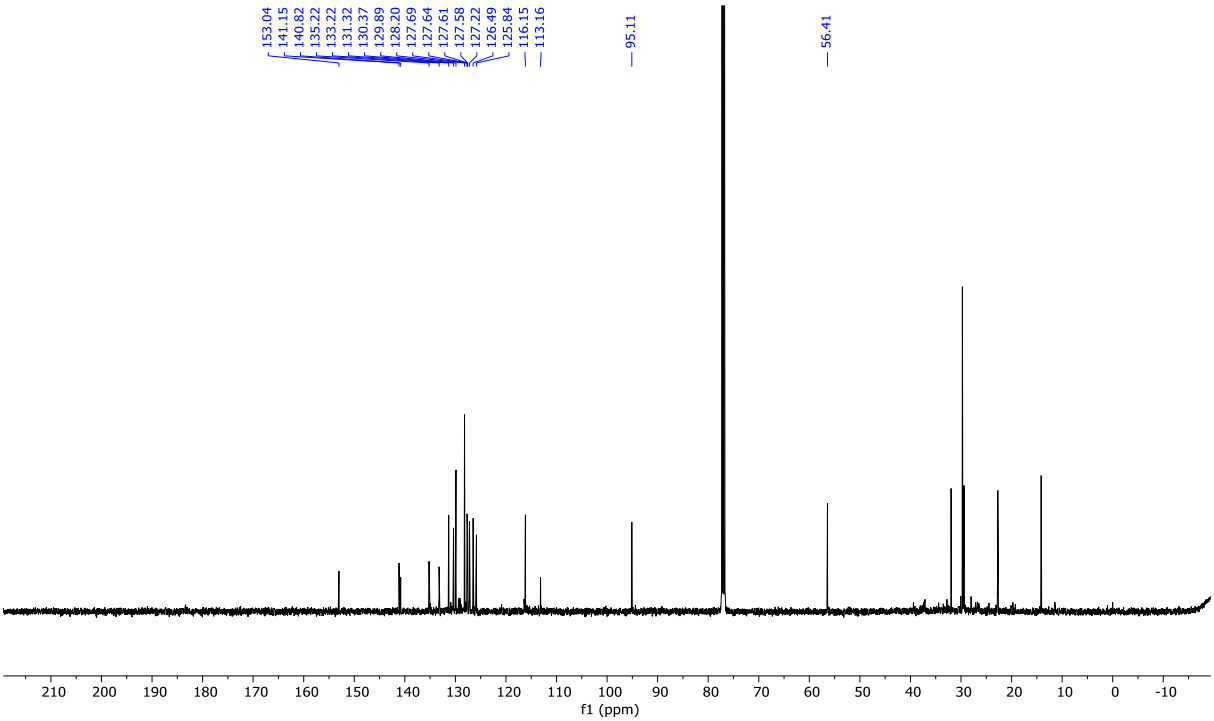


Compound 28

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.4 Hz, 1H), 7.46 (d, *J* = 2.1 Hz, 1H), 7.23 – 7.39 (m, 9H), 7.13 – 7.17 (m, 1H), 6.99 (d, *J* = 8.5 Hz, 1H), 6.79 – 6.94 (m, 2H), 5.14 (s, 2H), 3.42 (s, 3H).

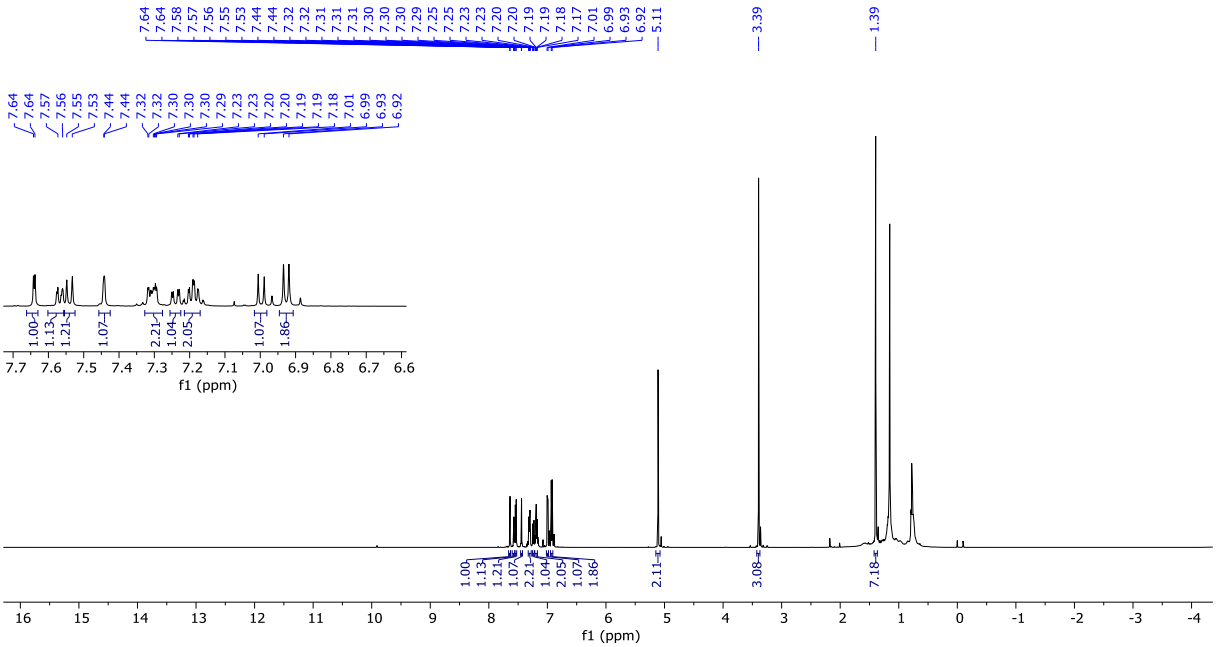


^{13}C NMR (126 MHz, $CDCl_3$) δ 153.04, 141.15, 140.82, 135.22, 133.22, 131.32, 130.37, 129.89, 128.20, 127.69, 127.64, 127.61, 127.58, 127.22, 126.49, 125.84, 116.15, 113.16, 95.11, 56.41.

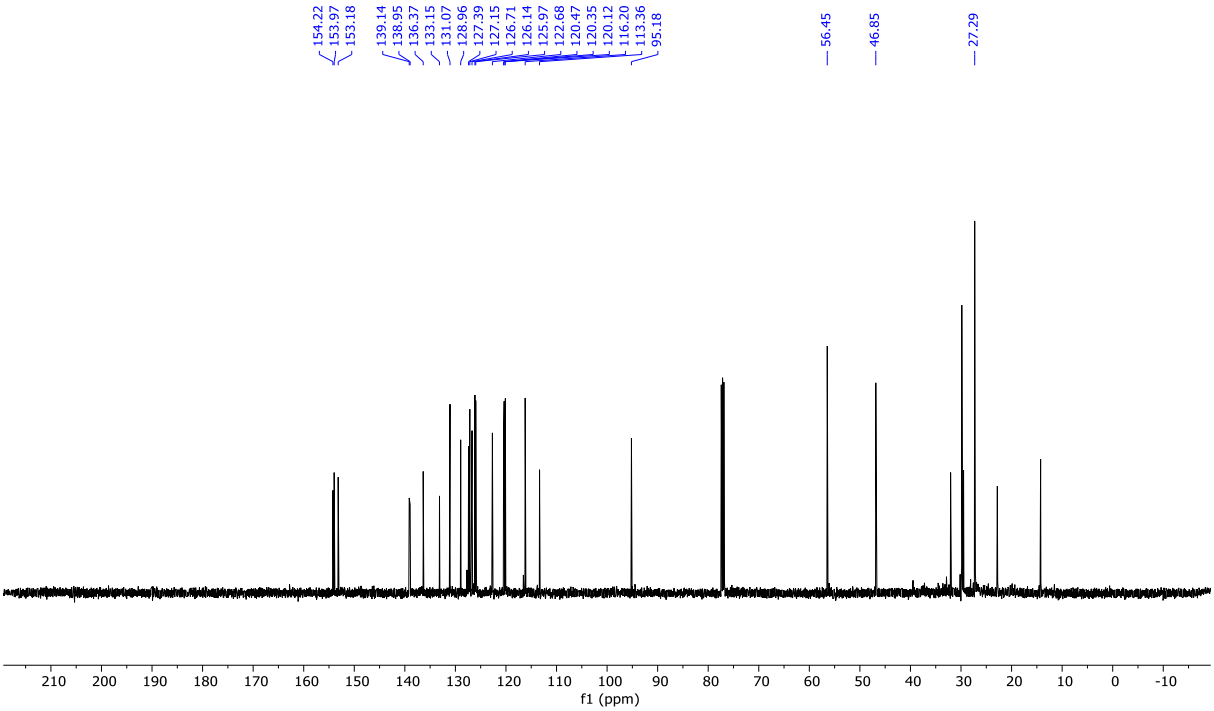


Compound 29

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64 (d, *J* = 2.1 Hz, 1H), 7.55 – 7.6 (m, 1H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.43 – 7.46 (m, 1H), 7.31 (s, 2H), 7.24 (dd, *J* = 2.1, 8.5 Hz, 1H), 7.17 – 7.21 (m, 2H), 7.00 (d, *J* = 8.5 Hz, 1H), 6.93 (d, *J* = 7.7 Hz, 2H), 5.11 (s, 2H), 3.39 (s, 3H), 1.39 (s, 6H).

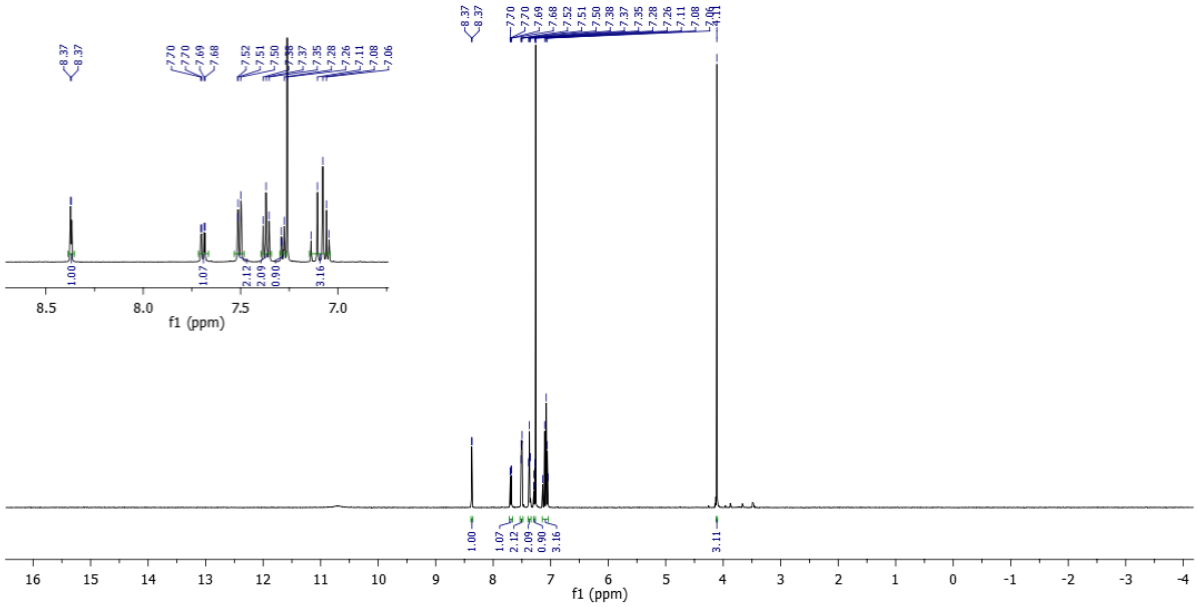


^{13}C NMR (126 MHz, $CDCl_3$, 27°C) δ 154.22, 153.97, 153.18, 139.14, 138.95, 136.37, 133.15, 131.07, 128.96, 127.39, 127.15, 126.71, 126.14, 125.97, 122.68, 120.47, 120.35, 120.12, 116.20, 113.36, 95.18, 56.45, 46.85, 27.29.

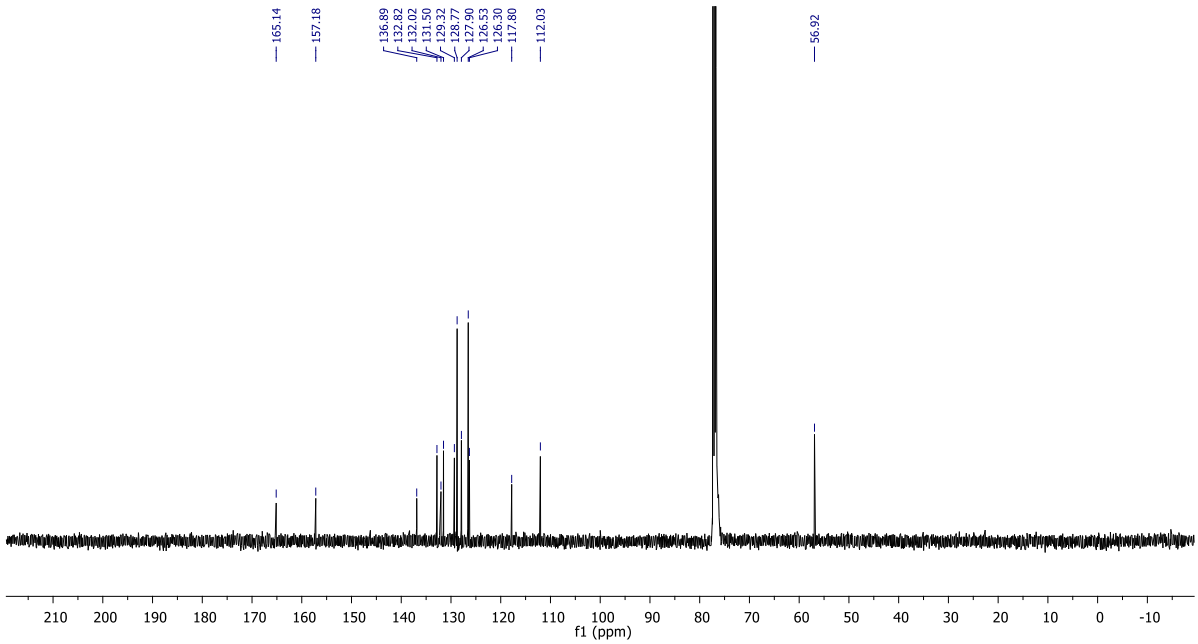


DC01

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (d, *J* = 2.4 Hz, 1H), 7.69 (dd, *J* = 8.6, 2.4 Hz, 1H), 7.51 (dd, *J* = 7.3, 1.2 Hz, 2H), 7.39 – 7.34 (m, 2H), 7.30 – 7.27 (m, 1H), 7.15 – 7.04 (m, 3H), 4.11 (s, 3H).

