

SI of SYNTHESIS AND PHARMACOLOGICAL ACTION OF HETEROCYCLIC  
BENZOXAZOLE DERIVATIVES

***N*-(2-(pyridin-2-yl)benzo[d]oxazol-5-yl)benzamide(4aa)**

<sup>1</sup>H NMR (500 MHz, DMSO)  $\delta$  10.49 (s, 1H), 8.84 (d,  $J$  = 4.2 Hz, 1H), 8.39 (d,  $J$  = 11.0 Hz, 2H), 8.10 (td,  $J$  = 7.8, 1.4 Hz, 1H), 8.01 (dd,  $J$  = 27.5, 7.2 Hz, 2H), 7.86 (s, 2H), 7.68 – 7.64 (m, 2H), 7.61 – 7.51 (m, 2H). <sup>13</sup>C NMR (126 MHz, DMSO)  $\delta$  166.17, 150.71, 147.41, 145.73, 141.85, 138.18, 137.08, 135.37, 132.13, 129.74, 128.92, 128.18, 126.70, 124.10, 120.13, 112.10, 111.49.

**2-phenyl-*N*-(2-(pyridin-2-yl)benzo[d]oxazol-5-yl)acetamide(4ab)**

<sup>1</sup>H NMR (500 MHz, DMSO)  $\delta$  10.46 (s, 1H), 8.82 (d,  $J$  = 4.1 Hz, 1H), 8.35 (d,  $J$  = 7.9 Hz, 1H), 8.26 (s, 1H), 8.08 (dd,  $J$  = 11.0, 4.4 Hz, 1H), 7.80 (d,  $J$  = 8.8 Hz, 1H), 7.67 – 7.62 (m, 2H), 7.38 (dd,  $J$  = 13.4, 6.0 Hz, 4H), 7.29 (t,  $J$  = 7.0 Hz, 1H), 3.72 (s, 2H). <sup>13</sup>C NMR (126 MHz, DMSO)  $\delta$  169.70, 162.46, 150.68, 147.05, 145.70, 141.90, 138.15, 137.19, 136.42, 129.65, 128.81, 127.05, 126.67, 124.07, 118.84, 111.62, 110.70, 43.80.

**2-methyl-*N*-(2-(pyridin-2-yl)benzo[d]oxazol-5-yl)benzamide(4ac)**

<sup>1</sup>H NMR (500 MHz, DMSO)  $\delta$  10.46 (s, 1H), 8.83 (d,  $J$  = 4.1 Hz, 1H), 8.38 (d,  $J$  = 10.0 Hz, 2H), 8.10 (t,  $J$  = 7.7 Hz, 1H), 7.87 – 7.82 (m, 4H), 7.69 – 7.65 (m, 1H), 7.47 (d,  $J$  = 6.6 Hz, 2H), 2.45 (s, 3H). <sup>13</sup>C NMR (126 MHz, DMSO)  $\delta$  166.27, 162.47, 150.71, 147.37, 145.73, 141.83, 138.24, 138.19, 137.13, 135.36, 132.70, 128.82, 128.66, 126.70, 125.34, 124.09, 120.10, 112.05, 111.47, 21.47.

**3-methyl-*N*-(2-(pyridin-2-yl)benzo[d]oxazol-5-yl)benzamide(4ad)**

<sup>1</sup>H NMR (500 MHz, DMSO)  $\delta$  10.55 (s, 1H), 8.83 (d,  $J$  = 4.1 Hz, 1H), 8.44 – 8.31 (m, 2H), 8.09 (td,  $J$  = 7.8, 1.5 Hz, 1H), 7.83 (q,  $J$  = 8.8 Hz, 2H), 7.67 (dd,  $J$  = 6.6, 4.9 Hz, 1H), 7.54 (d,  $J$  = 7.2 Hz, 1H), 7.44 (t,  $J$  = 7.1 Hz, 1H), 7.35 (t,  $J$  = 7.5 Hz, 2H), 2.45 (s, 3H). <sup>13</sup>C NMR (126 MHz, DMSO)  $\delta$  168.41, 162.49, 150.71, 147.29, 145.72, 141.89, 138.18, 137.64, 137.24, 135.78, 131.05, 130.18, 127.75, 126.69, 126.16, 124.09, 119.34, 111.57, 111.26, 19.82.

**4-methyl-*N*-(2-(pyridin-2-yl)benzo[d]oxazol-5-yl)benzamide(4ae)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.45 (s, 1H), 8.83 (d, *J* = 4.1 Hz, 1H), 8.41 – 8.35 (m, 2H), 8.09 (t, *J* = 7.6 Hz, 1H), 7.96 (d, *J* = 7.9 Hz, 2H), 7.90 – 7.81 (m, 2H), 7.66 (dd, *J* = 6.9, 5.0 Hz, 1H), 7.38 (d, *J* = 7.9 Hz, 2H), 2.42 (s, 3H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 165.96, 162.43, 150.69, 147.32, 145.73, 142.13, 141.82, 138.16, 137.18, 132.45, 129.42, 128.24, 126.67, 124.07, 120.14, 112.07, 111.41, 21.51.

***N*-(2-(pyridin-2-yl)benzo[d]oxazol-5-yl)-2-naphthamide(4af)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.83 (s, 1H), 8.84 (d, *J* = 4.2 Hz, 1H), 8.71 (s, 1H), 8.47 (d, *J* = 10.5 Hz, 1H), 8.39 (d, *J* = 7.8 Hz, 1H), 8.16 – 8.08 (m, 4H), 8.05 (d, *J* = 7.7 Hz, 1H), 7.95 (dd, *J* = 8.8, 1.5 Hz, 1H), 7.88 (d, *J* = 8.8 Hz, 1H), 7.72 – 7.61 (m, 3H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 166.22, 162.48, 150.71, 147.41, 145.74, 141.87, 138.18, 137.24, 134.81, 132.62, 129.49, 128.60, 128.51, 128.17, 127.81, 127.33, 126.69, 126.01, 124.99, 124.09, 120.19, 112.14, 111.50.

**4-methoxy-*N*-(2-(pyridin-2-yl)benzo[d]oxazol-5-yl)benzamide(4ag)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.32 (s, 1H), 8.83 (d, *J* = 4.0 Hz, 1H), 8.38 (d, *J* = 3.7 Hz, 2H), 8.10 (t, *J* = 7.6 Hz, 1H), 8.04 (d, *J* = 8.6 Hz, 2H), 7.84 (s, 2H), 7.67 (dd, *J* = 6.9, 5.1 Hz, 1H), 7.12 (d, *J* = 8.7 Hz, 2H), 3.89 (s, 3H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 165.52, 162.47, 162.43, 150.71, 147.28, 145.75, 141.84, 138.18, 137.26, 130.12, 127.36, 126.68, 124.08, 120.13, 114.15, 112.03, 111.41, 55.95.

***N*-(2-(pyridin-2-yl)benzo[d]oxazol-5-yl)-3-(trifluoromethyl)benzamide(4ah)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.82 (s, 1H), 8.83 (s, 1H), 8.39 (d, *J* = 9.9 Hz, 3H), 8.19 (s, 1H), 8.10 (t, *J* = 6.9 Hz, 1H), 8.01 (d, *J* = 6.9 Hz, 1H), 7.89 – 7.77 (m, 3H), 7.67 – 7.62 (m, 1H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 164.66, 162.56, 150.71, 147.60, 145.69, 141.85, 138.18, 136.71, 136.22, 133.34, 132.37, 130.23, 129.22, 128.68, 126.72, 124.80, 124.11, 120.33, 112.43, 111.56.

***N*-(2-(pyridin-2-yl)benzo[d]oxazol-5-yl)-4-(trifluoromethyl)benzamide(4ai)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.70 (s, 1H), 8.83 (d, *J* = 4.2 Hz, 1H), 8.43 – 8.35 (m, 2H), 8.22 (d, *J* = 8.0 Hz, 2H), 8.08 (tt, *J* = 12.1, 6.0 Hz, 1H), 7.96 (d, *J* = 8.1 Hz, 2H), 7.90 – 7.85 (m, 2H), 7.66 (dd, *J* = 6.9, 5.1 Hz, 1H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 166.68, 164.97, 162.56, 150.69, 147.59, 145.69, 141.86, 139.15, 138.15, 136.69, 130.58, 129.12, 126.70, 125.88, 124.10, 120.16, 112.26, 111.57.

**2-fluoro-*N*-(2-(pyridin-2-yl)benzo[d]oxazol-5-yl)benzamide(4aj)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.70 (s, 1H), 8.83 (s, 1H), 8.38 (s, 2H), 8.09 (s, 1H), 7.88 – 7.68 (m, 5H), 7.39 (d, *J* = 7.4 Hz, 2H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 163.37, 162.57, 150.71, 147.44, 145.68, 141.90, 138.19, 136.82, 133.12, 133.06, 130.44, 126.73, 125.08, 124.11, 119.44, 116.78, 116.61, 111.70, 111.42.

**3-fluoro-*N*-(2-(pyridin-2-yl)benzo[d]oxazol-5-yl)benzamide(4ak)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 8.83 (s, 1H), 8.38 (d, *J* = 11.4 Hz, 2H), 8.09 (t, *J* = 7.1 Hz, 1H), 7.92 – 7.79 (m, 4H), 7.65 (d, *J* = 6.2 Hz, 2H), 7.52 – 7.35 (m, 2H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 164.74, 163.42, 162.52, 161.48, 150.70, 147.52, 145.69, 141.84, 138.17, 136.79, 131.06, 126.70, 124.10, 120.20, 118.93, 116.09, 114.94, 112.25, 111.53.

**4-fluoro-*N*-(2-(pyridin-2-yl)benzo[d]oxazol-5-yl)benzamide(4al)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.56 (s, 1H), 8.83 (d, *J* = 4.2 Hz, 1H), 8.37 (d, *J* = 7.5 Hz, 2H), 8.10 (ddd, *J* = 9.1, 8.2, 3.5 Hz, 3H), 7.87 – 7.80 (m, 2H), 7.66 (dd, *J* = 7.1, 5.0 Hz, 1H), 7.41 (t, *J* = 8.8 Hz, 2H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 165.60, 165.05, 163.62, 162.49, 150.70, 147.43, 145.71, 141.84, 138.17, 136.98, 130.90, 126.69, 124.09, 120.18, 115.76, 112.18, 111.49.

**4-chloro-*N*-(2-(pyridin-2-yl)benzo[d]oxazol-5-yl)benzamide(4am)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.63 (s, 1H), 8.83 (d, *J* = 4.2 Hz, 1H), 8.37 (d, *J* = 9.4 Hz, 2H), 8.11 – 8.06 (m, 3H), 7.88 – 7.84 (m, 2H), 7.66 (t, *J* = 7.9 Hz, 3H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 165.04, 162.50, 150.70, 147.48, 145.70, 141.83, 138.17, 136.96, 136.89, 134.03, 130.17, 128.97, 126.70, 124.09, 120.18, 112.21, 111.50.

**4-bromo-*N*-(2-(pyridin-2-yl)benzo[d]oxazol-5-yl)benzamide(4an)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.69 (s, 1H), 8.83 (d, *J* = 4.1 Hz, 1H), 8.39 – 8.36 (m, 1H), 8.09 (dd, *J* = 10.9, 4.5 Hz, 1H), 8.01 (d, *J* = 8.4 Hz, 2H), 7.86 (s, 2H), 7.78 (d, *J* = 8.4 Hz, 2H), 7.66 (dd, *J* = 7.1, 5.1 Hz, 1H), 7.47 (d, *J* = 8.2 Hz, 1H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 165.17, 162.49, 150.70, 147.47, 145.70, 141.83, 138.17, 136.91, 134.40, 131.90, 130.37, 126.69, 125.88, 124.09, 120.20, 112.22, 111.49.

***N*-(2-(pyridin-2-yl)benzo[d]oxazol-5-yl)thiophene-2-carboxamide(4ao)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.46 (s, 1H), 8.83 (s, 1H), 8.40 – 8.32 (m, 2H), 8.10 (s, 2H), 7.92 – 7.79 (m, 3H), 7.67 (s, 1H), 7.28 (s, 1H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 162.53, 160.52, 150.70, 147.47, 145.70, 141.89, 140.37, 138.18, 136.59, 132.44, 129.73, 128.57, 126.71, 124.11, 120.15, 112.21, 111.57.

***N*-(2-(pyridin-3-yl)benzo[*d*]oxazol-5-yl)benzamide(4ba)**

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.48 (s, 1H), 9.34 (s, 1H), 8.79 (s, 1H), 8.52 (d, *J* = 6.9 Hz, 1H), 8.32 (s, 1H), 7.97 (d, *J* = 6.3 Hz, 2H), 7.79 (s, 2H), 7.65 – 7.52 (m, 4H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 165.72, 161.05, 152.39, 147.99, 146.70, 141.37, 136.61, 134.88, 131.69, 128.45, 127.71, 124.31, 122.85, 119.28, 111.43, 111.29, 110.82.

**2-phenyl-*N*-(2-(pyridin-3-yl)benzo[*d*]oxazol-5-yl)acetamide(4bb)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.48 (s, 1H), 9.36 (s, 1H), 8.83 (s, 1H), 8.55 (d, *J* = 6.8 Hz, 1H), 8.23 (s, 1H), 7.79 (d, *J* = 8.6 Hz, 1H), 7.70 – 7.58 (m, 2H), 7.41 – 7.23 (m, 5H), 3.72 (s, 2H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 169.71, 161.50, 152.81, 148.46, 146.82, 141.90, 137.20, 136.40, 135.23, 129.67, 128.83, 127.07, 124.82, 123.30, 118.43, 111.44, 110.41, 43.79.

**2-methyl-*N*-(2-(pyridin-3-yl)benzo[*d*]oxazol-5-yl)benzamide(4bc)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.56 (s, 1H), 9.41 (s, 1H), 8.87 (s, 1H), 8.63 (d, *J* = 6.9 Hz, 1H), 8.37 (s, 1H), 7.85 – 7.73 (m, 3H), 7.54 (d, *J* = 6.8 Hz, 1H), 7.44 (d, *J* = 7.0 Hz, 1H), 7.36 (d, *J* = 7.3 Hz, 2H), 2.45 (s, 3H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 168.41, 161.29, 152.17, 147.92, 147.05, 141.86, 137.60, 137.28, 135.92, 135.76, 131.05, 130.21, 127.75, 126.17, 125.12, 123.57, 119.01, 111.42, 110.98, 19.82.

**3-methyl-*N*-(2-(pyridin-3-yl)benzo[*d*]oxazol-5-yl)benzamide(4bd)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.55 (s, 1H), 9.39 (s, 1H), 8.84 (s, 1H), 8.57 (d, *J* = 7.2 Hz, 1H), 8.38 (s, 1H), 7.85 (s, 3H), 7.70 (d, *J* = 14.2 Hz, 2H), 7.45 (s, 1H), 7.17 (d, *J* = 20.4 Hz, 1H), 2.44 (s, 3H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 166.28, 161.48, 152.81, 148.47, 147.11, 141.83, 138.22, 137.17, 135.22, 132.68, 130.21, 128.80, 128.67, 125.35, 124.82, 123.33, 119.72, 111.79, 111.25, 21.47.

**4-methyl-*N*-(2-(pyridin-3-yl)benzo[*d*]oxazol-5-yl)benzamide(4be)**



<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.45 (s, 1H), 9.39 (s, 1H), 8.84 (s, 1H), 8.57 (d, *J* = 7.2 Hz, 1H), 8.37 (s, 1H), 7.95 (d, *J* = 7.3 Hz, 2H), 7.84 (s, 2H), 7.69 (s, 1H), 7.39 (d, *J* = 7.4 Hz, 2H), 3.37 (s, 3H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 165.96, 161.47, 152.81, 148.47, 147.09, 142.15, 141.83, 137.17, 135.22, 132.44, 129.43, 128.23, 124.82, 123.33, 119.75, 111.80, 111.23, 21.52.

***N*-(2-(pyridin-3-yl)benzo[*d*]oxazol-5-yl)-2-naphthamide(4bf)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.69 (s, 1H), 9.40 (s, 1H), 8.84 (s, 1H), 8.66 (s, 1H), 8.58 (d, *J* = 7.6 Hz, 1H), 8.43 (s, 1H), 8.10 (s, 4H), 7.88 (s, 2H), 7.68 (s, 3H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 166.20, 161.53, 152.82, 148.49, 147.18, 141.88, 137.15, 135.23, 134.80, 132.66, 132.58, 129.46, 128.55, 128.36, 128.18, 127.38, 124.94, 124.82, 123.33, 119.74, 119.64, 111.84, 111.33.

**4-methoxy-*N*-(2-(pyridin-3-yl)benzo[*d*]oxazol-5-yl)benzamide(4bg)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.34 (s, 1H), 9.38 (s, 1H), 8.83 (s, 1H), 8.56 (d, *J* = 6.8 Hz, 1H), 8.35 (s, 1H), 8.02 (s, 2H), 7.82 (s, 2H), 7.68 (s, 1H), 7.10 (s, 2H), 3.88 (s, 3H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 165.50, 162.43, 161.43, 152.78, 148.46, 147.02, 141.82, 137.26, 135.19, 130.12, 127.33, 124.80, 123.33, 119.72, 114.12, 111.76, 111.18, 55.93.

***N*-(2-(pyridin-3-yl)benzo[*d*]oxazol-5-yl)-3-(trifluoromethyl)benzamide(4bh)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.73 (s, 1H), 9.39 (s, 1H), 8.85 (s, 1H), 8.59 (s, 1H), 8.36 (s, 2H), 8.02 (d, *J* = 7.4 Hz, 1H), 7.90 – 7.81 (m, 4H), 7.70 (s, 1H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 164.65, 161.61, 152.86, 148.50, 147.36, 141.87, 138.72, 136.72, 136.24, 135.26, 132.37, 130.26, 129.82, 129.56, 128.68, 124.83, 123.29, 119.95, 112.15, 111.38.

***N*-(2-(pyridin-3-yl)benzo[*d*]oxazol-5-yl)-4-(trifluoromethyl)benzamide(4bi)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.72 (s, 1H), 9.39 (s, 1H), 8.84 (s, 1H), 8.56 (s, 1H), 8.37 (s, 1H), 8.22 (d, *J* = 7.6 Hz, 2H), 7.97 (d, *J* = 7.6 Hz, 2H), 7.85 (d, *J* = 8.8 Hz, 2H), 7.69 (s, 1H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 164.99, 161.61, 152.85, 148.49, 147.35, 141.86, 139.15, 136.70, 135.24, 132.03, 131.78, 129.12, 125.90, 124.82, 123.28, 119.78, 111.98, 111.39.

**2-fluoro-*N*-(2-(pyridin-3-yl)benzo[*d*]oxazol-5-yl)benzamide(4bj)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.68 (s, 1H), 9.39 (s, 1H), 8.84 (s, 1H), 8.57 (d, *J* = 6.9 Hz, 1H), 8.34 (s, 1H), 7.85 (d, *J* = 8.5 Hz, 1H), 7.77 – 7.63 (m, 4H), 7.40 (dd, *J* = 19.0, 8.9 Hz, 2H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 163.35, 161.62, 160.37, 152.86, 148.50, 147.20, 141.91, 136.81, 135.25, 133.07, 130.42, 125.12, 124.82, 123.28, 119.02, 116.79, 116.62, 111.51, 111.12.

**3-fluoro-*N*-(2-(pyridin-3-yl)benzo[d]oxazol-5-yl)benzamide(4bk)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.60 (s, 1H), 9.38 (s, 1H), 8.83 (s, 1H), 8.56 (d, *J* = 7.1 Hz, 1H), 8.36 (s, 1H), 7.90 – 7.82 (m, 4H), 7.65 (d, *J* = 24.3 Hz, 2H), 7.49 (s, 1H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 164.73, 163.39, 161.54, 152.81, 148.47, 147.27, 141.83, 137.65, 136.78, 135.21, 131.12, 124.79, 124.42, 123.28, 119.78, 119.10, 115.11, 111.95, 111.31.

**4-fluoro-*N*-(2-(pyridin-3-yl)benzo[d]oxazol-5-yl)benzamide(4bl)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.54 (s, 1H), 9.38 (s, 1H), 8.83 (s, 1H), 8.56 (d, *J* = 7.0 Hz, 1H), 8.35 (s, 1H), 8.12 (s, 2H), 7.83 (s, 2H), 7.68 (s, 1H), 7.42 (s, 2H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 165.02, 163.60, 161.50, 152.78, 148.45, 147.18, 141.82, 136.97, 135.23, 131.72, 130.91, 124.81, 123.31, 119.78, 115.93, 111.91, 111.26.

**4-chloro-*N*-(2-(pyridin-3-yl)benzo[d]oxazol-5-yl)benzamide(4bm)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.62 (s, 1H), 9.39 (d, *J* = 1.4 Hz, 1H), 8.86 – 8.83 (m, 1H), 8.58 – 8.56 (m, 1H), 8.36 (s, 1H), 8.07 (d, *J* = 8.5 Hz, 2H), 7.91 (d, *J* = 8.4 Hz, 1H), 7.84 (s, 1H), 7.70 – 7.66 (m, 2H), 7.41 (d, *J* = 8.3 Hz, 1H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 165.07, 161.57, 152.84, 148.50, 147.28, 141.87, 135.24, 134.05, 131.39, 130.18, 128.99, 128.05, 124.82, 123.33, 119.84, 111.99, 111.31.

**4-bromo-*N*-(2-(pyridin-3-yl)benzo[d]oxazol-5-yl)benzamide(4bn)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.57 (s, 1H), 9.38 (s, 1H), 8.84 (s, 1H), 8.56 (d, *J* = 7.0 Hz, 1H), 8.35 (s, 1H), 7.98 (d, *J* = 7.3 Hz, 2H), 7.82 (d, *J* = 13.6 Hz, 4H), 7.68 (s, 1H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 165.13, 161.54, 152.82, 148.48, 147.23, 141.84, 136.86, 135.22, 134.38, 131.92, 130.32, 125.90, 124.80, 123.29, 119.76, 111.91, 111.31.

***N*-(2-(pyridin-3-yl)benzo[d]oxazol-5-yl)thiophene-2-carboxamide(4bo)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.49 (s, 1H), 9.39 (s, 1H), 8.84 (s, 1H), 8.56 (s, 1H), 8.30 (s, 1H), 8.10 (s, 1H), 7.92 (s, 1H), 7.85 (d, *J* = 8.6 Hz, 1H), 7.78 (d, *J* = 8.7 Hz, 1H), 7.69 (s, 1H), 7.28 (s, 1H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 161.56, 160.50, 152.83, 148.49, 147.22, 141.88, 140.34, 136.59, 135.24, 132.46, 129.73, 128.58, 124.81, 123.30, 119.77, 111.94, 111.36.

***N*-(2-(pyridin-4-yl)benzo[*d*]oxazol-5-yl)benzamide(4ca)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.50 (s, 1H), 8.88 (d, *J* = 5.8 Hz, 2H), 8.40 (s, 1H), 8.17 – 8.10 (m, 2H), 8.03 (d, *J* = 7.2 Hz, 2H), 7.87 (s, 2H), 7.61 (dt, *J* = 12.2, 5.9 Hz, 3H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 166.21, 161.42, 151.37, 147.29, 141.80, 137.26, 135.33, 133.97, 132.16, 128.93, 128.18, 121.28, 120.44, 112.05, 111.51.

**2-phenyl-*N*-(2-(pyridin-4-yl)benzo[*d*]oxazol-5-yl)acetamide(4cb)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.52 (s, 1H), 8.86 (d, *J* = 6.1 Hz, 2H), 8.27 (s, 1H), 8.11 (d, *J* = 6.1 Hz, 2H), 7.82 (d, *J* = 8.9 Hz, 1H), 7.65 (d, *J* = 10.9 Hz, 1H), 7.42 – 7.34 (m, 4H), 7.29 (d, *J* = 7.0 Hz, 1H), 3.72 (s, 2H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 169.76, 161.39, 151.37, 146.93, 141.85, 137.39, 136.38, 133.94, 129.67, 128.82, 127.06, 121.26, 119.15, 111.68, 110.62, 43.78.

**2-methyl-*N*-(2-(pyridin-4-yl)benzo[*d*]oxazol-5-yl)benzamide(4cc)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.57 (s, 1H), 8.87 (s, 2H), 8.40 (s, 1H), 8.13 (d, *J* = 5.9 Hz, 2H), 7.84 (dd, *J* = 20.2, 8.8 Hz, 2H), 7.54 (d, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.2 Hz, 1H), 7.36 (t, *J* = 7.7 Hz, 2H), 1.94 (s, 3H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 172.49, 168.44, 161.43, 151.40, 147.16, 141.84, 137.41, 135.78, 133.95, 131.07, 130.23, 127.75, 126.18, 121.27, 119.63, 111.64, 111.18, 21.55.

**3-methyl-*N*-(2-(pyridin-4-yl)benzo[*d*]oxazol-5-yl)benzamide(4cd)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.47 (s, 1H), 8.88 (d, *J* = 6.0 Hz, 2H), 8.40 (s, 1H), 8.13 (d, *J* = 6.0 Hz, 2H), 7.87 – 7.79 (m, 4H), 7.50 – 7.41 (m, 2H), 2.45 (s, 3H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 166.31, 161.41, 151.39, 147.24, 141.79, 138.26, 137.30, 135.34, 133.96, 132.74, 128.84, 128.66, 125.34, 121.27, 120.38, 111.98, 111.52, 21.47.

**4-methyl-*N*-(2-(pyridin-4-yl)benzo[*d*]oxazol-5-yl)benzamide(4ce)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.44 (s, 1H), 8.87 (d, *J* = 6.0 Hz, 2H), 8.40 (s, 1H), 8.13 (d, *J* = 6.0 Hz, 2H), 7.95 (d, *J* = 8.1 Hz, 2H), 7.86 (s, 2H), 7.39 (d, *J* = 7.9 Hz, 2H), 2.43 (s, 3H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 166.00, 161.38, 151.38, 147.21, 142.19, 141.78, 137.34, 133.97, 132.41, 129.45, 128.23, 121.27, 120.42, 111.99, 111.48, 21.52.

***N*-(2-(pyridin-4-yl)benzo[*d*]oxazol-5-yl)-2-naphthamide(4cf)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.69 (s, 1H), 8.88 (d, *J* = 5.9 Hz, 2H), 8.65 (s, 1H), 8.46 (d, *J* = 1.3 Hz, 1H), 8.16 – 8.03 (m, 6H), 7.91 (dt, *J* = 18.0, 5.3 Hz, 2H), 7.71 – 7.64 (m, 2H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 166.24, 161.43, 151.35, 147.32, 141.84, 137.33, 134.83, 134.00, 132.63, 132.60, 129.46, 128.80, 128.56, 128.37, 128.19, 127.38, 124.93, 121.29, 120.46, 112.08, 111.55.

**4-methoxy-*N*-(2-(pyridin-4-yl)benzo[*d*]oxazol-5-yl)benzamide(4cg)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.34 (s, 1H), 8.88 (d, *J* = 5.7 Hz, 2H), 8.39 (s, 1H), 8.17 – 8.11 (m, 2H), 8.03 (d, *J* = 8.8 Hz, 2H), 7.86 (s, 2H), 7.12 (d, *J* = 8.8 Hz, 2H), 3.88 (s, 3H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 165.55, 162.49, 161.37, 151.38, 147.17, 141.79, 137.45, 133.99, 130.13, 127.31, 121.27, 120.44, 114.15, 111.99, 111.44, 55.95.

***N*-(2-(pyridin-4-yl)benzo[*d*]oxazol-5-yl)-3-(trifluoromethyl)benzamide(4ch)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.75 (s, 1H), 8.88 (d, *J* = 5.9 Hz, 2H), 8.36 (dd, *J* = 21.3, 13.1 Hz, 3H), 8.14 (d, *J* = 5.9 Hz, 2H), 8.03 (d, *J* = 7.7 Hz, 1H), 7.86 (dd, *J* = 20.6, 12.0 Hz, 3H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 164.70, 161.53, 154.77, 151.40, 147.49, 141.81, 136.84, 136.15, 133.93, 132.38, 130.29, 129.84, 128.80, 124.81, 121.30, 120.63, 112.37, 111.65.

***N*-(2-(pyridin-4-yl)benzo[*d*]oxazol-5-yl)-4-(trifluoromethyl)benzamide(4ci)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.71 (s, 1H), 8.86 (d, *J* = 6.0 Hz, 2H), 8.39 (s, 1H), 8.21 (d, *J* = 8.1 Hz, 2H), 8.11 (d, *J* = 6.0 Hz, 2H), 7.95 (d, *J* = 8.3 Hz, 2H), 7.86 (s, 2H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 164.99, 161.48, 151.35, 147.44, 141.78, 139.09, 136.86, 133.89, 132.06, 129.12, 125.89, 123.32, 121.25, 120.43, 112.17, 111.60.

**2-fluoro-*N*-(2-(pyridin-4-yl)benzo[*d*]oxazol-5-yl)benzamide(4cj)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.69 (s, 1H), 8.88 (d, *J* = 5.5 Hz, 2H), 8.38 (s, 1H), 8.14 (d, *J* = 5.6 Hz, 2H), 7.88 (d, *J* = 8.8 Hz, 1H), 7.82 – 7.73 (m, 2H), 7.64 (d, *J* = 6.6 Hz, 1H), 7.40 (dd, *J* = 19.6, 8.8 Hz, 2H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 163.39, 161.54, 151.41, 147.33, 141.86, 136.98, 133.92, 133.18, 130.45, 125.42, 125.11, 121.29, 119.72, 116.81, 116.63, 111.77, 111.35.

**3-fluoro-*N*-(2-(pyridin-4-yl)benzo[d]oxazol-5-yl)benzamide(4ck)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.67 (s, 1H), 8.88 (d, *J* = 4.1 Hz, 2H), 8.38 (s, 1H), 8.14 (d, *J* = 4.2 Hz, 2H), 7.88 (d, *J* = 8.7 Hz, 1H), 7.81 – 7.73 (m, 2H), 7.64 (d, *J* = 5.8 Hz, 1H), 7.40 (dd, *J* = 17.4, 9.2 Hz, 2H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 163.39, 161.54, 151.40, 147.35, 141.87, 136.98, 133.93, 133.17, 133.10, 130.43, 125.12, 121.29, 119.75, 116.80, 116.62, 111.75, 111.39.

**4-fluoro-*N*-(2-(pyridin-4-yl)benzo[d]oxazol-5-yl)benzamide(4cl)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.54 (s, 1H), 8.88 (d, *J* = 5.9 Hz, 2H), 8.39 (s, 1H), 8.15 – 8.09 (m, 4H), 7.87 (d, *J* = 7.4 Hz, 2H), 7.43 (t, *J* = 8.8 Hz, 2H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 165.08, 161.44, 151.39, 147.31, 141.79, 137.13, 133.94, 131.73, 130.90, 121.27, 120.47, 115.97, 115.79, 112.11, 111.55.

**4-chloro-*N*-(2-(pyridin-4-yl)benzo[d]oxazol-5-yl)benzamide(4cm)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.60 (s, 1H), 8.87 (d, *J* = 4.5 Hz, 2H), 8.38 (s, 1H), 8.12 (d, *J* = 5.8 Hz, 2H), 8.05 (d, *J* = 8.5 Hz, 2H), 7.86 (s, 2H), 7.66 (d, *J* = 8.5 Hz, 2H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 165.07, 161.45, 151.37, 147.37, 141.80, 137.08, 136.99, 134.02, 133.94, 130.16, 128.99, 121.27, 120.50, 112.18, 111.53.

**4-bromo-*N*-(2-(pyridin-4-yl)benzo[d]oxazol-5-yl)benzamide(4cn)**

<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.55 (s, 1H), 8.86 (s, 2H), 8.37 (s, 1H), 8.11 (d, *J* = 5.7 Hz, 2H), 7.97 (d, *J* = 8.4 Hz, 2H), 7.86 – 7.77 (m, 4H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 165.17, 161.43, 151.36, 147.34, 141.78, 137.01, 134.33, 133.91, 131.93, 130.32, 125.95, 121.26, 120.42, 112.11, 111.54.

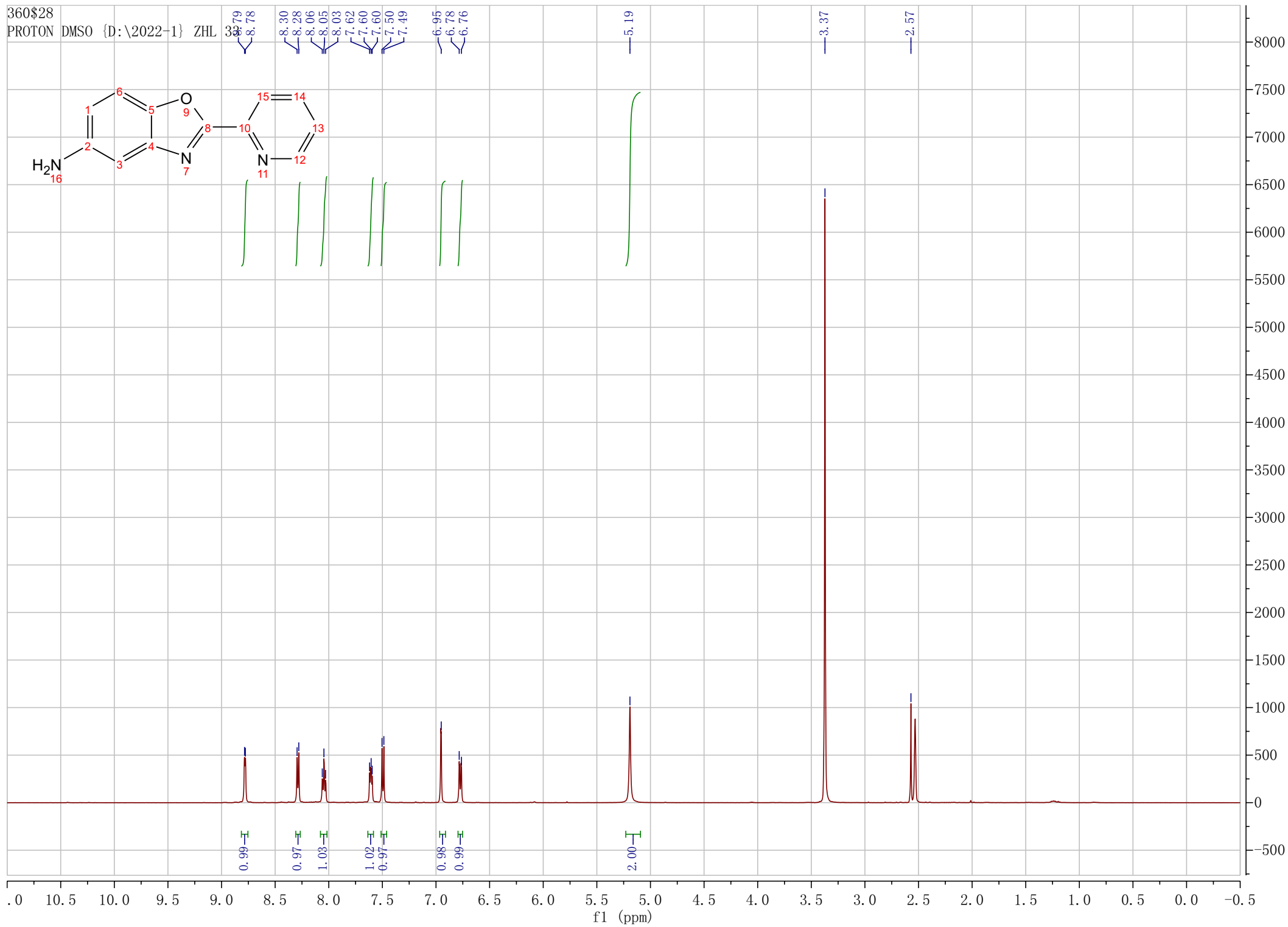
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<sup>1</sup>H NMR (500 MHz, DMSO) δ 10.48 (s, 1H), 8.88 (d, *J* = 6.0 Hz, 2H), 8.34 (s, 1H), 8.14 (d, *J* = 4.5 Hz, 2H), 8.09 (d, *J* = 3.6 Hz, 1H), 7.90 (dd, *J* = 18.6, 7.3 Hz, 2H), 7.81 (d, *J* = 8.9 Hz, 1H), 7.31 – 7.27 (m, 1H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 161.49,

160.54, 151.40, 147.36, 141.84, 140.29, 136.76, 133.95, 132.53, 129.77, 128.60,  
121.30, 120.47, 112.17, 111.63.

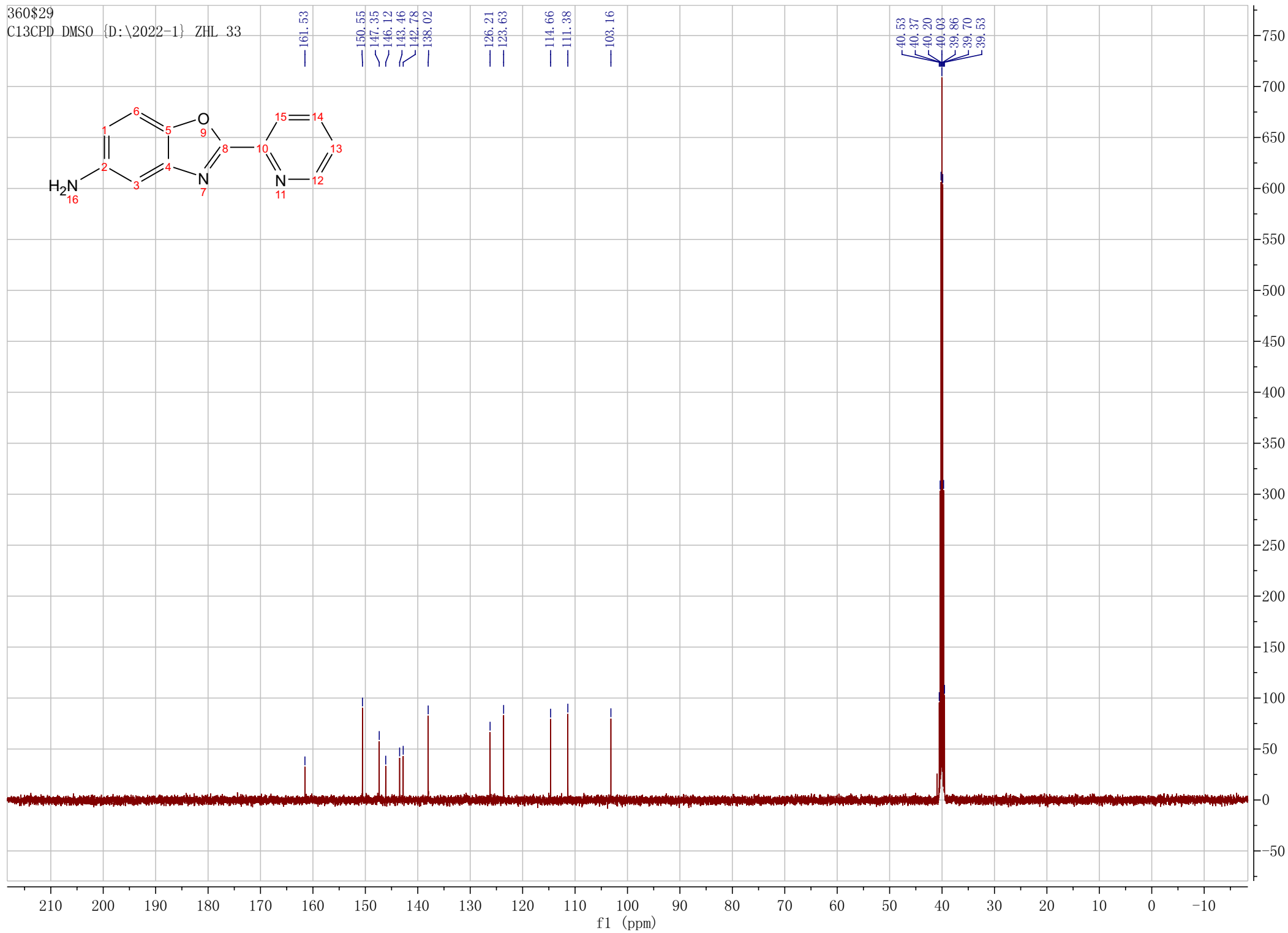
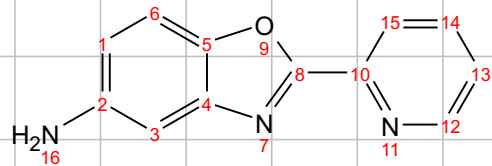
360\$28

PROTON DMSO {D:\2022-1} ZHL



360\$29

C13CPD DMSO {D:\2022-1} ZHL 33





360\$8

PROTON DMSO {D:\2021-3

31

79

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8.48

7.64

7.49

7.47

6.93

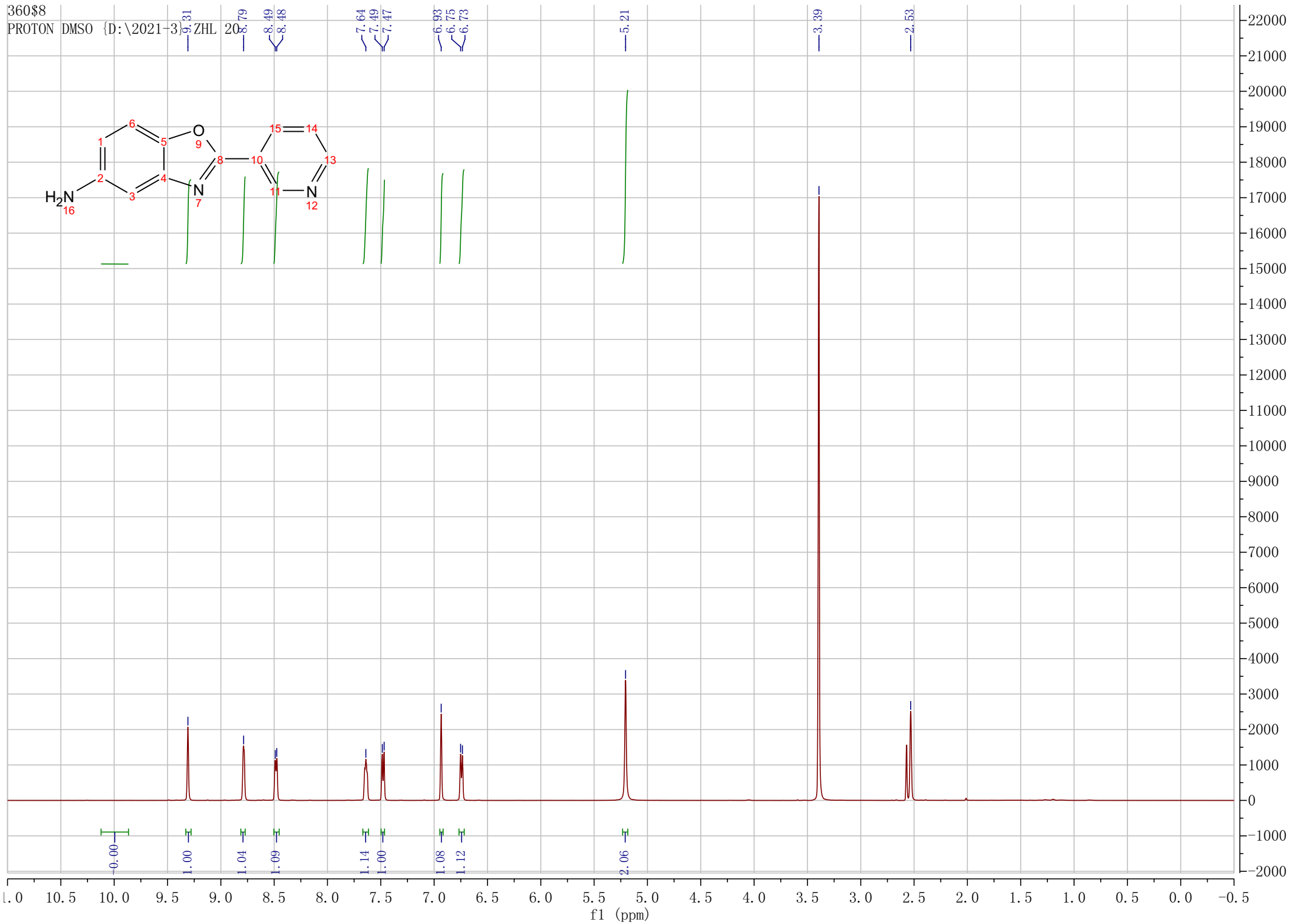
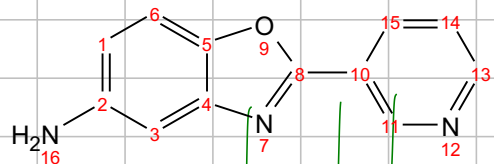
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6.73

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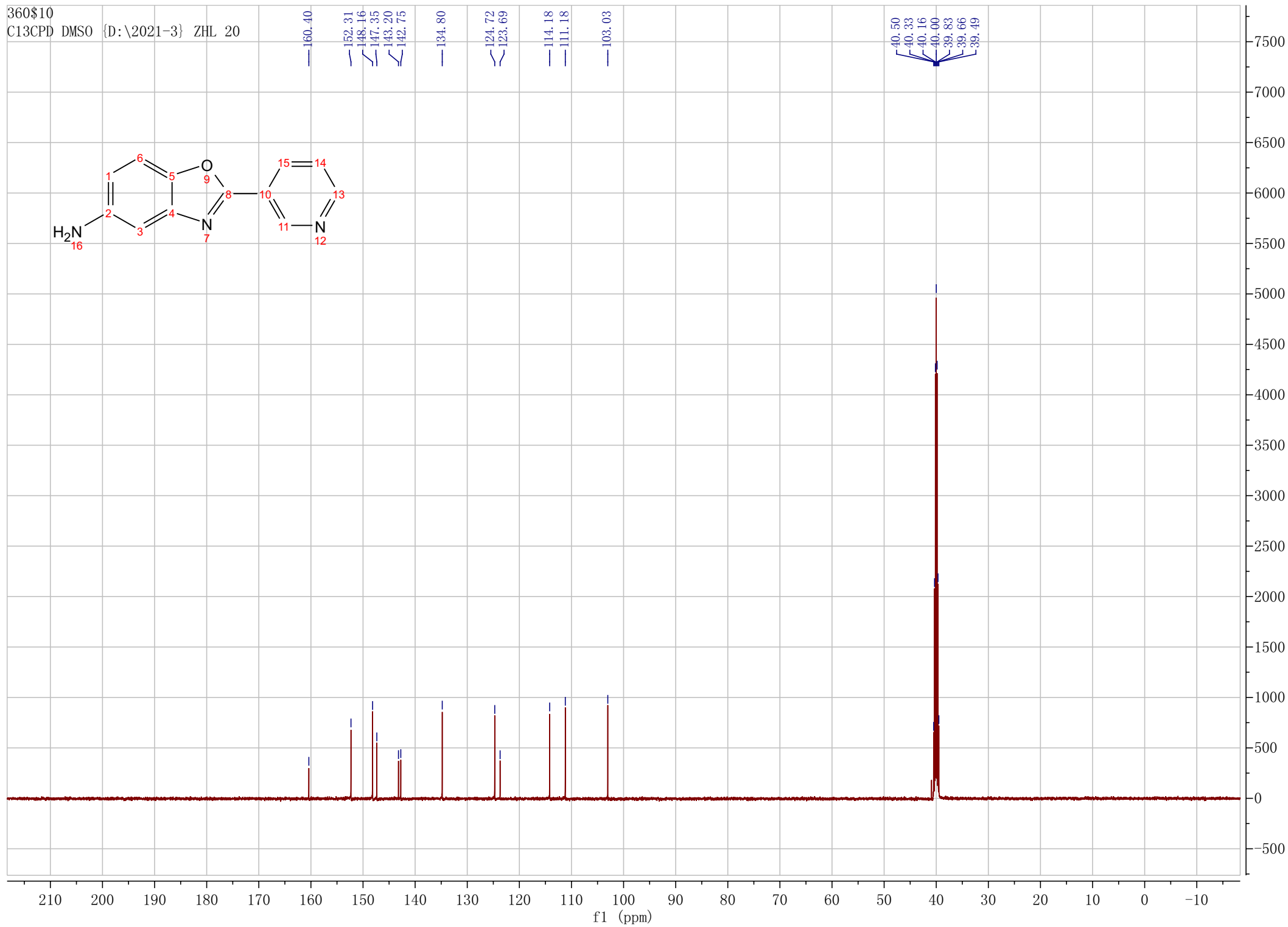
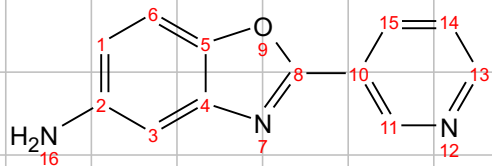
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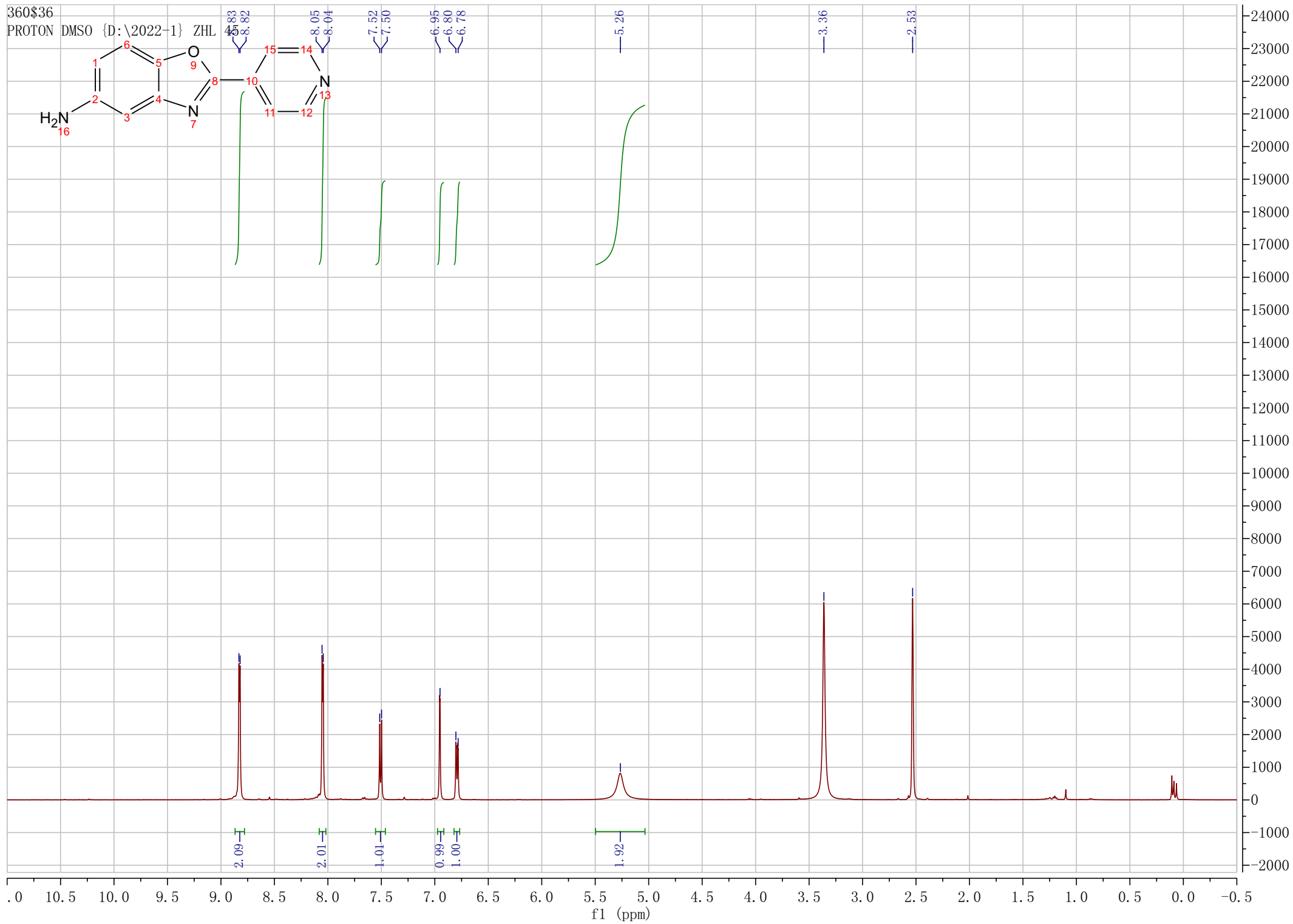
360\$10

