

# Quinacetophenone: A Simple Precursor for Synthesis of Phenoxazines

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## Supporting information

### 1-(2-hydroxy-3-(phenylamino)-10*H*-phenoxazin-1-yl)ethan-1-one (1D):



Red Solid; Yield- 60%, m.p = 240-242 °C, R<sub>f</sub> 0.4 (30:70 Ethyl acetate: Hexane); <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>): δ 11.31 (s, 1H), 9.55 (s, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.41 (d, *J* = 7.5 Hz, 2H), 7.35 (t, *J* = 7.8 Hz, 2H), 7.27 (t, *J* = 7.3 Hz, 1H), 7.22 (t, *J* = 7.4 Hz, 1H), 7.19 (d, *J* = 7.5 Hz, 2H), 5.81 (s, 1H), 2.31 (s, 3H), <sup>13</sup>C NMR (125 MHz, DMSO- *d*<sub>6</sub>): δ 199.77, 179.00, 178.79, 178.77, 148.09, 148.07, 139.74, 139.72, 129.83, 129.81, 129.20, 124.67, 124.40, 109.65, 96.93, 32.41. IR (neat, cm<sup>-1</sup>): 3290.74, 3047.55, 2803.77, 1649.96, 1565.33, 1488.15, 1329.90, 1287.72, HRMS *m/z* calculated for C<sub>20</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 333.1234 found 333.1235.

### 1-(2-hydroxy-10*H*-phenoxazin-1-yl)ethan-1-one (1C):



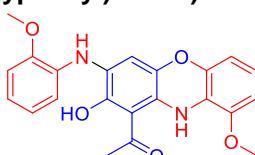
Red Solid; Yield- 20%, m.p = 156-158 °C, R<sub>f</sub> 0.3 (30:70 Ethyl acetate: Hexane); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 11.60 (s, 1H), 7.24 (t, *J* = 10 Hz, 2H), 7.17 (d, *J* = 10 Hz, 1H), 6.89 (m, 2H), 6.67 (d, *J* = 10 Hz, 2H), 2.51(s, 3H), <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 204.39, 156.27, 144.94, 144.75, 129.97, 129.26, 126.60, 124.56, 123.50, 120.59, 118.59, 116.23, 114.25, 29.70. IR (neat, cm<sup>-1</sup>): 3347.52, 2923.45, 2852.67, 1726.35, 1631.90, 1597.84, 1495.19, 1282.93, 1078.38. HRMS *m/z* calculated for C<sub>14</sub>H<sub>11</sub>NO<sub>3</sub> [M+H]<sup>+</sup>: 242.0817 found 242.0818.

### 1-(2-hydroxy-7-methyl-3-(p-tolylamino)-10*H*-phenoxazin-1-yl)ethan-1-one (2D):



Black Solid; Yield- 62%, m.p = 252-254 °C, R<sub>f</sub> 0.4 (30:70 Ethyl acetate: Hexane); <sup>1</sup>H NMR (500 MHz, DMSO- *d*<sub>6</sub>): δ 9.48 (s, 1H), 7.26 (s, 4H), 7.15 (d, *J* = 8.1 Hz, 2H), 7.06 (d, *J* = 8.3 Hz, 2H), 5.74 (s, 1H), 2.33 (s, 3H), 2.30 (s, 6H), <sup>13</sup>C NMR (125 MHz, DMSO- *d*<sub>6</sub>): δ 199.71, 178.72, 178.60, 148.30, 137.09, 136.07, 135.79, 135.42, 130.24, 129.65, 124.43, 124.31, 32.42, 21.08, 21.05. IR (neat, cm<sup>-1</sup>): 3233.68, 3211.48, 1693.66, 1477.80, 1347.01, 1260.66, 813.10, 716.63. HRMS *m/z* calculated for C<sub>22</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 361.1547 found 361.1550.

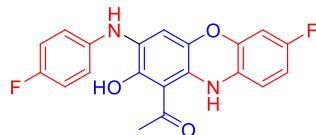
### 1-(2-hydroxy-9-methoxy-3-((2-methoxyphenyl)amino)-10*H*-phenoxazin-1-yl)ethan-1-one(3D):



Brown Solid; Yield 50%, m.p = 158-160 °C, R<sub>f</sub> 0.3 (30:70 Ethyl acetate: Hexane); <sup>1</sup>H NMR (500 MHz, DMSO- *d*<sub>6</sub>): δ 11.99 (bs, 1H), 9.01 (s, 1H), 7.37 (d, *J* = 7.8 Hz, 1H), 7.29 (t, *J* = 7.9 Hz, 1H), 7.24 (d, *J* = 7.8 Hz, 1H), 7.20 - 7.14 (m, 2H), 7.06 (s, 1H), 7.04 (d, *J* = 5.0 Hz, 1H), 6.93 (t, *J* = 7.6 Hz, 1H), 5.57 (s, 1H), 3.87 (s, 3H), 3.78 (s, 3H), 2.40 (s, 3H). <sup>13</sup>C NMR (125 MHz, DMSO- *d*<sub>6</sub>): δ 199.38, 178.29, 178.13, 152.69, 147.05, 128.40, 128.06, 127.67, 126.28, 125.75, 124.28, 121.34, 120.79, 112.65, 112.21, 108.76, 97.68, 56.32, 56.12,

32.53. IR (neat,  $\text{cm}^{-1}$ ): 3320.48, 3276.86, 2923.61, 2842.89, 1740.00, 1651.44, 1485.19, 1319.04, 1252.83, 844.34, 722.90. HRMS  $m/z$  calculated for  $\text{C}_{22}\text{H}_{20}\text{N}_2\text{O}_5$  [M+H]<sup>+</sup>: 393.1445 found 393.1448.

**1-(7-fluoro-3-((4-fluorophenyl)amino)-2-hydroxy-10*H*-phenoxazin-1-yl)ethan-1-one (4D):**



Orange Solid; Yield- 50%, m.p = 228-230 °C,  $R_f$  0.4 (30:70 Ethyl acetate: Hexane); <sup>1</sup>H NMR (500 MHz, DMSO-  $d_6$ ):  $\delta$  11.21 (s, 1H), 9.55 (s, 1H), 7.42 (dd,  $J$  = 8.0 Hz,  $J$  = 5.3 Hz, 2H), 7.30 (t,  $J$  = 8.7 Hz, 2H), 7.24 - 7.15 (m, 4H), 5.71 (s, 1H), 2.31 (s, 3H), <sup>13</sup>C NMR (125 MHz, DMSO-  $d_6$ ):  $\delta$  199.86, 178.94, 178.79, 160.57 (d,  $J$  = 243.33 Hz), 160.21 (d,  $J$  = 243.35 Hz), 148.40, 136.14, 134.38, 126.85, 126.79, 126.72, 126.65, 116.61 (d,  $J$  = 22.70 Hz), 115.96 (d,  $J$  = 22.81 Hz), 109.56, 96.68, 32.46. IR (neat,  $\text{cm}^{-1}$ ): 3303.13, 1738.54, 1578.02, 1358.11, 1216.92, 908.84, 831.11. HRMS  $m/z$  calculated for  $\text{C}_{20}\text{H}_{14}\text{F}_2\text{N}_2\text{O}_3$  [M+H]<sup>+</sup>: 369.1045 found 369.1047.

**1-(9-bromo-3-((2-bromophenyl)amino)-2-hydroxy-10*H*-phenoxazin-1-yl)ethan-1-one (5D):**



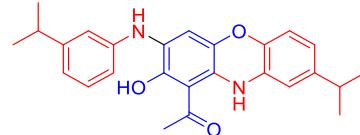
Brown Solid; Yield- 48%, m.p = 202-202 °C,  $R_f$  0.3 (30:70 Ethyl acetate: Hexane); <sup>1</sup>H NMR (500 MHz, DMSO-  $d_6$ ):  $\delta$  12.34 (s, 1H), 9.39 (s, 1H), 7.80 (d,  $J$  = 8.0 Hz, 1H), 7.68 (d,  $J$  = 8.0 Hz, 1H), 7.51 (t,  $J$  = 8.0 Hz, 1H), 7.46 (d,  $J$  = 6.5 Hz, 1H), 7.37 (t,  $J$  = 7.6 Hz, 1H), 7.32 (d,  $J$  = 7.0 Hz, 2H), 7.23 (t,  $J$  = 7.6 Hz, 1H), 5.19 (s, 1H), 2.44 (s, 3H), <sup>13</sup>C NMR (125 MHz, DMSO-  $d_6$ ):  $\delta$  200.27, 178.31, 178.02, 148.45, 138.84, 136.37, 133.95, 133.08, 129.49, 129.05, 128.65, 128.39, 127.95, 120.71, 119.56, 108.86, 98.03, 32.59. IR (neat,  $\text{cm}^{-1}$ ): 3277.84, 3003.17, 2779.41, 1737.20, 1356.93, 1288.47, 1027.99, 759.24, 661.20. HRMS  $m/z$  calculated for  $\text{C}_{20}\text{H}_{14}\text{Br}_2\text{N}_2\text{O}_3$  [M+H]<sup>+</sup>: 490.9429 found 490.9431

**1-(2-hydroxy-8-(trifluoromethyl)-3-((3-(trifluoromethyl)phenyl)amino)-10*H*-phenoxazin-1-yl)ethan-1-one (6D):**



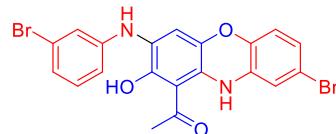
Violet Solid; Yield- 61%, m.p = 168-170 °C,  $R_f$  0.3 (30:70 Ethyl acetate: Hexane); <sup>1</sup>H NMR (500 MHz, DMSO-  $d_6$ ):  $\delta$  11.18 (s, 1H), 9.72 (s, 1H), 7.77 - 7.67 (m, 3H), 7.61 - 7.55 (m, 4H), 7.48 (d,  $J$  = 7.5 Hz, 1H), 5.90 (s, 1H), 2.31 (s, 3H), <sup>13</sup>C NMR (125 MHz, DMSO-  $d_6$ ):  $\delta$  199.75, 179.70, 179.18, 148.92, 147.45, 140.80, 139.15, 131.10, 130.67, 130.41, 129.84 (q,  $J$  = 31.99 Hz), 128.67, 127.85, 124.32 (q,  $J$  = 272.40 Hz), 124.30 (q,  $J$  = 272.54 Hz), 123.03 (q,  $J$  = 3.83 Hz), 122.45, 121.18, 120.87 (q,  $J$  = 3.85 Hz), 110.24, 97.72, 32.31. IR (neat,  $\text{cm}^{-1}$ ): 3271.46, 3236.94, 3073.67, 2823.71, 1736.45, 1326.88, 1218.26, 1073.13, 804.19, 689.87. HRMS  $m/z$  calculated for  $\text{C}_{22}\text{H}_{14}\text{F}_6\text{N}_2\text{O}_3$  [M+H]<sup>+</sup>: 469.0981 found 469.0997.

**1-(2-hydroxy-8-isopropyl-3-((3-isopropylphenyl)amino)-10*H*-phenoxazin-1-yl)ethan-1-one (7D):**



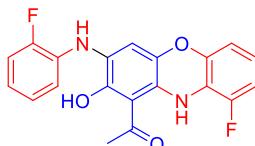
Black Solid; Yield - 54%, m.p = 169-171 °C,  $R_f$  0.4 (30:70 Ethyl acetate: Hexane); <sup>1</sup>H NMR (500 MHz, DMSO-  $d_6$ ):  $\delta$  11.09 (s, 1H), 9.49 (s, 1H), 7.37 (t,  $J$  = 7.8 Hz, 1H), 7.26 (d,  $J$  = 7.8 Hz, 2H), 7.20 (d,  $J$  = 7.8 Hz, 1H), 7.15 (d,  $J$  = 7.7 Hz, 1H), 7.10 (d,  $J$  = 7.7 Hz, 1H), 7.04 (s, 1H), 6.98 (d,  $J$  = 7.8 Hz, 1H), 5.78 (s, 1H), 2.90 (sept,  $J$  = 10 Hz, 1H), 2.86 (sept,  $J$  = 10 Hz, 1H), 2.27 (s, 3H), 1.22 (d,  $J$  = 6.9 Hz, 6H), 1.19 (d,  $J$  = 6.9 Hz, 6H), <sup>13</sup>C NMR (125 MHz, DMSO-  $d_6$ ):  $\delta$  199.40, 178.96, 178.64, 150.25, 149.44, 148.17, 139.54, 138.01, 129.71, 129.17, 124.80, 124.44, 122.43, 122.40, 122.33, 121.78, 109.63, 96.62, 33.77, 33.73, 32.45, 24.21, 24.06. IR (neat,  $\text{cm}^{-1}$ ): 3209.20, 290.50, 2866.69, 1698.65, 1436.93, 1346.93, 1278.25, 1000.71, 840.06, 697.90. HRMS  $m/z$  calculated for  $\text{C}_{26}\text{H}_{28}\text{N}_2\text{O}_3$  [M+H]<sup>+</sup>: 417.2173 found 417.2183.

**1-(8-bromo-3-((3-bromophenyl)amino)-2-hydroxy-10*H*-phenoxazin-1-yl)ethan-1-one (8D):**



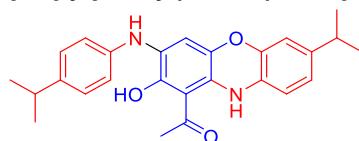
Red Solid; Yield- 43%, m.p = 215-217 °C, R<sub>f</sub> 0.3 (30:70 Ethyl acetate: Hexane); <sup>1</sup>H NMR (500 MHz, DMSO- *d*<sub>6</sub>): δ 11.07 (s, 1H), 9.60 (s, 1H), 7.61 (s, 1H), 7.47 - 7.38 (m, 5H), 7.31 (t, *J* = 8.0 Hz, 1H), 7.19 (d, *J* = 8.8 Hz, 1H), 5.86 (s, 1H), 2.32 (s, 3H), <sup>13</sup>C NMR (125 MHz, DMSO- *d*<sub>6</sub>): δ 199.81, 179.56, 179.04, 147.46, 139.92, 131.69, 131.08, 129.31, 128.87, 127.12, 126.8, 123.67, 123.0, 122.3, 121.74, 110.26, 97.69, 32.30. IR (neat, cm<sup>-1</sup>): 3300.03, 3000.28, 2950.35, 1737.20, 1653.44, 1310.23, 1215.30, 1000.25, 820.30, 650.80. HRMS *m/z* calculated for C<sub>20</sub>H<sub>14</sub>Br<sub>2</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 490.9429 found 490.9425.

