

## Electronic Supplementary Information

### An efficient regioselective synthesis of novel dispiropyrrolidine and dispiropyrrolizidine oxindole derivatives via azomethine ylide specific cycloaddition with alkyl indeno[1,2-*b*]quinoxalin-11-ylidene acetate dipolarophiles

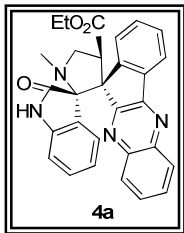
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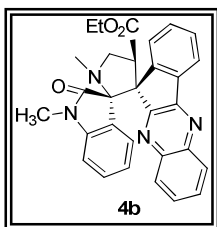
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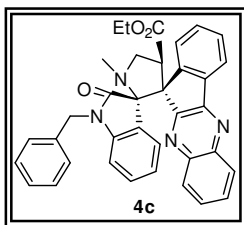
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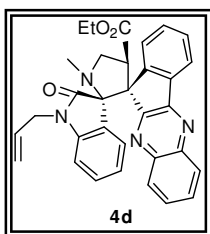
**Compound (4a):** Colorless solid, mp = 181-184 °C; IR (KBr): 1619, 1723, 1736 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 0.31 (t, 1H, *J* = 6.96 Hz), 2.31 (s, 3H), 3.273.33 (m, 1H), 3.52-3.58 (m, 1H), 3.91 (t, 1H, *J* = 10.24 Hz), 4.21 (dd, 1H, *J* = 6.88, 9.94 Hz), 5.13 (dd, 1H, *J* = 6.88, 10.70 Hz), 6.10 (d, 1H, *J* = 8.41 Hz), 6.40 (d, 1H, *J* = 7.64 Hz), 6.46 (t, 1H, *J* = 7.64 Hz), 6.87 (t, 1H, *J* = 8.02 Hz), 7.56 (t, 2H, *J* = 6.88 Hz), 7.62-7.67 (m, 2H), 7.73 (s, 3H), 8.01 (d, 1H, *J* = 7.64 Hz), 8.06 (t, 2H, *J* = 7.64 Hz), 8.13 (t, 1H, *J* = 7.64 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 13.1, 35.2, 47.3, 52.6, 60.1, 61.9, 78.6, 109.4, 121.8(2), 123.7, 126.0, 128.2, 128.6, 128.9, 129.3, 129.4, 129.6, 129.8, 130.9, 138.0, 141.3(2), 142.2, 146.2, 154.5, 158.4, 170.7, 177.4.; HRMS: *m/z* 477.1944 (M+H)<sup>+</sup> [Calcd 477.1921].



**Compound (4b):** Colorless solid, mp = 172-174 °C; IR (KBr): 1612, 1714, 1735 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 0.43 (t, 3H, *J* = 7.02 Hz), 2.29 (s, 3H), 2.71 (s, 3H), 3.42-3.72 (m, 3H), 4.54 (t, 1H, *J* = 9.2 Hz), 4.64 (t, 1H, *J* = 8.2 Hz), 6.40 (d, 1H, *J* = 7.76 Hz), 6.81 (t, 1H, *J* = 7.56 Hz), 7.07-7.13 (m, 2H), 7.44-7.53 (m, 2H), 7.61-7.70 (m, 2H), 7.90 (d, 1H, *J* = 8.24 Hz), 7.96-8.03 (m, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 13.2, 25.7, 35.7, 49.2, 53.8, 60.3, 62.6, 79.5, 107.6, 121.4, 121.5, 124.9, 127.1, 128.4, 128.5, 128.7, 129.0, 129.4(2), 130.4, 136.9, 140.7, 142.1, 143.5, 144.9, 154.2, 160.9, 170.1, 173.9.; HRMS: *m/z* 491.2072 (M+H)<sup>+</sup> [Calcd 491.2083].

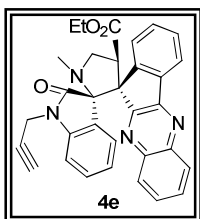


**Compound (4c):** Colorless solid, mp = 193-195 °C; IR (KBr): 1609, 1707, 1740 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 0.34 (t, 3H, *J* = 6.92 Hz), 2.34 (s, 3H), 3.44-3.50 (m, 1H), 3.58-3.64 (m, 1H), 3.72 (t, 1H, *J* = 10.00 Hz), 4.17 (d, 1H, *J* = 16.15 Hz), 4.57 (t, 1H, *J* = 9.23 Hz), 4.70 (t, 1H, *J* = 9.23 Hz), 4.79 (d, 1H, *J* = 15.68 Hz), 6.21 (d, 1H, *J* = 7.69 Hz), 6.40 (d, 2H, *J* = 8.46 Hz), 6.82 (t, 1H, *J* = 7.69 Hz), 6.96-7.04 (m, 2H), 7.24 (d, 1H, *J* = 7.69 Hz), 7.47-7.50 (m, 2H), 7.60 (t, 1H, *J* = 6.92, 8.46 Hz), 7.69 (t, 1H, *J* = 6.92, 8.46 Hz), 7.82 (d, 1H, *J* = 8.46 Hz), 8.02-8.08 (m, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 13.2, 35.9, 43.2, 49.5, 53.9, 60.4, 62.8, 79.5, 109.0, 121.7(2), 125.3, 126.2, 127.1, 127.5, 128.4, 128.6, 128.8(2), 129.0, 129.2, 129.5, 129.6, 130.9, 135.1, 137.1, 140.8, 142.2, 142.8, 145.2, 154.4, 160.7, 170.1, 173.9.; HRMS: *m/z* 567.2386 (M+H)<sup>+</sup> [Calcd 567.2391].

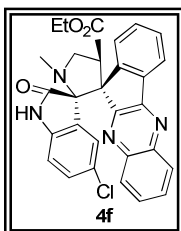


**Compound (4d):** Colorless solid, mp = 182-183°C; IR (KBr): 1637, 1712, 1739 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 0.43 (t, 3H, *J* = 6.88 Hz), 2.32 (s, 3H), 3.47-3.53 (m, 1H), 3.60-3.73 (m, 3H), 4.08-4.12 (m, 1H), 4.26 (d, 1H, *J* = 17.58 Hz), 4.57 (t, 1H, *J* = 8.41 Hz), 4.65-4.70 (m, 2H), 5.19-5.26 (m, 1H), 6.36 (d, 1H, *J* = 7.64 Hz), 6.77 (d, 1H, *J* = 7.64 Hz), 7.03 (t, 1H, *J* = 7.64 Hz), 7.13 (d, 1H, *J* = 7.64 Hz), 7.48-7.51 (m, 2H), 7.62-7.71 (m, 2H), 7.92-7.96 (m, 2H), 8.01-8.03 (m, 2H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 13.3, 35.9, 41.5, 49.2, 54.0, 60.4, 62.8, 79.7, 108.7, 116.5, 121.5, 121.7, 125.0, 127.3, 128.5, 128.6, 128.8, 129.0, 129.1, 129.5, 129.6, 130.6,

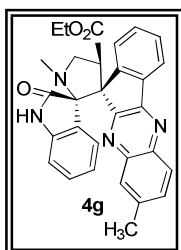
130.8, 137.0, 140.8, 142.2, 142.8, 145.0, 154.2, 161.2, 170.2, 173.7.; HRMS:  $m/z$  517.2241 (M+H)<sup>+</sup> [Calcd 517.2240].



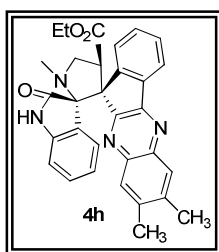
**Compound (4e):** Colorless solid, mp = 179-180°C; IR (KBr): 1646, 1719, 1738 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 0.43 (t, 3H,  $J$  = 6.88 Hz), 2.32 (s, 3H), 1.74 (t, 1H,  $J$  = 2.23 Hz), 3.46-3.53 (m, 1H), 3.60-3.66 (m, 1H), 3.72 (t, 1H,  $J$  = 9.5 Hz), 3.99 (m, 2H), 4.54 (t, 1H,  $J$  = 9.00 Hz), 4.65 (t, 1H,  $J$  = 9.00 Hz), 6.57 (d, 1H,  $J$  = 7.64 Hz), 6.86 (t, 1H,  $J$  = 7.64 Hz), 7.11-7.17 (m, 2H), 7.45-7.53 (m, 2H), 7.61-7.69 (m, 2H), 7.87 (d, 1H,  $J$  = 8.41 Hz), 7.95 (d, 1H,  $J$  = 7.64 Hz), 8.02(d, 1H,  $J$  = 6.88 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 13.3, 28.6, 35.9, 49.0, 54.0, 60.4, 62.9, 71.4, 76.3, 79.9, 108.8, 121.7, 122.0, 125.1, 127.3, 128.3, 128.6, 128.7, 129.1, 129.2, 129.5 (2), 130.8, 137.0, 140.8, 141.5, 142.2, 144.8, 154.2, 160.7, 170.2, 173.1.; HRMS:  $m/z$  515.2063 (M+H)<sup>+</sup> [Calcd 515.2083].



**Compound (4f):** Colorless solid, mp = 198-200 °C; IR (KBr): 1620, 1724, 1735 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>): δ 0.34 (t, 3H,  $J$  = 6.88 Hz), 2.26 (s, 3H), 3.37-3.41 (m, 1H), 3.50-3.53 (m, 1H), 3.65 (t, 1H,  $J$  = 9.94 Hz), 4.31 (t, 1H,  $J$  = 8.41 Hz), 4.63 (t, 1H,  $J$  = 8.41 Hz), 6.47 (d, 1H,  $J$  = 7.64 Hz), 7.09 (d, 1H,  $J$  = 8.41 Hz), 7.31 (s, 1H), 7.50-7.56 (m, 2H), 7.70-7.78 (m, 3H), 8.02-8.08 (m, 2H), 10.00 (s, 1H), <sup>13</sup>C NMR: (125 MHz, DMSO-*d*<sub>6</sub>): δ 13.3, 35.8, 49.3, 53.3, 60.3, 62.5, 79.6, 111.1, 121.6, 125.8, 127.6, 127.9, 128.7, 129.0, 129.1, 129.3, 129.4, 129.5, 130.4, 130.9, 136.6, 140.4, 140.7, 141.8, 145.1, 154.1, 160.0, 169.7, 174.8.; HRMS:  $m/z$  511.1550 (M+H)<sup>+</sup> [Calcd 511.1537].

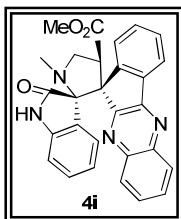


**Compound (4g):** Colorless solid, mp = 182-184°C; IR (KBr): 1616, 1722, 1736 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 0.37 (t, 3H,  $J$  = 6.88 Hz), 2.36 (s, 3H), 2.55 (s, 3H), 3.41-3.46 (m, 1H), 3.55-3.61 (m, 1H), 3.67 (t, 1H,  $J$  = 9.94 Hz), 4.47 (dd, 1H,  $J$  = 8.41, 9.94 Hz), 4.63 (dd, 1H,  $J$  = 8.41, 9.17 Hz), 6.38 (d, 1H,  $J$  = 6.88 Hz), 6.86 (t, 1H,  $J$  = 7.64 Hz), 7.04 (t, 1H,  $J$  = 7.64 Hz), 7.22 (d, 1H,  $J$  = 7.64 Hz), 7.31 (s, 1H), 7.42-7.44 (m, 3H), 7.70 (d, 1H,  $J$  = 8.41 Hz), 7.80 (s, 1H), 7.92-8.00 (m, 2H), <sup>13</sup>C NMR: (125 MHz, CDCl<sub>3</sub>): δ 13.2, 21.8, 36.0, 49.2, 53.8, 60.4, 62.7, 79.7, 109.7, 121.6, 125.9, 127.8, 128.4, 128.6, 129.0(2), 130.6, 130.7, 137.1, 139.2, 140.0, 140.5, 142.2, 144.9, 154.2, 159.4, 170.2, 175.8.; HRMS:  $m/z$  489.2088 (M+H)<sup>+</sup> [Calcd 491.2083].

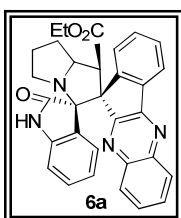


**Compound (4h):** Colorless solid, mp = 205-207 °C; IR (KBr): 1616, 1720, 1739 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 0.37 (t, 3H,  $J$  = 6.88 Hz), 2.31 (s, 3H), 2.43 (s, 3H), 2.45 (s, 3H), 3.42-3.47 (m, 1H), 3.54-3.60 (m, 1H), 3.67 (t, 1H,  $J$  = 9.94 Hz), 4.48 (t, 1H,  $J$  = 9.94 Hz), 4.61 (t, 1H,  $J$  = 9.17 Hz), 6.40 (d, 1H,  $J$  = 7.44 Hz), 6.83 (t, 1H,  $J$  = 7.64 Hz), 7.03 (t, 1H,  $J$  = 7.64 Hz), 7.14 (d, 1H,  $J$  = 7.64 Hz), 7.34-7.39 (m, 2H), 7.60 (s, 1H), 7.78 (s, 1H), 7.85 (s, 1H), 7.90 (d, 1H,  $J$  = 6.88 Hz), 7.95 (d, 1H,  $J$  = 6.88 Hz), <sup>13</sup>C NMR: (100 MHz,

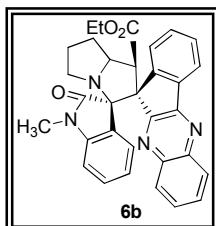
CDCl<sub>3</sub>):  $\delta$  13.0, 20.0, 20.1, 35.7, 49.0, 53.6, 60.1, 62.4, 79.5, 109.4, 121.2, 121.3, 125.6, 127.5, 127.8, 128.1, 128.5, 128.7, 128.8, 130.1, 137.1, 138.7, 139.4, 139.7, 140.3, 140.7, 144.4, 153.2, 159.4, 170.0, 175.6; HRMS:  $m/z$  505.2234 (M+H)<sup>+</sup> [Calcd 505.2240].



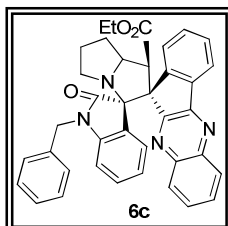
**Compound (4i):** Colorless solid, mp = 186-188 °C; IR (KBr): 1608, 1710, 1740 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  2.33 (s, 3H), 3.05 (s, 3H), 3.71 (t, 1H,  $J$  = 9.6 Hz), 4.52 (t, 1H,  $J$  = 9.4 Hz), 4.65 (t, 1H,  $J$  = 8.8 Hz), 6.38 (d, 1H,  $J$  = 8.56 Hz), 6.75 (t, 1H,  $J$  = 7.6 Hz), 6.98-7.06 (m, 2H), 7.14 (s, 1H), 7.42-7.47 (m, 2H), 7.61-7.70 (m, 2H), 7.89-8.04 (m, 4H); <sup>13</sup>C NMR: (100 MHz, CDCl<sub>3</sub>):  $\delta$  35.7, 49.1, 51.3, 53.9, 62.6, 79.7, 109.6, 121.5, 121.7, 125.4, 127.5, 128.0, 128.6, 128.7, 129.0, 129.1, 129.4, 129.5, 130.6, 136.8, 140.7, 142.2, 144.7, 154.0, 160.9, 170.7, 176.1.; HRMS:  $m/z$  463.1771 (M+H)<sup>+</sup> [Calcd 463.1770].



**Compound (6a):** Colorless solid, mp = 171-172 °C; IR (KBr): 1619, 1710, 1735 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  0.34 (t, 3H,  $J$  = 6.88 Hz), 2.17-2.35 (m, 4H), 2.69-2.75 (m, 1H), 2.85 (t, 1H,  $J$  = 8.41 Hz), 3.30-3.36 (m, 1H), 3.50-3.58 (m, 1H), 4.64-4.69 (m, 1H), 5.03 (d, 1H,  $J$  = 8.41 Hz), 6.36-6.49 (m, 3H), 6.84 (t, 1H,  $J$  = 7.64 Hz), 7.54-7.69 (m, 4H), 7.97 (s, 1H), 8.01 (d, 1H,  $J$  = 8.41 Hz), 8.07 (d, 2H,  $J$  = 7.64 Hz), 8.32 (d, 1H,  $J$  = 8.41 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  13.2, 30.6, 31.5, 47.7, 51.7, 60.0, 66.5, 66.9, 78.0, 109.3, 121.8, 122.0, 125.9, 126.1, 128.3, 128.6, 128.8, 129.1, 129.4, 129.7, 129.8, 131.2, 137.9, 140.5, 141.2, 142.1, 145.4, 154.3, 157.6, 170.3, 179.6.; HRMS:  $m/z$  503.2088 (M+H)<sup>+</sup> [Calcd 503.2078].

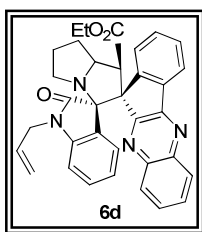


**Compound (6b):** Colorless solid, mp = 208-210 °C; IR (KBr): 1604, 1709, 1736 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  0.36 (t, 3H,  $J$  = 6.88 Hz), 2.15- 2.37 (m, 3H), 2.53-2.68 (m, 2H), 2.84 (t, 1H,  $J$  = 8.41 Hz), 3.04 (s, 1H), 3.32-3.38 (m, 1H), 3.51-3.58 (m, 1H), 4.65-4.70 (m, 1H), 5.02 (d, 1H,  $J$  = 8.41 Hz), 6.28 (d, 1H,  $J$  = 7.64 Hz), 6.44-6.50 (m, 2H), 7.03 (t, 1H,  $J$  = 7.64 Hz), 7.54 (t, 1H,  $J$  = 7.64 Hz), 7.65-7.71 (m, 3H), 8.01-8.14 (m, 3H), 8.33 (d, 1H,  $J$  = 7.64 Hz); <sup>13</sup>C NMR: (125 MHz, CDCl<sub>3</sub>):  $\delta$  13.2, 25.8, 30.7, 31.4, 47.8, 51.5, 60.0, 66.6, 67.5, 78.0, 107.4, 121.8, 121.9, 125.3, 125.4, 128.3, 128.7, 129.0, 129.1, 129.4, 129.6(2), 131.2, 137.7, 141.1, 142.2, 143.1, 145.4, 154.3, 157.7, 170.3, 177.9.; HRMS:  $m/z$  517.2234 (M+H)<sup>+</sup> [Calcd 517.2240].

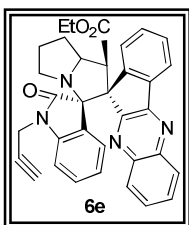


**Compound (6c):** Colorless solid, mp = 177-179 °C; IR (KBr): 1609, 1701, 1731 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  0.35 (t, 3H,  $J$  = 6.88), 2.14-2.40 (m, 3H), 2.52-2.73 (m, 2H), 2.87 (t, 1H,  $J$  = 8.41 Hz), 3.32-3.38 (m, 1H), 3.52-3.58 (m, 1H), 4.60-4.73 (m, 2H), 4.94 (d, 1H,  $J$  = 15.29 Hz), 5.12 (d, 1H,  $J$  = 8.41 Hz), 6.13 (d, 1H,  $J$  = 8.41 Hz), 6.44-6.47 (m, 2H), 6.74-6.78 (m, 1H), 6.96-7.02 (m, 4H), 7.10 (t, 1H,  $J$  = 6.88 Hz), 7.56 (t, 1H,  $J$  = 6.88, 7.64 Hz), 7.62-7.73 (m, 3H), 8.02-8.09 (m, 3H), 8.36 (d, 1H,  $J$  = 7.64 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  13.2, 30.6, 31.5, 43.8, 47.7, 51.9, 60.8, 66.6, 67.2, 77.6, 108.8, 122.0(2), 125.4, 125.7, 126.9, 127.3, 128.4,

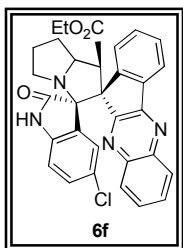
128.6, 128.8, 128.9, 129.1, 129.5, 1129.7, 130.0, 131.2, 135.6, 137.8, 141.2, 142.2, 142.7, 145.5, 154.4, 157.9, 170.3, 177.8.; HRMS:  $m/z$  593.2565 (M+H)<sup>+</sup> [Calcd 593.2547].



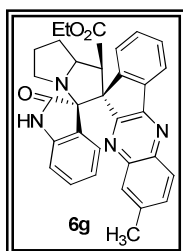
**Compound (6d):** Colorless solid, mp = 200-202°C; IR (KBr): 1639, 1718, 1733 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 0.35 (t, 3H,  $J$  = 6.88 Hz), 2.14-2.37 (m, 3H), 2.50-2.67 (m, 2H), 2.84 (t, 1H,  $J$  = 8.41 Hz), 3.31-3.37 (m, 1H), 3.51-3.58 (m, 1H), 4.16-4.28 (m, 2H), 4.65-4.70 (m, 1H), 4.89-4.93 (m, 2H), 5.06 (d, 1H,  $J$  = 8.41 Hz), 5.53-5.60 (m, 1H), 6.30 (d, 1H,  $J$  = 7.64 Hz), 6.45-6.49 (m, 2H), 6.85 (t, 1H,  $J$  = 7.64 Hz), 7.55 (t, 1H,  $J$  = 7.64 Hz), 7.66-7.71 (m, 3H), 8.01-8.12 (m, 3H), 8.34 (d, 1H,  $J$  = 8.41 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 13.2, 30.6, 31.4, 42.4, 47.7, 51.7, 60.0, 66.6, 67.3, 77.6, 108.5, 117.5, 121.8, 122.0, 125.3, 125.6, 128.3, 128.6, 128.9, 129.0, 129.4, 129.6, 129.8, 131.2, 131.6, 137.8, 141.0, 142.2, 142.6, 145.4, 154.4, 157.7, 170.3, 177.4.; HRMS:  $m/z$  543.2380 (M+H)<sup>+</sup> [Calcd 543.2396].



**Compound (6e):** Colorless solid, mp = 214-216 °C; IR (KBr): 1622, 1720, 1736 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 0.35 (t, 3H,  $J$  = 6.92 Hz), 1.71 (s, 1H), 2.12-2.37 (m, 3H), 2.49-2.66 (m, 2H), 2.84 (t, 1H,  $J$  = 8.41 Hz), 3.31-3.38 (m, 1H), 3.52-3.58 (m, 2H), 4.32-4.42 (m, 2H), 4.65-4.70 (m, 1H), 5.00 (d, 1H,  $J$  = 8.41 Hz), 6.48-6.54 (m, 3H), 6.92 (t, 1H,  $J$  = 7.69 Hz), 7.54 (t, 1H,  $J$  = 7.69 Hz), 7.63-7.68 (m, 3H), 7.99 (d, 1H,  $J$  = 8.46 Hz), 8.04 (d, 1H,  $J$  = 7.69 Hz), 8.15 (d, 1H,  $J$  = 7.69 Hz), 8.31 (d, 1H,  $J$  = 7.69 Hz); <sup>13</sup>CNMR: (125 MHz, CDCl<sub>3</sub>): δ 13.2, 28.9, 30.6, 31.5, 47.7, 51.7, 60.0, 66.6, 67.4, 71.9, 76.5, 77.9, 108.5, 121.9, 122.2, 125.2, 125.6, 128.2, 128.3, 128.8, 129.1, 129.4, 129.6, 130.3, 131.1, 137.8, 141.1, 141.3, 142.2, 145.3, 154.2, 157.5, 170.2, 176.9.; HRMS:  $m/z$  541.2260 (M+H)<sup>+</sup> [Calcd 541.2240].

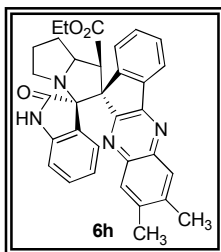


**Compound (6f):** Colorless solid, mp = 196-198 °C; IR (KBr): 1620, 1709, 1737 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 0.35 (t, 3H,  $J$  = 6.88 Hz), 2.11-2.49 (m, 4H), 2.67-2.72 (m, 1H), 2.88 (t, 1H,  $J$  = 8.41 Hz), 3.31-3.37 (m, 1H), 3.54-3.60 (m, 1H), 4.63-4.68 (m, 1H), 4.99 (d, 1H,  $J$  = 8.41 Hz), 6.31 (d, 1H,  $J$  = 8.41 Hz), 6.38 (s, 1H), 6.81-6.83 (m, 1H), 7.55-7.72 (m, 4H), 8.03 (d, 2H,  $J$  = 8.41 Hz), 8.07 (s, 1H), 8.11 (d, 1H,  $J$  = 7.64 Hz), 8.28 (d, 1H,  $J$  = 7.64 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 13.2, 28.9, 30.5, 31.5, 47.7, 51.6, 60.1, 66.6, 67.0, 78.1, 110.3, 122.3, 126.6, 127.2, 127.7, 128.1, 128.7, 128.9, 129.0, 129.7, 129.8, 131.3, 137.8, 138.9, 141.2, 142.2, 145.0, 154.3, 157.2, 165.4, 170.1, 179.3.; HRMS:  $m/z$  537.1699 (M+H)<sup>+</sup> [Calcd 537.1693].