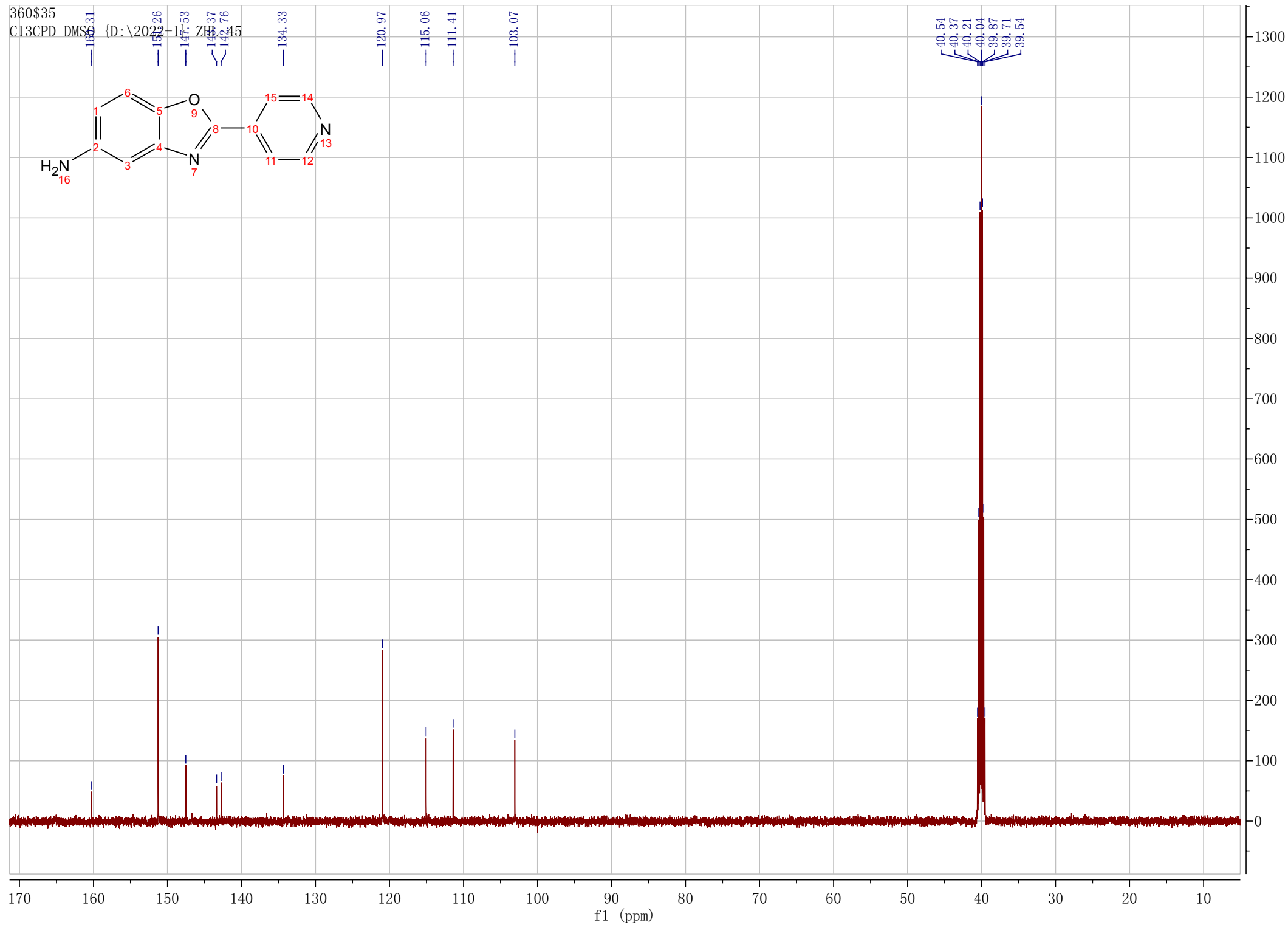
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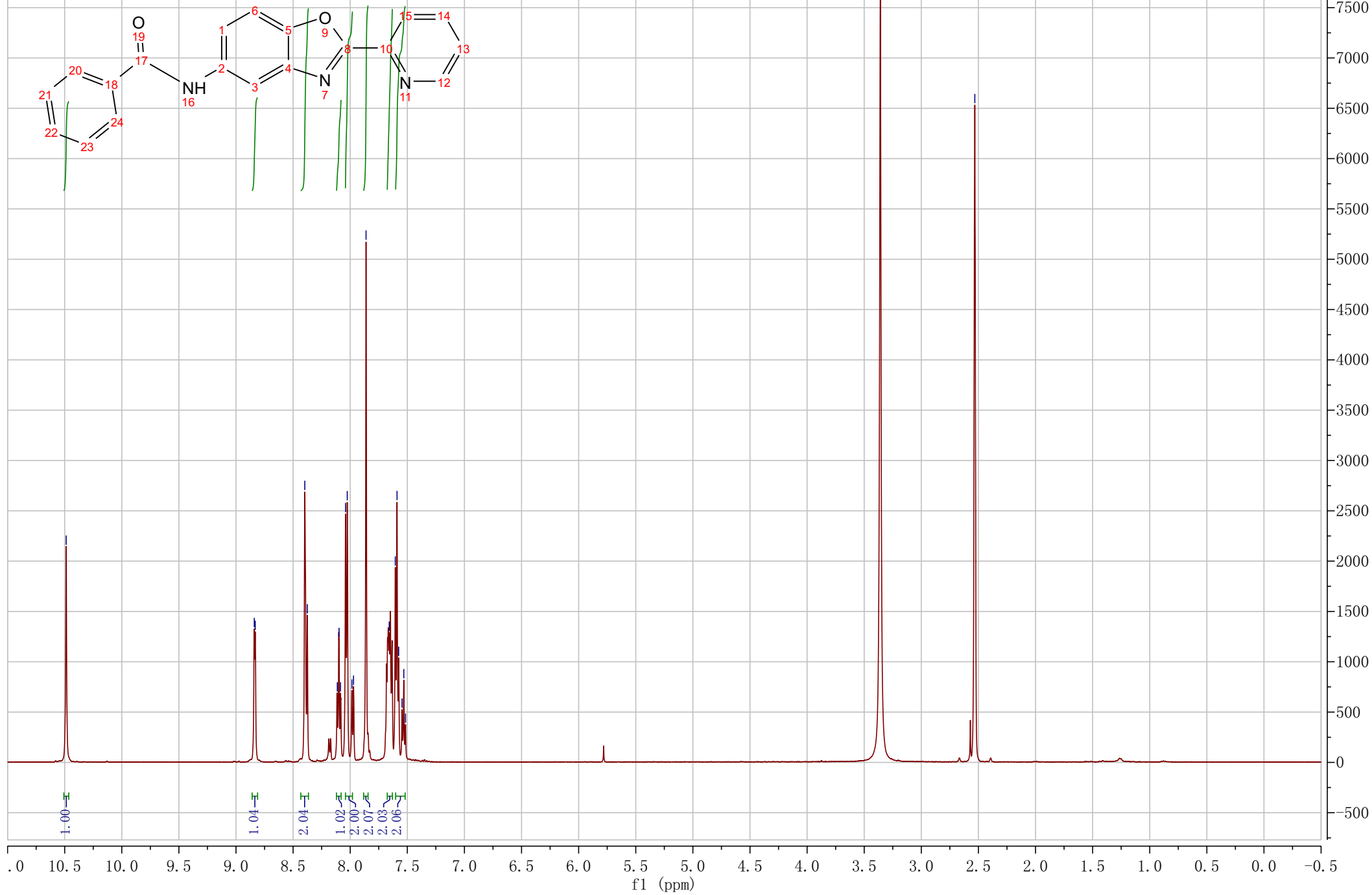
360\$36

PROTON DMSO {D:\2022-1} ZHL





360\$0  
PROTON DMSO {D:\2022-1} ZHL

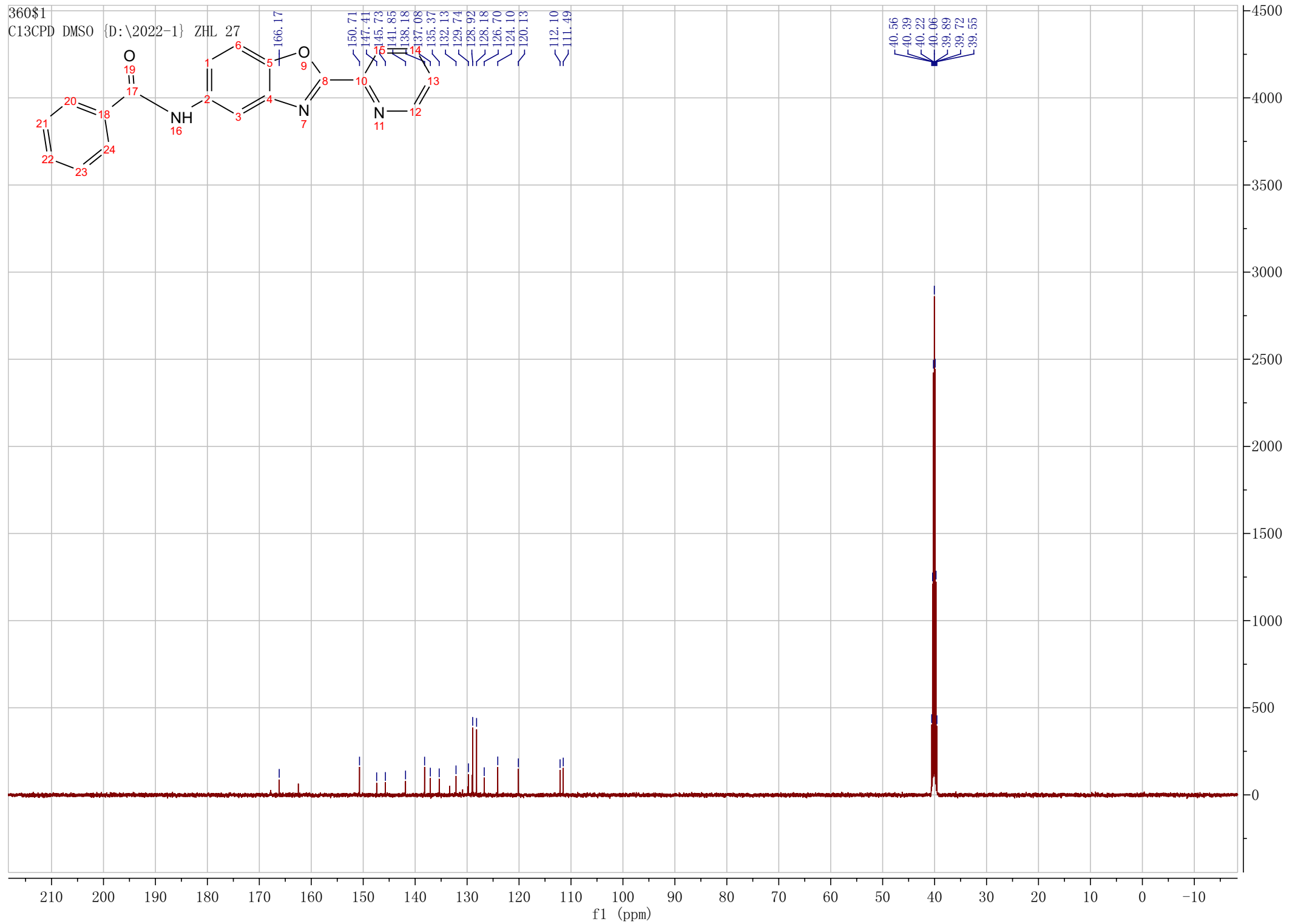


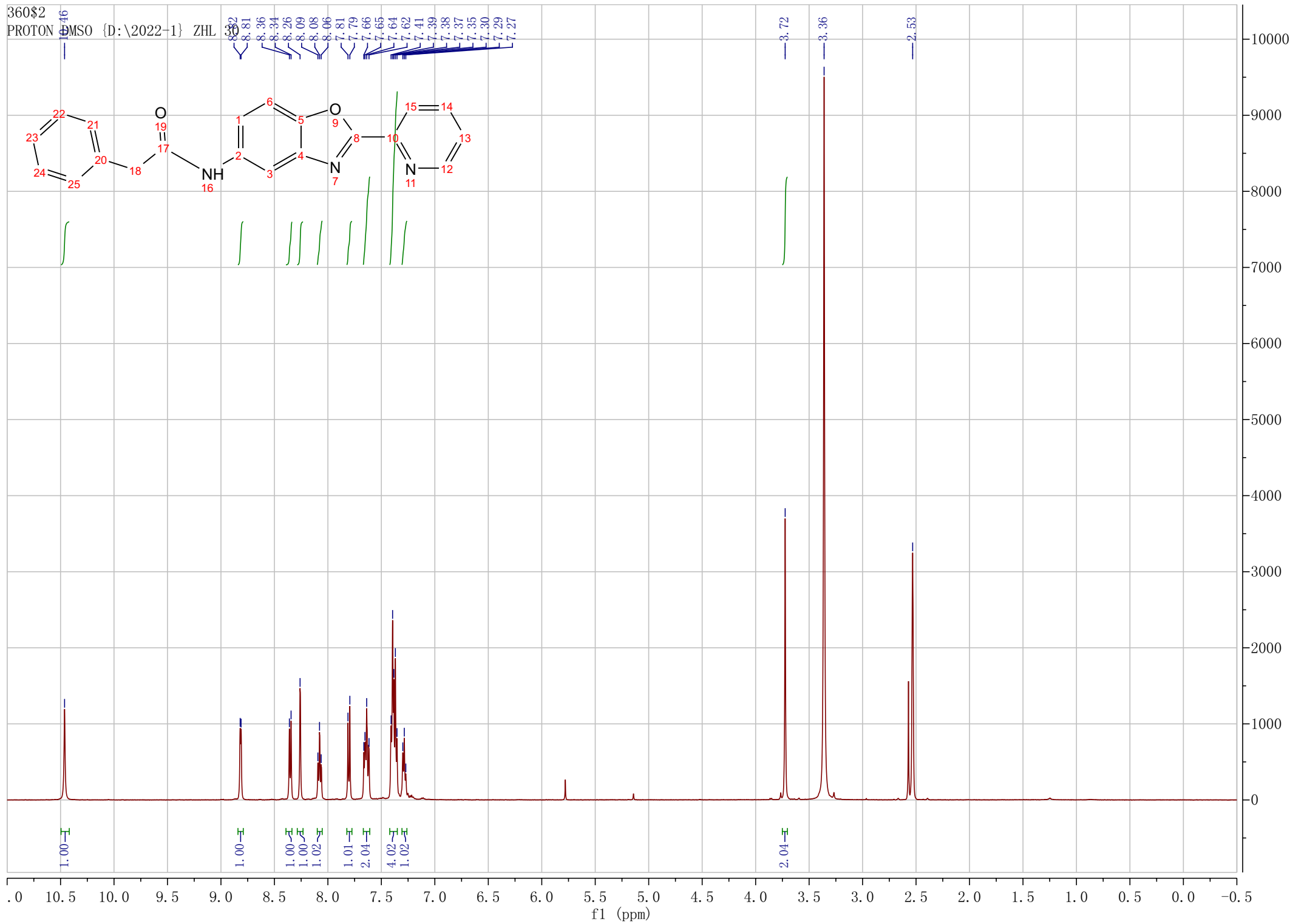
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{D: \2022-1}
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ZHL 27

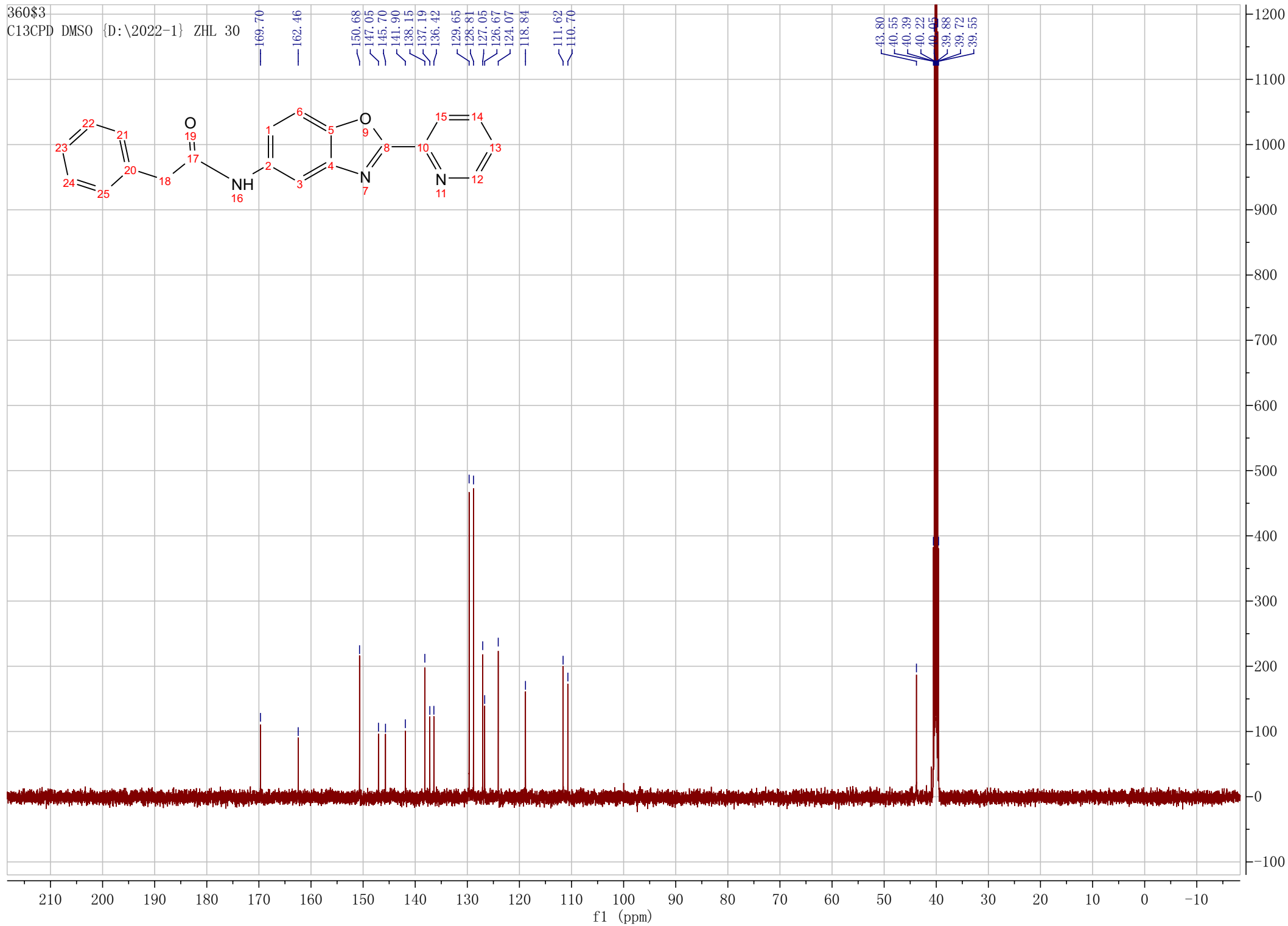
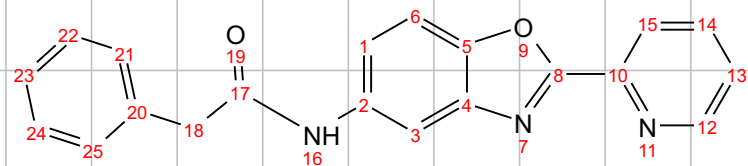
66.1



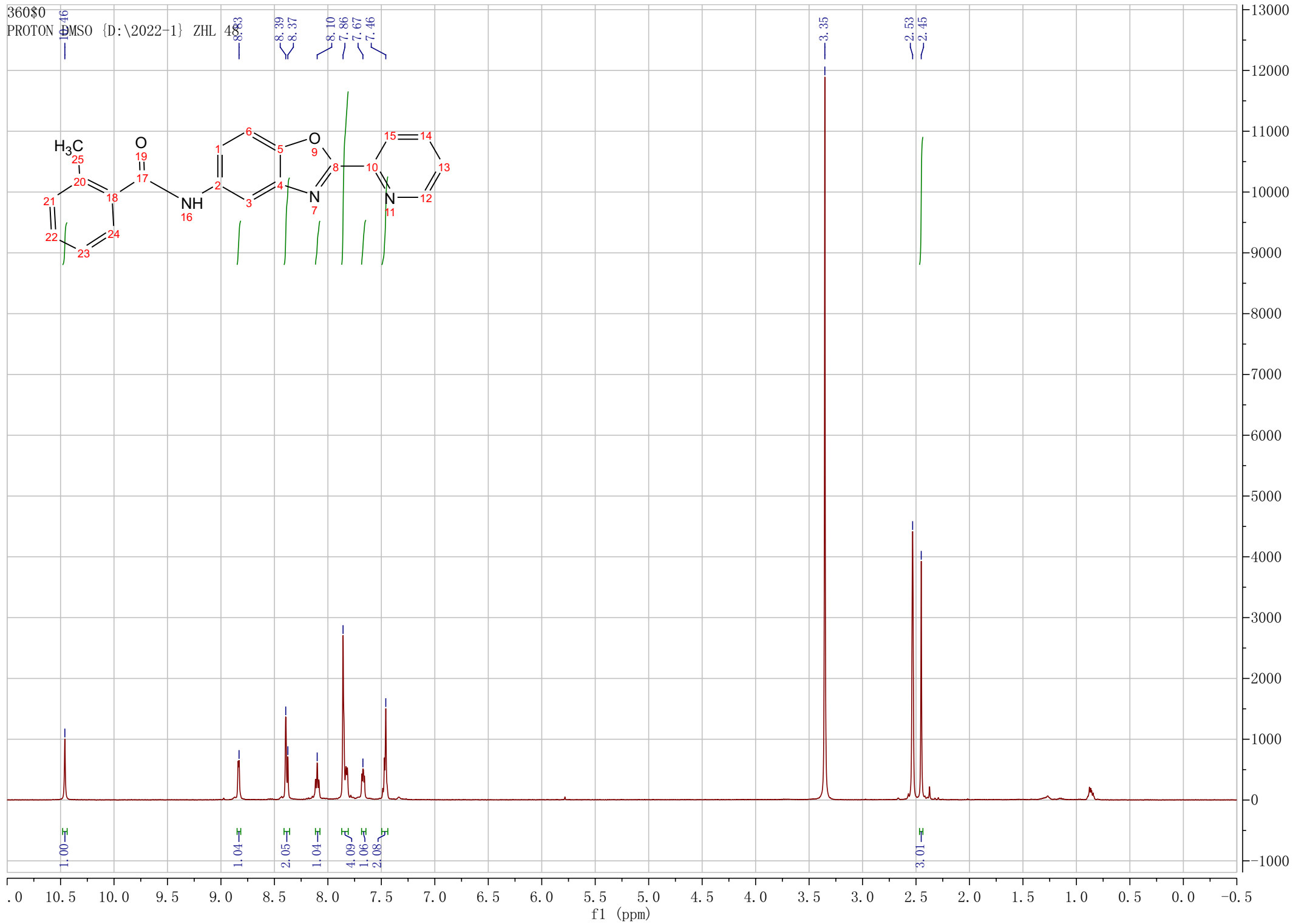


360\$3

C13CPD DMSO {D:\2022-1} ZHL 30

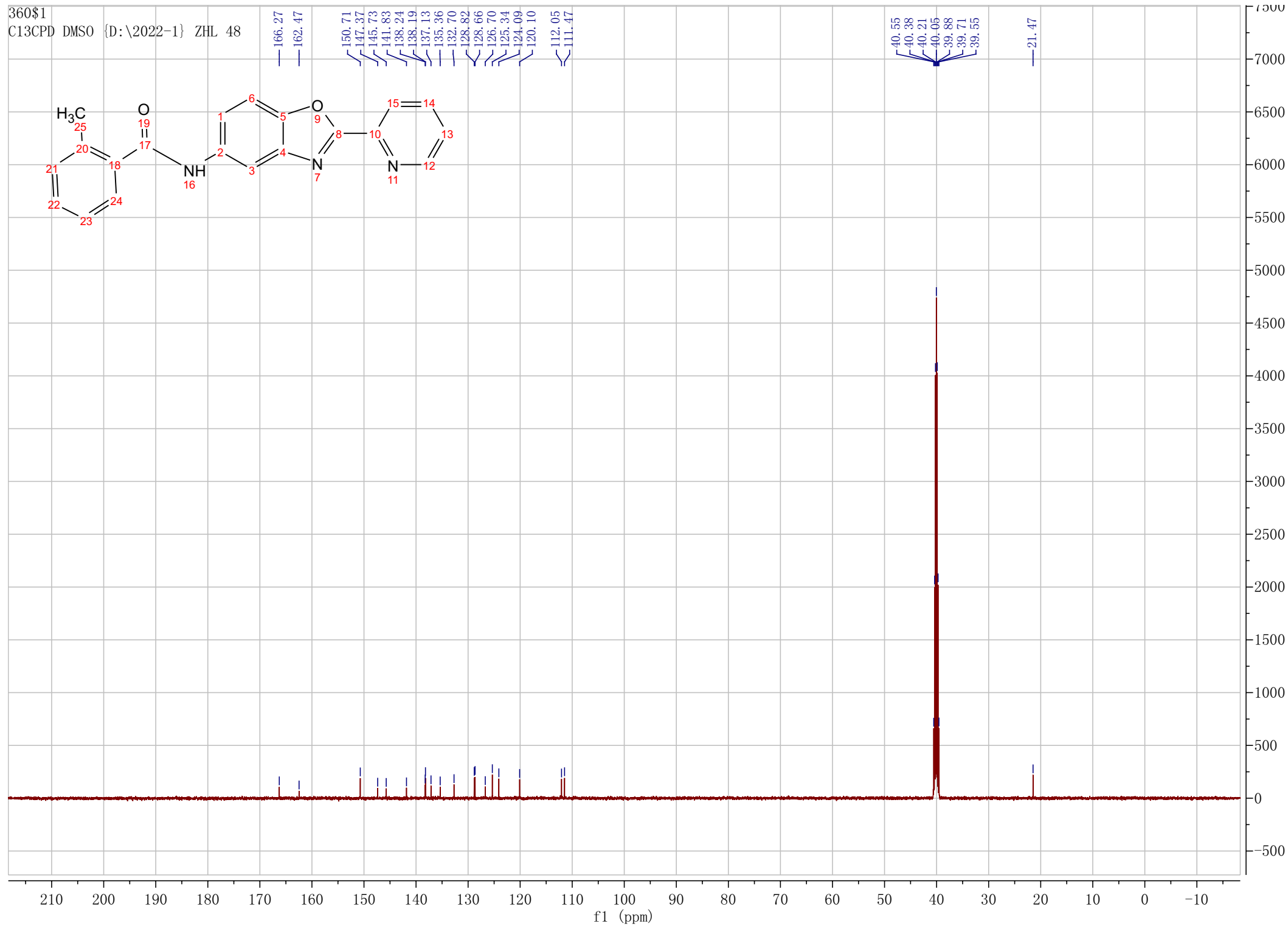


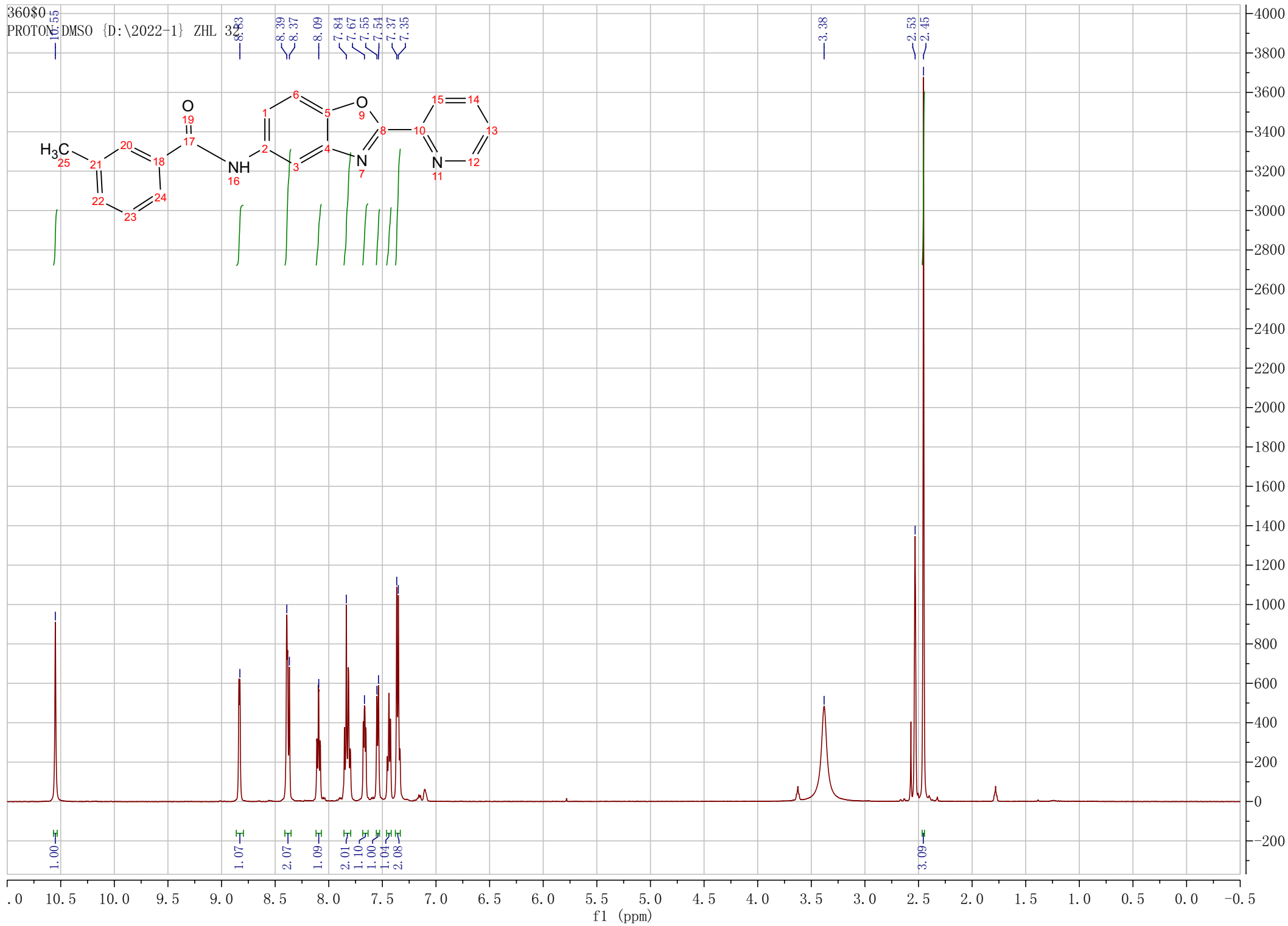


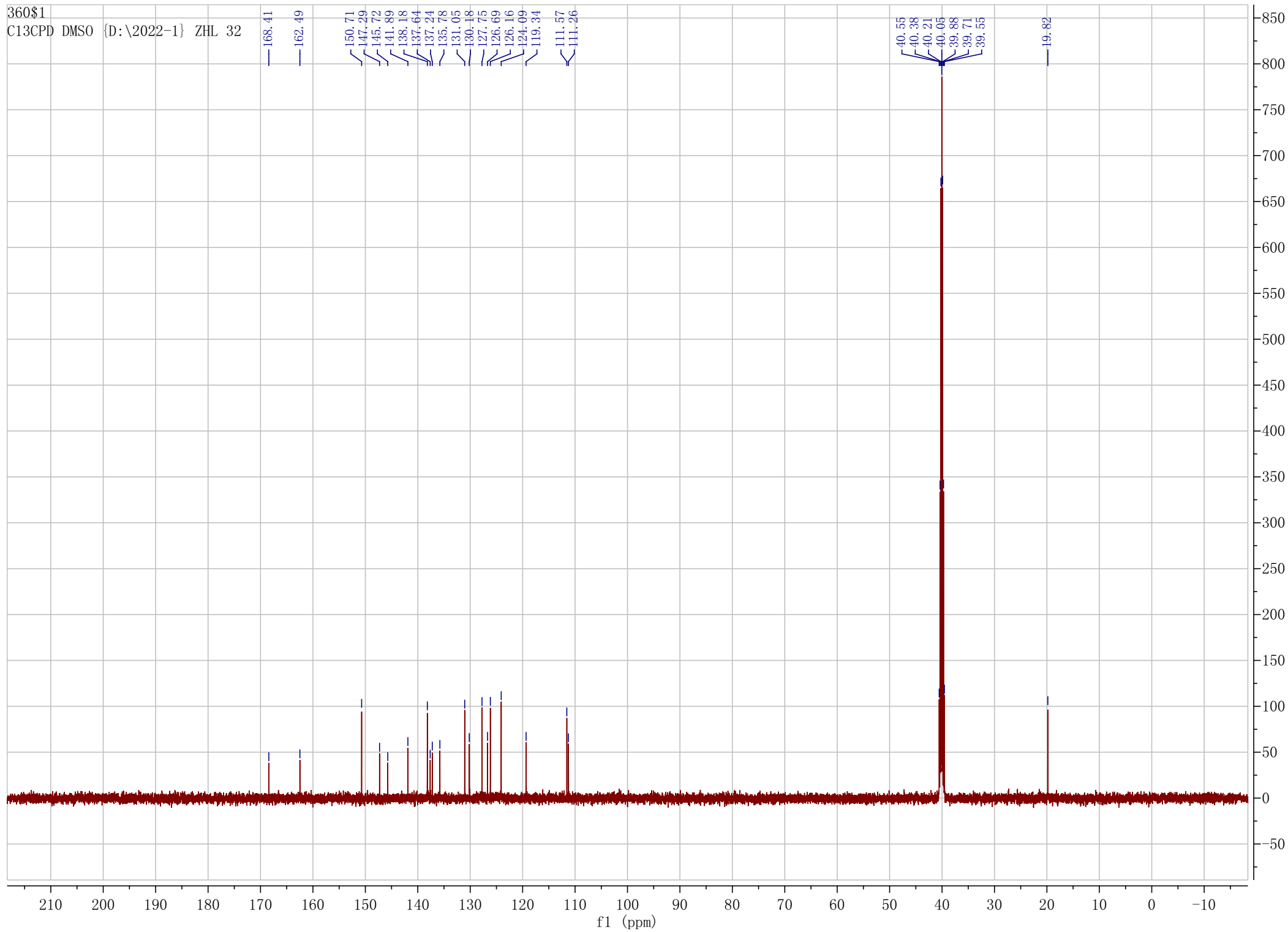


360\$1

C13CPD DMSO {D:\2022-1} ZHL 48

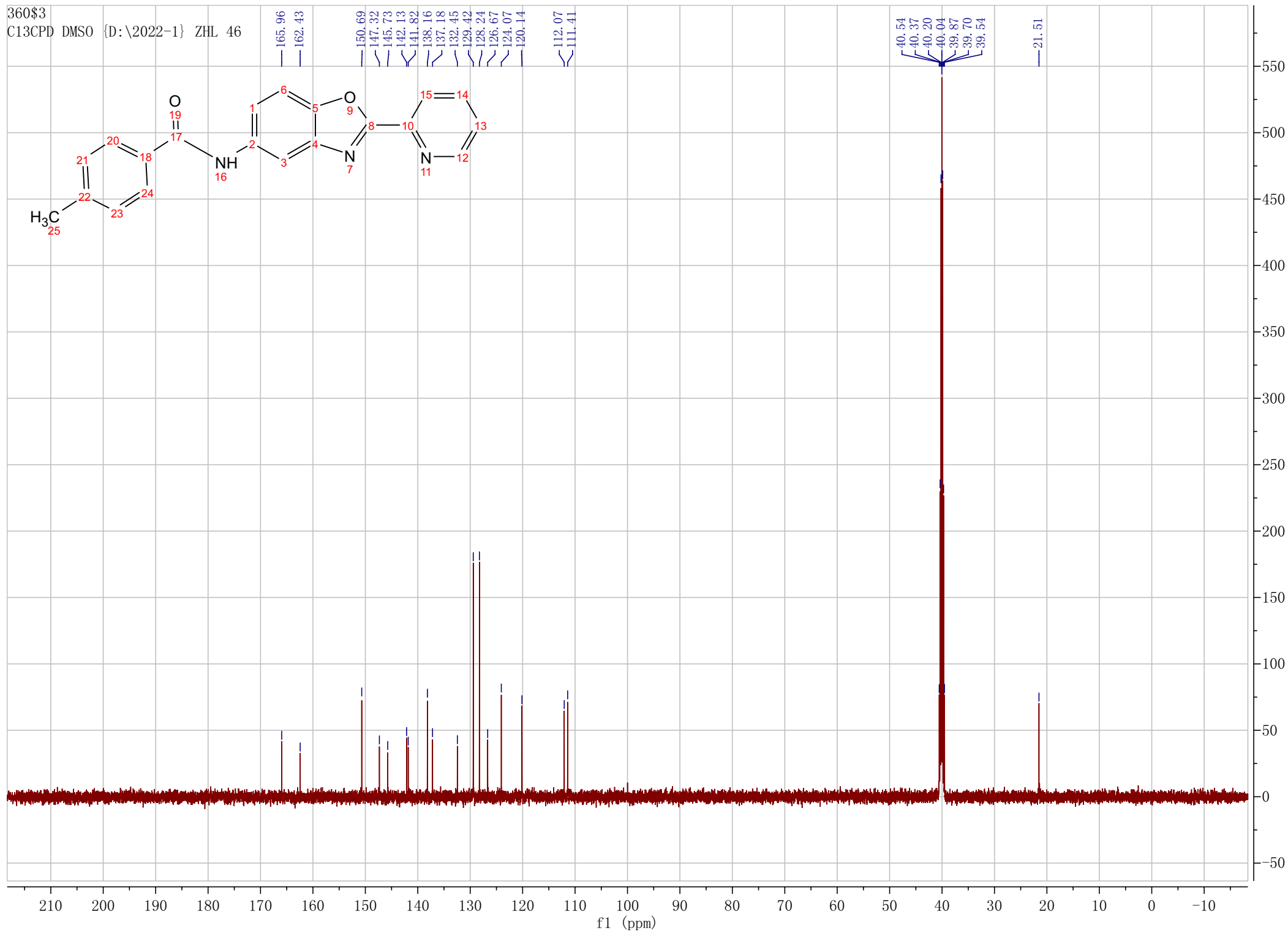


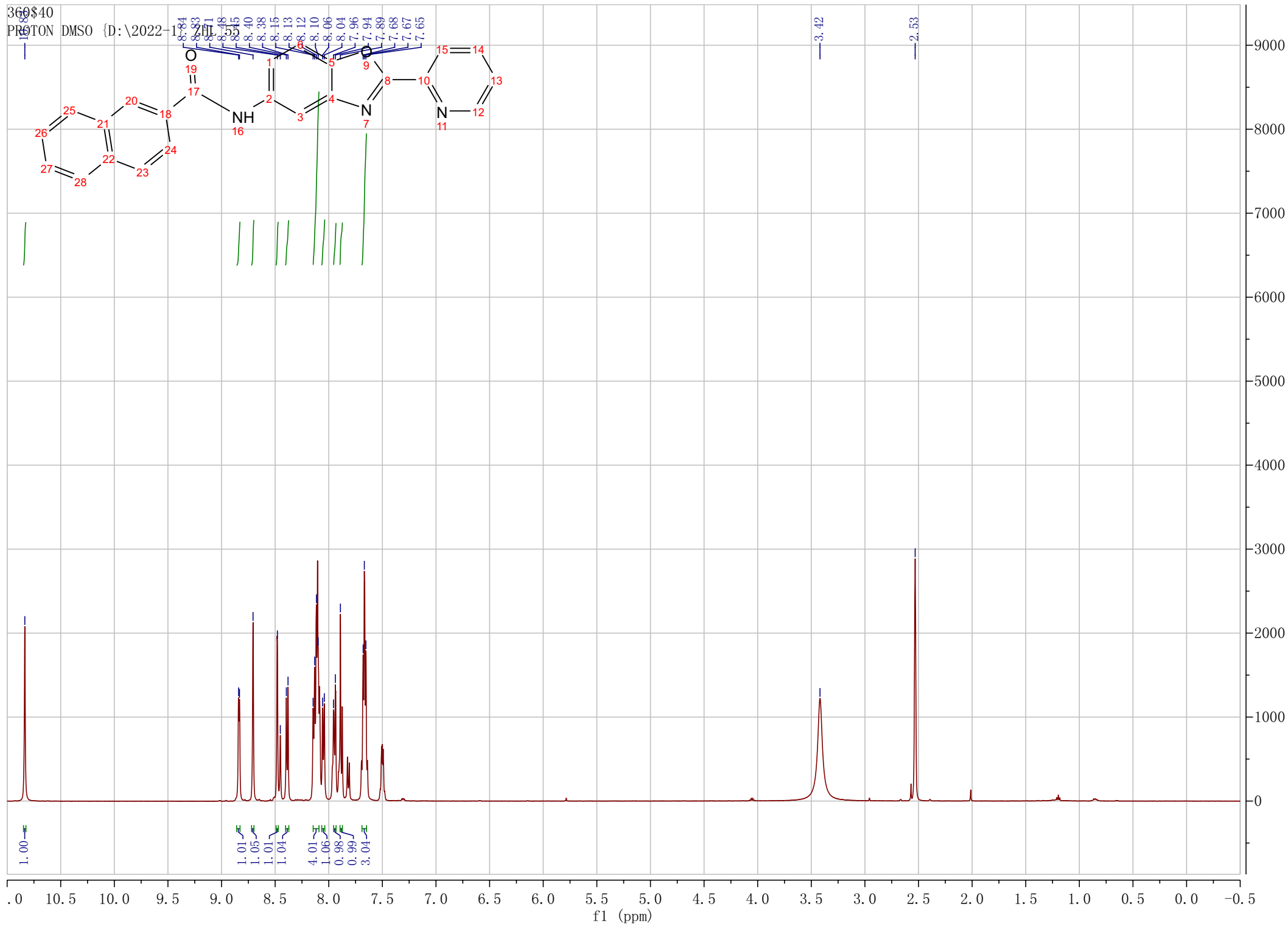




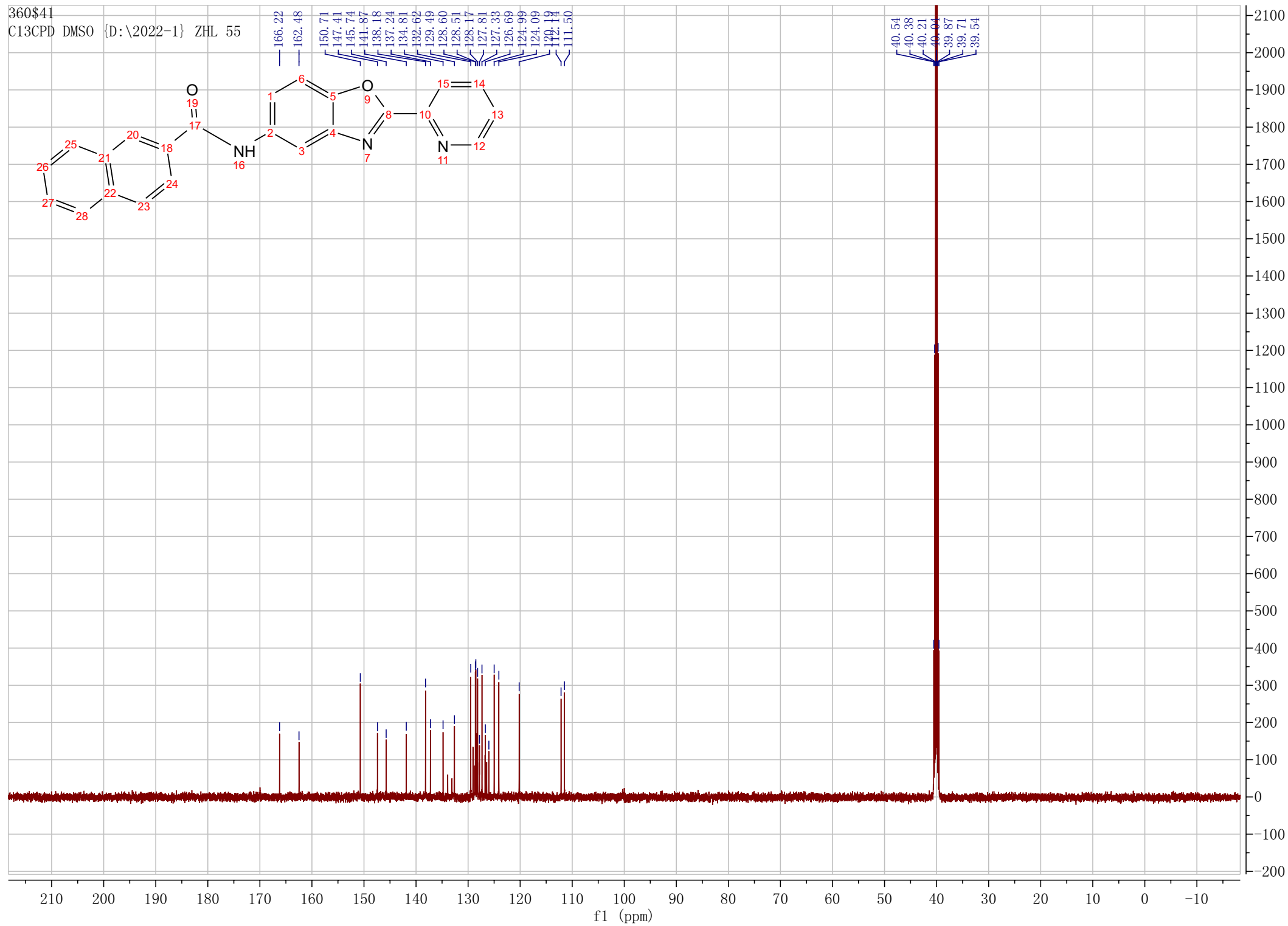
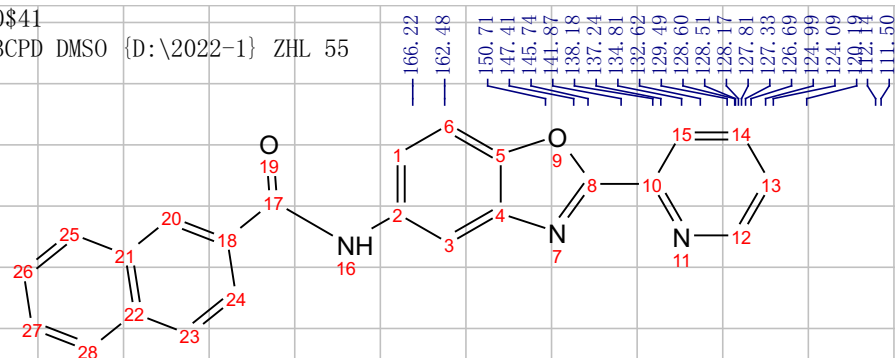


360\$3  
C13CPD DMSO {D:\2022-1} ZHL 46

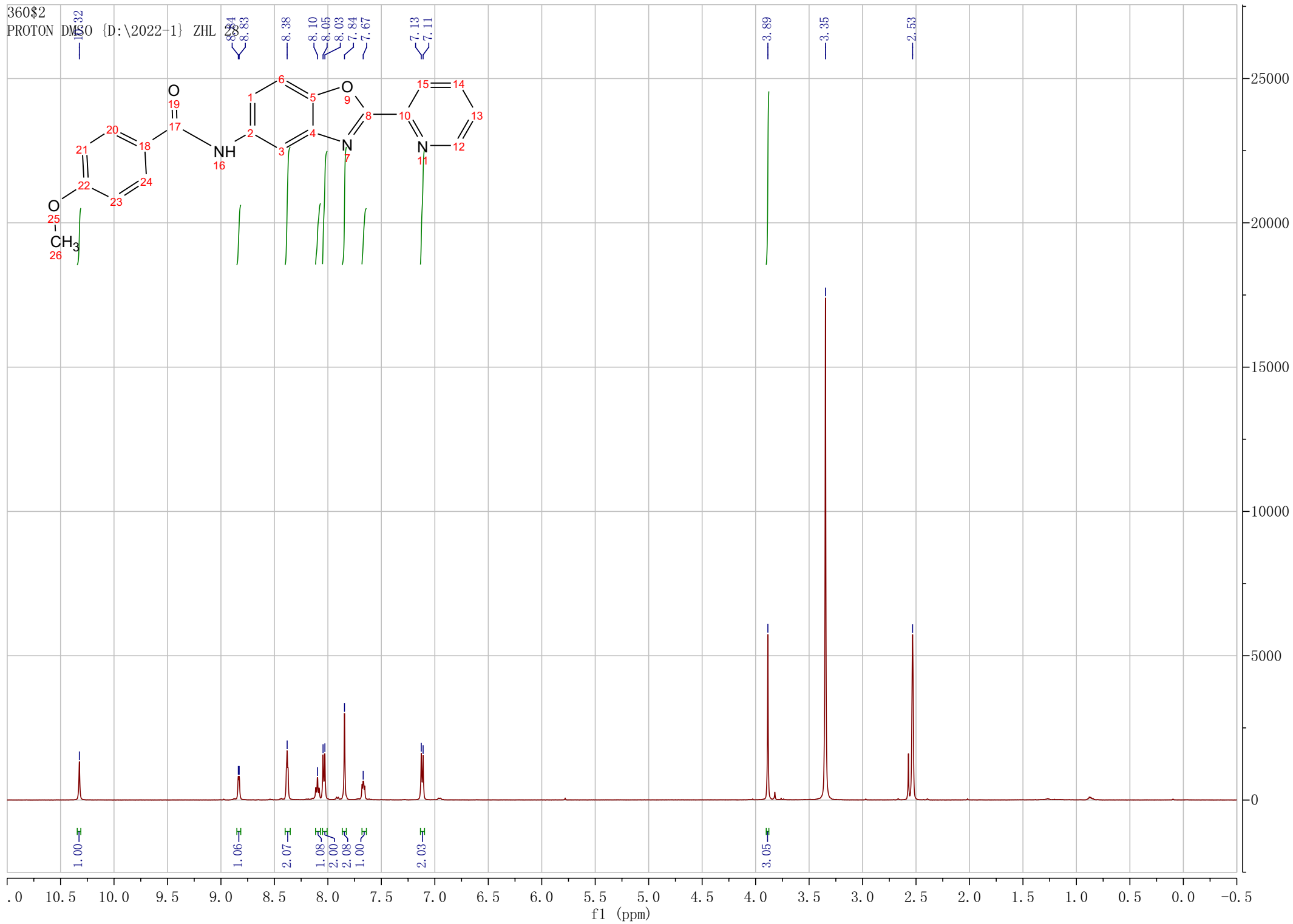




360\$41  
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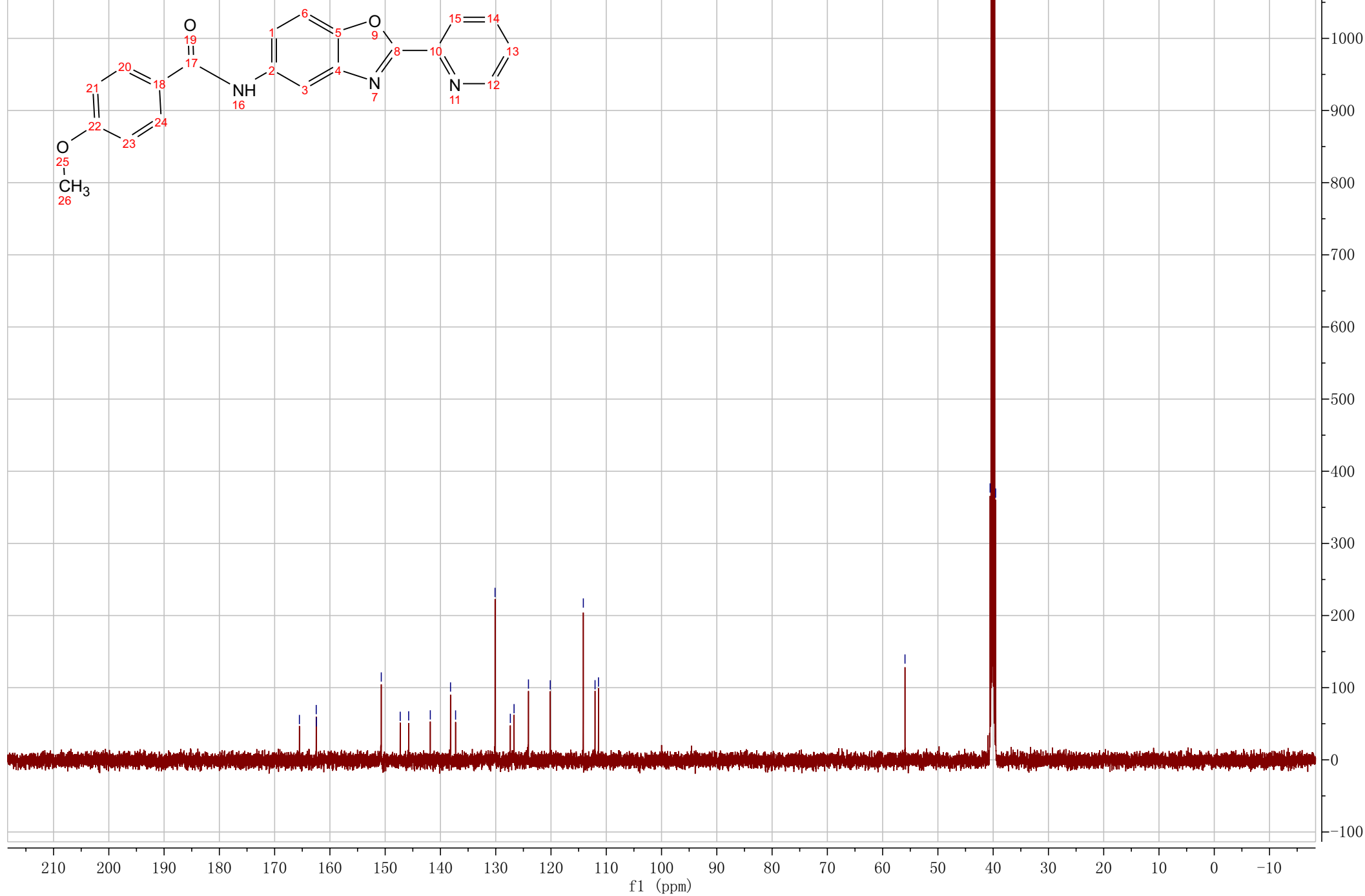