#### 1-(9-fluoro-3-((2-fluorophenyl)amino)-2-hydroxy-10*H*-phenoxazin-1-yl)ethan-1-one (9D):



Red Solid; Yield- 49%, m.p = 165-167 °C, R<sub>f</sub> 0.3 (30:70 Ethyl acetate: Hexane); <sup>1</sup>H NMR (500 MHz, DMSO- *d*<sub>6</sub>): δ 11.86 (broad s, 1H), 9.46 (s, 1H), 7.44 (t, *J* = 10 Hz, 1H), 7.41-7.39 (m, 2H), 7.35-7.29 (m, 3H), 7.27-7.23 (m, 1H), 7.19 (t, *J* = 8 Hz, 1H), 5.28 (s, 1H), 2.38 (s, 3H). <sup>13</sup>C NMR (125 MHz, DMSO- *d*<sub>6</sub>): δ 199.98, 178.54, 178.49, 156.56 (d, *J* = 249.20 Hz), 156.20 (d, *J* = 247.38 Hz), 148.68, 129.35, 128.98, 128.27, 127.70, 127.60, 127.31, 125.71, 125.37, 125.27, 125.03, 117.09 (d, *J* = 19.40 Hz), 116.25 (d, *J* = 19.50 Hz), 109.52, 97.78, 32.46. IR (neat, cm<sup>-1</sup>): 3320.03, 1725.38, 1615.21, 1429.80, 1370.20, 1250.38, 1005.65, 900.23, 825.32. HRMS *m/z* calculated for C<sub>20</sub>H<sub>14</sub>F<sub>2</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 369.1051 found 369.1095

#### 1-(2-hydroxy-7-isopropyl-3-((4-isopropylphenyl)amino)-10*H*-phenoxazin-1-yl)ethan-1-one (10D):



Black Solid; Yield- 58%, m.p = 163-165 °C, R<sub>f</sub> 0.4 (30:70 Ethyl acetate: Hexane); <sup>1</sup>H NMR (500 MHz, DMSO- *d*<sub>6</sub>): δ 11.39 (s, 1H), 9.52 (s, 1H), 7.31 (q, *J* = 8.7 Hz, 4H), 7.21 (d, *J* = 8.4 Hz, 2H), 7.08 (d, *J* = 8.4 Hz, 2H), 5.75 (s, 1H), 2.90 (septet, *J* = 10 Hz, 2H), 2.30 (s, 3H), 1.23 (s, 3H), 1.21 (s, 3H), 1.20 (s, 3H), <sup>13</sup>C NMR (125 MHz, DMSO- *d*<sub>6</sub>): δ 199.74, 178.72, 178.59, 148.25, 146.97, 146.68, 137.37, 135.71, 127.59, 127.00, 124.56, 124.36, 109.42, 98.68, 33.49, 33.43, 32.43, 24.28, 24.26. IR (neat, cm<sup>-1</sup>): 3217.84, 2960.86, 2869.21, 1738.65, 1554.37, 1343.98, 1285.96, 1053.72, 819.87, 721.11. HRMS *m/z* calculated for C<sub>26</sub>H<sub>28</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 417.2173 found 417.2190.

#### 1-(7-bromo-3-((4-bromophenyl)amino)-2-hydroxy-10*H*-phenoxazin-1-yl)ethan-1-one (11D):



Red Solid; Yield - 52%, m.p = 235-237 °C, R<sub>f</sub> 0.3 (30:70 Ethyl acetate: Hexane); <sup>1</sup>H NMR (500 MHz, DMSO- *d*<sub>6</sub>): δ 11.21 (s, 1H), 9.59 (s, 1H), 7.63 (d, *J* = 8.8 Hz, 2H), 7.53 (d, *J* = 8.7 Hz, 2H), 7.37 (d, *J* = 8.8 Hz, 2H), 7.14 (d, *J* = 8.7 Hz, 2H), 5.86 (s, 1H), 2.33 (s, 3H). <sup>13</sup>C NMR (125 MHz, DMSO- *d*<sub>6</sub>): δ 199.79, 179.28, 178.94, 147.50, 139.25, 137.56, 132.67, 132.04, 126.68, 126.20, 119.07, 118.36, 109.91, 97.52, 32.44. IR (neat, cm<sup>-1</sup>): 3255.59, 3084.73, 3053.98, 1737.20, 1294.59, 1218.58, 1013.87, 829.72, 709.77. HRMS *m/z* calculated for C<sub>20</sub>H<sub>14</sub>Br<sub>2</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 490.9425 found 490.9429

#### 1-(8-chloro-3-((3-chlorophenyl)amino)-2-hydroxy-10*H*-phenoxazin-1-yl)ethan-1-one (12D):



Red Solid; Yield- 50%, m.p = 190-192 °C, R<sub>f</sub> 0.4 (30:70 Ethyl acetate: Hexane); <sup>1</sup>H NMR (500 MHz, DMSO- *d*<sub>6</sub>): δ 11.09 (s, 1H), 9.60 (s, 1H), 7.48 (t, *J* = 8.0 Hz, 2H), 7.38 (dd, *J* = 15.8 Hz, *J* = 7.8 Hz, 2H), 7.32-7.26 (m, 3H), 7.15 (d, *J* = 7.2 Hz, 1H), 5.88 (s, 1H), 2.31 (s, 3H). <sup>13</sup>C NMR (125 MHz, DMSO- *d*<sub>6</sub>): δ 199.82, 179.53, 179.08, 148.85, 147.40, 141.38, 139.79, 134.04, 133.42, 131.43, 130.80, 126.47, 125.96, 124.43, 123.97, 123.31, 122.67, 110.27, 97.78, 32.28. IR (neat, cm<sup>-1</sup>): 3272.00, 2971.14, 2746.41, 1738.32, 1624.63, 1357.26, 1230.48, 881.77, 777.18. HRMS *m/z* calculated for C<sub>20</sub>H<sub>14</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 401.0454 found 401.0463.

#### 1-(7-chloro-3-((4-chlorophenyl)amino)-2-hydroxy-10*H*-phenoxazin-1-yl)ethan-1-one (13D):



Brick-red Solid; Yield- 55%, m.p = 240-242 °C, R<sub>f</sub> 0.4 (30:70 Ethyl acetate: Hexane); <sup>1</sup>H NMR (500 MHz, DMSO- *d*<sub>6</sub>): δ 11.20 (s, 1H), 9.60 (s, 1H), 7.51 (d, *J* = 8.8 Hz, 2H), 7.41 (dd, *J* = 14.2 Hz, *J* = 8.8 Hz, 4H), 7.20 (d, *J* = 8.7 Hz, 2H), 5.84 (s, 1H), 2.33 (s, 3H), <sup>13</sup>C NMR (125 MHz, DMSO- *d*<sub>6</sub>): δ 199.79, 179.27, 178.91, 147.63, 138.86, 137.13, 130.74, 130.14, 129.76, 129.12, 126.37, 125.93, 109.88, 97.42, 32.44. IR (neat, cm<sup>-1</sup>): 3289.00, 3076.75, 2971.19, 1905.01, 1737.11, 1594.00, 1330.55, 1286.56, 1010.03, 828.79, 624.96. HRMS *m/z* calculated for C<sub>20</sub>H<sub>14</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 401.0454 found 401.0462.

**1-(2-hydroxy-7-(trifluoromethyl)-3-((4-(trifluoromethyl)phenyl)amino)-10*H*-phenoxyazin-1-yl)ethan-1-one (14D):**



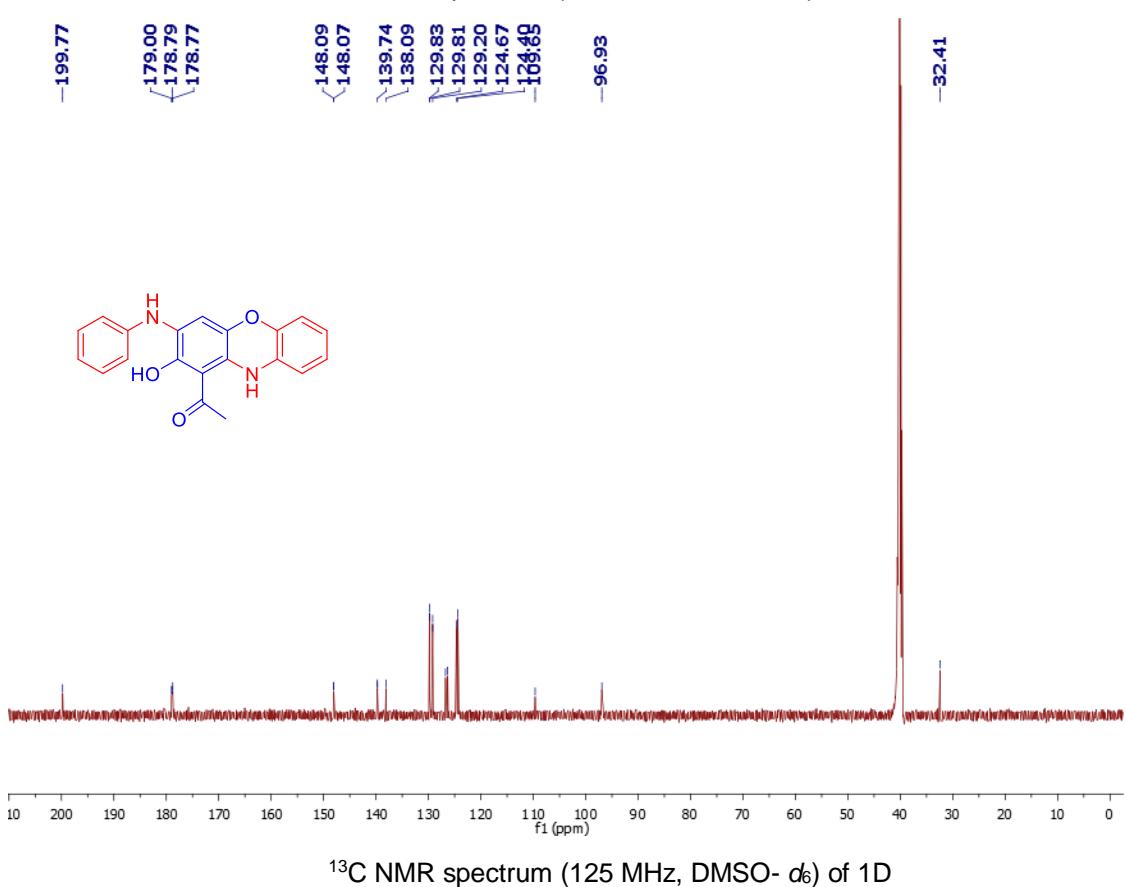
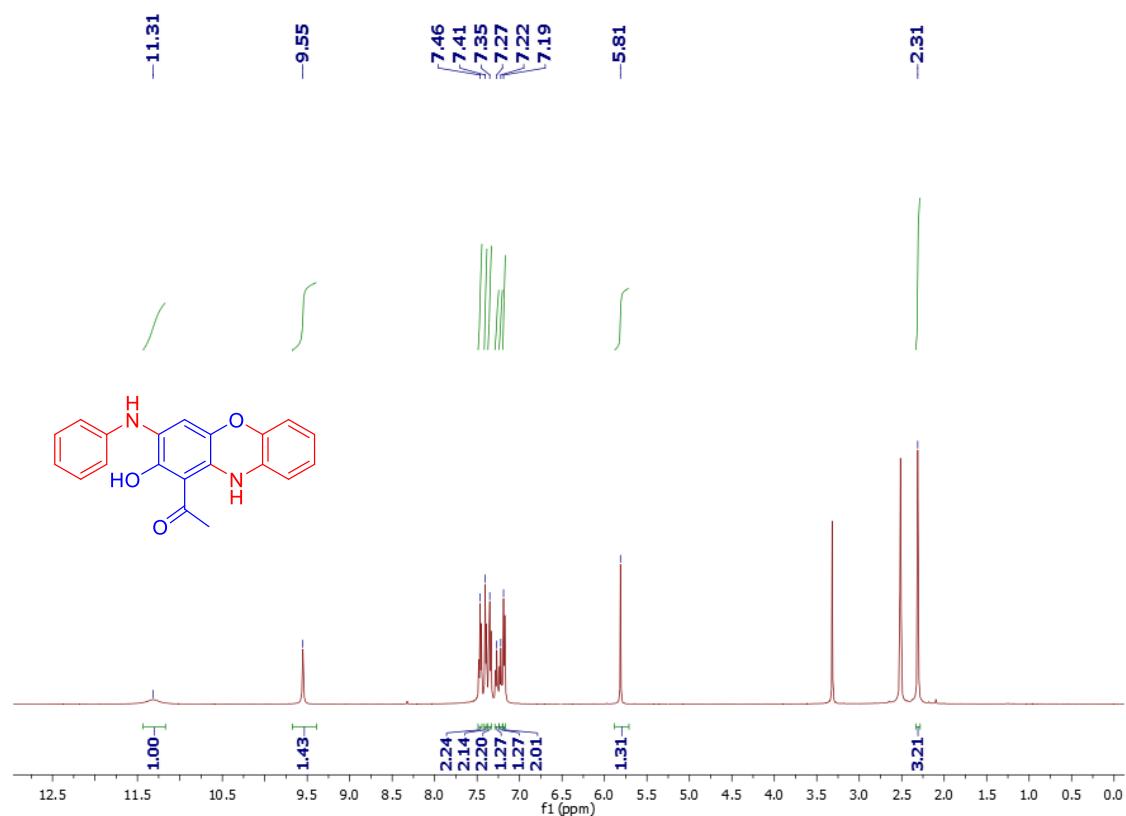
Red Solid; Yield- 53%, m.p = 190-192 °C, R<sub>f</sub> 0.4 (30:70 : Ethyl acetate: Hexane); <sup>1</sup>H NMR (500 MHz, DMSO- *d*<sub>6</sub>): δ 11.31 (s, 1H), 9.74 (s, 1H), 7.80 (d, *J* = 8.5 Hz, 2H), 7.71 (d, *J* = 8.4 Hz, 2H), 7.64 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.3 Hz, 2H), 6.06 (s, 1H), 2.35 (s, 3H), <sup>13</sup>C NMR (125 MHz, DMSO- *d*<sub>6</sub>): δ 199.87, 179.92, 179.28, 148.84, 146.79, 143.69, 142.11, 134.83, 133.66, 132.38, 128.75 (q, *J* = 34.11 Hz), 127.84, 126.96 (q, *J* = 3.75 Hz), 126.59, 126.30 (q, *J* = 3.34 Hz), 125.68 (q, *J* = 31.87 Hz), 124.98, 124.54 (q, *J* = 252.98 Hz), 124.03, 123.54, 110.61, 98.70, 32.39. IR (neat, cm<sup>-1</sup>): 3280.12, 2970.90, 1737.09, 1568.37, 1319.37, 1287.81, 1066.92, 827.05, 733.96. HRMS *m/z* calculated for C<sub>22</sub>H<sub>14</sub>F<sub>6</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 469.0981 found 469.0986.

