

## Supporting Information

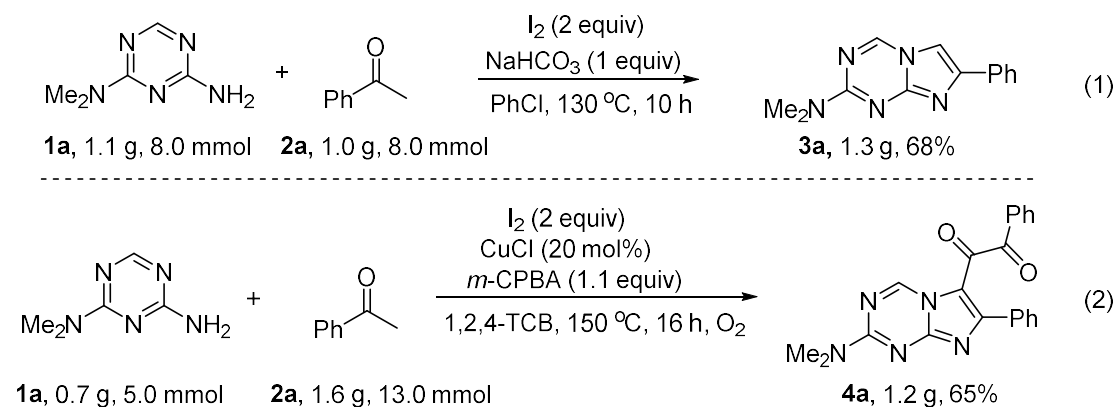
### Diversity-oriented synthesis of imidazo[1,2-a][1,3,5]triazine derivatives from 2-amine-[1,3,5]triazines with ketones

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### SI-Scheme 1. Gram-Scale Synthesis of **3a** and **4a**



### Experimental

Under otherwise noted, materials were obtained from commercial suppliers and used without further purification. <sup>1</sup>H NMR (500 MHz) and <sup>13</sup>C NMR (125 MHz) spectra were recorded on a Bruker Avance spectrometer in CDCl<sub>3</sub> with Me<sub>4</sub>Si as an internal standard. Data were reported as follows: chemical shift in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, br = broad and m = multiplet, coupling constant (Hz) and integration. Infrared spectra (IR) were obtained on FT-IR spectrometer; absorptions were reported in cm<sup>-1</sup>. HRMS and mass data were recorded by ESI on a TOF mass spectrometer.

### General procedure for the Synthesis of imidazo[1,2-a][1,3,5]triazines **3**

To a mixture of 1,3,5-triazine (0.50 mmol), ketone (0.50 mmol), NaHCO<sub>3</sub> (0.50 mmol) and I<sub>2</sub> (1.00 mmol) was added in PhCl (2 ml). The resulting mixture was then sealed and stirred at 130°C (oil bath). After completion of the reaction, the reaction mixture was cooled to room temperature, 10% Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> was added and the mixture was extracted with dichloromethane (3 × 15 mL). The organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The crude residue was obtained after evaporation of the solvent in vacuum, and the residue was purified by flash chromatography with petroleum ether/ethyl acetate as the eluent to give the pure product.

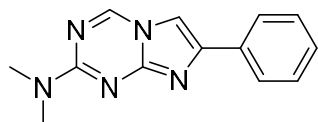
*Large-scale synthesis of 3a.* A Schlenk tube was charged with a stirring bar, and 1,3,5-triazine **1a** (1.1 g, 8.0 mmol), acetophenone **2a** (1.0 g, 8.0 mmol), NaHCO<sub>3</sub> (8.0 mmol), I<sub>2</sub> (16.0 mmol) and PhCl (15 ml) were added. The reaction was allowed to stir at 130 °C (oil bath) for 10 h. The crude product was separated by column chromatography with petroleum ether/ethyl acetate as the eluent to give a pure sample of **3a** in 68% yield (1.3 g).

### General procedure for the Synthesis of imidazo[1,2-a][1,3,5]triazines **4**

To a mixture of 1,3,5-triazine (0.50 mmol), ketone (1.35 mmol), CuCl (0.01 mmol), I<sub>2</sub> (1.00 mmol) and *m*-CPBA (0.56 mmol) was added in 1,2,4-TCB (4 ml) under O<sub>2</sub>. The resulting mixture was then sealed and stirred at 150 °C (oil bath). After completion of the reaction, the reaction mixture was cooled to room temperature, 10% Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> was added and the mixture was extracted with dichloromethane (3 × 15 mL). The organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The crude residue was obtained after evaporation of the solvent in vacuum, and the residue was purified by flash chromatography with dichloromethane /ethyl acetate as the eluent to give the pure product.

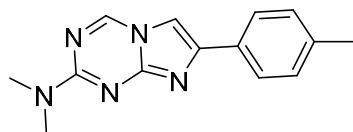
*Large-scale synthesis of 4a.* A Schlenk tube was charged with a stirring bar, and 1,3,5-triazine **1a** (0.7 g, 5.0 mmol), acetophenone **2a** (1.6 g, 13.0 mmol), CuCl (0.1 mmol), I<sub>2</sub> (10.0 mmol), *m*-CPBA (5.6 mmol), and 1,2,4-TCB (20 ml) were added. The reaction was allowed to stir at 150 °C (oil bath) for 16 h under O<sub>2</sub>. The crude product was separated by column chromatography with petroleum ether/ethyl acetate as the eluent to give a pure sample of **4a** in 65% yield (1.2 g).

***N,N*-dimethyl-7-phenylimidazo[1,2-*a*][1,3,5]triazin-2-amine (3a)**



98.5 mg, yellow solid, 82% yield, mp 286-287 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 8.68 (s, 1H), 8.00–7.92 (m, 2H), 7.45 (s, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.36–7.30 (m, 1H), 3.28 (s, 6H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 157.9, 150.8, 146.0, 145.2, 133.1, 128.6, 128.3, 126.0, 101.2, 37.2; IR (KBr, cm<sup>-1</sup>): 3476, 3028, 2929, 1640, 1587, 1466, 1411, 1351, 1229, 1176, 1069, 777, 718, 691, 596. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>13</sub>H<sub>14</sub>N<sub>5</sub> 240.1249, found 240.1266.

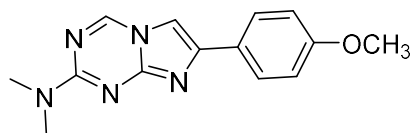
***N,N*-dimethyl-7-(*p*-tolyl)imidazo[1,2-*a*][1,3,5]triazin-2-amine (3b)**



88.4 mg, yellow solid, 70% yield, mp 290-291 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.65 (s, 1H), 7.83 (d, *J* = 8.0 Hz, 2H), 7.39 (s, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 3.26 (s, 6H), 2.37 (s, 3H); <sup>13</sup>C

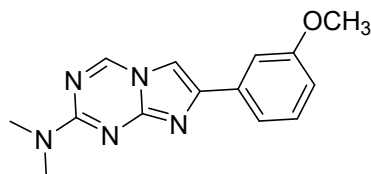
NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  157.9, 150.6, 145.6, 145.2, 138.3, 130.0, 129.3, 125.9, 100.9, 37.3, 21.3; IR (KBr, cm<sup>-1</sup>): 3446, 1642, 1586, 1494, 1464, 1412, 1183, 1065, 920, 824, 777, 767, 735. HRMS (ESI-TOF)  $m/z$  [M+H]<sup>+</sup> calcd for C<sub>14</sub>H<sub>16</sub>N<sub>5</sub> 254.1406, found 254.1410.

**7-(4-methoxyphenyl)-*N,N*-dimethylimidazo[1,2-*a*][1,3,5]triazin-2-amine (3c)**



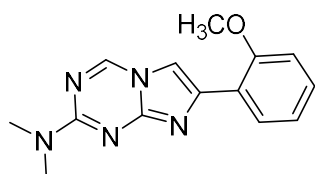
135.3 mg, yellow solid, 89% yield, mp 262-264 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  8.64 (s, 1H), 7.88 (d,  $J$  = 8.8 Hz, 2H), 7.34 (s, 1H), 6.94 (d,  $J$  = 8.8 Hz, 2H), 3.84 (s, 3H), 3.26 (s, 6H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  159.9, 157.9, 150.8, 145.9, 145.0, 127.3, 125.8, 114.0, 100.1, 55.3, 37.3; IR (KBr, cm<sup>-1</sup>): 3473, 3033, 2929, 2839, 1623, 1581, 1497, 1463, 1406, 1248, 1170, 1062, 1026, 833, 779, 742, 706. HRMS (ESI-TOF)  $m/z$  [M+H]<sup>+</sup> calcd for C<sub>14</sub>H<sub>16</sub>N<sub>5</sub>O 270.1355, found 270.1368.

**7-(3-methoxyphenyl)-*N,N*-dimethylimidazo[1,2-*a*][1,3,5]triazin-2-amine (3d)**



94.3 mg, light yellow solid, 70% yield, mp 224-226 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  8.66 (s, 1H), 7.60 (t,  $J$  = 1.7 Hz 1H), 7.45 (dd,  $J$  = 8.0, 1.7 Hz, Hz, 1H), 7.43 (s, 1H), 7.30 (t,  $J$  = 8.0 Hz, 1H), 6.88 (dd,  $J$  = 8.0, 1.7 Hz, 1H), 3.87 (s, 3H), 3.27 (s, 6H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  160.0, 157.9, 150.7, 145.8, 145.2, 134.4, 129.5, 118.2, 114.8, 110.8, 101.5, 55.4, 37.3; IR (KBr, cm<sup>-1</sup>): 3434, 2940, 1643, 1610, 1579, 1480, 1463, 1413, 1343, 1303, 1255, 1161, 1047, 921, 877, 800, 778, 763, 730, 677. HRMS (ESI-TOF)  $m/z$  [M+H]<sup>+</sup> calcd for C<sub>14</sub>H<sub>16</sub>N<sub>5</sub>O 270.1355, found 1359.

**7-(2-methoxyphenyl)-*N,N*-dimethylimidazo[1,2-*a*][1,3,5]triazin-2-amine (3e)**

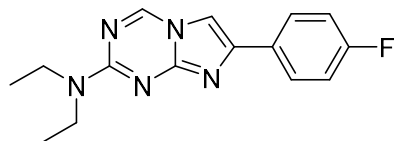


101.0 mg, yellow solid, 73% yield, mp 249-250 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  8.65 (s,



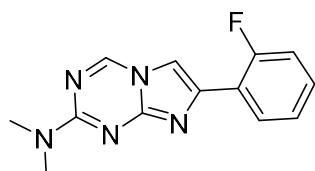
1H), 8.49 (dd,  $J = 7.8, 1.7$  Hz, 1H), 7.78 (s, 1H), 7.30 (td,  $J = 7.8, 1.7$  Hz, 1H), 7.08 (td,  $J = 7.8$  Hz, 1.7 Hz 1H), 6.96 (dd,  $J = 7.8, 1.7$  Hz, 1H), 3.97 (s, 3H), 3.27 (s, 6H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  158.0, 157.0, 149.5, 145.2, 141.3, 129.5, 128.8, 121.6, 120.9, 110.5, 105.8, 55.3, 37.2; IR (KBr,  $\text{cm}^{-1}$ ): 3427, 3155, 2933, 2796, 1635, 1584, 1467, 1410, 1242, 1171, 1061, 1022, 779, 765, 749, 739, 724. HRMS (ESI-TOF)  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{14}\text{H}_{16}\text{N}_5\text{O}$  270.1355, found 270.1367.

***N,N*-diethyl-7-(4-fluorophenyl)imidazo[1,2-*a*][1,3,5]triazin-2-amine (3f)**



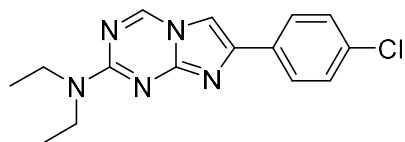
86.2 mg, yellow solid, 61% yield, mp 206-208 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.64 (s, 1H), 7.93–7.88 (m, 2H), 7.36 (s, 1H), 7.10–7.04 (m, 2H), 3.73-3.65 (m, 4H), 1.28-1.18 (m, 6H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  162.8 (d,  $J = 246.0$  Hz), 156.9, 151.0, 145.3 (d,  $J = 9.2$  Hz), 144.9, 129.2 (d,  $J = 3.0$  Hz), 127.7 (d,  $J = 6.1$  Hz), 127.6, 115.5 (d,  $J = 21.6$  Hz), 115.4 (d,  $J = 21.9$  Hz), 100.9, 42.6, 42.2, 13.7, 12.5; IR (KBr,  $\text{cm}^{-1}$ ): 3438, 2977, 2935, 1633, 1557, 1493, 1462, 1439, 1345, 1281, 1218, 1156, 1095, 852, 825, 779, 734, 698, 657, 521. HRMS (ESI-TOF)  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{15}\text{H}_{17}\text{FN}_5$  286.1468, found 286.1477.

**7-(2-fluorophenyl)-*N,N*-dimethylimidazo[1,2-*a*][1,3,5]triazin-2-amine (3g)**



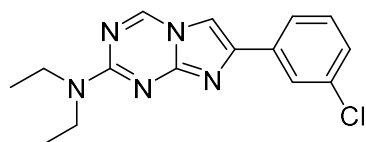
107.3 mg, yellow solid, 85% yield, mp 282-283 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.69 (s, 1H), 8.41 (td,  $J = 7.6, 1.9$  Hz, 1H), 7.65-7.63 (m, 1H), 7.32–7.28 (m, 1H), 7.24 (td,  $J = 7.6, 1.3$  Hz, 1H), 7.14-7.09 (m, 1H), 3.28 (s, 6H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  160.5 (d,  $J = 248.1$  Hz), 158.1, 150.0, 145.3, 139.5, 129.5 (d,  $J = 3.7$  Hz), 129.1 (d,  $J = 8.7$  Hz), 124.5 (d,  $J = 3.3$  Hz), 121.0 (d,  $J = 12.0$  Hz), 115.3 (d,  $J = 21.8$  Hz), 105.7 (d,  $J = 16.8$  Hz), 37.30; IR (KBr,  $\text{cm}^{-1}$ ): 3450, 3167, 3040, 2927, 1645, 1588, 1471, 1411, 1230, 1208, 1177, 1064, 778, 759, 744, 708. HRMS (ESI-TOF)  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{13}\text{H}_{13}\text{FN}_5$  258.1155, found 258.1158.

**7-(4-chlorophenyl)-*N,N*-diethylimidazo[1,2-*a*][1,3,5]triazin-2-amine (3h)**



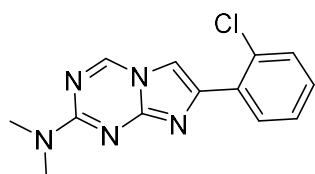
115.1 mg, yellow solid, 75% yield, mp 217-218 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.65 (s, 1H), 7.86 (d, *J* = 8.4 Hz, 2H), 7.39 (s, 1H), 7.36 (d, *J* = 8.4 Hz, 2H), 3.74-3.65 (m, 4H), 1.29-1.19 (m, 6H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 156.9, 151.0, 145.3, 144.6, 133.9, 131.6, 128.8, 127.2, 101.4, 42.7, 42.2, 13.7, 12.6; IR (KBr, cm<sup>-1</sup>): 3440, 2982, 2929, 1632, 1575, 1549, 1497, 1458, 1356, 1278, 1208, 1162, 1085, 830, 781, 731, 697, 502, 483. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>15</sub>H<sub>17</sub>ClN<sub>5</sub> 302.1172, found 302.1154.

**7-(3-chlorophenyl)-*N,N*-diethylimidazo[1,2-*a*][1,3,5]triazin-2-amine (3i)**



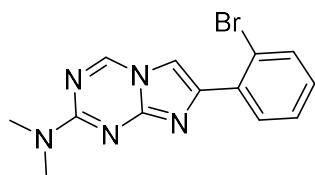
78.9 mg, yellow solid, 52% yield, mp 162-163 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.66 (s, 1H), 7.95 (t, *J* = 1.8 Hz, 1H), 7.80 (dt, *J* = 7.7, 1.8 Hz, 1H), 7.42 (s, 1H), 7.31 (t, *J* = 7.7 Hz, 1H), 7.27-7.25 (m, 1H), 3.65-3.73 (m, 4H), 1.27-1.20 (m, 6H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 156.9, 151.0, 145.4, 144.4, 135.0, 134.6, 129.8, 128.1, 126.1, 124.0, 101.8, 42.7, 42.2, 13.7, 12.6; IR (KBr, cm<sup>-1</sup>): 3460, 2970, 1634, 1601, 1565, 1548, 1499, 1473, 1454, 1437, 1359, 1278, 1210, 1163, 1087, 796, 780, 746, 722, 665. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>15</sub>H<sub>17</sub>ClN<sub>5</sub> 302.1172, found 302.1151.

**7-(2-chlorophenyl)-*N,N*-dimethylimidazo[1,2-*a*][1,3,5]triazin-2-amine (3j)**



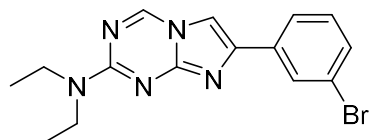
108.1 mg, yellow solid, 79% yield, mp 254-256 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 8.71 (s, 1H), 8.47 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.96 (s, 1H), 7.43 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.36 (td, *J* = 7.9, 1.1 Hz, 1H), 7.24 (td, *J* = 7.9, 1.6 Hz, 1H), 3.28 (s, 6H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 158.1, 149.6, 145.5, 141.8, 131.6, 131.3, 131.2, 130.3, 128.7, 127.0, 106.1, 37.3; IR (KBr, cm<sup>-1</sup>): 3430, 1645, 1586, 1547, 1506, 1463, 1411, 1340, 1179, 1043, 762, 733. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>13</sub>H<sub>13</sub>ClN<sub>5</sub> 274.0859, found 274.0867.

**7-(2-bromophenyl)-*N,N*-dimethylimidazo[1,2-*a*][1,3,5]triazin-2-amine (3k)**



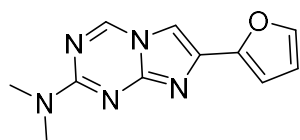
90.2 mg, light yellow solid, 57% yield, mp 232-234 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.72 (s, 1H), 8.36 (dd, *J* = 8.0, 1.7 Hz, 1H), 8.04 (s, 1H), 7.64 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.40 (td, *J* = 8.0, 1.1 Hz, 1H), 7.16 (td, *J* = 8.0, 1.7 Hz, 1H), 3.28 (s, 6H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 158.0, 149.6, 145.5, 143.0, 133.8, 133.3, 131.9, 129.0, 127.5, 121.0, 105.7, 37.3; IR (KBr, cm<sup>-1</sup>): 3444, 3138, 3049, 2928, 1650, 1585, 1459, 1414, 1296, 1217, 1176, 1020, 779, 758, 742, 732, 709. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>13</sub>H<sub>13</sub>BrN<sub>5</sub> 218.0354, found 218.0361.

**7-(3-bromophenyl)-*N,N*-diethylimidazo[1,2-*a*][1,3,5]triazin-2-amine (3l)**



82.7 mg, yellow solid, 48% yield, mp 158-160 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.67 (s, 1H), 8.14 (t, *J* = 1.6 Hz, 1H), 7.85 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.45–7.41 (m, 2H), 7.29–7.23 (m, 1H), 3.73-3.67 (m, 4H), 1.30-1.20 (m, 6H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 156.9, 151.0, 145.4, 144.3, 135.2, 131.0, 130.1, 129.0, 124.4, 122.8, 101.8, 42.7, 42.2, 13.7, 12.6; IR (KBr, cm<sup>-1</sup>): 3442, 2970, 1635, 1565, 1547, 1500, 1472, 1454, 1359, 1278, 1209, 1163, 1087, 796, 779, 719, 663. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>15</sub>H<sub>17</sub>BrN<sub>5</sub> 346.0667, found 346.0669.

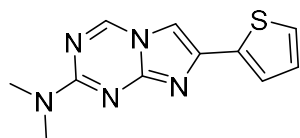
**7-(furan-2-yl)-*N,N*-dimethylimidazo[1,2-*a*][1,3,5]triazin-2-amine (3m)**



38.9 mg, brown solid, 34% yield, mp 285-286 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.66 (s, 1H), 7.47–7.40 (m, 1H), 7.35 (s, 1H), 6.99–6.92 (m, 1H), 6.51–6.47 (m, 1H), 3.26 (s, 6H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 158.0, 150.9, 149.3, 145.2, 142.2, 138.0, 111.7, 108.4, 100.8, 37.2; IR (KBr, cm<sup>-1</sup>): 3429, 3126, 3040, 2930, 1635, 1587, 1509, 1478, 1445, 1412, 1317, 1227, 1181, 1082, 1014, 948, 923, 888, 810, 780, 740, 677, 595, 497. HRMS (ESI-TOF) *m/z*

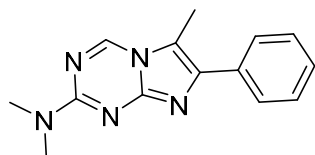
[M+H]<sup>+</sup> calcd for C<sub>11</sub>H<sub>12</sub>N<sub>5</sub>O 230.1042, found 230.1050.

***N,N*-dimethyl-7-(thiophen-2-yl)imidazo[1,2-*a*][1,3,5]triazin-2-amine (3n)**



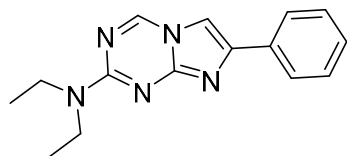
53.9 mg, brown solid, 44% yield, mp 250-251 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.62 (s, 1H), 7.50 (d, *J* = 3.5 Hz, 1H), 7.32 (s, 1H), 7.28 (d, *J* = 5.0 Hz, 1H), 7.06 (dd, *J* = 5.0, 3.5 Hz, 1H), 3.25 (s, 6H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 158.0, 150.7, 145.0, 141.1, 136.9, 127.7, 125.5, 124.5, 100.4, 37.3; IR (KBr, cm<sup>-1</sup>): 3458, 3118, 3029, 2928, 1638, 1589, 1515, 1465, 1410, 1280, 1207, 1166, 925, 848, 814, 778, 765, 722, 690, 661, 583. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>11</sub>H<sub>12</sub>N<sub>5</sub>S 246.0813, found 246.0811.

***N,N*,6-trimethyl-7-phenylimidazo[1,2-*a*][1,3,5]triazin-2-amine (3o)**



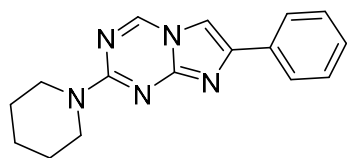
66.1 mg, yellow solid, 52% yield, mp 186-187 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.52 (s, 1H), 7.84–7.80 (m, 2H), 7.45–7.40 (m, 2H), 7.34–7.30 (m, 1H), 3.26 (s, 6H), 2.58 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 157.6, 149.4, 143.6, 141.2, 134.1, 128.4, 128.0, 127.5, 110.5, 37.2, 9.0; IR (KBr, cm<sup>-1</sup>): 3419, 1628, 1585, 1513, 1455, 1408, 1362, 1320, 1223, 1182, 1151, 1075, 1035, 770, 694. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>14</sub>H<sub>16</sub>N<sub>5</sub> 254.1406, found 254.1412.

***N,N*-diethyl-7-phenylimidazo[1,2-*a*][1,3,5]triazin-2-amine (3p)**



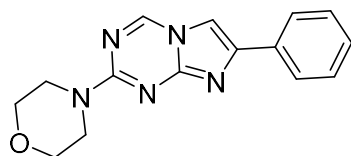
82.2 mg, yellow solid, 61% yield, mp 180-181 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.66 (s, 1H), 7.95 (d, *J* = 7.6 Hz, 2H), 7.43 (s, 1H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.34-7.30 (m, 1H), 3.74–3.66 (m, 4H), 1.29-1.21 (m, 6H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 156.9, 151.0, 145.8, 145.3, 133.1, 128.5, 128.2, 126.0, 101.2, 42.5, 42.2, 13.7, 12.6; IR (KBr, cm<sup>-1</sup>): 3416, 2956, 2930, 1631, 1562, 1550, 1497, 1466, 1436, 1373, 1348, 1282, 1244, 1163, 1071, 773, 712, 693. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>15</sub>H<sub>18</sub>N<sub>5</sub> 268.1562, found 268.1565.

### 7-phenyl-2-(piperidin-1-yl)imidazo[1,2-a][1,3,5]triazine (3q)



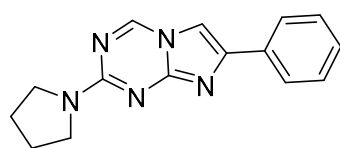
121.9 mg, yellow solid, 87% yield, mp 273-275 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.66 (s, 1H), 7.97–7.94 (m, 2H), 7.44 (s, 1H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.31–7.35 (m, 1H), 3.93–3.87 (m, 4H), 1.74–1.68 (m, 2H), 1.66–1.60 (m, 4H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 157.0, 150.9, 146.0, 145.4, 133.0, 128.6, 128.3, 126.0, 101.3, 45.3, 25.7, 24.7; IR (KBr, cm<sup>-1</sup>): 3428, 2940, 2850, 1633, 1548, 1495, 1464, 1443, 1365, 1349, 1244, 1198, 1070, 1017, 908, 850, 771, 748, 713, 692, 594. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>16</sub>H<sub>18</sub>N<sub>5</sub> 280.1562, found 280.1563.

### 4-(7-phenylimidazo[1,2-a][1,3,5]triazin-2-yl)morpholine (3r)



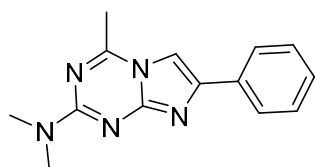
131.3 mg, yellow solid, 93% yield, mp 280-281 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.70 (s, 1H), 7.95–7.92 (m, 2H), 7.48 (s, 1H), 7.43–7.39 (m, 2H), 7.35–7.31 (m, 1H), 3.93 (t, *J* = 5.1 Hz, 4H), 3.77 (t, *J* = 5.1 Hz, 4H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 157.1, 150.4, 146.1, 145.7, 132.7, 128.6, 128.5, 126.0, 101.7, 66.7, 44.5; IR (KBr, cm<sup>-1</sup>): 3434, 2951, 2916, 2837, 1628, 1549, 1486, 1467, 1444, 1351, 1232, 1201, 1107, 1067, 931, 918, 774, 753, 731, 717, 691. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>15</sub>H<sub>16</sub>N<sub>5</sub>O 282.1355, found 282.1347.

### 7-phenyl-2-(pyrrolidin-1-yl)imidazo[1,2-a][1,3,5]triazine (3s)



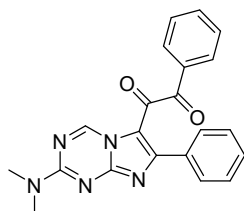
99.3 mg, yellow solid, 75% yield, mp 299-300 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.69 (s, 1H), 7.95 (d, *J* = 7.5 Hz, 2H), 7.45 (s, 1H), 7.40 (t, *J* = 7.5 Hz, 2H), 7.34–7.29 (m, 1H), 3.71-3.62 (m, 4H), 2.04-1.96 (m, 4H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 155.9, 150.7, 145.4, 132.8, 128.6, 128.3, 126.0, 101.3, 47.2, 47.0, 25.6, 25.2; IR (KBr, cm<sup>-1</sup>): 3439, 2962, 1633, 1580, 1505, 1458, 1349, 1294, 1205, 1070, 778, 719, 691, 505. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>15</sub>H<sub>16</sub>N<sub>5</sub> 266.1406, found 266.1402.

### *N,N*,4-trimethyl-7-phenylimidazo[1,2-a][1,3,5]triazin-2-amine (3t)



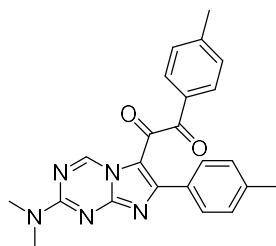
32.8 mg, light red solid, 26% yield, mp 164-165 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.96 (d, *J* = 7.4 Hz, 2H), 7.40 (t, *J* = 7.4 Hz, 2H), 7.35 (s, 1H), 7.32 (t, *J* = 7.4 Hz, 1H), 3.26 (s, 6H), 2.66 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 158.1, 154.7, 151.7, 145.1, 133.2, 128.5, 128.1, 125.9, 100.5, 37.1, 20.5; IR (KBr, cm<sup>-1</sup>): 3445, 2920, 1631, 1574, 1519, 1478, 1405, 1184, 1077, 1029, 772, 721, 699. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>14</sub>H<sub>16</sub>N<sub>5</sub> 254.1406, found 254.1421.

**1-(2-(dimethylamino)-7-phenylimidazo[1,2-a][1,3,5]triazin-6-yl)-2-phenylethane-1,2-dione (4a)**



144.5 mg, yellow solid, 78% yield, mp 267-268 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.02 (s, 1H), 7.76 (d, *J* = 7.7 Hz, 2H), 7.58 (t, *J* = 7.7 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 2H), 7.35 (d, *J* = 7.7 Hz, 2H), 7.28 (t, *J* = 7.7 Hz, 1H), 7.10 (t, *J* = 7.7 Hz, 2H), 3.40 (s, 3H), 3.34 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 191.3, 183.0, 161.5, 159.5, 154.4, 148.3, 134.2, 133.4, 132.3, 130.1, 129.9, 129.6, 128.6, 127.9, 116.0, 37.7, 37.3; IR (KBr, cm<sup>-1</sup>): 1681, 1650, 1633, 1585, 1525, 1479, 1393, 1360, 1256, 1221, 1132, 1008, 887, 790, 770, 724, 696. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>21</sub>H<sub>18</sub>N<sub>5</sub>O<sub>2</sub> 372.1460, found 372.1454.

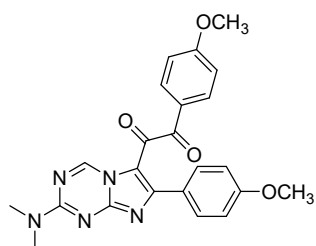
**1-(2-(dimethylamino)-7-(p-tolyl)imidazo[1,2-a][1,3,5]triazin-6-yl)-2-(p-tolyl)ethane-1,2-dione (4b)**



129.8 mg, yellow solid, 65% yield, mp 240-241 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.03 (s, 1H), 7.71 (d, *J* = 8.1 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 6.92 (d, *J* =

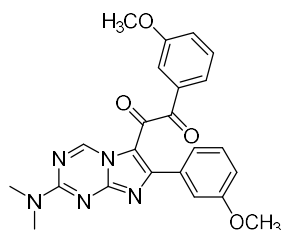
8.0 Hz, 2H), 3.40 (s, 3H), 3.34 (s, 3H), 2.45 (s, 3H), 2.29 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  190.9, 183.2, 161.3, 159.5, 154.3, 148.3, 145.3, 140.4, 131.1, 129.9, 129.8, 129.5, 129.3, 128.7, 115.8, 37.6, 37.3, 21.9, 21.4; IR (KBr,  $\text{cm}^{-1}$ ): 1681, 1651, 1634, 1587, 1486, 1393, 1336, 1261, 1220, 1130. HRMS (ESI-TOF)  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{23}\text{H}_{22}\text{N}_5\text{O}_2$  400.1773, found 400.1779.

**1-(2-(dimethylamino)-7-(4-methoxyphenyl)imidazo[1,2-a][1,3,5]triazin-6-yl)-2-(4-methoxyphenyl)ethane-1,2-dione (4c)**



129.3 mg, yellow solid, 60% yield, mp 168-169  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.01 (s, 1H), 7.79 (d,  $J = 8.9$  Hz, 2H), 7.35 (d,  $J = 8.7$  Hz, 2H), 6.90 (d,  $J = 8.9$  Hz, 2H), 6.64 (d,  $J = 8.7$  Hz, 2H), 3.89 (s, 3H), 3.76 (s, 3H), 3.38 (s, 3H), 3.33 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  190.1, 183.3, 164.4, 161.2, 160.9, 159.5, 154.3, 148.3, 132.1, 131.5, 126.7, 124.8, 115.7, 114.0, 113.4, 55.6, 55.3, 37.6, 37.3; IR (KBr,  $\text{cm}^{-1}$ ): 1668, 1651, 1633, 1601, 1574, 1558, 1487, 1393, 1334, 1259, 1218, 1180, 1130, 1031. HRMS (ESI-TOF)  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{23}\text{H}_{22}\text{N}_5\text{O}_4$  432.1672, found 432.1662.

**1-(2-(dimethylamino)-7-(3-methoxyphenyl)imidazo[1,2-a][1,3,5]triazin-6-yl)-2-(3-methoxyphenyl)ethane-1,2-dione (4d)**

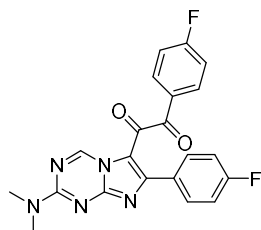


131.8 mg, yellow solid, 61% yield, mp 111-112  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.01 (s, 1H), 7.40 (d,  $J = 7.5$  Hz, 1H), 7.33 (t,  $J = 7.8$  Hz, 1H), 7.23-7.19 (m, 1H), 7.15-7.11 (m, 1H), 6.99 (t,  $J = 7.8$  Hz, 1H), 6.94-6.86 (m, 2H), 6.86-6.81 (m, 1H), 3.80 (s, 3H), 3.57 (s, 3H), 3.40 (s, 3H), 3.34 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  191.1, 182.8, 161.3, 159.8, 159.5, 159.1, 154.4, 148.2, 134.8, 133.6, 129.7, 129.1, 122.8, 122.6, 121.3, 117.2, 116.0, 113.8, 112.5, 55.5, 55.0, 37.7, 37.3; IR (KBr,  $\text{cm}^{-1}$ ): 1698, 1683, 1651, 1634, 1595, 1575, 1558, 1539,

1520, 1486, 1456, 1428, 1417, 1386, 1304, 1261, 1213, 1139, 1073, 1049, 899, 750, 720, 459.

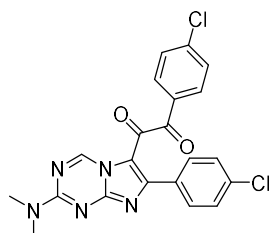
HRMS (ESI-TOF)  $m/z$   $[M+H]^+$  calcd for  $C_{23}H_{22}N_5O_4$  432.1672, found 432.1665.

**1-(2-(dimethylamino)-7-(4-fluorophenyl)imidazo[1,2-a][1,3,5]triazin-6-yl)-2-(4-fluorophenyl)ethane-1,2-dione (4e)**



127.0 mg, yellow solid, 63% yield, mp 126-127 °C;  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  9.99 (s, 1H), 7.85-7.82 (m, 2H), 7.35-7.32 (m, 2H), 7.14-7.01 (m, 2H), 6.89-6.80 (m, 2H), 3.40 (s, 3H), 3.34 (s, 3H);  $^{13}C$  NMR (125 MHz,  $CDCl_3$ )  $\delta$  189.8, 182.3, 166.4 (d,  $J = 258.1$  Hz), 163.9 (d,  $J = 251.1$  Hz), 160.3, 159.5, 154.4, 148.2, 132.3 (d,  $J = 9.7$  Hz), 131.9 (d,  $J = 8.7$  Hz), 129.8, 128.5, 116.1 (d,  $J = 22.1$  Hz), 115.9, 115.2 (d,  $J = 21.9$  Hz), 37.7, 37.3; IR (KBr,  $cm^{-1}$ ): 1669, 1636, 1597, 1568, 1532, 1495, 1448, 1395, 1339, 1244, 1215, 1132, 1071, 1021, 788, 750, 719, 687. HRMS (ESI-TOF)  $m/z$   $[M+H]^+$  calcd for  $C_{21}H_{16}F_2N_5O_2$  408.1272, found 408.1271.

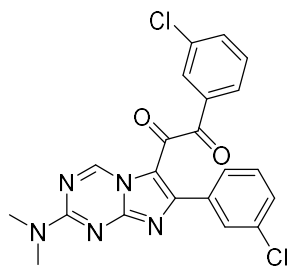
**1-(4-chlorophenyl)-2-(7-(4-chlorophenyl)-2-(dimethylamino)imidazo[1,2-a][1,3,5]triazin-6-yl)ethane-1,2-dione (4f)**



200.0 mg, yellow solid, 90% yield, mp 216-218 °C;  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  9.99 (s, 1H), 7.74 (d,  $J = 8.5$  Hz, 2H), 7.44 (d,  $J = 8.5$  Hz, 2H), 7.29 (d,  $J = 8.4$  Hz, 2H), 7.13 (d,  $J = 8.4$  Hz, 2H), 3.41 (s, 3H), 3.35 (s, 3H);  $^{13}C$  NMR (125 MHz,  $CDCl_3$ )  $\delta$  190.0, 182.0, 160.1, 159.5, 154.5, 148.2, 141.2, 136.6, 131.6, 131.2, 130.9, 130.7, 129.2, 128.3, 115.9, 37.7, 37.4; IR (KBr,  $cm^{-1}$ ): 1682, 1634, 1589, 1558, 1472, 1404, 1389, 1335, 1257, 1218, 1131, 1091. HRMS (ESI-TOF)  $m/z$   $[M+H]^+$  calcd for  $C_{21}H_{16}Cl_2N_5O_2$  440.0681, found 440.0680.

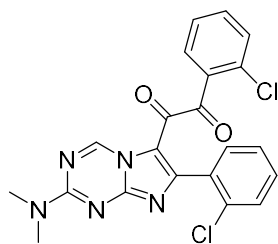
**1-(3-chlorophenyl)-2-(7-(3-chlorophenyl)-2-(dimethylamino)imidazo[1,2-a][1,3,5]triazin-6-yl)ethane-1,2-dione (4g)**





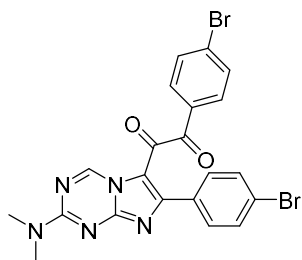
161.7 mg, yellow solid, 74% yield, mp 199-200 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 9.98 (s, 1H), 7.78–7.74 (m, 1H), 7.70 (d, *J* = 7.9 Hz, 1H), 7.59 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.42 (t, *J* = 7.9 Hz, 1H), 7.33–7.29 (m, 2H), 7.27–7.24 (m, 1H), 7.15 (t, *J* = 7.9 Hz, 1H), 3.41 (s, 3H), 3.35 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 189.8, 181.8, 159.6, 159.5, 154.4, 148.2, 135.3, 134.7, 134.4, 134.2, 133.9, 130.3, 130.2, 129.8, 129.5, 129.3, 128.0, 127.7, 115.9, 37.7, 37.4; IR (KBr, cm<sup>-1</sup>): 1674, 1642, 1580, 1519, 1505, 1470, 1456, 1410, 1385, 1334, 1246, 1207, 1175, 1136, 915, 789. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>21</sub>H<sub>16</sub>Cl<sub>2</sub>N<sub>5</sub>O<sub>2</sub> 440.0681, found 440.0686.

**1-(2-chlorophenyl)-2-(7-(2-chlorophenyl)-2-(dimethylamino)imidazo[1,2-a][1,3,5]triazin-6-yl)ethane-1,2-dione (4h)**



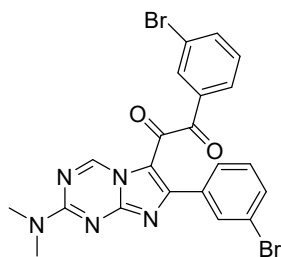
117.7 mg, yellow solid, 53% yield, mp 68-70 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 9.98 (s, 1H), 7.58 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.44 (td, *J* = 7.8, 1.6 Hz, 1H), 7.37 – 7.34 (m, 1H), 7.30 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.26 – 7.23 (m, 2H), 7.23 – 7.21 (m, 1H), 7.07 (td, *J* = 7.6, 1.6 Hz, 1H), 3.40 (s, 3H), 3.34 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 189.6, 181.1, 159.5, 157.6, 154.2, 148.1, 134.4, 134.3, 133.9, 132.6, 131.9, 131.7, 131.6, 131.0, 130.8, 129.5, 126.9, 126.0, 116.9, 37.6, 37.3; IR (KBr, cm<sup>-1</sup>): 1732, 1639, 1589, 1528, 1498, 1464, 1436, 1411, 1384, 1336, 1273, 1235, 1212, 1128, 1056, 1003, 894, 788, 747. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>21</sub>H<sub>17</sub>Cl<sub>2</sub>N<sub>5</sub>O<sub>2</sub> 440.0681, found 440.0688.

**1-(4-bromophenyl)-2-(7-(4-bromophenyl)-2-(dimethylamino)imidazo[1,2-a][1,3,5]triazin-6-yl)ethane-1,2-dione (4i)**



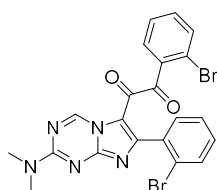
219.5 mg, yellow solid, 80% yield, mp 230-231 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  9.97 (s, 1H), 7.65 (d,  $J = 8.6$  Hz, 2H), 7.60 (d,  $J = 8.6$  Hz, 2H), 7.29 (d,  $J = 8.4$  Hz, 2H), 7.21 (d,  $J = 8.4$  Hz, 2H), 3.40 (s, 3H), 3.34 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  190.2, 182.0, 160.0, 159.5, 154.4, 148.2, 132.2, 132.0, 131.4, 131.3, 131.1, 131.0, 130.1, 125.0, 115.8, 37.8, 37.4; IR (KBr,  $\text{cm}^{-1}$ ): 1674, 1651, 1634, 1589, 1558, 1471, 1386, 1334, 1256, 1218, 1129, 1070, 1004. HRMS (ESI-TOF)  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{21}\text{H}_{16}\text{Br}_2\text{N}_5\text{O}_2$  527.9671, found 527.9683.