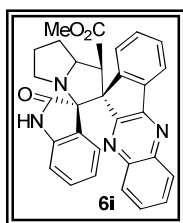


**Compound (6g):** Colorless solid, mp = 173-175 °C; IR (KBr): 1617, 1721, 1730 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 0.32 (t, 3H,  $J$  = 7.08 Hz), 2.15-2.51 (m, 7H), 2.71-2.89 (m, 2H), 3.27-3.35 (m, 1H), 3.49-3.57 (m, 1H), 4.63-4.69 (m, 1H), 5.01 (d, 1H,  $J$  = 8.4 Hz), 6.37-6.50 (m, 3H), 6.85 (t, 1H,  $J$  = 7.6 Hz), 7.45 (d, 1H,  $J$  = 8.72 Hz), 7.54 (t, 1H,  $J$  = 7.44 Hz), 7.63-7.67 (m, 2H), 7.76 (s, 1H), 7.85 (d, 1H,  $J$  = 8.44 Hz), 8.04 (d, 1H,  $J$  = 7.56 Hz), 8.31 (d, 1H,  $J$

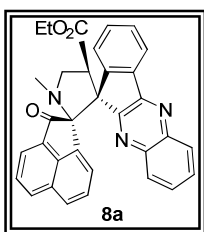
= 7.72 Hz);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  13.2, 21.8, 30.5, 31.5, 47.7, 51.7, 60.0, 66.5, 66.9, 78.0, 109.4, 121.8, 121.9, 126.0, 126.1, 127.9, 128.3, 129.0, 129.2, 129.3, 130.6, 130.8, 131.0, 131.6, 138.0, 140.1, 140.5, 142.1, 145.5, 154.2, 156.6, 170.3, 179.8.; HRMS:  $m/z$  517.2242 ( $\text{M}+\text{H}$ ) $^+$  [Calcd 517.2240].



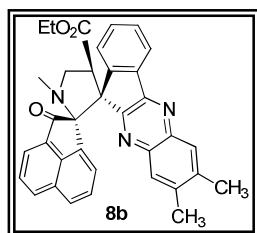
**Compound (6h):** Colorless solid, mp = 230-232 °C; IR (KBr): 1609, 1721, 1735  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  0.26 (t, 3H,  $J$  = 7.2 Hz), 1.47 (s, 3H), 2.15-2.50 (m, 7H), 2.81-2.93 (m, 2H), 3.18-3.26 (m, 1H), 3.44-3.52 (m, 1H), 4.62-4.68 (m, 1H), 5.02 (d, 1H,  $J$  = 8.4 Hz), 6.55-6.61 (m, 2H), 6.73 (d, 1H,  $J$  = 7.68 Hz), 6.87 (s, 1H), 6.93-6.98 (m, 1H), 7.44 (s, 1H), 7.56 (t, 1H,  $J$  = 7.44 Hz), 7.66 (t, 1H,  $J$  = 7.4 Hz), 8.07 (d, 1H,  $J$  = 7.48 Hz), 8.38 (d, 1H,  $J$  = 7.72 Hz), 9.84 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  13.0, 19.2, 20.0, 30.4, 31.5, 47.6, 52.4, 59.8, 66.3, 66.6, 77.7, 110.3, 121.4, 121.8, 126.3, 126.4, 127.2, 128.1, 128.4, 128.9, 129.2, 130.4, 138.3(2), 139.4, 139.7, 140.3, 141.4, 144.9, 153.1, 156.4, 170.3, 180.9.; HRMS:  $m/z$  531.2380 ( $\text{M}+\text{H}$ ) $^+$  [Calcd 531.2396].



**Compound (6i):** Colorless solid, mp = 205-207 °C; IR (KBr): 1607, 1705, 1739  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  2.13-2.54 (m, 4H), 2.68-2.88 (m, 2H), 2.99 (s, 3H), 4.63-4.69 (m, 1H), 5.07 (d, 1H,  $J$  = 8.4 Hz), 6.35-6.49 (m, 3H), 6.84 (t, 1H,  $J$  = 7.56 Hz), 7.53-7.69 (m, 4H), 7.90-8.08 (m, 4H), 8.30 (d, 1H,  $J$  = 7.8 Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  30.4, 31.4, 47.6, 51.3, 51.6, 66.5, 66.8, 77.9, 109.2, 121.8, 122.0, 125.7, 126.0, 128.1, 128.5, 128.8, 129.0, 129.3, 129.6, 129.7, 131.1, 137.6, 140.3, 141.2, 142.1, 145.3, 154.1, 157.3, 170.8, 179.5.; HRMS:  $m/z$  489.1934 ( $\text{M}+\text{H}$ ) $^+$  [Calcd 489.1927].

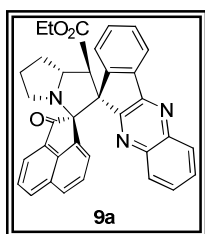


**Compound (8a):** Yellow solid, mp = 201-202 °C; IR (KBr): 1601, 1723, 1737  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  0.34 (t, 3H,  $J$  = 6.88 Hz), 2.34 (s, 3H), 3.38-3.41 (m, 1H), 3.57-3.60 (m, 1H), 3.80 (t, 1H,  $J$  = 9.94 Hz), 4.58 (dd, 1H,  $J$  = 7.64, 9.94 Hz), 4.81 (dd, 1H,  $J$  = 7.64, 9.94 Hz), 7.32 (t, 1H,  $J$  = 7.64 Hz), 7.41-7.52 (m, 3H), 7.55-7.63 (m, 4H), 7.67-7.73 (m, 2H), 7.78 (d, 1H,  $J$  = 7.64 Hz), 7.88 (d, 1H,  $J$  = 7.64 Hz), 7.95 (d, 1H,  $J$  = 7.64 Hz), 8.09 (d, 1H,  $J$  = 7.64 Hz);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  13.2, 36.0, 50.1, 54.2, 60.4, 63.6, 83.5, 120.9, 121.6, 124.3, 124.9, 127.5, 128.4, 128.6, 129.0, 129.1, 129.2, 129.3, 130.3, 130.8, 131.5, 132.0, 135.3, 136.8, 140.5, 141.3, 141.9, 145.2, 154.2, 160.0, 170.1, 201.8.; HRMS:  $m/z$  512.1983 ( $\text{M}+\text{H}$ ) $^+$  [Calcd 512.1969].

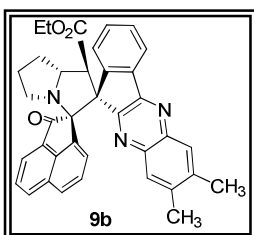


**Compound (8b):** Yellow solid, mp = 165-168 °C; IR (KBr): 1605, 1726, 1741  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  0.33 (t, 3H,  $J$  = 7.0 Hz), 2.33 (s, 3H), 2.38 (s, 6H), 3.34-3.42 (m, 1H), 3.52-3.60 (m, 1H), 3.78 (t, 1H,  $J$  = 10.00 Hz), 4.57 (t, 1H,  $J$  = 8.8 Hz), 4.77 (t, 1H,  $J$  = 8.4 Hz), 7.31-7.65 (m, 8H), 7.71 (d, 1H,  $J$  = 8 Hz), 7.79 (d, 1H,  $J$  = 7.92 Hz), 7.90 (d, 1H,  $J$  = 7.44 Hz), 8.05 (d, 1H,  $J$  = 7.68 Hz);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  13.1, 20.1(2), 35.9, 50.0, 54.2, 60.2, 63.2, 83.3, 120.7, 121.2, 124.2, 124.7, 127.4, 127.5, 127.9, 128.4,

128.8, 128.9, 130.2, 131.3, 132.0, 135.3, 137.1, 138.6, 139.4, 139.5, 140.6, 141.3, 144.8, 153.3, 159.1, 170.2, 202.0.; HRMS:  $m/z$  540.2263 (M+H)<sup>+</sup> [Calcd 540.2287].



**Compound (9a):** Yellow solid, mp = 214-216°C; IR (KBr): 1601, 1724, 1739 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 0.35 (t, 3H,  $J$  = 6.88 Hz), 2.13-2.34 (m, 3H), 2.59-2.69 (m, 1H), 2.80 (t, 1H,  $J$  = 8.41 Hz), 3.32-3.38 (m, 1H), 3.52-3.59 (m, 1H), 4.75-4.79 (m, 1H), 4.94 (d, 1H,  $J$  = 8.41 Hz), 6.82 (d, 1H,  $J$  = 7.64 Hz), 7.12 (t, 1H,  $J$  = 7.64 Hz), 7.39-7.47 (m, 2H), 7.54-7.57 (m, 3H), 7.68-7.74 (m, 2H), 7.81 (d, 1H,  $J$  = 6.88 Hz), 7.84-7.86 (m, 1H), 7.96-8.00 (m, 2H), 8.24 (d, 1H,  $J$  = 7.64 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 13.2, 30.5, 31.5, 46.9, 52.8, 60.0, 66.3, 68.2, 80.6, 119.5, 121.9, 122.2, 124.8, 127.7, 127.9, 128.2, 128.6, 129.3, 129.4, 129.5, 130.8, 131.3, 132.6, 135.9, 137.9, 140.7, 141.2, 141.8, 145.9, 154.1, 157.6, 170.2, 208.6.; HRMS:  $m/z$  538.2136 (M+H)<sup>+</sup> [Calcd 538.2125].



**Compound (9b):** Yellow solid, mp = 177-179 °C; IR (KBr): 1604, 1726, 1740 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 0.32 (t, 3H,  $J$  = 7.0 Hz), 2.16-2.41 (m, 9H), 2.57-2.81 (m, 3H), 3.29-3.35 (m, 1H), 3.49-3.56 (m, 1H), 4.73-4.79 (m, 1H), 4.90 (d, 1H,  $J$  = 8.56 Hz), 6.81 (d, 1H,  $J$  = 7.04 Hz), 7.11 (t, 1H,  $J$  = 7.84 Hz), 7.40-7.73 (m, 7H), 7.81 (d, 1H,  $J$  = 6.96 Hz), 7.96 (d, 1H,  $J$  = 7.6 Hz), 8.41 (d, 1H,  $J$  = 7.72 Hz); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 13.1, 20.1(2), 30.4, 31.4, 46.8, 52.7, 59.9, 66.5, 68.1, 80.6, 119.4, 121.5, 122.2, 124.6, 127.6, 127.8, 128.0, 128.6, 129.1, 130.0, 130.7, 132.6, 136.0, 138.1, 138.8, 139.5, 139.7, 140.5, 141.2, 145.6, 153.1, 156.5, 170.2, 208.6.; HRMS:  $m/z$  566.2446 (M+H)<sup>+</sup> [Calcd 566.2444].

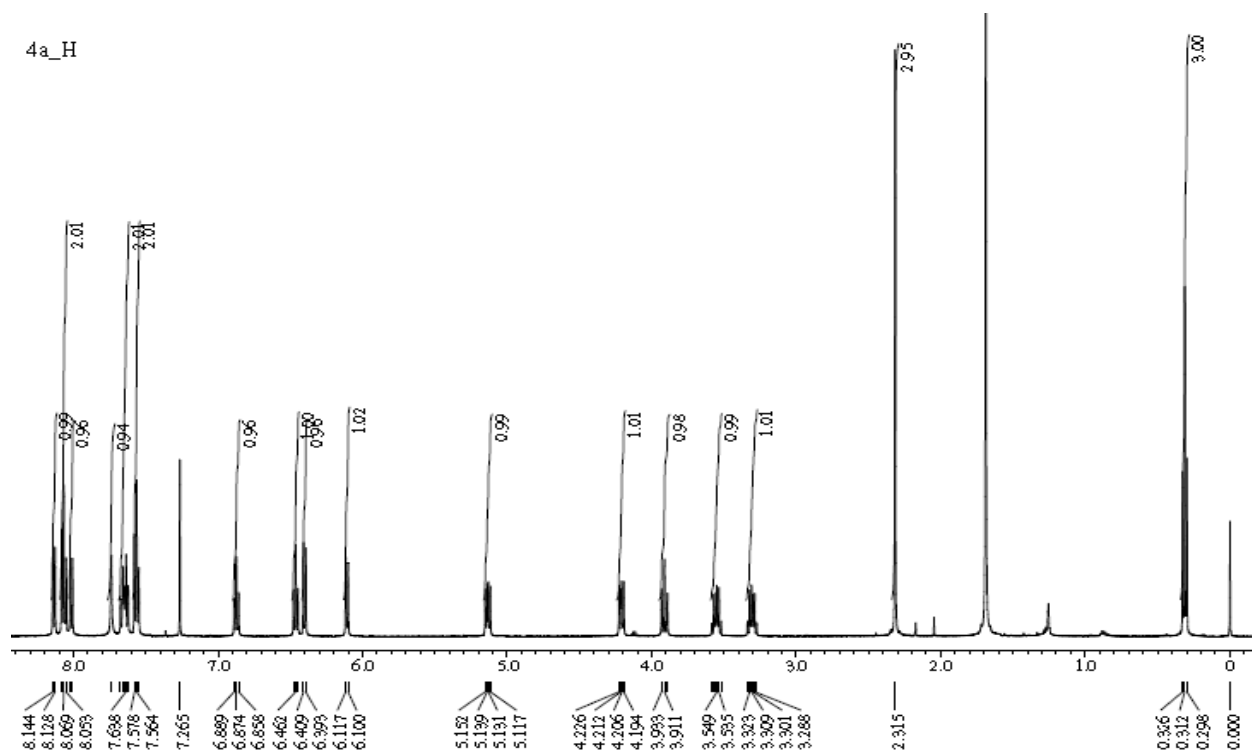


Figure S1. <sup>1</sup>H NMR spectrum of 4a

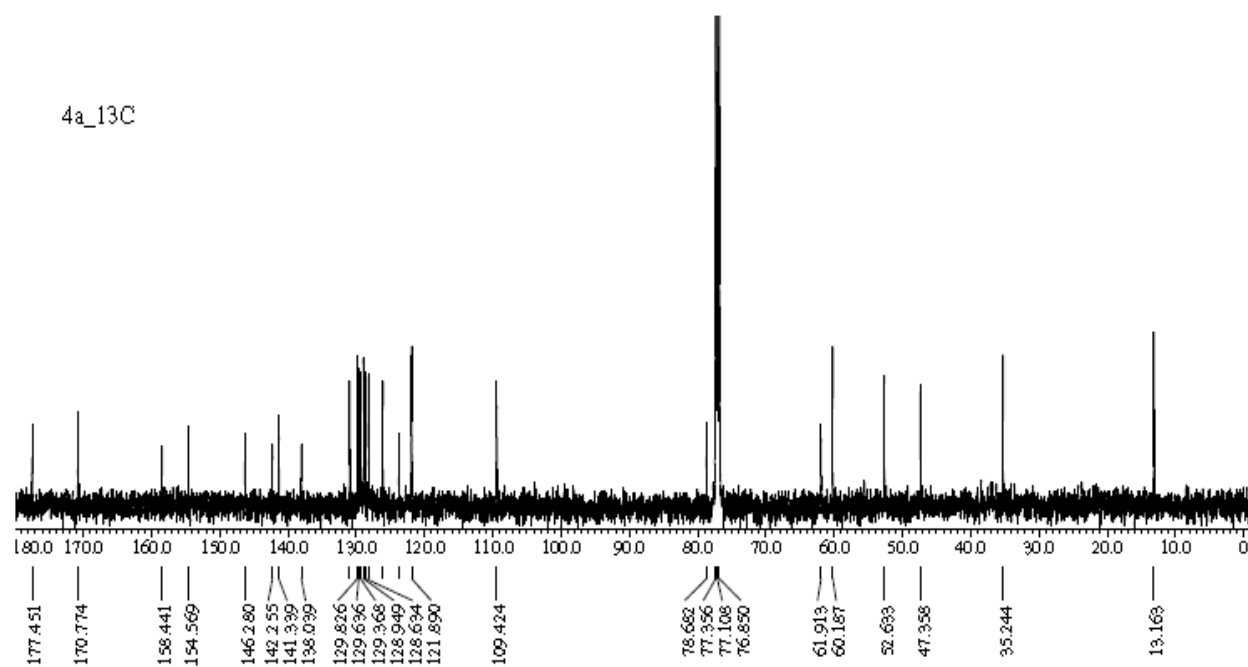
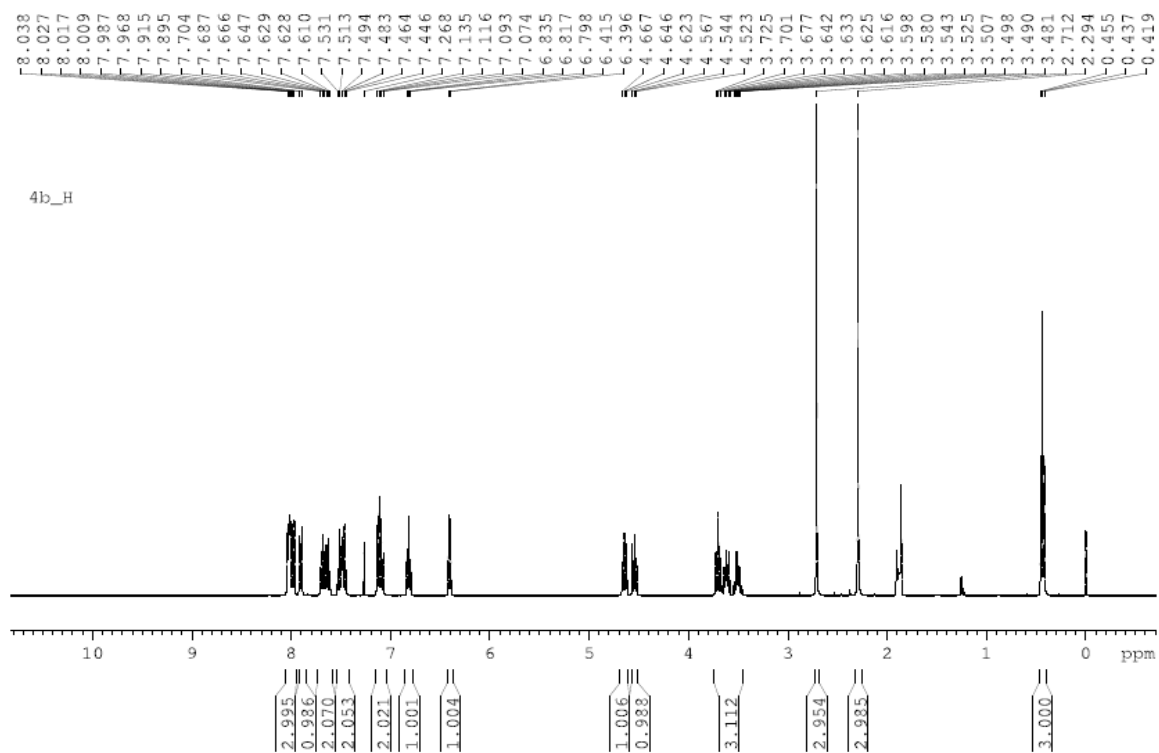
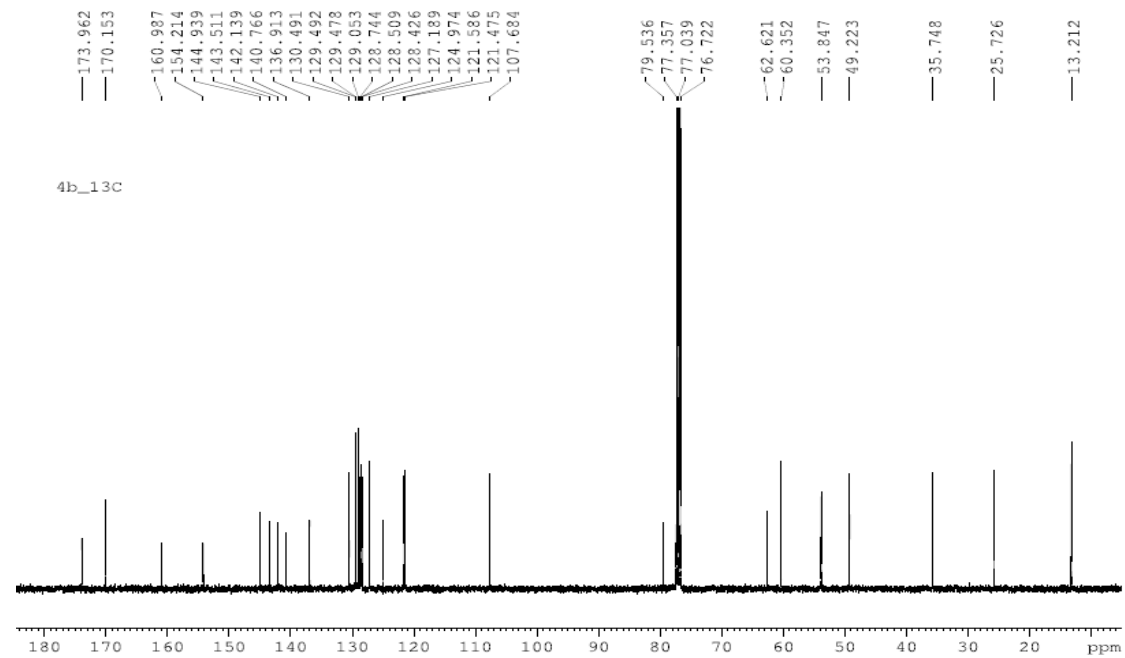