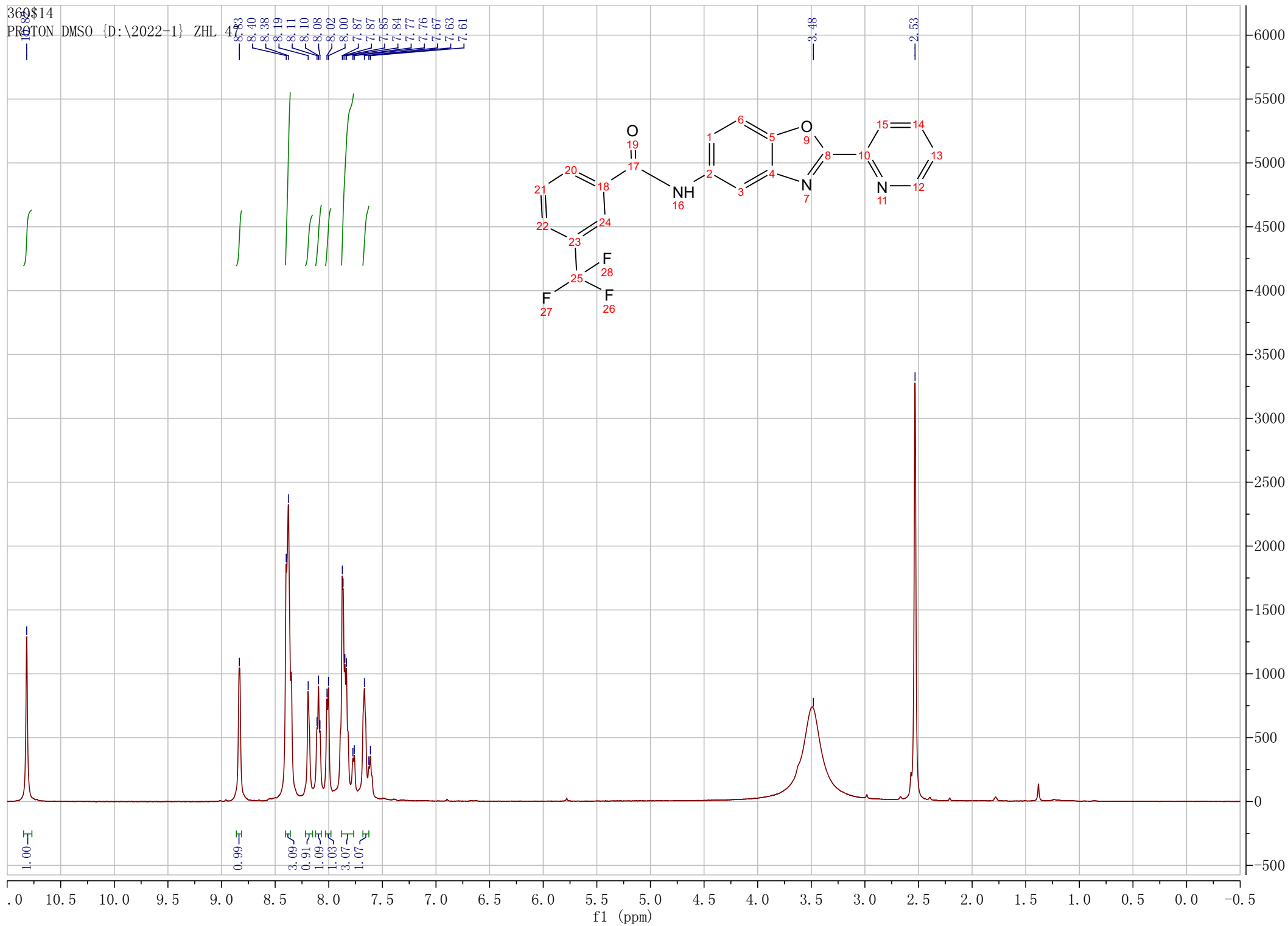
360\$3

C13CPD DMSO {D:\2022-1} ZHL 28



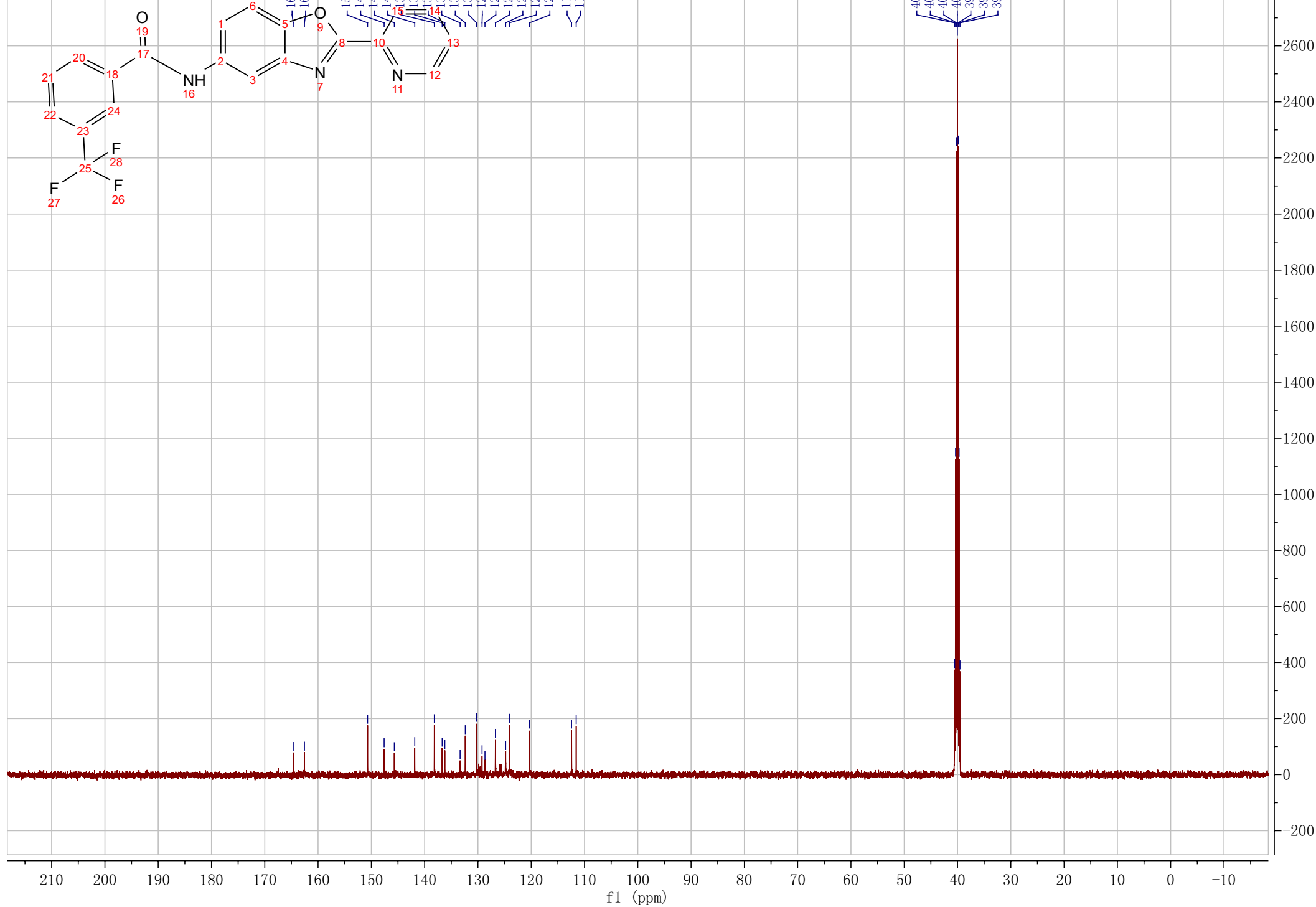
369\$14

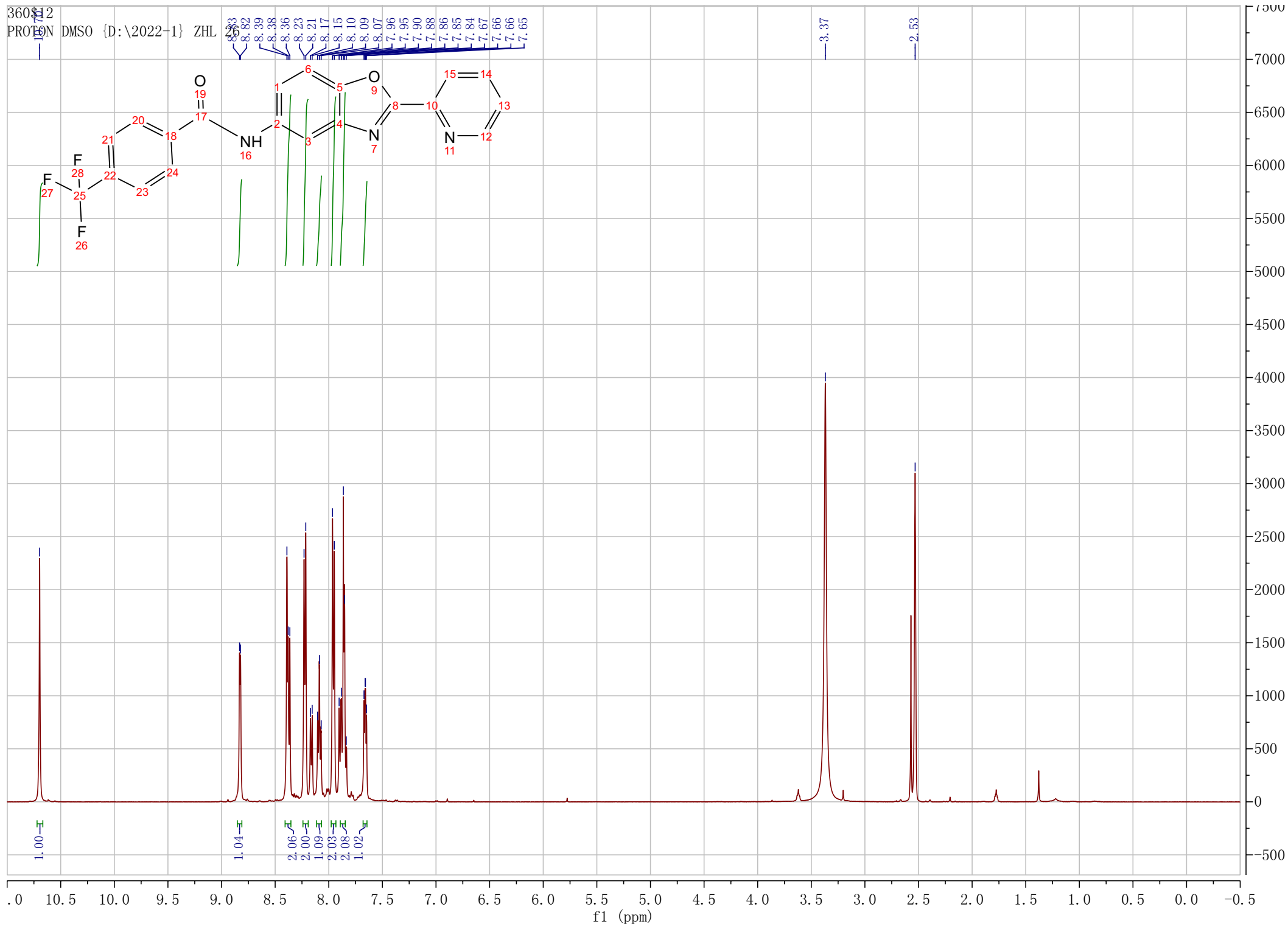
PROTON DMSO {D:\2022-1} ZHL 4



360\$15

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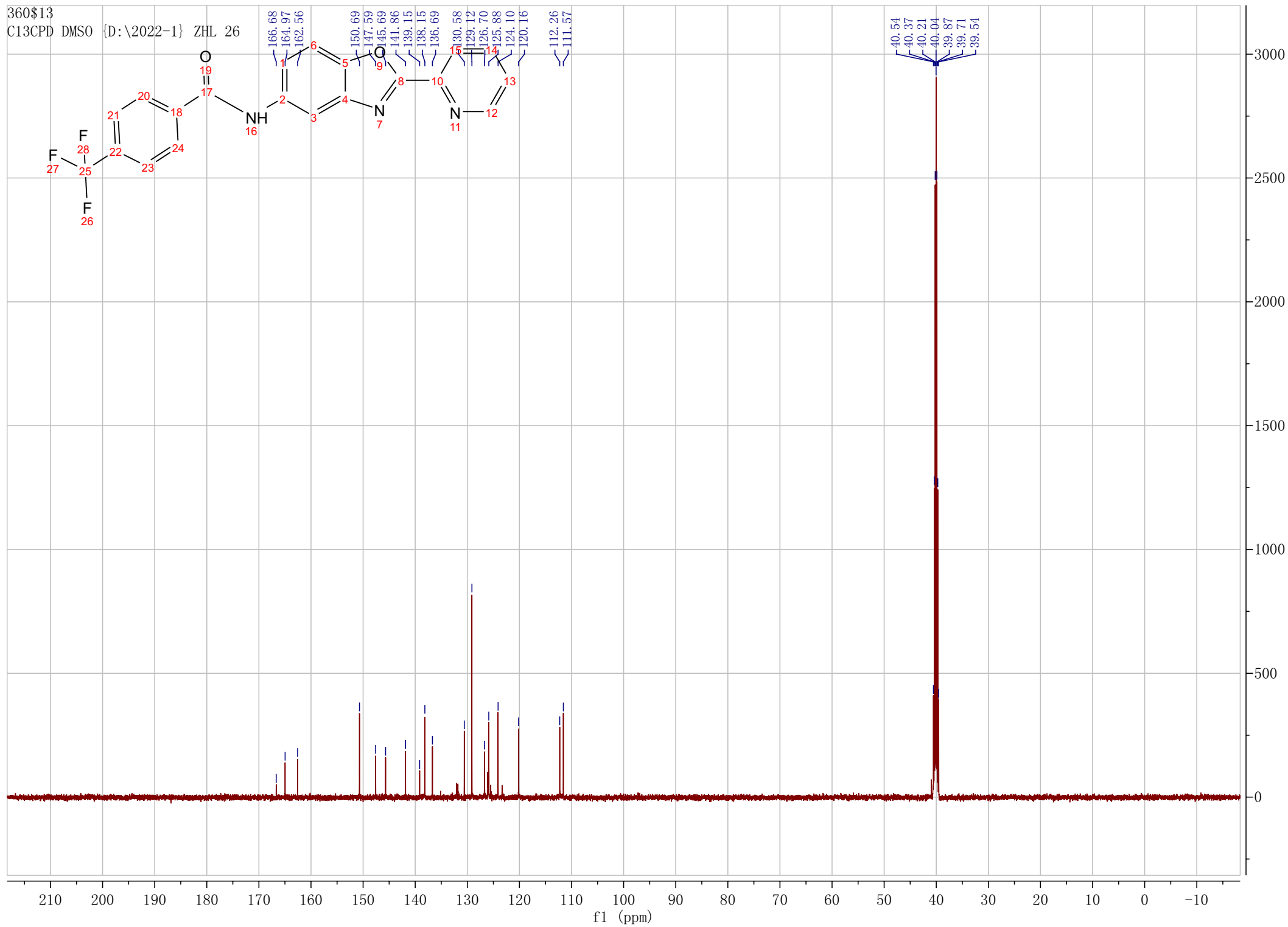


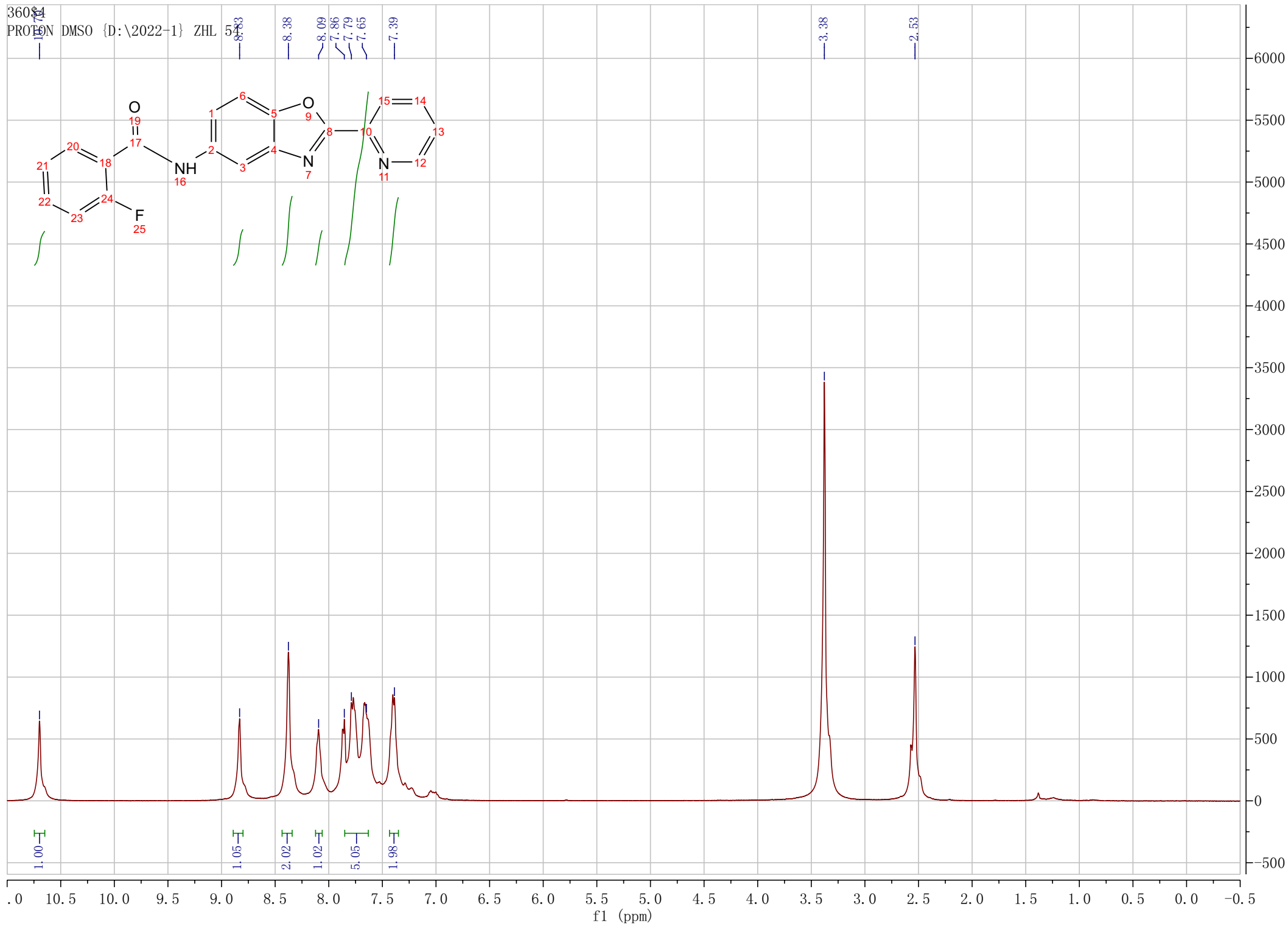


360\$13

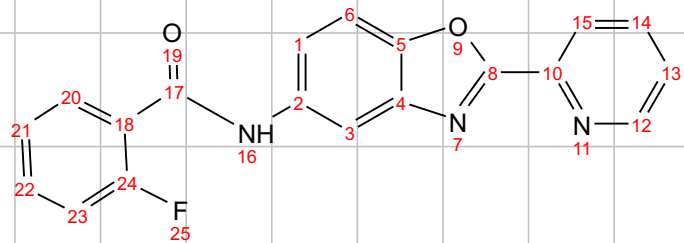
C13CPD DMSO {D:\2022-1}

ZHL 26



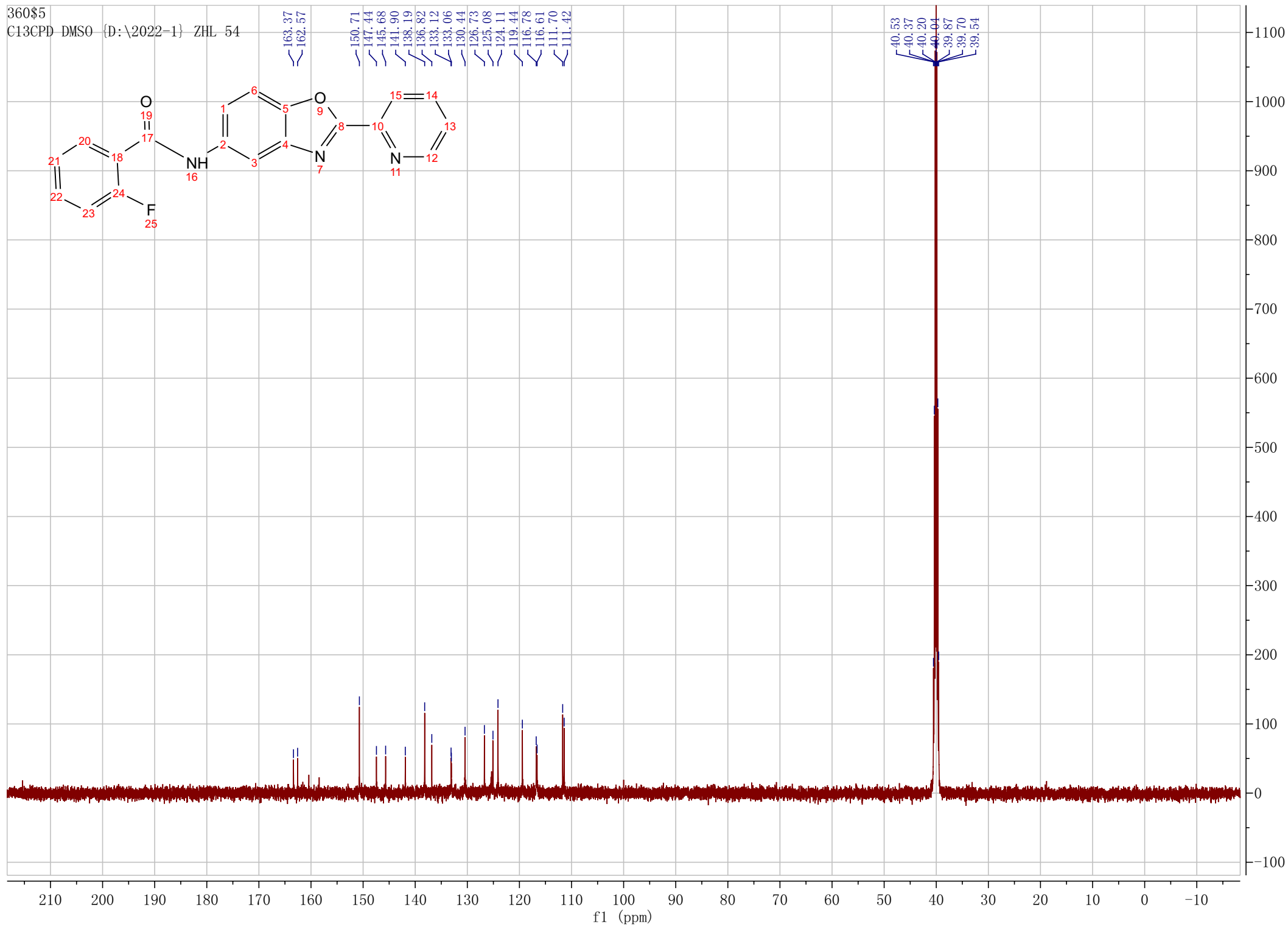


360\$5  
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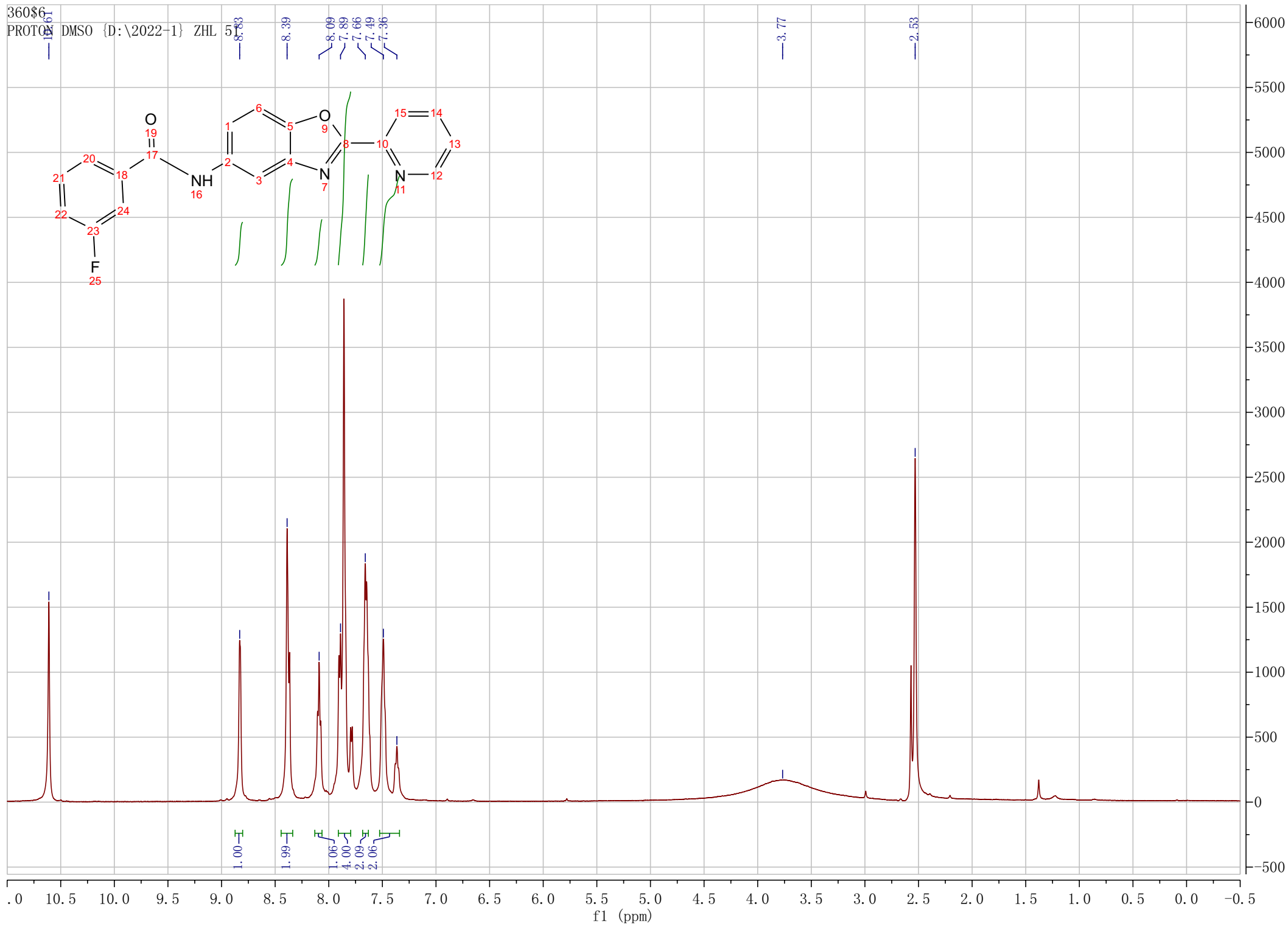


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111.42

40.53  
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39.54

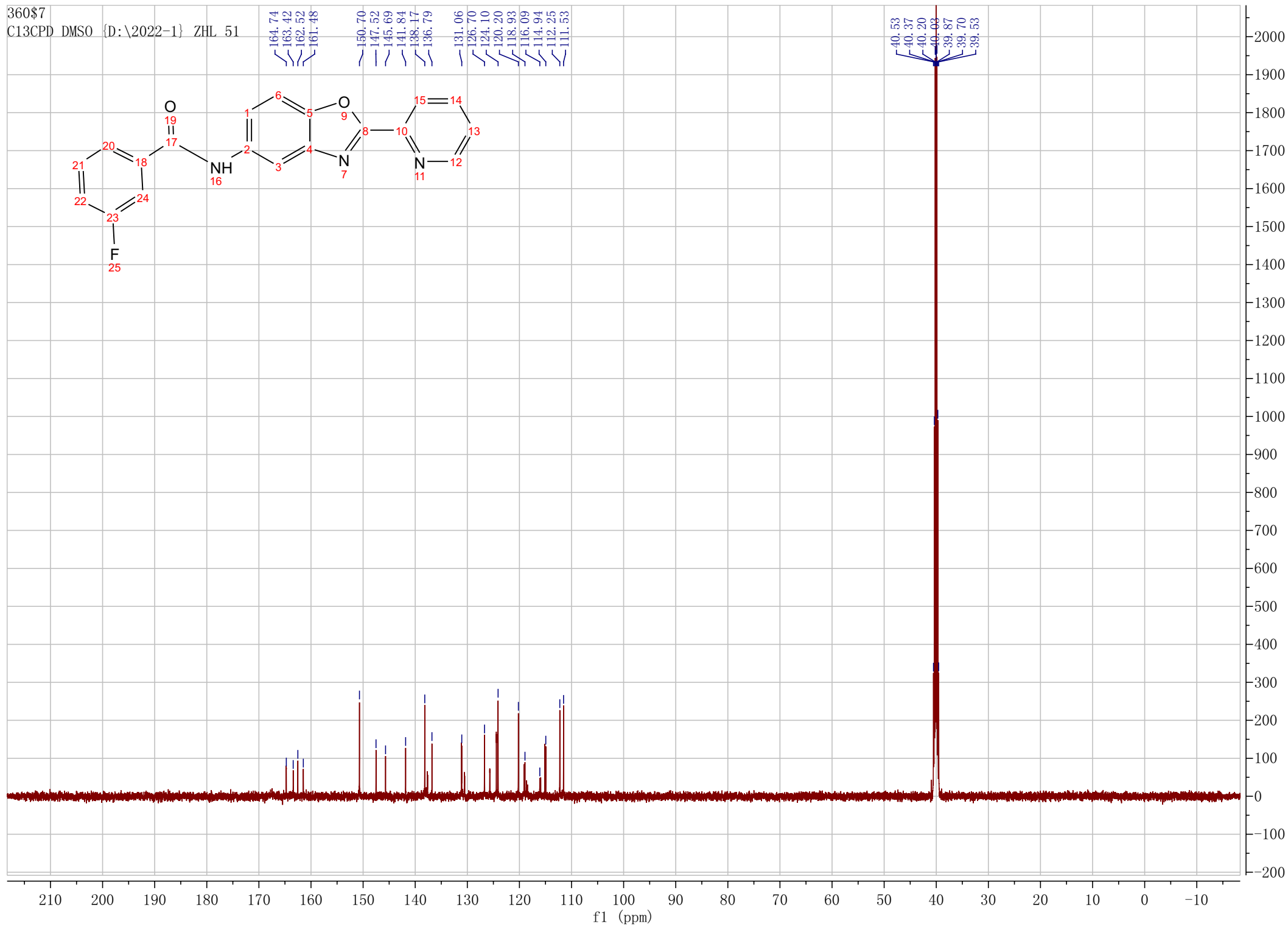




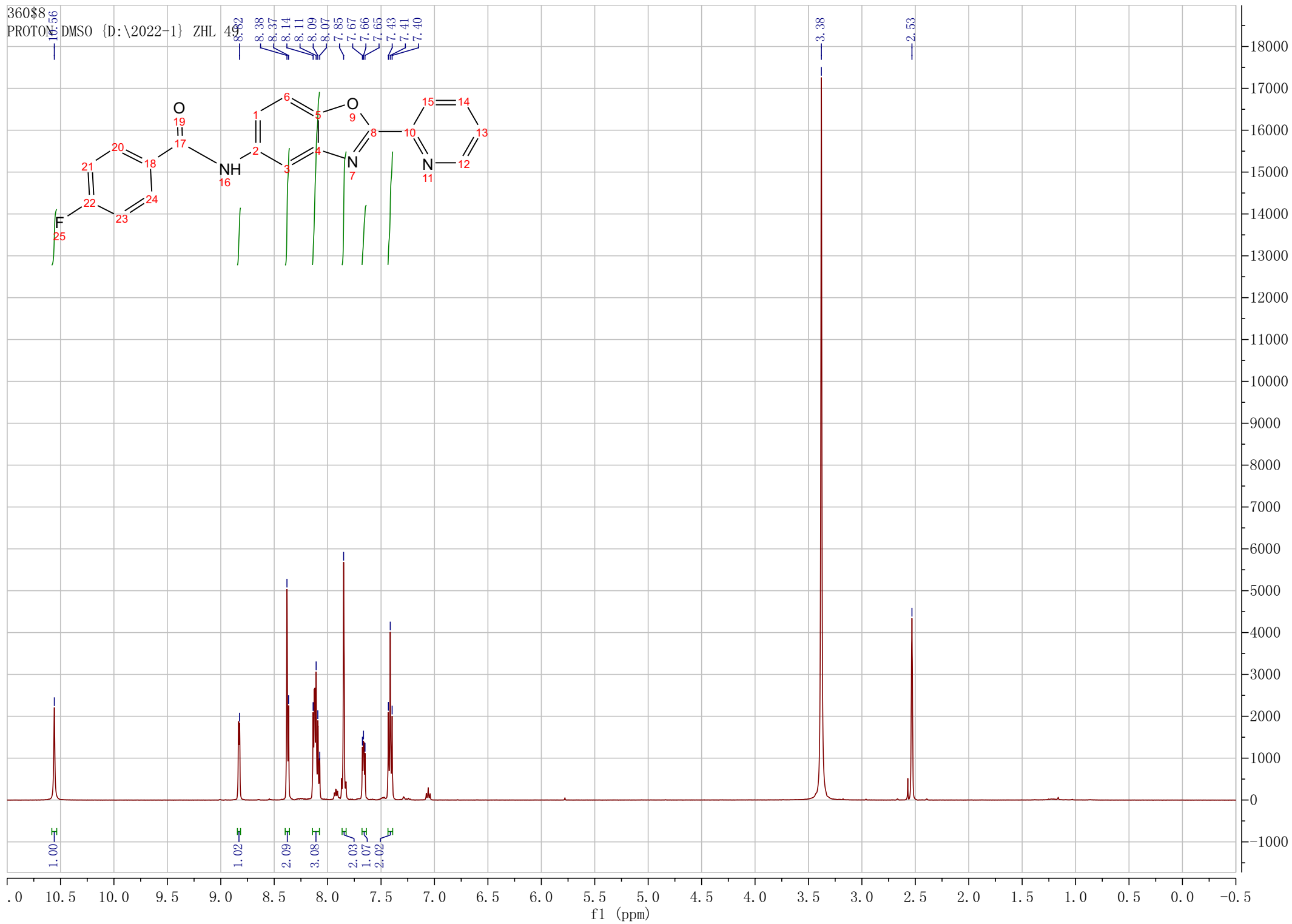


360\$7

C13CPD DMSO {D:\2022-1} ZHL 51

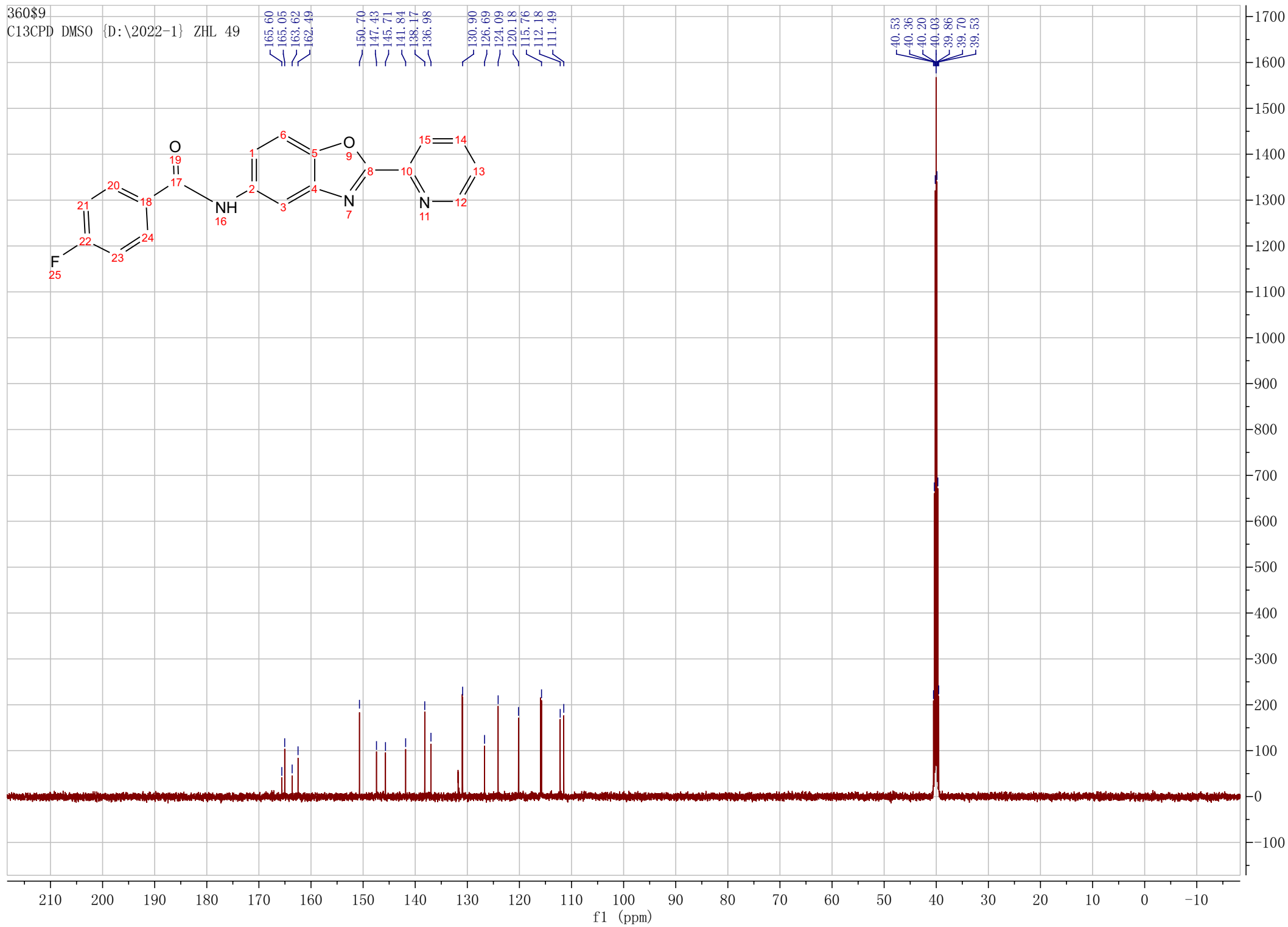


360\$8  
PROTON DMSO {D:\2022-1} ZHL 492



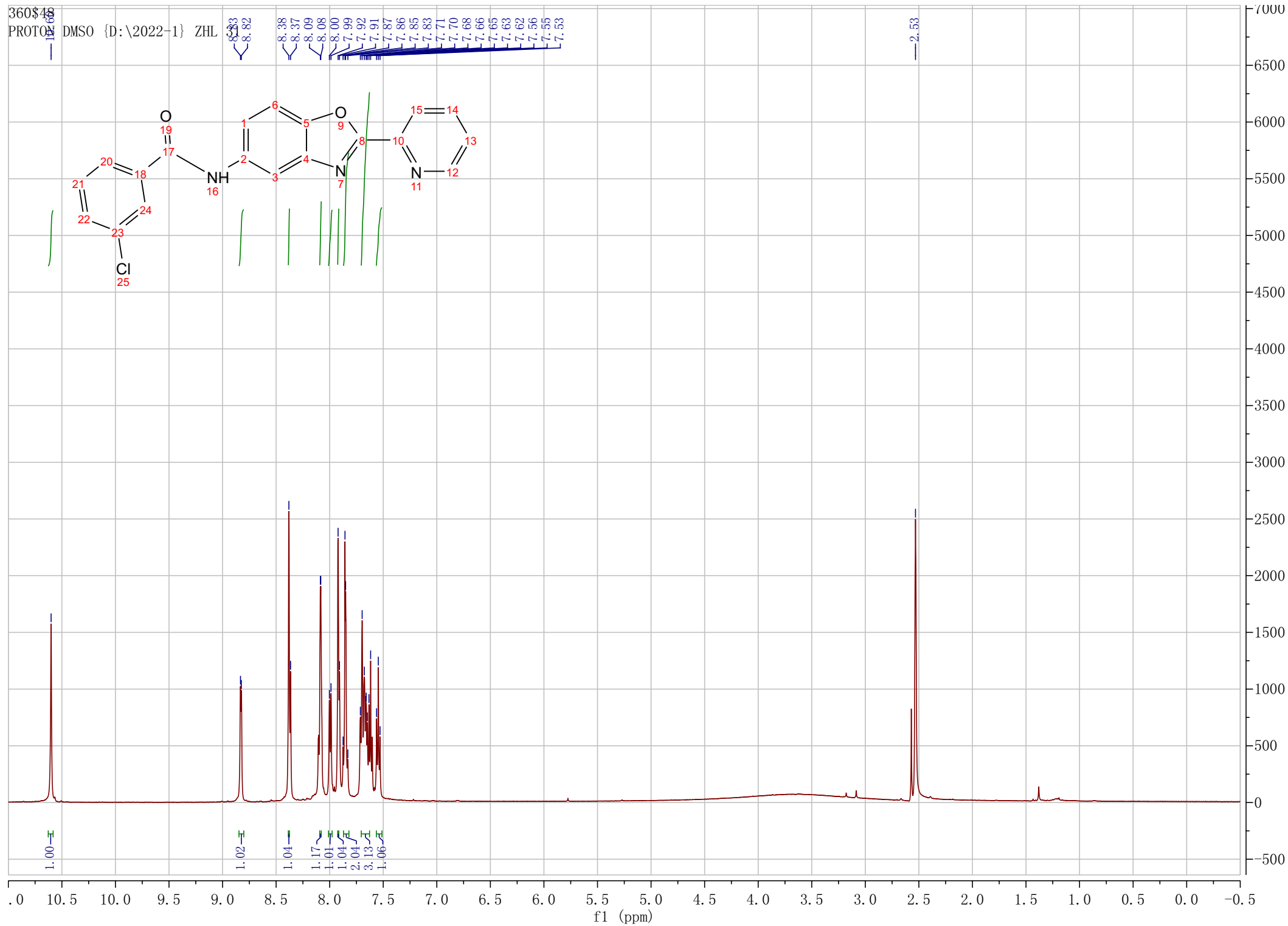
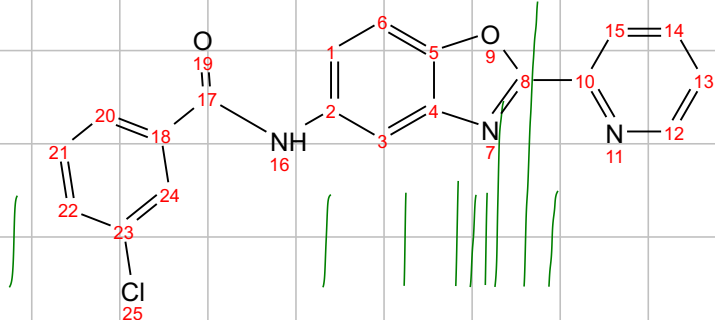
360\$9

C13CPD DMSO {D:\2022-1} ZHL 49



360\$48

PROTON	DMSO	{D:\2022-1}	ZHL
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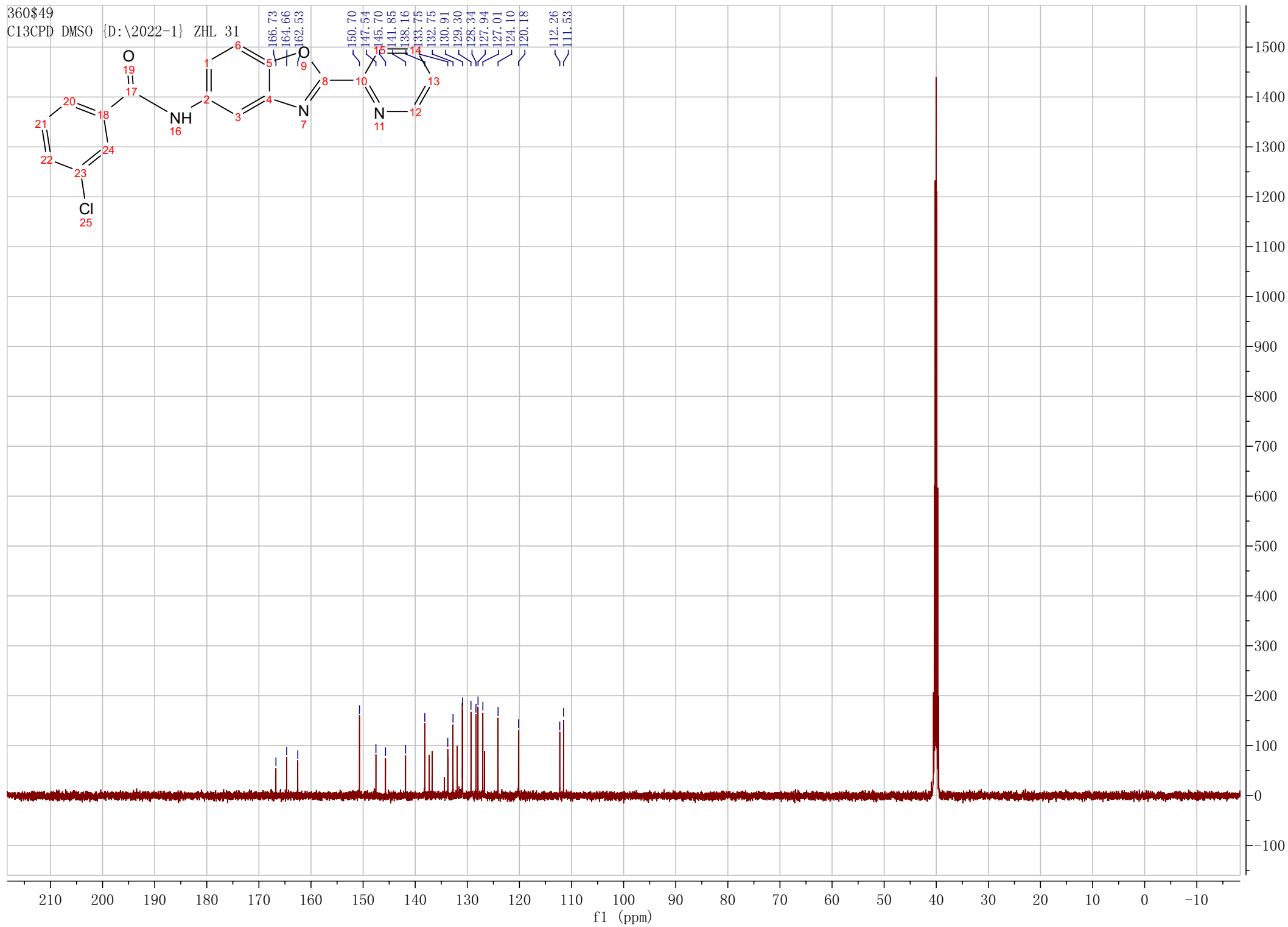


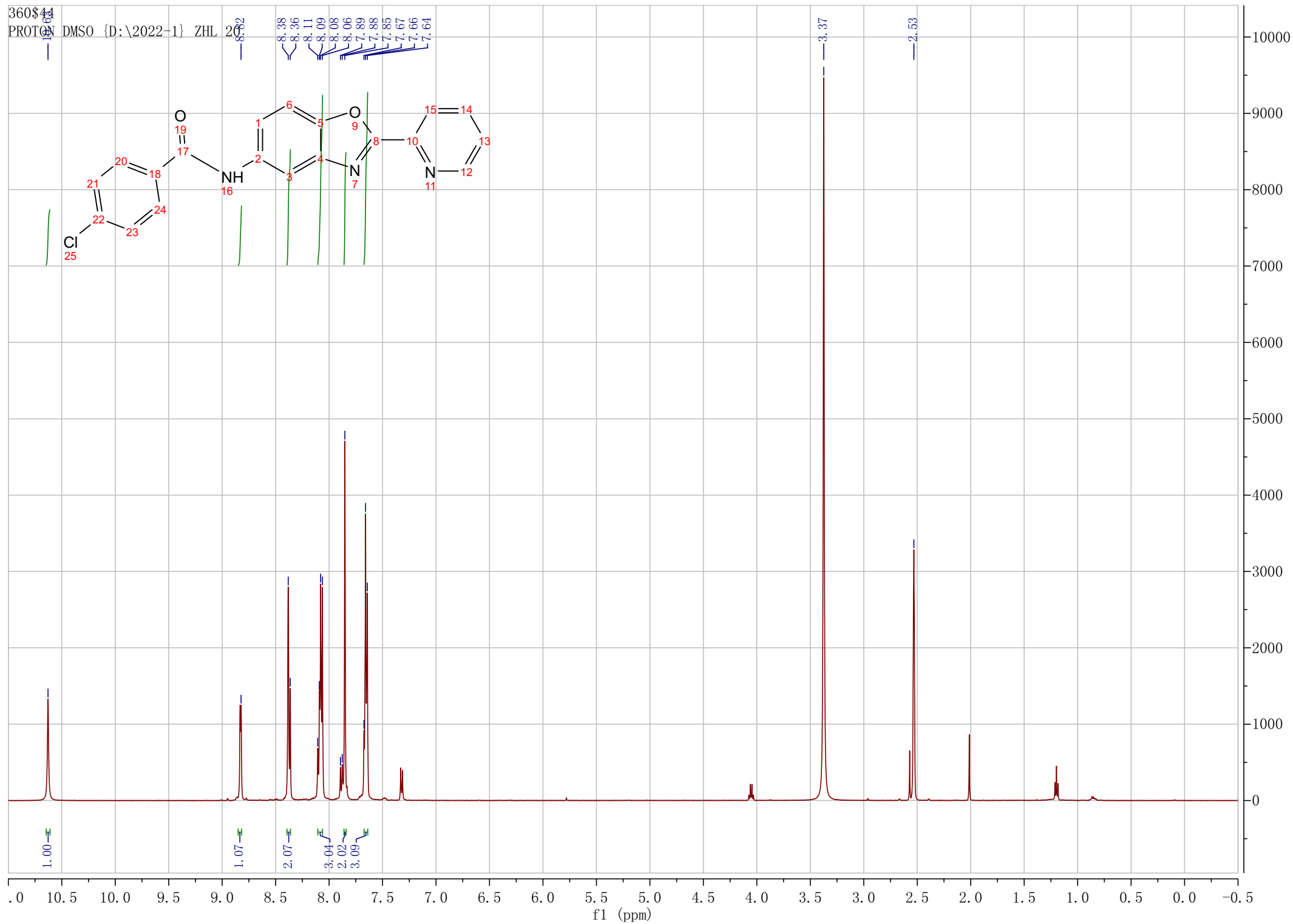
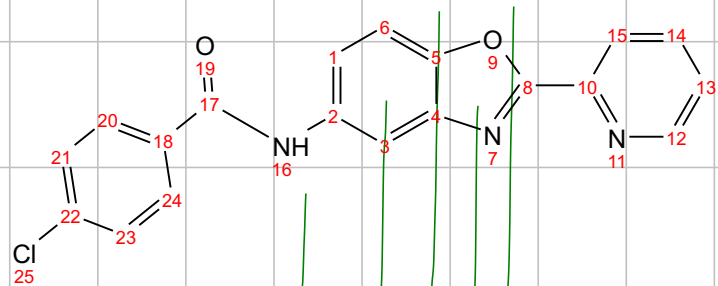
360\$49

C13CPD DMSO

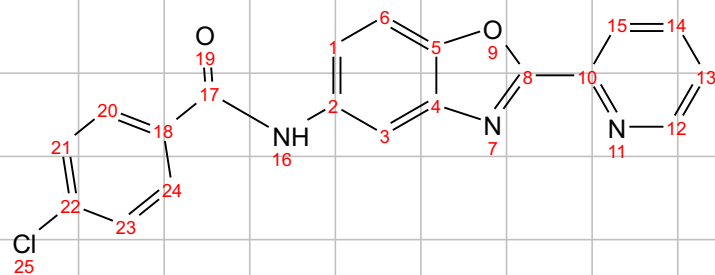
{D:\2022-1}

ZHL 31



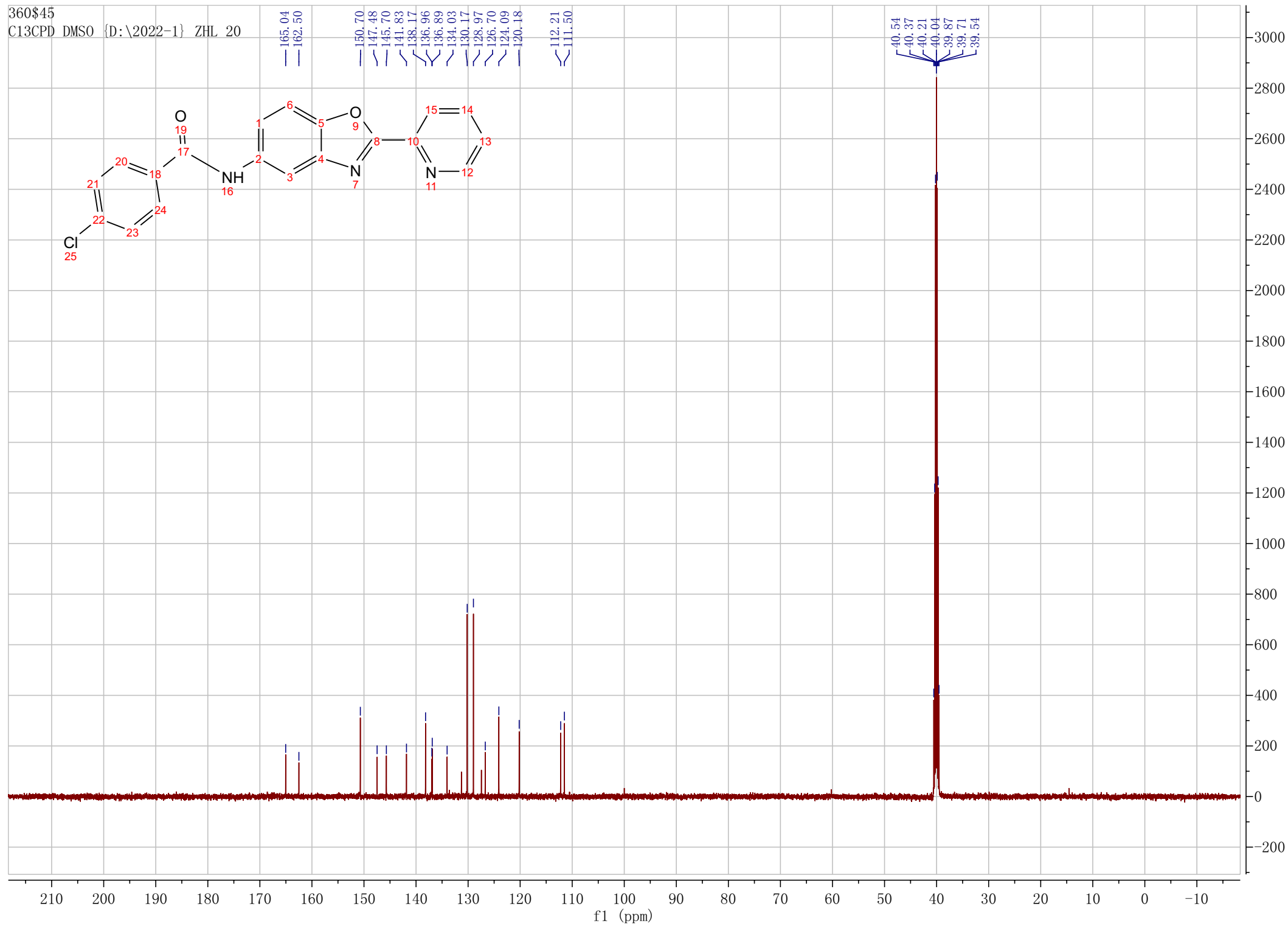
[illegible]