**1-(3-bromophenyl)-2-(7-(3-bromophenyl)-2-(dimethylamino)imidazo[1,2-a][1,3,5]triazin-6-yl)ethane-1,2-dione (4j)**



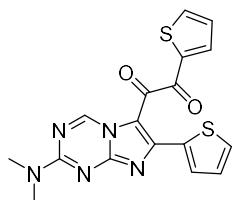
161.4 mg, yellow solid, 61% yield, mp 192-193 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  9.97 (s, 1H), 7.91 (t,  $J = 1.7$  Hz, 1H), 7.77–7.71 (m, 2H), 7.49–7.44 (m, 1H), 7.41–7.36 (m, 2H), 7.36–7.33 (m, 1H), 7.10 (t,  $J = 7.8$  Hz, 1H), 3.41 (s, 3H), 3.34 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  189.8, 181.7, 159.7, 159.5, 154.5, 148.2, 137.3, 134.9, 134.2, 133.2, 132.7, 132.3, 130.5, 129.8, 128.4, 128.2, 123.3, 122.2, 115.9, 37.7, 37.4; IR (KBr,  $\text{cm}^{-1}$ ): 1674, 1651, 1639, 1576, 1558, 1519, 1505, 1464, 1409, 1384, 1335, 1244, 1208, 1173, 1131, 1071, 1007, 905. HRMS (ESI-TOF)  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{21}\text{H}_{16}\text{Br}_2\text{N}_5\text{O}_2$  527.9671, found 527.9685.

**1-(2-bromophenyl)-2-(7-(2-bromophenyl)-2-(dimethylamino)imidazo[1,2-a][1,3,5]triazin-6-yl)ethane-1,2-dione (4k)**



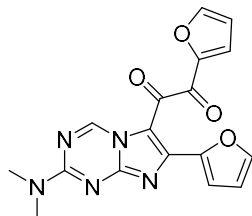
169.7 mg, yellow solid, 64% yield, mp 183-184 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 9.99 (s, 1H), 7.61–7.54 (m, 2H), 7.48–7.43 (m, 1H), 7.35 (td, *J* = 7.6, 1.8 Hz, 1H), 7.32-7.28 (m, 2H), 7.17–7.13 (m, 2H), 3.40 (s, 3H), 3.35 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 190.1, 180.8, 159.5, 158.8, 154.1, 148.1, 134.6, 134.2, 133.5, 133.4, 133.3, 132.7, 131.7, 130.9, 127.4, 126.7, 123.5, 122.5, 117.1, 37.7, 37.3; IR (KBr, cm<sup>-1</sup>): 1716, 1682, 1652, 1639, 1586, 1558, 1539, 1506, 1471, 1456, 1387, 1340, 1240, 1215, 1125, 1047, 1004, 893, 762, 743. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>21</sub>H<sub>16</sub>Br<sub>2</sub>N<sub>5</sub>O<sub>2</sub> 527.9671, found 527.9680.

**1-(2-(dimethylamino)-7-(thiophen-2-yl)imidazo[1,2-a][1,3,5]triazin-6-yl)-2-(thiophen-2-yl)ethane-1,2-dione (4l)**



110.4 mg, brown solid, 58% yield, mp 262-264 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 9.91 (s, 1H), 7.82–7.80 (m, 1H), 7.79–7.75 (m, 1H), 7.44 (d, *J* = 4.8 Hz, 1H), 7.20 (d, *J* = 4.3 Hz, 1H), 7.17 (t, *J* = 4.3 Hz, 1H), 6.89 (t, *J* = 4.8 Hz, 1H), 3.39 (s, 3H), 3.34 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 183.8, 180.9, 159.5, 154.3, 154.0, 148.1, 140.5, 136.5, 135.8, 134.4, 131.2, 130.5, 128.6, 127.4, 115.0, 37.7, 37.4; IR (KBr, cm<sup>-1</sup>): 1630, 1592, 1572, 1483, 1409, 1384, 1351, 1320, 1265, 1214, 1160, 1112, 1077, 1055, 831, 740, 716. HRMS (ESI-TOF) *m/z* [M+H]<sup>+</sup> calcd for C<sub>17</sub>H<sub>14</sub>N<sub>5</sub>O<sub>2</sub>S<sub>2</sub> 384.0589, found 384.0585.

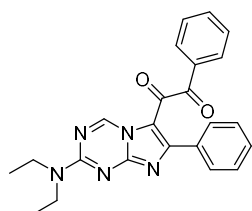
**1-(2-(dimethylamino)-7-(furan-2-yl)imidazo[1,2-a][1,3,5]triazin-6-yl)-2-(furan-2-yl)ethane-1,2-dione (4m)**



46.8 mg, brown solid, 26% yield, mp 245-246 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 9.90 (s, 1H), 7.76-7.73 (m, 1H), 7.39 (d, *J* = 3.4 Hz, 1H), 7.26 (d, *J* = 3.4 Hz, 1H), 7.19-7.16 (m, 1H), 6.65 (dd, *J* = 3.6, 1.6 Hz, 1H), 6.49 (dd, *J* = 3.6, 1.6 Hz, 1H), 3.38 (s, 3H), 3.33 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 181.4, 179.1, 159.5, 154.7, 150.5, 148.2, 148.1, 147.9, 147.5, 144.7,

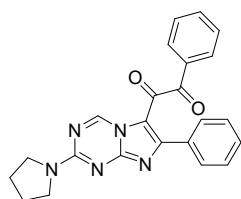
121.0, 115.4, 113.6, 112.7, 112.6, 37.7, 37.3; IR (KBr,  $\text{cm}^{-1}$ ): 1467, 1634, 1595, 1504, 1462, 1405, 1366, 1331, 1218, 1135, 1037, 1005, 945, 884, 849, 776, 728, 437. HRMS (ESI-TOF)  $m/z$   $[M+H]^+$  calcd for  $\text{C}_{17}\text{H}_{14}\text{N}_5\text{O}_4$  352.1046, found 352.1034..

**1-(2-(diethylamino)-7-phenylimidazo[1,2-a][1,3,5]triazin-6-yl)-2-phenylethane-1,2-dione (4n)**



161.0 mg, yellow solid, 80% yield, mp 72.4-74.4 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.03 (s, 1H), 7.77-7.72 (m, 2H), 7.60-7.55 (m, 1H), 7.40 (t,  $J = 7.8$  Hz, 2H), 7.37-7.34 (m, 2H), 7.30-7.28 (m, 1H), 7.10 (t,  $J = 7.8$  Hz, 2H), 3.80 (q,  $J = 7.1$  Hz, 2H), 3.77 (q,  $J = 7.1$  Hz, 2H), 1.30 (t,  $J = 7.1$  Hz, 3H), 1.29 (t,  $J = 7.1$  Hz, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  191.4, 182.9, 161.4, 158.6, 154.6, 148.4, 134.2, 133.4, 132.3, 130.1, 129.9, 129.6, 128.6, 127.9, 116.0, 43.2, 42.7, 13.4, 12.5; IR (KBr,  $\text{cm}^{-1}$ ): 1682, 1635, 1568, 1526, 1496, 1476, 1441, 1392, 1357, 1336, 1254, 1234, 1199, 1131, 1079, 1006, 878, 789, 718. HRMS (ESI-TOF)  $m/z$   $[M+H]^+$  calcd for  $\text{C}_{23}\text{H}_{22}\text{N}_5\text{O}_2$  400.1773, found 400.1779.

**1-phenyl-2-(7-phenyl-2-(pyrrolidin-1-yl)imidazo[1,2-a][1,3,5]triazin-6-yl)ethane-1,2-dione (4o)**

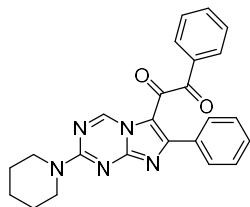


132.3 mg, yellow solid, 66% yield, mp 175-176 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.04 (s, 1H), 7.77 (d,  $J = 7.4$  Hz, 2H), 7.58 (t,  $J = 7.4$  Hz, 1H), 7.41 (t,  $J = 7.4$  Hz, 2H), 7.36 (d,  $J = 7.6$  Hz, 2H), 7.28 (t,  $J = 7.6$  Hz, 1H), 7.10 (t,  $J = 7.6$  Hz, 2H), 3.79 (t,  $J = 6.6$  Hz, 2H), 3.75 (t,  $J = 6.6$  Hz, 2H), 2.10 - 2.05 (m, 4H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  191.3, 182.9, 161.5, 157.4, 154.4, 148.4, 134.2, 133.4, 132.3, 130.1, 129.9, 129.7, 128.6, 127.9, 115.9, 47.7, 47.3, 25.4, 25.1; IR (KBr,  $\text{cm}^{-1}$ ): 1682, 1634, 1593, 1573, 1525, 1495, 1479, 1455, 1393, 1336, 1251, 1222, 1173, 1133, 1072, 1007, 888, 850, 781, 748, 726, 714, 697, 666, 620. HRMS

(ESI-TOF)  $m/z$   $[M+H]^+$  calcd for  $C_{23}H_{20}N_5O_2$  398.1617, found 398.1631.

**1-phenyl-2-(7-phenyl-2-(piperidin-1-yl)imidazo[1,2-a][1,3,5]triazin-6-yl)ethane-1,2-dione**

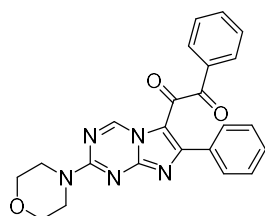
**(4p)**



146.4 mg, yellow solid, 71% yield, mp 108-110 °C;  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  10.00 (s, 1H), 7.75 (d,  $J = 7.4$  Hz, 2H), 7.58 (t,  $J = 7.4$  Hz, 1H), 7.41 (t,  $J = 7.4$  Hz, 2H), 7.35 (d,  $J = 6.8$  Hz, 2H), 7.29 (t,  $J = 6.8$  Hz, 1H), 7.11 (t,  $J = 6.8$  Hz, 2H), 4.04-3.95 (m, 4H), 1.78-1.66 (m, 6H);  $^{13}C$  NMR (125 MHz,  $CDCl_3$ )  $\delta$  191.3, 183.0, 161.5, 158.4, 154.7, 148.5, 134.2, 133.4, 130.1, 129.9, 129.7, 129.6, 128.6, 128.0, 116.0, 46.1, 45.3, 26.2, 25.6, 24.5; IR (KBr,  $cm^{-1}$ ): 1722, 1714, 1674, 1651, 1634, 1598, 1568, 1530, 1495, 1448, 1393, 1361, 1338, 1243, 1214, 1132, 1071, 1023, 750, 719, 668, 648. HRMS (ESI-TOF)  $m/z$   $[M+H]^+$  calcd for  $C_{24}H_{22}N_5O_2$  412.1773, found 412.1768.

**1-(2-morpholino-7-phenylimidazo[1,2-a][1,3,5]triazin-6-yl)-2-phenylethane-1,2-dione**

**(4q)**



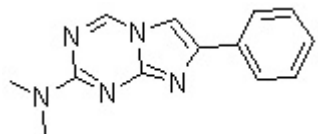
99.6 mg, yellow solid, 48% yield, mp 102-104 °C;  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  10.04 (s, 1H), 7.78 – 7.74 (m, 2H), 7.61 – 7.57 (m, 1H), 7.44 – 7.40 (m, 2H), 7.37 – 7.33 (m, 2H), 7.32 – 7.28 (m, 1H), 7.13 – 7.09 (m, 2H), 4.09 – 4.02 (m, 4H), 3.84 – 3.80 (m, 4H).  $^{13}C$  NMR (125 MHz,  $CDCl_3$ )  $\delta$  191.1, 183.3, 161.4, 158.7, 154.2, 148.8, 134.3, 133.3, 132.1, 130.2, 129.9, 129.6, 128.7, 128.0, 116.2, 66.8, 66.5, 45.2, 44.4; IR (KBr,  $cm^{-1}$ ): 1481, 1634, 1592, 1587, 1524, 11494, 1476, 1446, 1393, 1352, 1336, 1243, 1178, 1134, 1118, 1068, 992, 913, 786, 720, 699, 616. HRMS (ESI-TOF)  $m/z$   $[M+H]^+$  calcd for  $C_{23}H_{20}N_5O_3$  414.1566, found 414.1567.

191008

ZWQ190716-a

CDC13

1008



**3a**

8.6788

7.9695

7.9668

7.9526

7.4498

7.4320

7.4173

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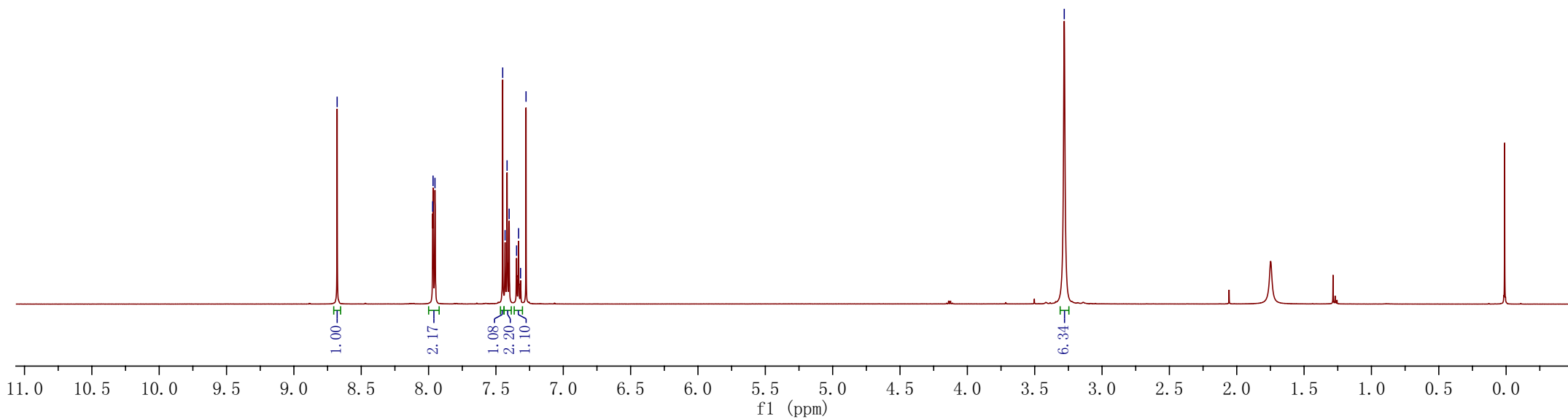
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7.3319

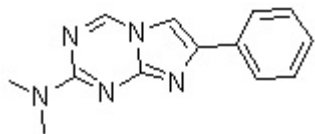
7.3171

7.2765

3.2805



200903  
ZWQ200801 CDC13 0903



**3a**

— 157.9438

— 150.7538

— 146.0105

— 145.1684

— 133.0856

— 128.5670

— 128.2538

— 125.9962

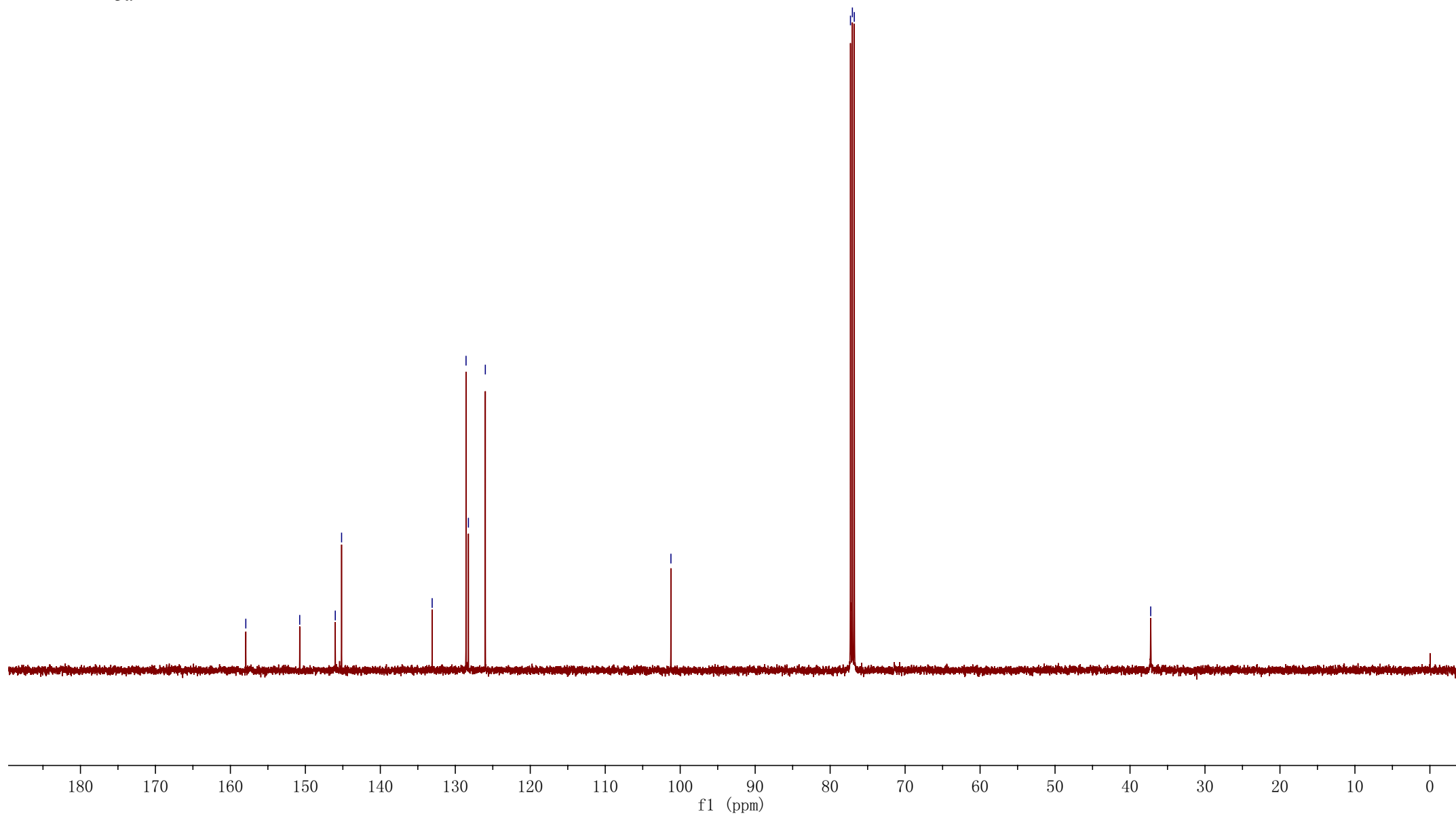
— 101.2376

— 77.2874

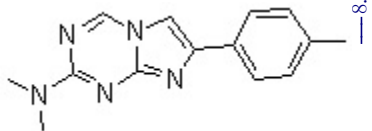
— 77.0331

— 76.7791

— 37.2407



ZWQ200817-a CDCl3

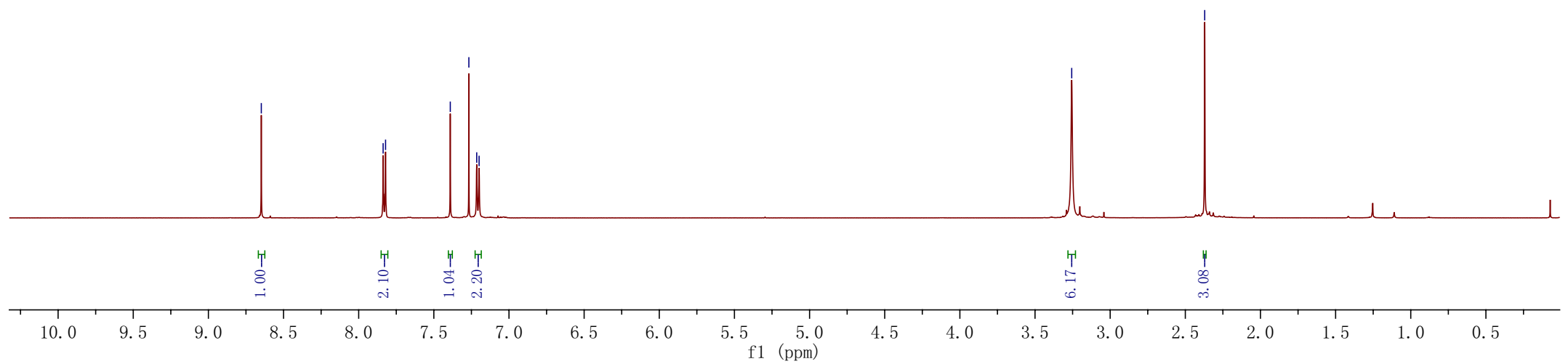


**3b**

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7.2670  
7.2147  
7.1989

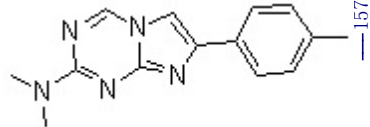
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2.3710

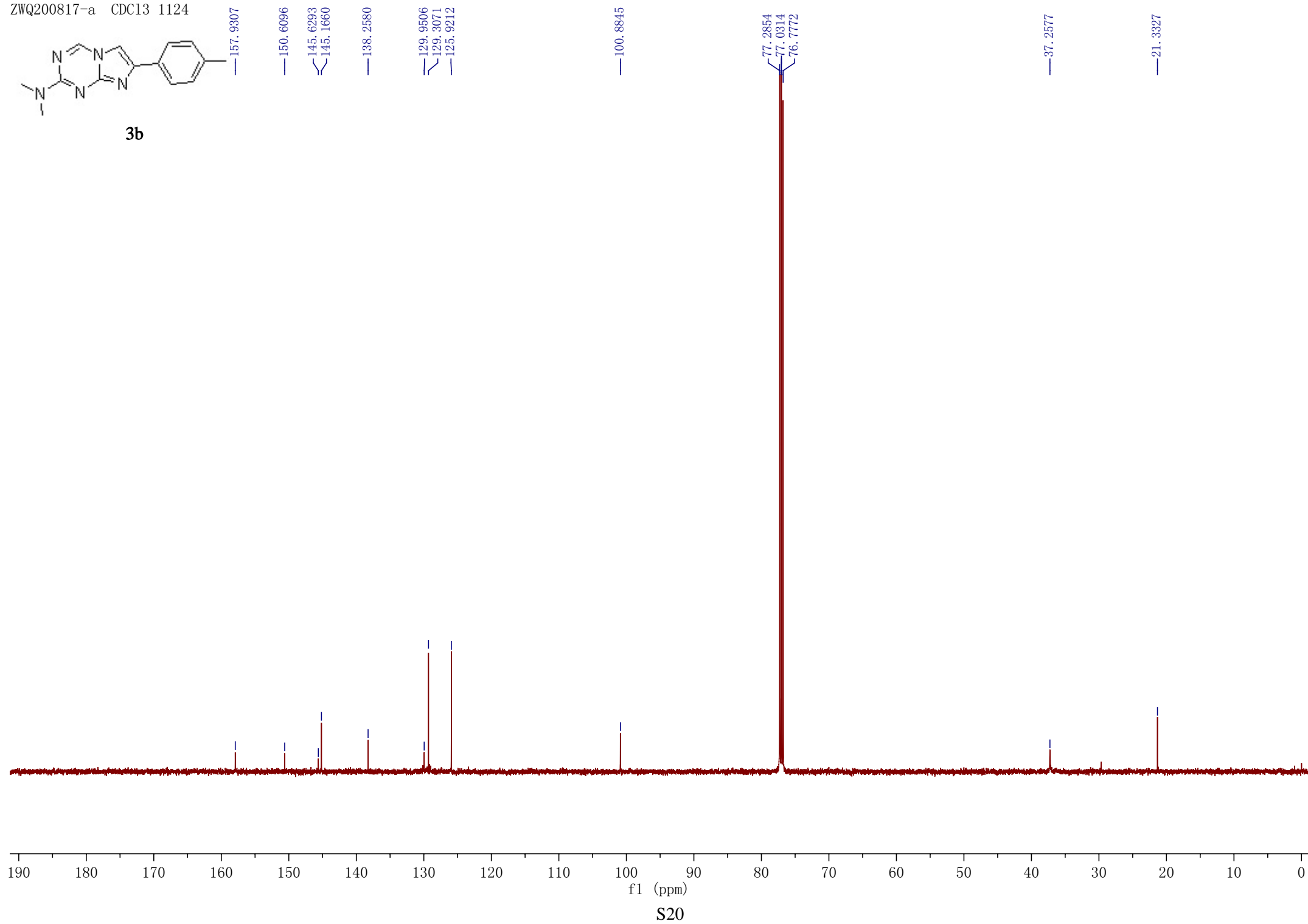




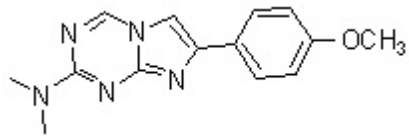
ZWQ200817-a CDC13 1124



3b



200903  
ZWQ200817-b CDC13 0903



3c

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7.2760

6.9470  
6.9294

3.8446

3.2626

1.00

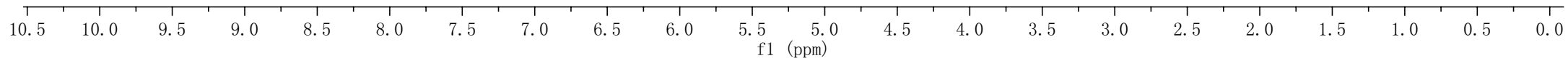
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1.06

2.12

3.22

6.27

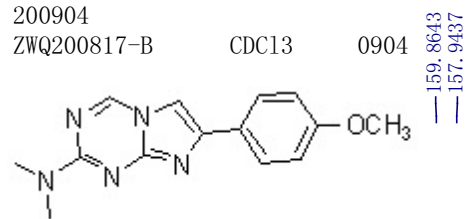


200904

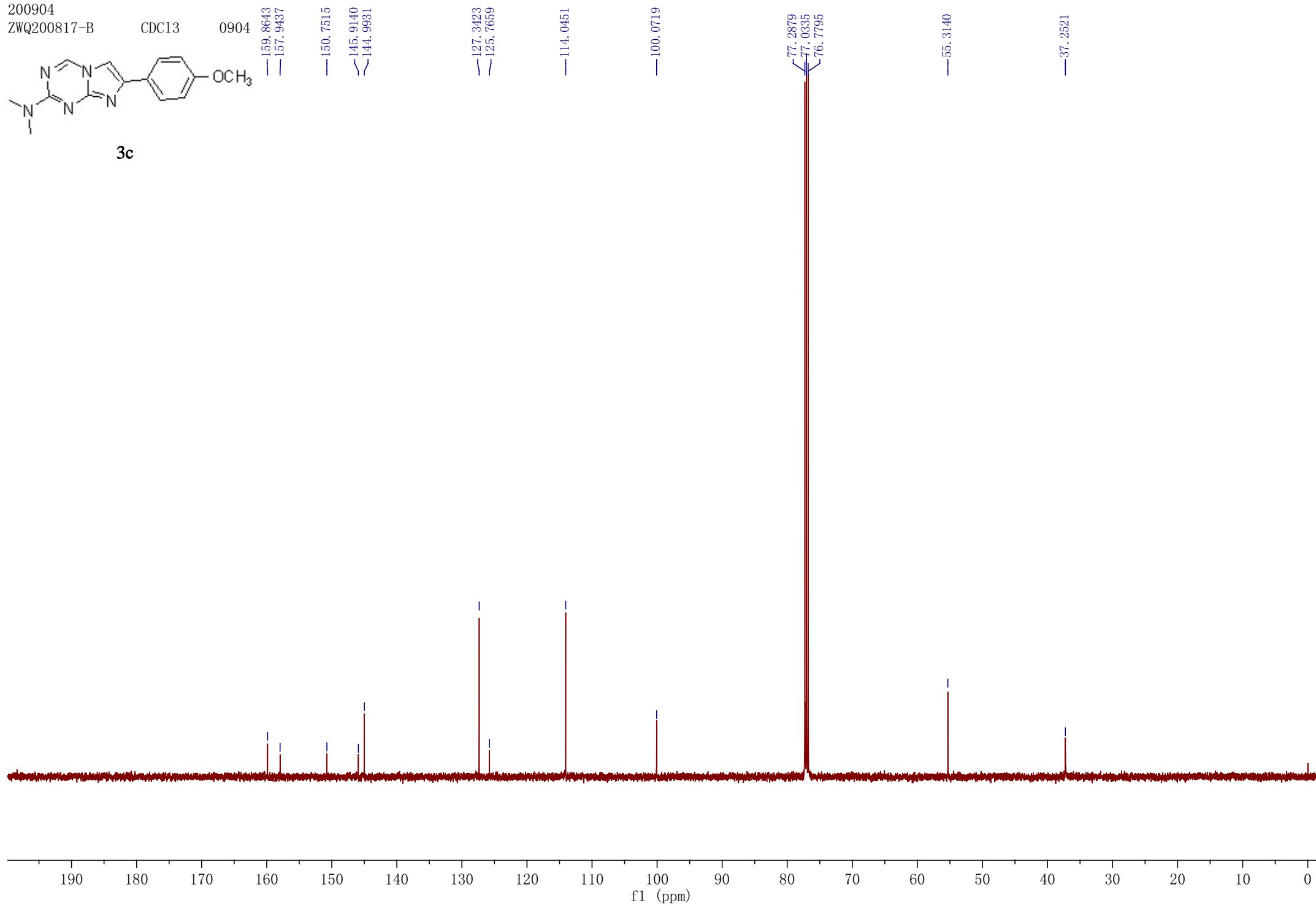
ZWQ200817-B

CDC13

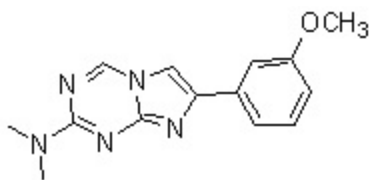
0904



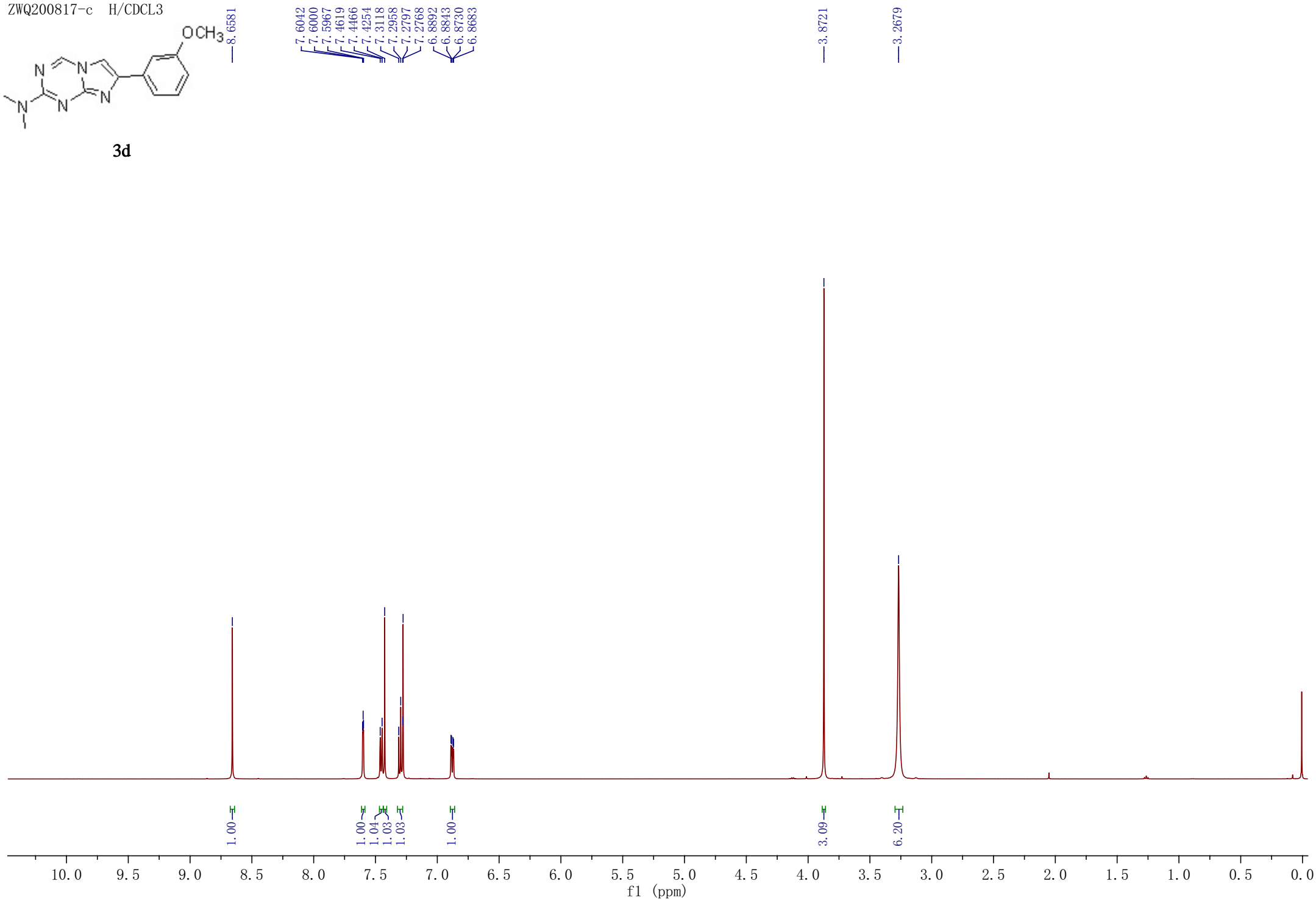
3c



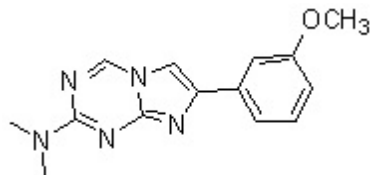
ZWQ200817-c H/CDCL3



**3d**



ZWQ200817-c CDC13 0104



3d

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—157.9105

—150.6510

—145.7767  
—145.1622

—134.4453

—129.4872

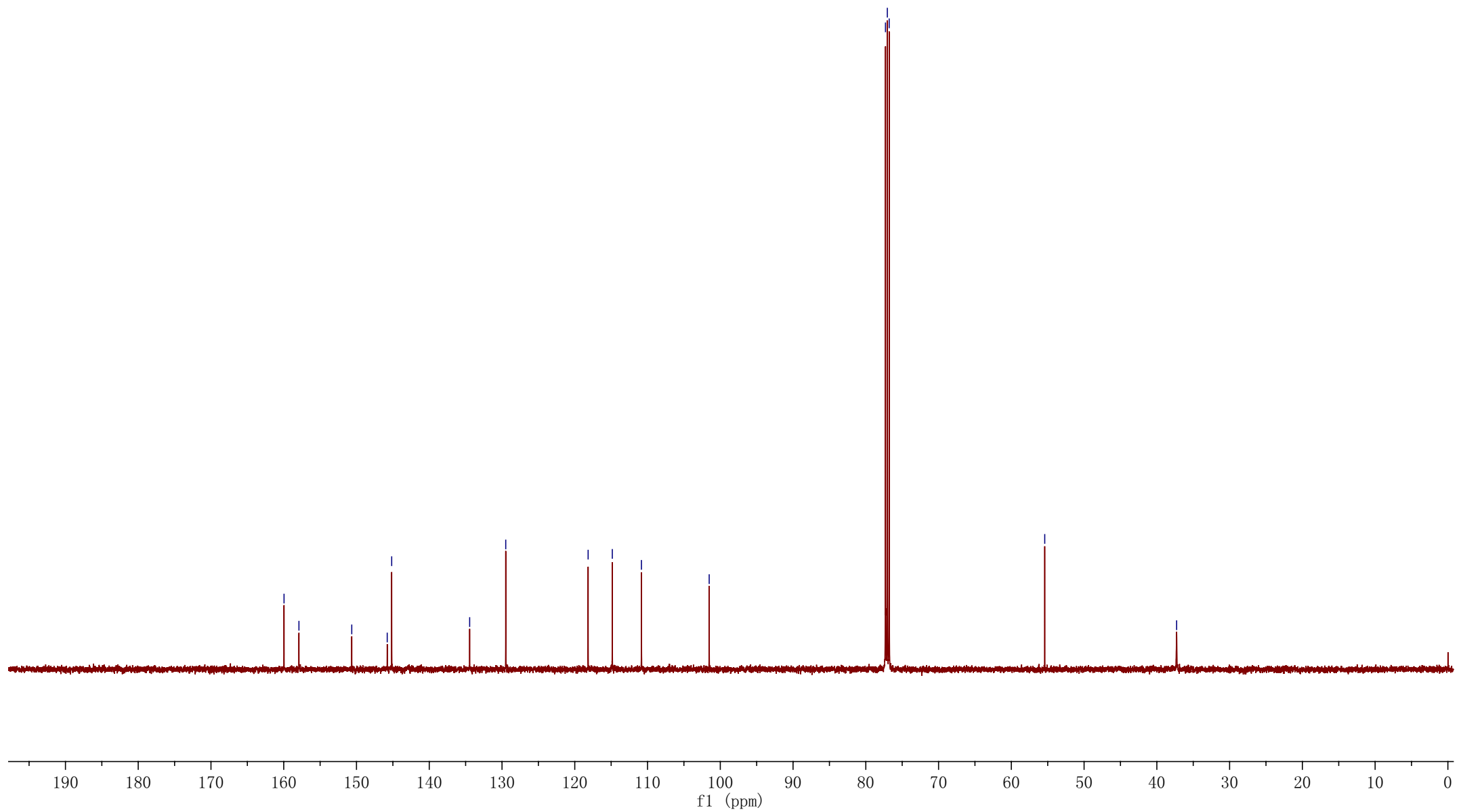
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—101.5250

—77.2958  
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—76.7877

—55.4066

—37.2815



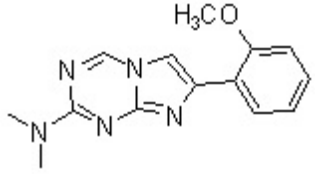
200831  
ZWQ200825-C CDCL3 0831

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8.4820

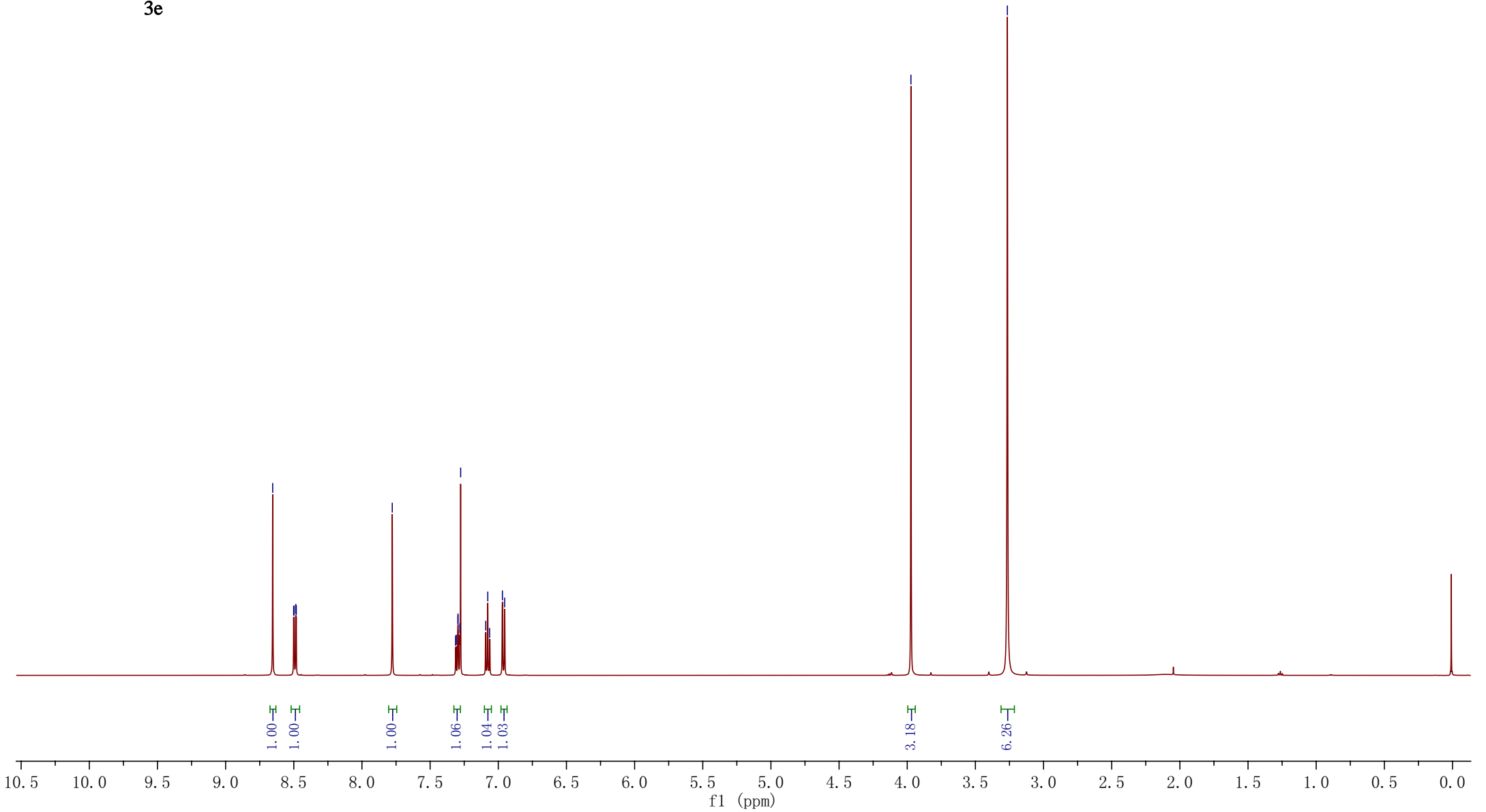
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7.0635  
6.9696  
6.9532

