

## Supporting Information

### Ruthenium (II)-Catalyzed C-H Alkenylation/Annulation Cascade for the Rapid Synthesis of Benzoimidazoisindoles

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## General Remarks

Solvents were distilled before use. All the reactions were performed under open air atmosphere with unpurified reagents and dry solvents. Analytical thin-layer chromatography (TLC) was performed using 0.25 mm silica gelcoated Kieselgel 60 F254 plates. Flash chromatography was performed using the indicated solvent and silica gel 60 (Merck, 230-400 mesh). <sup>1</sup>H NMR (300 & 400 MHz) and <sup>13</sup>C NMR (75 & 100 MHz) spectra were recorded on a Bruker DX-300 spectrometer. Chemical shifts are reported in parts per million (ppm) on the δ scale from an internal standard. High-resolution mass spectra (HRMS) were recorded on a JEOL TMS-HX 110 mass spectrometer.

## Spectral data of compounds 3:

### Methyl 2-(3-methyl-11*H*-benzo[4,5]imidazo[2,1-*a*]isoindol-11-yl) acetate (3b)

Yellow solid, yield = 78 %; mp = 122-124 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.87 – 7.80 (m, 2H), 7.46-7.39 (m, 2H), 7.30-7.25 (m, 5H), 5.69 (t, *J* = 6.5 Hz, 1H), 3.80 (s, 3H), 3.14 (dd, *J* = 16.4, 4.0 Hz, 1H), 2.85 (dd, *J* = 16.4, 4.0 Hz, 1H), 2.48 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 171.1, 148.8, 144.7, 139.6, 132.2, 130.9, 128.9, 123.4, 122.9, 122.7, 122.4, 120.8, 109.9, 55.9, 52.5, 39.0, 21.6; LRMS (ESI<sup>+</sup>) *m/z* : 293.2 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>18</sub>H<sub>17</sub>N<sub>2</sub>O<sub>2</sub> (M+H)<sup>+</sup> *m/z*: 293.1285; Found 293.1288; IR (cm<sup>-1</sup>, neat): 3143, 2787, 1975, 1658, 1570, 1517, 1473, 1394.

### Methyl 2-(2-methyl-11*H*-benzo[4,5]imidazo[2,1-*a*]isoindol-11-yl) acetate (3c)

White solid, yield = 93 %; mp = 103-105 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.89 (d, *J* = 7.6 Hz, 1H), 7.81-7.76 (m, 1H), 7.40-7.35 (m, 1H), 7.33-7.28 (m, 2H), 7.26-7.20 (m, 3H), 5.66 (t, *J* = 7.6 Hz, 1H), 3.78 (d, *J* = 1.2 Hz, 3H), 3.10 (dd, *J* = 16.6, 8.0 Hz, 1H), 2.85 (dd, *J* = 16.6, 8.0 Hz, 1H), 2.43 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 170.9, 157.6, 148.7, 147.6, 140.5, 132.0, 130.1, 126.0, 124.1, 122.6, 122.1, 121.8, 120.5, 109.6, 55.8, 52.4, 38.8, 21.9; LRMS (ESI<sup>+</sup>) *m/z*: 293.2 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>18</sub>H<sub>17</sub>N<sub>2</sub>O<sub>2</sub> (M+H)<sup>+</sup> *m/z*: 293.1285; Found 293.1295; IR (cm<sup>-1</sup>, neat) : 3136, 2785, 1967, 1826, 1583, 1508, 1400.

### Methyl 2-(2-chloro-11*H*-benzo[4,5]imidazo[2,1-*a*]isoindol-11-yl) acetate (3d)

Brown solid, yield = 71 %; mp = 133-135 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.96 (d, *J* = 8.1 Hz, 1H), 7.85-7.81 (m, 1H), 7.59-7.57 (m, 1H), 7.51 (dd, *J* = 8.1, 1.9 Hz, 1H), 7.44-7.41 (m, 1H),

7.30- 7.27 (m, 2H), 5.72 (t,  $J = 6.4$  Hz, 1H), 3.82 (s, 3H), 3.22 (dd,  $J = 16.4$ , 8 Hz, 1H), 2.88 (dd,  $J = 16.4$ , 8.0 Hz, 1H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  170.6, 156.3, 148.8, 148.6, 135.9, 129.8, 127.3, 124.3, 123.2, 123.0, 122.6, 120.8, 109.7, 55.7, 52.5, 38.4, 29.7; LRMS ( $\text{ESI}^+$ )  $m/z$ : 313.2 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS: calcd for  $\text{C}_{17}\text{H}_{14}\text{ClN}_2\text{O}_2$  ( $\text{M}+\text{H}$ ) $^+$   $m/z$ : 313.0738; Found 313.0741; IR ( $\text{cm}^{-1}$ , neat) : 3143, 2761, 1990, 1652, 1566, 1506.

**Methyl 2-(2-(trifluoromethyl)-11H-benzo[4,5]imidazo[2,1-a]isoindol- 11-yl)acetate (3e)**

White solid, yield = 81 %; mp = 191-194 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.15 (d,  $J = 7.9$  Hz, 1H), 7.91-7.77 (m, 3H), 7.47 (dt,  $J = 6.2$ , 2.8 Hz, 1H), 7.32 (dt,  $J = 5.9$ , 2.8 Hz, 2H), 5.80 (t,  $J = 6.2$  Hz, 1H), 3.82 (s, 3H), 3.24 (dd,  $J = 16.9$ , 5.8 Hz, 1H), 2.92 (dd,  $J = 16.9$ , 7.2 Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.5, 155.8, 148.7, 147.6, 132.2, 131.9, 131.7 (q,  $J_{\text{C-F}} = 32.8$  Hz), 126.8 (q,  $J_{\text{C-F}} = 3.7$  Hz), 123.8 (q,  $J_{\text{C-F}} = 272.7$  Hz), 123.6, 122.9, 122.3, 121.2, 120.9, 110.0, 56.0, 52.6, 38.4; LRMS ( $\text{ESI}^+$ )  $m/z$ : 347.2 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS: calcd for  $\text{C}_{18}\text{H}_{14}\text{F}_3\text{N}_2\text{O}_2$  ( $\text{M}+\text{H}$ ) $^+$   $m/z$ : 347.1002; Found 347.1012; IR ( $\text{cm}^{-1}$ , neat) : 3126, 3030, 2738, 1990, 1967, 1826, 1598, 1494, 1407.

**Methyl 2-(2-methoxy-11H-benzo[4,5]imidazo[2,1-a]isoindol-11-yl) acetate (3f)**

Yellow solid, Yield = 66 %; mp = 139-141 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.94 (d,  $J = 8.4$  Hz, 1H), 7.81-7.76 (m, 1H), 7.41-7.36 (m, 1H), 7.27-7.21 (m, 3H), 7.08 (m, 1H), 7.04 (dd,  $J = 8.4$ , 2.3 Hz, 1H), 5.67 (t,  $J = 6.4$ , 1H), 3.88 (s, 3H), 3.80 (s, 3H), 3.16 (dd,  $J = 16.7$ , 6.3 Hz, 1H), 2.86 (dd,  $J = 16.7$ , 6.4 Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.9, 161.5, 149.4, 129.5, 125.7, 123.2, 122.5, 122.1, 121.2, 120.4, 114.8, 109.8, 109.4, 77.2, 55.8, 55.7, 52.4, 38.8; LRMS ( $\text{ESI}^+$ )  $m/z$ : 309.3 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS: calcd for  $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}_3$  ( $\text{M}+\text{H}$ ) $^+$   $m/z$ : 309.1234; Found 309.1233; IR ( $\text{cm}^{-1}$ , neat) : 3143, 2866, 2717, 1994, 1820, 1654, 1568, 1516.

**Ethyl-2-(2-(trifluoromethyl)-11H-benzo[4,5]imidazo[2,1-a]isoindol-11-yl) acetate (3g)**

Yellow liquid, Yield = 75 %;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.51 (d,  $J = 8.0$  Hz, 1H), 7.94-7.87 (m, 2H), 7.83 (d,  $J = 8.0$  Hz, 1H), 7.63-7.58 (m, 1H), 7.47-7.39 (m, 2H), 6.00 (t,  $J = 6.2$  Hz, 1H), 4.29-4.17 (m, 2H), 3.29 (dd,  $J = 17.0$ , 5.3 Hz, 1H), 3.05 (dd,  $J = 17.0$ , 6.8 Hz, 1H), 1.24-1.20 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  168.5, 151.9, 147.8, 135.5, 135.0 (q,  $J = 32.8$  Hz), 128.7, 127.8 (q,  $J = 3.5$  Hz), 127.3, 127.1, 125.8 (q,  $J = 272.2$  Hz), 127.0, 126.1, 120.9 (q,  $J = 3.8$  Hz), 117.1, 112.0, 62.3, 59.6, 37.1, 14.0; LRMS ( $\text{ESI}^+$ )  $m/z$ : 361.1 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS: calcd for

$C_{19}H_{16}F_3N_2O_2$  (M+H)<sup>+</sup> *m/z*: 361.1158; Found 361.1159; IR (cm<sup>-1</sup>, neat) : 3134, 2754, 1992, 1828, 1793, 1647, 1585, 1506.

**Ethyl-2-(2-chloro-11*H*-benzo[4,5]imidazo[2,1-*a*]isoindol-11-yl)acetate (3h)**

Yellow solid, yield = 65 %; mp = 130-132 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.94 (d, *J* = 8.1 Hz, 1H), 7.79-7.77 (m, 1H), 7.58-7.57 (m, 1H), 7.47 (dd, *J* = 8.2, 1.8 Hz, 1H), 7.46-7.42 (m, 1H), 7.28 (dd, *J* = 6.1, 3.2 Hz, 2H), 5.71 (t, *J* = 6.3 Hz, 1H), 4.27-4.22 (q, *J* = 7.1 Hz, 2H), 3.18 (dd, *J* = 16.8, 5.5 Hz, 1H), 2.88 (dd, *J* = 16.8, 7.2 Hz, 1H), 1.24 (t, *J* = 7.1 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 168.6, 152.5, 148.9, 131.1, 128.6, 127.6, 126.6, 126.5, 124.4, 124.2, 121.3, 117.0, 111.7, 62.2, 59.1, 37.2, 14.0; LRMS (ESI<sup>+</sup>) *m/z*: 327.2 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>18</sub>H<sub>16</sub>ClN<sub>2</sub>O<sub>2</sub> *m/z*: 327.0895; Found 327.0887; IR (cm<sup>-1</sup>, neat): 3134, 3028, 2823, 2748, 1994, 1820, 1502, 1406.

**Ethyl-2-(2-methyl-11*H*-benzo[4,5]imidazo[2,1-*a*]isoindol-11-yl)acetate (3i)**

Yellow solid, Yield = 85 %; mp = 115-118 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.34 (d, *J* = 7.8 Hz, 1H), 7.93-7.87 (m, 1H), 7.58-7.53 (m, 1H), 7.43-7.36 (m, 4H), 5.87 (t, *J* = 6.1 Hz, 1H), 4.22 (q, *J* = 7.1 Hz, 2H), 3.17 (dd, *J* = 16.9, 5.9 Hz, 1H), 3.04 (dd, *J* = 16.9, 6.4 Hz, 1H), 2.50 (s, 3H), 1.21 (t, *J* = 7.1 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 170.0, 156.4, 147.7, 141.8, 131.0, 130.5, 124.2, 124.1, 123.7, 123.4, 123.1, 119.4, 110.3, 61.6, 56.8, 38.5, 22.0, 14.0; LRMS (ESI<sup>+</sup>) *m/z*: 307.3 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>19</sub>H<sub>19</sub>N<sub>2</sub>O<sub>2</sub> (M+H)<sup>+</sup> *m/z*: 307.1441; Found 307.1442; IR (cm<sup>-1</sup>, neat): 3134, 2947, 2862, 2754, 1992, 1890, 1828, 1664, 1519.

**Cyclohexyl 2-(11*H*-benzo[4,5]imidazo[2,1-*a*]isoindol-11-yl)acetate (3j)**

Yellow solid, yield = 62 %; mp = 199-202 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.05-8.00 (m, 1H), 7.84-7.79 (m, 1H), 7.56-7.52 (m, 1H), 7.52-7.43 (m, 3H), 7.27-7.23 (m, 3H), 5.70 (t, *J* = 6.2 Hz, 1H), 4.84 (m, 1H), 3.14 (dd, *J* = 16.5, 5.7 Hz, 1H), 2.90 (dd, *J* = 16.5, 6.8 Hz, 1H), 1.82-1.75 (m, 2H), 1.69-1.61 (m, 2H), 1.50 (d, *J* = 12.6 Hz, 1H), 1.38-1.24 (m, 5H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 169.6, 157.5, 148.5, 147.3, 132.0, 129.8, 129.2, 128.8, 123.5, 122.8, 122.3, 122.1, 120.6, 109.9, 74.1, 56.1, 39.1, 31.4, 31.4, 25.2, 23.6, 23.6; LRMS (ESI<sup>+</sup>) *m/z* : 347.2 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>22</sub>H<sub>23</sub>N<sub>2</sub>O<sub>2</sub> *m/z*: 347.1754; Found 347.1759; IR (cm<sup>-1</sup>, neat): 3236, 2754, 2754, 1867, 1832, 1570, 1508.

**Butyl 2-(11*H*-benzo[4,5]imidazo[2,1-*a*]isoindol-11-yl)acetate (3k)**

Yellow liquid, Yield = 67 %; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.04 (d, *J* = 7.4 Hz, 1H), 7.87-7.80 (m, 1H), 7.57-7.41 (m, 4H), 7.30-7.23 (m, 3H), 5.71 (t, *J* = 6.4 Hz, 1H), 4.17 (t, *J* = 6.7 Hz, 2H), 3.12 (dd, *J* = 16.6, 5.9 Hz, 1H), 2.90 (dd, *J* = 16.6, 6.8 Hz, 1H), 1.56 (p, *J* = 6.9 Hz, 2H), 1.28 (m, 2H), 0.89 (t, *J* = 7.4 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 170.4, 157.4, 148.6, 147.3, 132.0, 129.9, 129.2, 128.7, 123.5, 122.9, 122.3, 122.1, 120.6, 109.8, 65.4, 56.0, 38.8, 30.4, 19.0, 13.6; LRMS (ESI<sup>+</sup>) *m/z*: 321.3 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>20</sub>H<sub>21</sub>N<sub>2</sub>O<sub>2</sub> (M+H)<sup>+</sup> *m/z*: 321.1598; Found 321.1602; IR (cm<sup>-1</sup>, neat): 3147, 3006, 1830, 1652, 1570, 1504.

