

## Supporting Information

### Design, synthesis, biological activities and 3D-QSAR studies of quinazolinone derivatives containing hydrazone structural units

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**(E)-3-methyl-2-((4-((2-(4-cyanophenyl)hydrazono)methyl)phenoxy)methyl)quihzolin-4(3H)-one(7a)**

Yellow solid, m.p.202–203°C, yield 58%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ10.97 (s, 1H), 8.12 (d, *J* = 7.8 Hz, 1H), 7.92 (s, 1H), 7.79 (t, *J* = 7.2 Hz, 1H), 7.63 (d, *J* = 9.1 Hz, 3H), 7.56 (d, *J* = 9.2 Hz, 2H), 7.53–7.48 (m, 2H), 7.11 (d, *J* = 7.9 Hz, 2H), 6.71 (d, *J* = 8.7 Hz, 1H), 5.30 (s, 2H), 3.59 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8, 158.8, 152.8, 149.2, 146.9, 140.3, 134.9, 134.1, 129.1, 128.2, 127.8, 127.6, 126.7, 120.8, 120.7, 115.8, 112.4, 99.3, 69.2, 30.5; HRMS (ESI) *m/z* [M+H]<sup>+</sup>calcd for C<sub>24</sub>H<sub>20</sub>N<sub>5</sub>O<sub>2</sub>: 409.1612, found: 410.1603.

**(E)-3-methyl-2-((4-((2-(4-nitrophenyl)hydrazono)methyl)phenoxy)methyl)quihzolin-4(3H)-one(7b)**

Yellow solid, m.p.237–238°C, yield 62%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ11.19 (s, 1H), 8.17–8.03 (m, 3H), 7.97 (s, 1H), 7.83–7.76 (m, 1H), 7.65 (dd, *J* = 17.8, 8.6 Hz, 3H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.14 (t, *J* = 12.2 Hz, 4H), 5.32 (s, 2H), 3.59 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8, 159.1, 152.8, 151.2, 146.9, 142.1, 138.5, 134.9, 128.7, 128.50, 127.8, 127.6, 126.7, 126.7, 120.8, 115.9, 111.6, 69.2, 30.5; HRMS (ESI) *m/z* [M+H]<sup>+</sup>calcd for C<sub>23</sub>H<sub>20</sub>N<sub>5</sub>O<sub>4</sub>: 430.1510, found: 430.1500.

**(E)-2-((4-((2-(4-bromophenyl)hydrazono)methyl)phenoxy)methyl)-3-methylquihzolin-4(3H)-one(7c)**

Yellow solid, m.p.217–218°C, yield 67%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ10.35 (s, 1H), 8.17 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.89–7.78 (m, 2H), 7.59 (ddd, *J* = 15.6, 15.1, 7.7 Hz, 4H), 7.35 (d, *J* = 8.8 Hz, 2H), 7.15 (d, *J* = 8.8 Hz, 2H), 7.00 (d, *J* = 8.8 Hz, 2H), 5.33 (s, 2H), 3.63 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8, 158.3, 152.9, 146.9, 145.2, 137.7, 134.9, 132.2, 129.6, 127.8, 127.7, 126.7, 120.8, 115.8, 114.2, 109.6, 69.3, 30.5; HRMS (ESI) *m/z* [M+H]<sup>+</sup>calcd for C<sub>23</sub>H<sub>20</sub>BrN<sub>4</sub>O<sub>2</sub>: 463.0764, found: 430.0755.

**(E)-3-methyl-2-((4-((2-(*p*-tolyl)hydrazono)methyl)phenoxy)methyl)quihzolin-4(3H)-one(7d)**

Yellow solid, m.p. 180–181°C, yield 53%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ10.05 (s, 1H), 8.16 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.86–7.77 (m, 2H), 7.68 (d, *J* = 7.8 Hz, 1H), 7.61–7.53 (m, 3H), 7.13 (d, *J* = 8.8 Hz, 2H), 7.01 (d, *J* = 8.3 Hz, 2H), 6.95 (d, *J* = 8.5 Hz, 2H),

5.32 (s, 2H), 3.63 (s, 3H), 2.20 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8, 158.0, 152.9, 147.0, 143.8, 136.1, 135.0, 130.2, 130.0, 127.9, 127.7, 127.4, 127.4, 127.4, 126.8, 120.8, 115.8, 112.4, 69.4, 30.6, 20.8; HRMS (ESI) m/z [M+H]<sup>+</sup>calcd for C<sub>24</sub>H<sub>23</sub>N<sub>4</sub>O<sub>2</sub>: 399.1815, found: 399.1807.

**(E)-2-((4-((2-(4-fluorophenyl)hydrazono)methyl)phenoxy)methyl)-3-methylquinoxalin-4(3H)-one(7e)**

Brown solid, m.p.206–207°C, yield 55%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ10.15 (s, 1H), 8.12 (d, *J* = 7.8 Hz, 1H), 7.81 –7.74 (m, 2H), 7.64 (d, *J* = 8.1 Hz, 1H), 7.57 (d, *J* = 8.5 Hz, 2H), 7.52 (d, *J* = 7.5 Hz, 1H), 7.10 (d, *J* = 8.6 Hz, 2H), 7.00 (d, *J* = 7.6 Hz, 4H), 5.29 (s, 2H), 3.59 (s, 3H).; <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8, 158.1, 152.9, 146.9, 142.7, 136.8, 134.9, 129.9, 127.8, 127.6, 127.5, 126.7, 120.8, 116.1, 115.8, 113.2, 69.3, 30.5; HRMS (ESI) m/z [M+H]<sup>+</sup>calcd for C<sub>23</sub>H<sub>20</sub>FN<sub>4</sub>O<sub>2</sub>: 403.1565, found: 430.1555.

**(E)-2-((4-((2-(4-chlorophenyl)hydrazono)methyl)phenoxy)methyl)-3-methylquinoxalin-4(3H)-one(7f)**

Brown solid, m.p.211–212°C, yield 49%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ10.31 (s, 1H), 8.13 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.81 – 7.76 (m, 2H), 7.55 (ddd, *J* = 18.6, 15.1, 10.7 Hz, 4H), 7.19 (d, *J* = 8.9 Hz, 2H), 7.11 (d, *J* = 8.8 Hz, 2H), 7.00 (d, *J* = 8.9 Hz, 2H), 5.29 (s, 2H), 3.59 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8, 158.3, 152.9, 146.9, 144.9, 137.6, 134.9, 129.7, 129.3, 127.8, 127.6, 126.7, 122.1, 115.8, 113.7, 69.3, 30.5; HRMS (ESI) m/z [M+H]<sup>+</sup>calcd for C<sub>23</sub>H<sub>20</sub>ClN<sub>4</sub>O<sub>2</sub>: 419.1269, found: 419.1260.

**(E)-3-methyl-2-((4-((2-(3-fluorophenyl)hydrazono)methyl)phenoxy)methyl)quinoxalin-4(3H)-one(7g)**

Yellow solid, m.p.213–214°C, yield 47%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ10.44 (s, 1H), 8.16 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.86 – 7.81 (m, 2H), 7.68 (d, *J* = 7.7 Hz, 1H), 7.64 (d, *J* = 8.8 Hz, 2H), 7.59 – 7.54 (m, 1H), 7.21 (d, *J* = 6.9 Hz, 1H), 7.15 (d, *J* = 8.9 Hz, 2H), 6.84 (dt, *J* = 11.8, 2.2 Hz, 1H), 6.80 (d, *J* = 8.2 Hz, 1H), 6.53 – 6.46 (m, 1H), 5.33 (s, 2H), 3.63 (s, 3H).; <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8, 158.4, 152.9, 148.0, 147.9, 146.9, 138.0, 134.9, 131.2, 131.1, 129.6, 127.8, 127.8, 127.6, 126.7, 120.8, 115.8, 108.5, 105.0, 104.8, 98.9, 98.6, 69.3, 30.5; HRMS (ESI) m/z [M+H]<sup>+</sup>calcd for C<sub>23</sub>H<sub>20</sub>FN<sub>4</sub>O<sub>2</sub>: 403.1565, found: 403.1556.

**(E)-2-((4-((2-(3-chlorophenyl)hydrazono)methyl)phenoxy)methyl)-3-methylquihzolin-4(3H)-one(7h)**

Yellow solid, m.p.214–215°C, yield 51%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ10.37 (s, 1H), 8.13 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.82 – 7.78 (m, 2H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.60 (d, *J* = 8.8 Hz, 2H), 7.55 – 7.51 (m, 1H), 7.17 (t, *J* = 8.0 Hz, 1H), 7.12 (d, *J* = 8.8 Hz, 2H), 7.04 (t, *J* = 2.1 Hz, 1H), 6.90 (dd, *J* = 7.9, 1.6 Hz, 1H), 6.70 (ddd, *J* = 7.8, 2.0, 0.8 Hz, 1H), 5.30 (s, 2H), 3.59 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8, 158.4, 152.9, 147.4, 146.9, 138.2, 134.9, 134.3, 131.2, 129.5, 127.8, 127.6, 126.7, 120.8, 118.3, 115.8, 111.5, 111.0, 69.3, 30.5; HRMS (ESI) *m/z* [M+H]<sup>+</sup>calcd for C<sub>23</sub>H<sub>20</sub>ClN<sub>4</sub>O<sub>2</sub>: 419.1269, found: 419.1260.

**(E)-2-((4-((2-(3-bromophenyl)hydrazono)methyl)phenoxy)methyl)-3-methylquiHzolin-4(3H)-one(7i)**

Yellow solid, m.p.212–213°C, yield 48%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ10.36 (s, 1H), 8.13 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.81 – 7.77 (m, 2H), 7.65 – 7.62 (m, 1H), 7.59 (s, 2H), 7.53 (ddd, *J* = 8.1, 7.2, 1.1 Hz, 1H), 7.18 (s, 1H), 7.10 (s, 3H), 6.95 – 6.93 (m, 1H), 6.83 (ddd, *J* = 7.9, 1.9, 0.8 Hz, 1H), 5.29 (s, 2H), 3.59 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8, 158.4, 152.9, 147.5, 146.9, 138.3, 134.9, 131.5, 129.5, 127.8, 127.6, 126.7, 122.9, 121.1, 120.8, 115.8, 114.4, 111.4, 69.3, 30.5; HRMS (ESI) *m/z* [M+H]<sup>+</sup>calcd for C<sub>23</sub>H<sub>20</sub>BrN<sub>4</sub>O<sub>2</sub>: 463.0764, found: 467.0754.

**(E)-3-methyl-2-((4-((2-phenylhydrazono)methyl)phenoxy)methyl)quihzolin-4(3H)-one(7j)**

Yellow solid, m.p. 198–199°C, yield 84%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ10.21 (s, 1H), 8.21 (s, 1H), 7.88 – 7.79 (m, 2H), 7.68 (d, *J* = 8.1Hz, 1H), 7.64 – 7.54 (m, 3H), 7.21 (t, *J* = 7.8Hz, 2H), 7.15 (d, *J* = 8.7Hz, 2H), 7.05 (d, *J* = 8.1Hz, 2H), 6.72 (t, *J* = 7.3Hz, 1H), 5.33 (s, 2H), 3.63 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8, 158.1, 152.9, 146.9, 145.9, 136.7, 134.9, 130.0, 129.5, 127.8, 127.6, 127.7, 126.7, 120.8, 118.9, 118.1, 115.8, 112.3, 69.3, 30.5; HRMS (ESI) *m/z* [M+H]<sup>+</sup>calcd for C<sub>23</sub>H<sub>21</sub>N<sub>4</sub>O<sub>2</sub>: 385.1659, found: 385.1650.

**(E)-3-methyl-2-((4-((2-(2,4,6-trichlorophenyl)hydrazono)methyl)phenoxy)methyl)quihzolin-4(3H)-one(7k)**

White solid, m.p. 178–179°C, yield 72%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ9.47 (s, 1H), 8.16 (d, *J* = 7.2Hz, 1H), 8.03 (s, 2H), 7.87 – 7.79 (m, 1H), 7.67 (d, *J* = 8.1Hz, 1H), 7.61 (s, 2H), 7.56 (d, *J* = 8.6Hz, 3H), 7.14 (d, *J* = 8.7Hz, 2H), 5.33 (s, 2H), 3.63 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8, 158.5, 152.8, 146.9, 140.3, 138.1, 134.9, 129.4, 129.3, 128.8, 127.8, 127.7, 127.6, 127.3, 127.0, 126.7, 120.8, 115.8, 69.2, 30.5; HRMS (ESI) *m/z* [M+H]<sup>+</sup>calcd for C<sub>23</sub>H<sub>18</sub>N<sub>4</sub>O<sub>2</sub>Cl<sub>3</sub>: 487.0490, found: 487.0485.

**(E)-2-((4-((2-(3,4-dichlorophenyl)hydrazono)methyl)phenoxy)methyl)-3-methylquinoxalin-4(3H)-one(7l)**

White solid, m.p.239–240°C, yield 57%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ10.51 (s, 1H), 8.13 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.82 (s, 1H), 7.81 – 7.77 (m, 1H), 7.64 (s, 1H), 7.61 (d, *J* = 8.8 Hz, 2H), 7.55 – 7.51 (m, 1H), 7.36 (d, *J* = 8.8 Hz, 1H), 7.19 (d, *J* = 2.5 Hz, 1H), 7.12 (d, *J* = 8.8 Hz, 2H), 6.93 (dd, *J* = 8.8, 2.5 Hz, 1H), 5.30 (s, 2H), 3.59 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8,158.5, 152.9, 146.99, 146.0, 139.0, 134.9, 132.0, 131.3, 129.3, 127.95, 127.8, 127.6, 126.7, 120.8, 119.5, 115.8, 113.1, 112.6, 69.3, 30.5; HRMS (ESI) *m/z* [M+H]<sup>+</sup>calcd for C<sub>23</sub>H<sub>19</sub>Cl<sub>2</sub>N<sub>4</sub>O<sub>2</sub>: 453.0880, found: 453.0872.

**(E)-2-((4-((2-(3,4-difluorophenyl)hydrazono)methyl)phenoxy)methyl)-3-methylquinoxalin-4(3H)-one(7m)**

White solid, m.p.229–230°C, yield 58%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ10.34 (s, 1H), 8.12 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.80 (s, 2H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 8.7 Hz, 2H), 7.55 – 7.49 (m, 1H), 7.21 (dd, *J* = 19.5, 9.1 Hz, 1H), 7.11 (d, *J* = 8.8 Hz, 2H), 6.98 (dd, *J* = 11.9, 5.9 Hz, 1H), 6.72 (d, *J* = 9.0 Hz, 1H), 5.29 (s, 2H), 3.59 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8, 158.4, 152.9, 146.9, 138.0, 134.9, 129.5, 127.8, 127.68, 126.78, 120.8, 118.3, 118.1, 115.8, 107.9, 101.7, 101.5, 69.3, 30.5; HRMS (ESI) *m/z* [M+H]<sup>+</sup>calcd for C<sub>23</sub>H<sub>19</sub>F<sub>2</sub>N<sub>4</sub>O<sub>2</sub>: 421.1471, found: 421.1461.

**(E)-2-((4-((2-(2-fluorophenyl)hydrazono)methyl)phenoxy)methyl)-3-methylquinoxalin-4(3H)-one(7n)**

Yellow solid, m.p.184–185°C, yield 62%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ10.08 (s, 1H), 8.18 – 7.99 (m, 2H), 7.79 (d, *J* = 7.2 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.56 (dd, *J* = 25.1, 7.9 Hz, 3H), 7.47 (s, 1H), 7.12 (d, *J* = 8.4 Hz, 2H), 7.05 (d, *J* = 7.4 Hz, 2H), 6.70 (d, *J* = 5.0 Hz, 1H), 5.30 (s, 2H), 3.59 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8,

158.4, 152.9, 146.9, 139.6, 134.9, 134.2, 134.1, 129.7, 127.8, 127.8, 127.6, 126.7, 125.4, 125.4, 120.8, 118.7, 118.7, 115.8, 114.2, 69.3, 30.5; HRMS (ESI)  $m/z$   $[M+H]^+$  calcd for  $C_{23}H_{20}FN_4O_2$ : 403.1565, found: 403.1559.

**(E)-2-((4-((2-(2-chlorophenyl)hydrazono)methyl)phenoxy)methyl)-3-methylquinoxalin-4(3H)-one(7o)**

Red solid, m.p. 180–181°C, yield 54%;  $^1H$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$  9.73 (s, 1H), 8.21 (s, 1H), 8.13 (dd,  $J = 8.0, 1.2$  Hz, 1H), 7.80 (dd,  $J = 11.9, 4.9$  Hz, 1H), 7.62 (dd,  $J = 22.6, 8.4$  Hz, 3H), 7.51 (dd,  $J = 12.8, 4.6$  Hz, 2H), 7.28 (dd,  $J = 7.9, 1.3$  Hz, 1H), 7.23 – 7.18 (m, 1H), 7.13 (d,  $J = 8.8$  Hz, 2H), 6.73 (d,  $J = 7.7, 1.4$  Hz, 1H), 5.31 (s, 2H), 3.60 (s, 3H);  $^{13}C$  NMR (101 MHz, DMSO- $d_6$ )  $\delta$  161.8, 158.6, 152.9, 146.9, 142.0, 140.6, 134.9, 129.8, 129.5, 128.5, 127.9, 127.8, 127.7, 126.7, 120.8, 119.8, 116.4, 115.8, 114.4, 69.3, 30.5; HRMS (ESI)  $m/z$   $[M+H]^+$  calcd for  $C_{23}H_{20}ClN_4O_2$ : 419.1269, found: 419.1262.

**(E)-2-((4-((2-(2-bromophenyl)hydrazono)methyl)phenoxy)methyl)-3-methylquinoxalin-4(3H)-one(7p)**

Yellow solid, m.p. 162–163°C, yield 61%;  $^1H$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$  9.49 (s, 1H), 8.23 (s, 1H), 8.13 (dd,  $J = 8.0, 1.1$  Hz, 1H), 7.80 (ddd,  $J = 8.5, 7.2, 1.5$  Hz, 1H), 7.64 (d,  $J = 7.8$  Hz, 1H), 7.60 (d,  $J = 8.8$  Hz, 2H), 7.53 (td,  $J = 7.7, 1.1$  Hz, 1H), 7.49 (dd,  $J = 8.2, 1.4$  Hz, 1H), 7.43 (dd,  $J = 7.9, 1.4$  Hz, 1H), 7.27 – 7.22 (m, 1H), 7.13 (d,  $J = 8.8$  Hz, 2H), 6.70 – 6.64 (m, 1H), 5.31 (s, 2H), 3.60 (s, 3H);  $^{13}C$  NMR (101 MHz, DMSO- $d_6$ )  $\delta$  162.8, 161.8, 158.6, 152.9, 146.99, 143.09, 140.89, 134.99, 133.09, 129.5, 129.0, 128.0, 127.8, 127.6, 126.7, 120.8, 120.5, 115.8, 114.8, 106.4, 69.3, 30.5; HRMS (ESI)  $m/z$   $[M+H]^+$  calcd for  $C_{23}H_{20}BrN_4O_2$ : 463.0764, found: 463.0756.

**(E)-2-((4-((2-(2,4-difluorophenyl)hydrazono)methyl)phenoxy)methyl)-3-methylquinoxalin-4(3H)-one(7q)**

White solid, m.p. 237–238°C, yield 57%;  $^1H$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$  10.03 (s, 1H), 8.13 (d,  $J = 7.9$  Hz, 1H), 8.03 (s, 1H), 7.83 – 7.77 (m, 1H), 7.64 (d,  $J = 8.1$  Hz, 1H), 7.58 (d,  $J = 8.7$  Hz, 2H), 7.54 (t,  $J = 7.6$  Hz, 1H), 7.44 (d,  $J = 6.0$  Hz, 1H), 7.19 – 7.14 (m, 1H), 7.12 (d,  $J = 8.8$  Hz, 2H), 6.95 (t,  $J = 8.6$  Hz, 1H), 5.30 (s, 2H), 3.59 (s, 3H);  $^{13}C$  NMR (101 MHz, DMSO- $d_6$ )  $\delta$  161.8, 158.4, 152.9, 146.9, 139.6, 135.0, 129.6, 127.8, 127.7,

126.7, 120.7, 115.8, 69.2, 30.5; HRMS (ESI)  $m/z$   $[M+H]^+$ calcd for  $C_{23}H_{19}F_2N_4O_2$ : 421.1471, found: 421.1462.

**(E)-2-((4-((2-(2,4-dichlorophenyl)hydrazono)methyl)phenoxy)methyl)-3-methylquinoxalin-4(3H)-one(7r)**

White solid, m.p. 143–144°C, yield 48%;  $^1H$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$ 10.34 (s, 1H), 8.12 (dd,  $J = 7.9, 1.0$  Hz, 1H), 7.80 (s, 2H), 7.63 (d,  $J = 8.0$  Hz, 1H), 7.60 (d,  $J = 8.7$  Hz, 2H), 7.55 – 7.49 (m, 1H), 7.21 (dd,  $J = 19.5, 9.1$  Hz, 1H), 7.11 (d,  $J = 8.8$  Hz, 2H), 6.98 (dd,  $J = 11.9, 5.9$  Hz, 1H), 6.72 (d,  $J = 9.0$  Hz, 1H), 5.29 (s, 2H), 3.59 (s, 3H);  $^{13}C$  NMR (101 MHz, DMSO- $d_6$ )  $\delta$ 161.8, 158.9, 152.9, 146.9, 143.1, 142.2, 134.9, 133.2, 131.2, 129.1, 128.3, 127.9, 127.7, 126.7, 120.8, 119.0, 115.9, 115.0, 113.3, 69.2, 30.5; HRMS (ESI)  $m/z$   $[M+H]^+$ calcd for  $C_{17}H_{18}FN_4O_2$ : 453.0874, found: 453.0880.

**(E)-3-methyl-2-((4-((2-(4-(trifluoromethyl)phenyl)hydrazono)methyl)phenoxy)methyl)quinoxalin-4(3H)-one(7s)**

Yellow solid, m.p. 213–214°C, yield 63%;  $^1H$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$ 10.68 (d,  $J = 24.4$  Hz, 1H), 8.13 (d,  $J = 8.0$  Hz, 1H), 7.94 – 7.77 (m, 2H), 7.72 – 7.60 (m, 3H), 7.57 – 7.45 (m, 3H), 7.14 (dd,  $J = 16.0, 8.4$  Hz, 4H), 5.33 (d,  $J = 23.8$  Hz, 2H), 3.61 (t,  $J = 12.4$  Hz, 3H);  $^{13}C$  NMR (101 MHz, DMSO- $d_6$ )  $\delta$ 161.8, 158.6, 152.9, 148.9, 146.9, 139.2, 134.9, 129.3, 128.0, 127.8, 127.6, 126.9, 126.7, 120.8, 115.8, 111.9, 79.6, 69.2, 30.5; HRMS (ESI)  $m/z$   $[M+H]^+$ calcd for  $C_{24}H_{20}F_3N_4O_2$ : 453.1533, found: 453.1525.

**(E)-3-methyl-2-((4-((2-(o-tolyl)hydrazono)methyl)phenoxy)methyl)quinazolin-4(3H)-one(7t)**

yellow solid, m.p. 213–214°C, yield 63%;  $^1H$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$ 9.37 (s, 1H), 8.15 – 8.11 (m, 1H), 8.07 (s, 1H), 7.82 – 7.78 (m, 1H), 7.65 (d,  $J=7.6$  Hz, 1H), 7.58 (d,  $J=8.8$  Hz, 2H), 7.56 – 7.51 (m, 1H), 7.36 (d,  $J=7.6$  Hz, 1H), 7.12 (d,  $J=8.8$  Hz, 2H), 7.06 (t,  $J=7.7$  Hz, 1H), 7.00 (d,  $J=7.3$  Hz, 1H), 6.64 (td,  $J=7.3, 1.1$  Hz, 1H), 5.30 (s, 2H), 3.60 (s, 3H), 2.17 (s, 3H);  $^{13}C$  NMR (101 MHz, DMSO- $d_6$ )  $\delta$ 161.7, 158.1, 152.9, 146.9, 143.8, 138.3, 134.9, 130.7, 130.0, 127.8, 127.6, 127.5, 127.1, 126.7, 120.9, 120.7, 118.9, 115.7, 112.3, 69.2, 30.5, 17.9; HRMS (ESI)  $m/z$   $[M+H]^+$ calcd for  $C_{24}H_{22}N_4O_2$ : 399.1815, found: 399.1808.

**(E)-3-methyl-2-((4-((2-(pyridin-4-yl)hydrazono)methyl)phenoxy)methyl)quihzolin-4(3H)-one(8a)**

White solid, m.p. 197–198°C, yield 68%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ11.95 (s, 1H), 9.08 (d, *J* = 1.6 Hz, 1H), 8.77 (dd, *J* = 4.7, 1.4 Hz, 1H), 8.42 (s, 1H), 8.33–8.21 (m, 1H), 8.19 – 8.14 (m, 1H), 7.89–7.79 (m, 1H), 7.74 (d, *J* = 8.7 Hz, 2H), 7.67 (d, *J* = 8.1 Hz, 1H), 7.60–7.54 (m, 2H), 7.23 (d, *J* = 8.7 Hz, 2H), 5.38 (s, 2H), 3.64 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ162.0, 161.7, 159.8, 152.7, 152.7, 149.0, 148.6, 146.9, 135.9, 134.9, 129.7, 129.3, 128.8, 128.1, 127.8, 127.6, 126.7, 124.1, 120.8, 115.9, 69.1, 30.4; HRMS (ESI) *m/z* [M+H]<sup>+</sup>calcd for C<sub>23</sub>H<sub>20</sub>N<sub>5</sub>O<sub>4</sub>: 414.1561, found: 414.1555.

**(E)-3-methyl-2-((4-((2-(pyridin-3-yl)hydrazono)methyl)phenoxy)methyl)quihzolin-4(3H)-one(8b)**

White solid, m.p.231–232°C, yield 65%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ11.99 (s, 1H), 8.79 (d, *J* = 5.9 Hz), 8.44 (s, 1H), 8.20–8.15 (m, 1H), 7.83 (d, *J* = 6.0 Hz, 3H), 7.74 (d, *J* = 8.7 Hz, 2H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.24 (d, *J* = 8.8 Hz, 2H), 5.39 (s, 2H), 3.64 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.9, 161.7, 159.9, 152.7, 151.0, 150.8, 150.7, 150.0, 149.2, 146.9, 141.0, 134.9, 129.4, 128.9, 128.0, 127.8, 127.6, 126.7, 123.6, 122.0, 121.8, 121.5, 120.8, 115.9, 69.1, 30.4; HRMS (ESI) *m/z* [M+H]<sup>+</sup>calcd for C<sub>23</sub>H<sub>20</sub>N<sub>5</sub>O<sub>4</sub>: 414.1561, found: 414.1556.

**(E)-N-(3,4-difluorophenyl)-2-(4-((3-methyl-4-oxo-3,4-dihydroquihzolin-2-yl)methoxy)benzylidene)hydrazine-1-carboxamide(9a)**

White solid, m.p.237–238°C, yield 55%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ10.72 (s, 1H), 9.03 (s, 1H), 8.13 (d, *J* = 8.0 Hz, 1H), 7.87 (s, 1H), 7.82 – 7.75 (m, 5H), 7.63 (d, *J* = 8.2 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.45 (d, *J* = 9.1 Hz, 1H), 7.32 (dd, *J* = 19.7, 9.2 Hz, 1H), 7.14 (d, *J* = 8.8 Hz, 2H), 5.33 (s, 2H), 3.60 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8, 159.2, 153.5, 152.8, 146.9, 141.4, 134.9, 129.1, 128.3, 127.8, 127.6, 126.7, 120.7, 117.5, 117.3, 116.4, 115.6, 109.2, 109.0, 69.2, 30.5; HRMS (ESI) *m/z* [M+H]<sup>+</sup>calcd for C<sub>24</sub>H<sub>20</sub>F<sub>2</sub>N<sub>5</sub>O<sub>3</sub>: 464.1528, found: 464.1526.

**(E)-N-(3-fluorophenyl)-2-(4-((3-methyl-4-oxo-3,4-dihydroquihzolin-2-yl)methoxy)benzylidene)hydrazine-1-carboxamide(9b)**



White solid, m.p.222–223°C, yield 42%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ10.86 (s, 1H), 9.17 (s, 1H), 8.13 (d, *J* = 8.0 Hz, 1H), 7.89 (s, 1H), 7.79 (dd, *J* = 13.8, 7.6 Hz, 3H), 7.64 – 7.57 (m, 2H), 7.52 (d, *J* = 7.9 Hz, 1H), 7.45 (d, *J* = 8.1 Hz, 1H), 7.27 (dd, *J* = 15.4, 8.0 Hz, 1H), 7.14 (d, *J* = 8.6 Hz, 2H), 6.77 (t, *J* = 7.8 Hz, 1H), 5.33 (s, 2H), 3.60 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8, 159.2, 153.4, 152.8, 146.9, 141.3, 134.9, 130.4, 130.3, 129.1, 128.4, 127.8, 127.6, 126.7, 120.8, 115.6, 109.1, 108.9, 106.8, 106.5, 69.2, 30.5; HRMS (ESI) *m/z* [M+H]<sup>+</sup>calcd for C<sub>24</sub>H<sub>21</sub>FN<sub>5</sub>O<sub>3</sub>: 446.1623, found: 446.1619.

**(E)-N-(2-fluorophenyl)-2-(4-((3-methyl-4-oxo-3,4-dihydroquihzolin-2-yl)methoxy)benzylidene)hydrazine-1-carboxamide(9c)**

White solid, m.p.239–240°C, yield 49%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ10.79 (s, 1H), 8.63 (s, 1H), 8.13 (d, *J* = 8.0 Hz, 1H), 7.89 (s, 1H), 7.86 (t, *J* = 8.0 Hz, 1H), 7.82 – 7.77 (m, 1H), 7.69 (d, *J* = 8.8 Hz, 2H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.25 – 7.20 (m, 1H), 7.17 – 7.11 (m, 3H), 7.11 – 7.06 (m, 1H), 5.32 (s, 2H), 3.59 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8, 159.3, 153.2, 152.8, 146.9, 141.4, 134.9, 128.8, 128.3, 127.8, 127.6, 126.7, 124.8, 120.8, 115.8, 115.6, 69.2, 30.5; HRMS (ESI) *m/z* [M+H]<sup>+</sup>calcd for C<sub>24</sub>H<sub>21</sub>FN<sub>5</sub>O<sub>3</sub>: 446.1623, found: 446.1617.

**(E)-N-(4-methoxyphenyl)-2-(4-((3-methyl-4-oxo-3,4-dihydroquihzolin-2-yl)methoxy)benzylidene)hydrazine-1-carboxamide(9d)**

White solid, m.p.198–199°C, yield 55%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ10.50 (s, 1H), 8.70 (s, 1H), 8.13 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.85 (s, 1H), 7.79 (dd, *J* = 18.3, 8.6 Hz, 3H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 7.0 Hz, 1H), 7.49 (d, *J* = 9.0 Hz, 2H), 7.13 (d, *J* = 8.8 Hz, 2H), 6.84 (d, *J* = 9.0 Hz, 2H), 5.32 (s, 2H), 3.69 (s, 3H), 3.60 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ161.8, 159.1, 155.3, 153.8, 152.8, 146.9, 140.5, 134.9, 132.6, 129.0, 128.6, 127.8, 127.6, 126.7, 122.2, 120.8, 115.6, 114.0, 69.2, 55.6, 30.5; HRMS (ESI) *m/z* [M+H]<sup>+</sup>calcd for C<sub>25</sub>H<sub>24</sub>N<sub>5</sub>O<sub>4</sub>: 458.1823, found: 458.1818.