3.9729

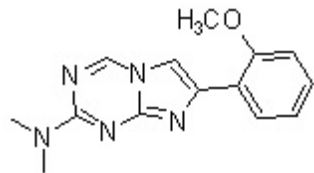
3.2656



3e



200902  
ZWQ200825-c CDC13 0902



3e

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149.4847

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141.3035

129.5017  
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121.6235  
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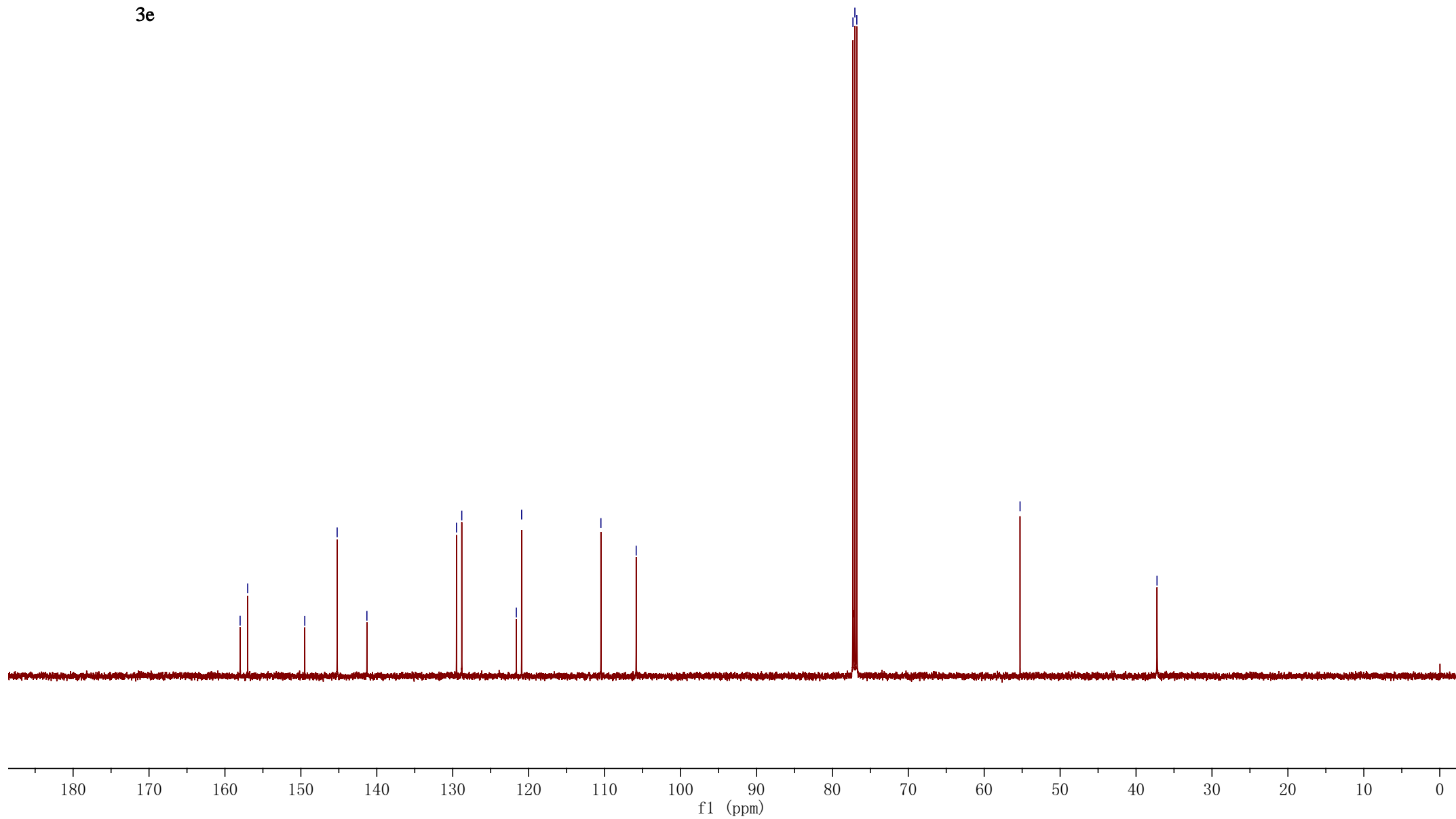
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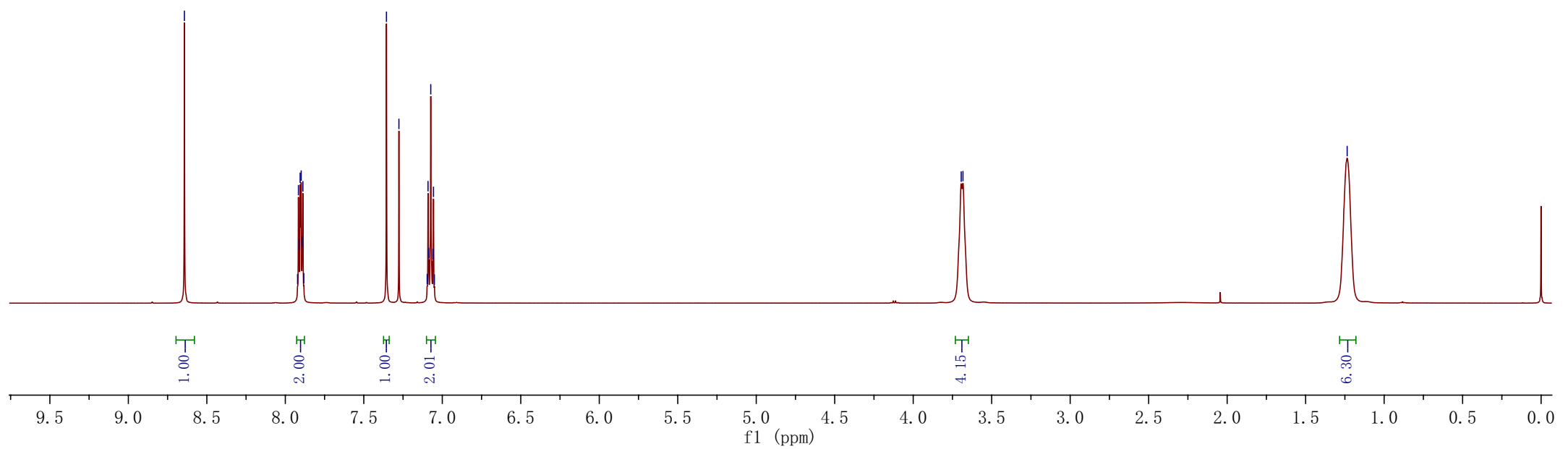
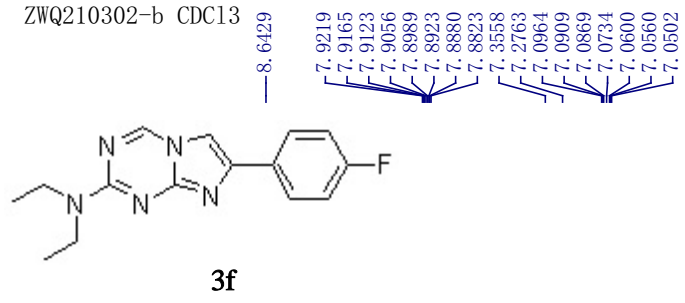
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77.2878  
77.0334  
76.7793

55.2777

37.2398







ZWQ210302-b CDC13

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144.8816

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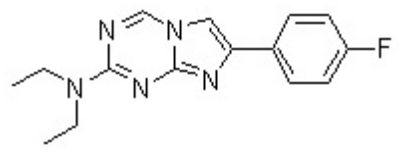
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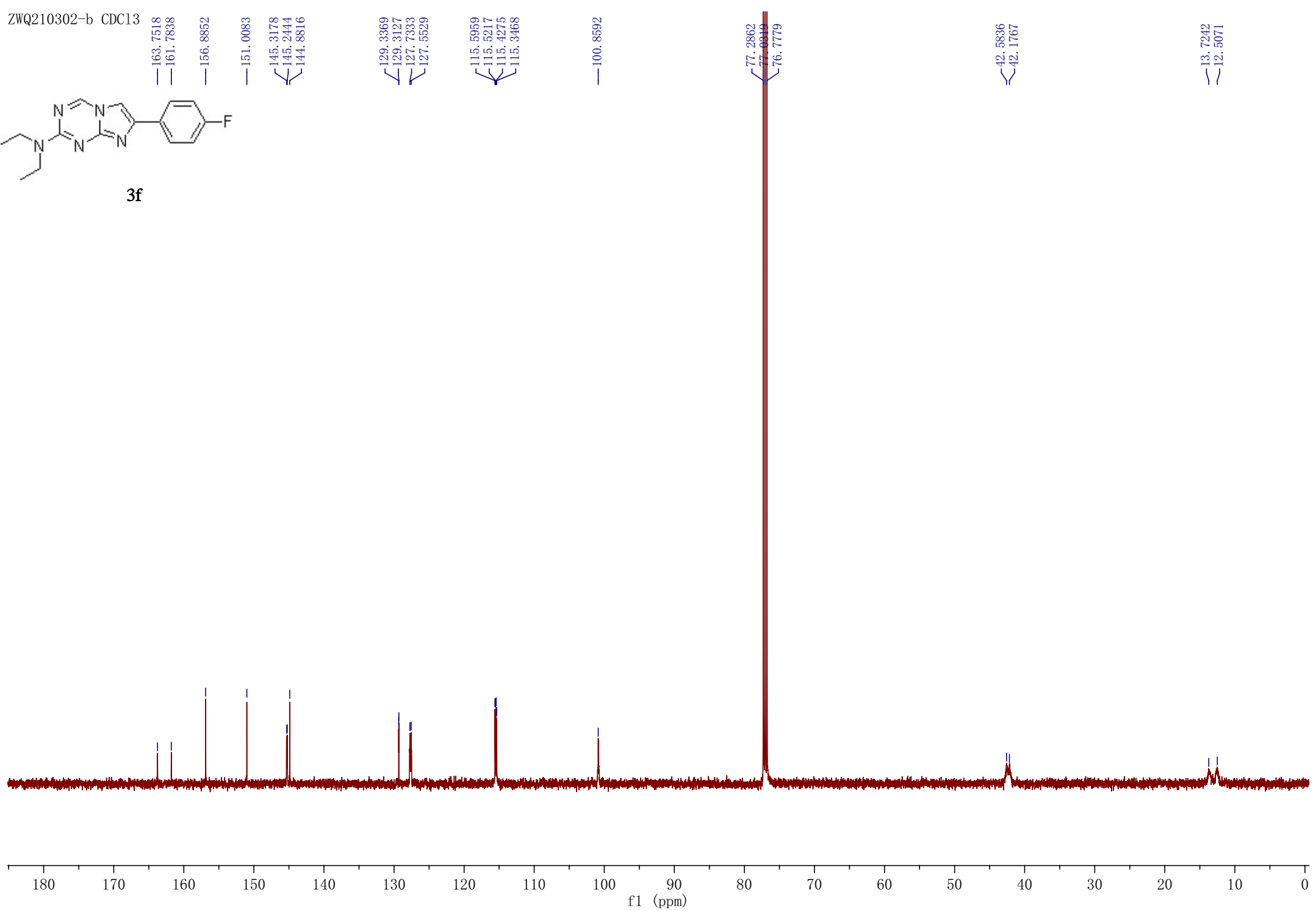
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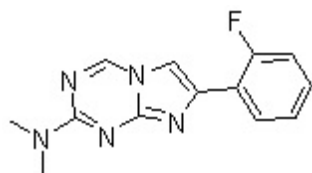
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3f



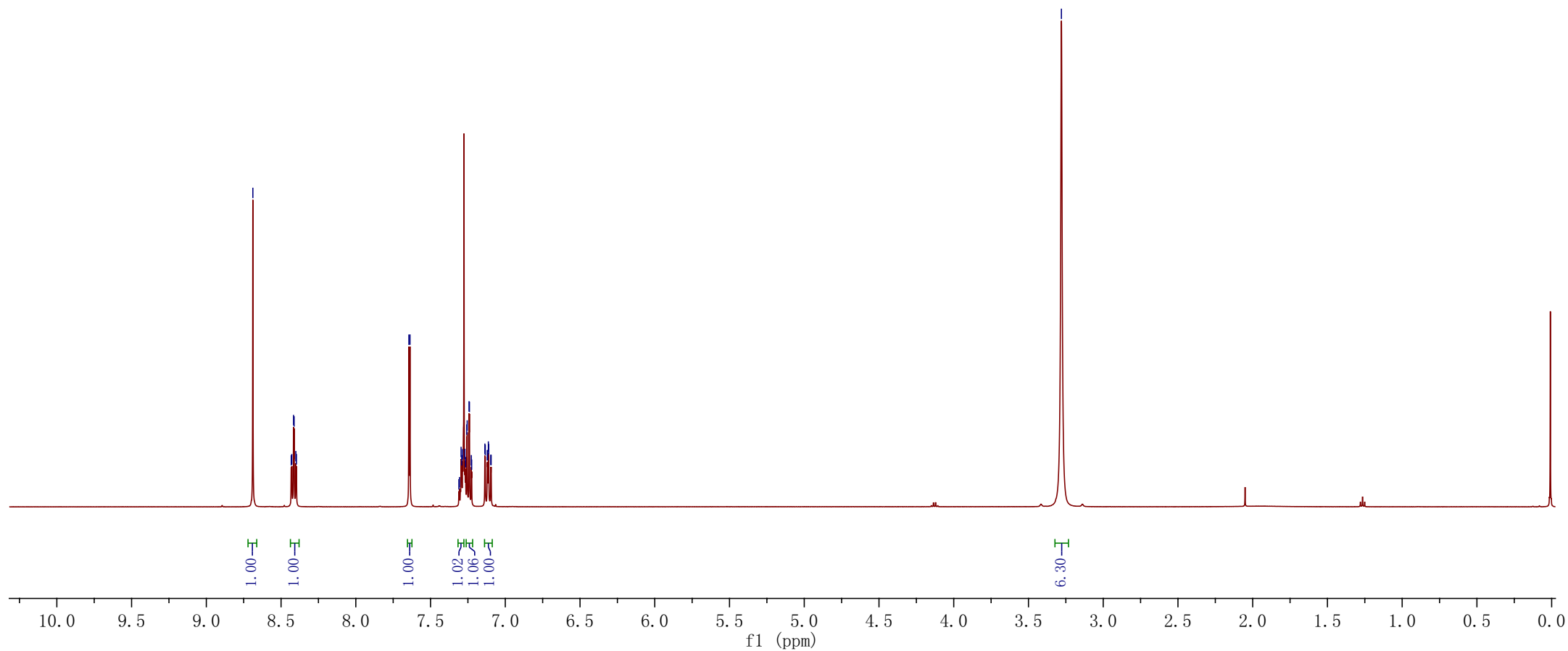


3g

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8.4127  
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8.3972

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7.2698  
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7.2275  
7.2250  
7.1364  
7.1340  
7.1202  
7.1179  
7.1132  
7.1106  
7.0972  
7.0947

3.2796



ZWQ200827-a CDC13 0904

161.5095  
159.5244  
158.0701

150.0401

145.3394

139.4479

129.4748

129.4457

129.1712

129.1019

124.4757

124.4497

121.0116

120.9156

115.4443

115.2697

105.7191

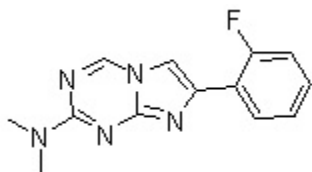
105.5857

77.2852

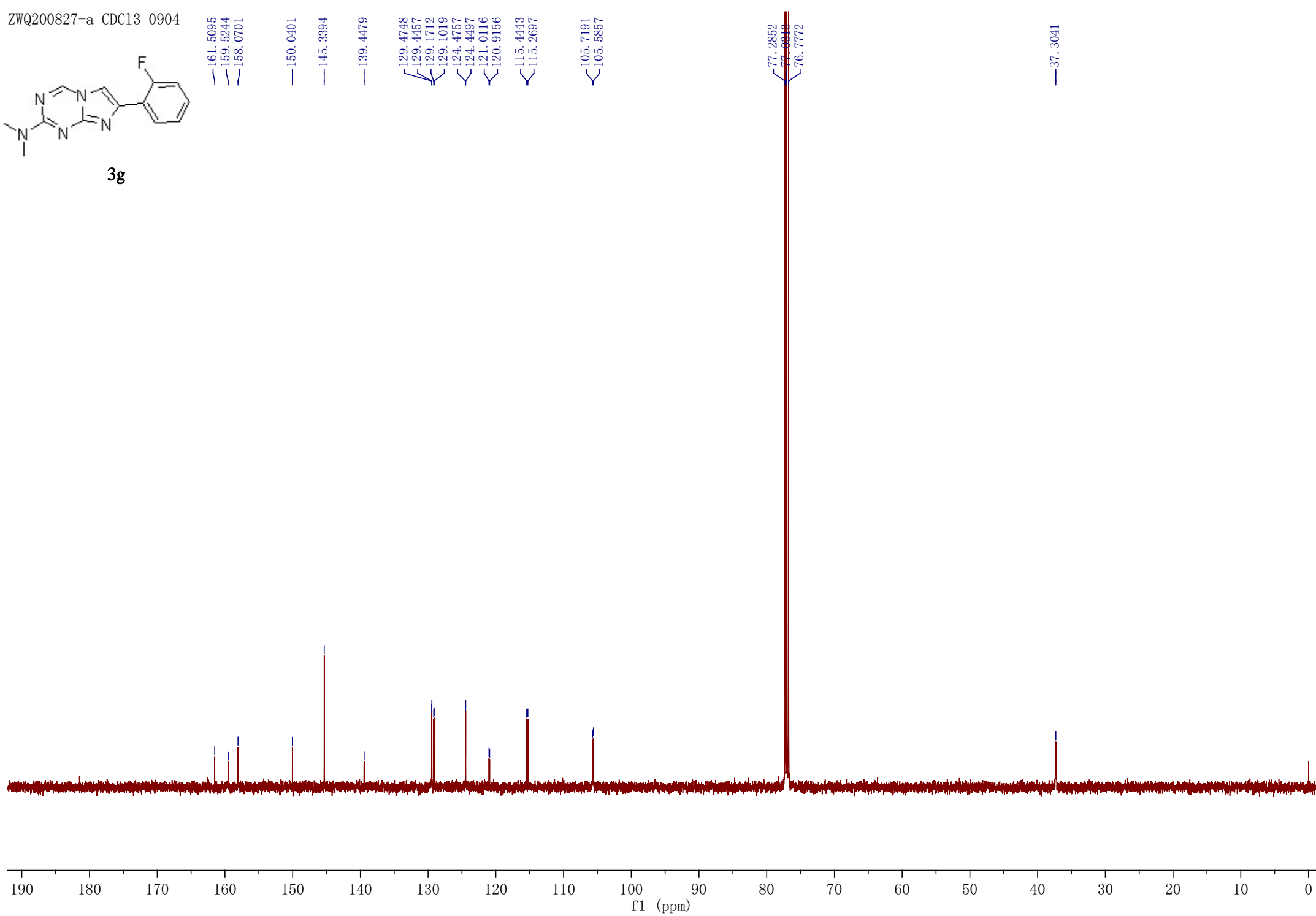
77.0319

76.7772

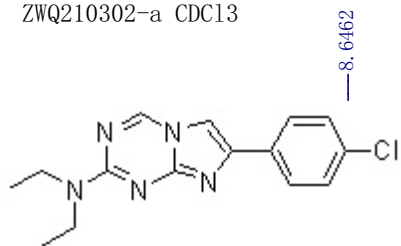
37.3041



3g



S30



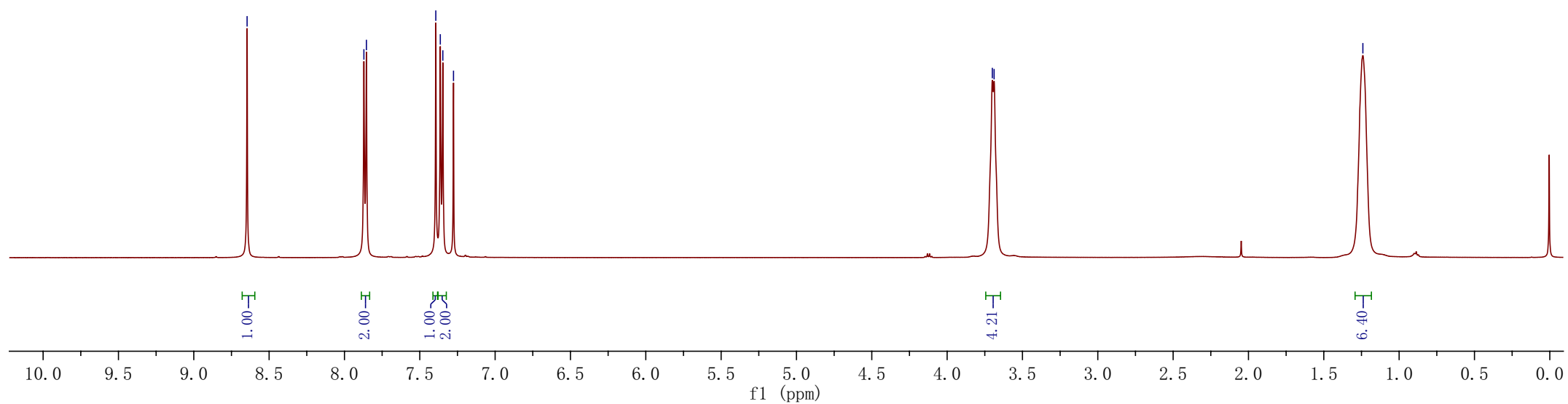
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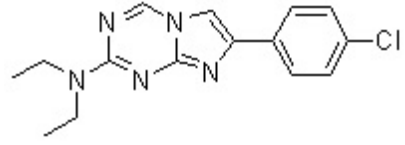
7.8710  
7.8542

7.3937  
7.3639  
7.3471  
7.2763

3.7000  
3.6882

1.2407





3h

156.9202  
151.0811  
145.3394  
144.6273

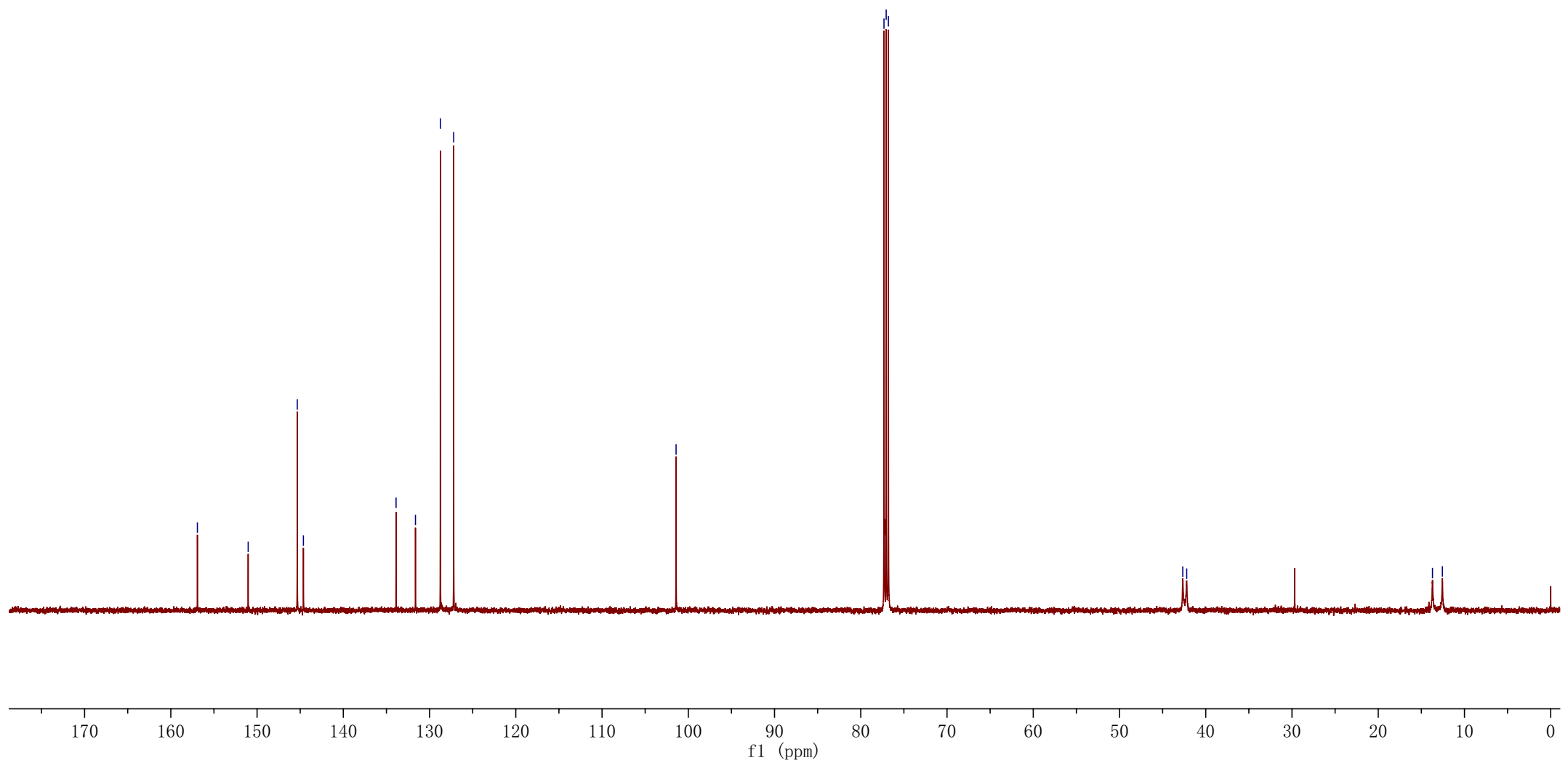
133.8834  
131.6340  
128.7476  
127.2043

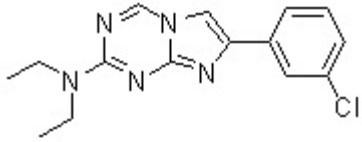
101.4159

77.3077  
77.0536  
76.7993

42.6624  
42.2073

13.7085  
12.5632



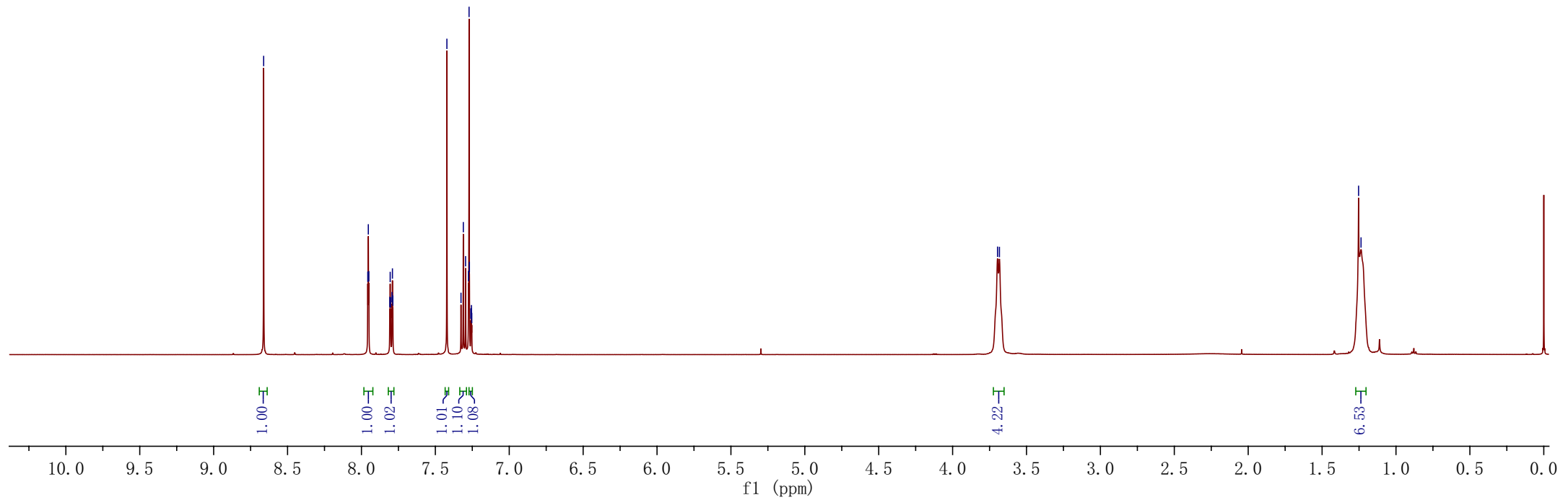


3i

8.6617  
7.9571  
7.9535  
7.9501  
7.8083  
7.8055  
7.8028  
7.7931  
7.7903  
7.7875  
7.4219  
7.3264  
7.3107  
7.2954  
7.2758  
7.2719  
7.2695  
7.2599  
7.2574  
7.2558  
7.2534

3.6961  
3.6832

1.2531  
1.2365



ZWQ210304-a CDC13

156.9326

151.0130

145.4050  
144.3806

134.9530  
134.6063

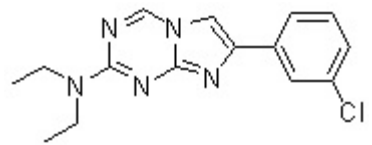
129.8143  
128.1105  
126.0800  
123.9820

101.8173

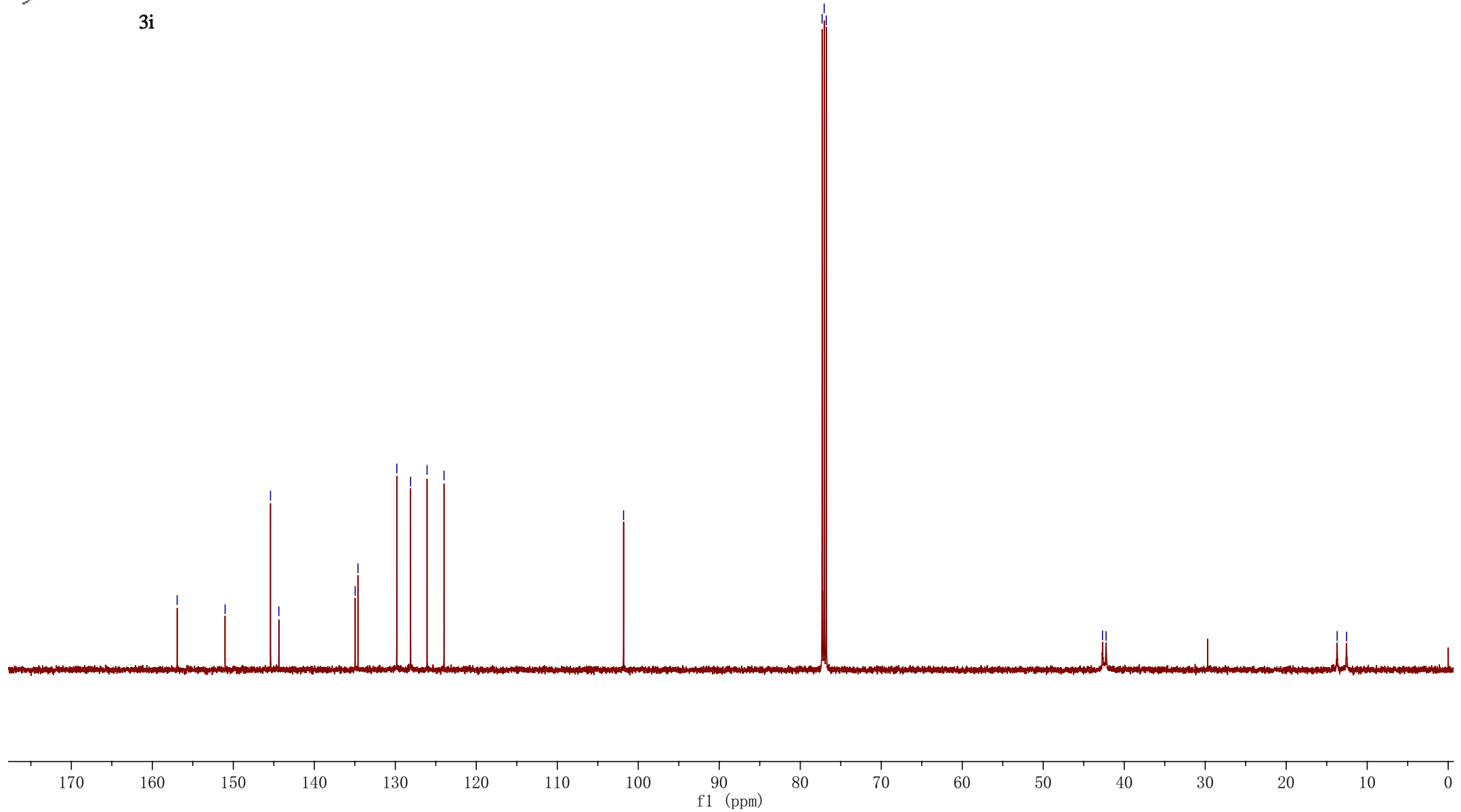
77.3033  
77.0490  
76.7949

42.6819  
42.2427

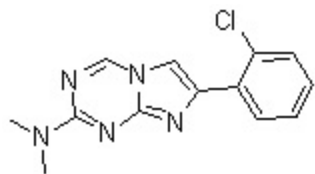
13.7109  
12.5493



3i

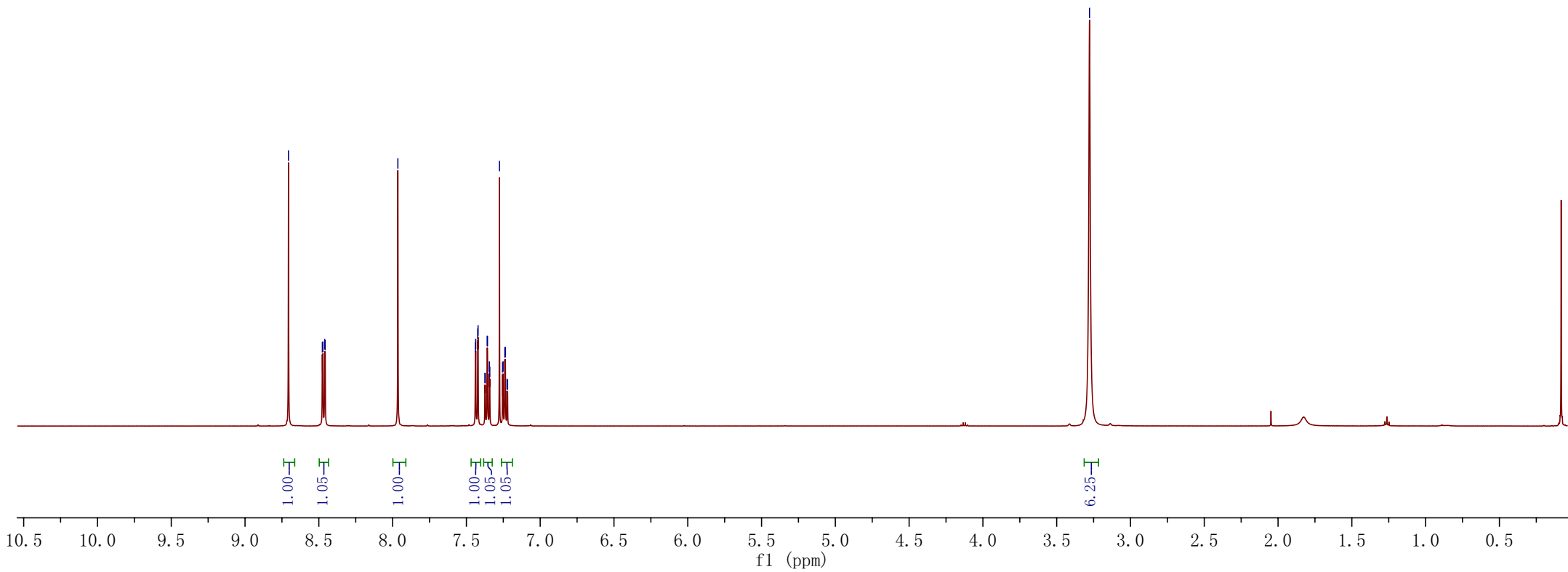


200831  
ZWQ200825-B CDCL3 0831



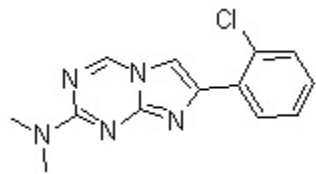
3j

8.7055  
8.4761  
8.4728  
8.4603  
8.4570  
7.9644  
7.4390  
7.4368  
7.4231  
7.4209  
7.3744  
7.3720  
7.3586  
7.3575  
7.3440  
7.3416  
7.2760  
7.2549  
7.2515  
7.2394  
7.2364  
7.2243  
7.2209  
3.2776





200902  
ZWQ200825-b CDC13 0902



3j

158.0707

149.5682

145.4527

141.8223

131.5546

131.3211

131.2743

130.2905

128.6689

126.9507

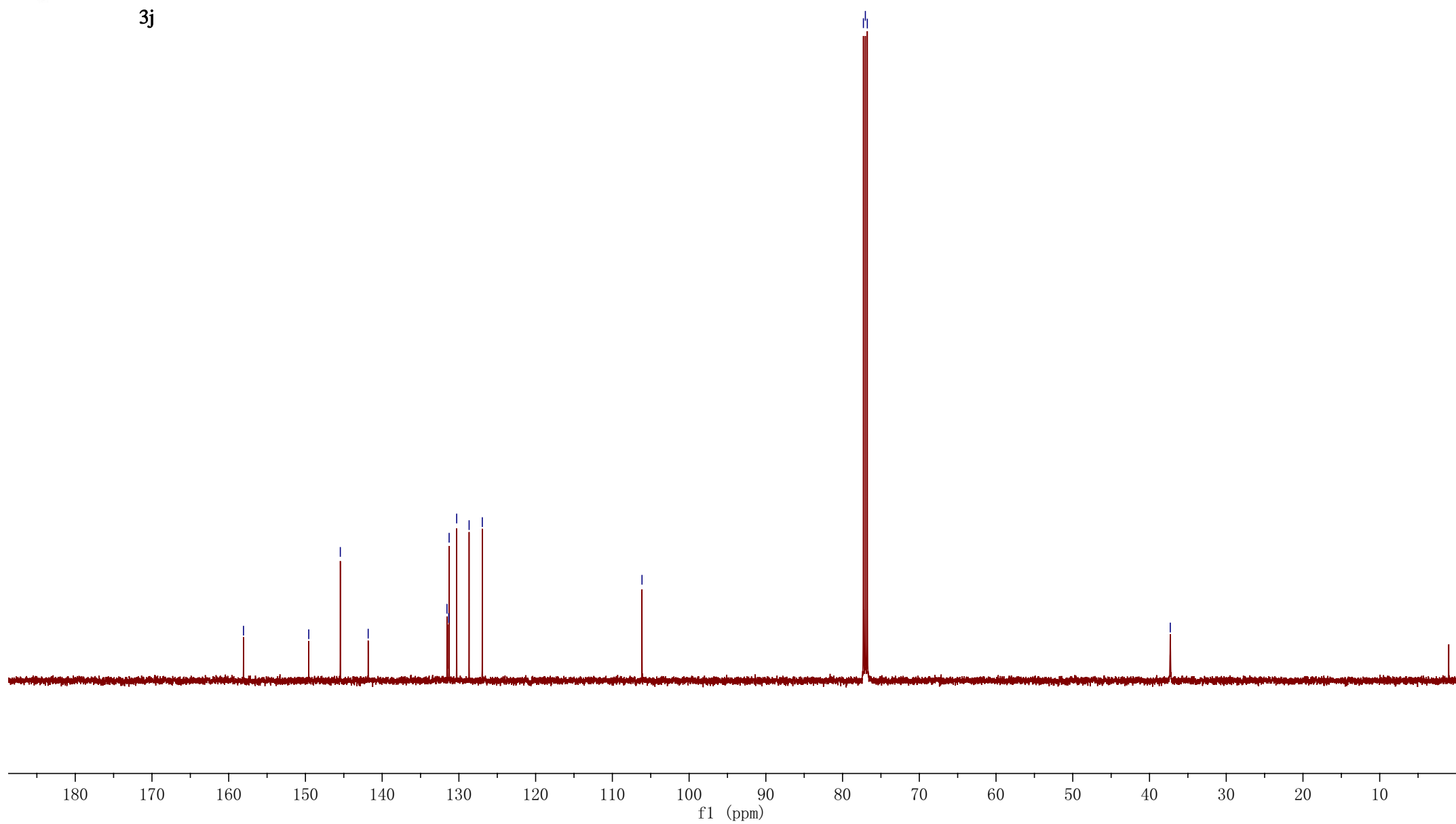
106.1368

77.2838

77.0296

76.7755

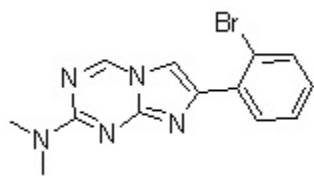
37.2920



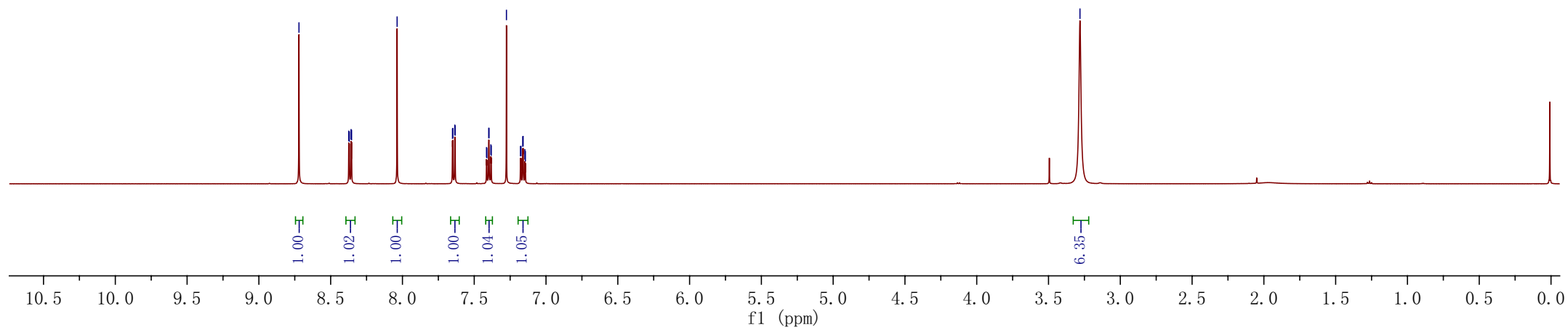
200907  
ZWQ200827-b

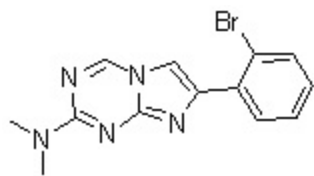
CDC13

0907  
8.7207  
8.3737  
8.3703  
8.3579  
8.3545  
8.0371  
7.6514  
7.6492  
7.6354  
7.6332  
7.4144  
7.4120  
7.3983  
7.3977  
7.3840  
7.3816  
7.2756  
7.1778  
7.1743  
7.1620  
7.1595  
7.1473  
7.1437  
3.2809