360\$45  
C13CPD DMSO {D:\2022-1} ZHL 20

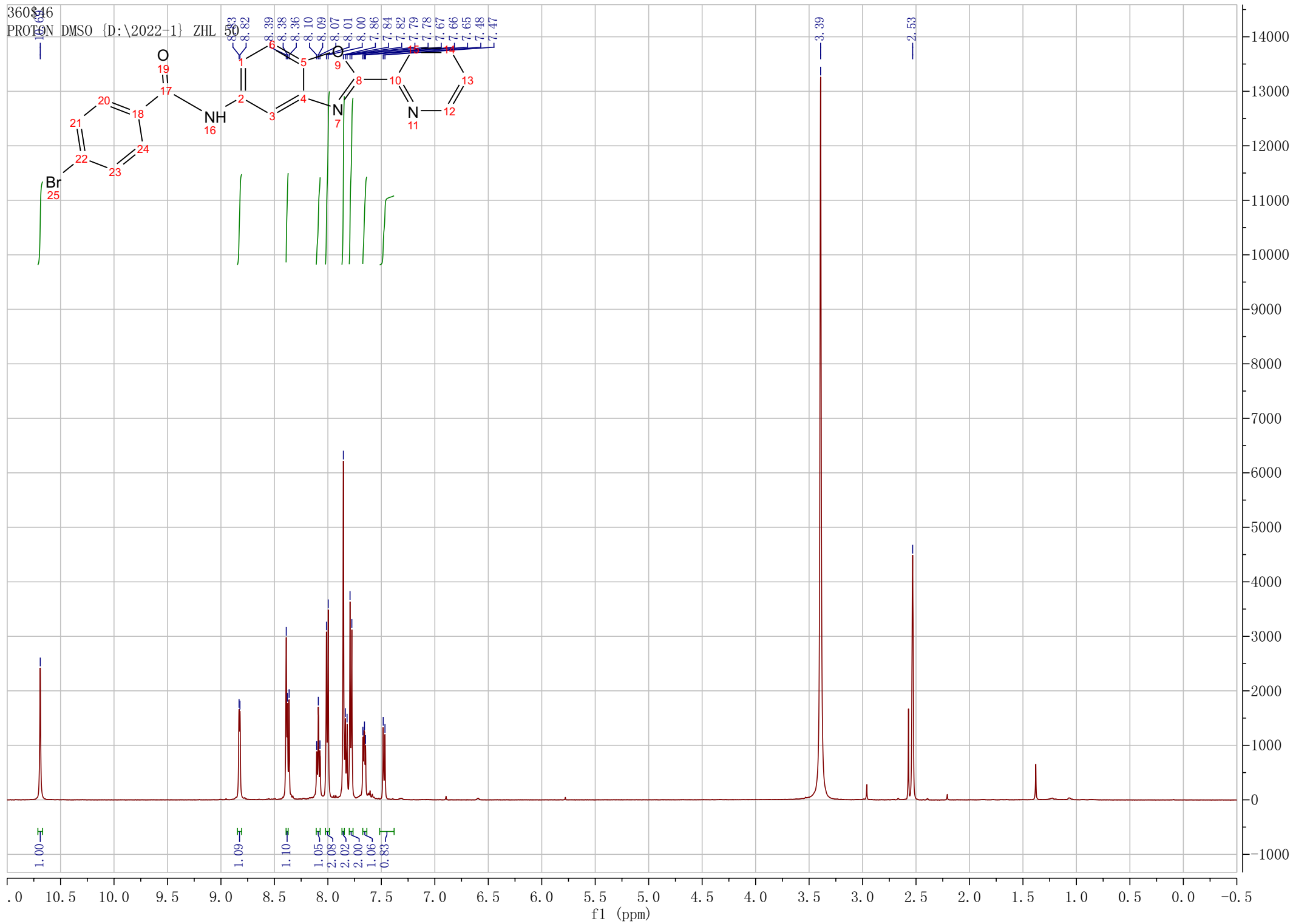


165.04  
162.50  
150.70  
147.48  
145.70  
141.83  
138.17  
136.96  
136.89  
134.03  
130.17  
128.97  
126.70  
124.09  
120.18  
112.21  
111.50

40.54  
40.37  
40.21  
40.04  
39.87  
39.71  
39.54

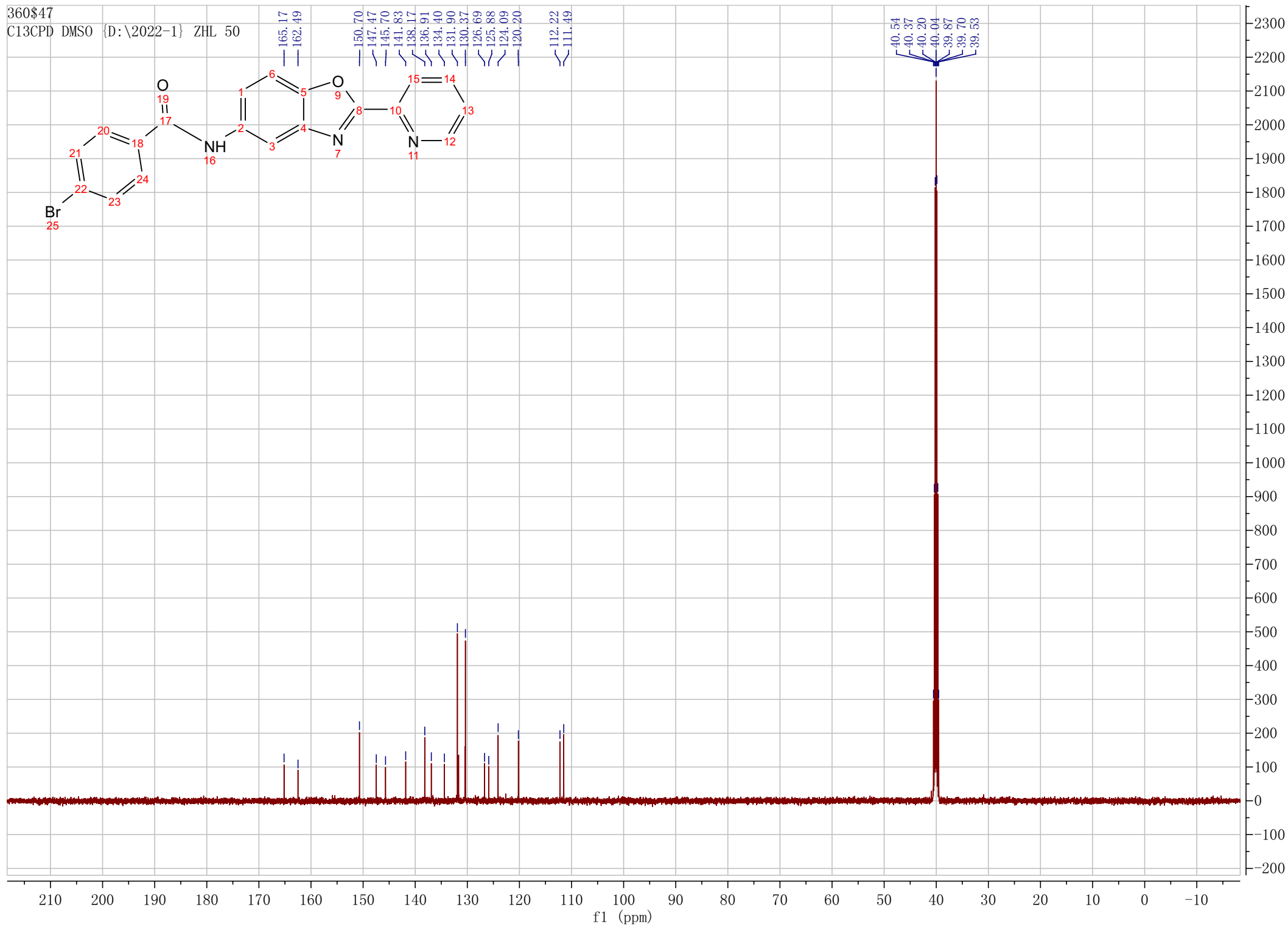


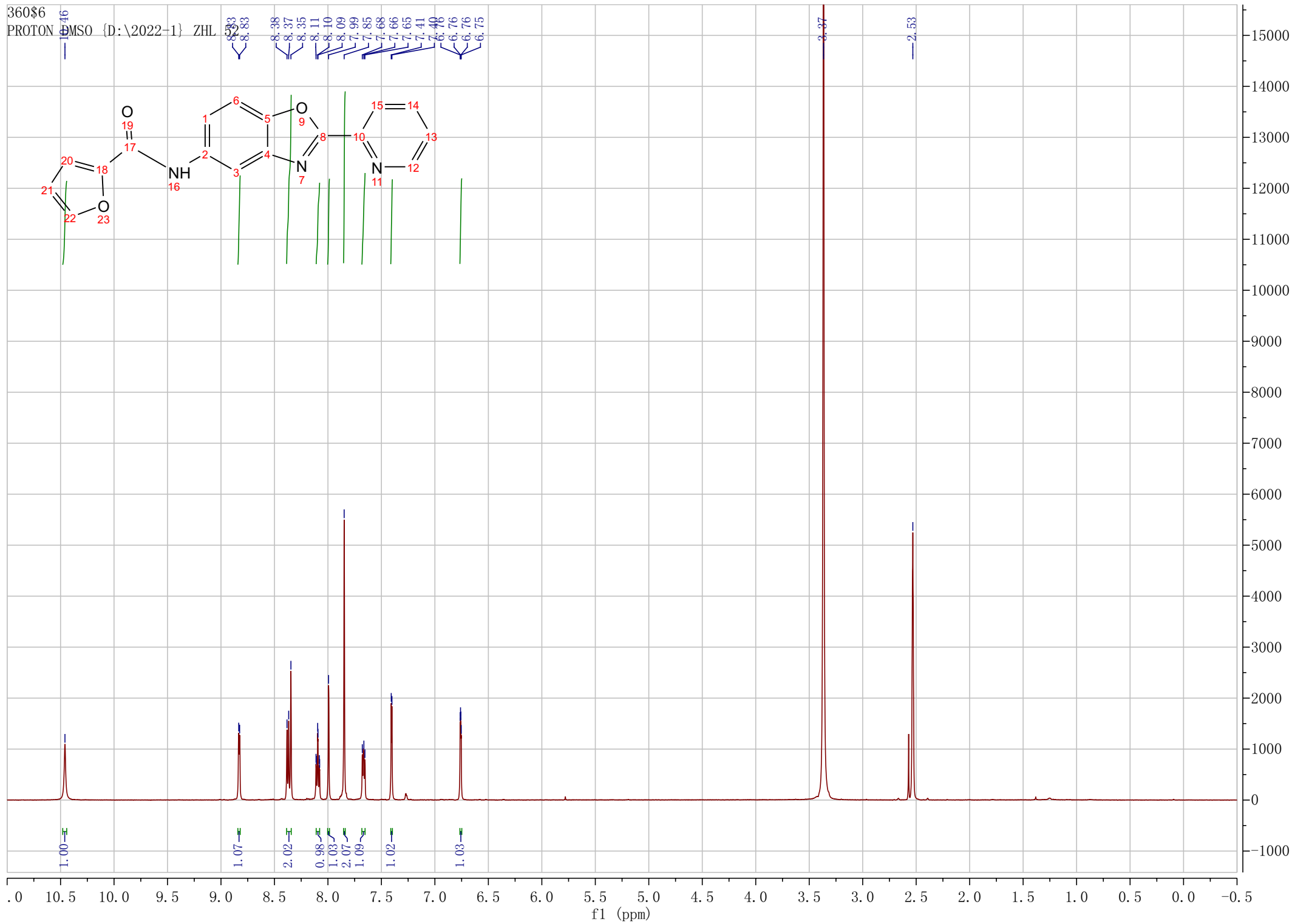




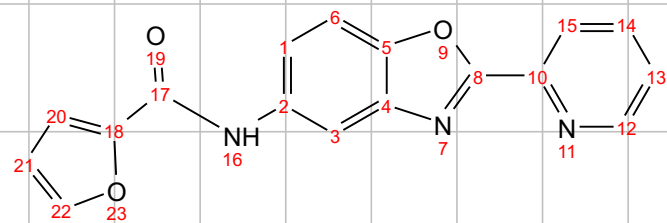
360\$47

C13CPD DMSO {D:\2022-1} ZHL 50



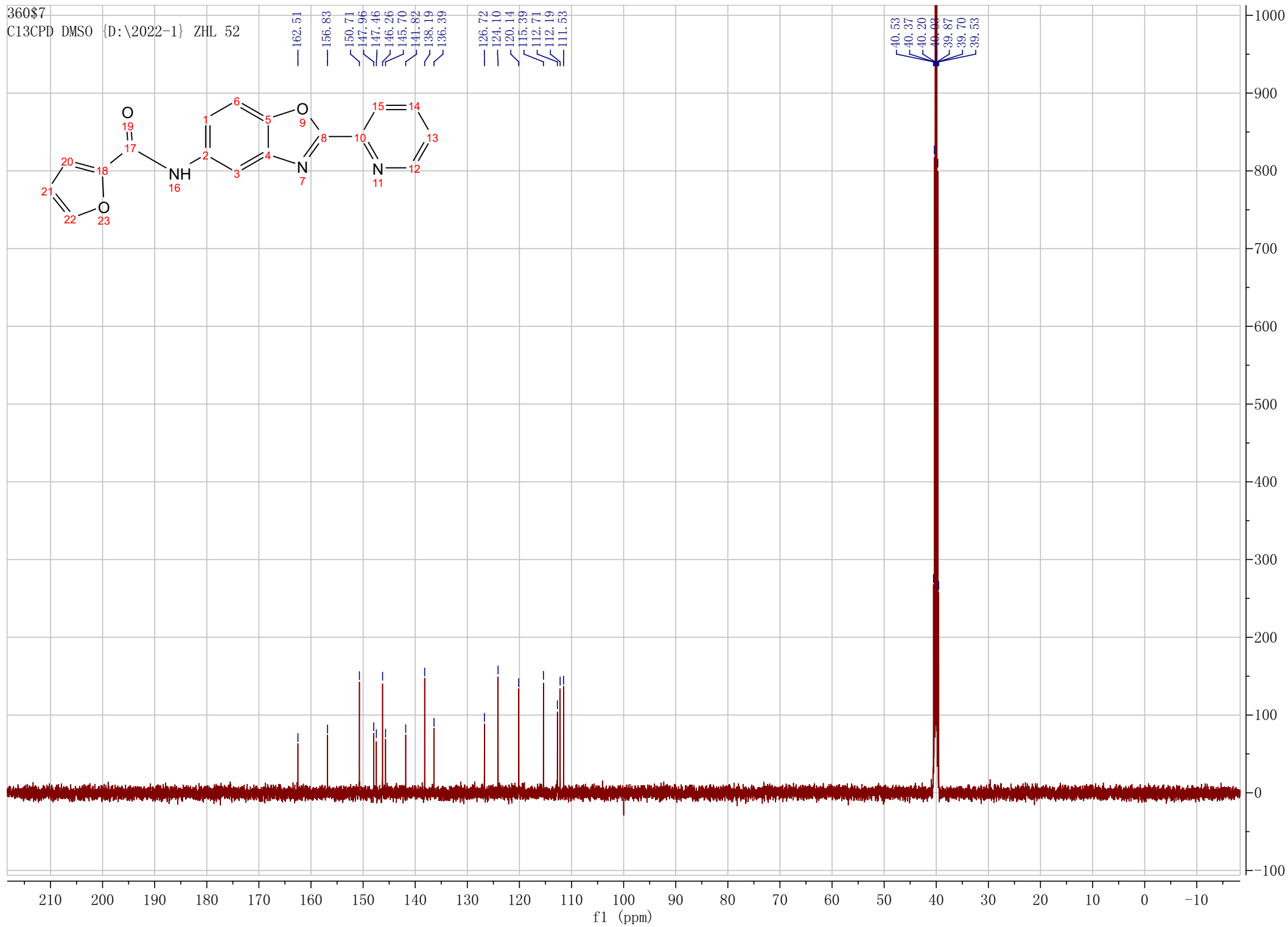


360\$7  
C13CPD DMSO {D:\2022-1} ZHL 52



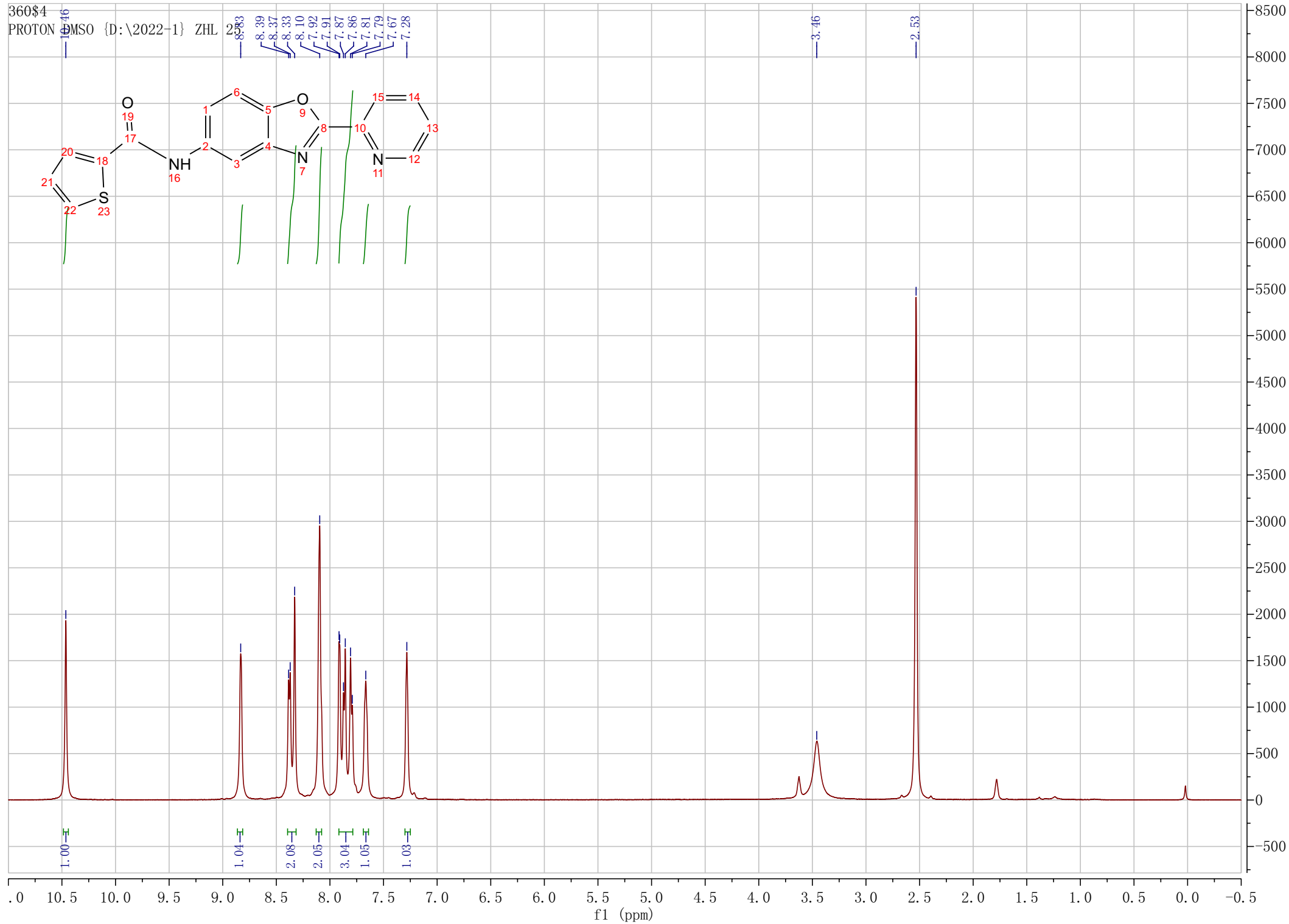
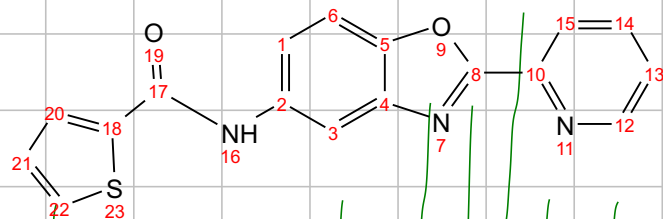
162.51  
156.83  
150.71  
147.96  
147.46  
146.26  
145.70  
141.82  
138.19  
136.39  
126.72  
124.10  
120.14  
115.39  
112.71  
112.19  
111.53

40.53  
40.37  
40.20  
40.02  
39.87  
39.70  
39.53



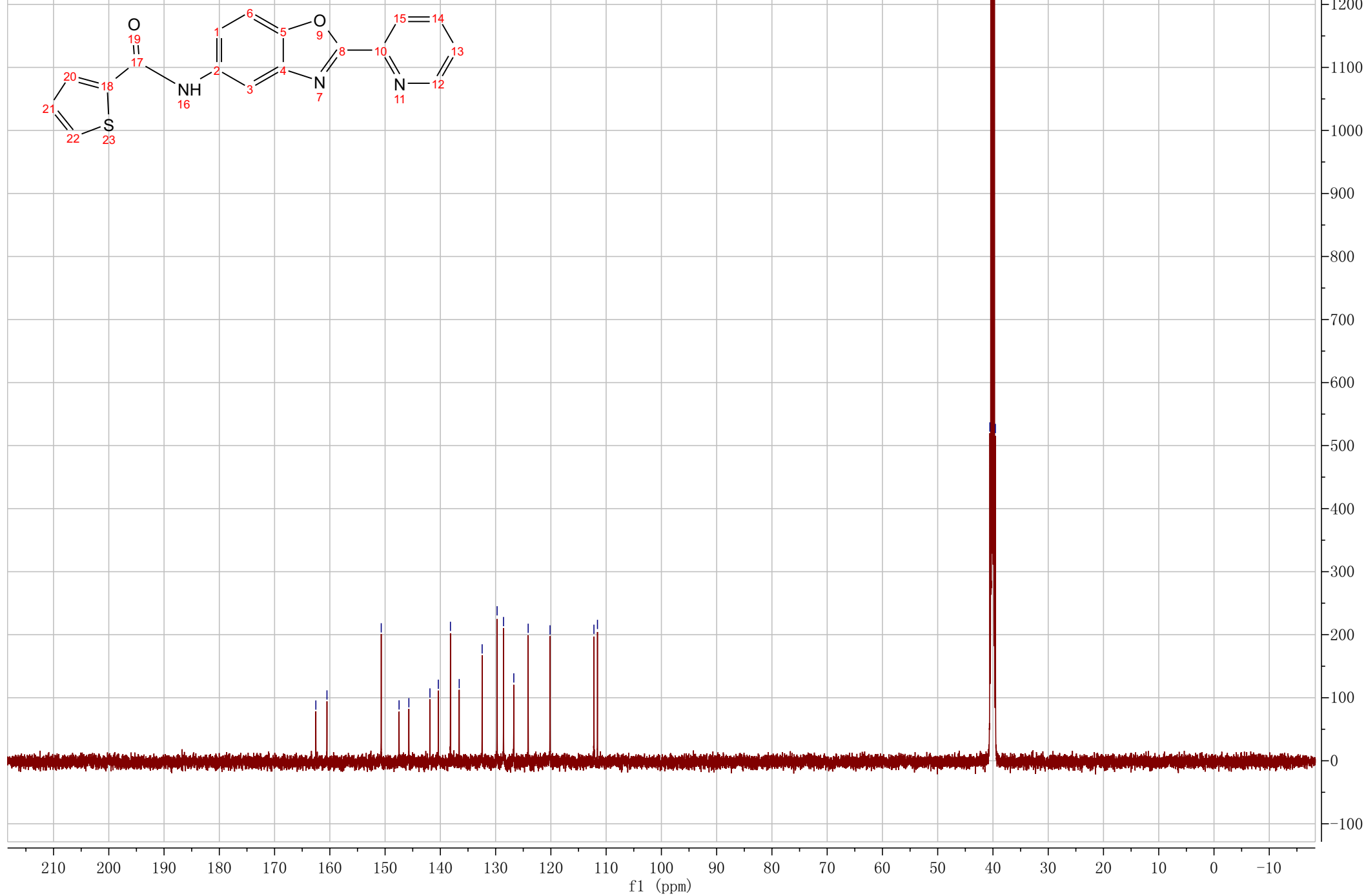
360\$4

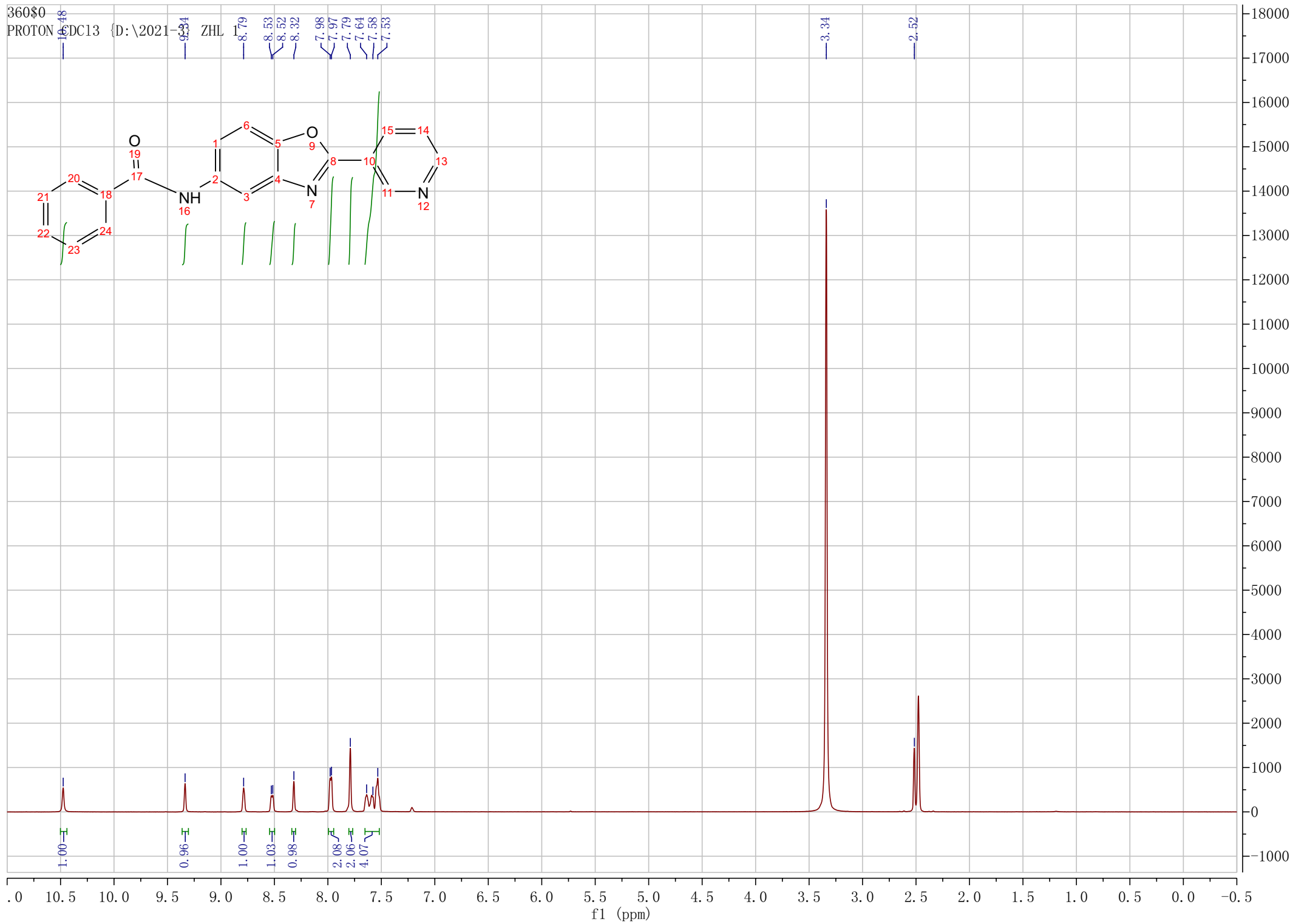
PROTON	DMSO	{D:\2022-1}	ZHL
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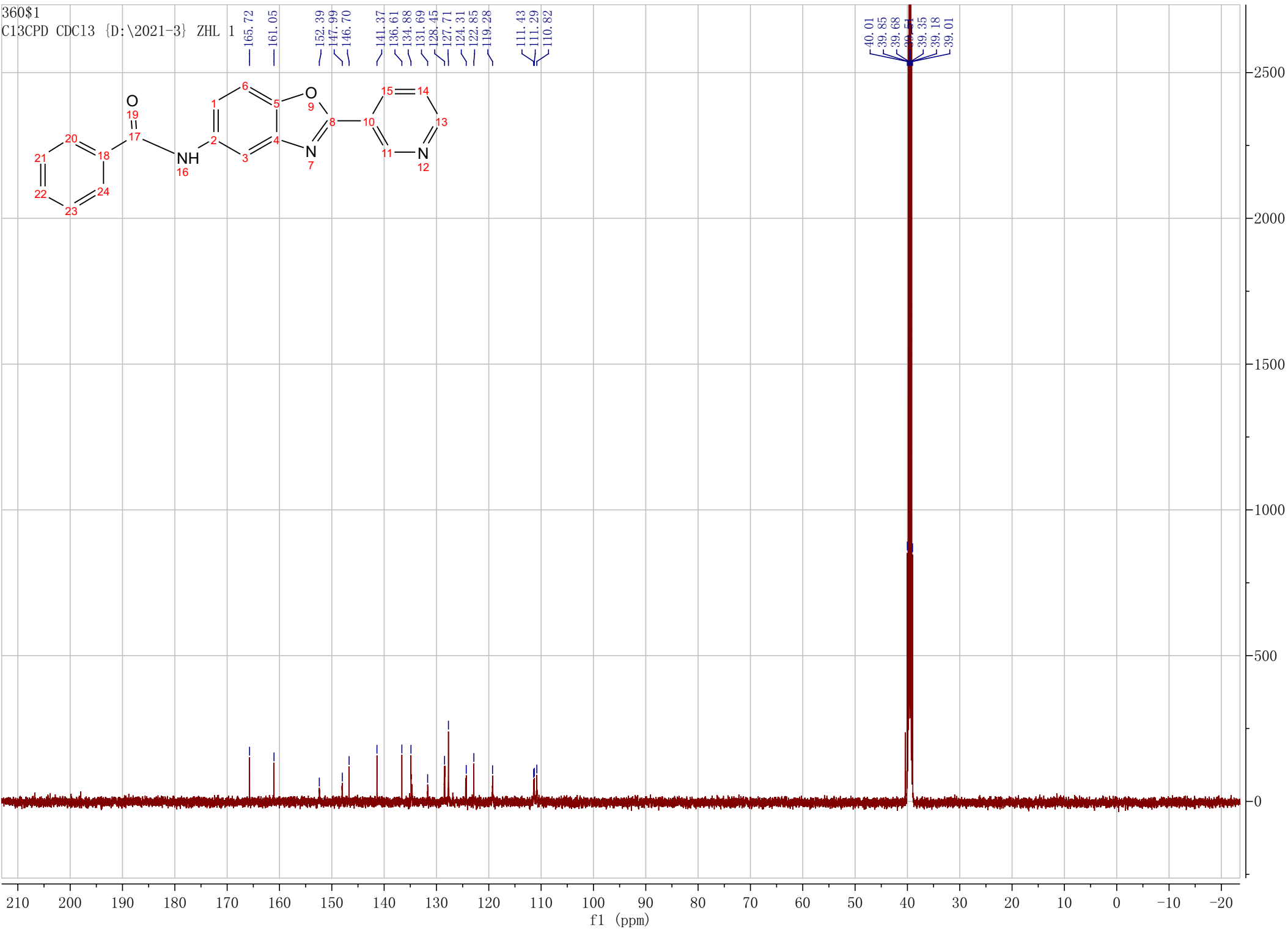
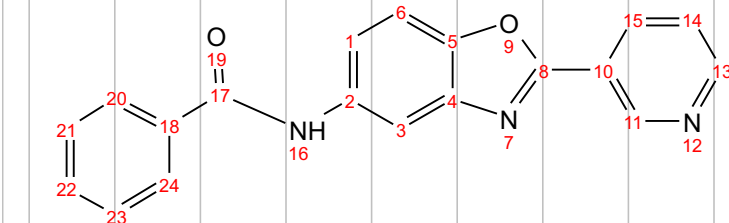
360\$5

C13CPD DMSO {D:\2022-1} ZHL 25

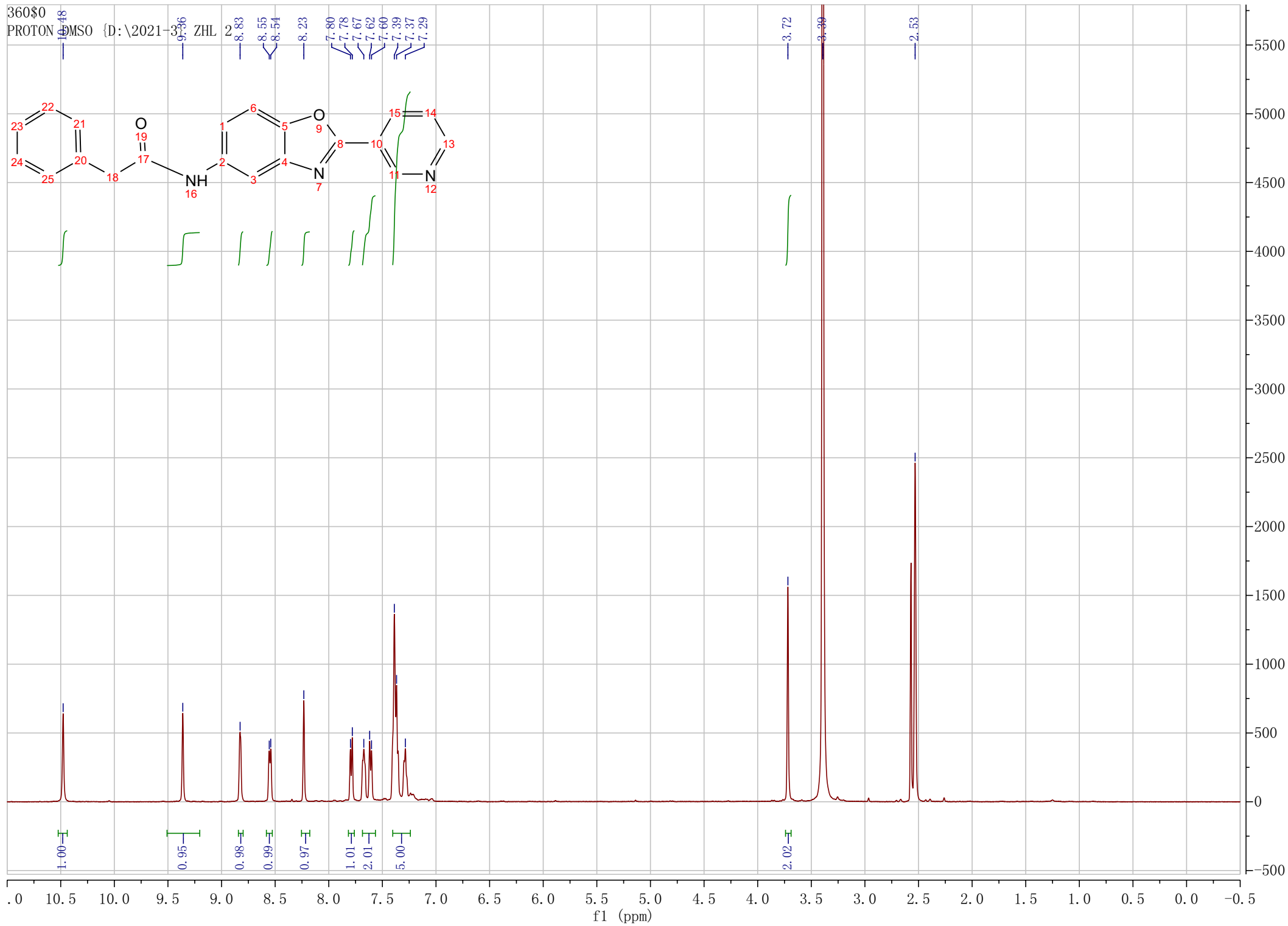




360\$1  
C13CPD CDC13 {D:\2021-3} ZHL 1

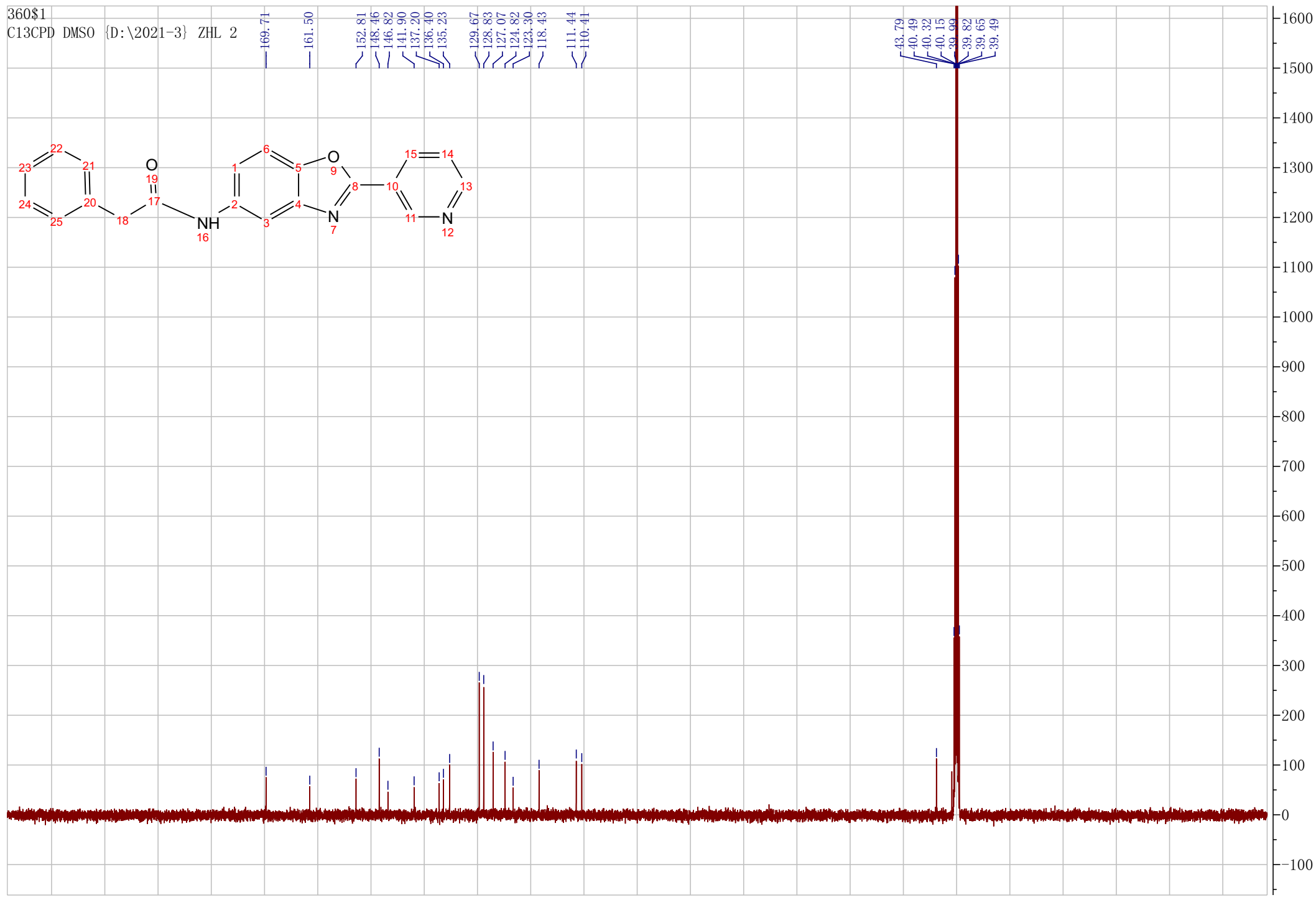


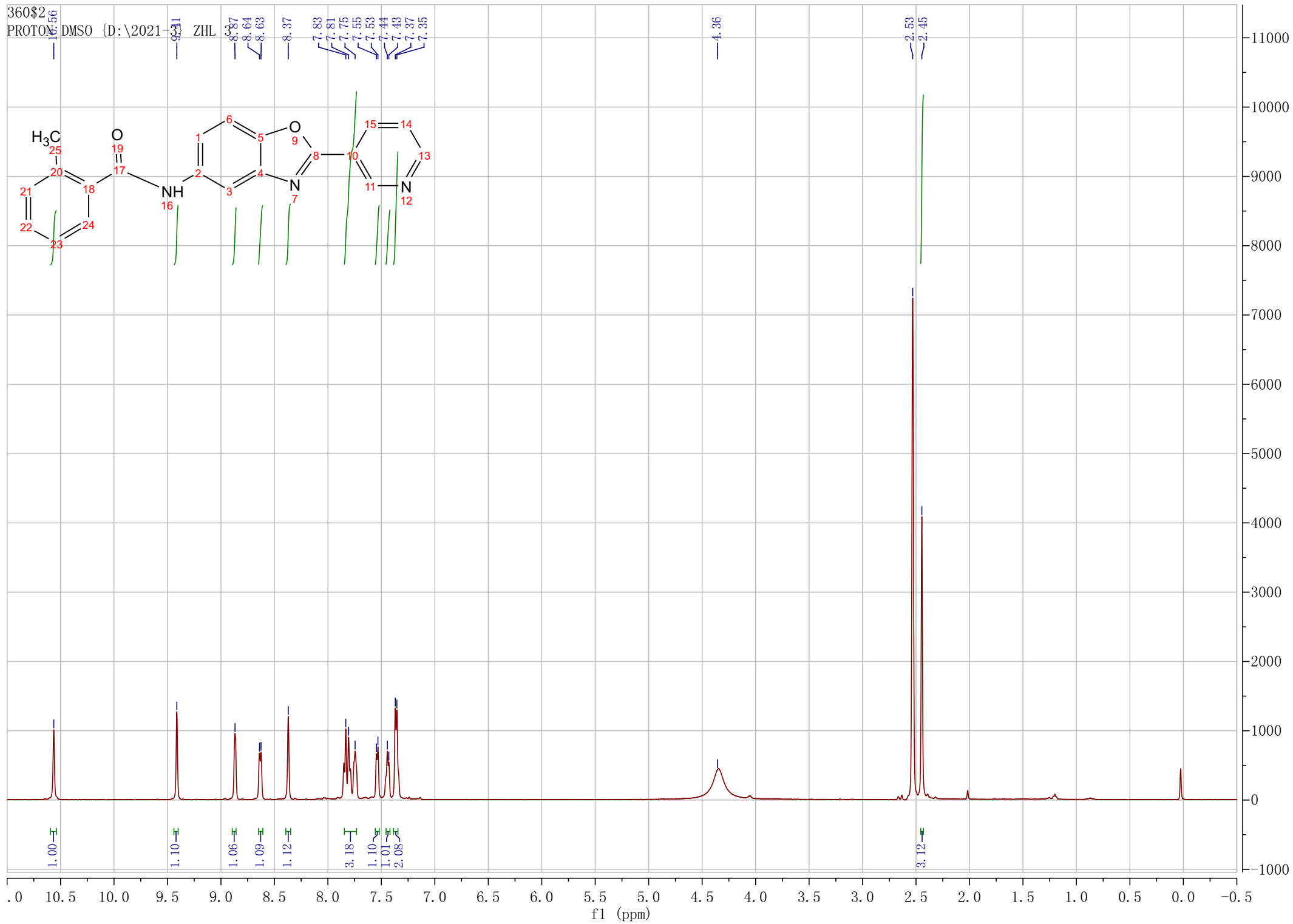




360\$1

C13CPD DMSO {D:\2021-3} ZHL 2

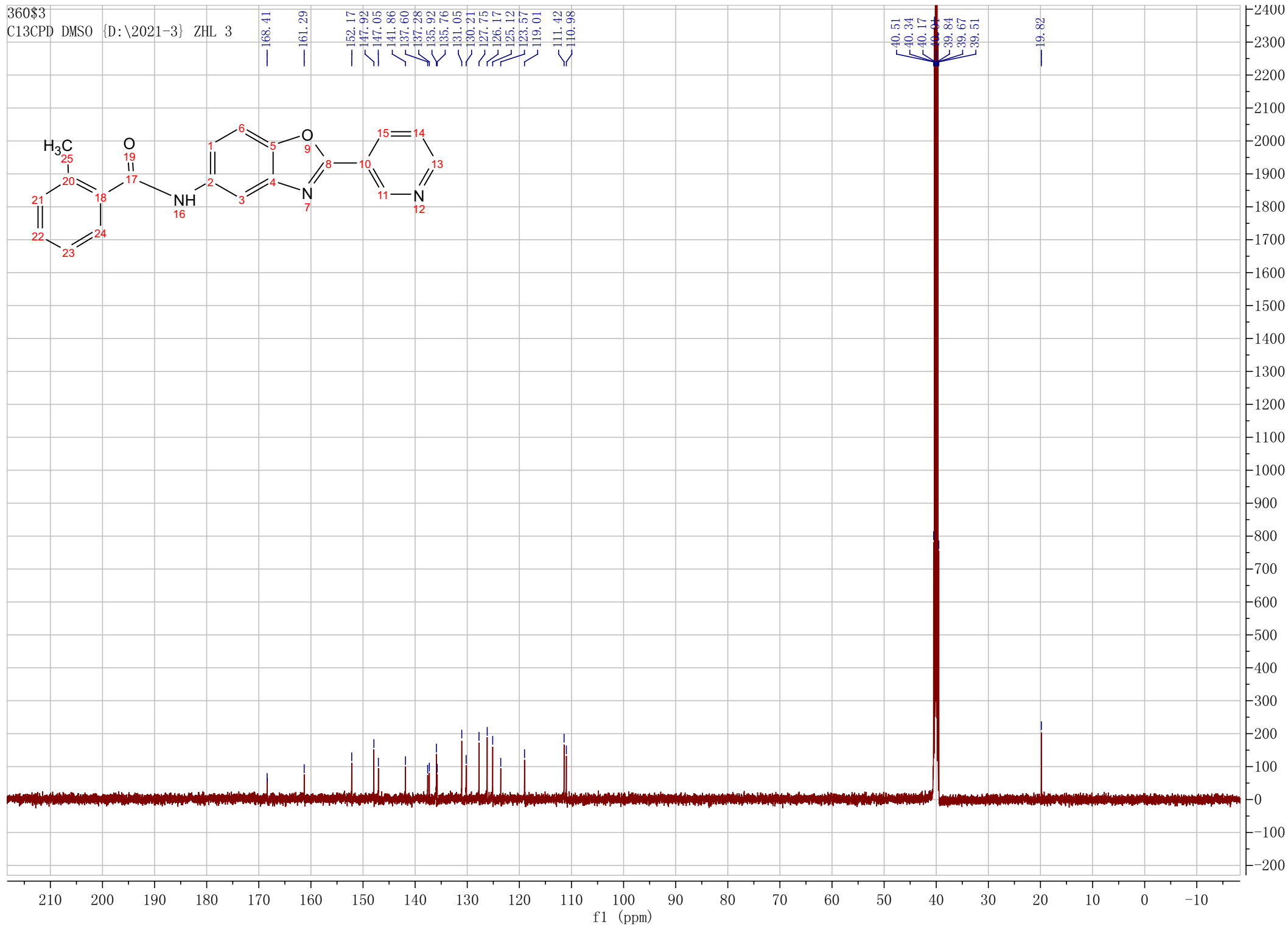


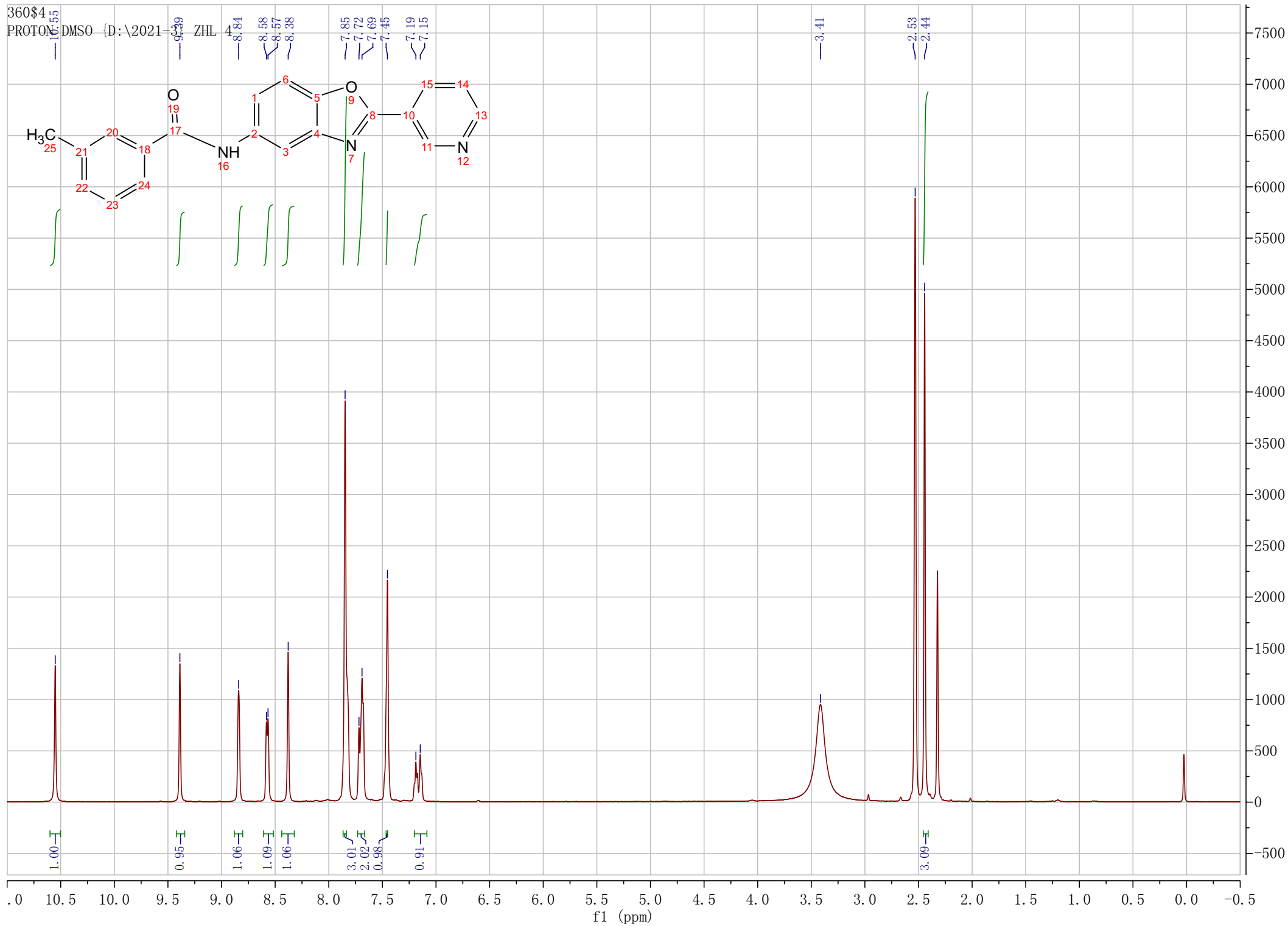


360\$3

C13CPD DMSO

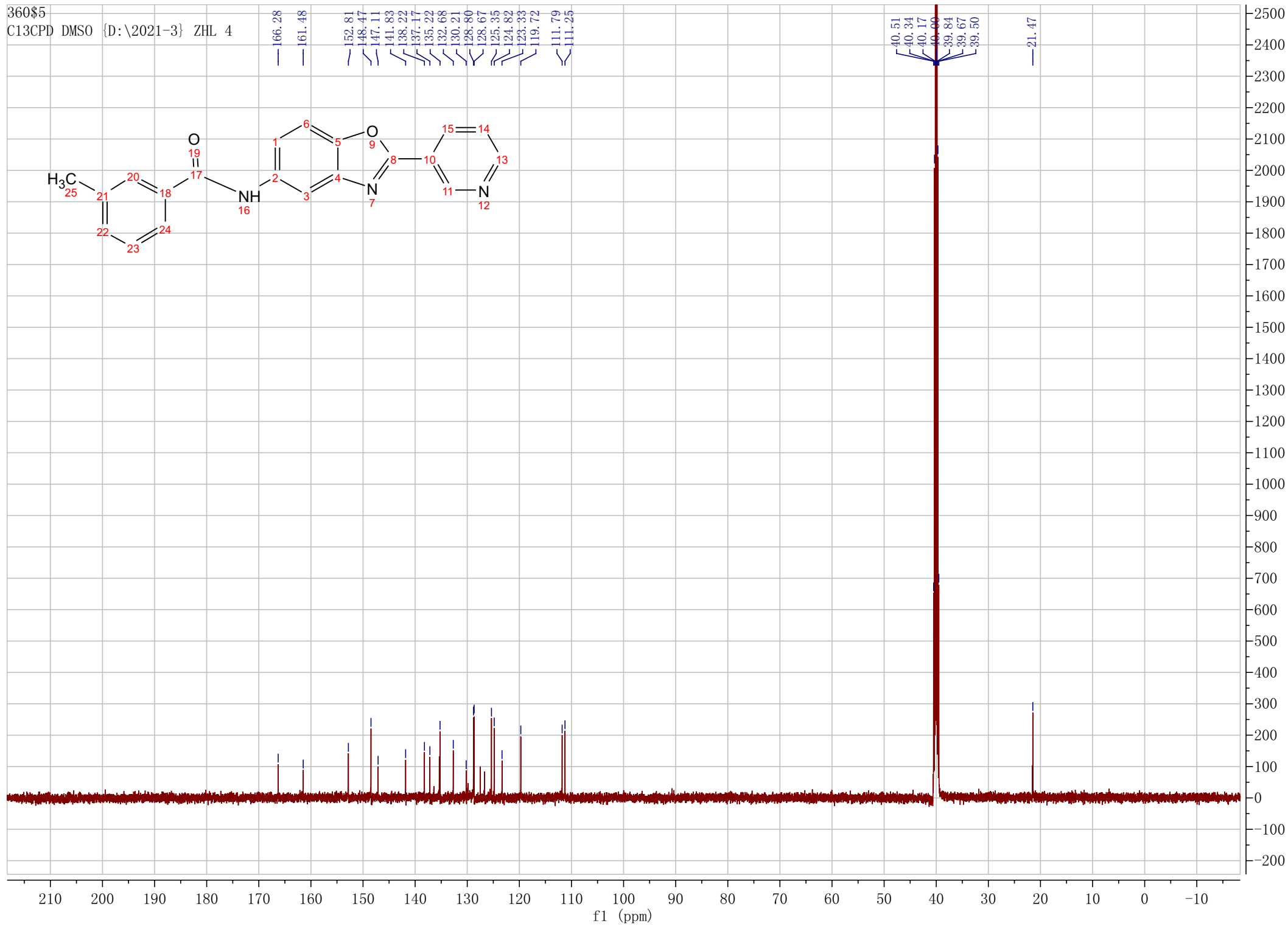
{D:\2021-3} ZHL 3

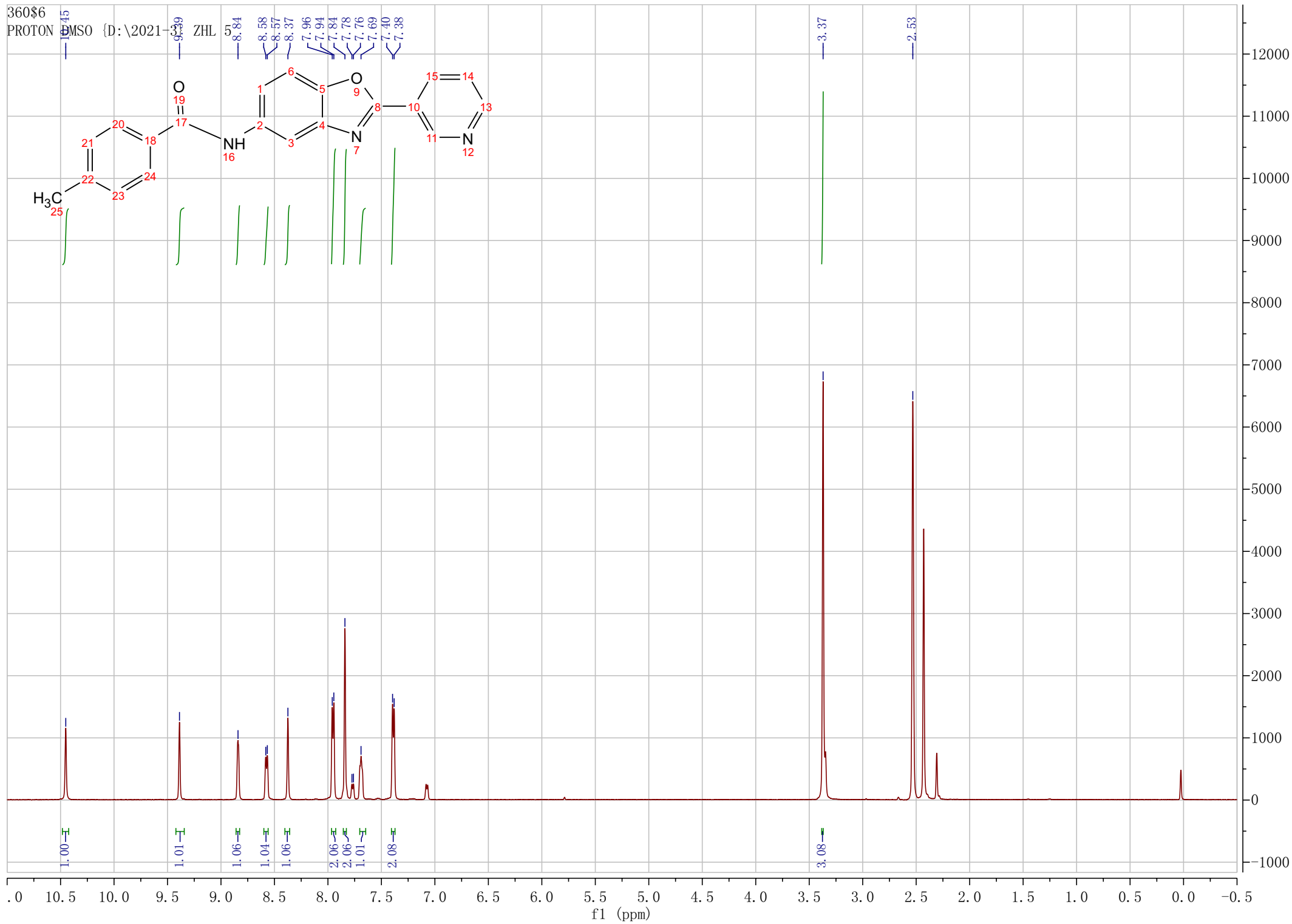




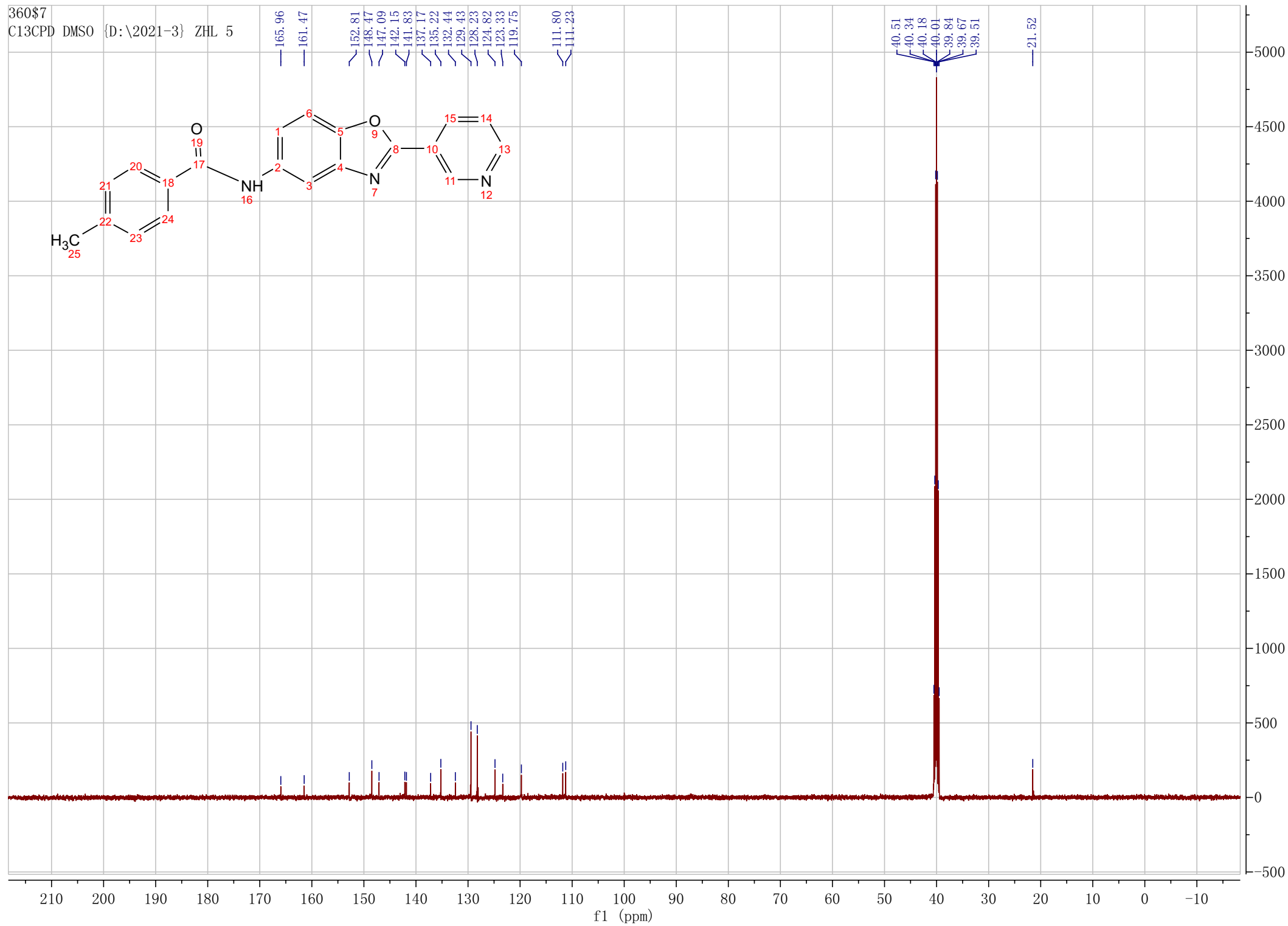
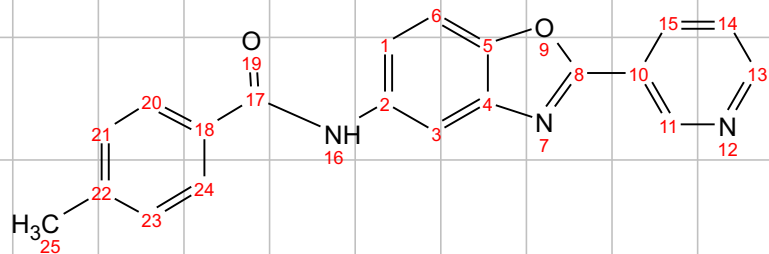
360\$5