**(E)-N-(3-chloro-4-(trifluoromethyl)phenyl)-2-(4-((3-methyl-4-oxo-3,4-dihydroquihzolin-2-yl)methoxy)benzylidene)hydrazine-1-carboxamide(9e)**

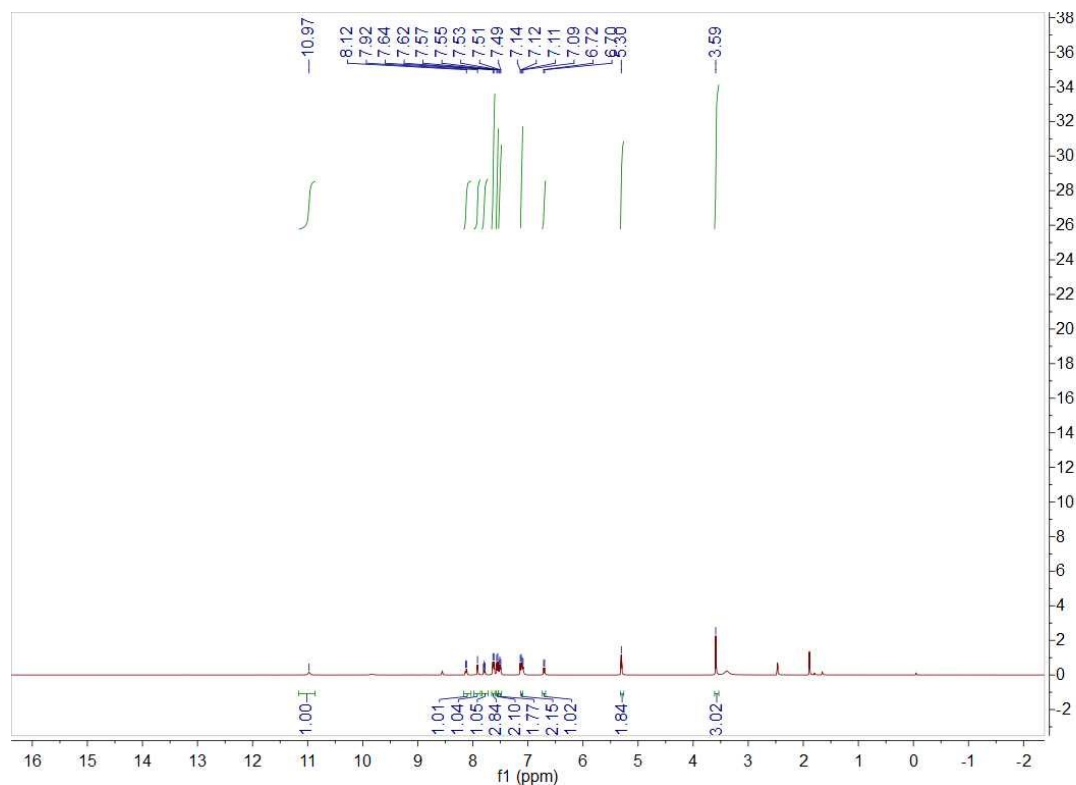
White solid, m.p.228–229°C, yield 53%; <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ10.83 (s, 1H), 9.27 (s, 1H), 8.25 (s, 1H), 8.12 (d, *J* = 7.9 Hz, 1H), 8.01 (d, *J* = 8.8 Hz, 1H), 7.89 (s, 1H), 7.80 (d, *J* = 8.6 Hz, 3H), 7.70 – 7.51 (m, 3H), 7.16 (s, 2H), 5.33 (s, 2H), 3.59 (s, 3H);

$^{13}\text{C}$  NMR (101 MHz, DMSO- $d_6$ )  $\delta$ 161.8, 159.3, 153.5, 152.8, 146.9, 141.7, 139.4, 134.9, 132.1, 129.2, 128.2, 127.8, 127.6, 126.7, 124.9, 120.7, 115.6, 69.2, 30.5; HRMS (ESI)  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{25}\text{H}_{24}\text{ClF}_3\text{N}_5\text{O}_3$ : 530.1201, found: 530.1196.

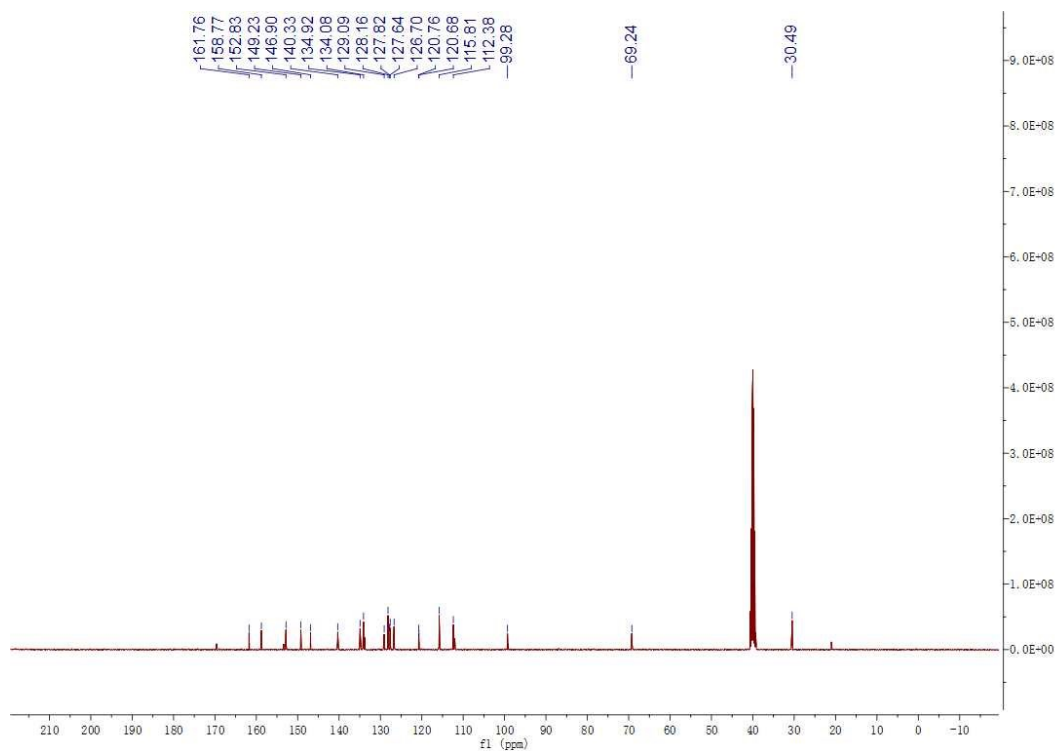
**(E)-N-(4-fluorophenyl)-2-(4-((3-methyl-4-oxo-3,4-dihydroquinolin-2-yl)methoxy)benzylidene)hydrazine-1-carboxamide(9f)**

White solid, m.p.232–233°C, yield 57%;  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$ 10.61 (s, 1H), 8.89 (s, 1H), 8.13 (d,  $J = 7.9$  Hz, 1H), 7.87 (s, 2H), 7.78 (d,  $J = 8.8$  Hz, 2H), 7.63 (d,  $J = 7.2$  Hz, 3H), 7.53 (t,  $J = 7.2$  Hz, 1H), 7.22 – 7.07 (m, 4H), 5.32 (s, 2H), 3.60 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz, DMSO- $d_6$ )  $\delta$ 161.8, 159.4, 159.1, 157.0, 153.7, 152.8, 146.9, 140.9, 136.0, 134.9, 129.1, 128.4, 127.8, 127.6, 126.7, 122.2, 122.2, 120.7, 115.6, 115.5, 115.2, 69.2, 30.5; HRMS (ESI)  $m/z$   $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{24}\text{H}_{21}\text{FN}_5\text{O}_3$ : 446.1623, found: 446.1618.

**4.  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, and HRMS spectra of title compounds 7–9**

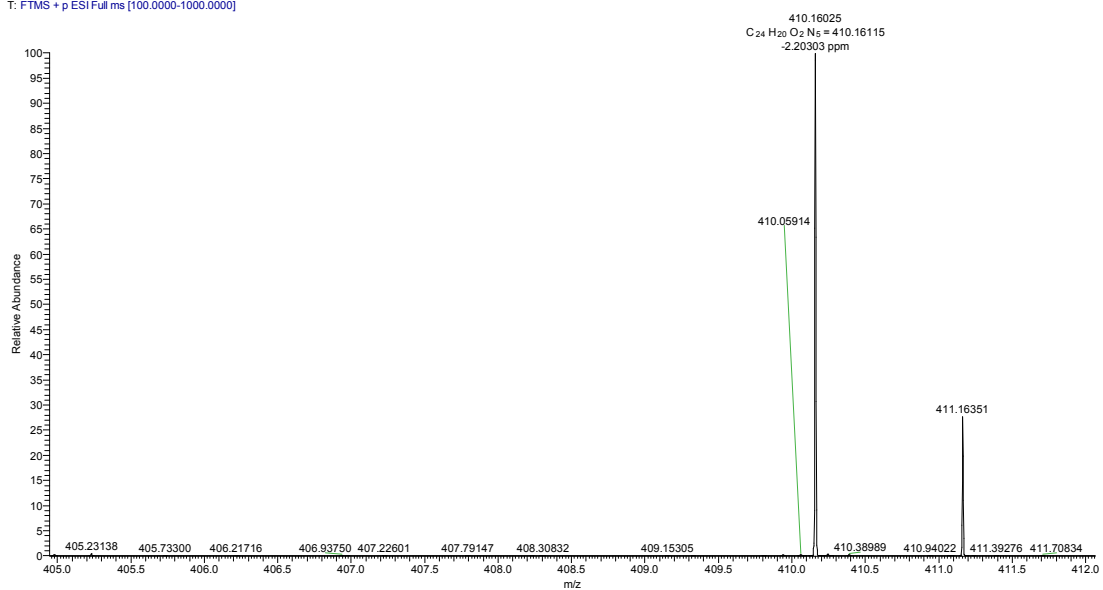


**Fig. S1**  $^1\text{H}$  NMR spectrum of title compound 7a

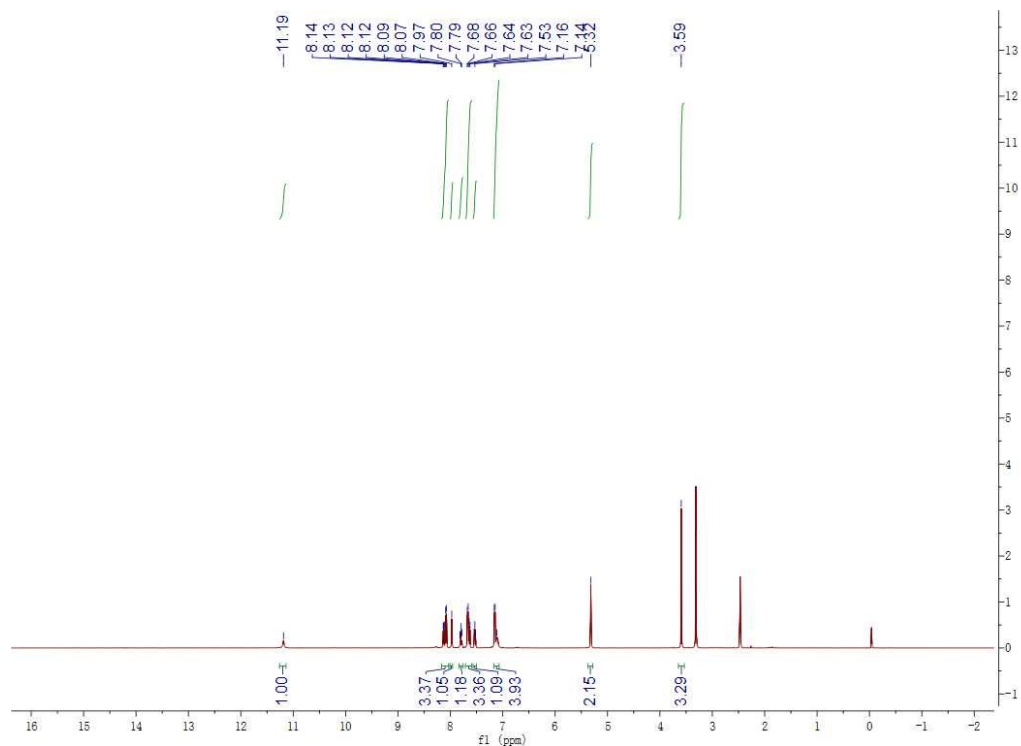


**Fig. S2**  $^{13}\text{C}$  NMR spectrum of title compound **7a**

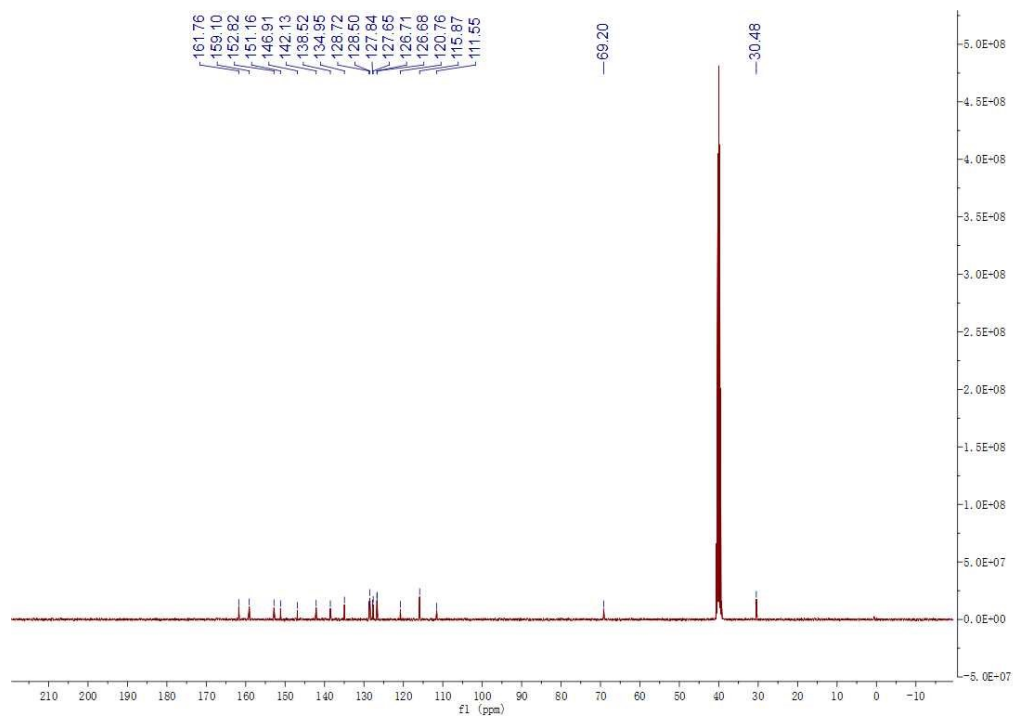
2019112969 #37 RT: 0.38 AV: 1 NL: 7.91E7  
T: FTMS + p ESI Full ms [100.0000-1000.0000]



**Fig. S3** HRMS spectrum of title compound **7a**



**Fig. S4**  $^1\text{H}$  NMR spectrum of title compound **7b**



**Fig. S5**  $^{13}\text{C}$  NMR spectrum of title compound **7b**

2019112970 #39 RT: 0.41 AV: 1 NL: 1.46E7  
T: FTMS + p ESI Full ms [100.0000-1000.0000]

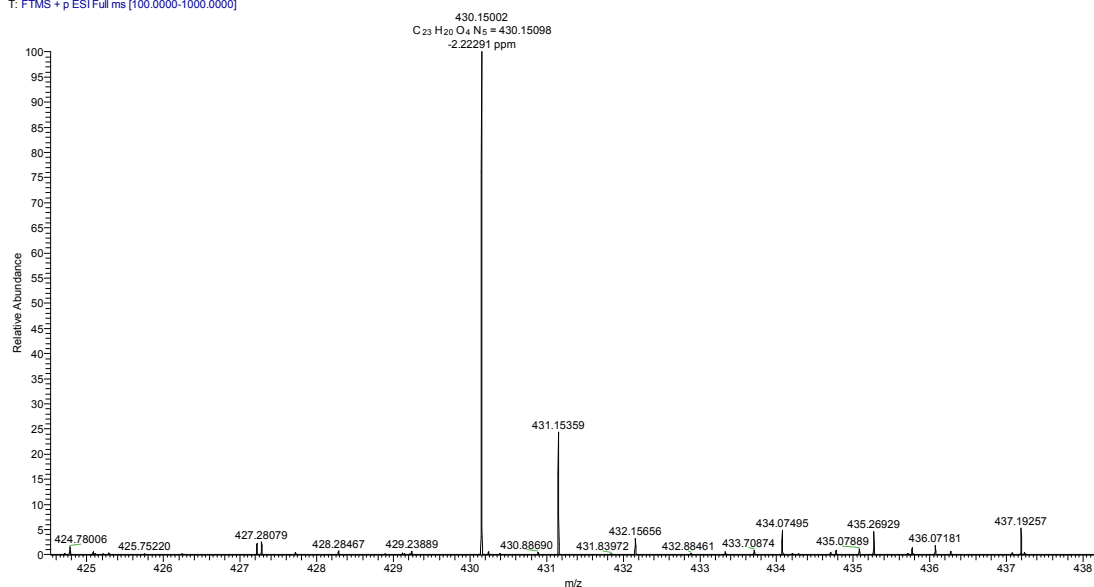


Fig. S6 HRMS spectrum of title compound 7b

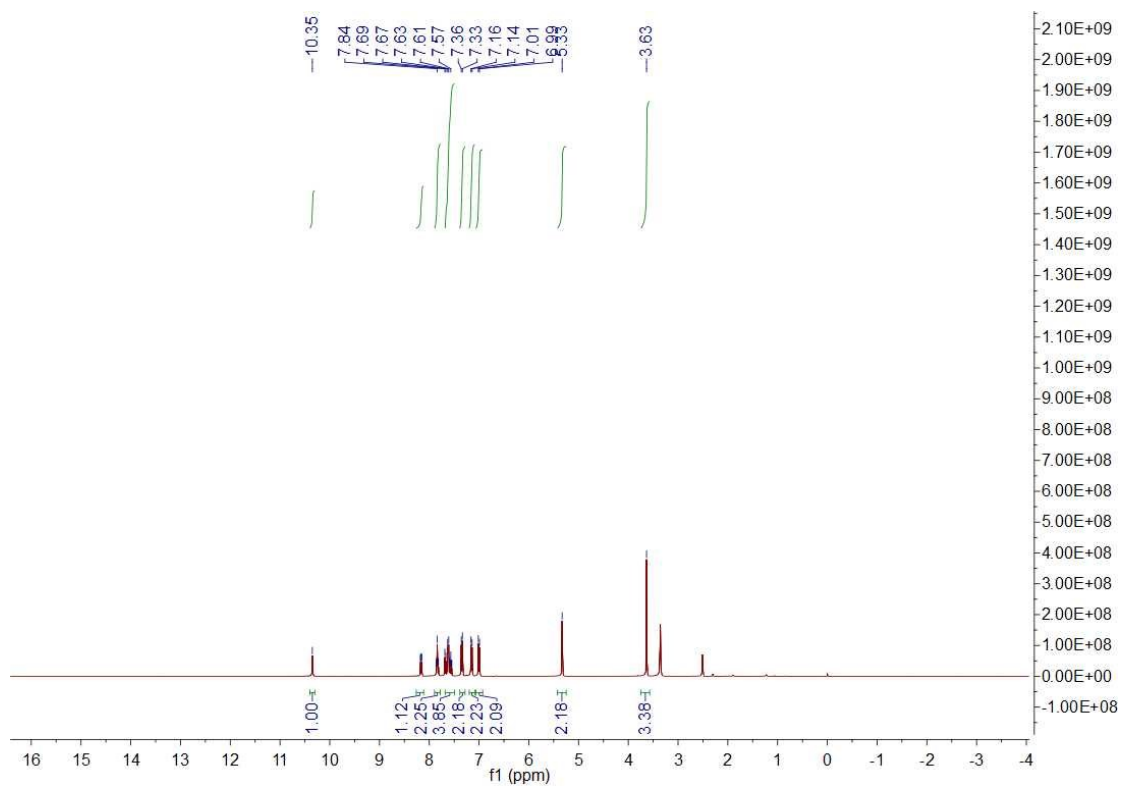


Fig. S7 <sup>1</sup>H NMR spectrum of title compound 7c

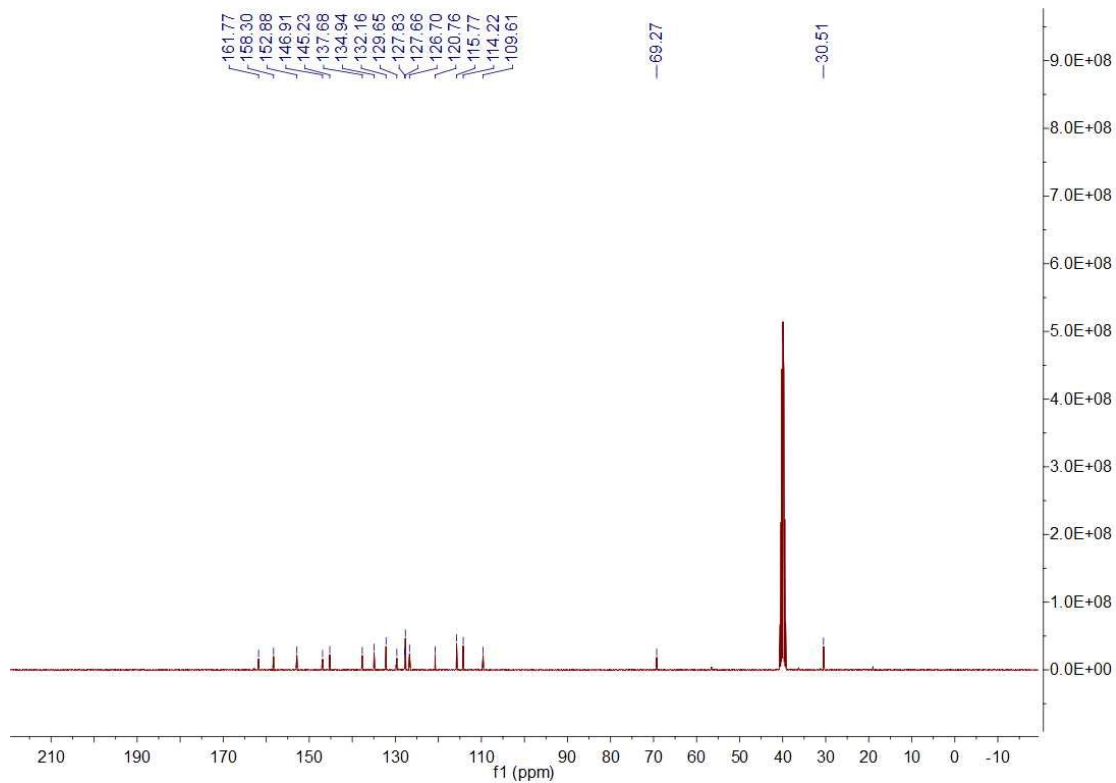


Fig. S8  $^{13}\text{C}$  NMR spectrum of title compound **7c**

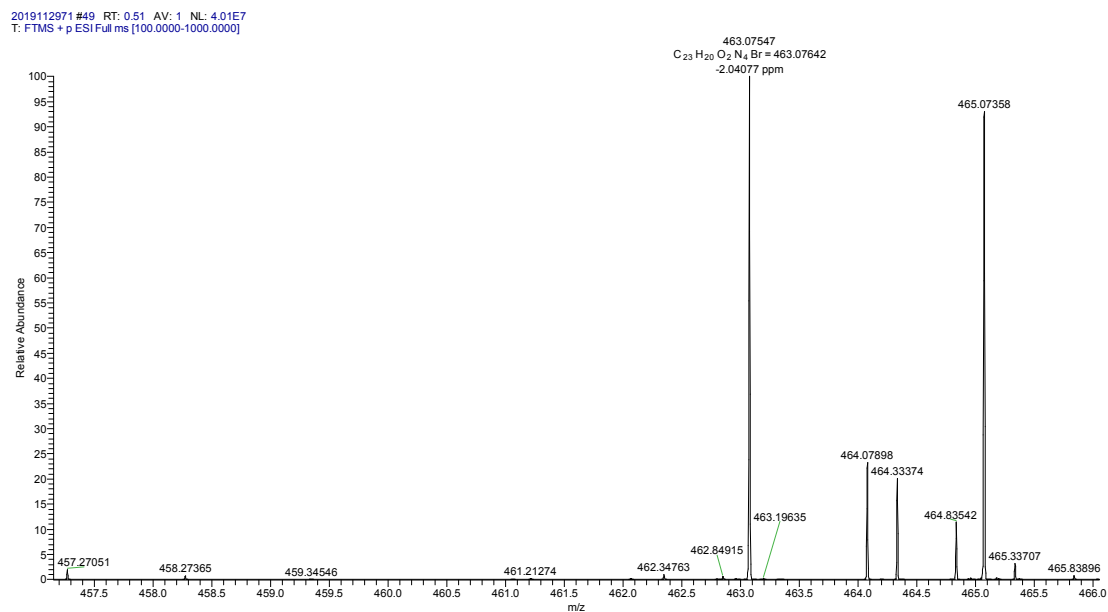
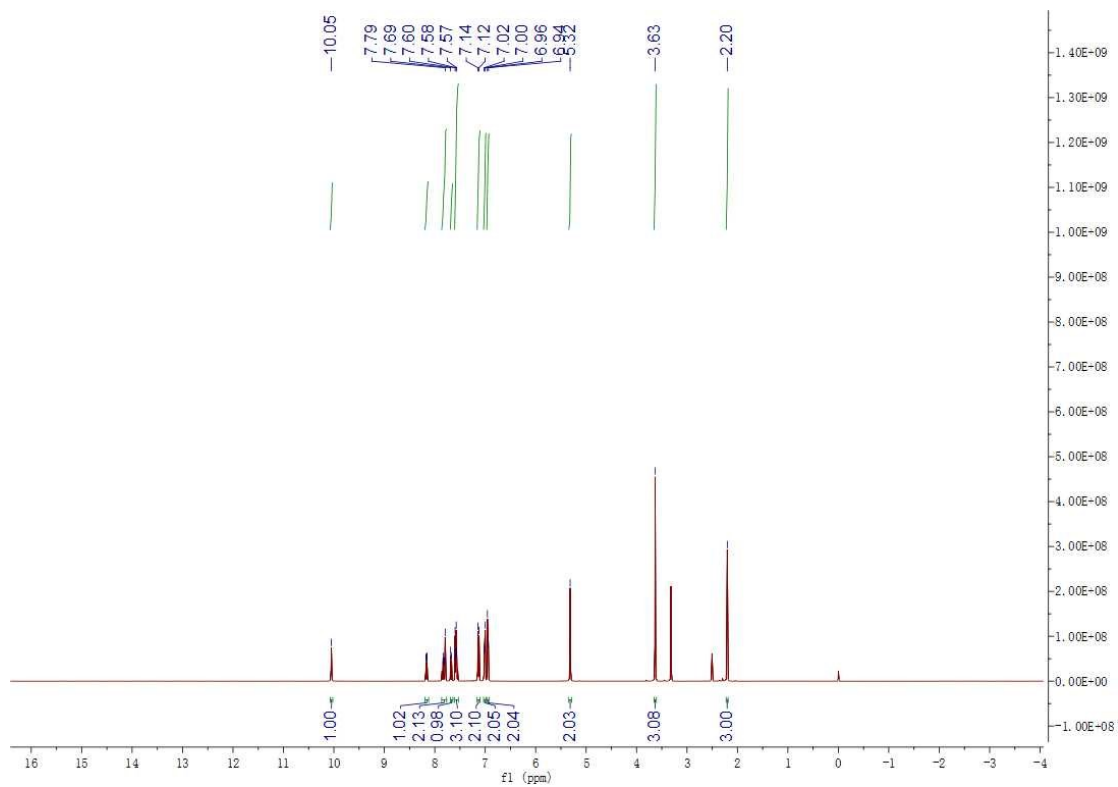
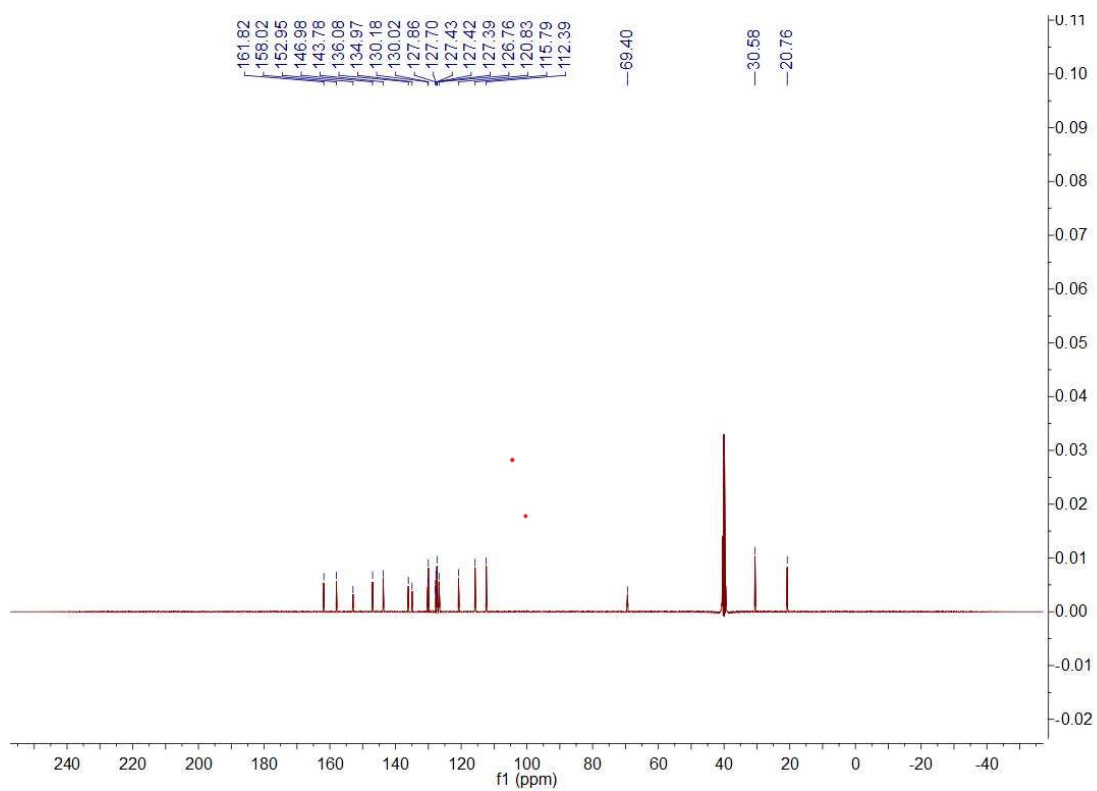