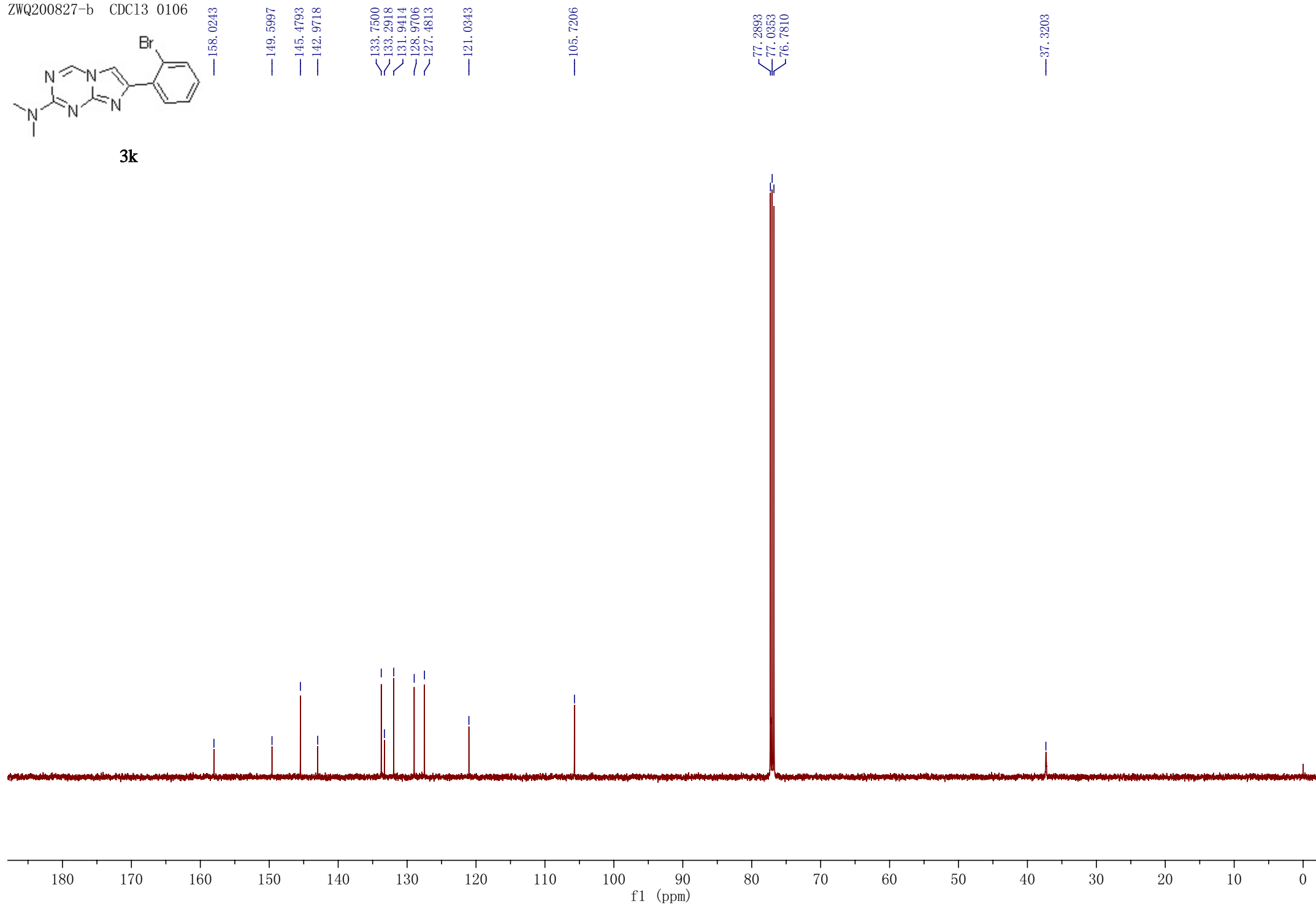


3k

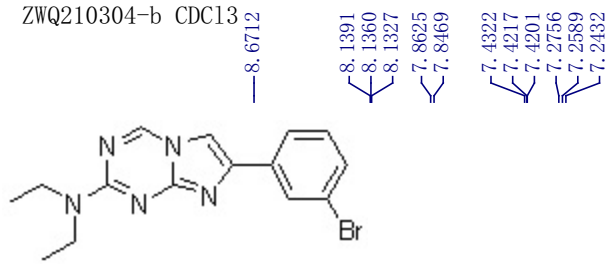




3k



ZWQ210304-b CDC13



31

8.6712

8.1391  
8.1360  
8.1327

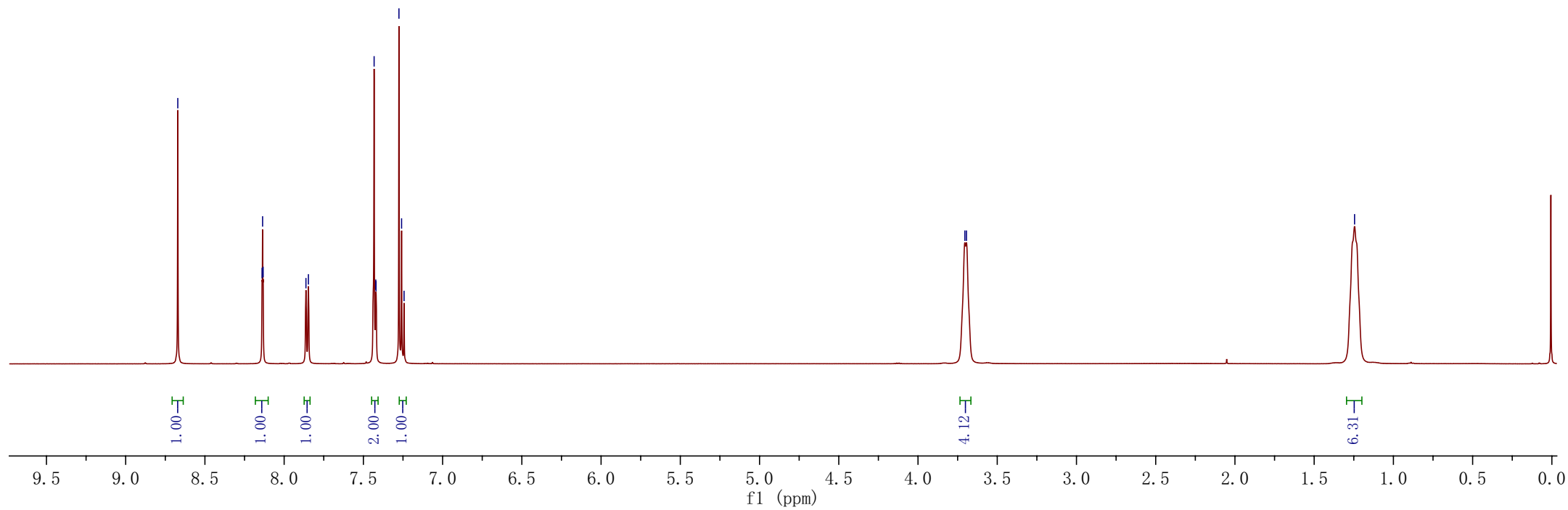
7.8625  
7.8469

7.4322  
7.4217  
7.4201

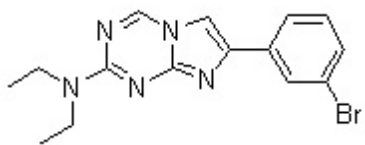
7.2756  
7.2589  
7.2432

3.7045  
3.6943

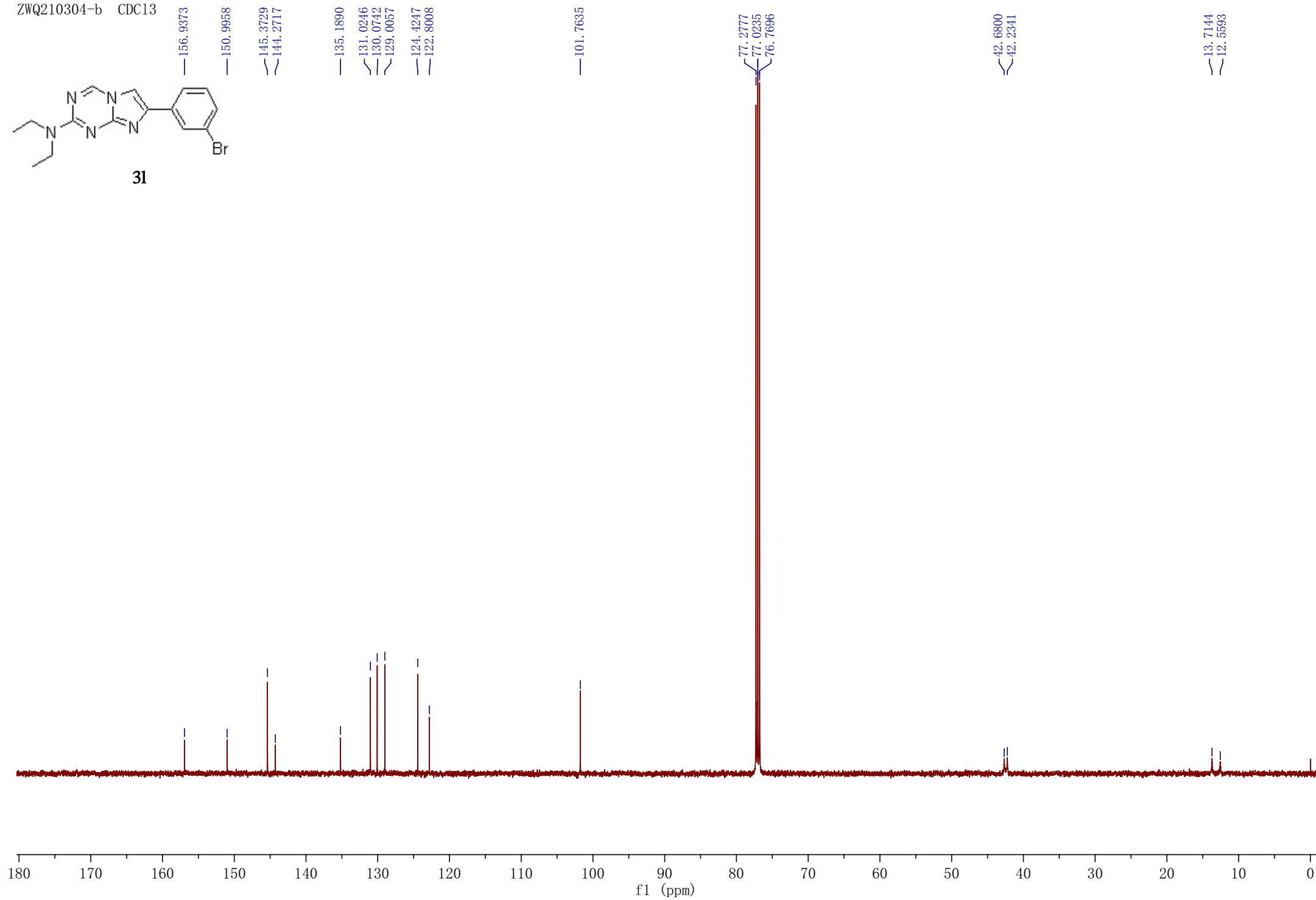
1.2451



ZWQ210304-b CDC13

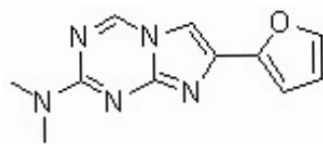


**31**



S40

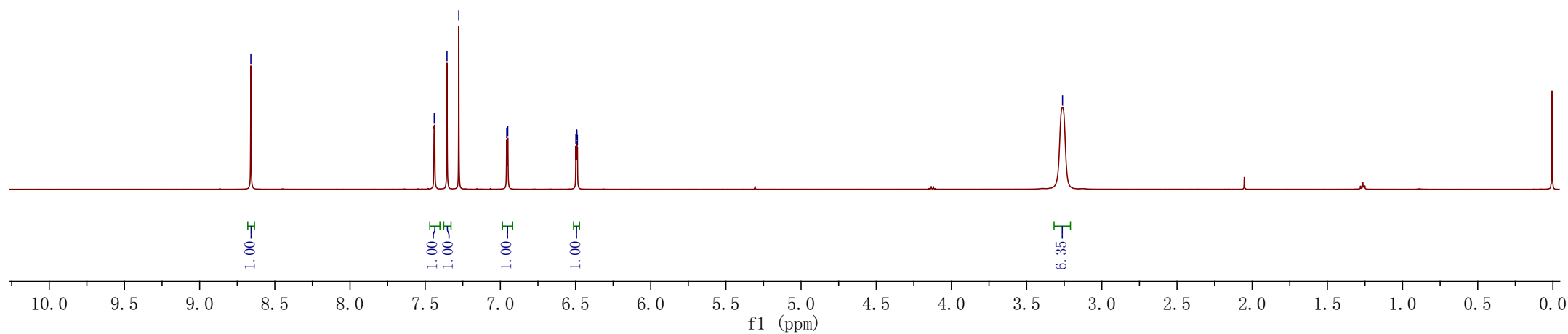
ZWQ200908-b CDC13 1230



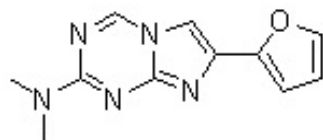
**3m**

7.4396  
7.4377  
7.3549  
7.2765  
6.9574  
6.9508  
6.4976  
6.4941  
6.4910  
6.4875

3.2614



ZWQ200908-b CDCL3 1231



**3m**

— 158.0188

— 150.8528

— 149.2869

— 145.1769

— 142.2290

— 138.0025

— 111.7004

— 108.3864

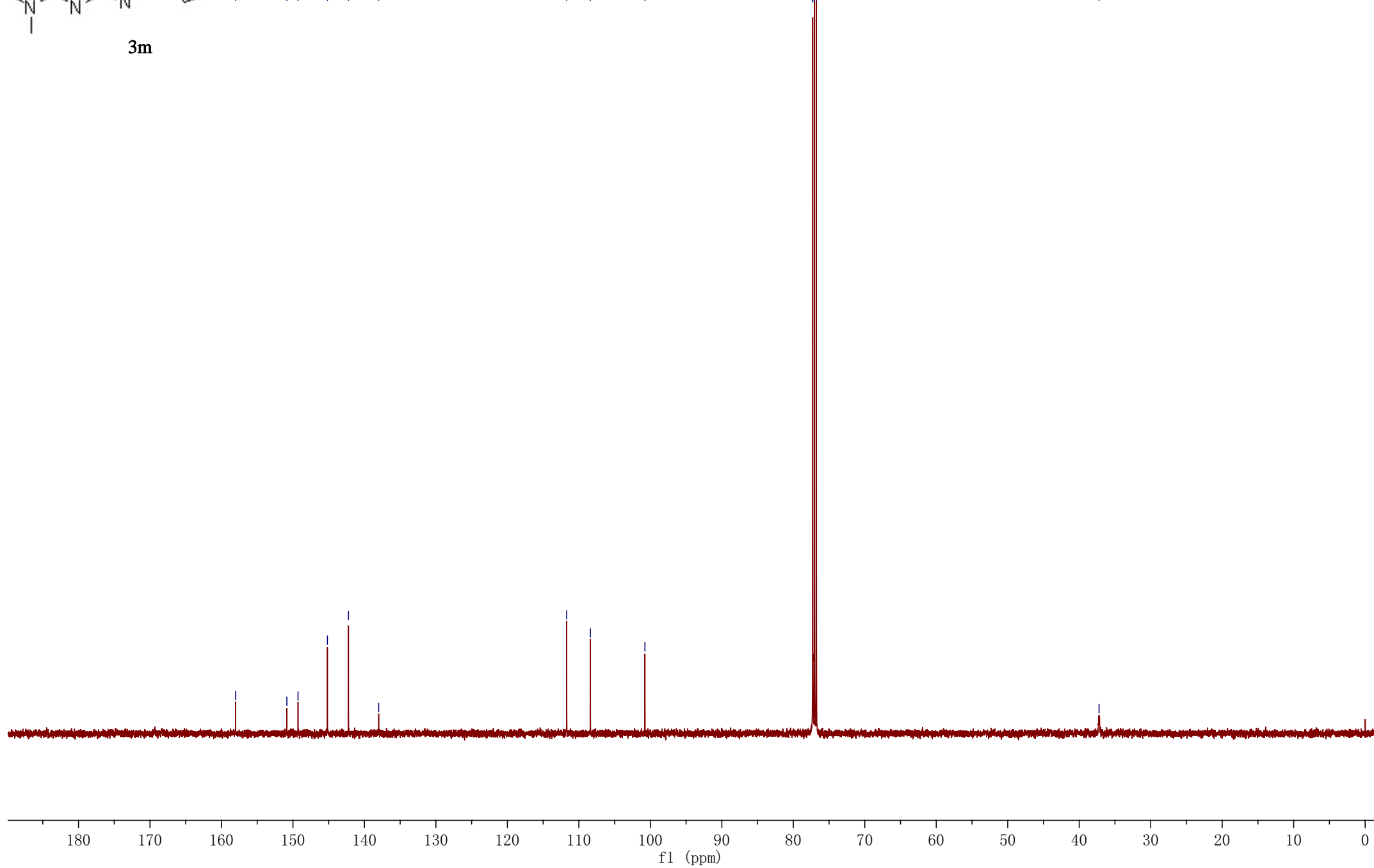
— 100.7557

— 77.2829

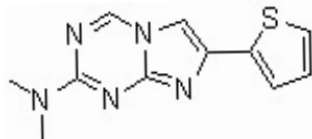
— 77.0286

— 76.7746

— 37.2278



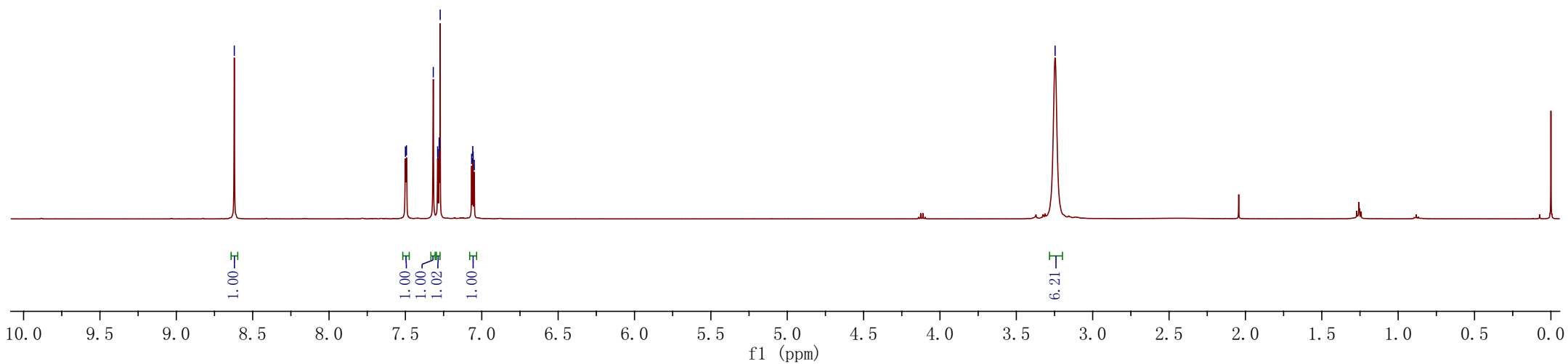
ZWQ200928-b CDC13



**3n**

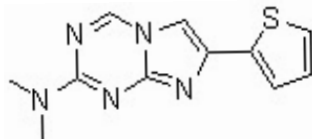
7.5000  
7.4930  
7.3175  
7.2890  
7.2878  
7.2790  
7.2775  
7.2723  
7.0663  
7.0589  
7.0565  
7.0491

3.2462





ZWQ200928-b CDC13



**3n**

—157.9782

—150.6569

—144.9759

—141.1191

—136.8756

—127.7053

—125.4595

—124.4654

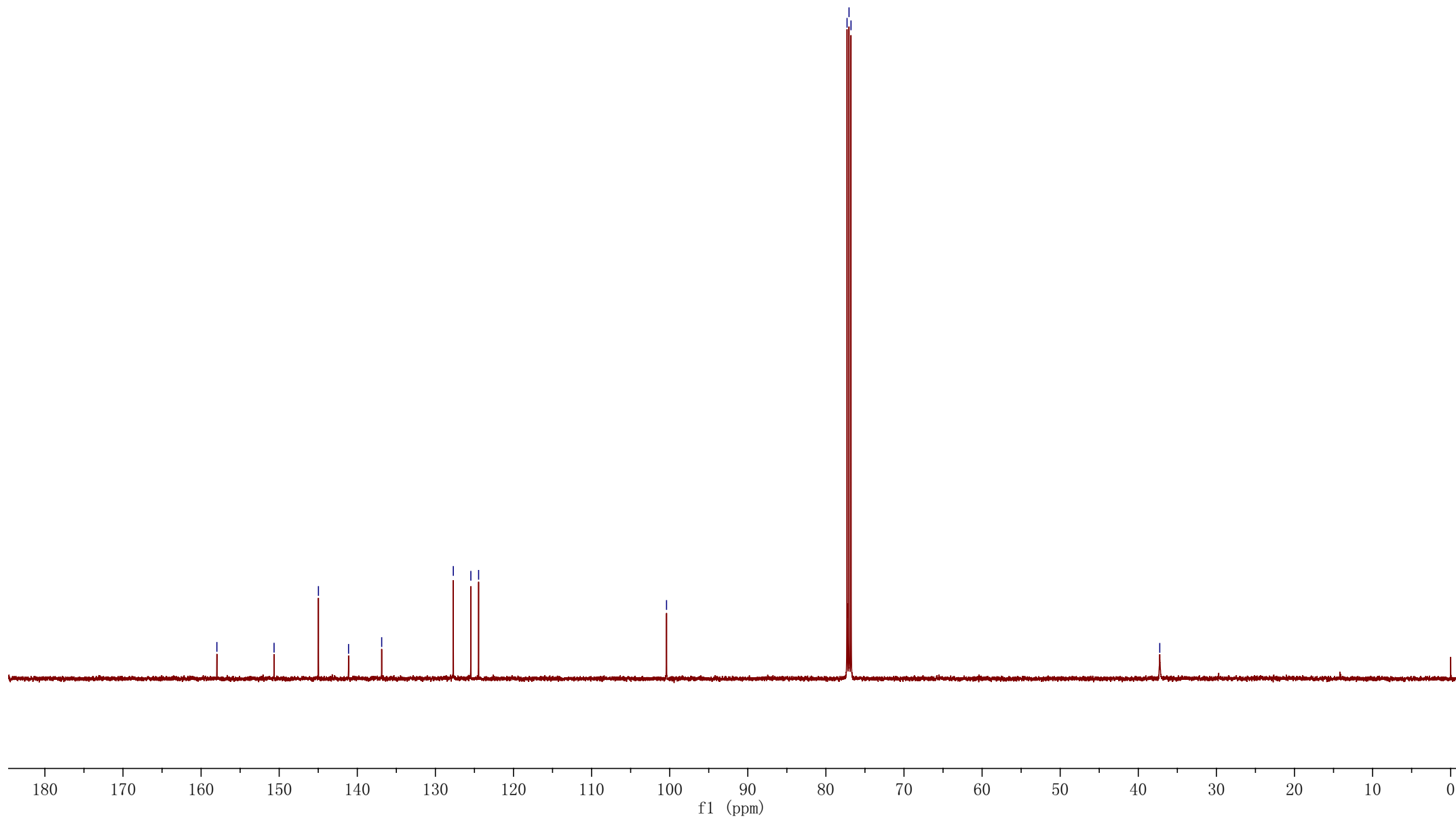
—100.4049

77.2916

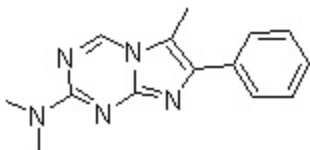
77.0376

76.7834

—37.2504



ZWQ200918-c CDC13



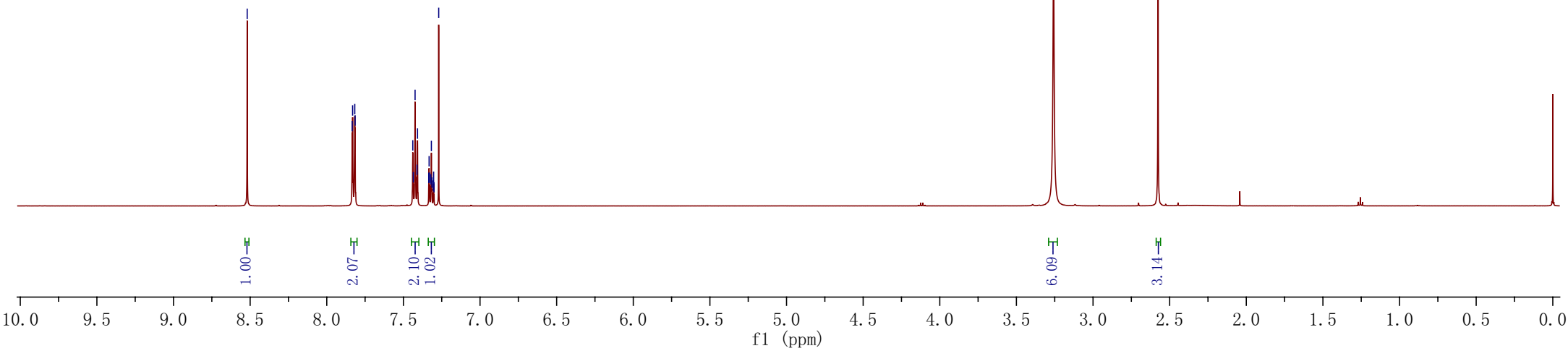
3o

8.5193

7.8341  
7.8315  
7.8173  
7.8151  
7.4387  
7.4352  
7.4238  
7.4112  
7.4080  
7.3347  
7.3322  
7.3297  
7.3209  
7.3175  
7.3139  
7.3051  
7.3027  
7.3002  
7.2696

3.2577

2.5759



1.00

2.07

2.10

1.02

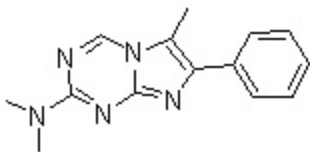
6.09

3.14

f1 (ppm)

S45

ZWQ200918-c CDC13



3o

—157.6468

—149.4414

—143.6053

—141.1901

—134.0657

—128.3817

—128.0384

—127.5154

—110.5112

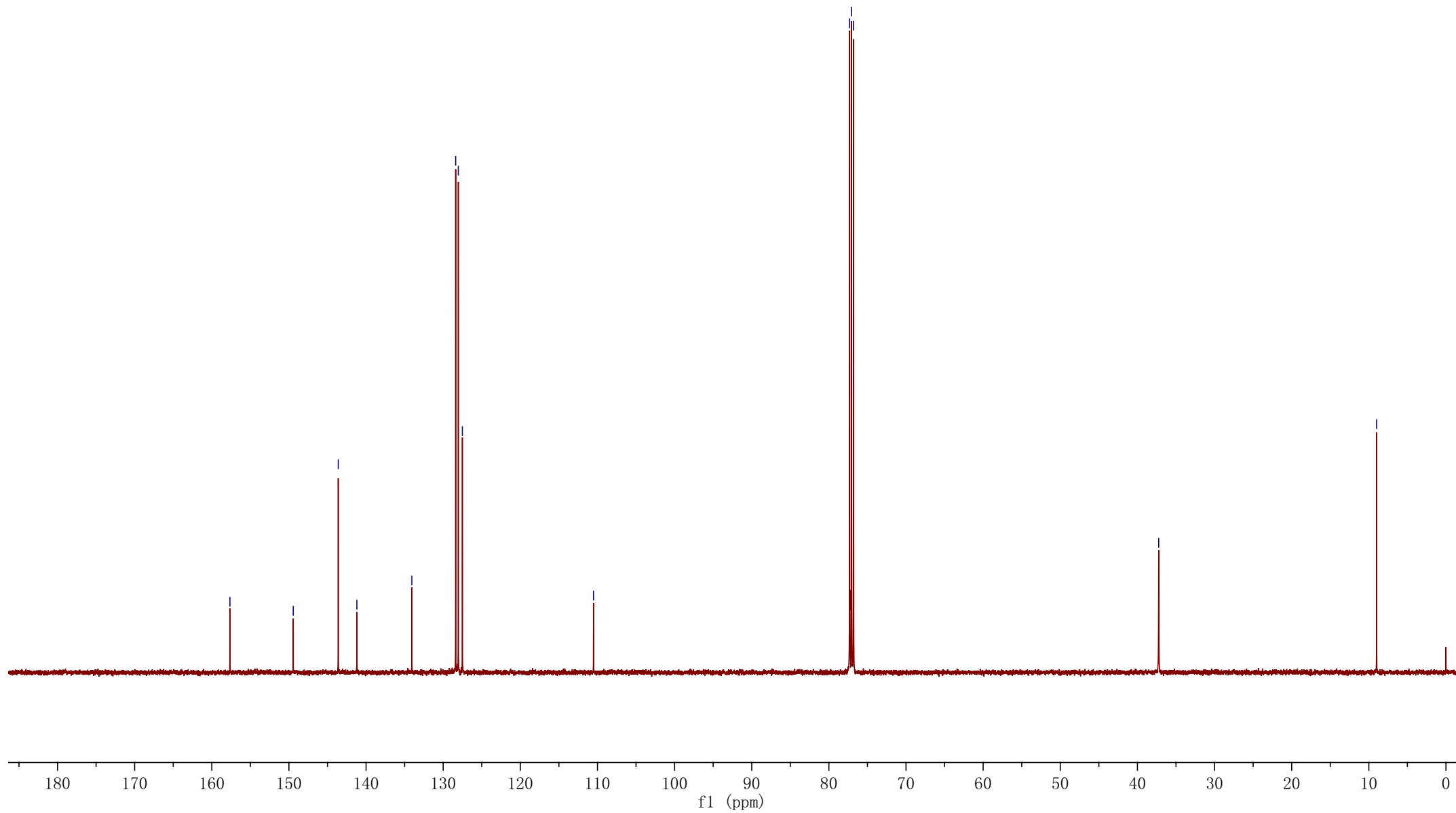
—77.3129

—77.0588

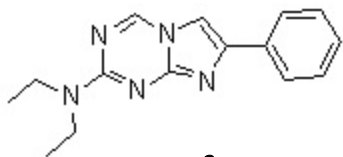
—76.8046

—37.2406

—8.9878



201010  
ZWQ200915-b CDC13 1010



3p

8.6607

7.9583

7.9430

7.4290

7.4157

7.4007

7.3850

7.3306

7.3158

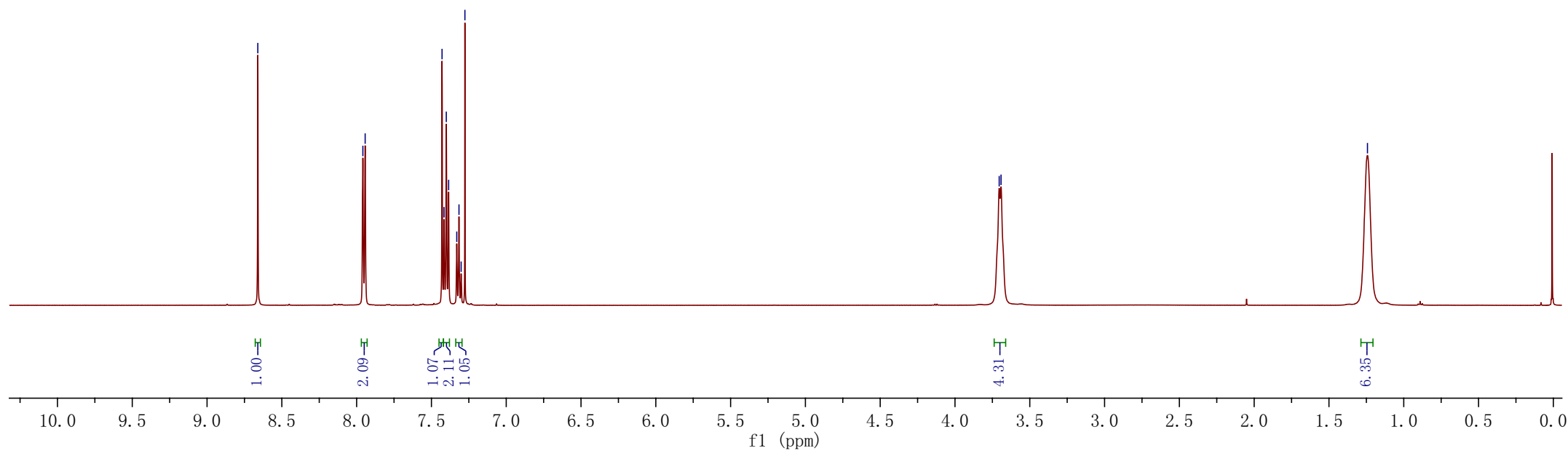
7.3013

7.2762

3.7045

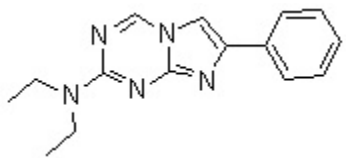
3.6921

1.2426



201013  
ZWQ200915-b CDC13

1013  
156.8934



3p

150.9707

145.7889  
145.3218

133.0849

128.5430  
128.2038

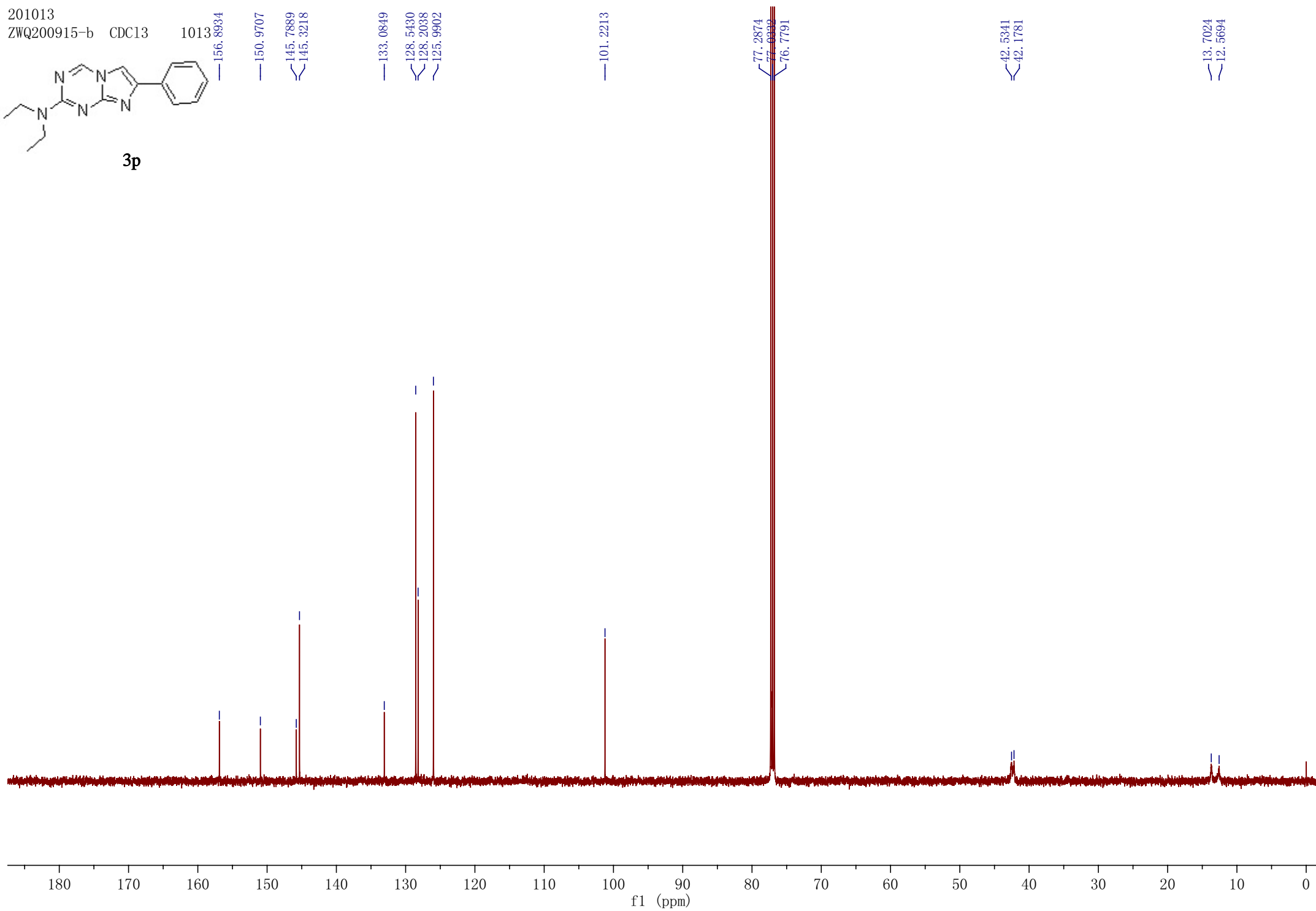
125.9902

101.2213

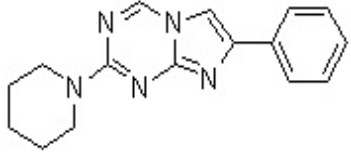
77.2874  
77.0000  
76.7791

42.5341  
42.1781

13.7024  
12.5694



201019  
ZWQ200911-a CDC13 1019



3q

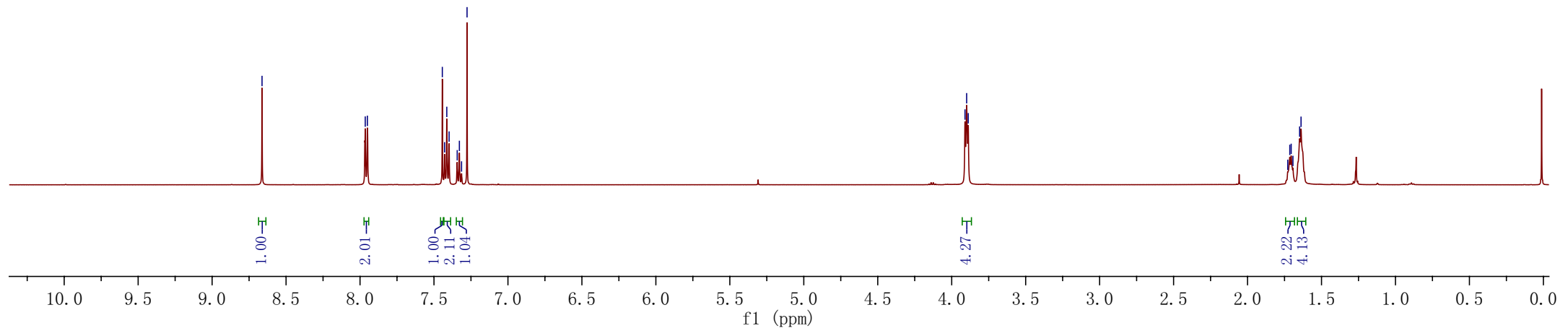
8.6625

7.9647  
7.9502

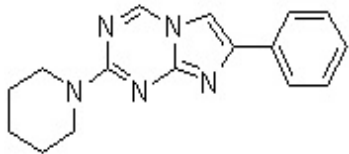
7.4436  
7.4283  
7.4135  
7.3979  
7.3430  
7.3283  
7.3136  
7.2765