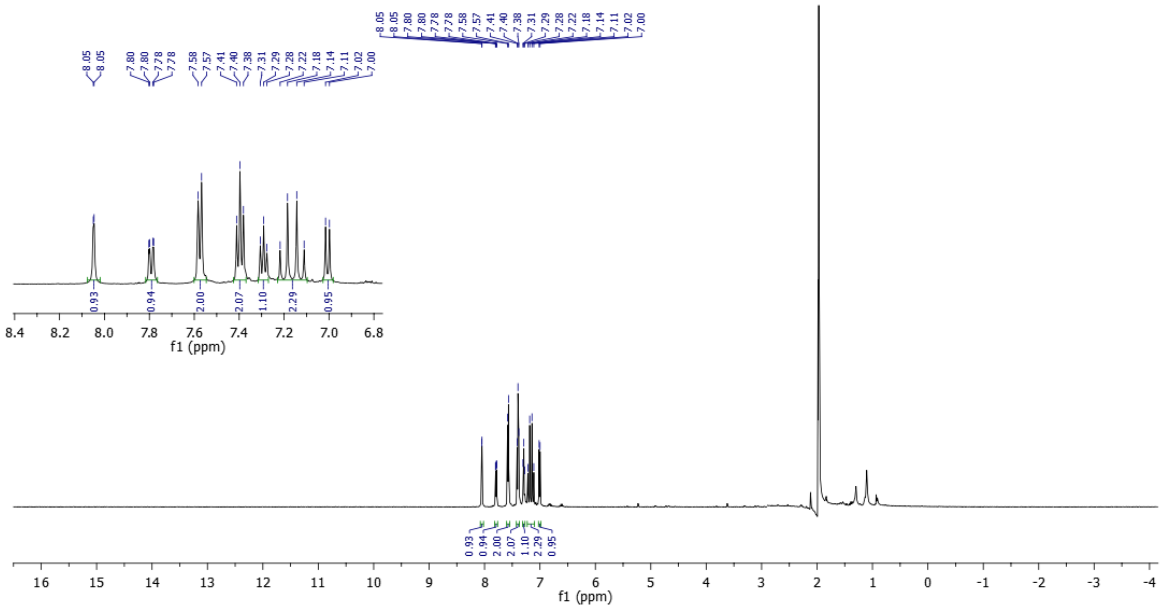


^{13}C NMR (126 MHz, $CDCl_3$) δ 165.14, 157.18, 136.89, 132.82, 132.02, 131.50, 129.32, 128.77, 127.90, 126.53, 126.30, 117.80, 112.03, 56.92.

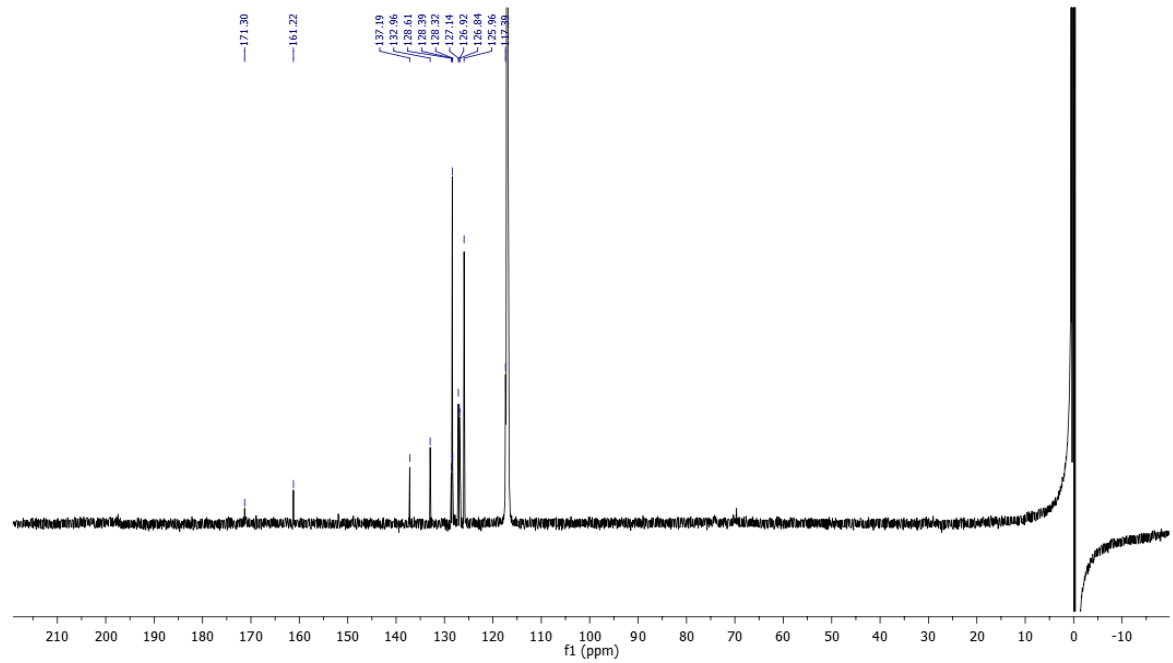


DC02

^{1}H NMR (500 MHz, CD_3CN) δ 8.05 (d, *J* = 1.7 Hz, 1H), 7.79 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.58 (d, *J* = 7.6 Hz, 2H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.29 (t, *J* = 7.3 Hz, 1H), 7.16 (dd, *J* = 37.0, 16.5 Hz, 2H), 7.01 (d, *J* = 8.7 Hz, 1H).

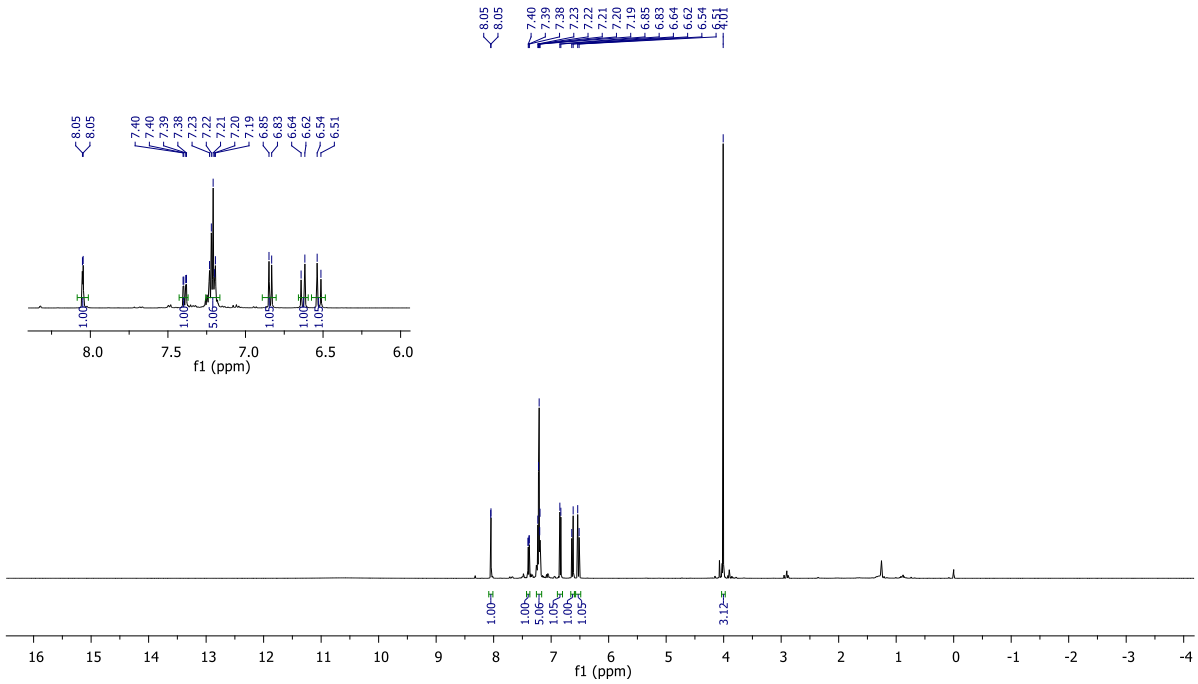


^{13}C NMR (126 MHz, CD_3CN) δ 171.30, 161.22, 137.19, 132.96, 128.61, 128.39, 128.32, 127.14, 126.92, 126.84, 125.96, 117.39 (probabily last peak under solvent peak).

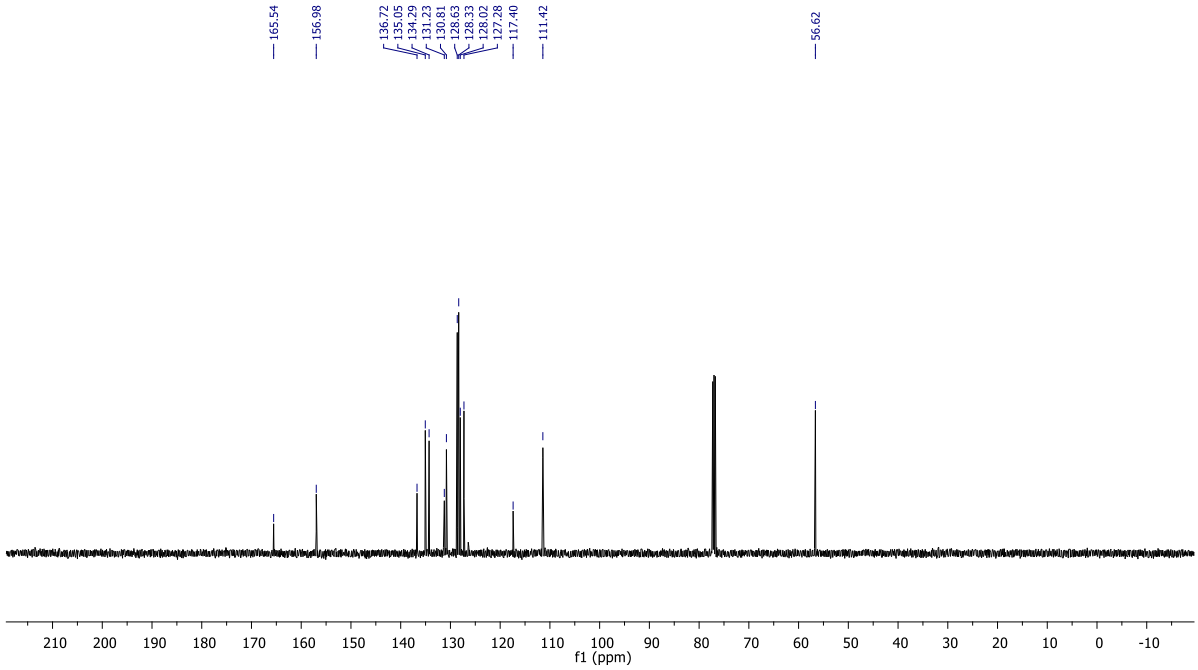


DC03

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (d, *J* = 2.3 Hz, 1H), 7.39 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.26 – 7.16 (m, 5H), 6.84 (d, *J* = 8.7 Hz, 1H), 6.63 (d, *J* = 12.1 Hz, 1H), 6.53 (d, *J* = 12.2 Hz, 1H), 4.01 (s, 3H).

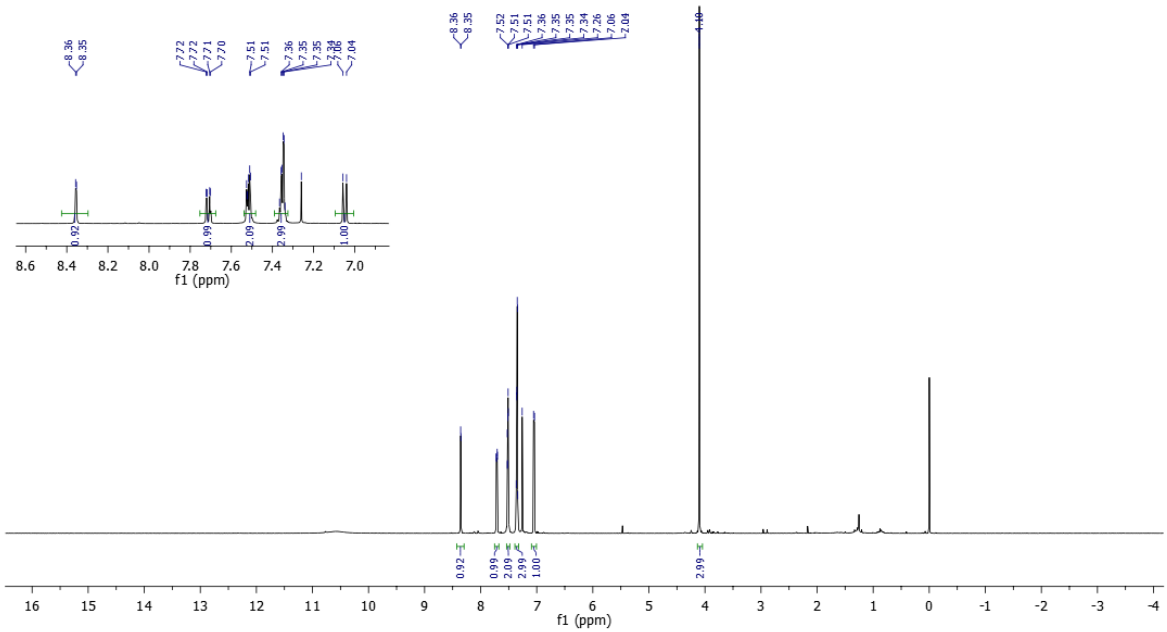


^{13}C NMR (126 MHz, $CDCl_3$) δ 165.54, 156.98, 136.72, 135.05, 134.29, 131.23, 130.81, 128.63, 128.33, 128.02, 127.28, 117.40, 111.42, 56.62.