Fig. S9 HRMS spectrum of title compound **7c**



**Fig. S10**  $^1\text{H}$  NMR spectrum of title compound **7d**



**Fig. S11**  $^{13}\text{C}$  NMR spectrum of title compound **7d**

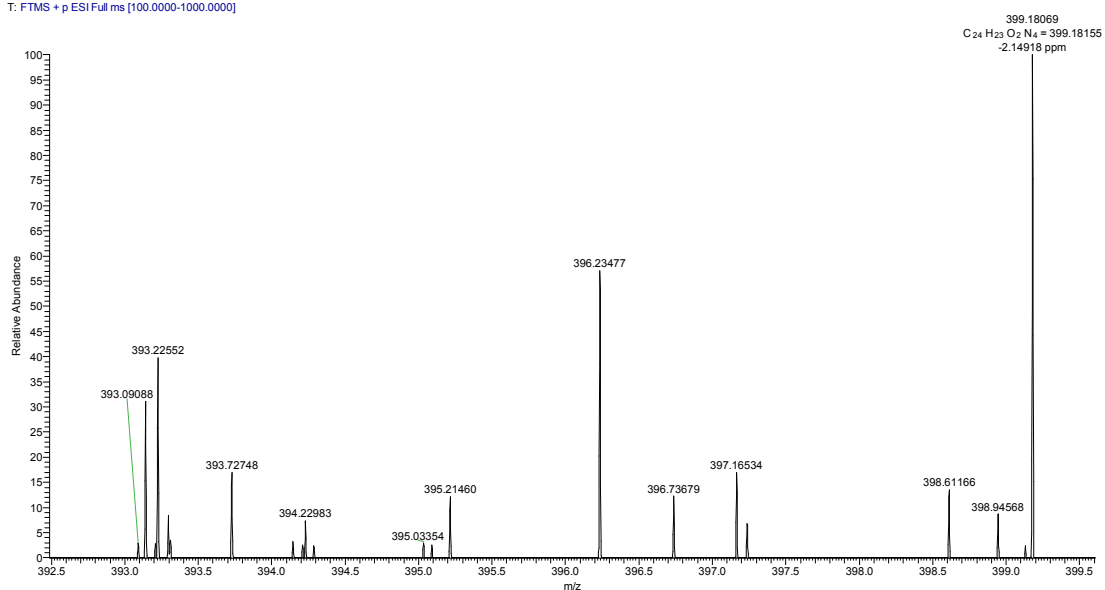


Fig. S12 HRMS spectrum of title compound 7d

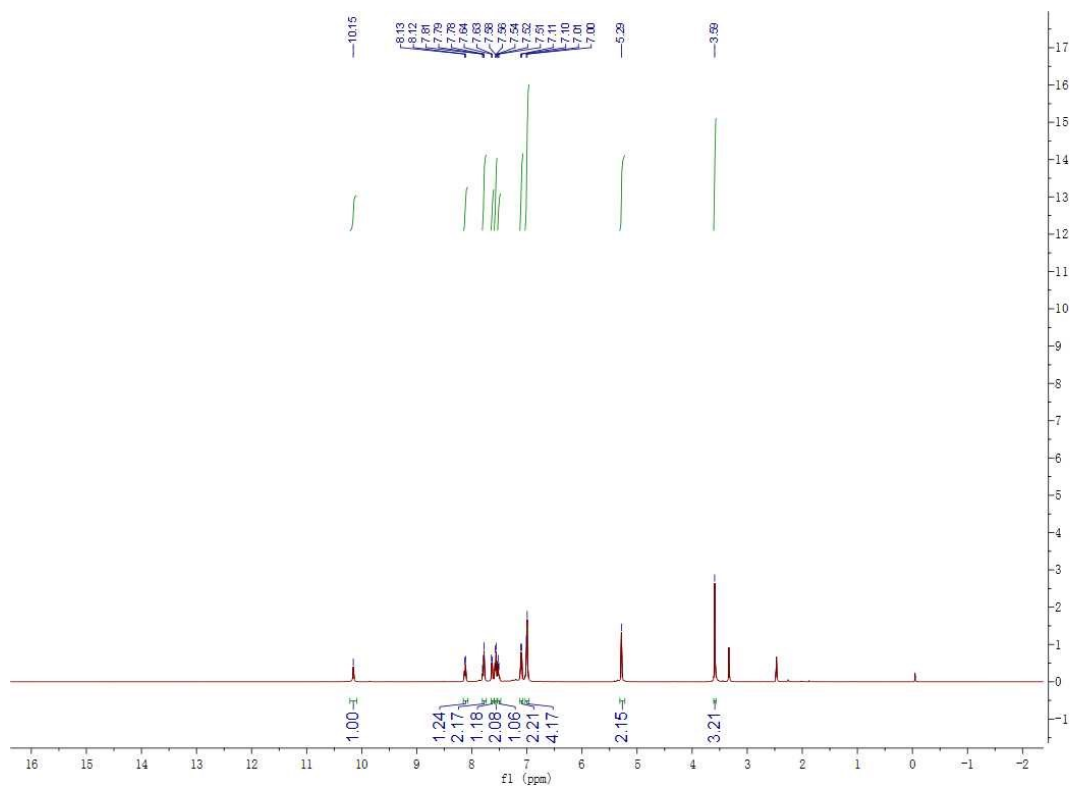
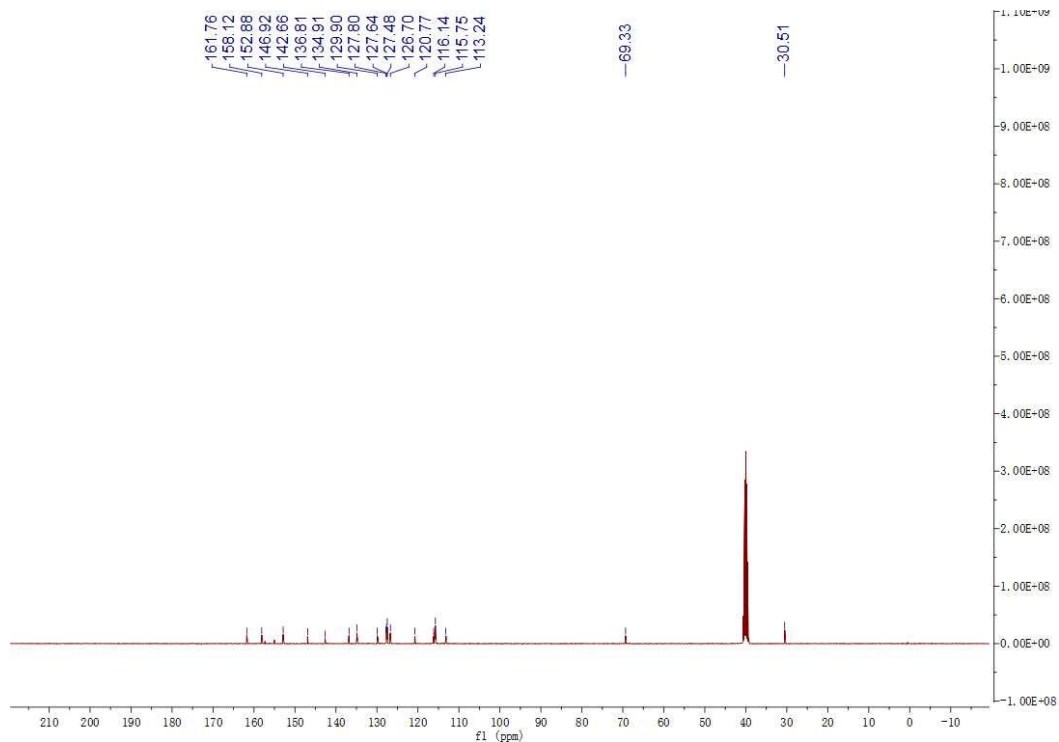


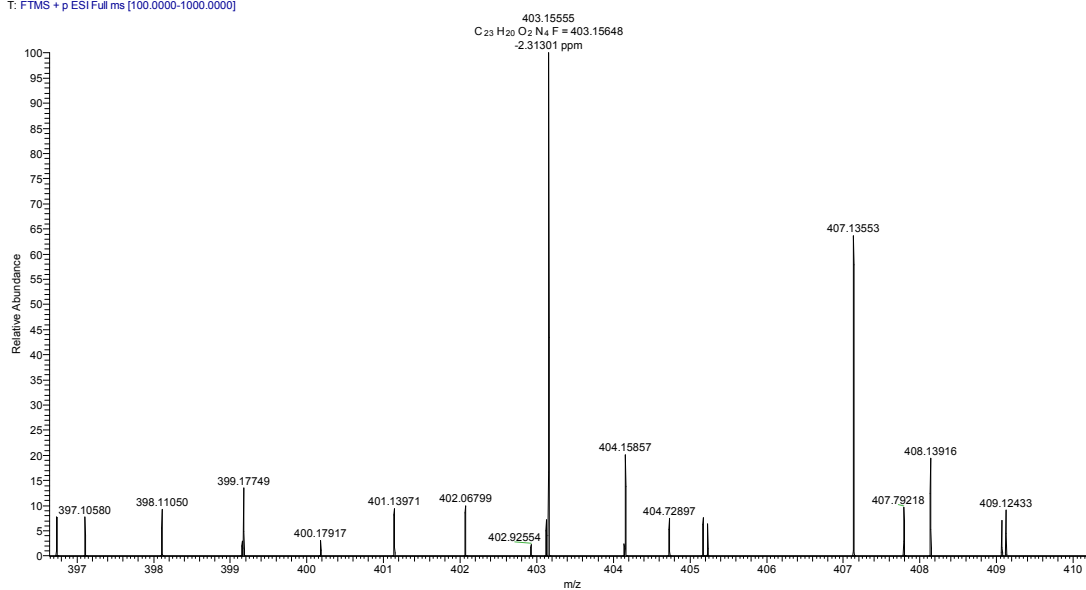
Fig. S13 <sup>1</sup>H NMR spectrum of title compound 7e



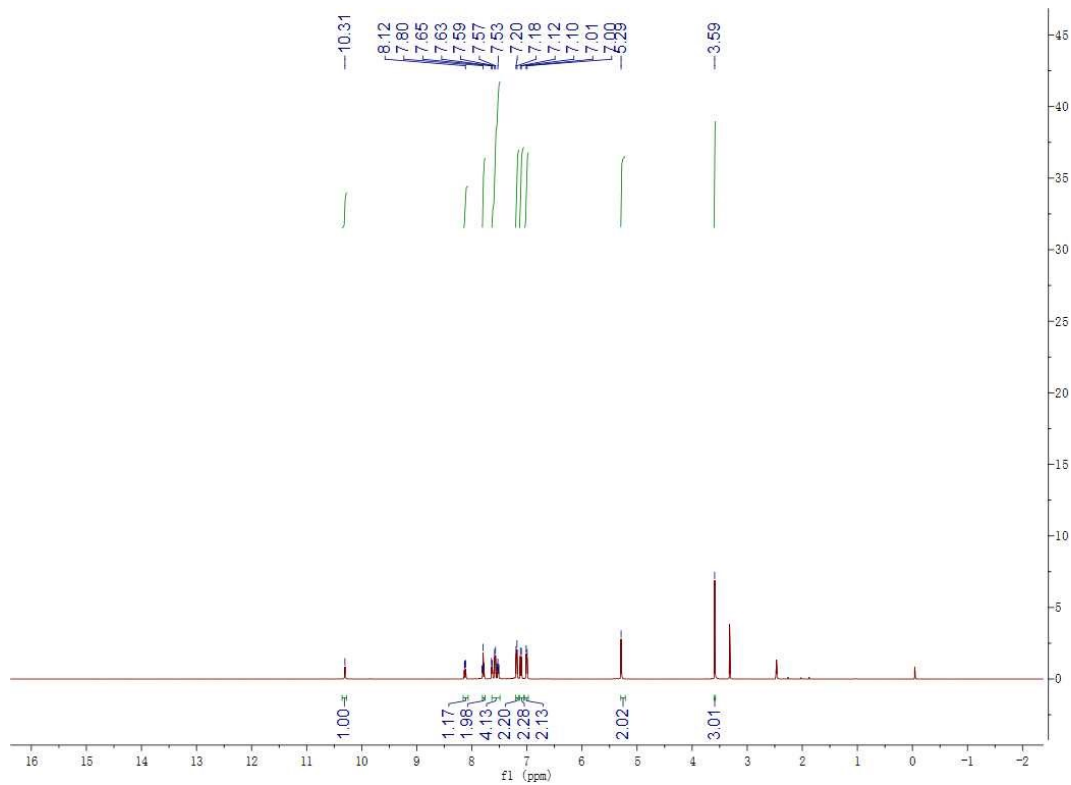


**Fig. S14**  $^{13}\text{C}$ NMR spectrum of title compound **7e**

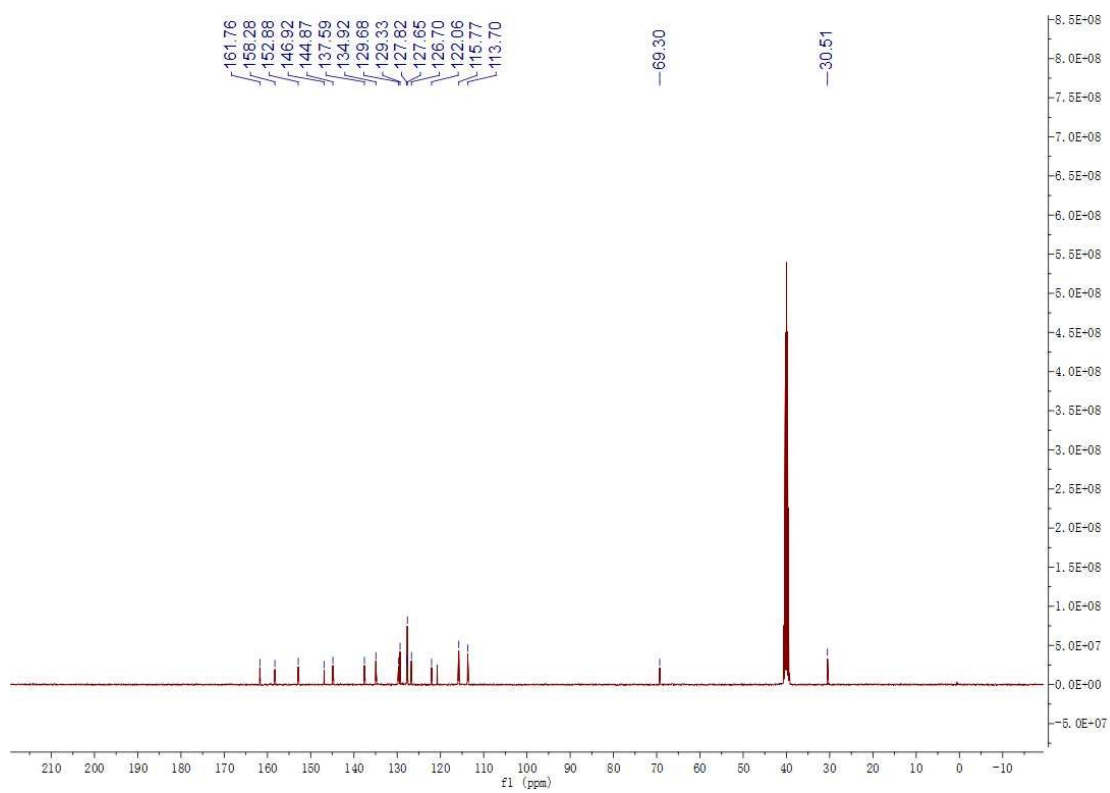
2019112973 #35 RT: 0.36 AV: 1 NL: 4.25E6  
T: FTMS + p ESI Full ms [100.0000-1000.0000]



**Fig. S15** HRMS spectrum of title compound **7e**



**Fig. S16**  $^1\text{H}$  NMR spectrum of title compound **7f**



**Fig. S17**  $^{13}\text{C}$  NMR spectrum of title compound **7f**

2019112974 #47 RT: 0.48 AV: 1 NL: 1.22E8  
T: FTMS + p ESI Full ms [100.0000-1000.0000]

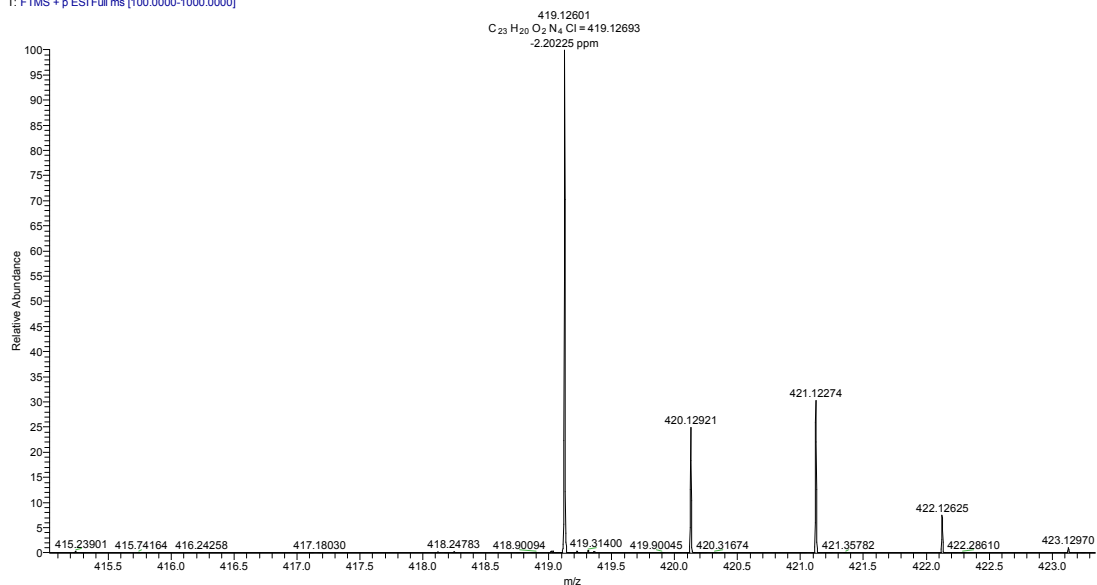


Fig. S18 HRMS spectrum of title compound 7f

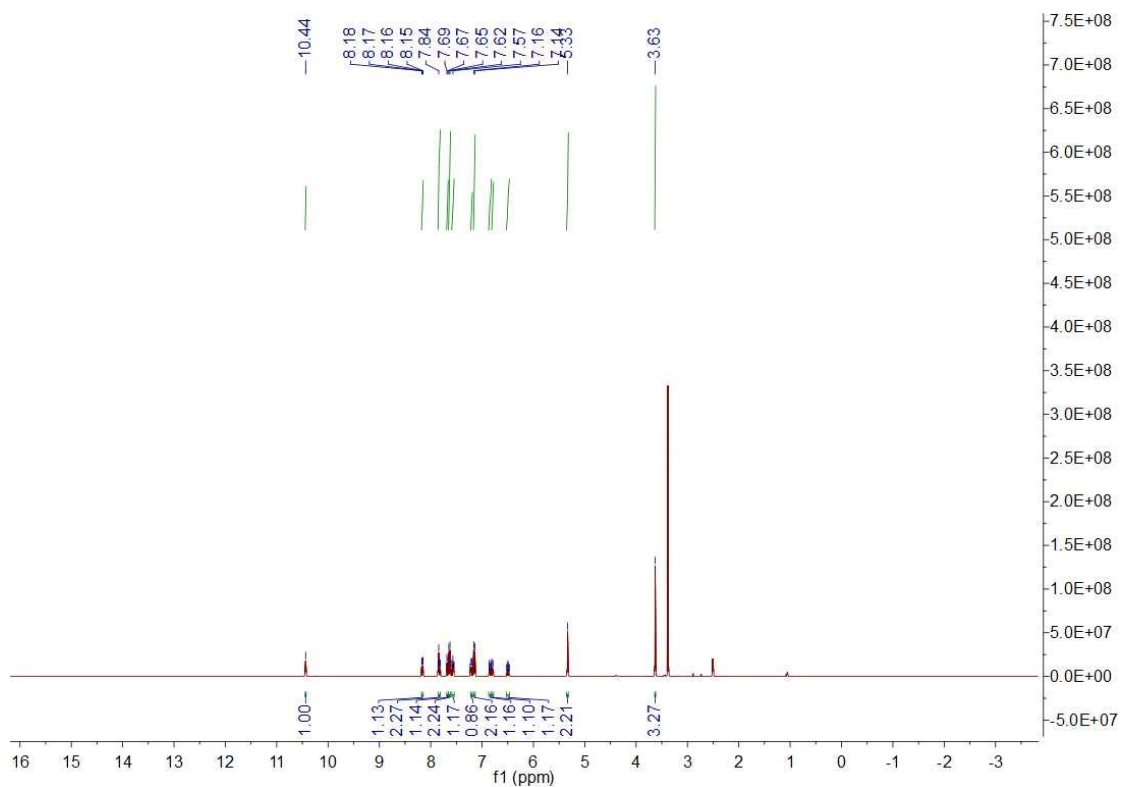
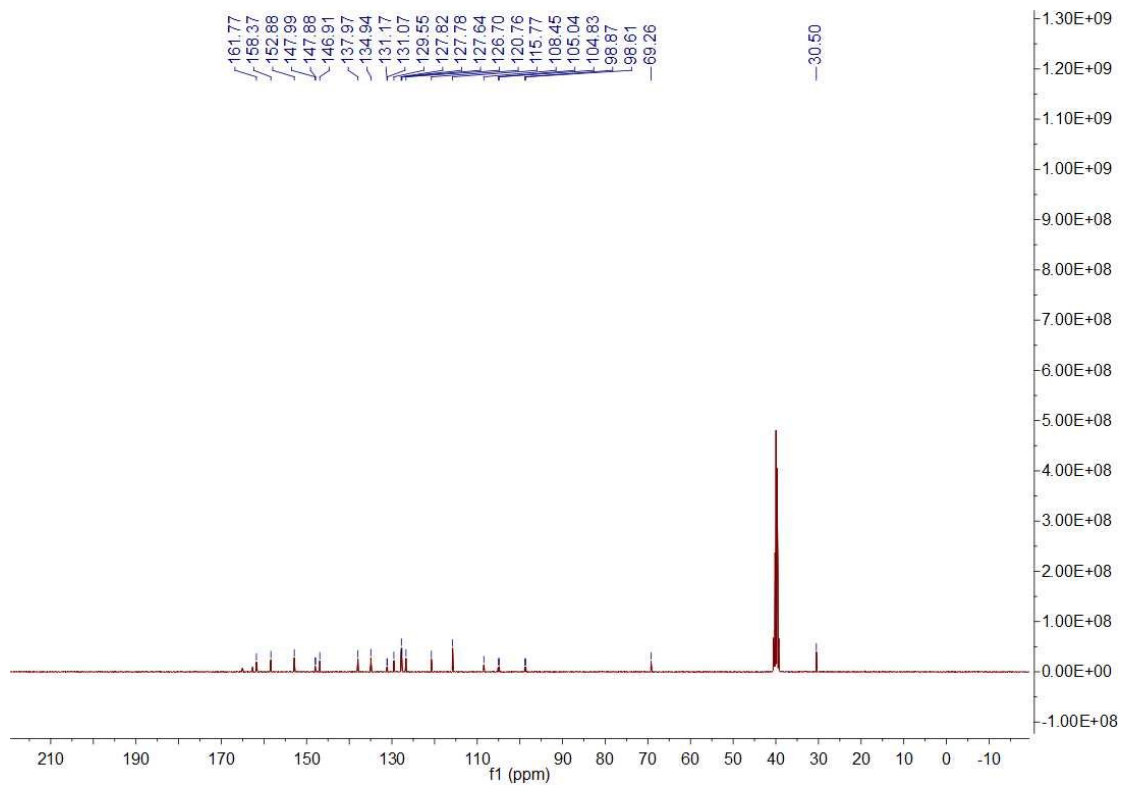
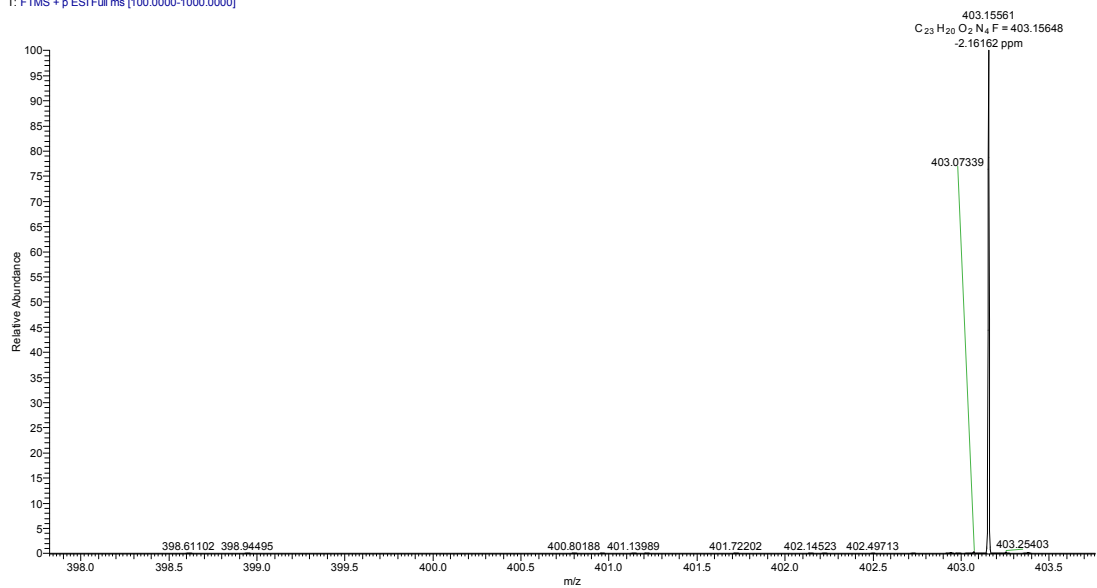


Fig. S19 <sup>1</sup>H NMR spectrum of title compound 7g



**Fig. S20**  $^{13}\text{C}$ NMR spectrum of title compound **7g**

2019112975 #41 RT: 0.42 AV: 1 NL: 2.68E8  
T: FTMS + p ESI Full ms [100.0000-1000.0000]