3.9102  
3.8990  
3.8883

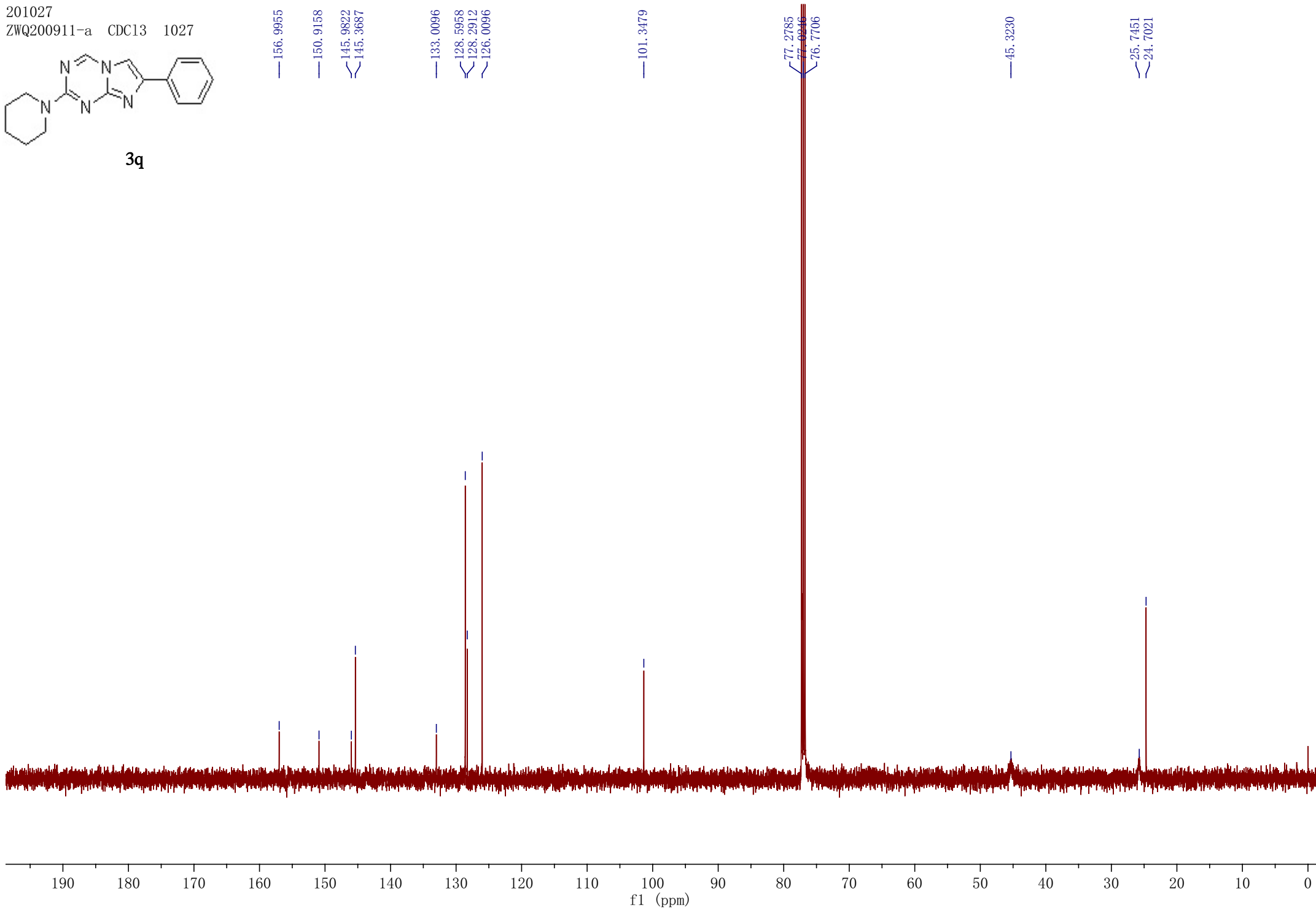
1.7282  
1.7143  
1.7051  
1.6931  
1.6478  
1.6383



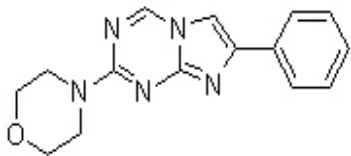
201027  
ZWQ200911-a CDC13 1027



3q



ZWQ200916-a CDC13

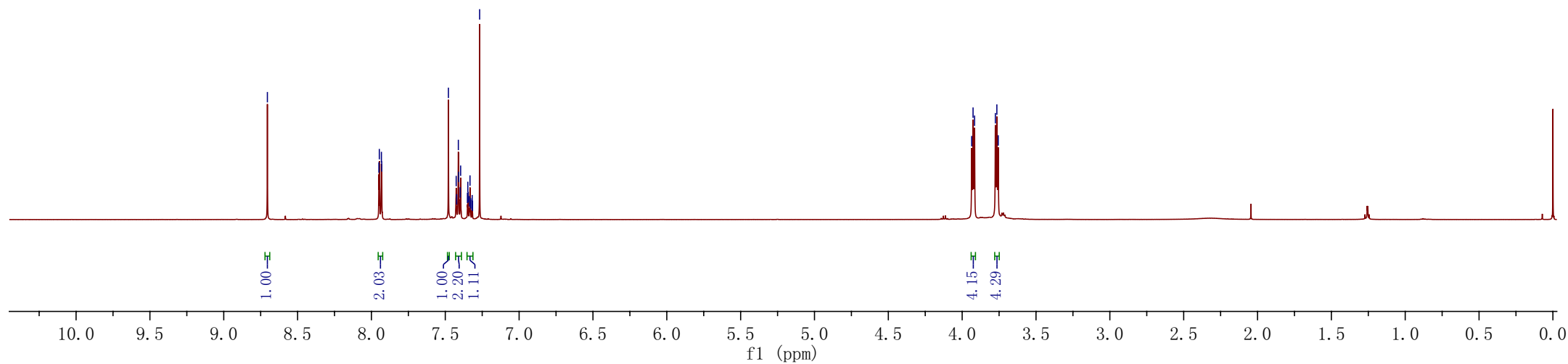


3r

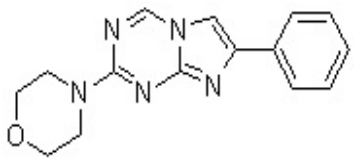
8.7045

7.9494  
7.9466  
7.9325  
7.9304  
7.4787  
7.4261  
7.4228  
7.4115  
7.4092  
7.3989  
7.3960  
7.3498  
7.3472  
7.3447  
7.3364  
7.3325  
7.3285  
7.3203  
7.3178  
7.3154  
7.2674

3.9855  
3.9262  
3.9160  
3.7753  
3.7651  
3.7557

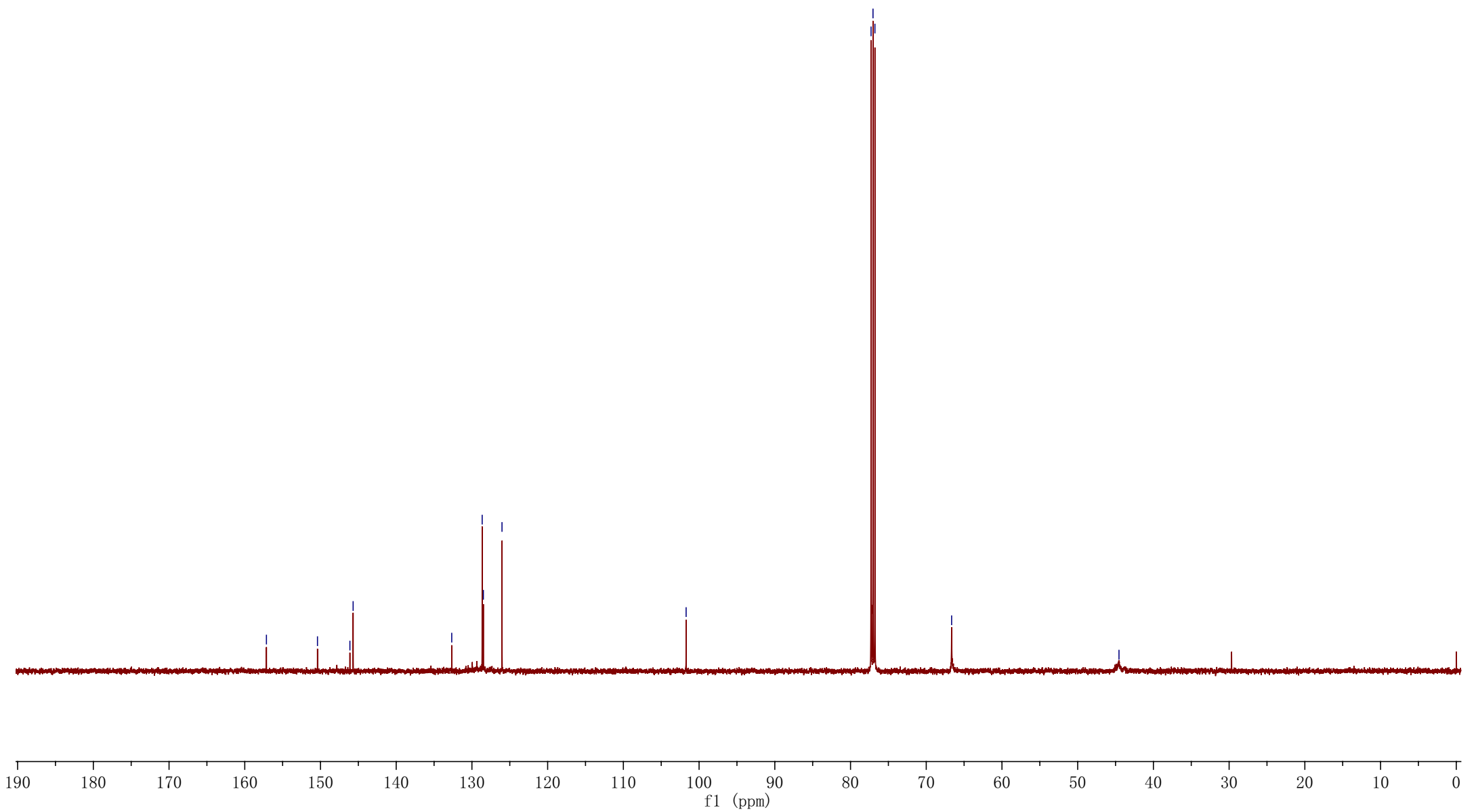




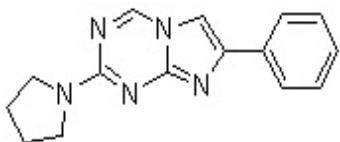


3r

- 157.1397
- 150.3969
- 146.1139
- 145.6890
- 132.6658
- 128.6456
- 128.4876
- 126.0283
- 101.7115
- 77.2856
- 77.0315
- 76.7774
- 66.6467
- 44.5447



ZWQ200917-b CDC13



3s

8.6905

7.9582

7.9432

7.4519

7.4167

7.4020

7.3874

7.3307

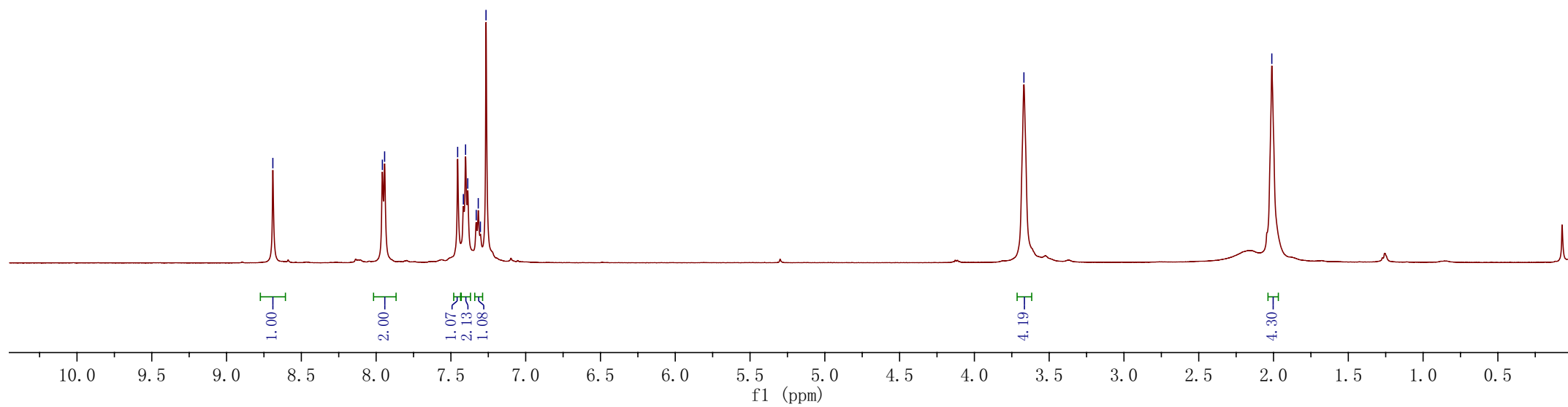
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7.3029

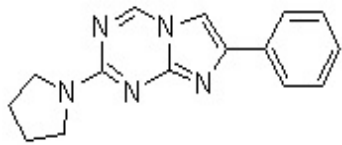
7.2653

3.6688

2.0114



ZWQ200917-b CDC13 1124



**3s**

155.9307

150.6576

145.3830

132.7773

128.6148

128.3372

126.0218

101.3045

77.2847

77.0808

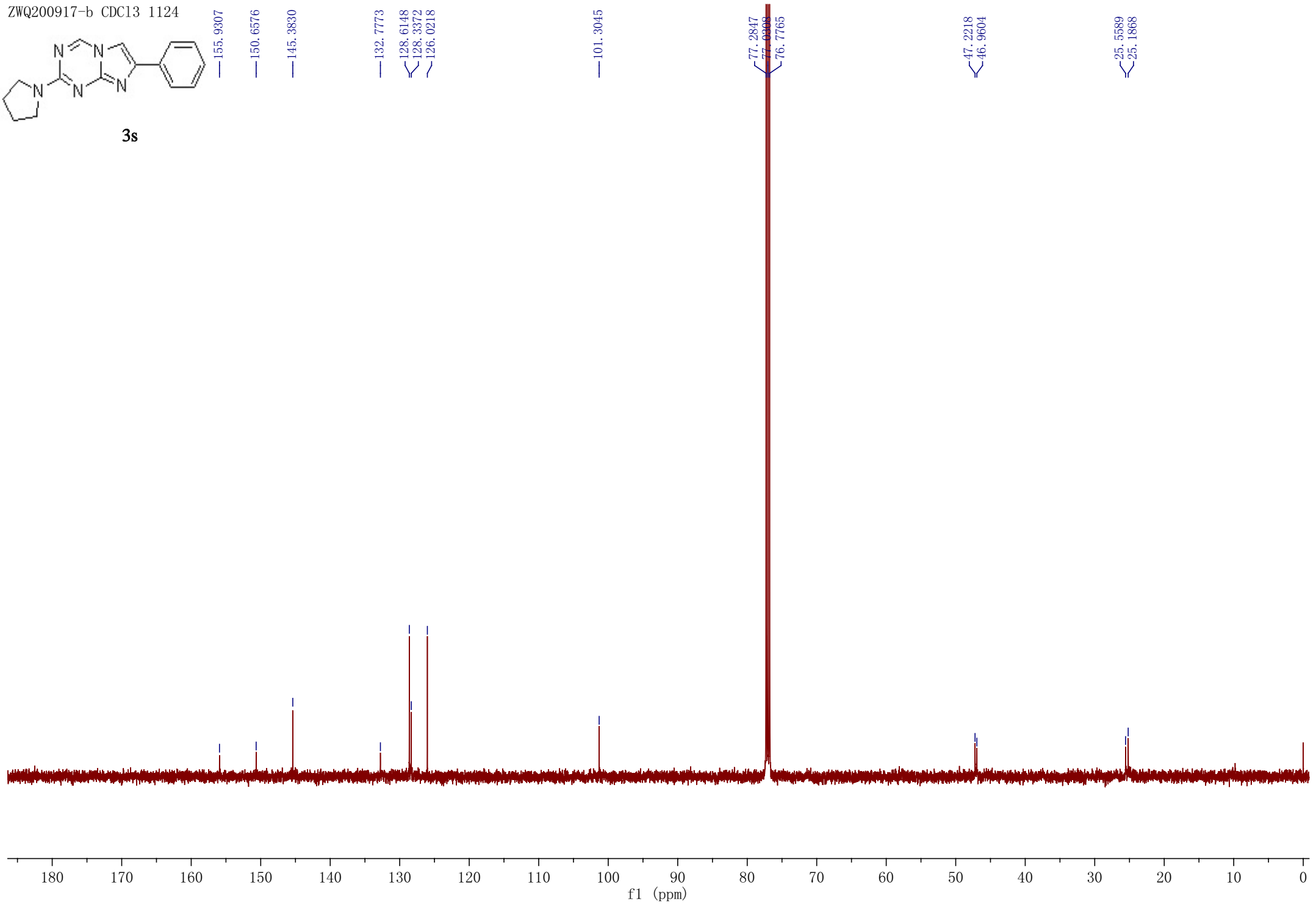
76.7765

47.2218

46.9604

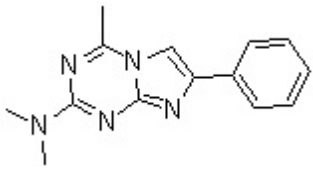
25.5589

25.1868



ZWQ201006 CDC13

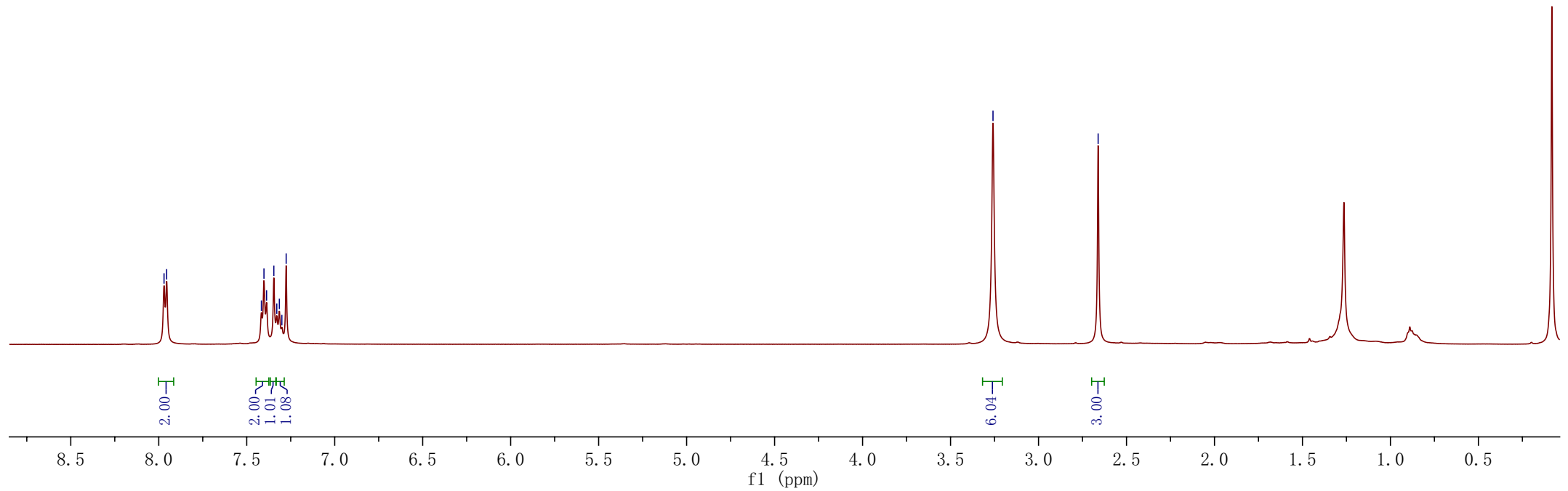
7.9700  
7.9551  
7.4167  
7.4020  
7.3873  
7.3459  
7.3292  
7.3145  
7.3003  
7.2759



3t

3.2587

2.6612



ZWQ201006 CDC13

158.0915  
154.7088  
151.6768

145.1182

133.1502

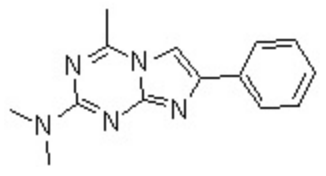
128.5305  
128.1333  
125.9211

100.5355

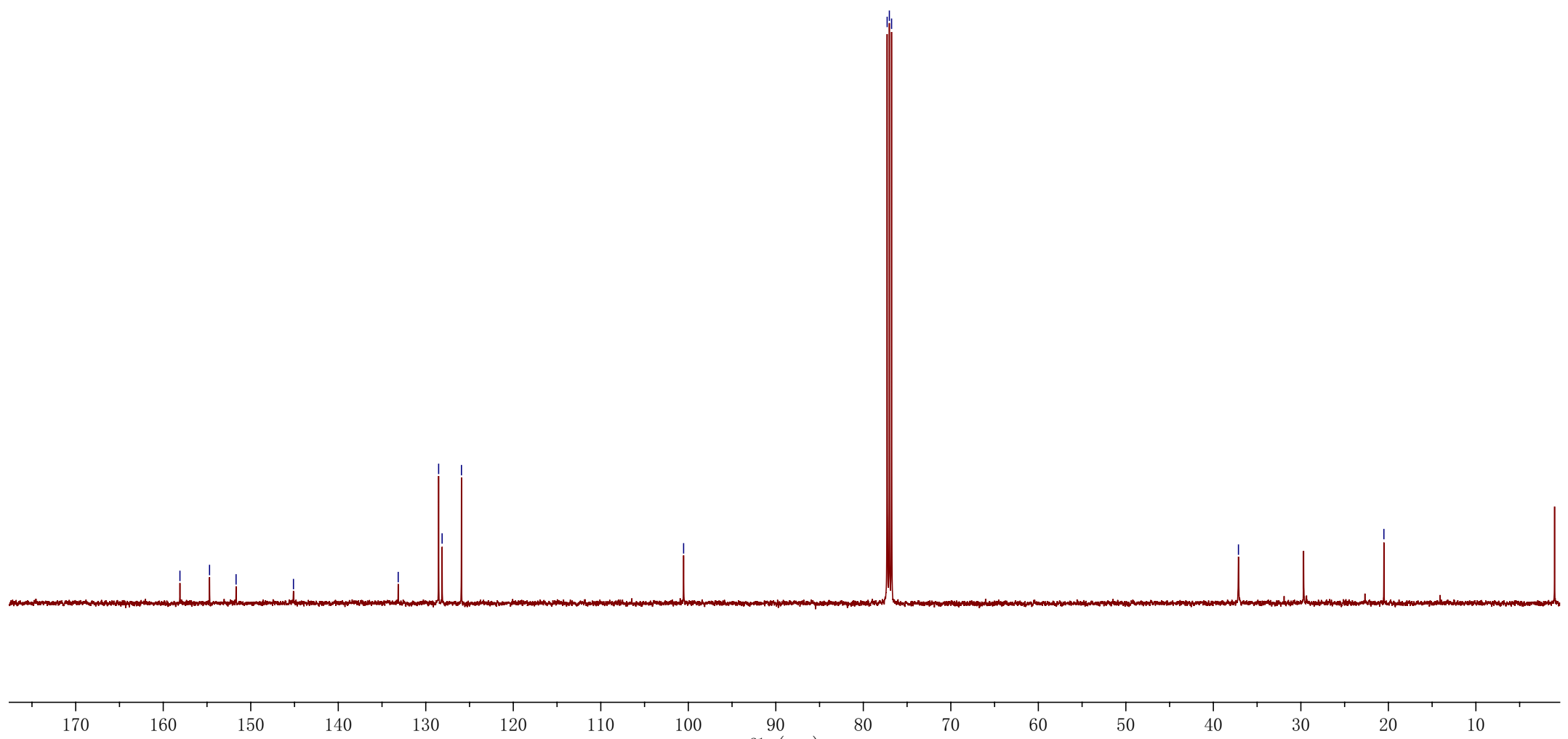
77.2772  
77.0232  
76.7691

37.1320

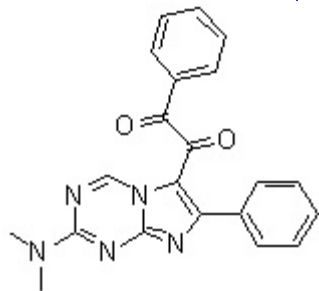
20.5113



3t



200620  
ZWQ-TM CDC13 0620

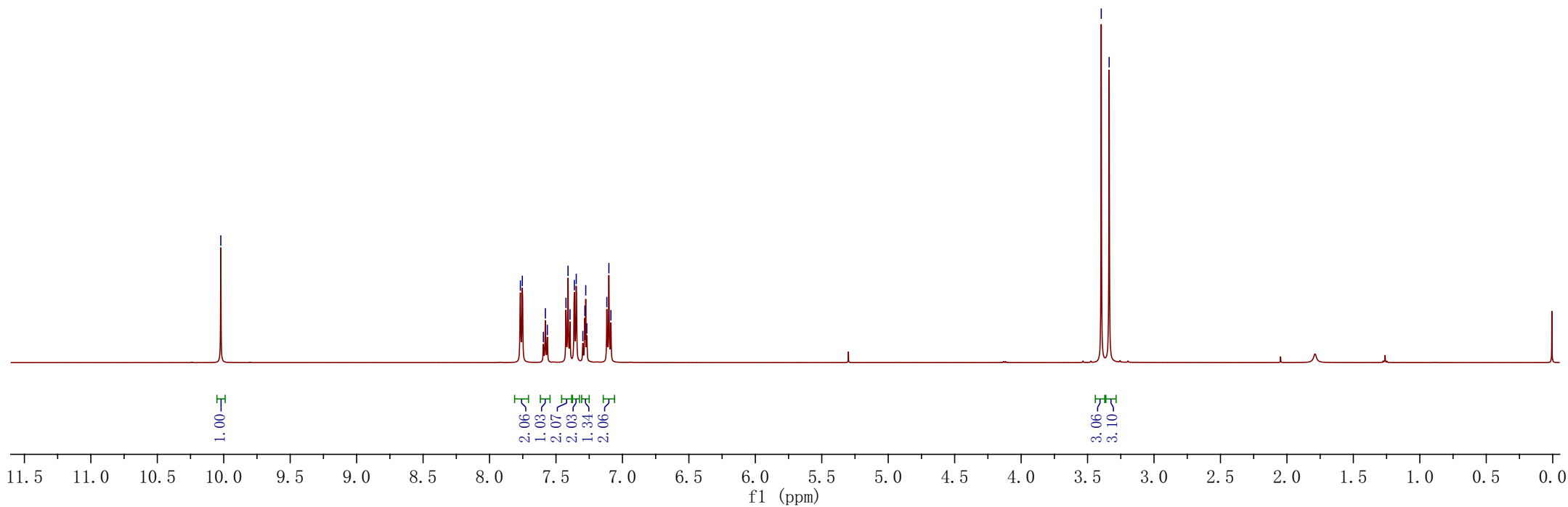


**4a**

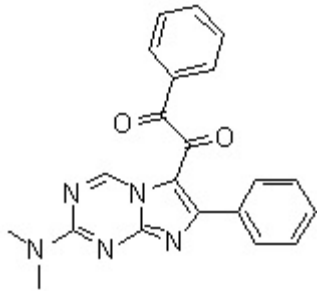
10.0222

7.7678  
7.7532  
7.5947  
7.5798  
7.5650  
7.4250  
7.4096  
7.3942  
7.3619  
7.3475  
7.2979  
7.2829  
7.2760  
7.2680  
7.1173  
7.1019  
7.0866

3.3970  
3.3376

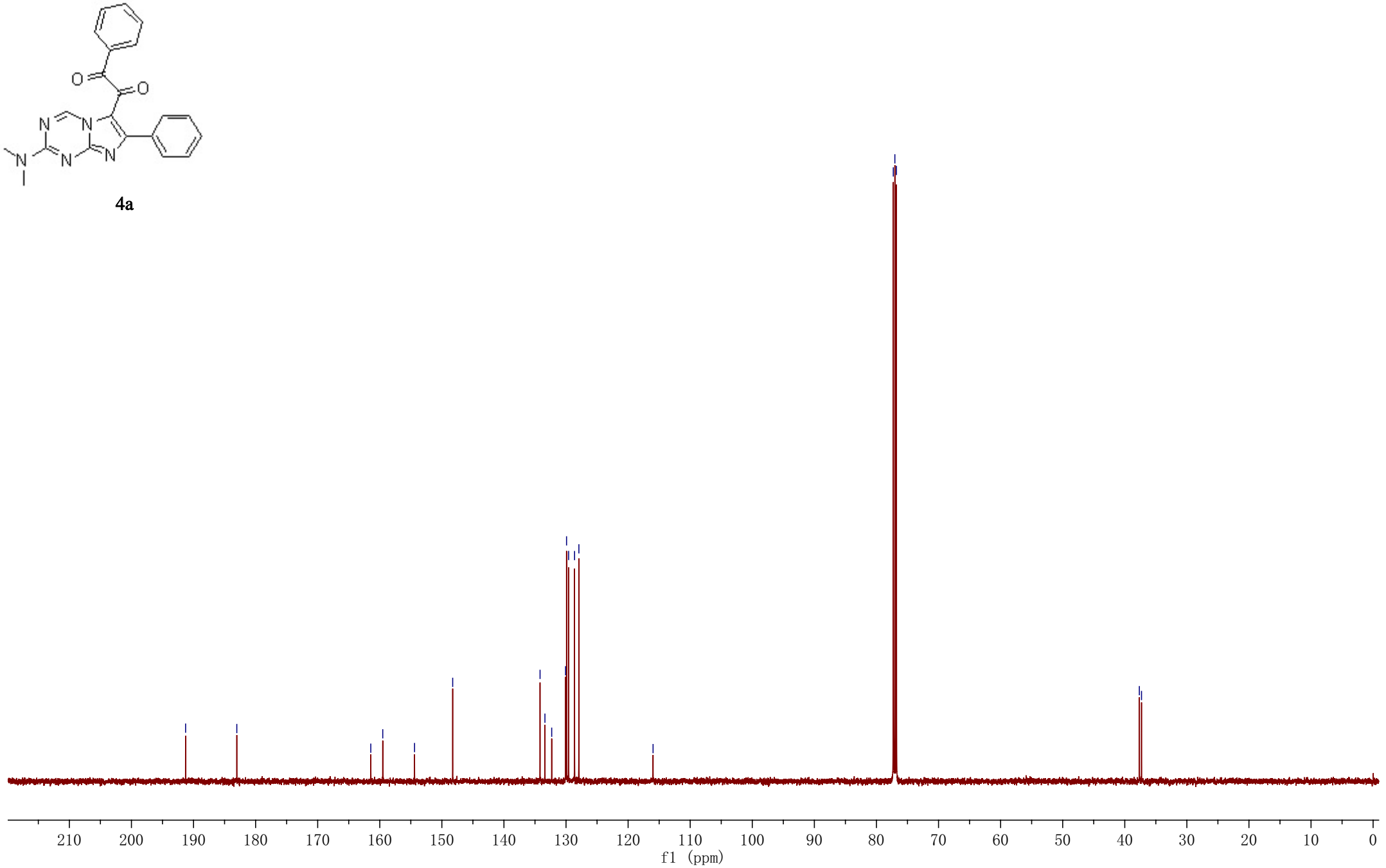


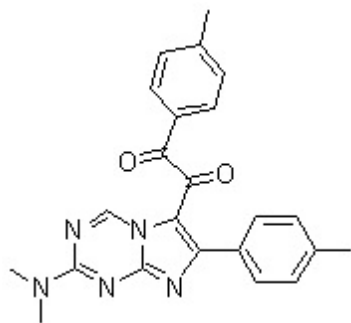
200624  
ZWQ-TM CDC13 0624



4a

191.2757  
183.0265  
161.4478  
159.5194  
154.3998  
148.2535  
134.1832  
133.3979  
132.3055  
130.0756  
129.9160  
129.5825  
128.6263  
127.9283  
115.9806  
77.2862  
77.0321  
76.7780  
37.6539  
37.3047





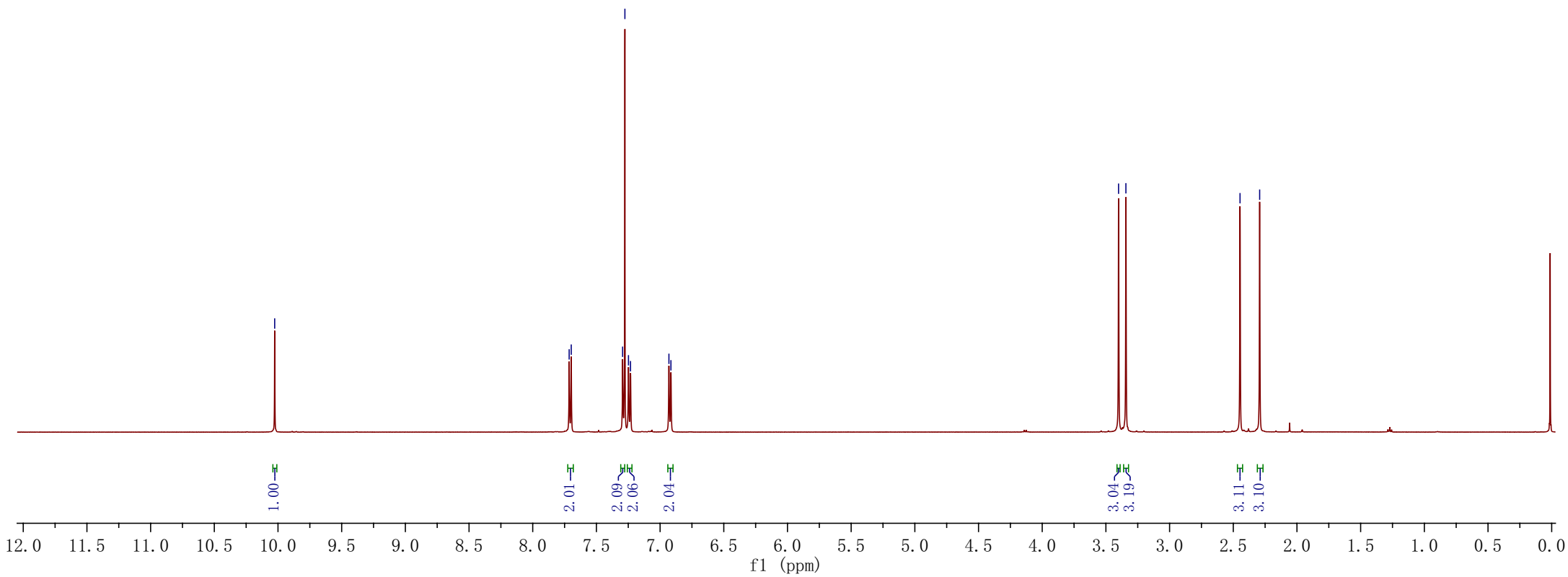
4b

10.0259

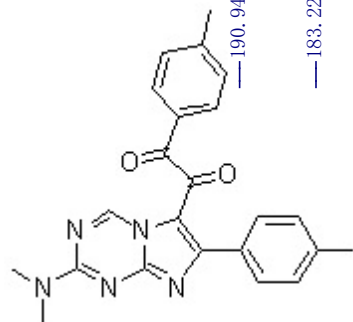
7.7139  
7.6976  
7.2943  
7.2764  
7.2483  
7.2322  
6.9307  
6.9150