**1-(2-hydroxy-8-methoxy-3-((3-methoxyphenyl)amino)-10*H*-phenoxyazin-1-yl)ethan-1-one (15D):**

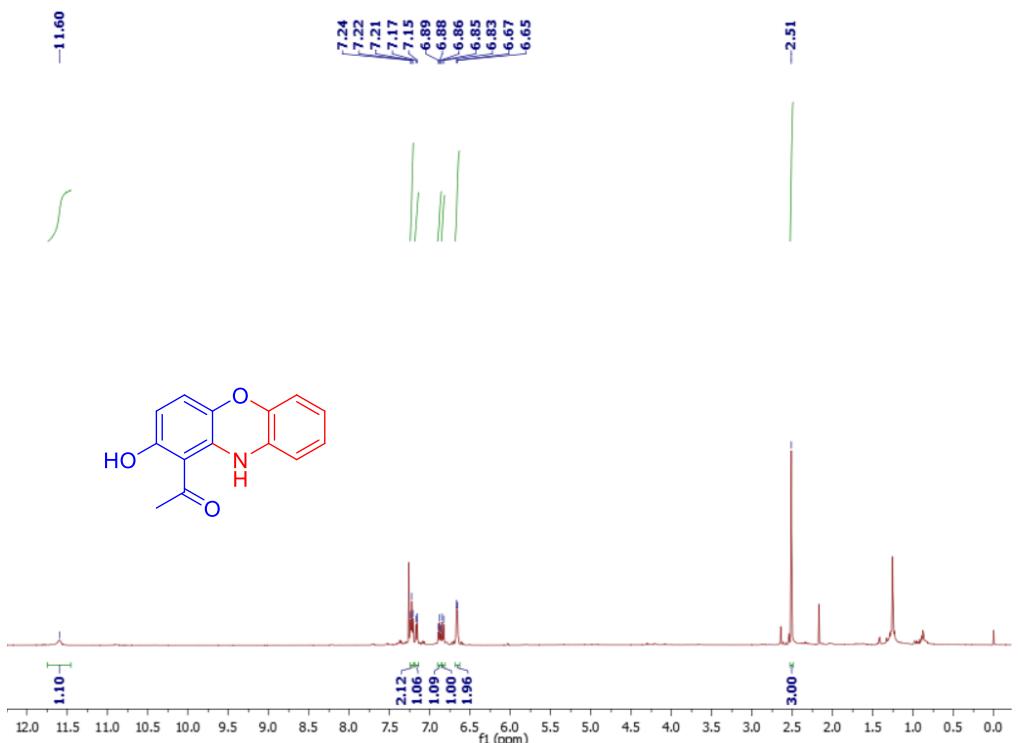


Brown Solid; Yield- 48%, m.p = 161-163 °C, R<sub>f</sub> = 0.3 (30:70 Ethyl acetate: Hexane: Ethyl acetate); <sup>1</sup>H NMR (500 MHz, DMSO- *d*<sub>6</sub>): δ 11.03 (s, 1H), 9.48 (s, 1H), 7.36 (t, *J* = 8.1 Hz, 1H), 7.24 (t, *J* = 8.0 Hz, 1H), 6.98 (d, *J* = 7.2 Hz, 2H), 6.86 – 6.83 (m, 1H), 6.80 (d, *J* = 5.0 Hz, 1H), 6.79 (s, 1H), 6.74 (d, *J* = 8.5 Hz, 1H), 5.85 (s, 1H), 3.78 (s, 3H), 3.75 (s, 3H), 2.28 (s, 3H). <sup>13</sup>C NMR (125 MHz, DMSO- *d*<sub>6</sub>): δ 199.59, 179.15, 178.79, 160.41, 159.97, 147.82, 140.83, 139.28, 130.61, 130.00, 116.82, 116.21, 112.45, 111.89, 110.39, 110.19, 55.75, 55.70, 32.28. IR (neat, cm<sup>-1</sup>): 3291.26, 2971.35, 2922.74, 2838.76, 1738.76, 1588.89, 1356.29, 1275.75, 1047.87, 866.65. HRMS *m/z* calculated for C<sub>22</sub>H<sub>20</sub>N<sub>2</sub>O<sub>5</sub> [M+H]<sup>+</sup>: 393.1450 found 393.1445

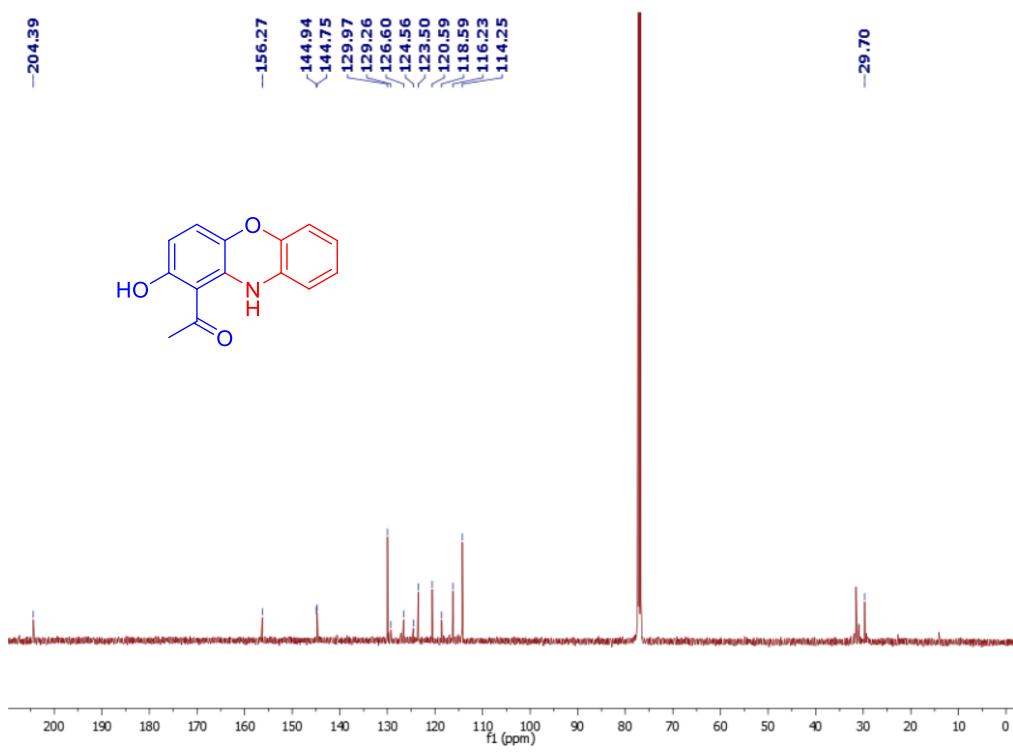
**1-(2-hydroxy-3-(phenylamino)-10*H*-phenoxyazin-1-yl)ethan-1-one (1D):**



**1-(2-hydroxy-10H-phenoxazin-1-yl)ethan-1-one (1C):**

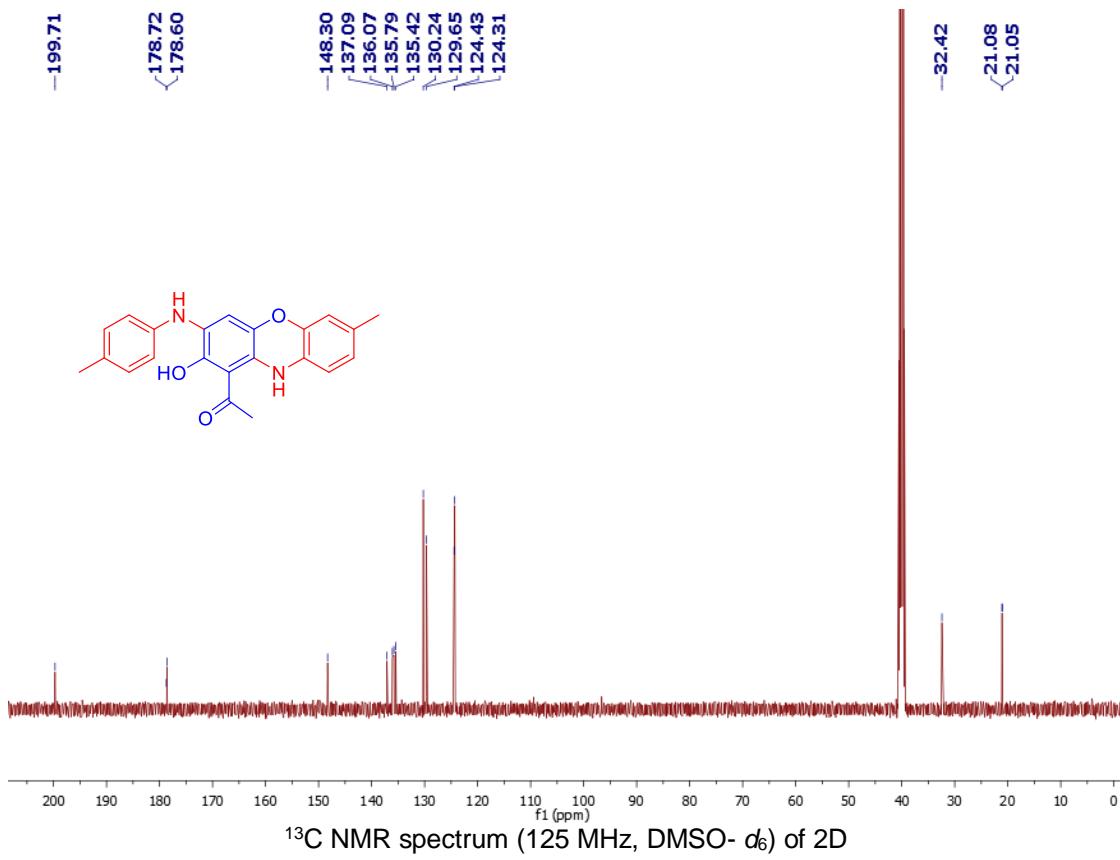
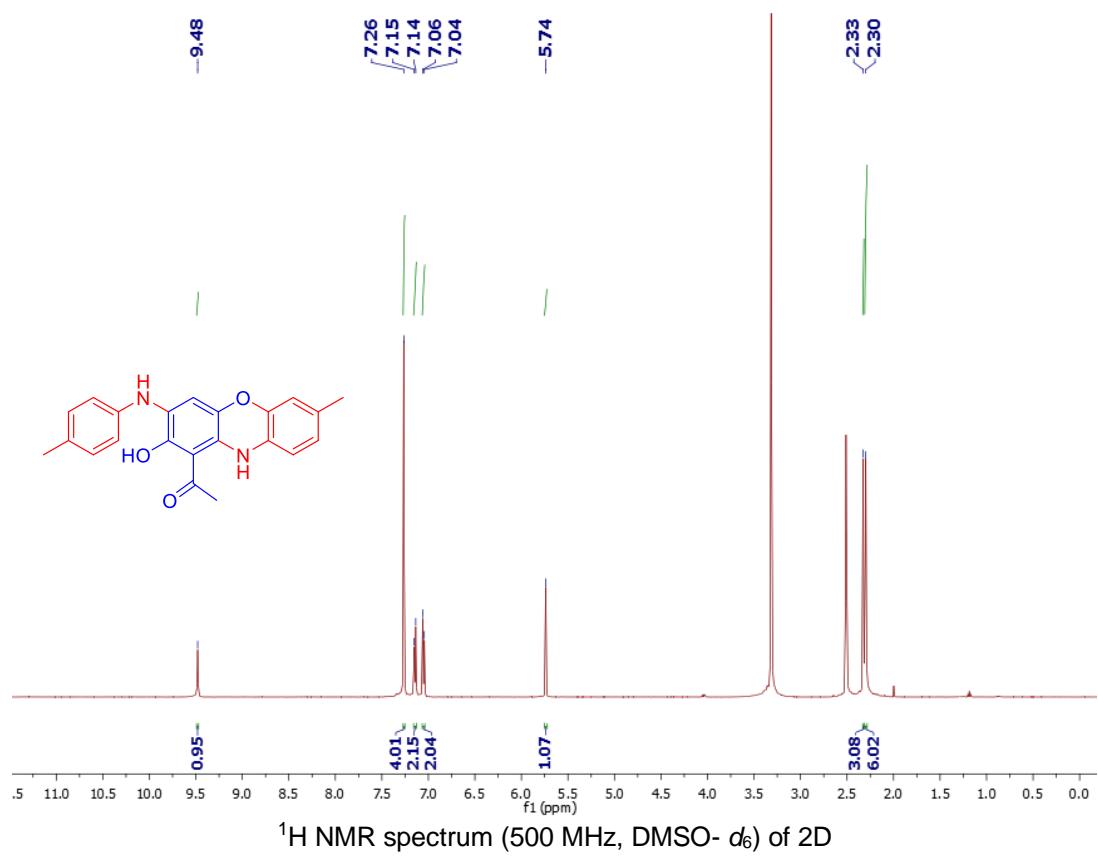


<sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of 1C

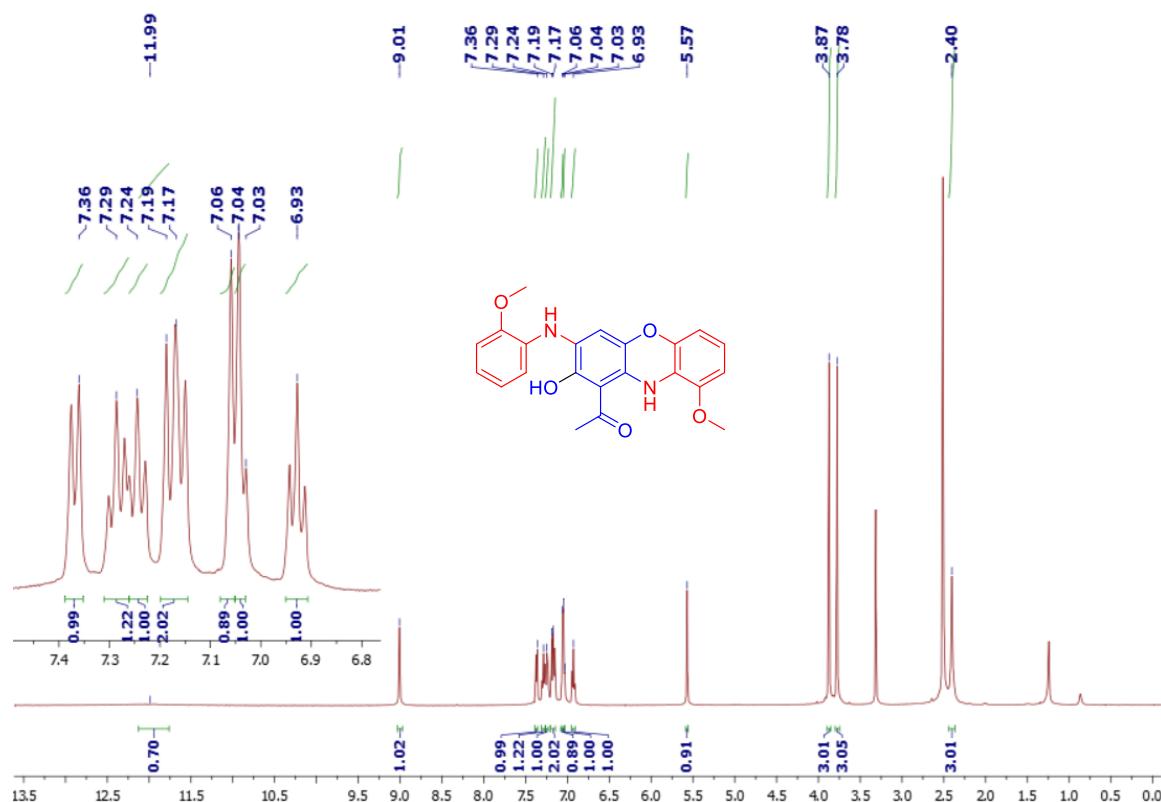


<sup>13</sup>C NMR spectrum (125 MHz, CDCl<sub>3</sub>) of 1C

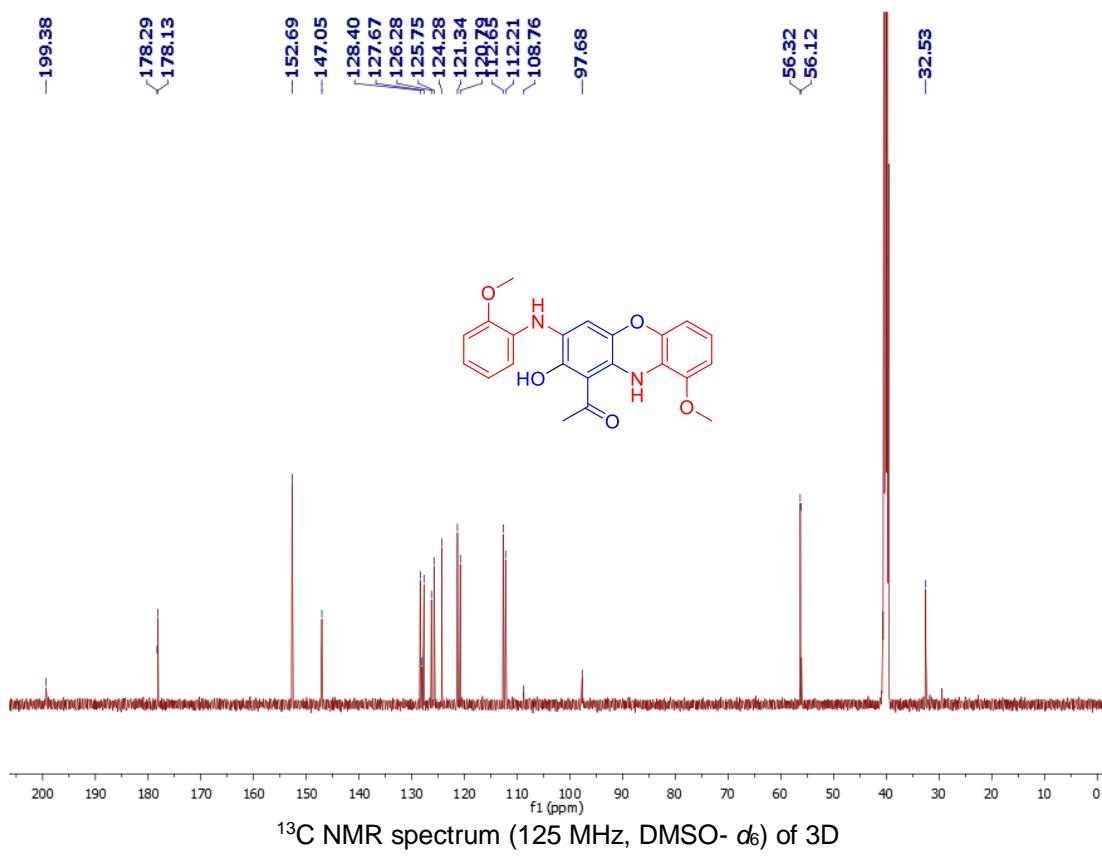
**1-(2-hydroxy-7-methyl-3-(p-tolylamino)-10*H*-phenoazin-1-yl)ethan-1-one (2D):**