**Fig. S21** HRMS spectrum of title compound **7g**

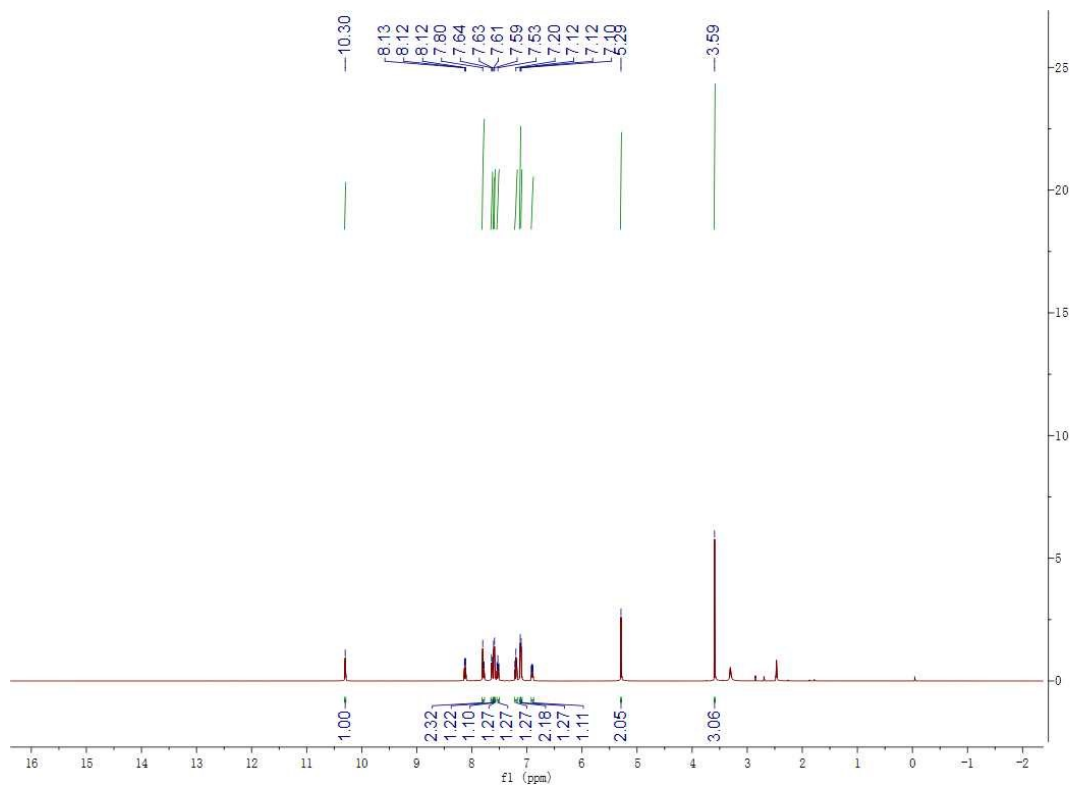


Fig. S22  $^1\text{H}$  NMR spectrum of title compound **7h**

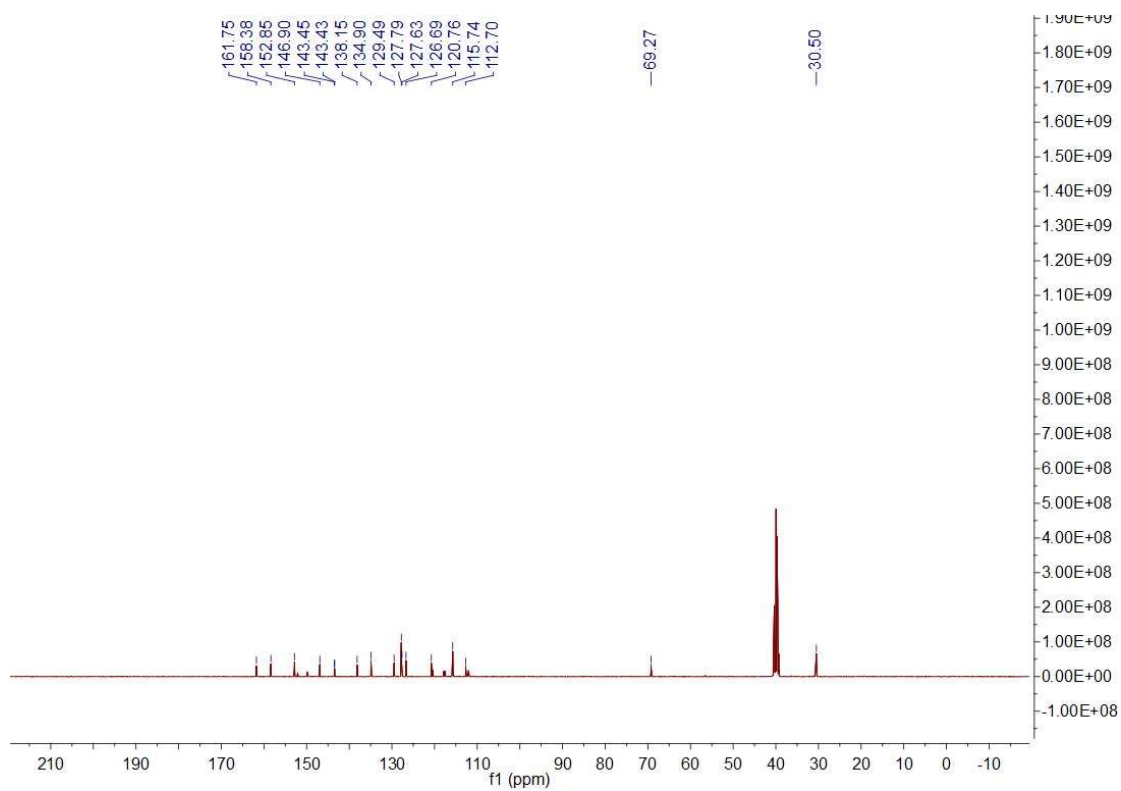


Fig. S23  $^{13}\text{C}$  NMR spectrum of title compound **7h**

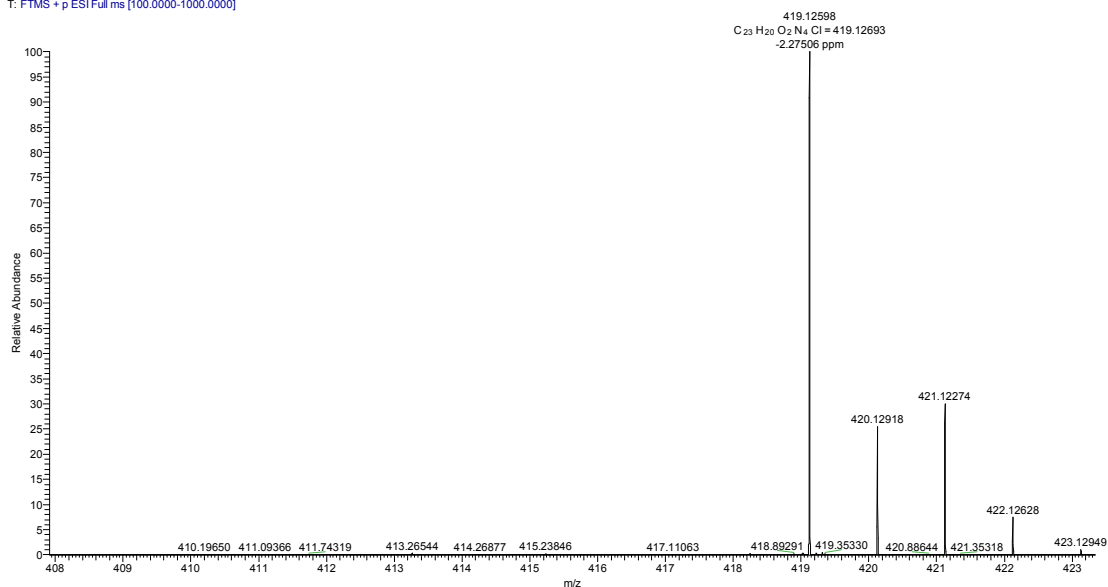


Fig. S24 HRMS spectrum of title compound 7h

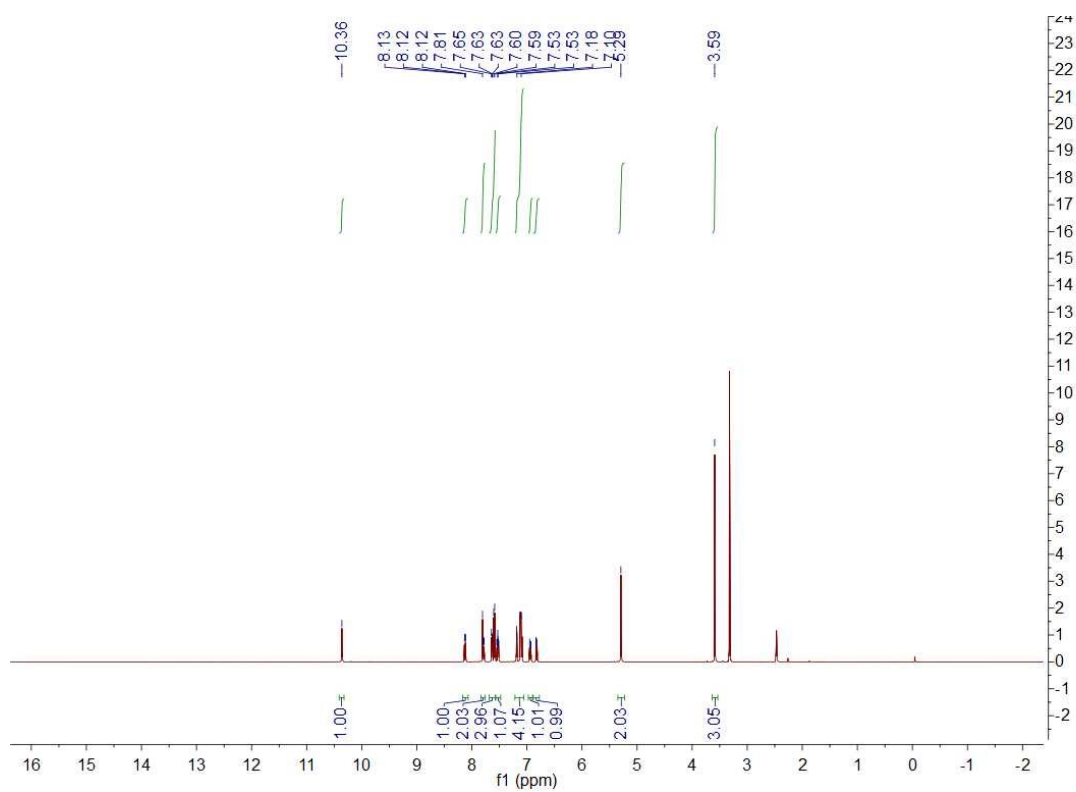


Fig. S25 <sup>1</sup>H NMR spectrum of title compound 7i

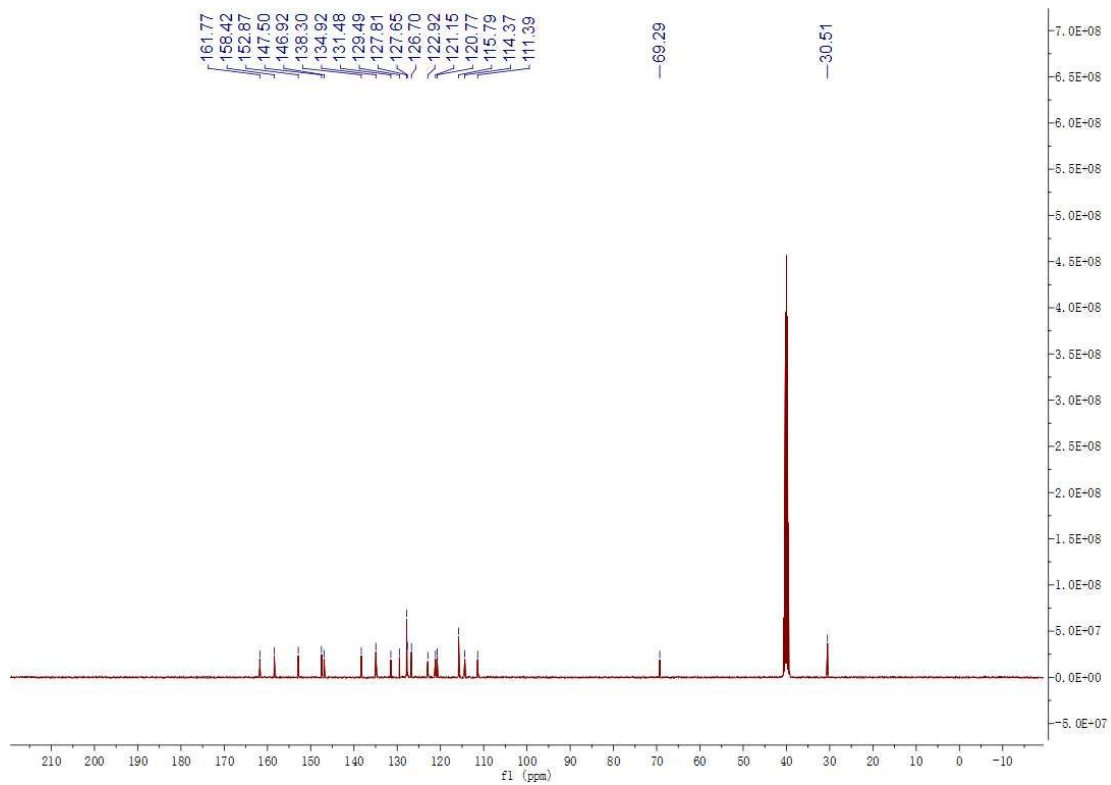


Fig. S26  $^{13}\text{C}$ NMR spectrum of title compound 7i

2019112977 #49 RT: 0.50 AV: 1 NL: 9.16E7  
T: FTMS + p ESI Full ms [100.0000-1000.0000]

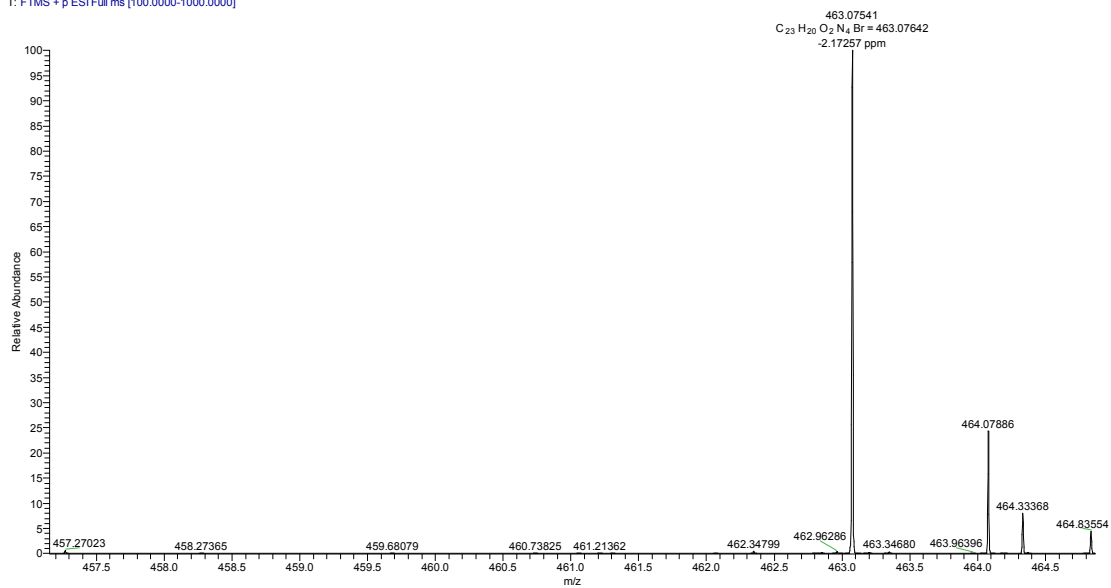


Fig. S27 HRMS spectrum of title compound 7i

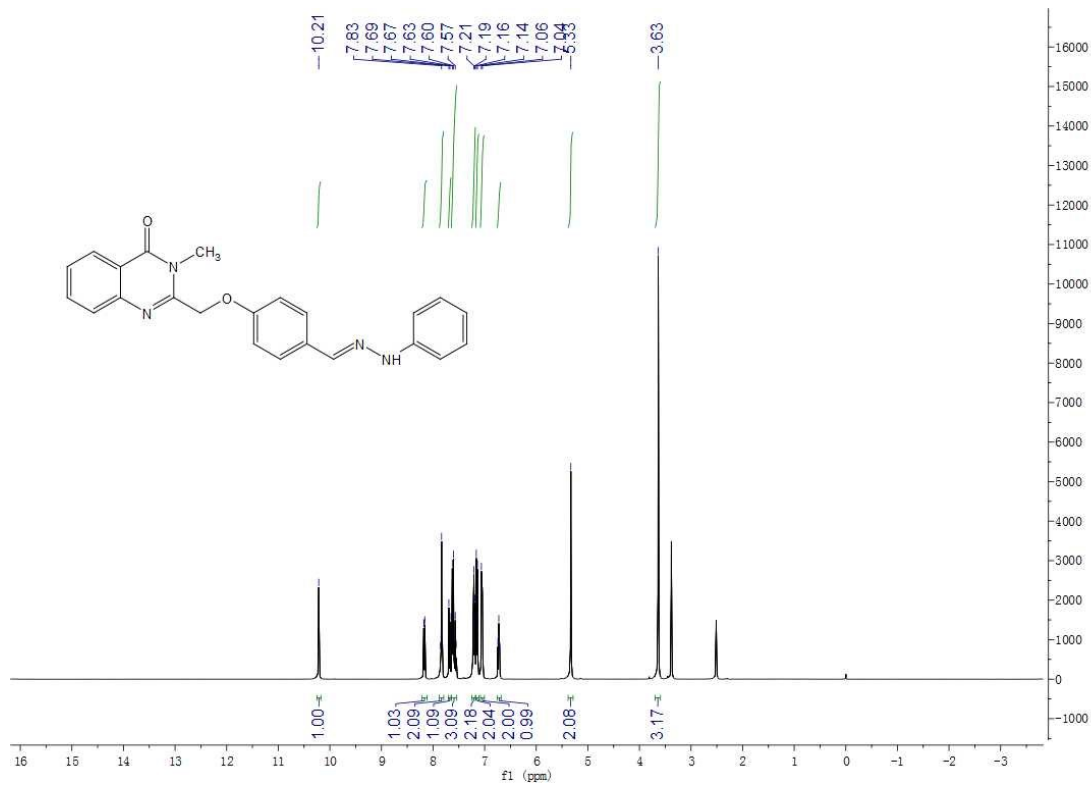


Fig. S28 <sup>1</sup>H NMR spectrum of title compound 7j

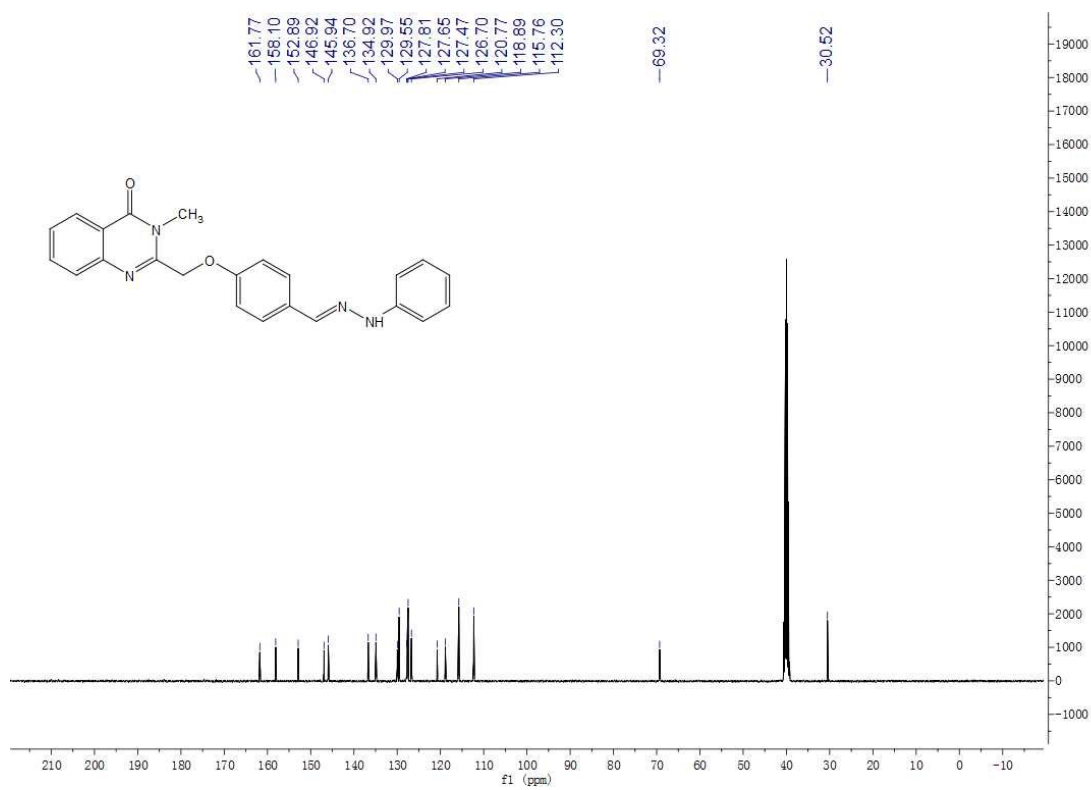


Fig. S29 <sup>13</sup>C NMR spectrum of title compound 7j



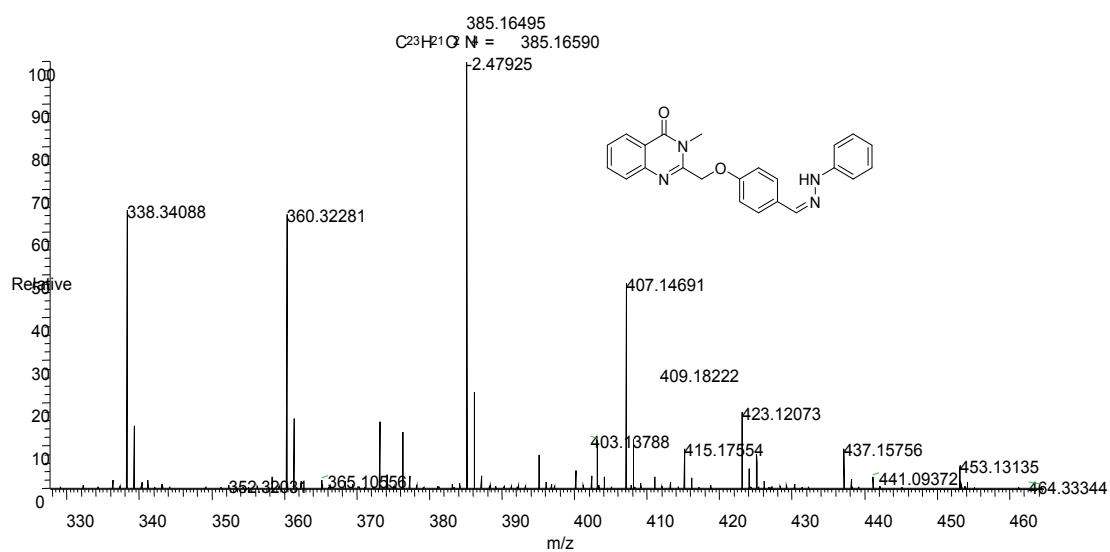


Fig. S30 HRMS spectrum of title compound 7j

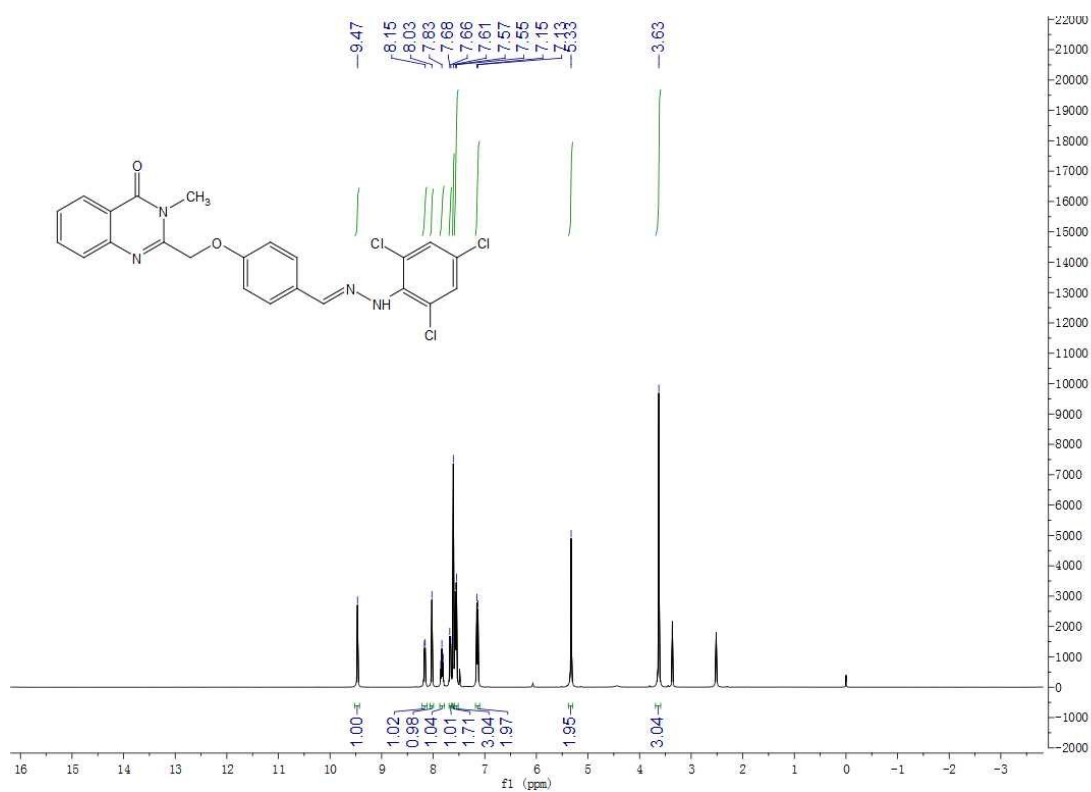
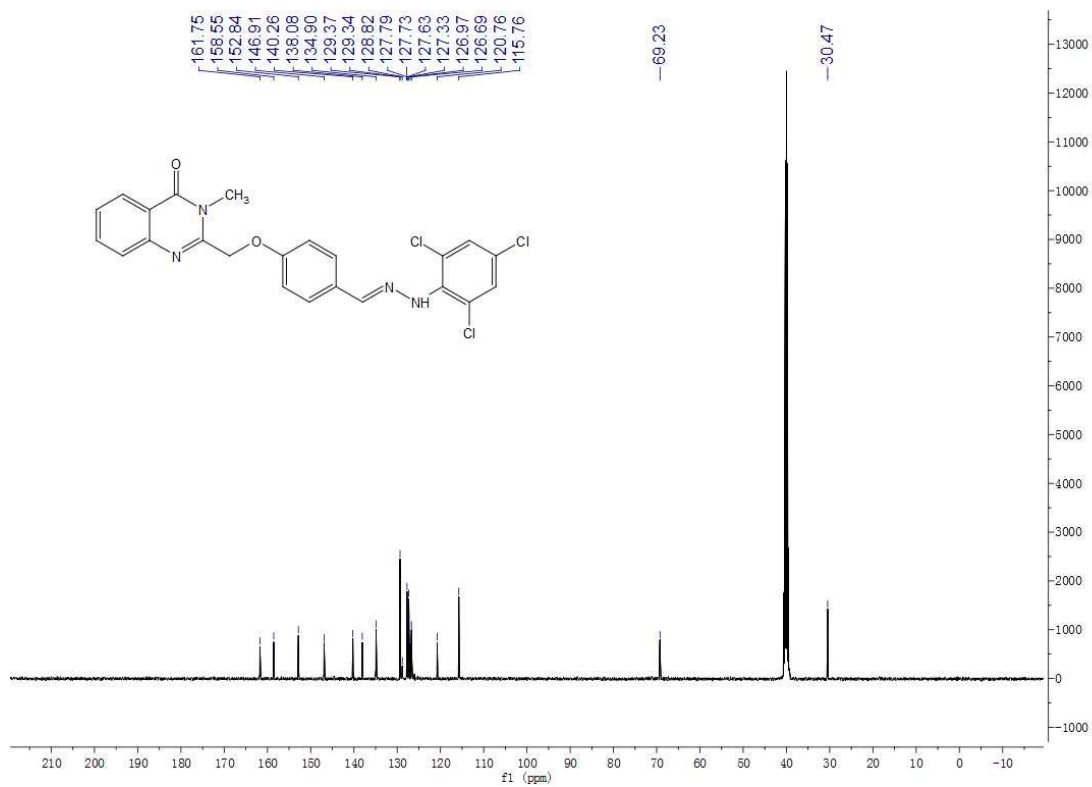
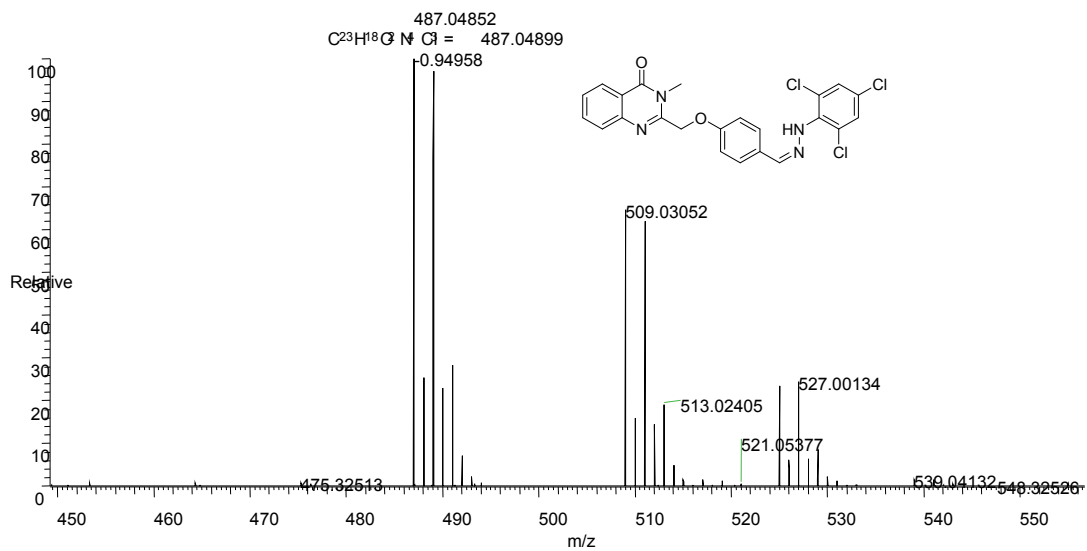


Fig. S31 <sup>1</sup>H NMR spectrum of title compound 7k



**Fig. S32** <sup>13</sup>CNMR spectrum of title compound **7k**



**Fig. S33** HRMS spectrum of title compound **7k**

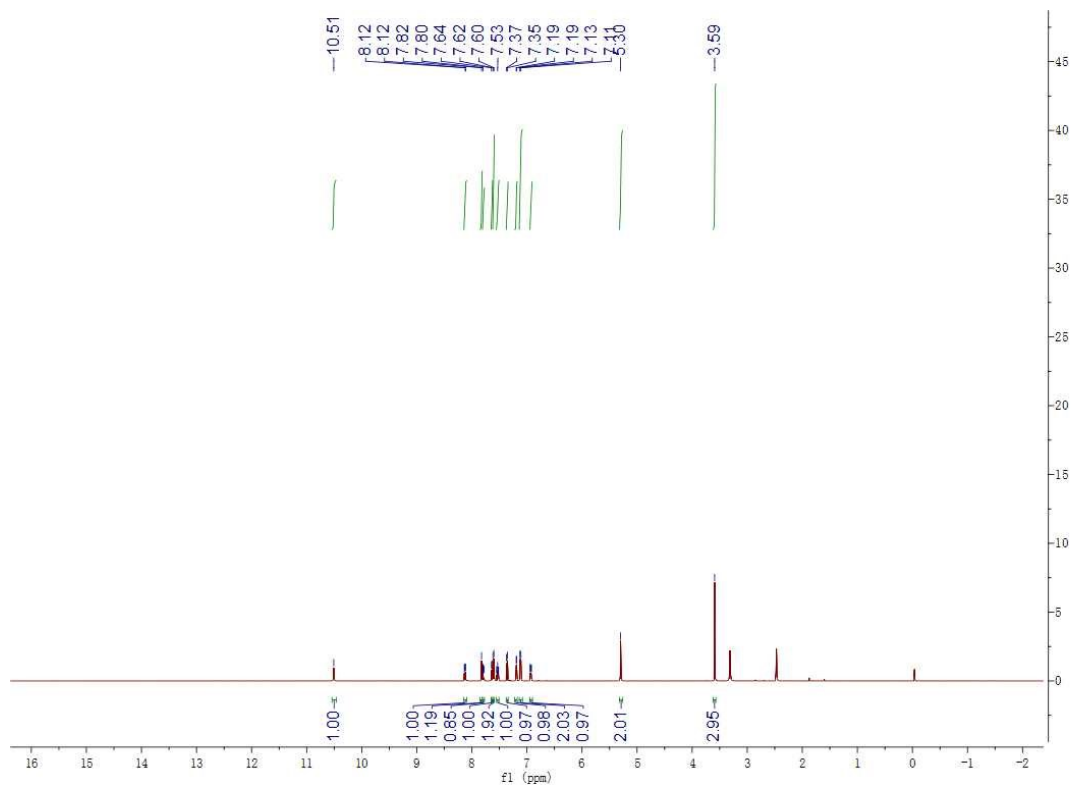


Fig. S34  $^1\text{H}$  NMR spectrum of title compound 71

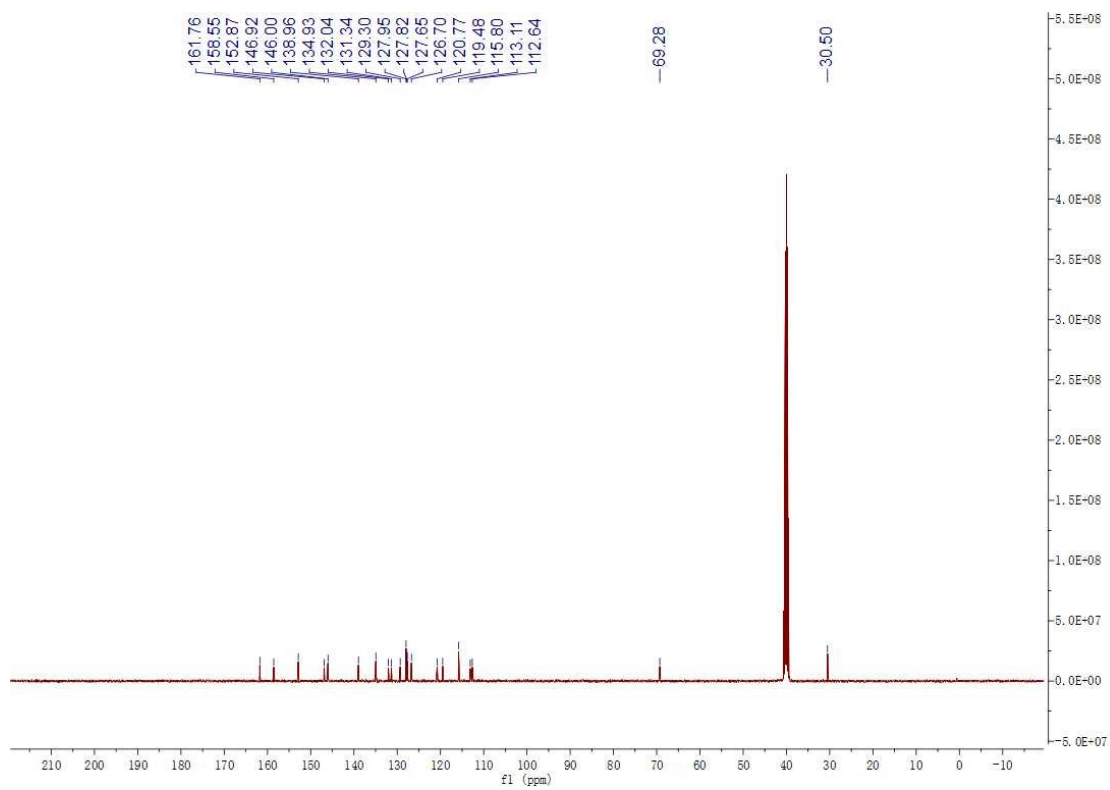


Fig. S35  $^{13}\text{C}$  NMR spectrum of title compound 71

2019112980 #61 RT: 0.63 AV: 1 NL: 1.25E7  
T: FTMS + p ESI Full ms [100.0000-1000.0000]