Figure S2. <sup>13</sup>C NMR spectrum of 4a





**Figure S3.** <sup>1</sup>H NMR spectrum of **4b**



**Figure S4.** <sup>13</sup>C NMR spectrum of **4b**

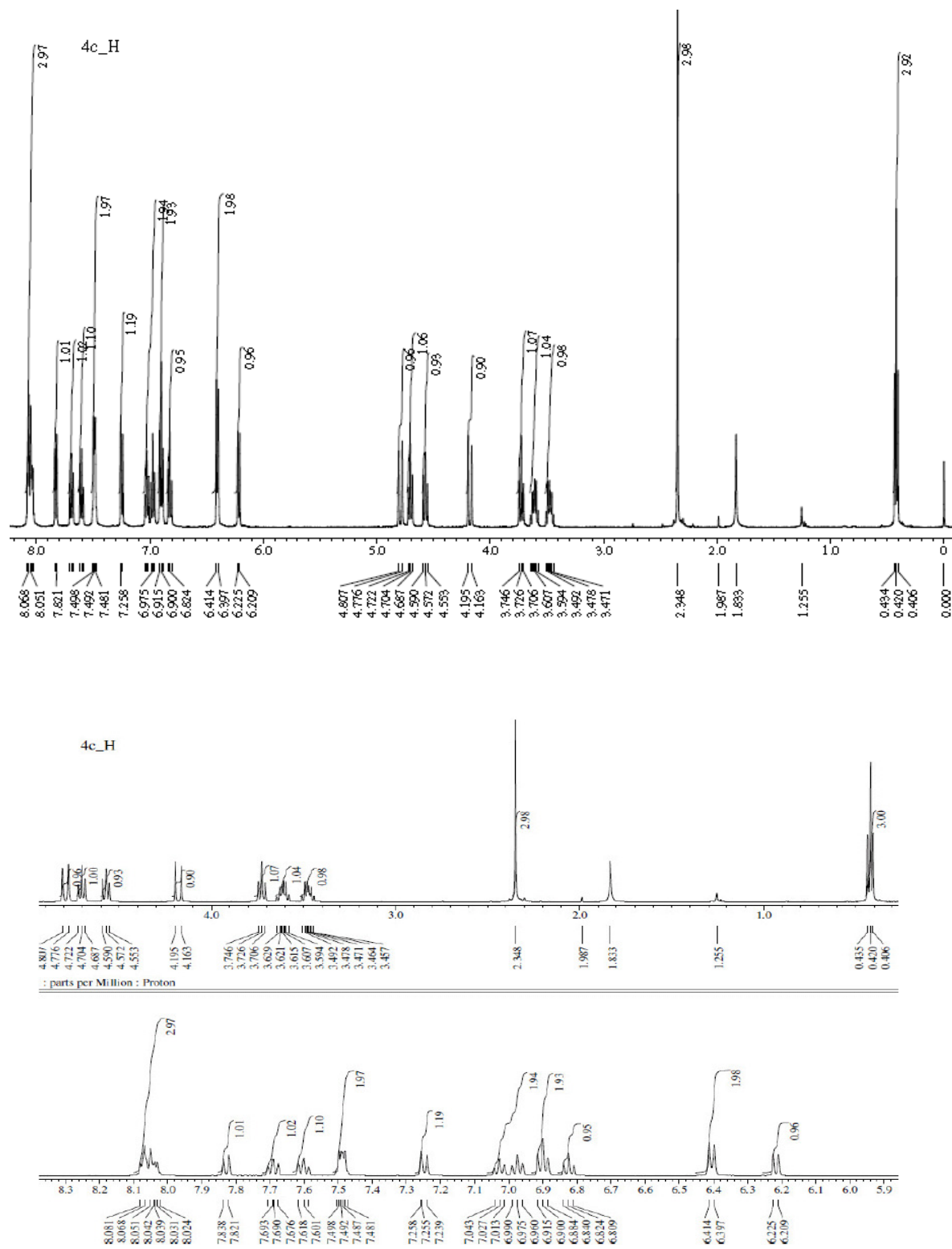


Figure S5. <sup>1</sup>H NMR spectrum of 4c

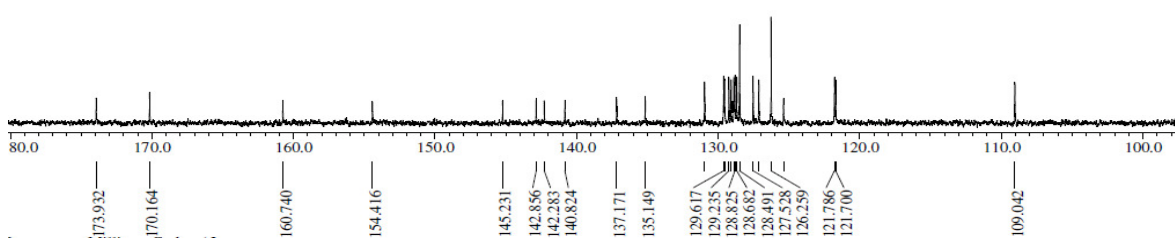
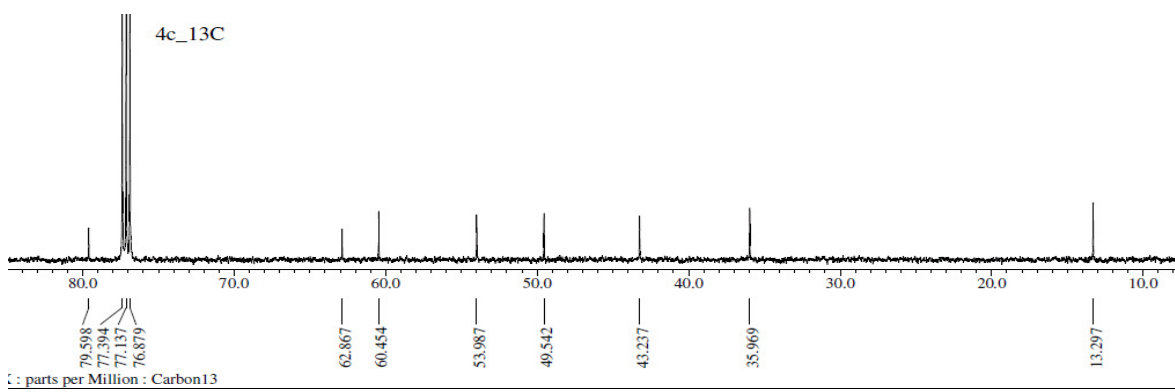
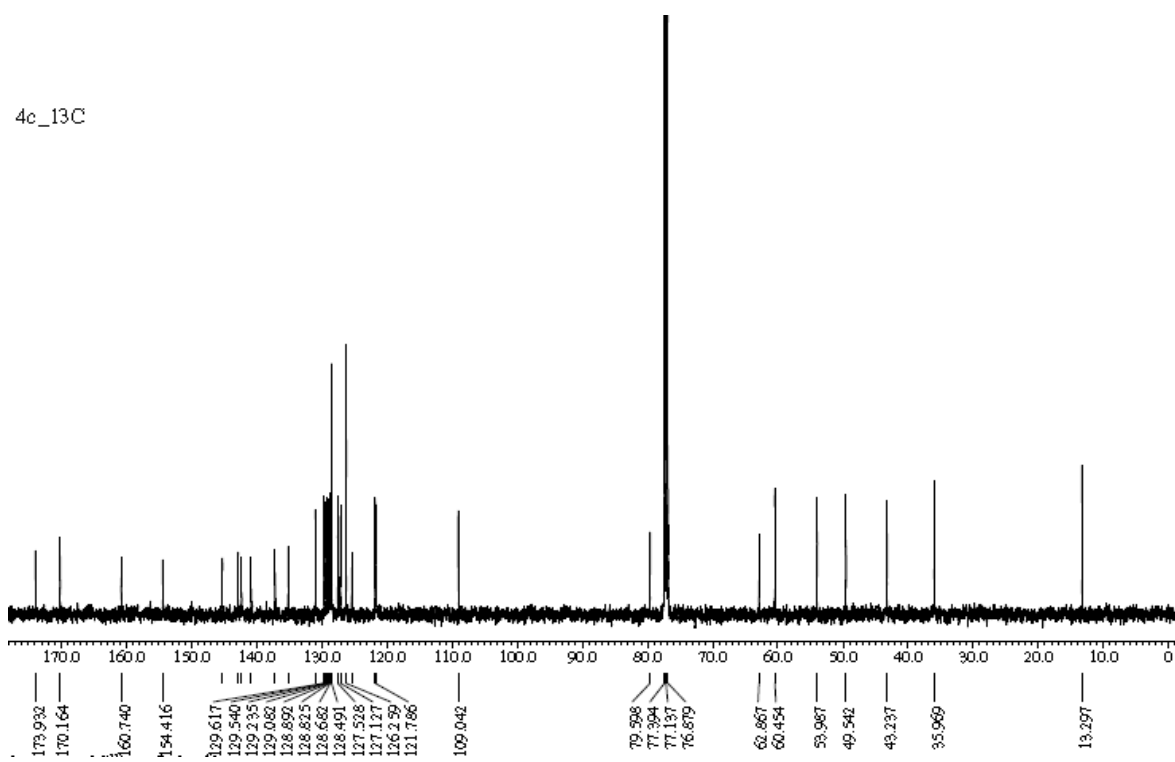


Figure S6.  $^{13}\text{C}$  NMR spectrum of **4c**

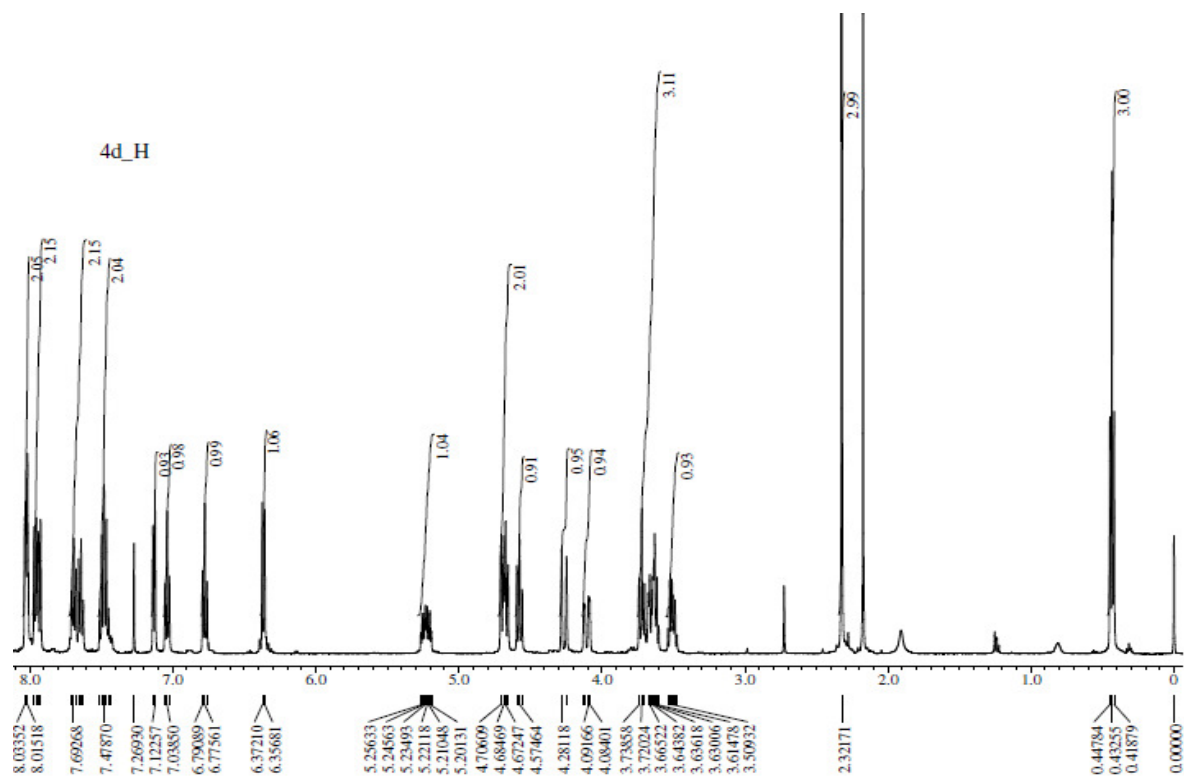


Figure S7.  $^1\text{H}$  NMR spectrum of **4d**

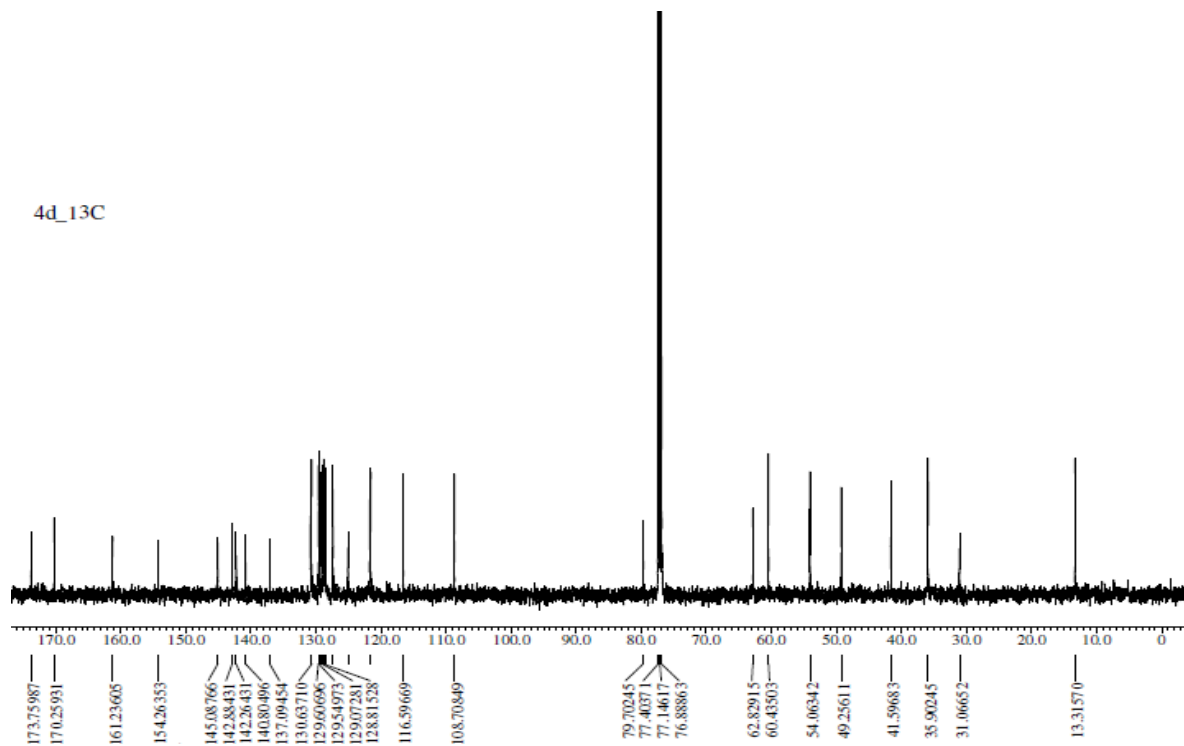
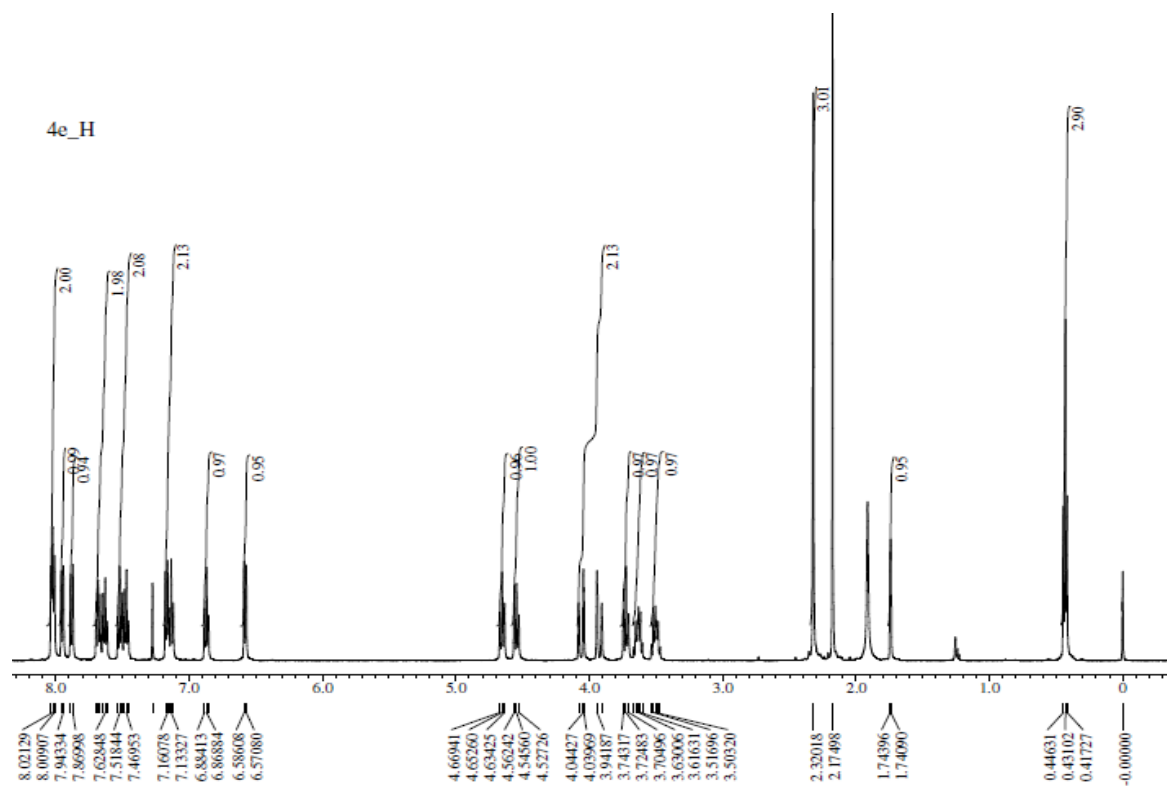
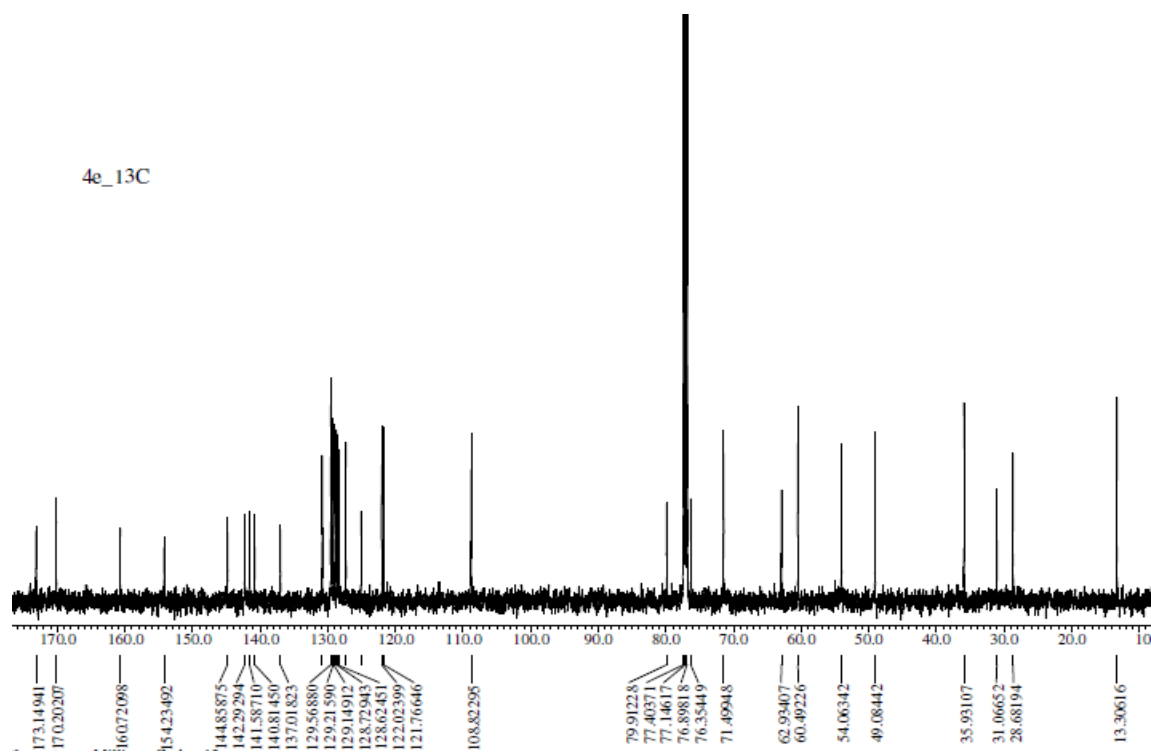


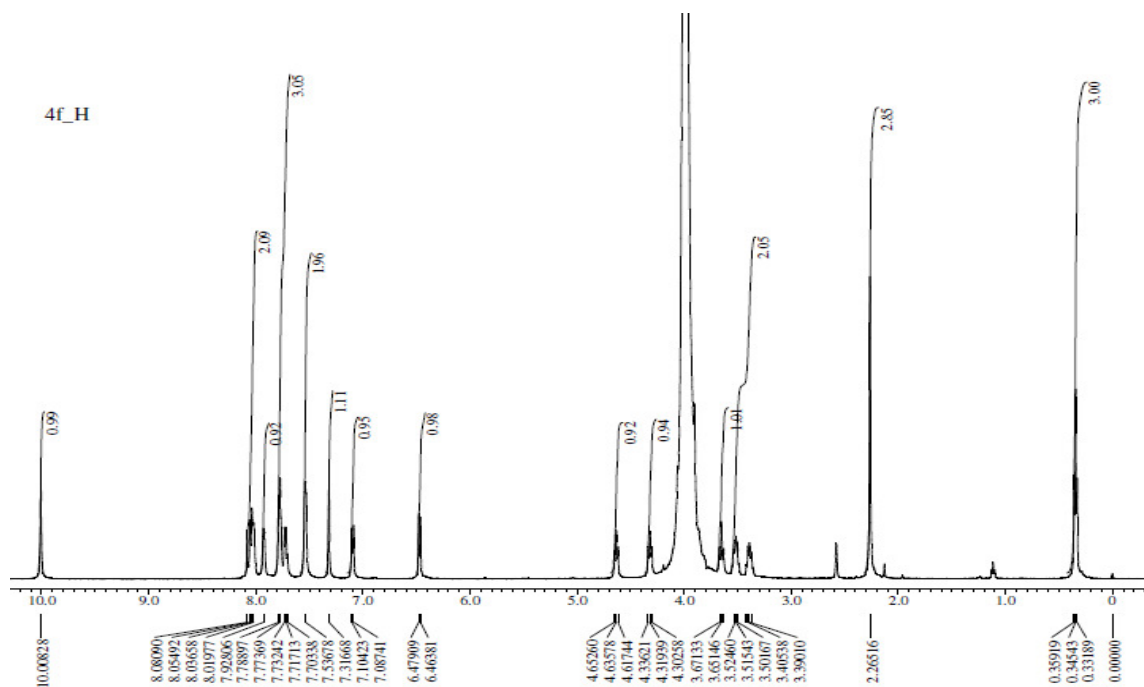
Figure S8  $^{13}\text{C}$  NMR spectrum of **4d**



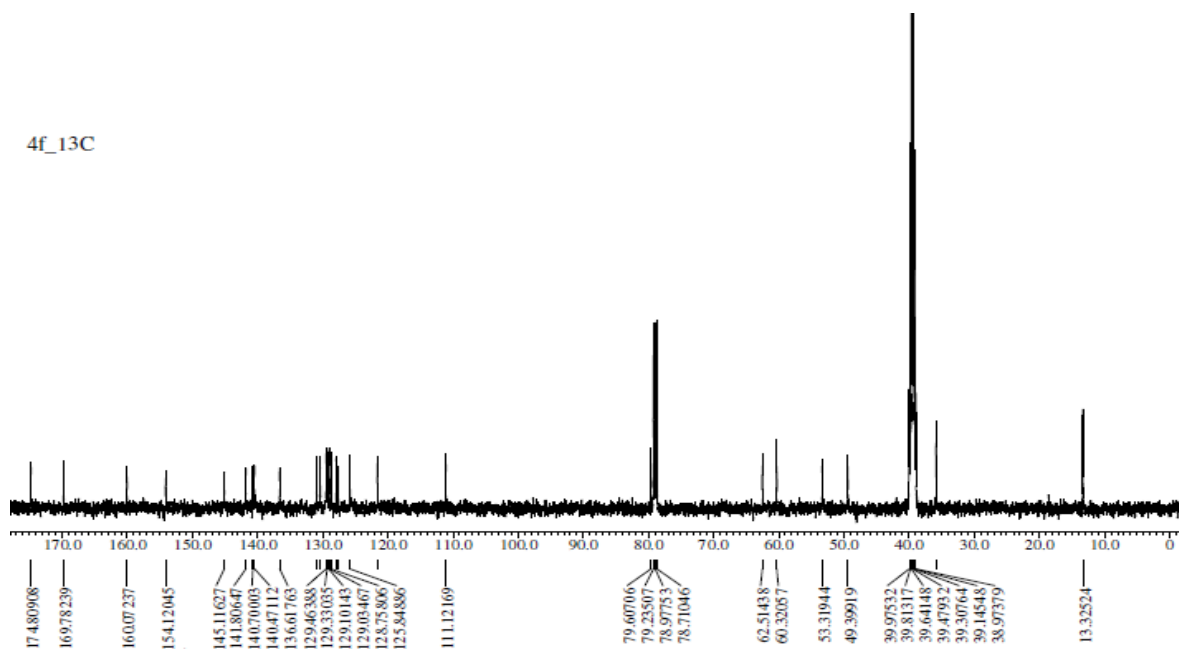
**Figure S9.**  $^1\text{H}$  NMR spectrum of **4e**