**Ethyl 2-(11*H*-benzo[4,5]imidazo[2,1-*a*]isoindol-11-yl)acetate (3l)**

Yellow liquid, yield = 65 %; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.05 (d, *J* = 7.3 Hz, 1H), 7.85-7.80 (m, 1H), 7.58-7.41 (m, 4H), 7.30-7.23 (m, 3H), 5.71 (t, *J* = 6.4 Hz, 1H), 4.23 (m, 2H), 3.14 (dd, *J* = 16.6, 5.9 Hz, 1H), 2.89 (dd, *J* = 16.6, 6.8 Hz, 1H), 1.23 (t, *J* = 7.1 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 170.3, 157.5, 148.6, 147.3, 132.0, 129.9, 129.2, 128.8, 123.5, 122.8, 122.3, 122.1, 120.7, 109.8, 61.4, 56.0, 38.9, 14.1; LRMS (ESI<sup>+</sup>) *m/z*: 293.2 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>18</sub>H<sub>17</sub>N<sub>2</sub>O<sub>2</sub> (M+H)<sup>+</sup> *m/z*: 293.1285; Found 293.1284; IR (cm<sup>-1</sup>, neat): 3145, 2781, 1994, 1830, 1652, 1570, 1517.

**Tert-butyl 2-(11*H*-benzo[4,5]imidazo[2,1-*a*]isoindol-11-yl)acetate (3m)**

Yellow solid, yield = 50 %; mp = 199-202 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.04 (d, *J* = 7.3 Hz, 1H), 7.86-7.80 (m, 1H), 7.59-7.45 (m, 4H), 7.30-7.25 (m, 3H), 5.67 (t, *J* = 6.0 Hz, 1H), 3.10 (dd, *J* = 16.4, 5.5 Hz, 1H), 2.91 (dd, *J* = 16.4, 6.6 Hz, 1H), 1.37 (s, 9H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 169.3, 157.5, 148.6, 147.4, 132.1, 129.8, 129.1, 128.9, 123.5, 122.7, 122.2, 122.0, 120.6, 110.0, 82.0, 56.0, 39.7, 27.8; LRMS (ESI<sup>+</sup>) *m/z*: 321.3 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>20</sub>H<sub>21</sub>N<sub>2</sub>O<sub>2</sub> (M+H)<sup>+</sup> *m/z*: 321.1598; Found 321.1611; IR (cm<sup>-1</sup>, neat): 3026, 2835, 1865, 1795, 1656, 1568, 1519, 1407.

**Benzyl 2-(11*H*-benzo[4,5]imidazo[2,1-*a*]isoindol-11-yl)acetate (3n)**

Yellow liquid, yield = 62 %; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.03 (d, *J* = 7.6 Hz, 1H), 7.83 (d, *J* = 8.1 Hz, 1H), 7.56-7.18 (m, 11H), 5.73 (t, *J* = 6.4 Hz, 1H), 5.23 (s, 2H), 3.20 (dd, *J* = 16.6, 5.9 Hz, 1H), 2.94 (dd, *J* = 16.6, 6.9 Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 170.2, 157.4, 148.6, 147.2,

135.0, 132.0, 129.9, 129.3, 128.7, 128.7, 128.6, 128.6, 123.5, 122.9, 122.3, 122.1, 120.7, 109.8, 67.3, 55.9, 38.9; LRMS (ESI<sup>+</sup>)  $m/z$ : 355.2 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>23</sub>H<sub>19</sub>N<sub>2</sub>O<sub>2</sub> (M+H)<sup>+</sup>  $m/z$  : 355.1441, Found 355.1446; IR (cm<sup>-1</sup>, neat): 3147, 2829, 2783, 2756, 2023, 1834, 1654, 1570, 1512.

**Methyl-11-(2-methoxy-2-oxoethyl)-11H-benzo[4,5]imidazo[2,1-a]isoindole-7-carboxylate (3o)**

Inseparable mixture, yellow liquid, yield = 53 % ; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.53 (d,  $J$  = 1.0 Hz, 1H), 8.17 – 8.15 (m, 1H), 8.08 (d,  $J$  = 6.6 Hz, 2H), 8.03-7.99 (m, 2H), 7.84 (d,  $J$  = 8.6 Hz, 1H), 7.60 -7.54 (m, 6H), 7.46 (d,  $J$  = 8.5 Hz, 1H), 5.85-5.73 (m, 2H), 3.96 (d,  $J$  = 2.6 Hz, 6H), 3.84 (s, 3H), 3.80 (s, 3H), 3.21-3.12 (m, 2H), 2.98-2.92 (m, 2H); LRMS (ESI<sup>+</sup>)  $m/z$  : 337.2 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>19</sub>H<sub>17</sub>N<sub>2</sub>O<sub>4</sub> (M+H)<sup>+</sup>  $m/z$ : 337.1183; Found 337.1184; IR (cm<sup>-1</sup>, neat) : 3134, 3093, 2756, 1994, 1847, 1641, 1502,

**Methyl-2-(7-methyl-11H-benzo[4,5]imidazo[2,1-a]isoindol-11-yl)acetate (3p)**

Inseparable mixture, yellow liquid, yield = 50 %; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.03-7.99 (m, 2H), 7.69 (d,  $J$  = 8.2 Hz, 1H), 7.60-7.59 (m, 1H), 7.54-7.45 (m, 6H), 7.29 (d,  $J$  = 8.2 Hz, 1H), 7.21-7.20 (m, 1H), 7.10-7.06 (m, 2H), 5.74-5.60 (m, 2H), 3.80 (s, 3H), 3.79 (s, 3H), 3.20- 3.09 (m, 2H), 2.89-2.81 (m, 2H), 2.49 (s, 3H), 2.48 (s, 3H); LRMS (ESI<sup>+</sup>)  $m/z$ : 293.2 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>18</sub>H<sub>17</sub>N<sub>2</sub>O<sub>2</sub> (M+H)<sup>+</sup>  $m/z$ : 293.1285; Found 293.1286; IR (cm<sup>-1</sup>, neat): 3143, 2781, 1996, 1909, 1654, 1506.

**Methyl 2-(7-nitro-11H-benzo[4,5]imidazo[2,1-a]isoindol-11-yl)acetate (3q)**

Inseparable mixture, yellow solid, yield = 60 %; mp = 145-148 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.71 (d,  $J$  = 2.2 Hz, 1H), 8.41 (d,  $J$  = 2.2 Hz, 1H), 8.25-8.20 (m, 2H), 8.12-8.07 (m, 2H), 7.86 (d,  $J$  = 8.9 Hz, 1H), 7.65-7.57 (m, 6H), 7.53 (d,  $J$  = 9.0 Hz, 1H), 5.84 (dt,  $J$  = 12.5, 6.3 Hz, 2H), 3.86 (s, 3H), 3.81 (s, 3H), 3.14-3.00 (m, 4H); LRMS (ESI<sup>+</sup>)  $m/z$ : 324.2 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>17</sub>H<sub>14</sub>N<sub>3</sub>O<sub>4</sub> (M+H)<sup>+</sup>  $m/z$ : 324.0979; Found 324.0981; IR (cm<sup>-1</sup>, neat): 3136, 3026, 2785, 1849, 1838, 1649, 1568, 1398

**Methyl 2-(7-fluoro-11H-benzo[4,5]imidazo[2,1-a]isoindol-11-yl)acetate (3r)**

Brown solid, yield = 51 %; mp = 126-129 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.02 (d, *J* = 7.1 Hz, 1H), 7.75 – 7.71 (m, 1H), 7.57 – 7.51 (m, 3H), 7.16 (dd, *J* = 8.7, 2.5 Hz, 1H), 7.04 – 7.00 (m, 1H), 5.73 (t, *J* = 6.4 Hz, 1H), 3.82 (s, 3H), 3.07 (dd, *J* = 16.7, 6.5 Hz, 1H), 2.94 (dd, *J* = 16.8, 6.3 Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 170.9, 146.9, 145.0, 130.0, 129.4, 128.5, 123.5, 122.2, 122.0, 121.2, 121.1, 110.6, 110.4, 97.1, 96.8, 56.1, 52.5, 38.7; LRMS (ESI<sup>+</sup>) *m/z*: 297.1 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>17</sub>H<sub>14</sub>FN<sub>2</sub>O<sub>2</sub> (M+H)<sup>+</sup> *m/z*: 297.1034; Found 297.1035; IR (cm<sup>-1</sup>, neat) : 3147, 2879, 2756, 1998, 1905, 1830, 1780, 1652, 1508

**Methyl 2-(7-chloro-11*H*-benzo[4,5]imidazo[2,1-*a*]isoindol-11-yl) acetate (3s)**

Yellow solid, yield = 70 %; mp = 122-125 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.04 (d, *J* = 7.2 Hz, 1H), 7.73 (d, *J* = 8.7 Hz, 1H), 7.58 – 7.48 (m, 3H), 7.45 (d, *J* = 2.1 Hz, 1H), 7.25 (m, 1H), 5.73 (t, *J* = 6.4 Hz, 1H), 3.82 (s, 3H), 3.10 (dd, *J* = 16.7, 6.3 Hz, 1H), 2.93 (dd, *J* = 16.7, 6.6 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 170.8, 147.3, 147.1, 130.2, 129.4, 128.6, 128.3, 123.6, 123.0, 122.3, 121.4, 110.0, 56.2, 52.5, 38.7; LRMS (ESI<sup>+</sup>) *m/z*: 313.2 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>17</sub>H<sub>14</sub>ClN<sub>2</sub>O<sub>2</sub> (M+H)<sup>+</sup> *m/z*: 313.0738; Found 313.0747; IR (cm<sup>-1</sup>, neat): 3143, 3035, 2881, 2796, 1909, 1834, 1643, 1597, 1502

**Methyl 2-(7-bromo-11*H*-benzo[4,5]imidazo[2,1-*a*]isoindol-11-yl)acetate (3t)**

Brown solid, yield = 62 %; mp = 134-137 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.04 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.69 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.60 – 7.49 (m, 4H), 7.37 (dd, *J* = 8.6, 1.9 Hz, 1H), 5.71 (t, *J* = 6.4 Hz, 1H), 3.81 (s, 3H), 3.09 (dd, *J* = 16.6, 6.3 Hz, 1H), 2.92 (dd, *J* = 16.6, 6.5 Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 170.7, 147.1, 130.4, 129.5, 125.7, 123.5, 123.1, 122.4, 121.7, 121.2, 113.0, 110.1, 56.3, 56.3, 52.5, 38.7, 38.6; LRMS (ESI<sup>+</sup>) *m/z*: 357.0 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>17</sub>H<sub>14</sub>BrN<sub>2</sub>O<sub>2</sub> (M+H)<sup>+</sup> *m/z*: 357.0233; Found 357.0235; IR (cm<sup>-1</sup>, neat) : 3141, 3039, 2792, 1998, 1907, 1834, 1660, 1502

**Methyl 2-(6-methyl-11*H*-benzo[4,5]imidazo[2,1-*a*]isoindol-11-yl)acetate (3u)**

Yellow solid, yield = 65 %; mp = 102-105 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.15 (d, *J* = 7.5 Hz, 1H), 7.57 – 7.46 (m, 3H), 7.28 (d, *J* = 7.9 Hz, 1H), 7.18 (t, *J* = 7.7 Hz, 1H), 7.10 (d, *J* = 7.3 Hz, 1H), 5.73 (t, *J* = 6.5 Hz, 1H), 3.80 (s, 3H), 3.19 (dd, *J* = 16.7, 5.8 Hz, 1H), 2.85 (dd, *J* = 16.7, 7.1 Hz, 1H), 2.74 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 170.9, 147.2, 130.7, 129.8, 129.3, 123.5, 122.9, 122.9, 122.3, 107.3, 55.9, 52.4, 38.7, 29.9, 17.1; LRMS (ESI<sup>+</sup>) *m/z*: 293.2 (M+H)<sup>+</sup>;

HRMS: calcd for C<sub>18</sub>H<sub>17</sub>N<sub>2</sub>O<sub>2</sub> (M+H)<sup>+</sup> *m/z*: 293.1285; Found 293.1287; R (cm<sup>-1</sup>, neat): 3136, 3006, 2881, 2760, 1998, 1838, 1641, 1571, 1512

**Methyl (E)-3-(2-(1*H*-benzo[*d*]imidazol-2-yl)furan-3-yl)acrylate (4b)**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.90 – 7.84 (m, 1H), 7.82 – 7.78 (m, 1H), 7.62 – 7.52 (m, 4H), 7.44 – 7.34 (m, 3H), 6.42 (d, *J* = 16.0 Hz, 1H), 3.70 (s, 3H), 3.62 (s, 3H); LRMS (ESI<sup>+</sup>) *m/z*: 269.1 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>15</sub>H<sub>13</sub>N<sub>2</sub>O<sub>3</sub> (M+H)<sup>+</sup> *m/z*: 269.0921; Found 269.0921.

**Methyl (E)-3-(2-(1*H*-benzo[*d*]imidazol-2-yl)thiophen-3-yl)acrylate (4c)**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.85 (d, *J* = 8.0 Hz, 1H), 7.54 (d, *J* = 5.4 Hz, 1H), 7.44 – 7.33 (m, 5H), 7.10 (d, *J* = 5.4 Hz, 1H), 3.83 (s, 3H); LRMS (ESI<sup>+</sup>) *m/z*: 285.1 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>15</sub>H<sub>13</sub>N<sub>2</sub>O<sub>2</sub>S (M+H)<sup>+</sup> *m/z*: 285.0692.0921; Found 285.0694.