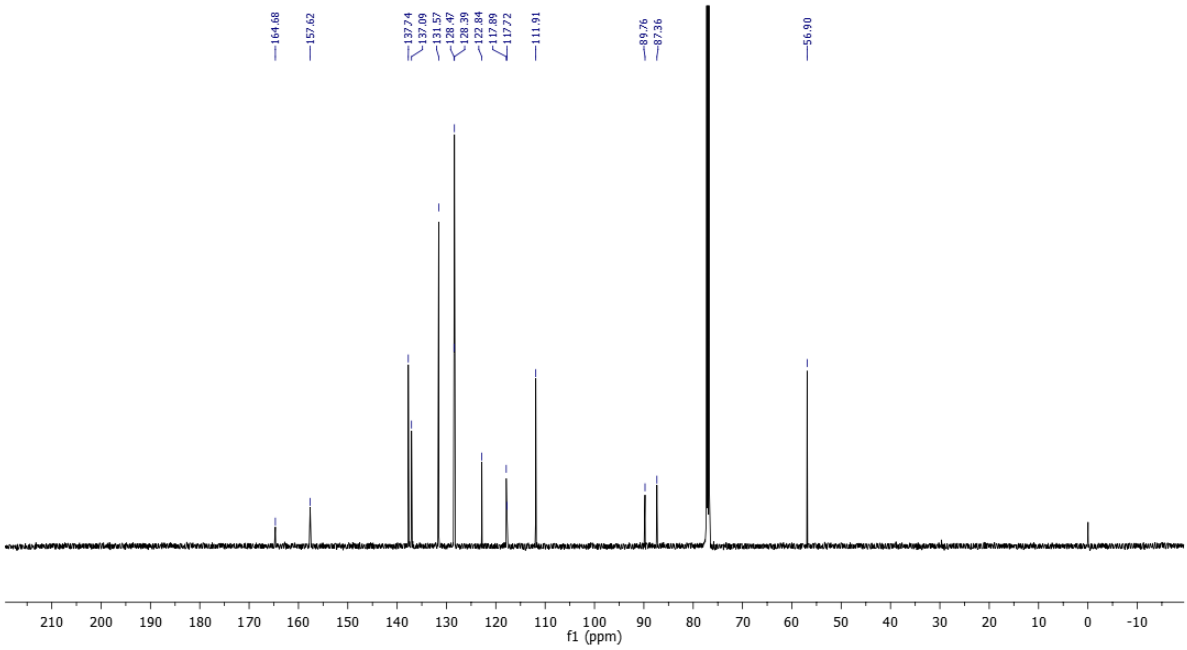


DC04

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (d, *J* = 2.1 Hz, 1H), 7.71 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.57 – 7.48 (m, 2H), 7.39 – 7.32 (m, 3H), 7.05 (d, *J* = 8.6 Hz, 1H), 4.10 (s, 3H).

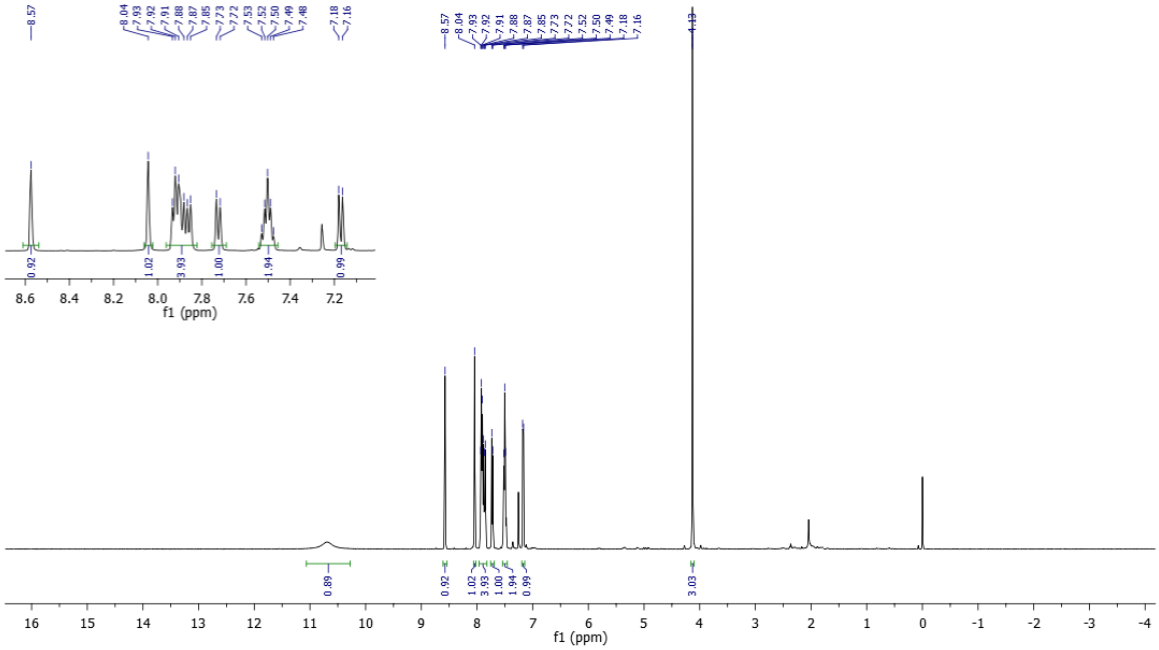


^{13}C NMR (126 MHz, $CDCl_3$) δ 164.68, 157.62, 137.74, 137.09, 131.57, 128.47, 128.39, 122.84, 117.89, 117.72, 111.91, 89.76, 87.36, 56.90.

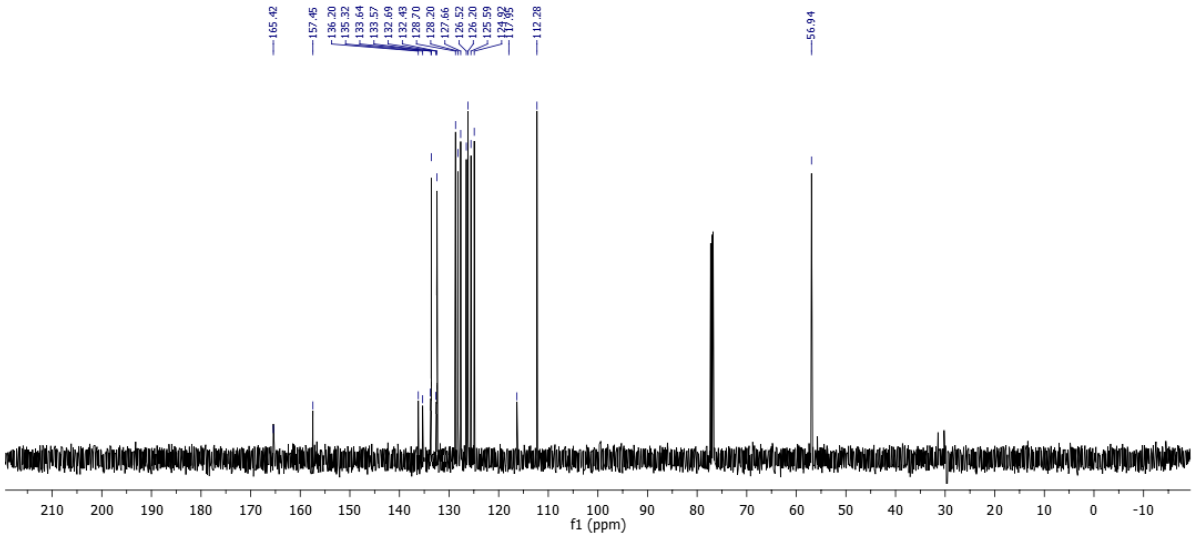


DC05

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.70 (s, 1H), 8.57 (s, 1H), 8.04 (s, 1H), 7.96 – 7.82 (m, 4H), 7.73 (d, *J* = 8.5 Hz, 1H), 7.50 (t, *J* = 6.8 Hz, 2H), 7.17 (d, *J* = 8.6 Hz, 1H), 4.13 (s, 3H).

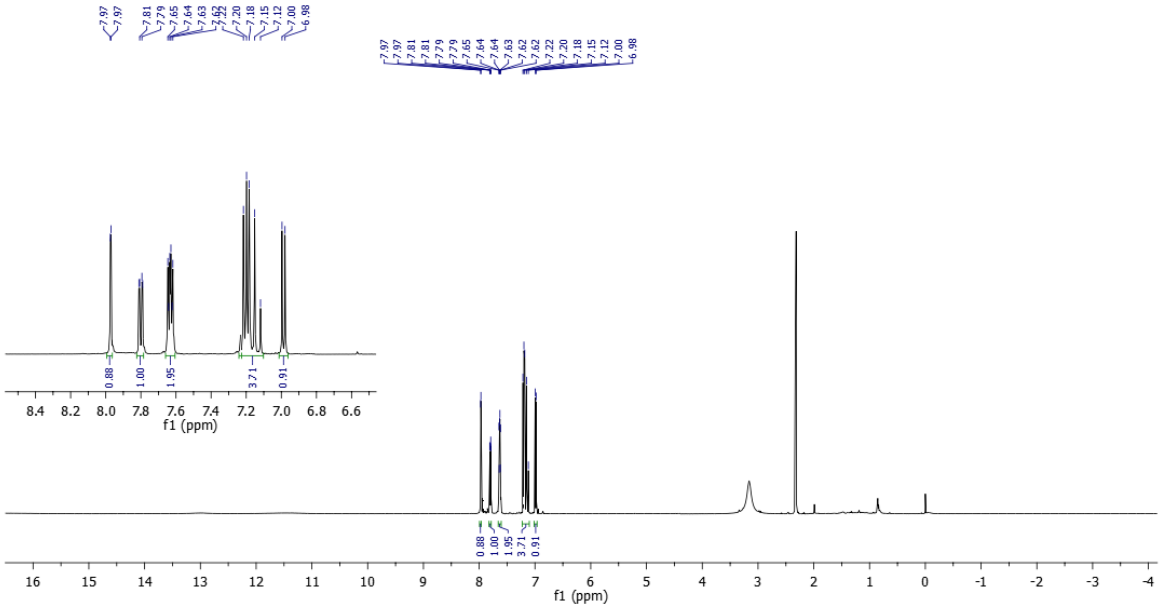


^{13}C NMR (126 MHz, $CDCl_3$) δ 165.42, 157.45, 136.20, 135.32, 133.64, 133.57, 132.69, 132.43, 128.70, 128.20, 127.66, 126.52, 126.20, 125.59, 124.92, 117.95, 112.28, 56.94.

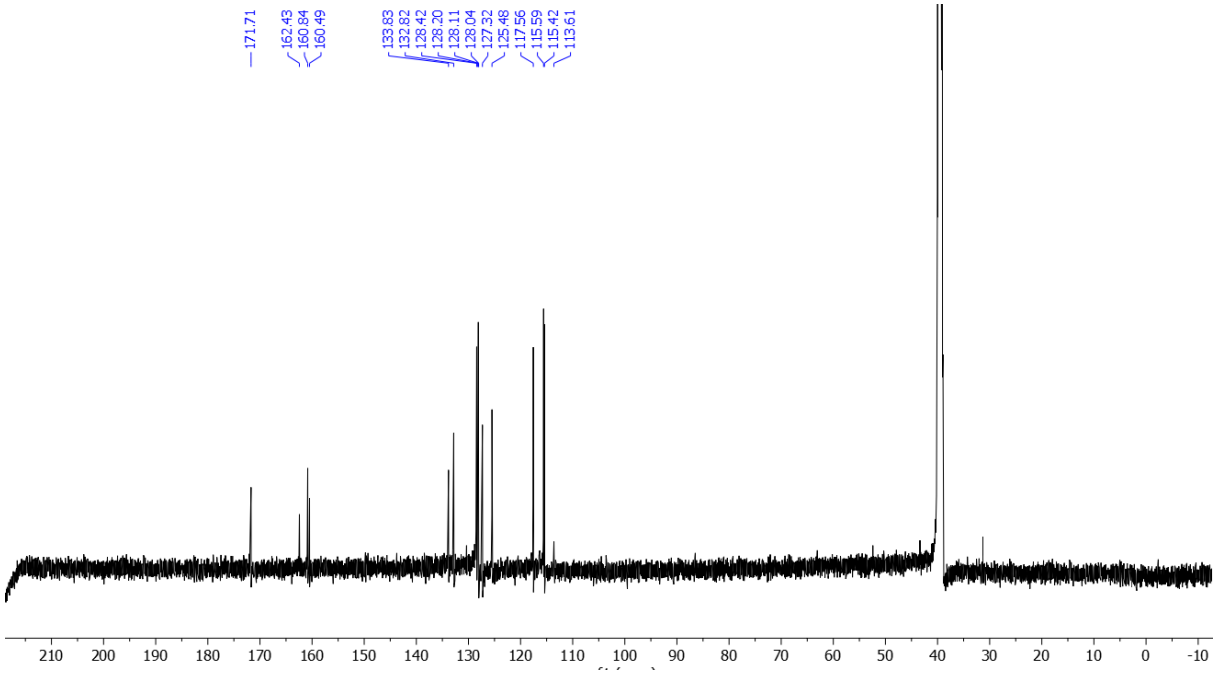


DC07

^{1}H NMR (500 MHz, DMSO) δ 7.97 (d, *J* = 2.3 Hz, 1H), 7.80 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.66 – 7.61 (m, 2H), 7.23 – 7.10 (m, 4H), 6.99 (d, *J* = 8.6 Hz, 1H).