3.4006  
3.3430

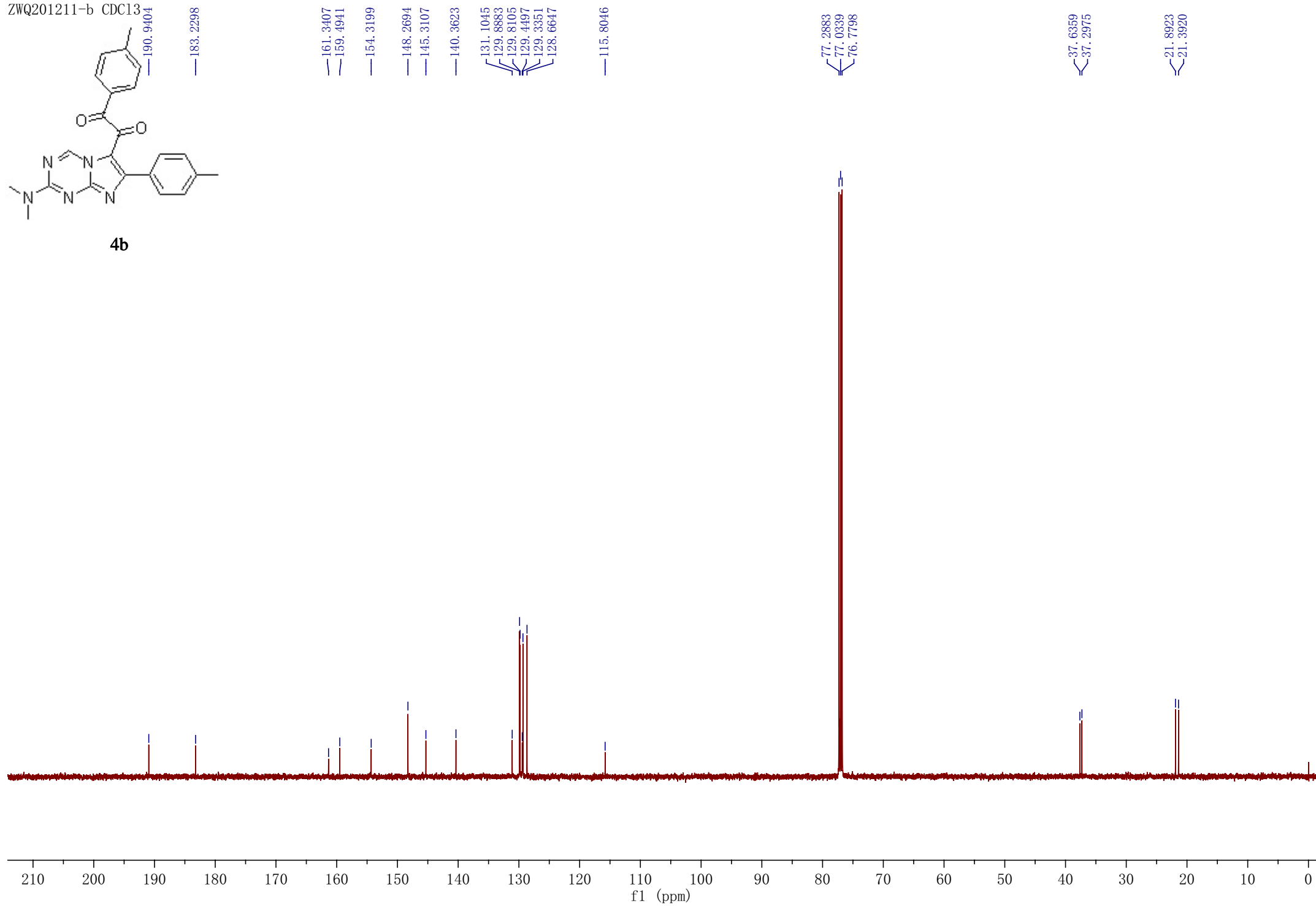
2.4469  
2.2928

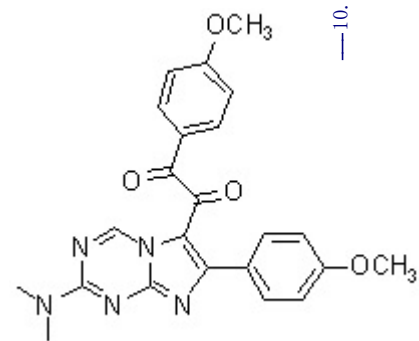






4b





4c

10.0076

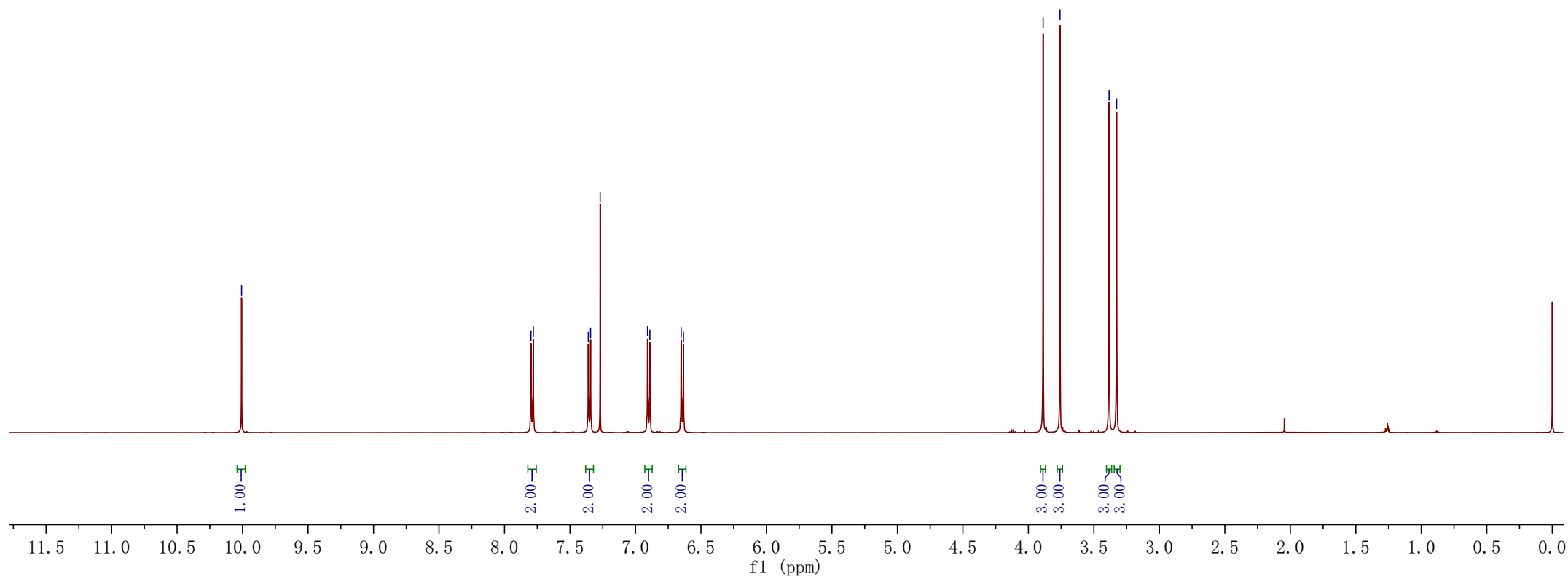
7.7980  
7.7803

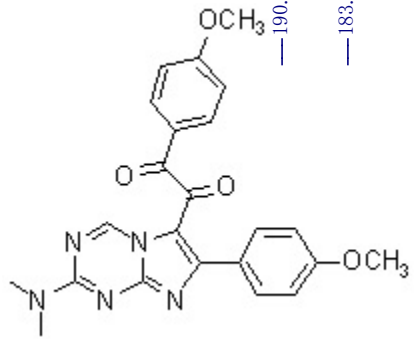
7.3603  
7.3429  
7.2697

6.9080  
6.8903  
6.6514  
6.6339

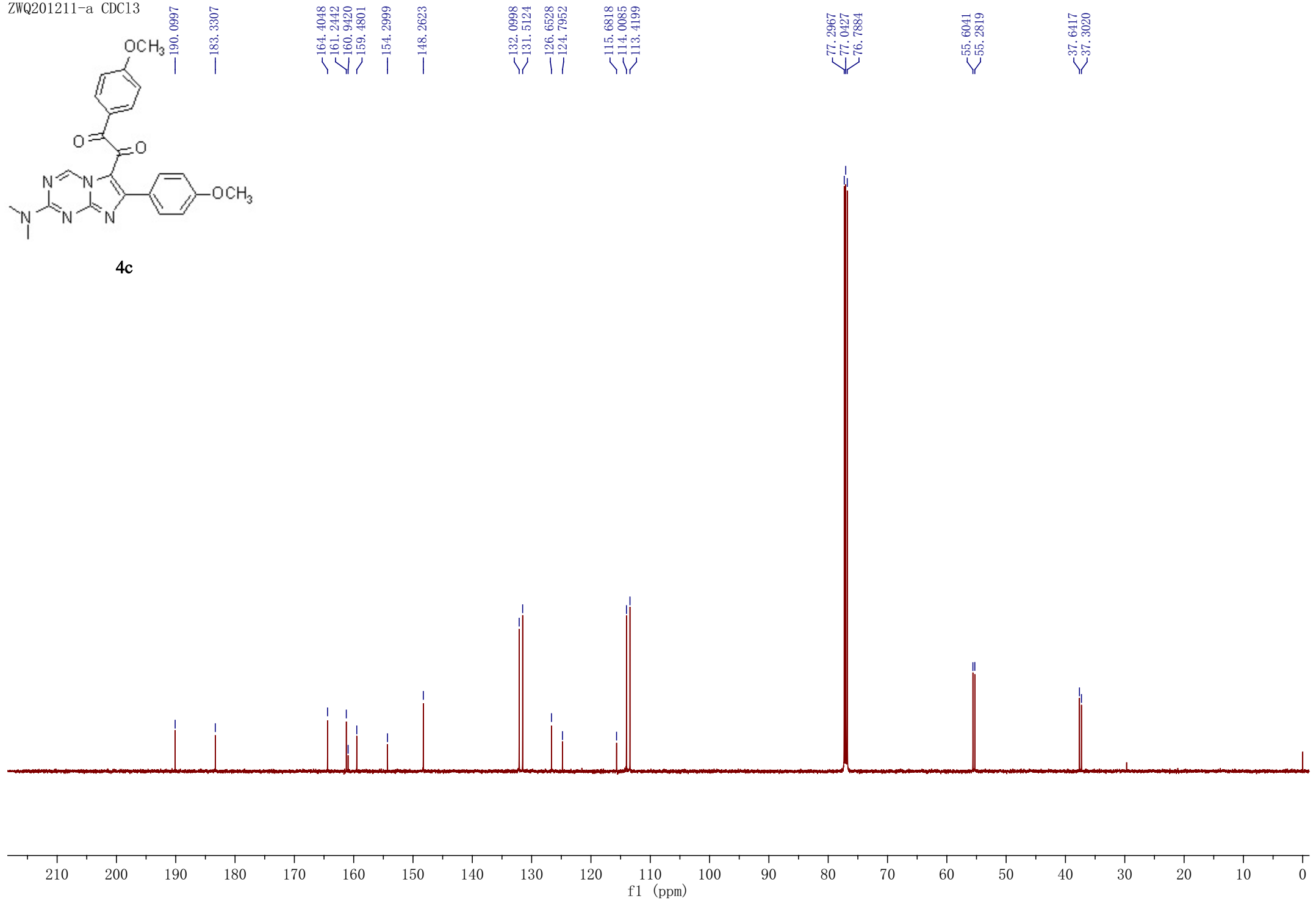
3.8874  
3.7584

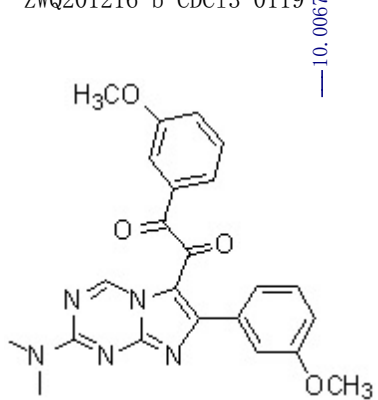
3.3839  
3.3264



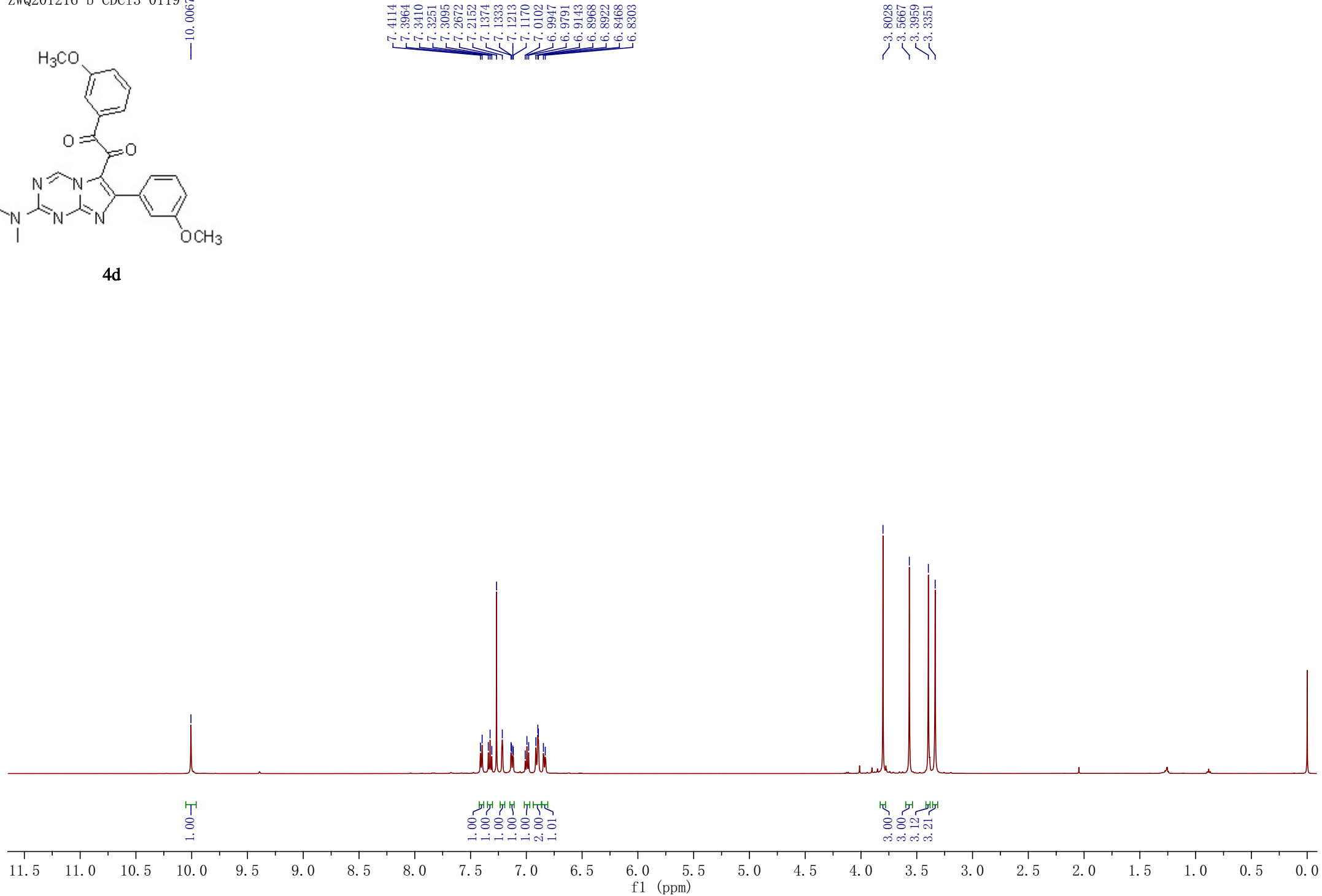


4c

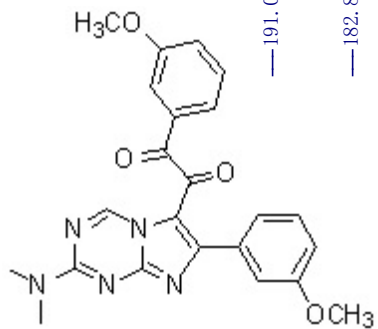




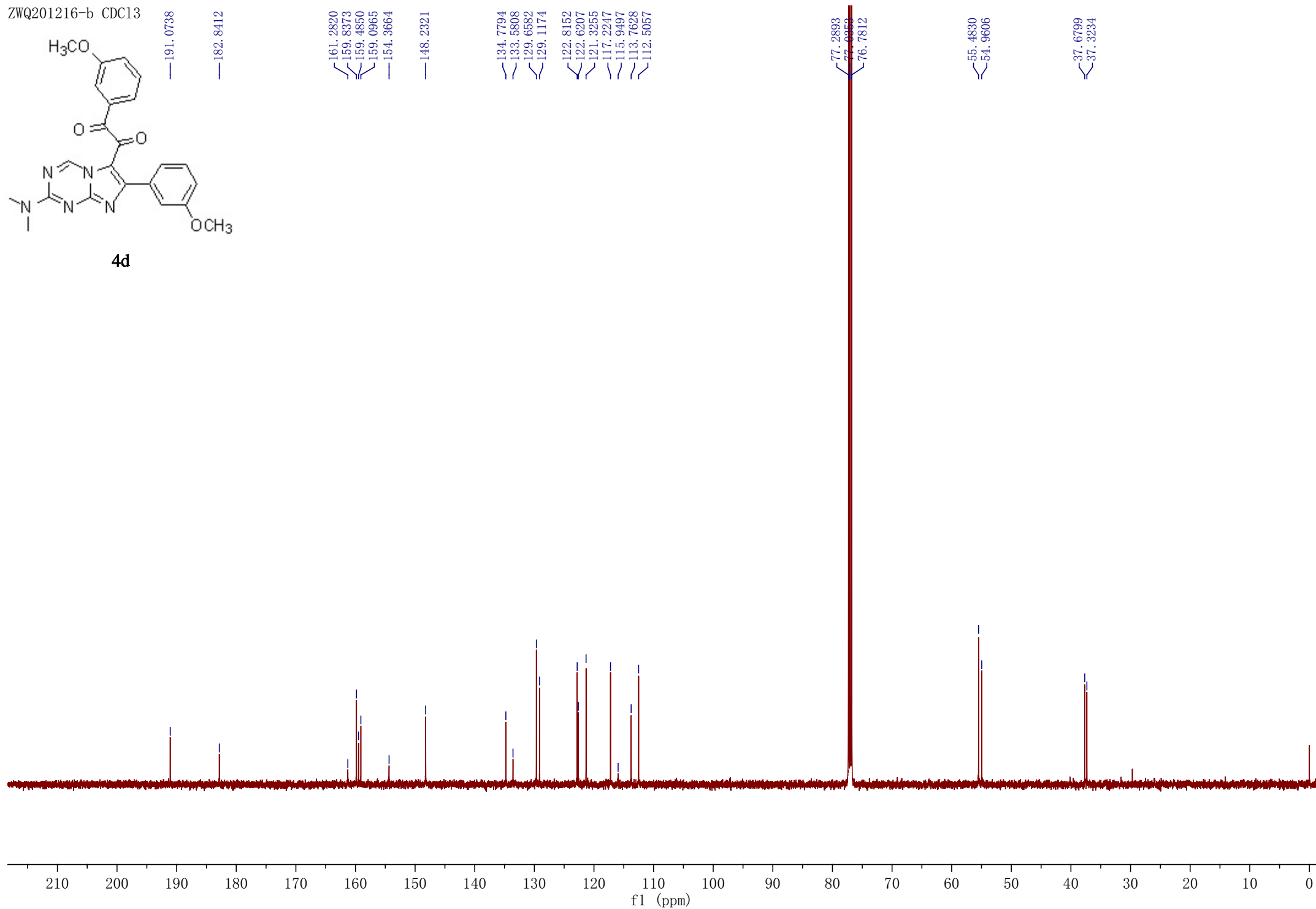
4d

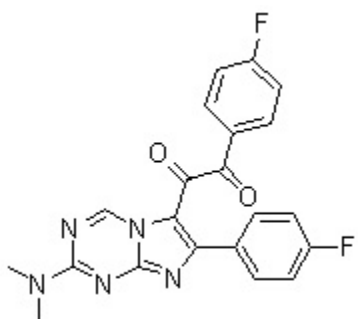


ZWQ201216-b CDC13

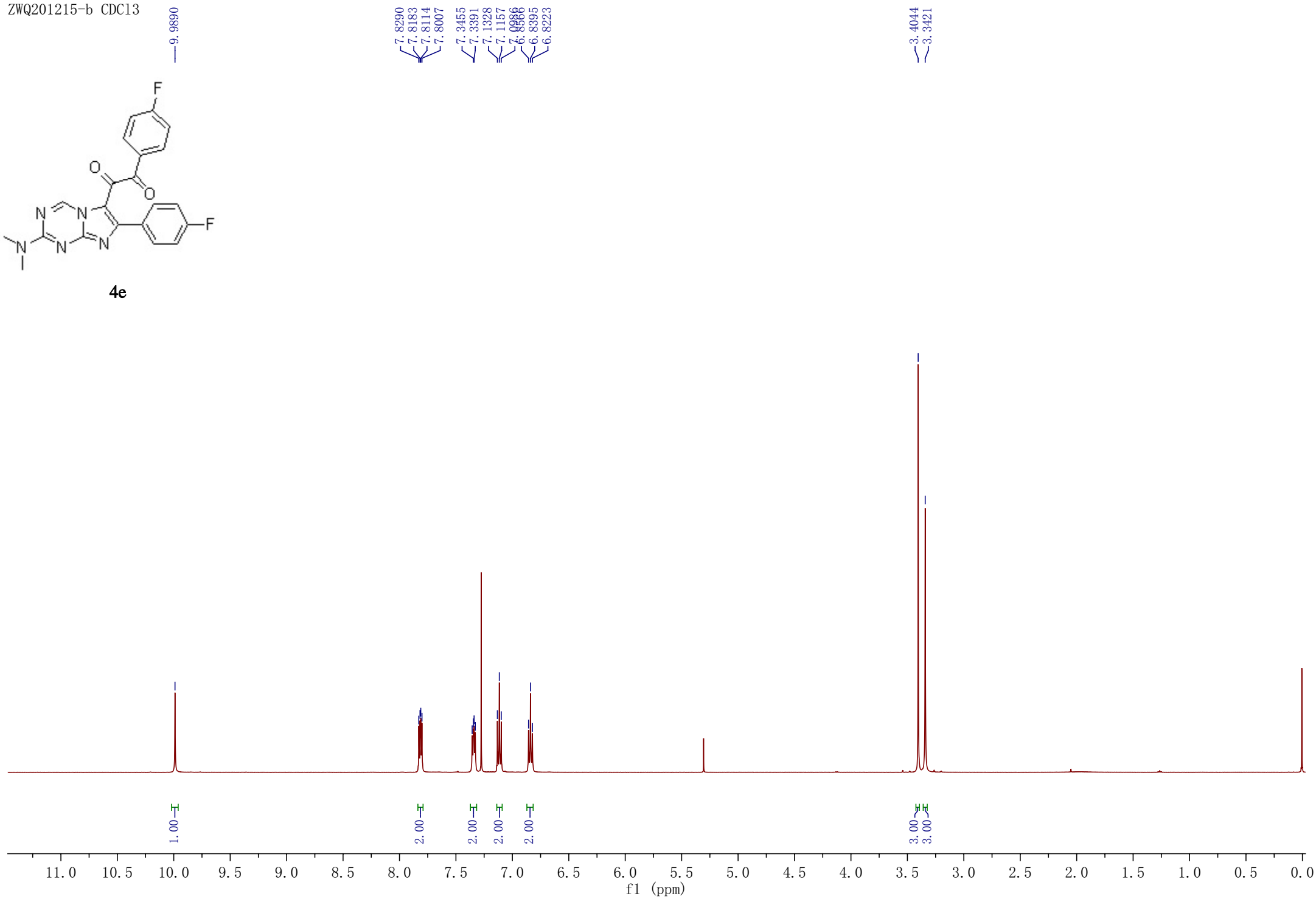


4d

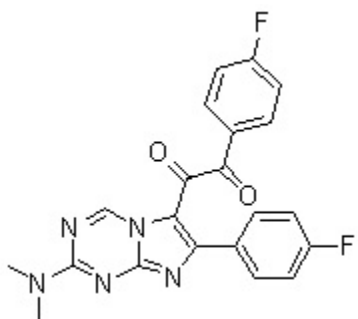




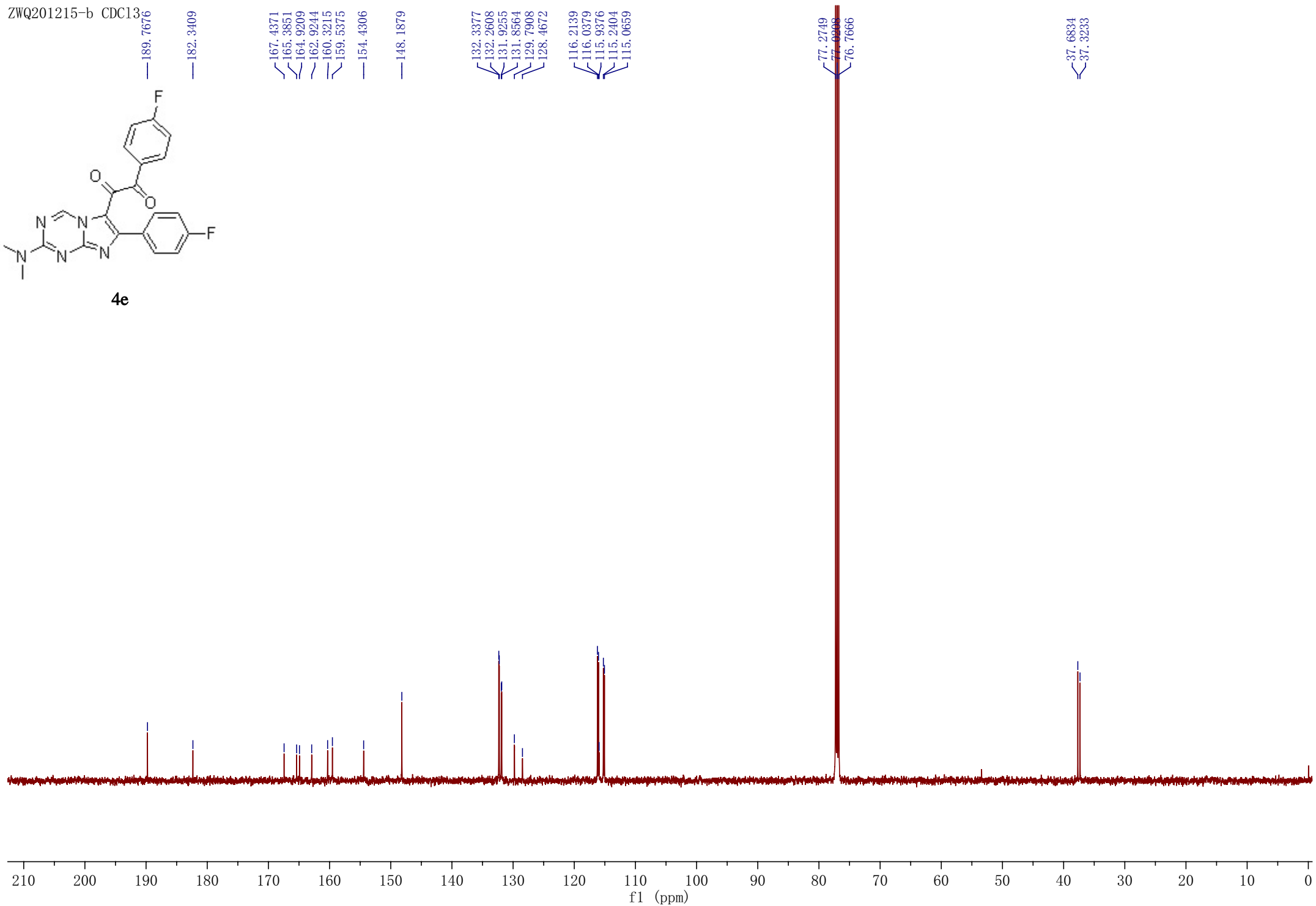
4e

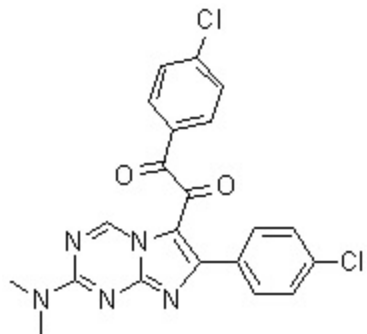


ZWQ201215-b CDC13



4e



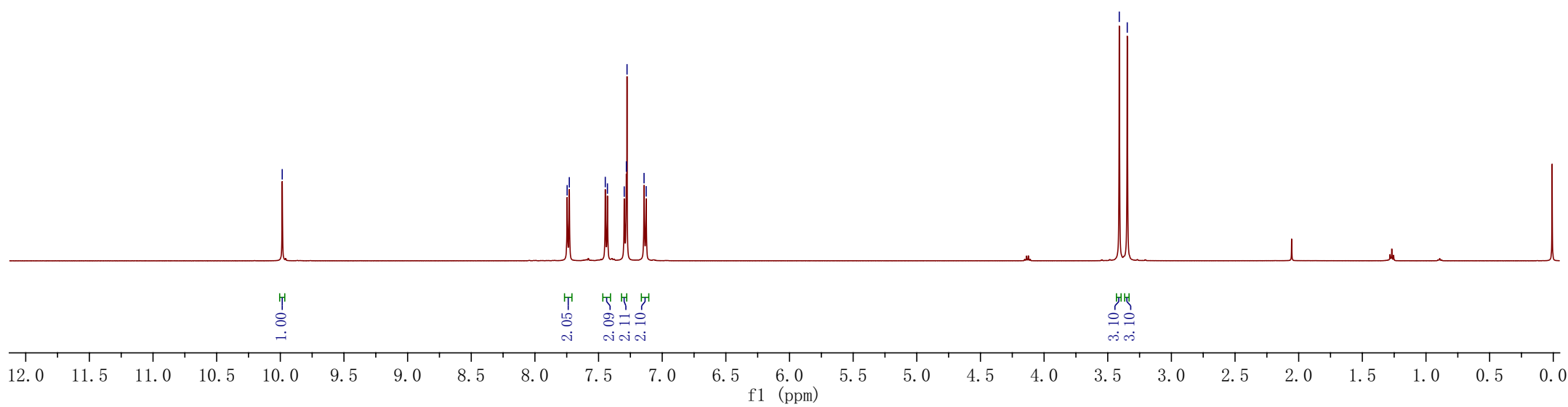


4f

9.9850

7.7468  
7.7298  
7.4471  
7.4302  
7.2883  
7.2814  
7.2762  
7.1427  
7.1260

3.4093  
3.3467



1.00H

2.05H

2.09H

2.11H

2.10H

3.10H

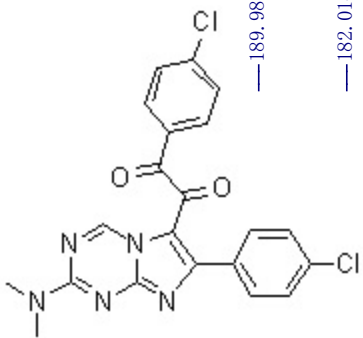
3.10H

f1 (ppm)

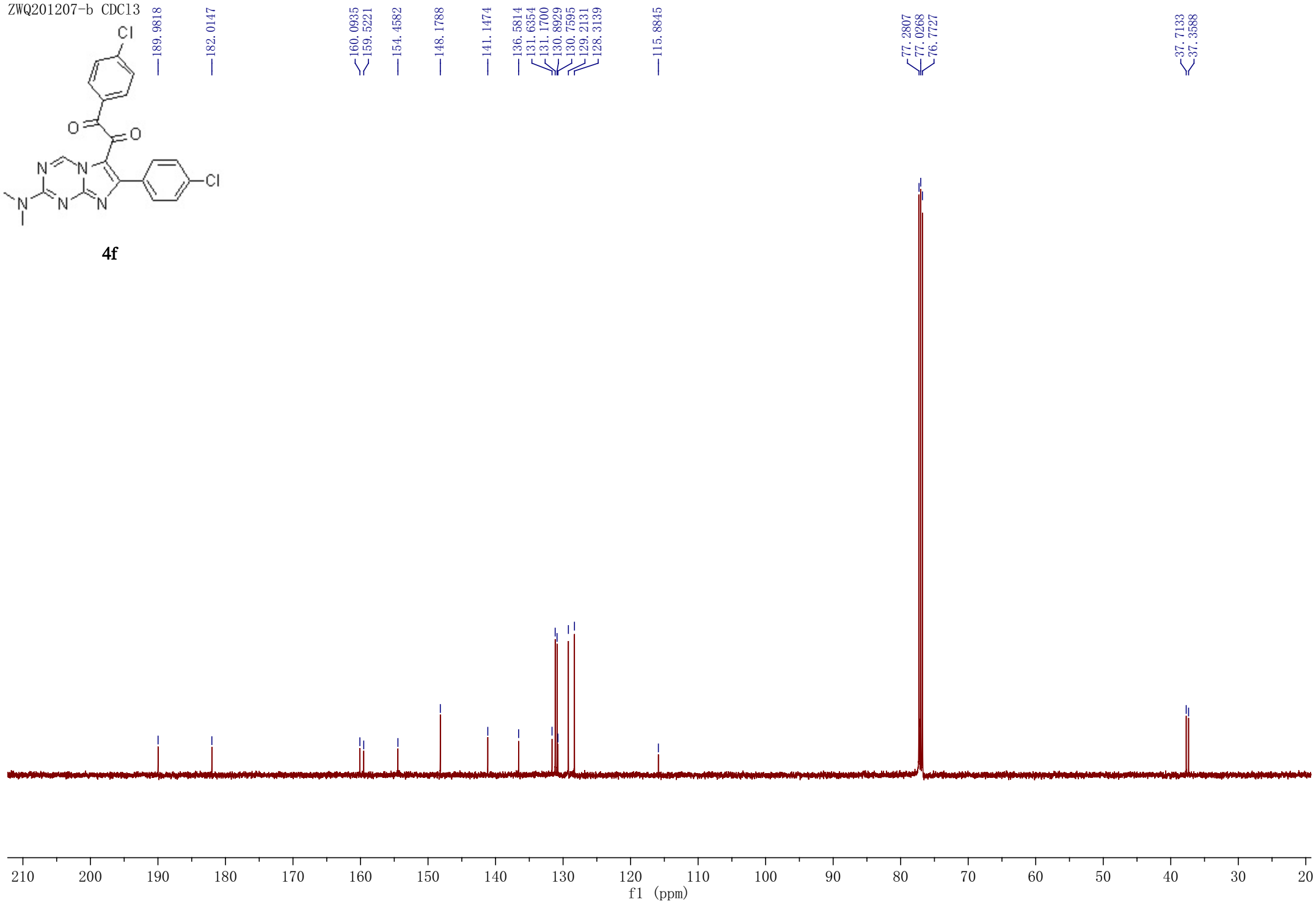
S67

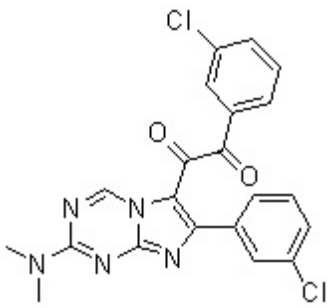


ZWQ201207-b CDC13



4f

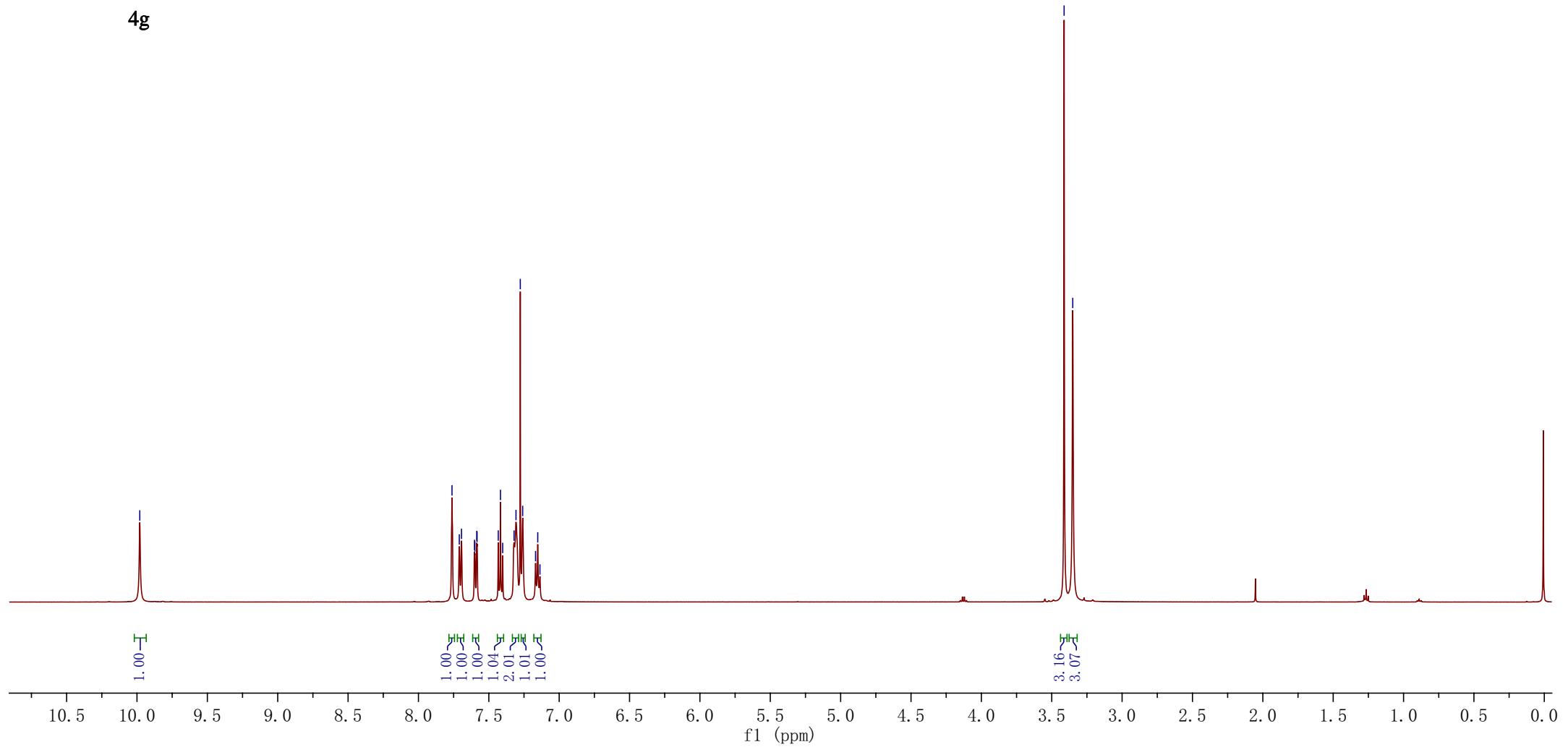




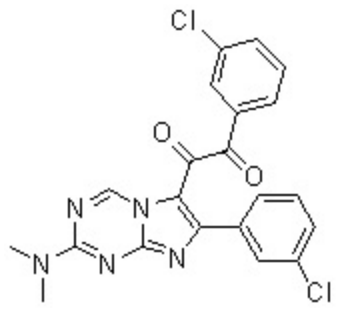
4g

7.7616  
7.7097  
7.6942  
7.6016  
7.5994  
7.5857  
7.5834  
7.4329  
7.4172  
7.4014  
7.3206  
7.3070  
7.2763  
7.2594  
7.1678  
7.1523  
7.1367

3.4120  
3.3507

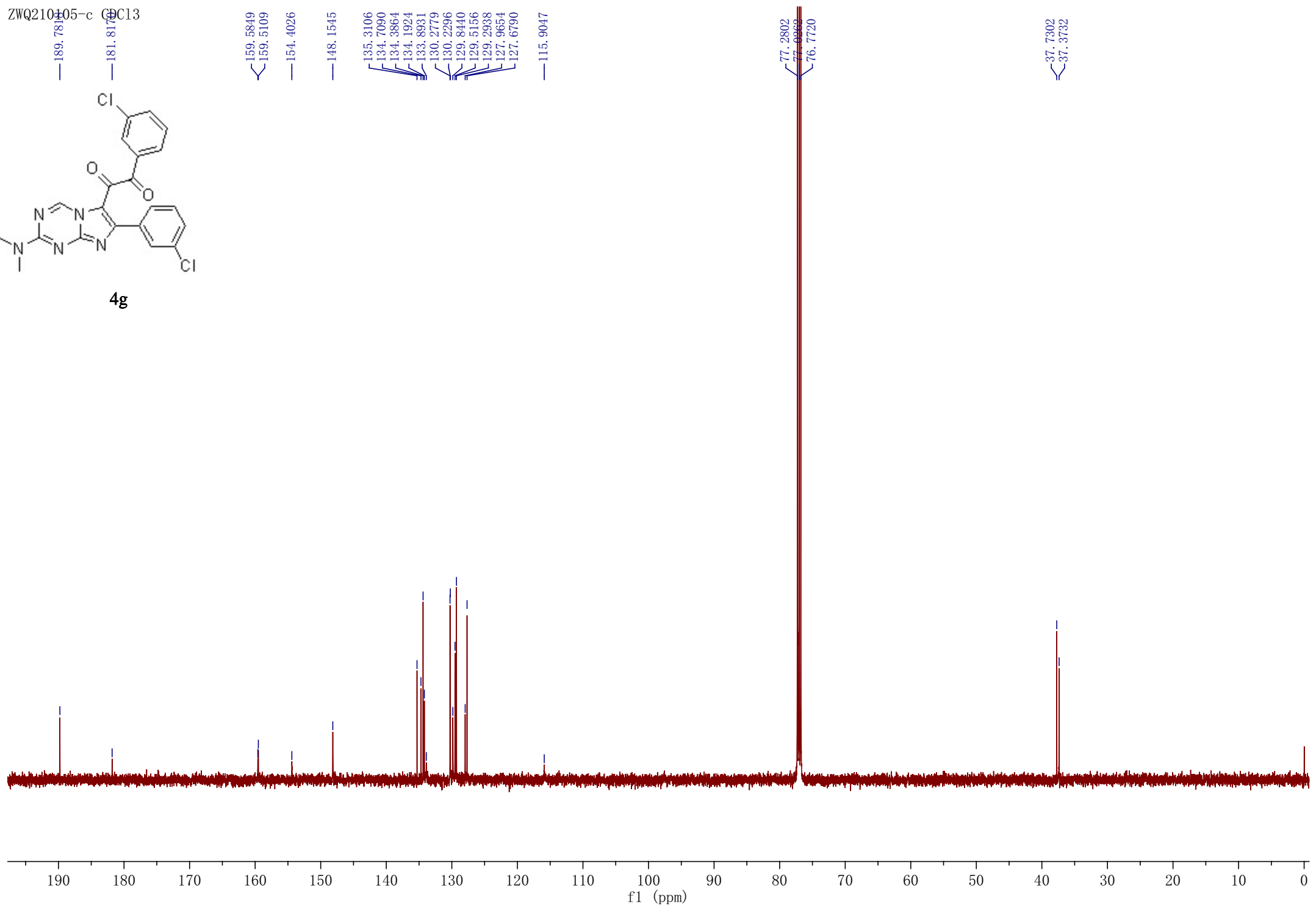


ZWQ210105-c CDCl3



4g

- 189.781
- 181.817
- 159.5849
- 159.5109
- 154.4026
- 148.1545
- 135.3106
- 134.7090
- 134.3864
- 134.1924
- 133.8931
- 130.2779
- 130.2296
- 129.8440
- 129.5156
- 129.2938
- 127.9654
- 127.6790
- 115.9047



- 77.2802
- 77.0959
- 76.7720

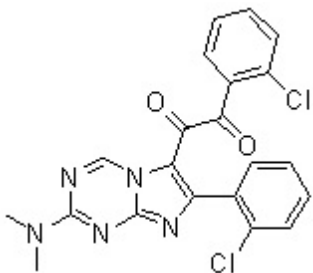
- 37.7302
- 37.3732

ZWQ210115-b CDC13

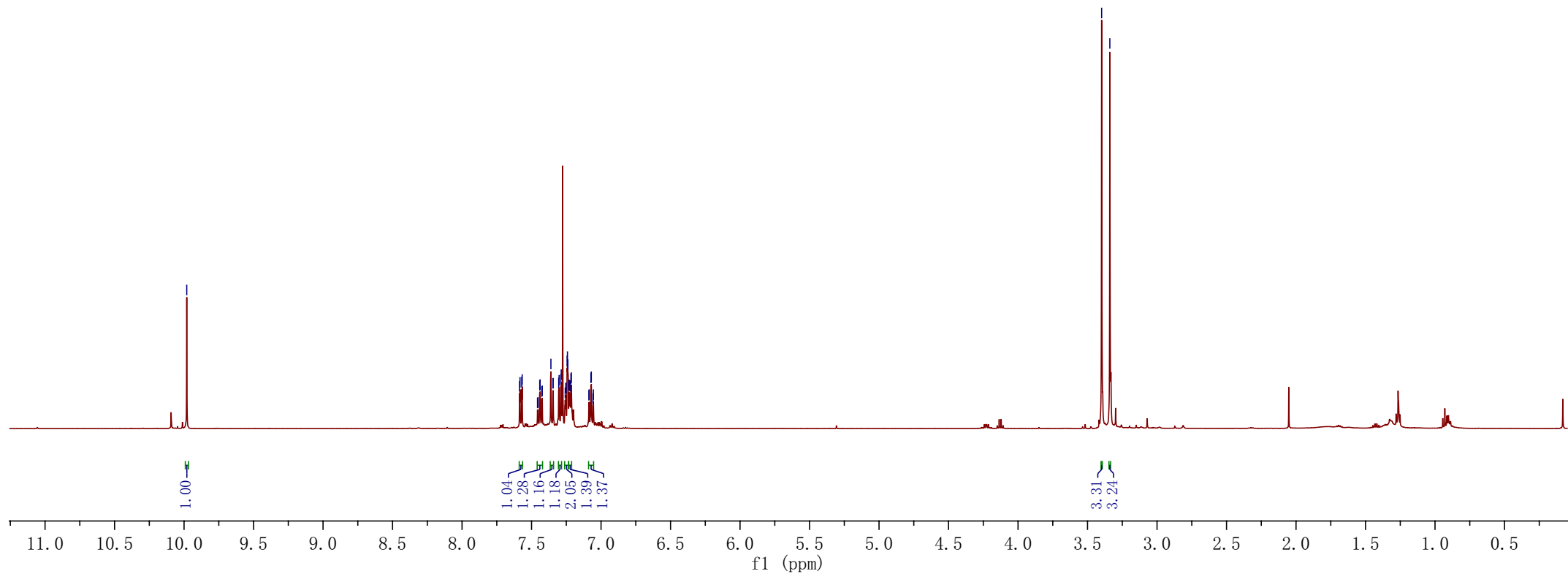
9.9806

7.5862  
7.5830  
7.5705  
7.5673  
7.4570  
7.4537  
7.4411  
7.4382  
7.4263  
7.4230  
7.3607  
7.3462  
7.3447  
7.3045  
7.3017  
7.2894  
7.2865  
7.2578  
7.2536  
7.2516  
7.2441  
7.2416  
7.2385  
7.2312  
7.2281  
7.2233  
7.2214  
7.2167  
7.2137  
7.0875  
7.0847  
7.0726  
7.0700  
7.0577  
7.0551