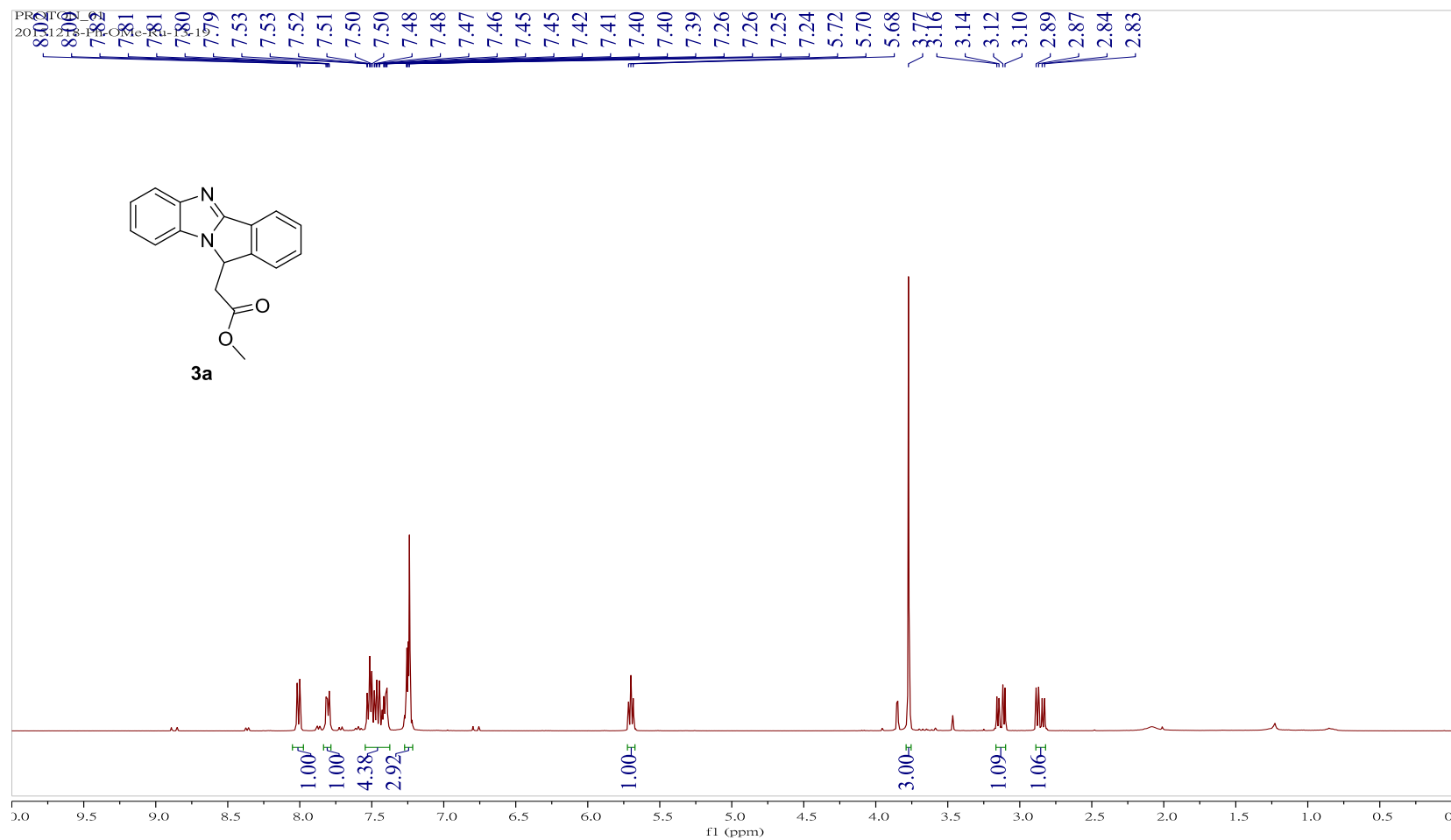
**Methyl (E)-3-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)phenyl)acrylate (6a)**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.90 – 7.84 (m, 1H), 7.82 – 7.78 (m, 1H), 7.62 – 7.52 (m, 4H), 7.44 – 7.34 (m, 3H), 6.42 (d, *J* = 16.0 Hz, 1H), 3.70 (s, 3H), 3.62 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 166.8, 151.8, 141.6, 134.5, 131.4, 130.3, 129.9, 126.8, 123.1, 122.7, 120.4, 120.1, 109.7, 51.7, 31.0; LRMS (ESI<sup>+</sup>) *m/z*: 293.2 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>18</sub>H<sub>17</sub>N<sub>2</sub>O<sub>2</sub> (M+H)<sup>+</sup> *m/z*: 293.1285; Found 293.1285.

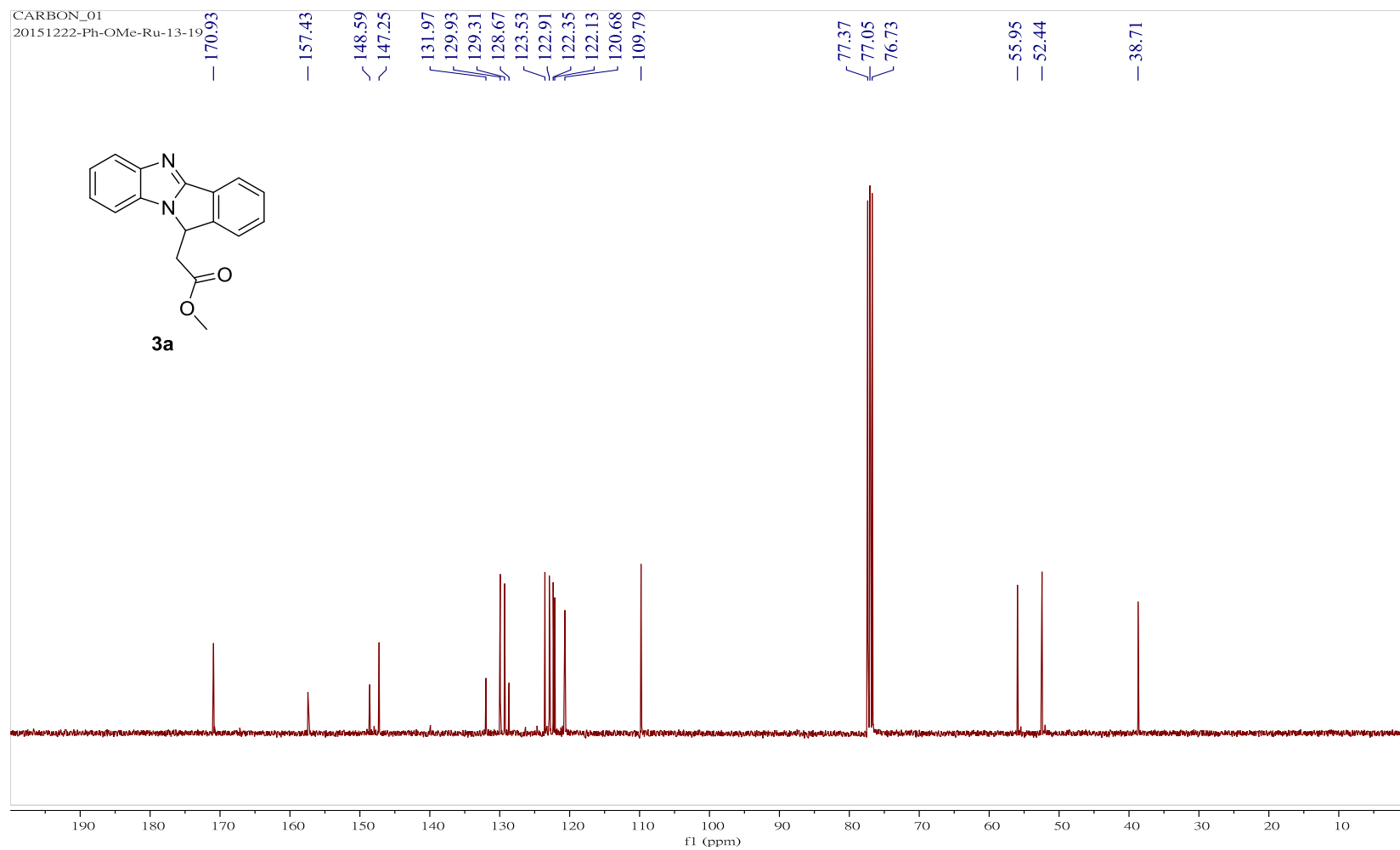
**Methyl 3-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)phenyl)propanoate (7a)**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.88 – 7.81 (m, 1H), 7.47 – 7.32 (m, 7H), 3.64 (s, 3H), 3.55 (s, 3H), 2.94 (t, *J* = 7.7 Hz, 2H), 2.54 (t, *J* = 7.7 Hz, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 173.1, 152.8, 140.7, 135.3, 130.5, 130.1, 129.4, 126.3, 122.80, 122.4, 119.8, 109.6, 51.5, 34.9, 30.7, 28.3; LRMS (ESI<sup>+</sup>) *m/z*: 295.2 (M+H)<sup>+</sup>; HRMS: calcd for C<sub>18</sub>H<sub>19</sub>N<sub>2</sub>O<sub>2</sub> (M+H)<sup>+</sup> *m/z*: 295.1441; Found 295.1447.





$^1\text{H}$  NMR Spectrum (400 MHz) of compound **3a** in  $\text{CDCl}_3$

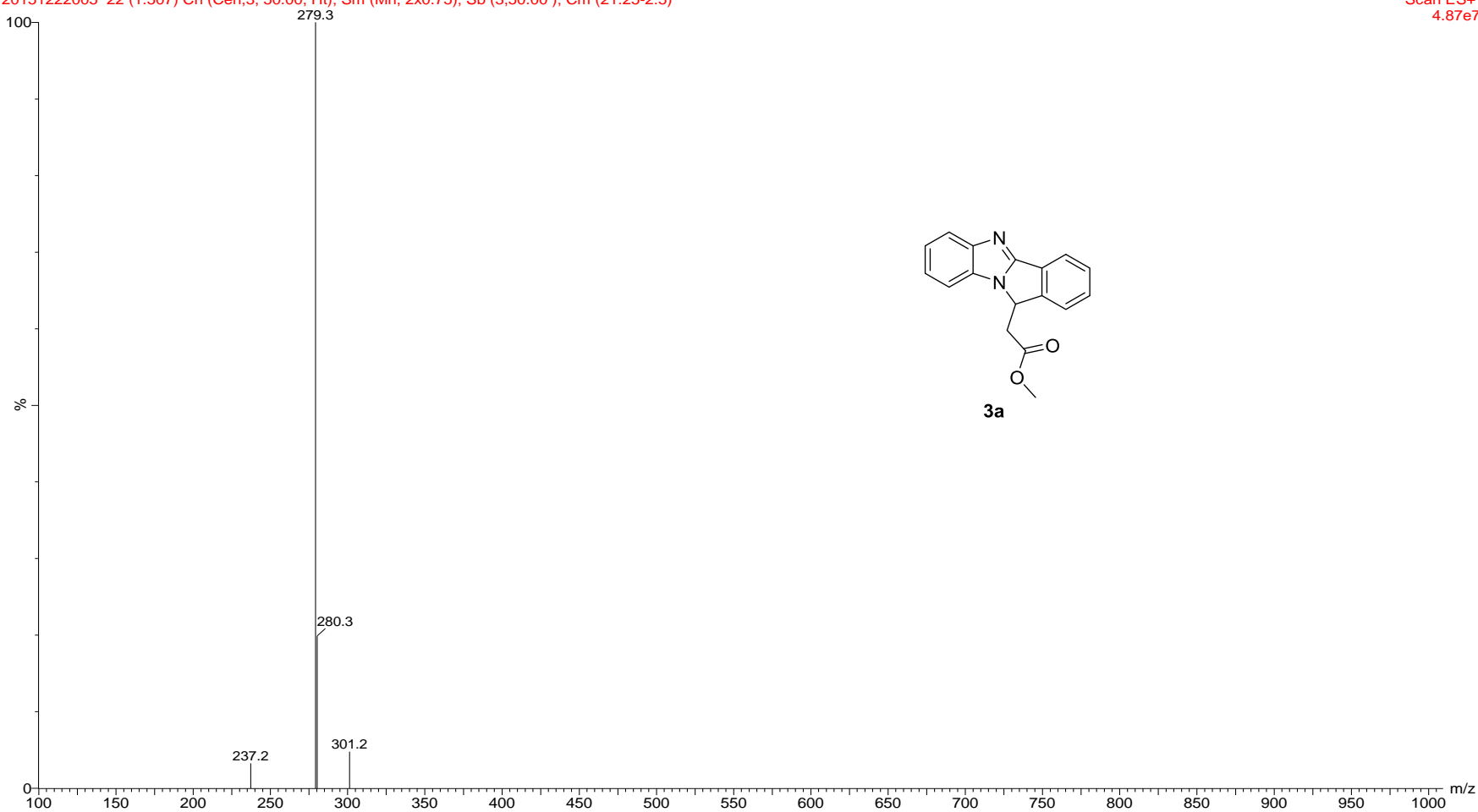


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3a** in  $\text{CDCl}_3$

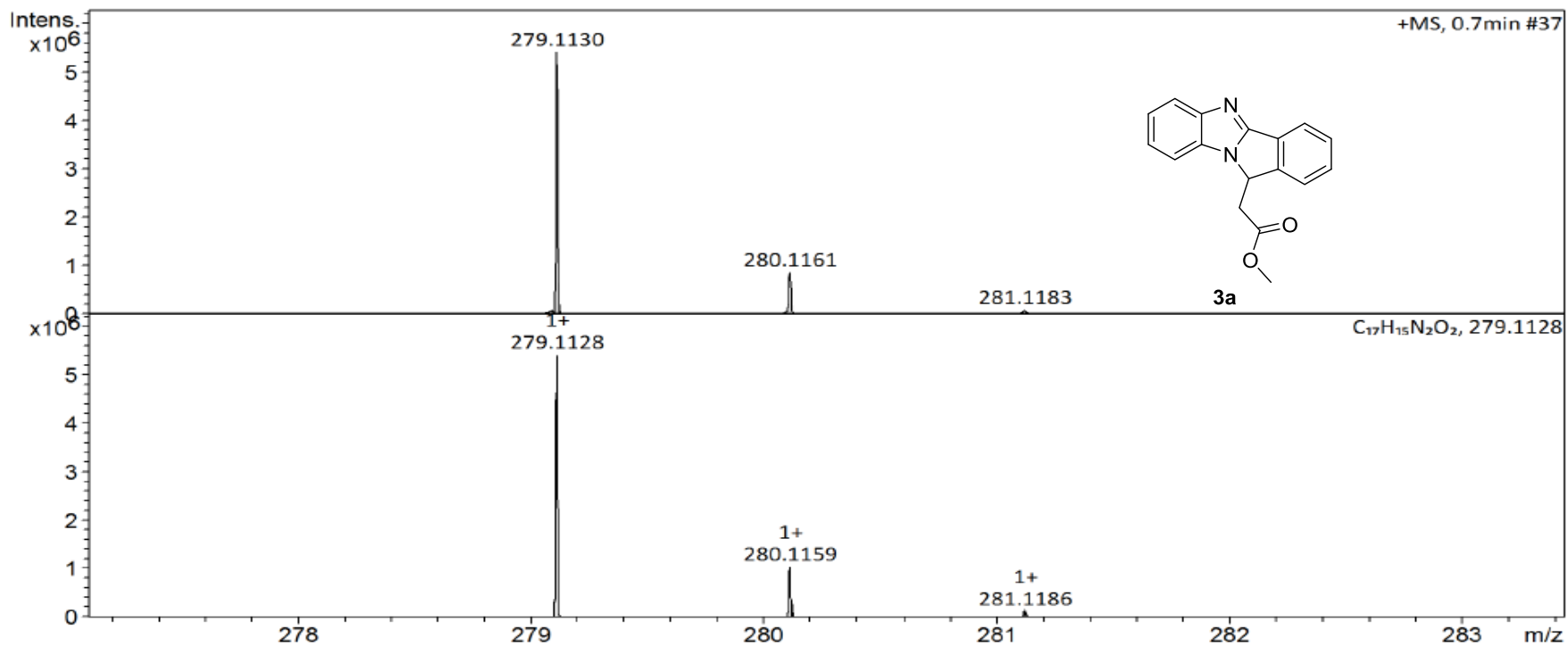
**Ph-OMe-Ru--20**

20151222005 22 (1.507) Cn (Cen,3, 50.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00 ); Cm (21:25-2:5)