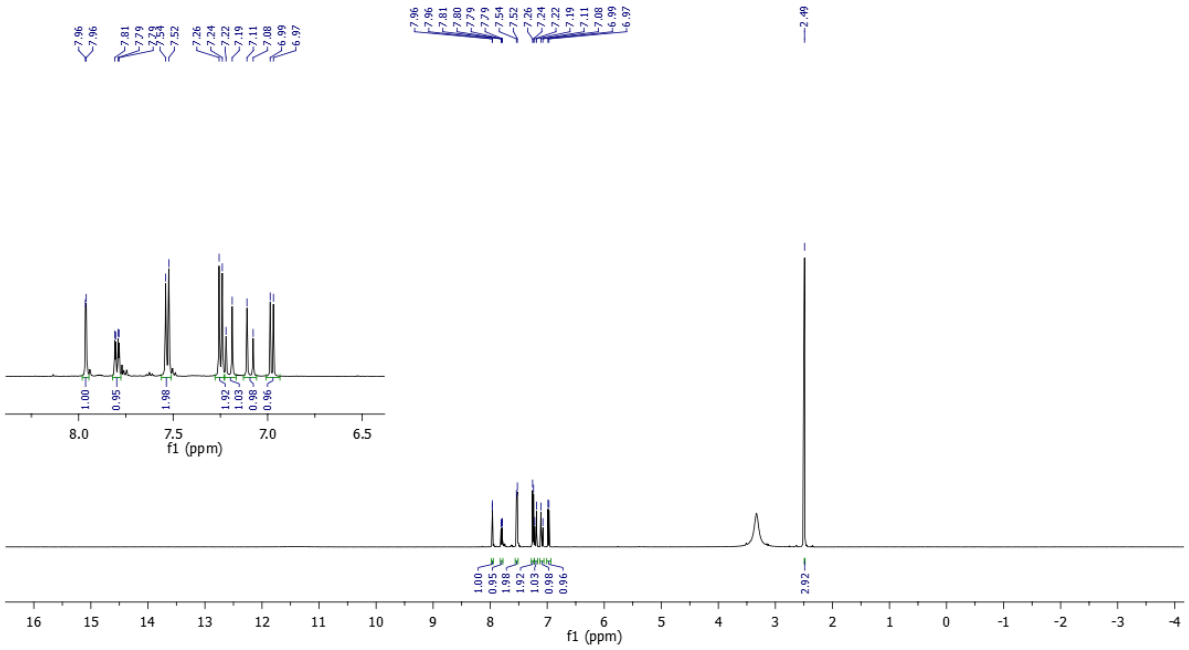


^{13}C NMR (126 MHz, DMSO) δ 171.71, 161.45 (d, *J* = 236.6 Hz), 160.84, 133.83, 132.82, 128.42, 128.20, 128.08 (d, *J* = 7.3 Hz), 127.32, 125.48, 117.56, 115.51 (d, *J* = 21.0 Hz), 113.61.

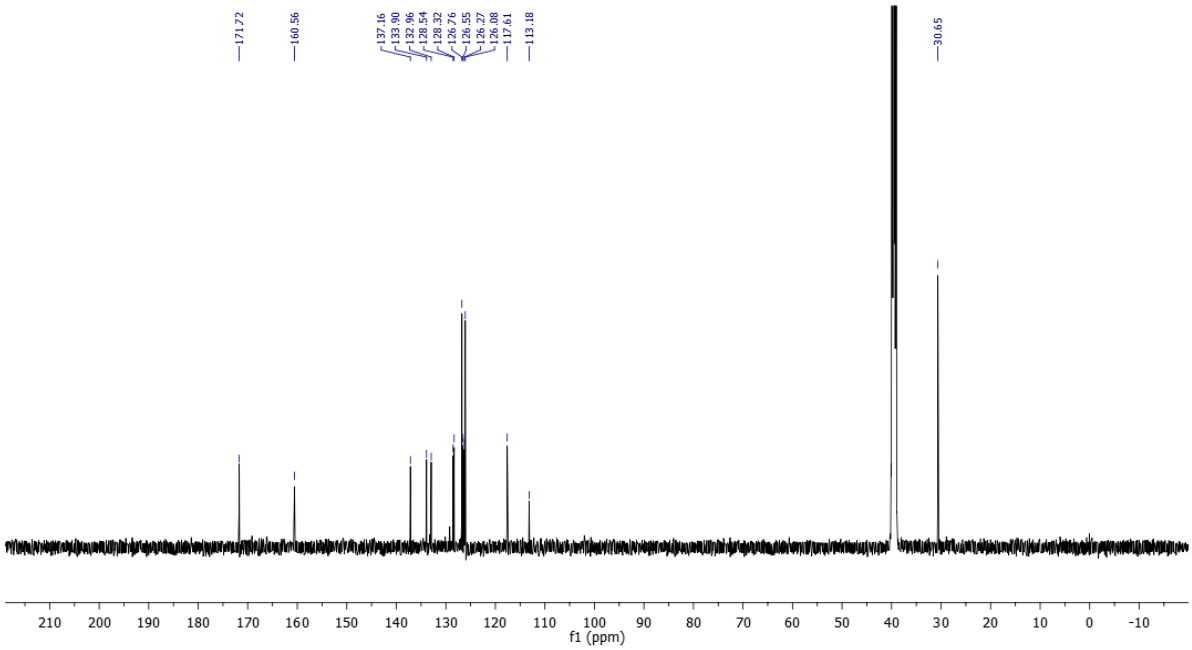


DC08

^{1}H NMR (500 MHz, DMSO) δ 7.96 (d, *J* = 2.3 Hz, 1H), 7.80 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.56 – 7.49 (m, 2H), 7.28 – 7.23 (m, 2H), 7.20 (d, *J* = 16.5 Hz, 1H), 7.09 (d, *J* = 16.5 Hz, 1H), 6.98 (d, *J* = 8.6 Hz, 1H), 2.49 (s, 3H).

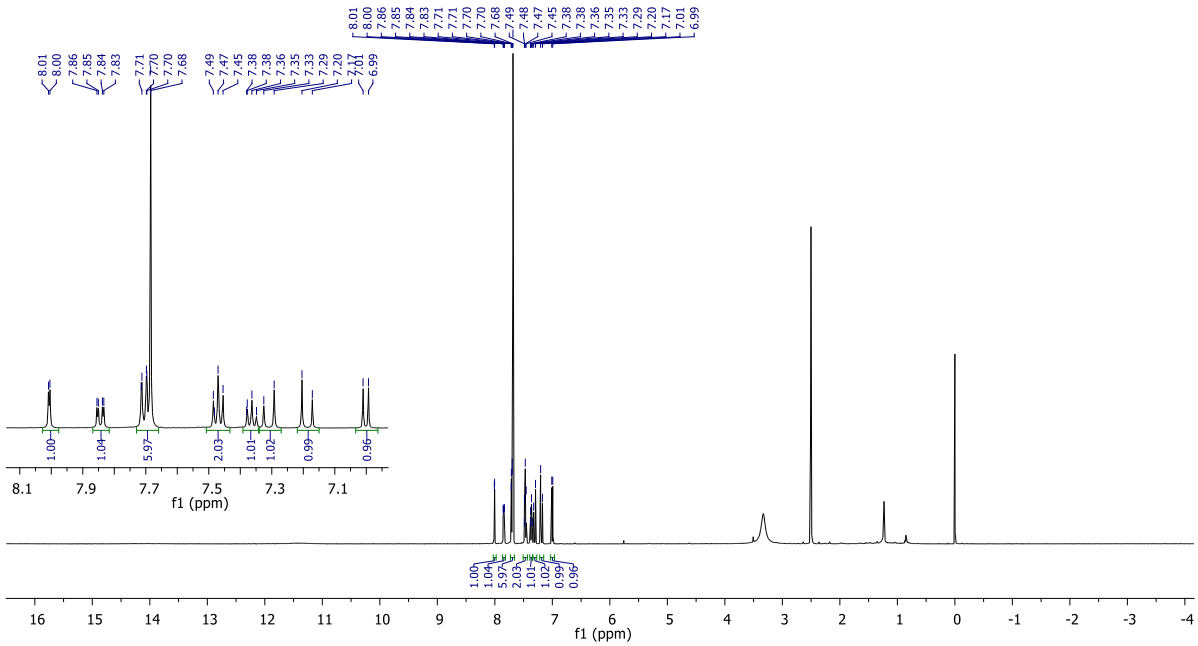


^{13}C NMR (126 MHz, DMSO) δ 171.72, 160.56, 137.16, 133.90, 132.96, 128.54, 128.32, 126.76, 126.55, 126.27, 126.08, 117.61, 113.18, 30.65.

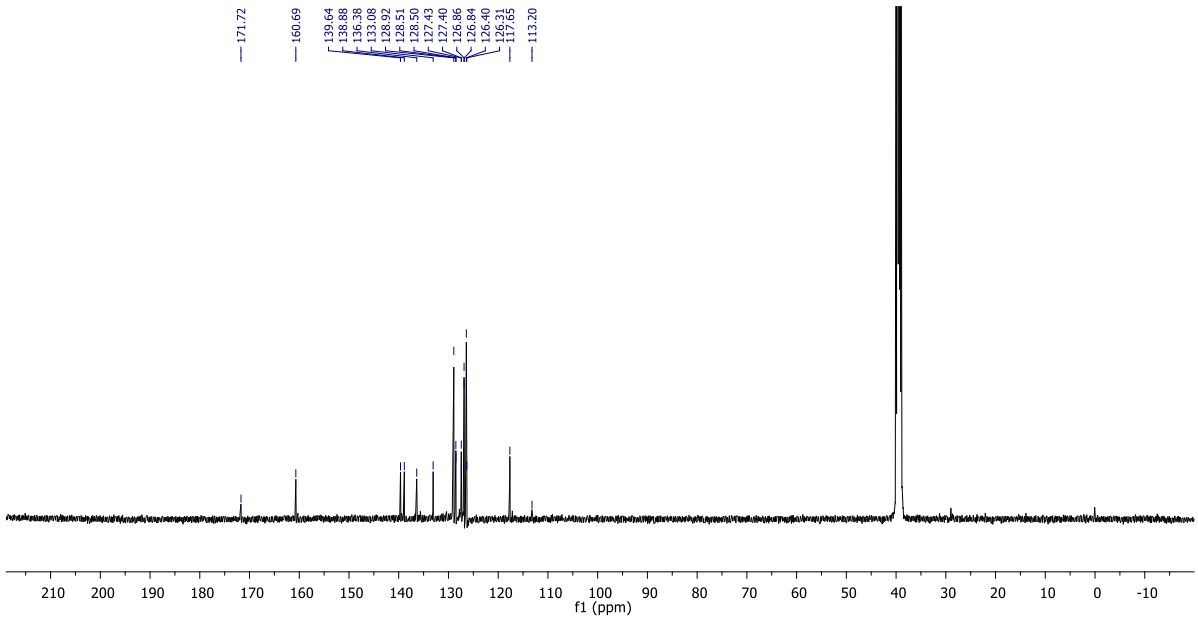


DC10

^{1}H NMR (500 MHz, DMSO) δ 8.01 (d, *J* = 2.2 Hz, 1H), 7.84 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.73 – 7.66 (m, 6H), 7.51 – 7.43 (m, 2H), 7.39 – 7.34 (m, 1H), 7.31 (d, *J* = 16.5 Hz, 1H), 7.19 (d, *J* = 16.5 Hz, 1H), 7.00 (d, *J* = 8.6 Hz, 1H).

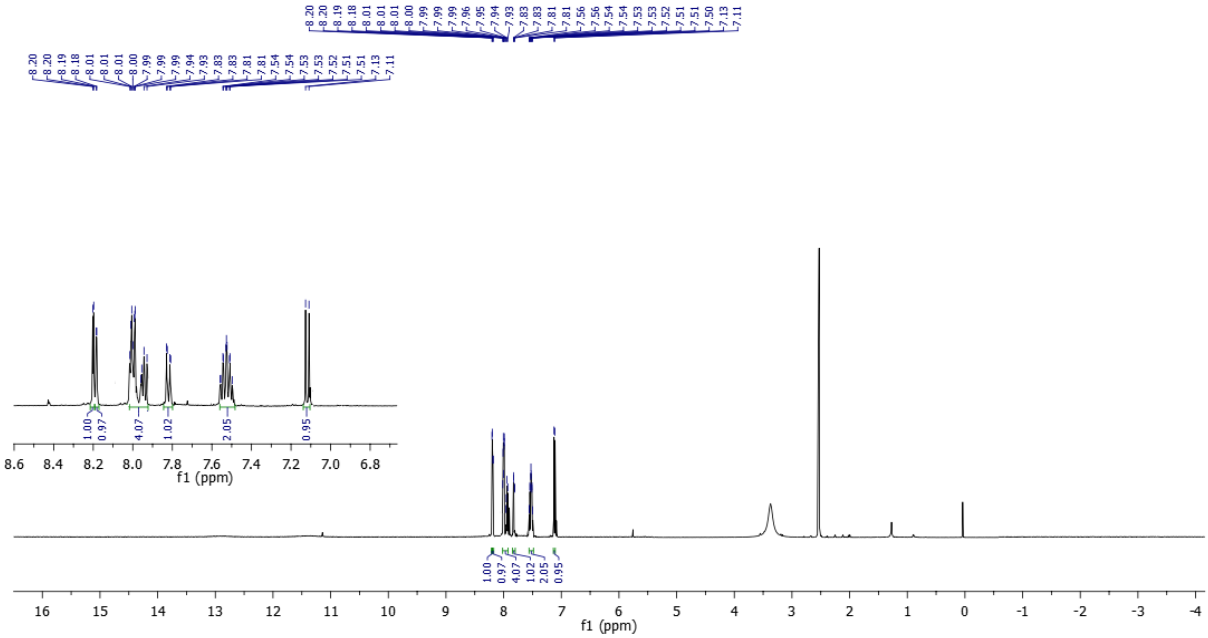


^{13}C NMR (126 MHz, DMSO) δ 171.72, 160.69, 139.64, 138.88, 136.38, 133.08, 128.92, 128.51, 128.50, 127.43, 127.40, 126.86, 126.84, 126.40, 126.31, 117.65, 113.20.