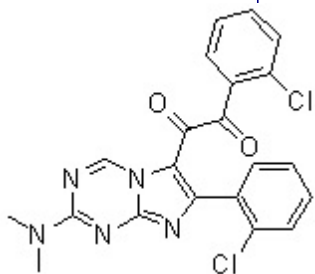
3.3986  
3.3394



4h



ZWQ210115-b CDC13



4h

189.6025

181.1389

159.4531

157.5962

154.2197

148.0853

134.4172

134.3429

133.9125

132.5665

131.8896

131.6604

131.6045

130.9785

130.7655

129.4703

126.9814

126.0223

116.9017

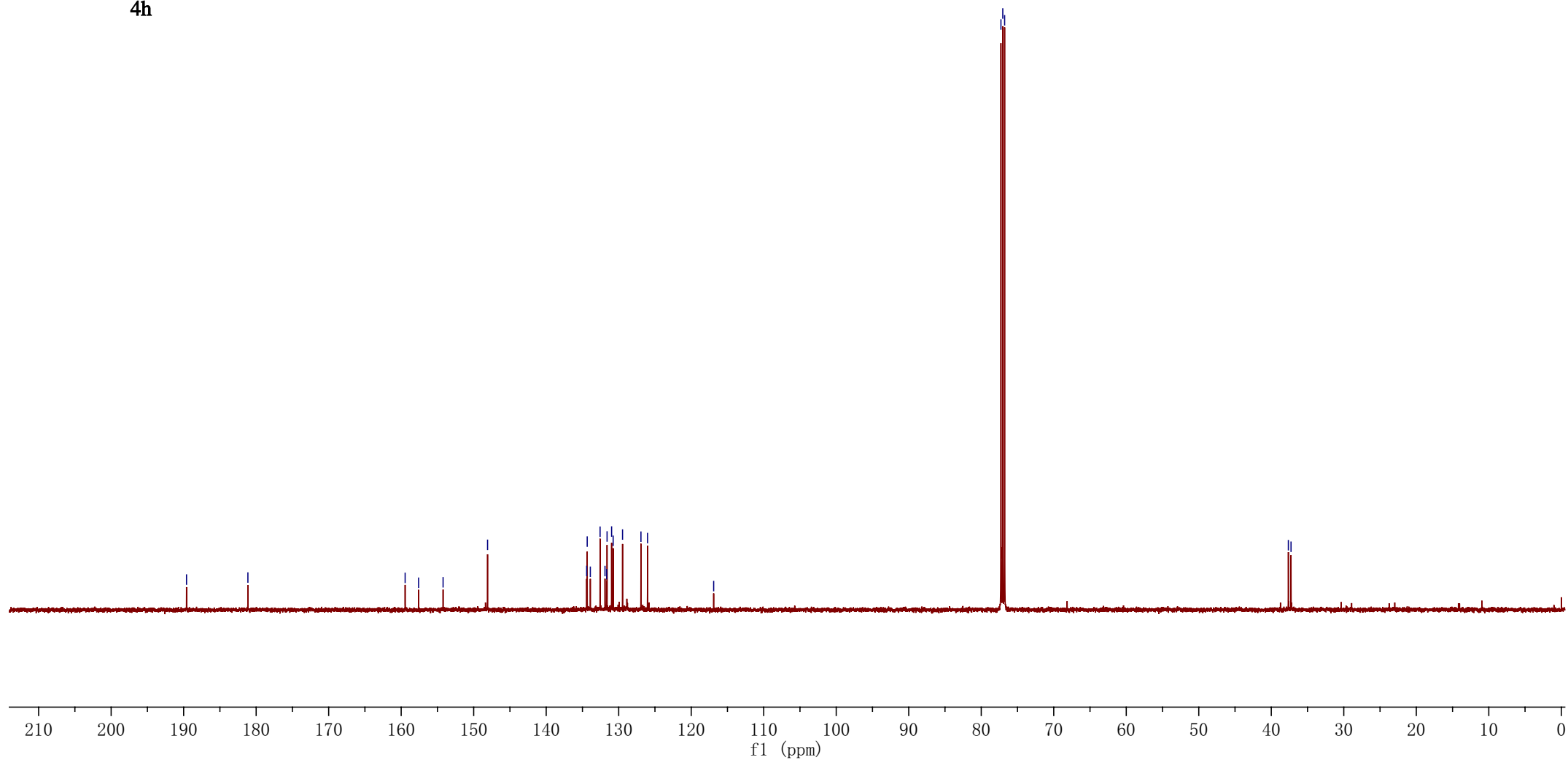
77.2829

77.0286

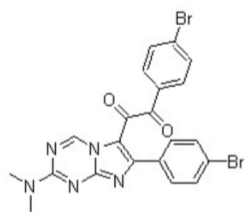
76.7745

37.6434

37.2743



ZWQ201215-a CDCl3

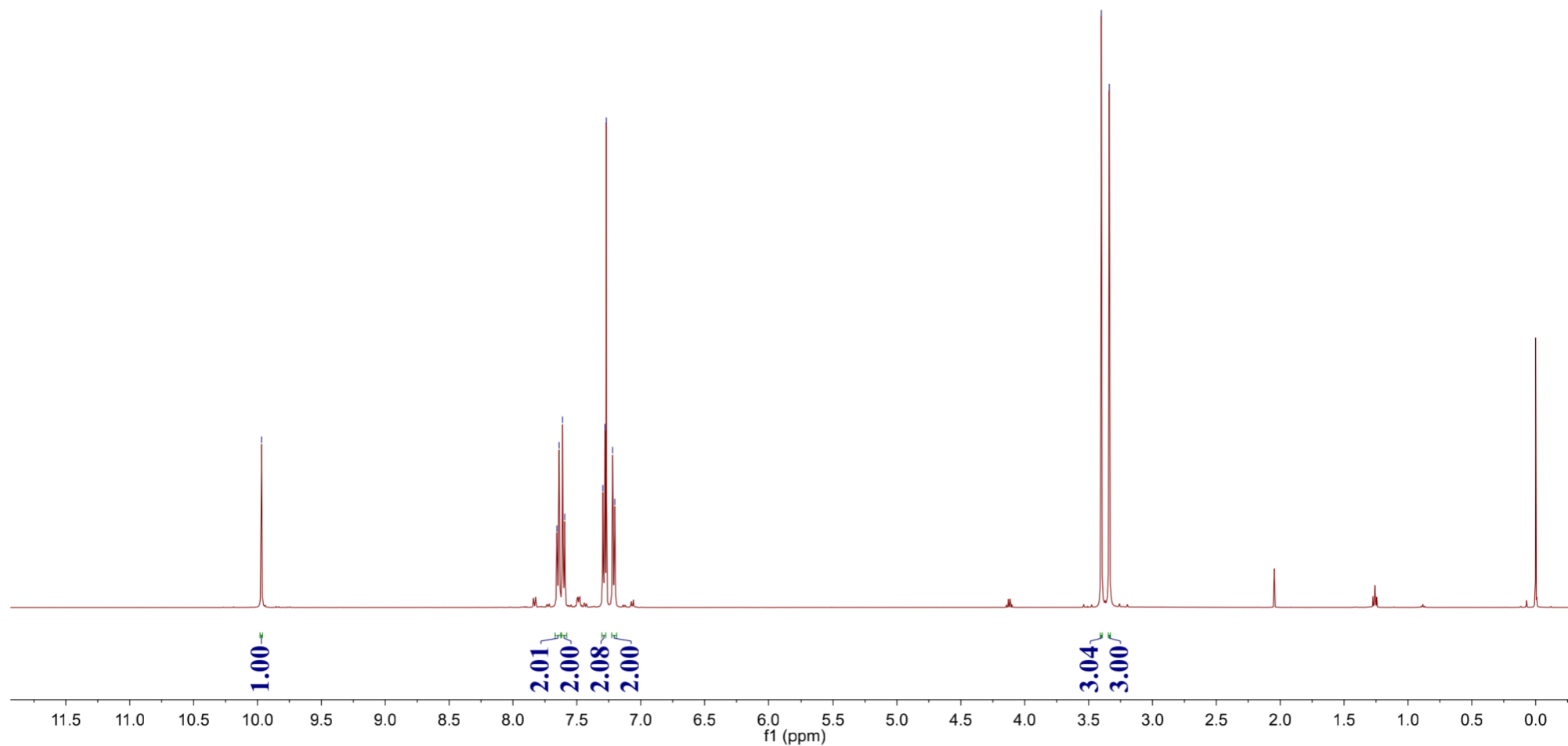


4i

9.9686

7.6559  
7.6391  
7.6114  
7.5943  
7.2965  
7.2800  
7.2689  
7.2195  
7.2026

3.4002  
3.3381



— 190.1902

— 181.9656

— 160.0087  
— 159.5072

— 154.4253

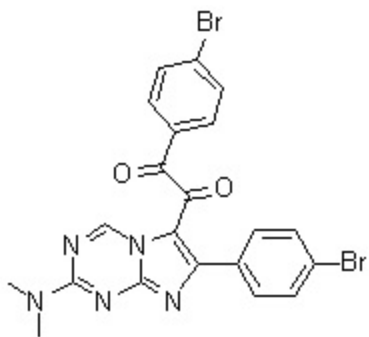
— 148.1921

— 132.2378  
— 132.0066  
— 131.3990  
— 131.3098  
— 131.1164  
— 130.9651  
— 130.8853  
— 125.0379

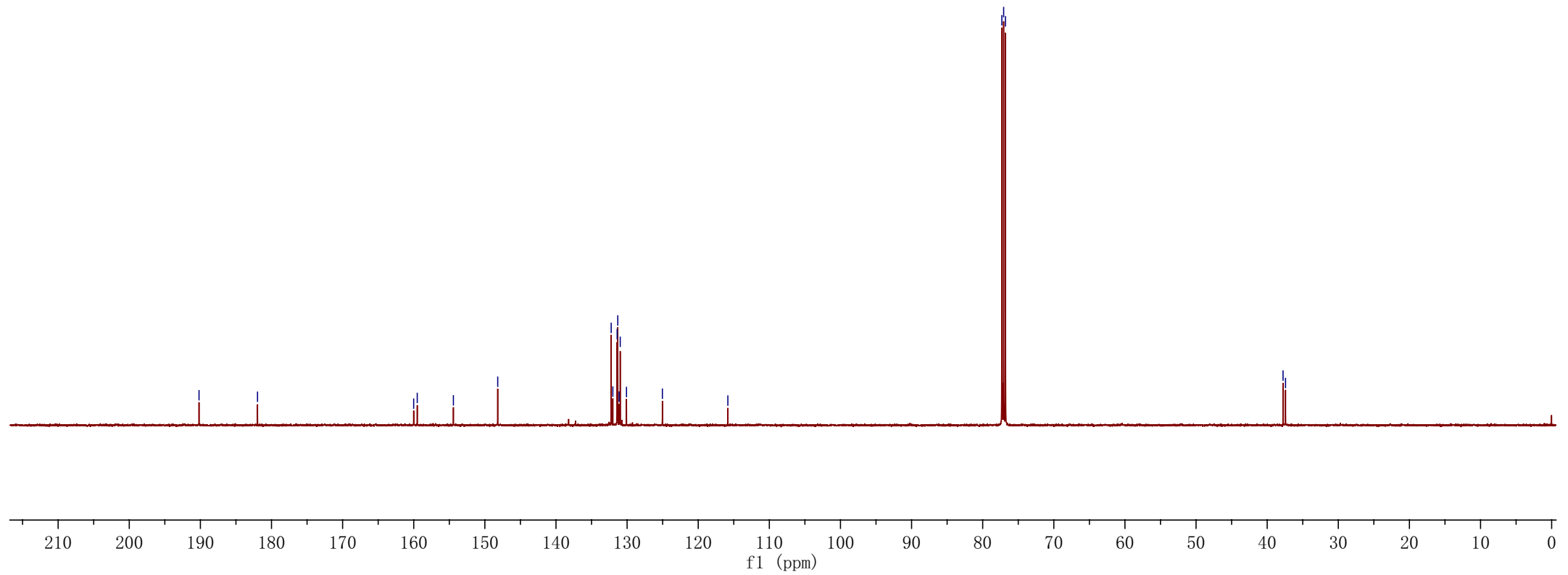
— 115.8335

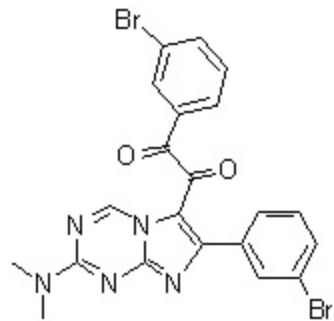
— 77.3082  
— 77.0541  
— 76.7999

— 37.7679  
— 37.4221



**4i**



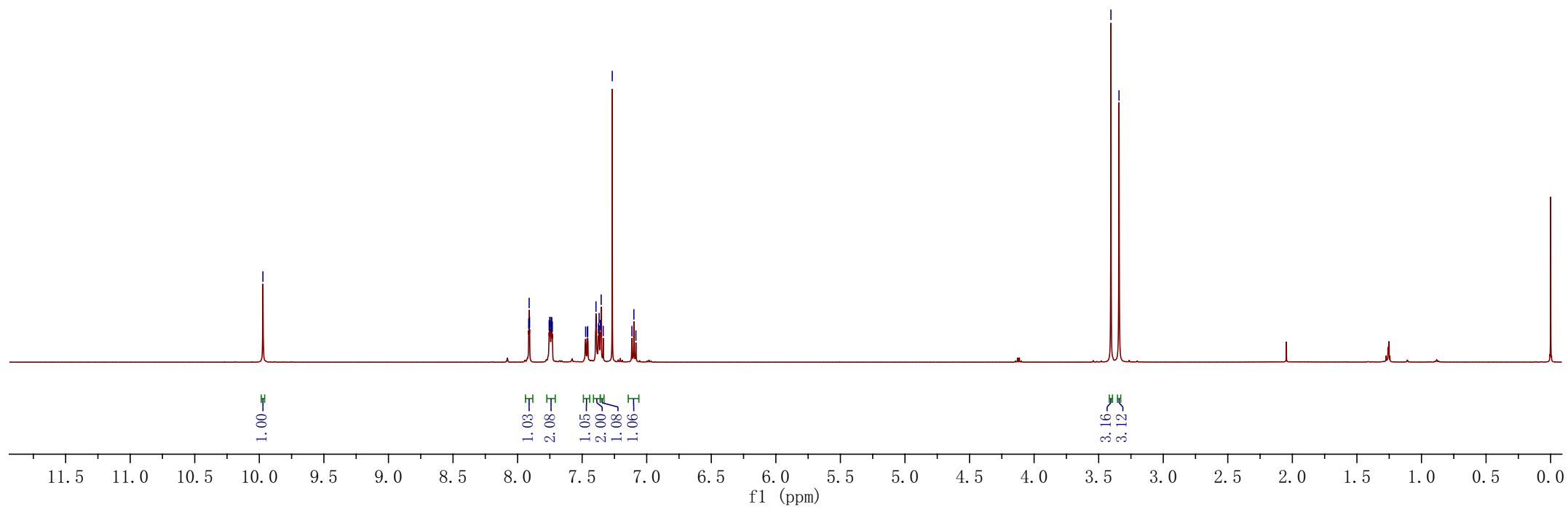


4j

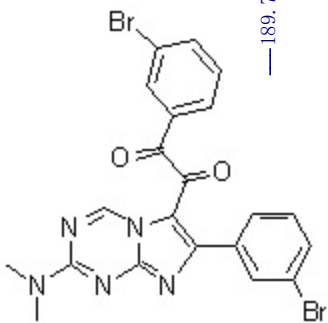
9.9722

7.9137  
7.9104  
7.9070  
7.7555  
7.7509  
7.7469  
7.7401  
7.7373  
7.7349  
7.7309  
7.4731  
7.4586  
7.4568  
7.3928  
7.3896  
7.3736  
7.3684  
7.3581  
7.3526  
7.3369  
7.2668  
7.1150  
7.0993  
7.0836

3.4051  
3.3425







189.7509

181.7283

159.6685

159.5069

154.4770

148.1567

137.3226

134.8534

133.1871

132.6505

132.2780

130.4879

129.7568

128.3689

128.1734

123.3696

122.2046

115.9174

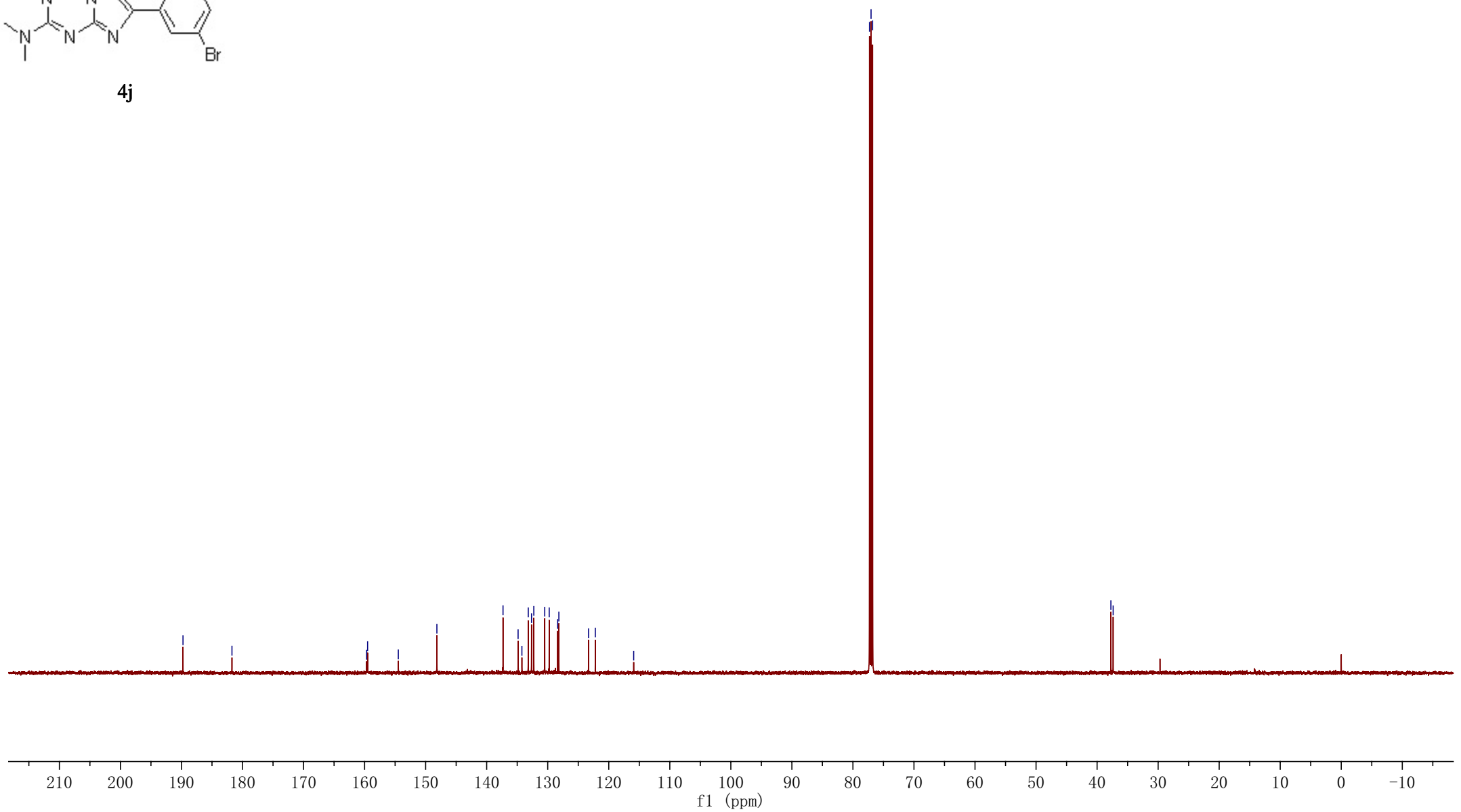
77.2844

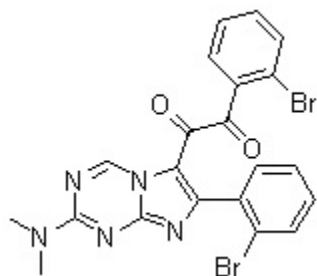
77.0304

76.7763

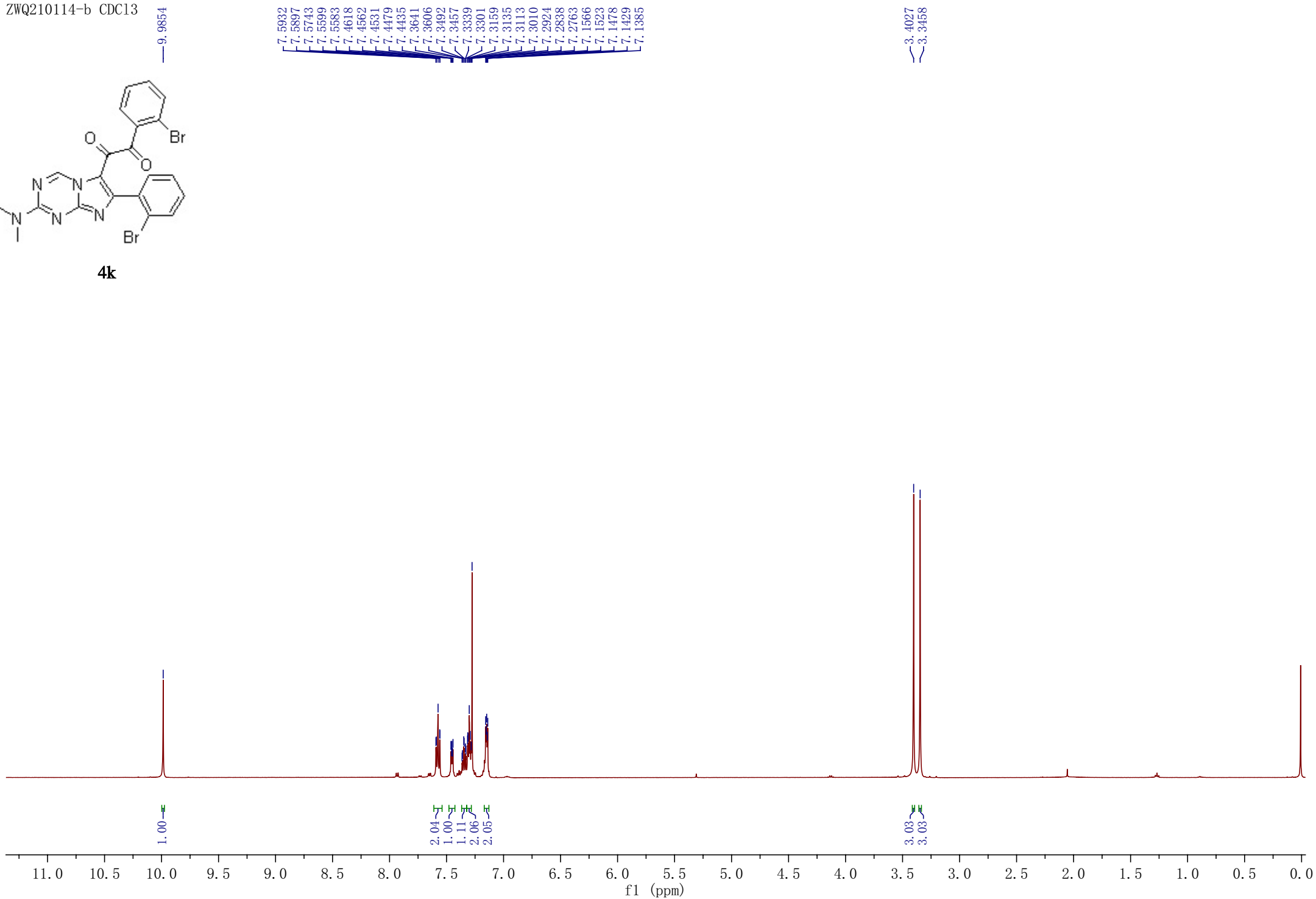
37.7367

37.3690

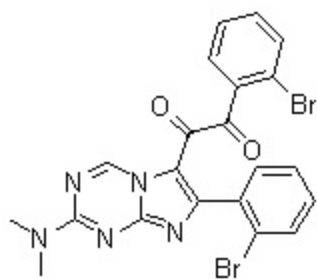




4k



ZWQ210114-b CDC13



4k

190.0994

180.7737

159.4702  
158.8074

154.1023

148.1170

134.6095

134.2169

133.5041

133.4349

133.3466

132.6757

131.6454

130.8764

127.4126

126.6483

123.4480

122.5347

117.0470

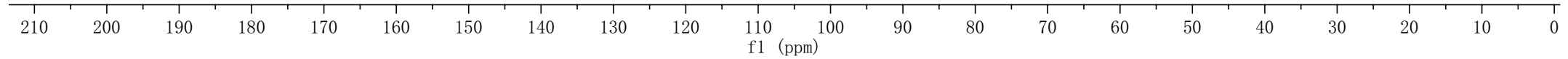
77.2797

77.0056

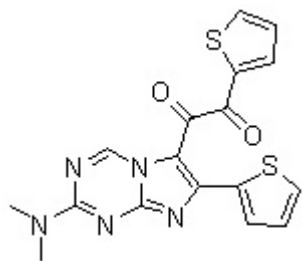
76.7715

37.6637

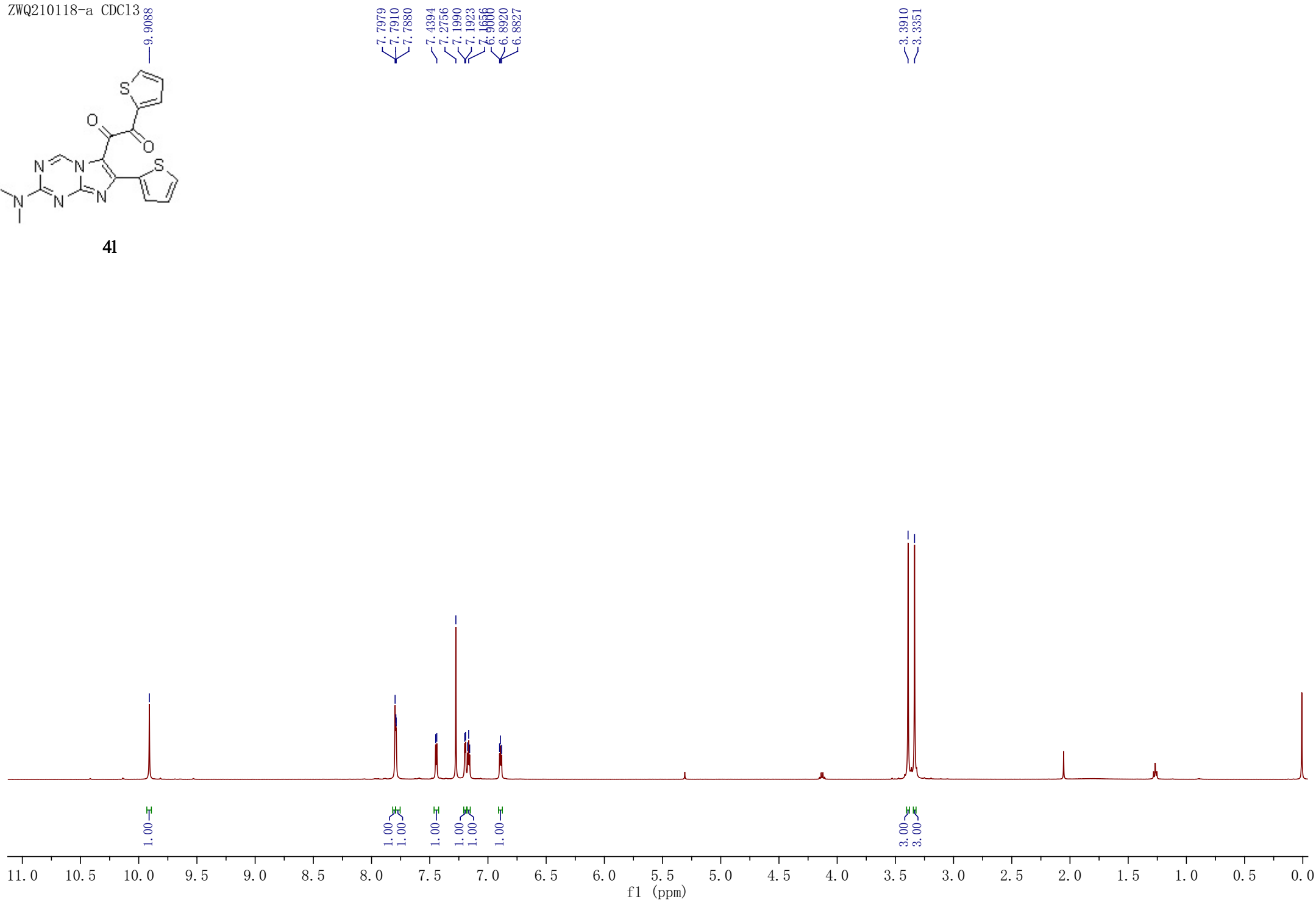
37.3065



ZWQ210118-a CDC13



41



S79

ZWQ210118-a CDC13

183.7981  
180.9033

159.5172

154.3014  
153.9967

148.0714

140.4996  
136.4916

135.8037  
134.3842

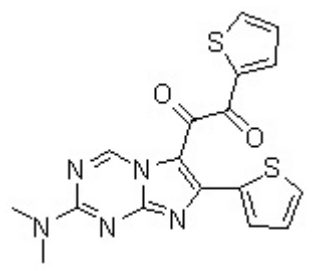
131.2419  
130.5379

128.5791  
127.3792

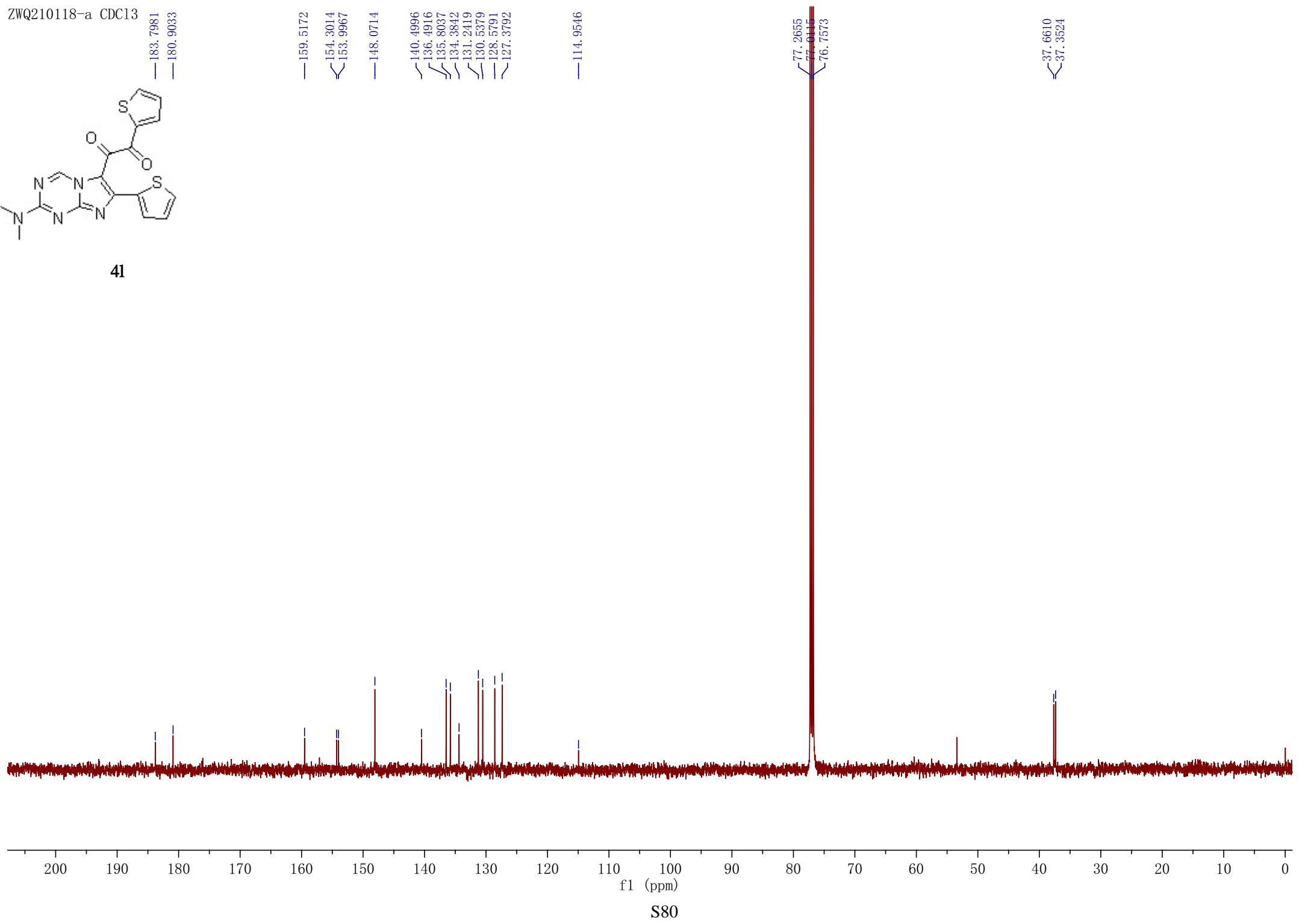
114.9546

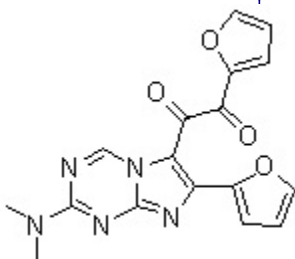
77.2655  
77.0115  
76.7573

37.6610  
37.3524



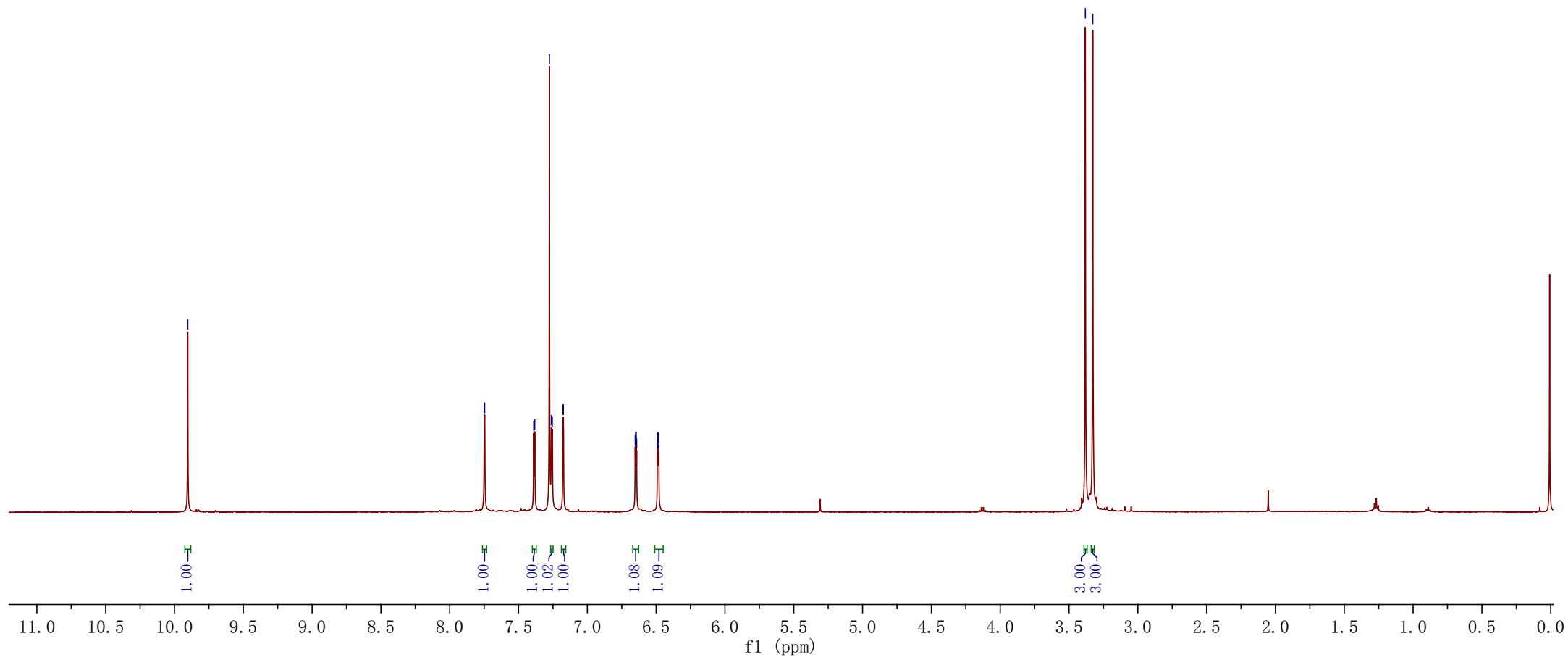
41



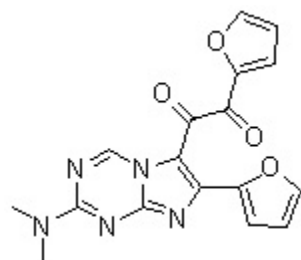


4m

7.7481  
7.7462  
7.3825  
7.2758  
7.2613  
7.2550  
7.1762  
6.6448  
6.6416  
6.4907  
6.4872  
6.4838  
6.4804  
3.3814  
3.3275



ZWQ210109-c CDC13



4m

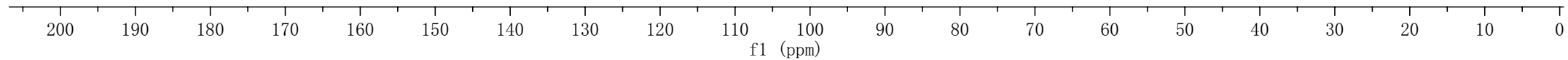
181.3701  
179.0653

159.5015  
154.6711  
150.4721  
148.1822  
148.1537  
147.9167  
147.4589  
144.7058

120.9523  
115.4067  
113.6077  
112.6858  
112.6195

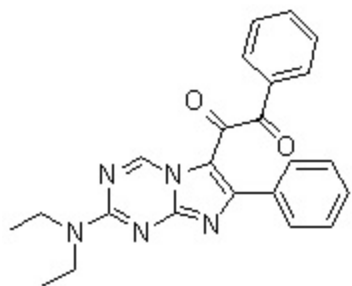
77.2660  
77.0199  
76.7578

37.6453  
37.3102



ZWQ210109-a CDC13

10.0279

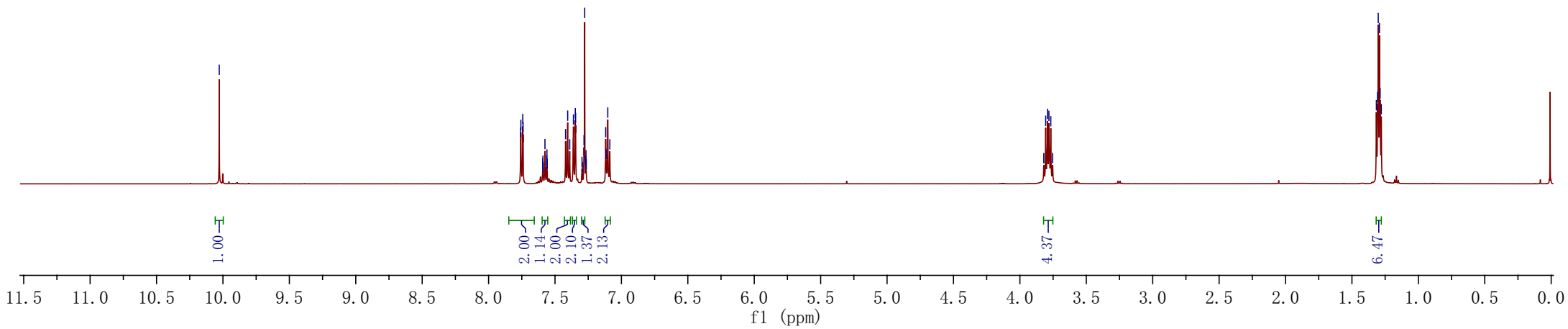


4n

7.7589  
7.7570  
7.7427  
7.7402  
7.5927  
7.5906  
7.5882  
7.5756  
7.5631  
7.5608  
7.5584  
7.4205  
7.4045  
7.3893  
7.3613  
7.3472  
7.3448  
7.2967  
7.2943  
7.2816  
7.2764  
7.2690  
7.2667  
7.2645  
7.1183  
7.1153  
7.1026  
7.0872