**Figure S10.**  $^{13}\text{C}$  NMR spectrum of **4e**



**Figure S11.** <sup>1</sup>H NMR spectrum of **4f**



**Figure S12.** <sup>13</sup>C NMR spectrum of **4f**

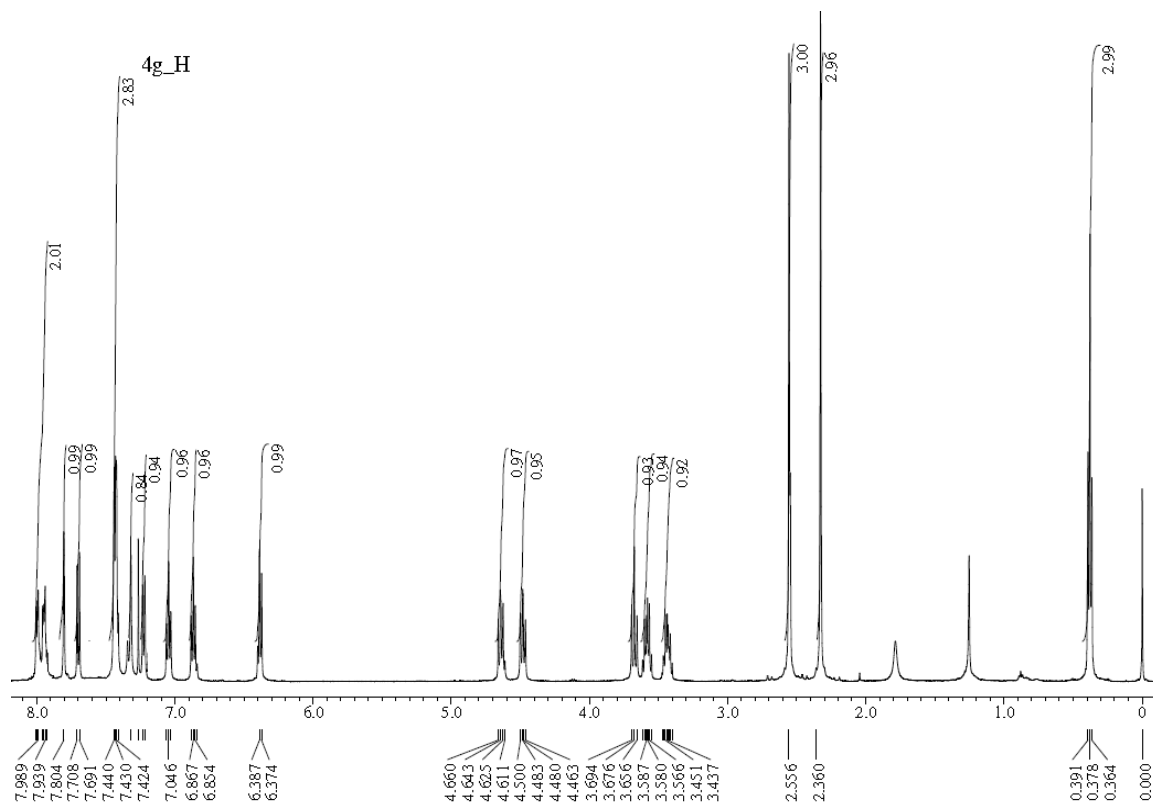


Figure S13.. <sup>1</sup>H NMR spectrum of 4g

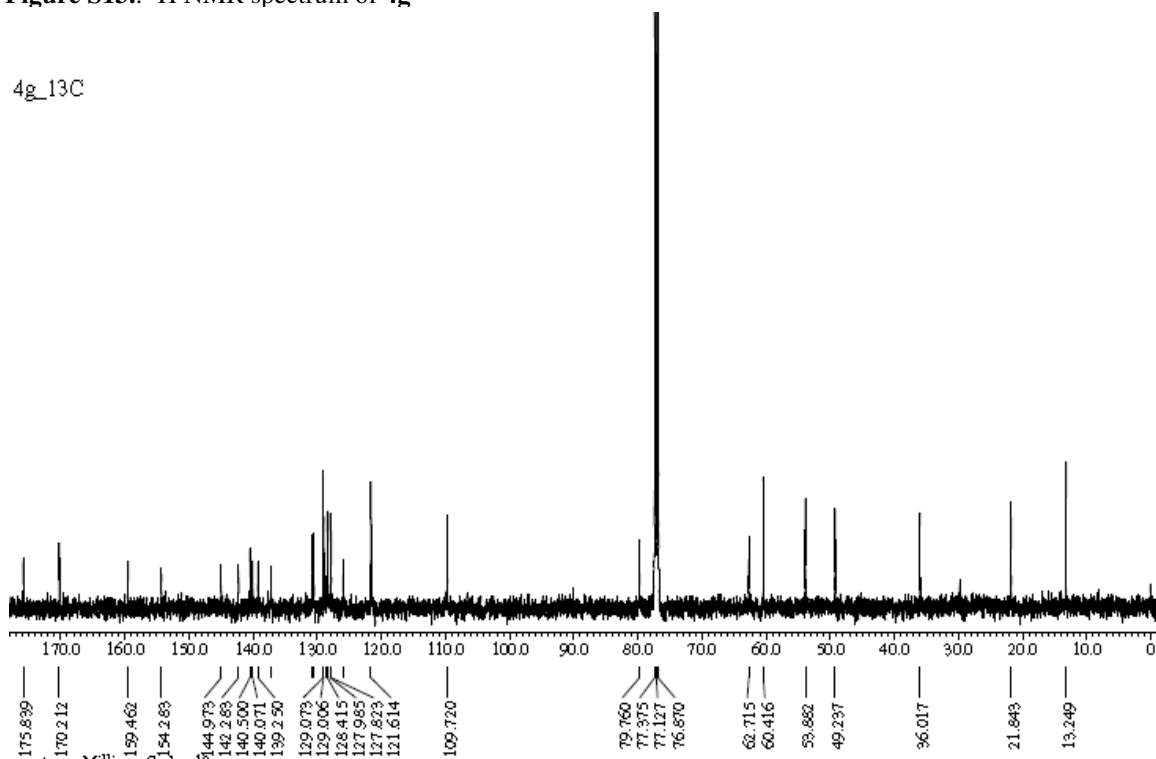


Figure S14. <sup>13</sup>C NMR spectrum of 4g

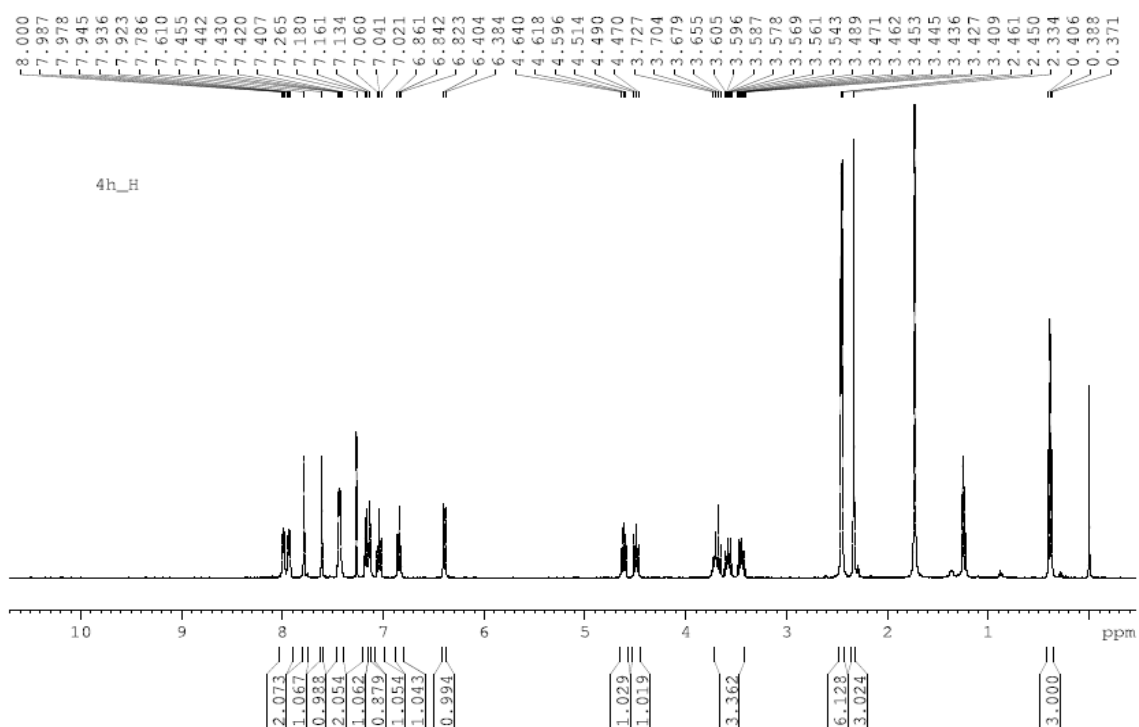


Figure S15. <sup>1</sup>H NMR spectrum of 4h

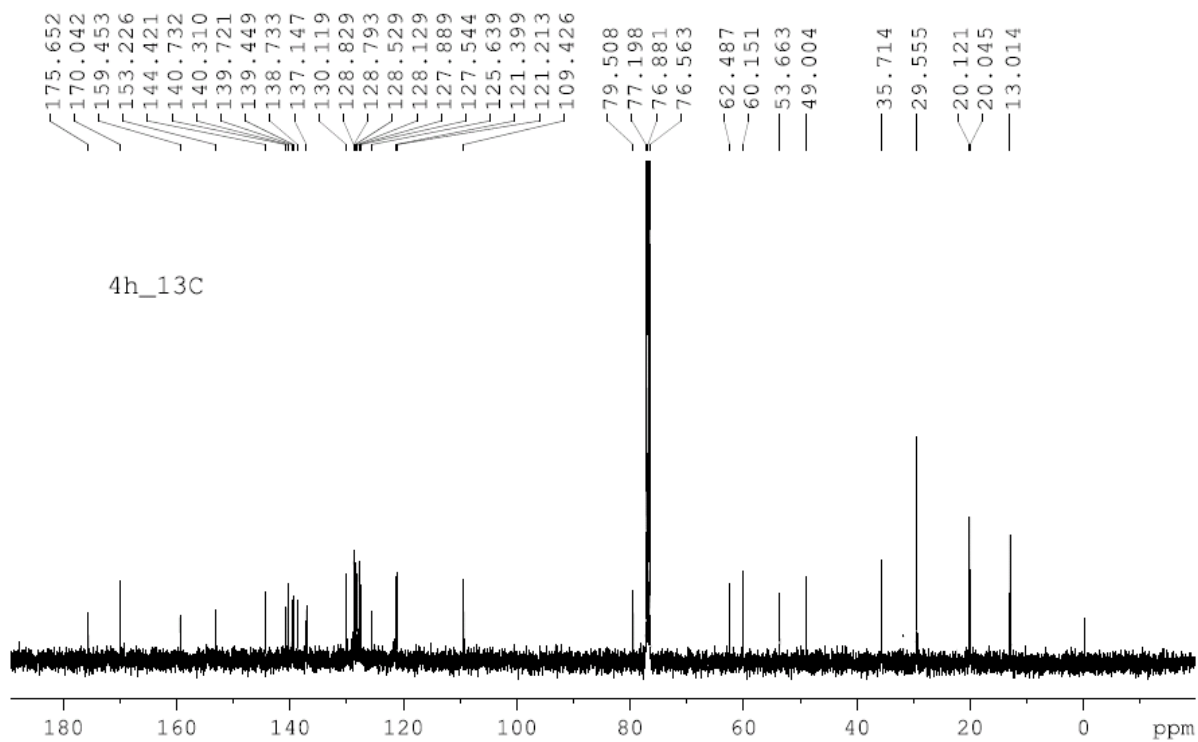
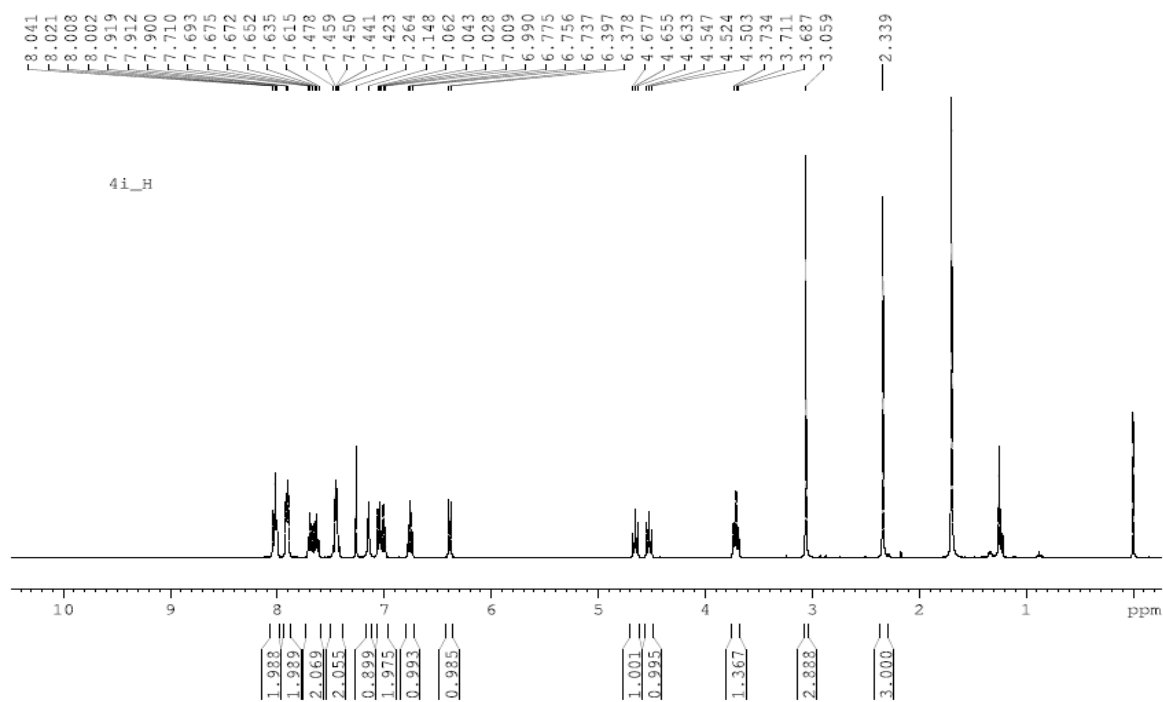
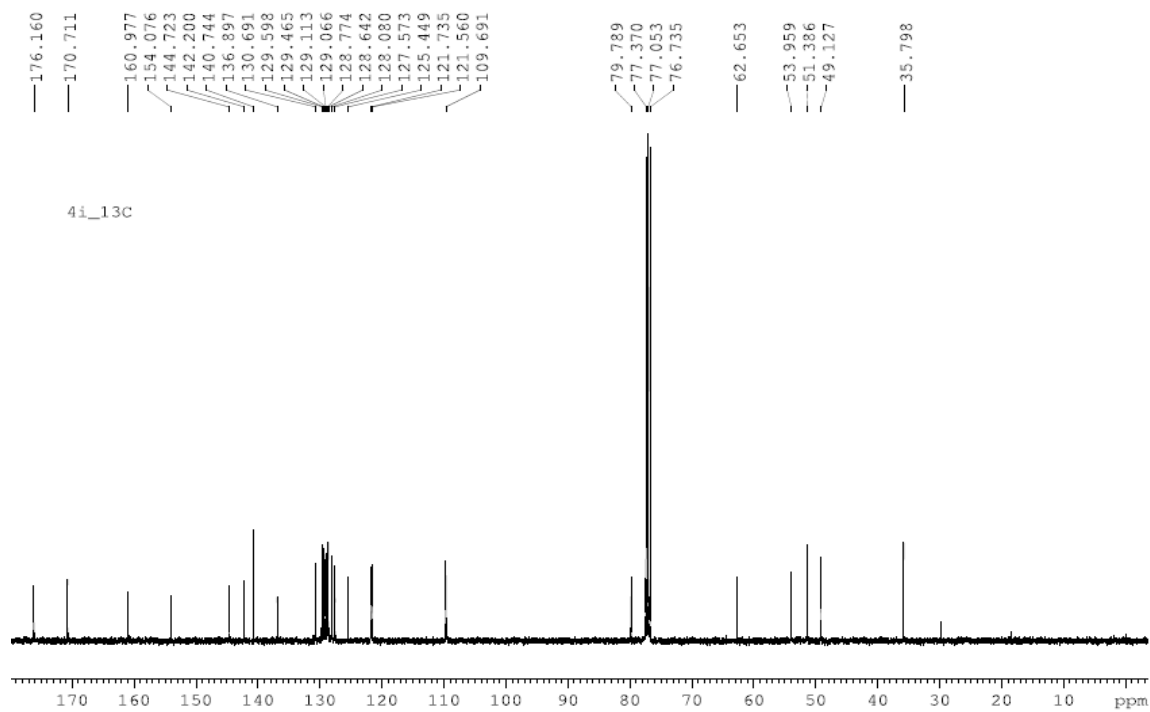