Scan ES+  
4.87e7

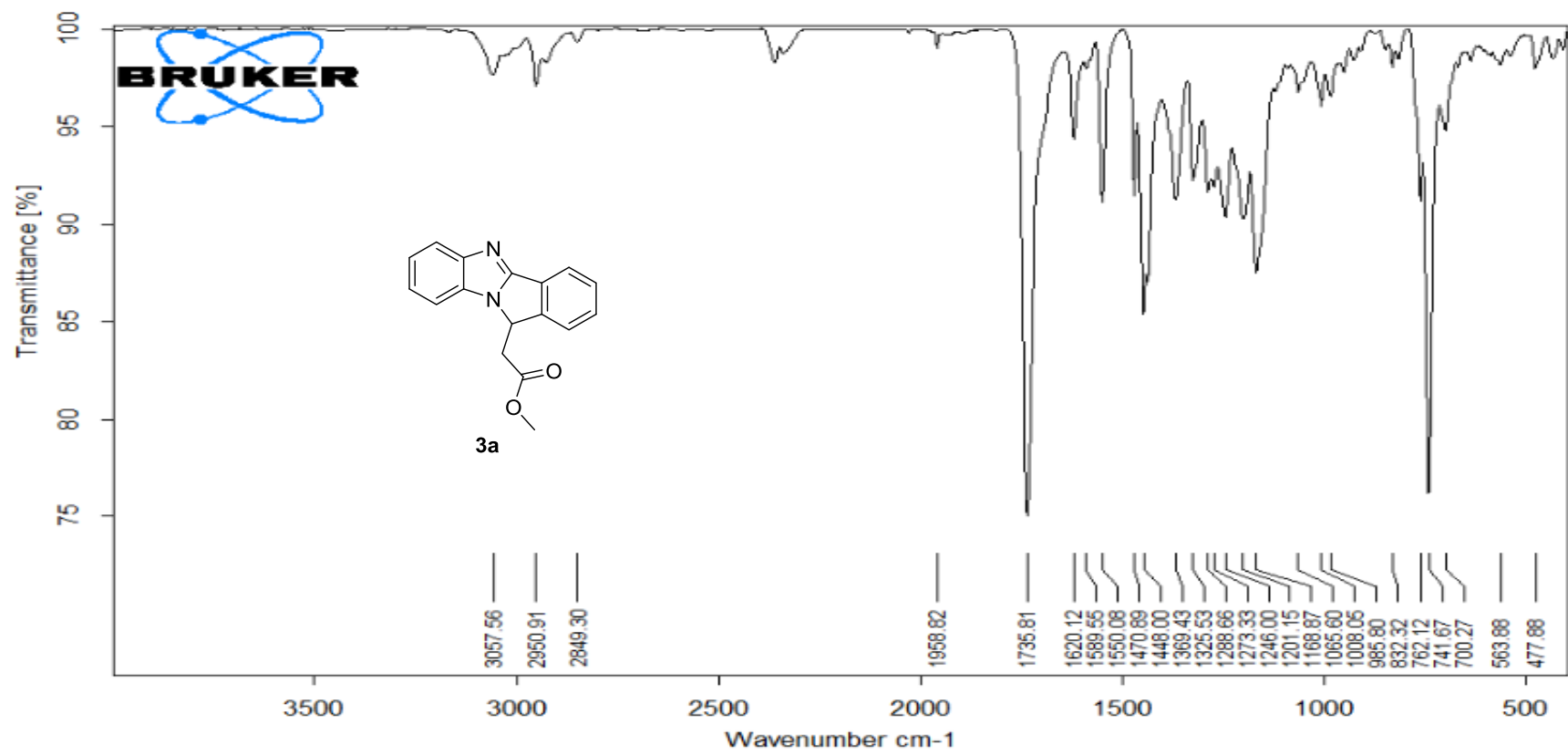


ESI<sup>+</sup> Mass spectrum of compound **3a**

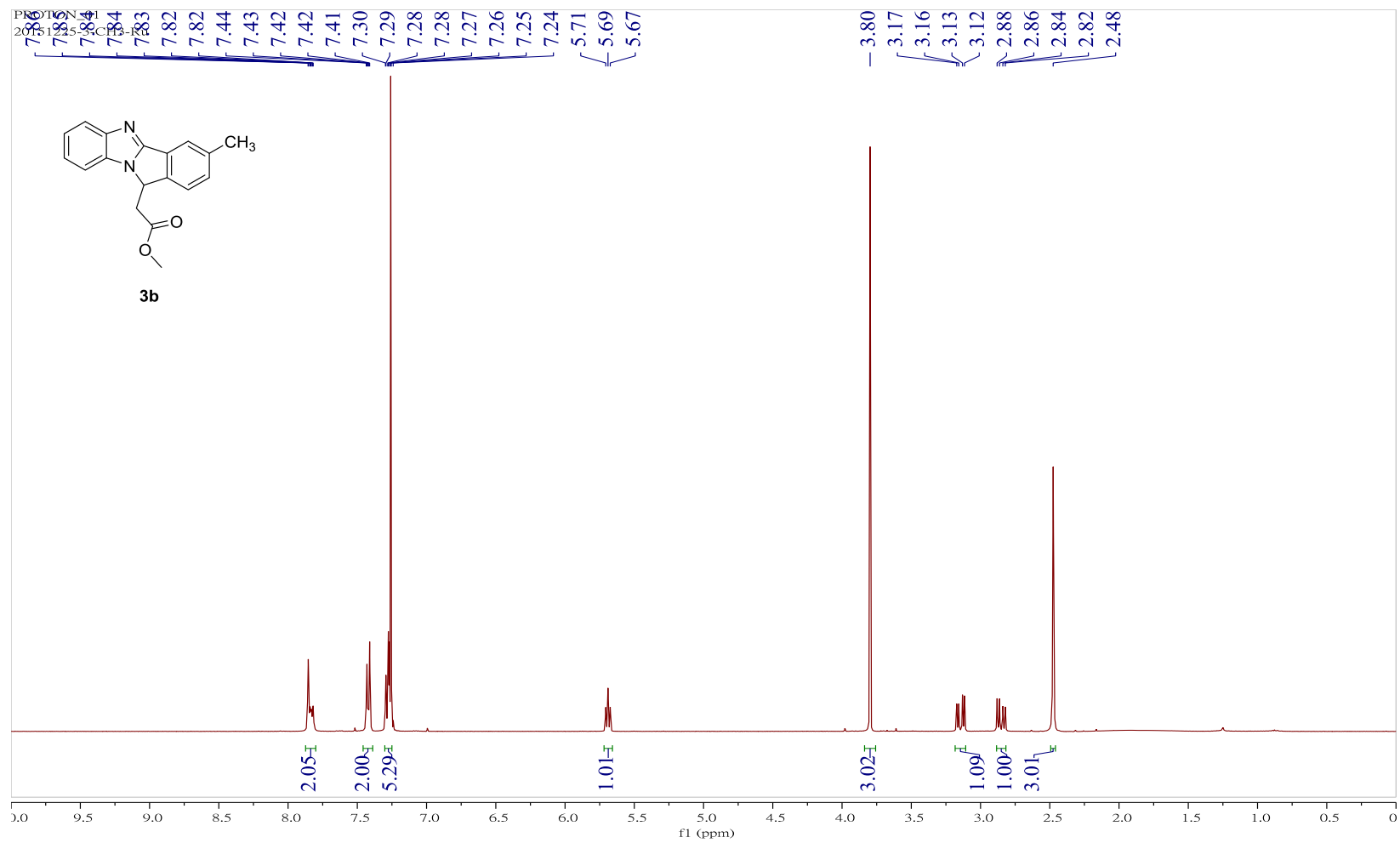


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
279.1130	1	C <sub>17</sub> H <sub>15</sub> N <sub>2</sub> O <sub>2</sub>	279.1128	0.7	19.4	1	100.00	11.5	even	ok	M+H

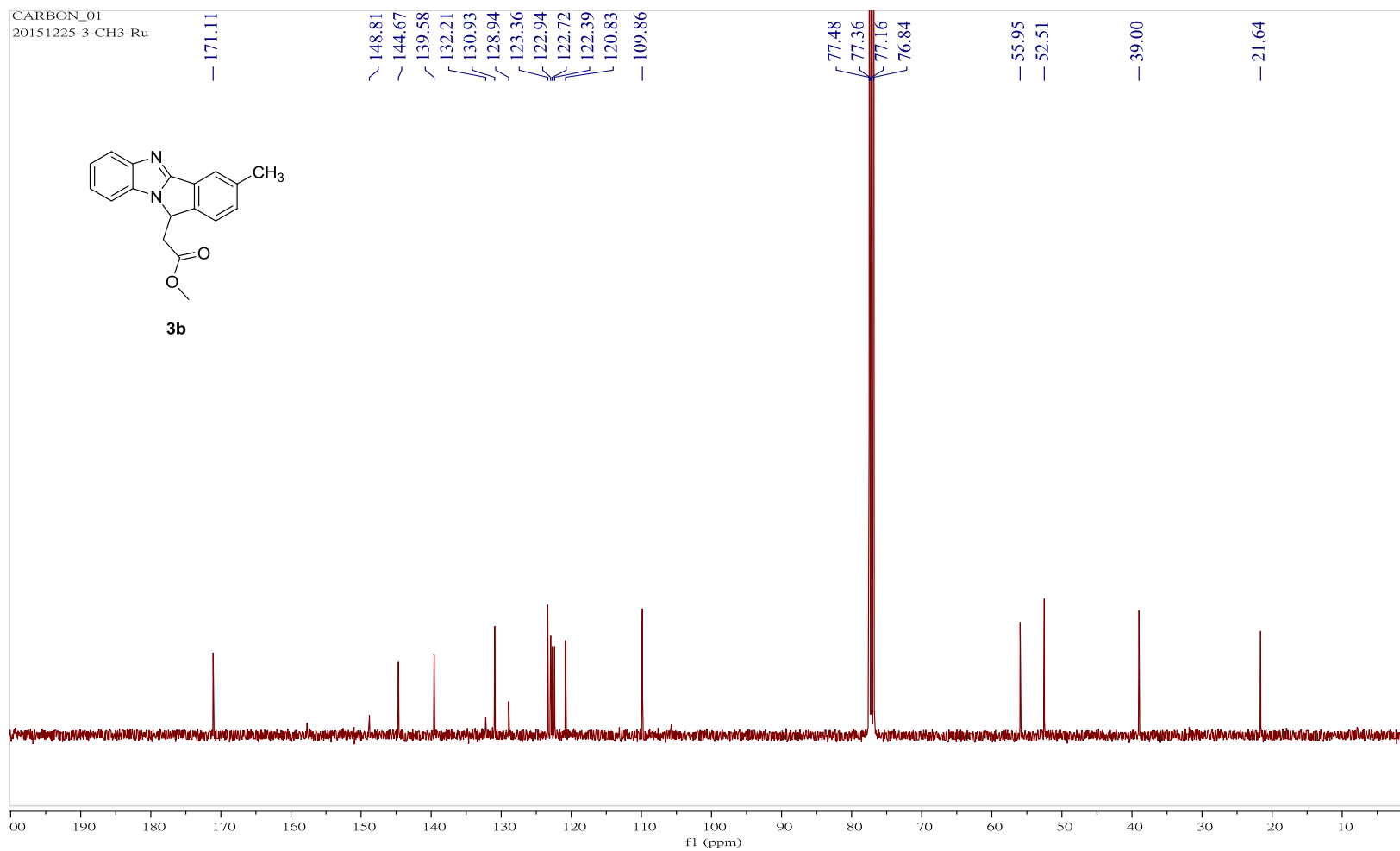
High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3a**