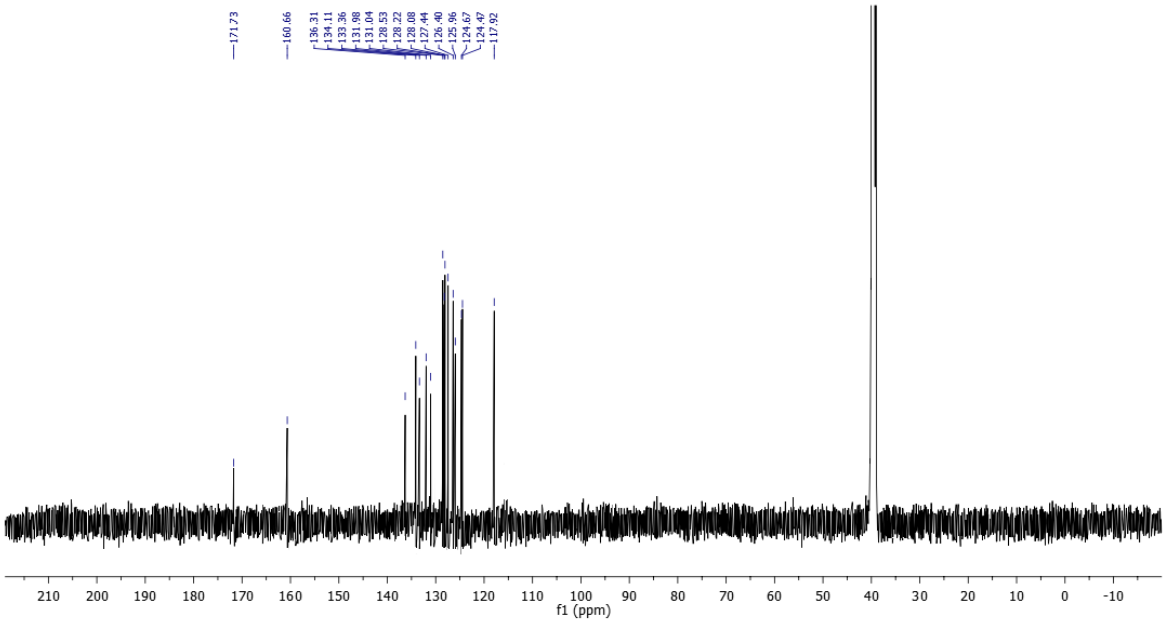


DC11

^{1}H NMR (500 MHz, DMSO) δ 8.20 (d, *J* = 2.4 Hz, 1H), 8.18 (d, *J* = 1.4 Hz, 1H), 8.02 – 7.92 (m, 4H), 7.82 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.56 – 7.48 (m, 2H), 7.12 (d, *J* = 8.6 Hz, 1H).

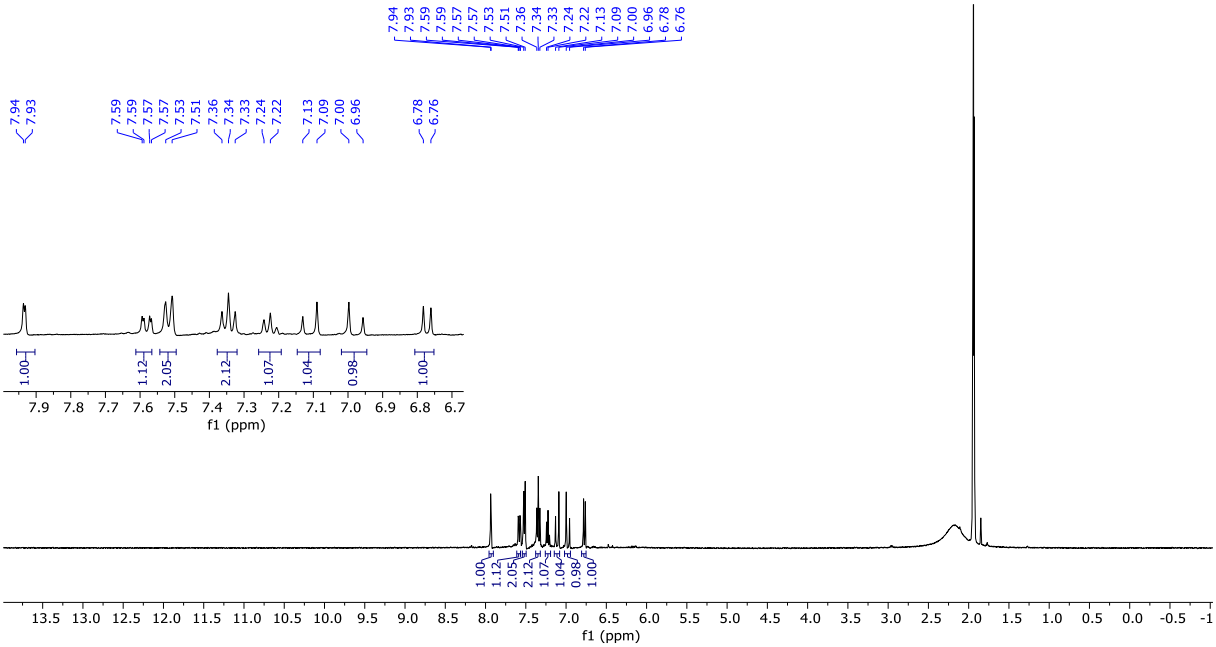


^{13}C NMR (126 MHz, DMSO) δ 171.73, 160.66, 136.31, 134.11, 133.36, 131.98, 131.04, 128.53, 128.22, 128.08, 127.44, 126.40, 125.96, 124.67, 124.47, 117.92 (one of the carbon peaks is not visible)

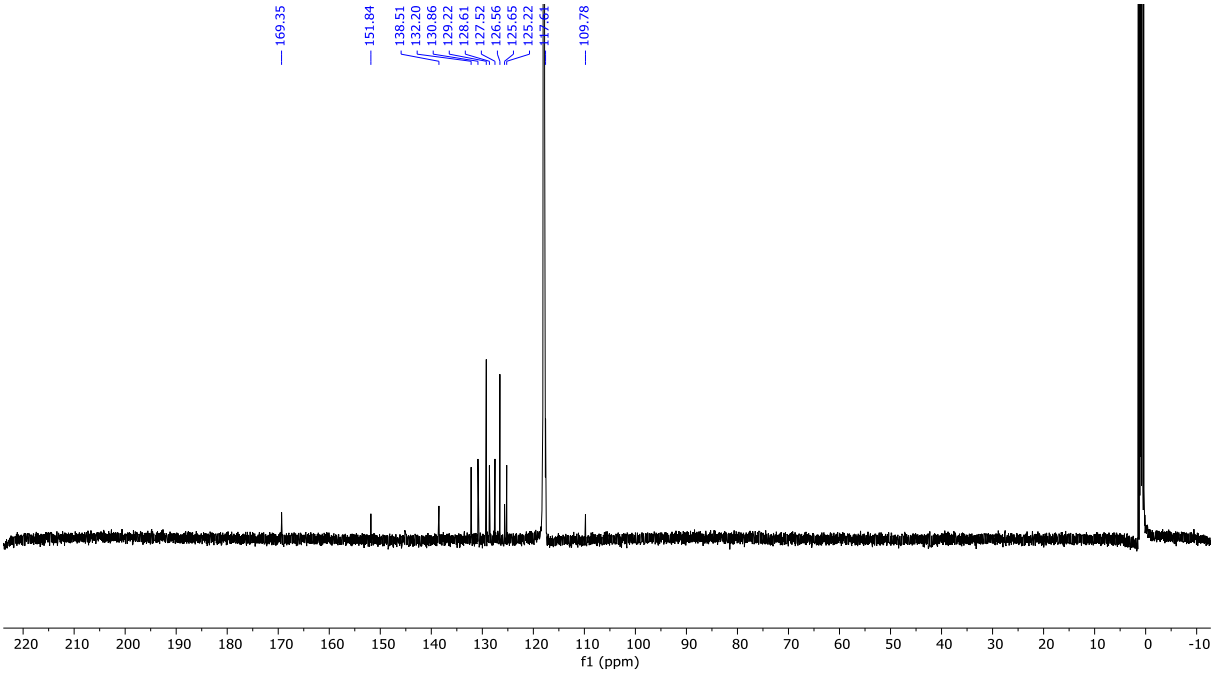


DC12

^{1}H NMR (400 MHz, CD_3CN) δ 7.93 (d, *J* = 2.1 Hz, 1H), 7.58 (dd, *J* = 2.1, 8.7 Hz, 1H), 7.52 (d, *J* = 7.4 Hz, 2H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.23 (d, *J* = 7.3 Hz, 1H), 7.11 (d, *J* = 16.4 Hz, 1H), 6.98 (d, *J* = 16.5 Hz, 1H), 6.77 (d, *J* = 8.6 Hz, 1H).

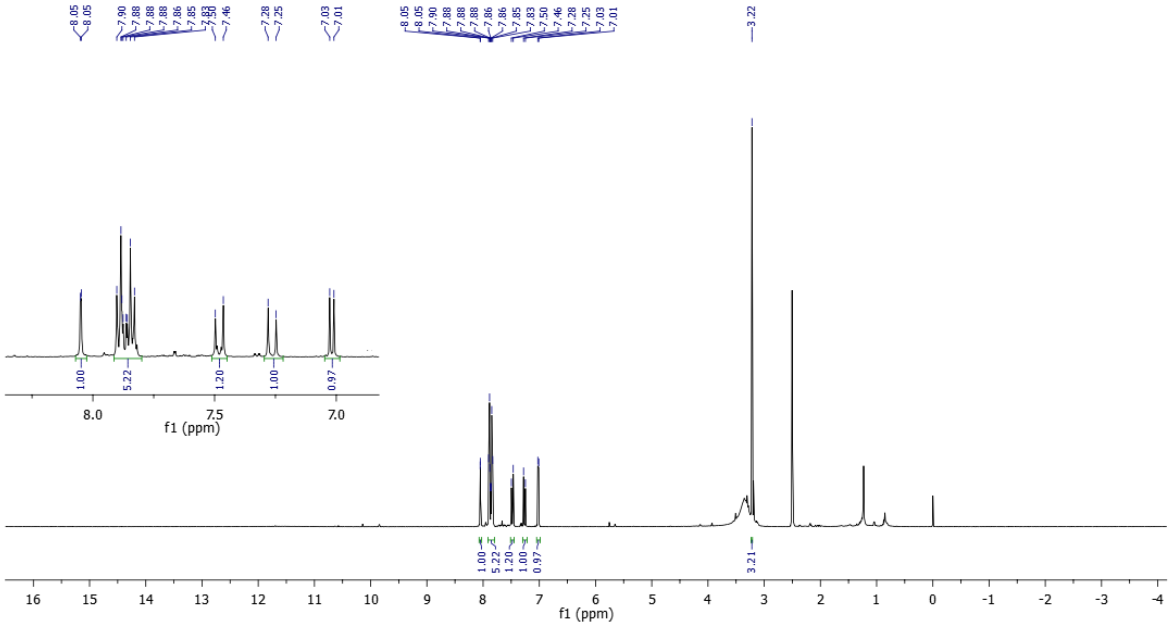


^{13}C NMR (126 MHz, CD_3CN) δ 169.35, 151.84, 138.51, 132.20, 130.86, 129.22, 128.61, 127.52, 126.56, 125.65, 125.22, 117.61, 109.78.

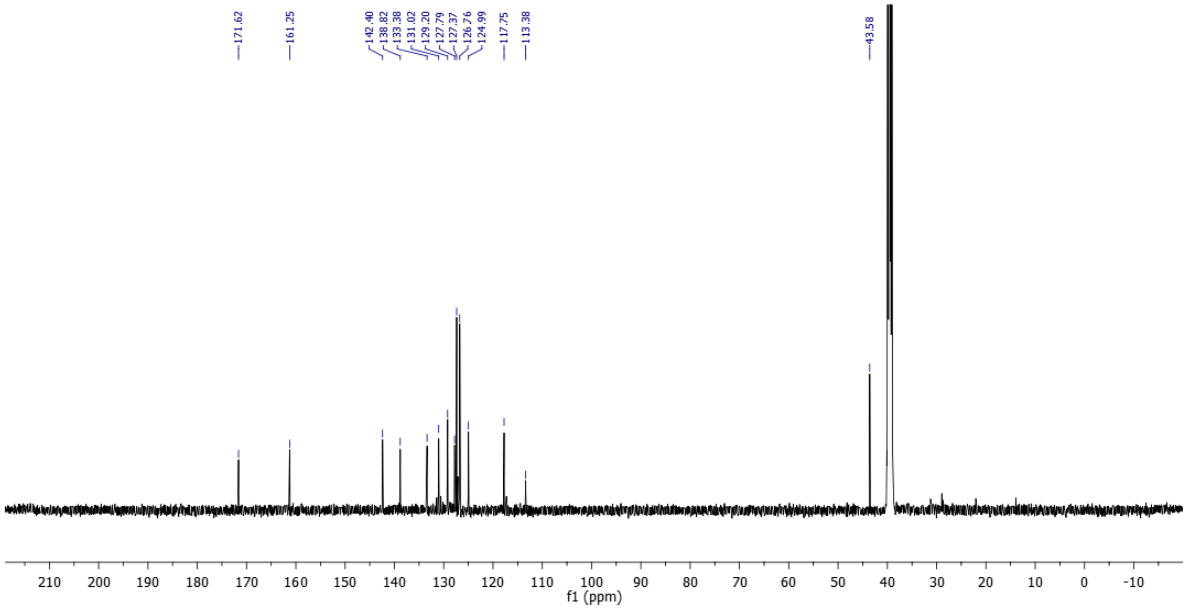


DC13

^{1}H NMR (500 MHz, DMSO) δ 8.05 (d, *J* = 2.2 Hz, 1H), 7.91 – 7.80 (m, 5H), 7.48 (d, *J* = 16.5 Hz, 1H), 7.26 (d, *J* = 16.5 Hz, 1H), 7.02 (d, *J* = 8.6 Hz, 1H), 3.22 (s, 3H).