Figure S26. <sup>13</sup>C NMR spectrum of 4h





**Figure S47.**  $^1\text{H}$  NMR spectrum of **4i**



**Figure S58.**  $^{13}\text{C}$  NMR spectrum of **4i**

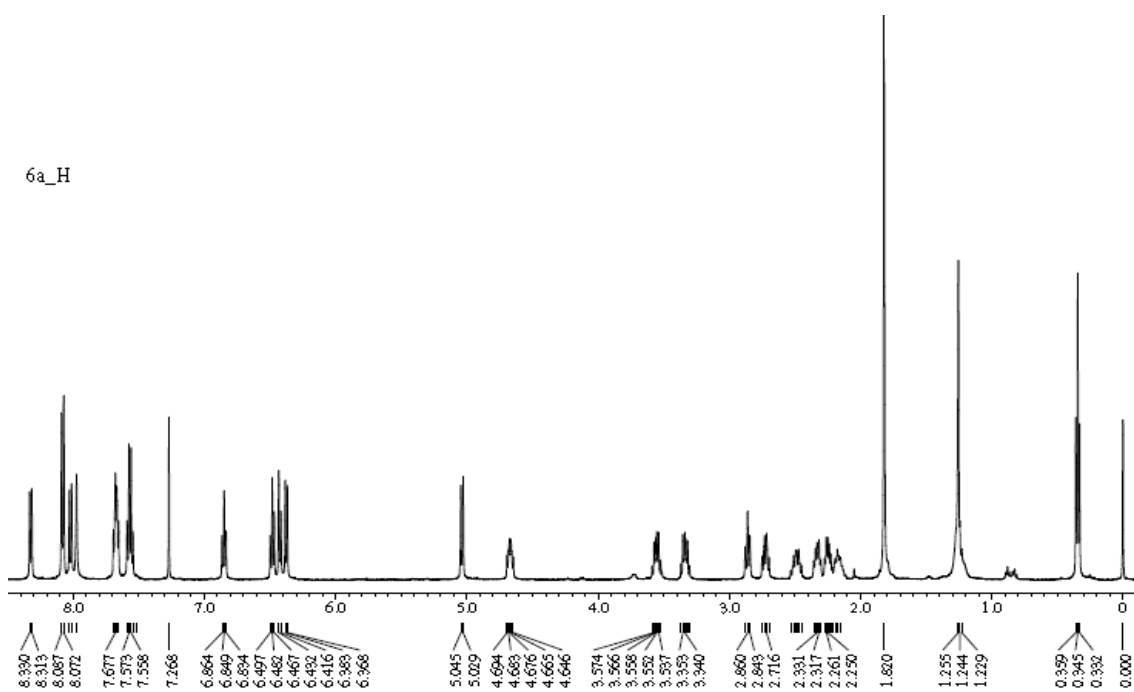


Figure S69.  $^1\text{H}$  NMR spectrum of **6a**

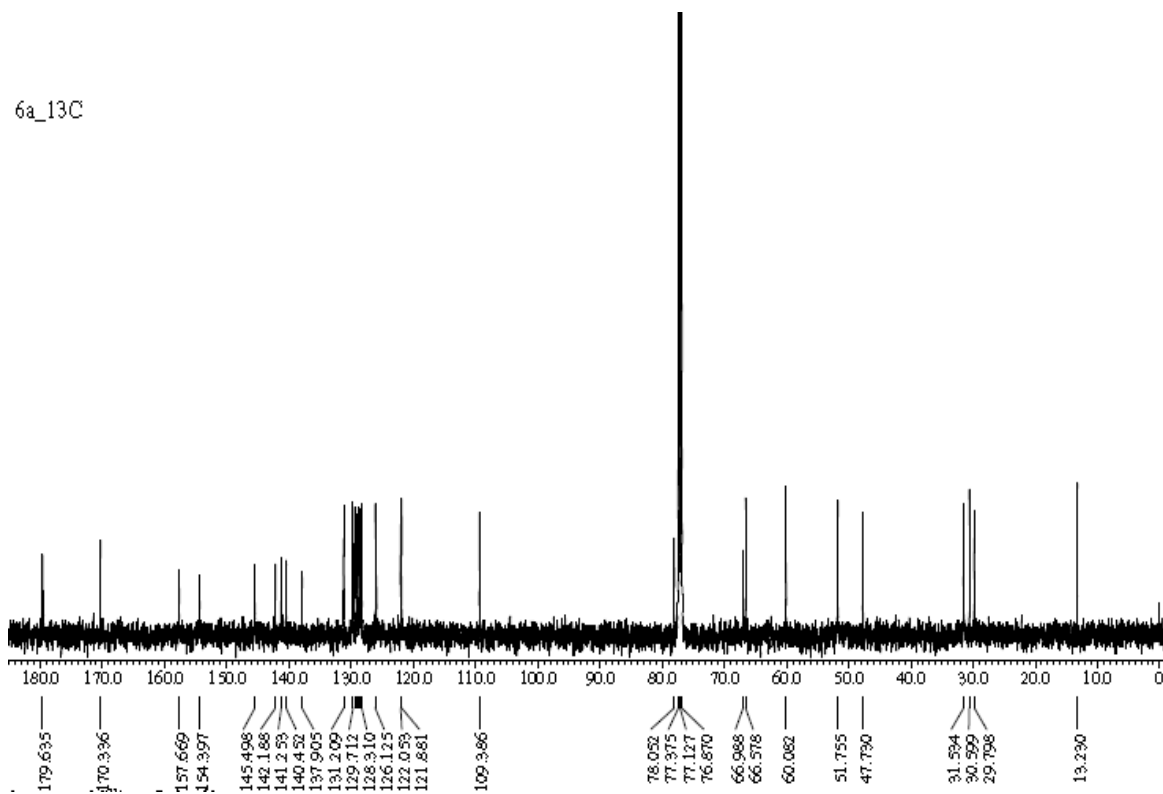


Figure S20.  $^{13}\text{C}$  NMR spectrum of **6a**

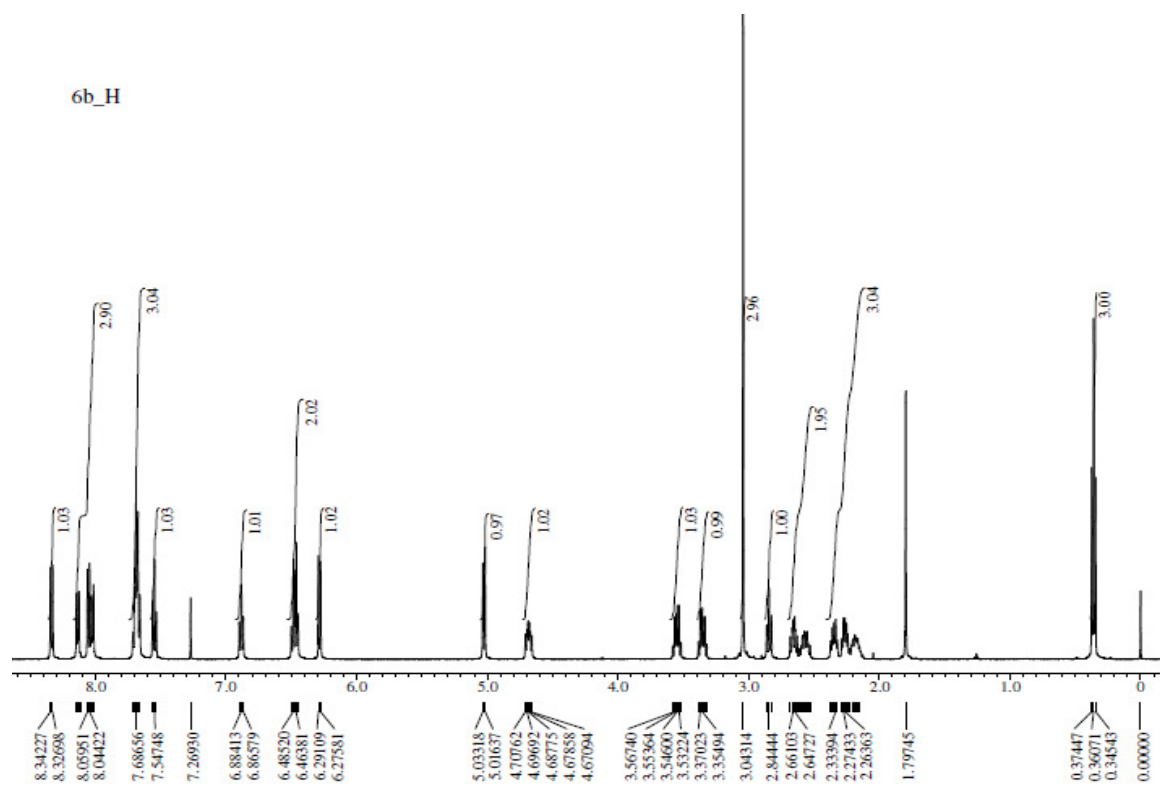


Figure S21. <sup>1</sup>H NMR spectrum of 6b

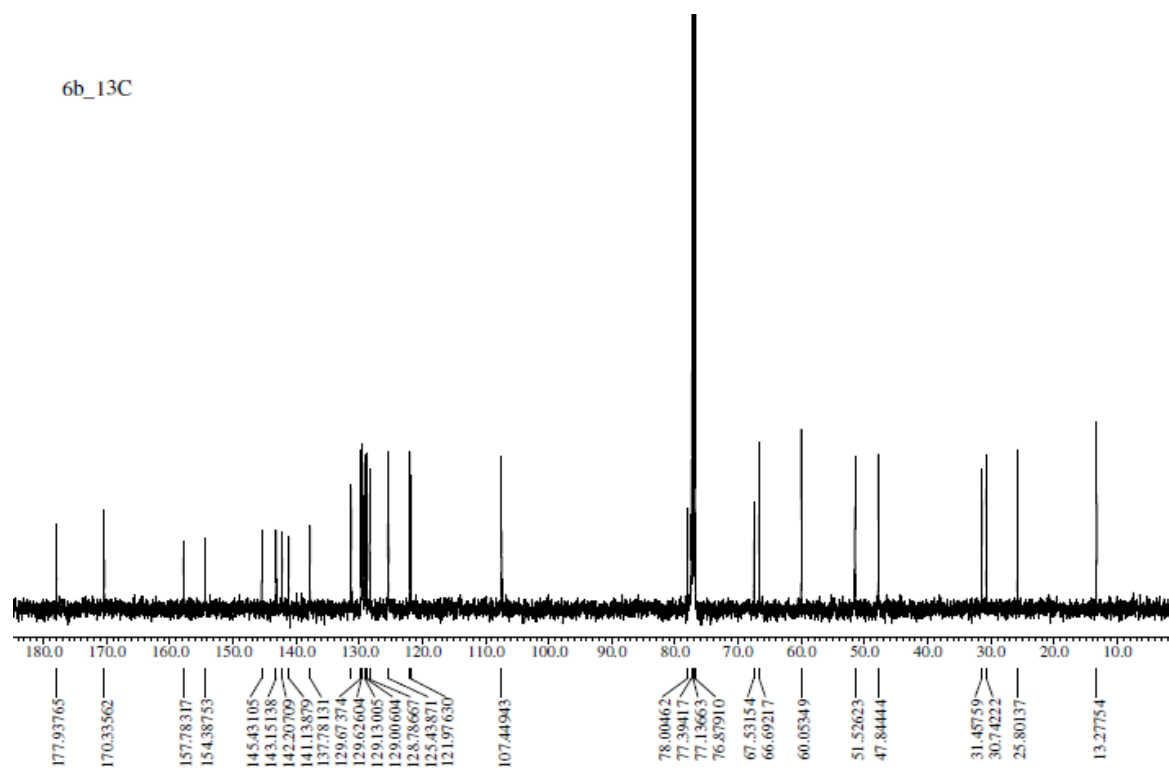


Figure S22. <sup>13</sup>C NMR spectrum of 6b

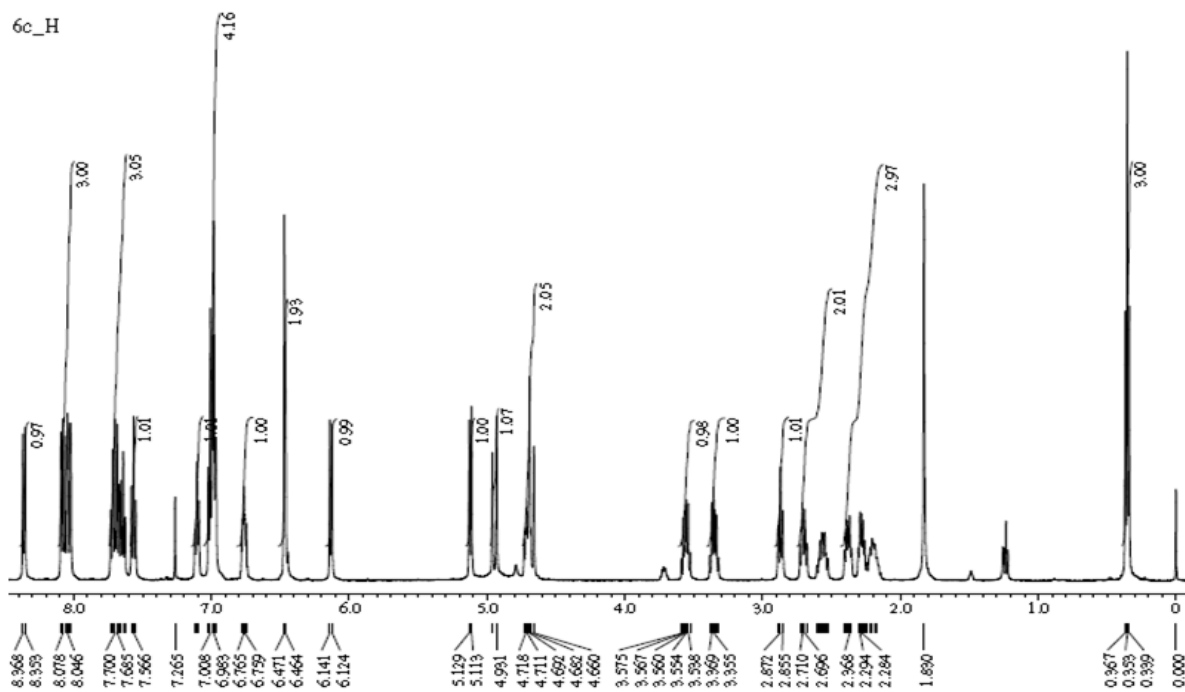


Figure S23. <sup>1</sup>H NMR spectrum of 6c

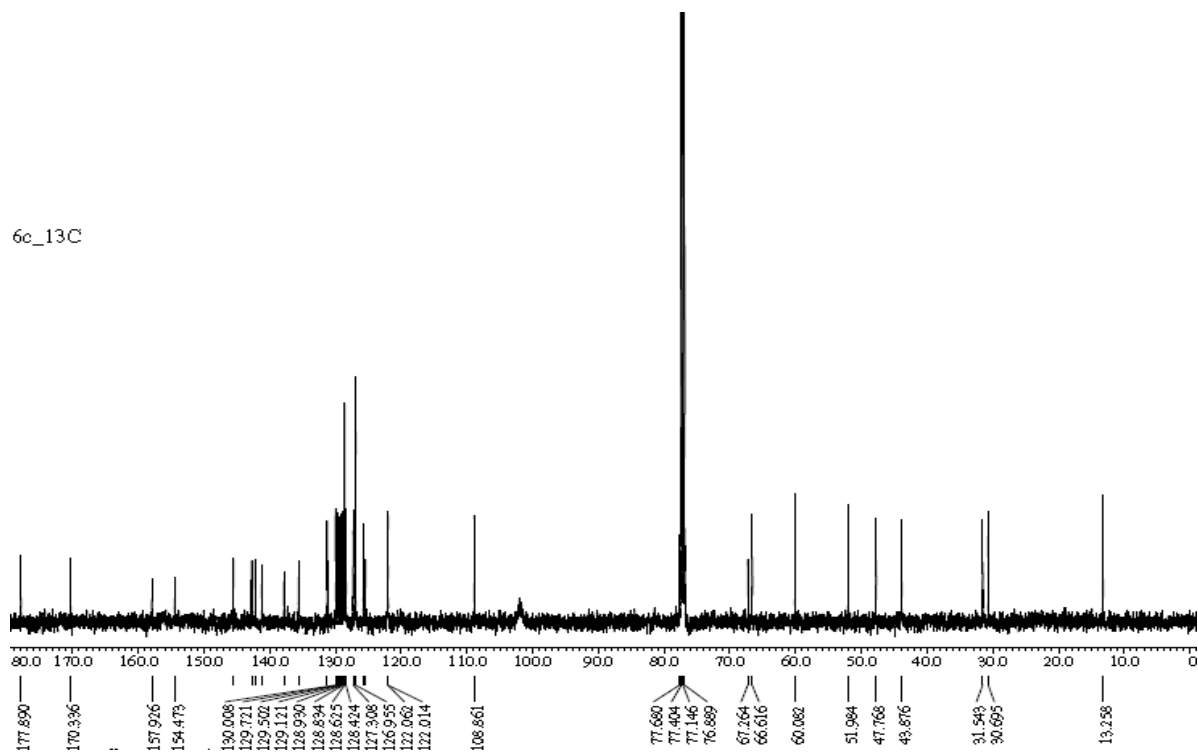


Figure S24. <sup>13</sup>C NMR spectrum of 6c

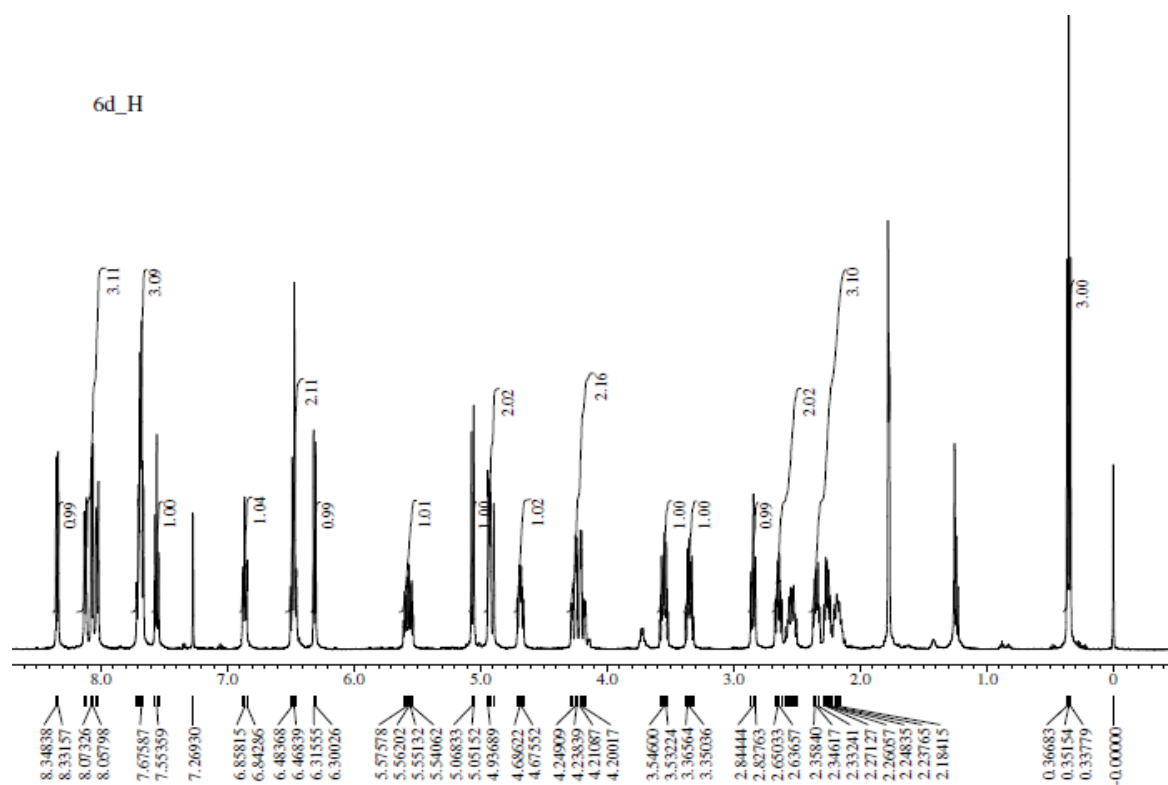


Figure S25. <sup>1</sup>H NMR spectrum of 6d

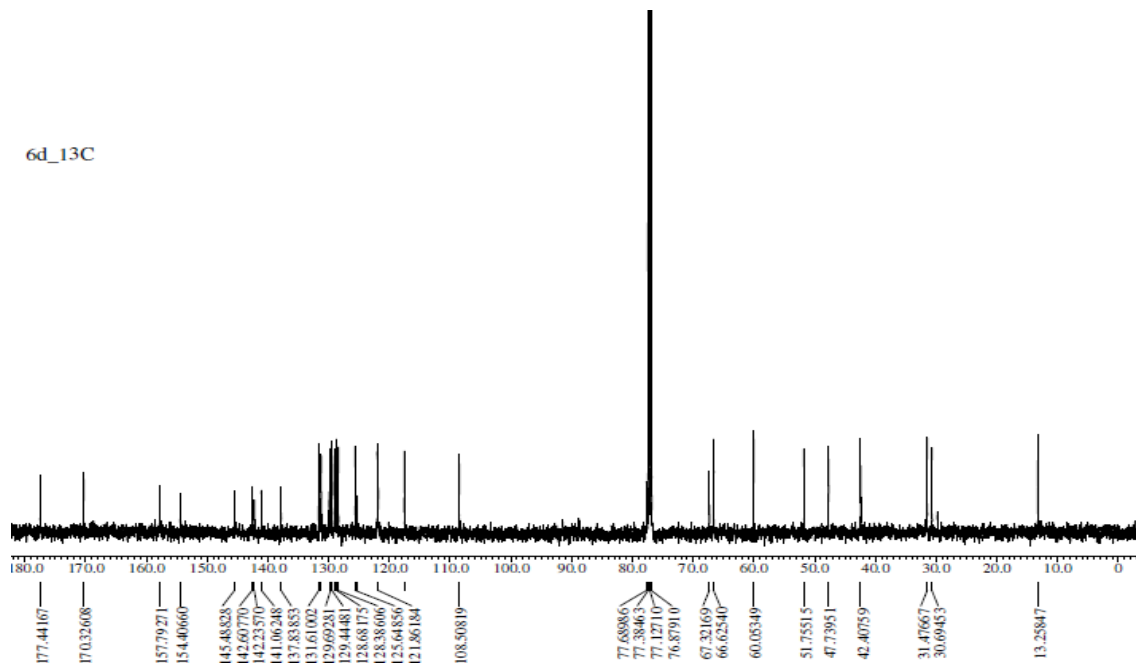
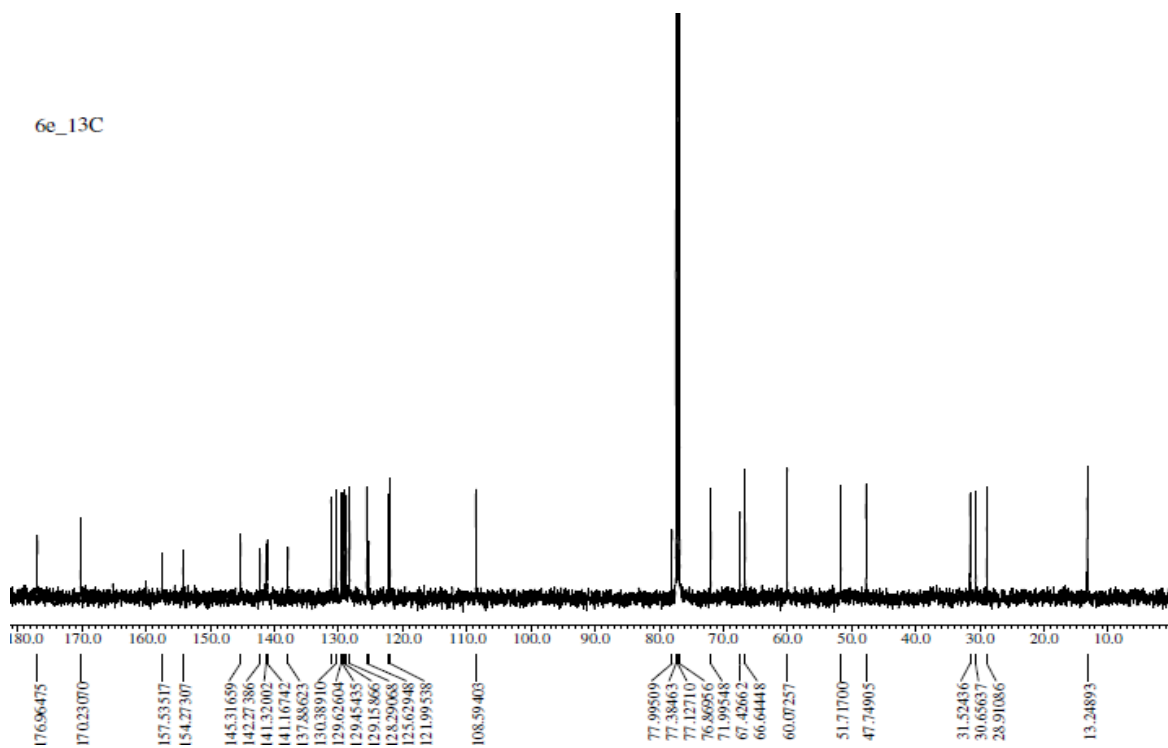
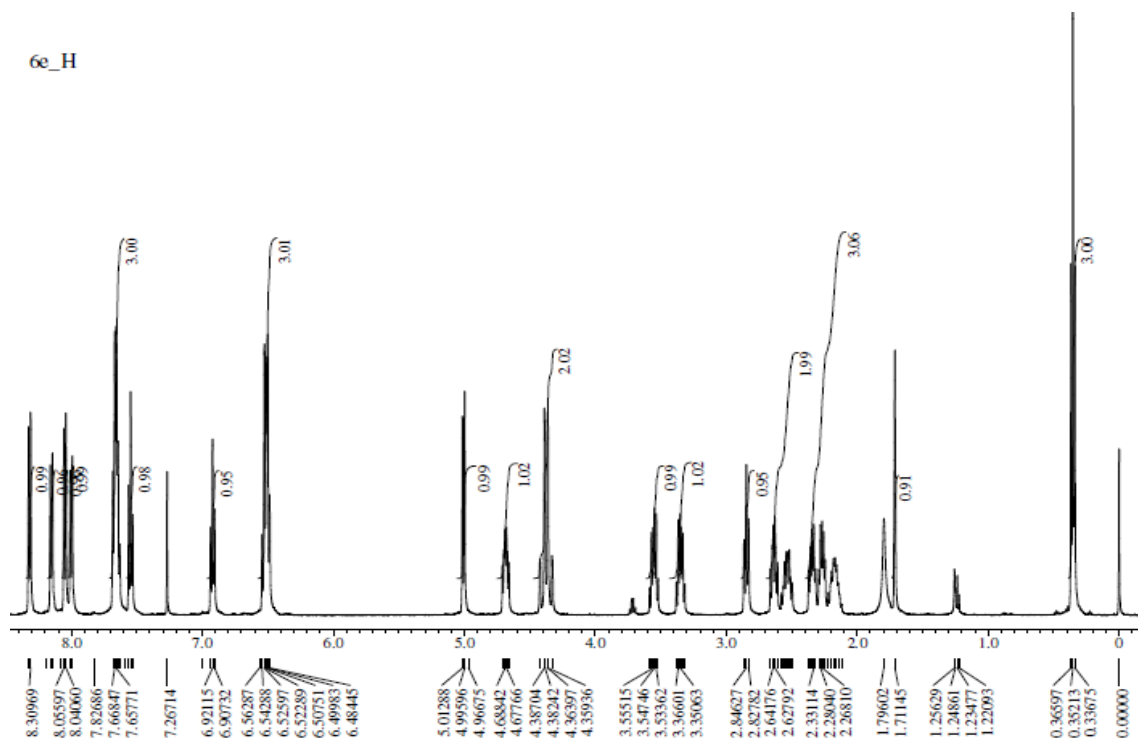