C13CPD DMSO {D:\2021-3} ZHL 4





360\$7  
C13CPD DMSO {D:\2021-3} ZHL 5

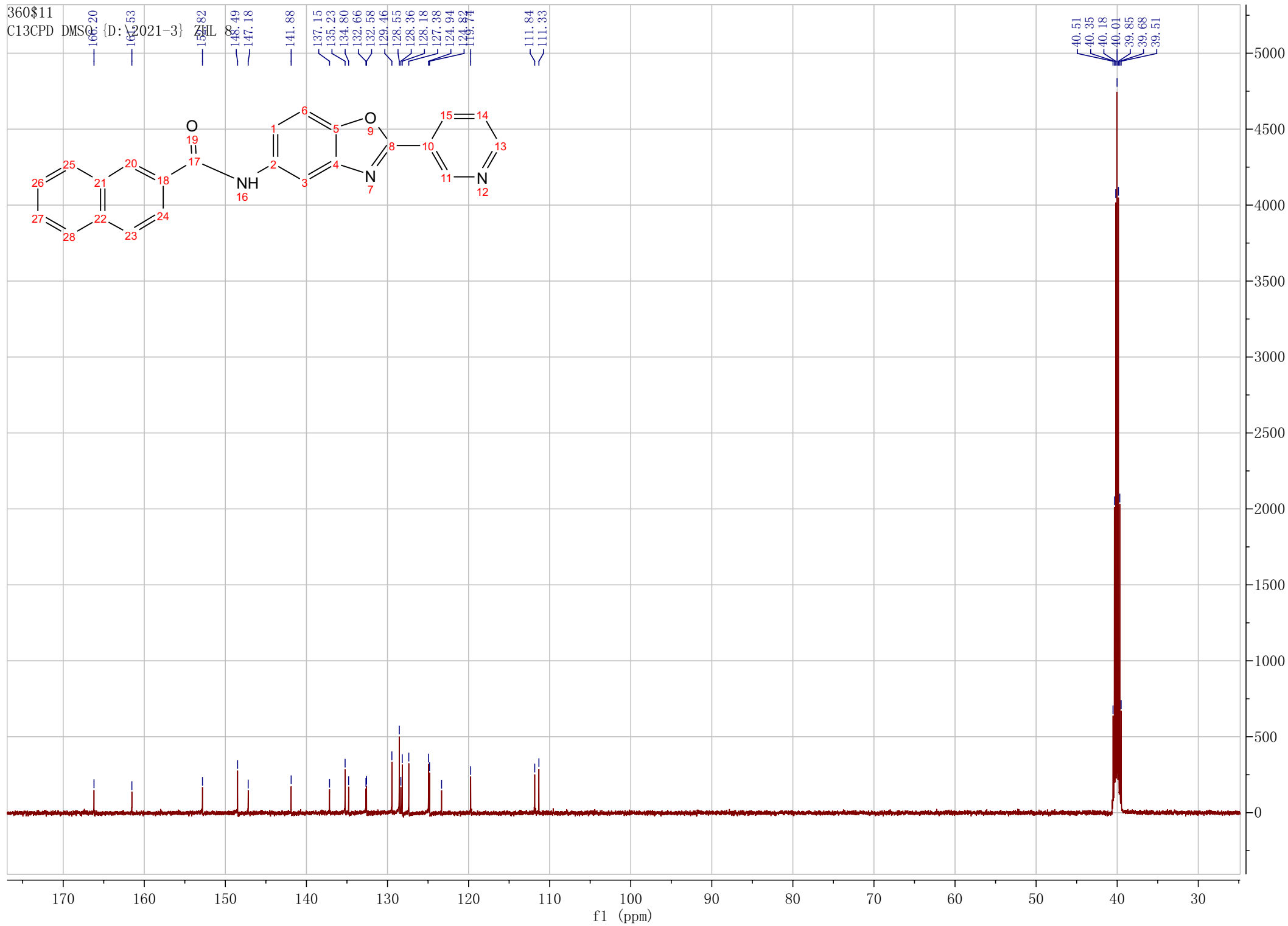






360\$11

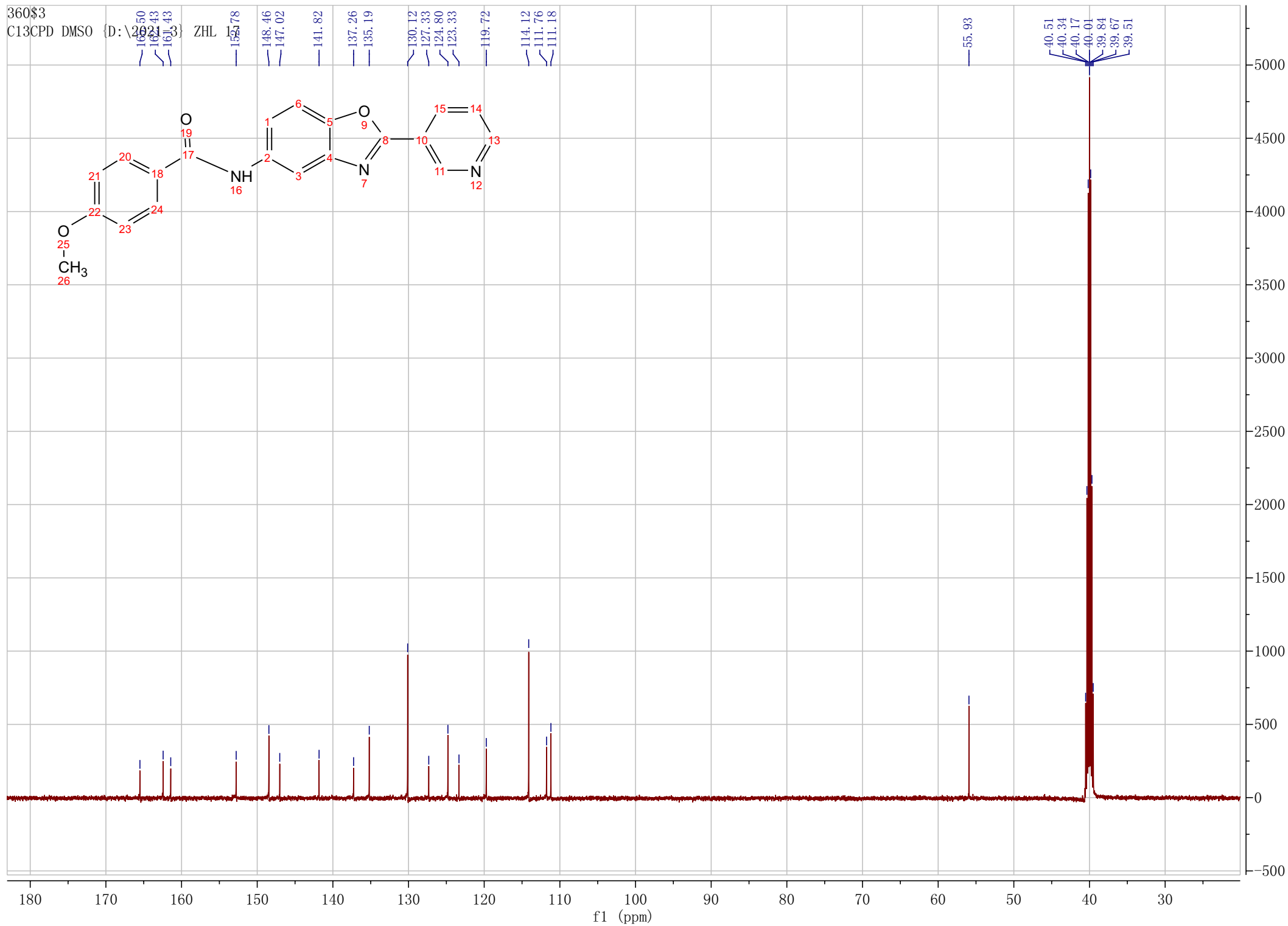
C13CPD DMSO {D:\2021-3}

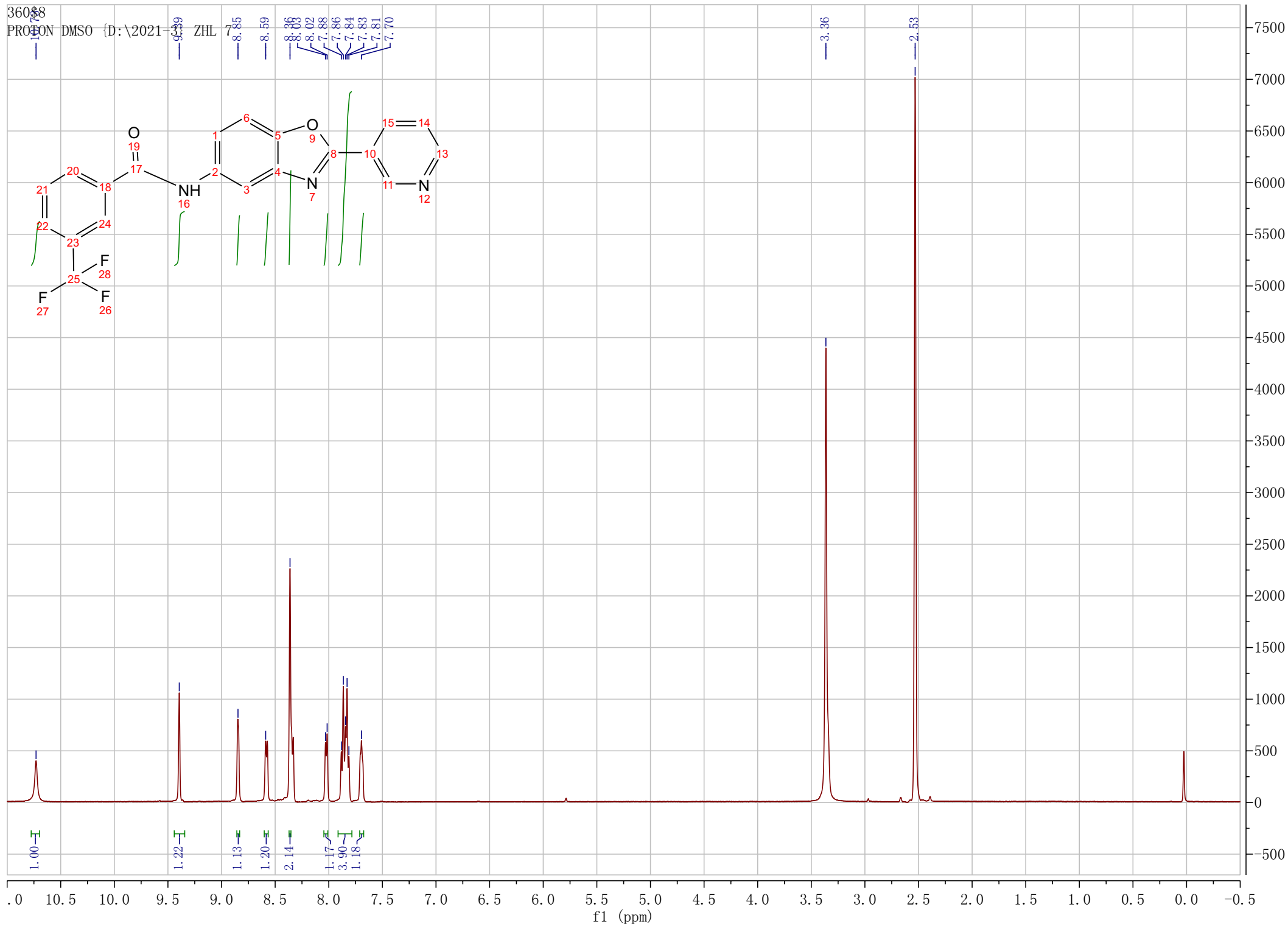


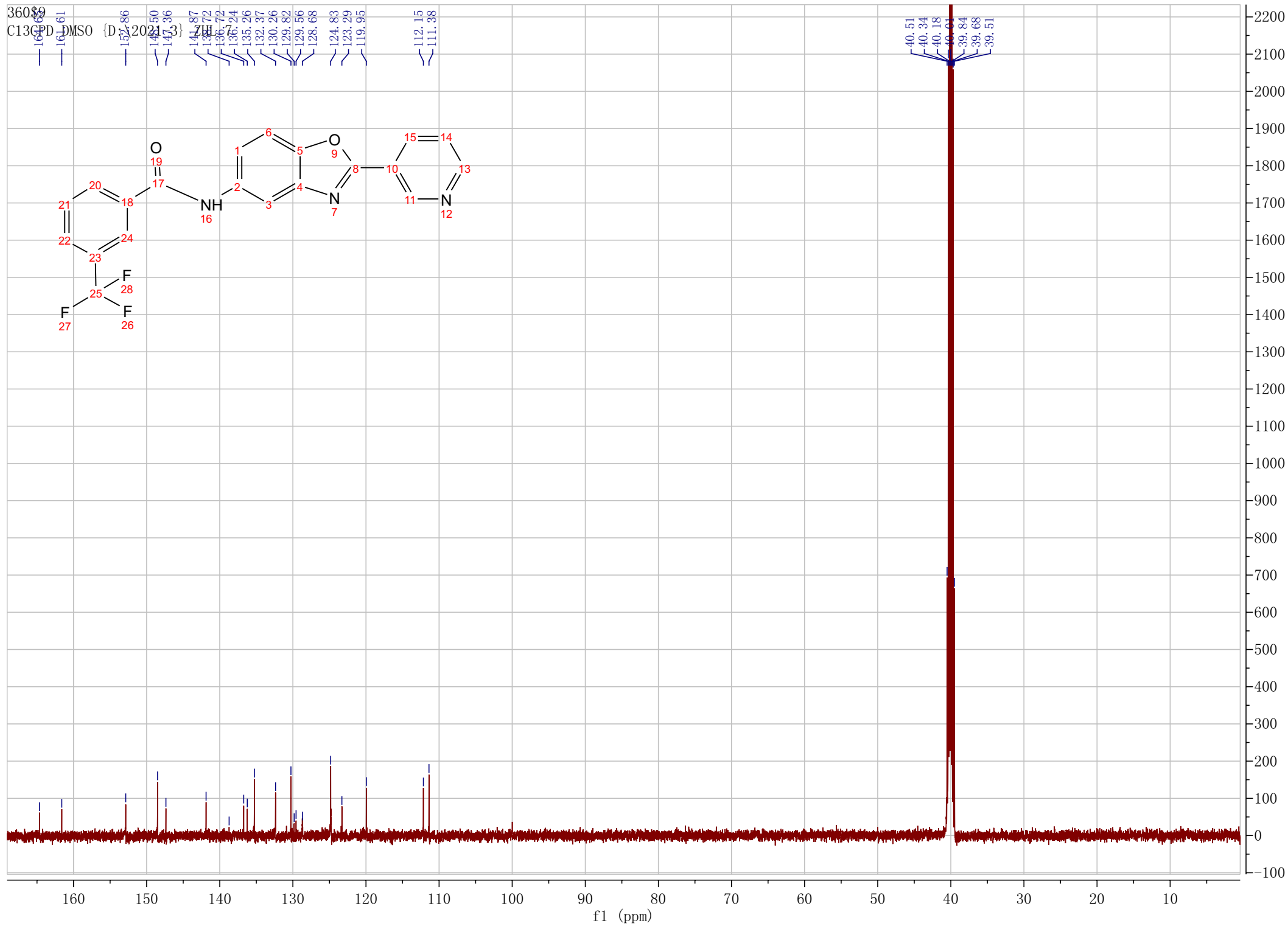


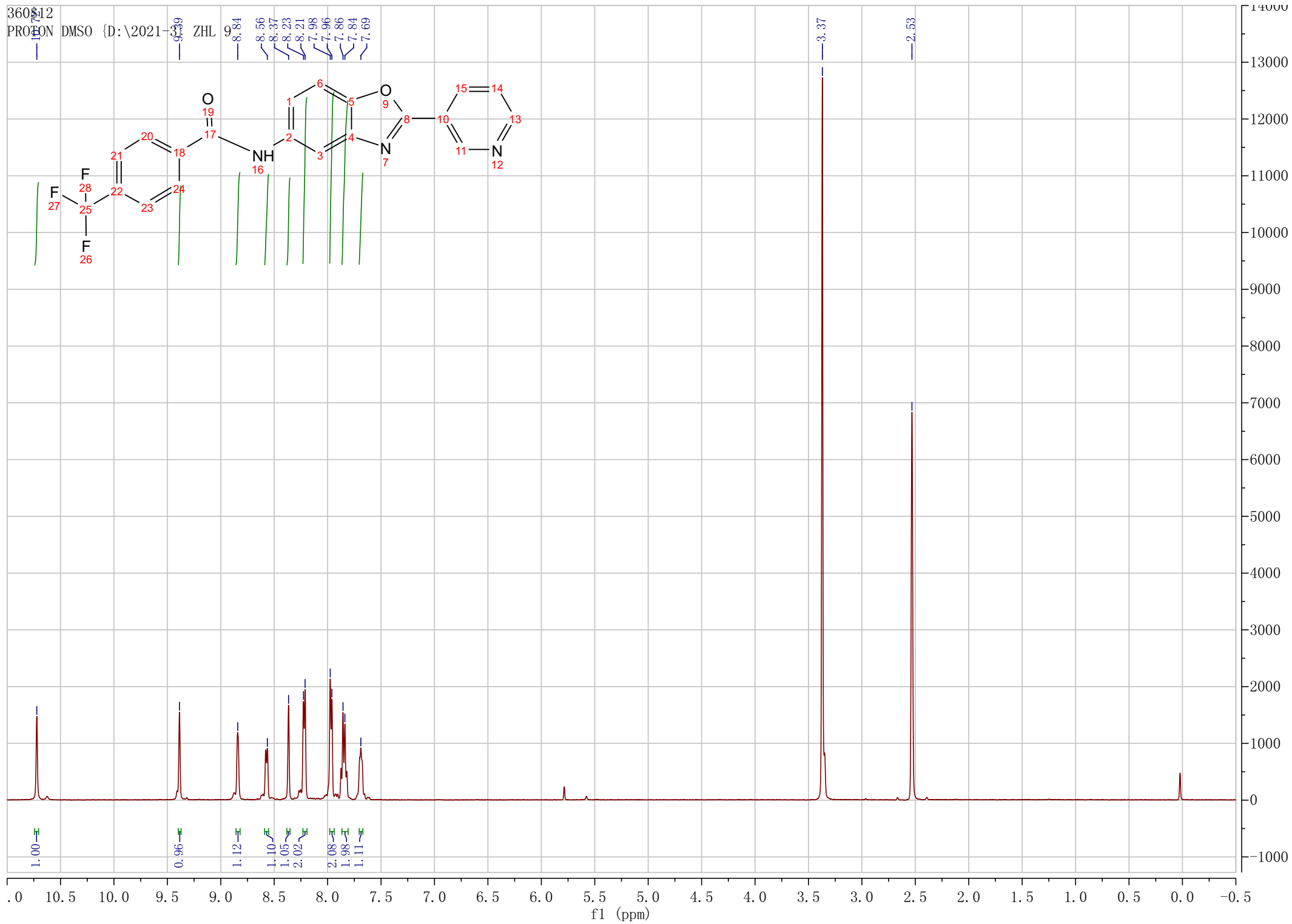
360\$3

C13CPD DMSO {D:\2021\3}

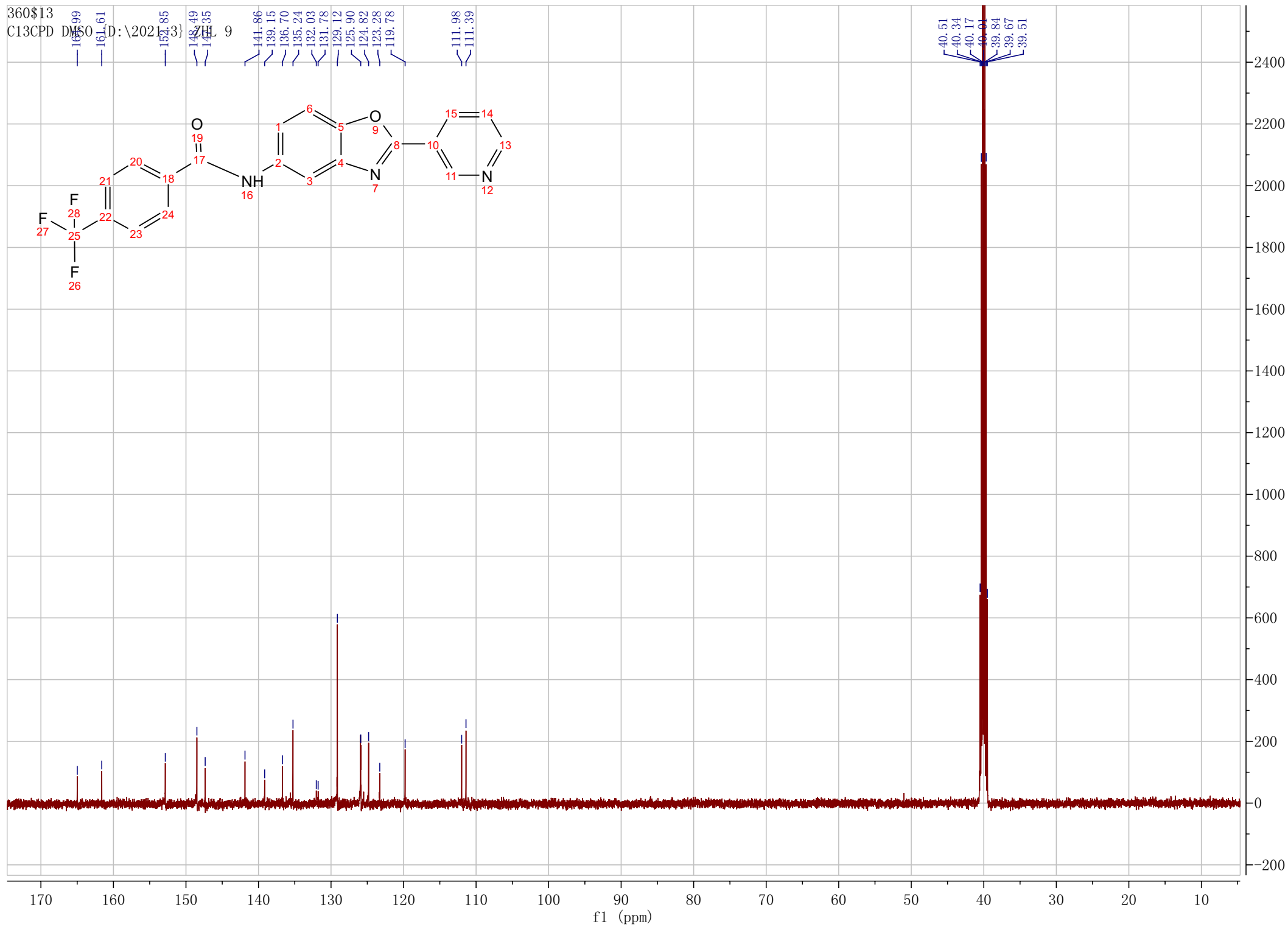






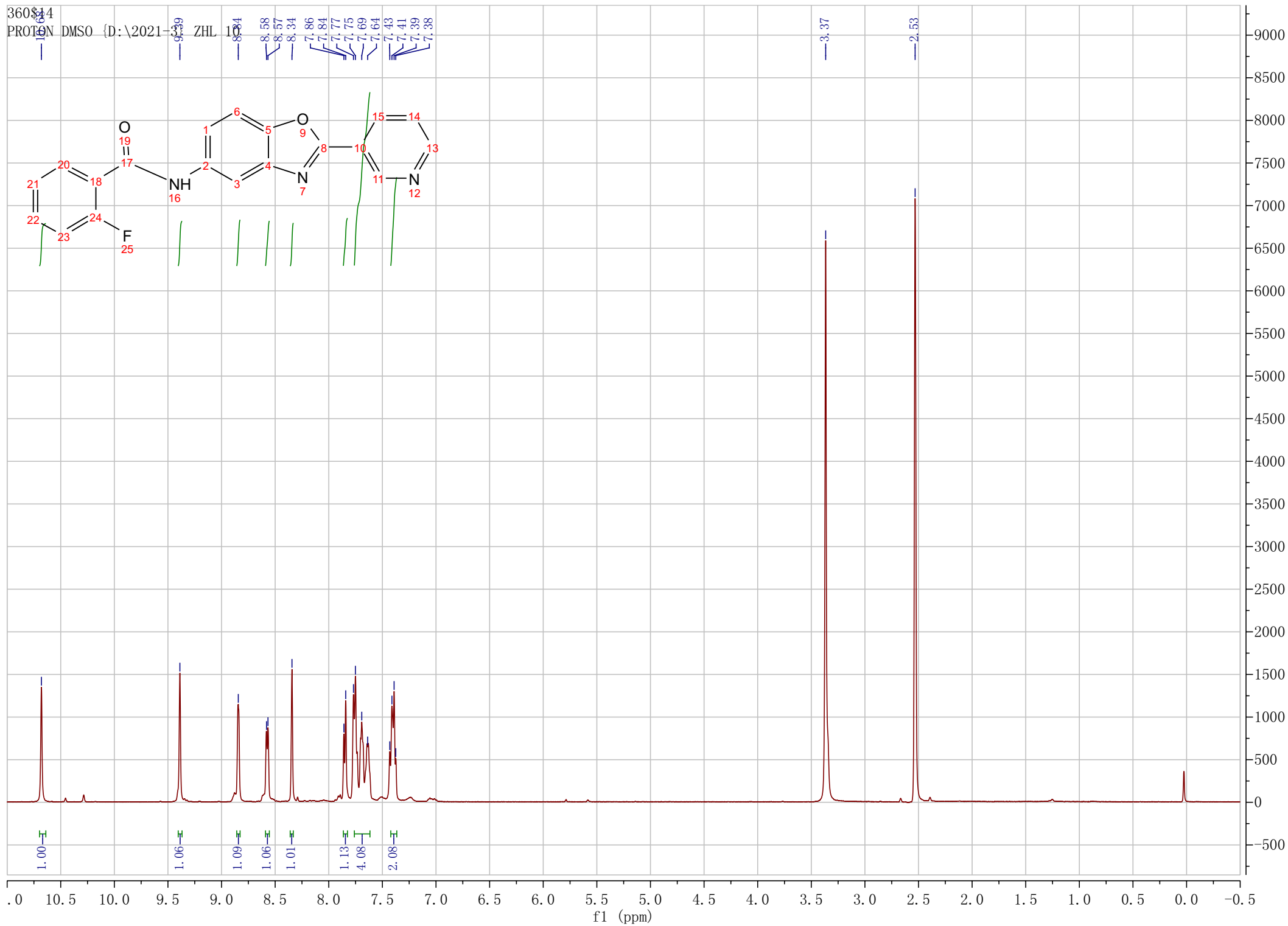


360\$13

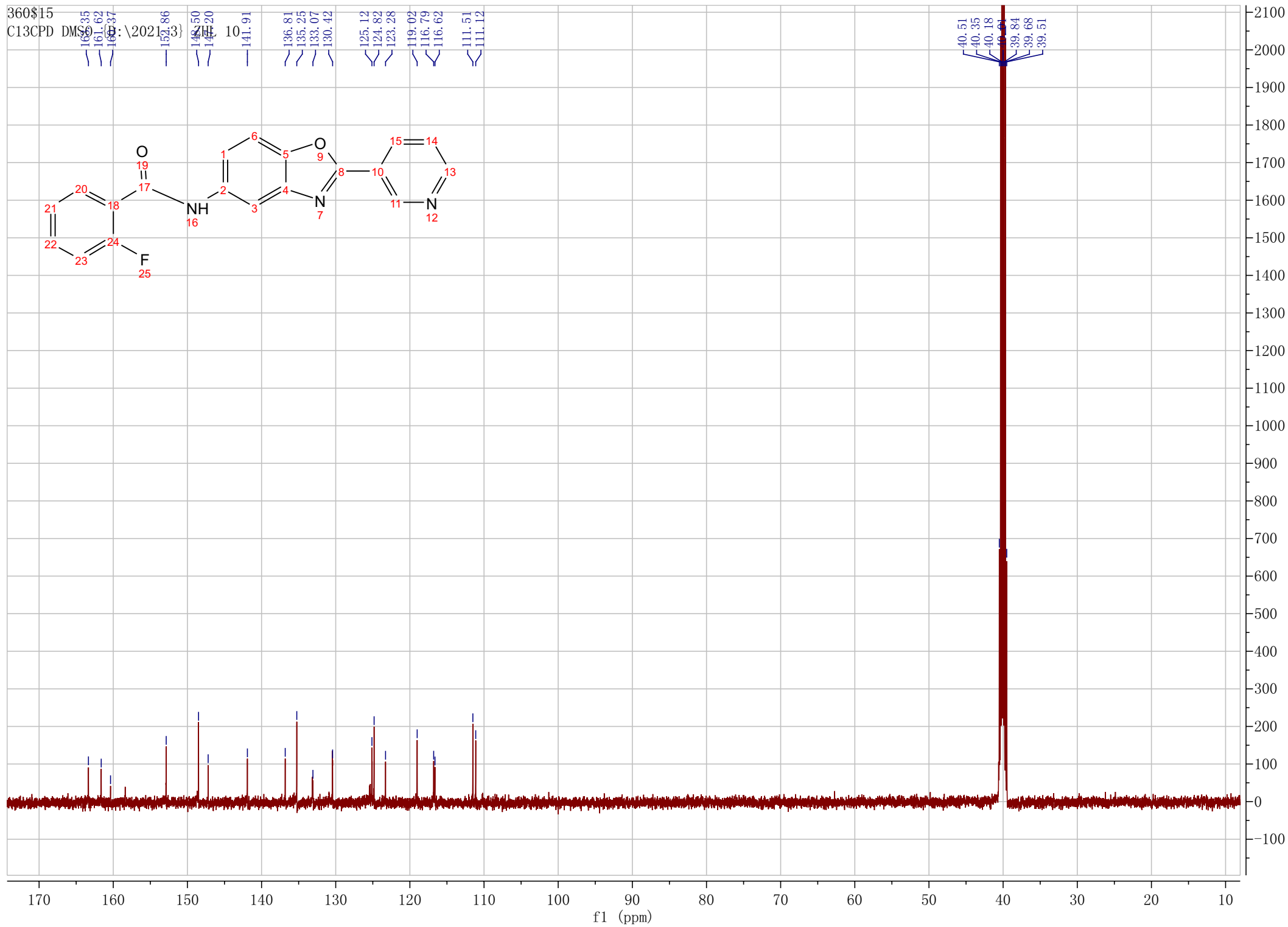
C13CPD DMSO-D<sub>6</sub> ID:\2021\3\211 9

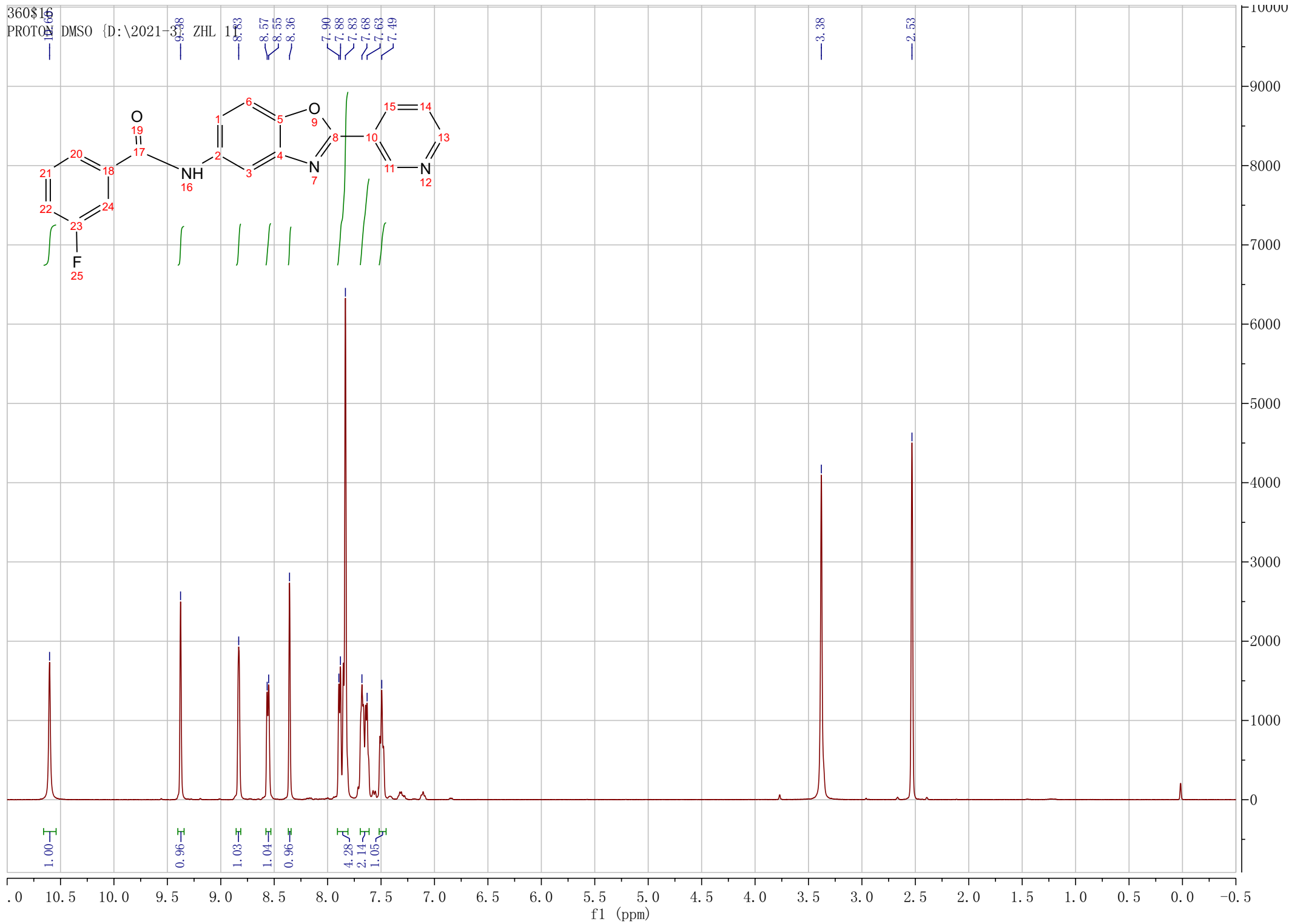


360\$14  
PROTON DMSO {D:\2021-



360\$15

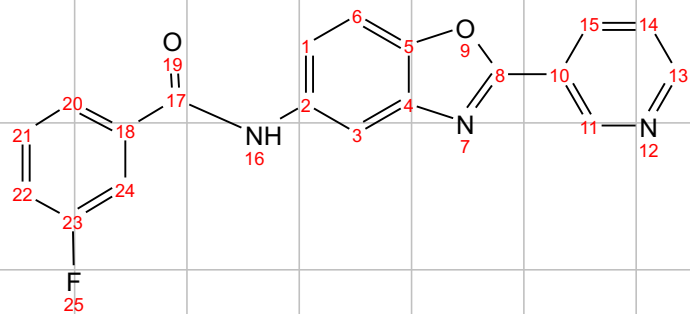
C13CPD DMSO-d<sub>6</sub> 20210331



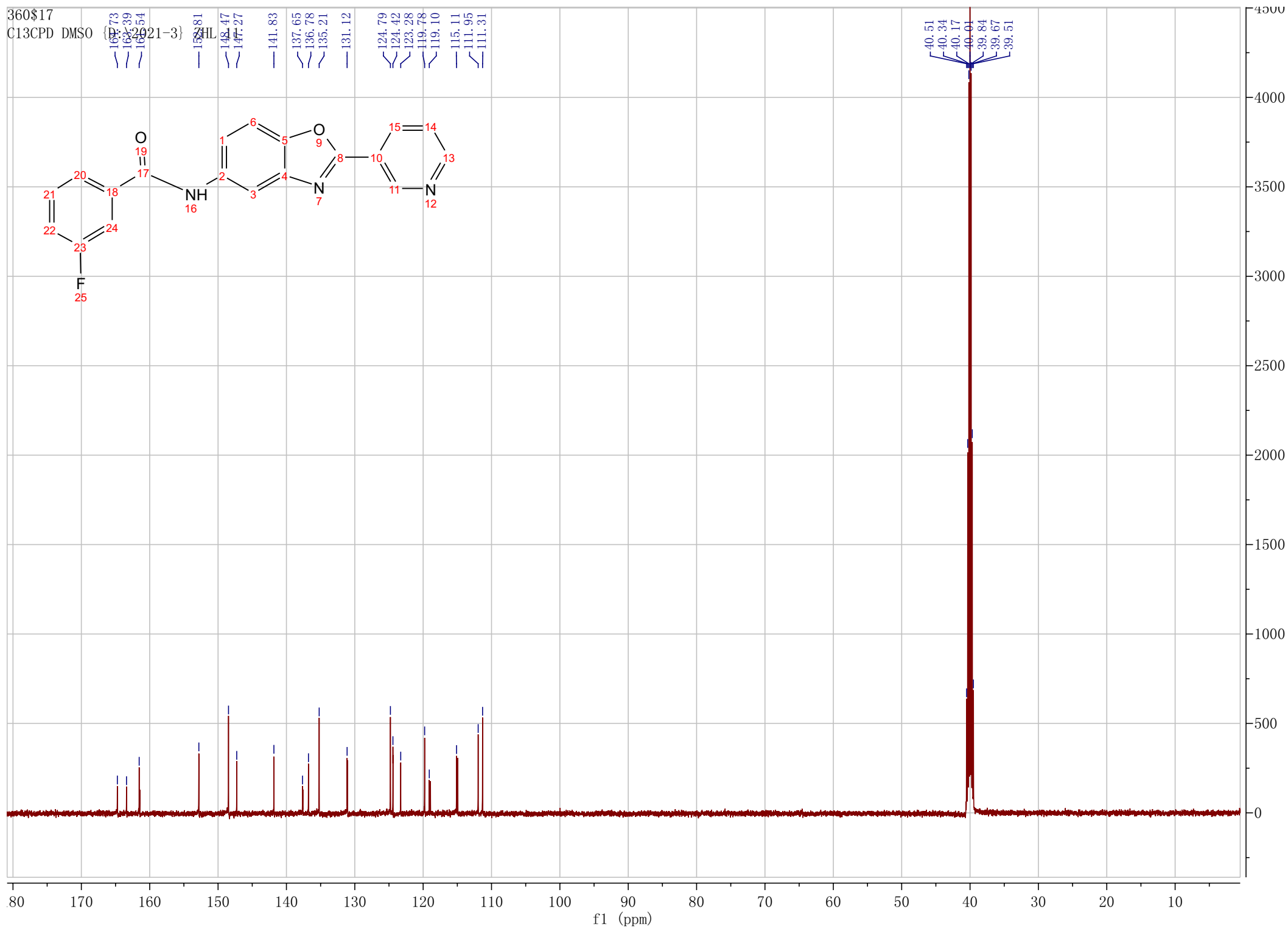
360\$17

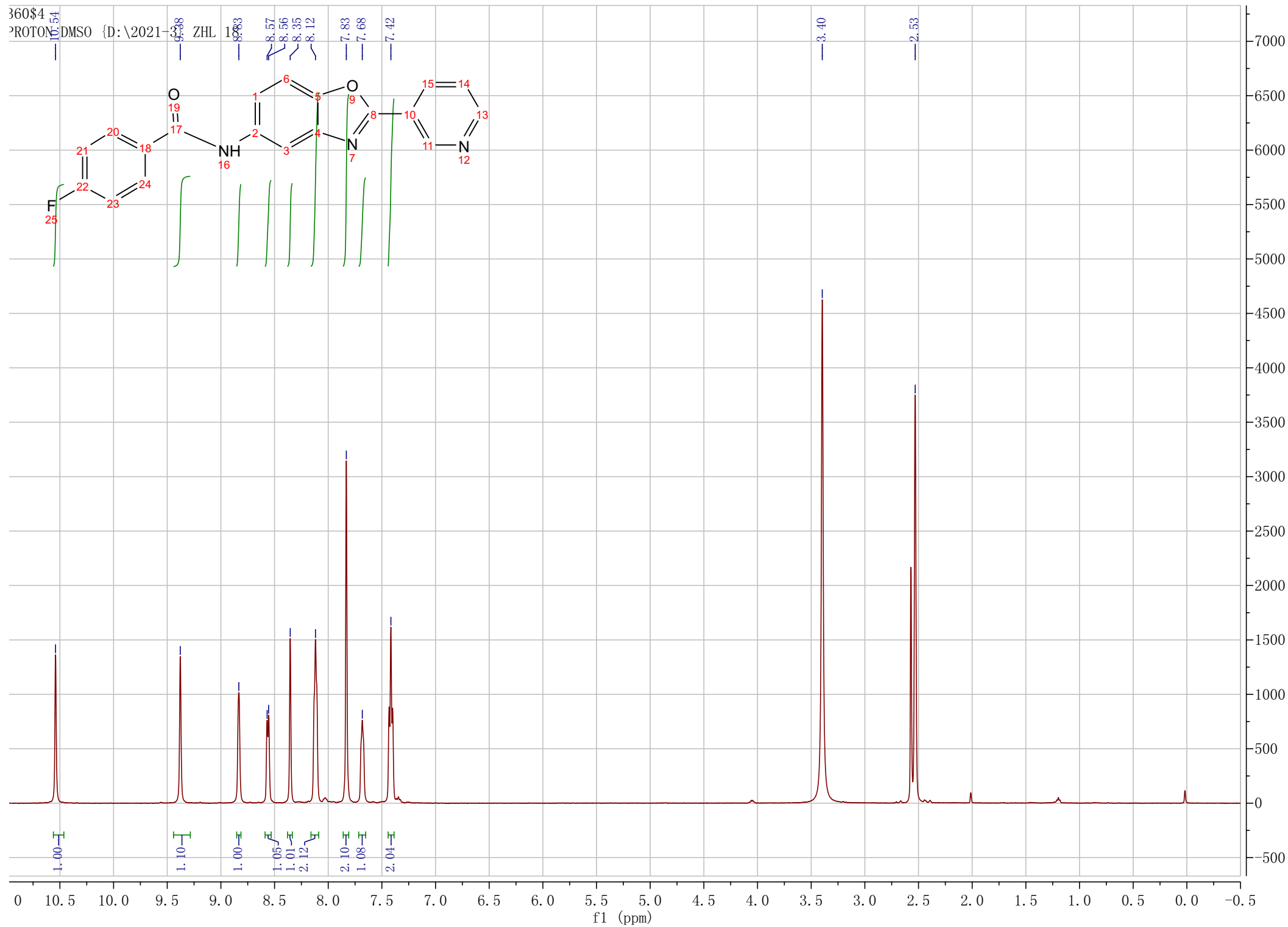
C13CPD DMSO

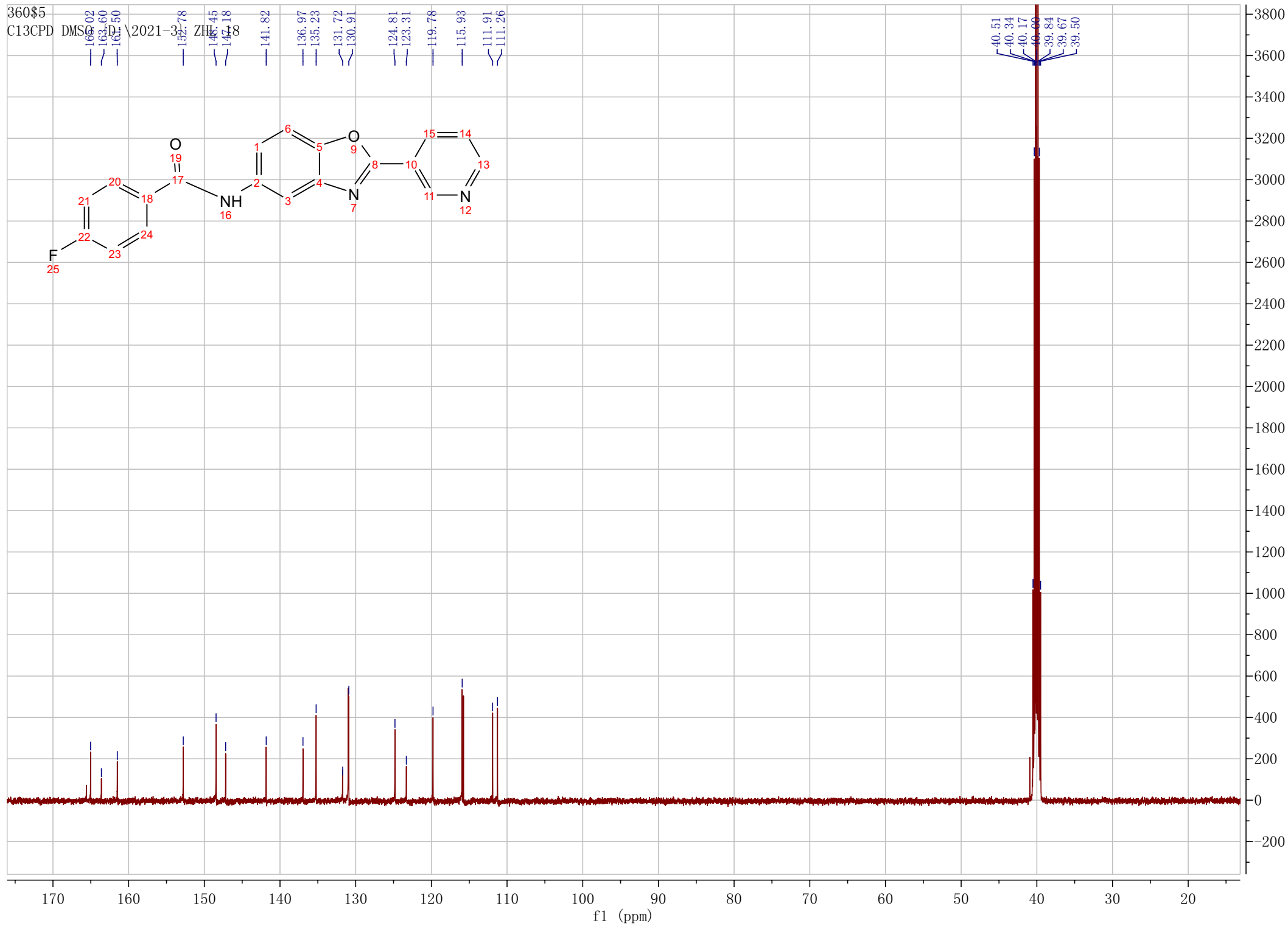
{163.73, 163.39, 162.54, 158.21-3}  
158.81  
148.47  
147.27  
141.83  
137.65  
136.78  
135.21  
131.12  
124.79  
124.42  
123.28  
119.78  
119.10  
115.11  
111.95  
111.31