IR spectrum of compound of **3a**



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **3b** in CDCl<sub>3</sub>

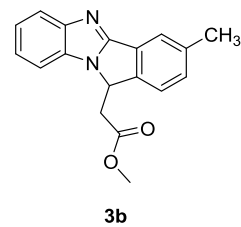
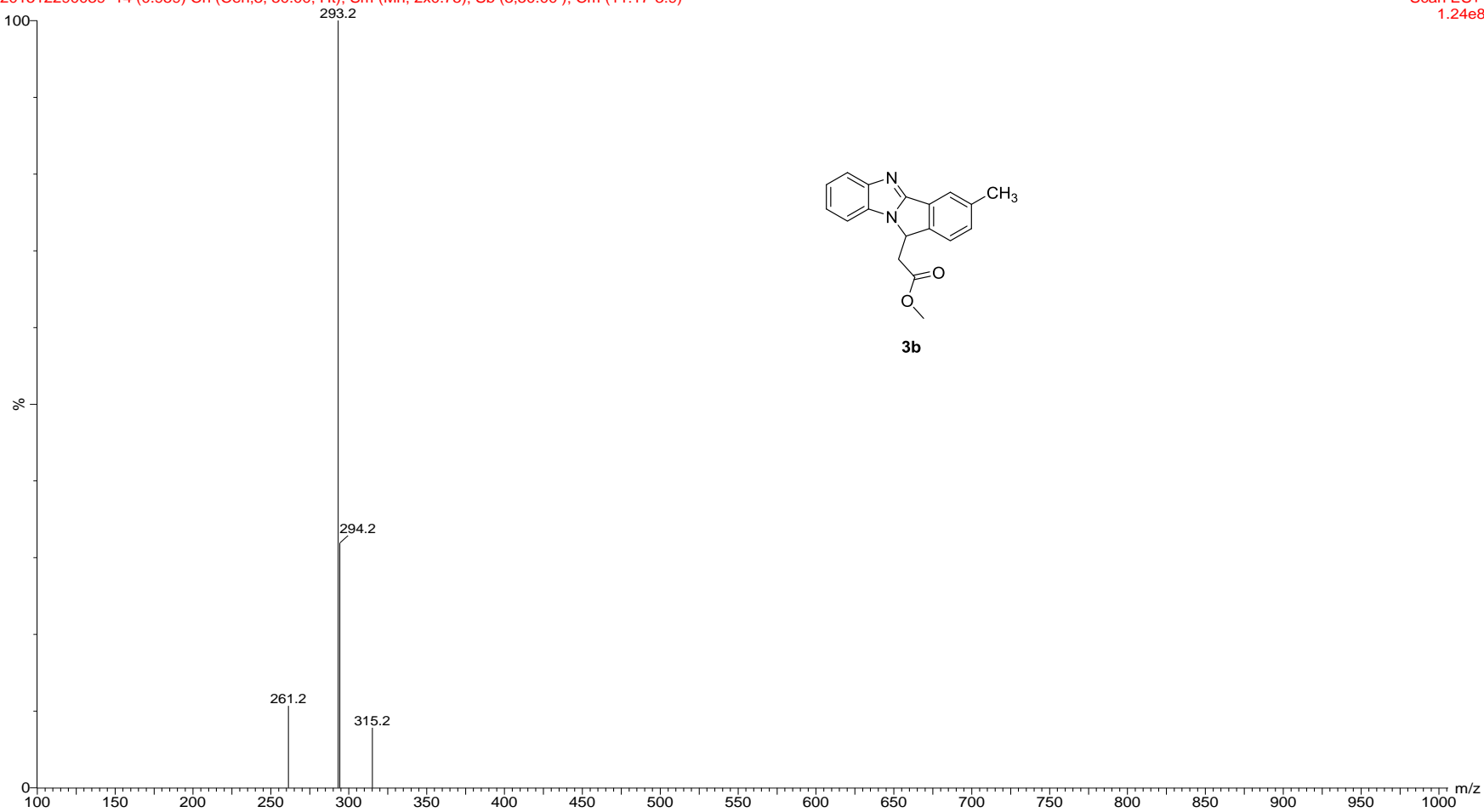


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3b**  $\text{CDCl}_3$

**3-CH3-Ru pen-out**

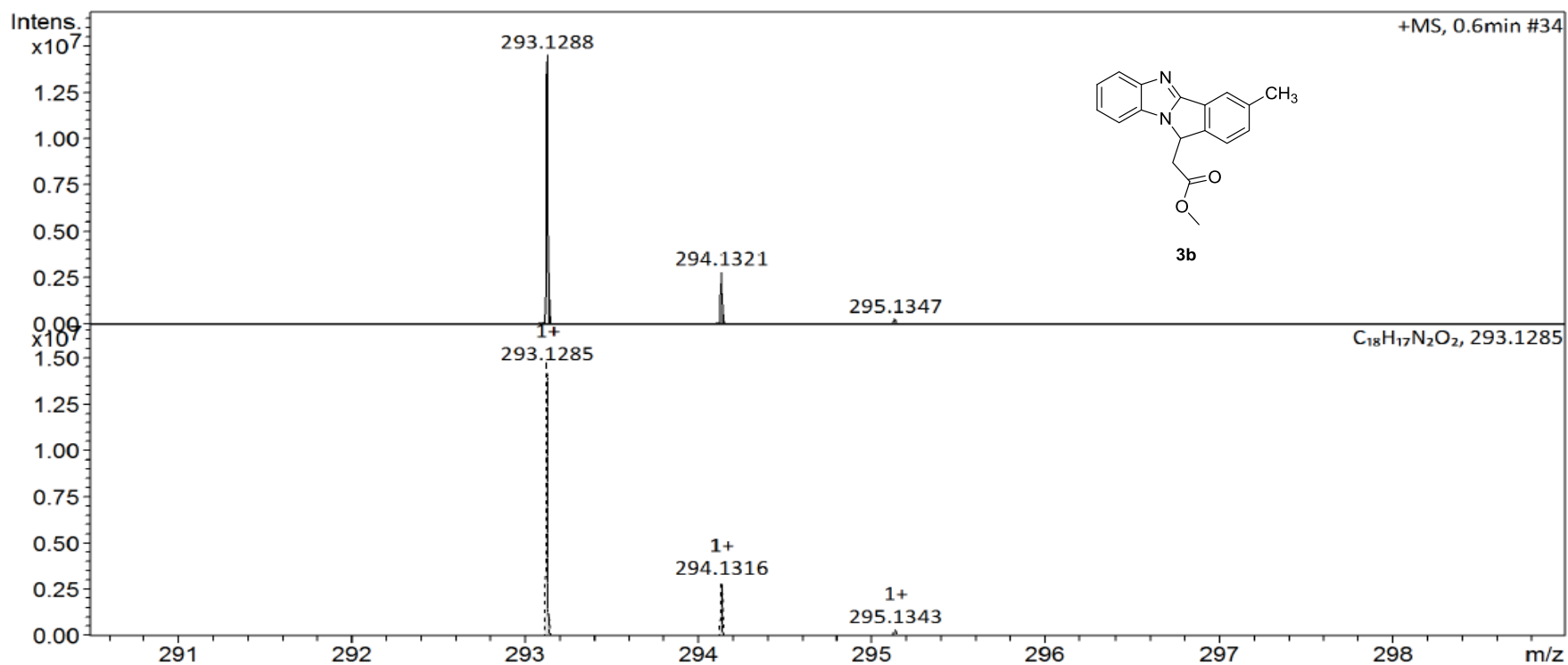
201512290039 14 (0.959) Cn (Cen,3, 50.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00); Cm (11:17-3:9)

Scan ES+  
1.24e8



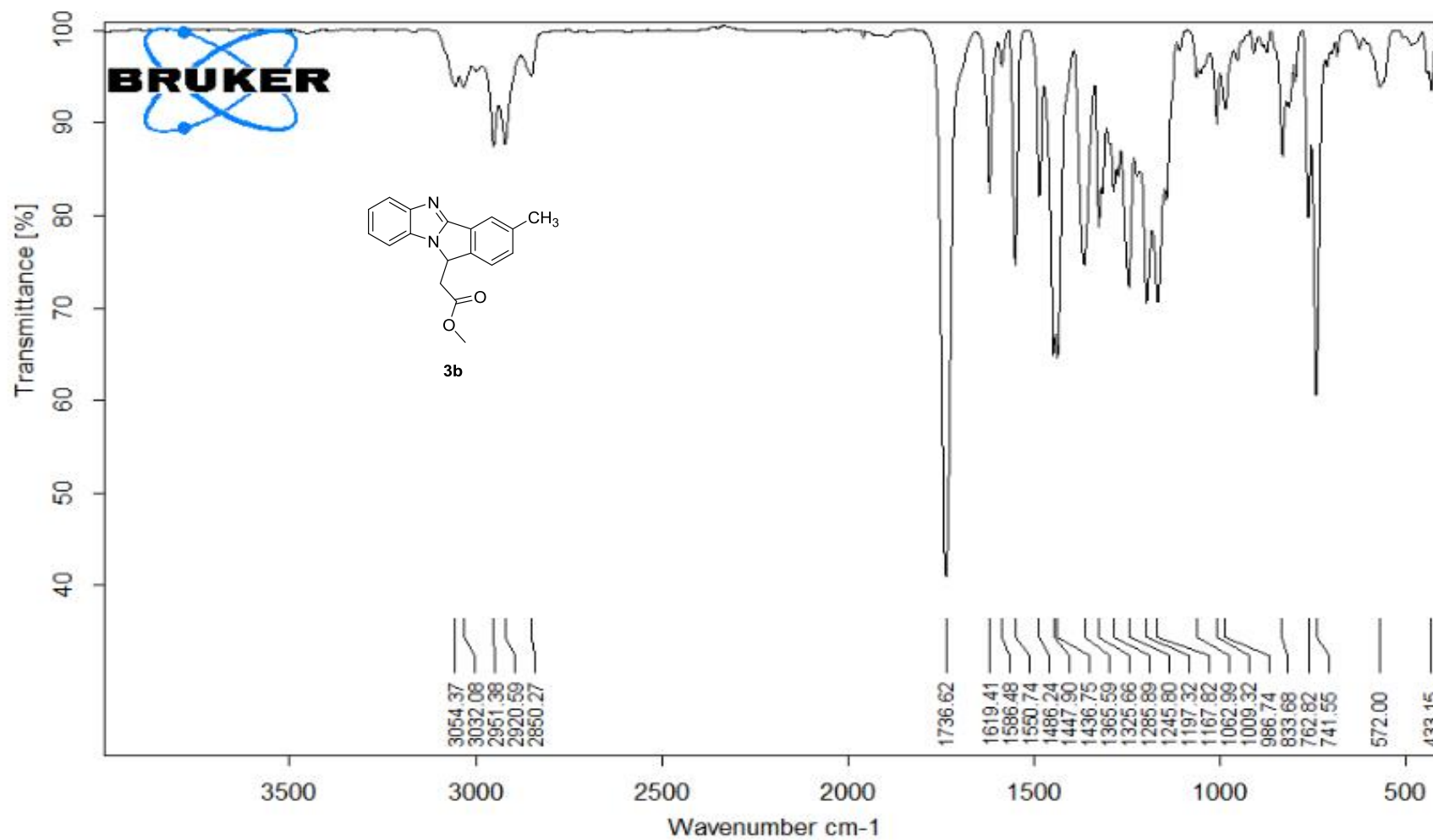
ESI<sup>+</sup> Mass spectrum of compound **3b**



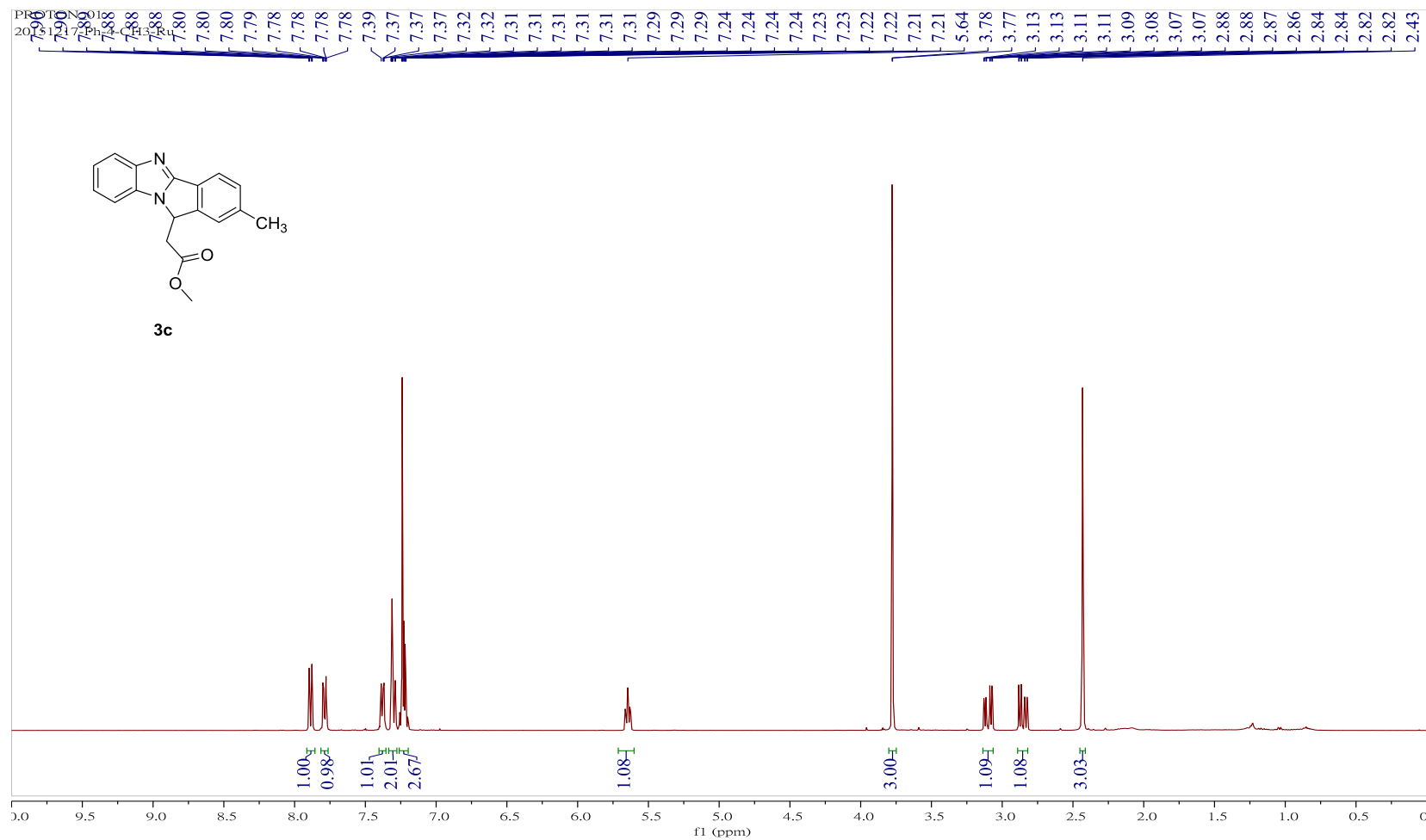


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
293.1288	1	C <sub>18</sub> H <sub>17</sub> N <sub>2</sub> O <sub>2</sub>	293.1285	1.0	6.5	1	100.00	11.5	even	ok	M+H