Figure S26. <sup>13</sup>C NMR spectrum of 6d



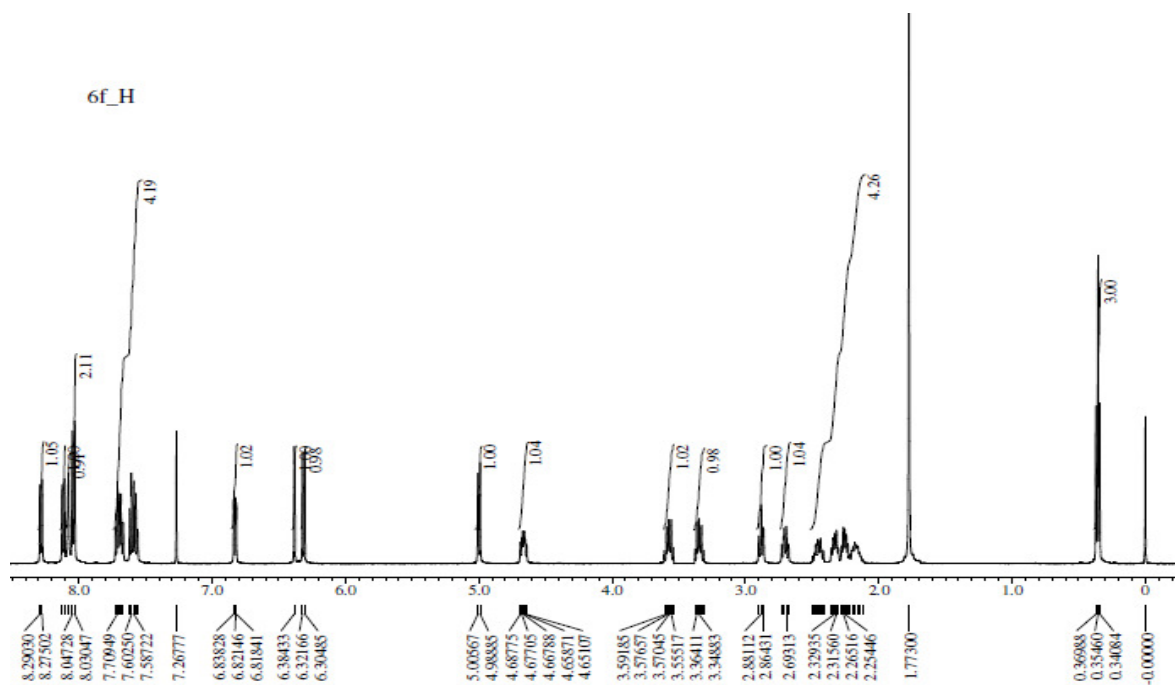


Figure S29. <sup>1</sup>H NMR spectrum of 6f

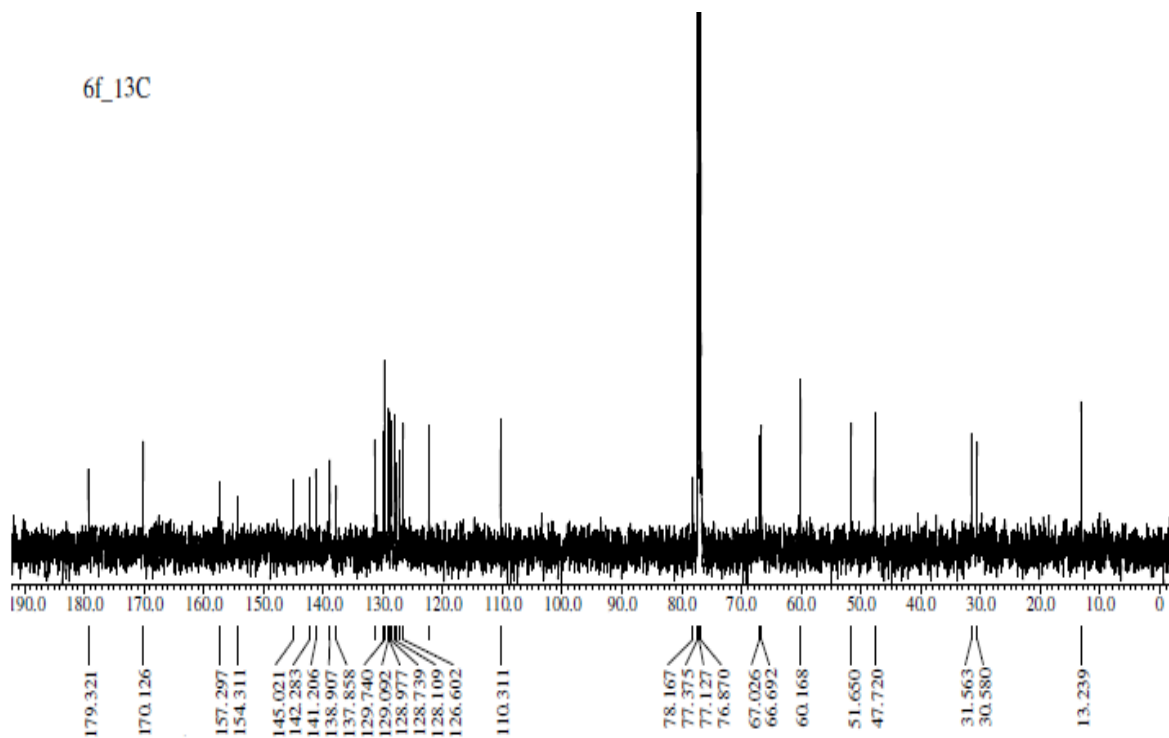


Figure S30. <sup>13</sup>C NMR spectrum of 6f

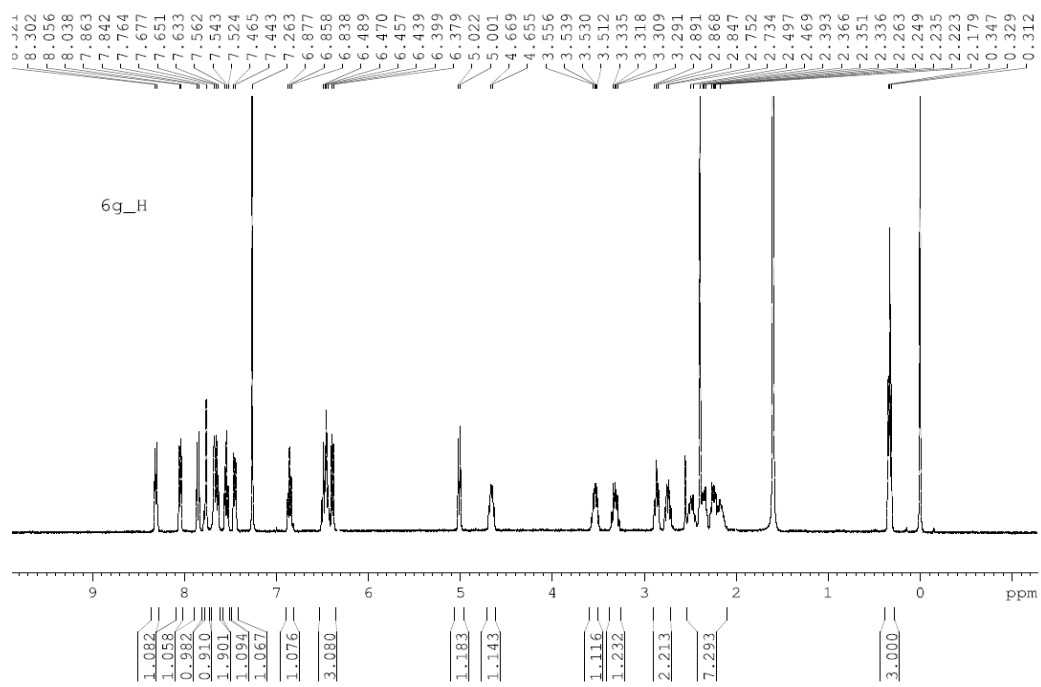


Figure S37.  $^1\text{H}$  NMR spectrum of **6g**

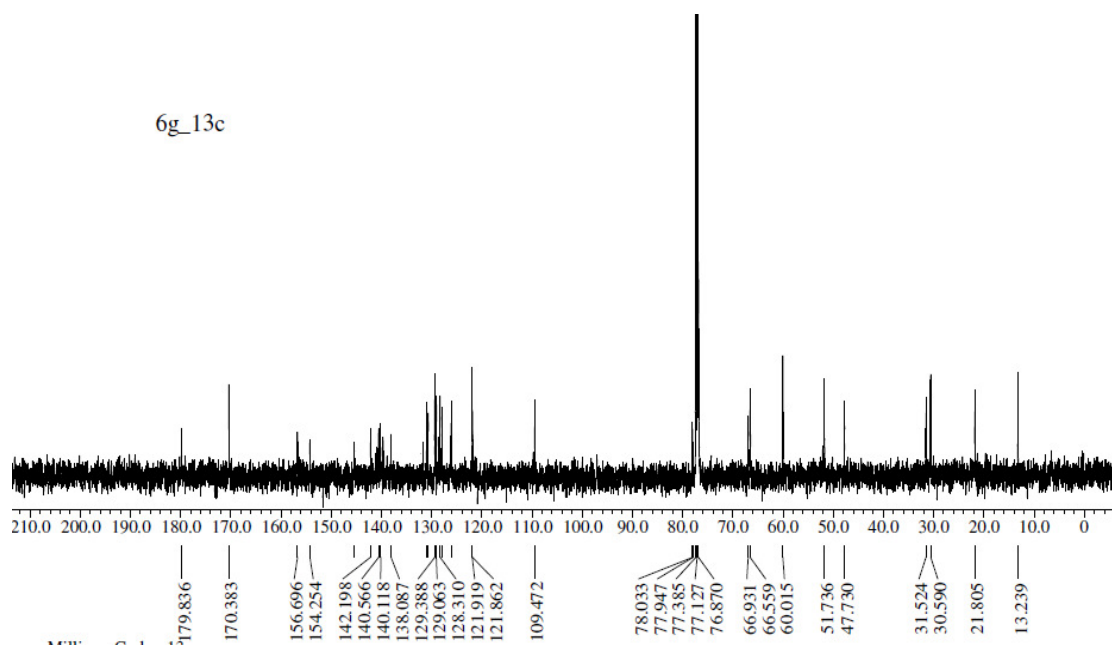


Figure S32.  $^{13}\text{C}$  NMR spectrum of **6g**



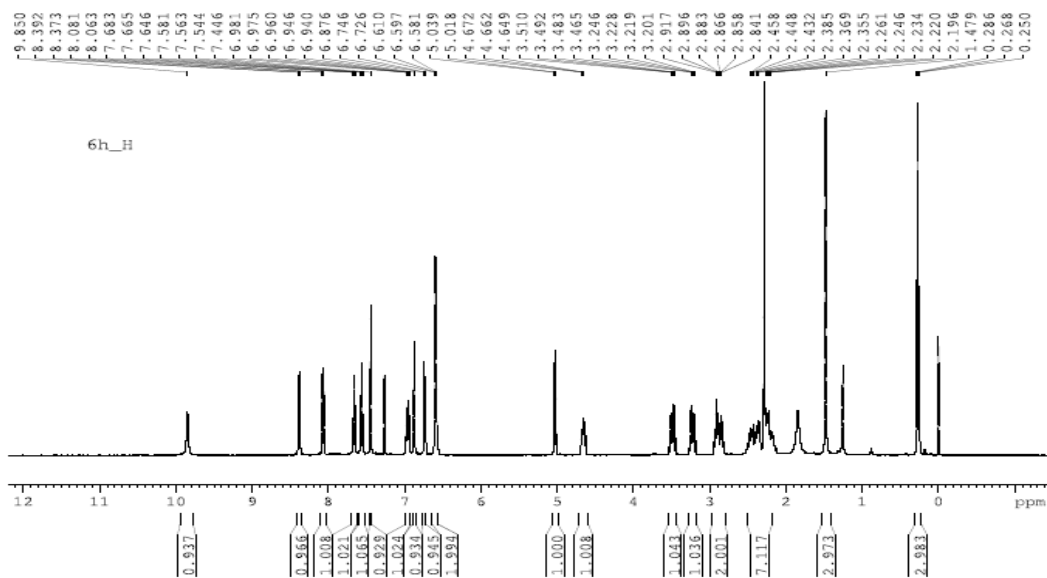


Figure S33. <sup>1</sup>H NMR spectrum of 6h

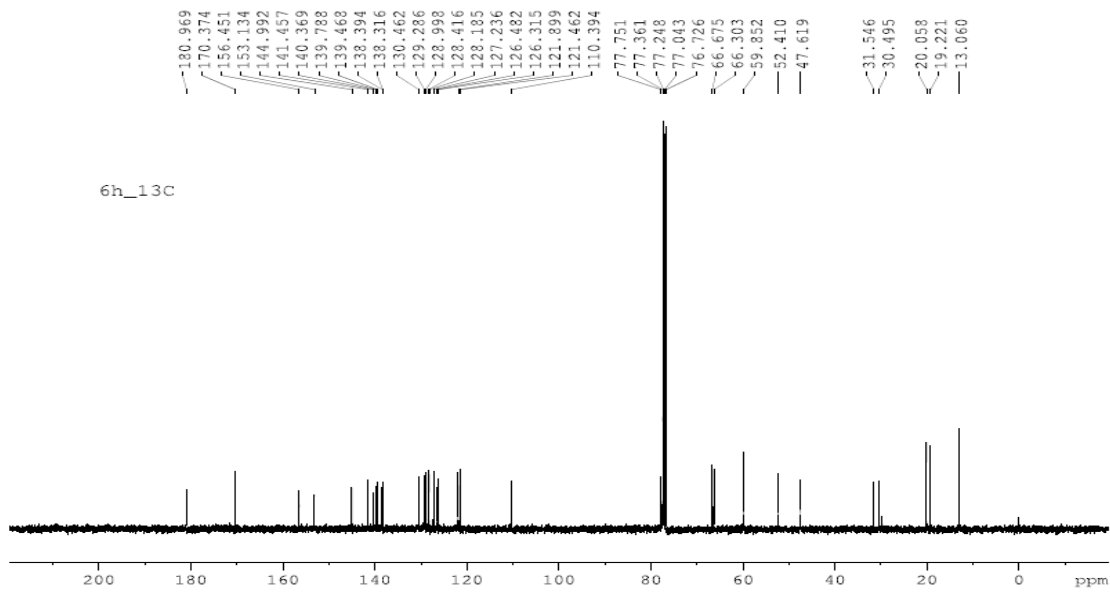
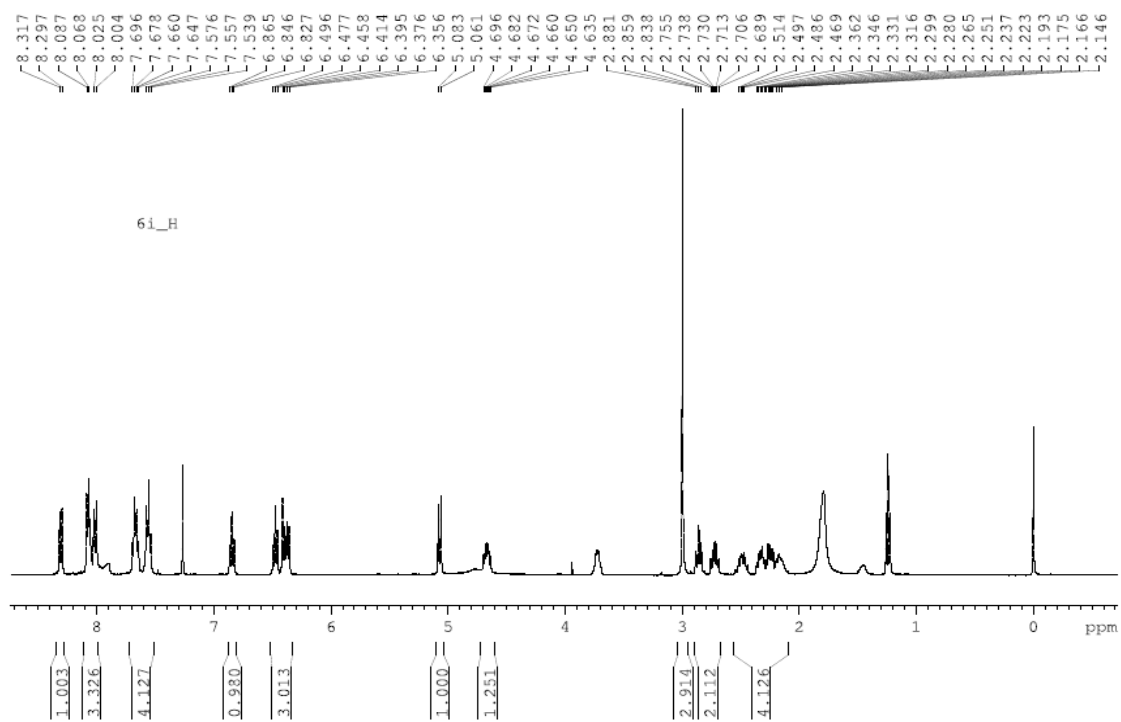
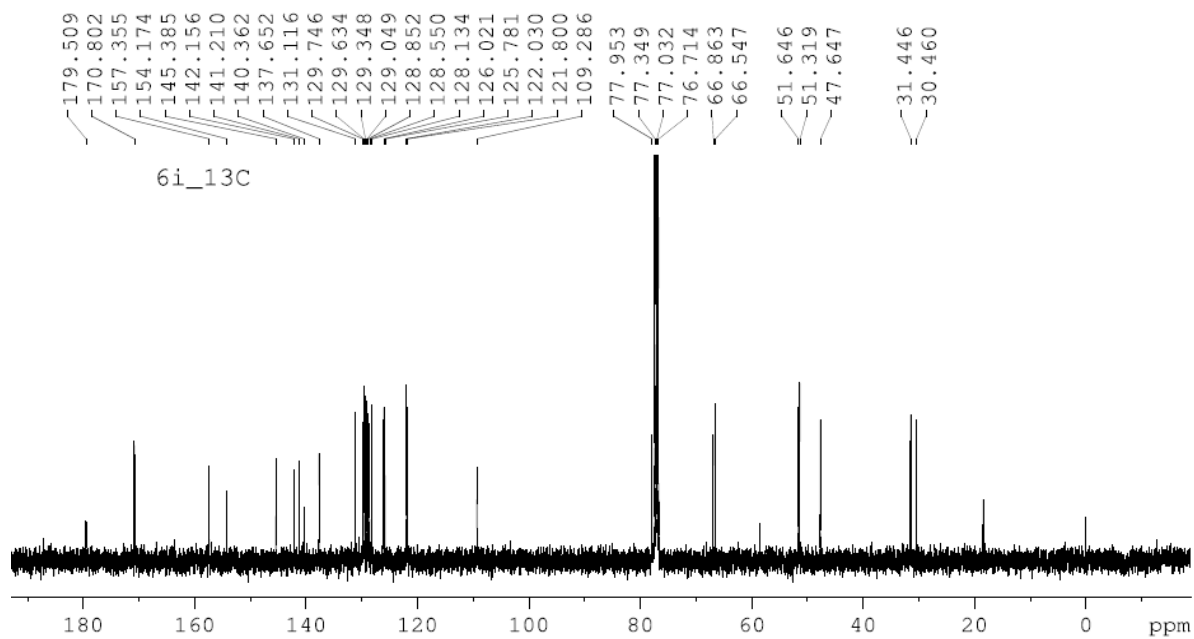


Figure S34. <sup>13</sup>C NMR spectrum of 6h



**Figure S35.**  $^1\text{H}$  NMR spectrum of **6i**



**Figure S36.**  $^{13}\text{C}$  NMR spectrum of **6i**

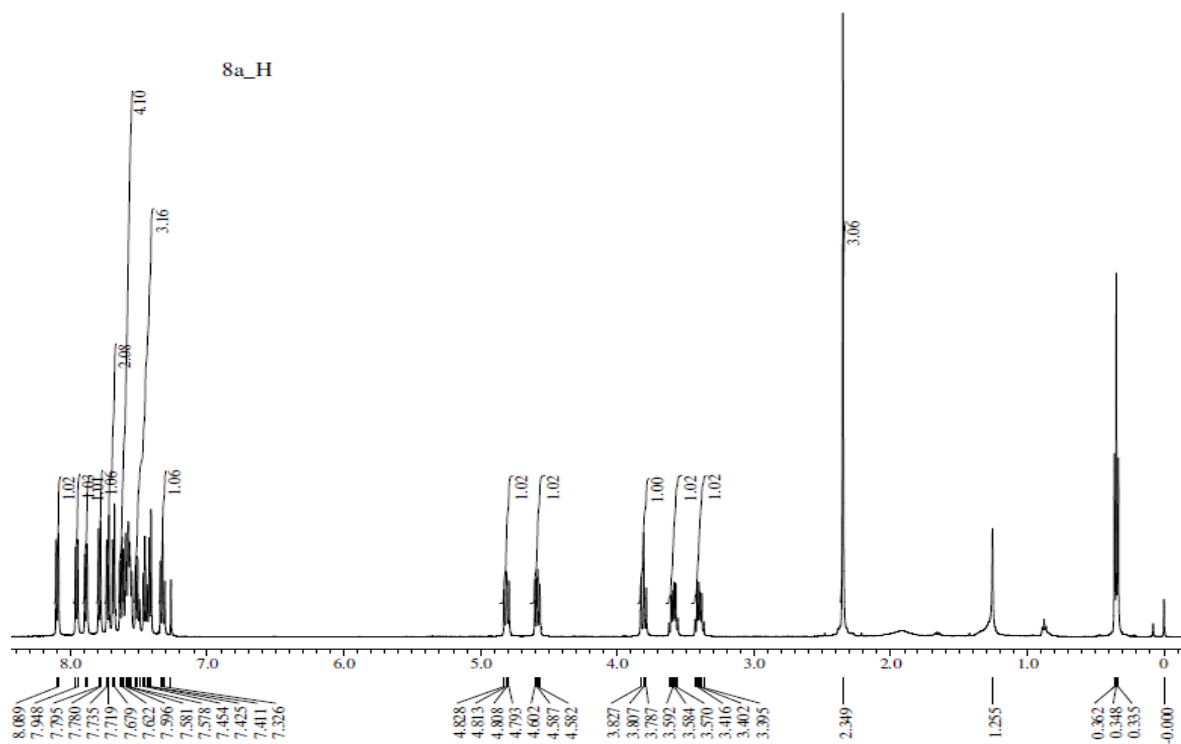


Figure S37.. <sup>1</sup>H NMR spectrum of 8a

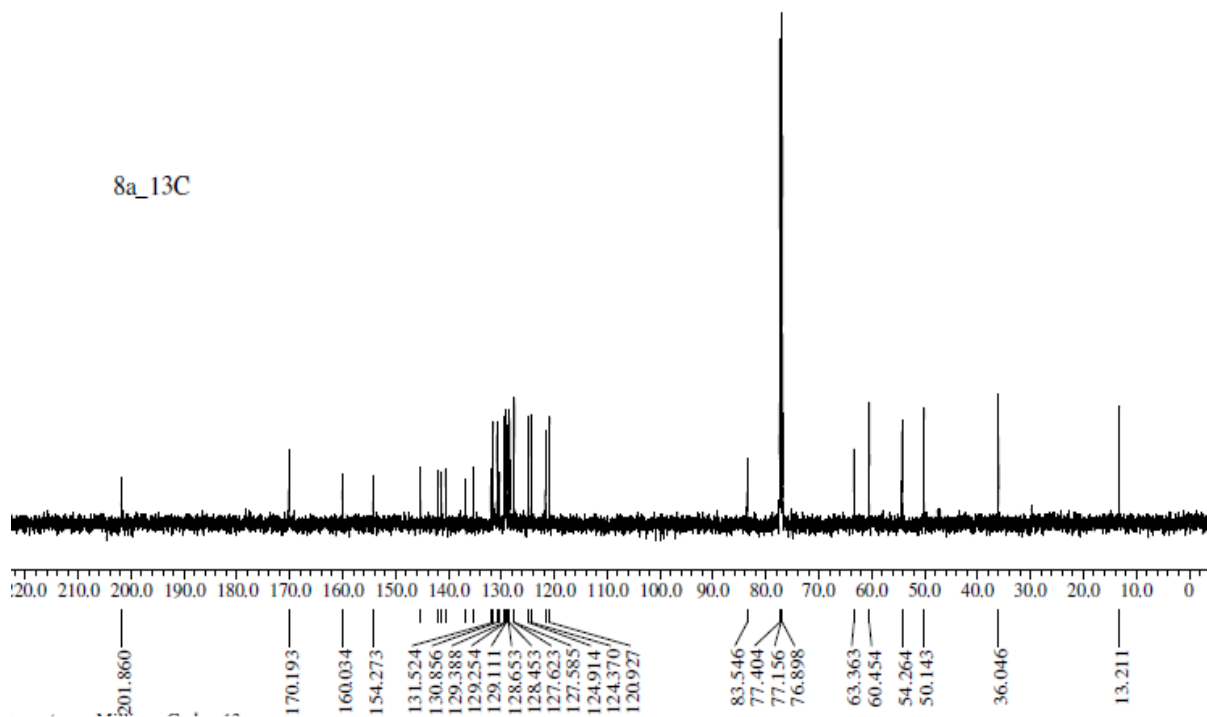
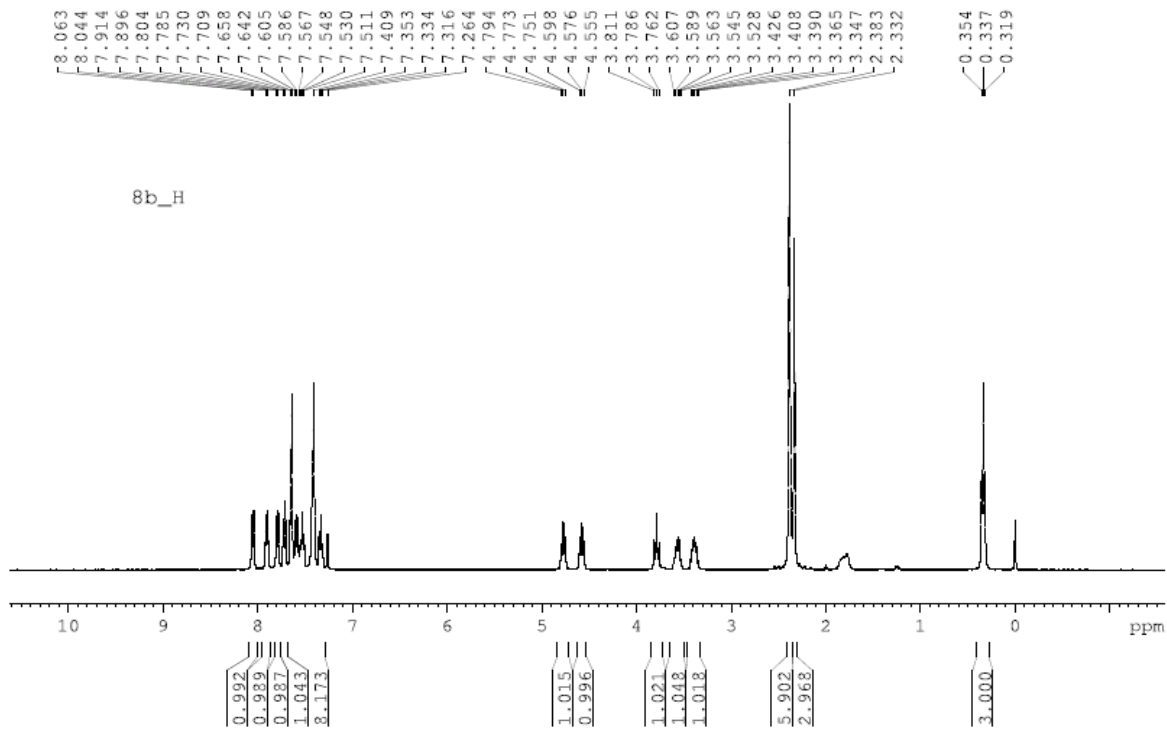
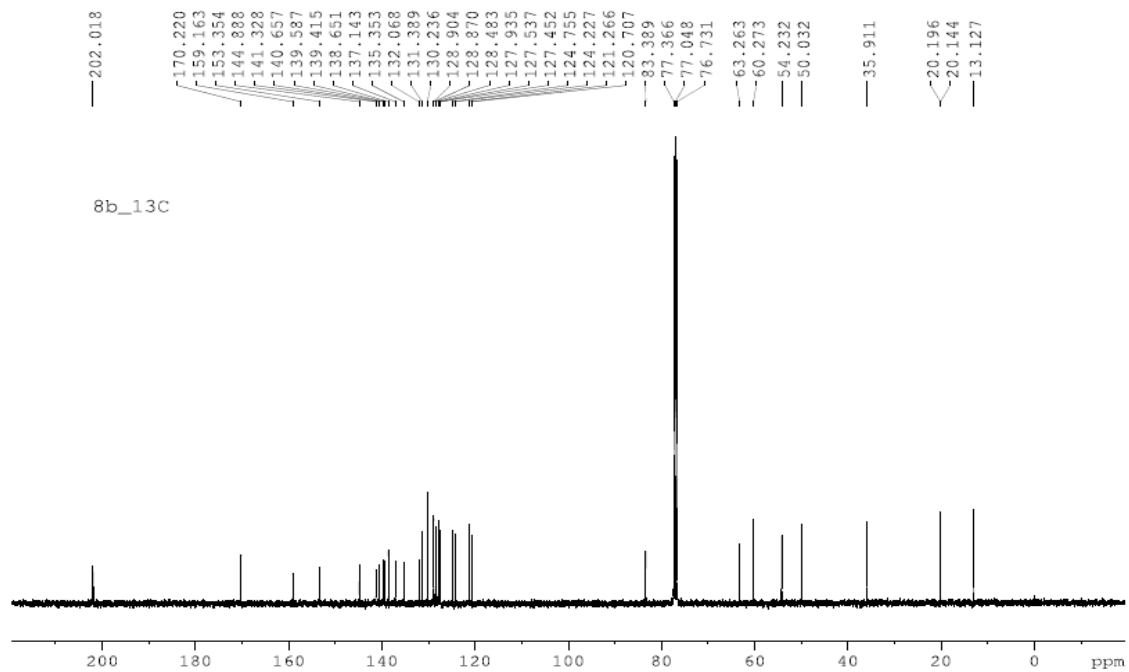