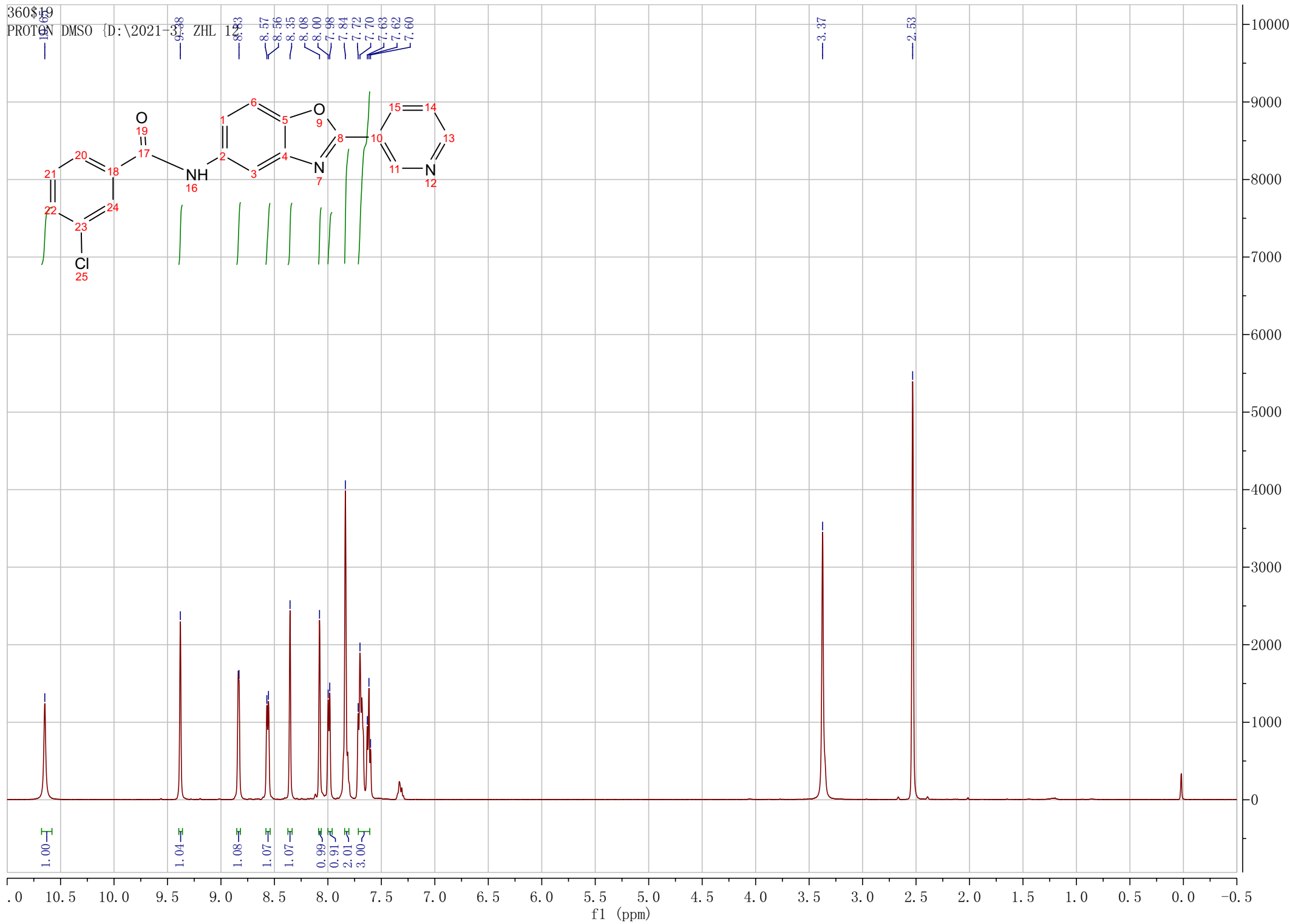


40.51  
40.34  
40.17  
40.01  
39.84  
39.67  
39.51







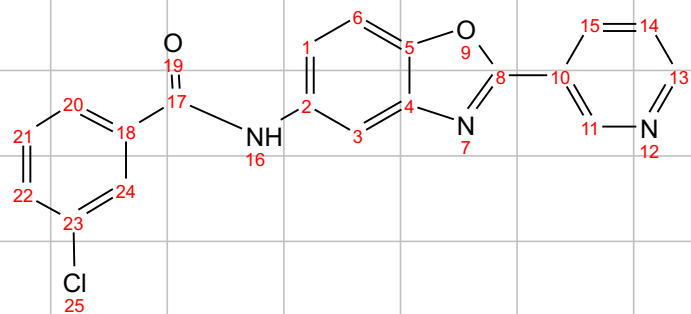


360\$20

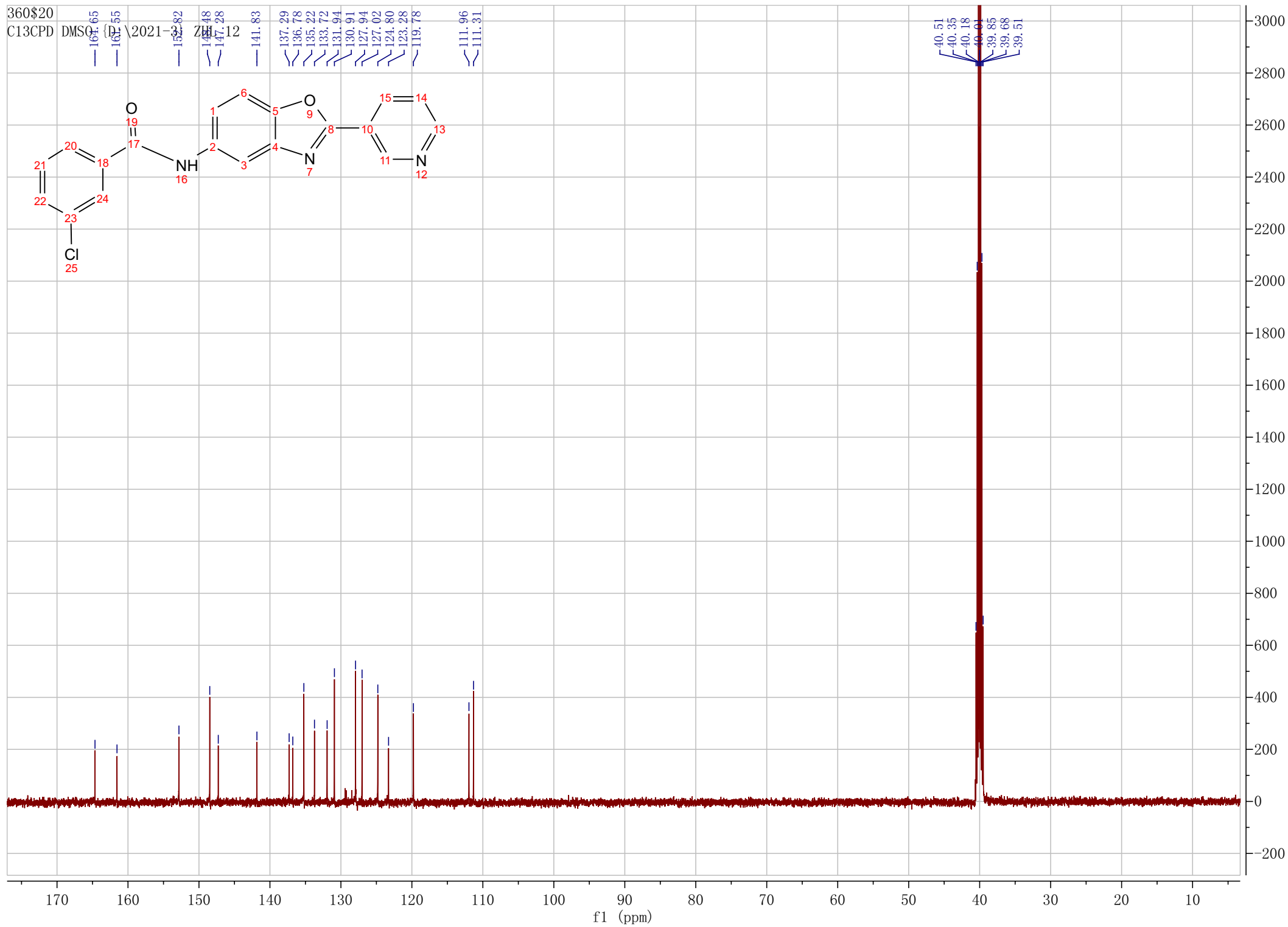
C13CPD

DMSO-d<sub>6</sub> 2021-3-11 ZHL-12

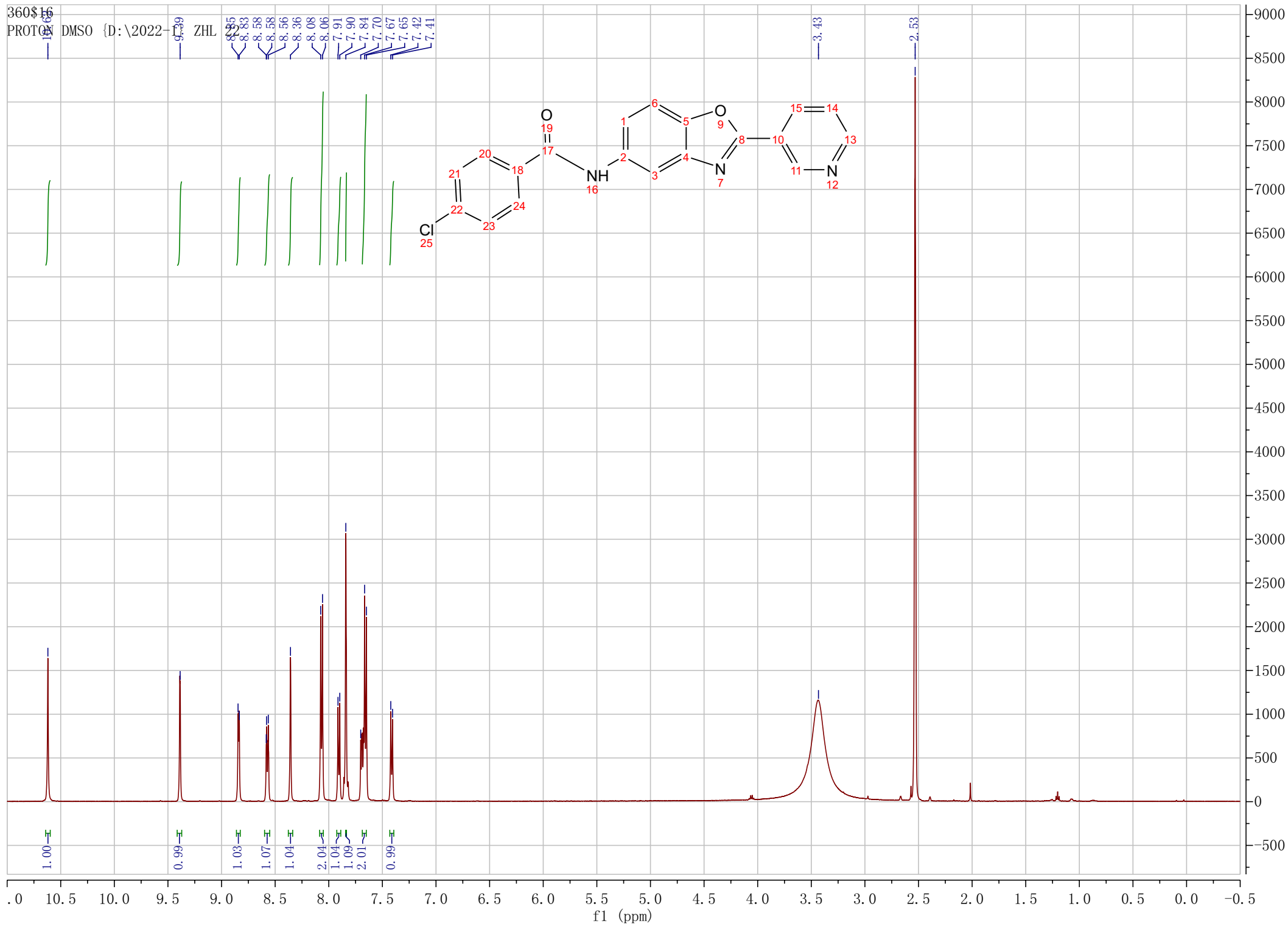
161.65	161.55	153.82	148.18	147.28	141.83	137.29	136.78	135.22	133.72	131.94	130.91	127.94	127.02	124.80	123.28	119.78	111.96	111.31
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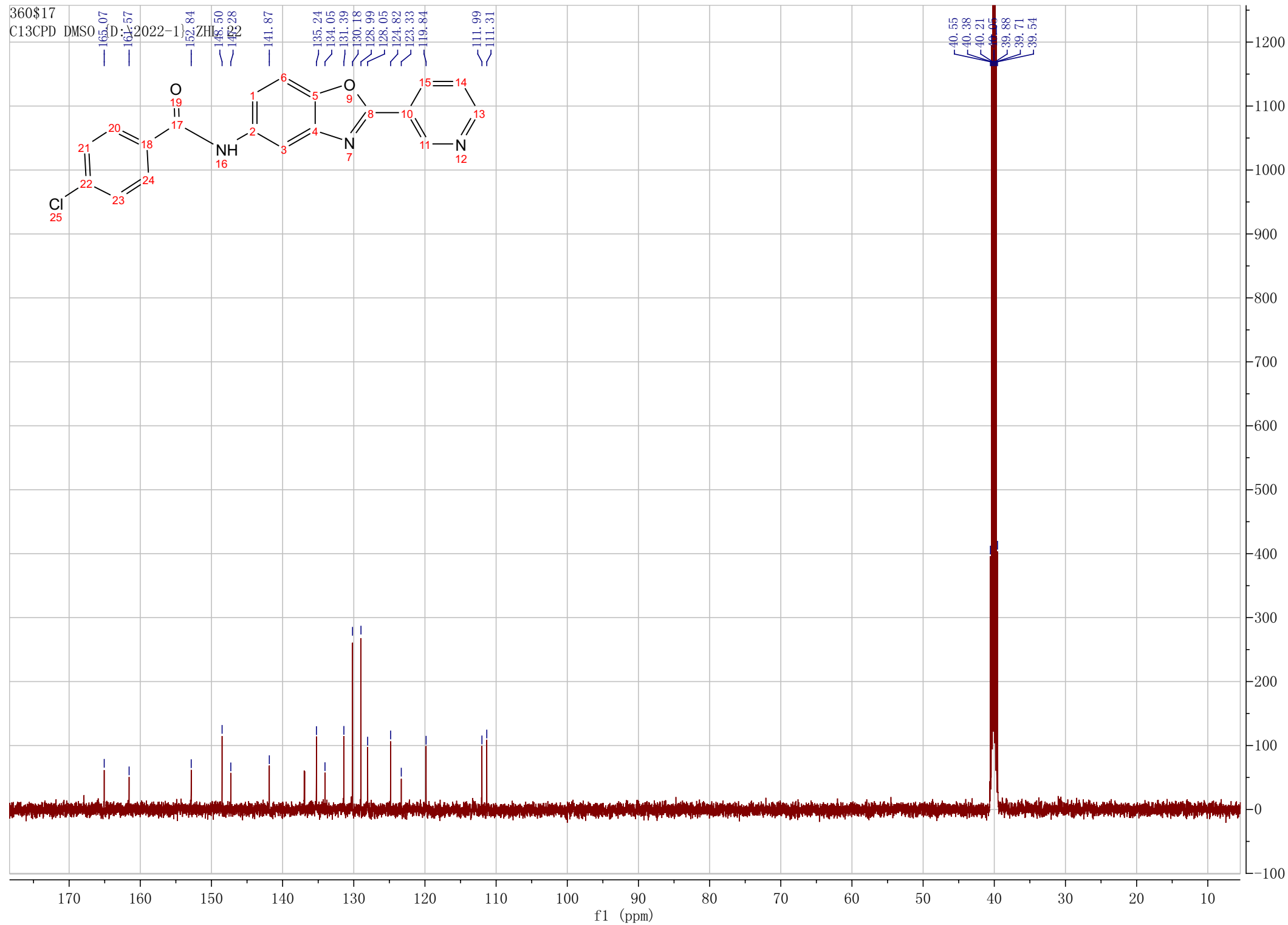


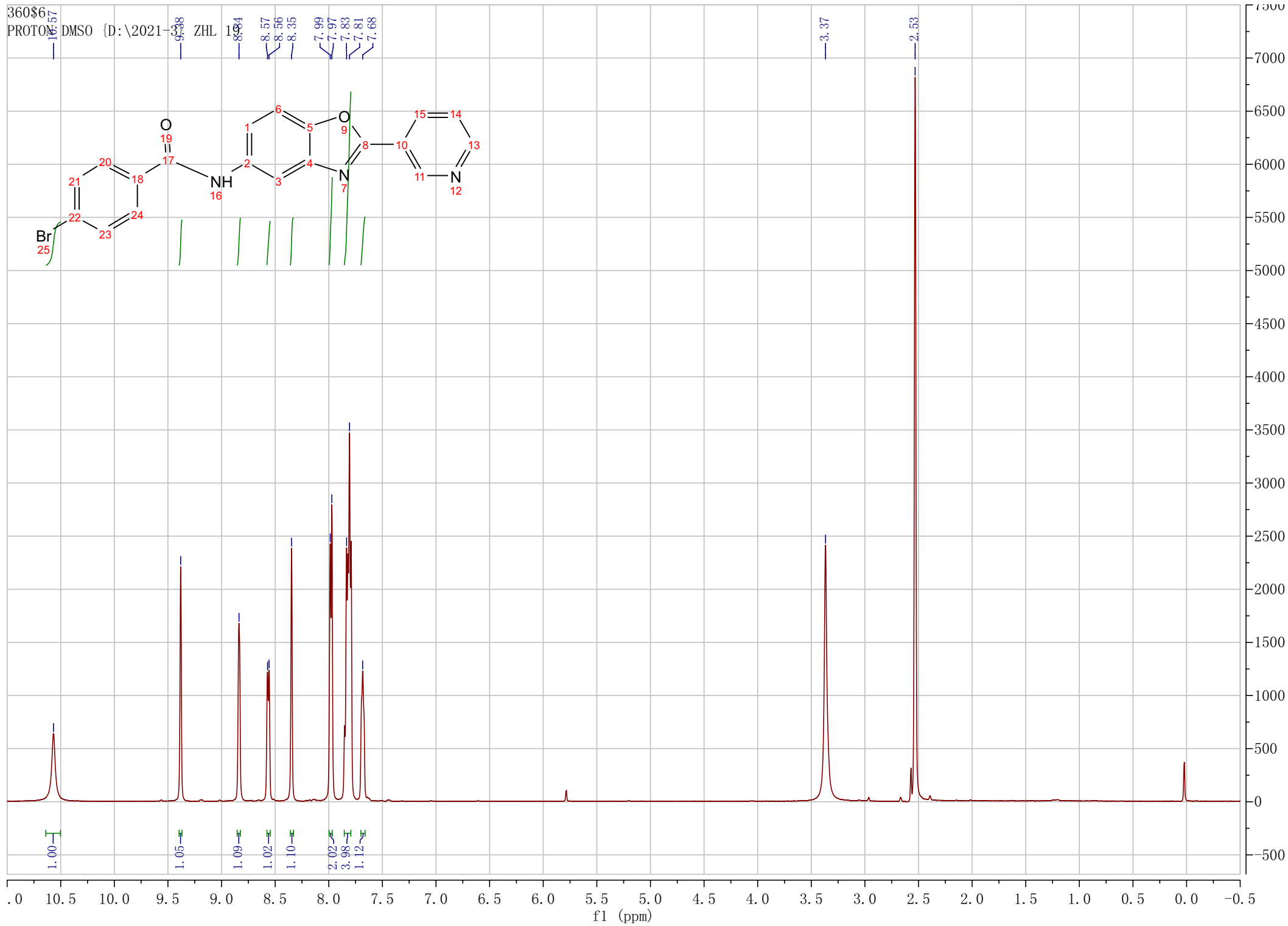
40.51	40.35	40.18	39.85	39.68	39.51
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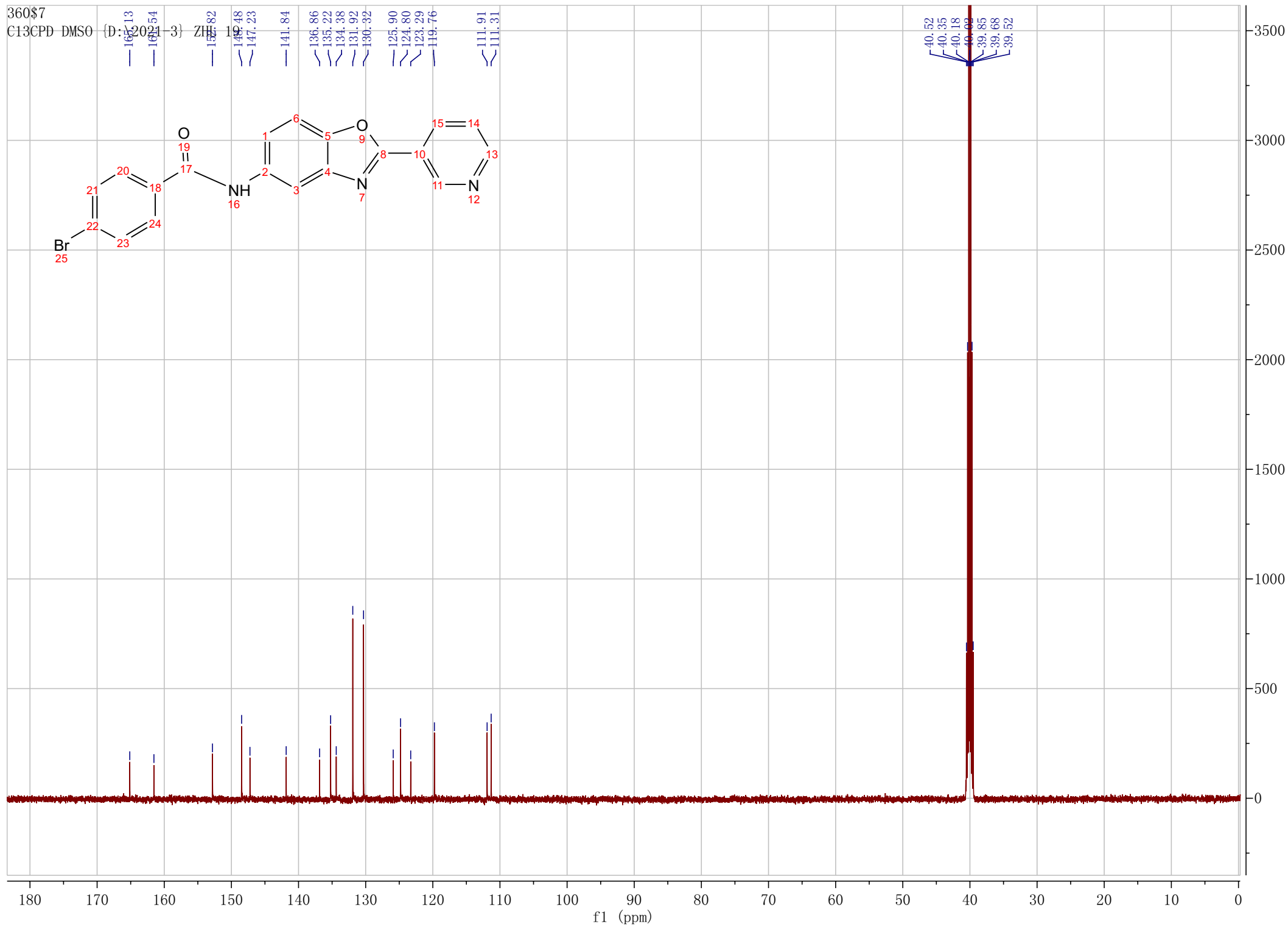
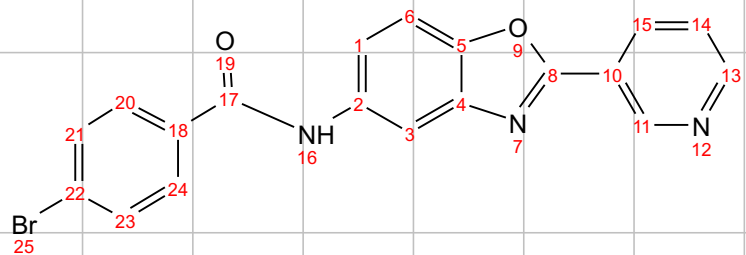




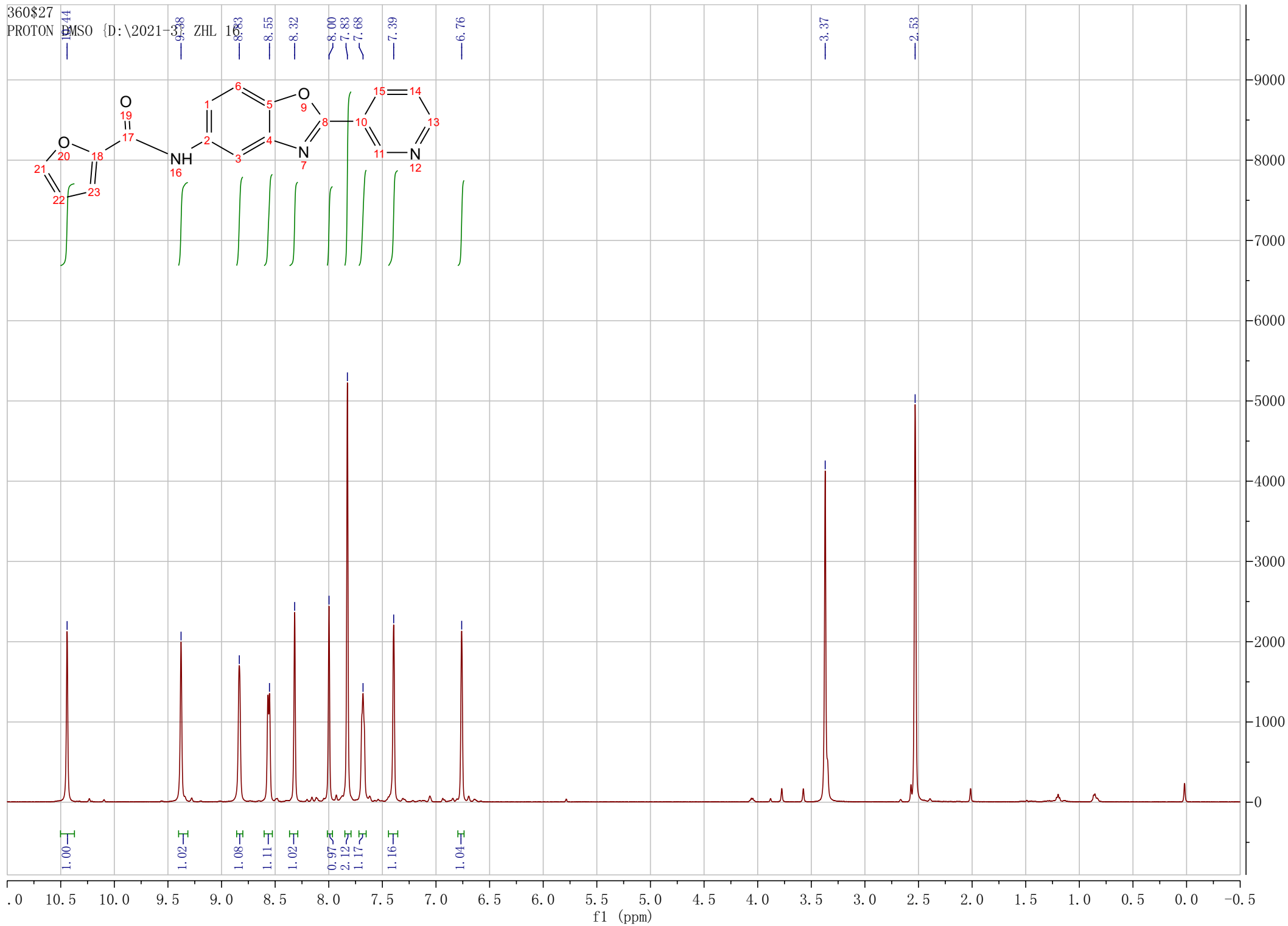


360\$7

C13CPD DMSO {D:\2021-3} ZH-19

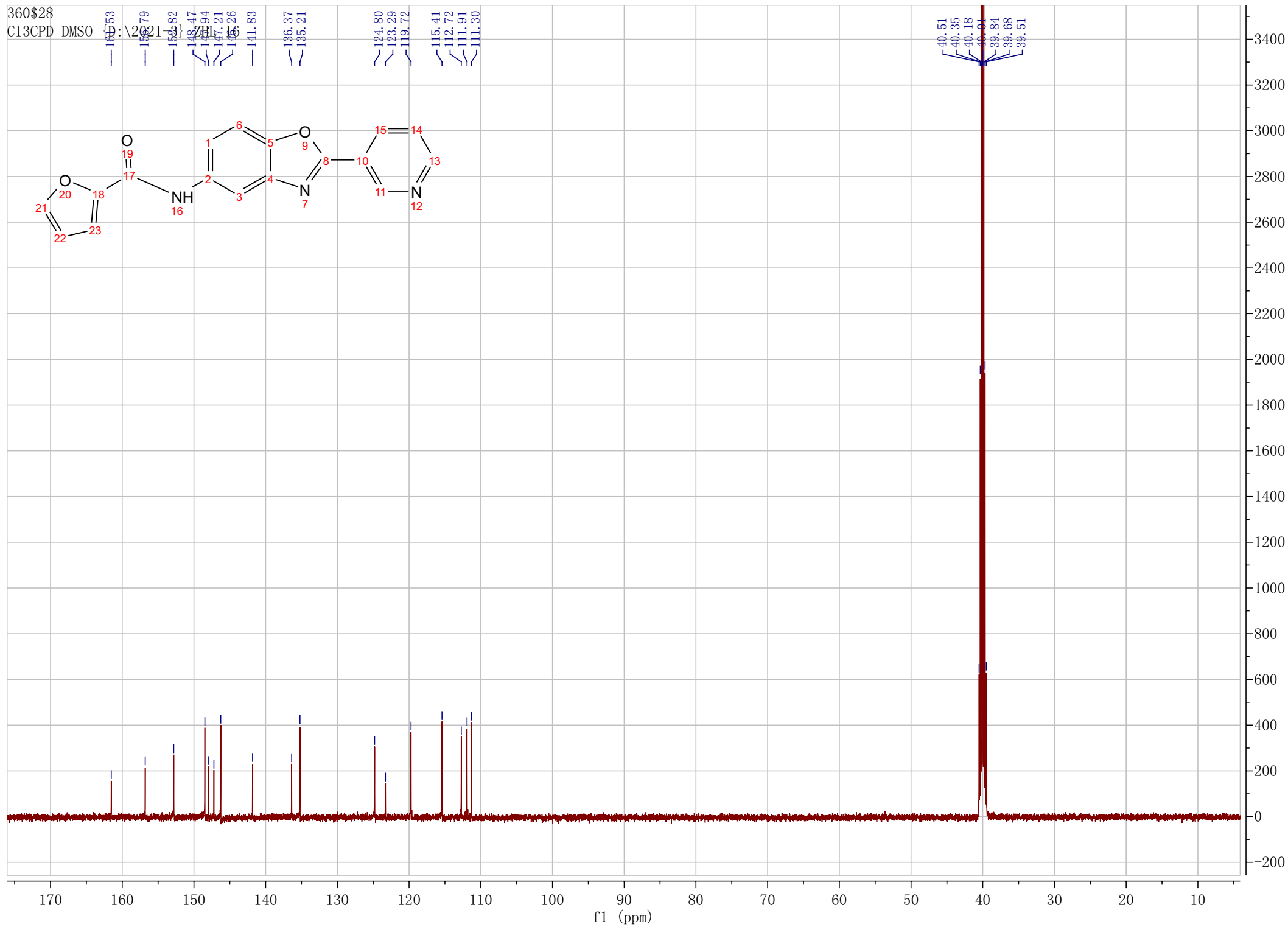


360\$27  
PROTON



360\$28

C13CPD DMSO

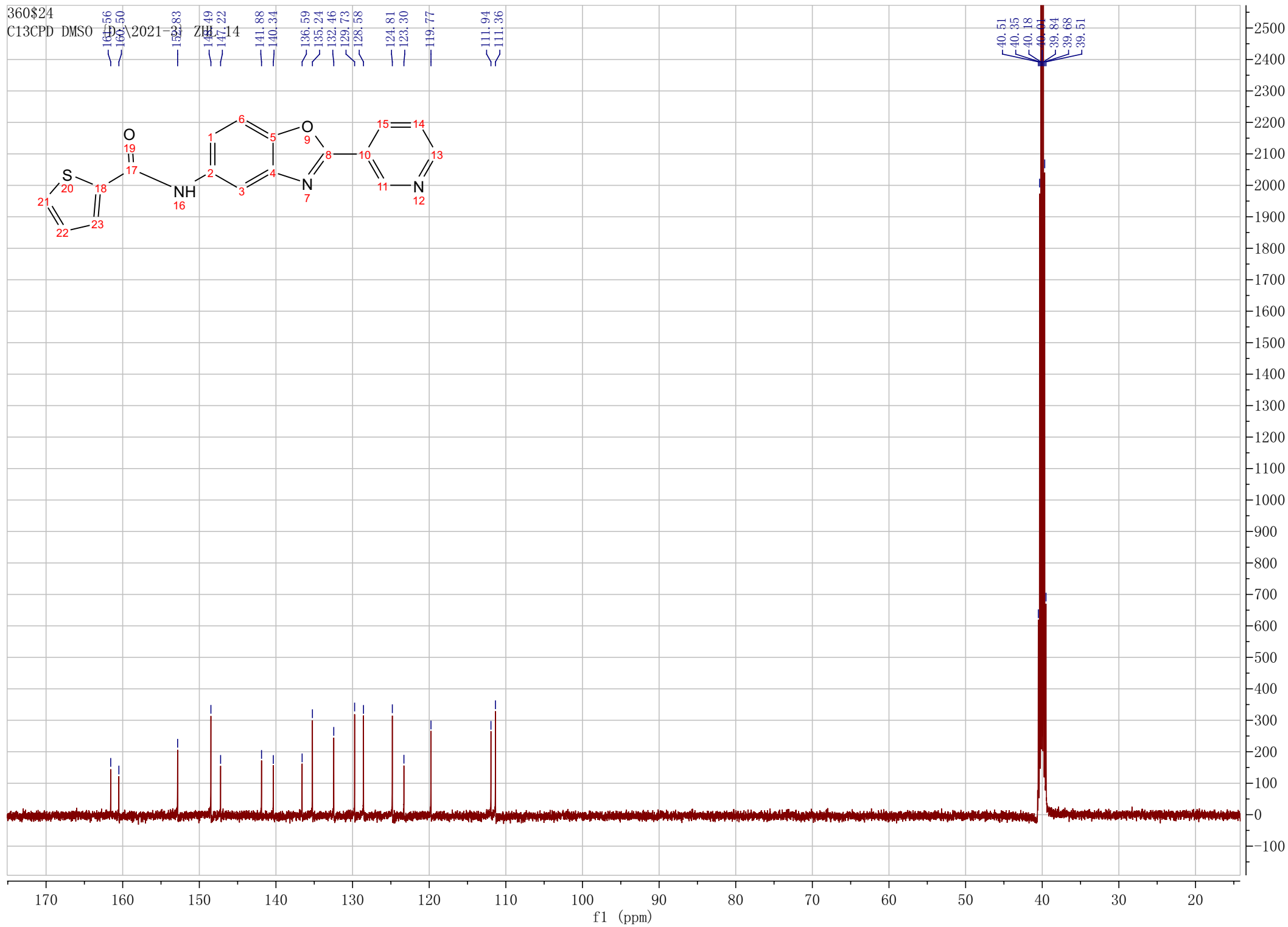
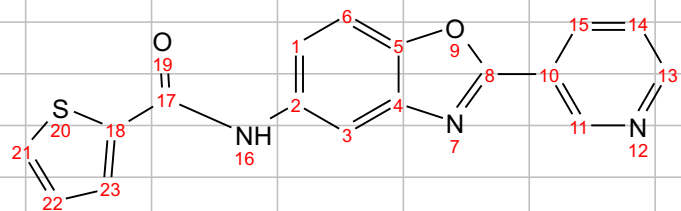