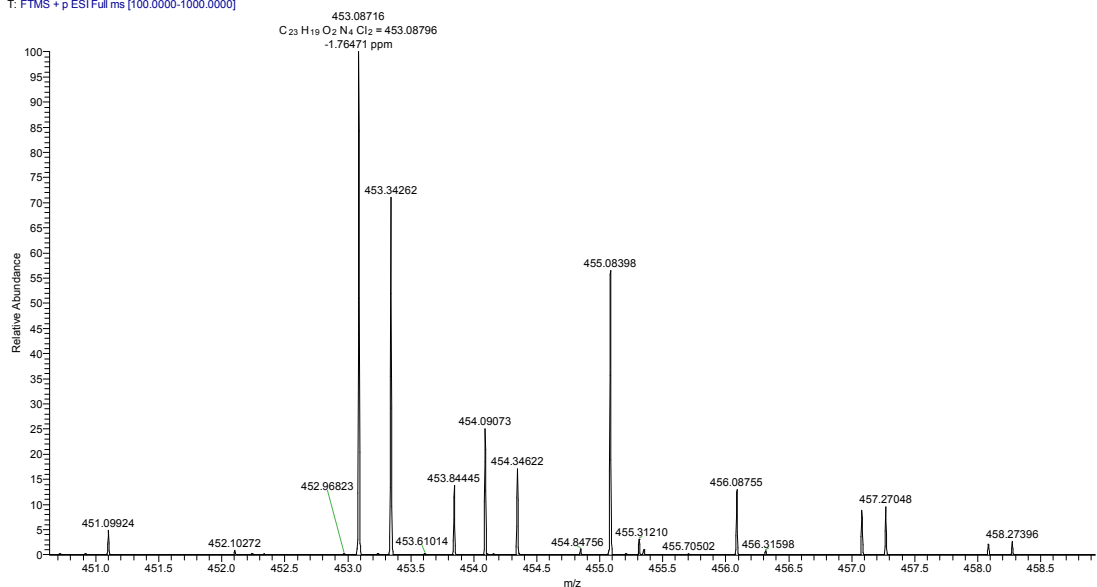


Fig. S36 HRMS spectrum of title compound 7l

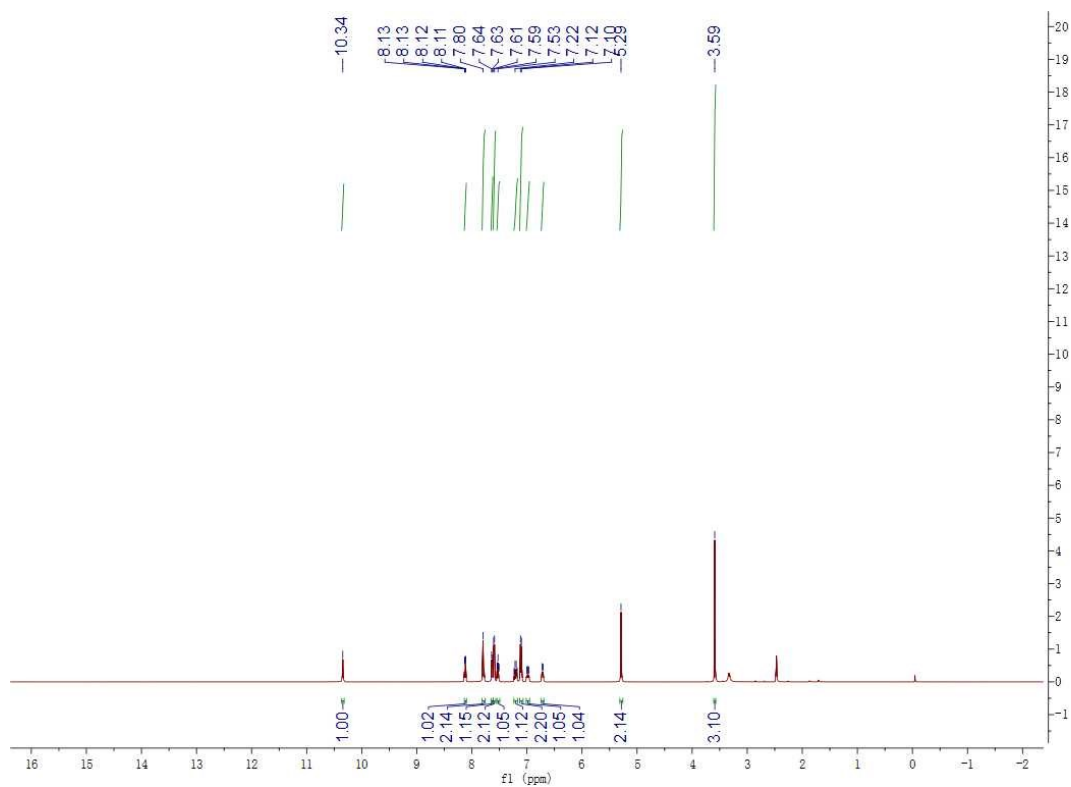


Fig. S37 <sup>1</sup>H NMR spectrum of title compound 7m

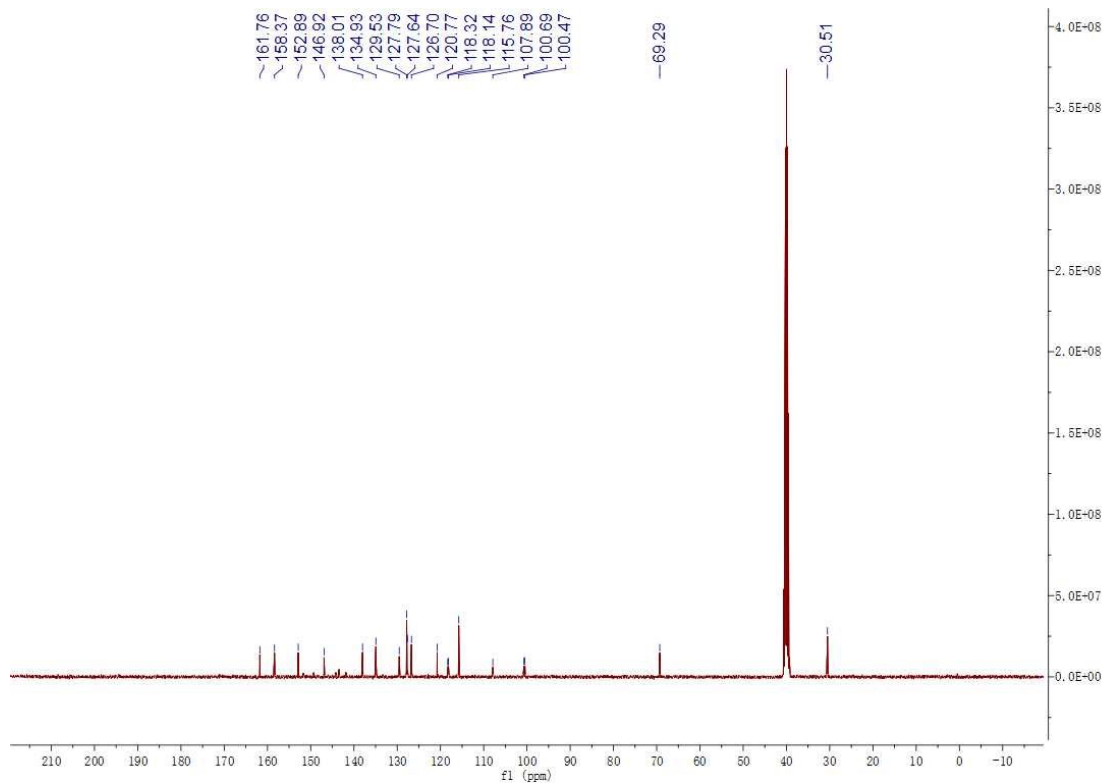


Fig. S38  $^{13}\text{C}$  NMR spectrum of title compound 7m

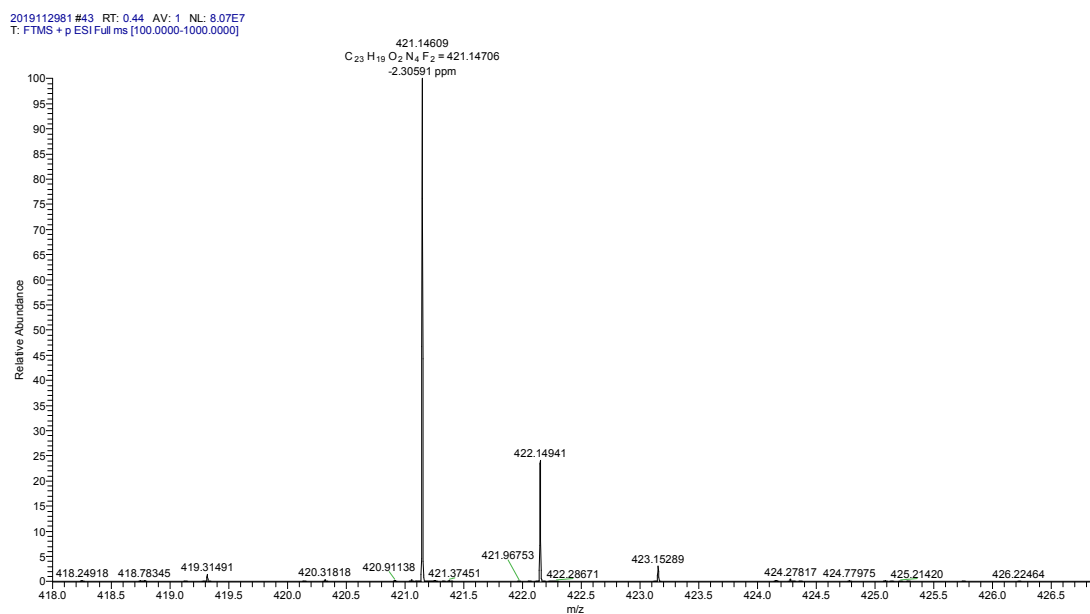


Fig. S39 HRMS spectrum of title compound 7m

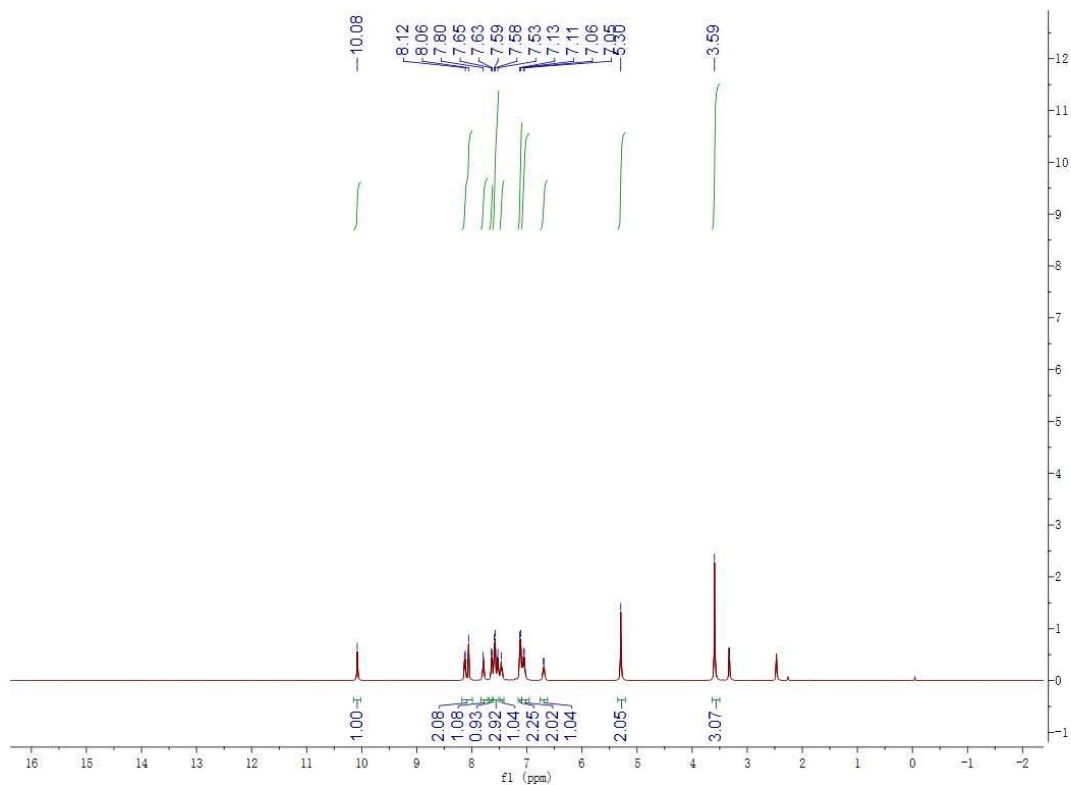


Fig. S40  $^1\text{H}$  NMR spectrum of title compound 7n

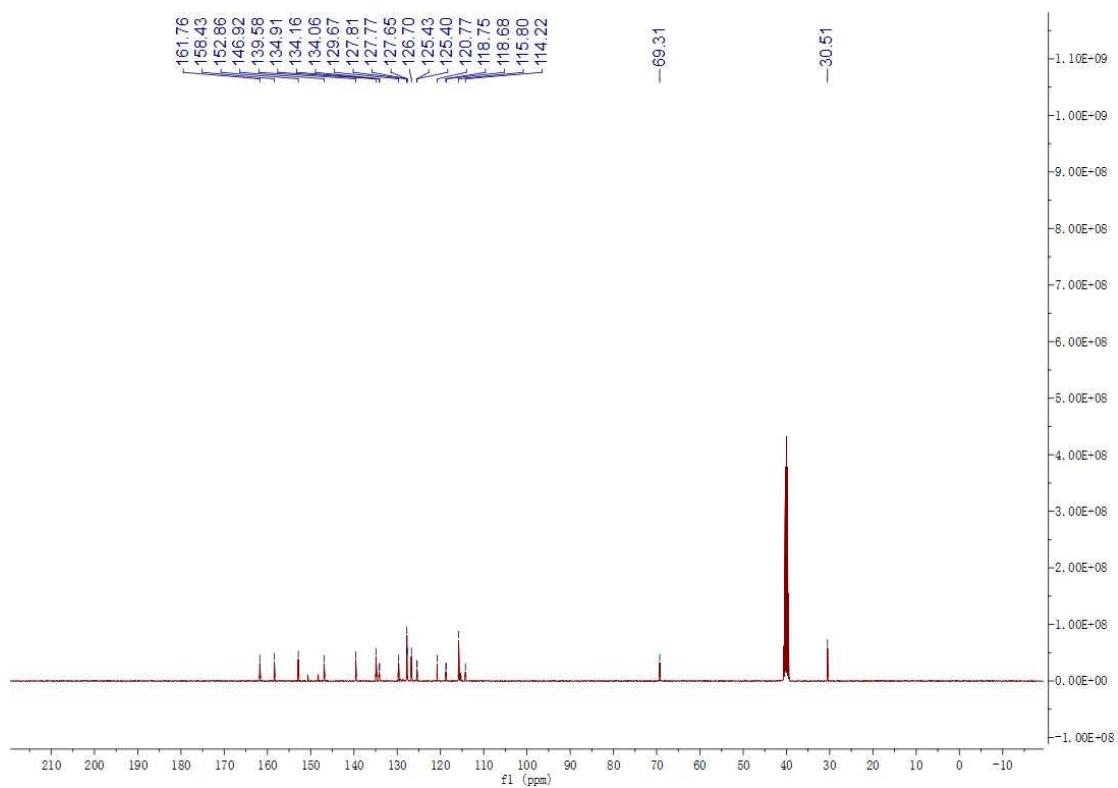


Fig. S41  $^{13}\text{C}$  NMR spectrum of title compound 7n

2019112982 #43 RT: 0.44 AV: 1 NL: 7.73E7  
T: FTMS + p ESI Full ms [100.0000-1000.0000]

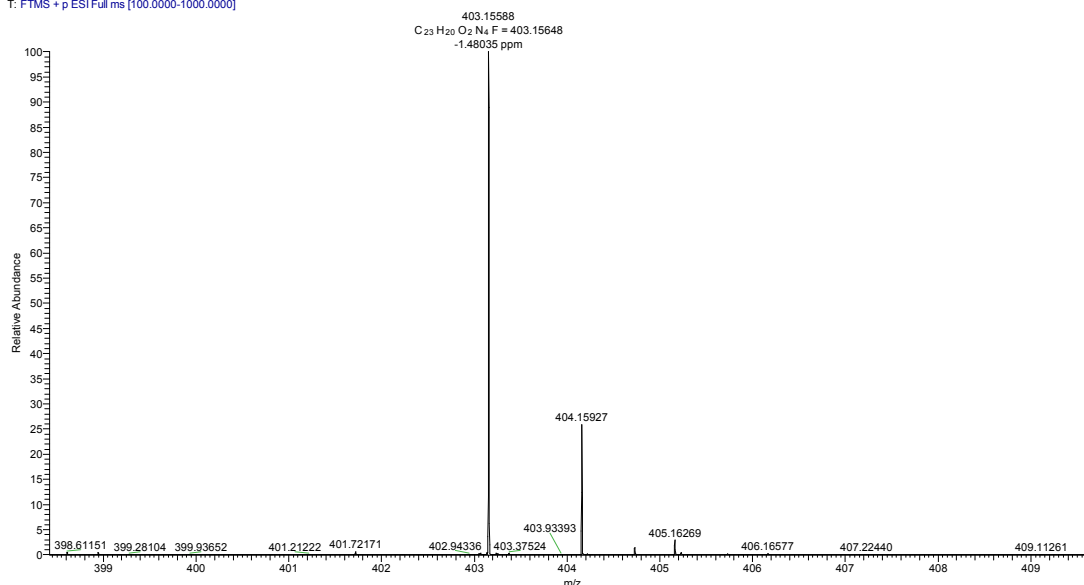


Fig. S42 HRMS spectrum of title compound 7n

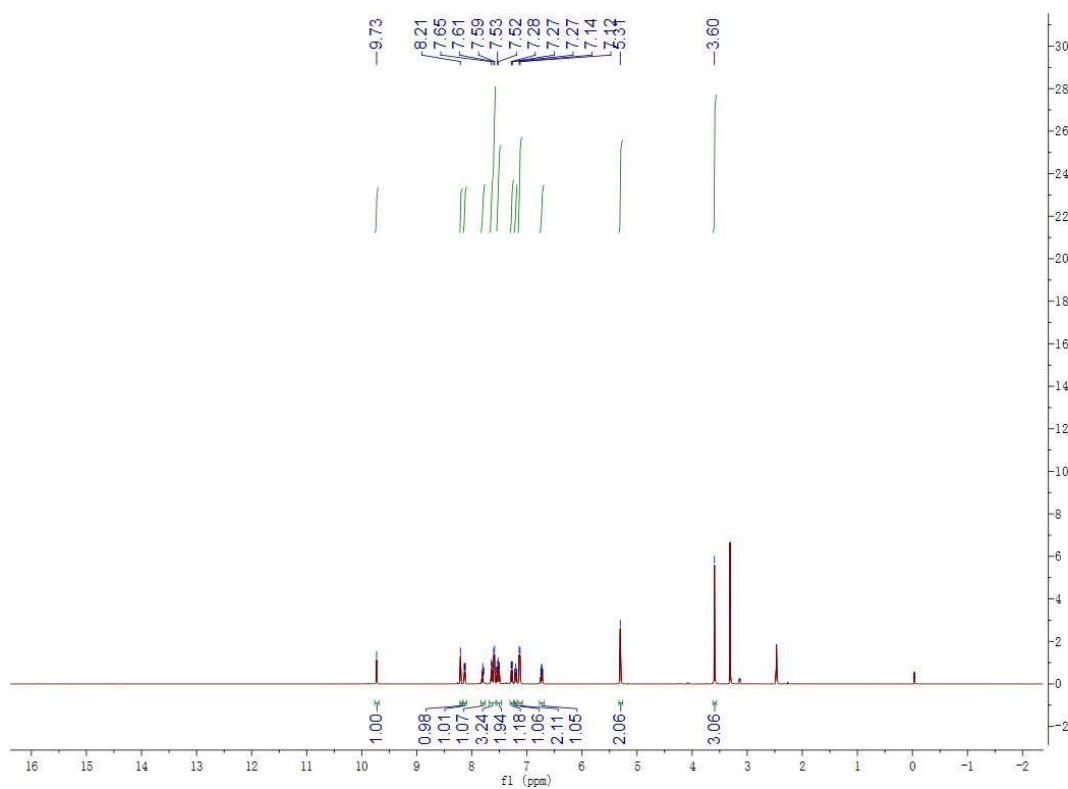
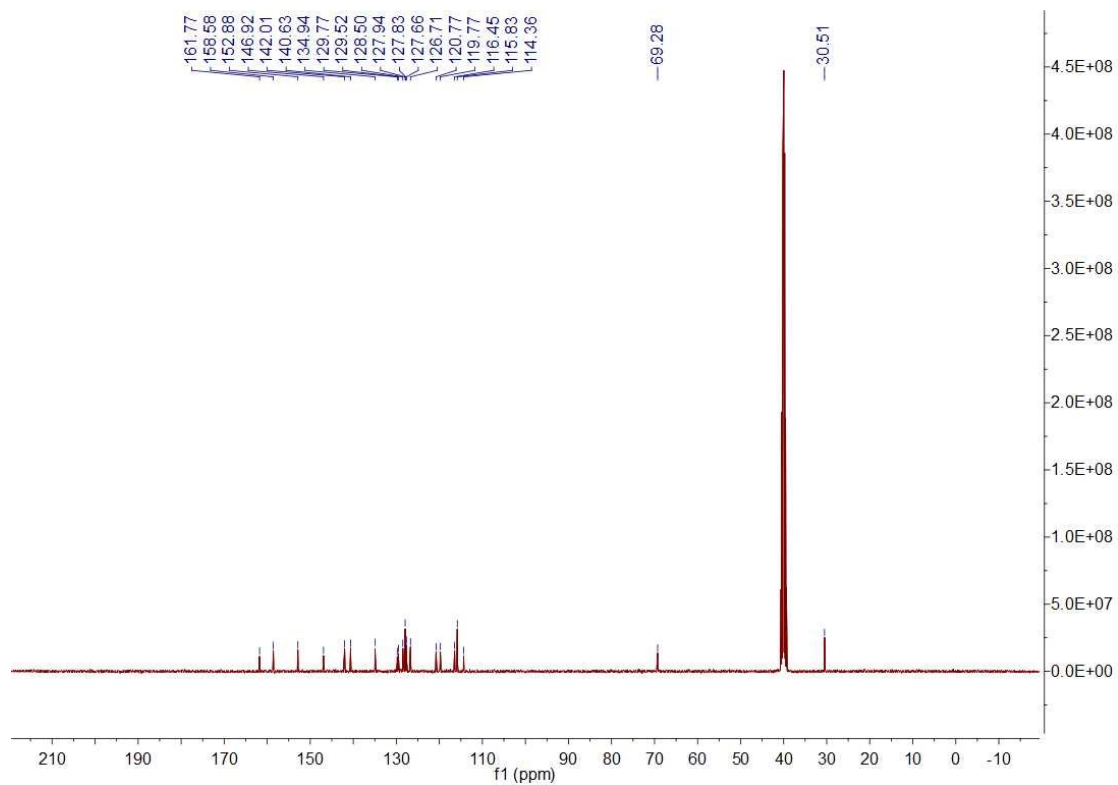
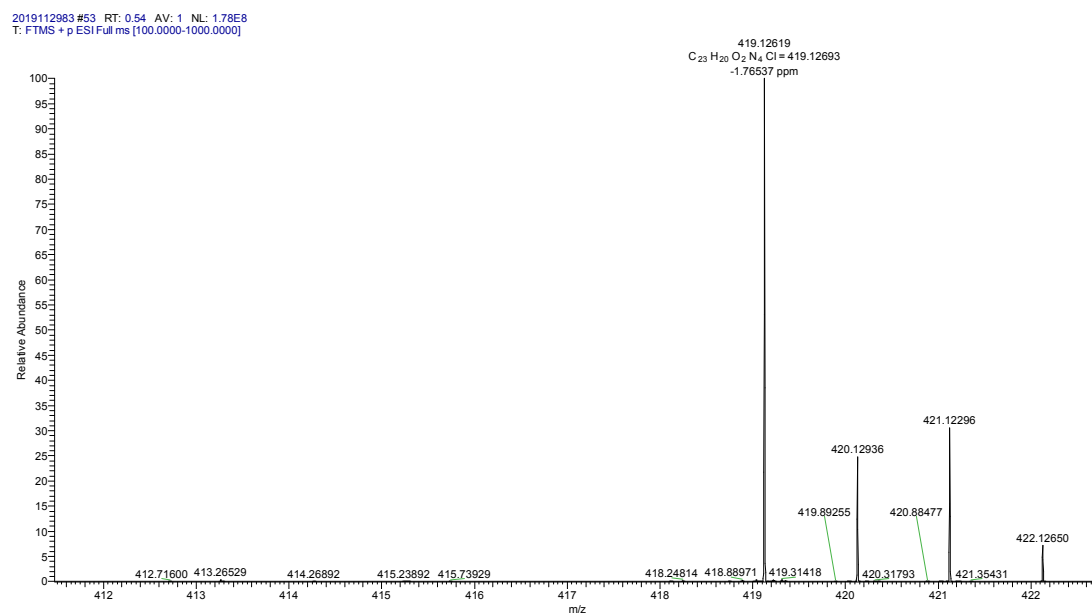