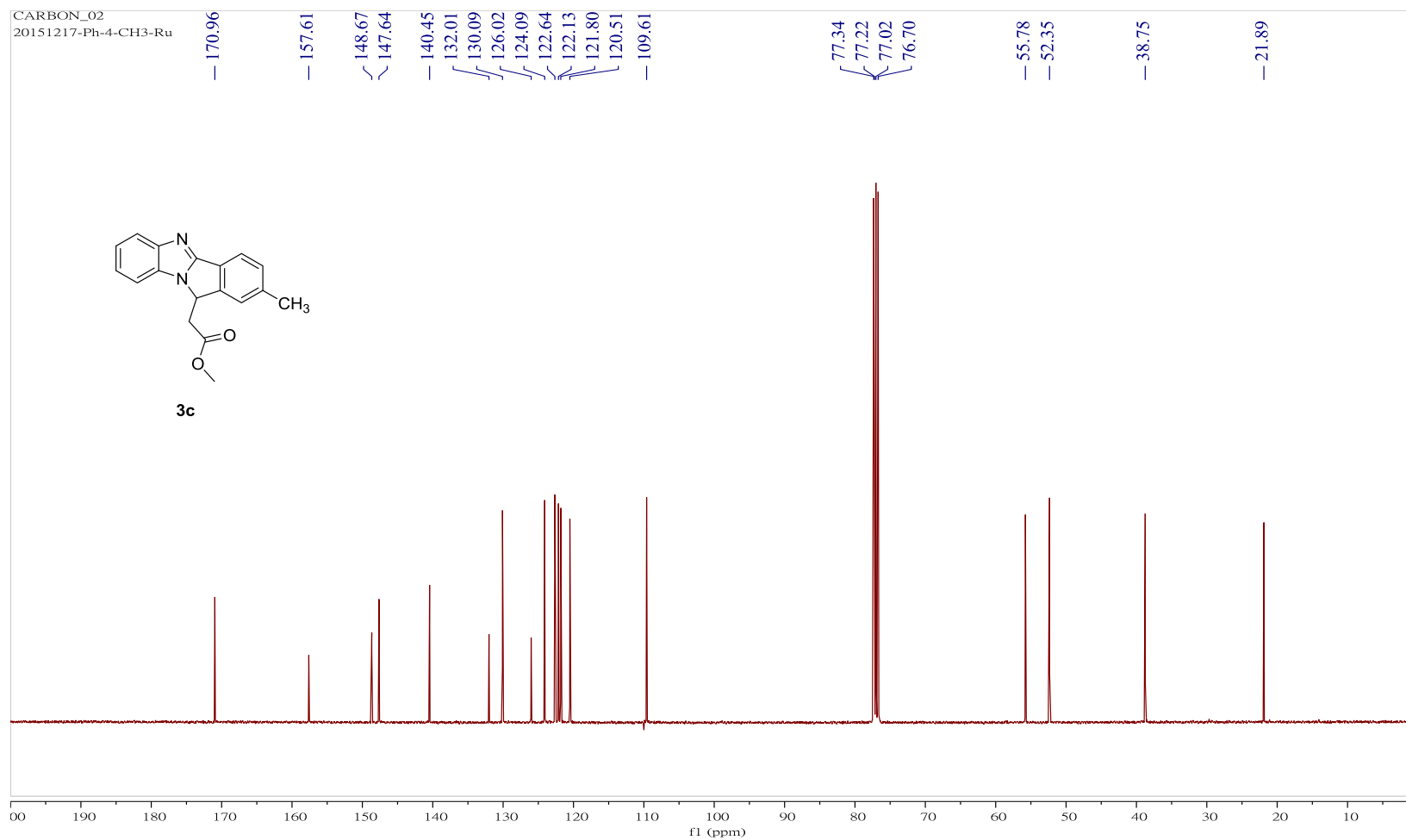
High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3b**



IR spectrum of compound of **3b**



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **3c** in CDCl<sub>3</sub>

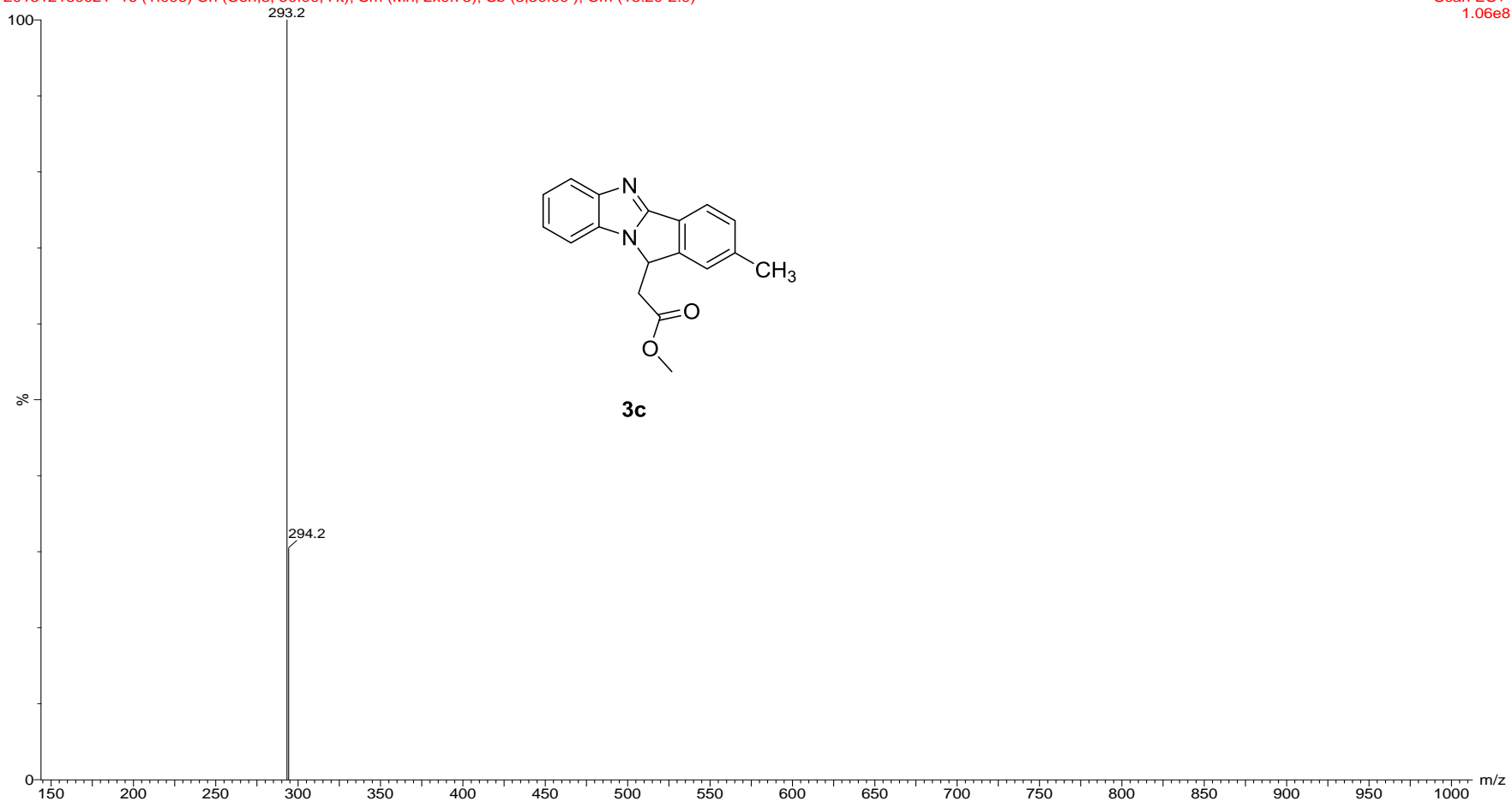


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3c**CDCl<sub>3</sub>

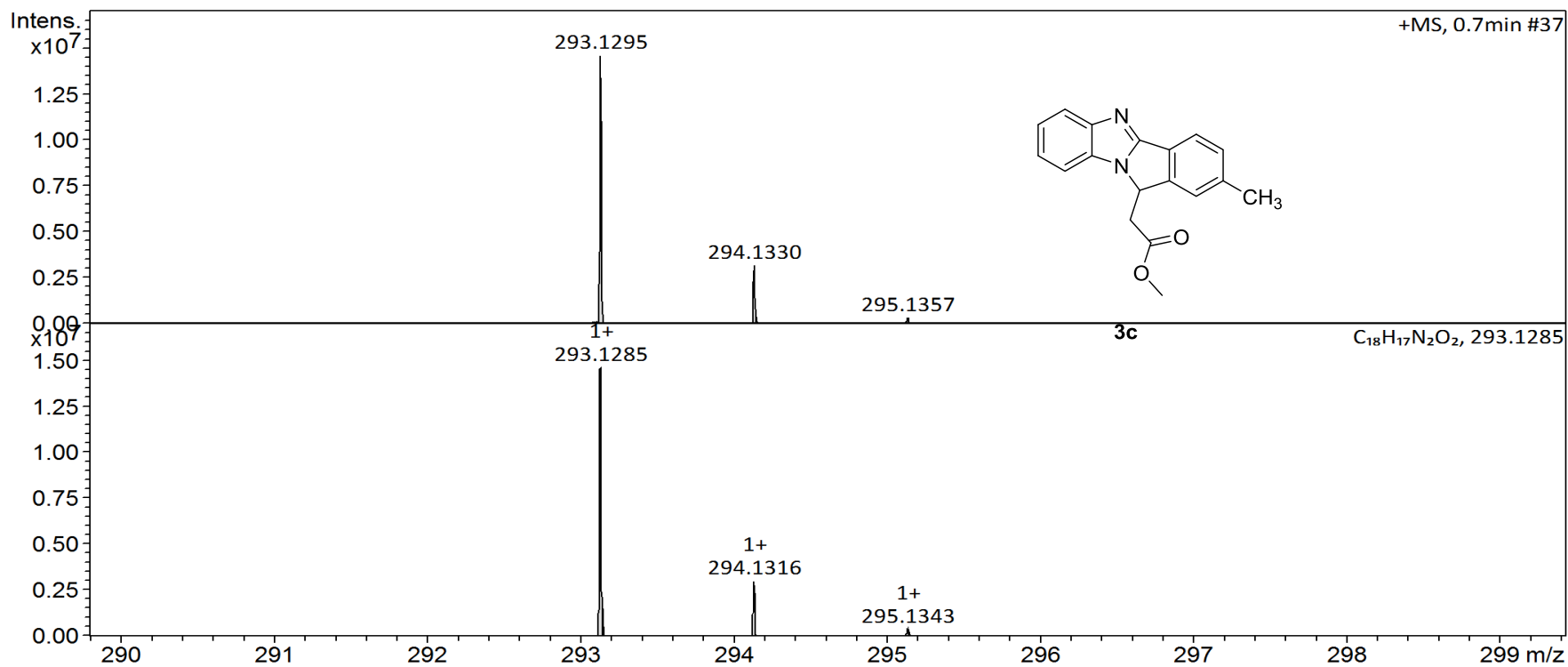
4-CH3-Ru

201512180021 16 (1.096) Cn (Cen,3, 50.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00 ); Cm (15:20-2:9)