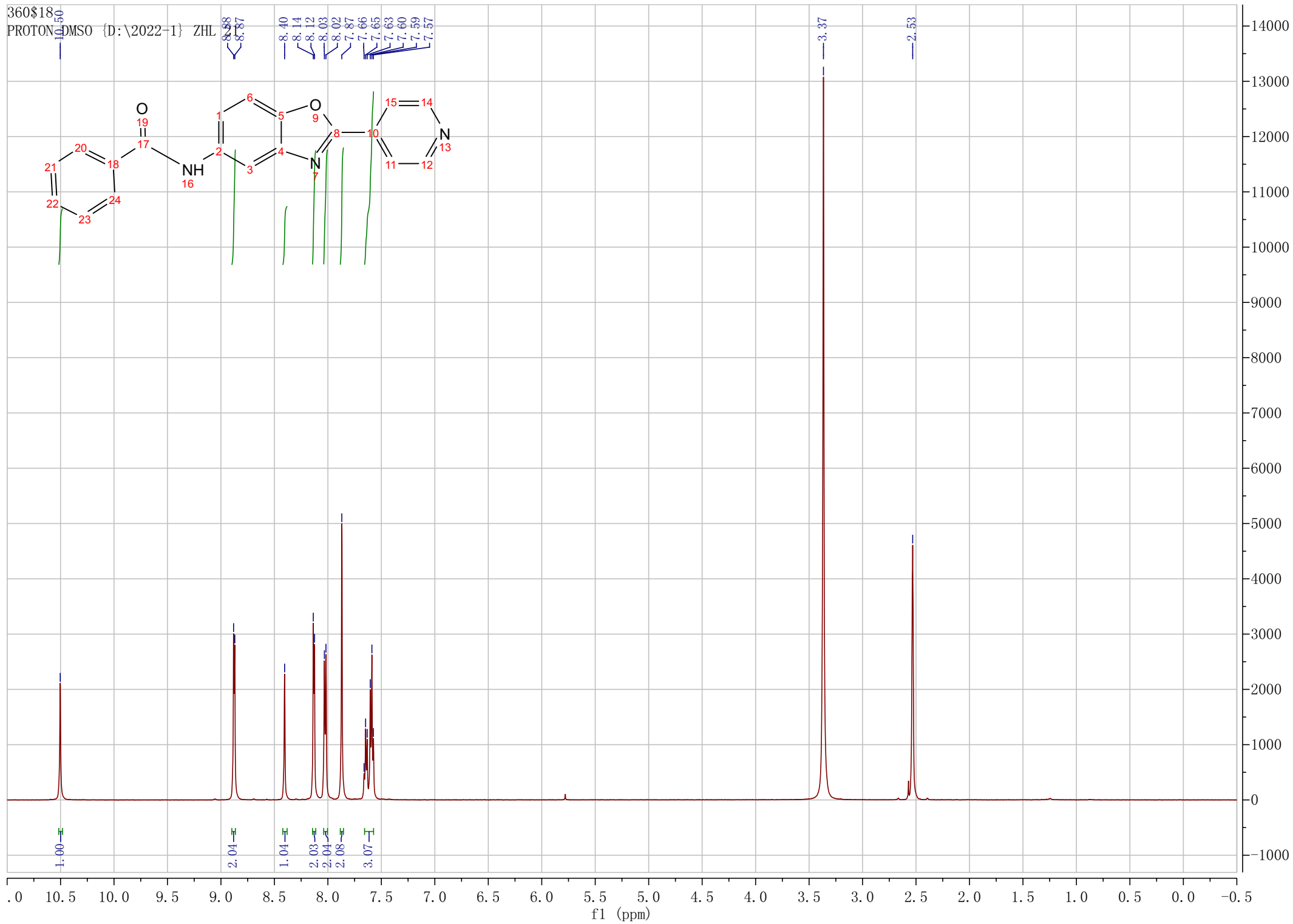
360\$24

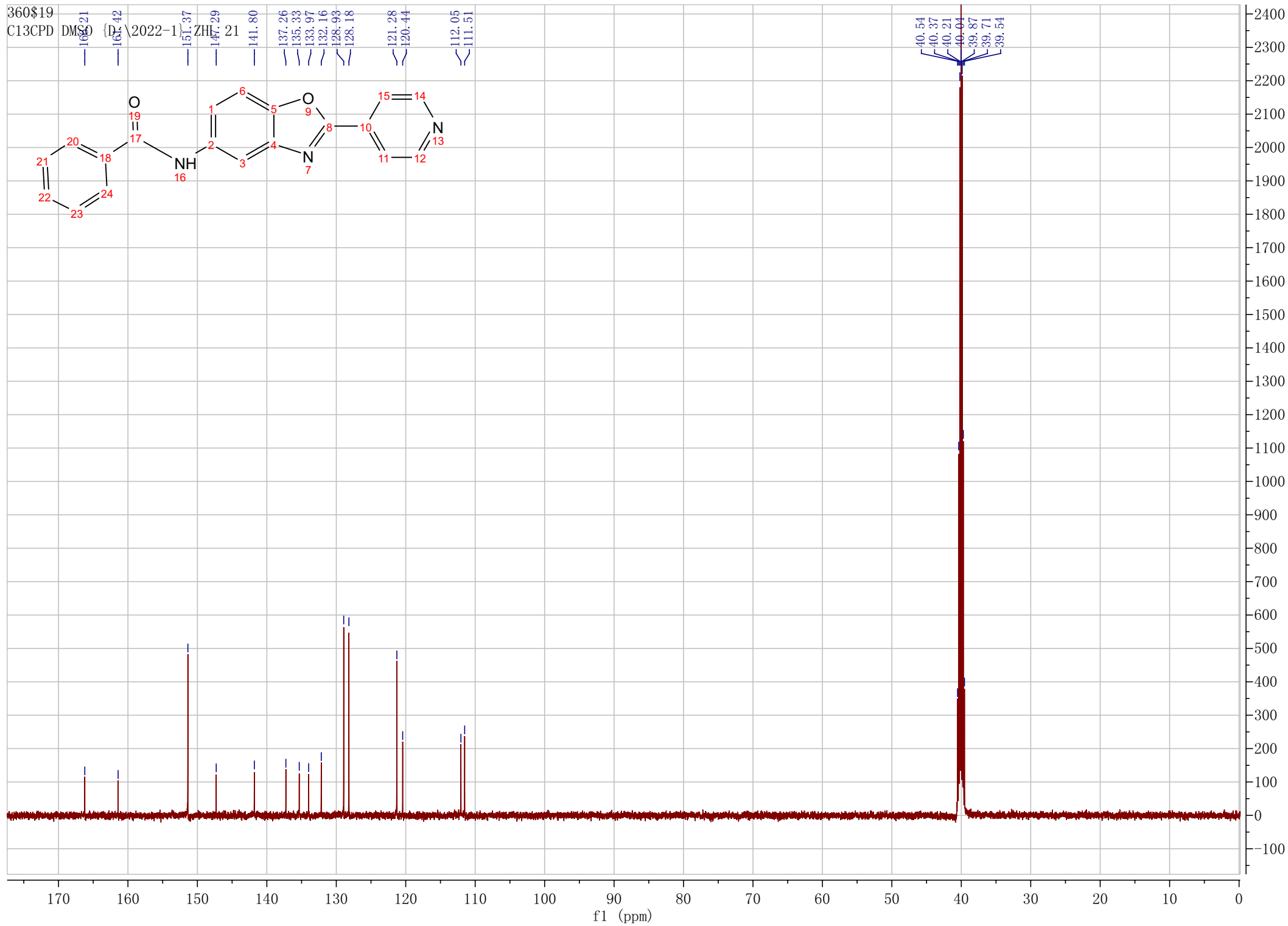
C13CPD DMSO

D-2021-21 ZH



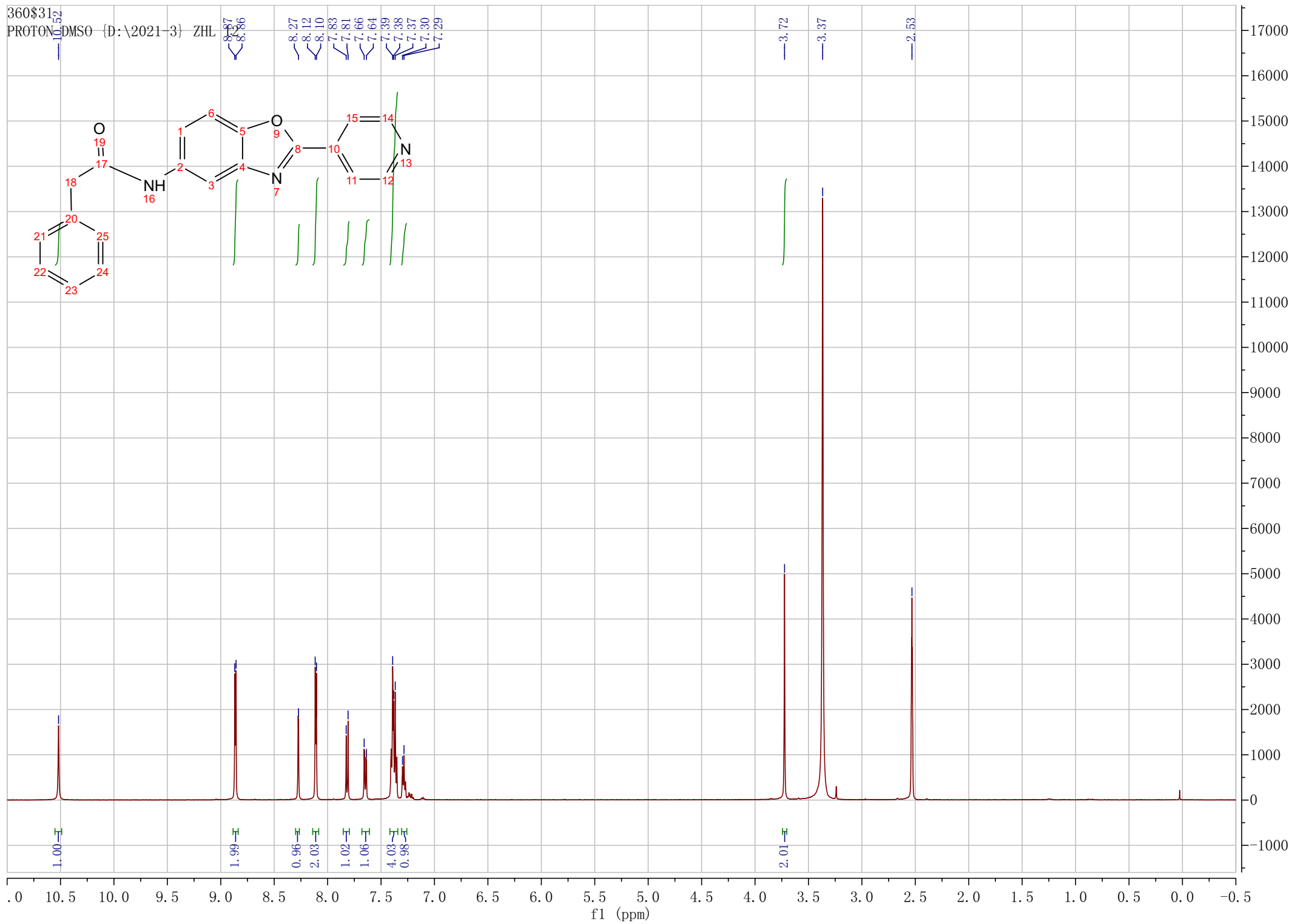






360\$31

PROTON DMSO-{D:\2021-3}-ZHL



360\$32

C13CPD DMSO {D:\2021-3}

ZHE

126.93

141.85

137.39

136.38

133.94

129.67

128.82

127.06

121.26

119.15

111.68

110.62

43.78

40.52

40.36

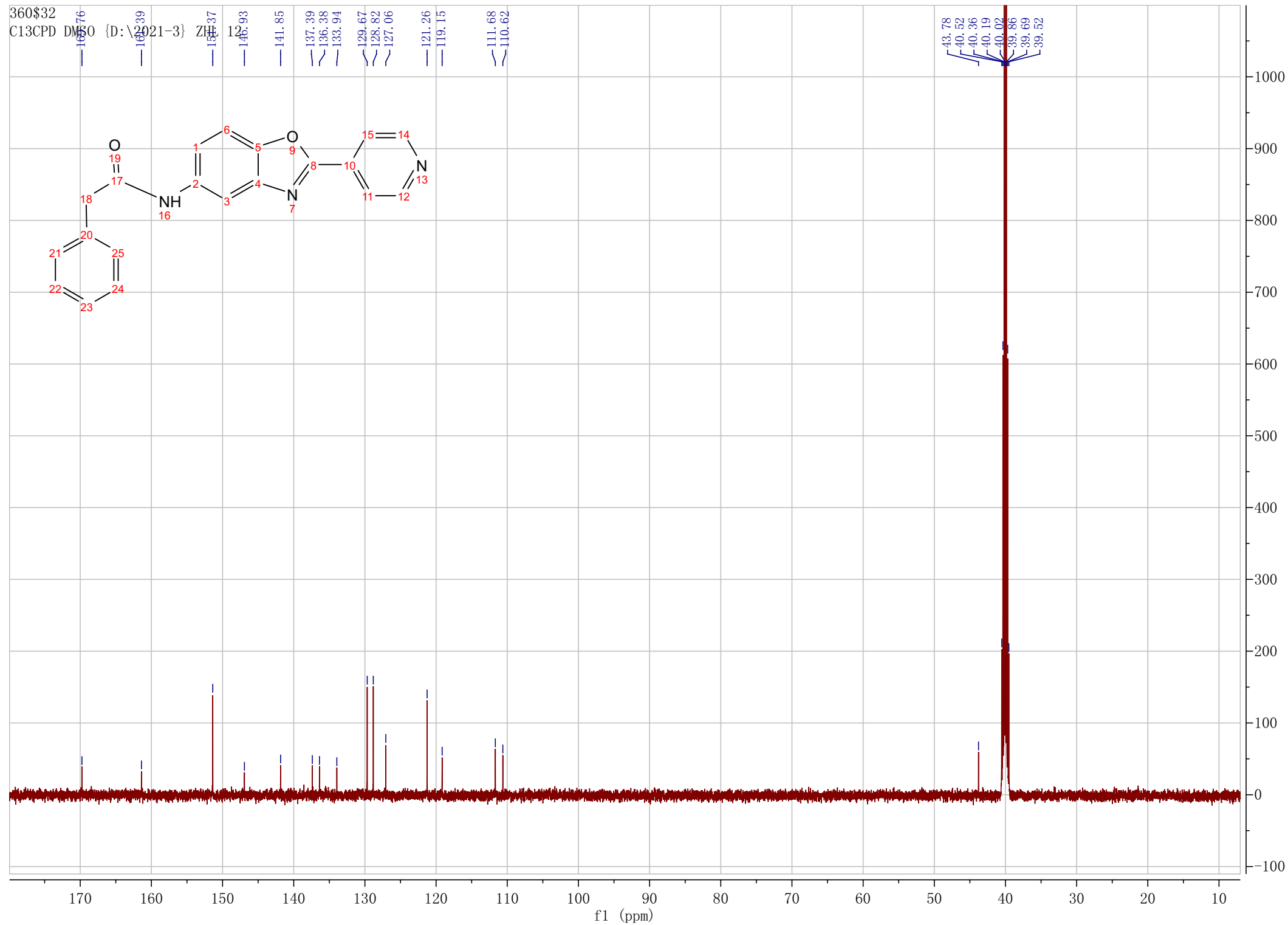
40.19

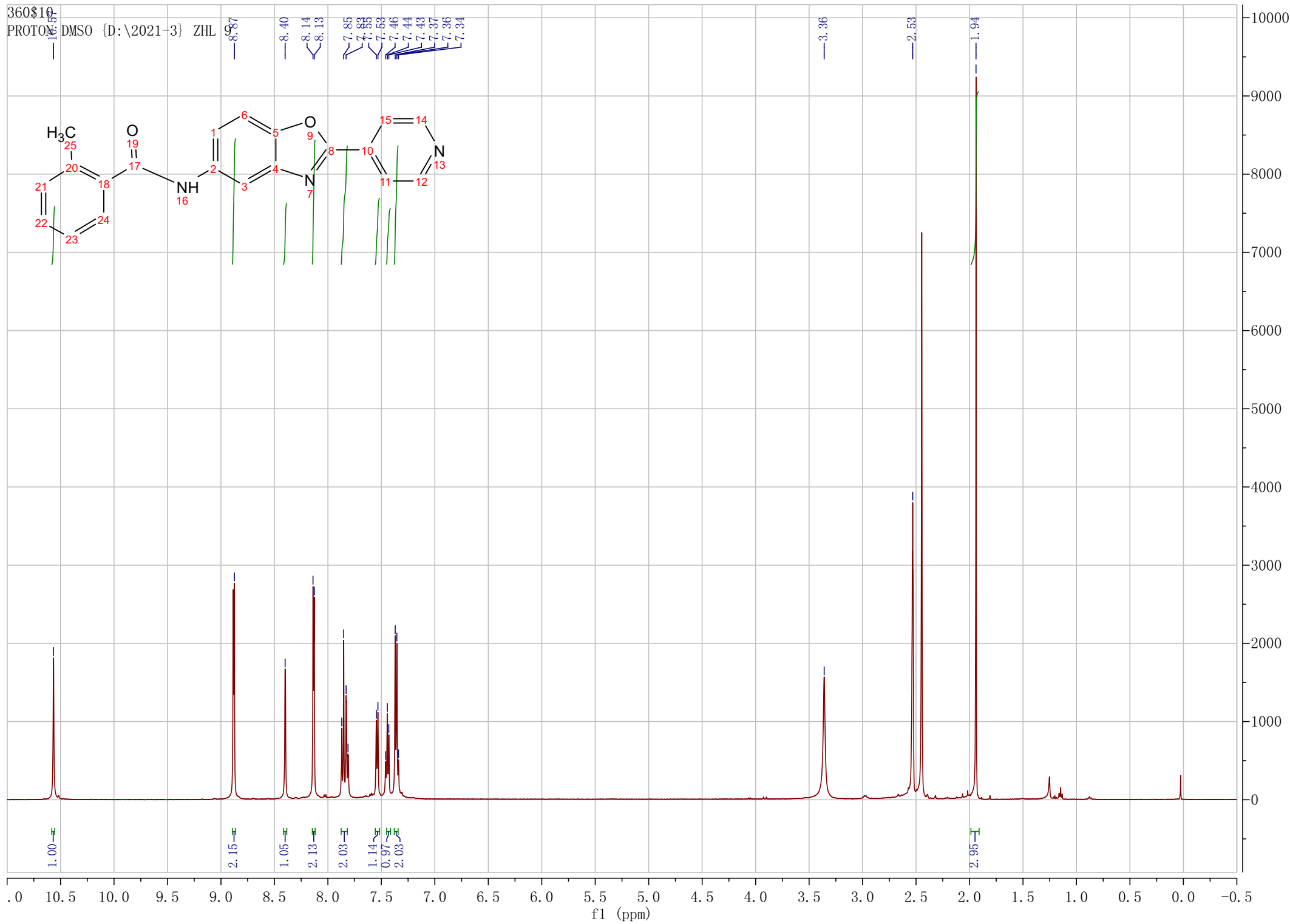
40.02

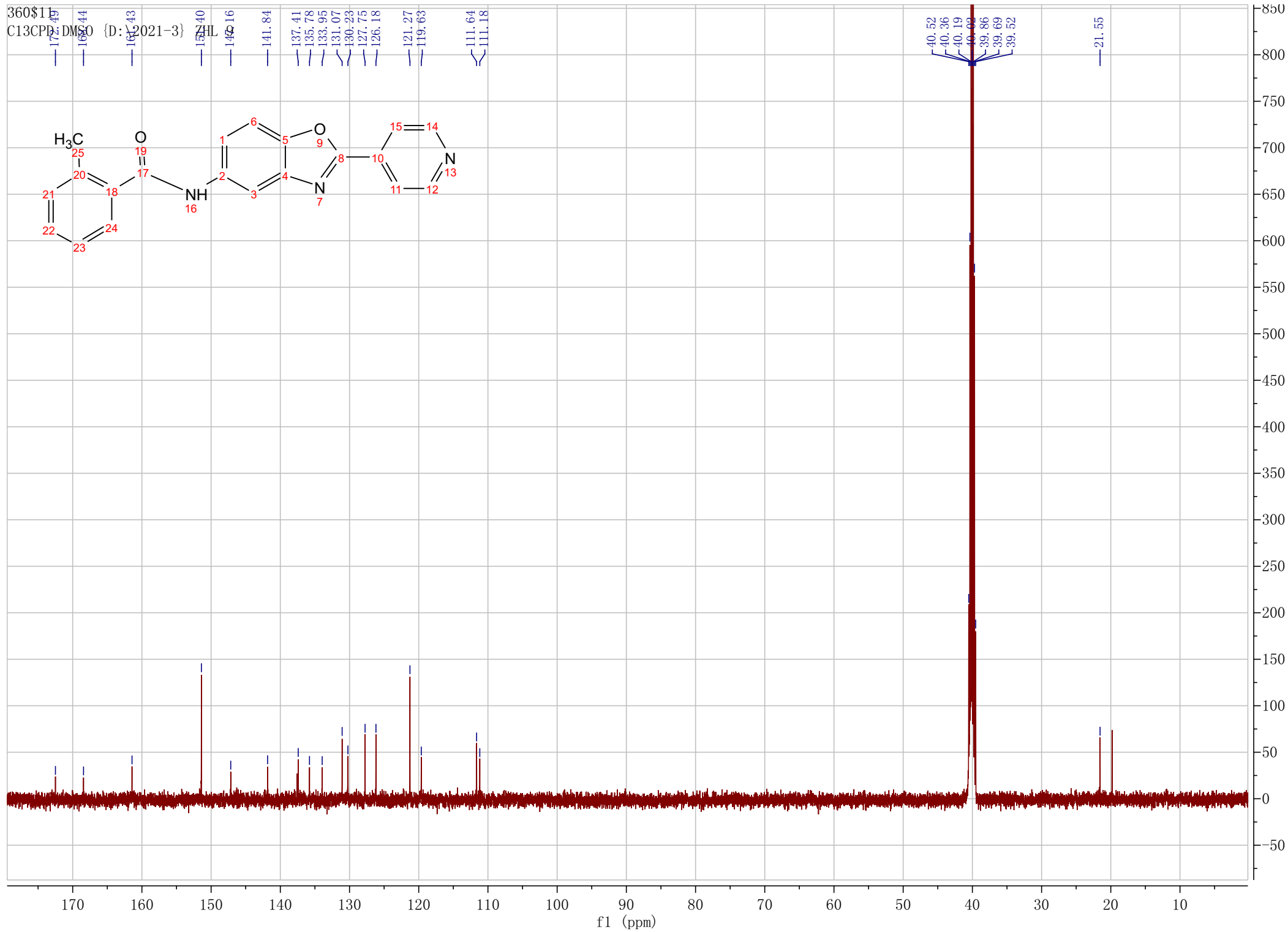
39.86

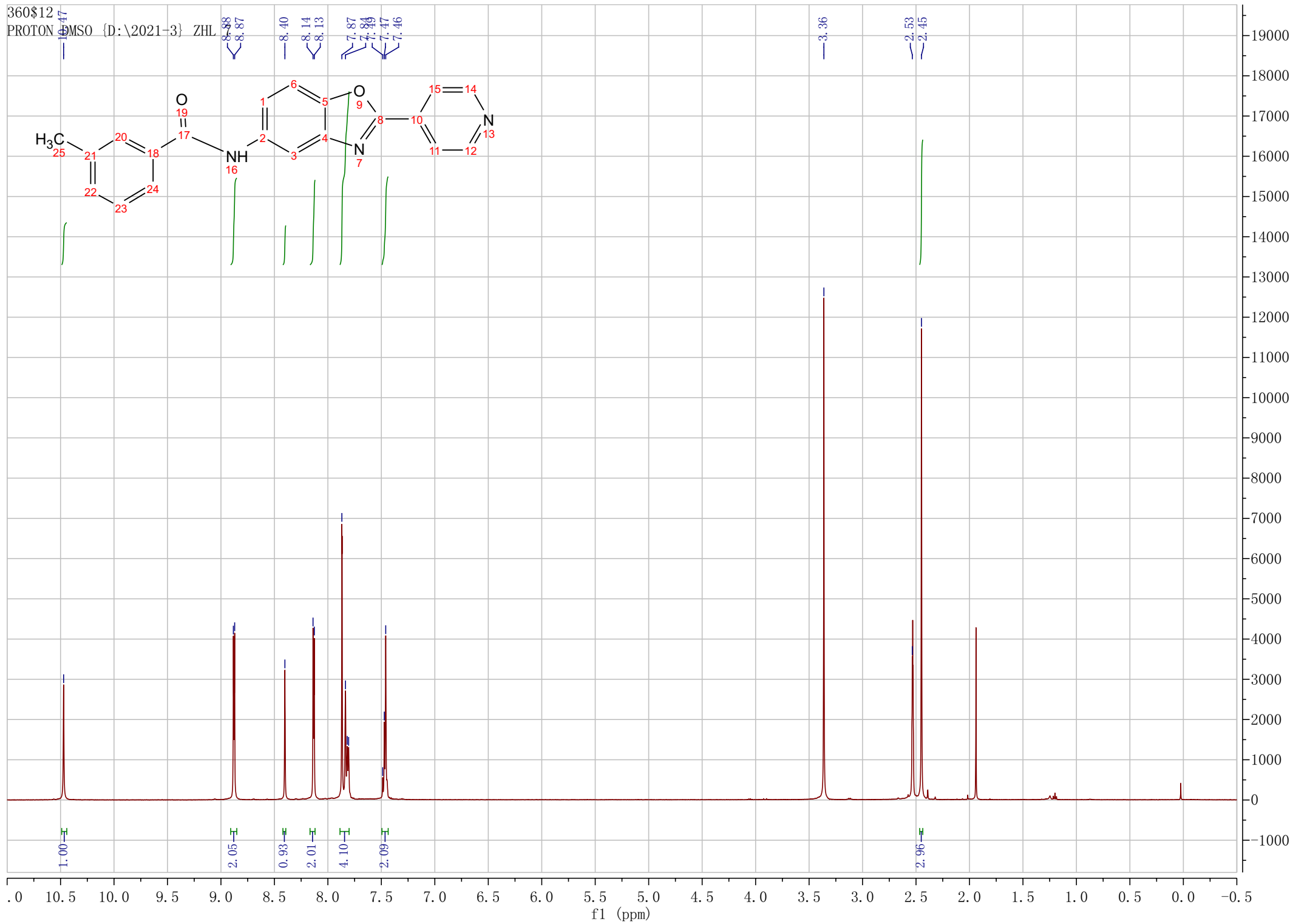
39.69

39.52

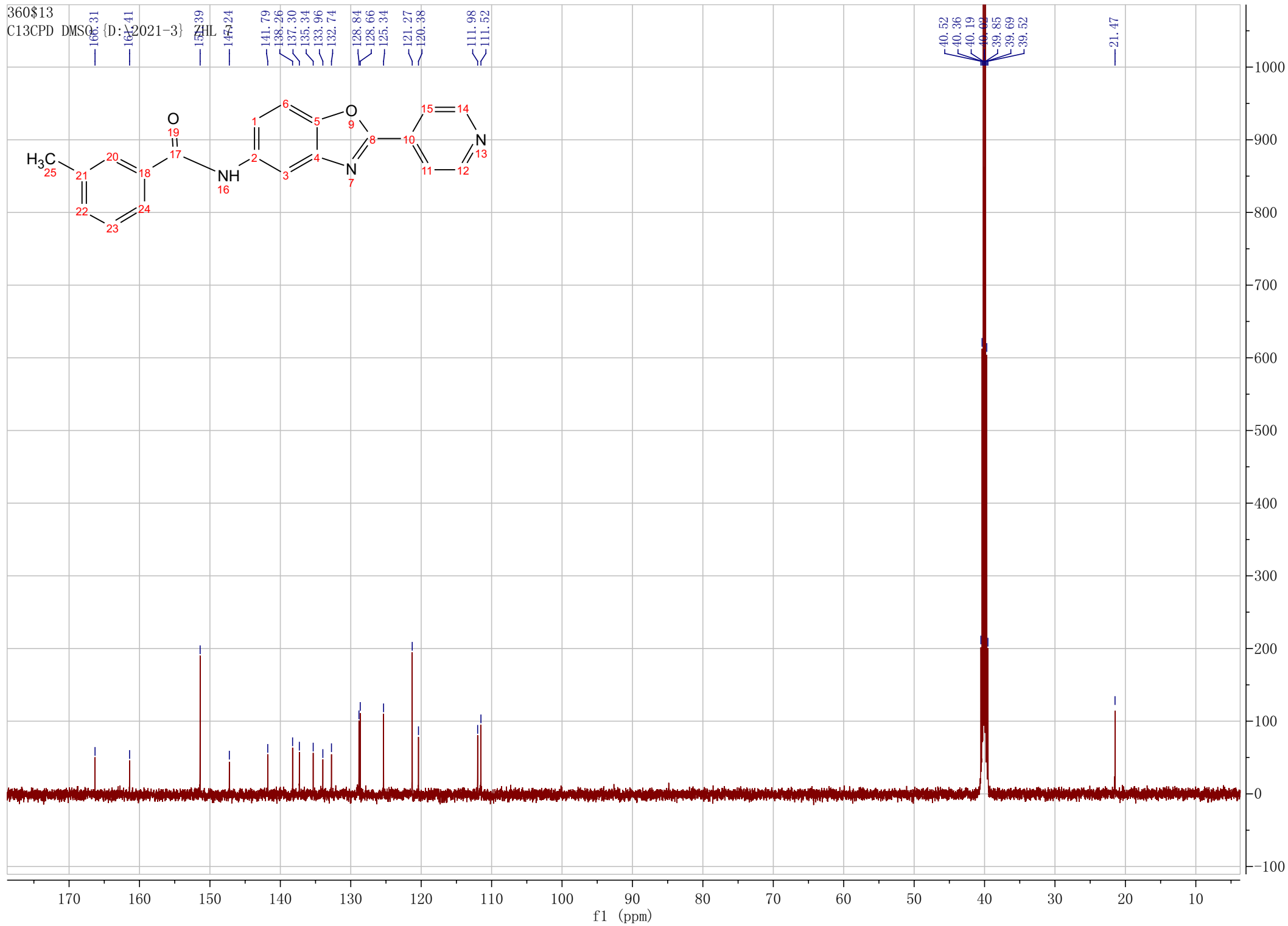




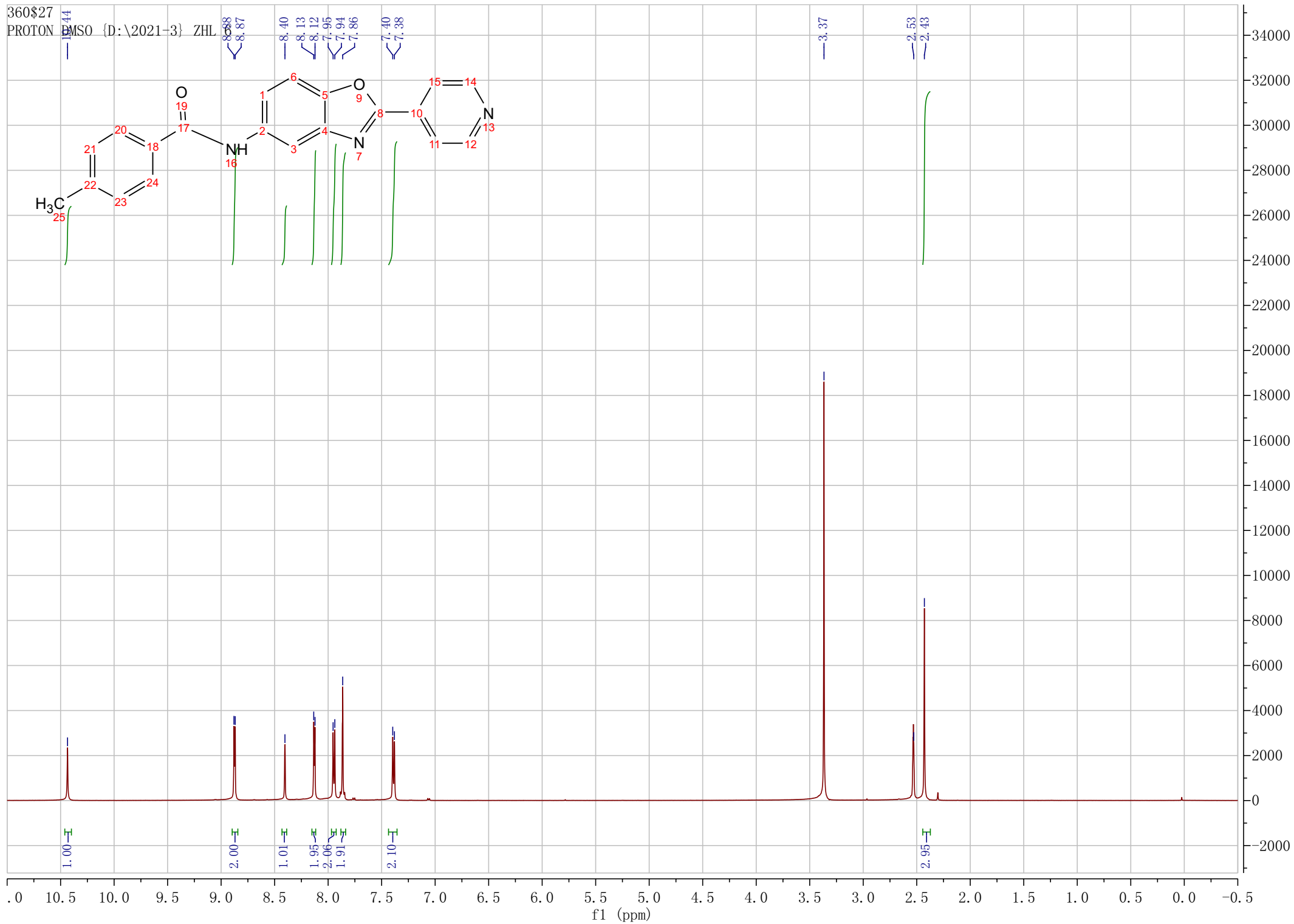




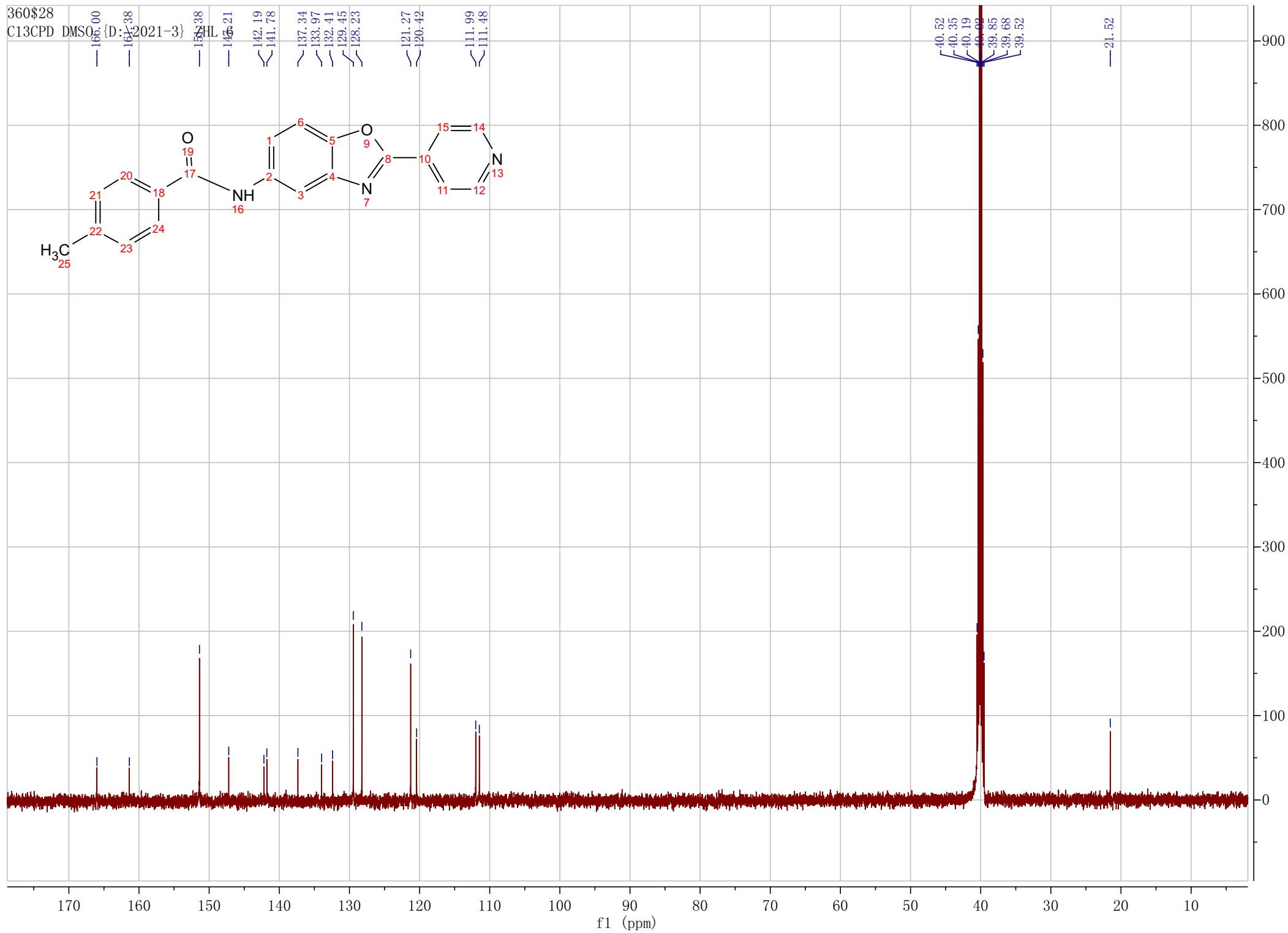
360\$13  
C13CPD DMSO {D: 2021-3}

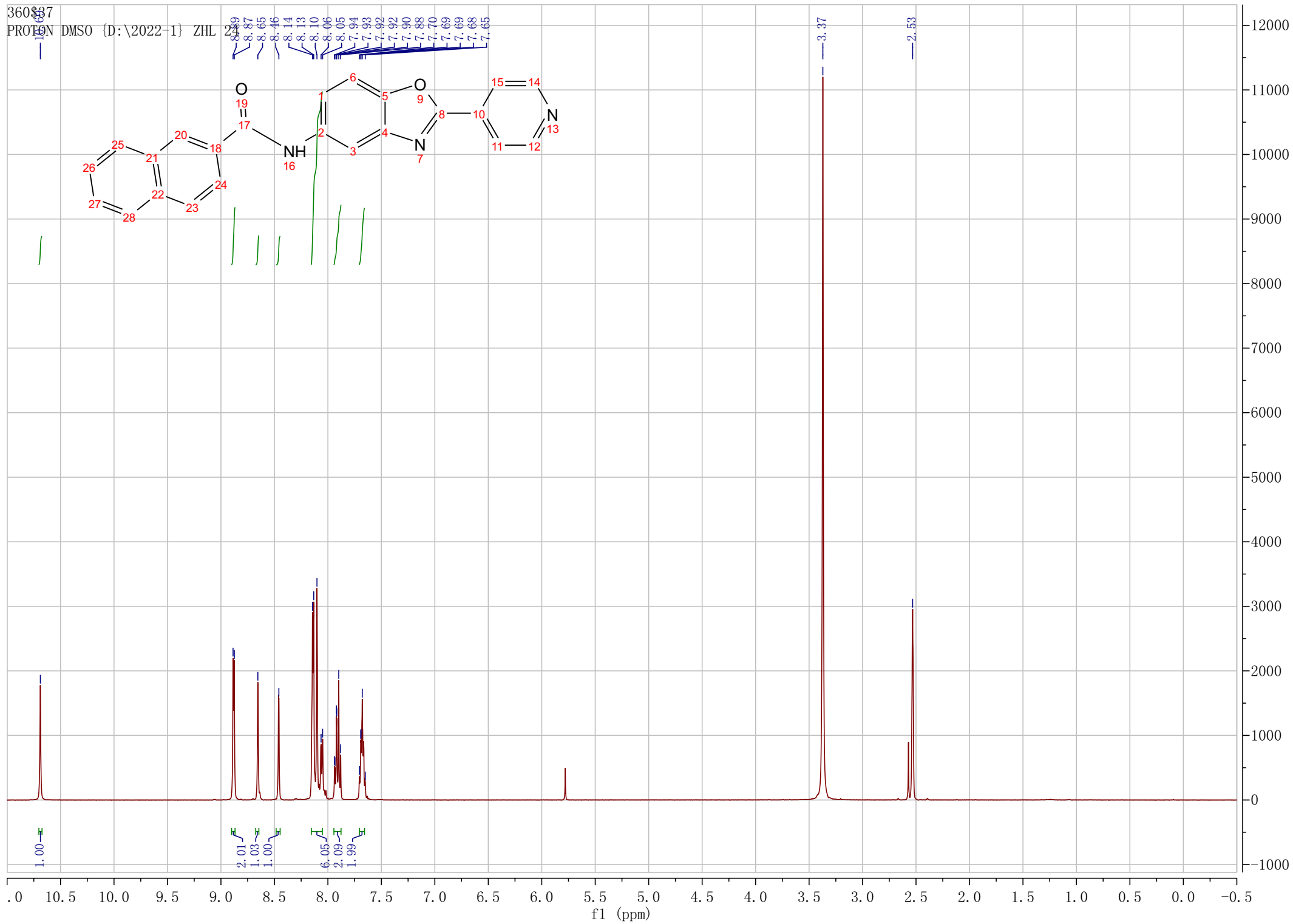






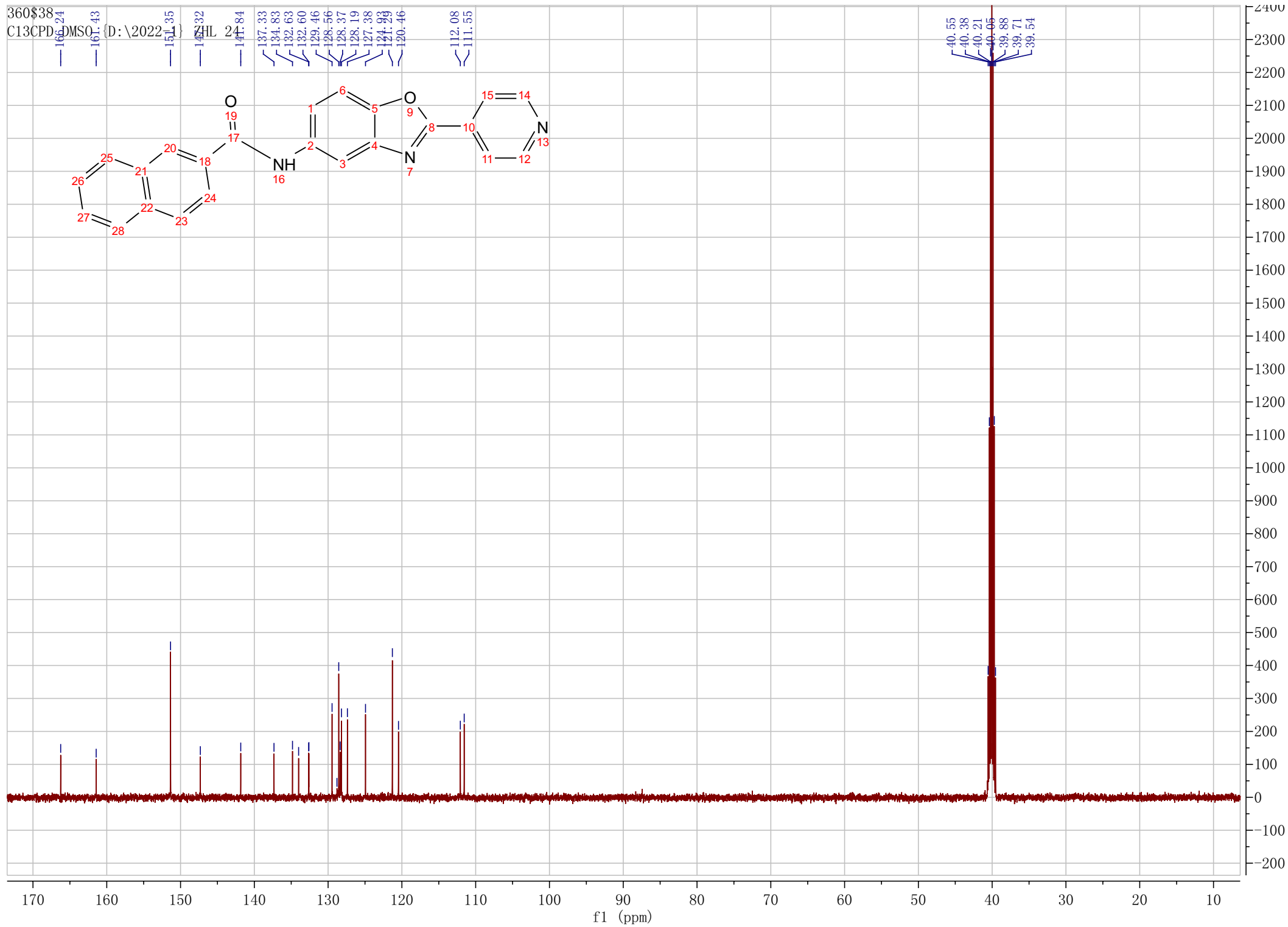
360\$28

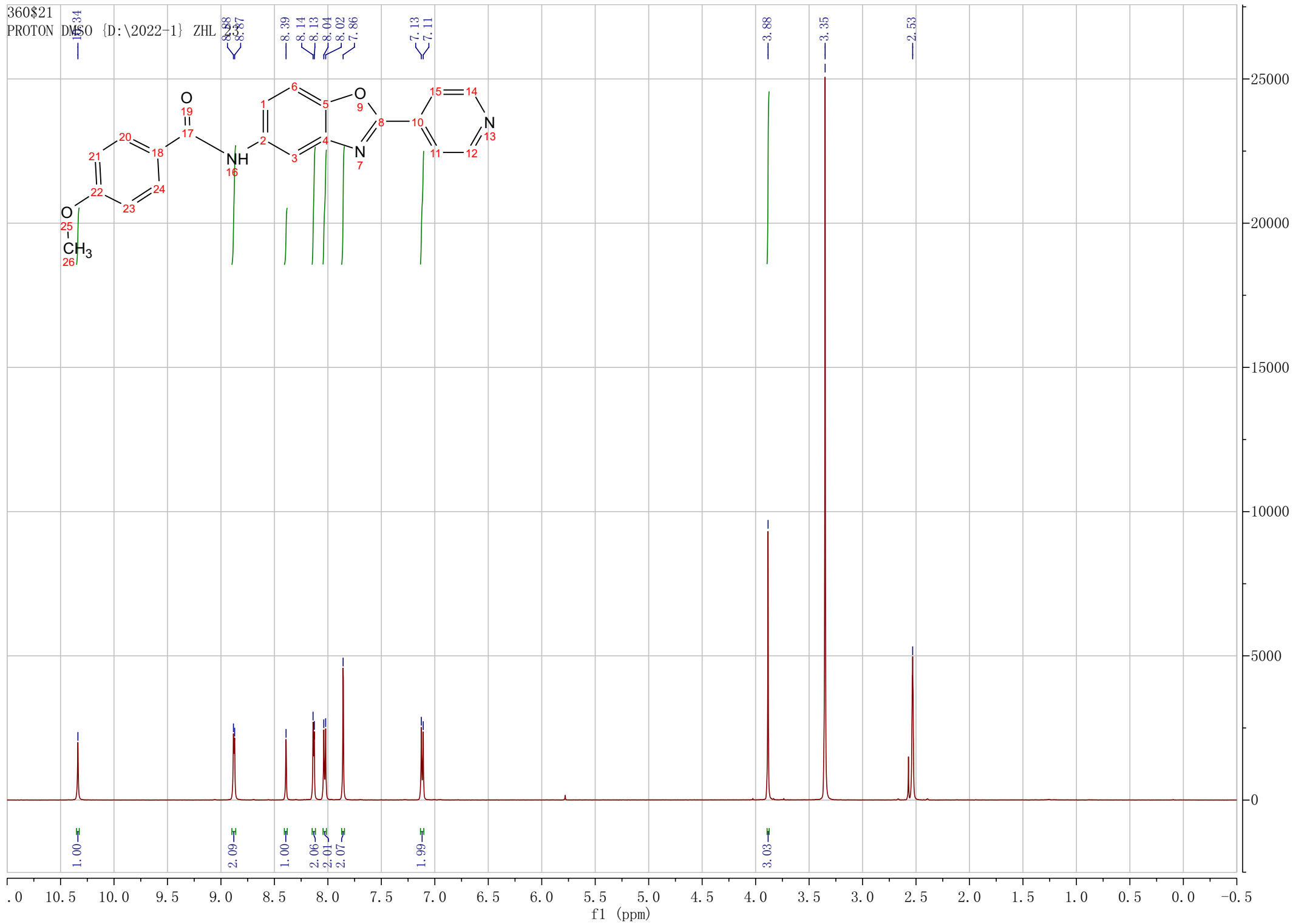
C13CPD DMSO-{D:<sub>6</sub>}-2021-3}

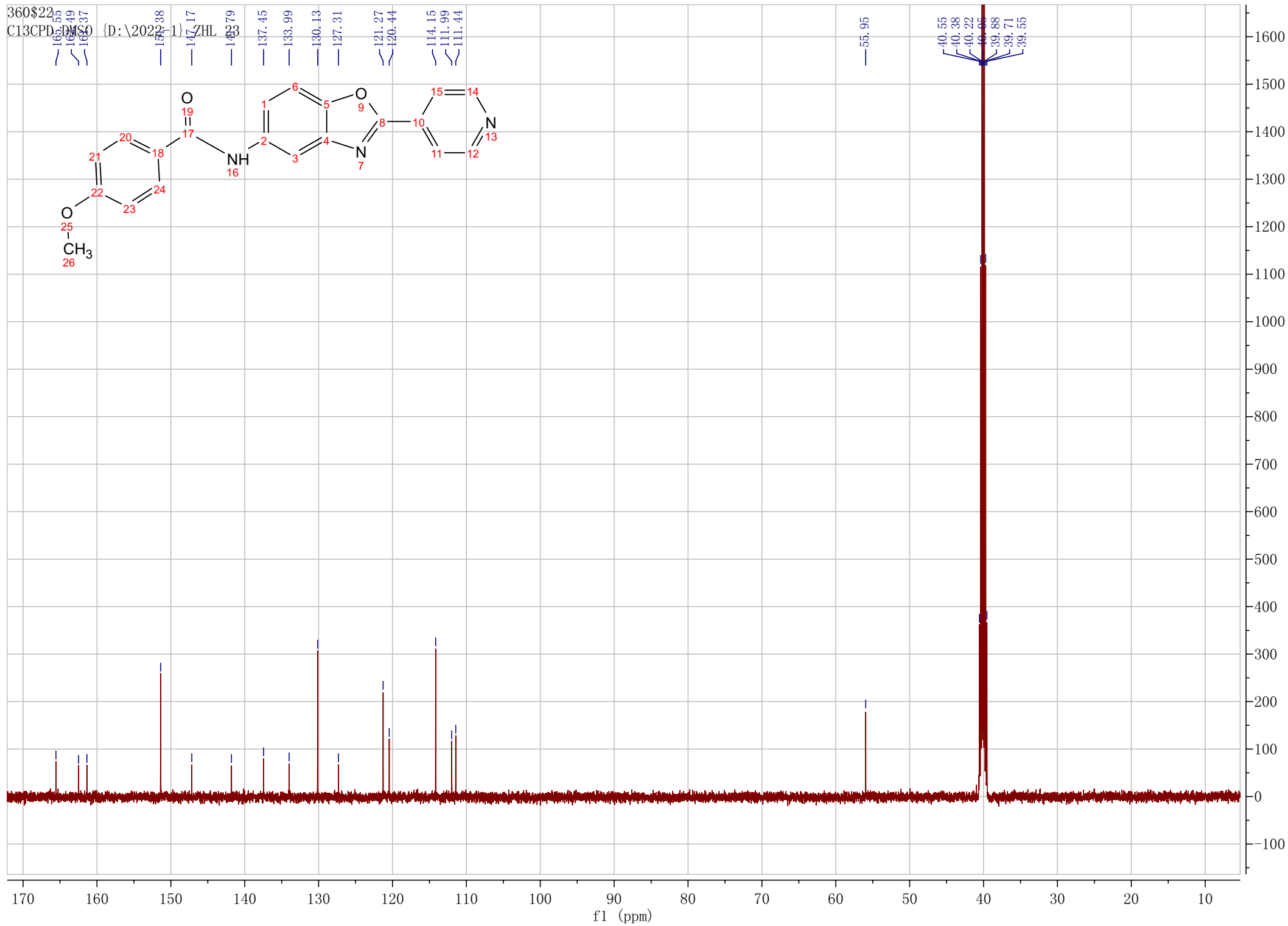


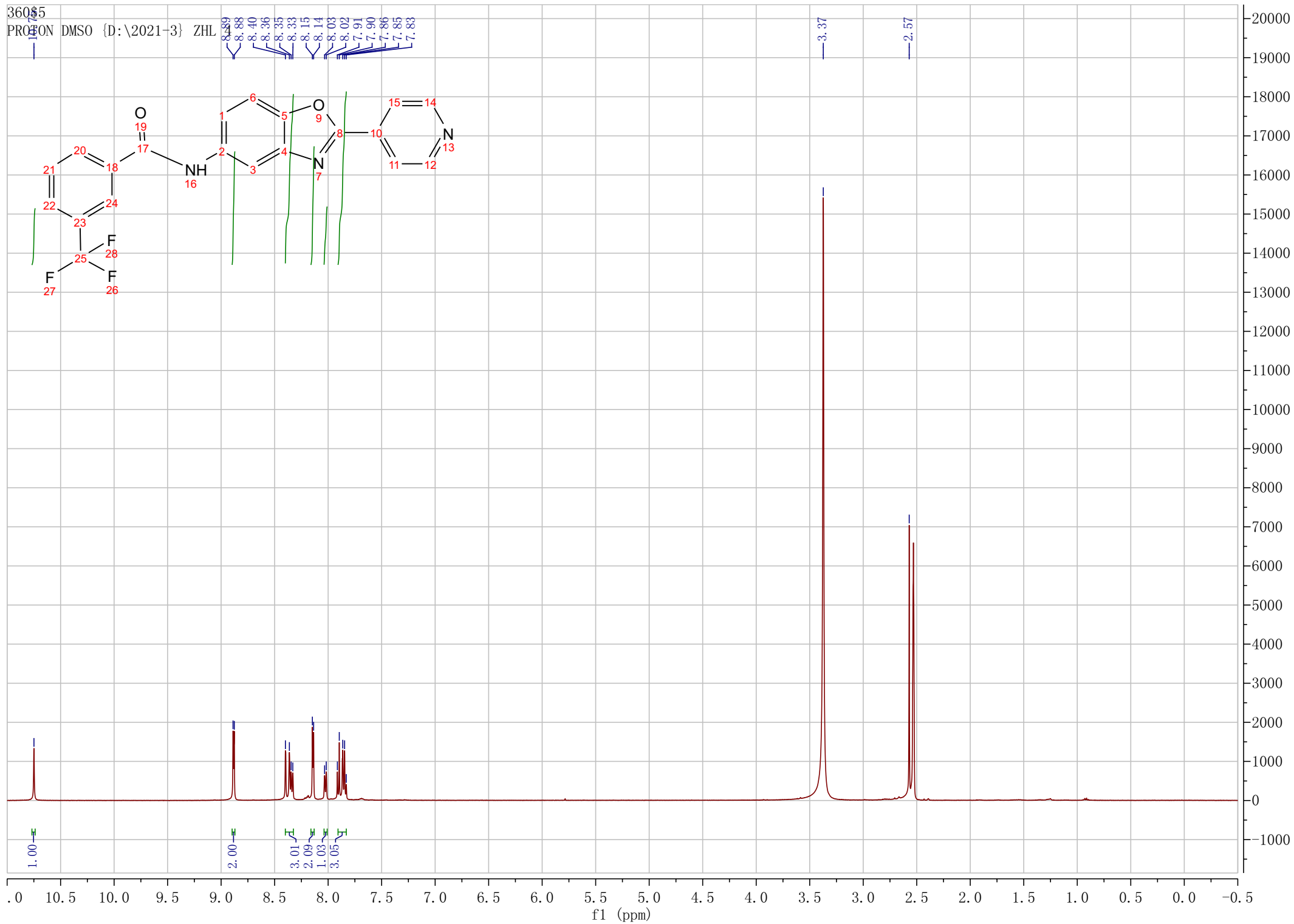
360\$38

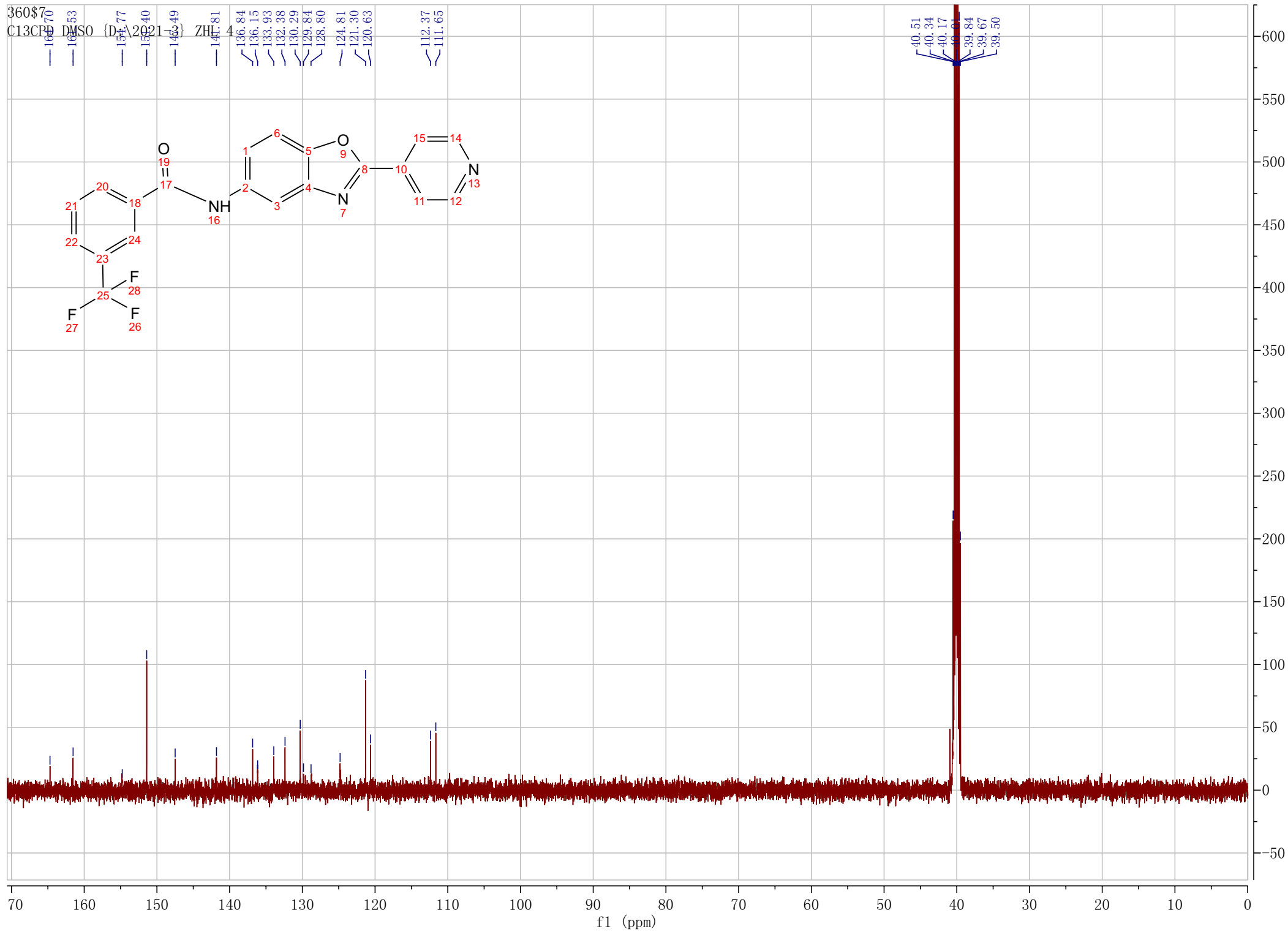
C13CPD.DMSO-{D:\2022\1}



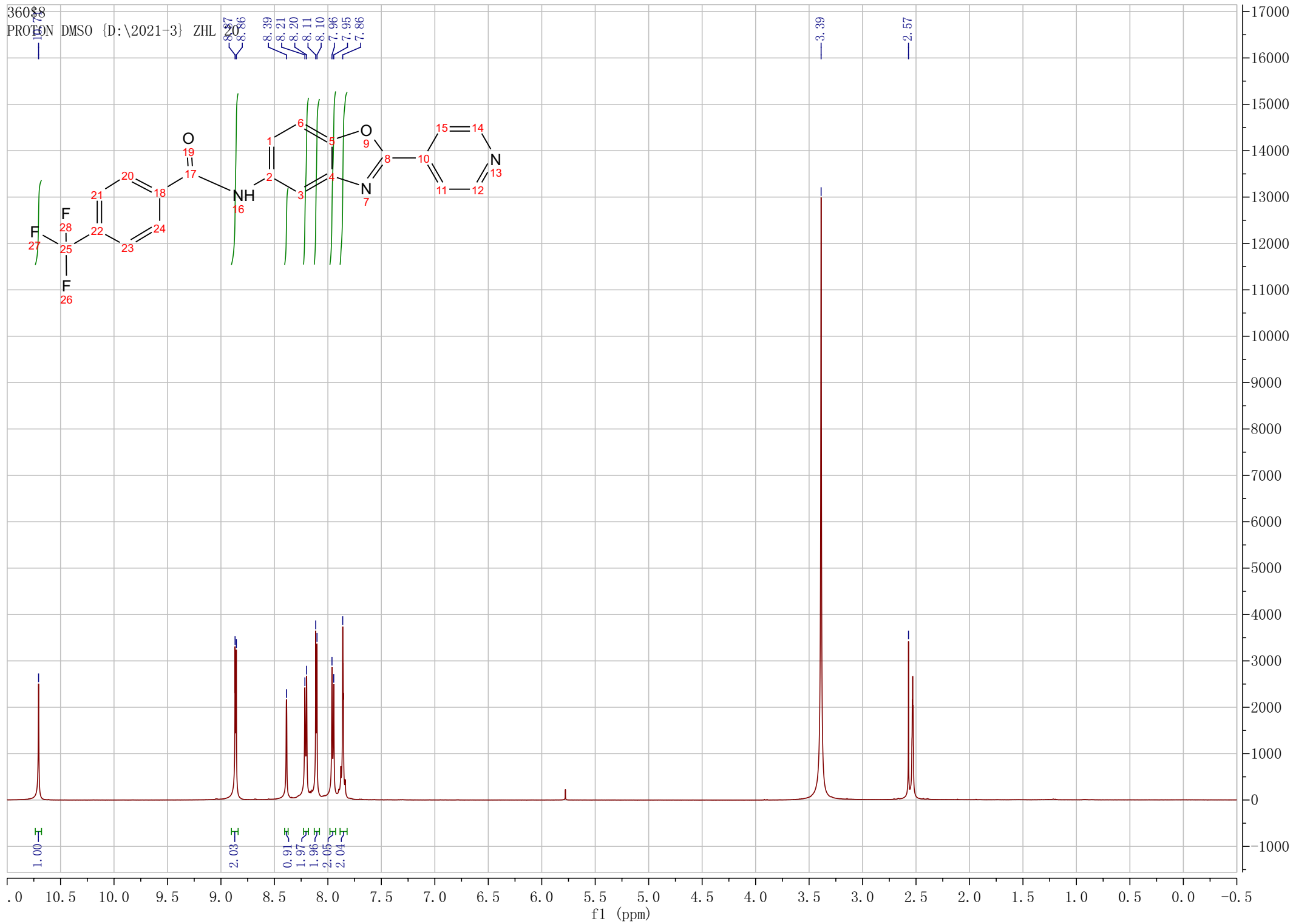




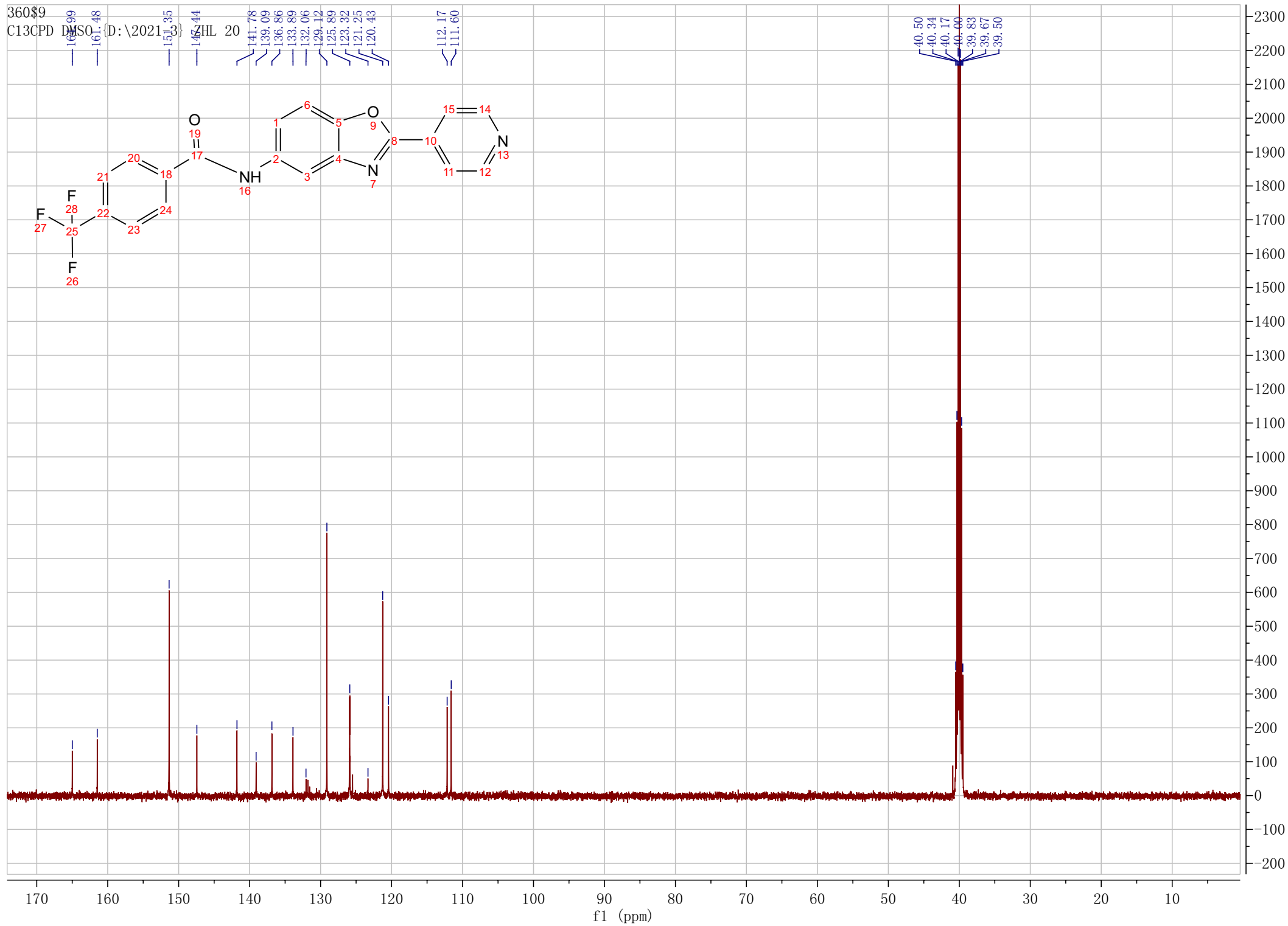


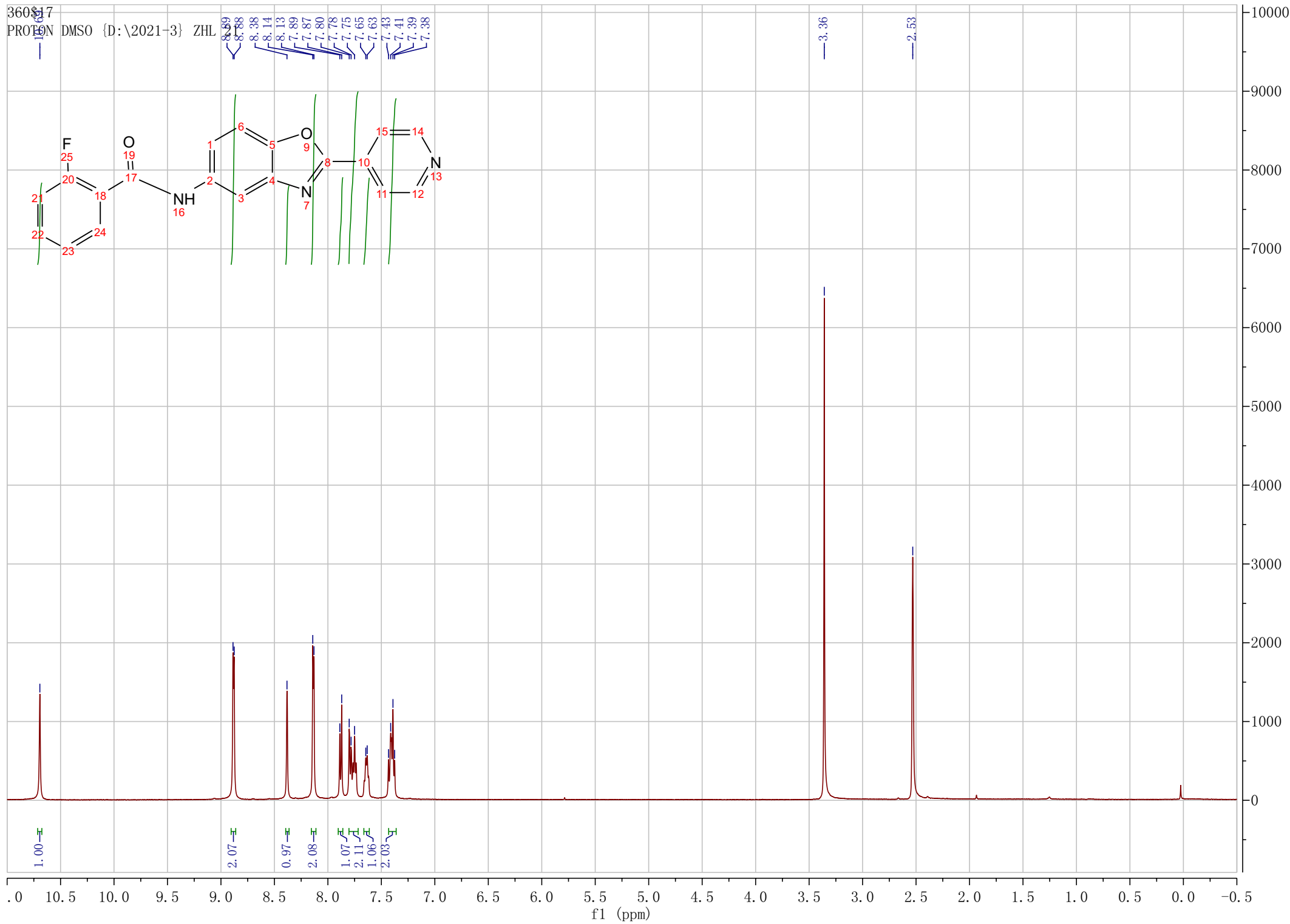