**1-(2-hydroxy-9-methoxy-3-((2-methoxyphenyl)amino)-10*H*-phenoxyazin-1-yl)ethan-1-one(3D):**

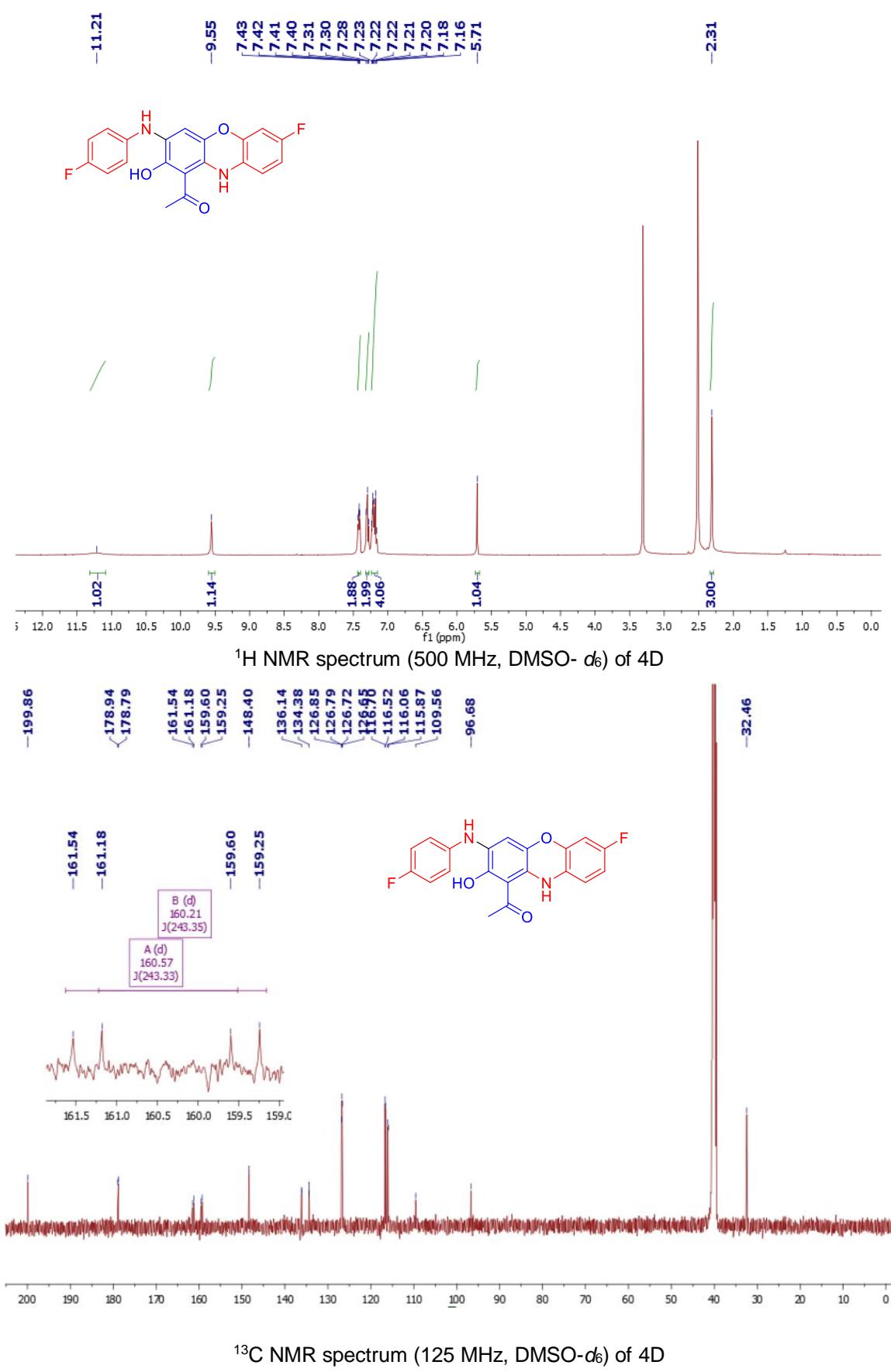


$^1\text{H}$  NMR spectrum (500 MHz, DMSO-  $d_6$ ) of 3D

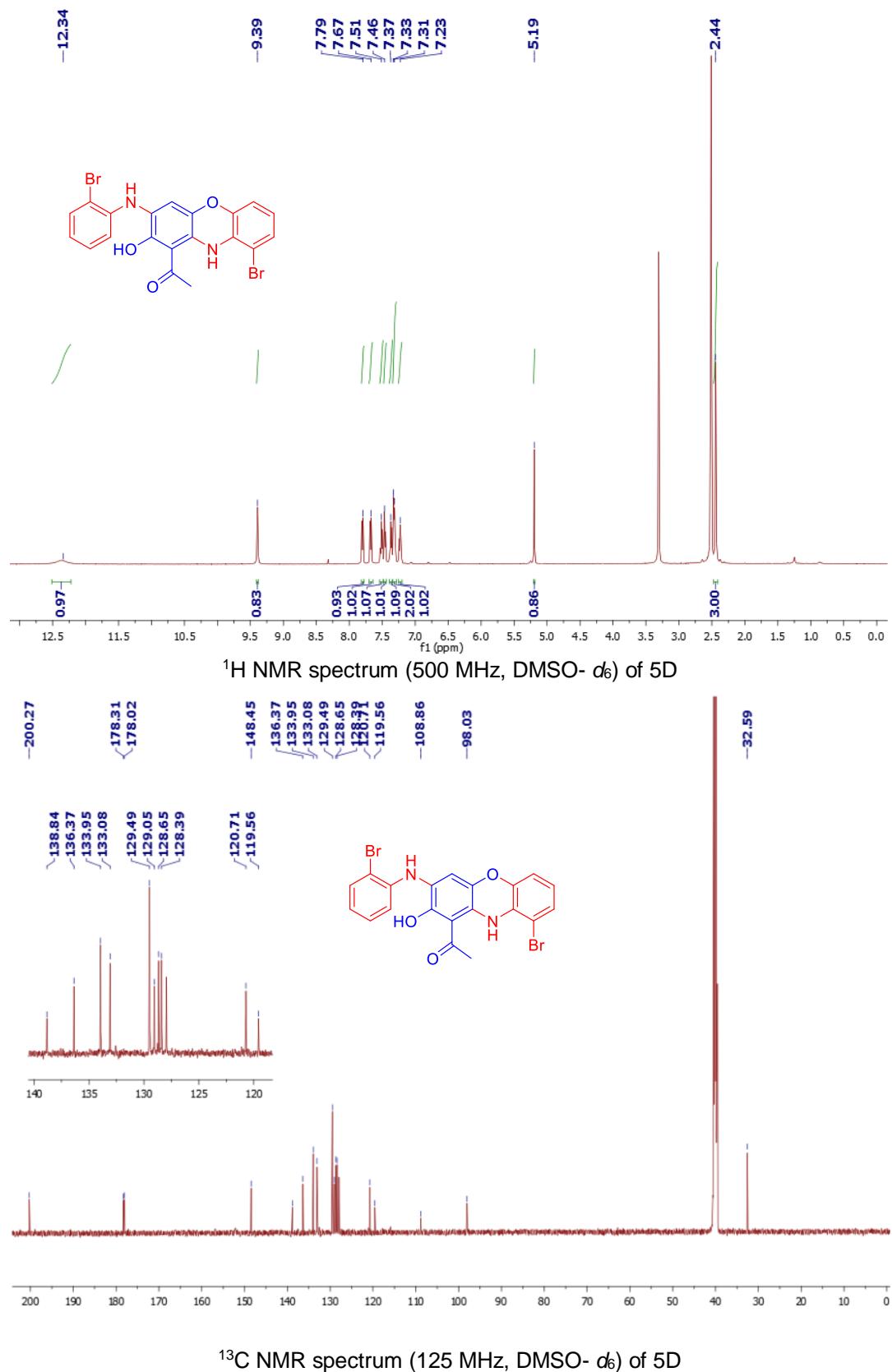


$^{13}\text{C}$  NMR spectrum (125 MHz, DMSO-  $d_6$ ) of 3D

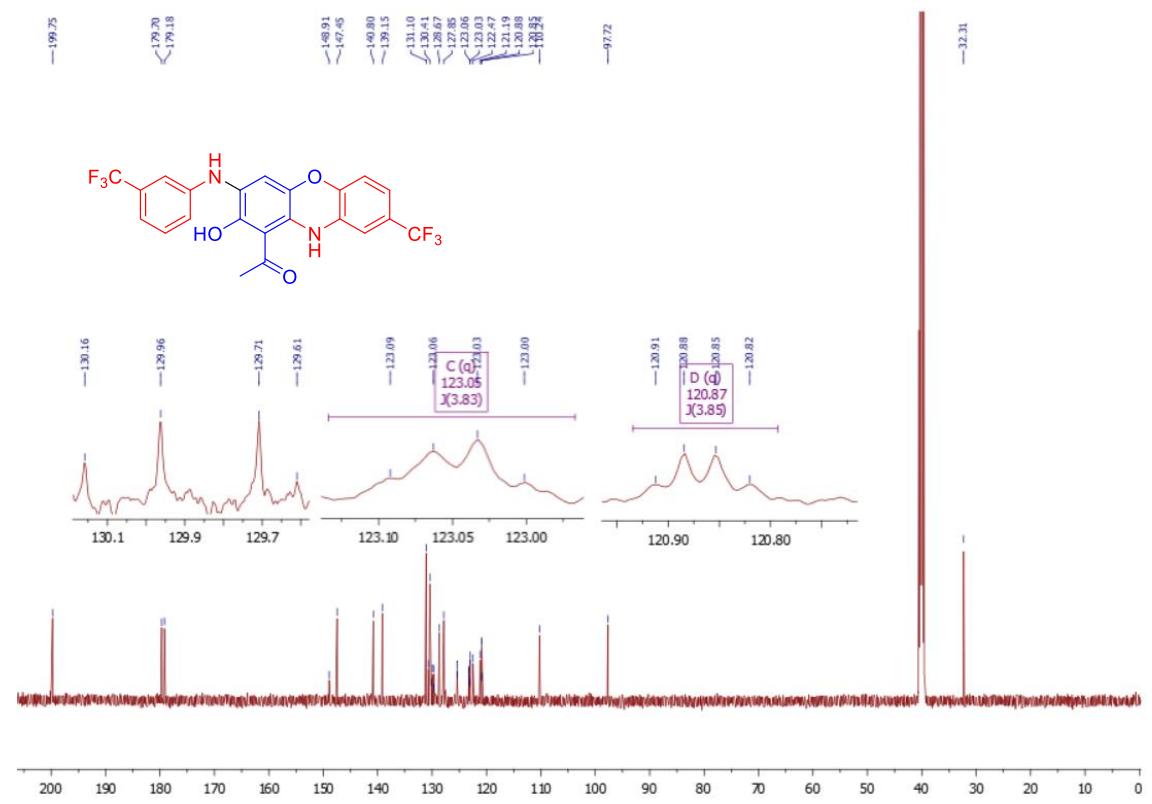
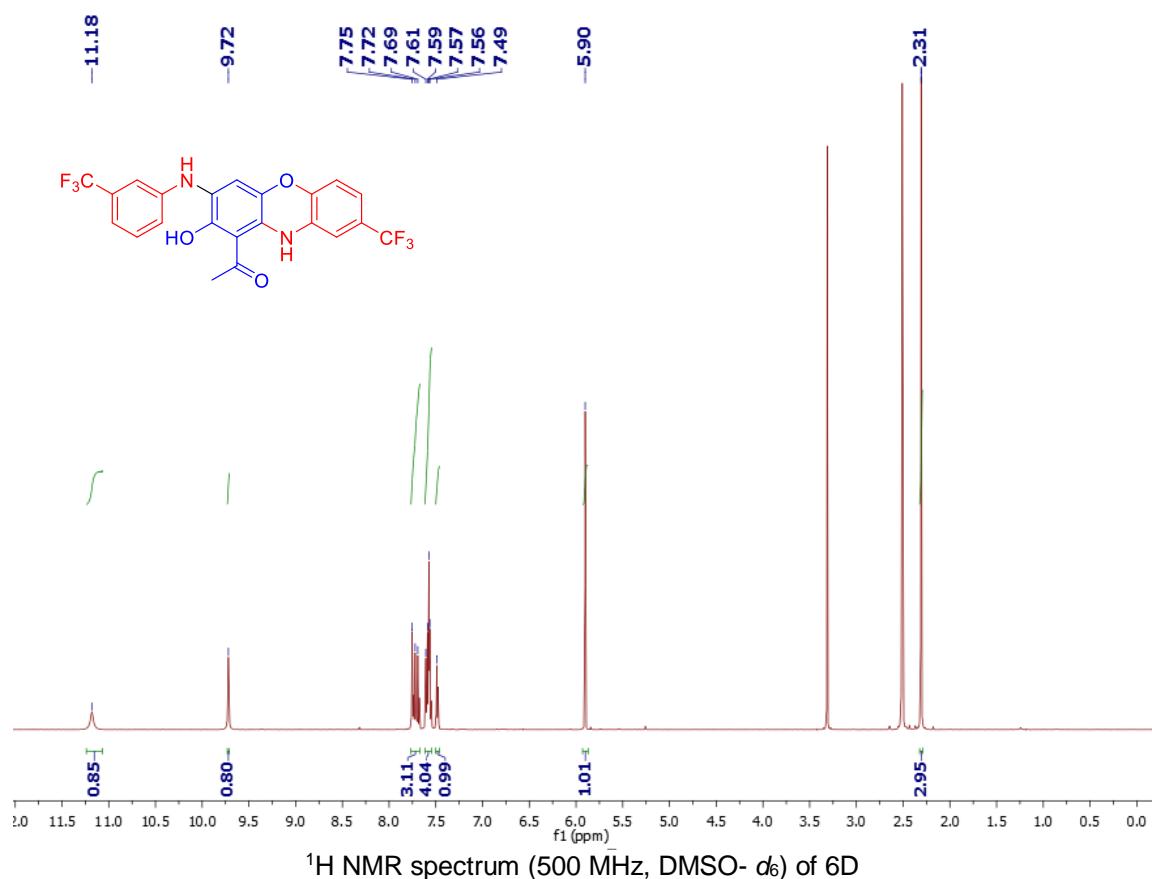
**1-(7-fluoro-3-((4-fluorophenyl)amino)-2-hydroxy-10H-phenoxazin-1-yl)ethan-1-one  
(4D):**



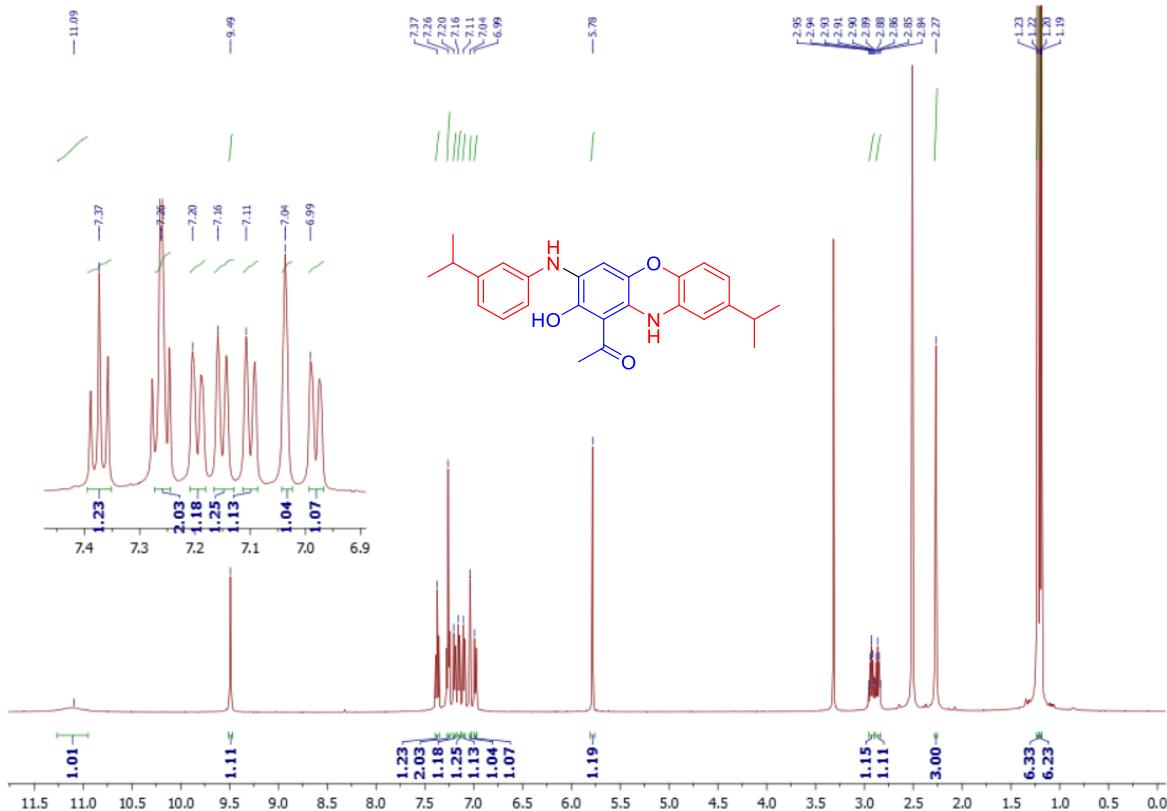
**1-(9-bromo-3-((2-bromophenyl)amino)-2-hydroxy-10*H*-phenoxazin-1-yl)ethan-1-one (5D):**



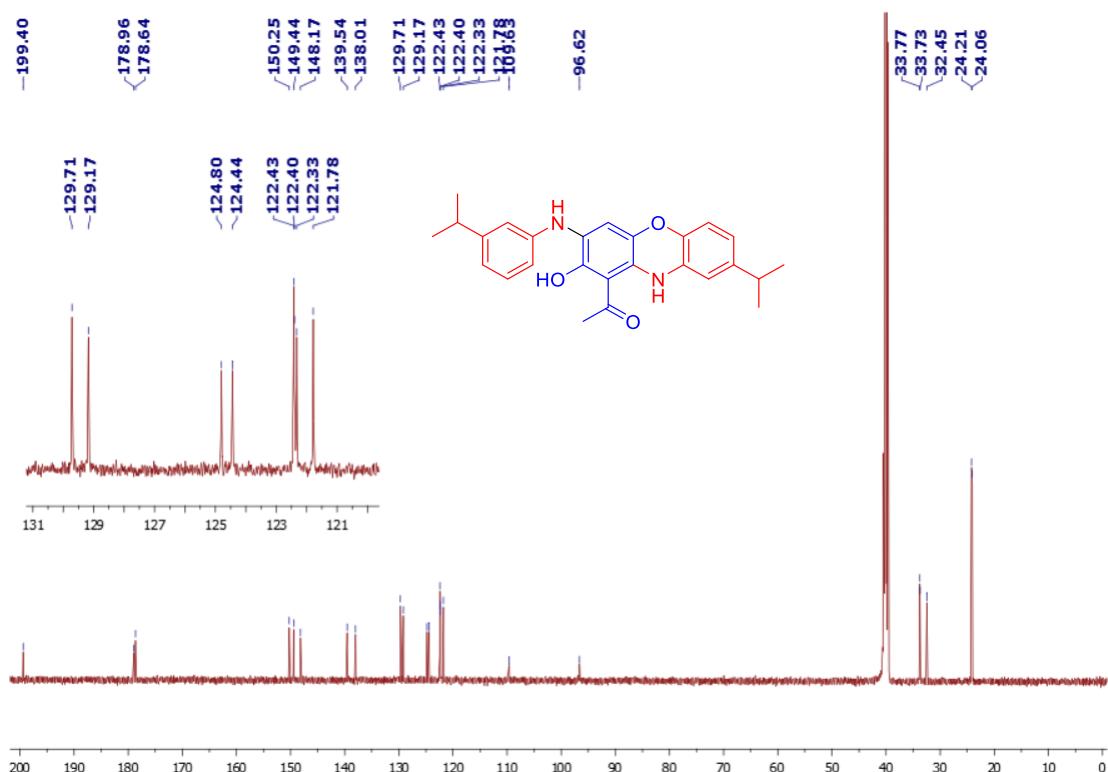
**1-(2-hydroxy-8-(trifluoromethyl)-3-((3-(trifluoromethyl)phenyl)amino)-10*H*-phenoxazin-1-yl)ethan-1-one (6D):**