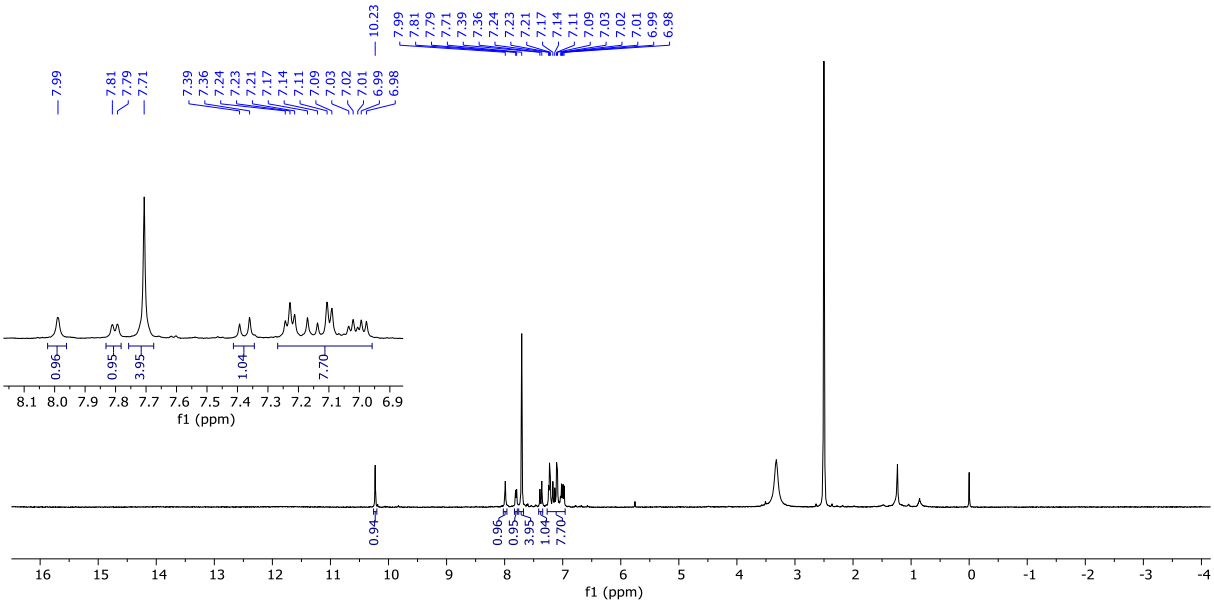


^{13}C NMR (126 MHz, DMSO) δ 171.62, 161.25, 142.40, 138.82, 133.38, 131.02, 129.20, 127.79, 127.37, 126.76, 124.99, 117.75, 113.38, 43.58.

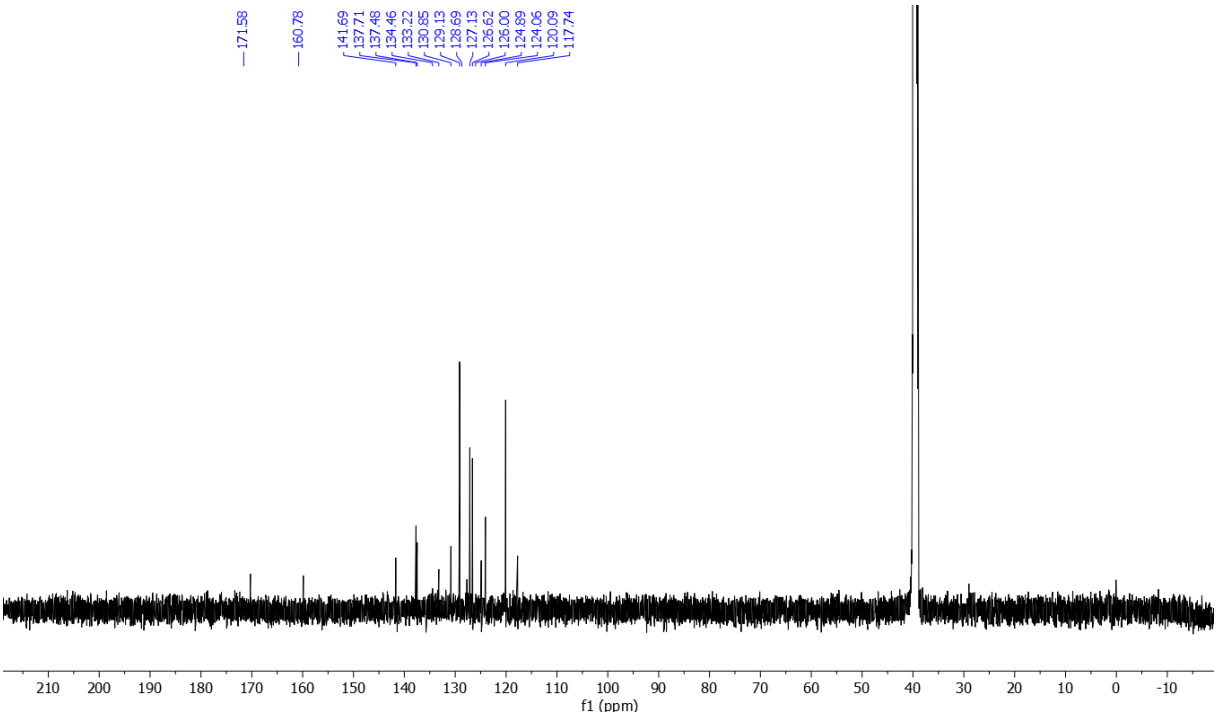


DC14

^{1}H NMR (500 MHz, DMSO) δ 10.23 (s, 1H), 7.99 (s, 1H), 7.80 (d, *J* = 8.4 Hz, 1H), 7.71 (s, 4H), 7.38 (d, *J* = 16.4 Hz, 1H), 6.96 – 7.27 (m, 7H).

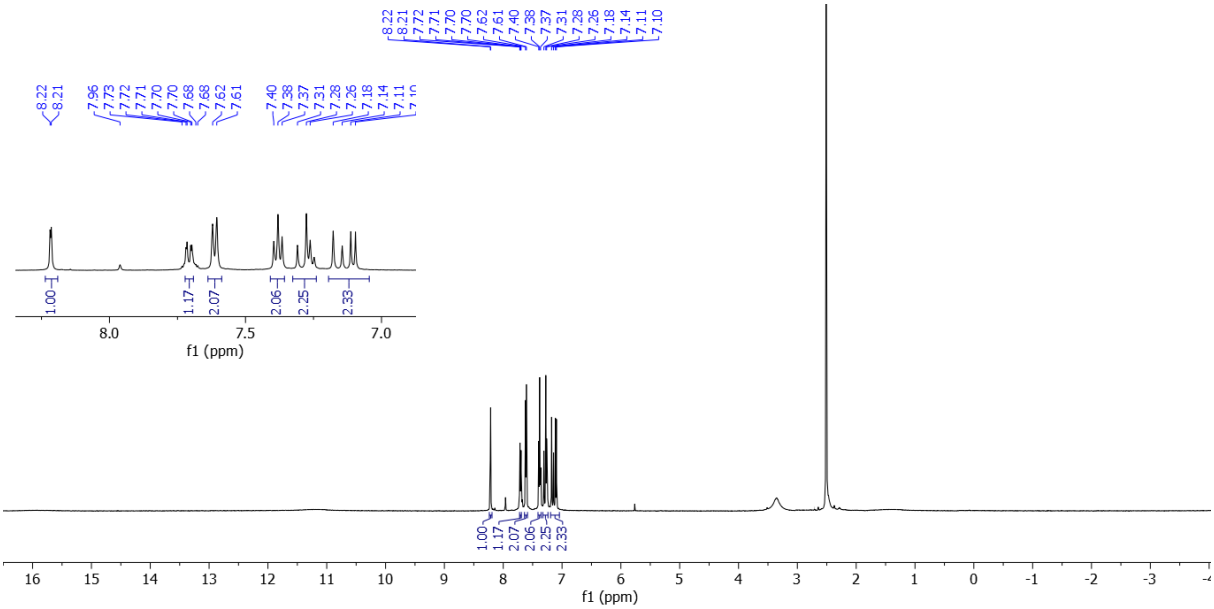


^{13}C NMR (126 MHz, DMSO, 27°C) δ 171.58, 160.78, 141.69, 137.71, 137.48, 134.46, 133.22, 130.85, 129.13, 128.69, 127.13, 126.62, 126.00, 124.89, 124.06, 120.09, 117.74.

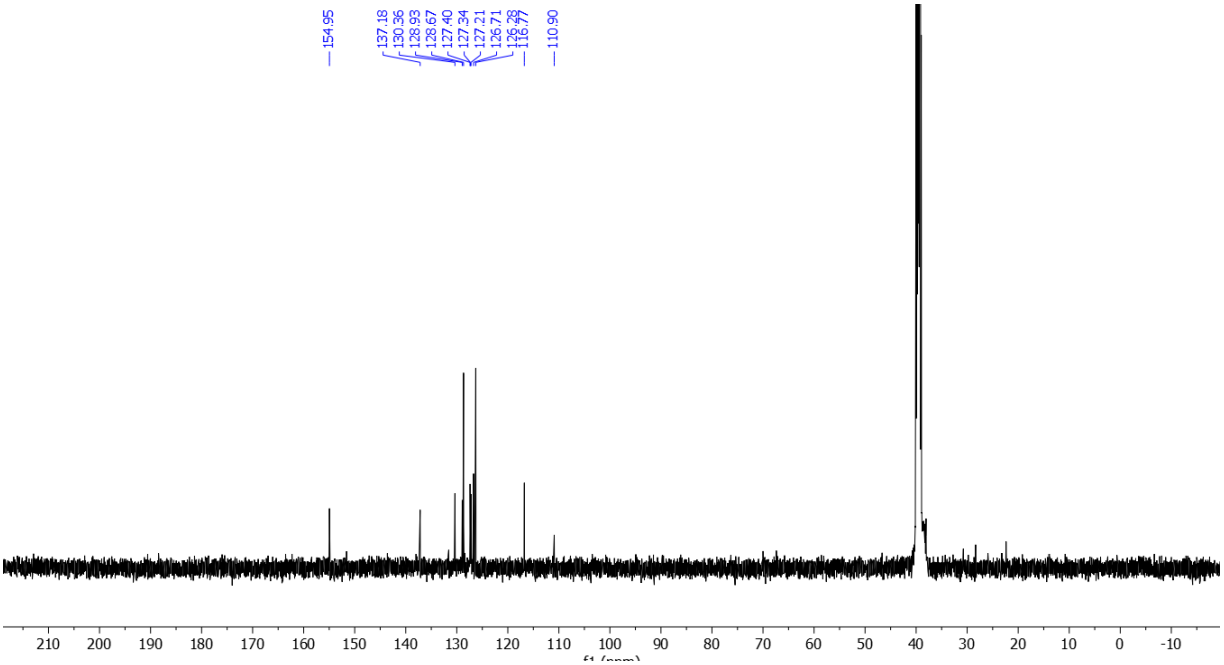


DC15

^{1}H NMR (500 MHz, DMSO) δ 8.22 (d, *J* = 2.1 Hz, 1H), 7.71 (dd, *J* = 2.1, 8.7 Hz, 1H), 7.61 (d, *J* = 7.5 Hz, 2H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.24 – 7.33 (m, 2H), 7.04 – 7.19 (m, 2H).

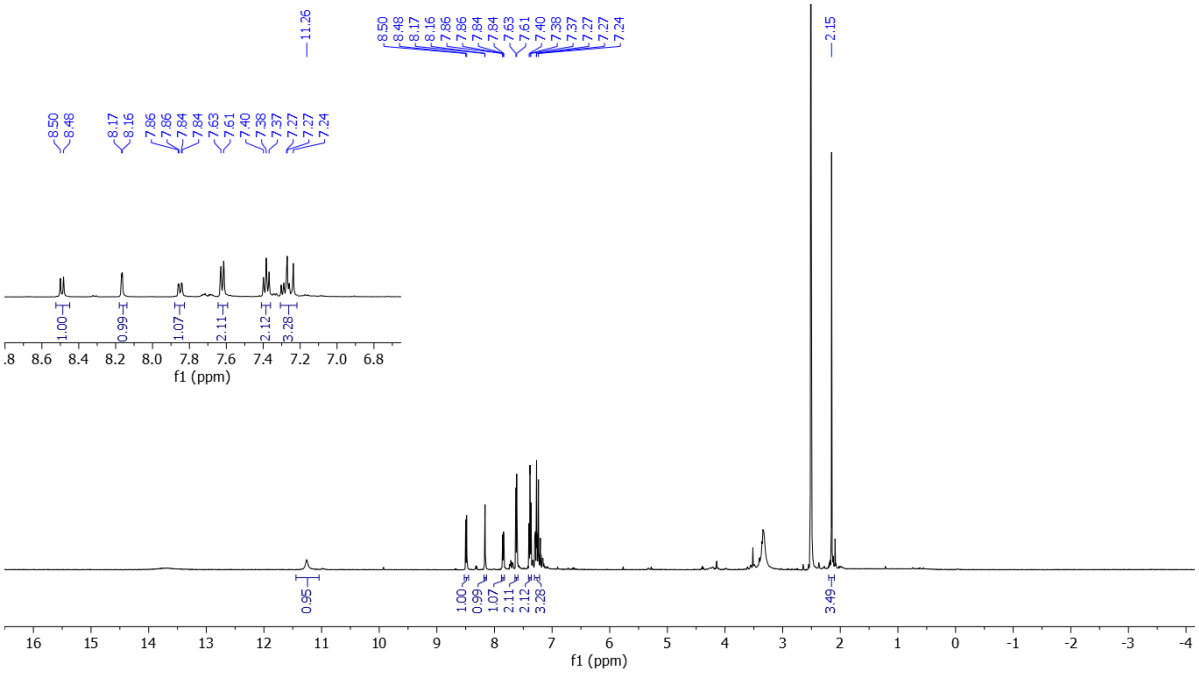


^{13}C NMR (126 MHz, DMSO) δ 154.95, 137.18, 130.36, 128.93, 128.67, 127.40, 127.34, 127.21, 126.71, 126.28, 116.77, 110.90.