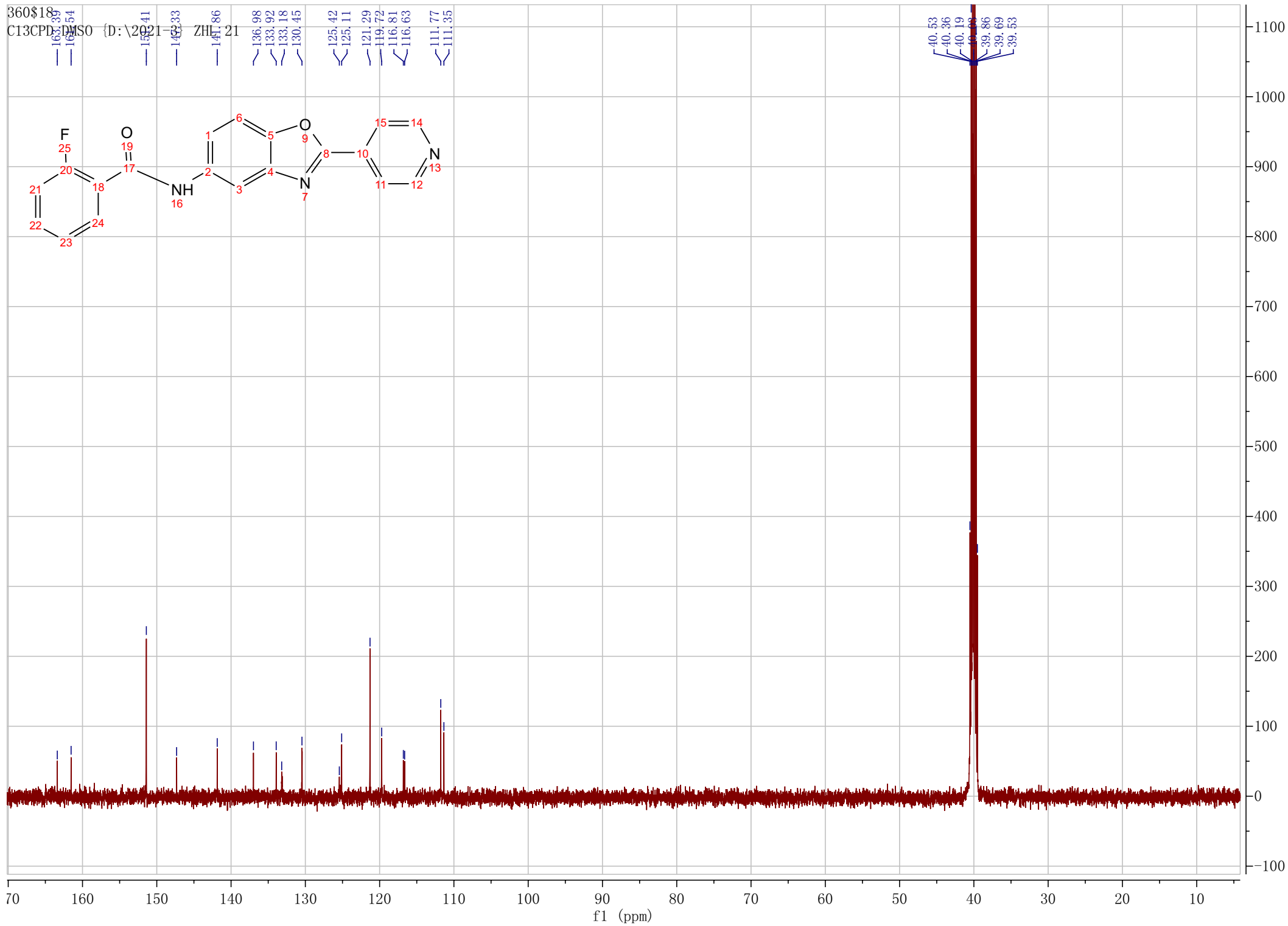


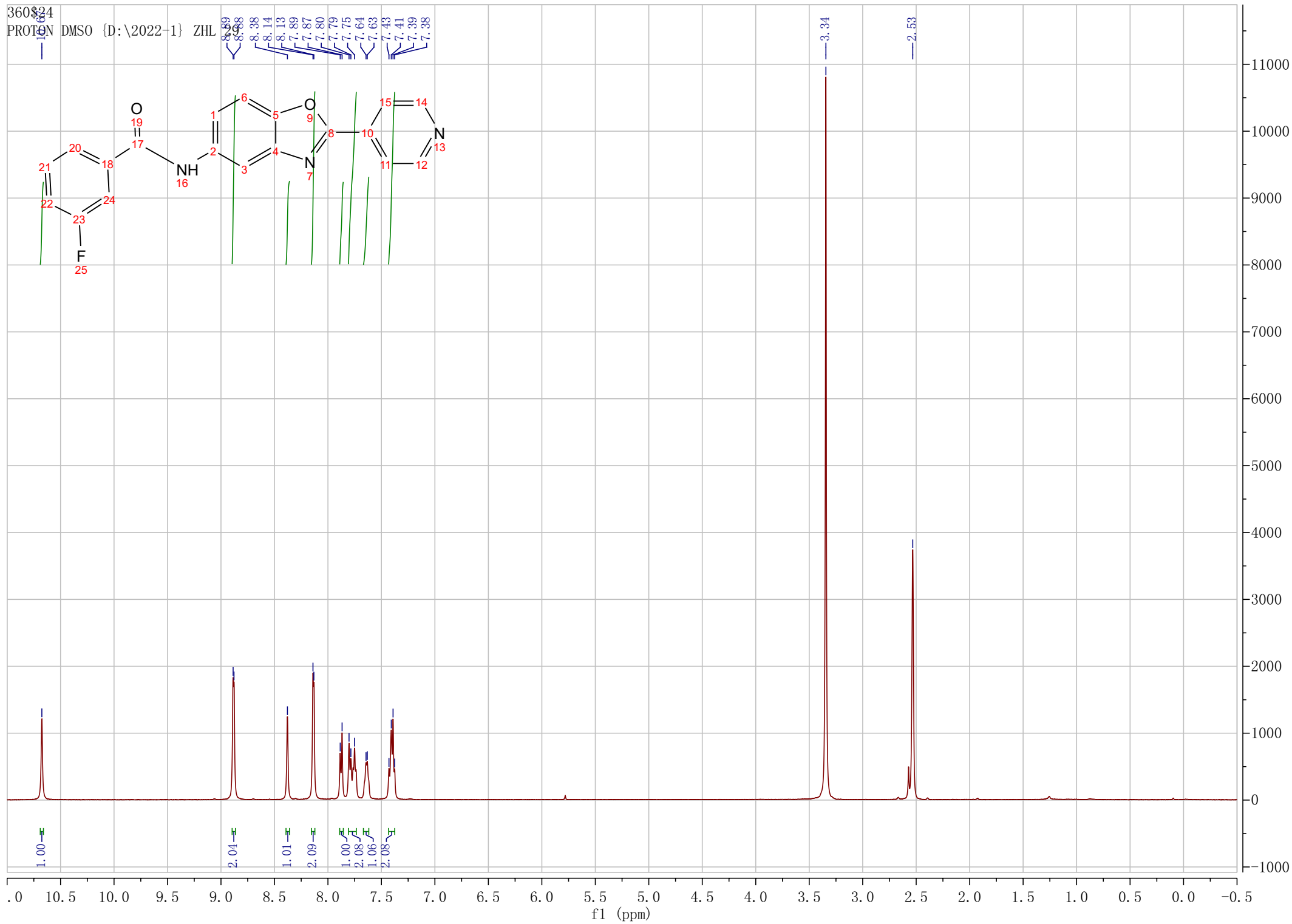


360\$9

C13CPD DMSO-d<sub>6</sub> {D:\2021\3}

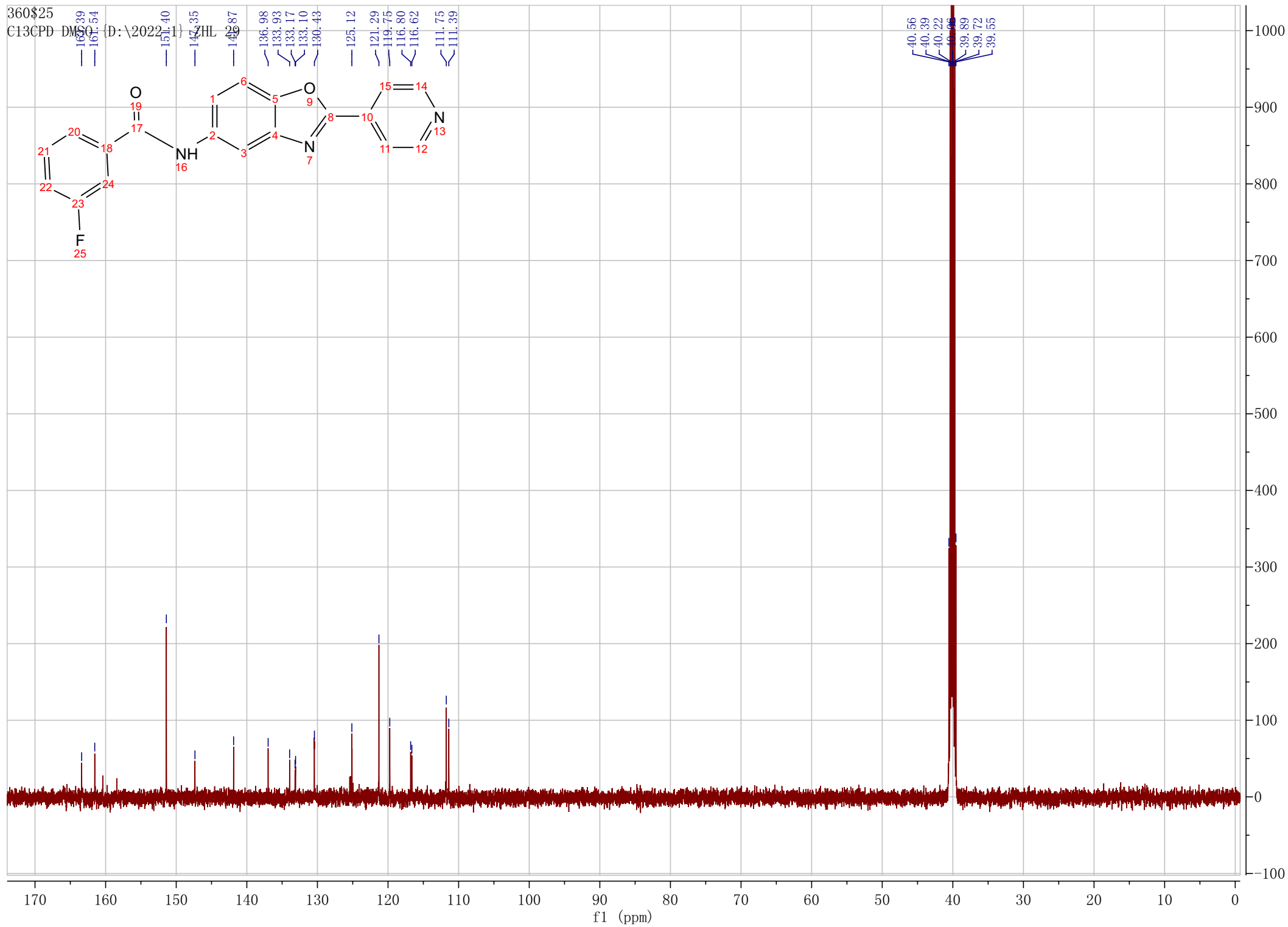






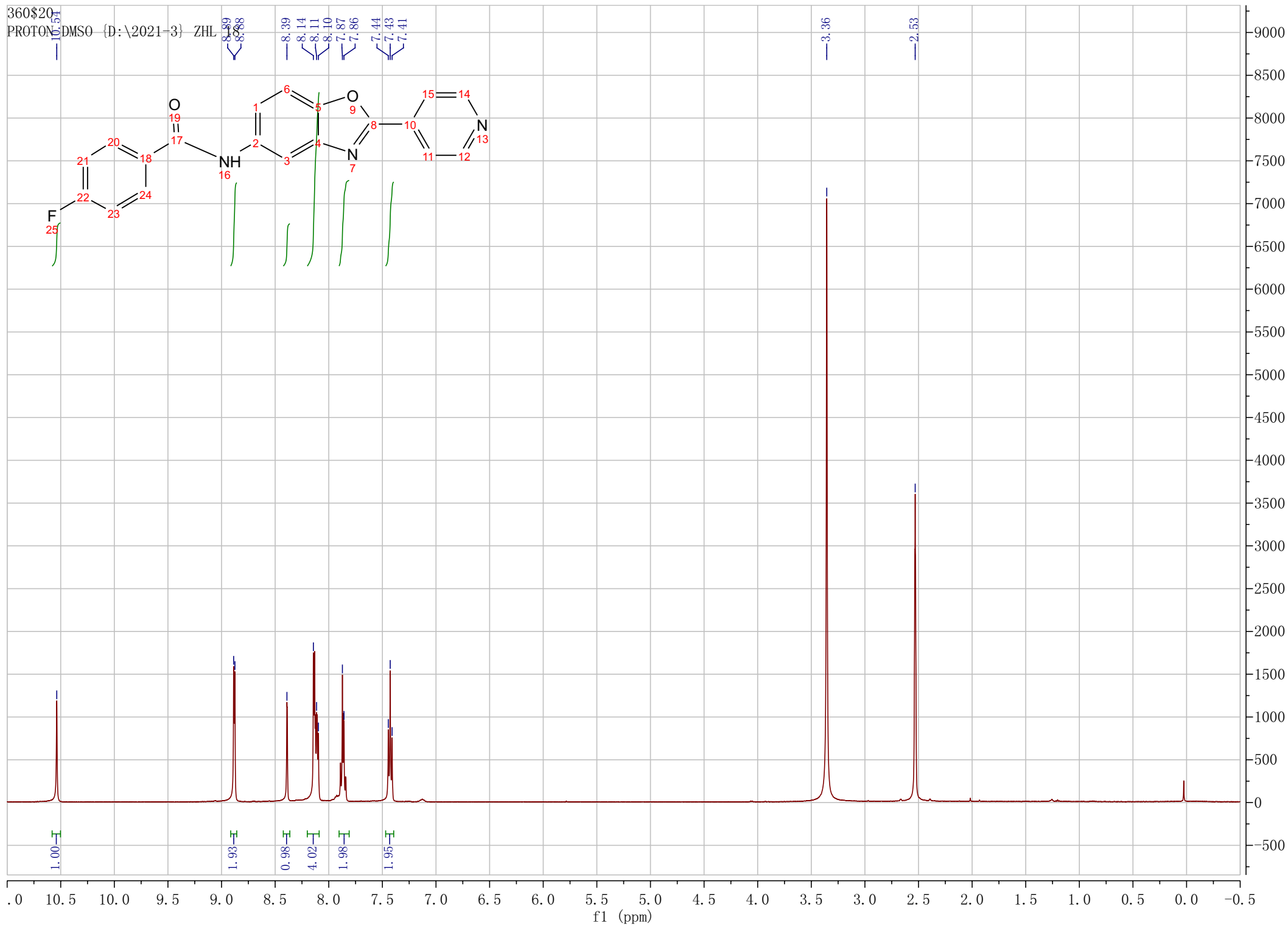
360\$25

C13CPD - DMSO - (D:\2022-11-17)

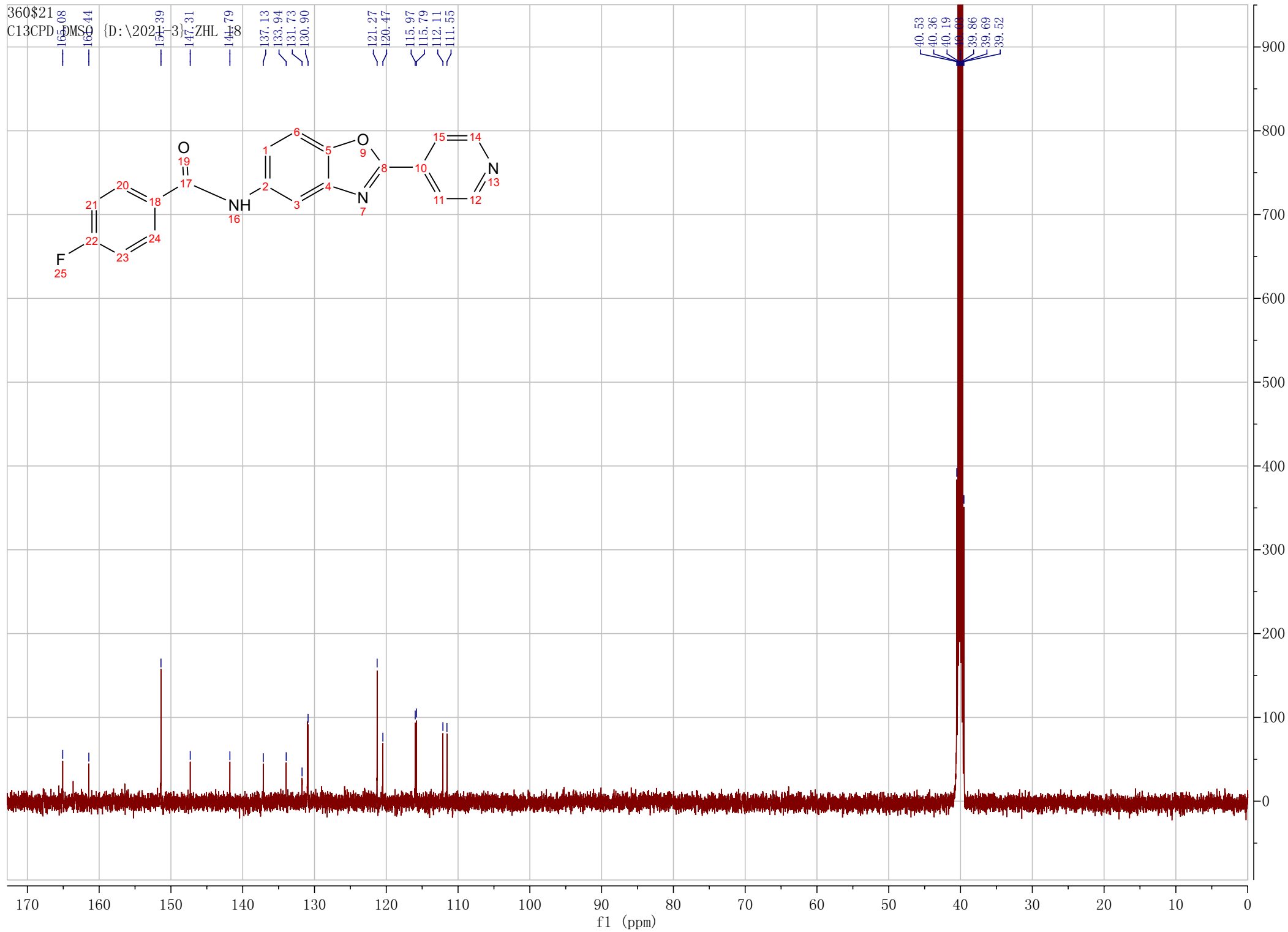


360\$20

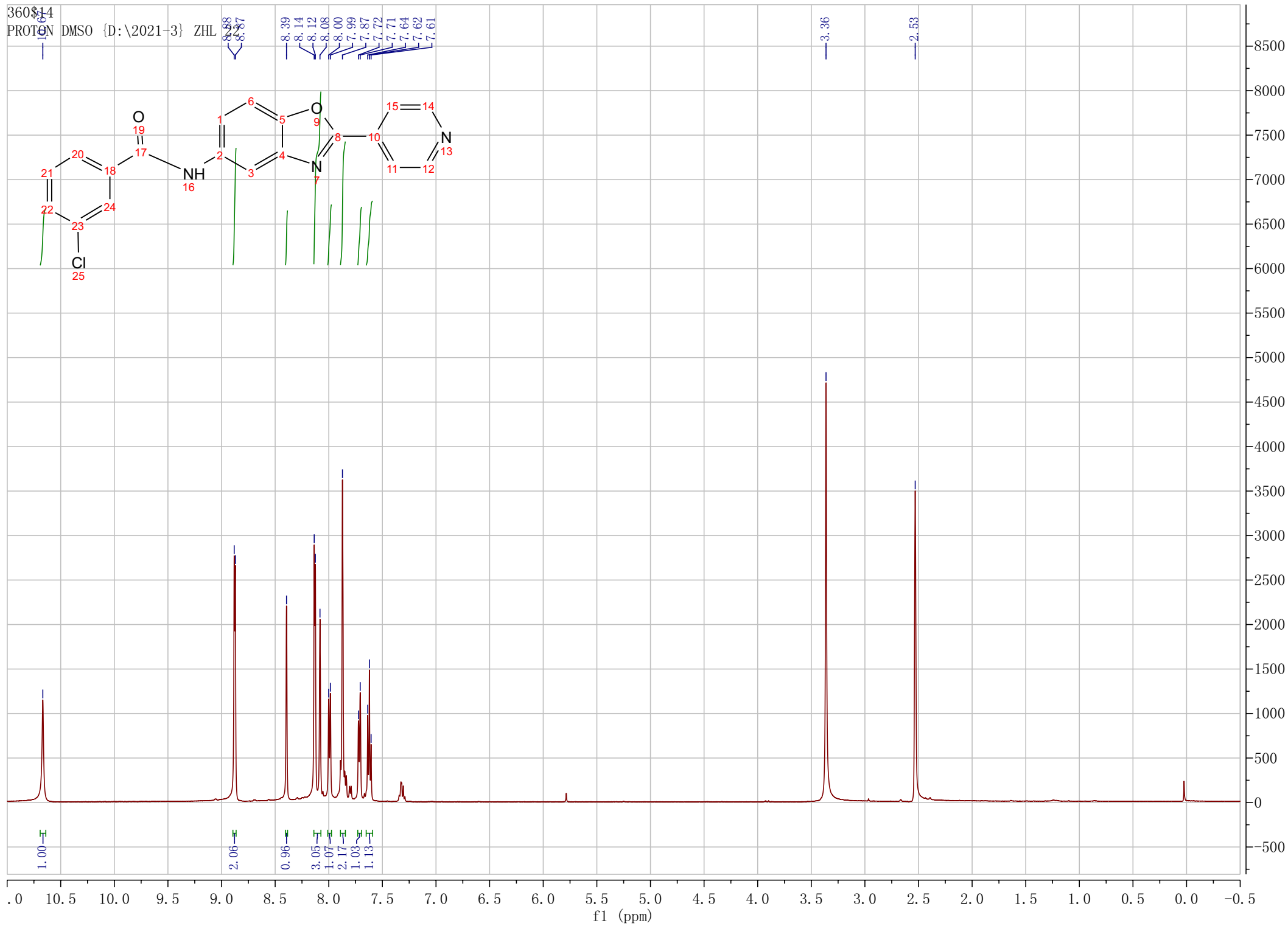
PROTON DMSO -{D:\2021-3} ZHL

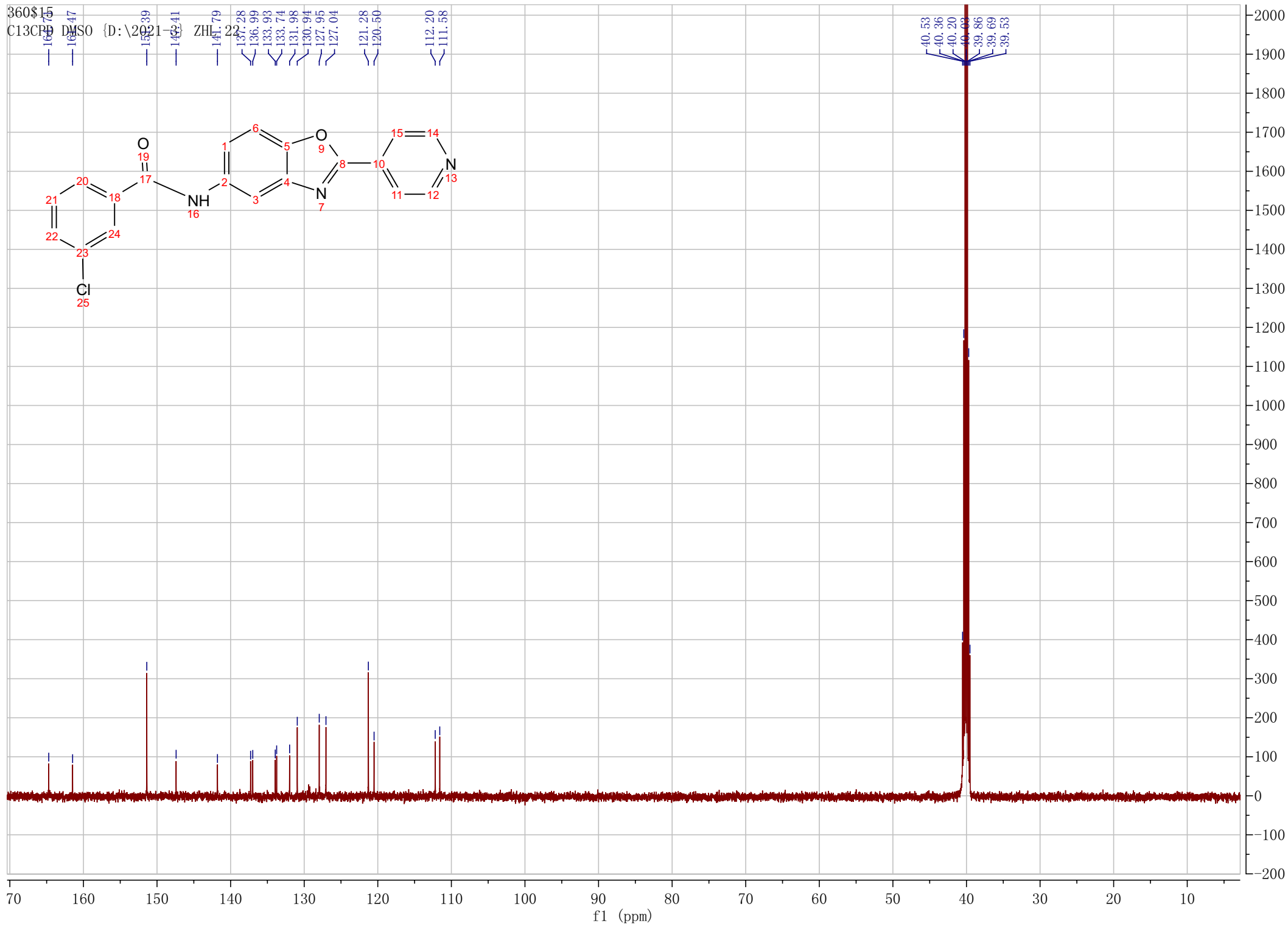


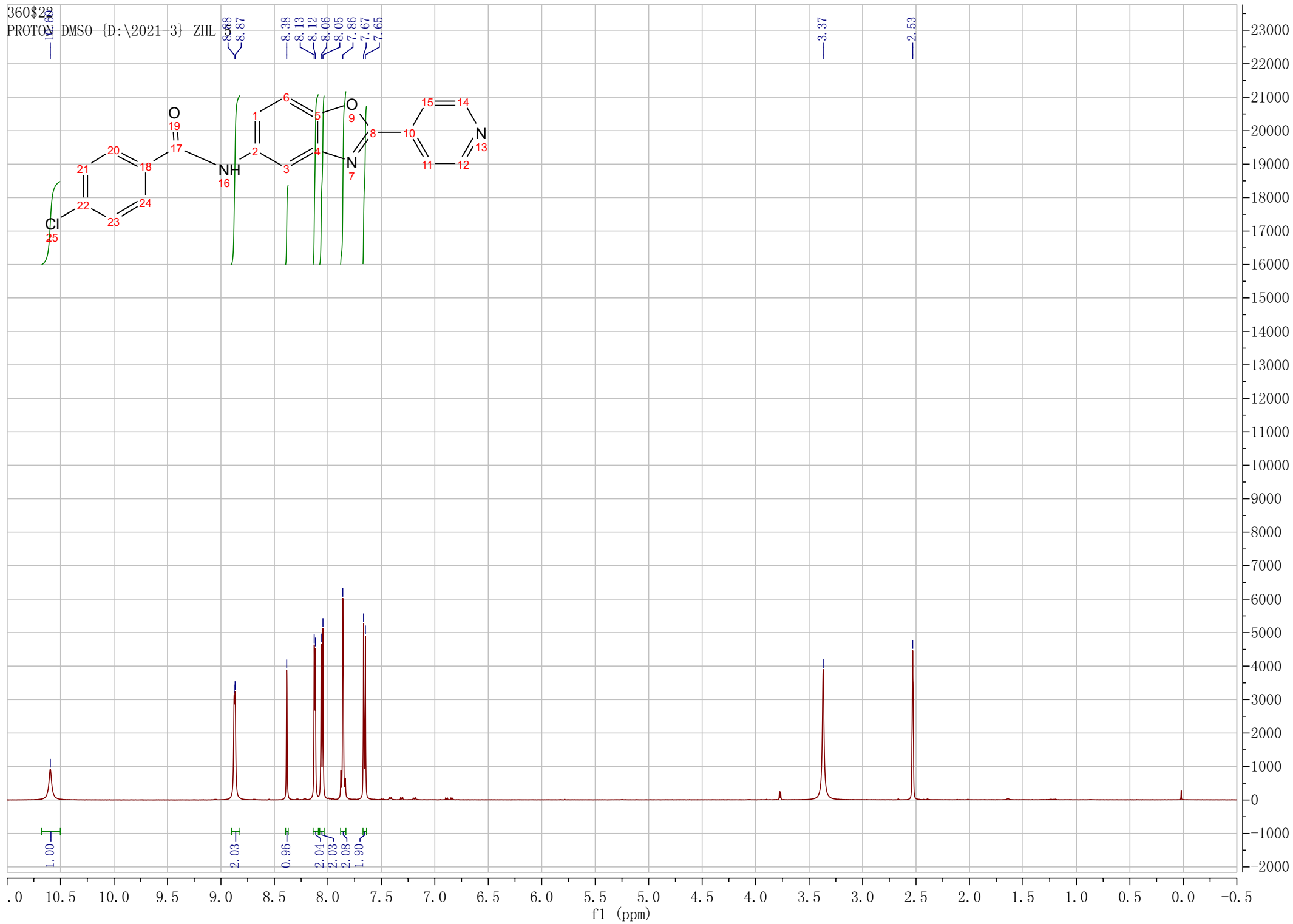
360\$21  
C13CPD





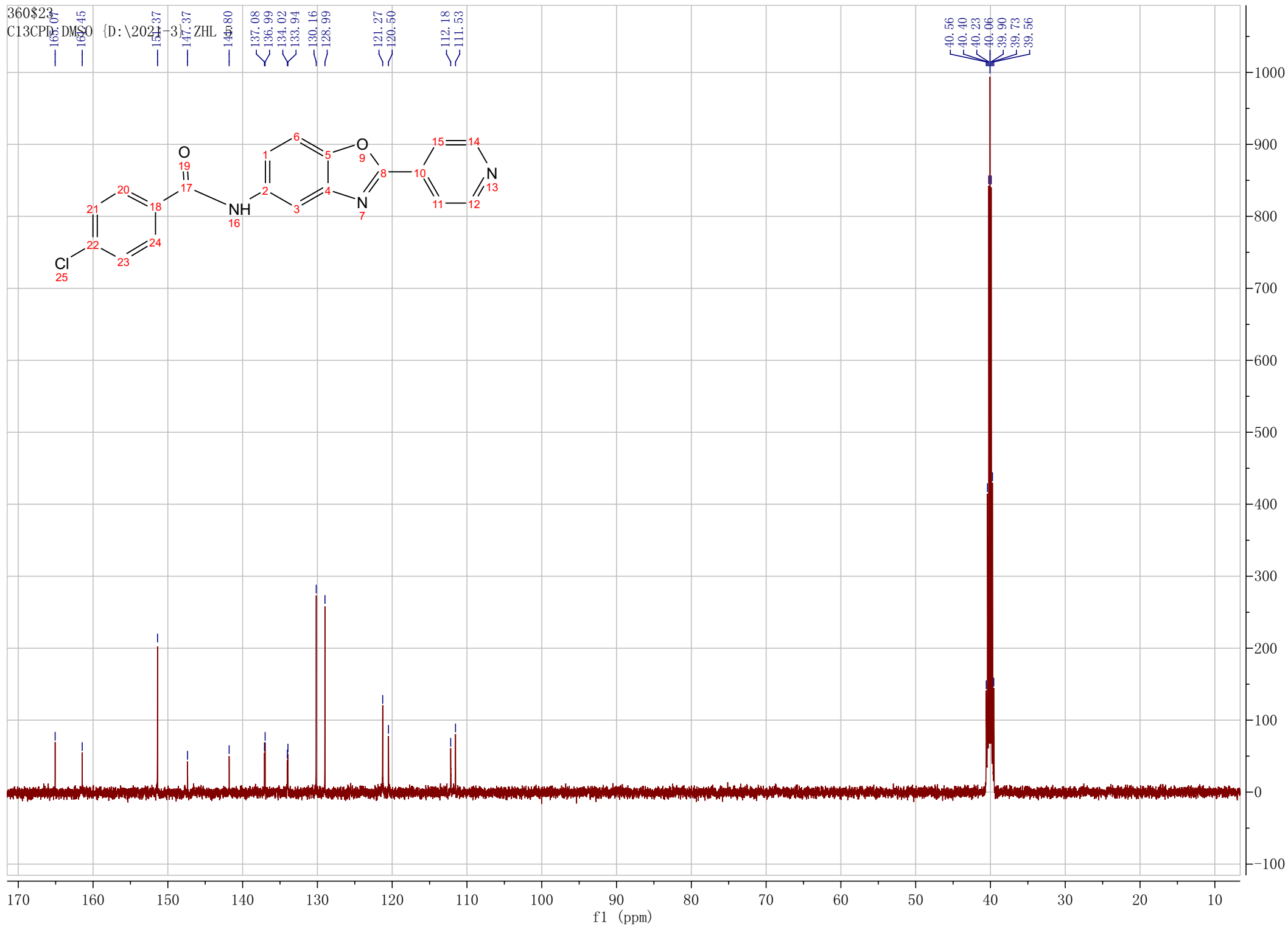
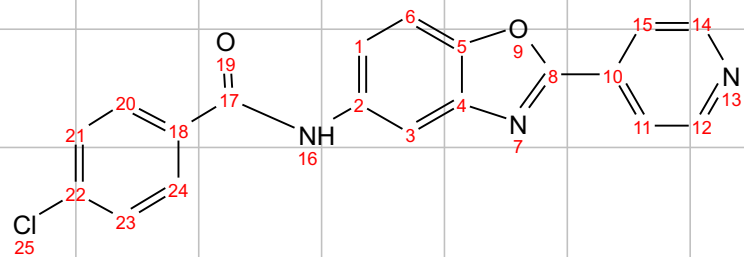




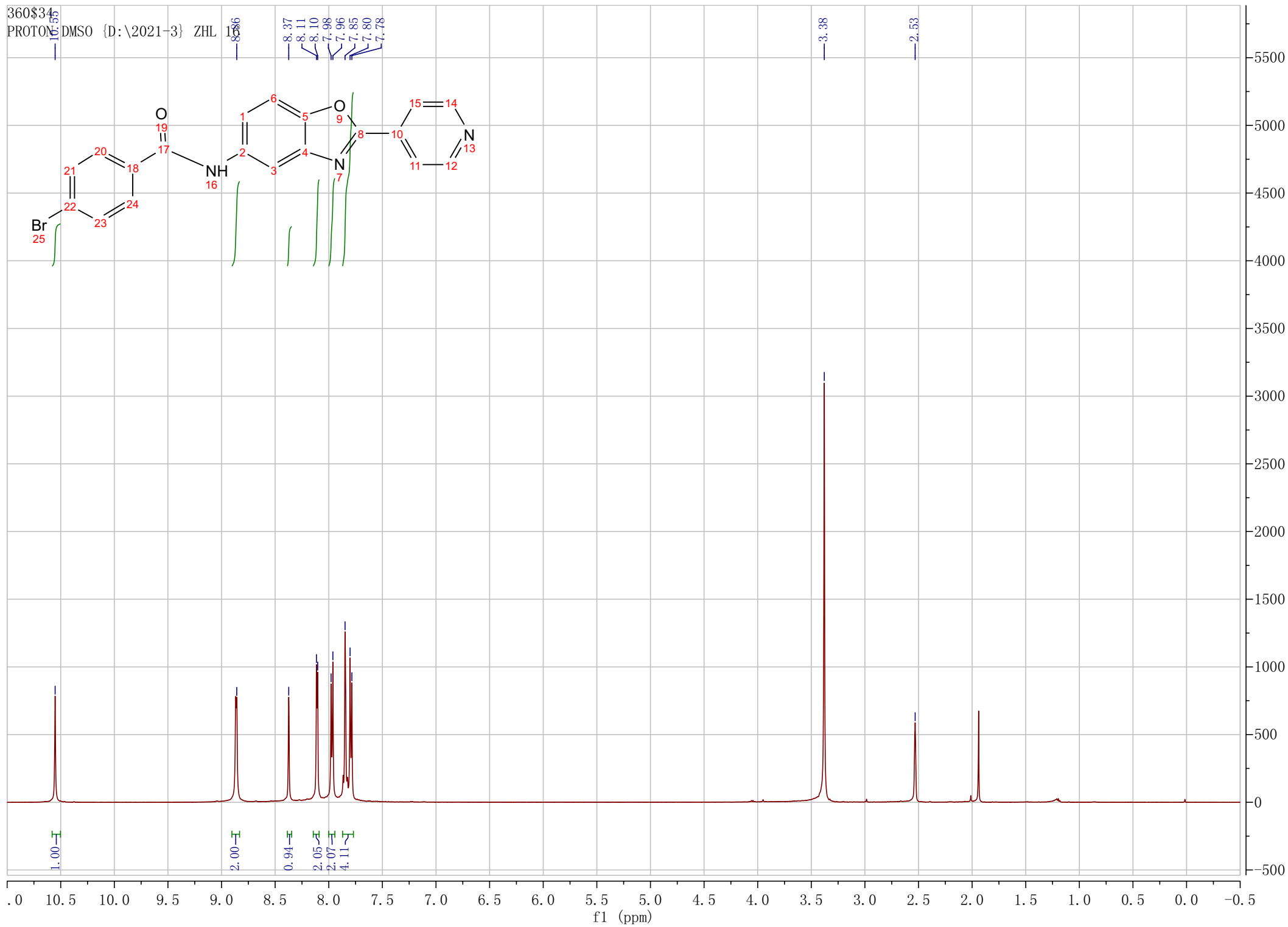


360\$23  
C13CPD.DMSO

{D:\2021-3  
ZHL



360\$34  
PROTON DMSO {D:\2021-3} ZHL



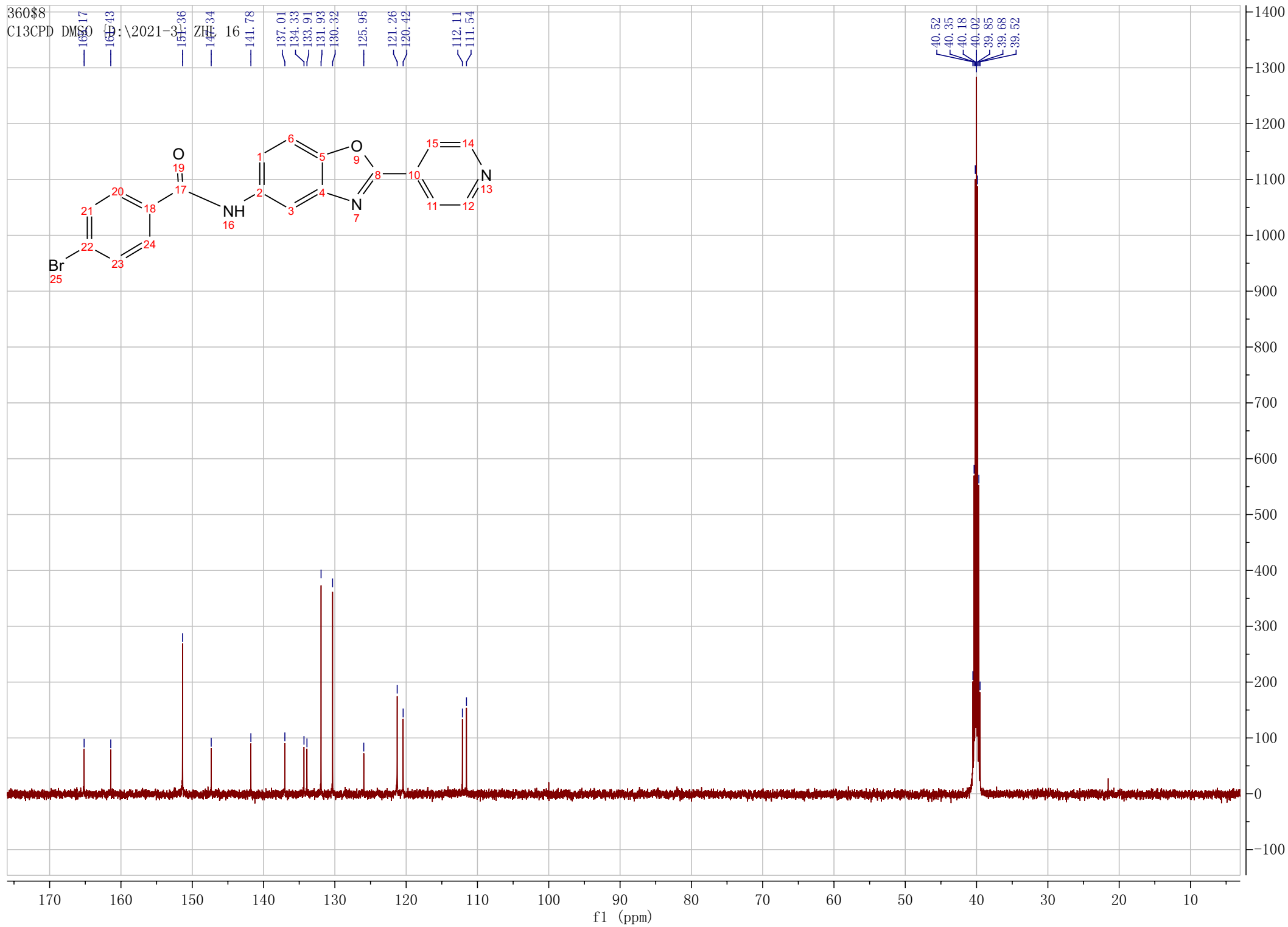
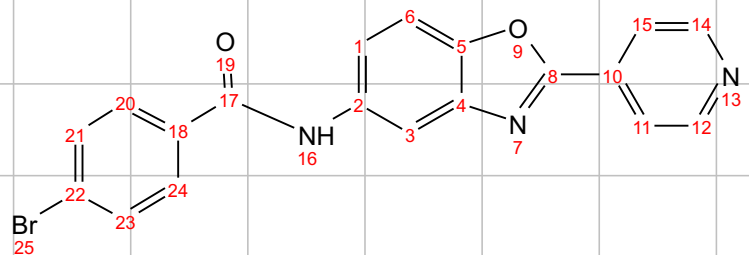
360\$8

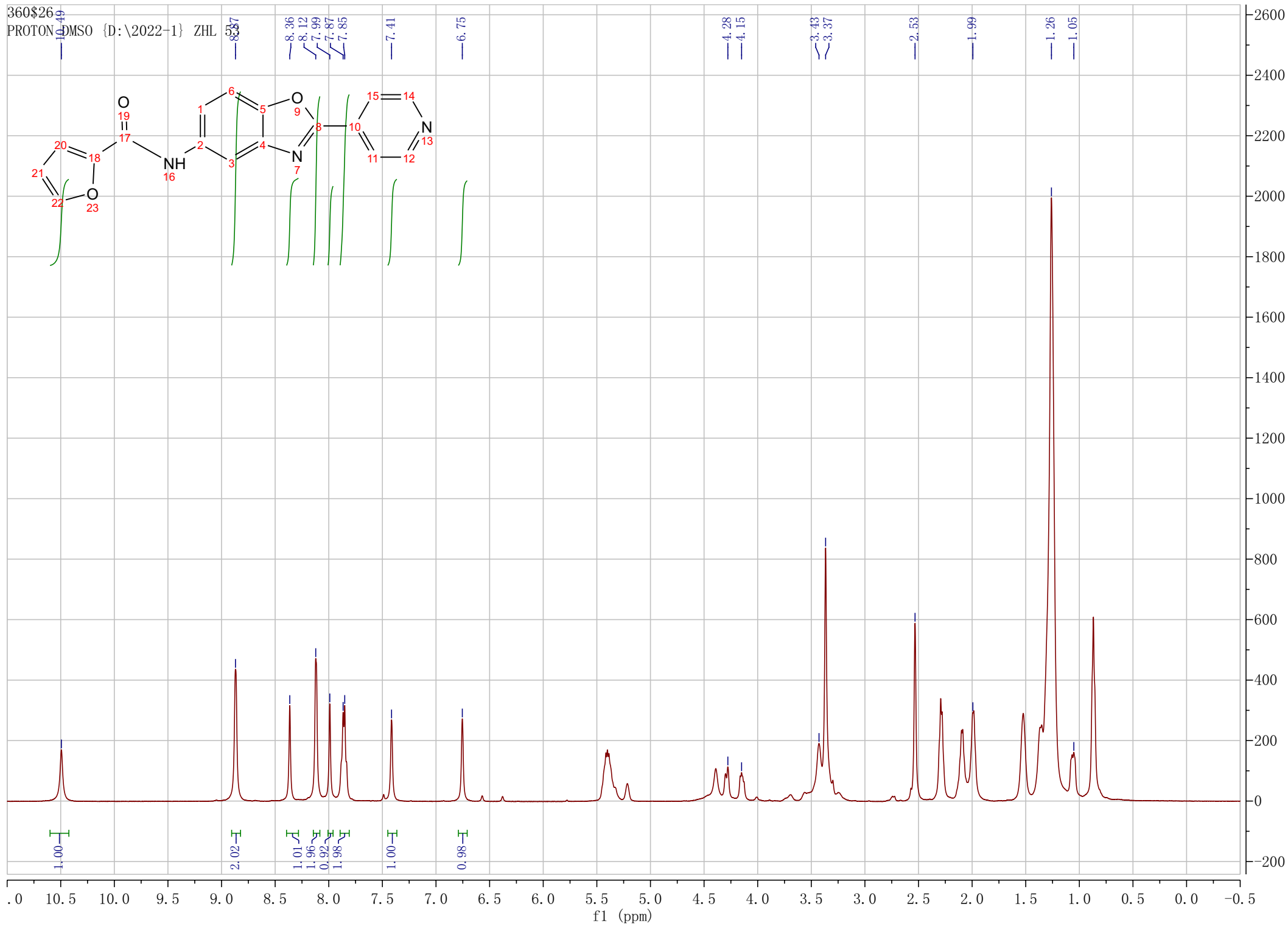
C13CPD

DMSO-d<sub>6</sub>

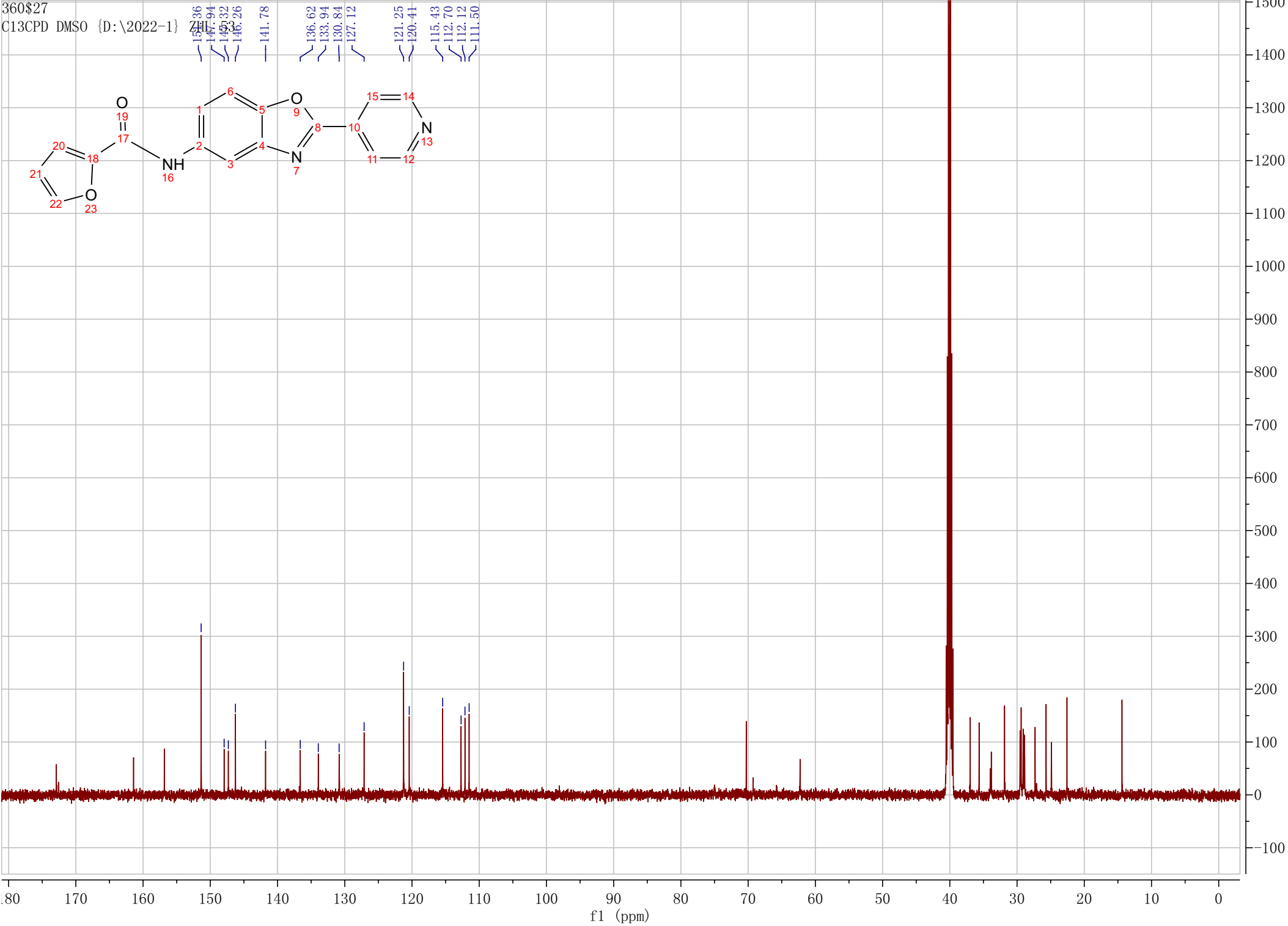
2021-3-19

ZHE 16





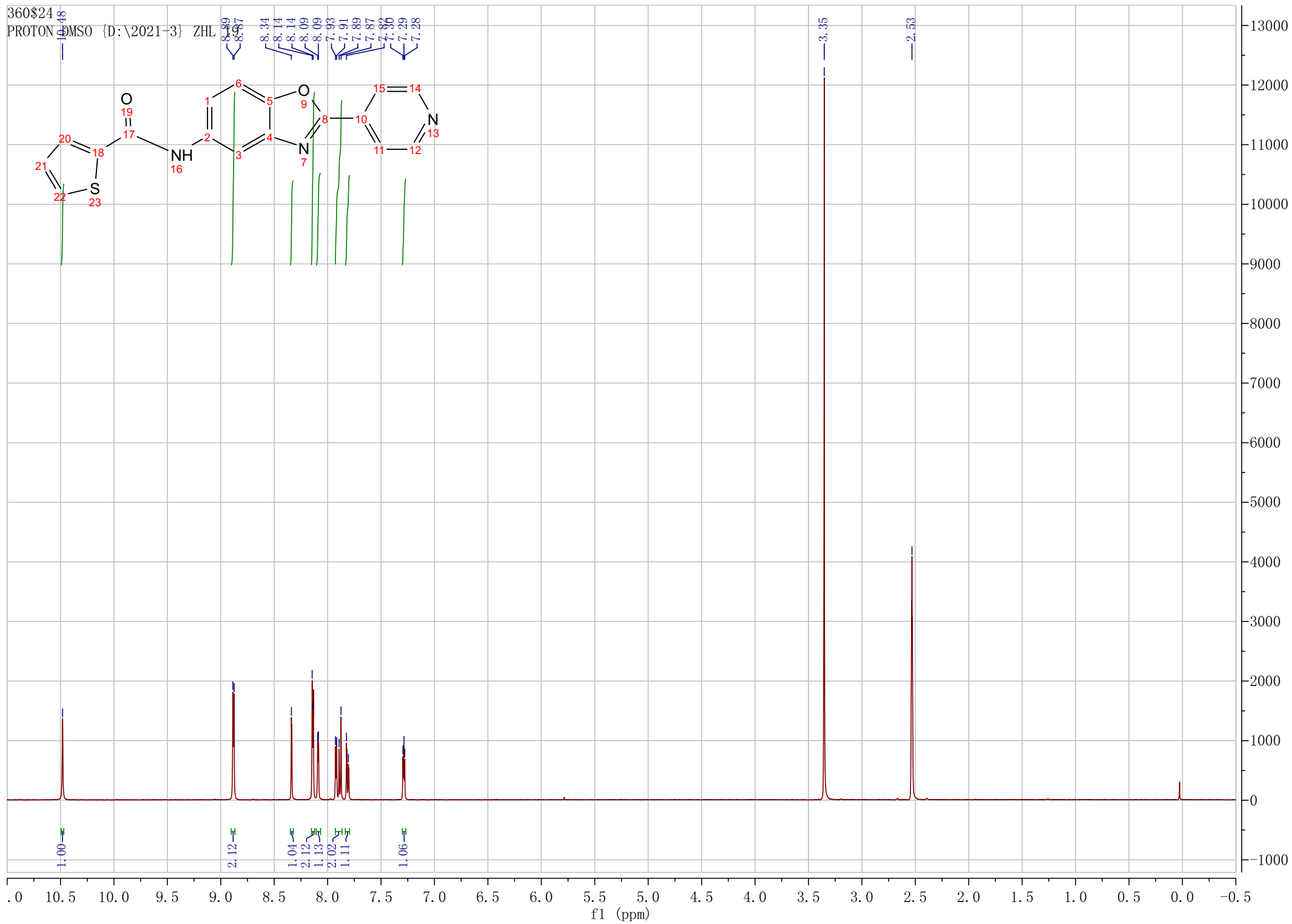
360\$27  
C13CPD DMSO {D:\2022-1}





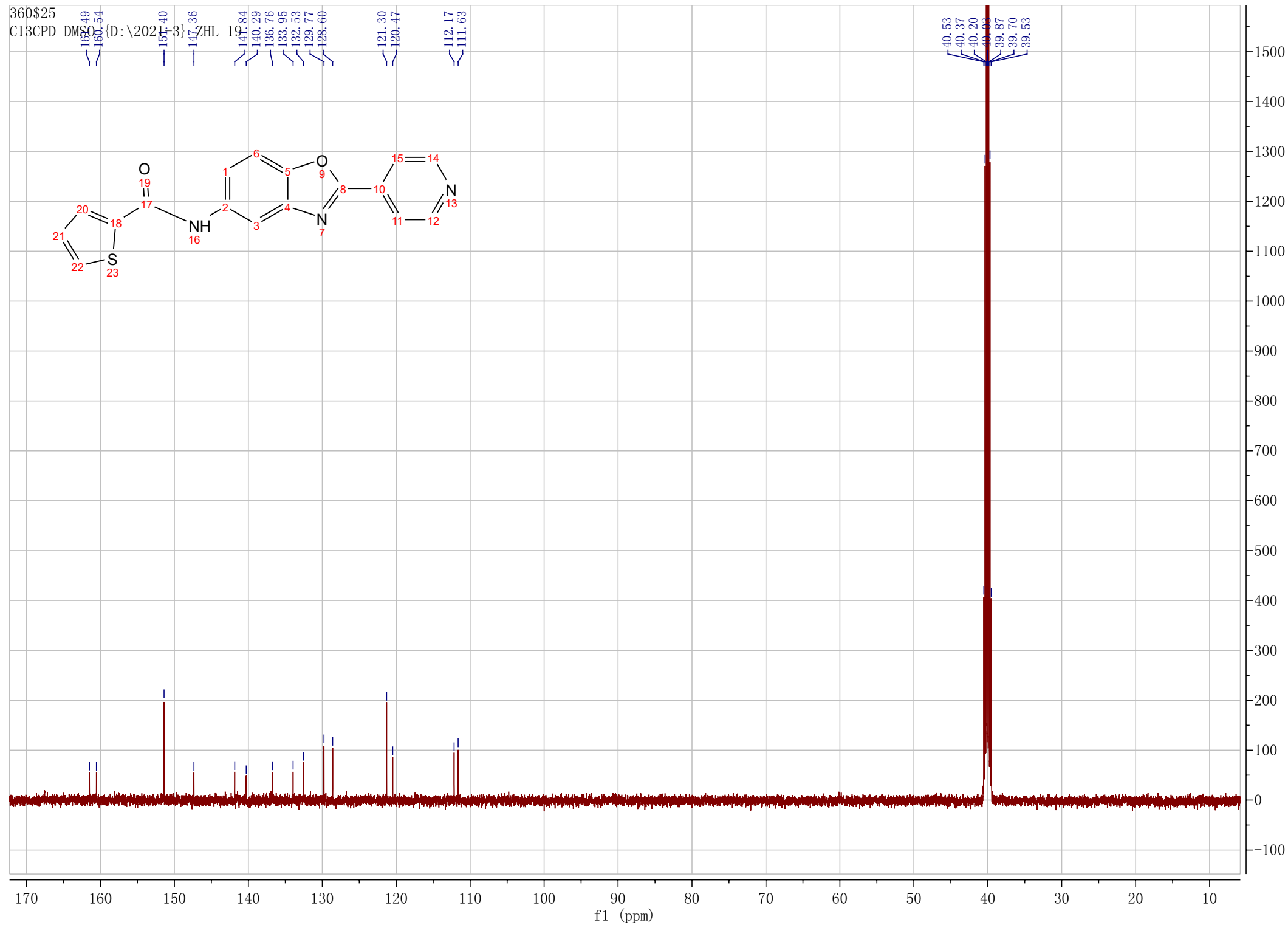
360\$24

PROTON DMSO {D:\2021-3} ZHL



360\$25

C13CPD DMSO-{D:\2021-3}



360\$36

PROTON DMSO {D:\2022-1} ZHL