**1-(2-hydroxy-8-isopropyl-3-((3-isopropylphenyl)amino)-10*H*-phenoxazin-1-yl)ethan-1-one (7D):**

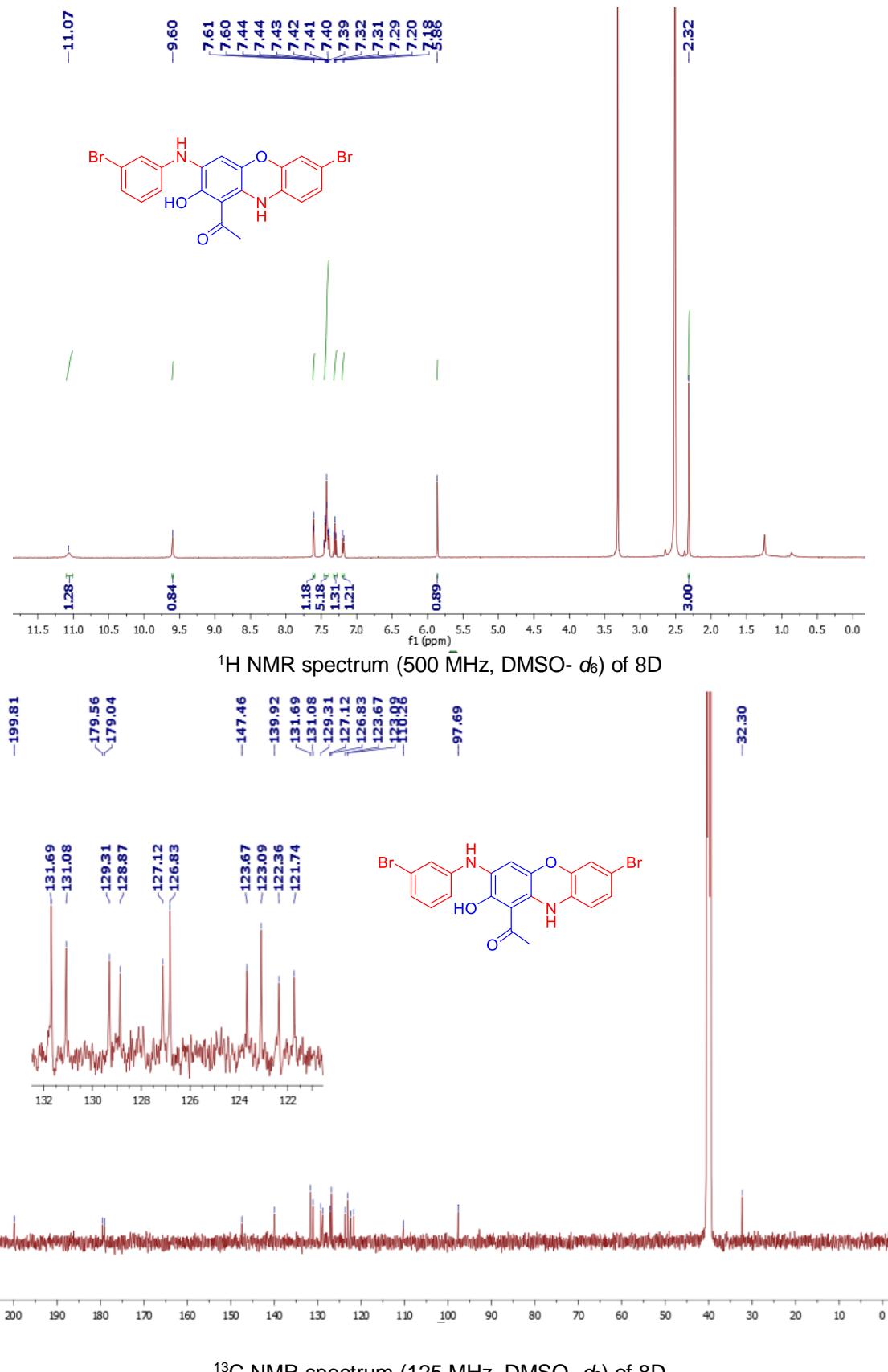


<sup>1</sup>H NMR spectrum (500 MHz, DMSO- d<sub>6</sub>) of 7D

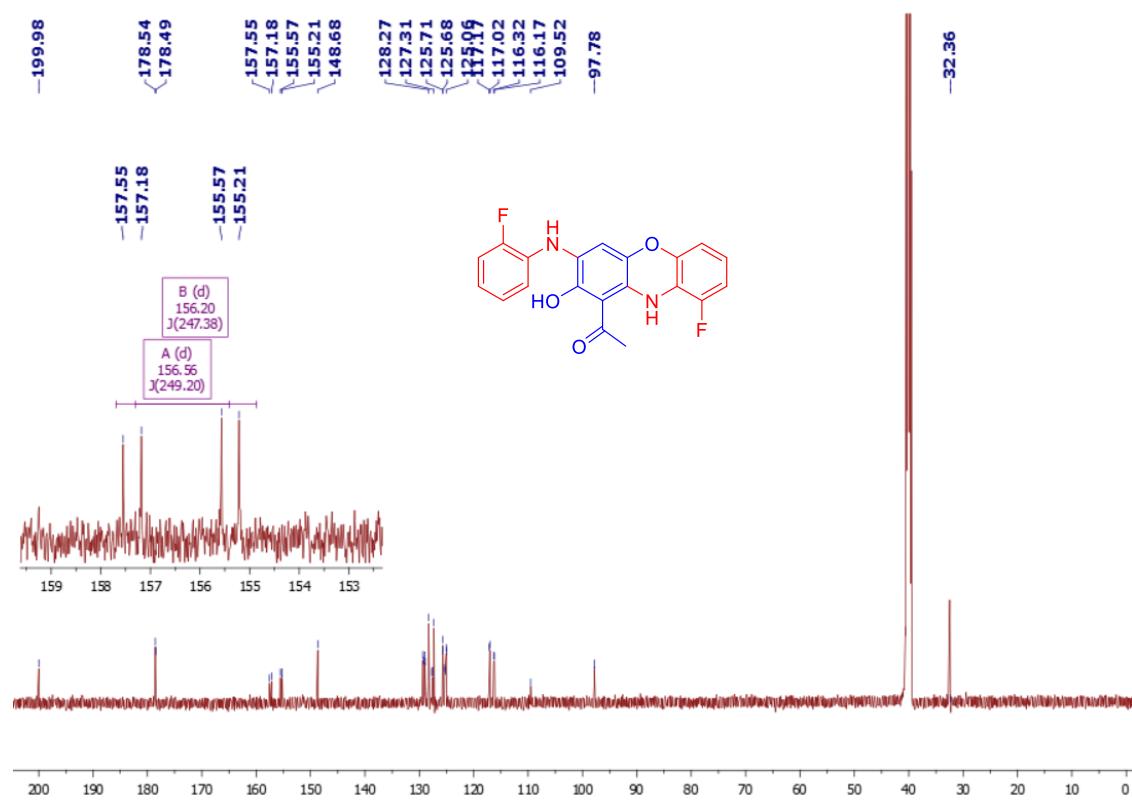
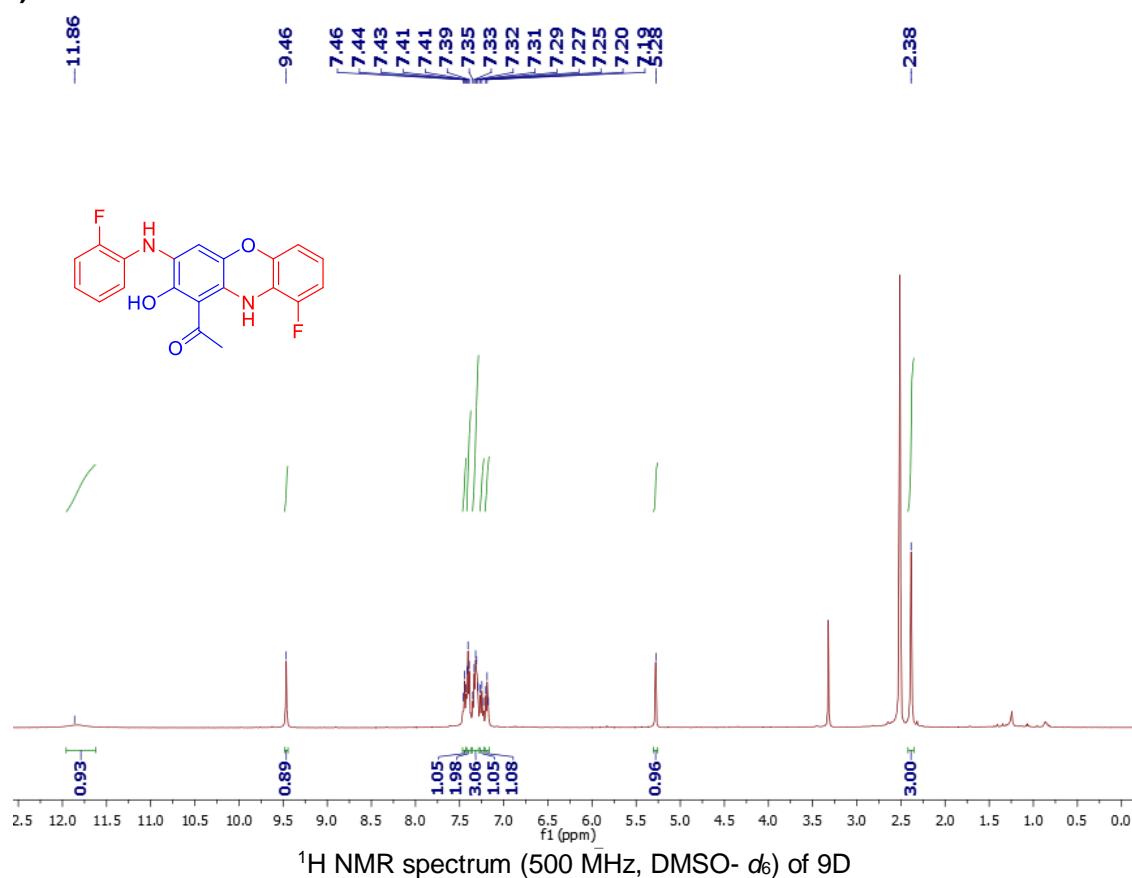


<sup>13</sup>C NMR spectrum (125 MHz, DMSO- *d*<sub>6</sub>) of 7D

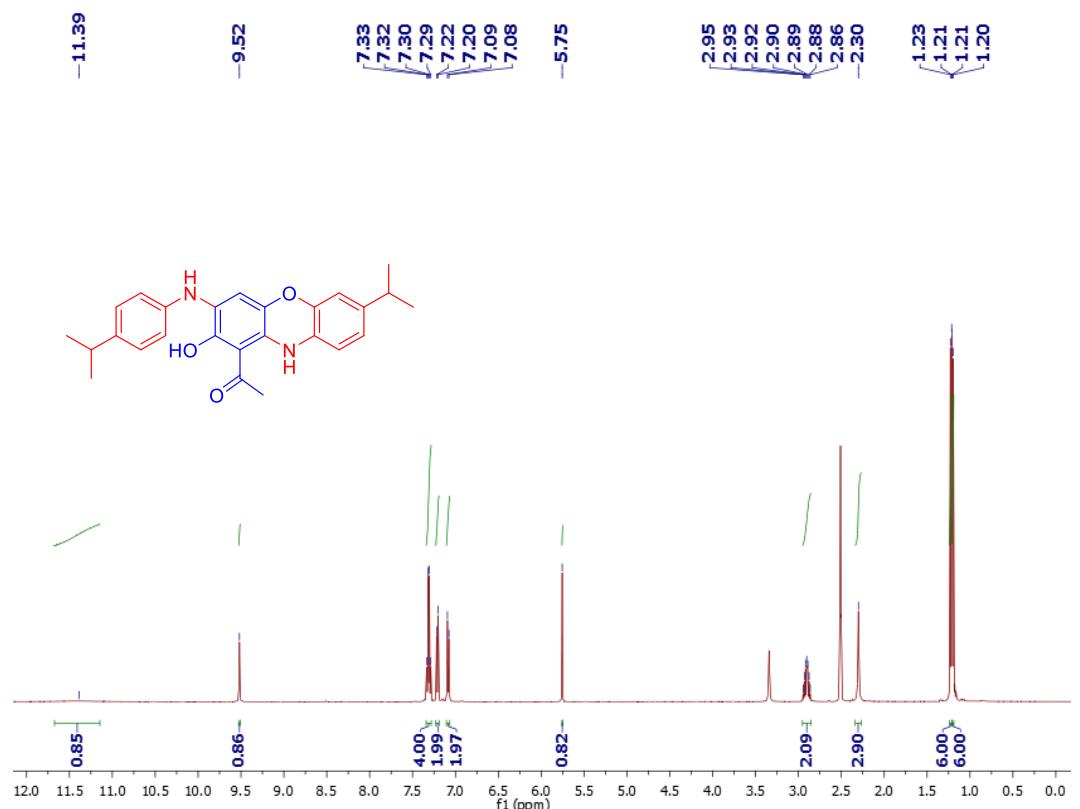
**1-(8-bromo-3-((3-bromophenyl)amino)-2-hydroxy-10*H*-phenoxazin-1-yl)ethan-1-one (8D):**



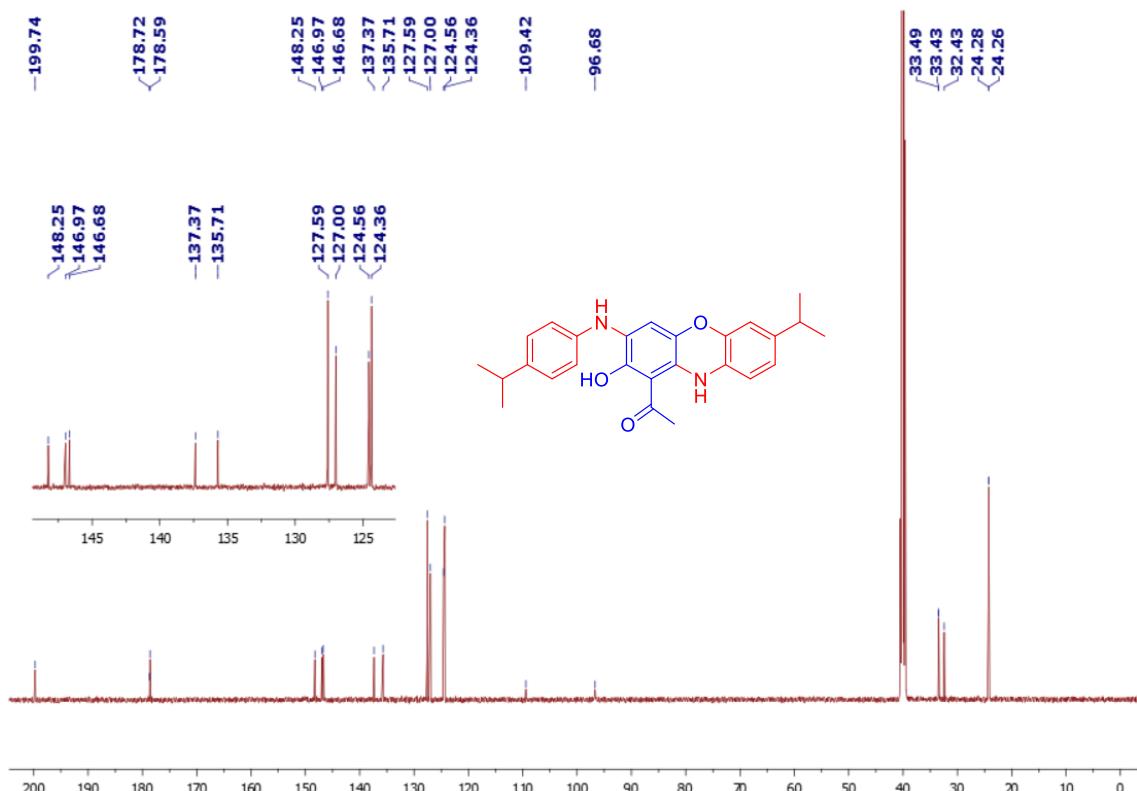
**1-(9-fluoro-3-((2-fluorophenyl)amino)-2-hydroxy-10H-phenoxazin-1-yl)ethan-1-one (9D):**



**1-(2-hydroxy-7-isopropyl-3-((4-isopropylphenyl)amino)-10*H*-phenoazin-1-yl)ethan-1-one (10D):**

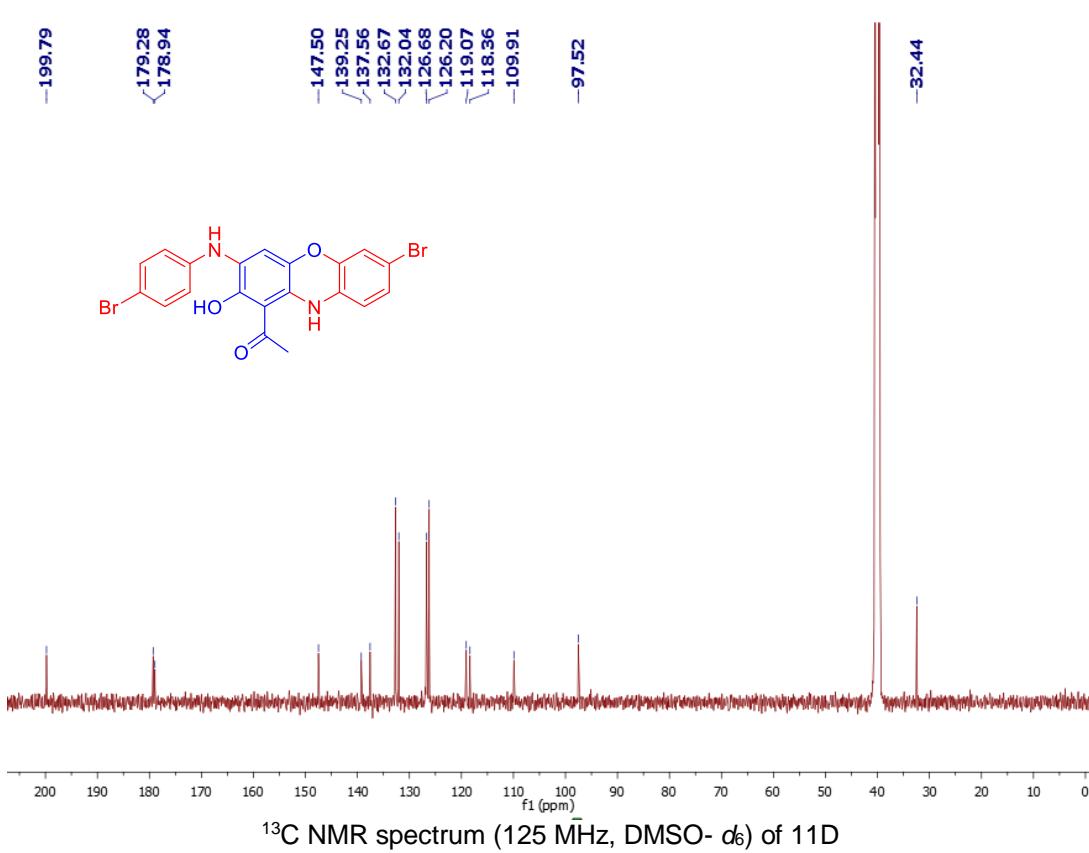
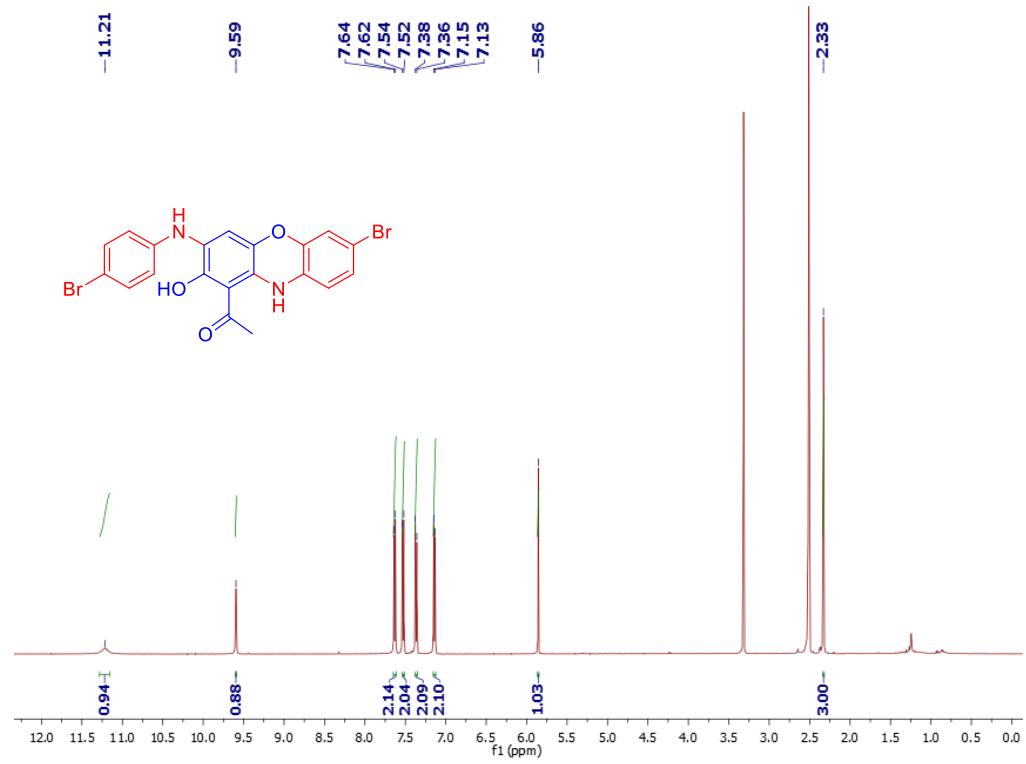