Scan ES+  
1.06e8

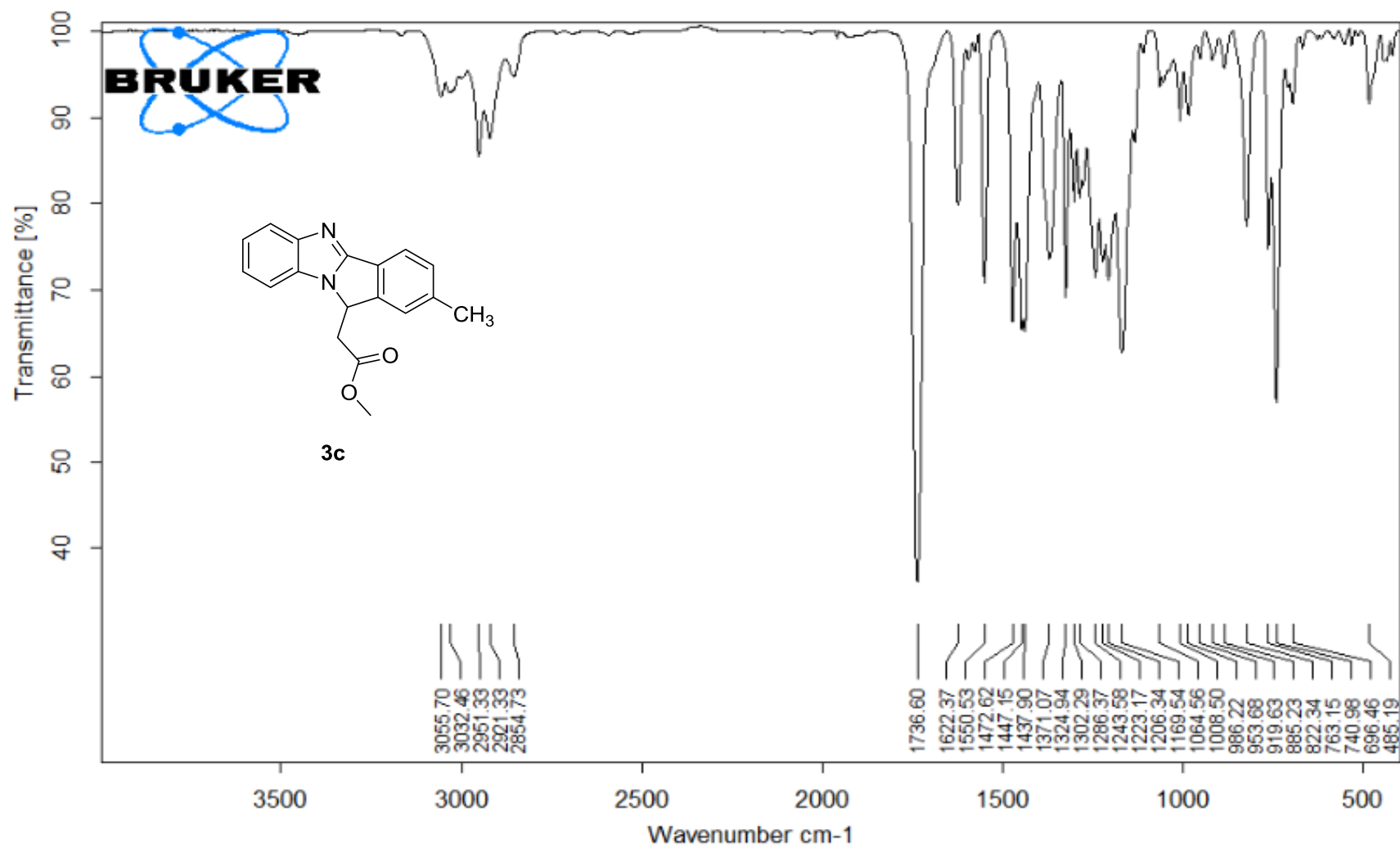


ESI<sup>+</sup> Mass spectrum of compound **3c**

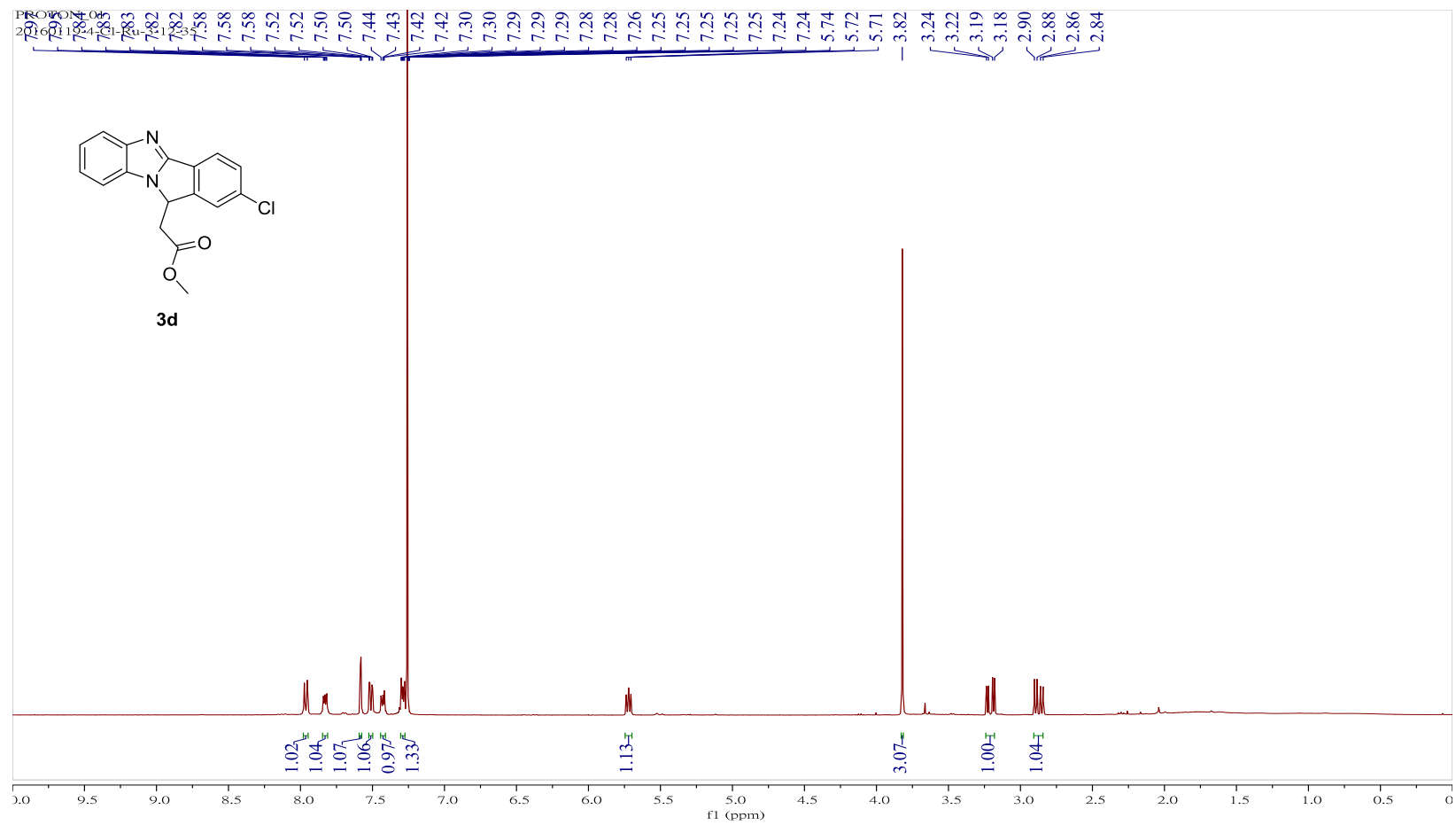


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
293.1295	1	C <sub>18</sub> H <sub>17</sub> N <sub>2</sub> O <sub>2</sub>	293.1285	3.6	6.8	1	100.00	11.5	even	ok	M+H