Fig. S43 <sup>1</sup>H NMR spectrum of title compound 7o

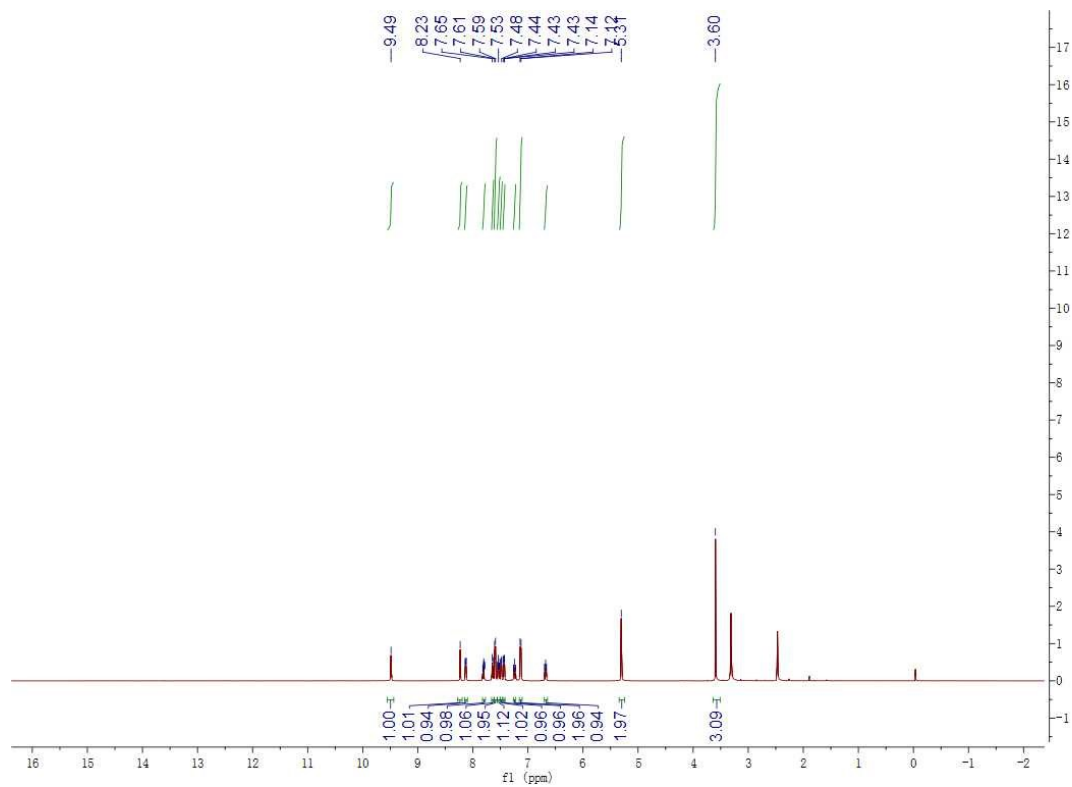


**Fig. S44** <sup>13</sup>C NMR spectrum of title compound **7o**

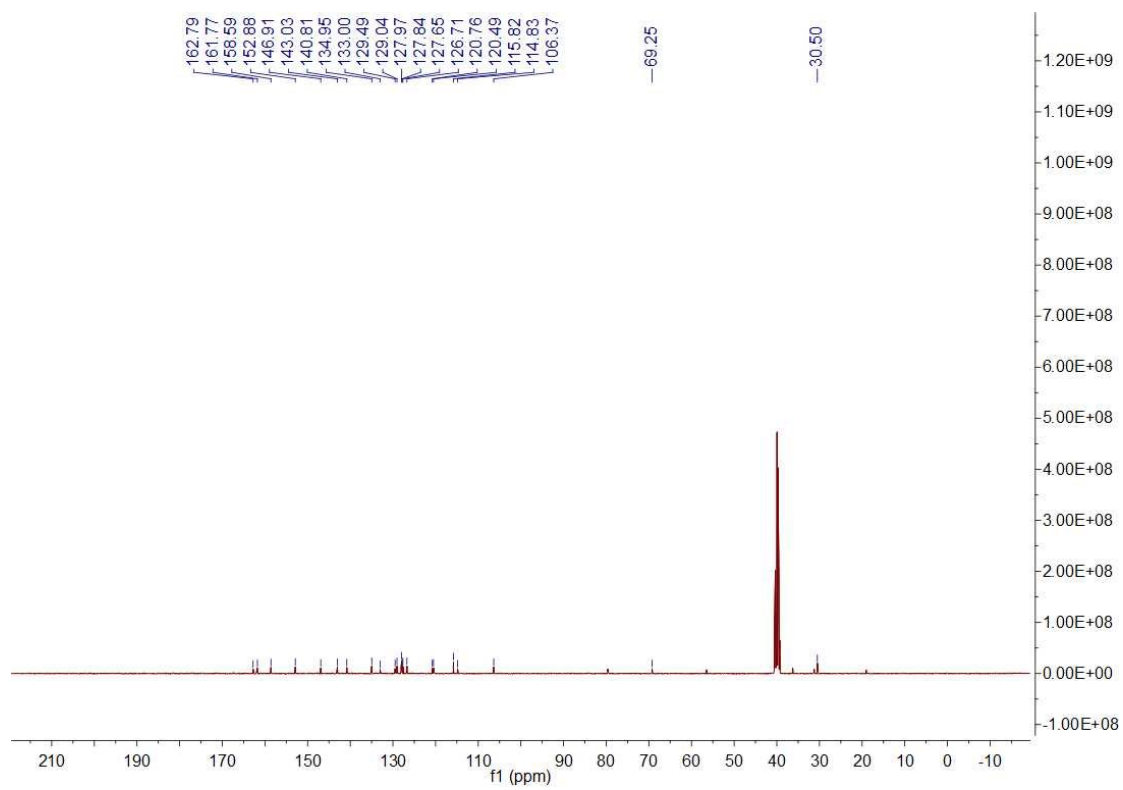


**Fig. S45** HRMS spectrum of title compound **7o**





**Fig. S46**  $^1\text{H}$  NMR spectrum of title compound **7p**



**Fig. S47**  $^{13}\text{C}$  NMR spectrum of title compound **7p**

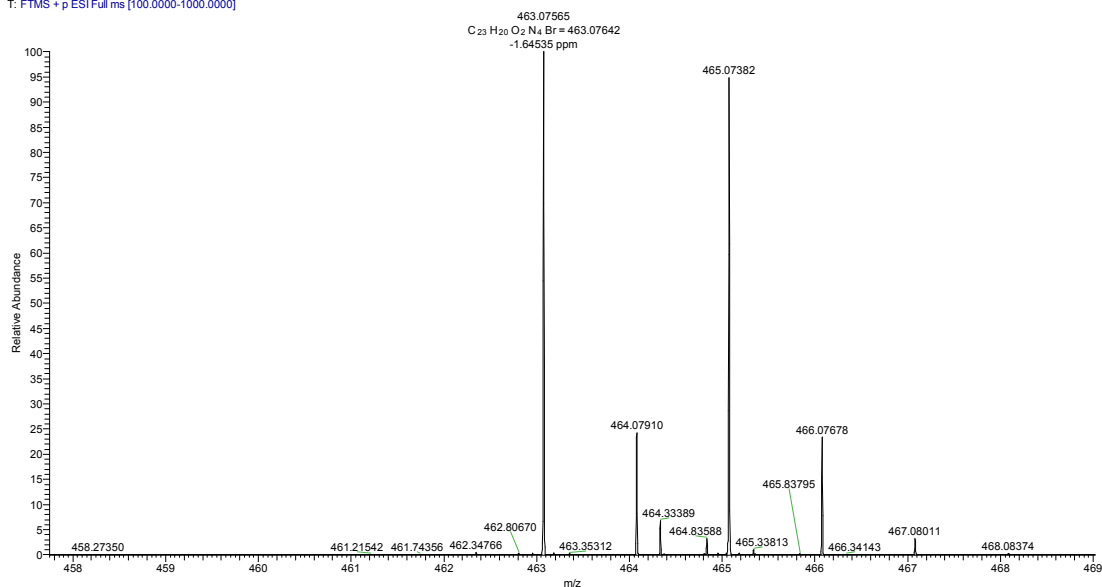


Fig. S48 HRMS spectrum of title compound 7p

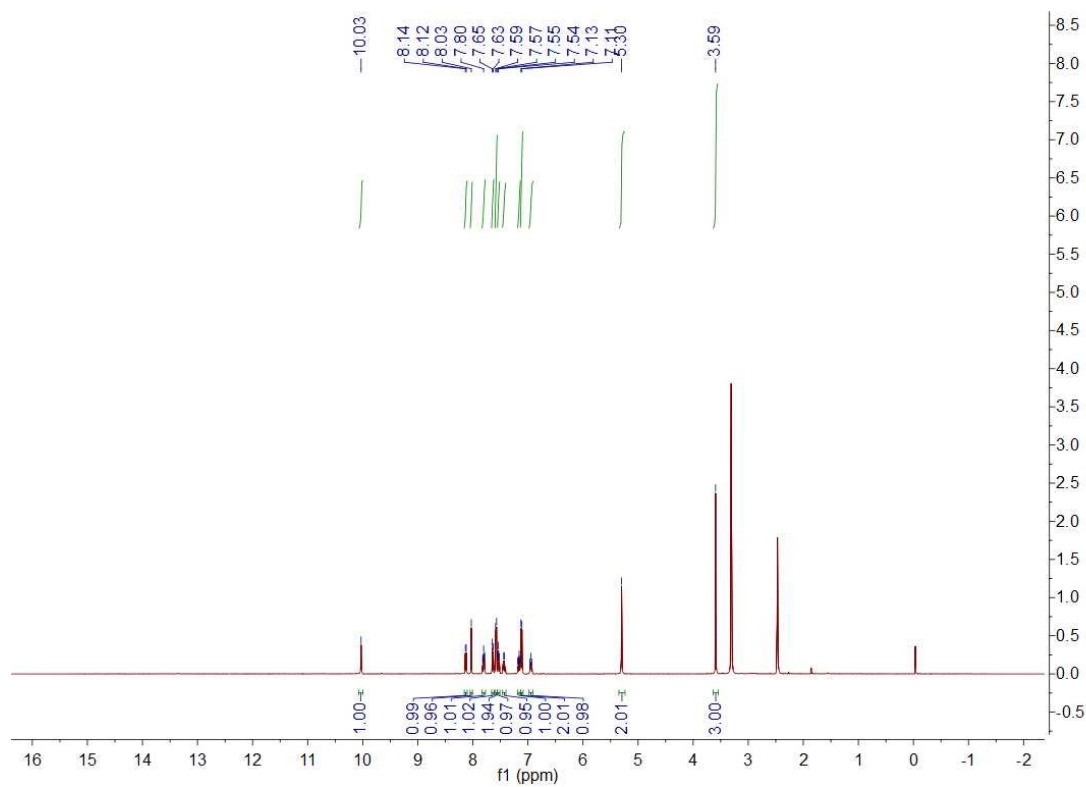
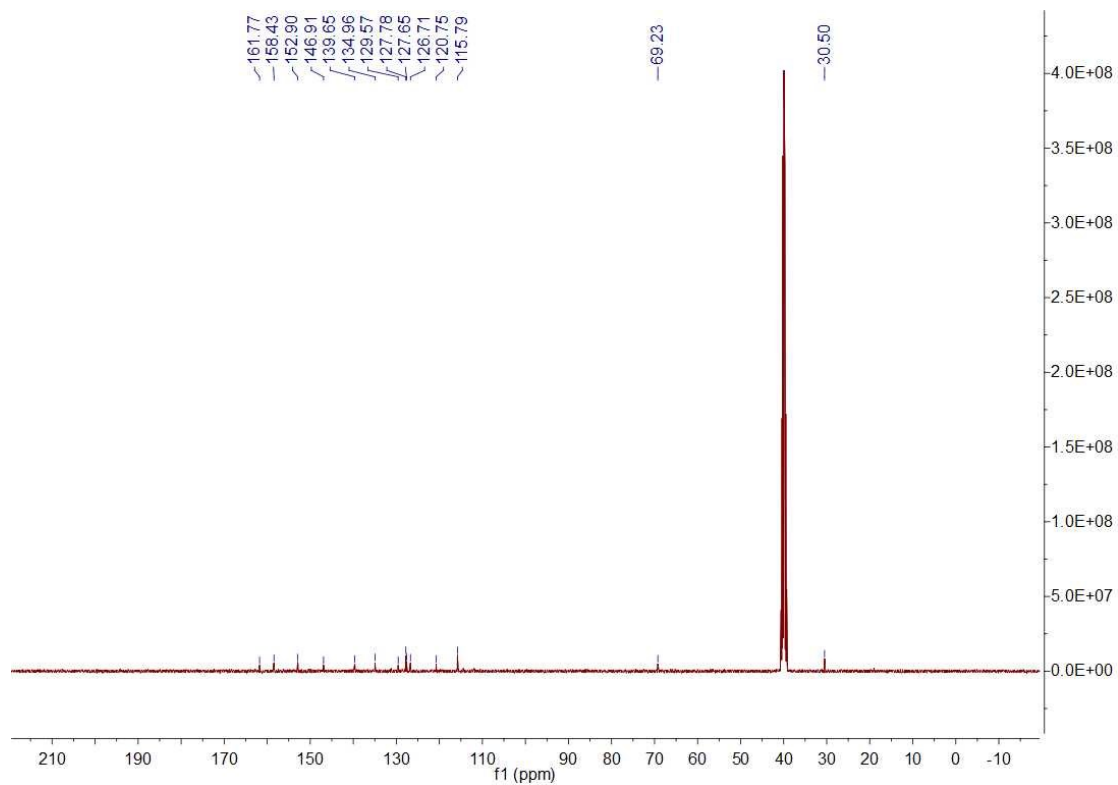
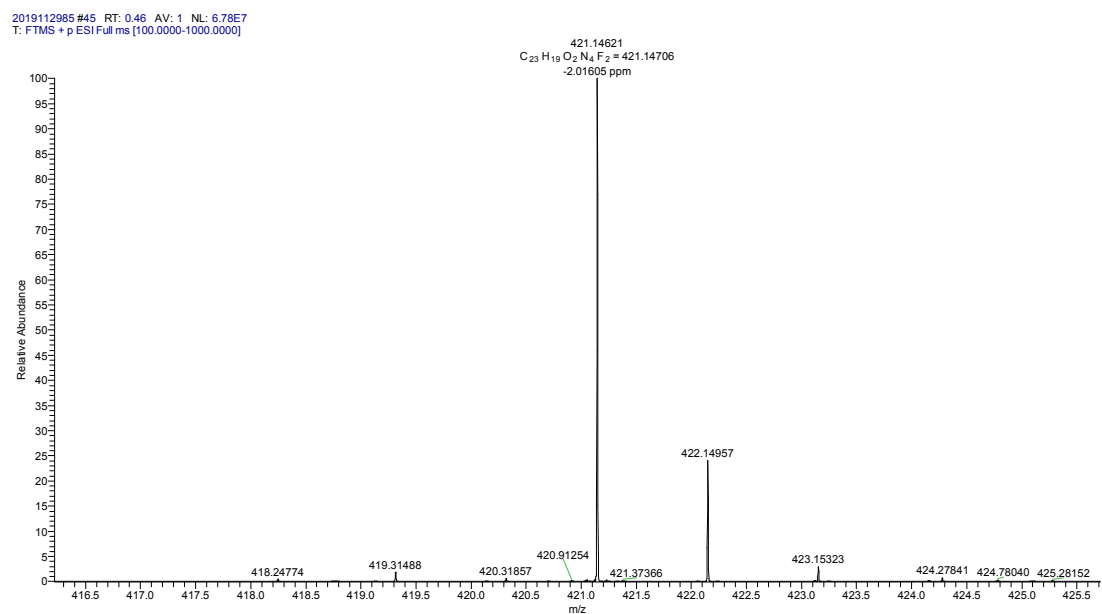


Fig. S49 <sup>1</sup>H NMR spectrum of title compound 7q



**Fig. S50**  $^{13}\text{C}$  NMR spectrum of title compound **7q**



**Fig. S51** HRMS spectrum of title compound **7q**

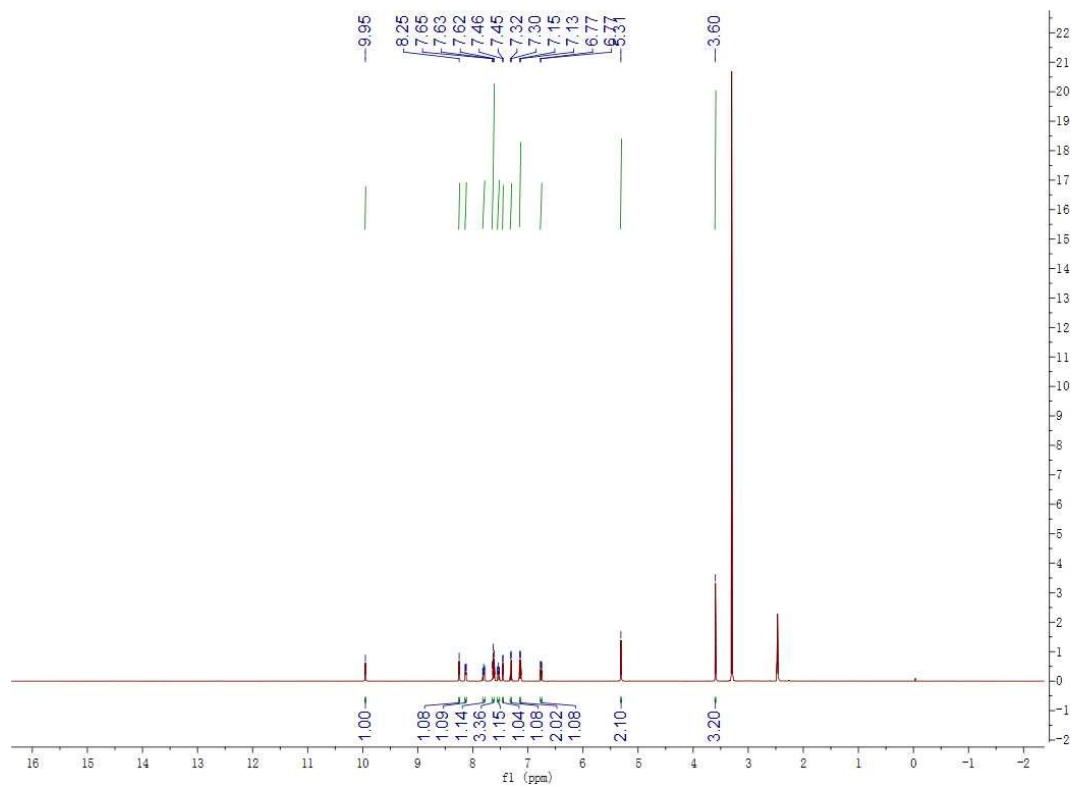


Fig. S52 <sup>1</sup>H NMR spectrum of title compound 7r

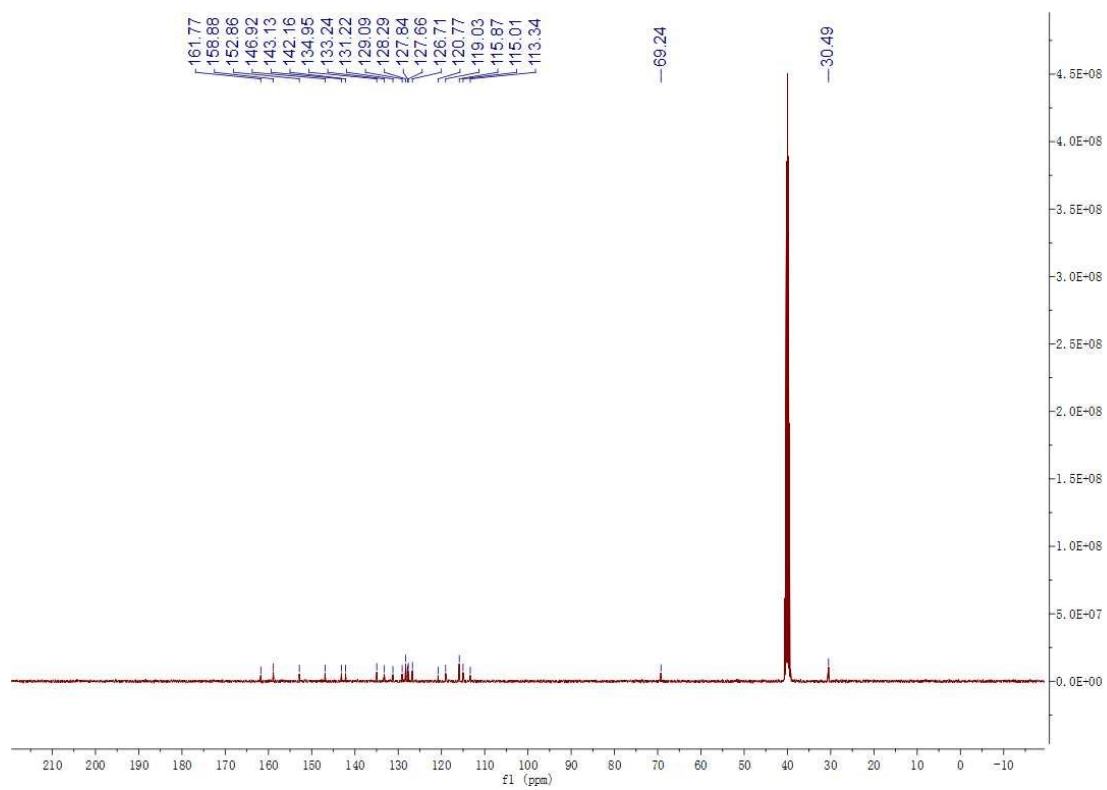


Fig. S53 <sup>13</sup>C NMR spectrum of title compound 7r

2019112986 #85 RT: 0.87 AV: 1 NL: 1.29E7  
T: FTMS + p ESI Full ms [100.0000-1000.0000]