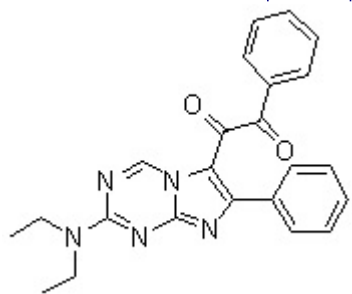
3.8199  
3.8058  
3.7916  
3.7814  
3.7673  
3.7532

1.3162  
1.3071  
1.3021  
1.2980  
1.2879  
1.2789

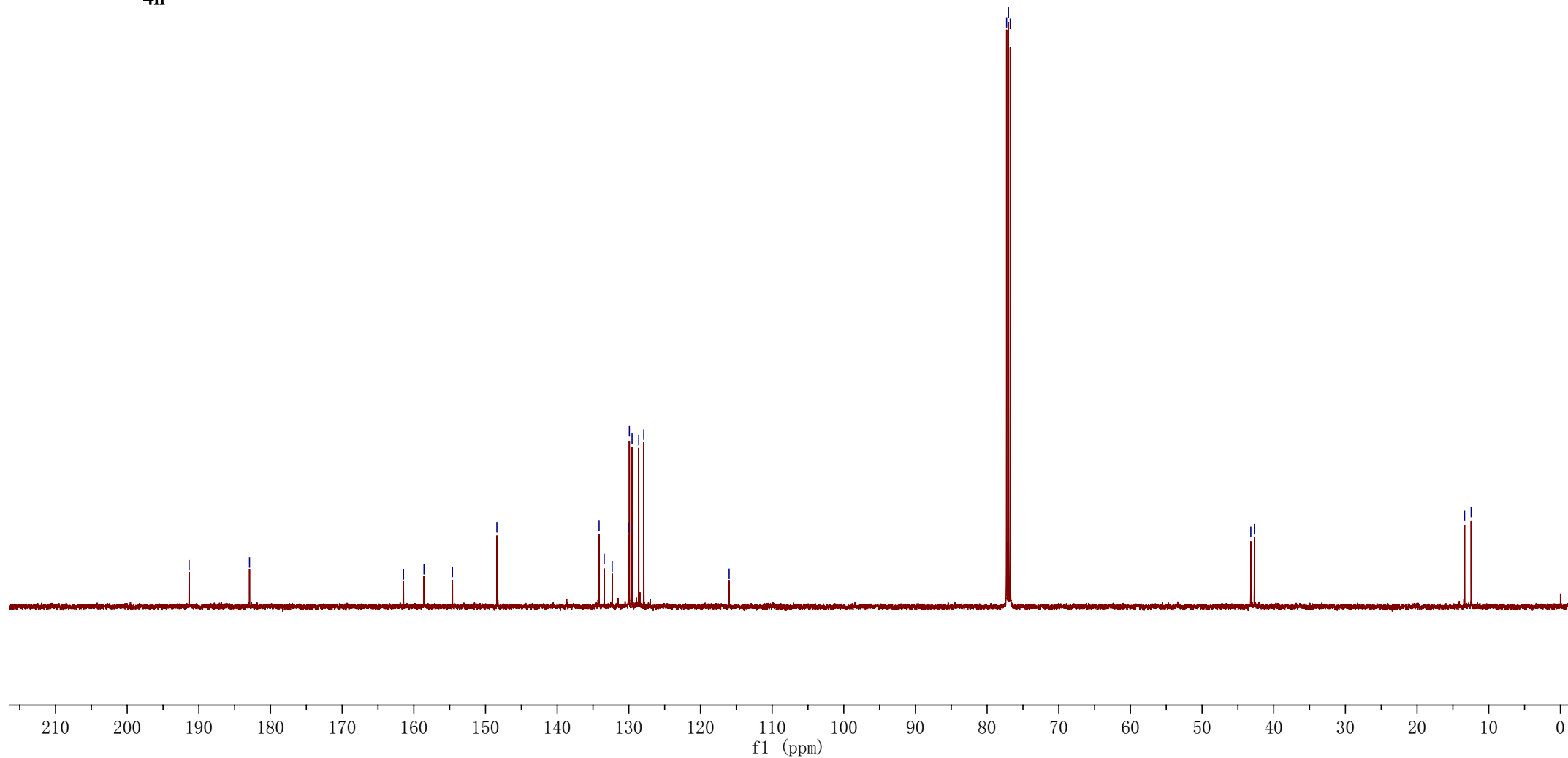


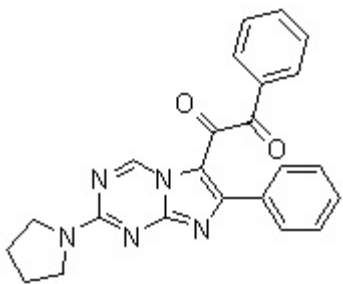


ZWQ210109-a CDC13



4n



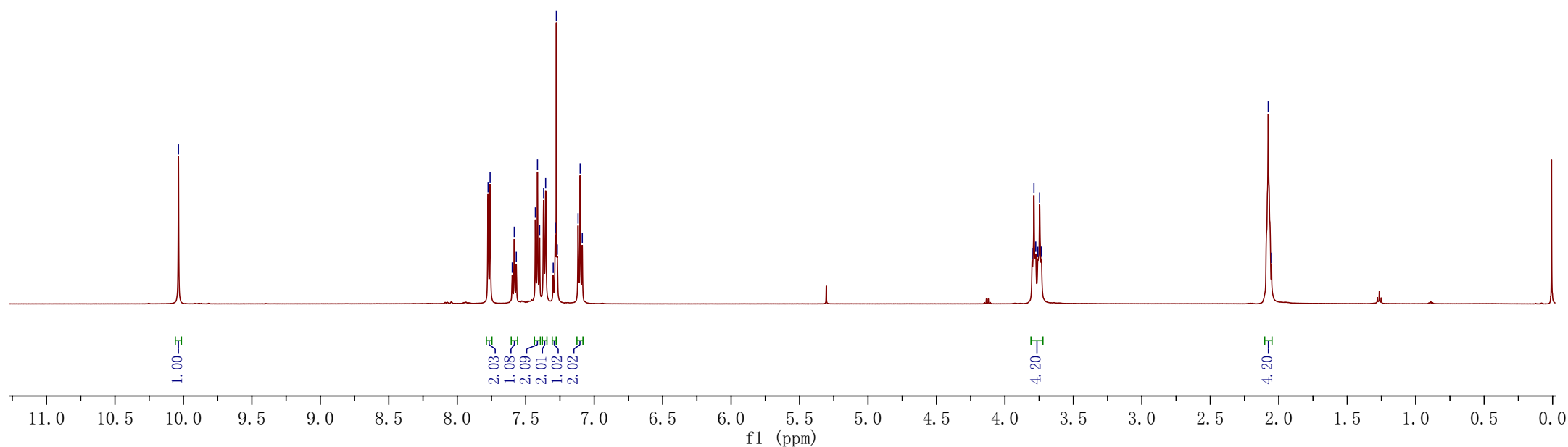


4o

7.7746  
7.7600  
7.5983  
7.5835  
7.5687  
7.4296  
7.4141  
7.3985  
7.3689  
7.3544  
7.2991  
7.2840  
7.2762  
7.2695  
7.1176  
7.1023  
7.0869

3.8013  
3.7879  
3.7747  
3.7594  
3.7463  
3.7332

2.0767  
2.0527



ZWQ210108-c CDC13

191.3271

182.9414

161.4883

157.3529

154.4206

148.3884

134.1534

133.4158

132.3440

130.0908

129.9338

129.6606

128.6424

127.9321

115.9029

77.2923

77.0281

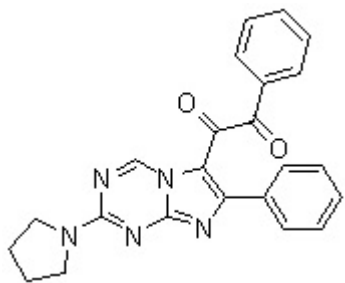
76.7840

47.6819

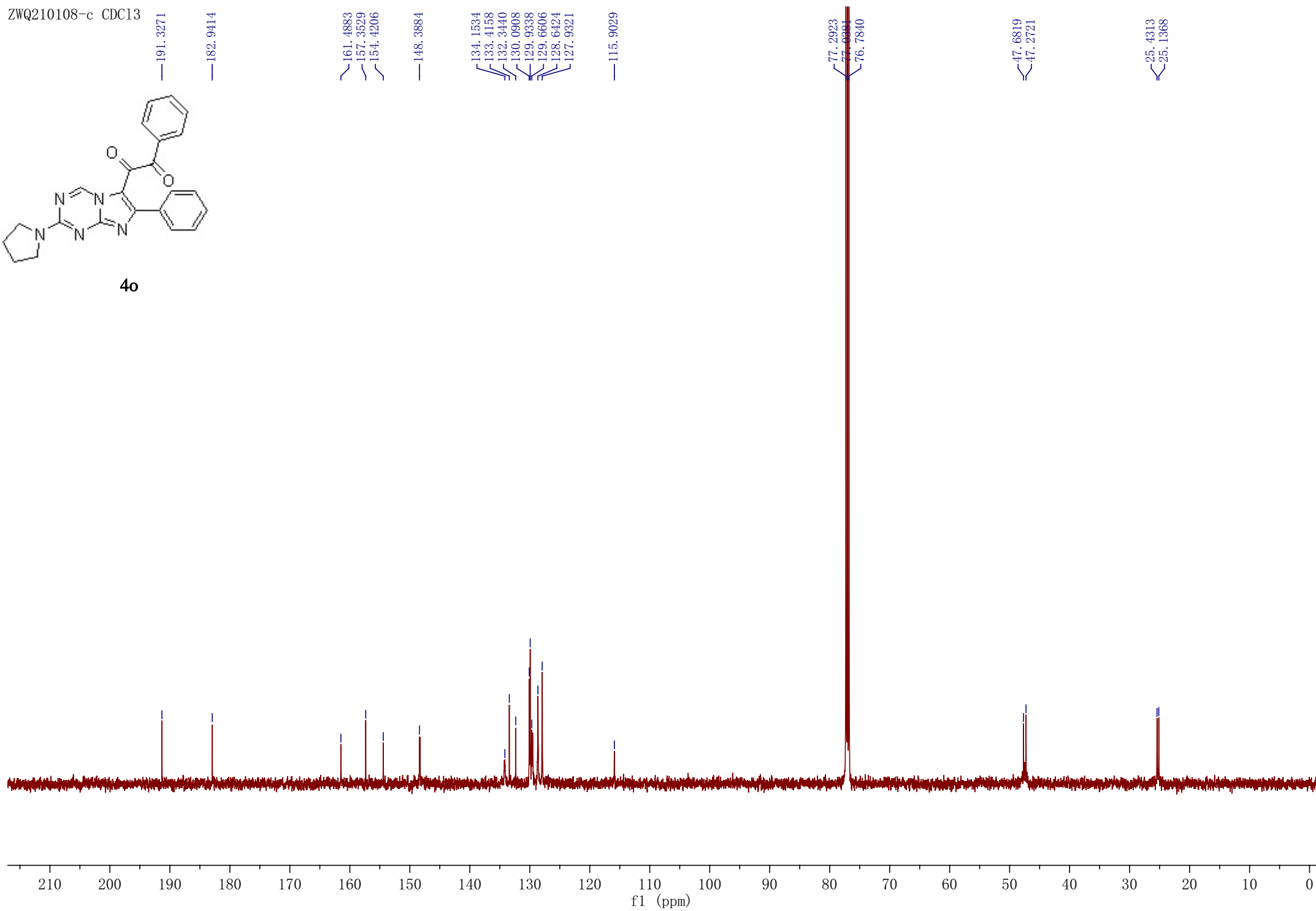
47.2721

25.4313

25.1368



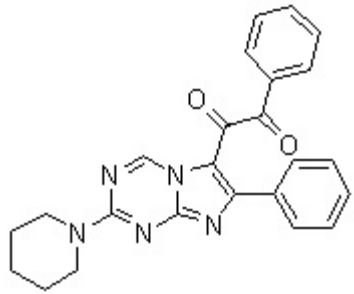
4o



f1 (ppm)

S86

ZWQ210108-b CDC13

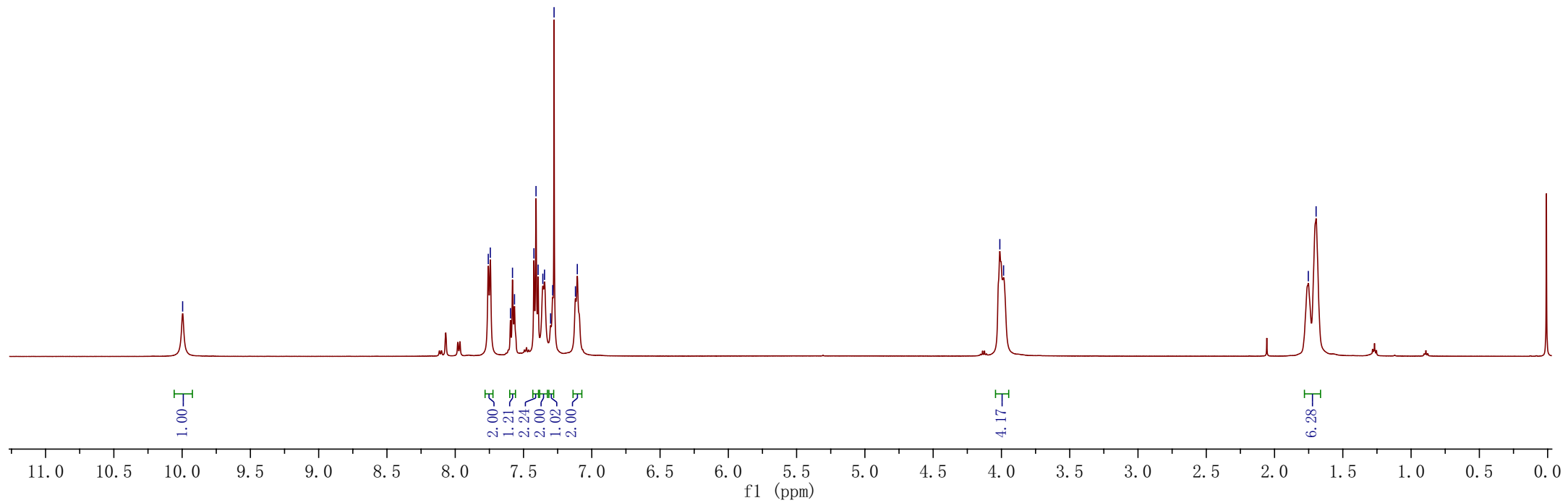


4p

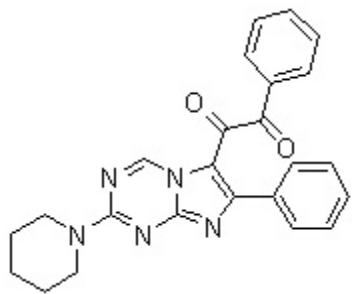
7.7579  
7.7431  
7.5954  
7.5806  
7.5659  
7.4237  
7.4084  
7.3930  
7.3584  
7.3461  
7.3014  
7.2863  
7.2762  
7.1196  
7.1060

4.0117  
3.9842

1.7526  
1.6956



ZWQ210108-b CDC13



4p

191.3171  
183.0105

161.4492  
158.3459  
154.6802

148.4978

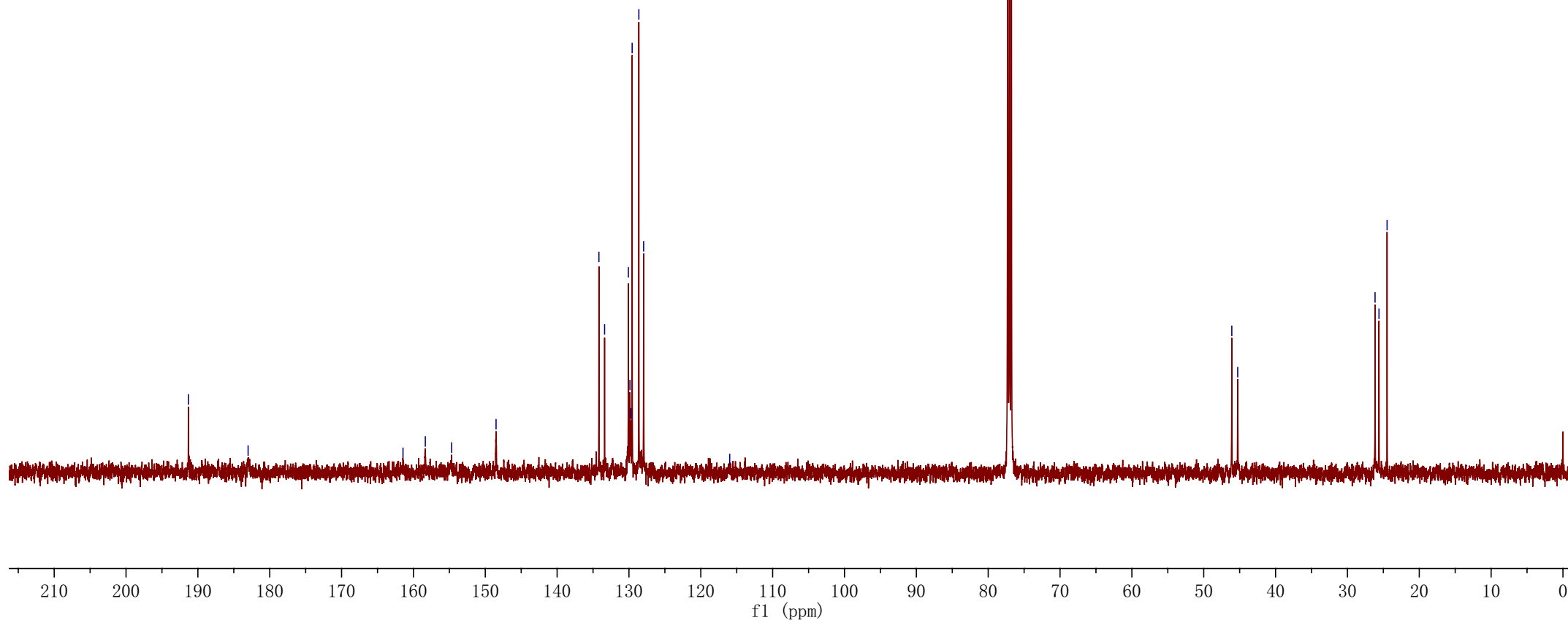
134.1811  
133.3905  
130.0821  
129.8643  
129.7354  
129.5561  
128.6224  
127.9559

115.9770

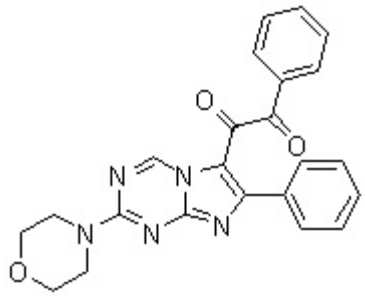
77.2873  
77.0291  
76.7791

46.0917  
45.2688

26.1528  
25.6068  
24.4805



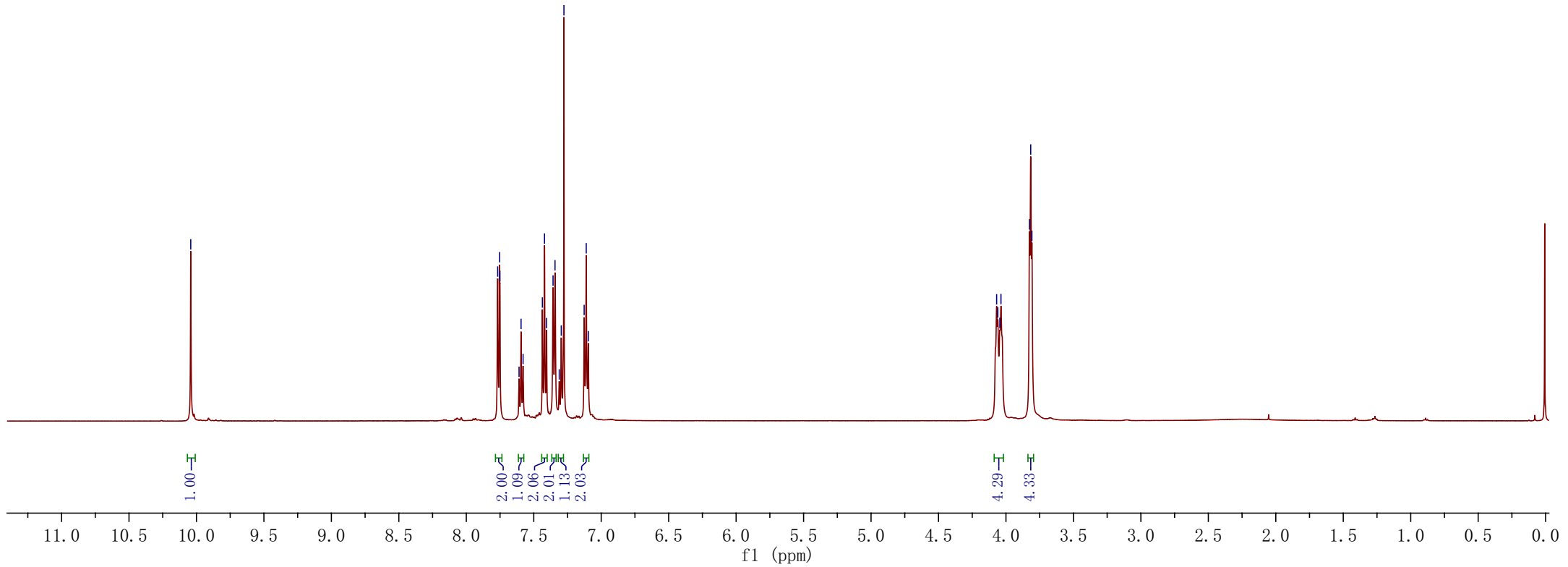
ZWQ210105-b CDCL3



4q

7.7673  
7.7528  
7.7510  
7.6090  
7.5941  
7.5793  
7.4360  
7.4204  
7.4048  
7.3569  
7.3424  
7.3110  
7.2961  
7.2763  
7.1263  
7.1110  
7.0956

4.0692  
4.0602  
4.0453  
4.0370  
3.8259  
3.8165  
3.8077



ZWQ210105-b CDC13

191.1362

183.2835

161.3923

158.6697

154.2208

148.7706

134.2847

133.2984

132.1275

130.1975

129.8935

129.5765

128.6712

127.9988

116.1989

77.2813

77.0000

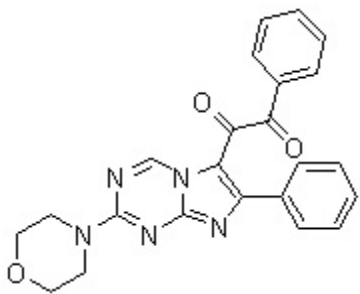
76.7732

66.7632

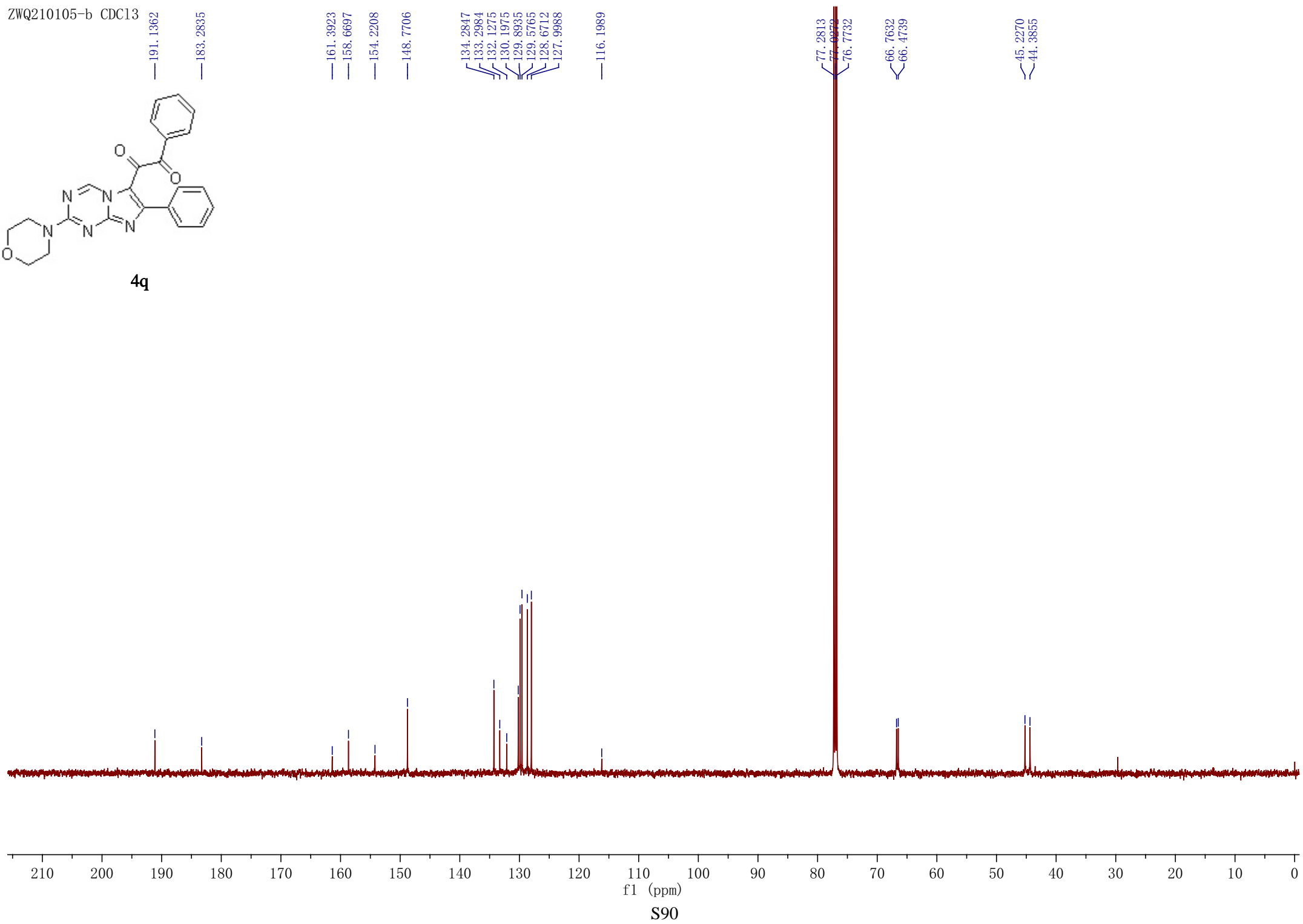
66.4739

45.2270

44.3855



4q



f1 (ppm)

S90

## checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.      CIF dictionary      Interpreting this report

### Datablock: mo\_201210\_zwq\_1\_0m

---

Bond precision:    C-C = 0.0045 A                      Wavelength=0.71073

Cell:                      a=7.3250(4)              b=12.3657(5)              c=27.8190(12)  
                                    alpha=90                      beta=90                      gamma=90

Temperature:              170 K

	Calculated	Reported
Volume	2519.810	2519.8(2)
Space group	P b c a	?
Hall group	-P 2ac 2ab	?
Moiety formula	C13 H12 Br N5	?
Sum formula	C13 H12 Br N5	C13 H12 Br N5
Mr	318.18	318.19
Dx,g cm-3	1.677	1.677
Z	8	8
Mu (mm-1)	3.256	3.256
F000	1280.0	1280.0
F000'	1278.06	
h,k,lmax	8,14,33	8,14,33
Nref	2219	2221
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 1.001                      Theta(max)= 25.000

R(reflections)= 0.0375( 2056)              wR2(reflections)= 0.0856( 2221)

S = 1.076                                      Npar= 174

---

The following ALERTS were generated. Each ALERT has the format  
**test-name\_ALERT\_alert-type\_alert-level.**  
Click on the hyperlinks for more details of the test.

---



## Alert level A

SYMM001\_ALERT\_1\_A \_symmetry\_cell\_setting is missing  
The cell setting should be one of the following  
\* triclinic  
\* monoclinic  
\* orthorhombic  
\* tetragonal  
\* rhombohedral  
\* trigonal  
\* hexagonal  
\* cubic  
The following tests will not be performed.  
SYMMS\_01,SYMMS\_02  
EXPT005\_ALERT\_1\_A \_exptl\_crystal\_description is missing  
Crystal habit description.  
The following tests will not be performed.  
CRYSR\_01

DIFF003\_ALERT\_1\_A \_diffrn\_measurement\_device\_type is missing  
Diffractometer make and type. Replaces \_diffrn\_measurement\_type.  
PLAT122\_ALERT\_1\_A No \_symmetry\_space\_group\_name\_H-M Given ..... Please Do !  
PLAT183\_ALERT\_1\_A Missing \_cell\_measurement\_reflms\_used Value .... Please Do !  
PLAT184\_ALERT\_1\_A Missing \_cell\_measurement\_theta\_min Value ..... Please Do !  
PLAT185\_ALERT\_1\_A Missing \_cell\_measurement\_theta\_max Value ..... Please Do !  
PLAT699\_ALERT\_1\_A Missing \_exptl\_crystal\_description Value ..... Please Do !

---

## Alert level C

PLAT052\_ALERT\_1\_C Info on Absorption Correction Method Not Given Please Do !  
PLAT053\_ALERT\_1\_C Minimum Crystal Dimension Missing (or Error) ... Please Check  
PLAT054\_ALERT\_1\_C Medium Crystal Dimension Missing (or Error) ... Please Check  
PLAT055\_ALERT\_1\_C Maximum Crystal Dimension Missing (or Error) ... Please Check

---

## Alert level G

PLAT005\_ALERT\_5\_G No Embedded Refinement Details Found in the CIF Please Do !  
PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 8.53 Why ?  
PLAT093\_ALERT\_1\_G No s.u.'s on H-positions, Refinement Reported as mixed Check  
PLAT104\_ALERT\_1\_G The Reported Crystal System is Inconsistent with Pbca Check  
PLAT899\_ALERT\_4\_G SHELXL97 is Deprecated and Succeeded by SHELXL/ 2018 Note

---

8 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
5 **ALERT level G** = General information/check it is not something unexpected

14 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
1 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

---

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

### **Publication of your CIF in IUCr journals**

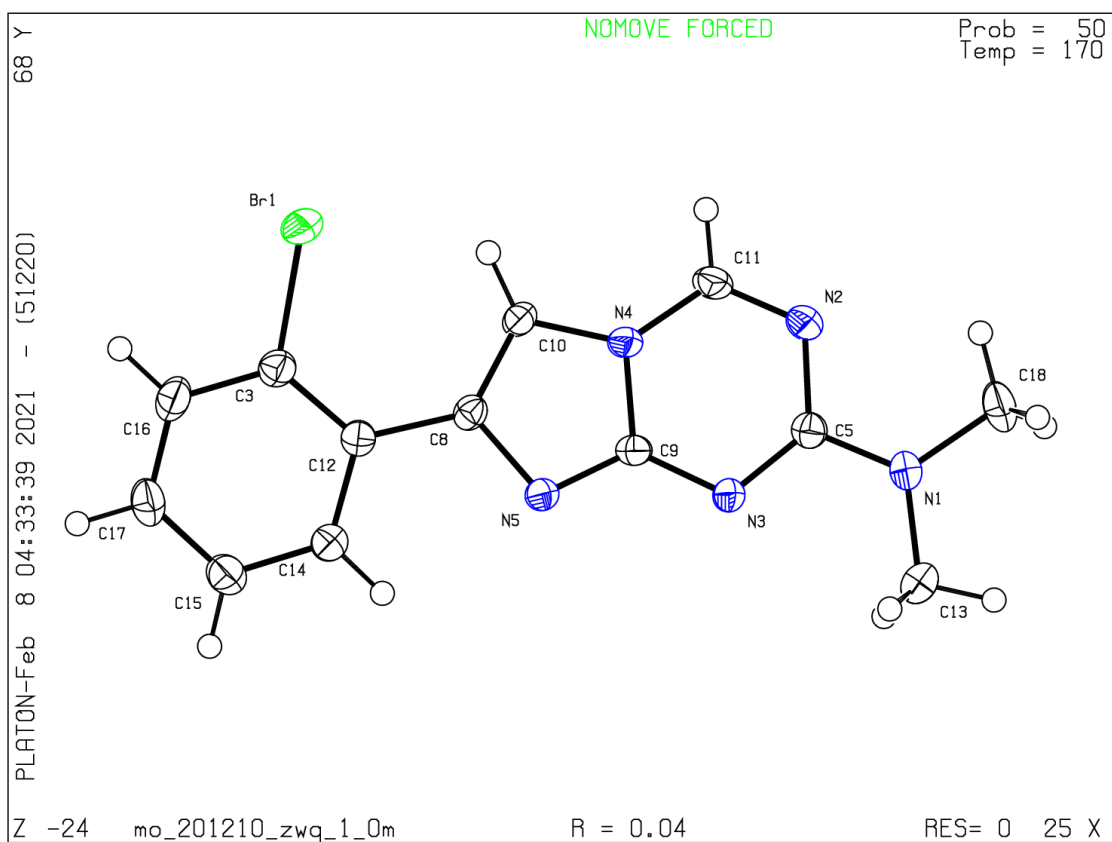
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

### **Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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**PLATON version of 05/12/2020; check.def file version of 05/12/2020**



**Crystallization:** Crystals of compound **3k** suitable for X-ray analysis were grown from the solvent of chloroform by slow evaporation method **Figure**. Molecular structure of **3k** showing thermal ellipsoid at the 30% probability level

## checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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No syntax errors found.      CIF dictionary      Interpreting this report

### Datablock: y

---

Bond precision:    C-C = 0.0019 Å                      Wavelength=0.71073

Cell:                      a=11.231(2)              b=7.9355(16)              c=39.428(8)  
                                    alpha=90              beta=90                      gamma=90

Temperature:              293 K

	Calculated	Reported
Volume	3513.965	3514.1(12)
Space group	P b c a	?
Hall group	-P 2ac 2ab	?
Moiety formula	C21 H17 N5 O2	?
Sum formula	C21 H17 N5 O2	C21 H17 N5 O2
Mr	371.40	371.40
Dx,g cm-3	1.404	1.404
Z	8	8
Mu (mm-1)	0.095	0.095
F000	1552.0	1552.0
F000'	1552.60	
h,k,lmax	14,10,50	14,10,50
Nref	3910	3895
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.996                      Theta(max)= 27.160

R(reflections)= 0.0406( 3331)              wR2(reflections)= 0.1178( 3895)

S = 1.139                                      Npar= 256

---

The following ALERTS were generated. Each ALERT has the format  
**test-name\_ALERT\_alert-type\_alert-level**.  
Click on the hyperlinks for more details of the test.

---

## Alert level A

SYMM001\_ALERT\_1\_A \_symmetry\_cell\_setting is missing  
The cell setting should be one of the following

- \* triclinic
- \* monoclinic
- \* orthorhombic
- \* tetragonal
- \* rhombohedral
- \* trigonal
- \* hexagonal
- \* cubic

The following tests will not be performed.

SYMMS\_01, SYMMS\_02

EXPT005\_ALERT\_1\_A \_exptl\_crystal\_description is missing  
Crystal habit description.

The following tests will not be performed.

CRYSR\_01

DIFF003\_ALERT\_1\_A \_diffrn\_measurement\_device\_type is missing

Diffractometer make and type. Replaces \_diffrn\_measurement\_type.

PLAT122_ALERT_1_A	No _symmetry_space_group_name_H-M Given .....	Please Do !
PLAT183_ALERT_1_A	Missing _cell_measurement_reflms_used Value ....	Please Do !
PLAT184_ALERT_1_A	Missing _cell_measurement_theta_min Value .....	Please Do !
PLAT185_ALERT_1_A	Missing _cell_measurement_theta_max Value .....	Please Do !
PLAT699_ALERT_1_A	Missing _exptl_crystal_description Value .....	Please Do !

---

## Alert level C

PLAT052_ALERT_1_C	Info on Absorption Correction Method Not Given	Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...	Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...	Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...	Please Check
PLAT199_ALERT_1_C	Reported _cell_measurement_temperature ..... (K)	293 Check
PLAT200_ALERT_1_C	Reported _diffrn_ambient_temperature ..... (K)	293 Check
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C5 - C9 .	1.53 Ang.

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## Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed Check
PLAT104_ALERT_1_G	The Reported Crystal System is Inconsistent with	Pbca Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C13	2.98 Ang.
	1/2-x, -1/2+y, z =	8_655 Check
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL/	2018 Note

---

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7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
5 **ALERT level G** = General information/check it is not something unexpected

16 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data  
2 **ALERT type 2** Indicator that the structure model may be wrong or deficient  
0 **ALERT type 3** Indicator that the structure quality may be low  
1 **ALERT type 4** Improvement, methodology, query or suggestion  
1 **ALERT type 5** Informative message, check

---

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### **Publication of your CIF in IUCr journals**

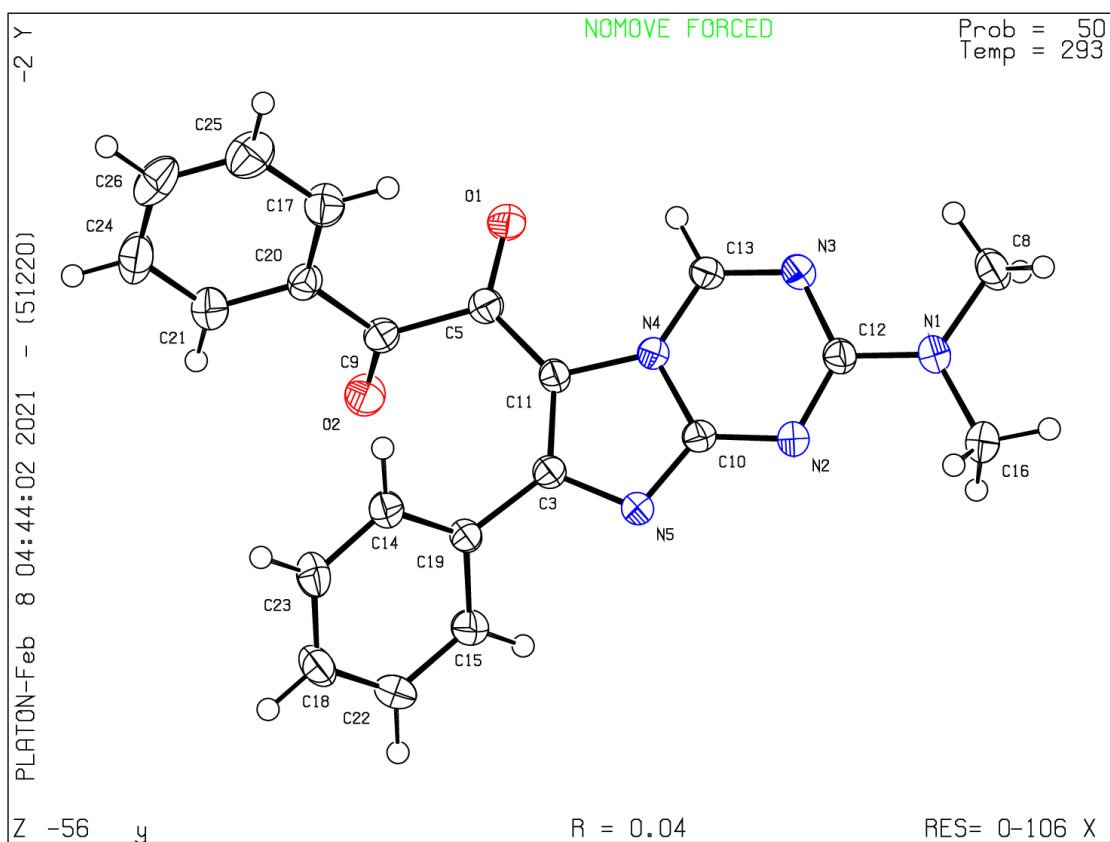
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**PLATON version of 05/12/2020; check.def file version of 05/12/2020**



**Crystallization:** Crystals of compound **4a** suitable for X-ray analysis were grown from the solvent of chloroform by slow evaporation method

**Figure.** Molecular structure of **4a** showing thermal ellipsoid at the 30% probability level

**X-Ray Data Collection and Structure Refinement Details:**

Diffraction was performed on a Bruker D8 Venture area detector diffractometer using graphite-monochromated Mo K $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) at 293(2) K,  $\varphi$  and  $\omega$  scan technique. An empirical absorption correction was applied using the SADABS program. The structure was solved by direct methods, completed by subsequent difference Fourier syntheses, and refined anisotropically for all nonhydrogen atoms by full-matrix least-squares calculations based on F 2 using the SHELXTL program package. The hydrogen atom coordinates were calculated with SHELXTL by using an appropriate riding model with varied thermal parameters. The residual electron densities of solvent were squeezed by using PLATON.3 All crystal structural pictures drawn by IUCr web.