$^1\text{H}$  NMR spectrum (500 MHz, DMSO-  $d_6$ ) of 10D

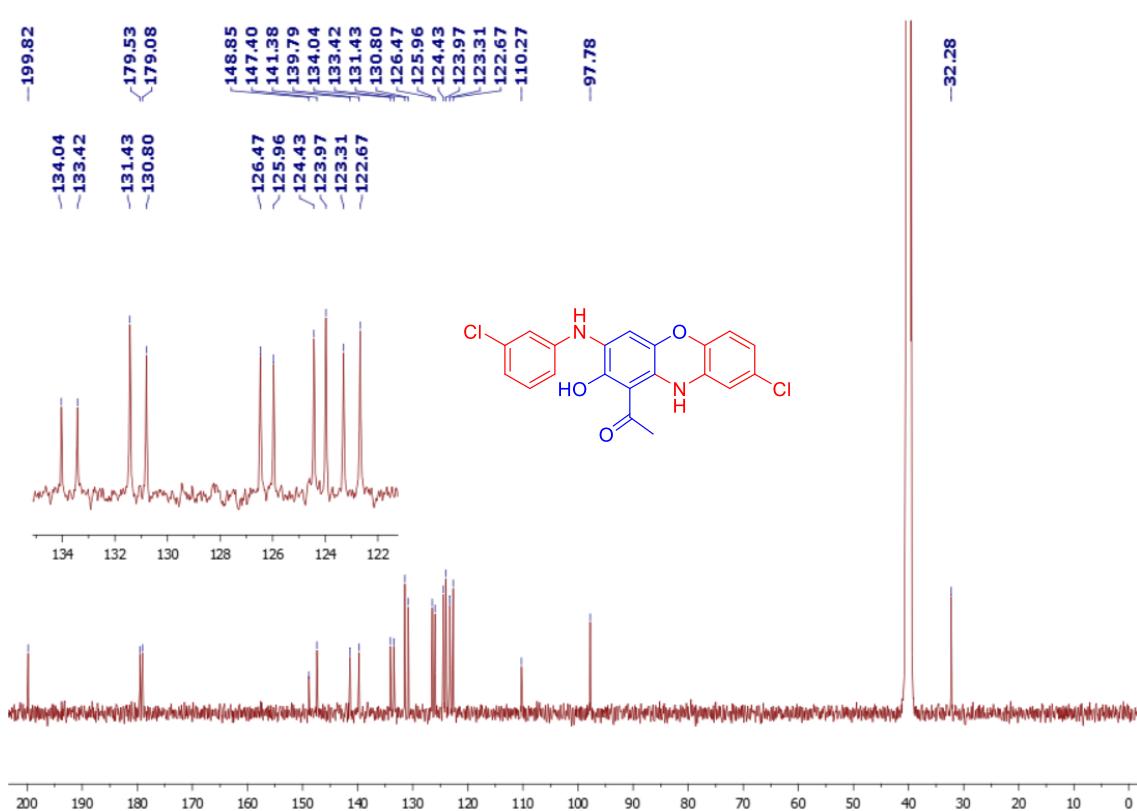
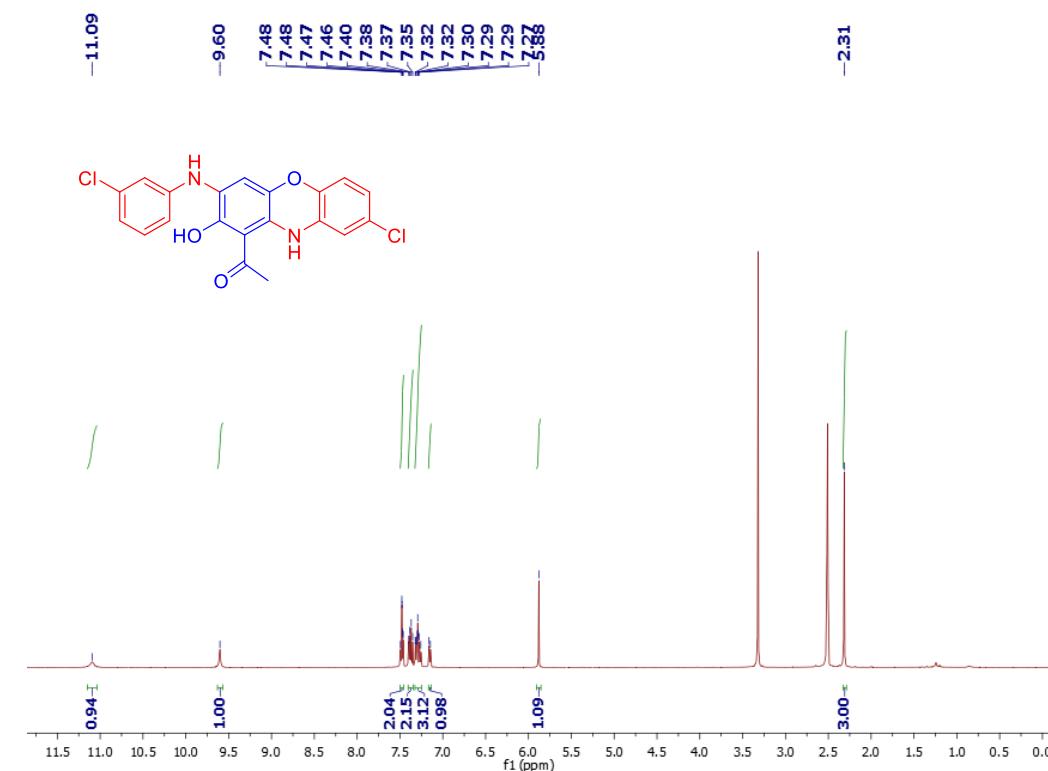


$^{13}\text{C}$  NMR spectrum (125 MHz, DMSO-  $d_6$ ) of 10D

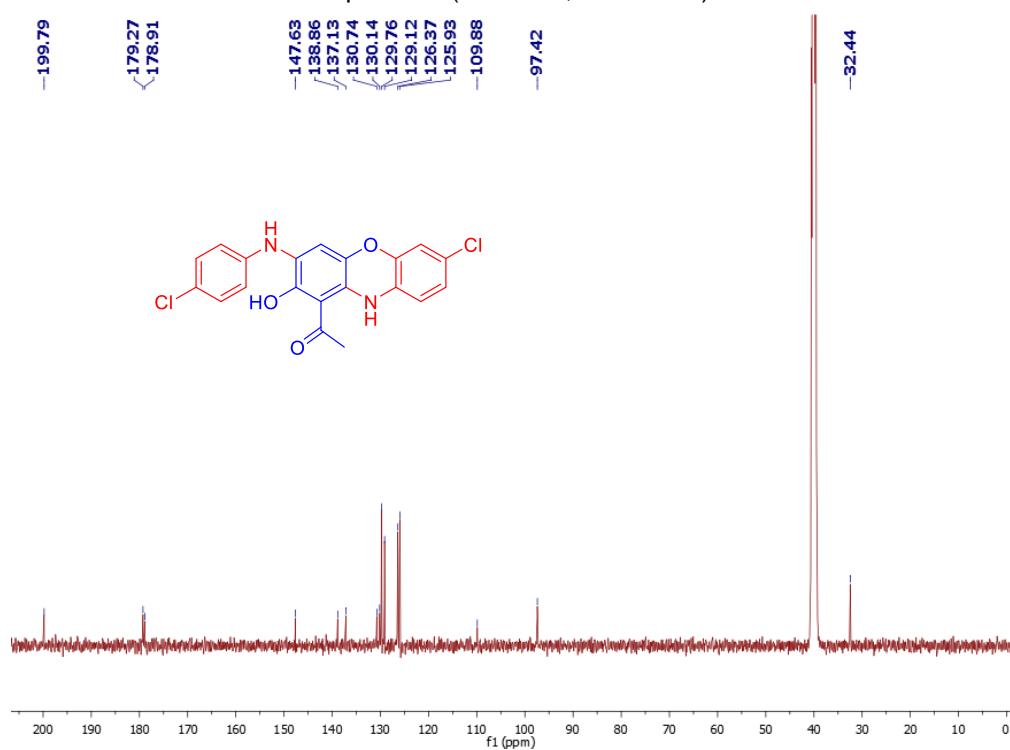
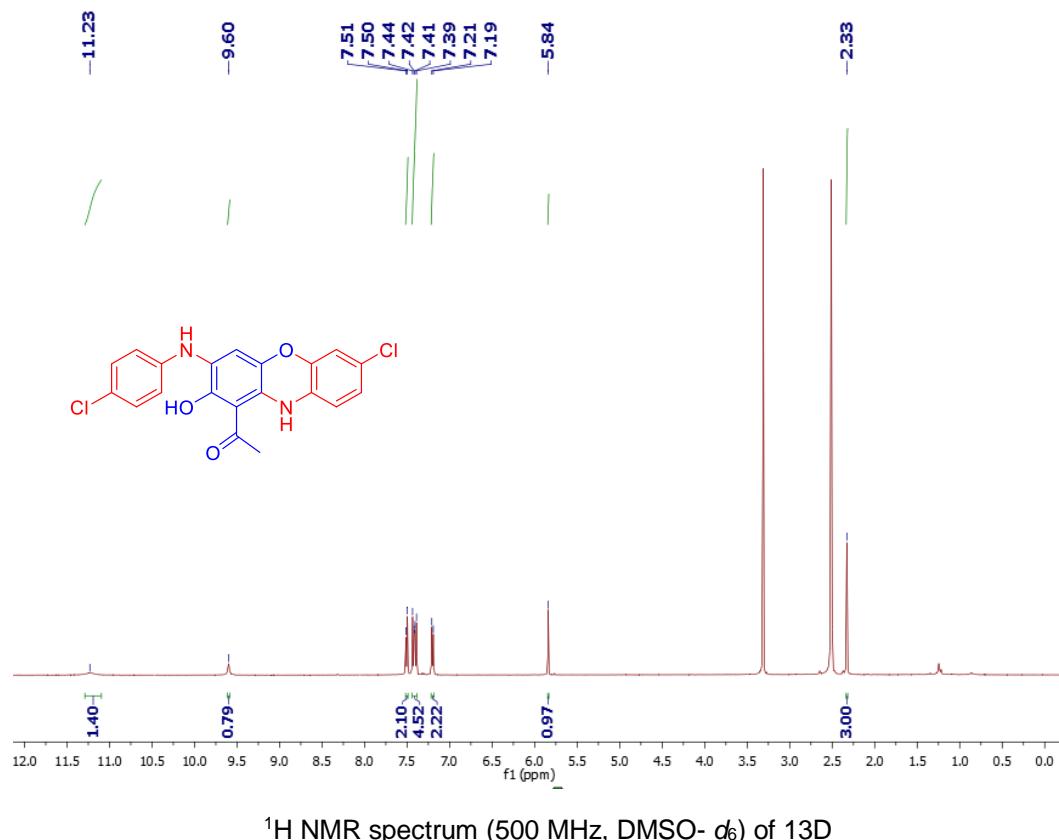
**1-(7-bromo-3-((4-bromophenyl)amino)-2-hydroxy-10*H*-phenoxazin-1-yl)ethan-1-one  
(11D):**