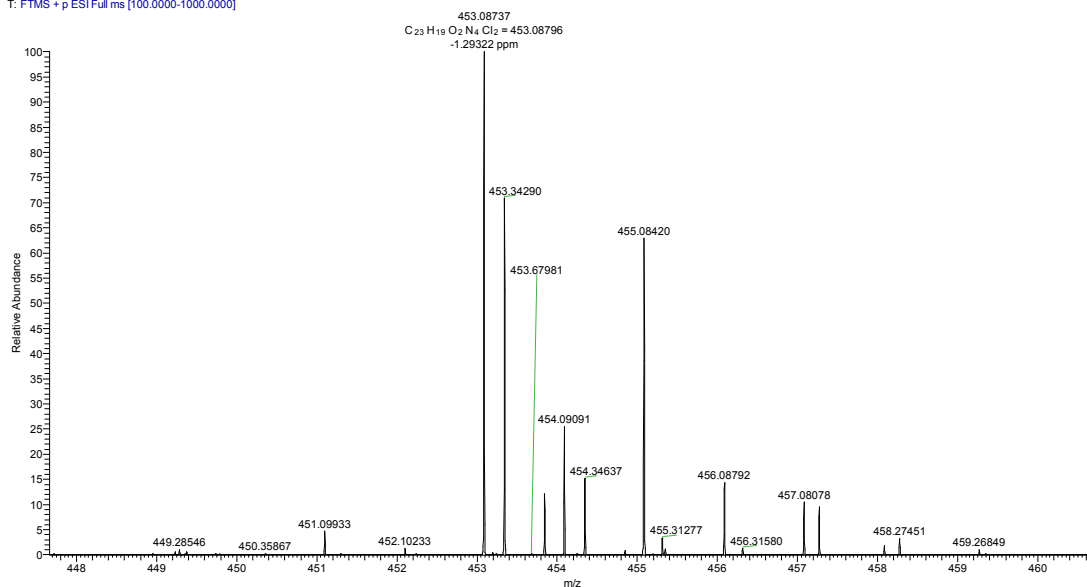


Fig. S54 HRMS spectrum of title compound 7r

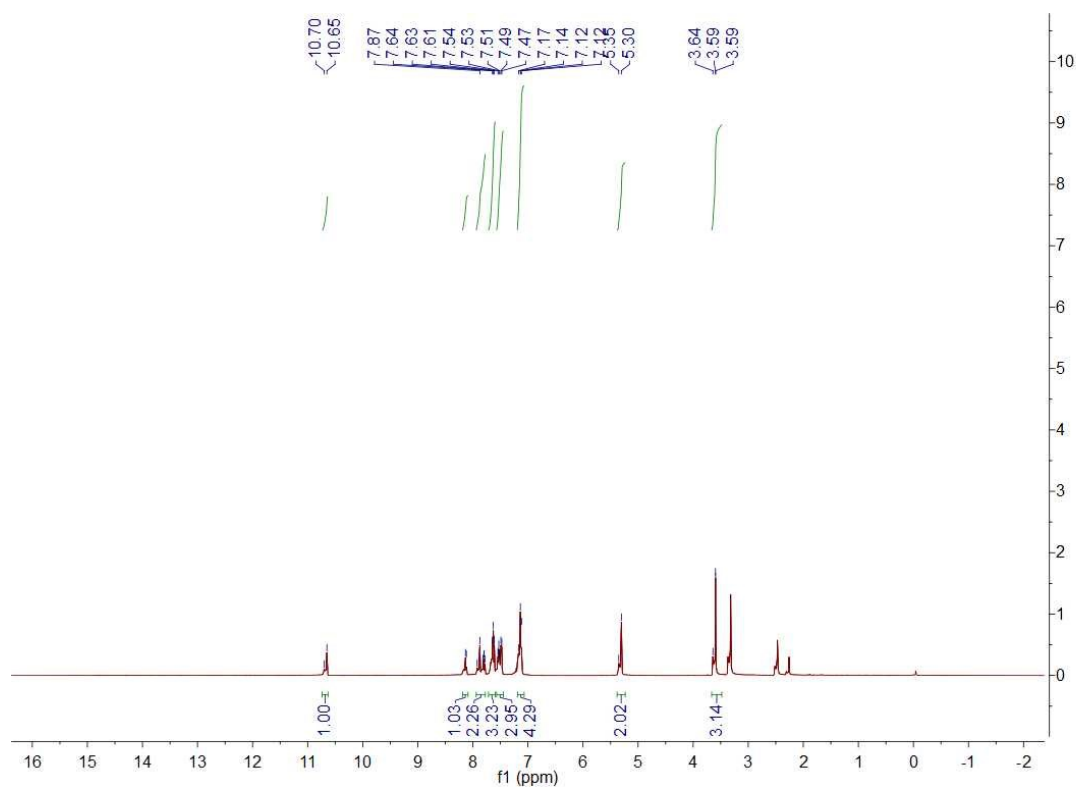


Fig. S55 <sup>1</sup>H NMR spectrum of title compound 7s

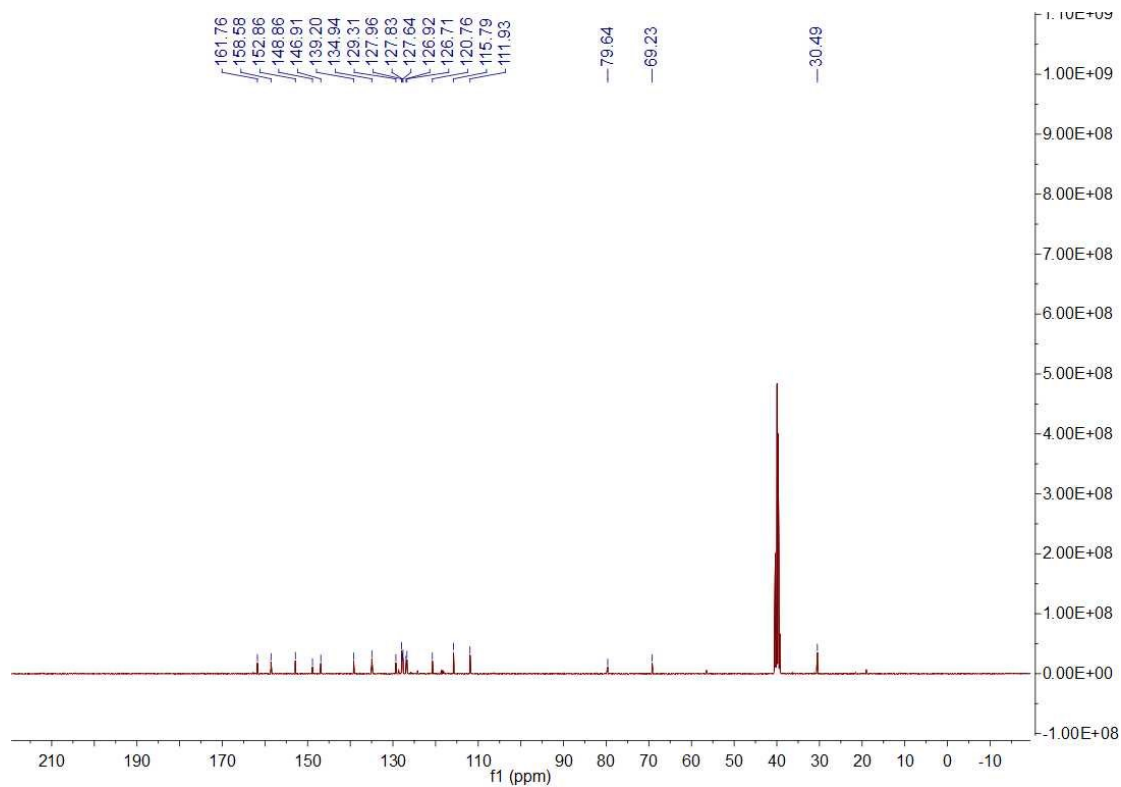


Fig. S56 <sup>13</sup>CNMR spectrum of title compound 7s

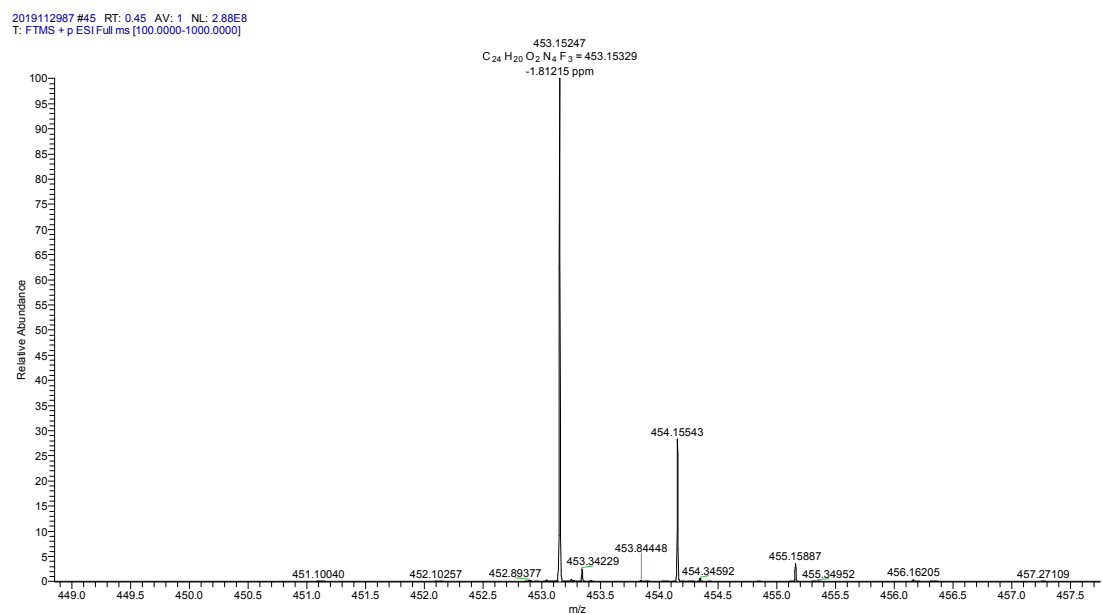


Fig. S57 HRMS spectrum of title compound 7s

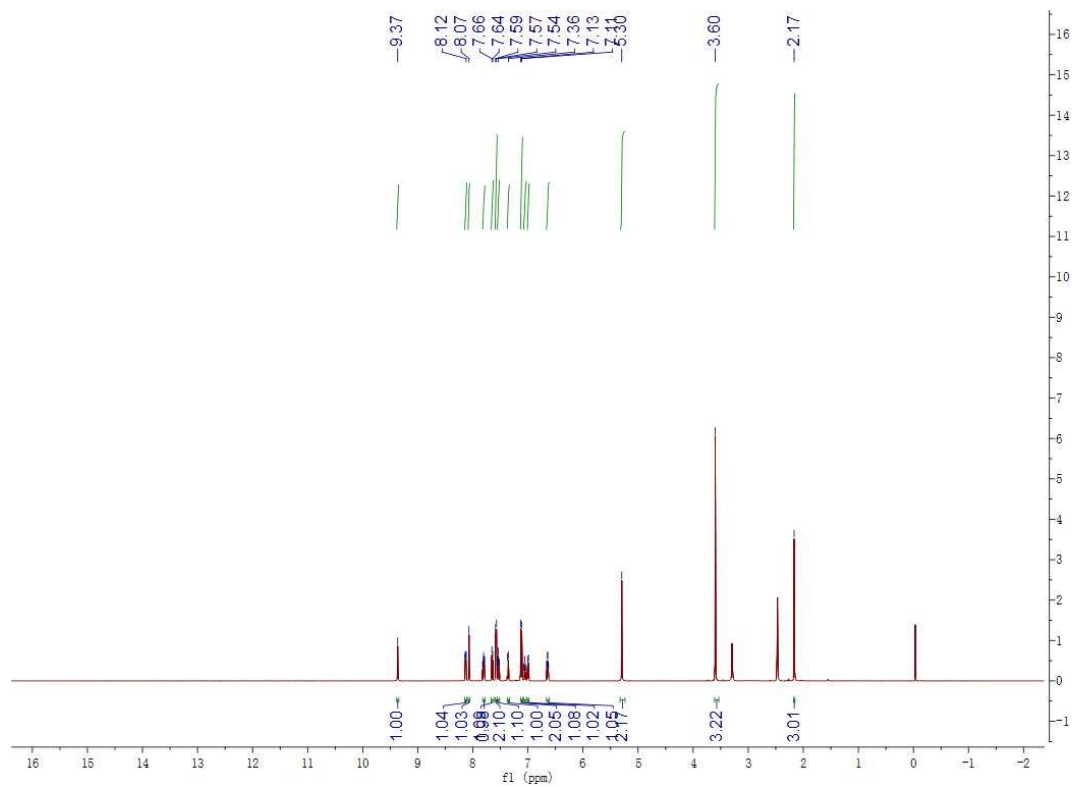


Fig. S58  $^1\text{H}$  NMR spectrum of title compound **7t**

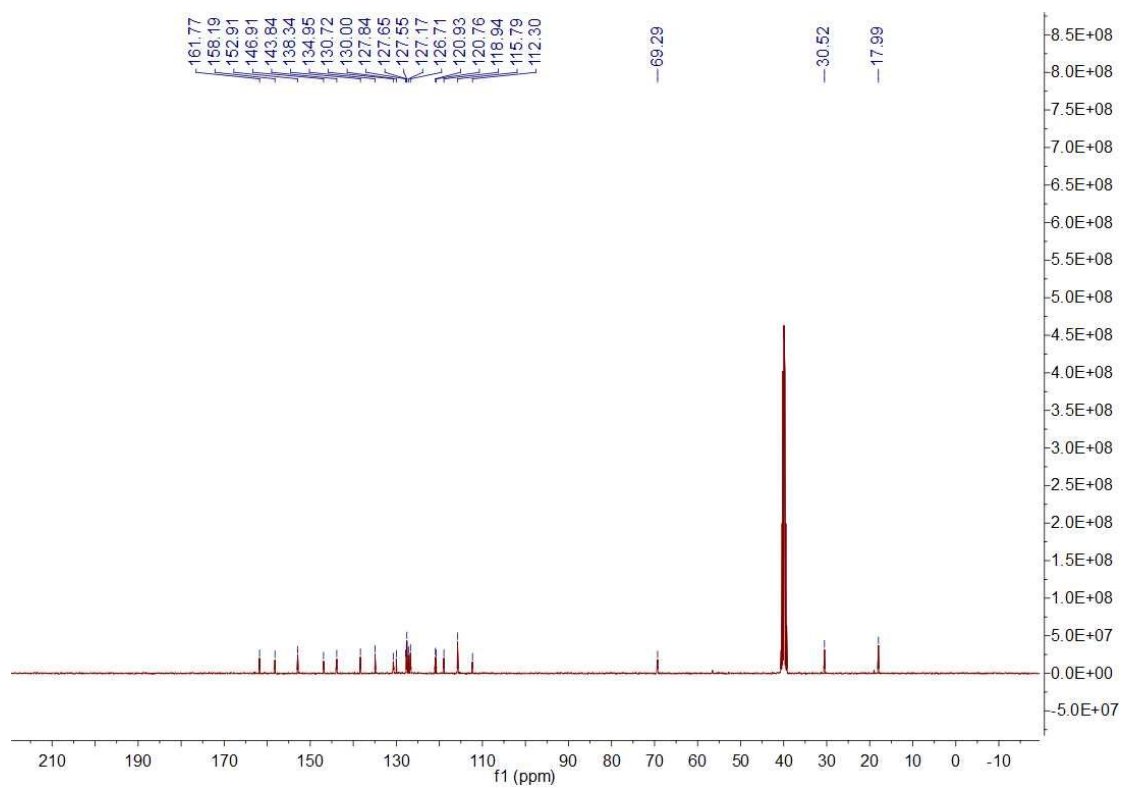


Fig. S59  $^{13}\text{C}$  NMR spectrum of title compound **7t**

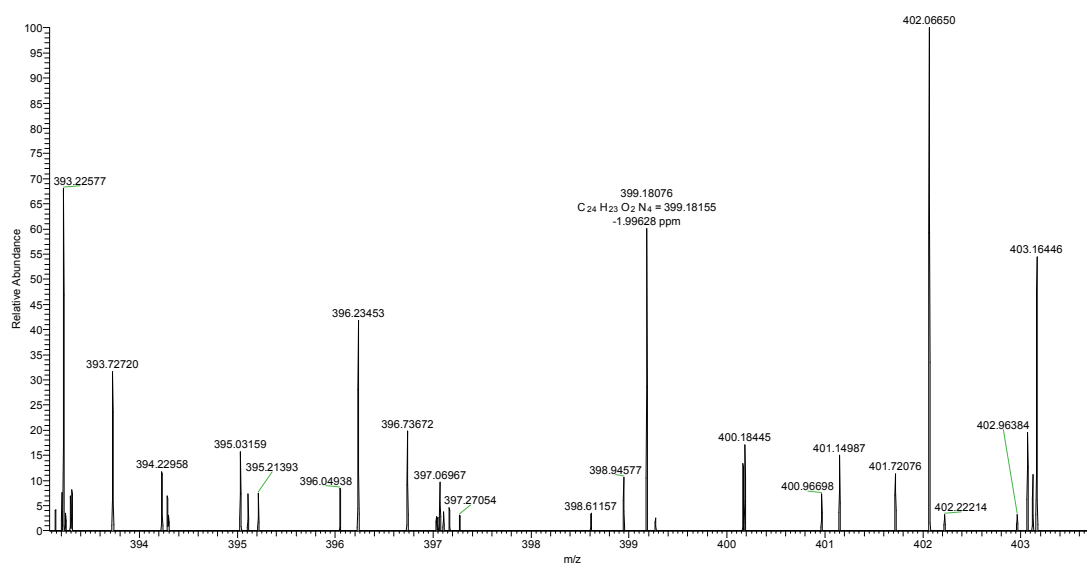


Fig. S60 HRMS spectrum of title compound 7t

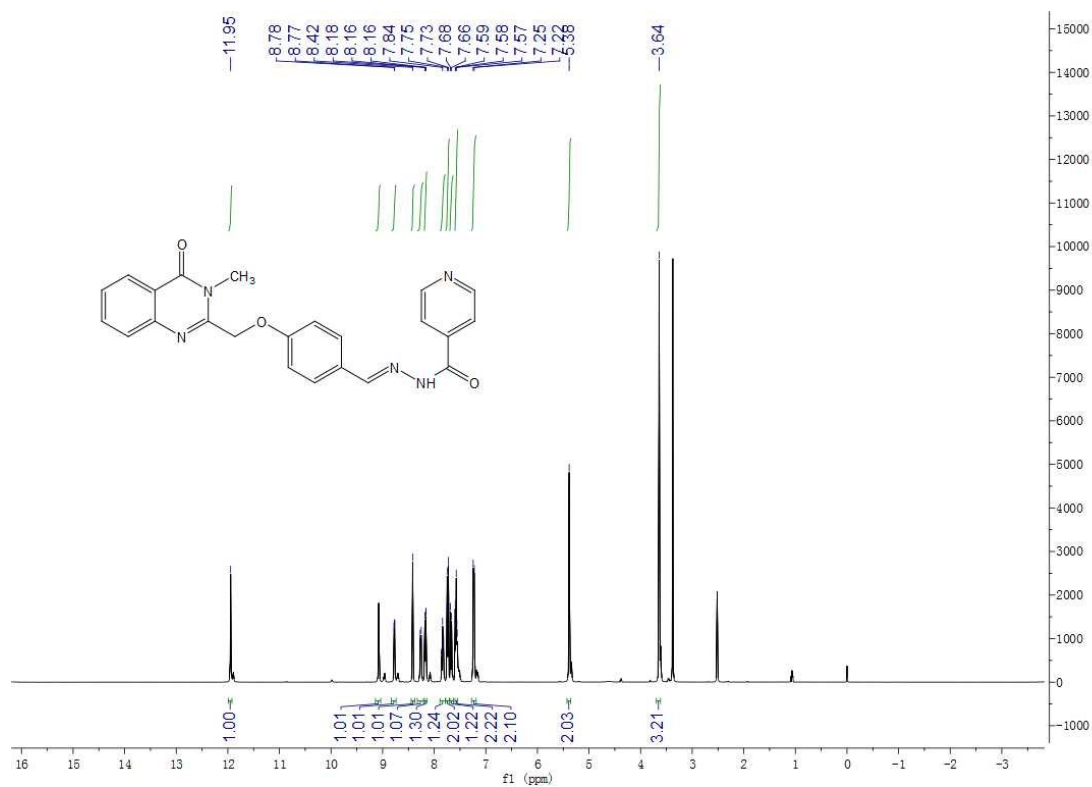
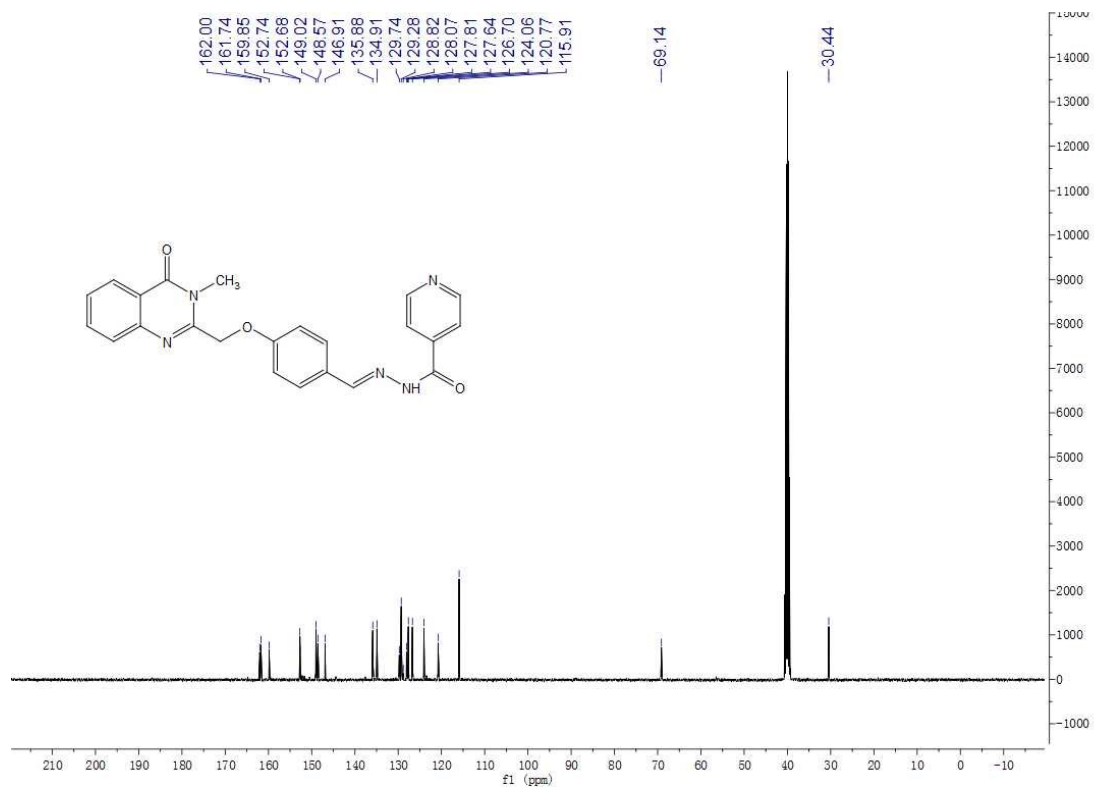
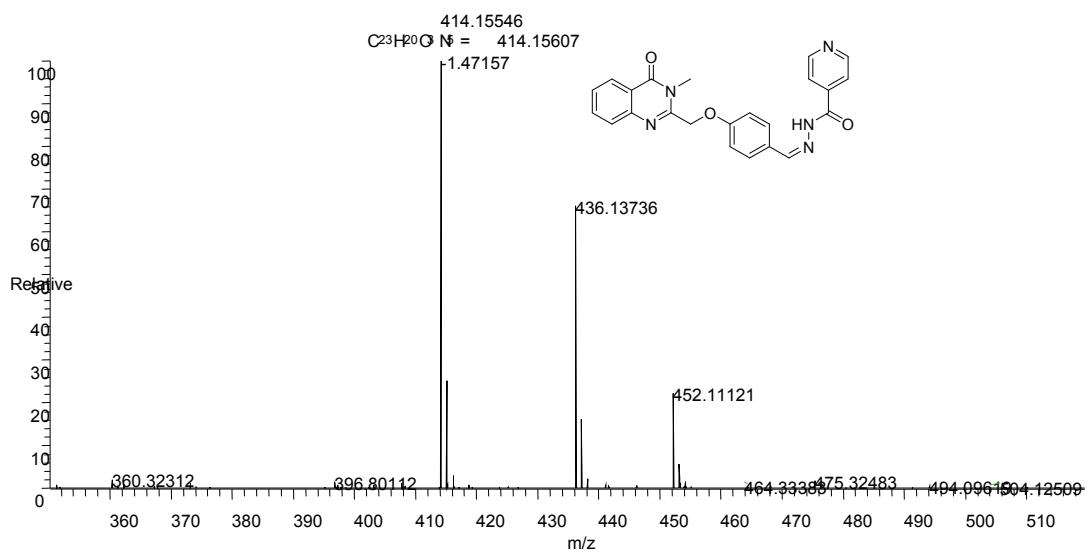


Fig. S61 <sup>1</sup>H NMR spectrum of title compound 8a





**Fig. S62**  $^{13}\text{C}$  NMR spectrum of title compound **8a**



**Fig. S63** HRMS spectrum of title compound **8a**

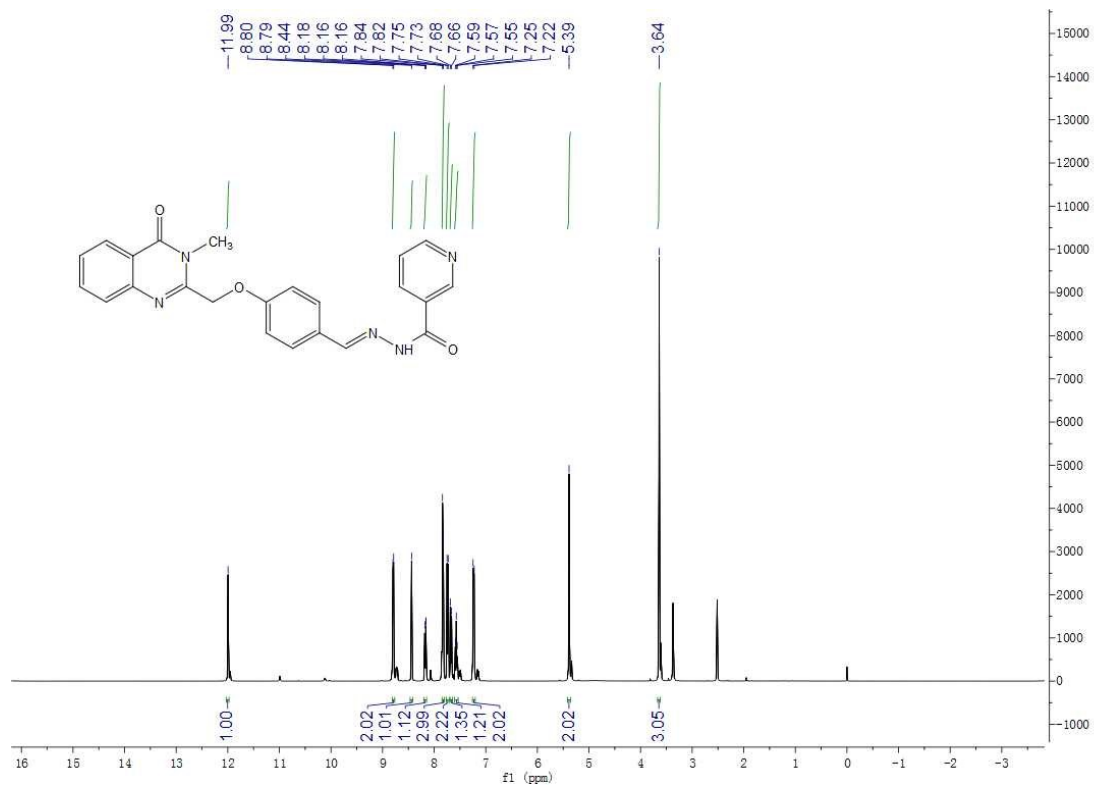


Fig. S64 <sup>1</sup>H NMR spectrum of title compound **8b**

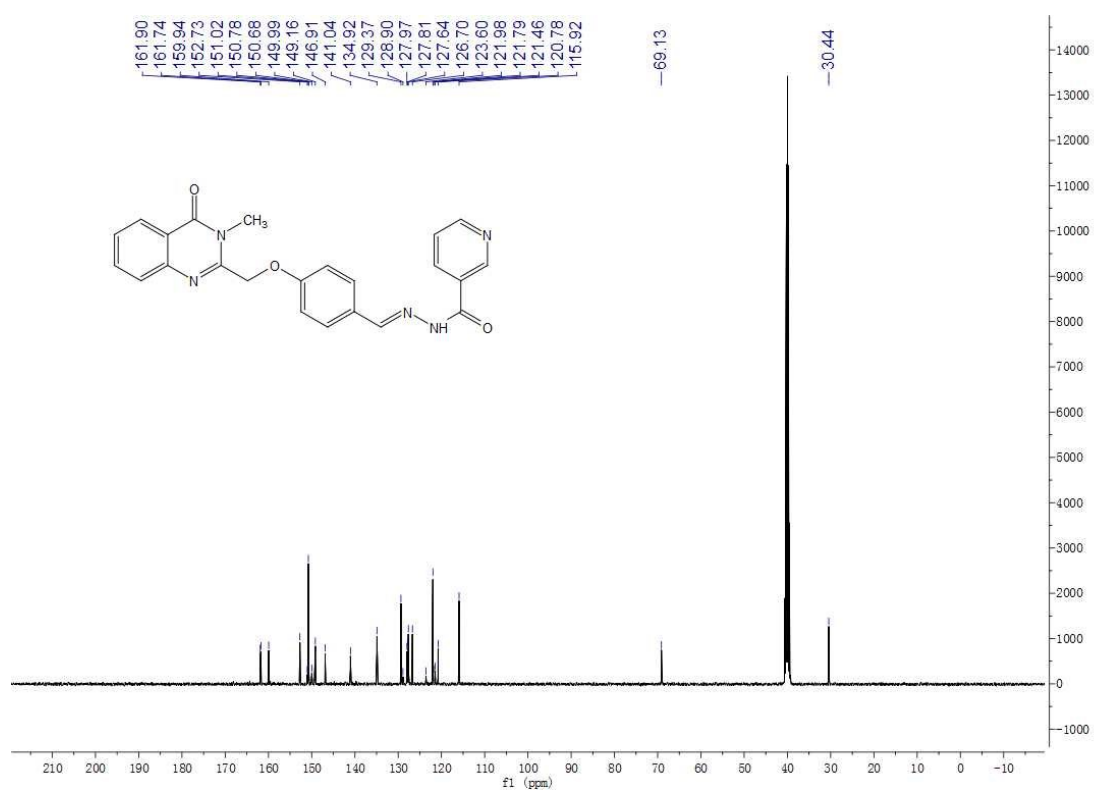
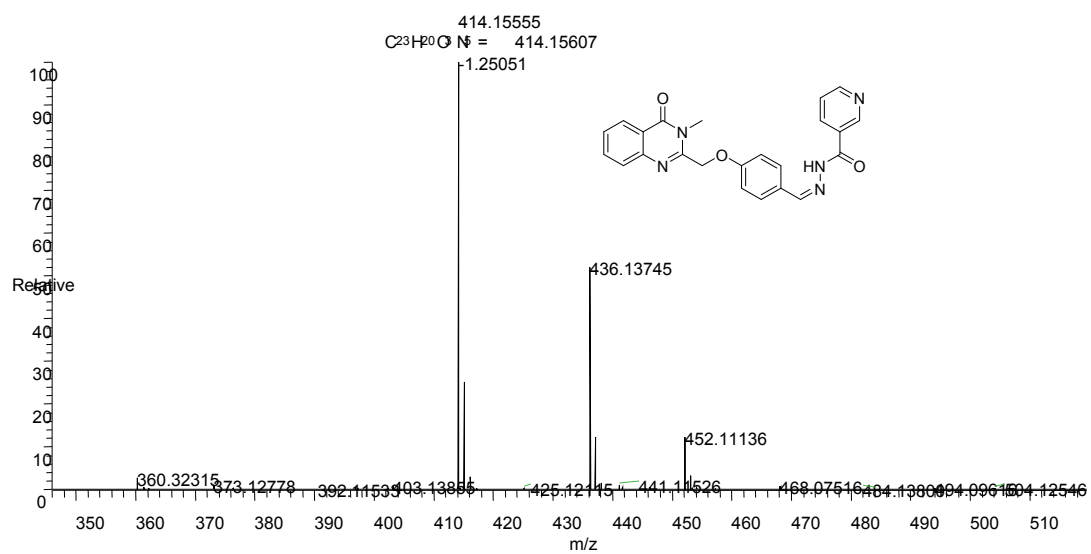
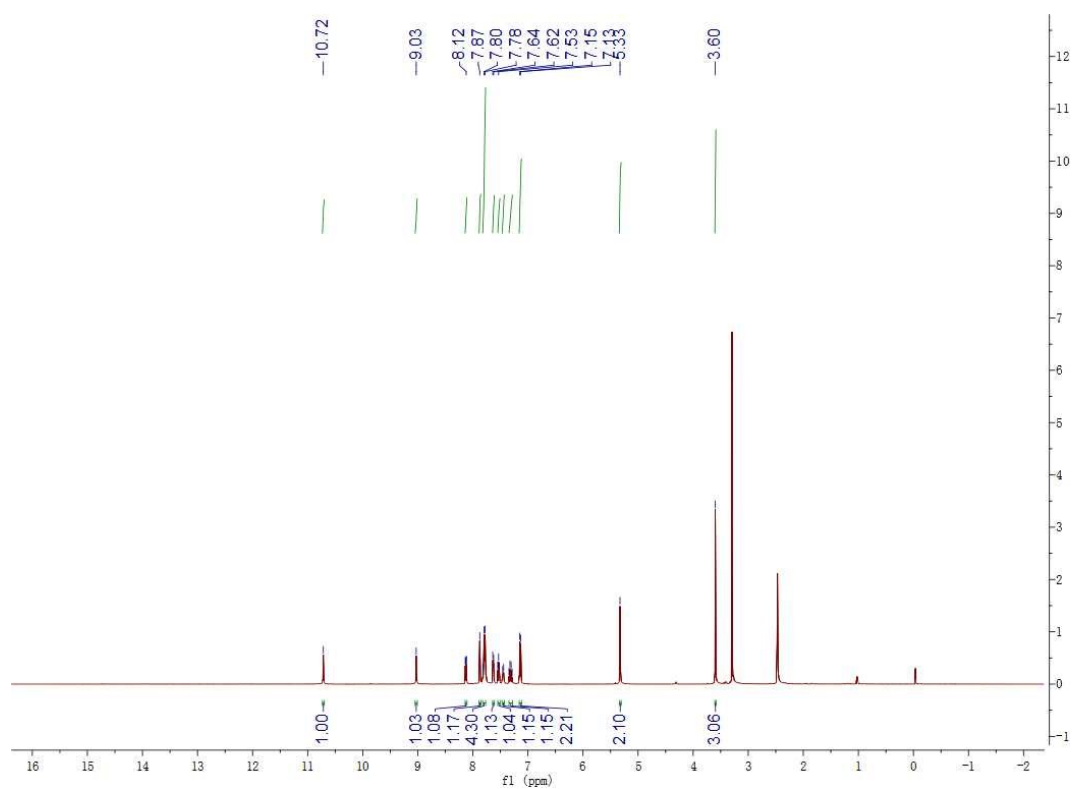


Fig. S65 <sup>13</sup>C NMR spectrum of title compound **8b**



**Fig. S66** HRMS spectrum of title compound **8b**



**Fig. S67**  $^1\text{H}$  NMR spectrum of title compound **9a**

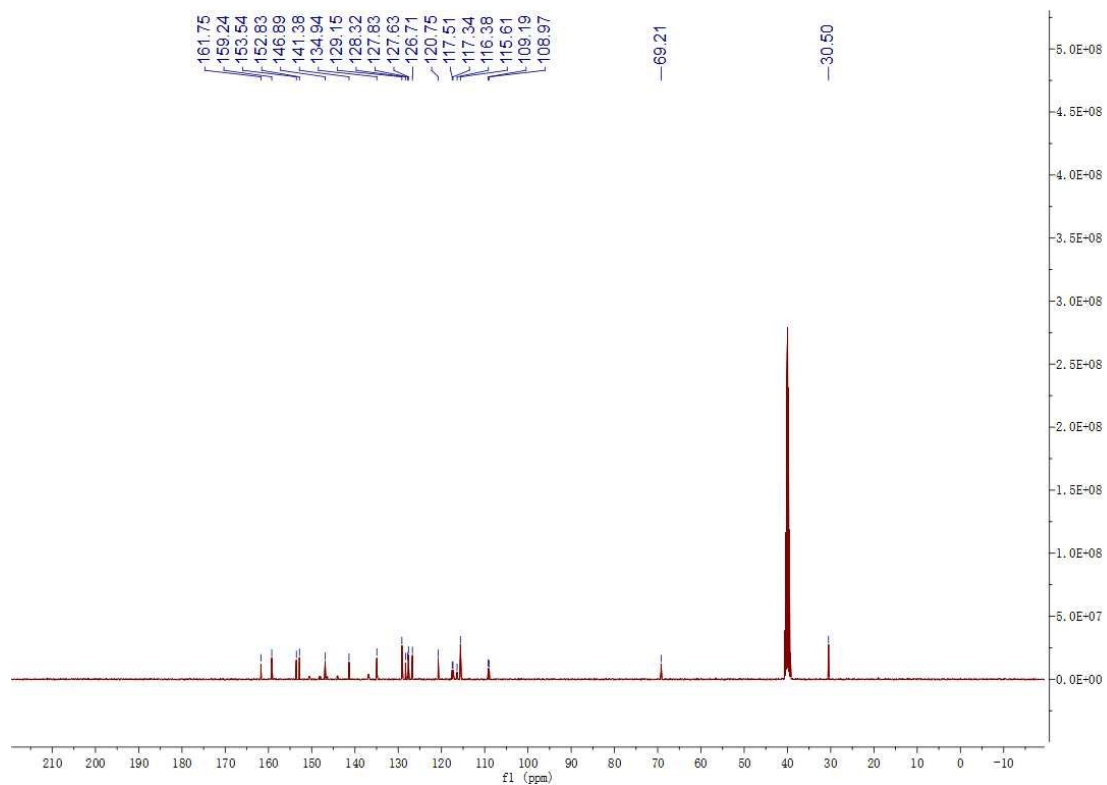


Fig. S68  $^{13}\text{C}$  NMR spectrum of title compound 9a

20191129103 #37 RT: 0.37 AV: 1 NL: 2.88E7  
T: FTMS + p ESI Full ms [100.0000-1000.0000]

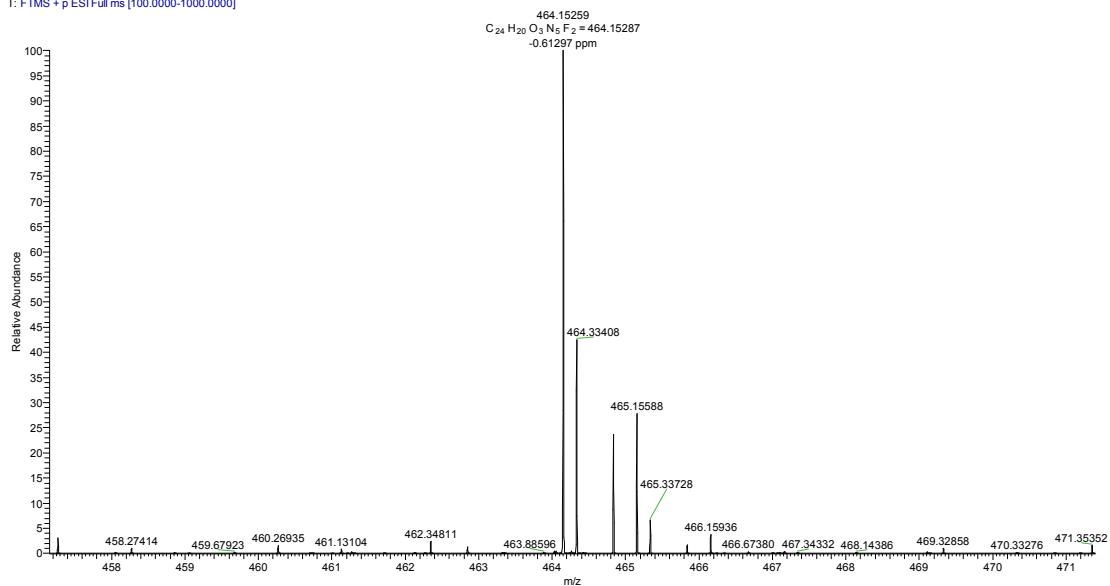
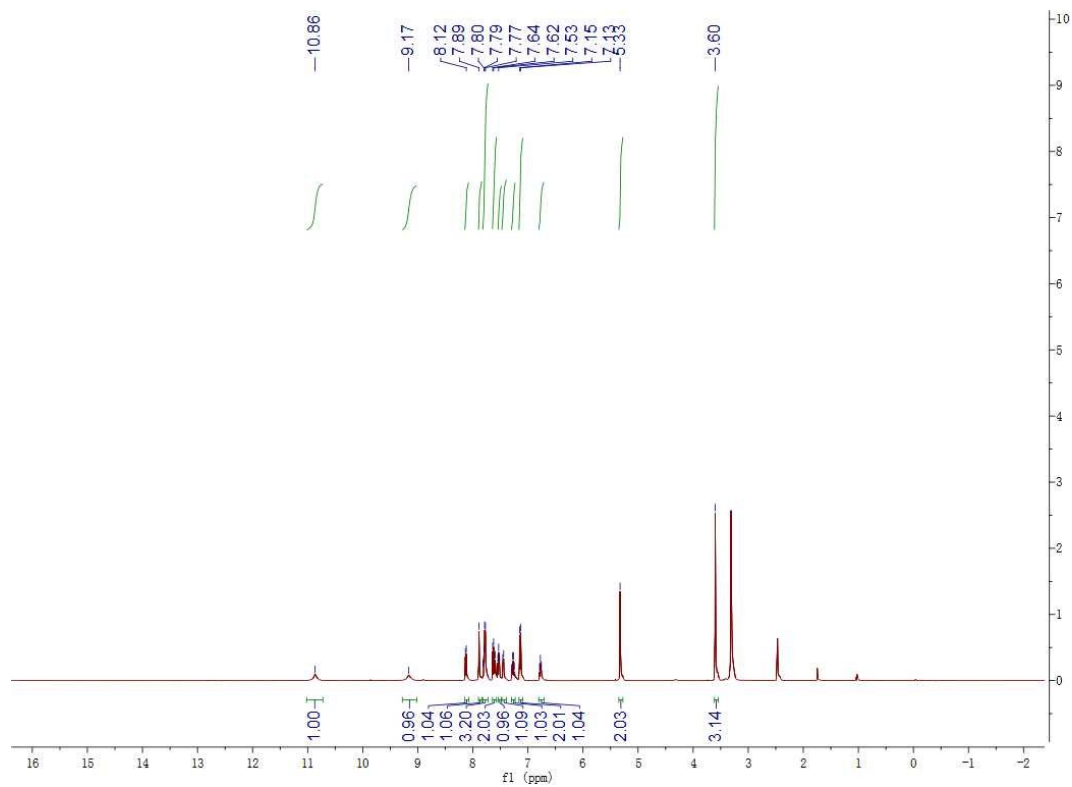
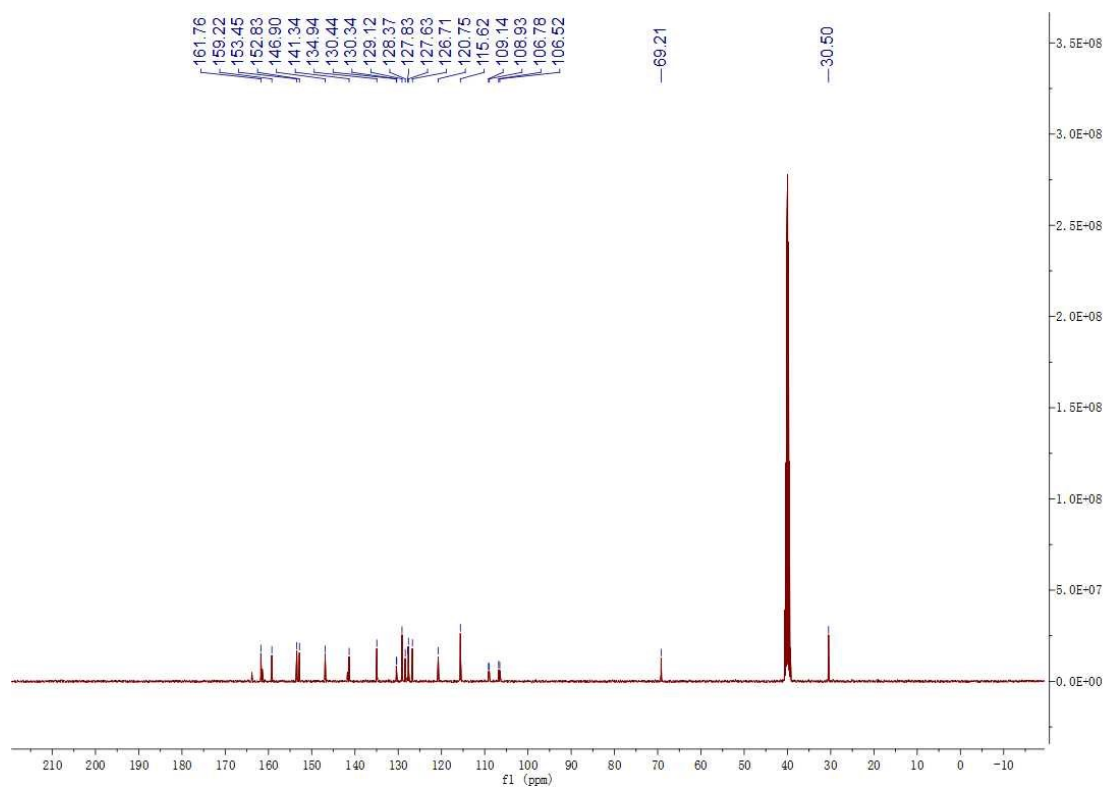


Fig. S69 HRMS spectrum of title compound 9a



**Fig. S70**  $^1\text{H}$  NMR spectrum of title compound **9b**



**Fig. S71**  $^{13}\text{C}$  NMR spectrum of title compound **9b**

20191129104 #37 RT: 0.37 AV: 1 NL: 7.90E7  
T: FTMS + p ESI Full ms [100.0000-1000.0000]