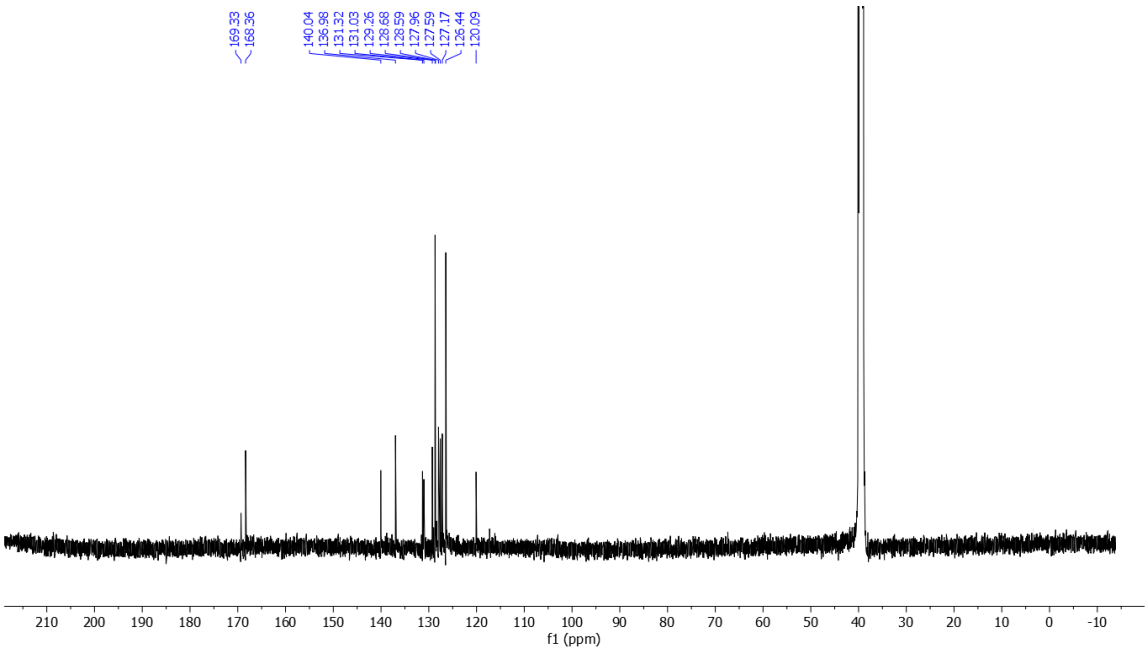


DC16

^{1}H NMR (500 MHz, DMSO) δ 11.26 (s, 1H), 8.49 (d, *J* = 8.7 Hz, 1H), 8.17 (d, *J* = 2.0 Hz, 1H), 7.85 (dd, *J* = 2.0, 8.7 Hz, 1H), 7.62 (d, *J* = 7.4 Hz, 2H), 7.38 (t, *J* = 7.7 Hz, 2H), 7.19 – 7.32 (m, 4H), 2.15 (s, 3H).

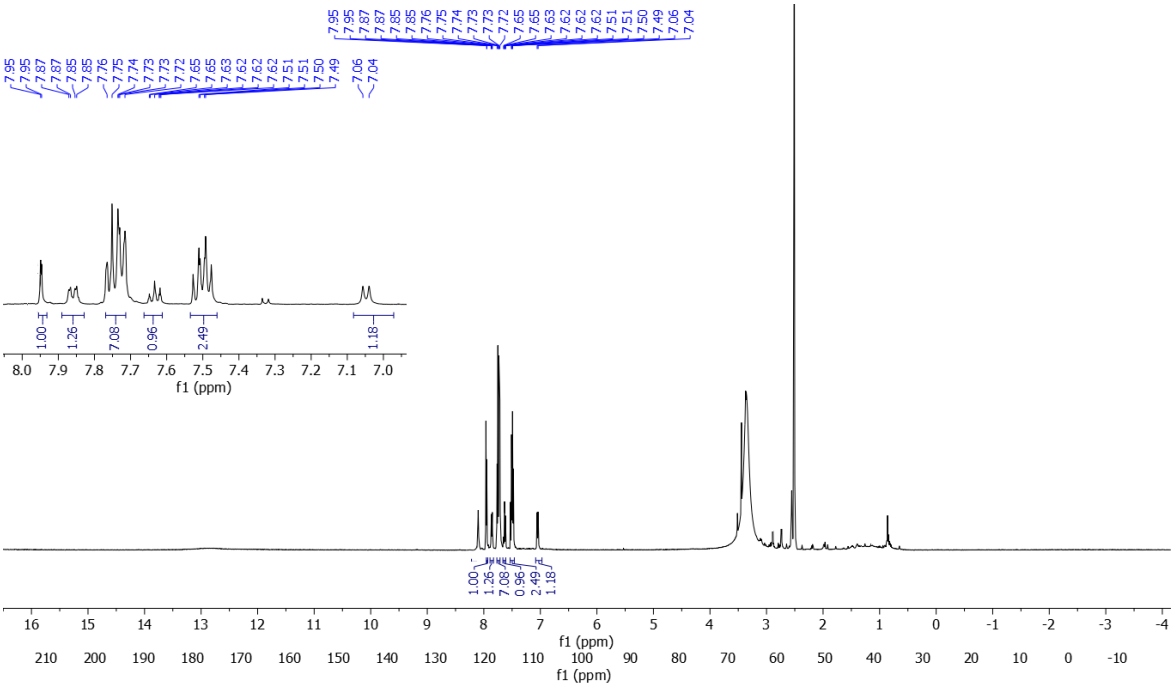


^{13}C NMR (126 MHz, DMSO) δ 169.33, 168.36, 140.04, 136.98, 131.32, 131.03, 129.26, 128.68, 128.36, 127.96, 127.59, 127.17, 126.44, 120.09, 25.01.

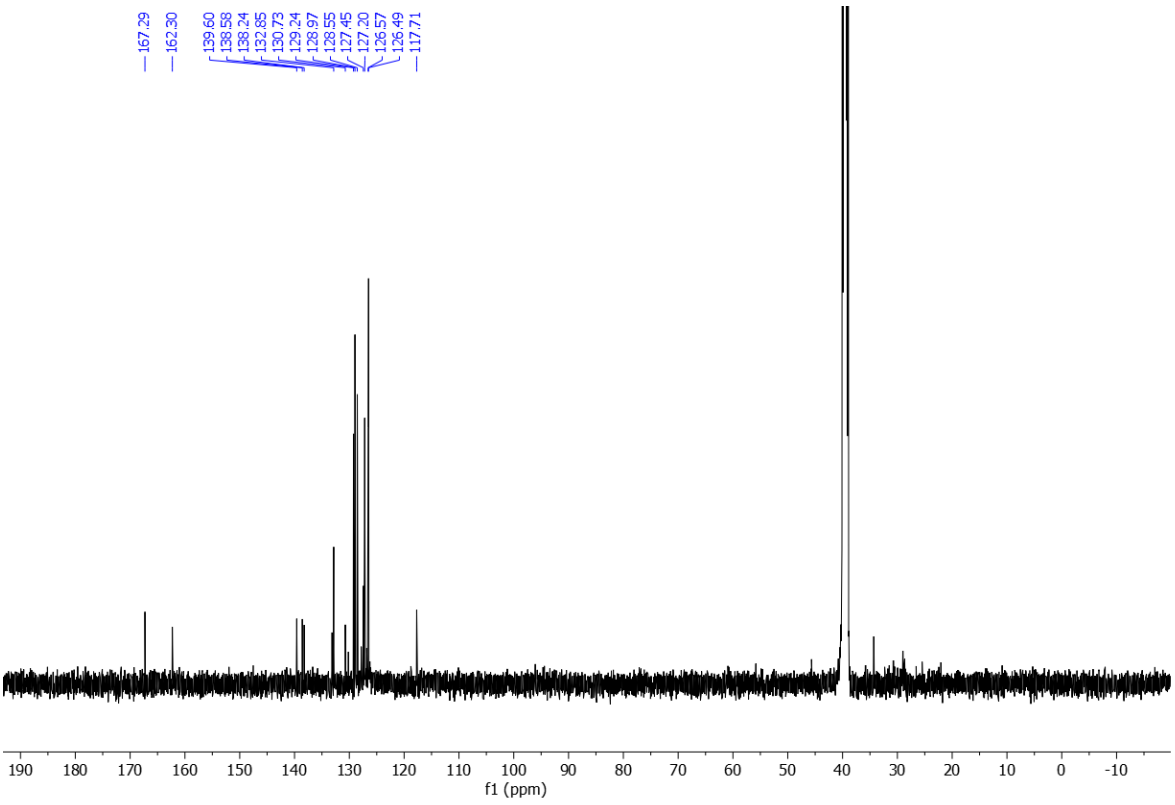


DC17

^{1}H NMR (500 MHz, DMSO) δ 7.95 (d, *J* = 1.3 Hz, 1H), 7.86 (dd, *J* = 2.3, 8.6 Hz, 1H), 7.71 – 7.77 (m, 6H), 7.61 – 7.66 (m, 1H), 7.46 – 7.53 (m, 2H), 7.05 (d, *J* = 8.5 Hz, 1H).

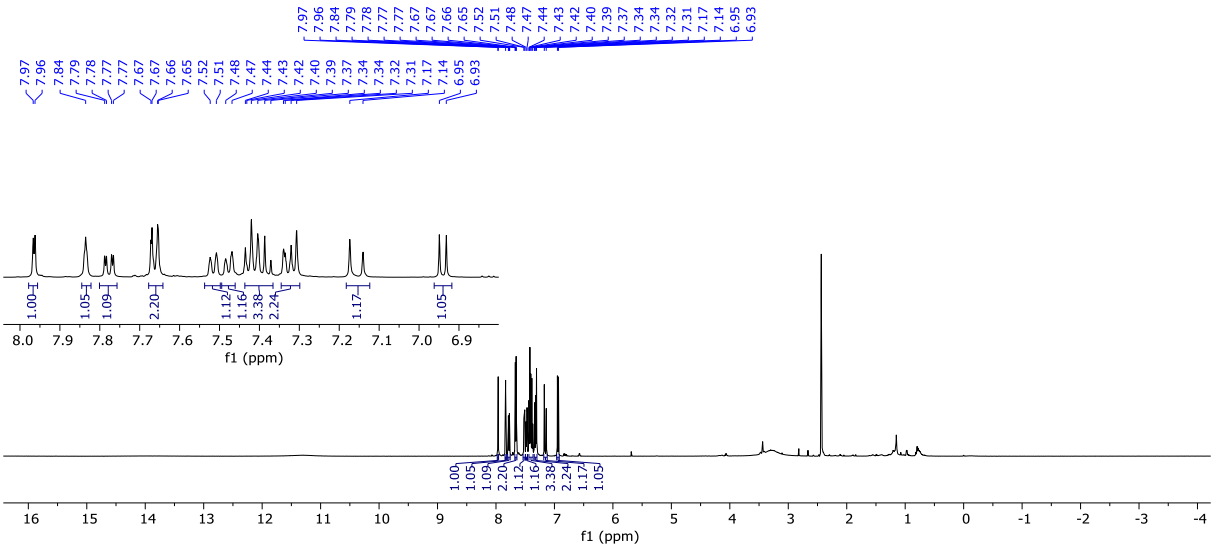


^{13}C NMR (126 MHz, DMSO, 27°C) δ 167.29, 162.30, 139.60, 138.58, 138.24, 132.85, 130.73, 129.24, 128.97, 128.55, 127.45, 127.20, 126.57, 126.49, 117.71.

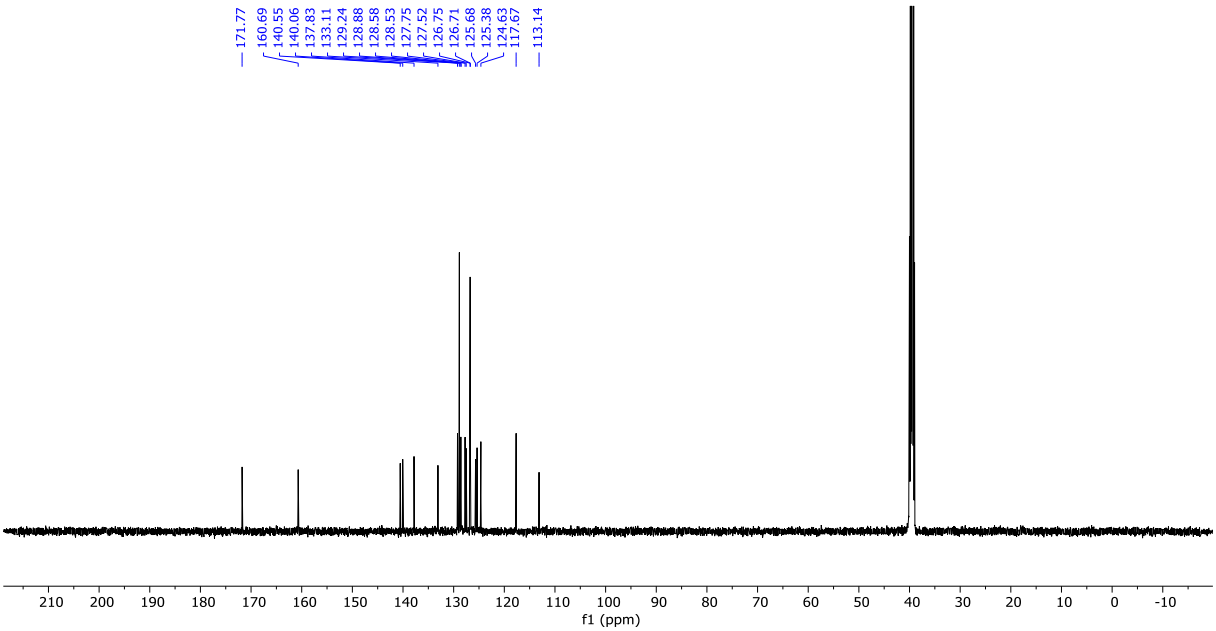


DC18

^{1}H NMR (500 MHz, DMSO) δ 7.96 (d, *J* = 2.2 Hz, 1H), 7.84 (s, 1H), 7.78 (dd, *J* = 2.3, 8.7 Hz, 1H), 7.66 (dd, *J* = 1.0, 8.1 Hz, 2H), 7.52 (d, *J* = 7.7 Hz, 1H), 7.48 (d, *J* = 7.9 Hz, 1H), 7.37 – 7.44 (m, 3H), 7.3 – 7.35 (m, 2H), 7.16 (d, *J* = 16.5 Hz, 1H), 6.94 (d, *J* = 8.6 Hz, 1H).