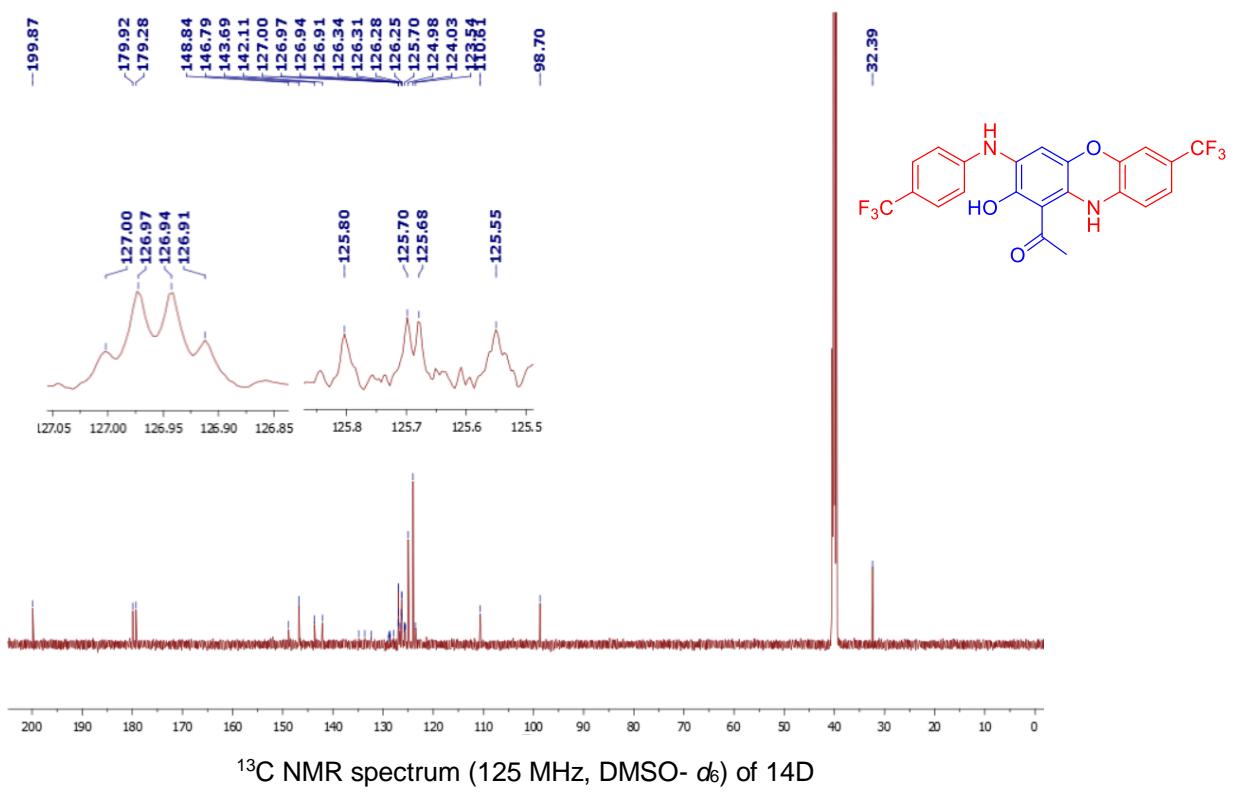
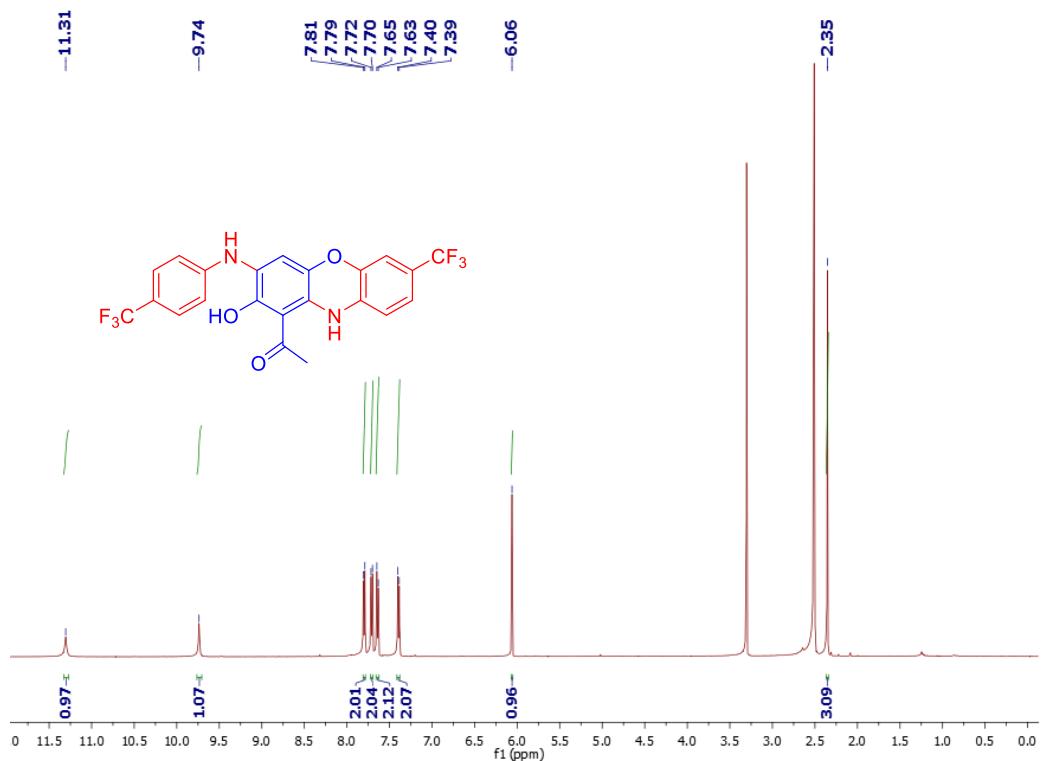
**1-(8-chloro-3-((3-chlorophenyl)amino)-2-hydroxy-10*H*-phenoxazin-1-yl)ethan-1-one  
(12D):**



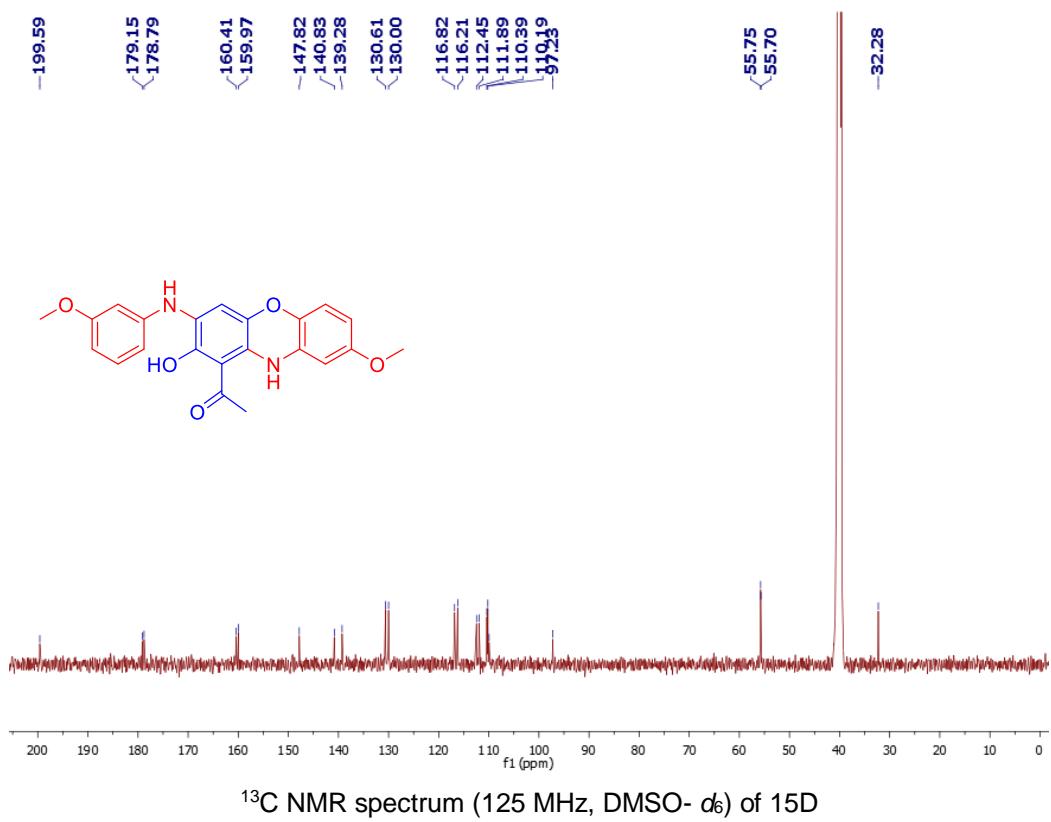
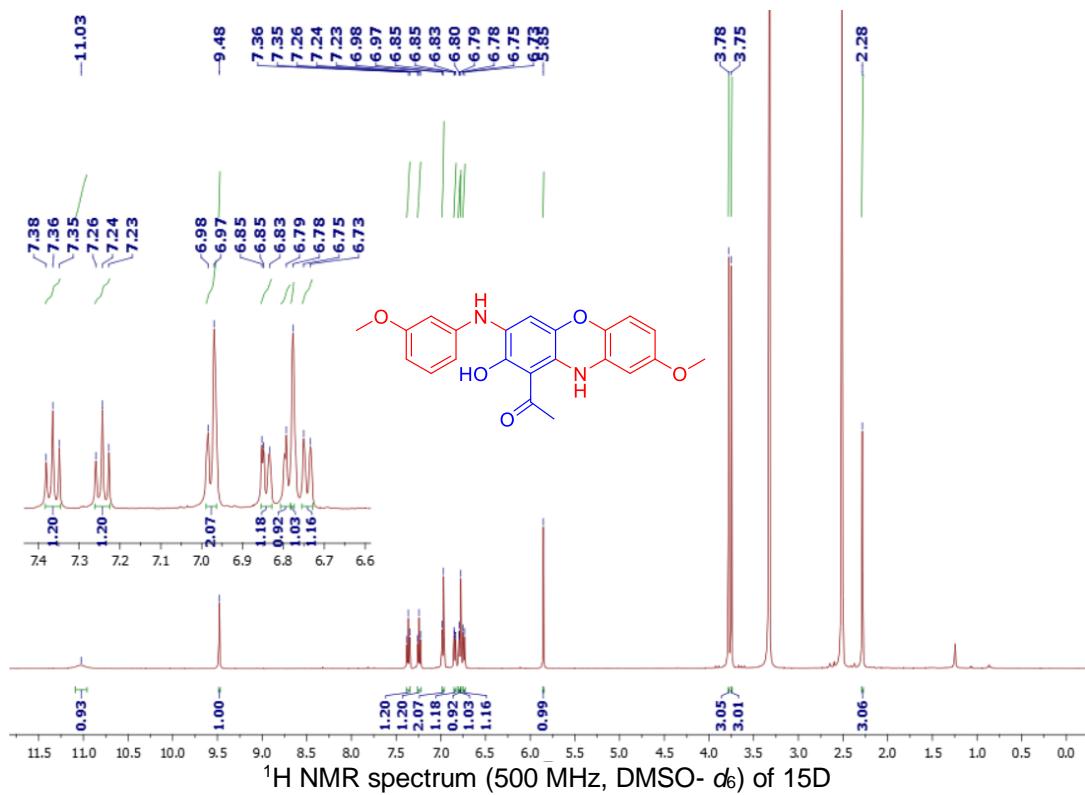
**1-(7-chloro-3-((4-chlorophenyl)amino)-2-hydroxy-10*H*-phenoxazin-1-yl)ethan-1-one  
(13D):**



**1-(2-hydroxy-7-(trifluoromethyl)-3-((4-(trifluoromethyl)phenyl)amino)-10*H*-phenoazin-1-yl)ethan-1-one (14D):**

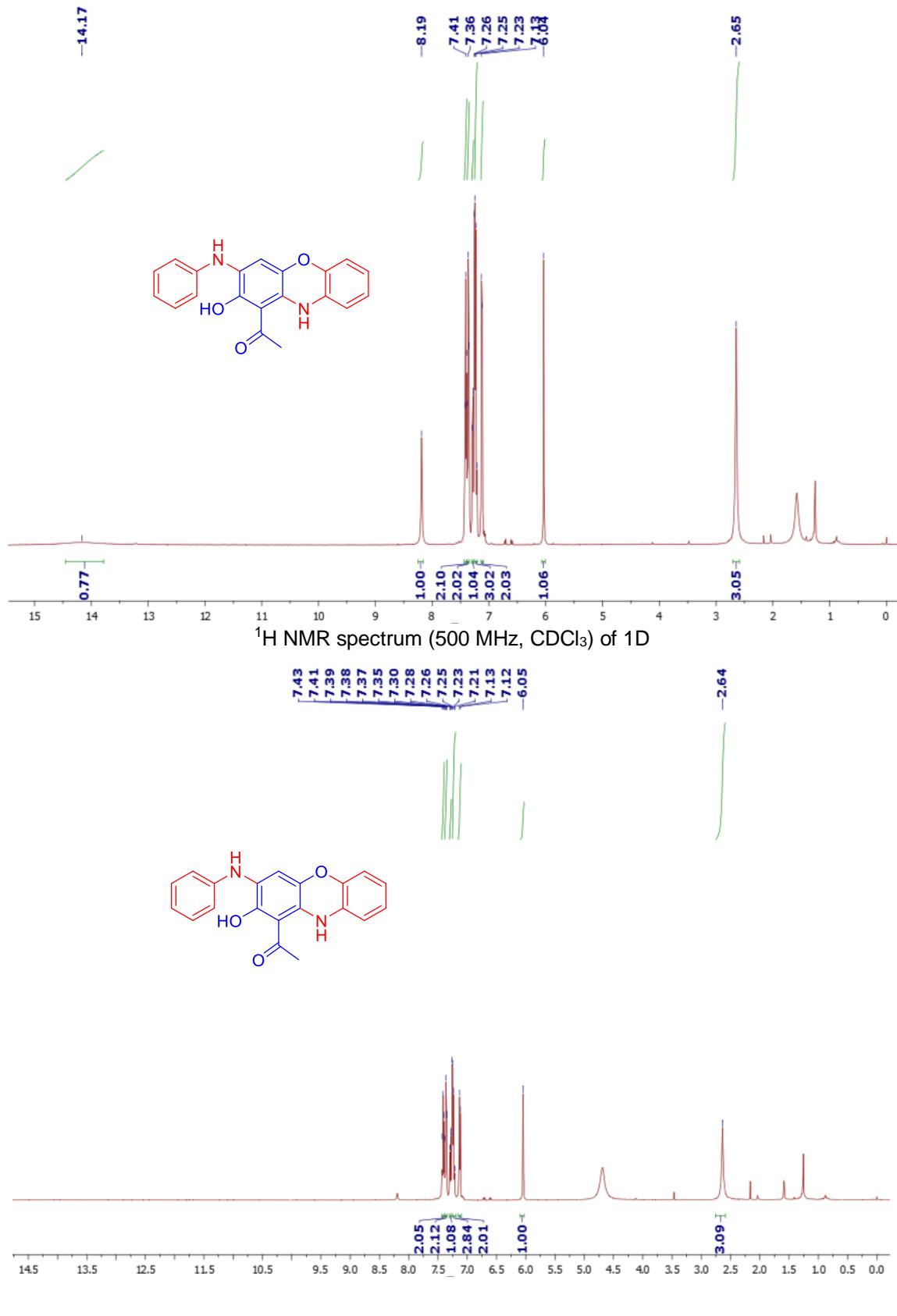


**1-(2-hydroxy-8-methoxy-3-((3-methoxyphenyl)amino)-10*H*-phenoxyazin-1-yl)ethan-1-one (15D):**



## D<sub>2</sub>O exchange experiment of compound 1D

#### **1-(2-hydroxy-3-(phenylamino)-10*H*-phenoxazin-1-yl)ethan-1-one (1D):**



<sup>1</sup>H NMR spectrum D<sub>2</sub>O exchange experiment (500 MHz, CDCl<sub>3</sub>) of 1D