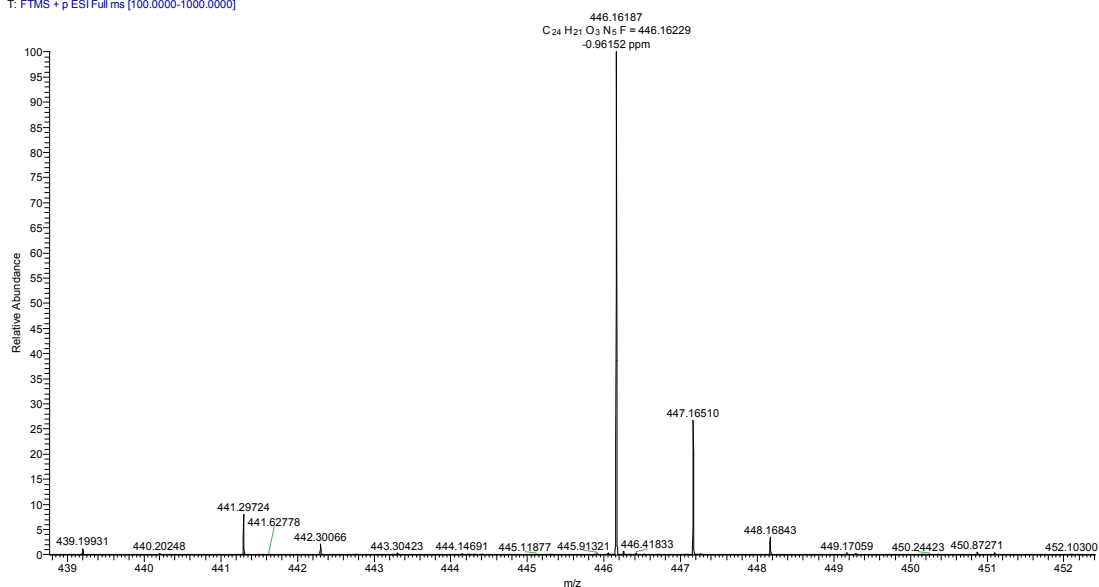


Fig. S72 HRMS spectrum of title compound 9b

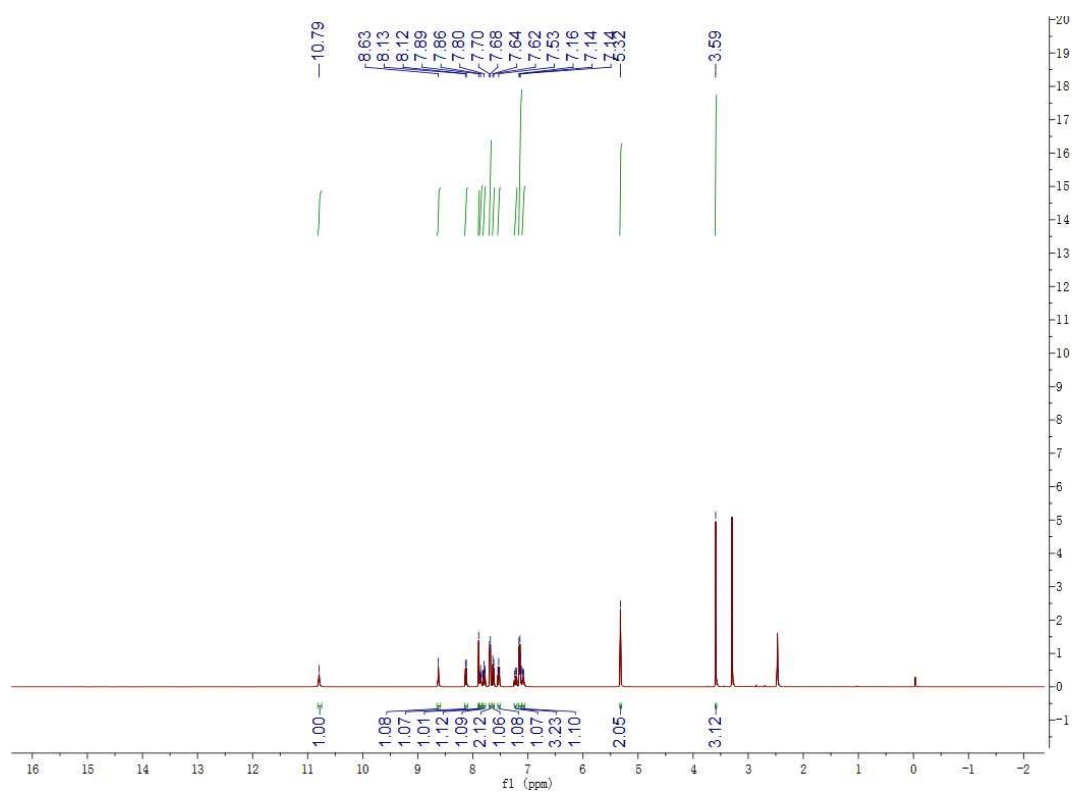


Fig. S73  $^1\text{H}$  NMR spectrum of title compound 9c

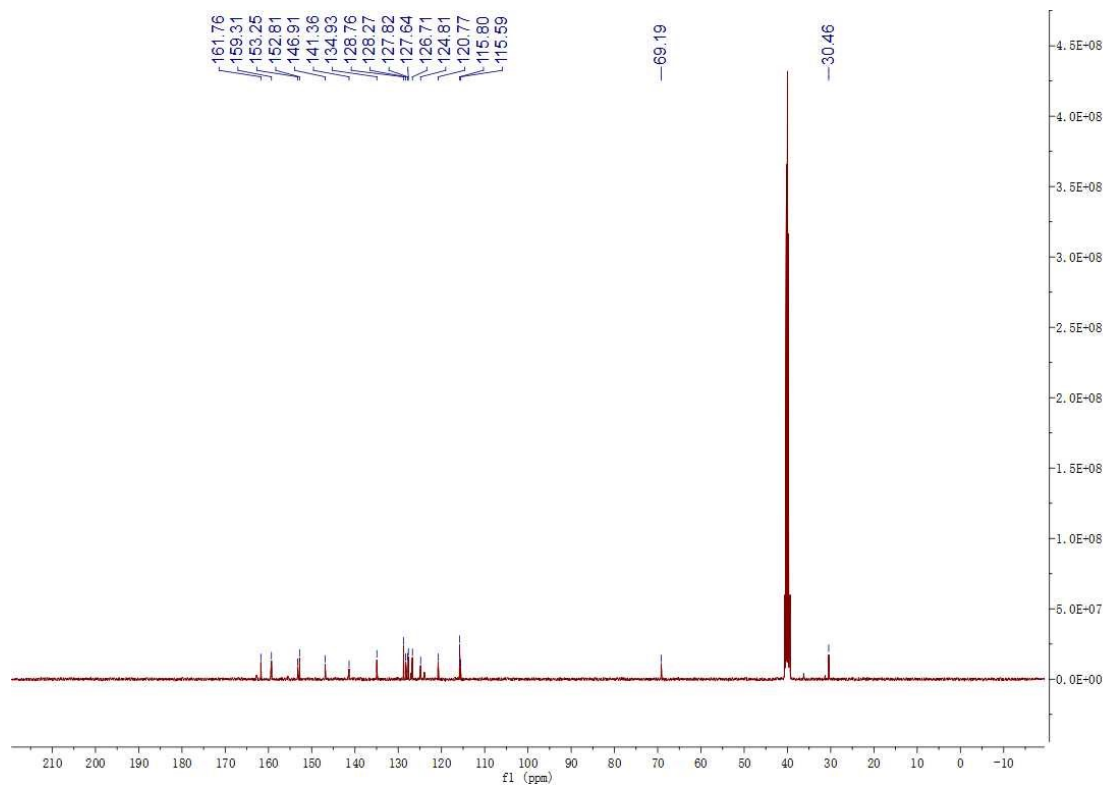


Fig. S74  $^{13}\text{C}$  NMR spectrum of title compound 9c

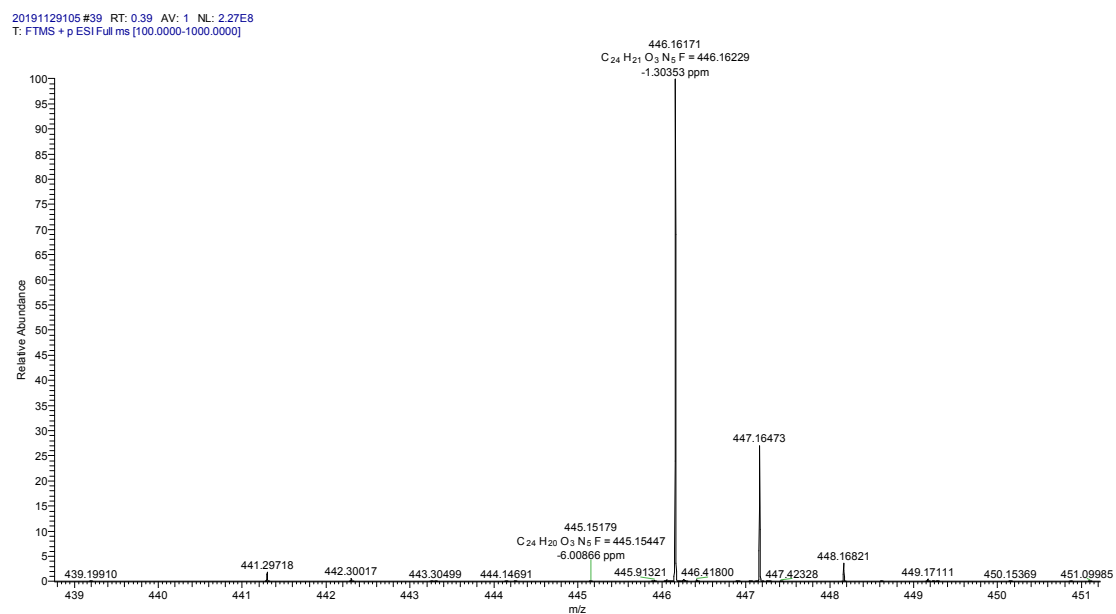


Fig. S75 HRMS spectrum of title compound 9c

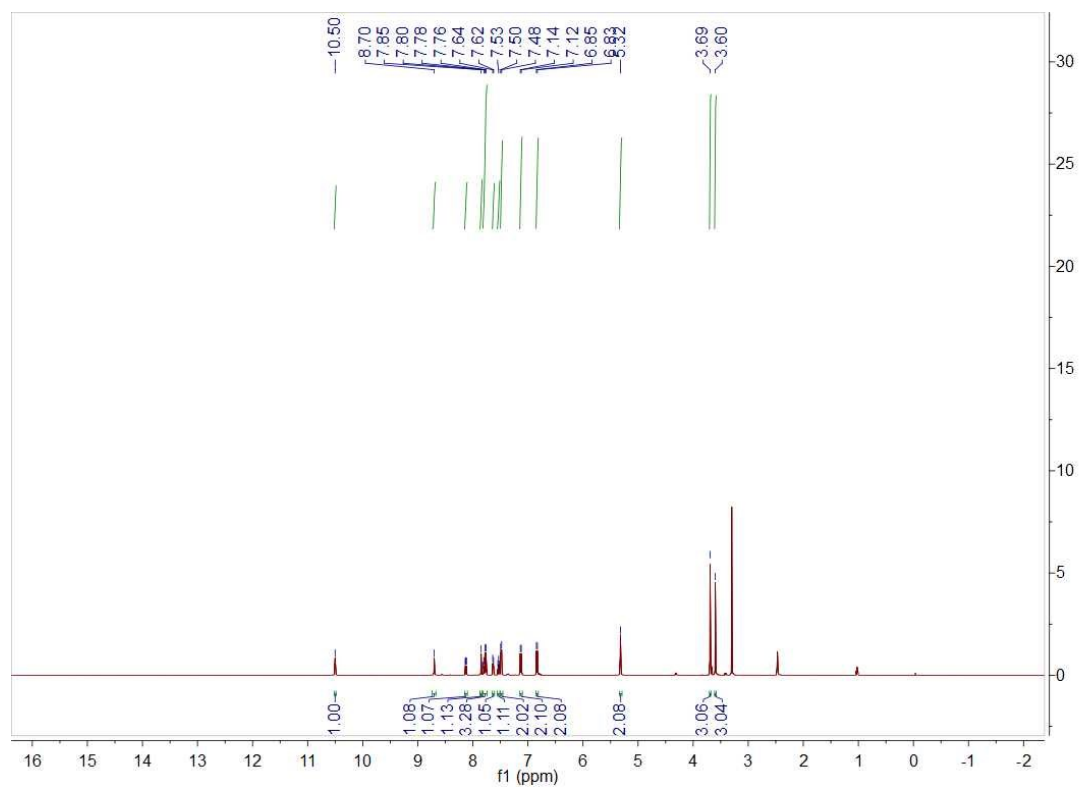


Fig. S76  $^1\text{H}$  NMR spectrum of title compound 9d

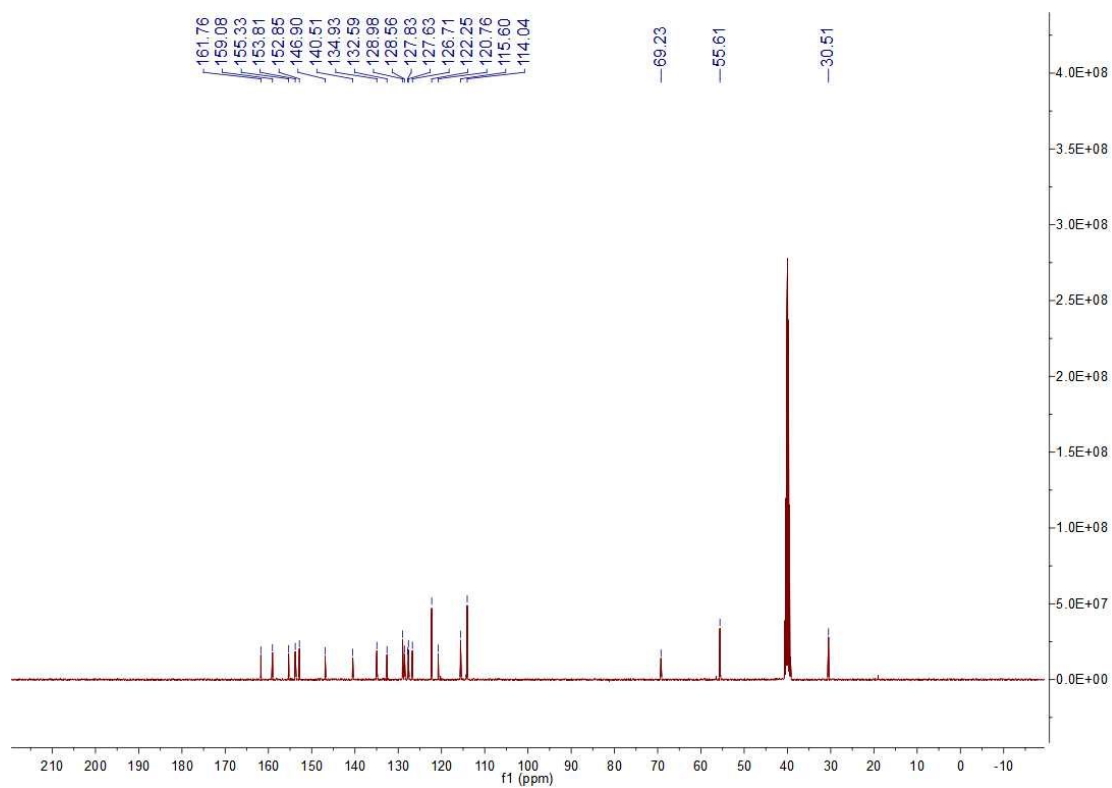


Fig. S77  $^{13}\text{C}$  NMR spectrum of title compound 9d



20191129107 #35 RT: 0.35 AV: 1 NL: 1.07E8  
T: FTMS + p ESI Full ms [100.0000-1000.0000]

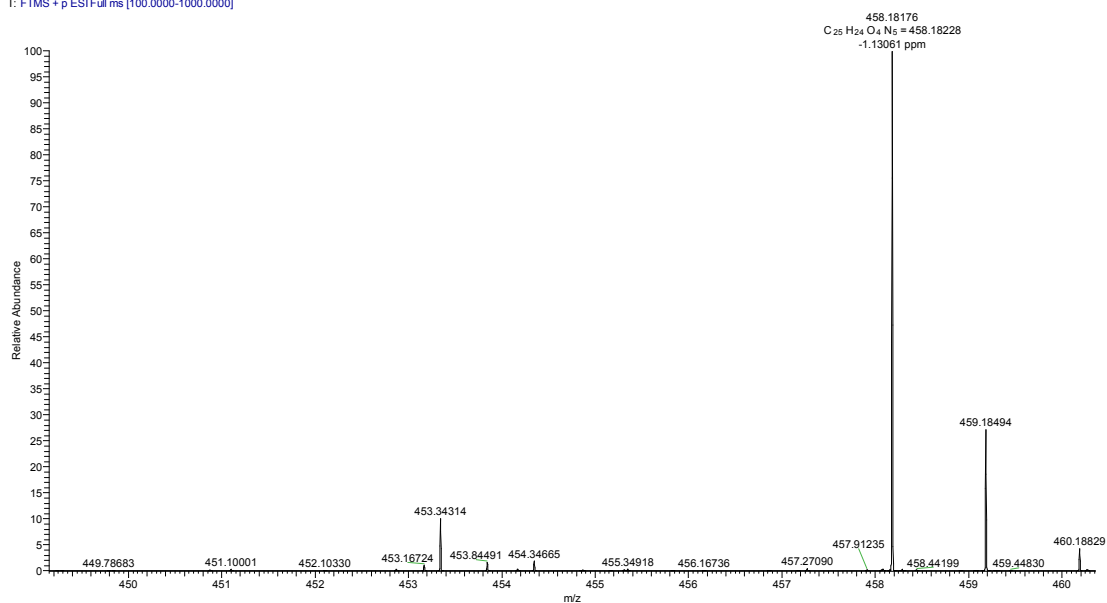


Fig. S78 HRMS spectrum of title compound 9d

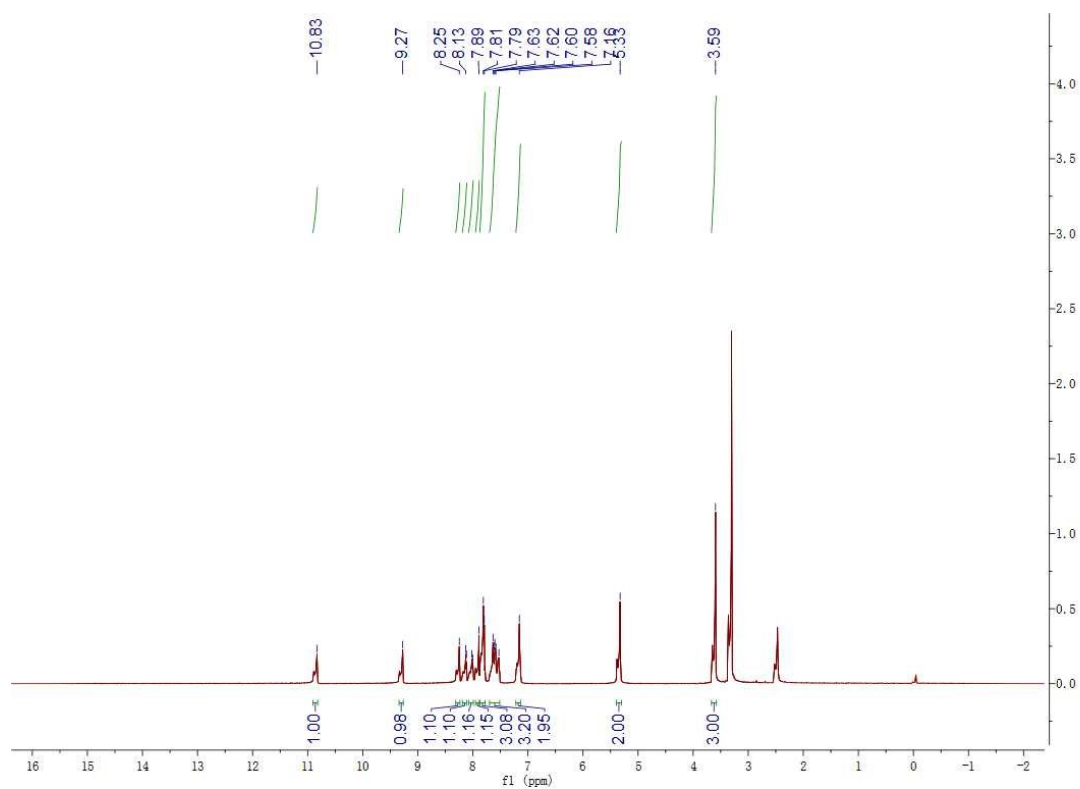
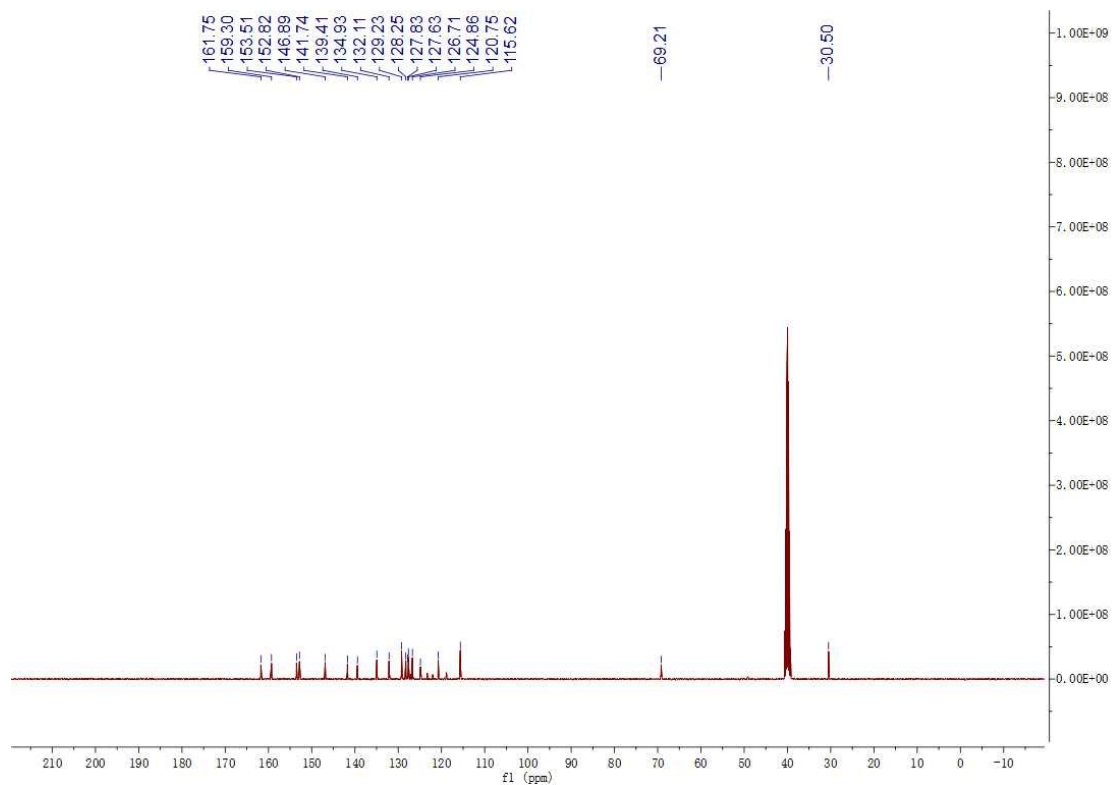
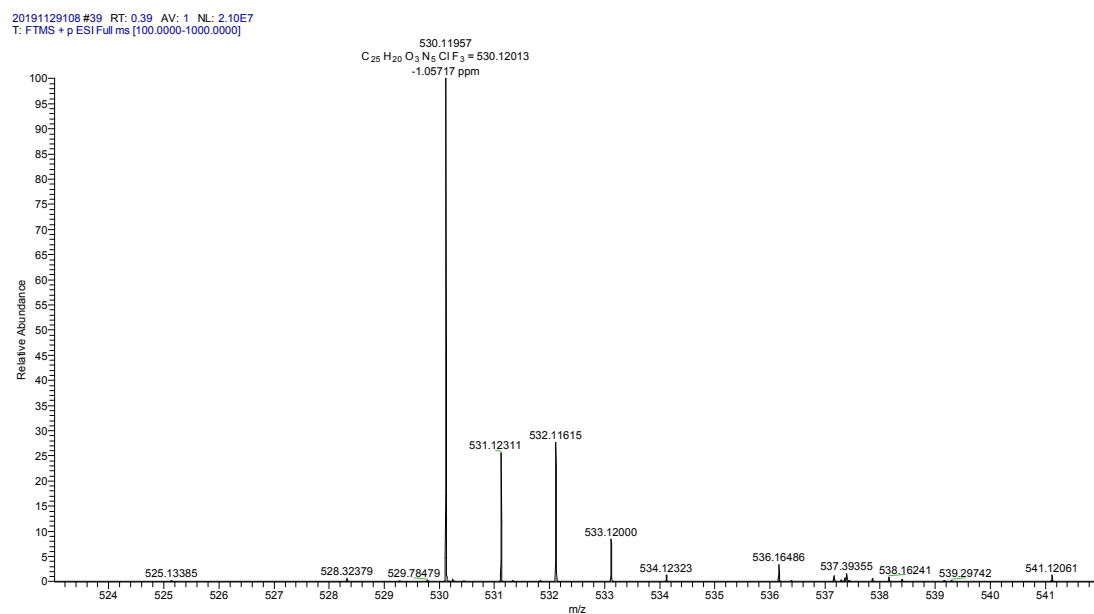


Fig. S79 <sup>1</sup>H NMR spectrum of title compound 9e



**Fig. S80**  $^{13}\text{C}$  NMR spectrum of title compound **9e**



**Fig. S81** HRMS spectrum of title compound **9e**

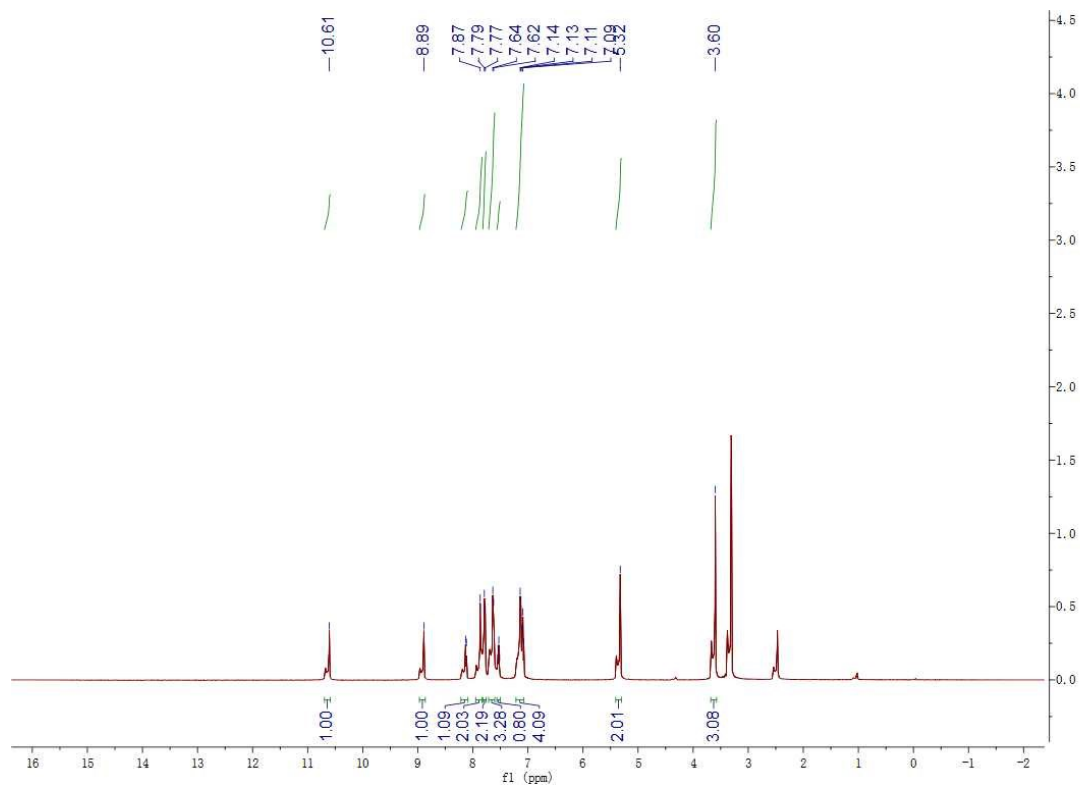


Fig. S82  $^1\text{H}$  NMR spectrum of title compound 9f

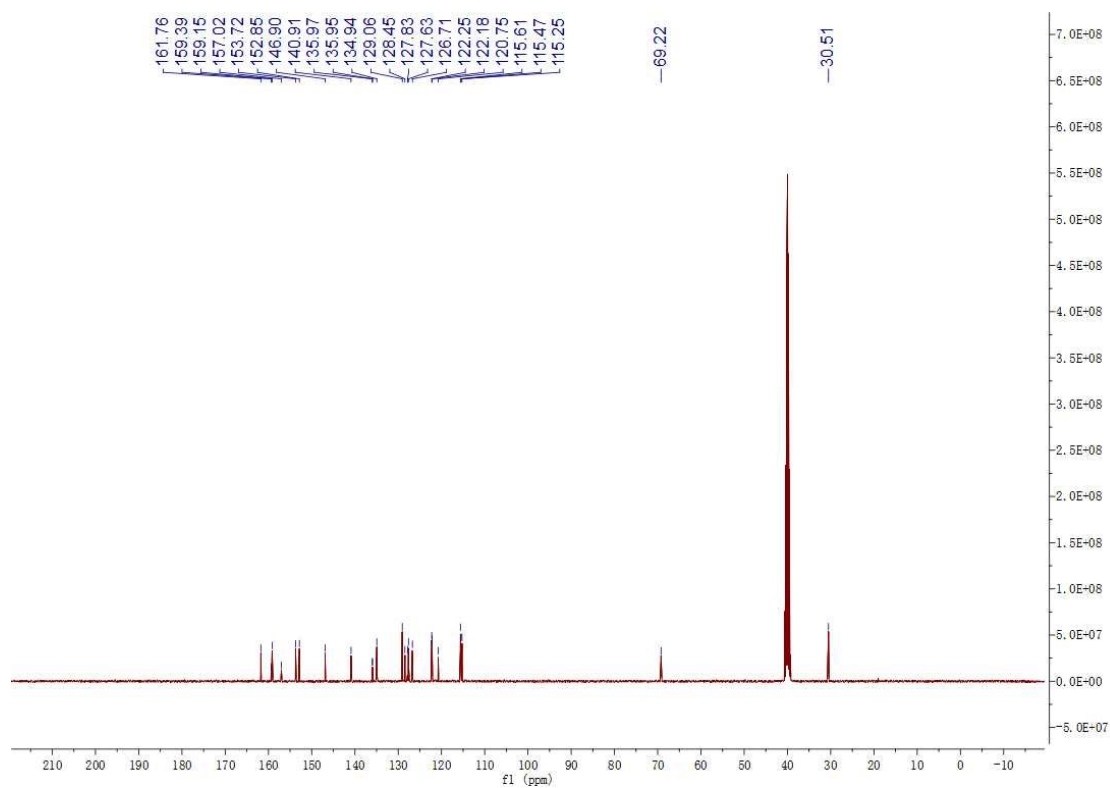


Fig. S83  $^{13}\text{C}$  NMR spectrum of title compound 9f

20191129109 #33 RT: 0.33 AV: 1 NL: 6.30E7  
T: FTMS + p ESI Full ms [100.0000-1000.0000]

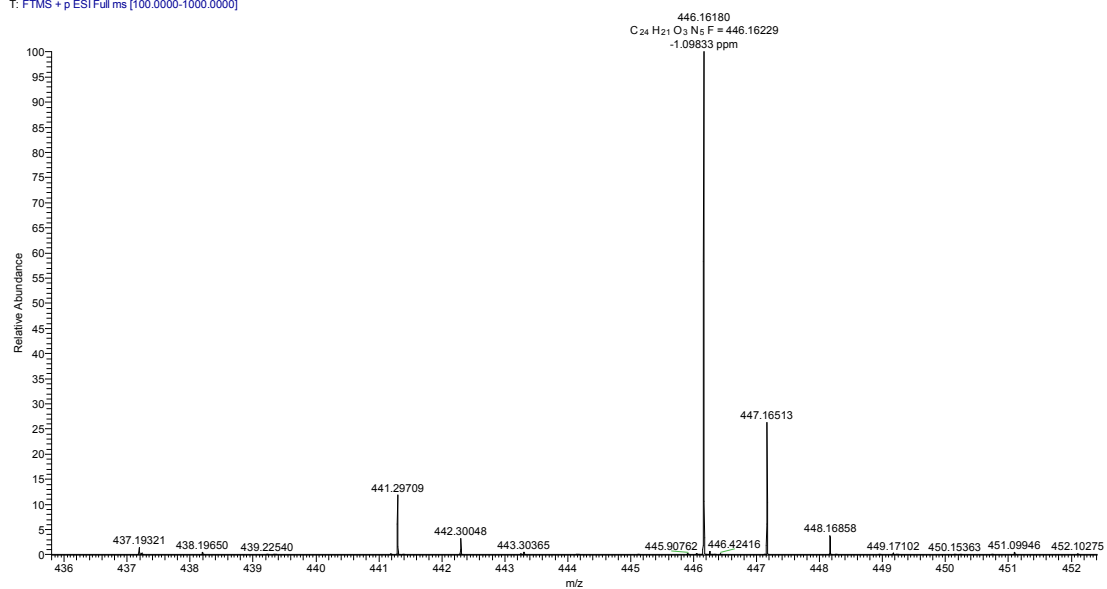


Fig. S84 HRMS spectrum of title compound 9f