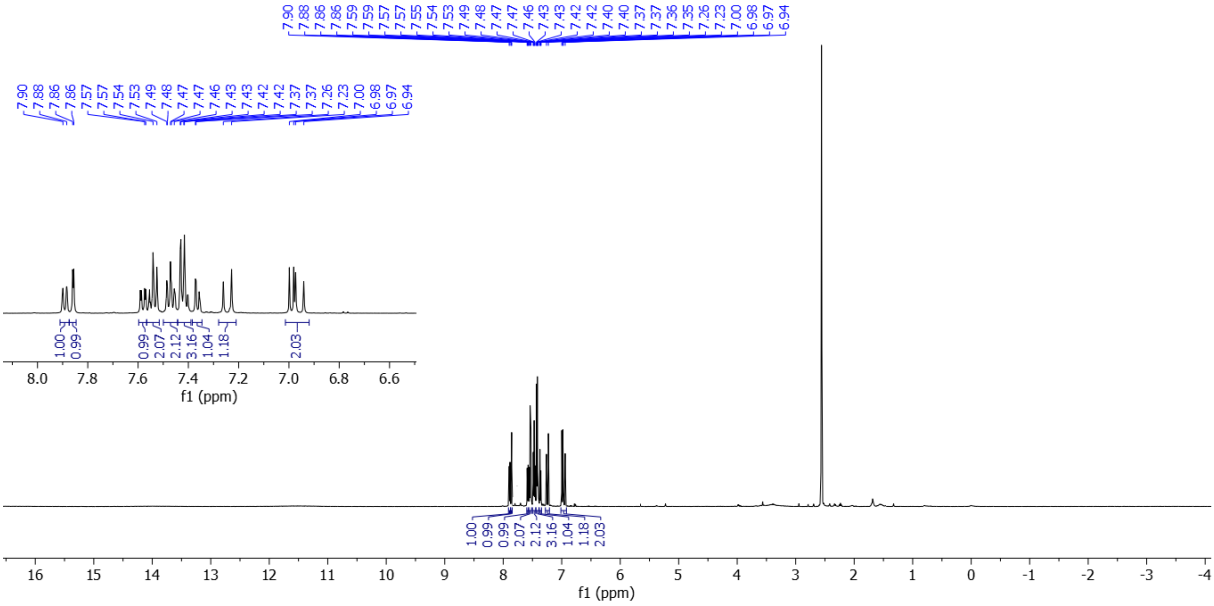


^{13}C NMR (126 MHz, DMSO, 27°C) δ 171.77, 160.69, 140.55, 140.06, 137.83, 133.11, 129.24, 128.88, 128.58, 128.53, 127.75, 127.52, 126.75, 126.71, 125.68, 125.38, 124.63, 117.67, 113.14.

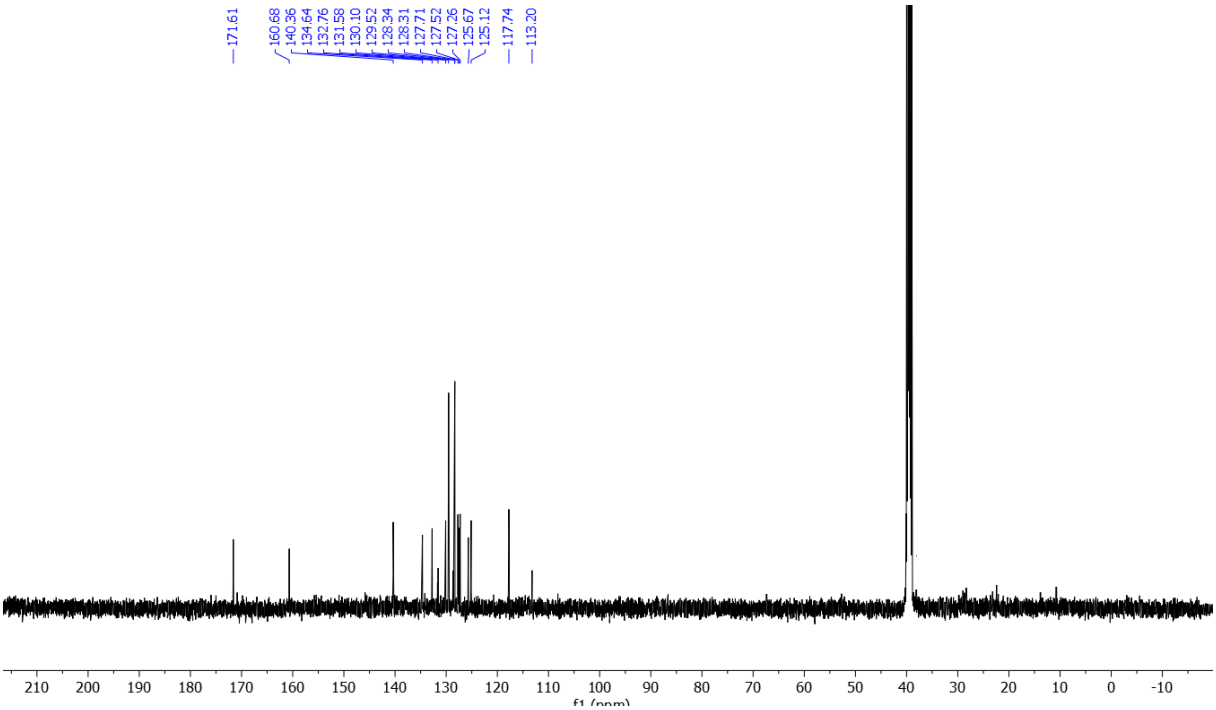


DC19

^{1}H NMR (500 MHz, DMSO) δ 7.89 (d, *J* = 7.5 Hz, 1H), 7.86 (d, *J* = 2.2 Hz, 1H), 7.51 – 7.6 (m, 3H), 7.44 – 7.5 (m, 2H), 7.39 – 7.44 (m, 3H), 7.36 (dd, *J* = 1.4, 7.6 Hz, 1H), 7.24 (d, *J* = 16.4 Hz, 1H), 6.92 – 7.01 (m, 2H).

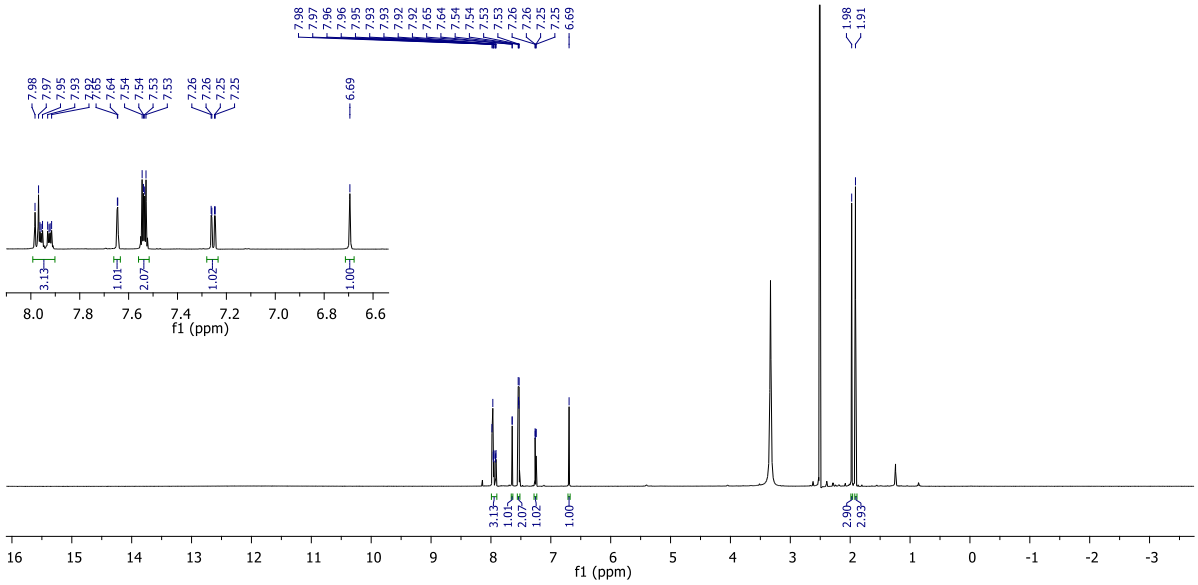


^{13}C NMR (126 MHz, DMSO) δ 171.61, 160.68, 140.36, 134.64, 132.76, 131.58, 130.10, 129.52, 128.34, 128.31, 127.71, 127.52, 127.26, 125.67, 125.12, 117.74, 113.20.

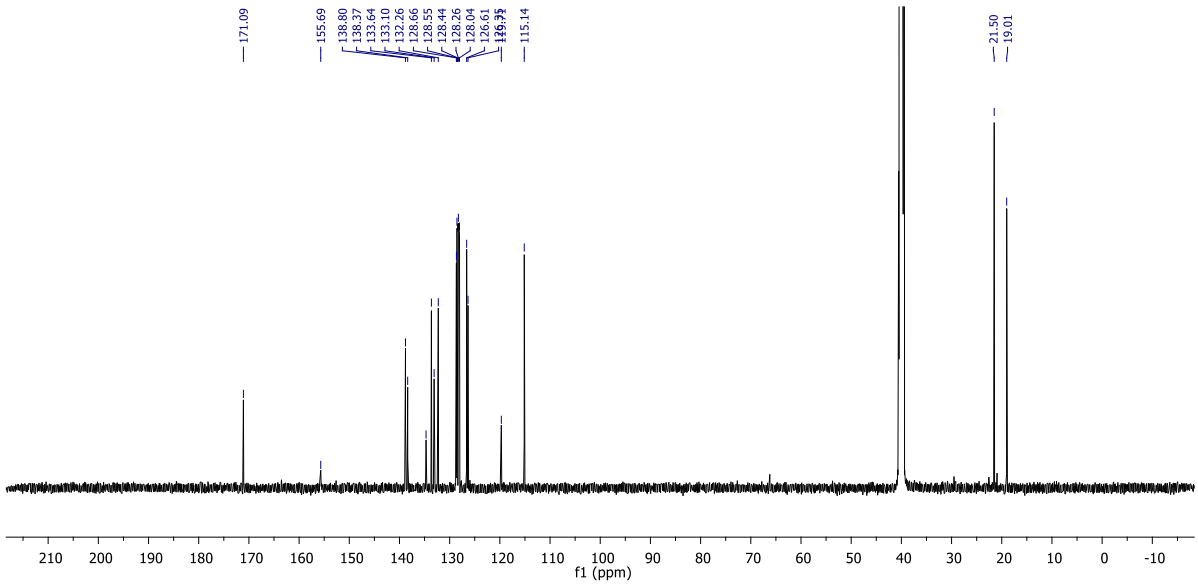


DC20

^{1}H NMR (600 MHz, DMSO) δ 7.99 – 7.90 (m, 3H), 7.65 (d, *J* = 0.9 Hz, 1H), 7.56 – 7.52 (m, 2H), 7.25 (dd, *J* = 8.3, 1.7 Hz, 1H), 6.69 (s, 1H), 1.98 (s, 3H), 1.91 (s, 3H).

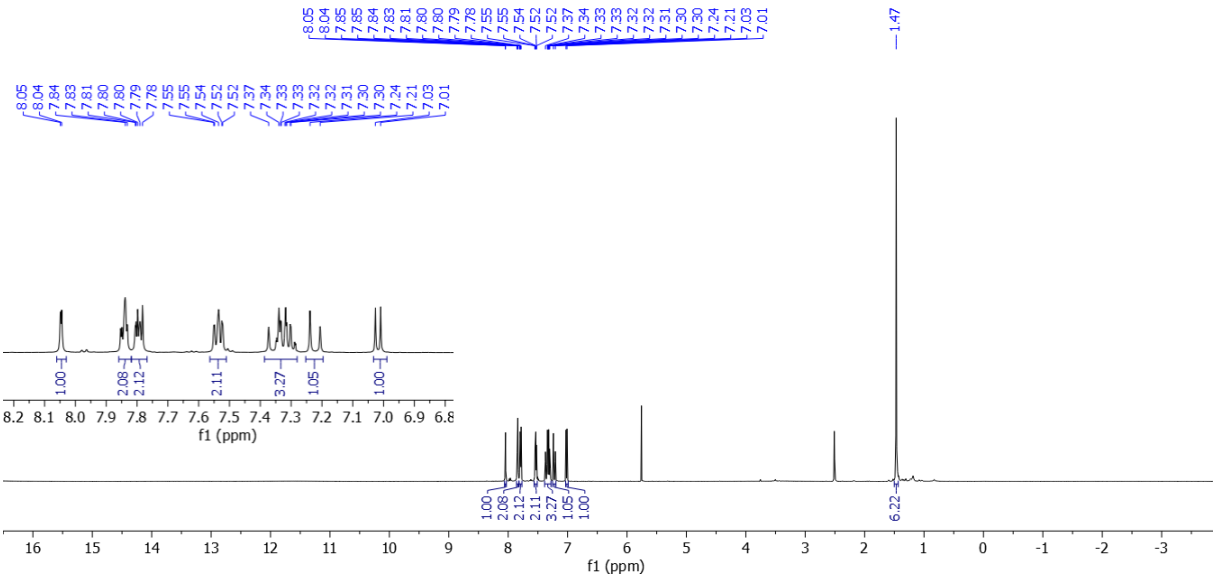


^{13}C NMR (151 MHz, DMSO) δ 171.09, 155.69 138.80, 138.37, 134.71, 133.64, 133.10, 132.26, 128.66, 128.55, 128.44, 128.26, 128.04, 126.61, 126.35, 119.71, 115.14, 21.50, 19.01



DC21

^{1}H NMR (500 MHz, DMSO) δ 8.05 (d, *J* = 2.2 Hz, 1H), 7.82 – 7.86 (m, 2H), 7.77 – 7.82 (m, 2H), 7.51 – 7.56 (m, 2H), 7.28 – 7.39 (m, 3H), 7.22 (d, *J* = 16.4 Hz, 1H), 7.02 (d, *J* = 8.6 Hz, 1H), 1.47 (s, 6H).



^{13}C NMR (126 MHz, DMSO) δ 171.82, 160.63, 153.80, 153.52, 138.34, 137.95, 136.52, 132.96, 128.71, 128.45, 127.24, 127.21, 127.04, 126.84, 125.94, 122.73, 120.29, 120.27, 120.04, 117.69, 113.17, 26.86.