Figure S38.. <sup>13</sup>C NMR spectrum of 8a



**Figure S39.** <sup>1</sup>H NMR spectrum of **8b**



**Figure S40.** <sup>13</sup>C NMR spectrum of **8b**

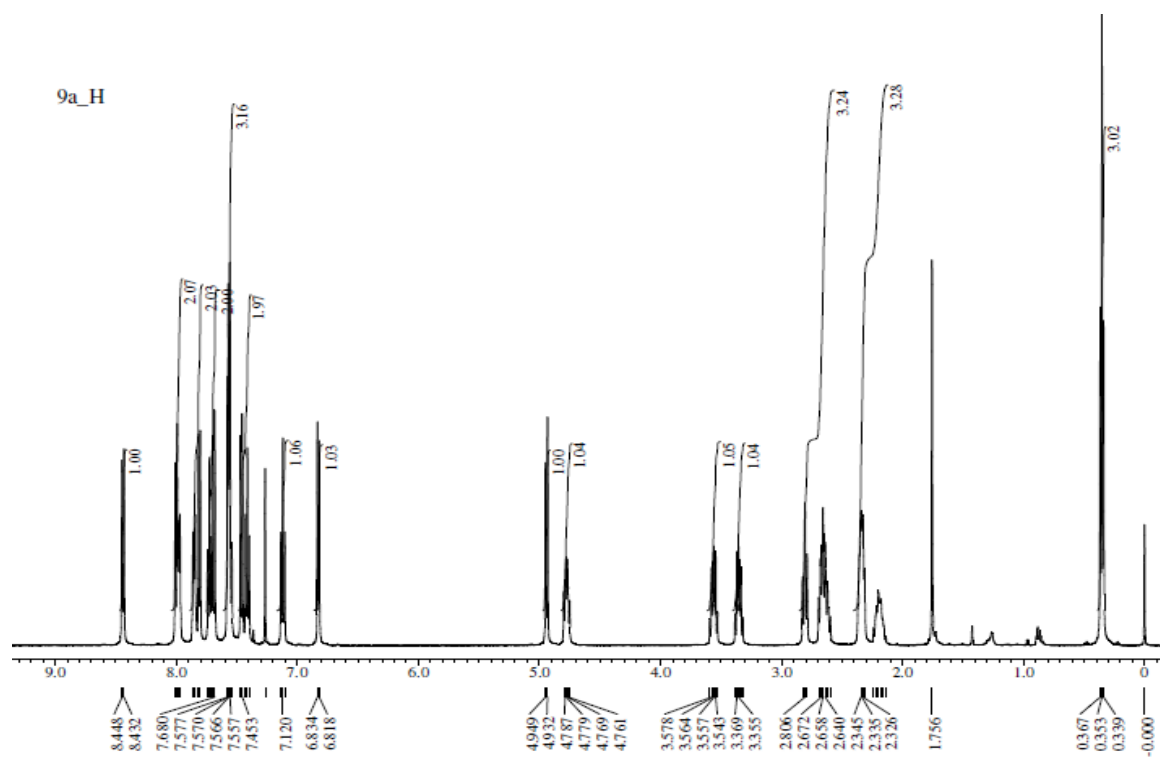


Figure S41. <sup>1</sup>H NMR spectrum of 9a

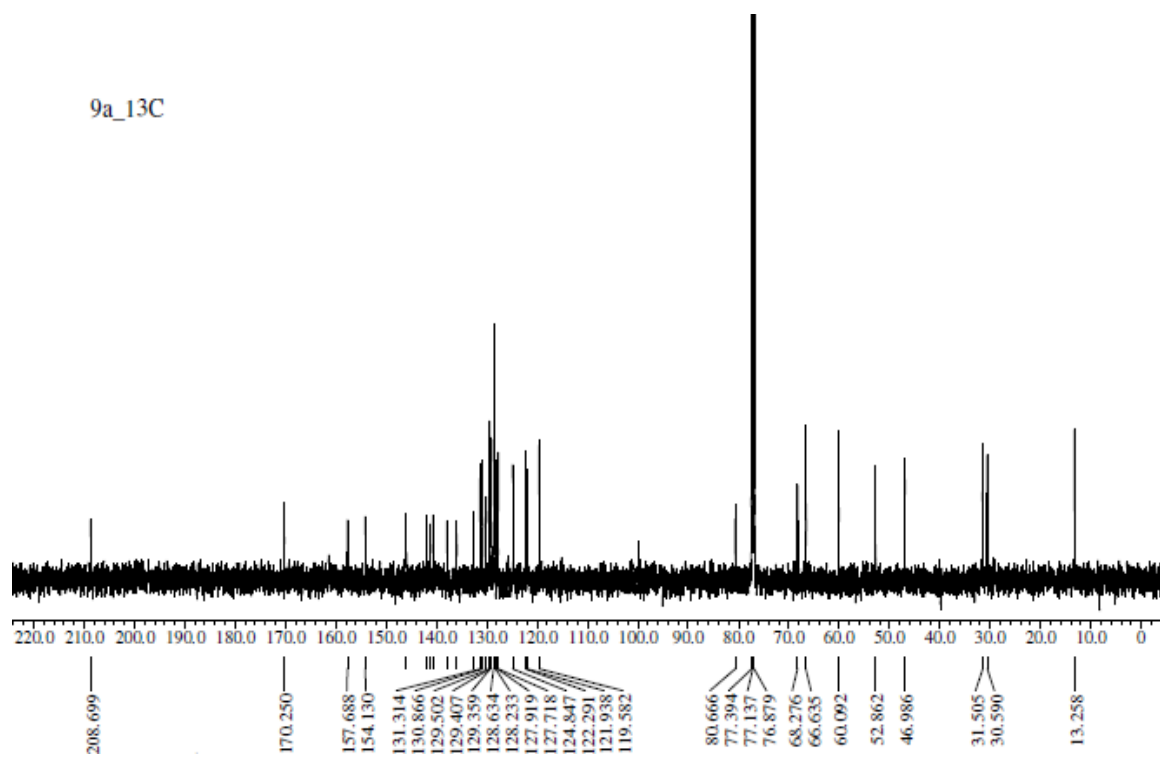


Figure S42. <sup>13</sup>C NMR spectrum of 9a

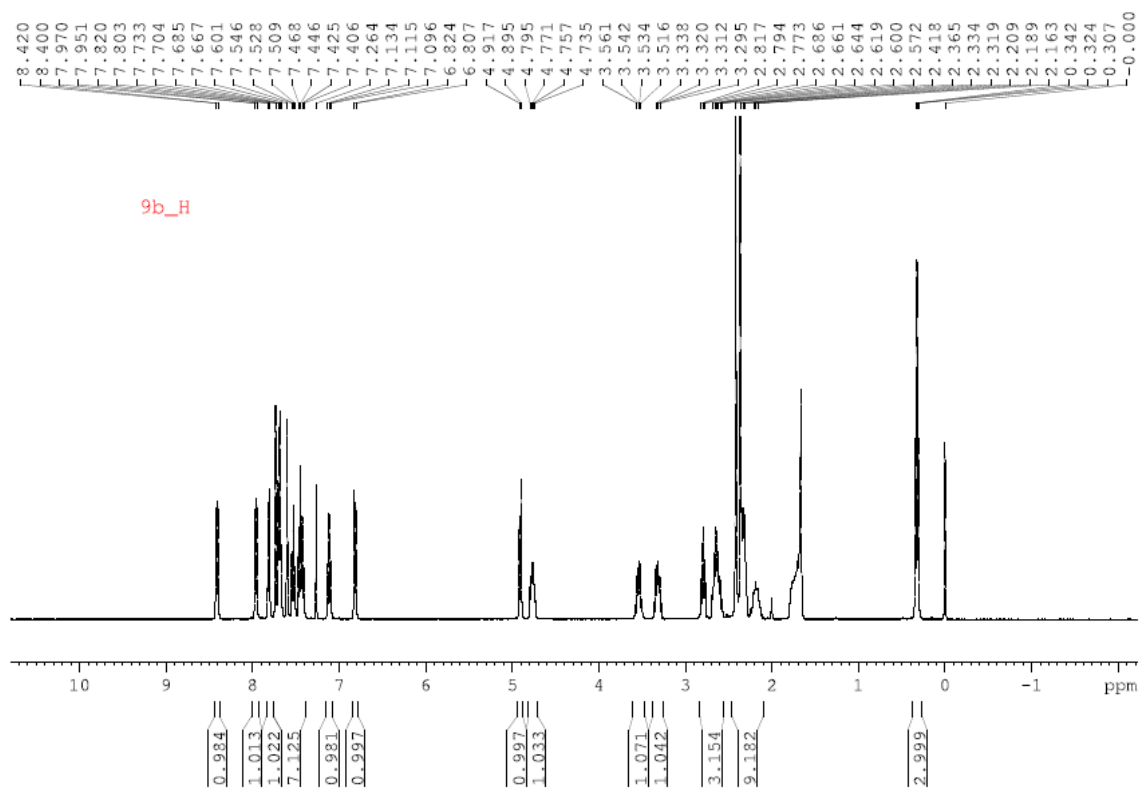


Figure S43.  $^1\text{H}$  NMR spectrum of **9b**

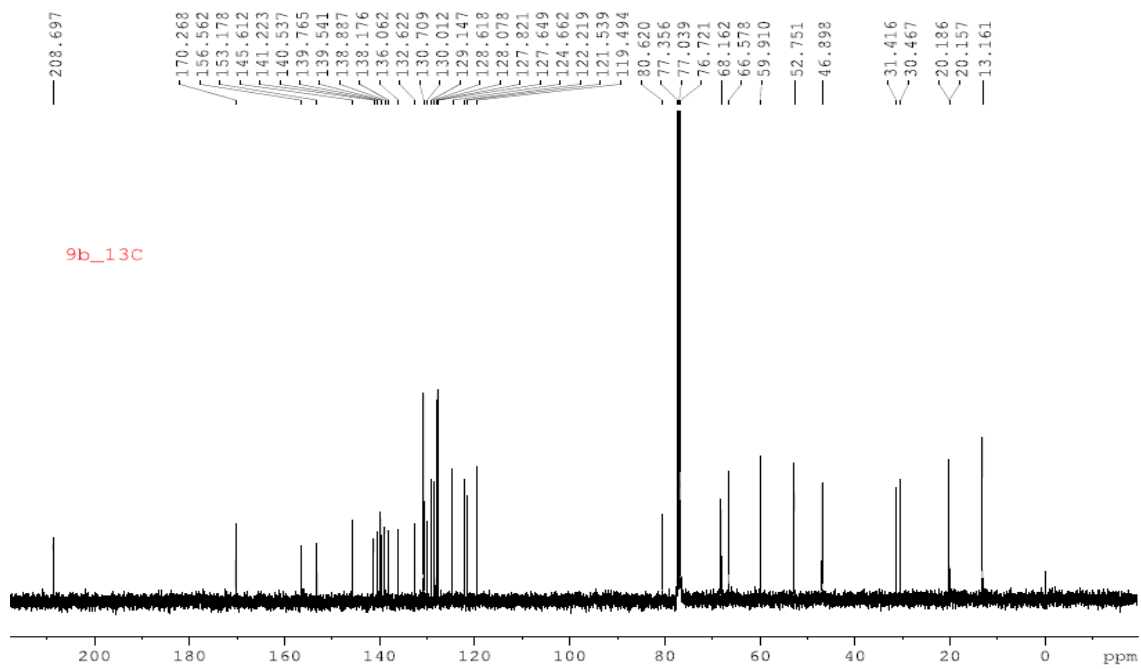


Figure S44.  $^{13}\text{C}$  NMR spectrum of **9b**

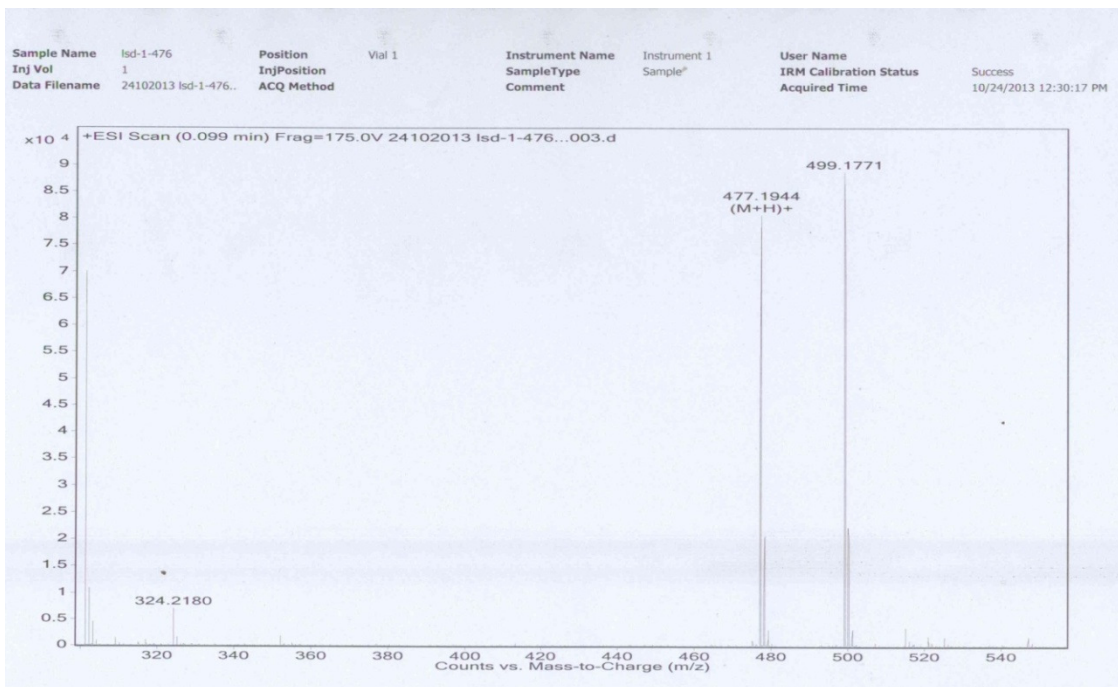


Figure S45. HRMS spectra of 4a

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Single Mass Analysis (displaying only valid results)

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

QTOF MICRO

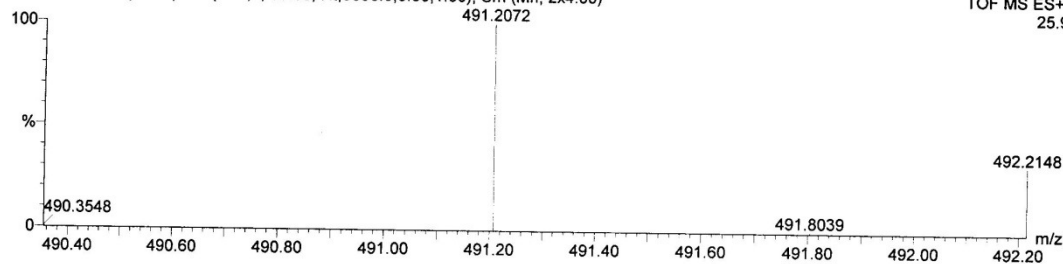
DEPARTMENT OF CHEMISTRY IITM

26-Oct-2013 16:13:33

EXT-LSD-4B 89 (1.658) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00)

TOF MS ES+

25.9



Minimum:

Maximum: 200.0 5.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
491.2072	491.2083	-1.2	-2.4	19.5	1	C30 H27 N4 O3

Figure S46. HRMS spectra of 4b

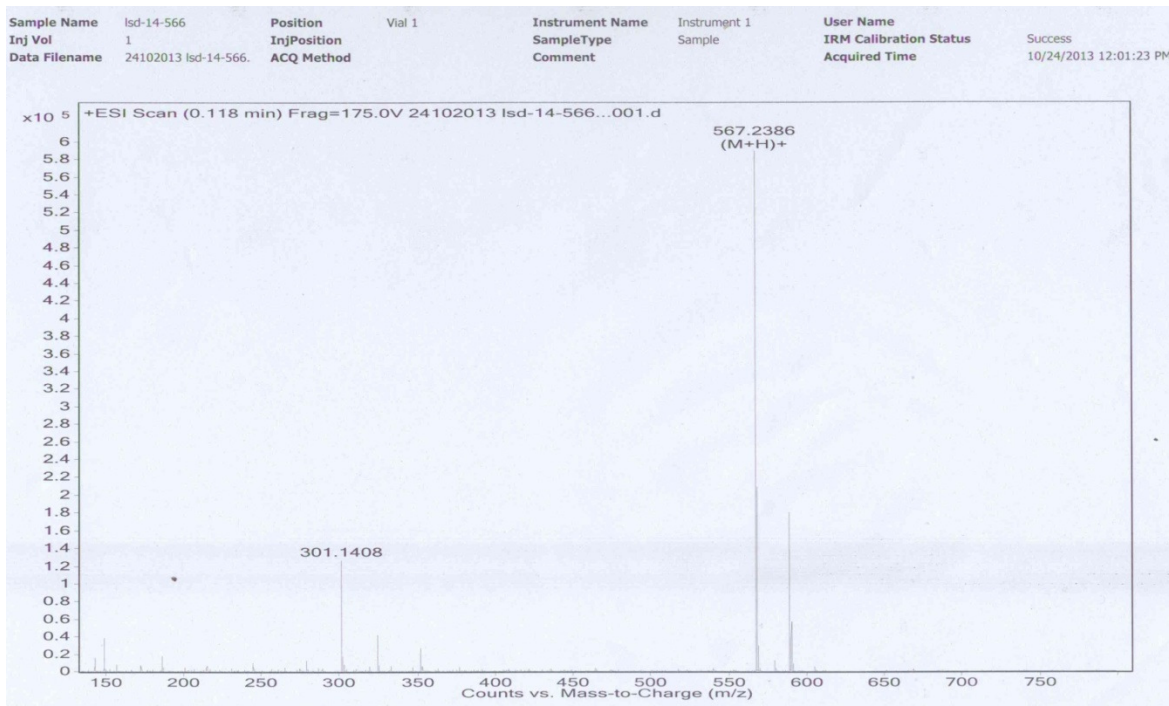


Figure S47. HRMS spectra of **4c**

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Single Mass Analysis (displaying only valid results)

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

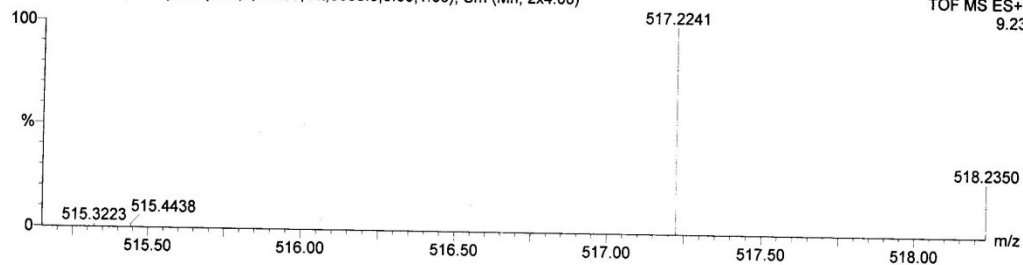
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

QTOF MICRO DEPARTMENT OF CHEMISTRY IITM  
 EXT-LSD-4D 77 (1.434) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00)

26-Oct-2013 16:16:26  
 TOF MS ES+  
 9.23



Minimum:				-1.5		
Maximum:		200.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
517.2241	517.2240	0.2	0.3	20.5	1	C32 H29 N4 O3

Figure S48. HRMS spectra of **4d**



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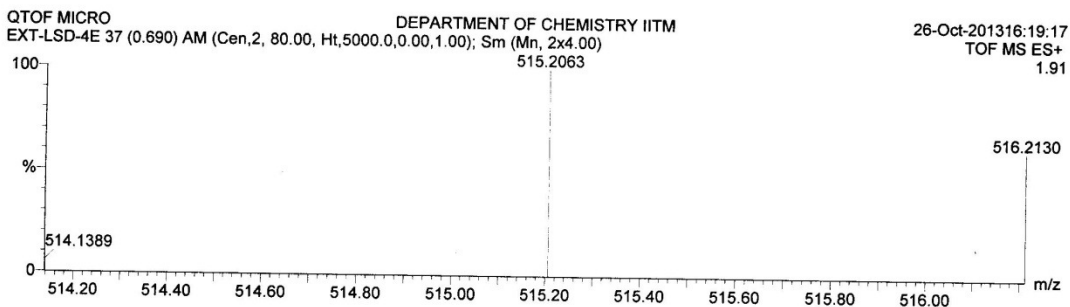
### Single Mass Analysis (displaying only valid results)

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)



Minimum:				-1.5					
Maximum:		200.0	5.0	50.0					
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula			
515.2063	515.2083	-2.0	-3.9	21.5	1	C32	H27	N4	O3

Figure S49. HRMS spectra of 4e

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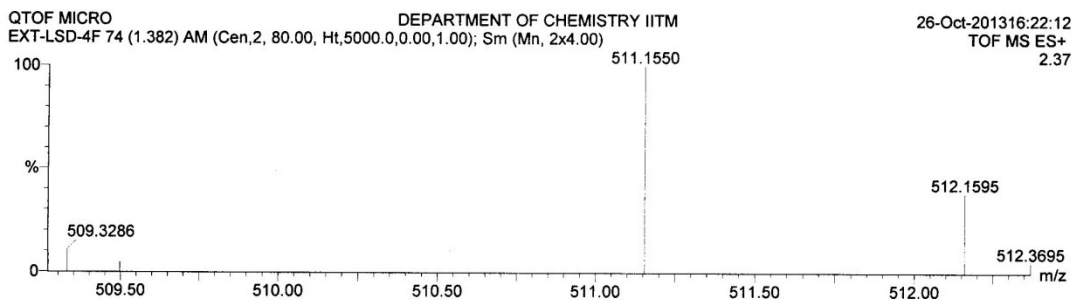
### Single Mass Analysis (displaying only valid results)

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

29 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)



Minimum:				-1.5					
Maximum:		200.0	5.0	50.0					
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula			
511.1550	511.1537	1.3	2.6	19.5	1	C29	H24	N4	O3 C1

Figure S50. HRMS spectra of 4f

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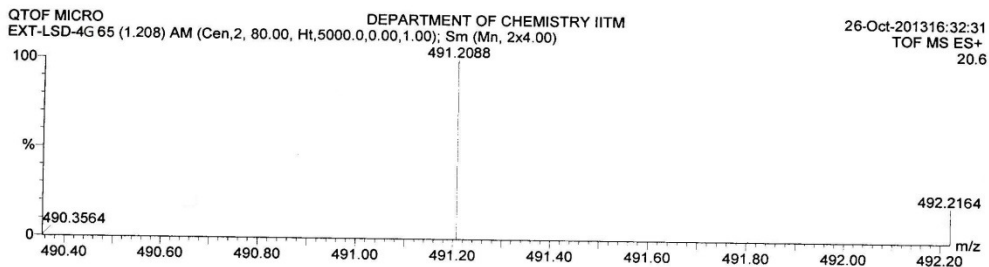
#### Single Mass Analysis (displaying only valid results)

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)



Minimum:				-1.5		
Maximum:	200.0	5.0		50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
491.2088	491.2083	0.5	1.0	19.5	1	C30 H27 N4 O3

Figure S51. HRMS spectra of 4g

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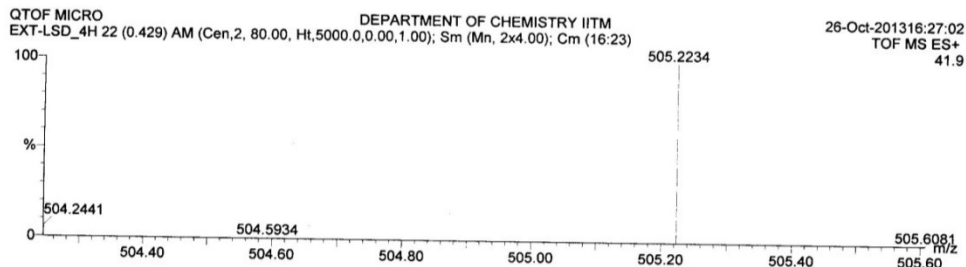
#### Single Mass Analysis (displaying only valid results)

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)



Minimum:				-1.5		
Maximum:	200.0	5.0		50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
505.2234	505.2240	-0.6	-1.2	19.5	1	C31 H29 N4 O3

Figure S52. HRMS spectra of 4h

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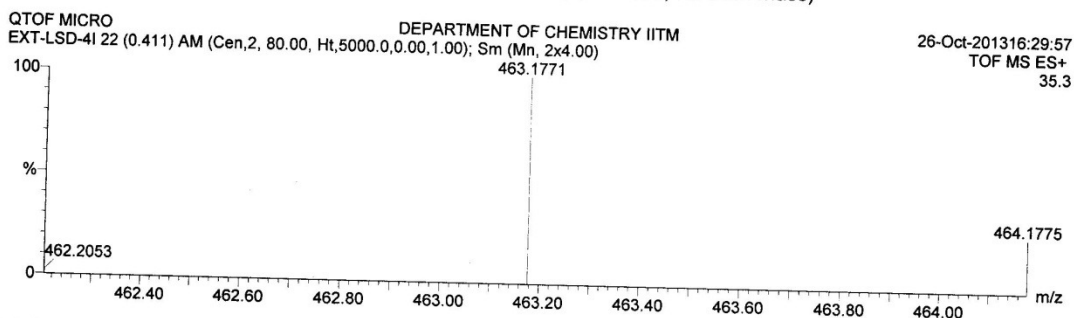
### Single Mass Analysis (displaying only valid results)

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)



Minimum:						
Maximum:	200.0	5.0	-1.5			
			50.0			
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
463.1771	463.1770	0.1	0.2	19.5	1	C28 H23 N4 O3

Figure S53. HRMS spectra of **4i**

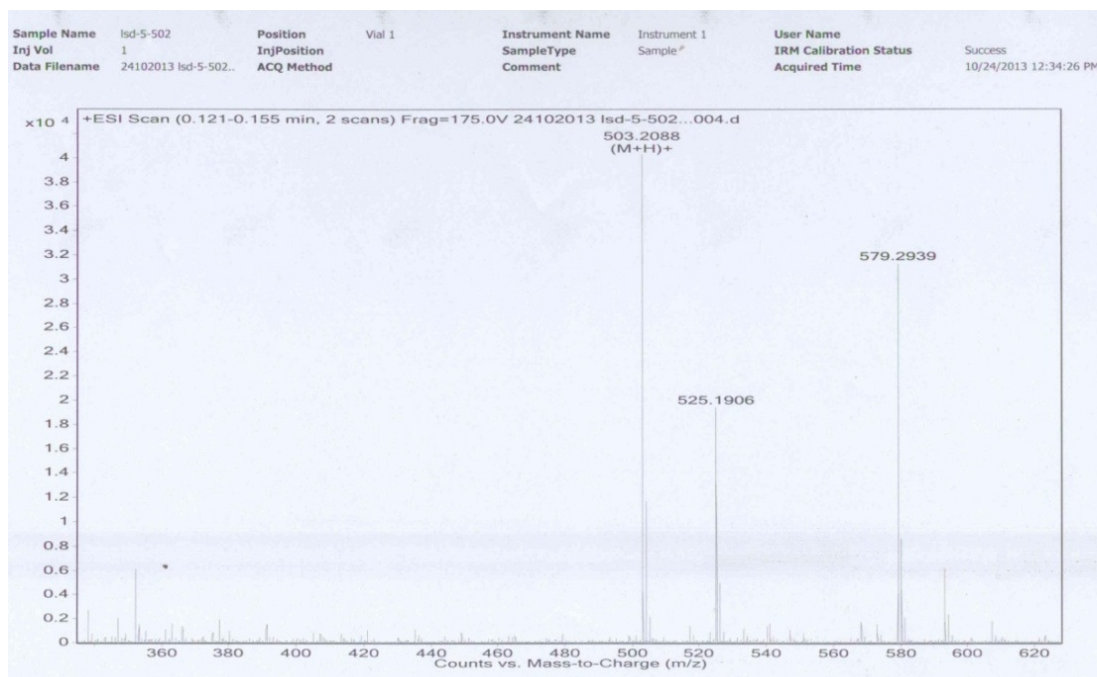


Figure S54. HRMS spectra of **6a**

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#### Single Mass Analysis (displaying only valid results)

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

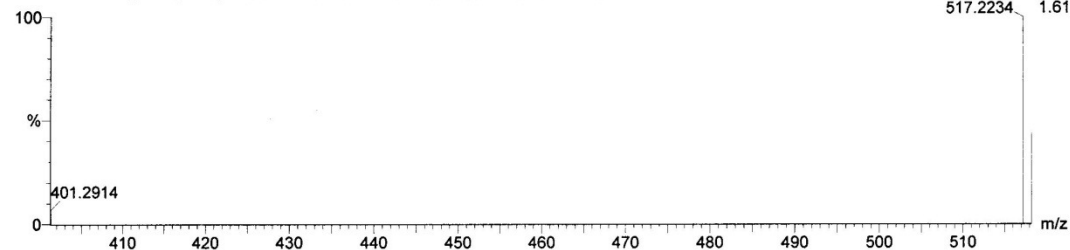
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

QTOF MICRO DEPARTMENT OF CHEMISTRY IITM  
EXT-LSD-6B 81 (1.509) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00)

26-Oct-2013 15:46:39  
TOF MS ES+  
517.2234 1.61



Minimum: -1.5  
Maximum: 200.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
517.2234	517.2240	-0.5	-1.0	20.5	1	C32 H29 N4 O3

Figure S55. HRMS spectra of **6b**

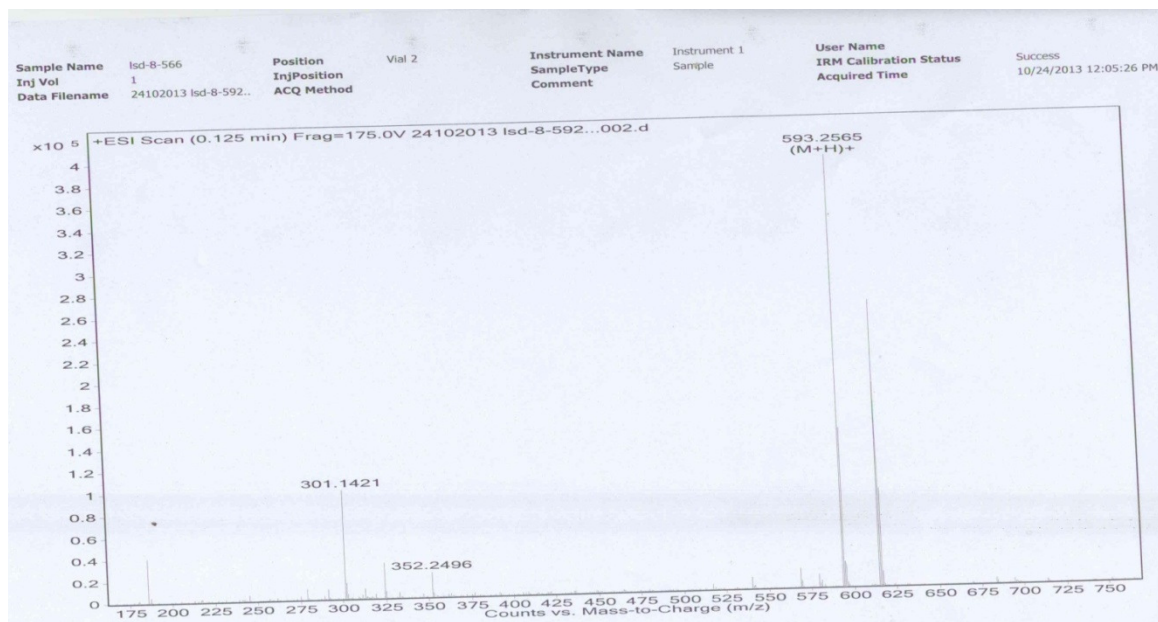


Figure S56. HRMS spectra of **6c**

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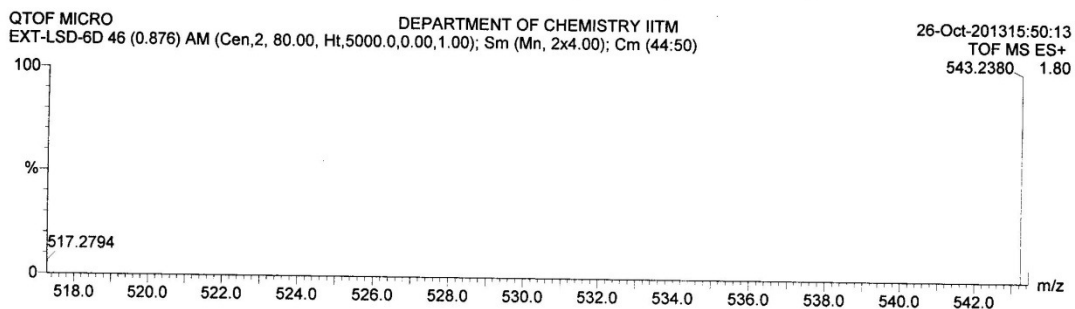
#### Single Mass Analysis (displaying only valid results)

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)



Minimum:				-1.5		
Maximum:	200.0	5.0		50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
543.2380	543.2396	-1.6	-3.0	21.5	1	C34 H31 N4 O3

Figure S57. HRMS spectra of 6d

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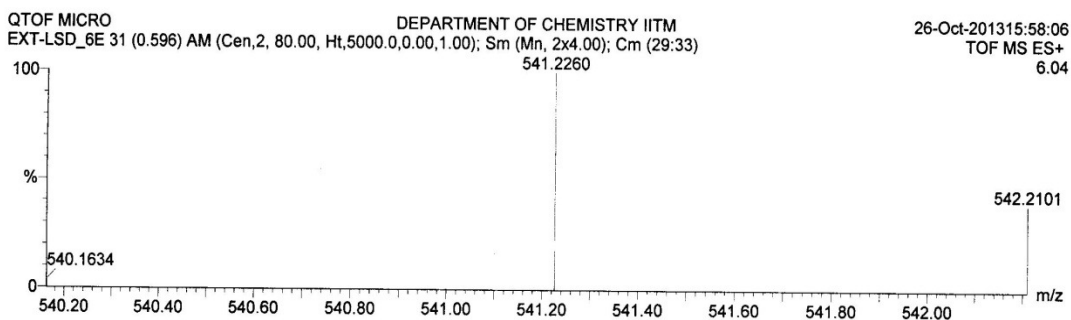
#### Single Mass Analysis (displaying only valid results)

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)



Minimum:				-1.5		
Maximum:	200.0	5.0		50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
541.2260	541.2240	2.0	3.8	22.5	1	C34 H29 N4 O3

Figure S58. HRMS spectra of 6e

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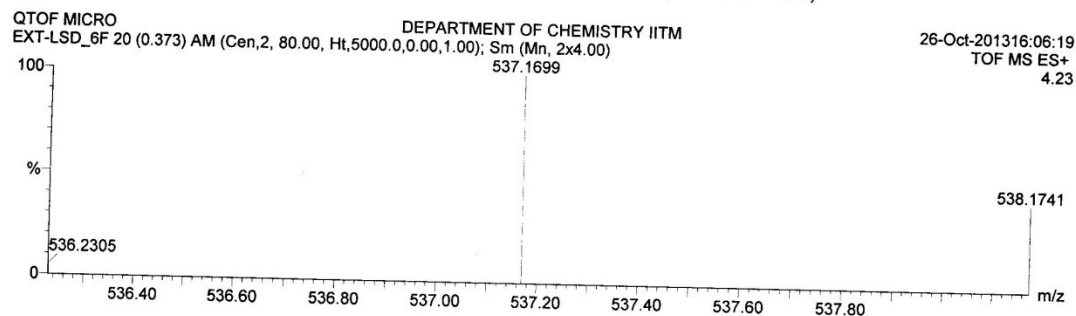
#### Single Mass Analysis (displaying only valid results)

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

28 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)



Minimum:				-1.5				
Maximum:		200.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula		
537.1699	537.1693	0.5	1.0	20.5	1	C31	H26	N4 O3 C1

Figure S59. HRMS spectra of 6f

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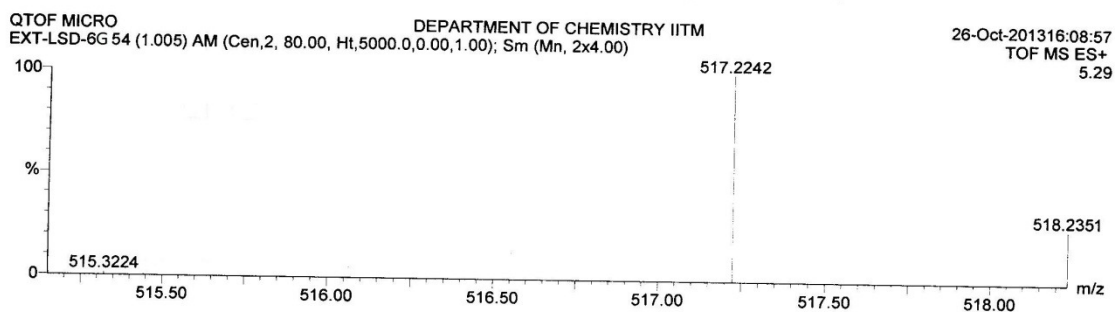
#### Single Mass Analysis (displaying only valid results)

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)



Minimum:				-1.5				
Maximum:		200.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula		
517.2242	517.2240	0.2	0.4	20.5	1	C32	H29	N4 O3

Figure S60. HRMS spectra of 6g

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#### Single Mass Analysis (displaying only valid results)

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

QTOF MICRO

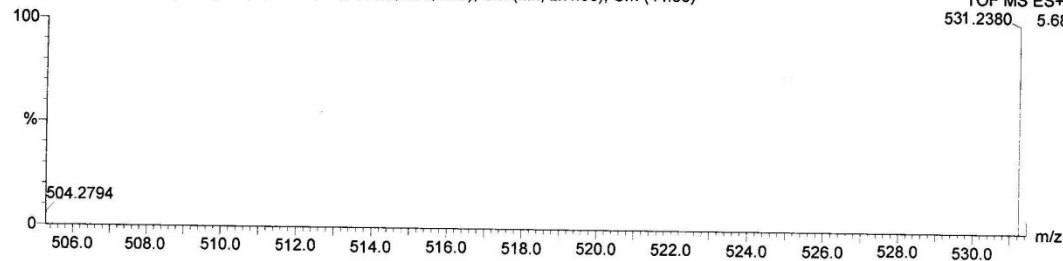
DEPARTMENT OF CHEMISTRY IITM

EXT-LSD-6H 36 (0.676) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00); Cm (44:50)

26-Oct-201315:33:25

TOF MS ES+

531.2380 5.68



Minimum:

Maximum: 200.0 5.0 -1.5

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
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531.2380	531.2396	-1.6	-3.1	20.5	1	C33 H31 N4 O3
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Figure S61. HRMS spectra of 6h

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#### Single Mass Analysis (displaying only valid results)

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

QTOF MICRO

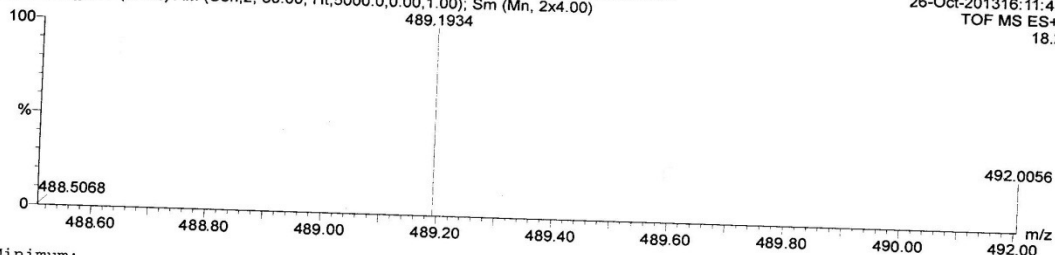
DEPARTMENT OF CHEMISTRY IITM

EXT-LSD\_6I 7 (0.130) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00)

26-Oct-201316:11:41

TOF MS ES+

18.2



Minimum:

Maximum: 200.0 5.0 -1.5

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
------	------------	-----	-----	-----	-------	---------

489.1934	489.1927	0.8	1.6	20.5	1	C30 H25 N4 O3
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Figure S62. HRMS spectra of 6i

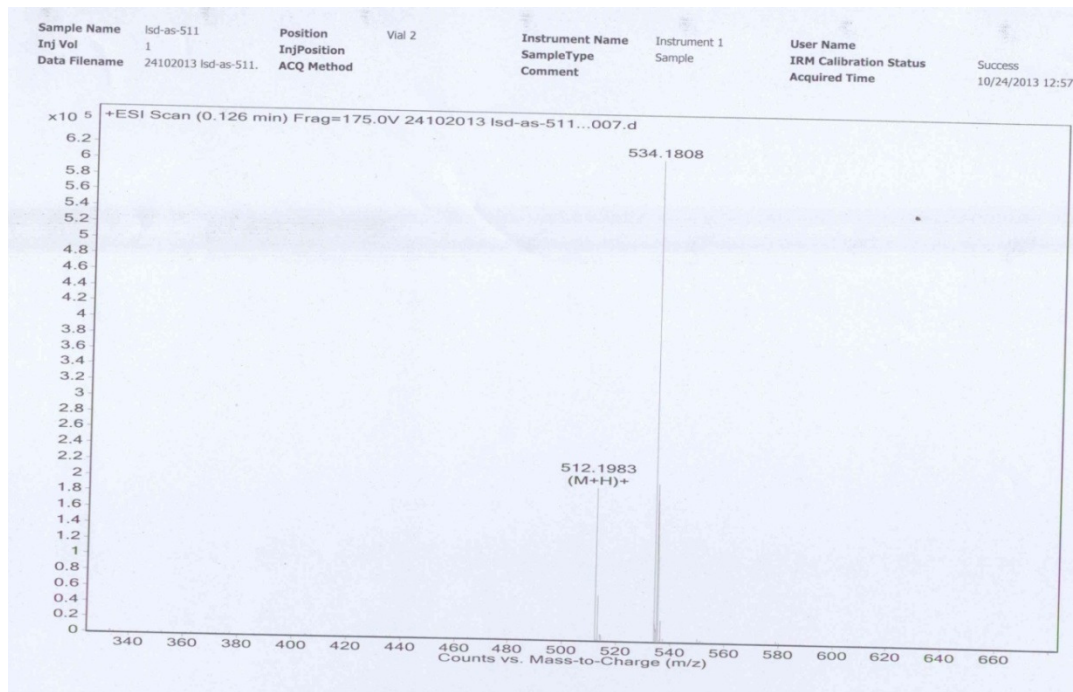


Figure S63. HRMS spectra of 8a

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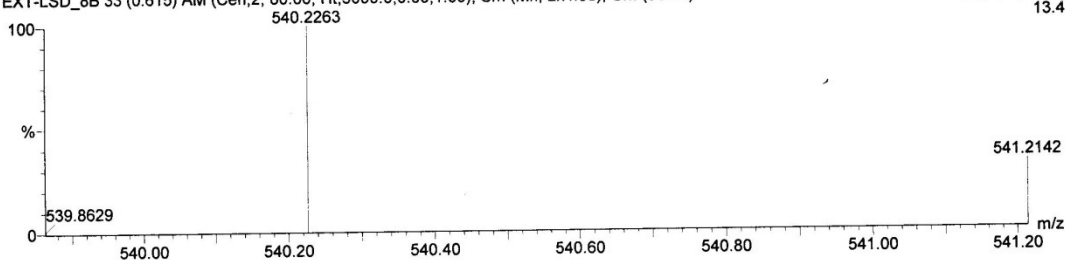
Single Mass Analysis (displaying only valid results)

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0  
 Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions  
 7 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

QTOF MICRO DEPARTMENT OF CHEMISTRY IITM  
 EXT-LSD\_8B 33 (0.615) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00); Cm (32:44)

26-Oct-2013 16:36:57  
 TOF MS ES+  
 13.4



Minimum: -1.5  
 Maximum: 200.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
540.2263	540.2287	-2.5	-4.6	22.5	1	C35 H30 N3 O3

Figure S64. HRMS spectra of 8b



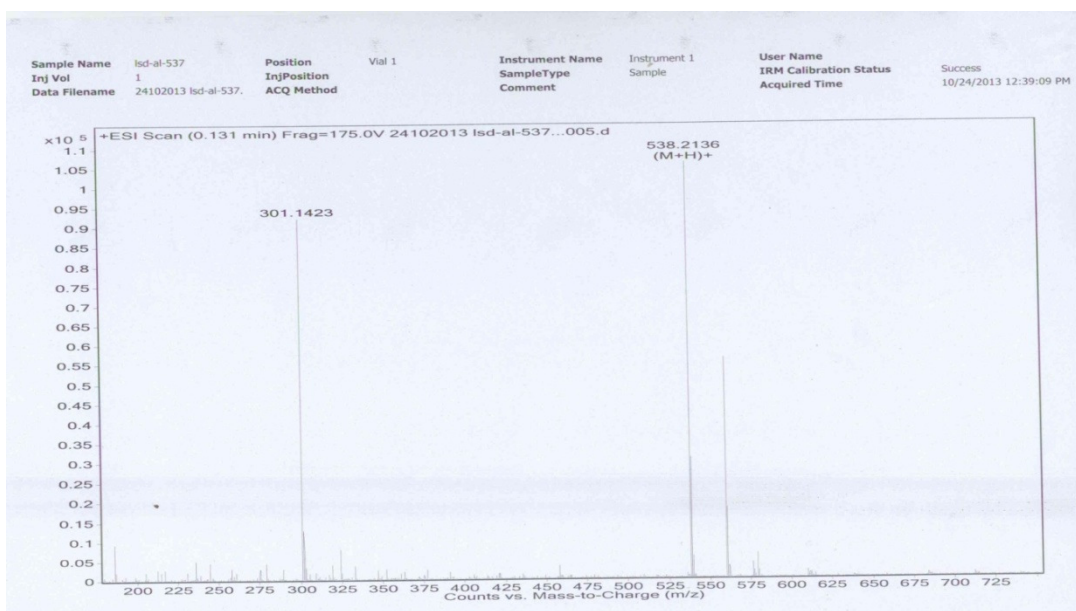


Figure S65. HRMS spectra of 9a

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Single Mass Analysis (displaying only valid results)

Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

7 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

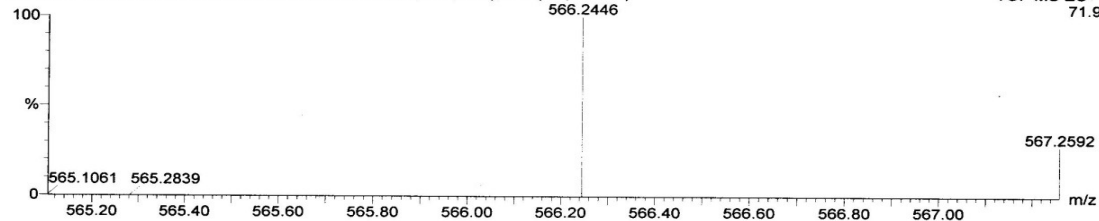
QTOF MICRO

DEPARTMENT OF CHEMISTRY IITM

26-Oct-2013 16:41:31

EXT-LSD-9B 173 (3.243) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x4.00)

TOF MS ES+



Minimum:

Maximum: 200.0 5.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
566.2446	566.2444	0.2	0.4	23.5	1	C37 H32 N3 O3

Figure S66. HRMS spectra of 9b