High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3c**

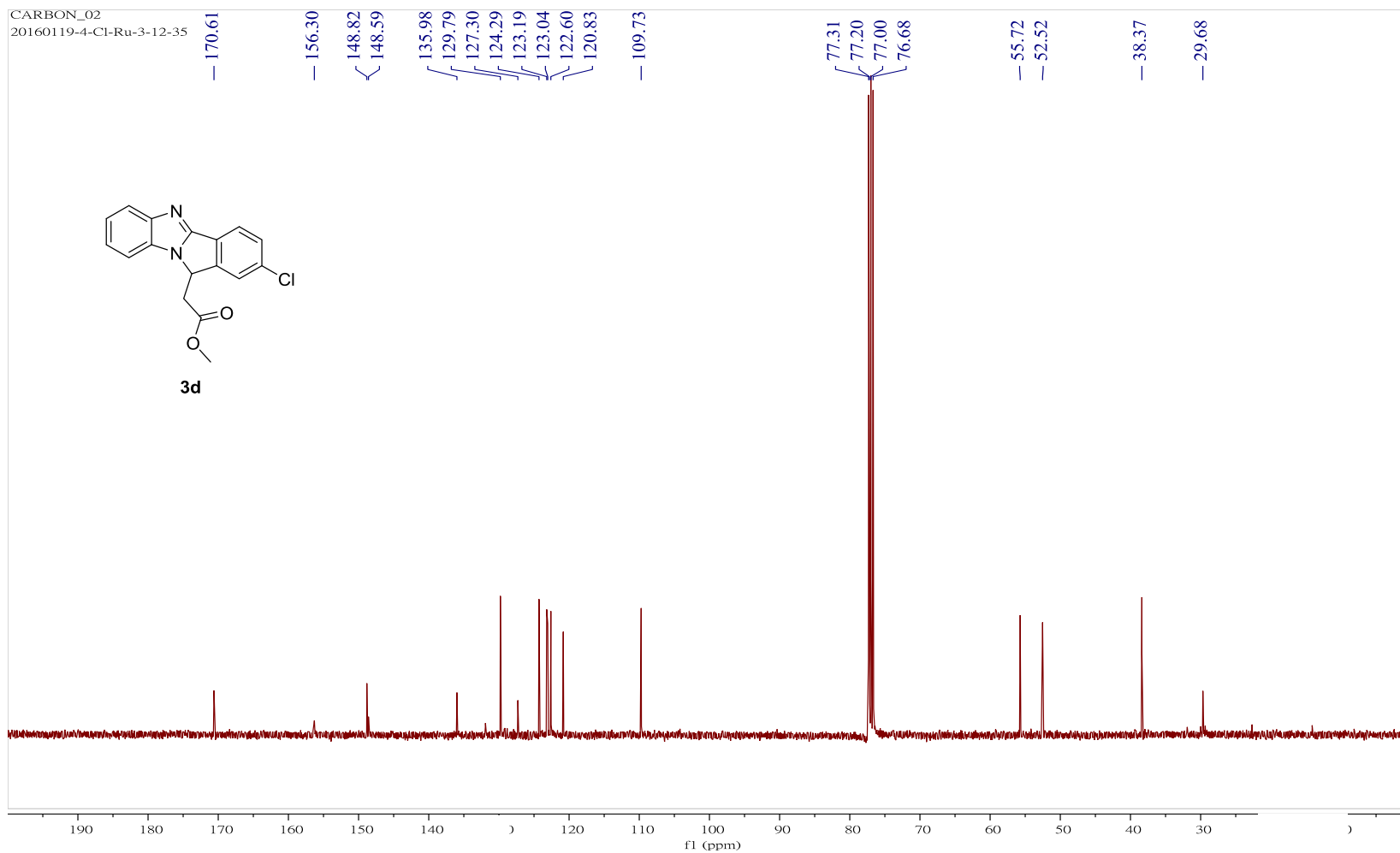


IR spectrum of compound of **3c**



$^1\text{H}$  NMR Spectrum (400 MHz) of compound **3d** in  $\text{CDCl}_3$



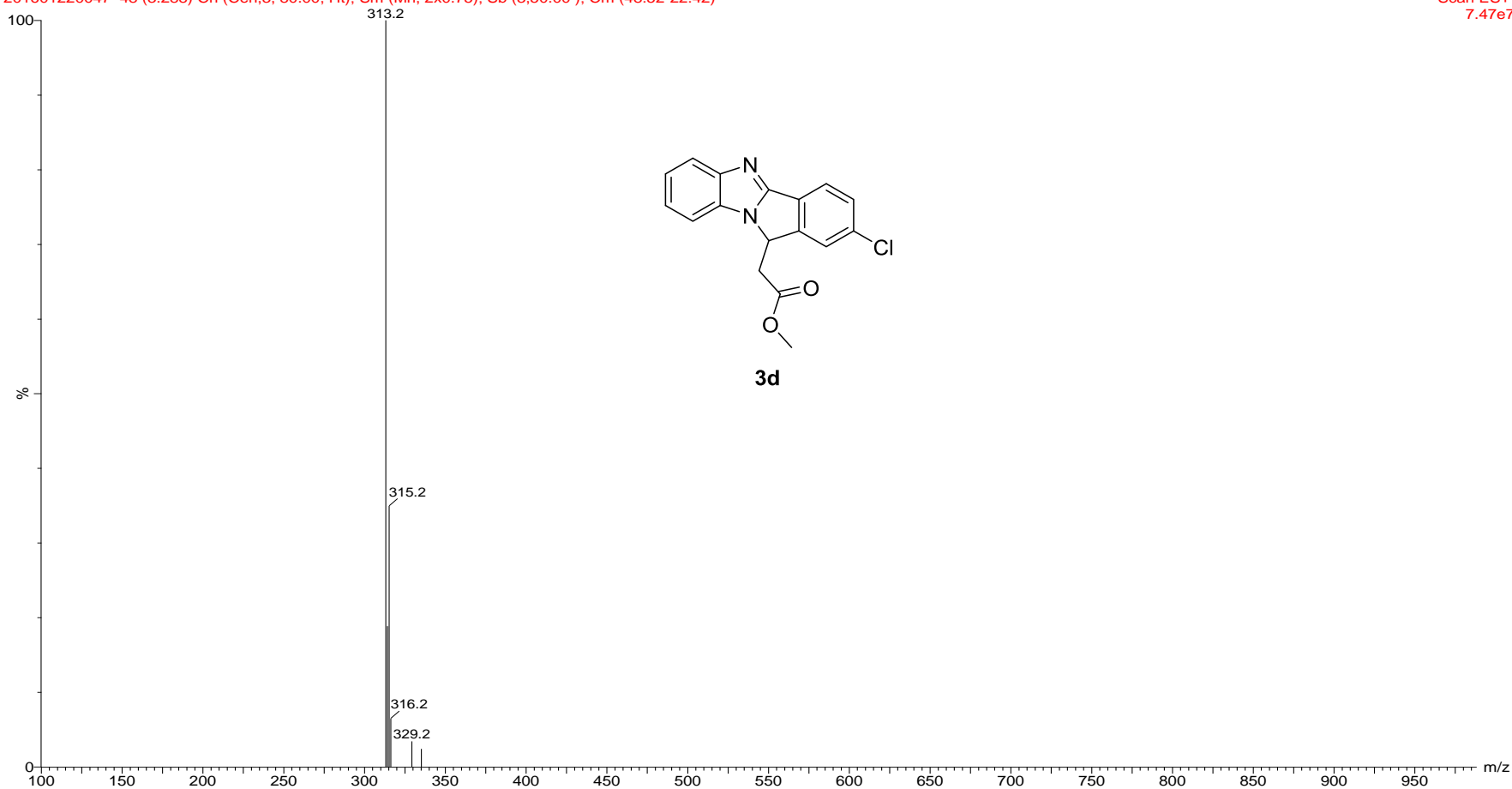


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3d**  $\text{CDCl}_3$

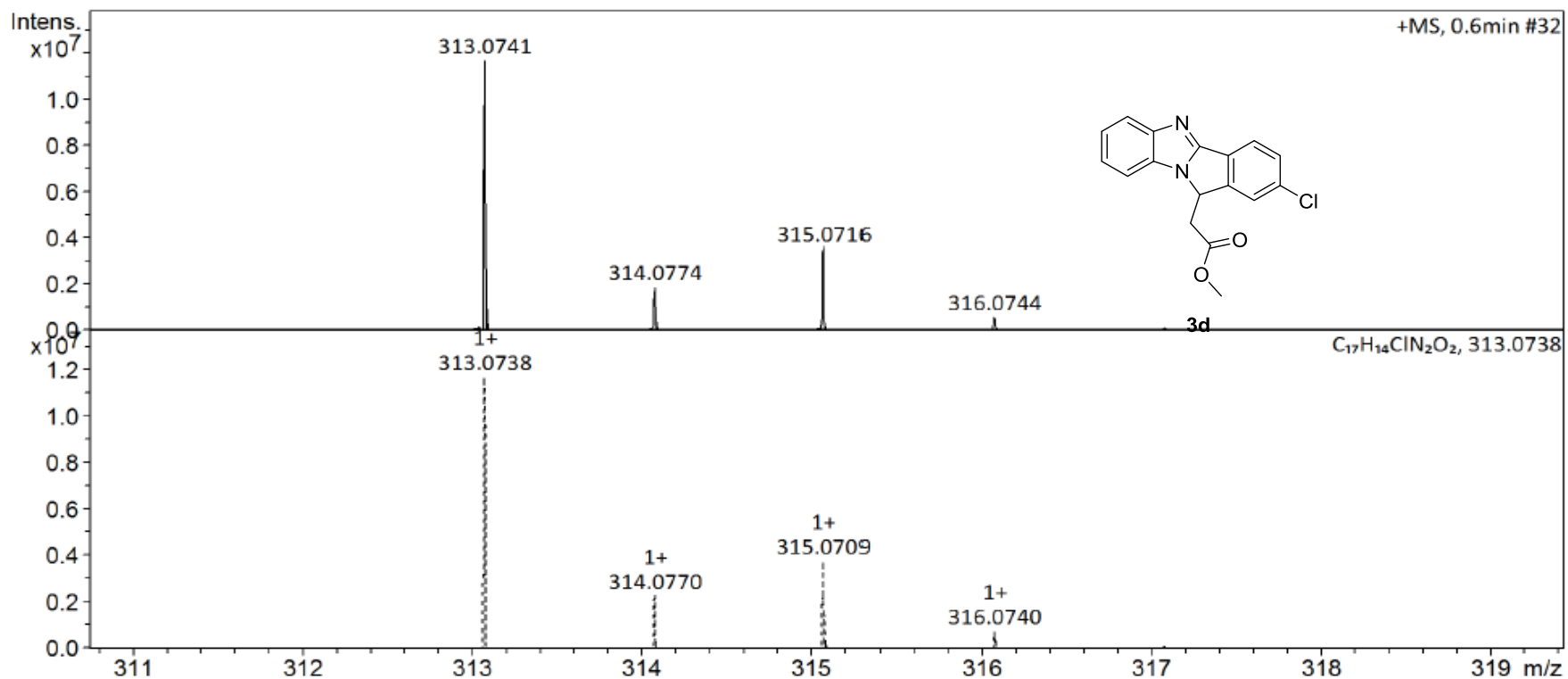
**4-Cl-Ru**

201601220047 48 (3.288) Cn (Cen,3, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00 ); Cm (48:52-22:42)

Scan ES+  
7.47e7

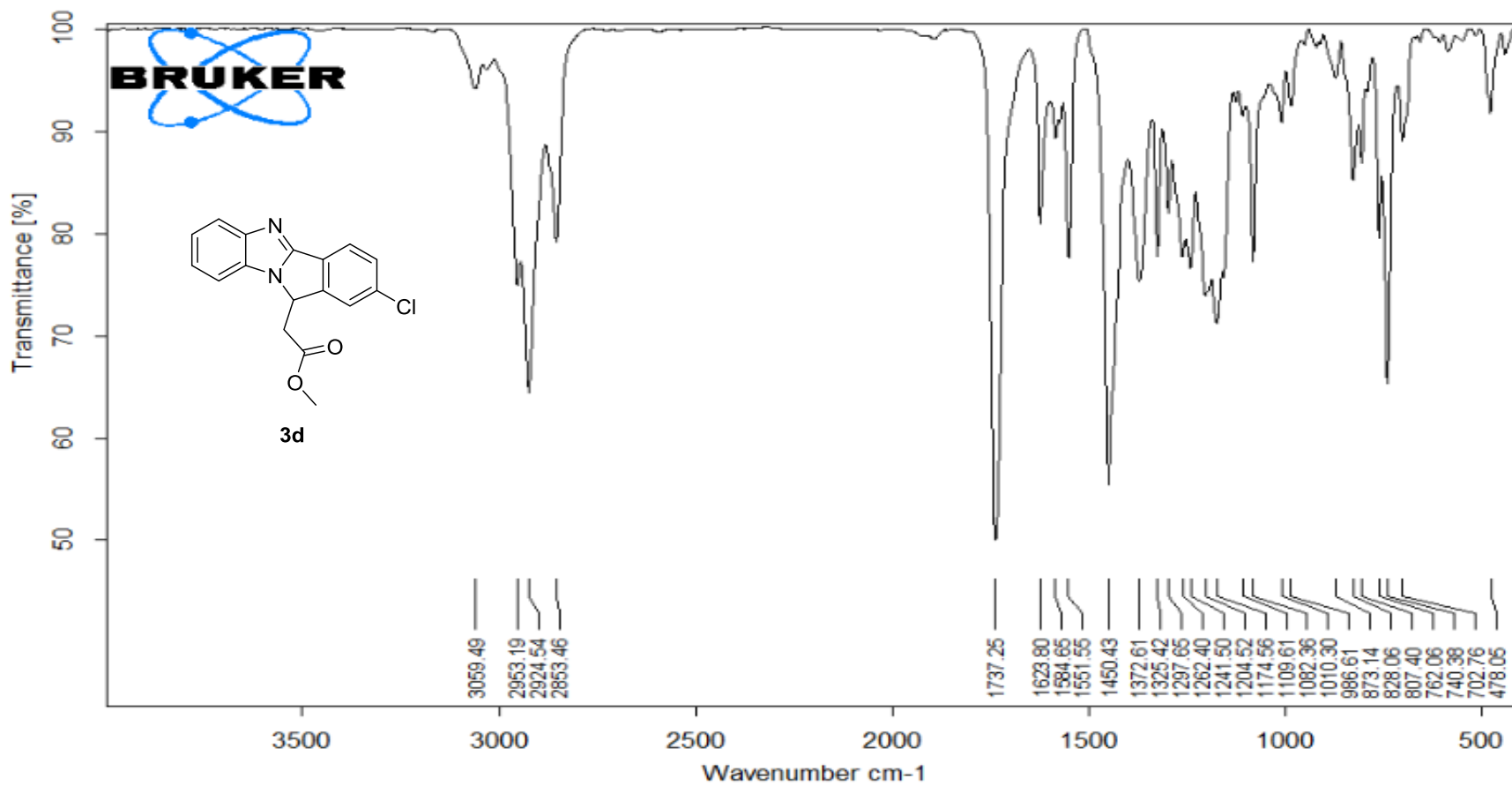


ESI<sup>+</sup> Mass spectrum of compound **3d**

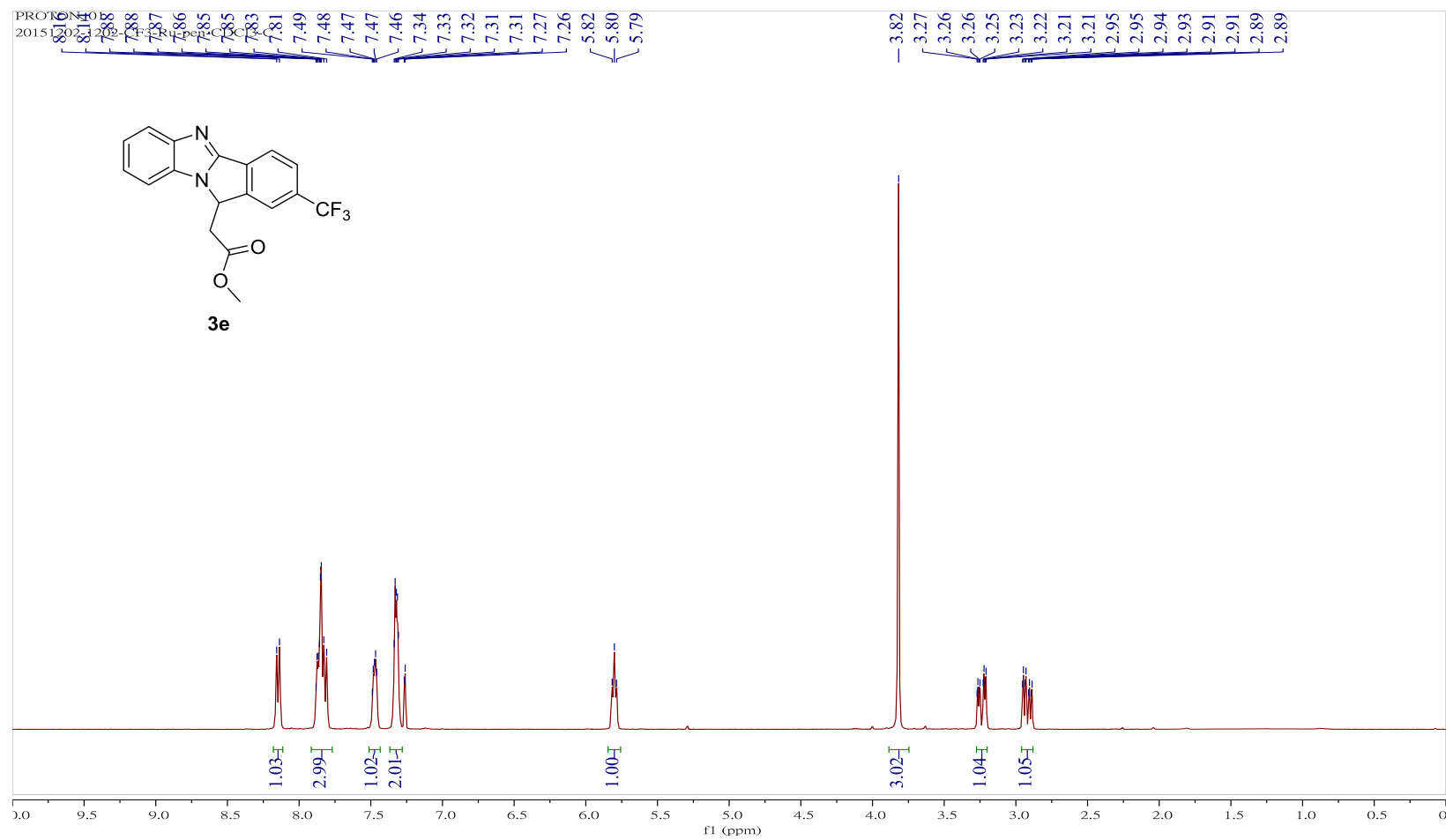


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
313.0741	1	C <sub>17</sub> H <sub>14</sub> ClN <sub>2</sub> O <sub>2</sub>	313.0738	0.7	23.5	1	100.00	11.5	even	ok	M+H

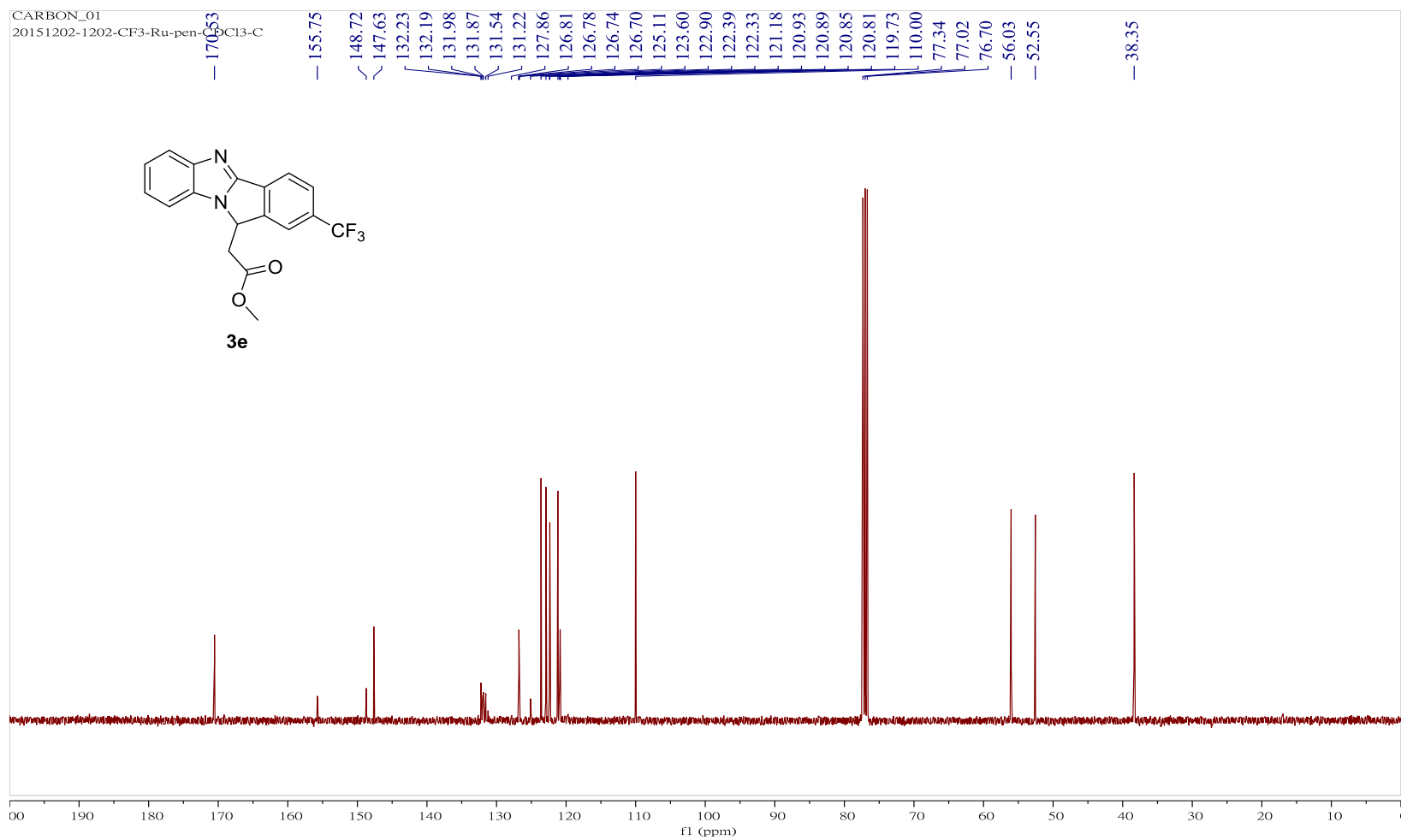
High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3d**



IR spectrum of compound of **3d**



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **3e** in CDCl<sub>3</sub>

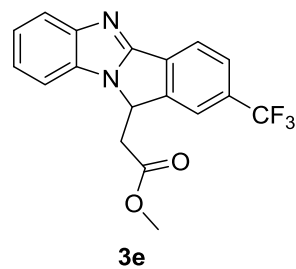
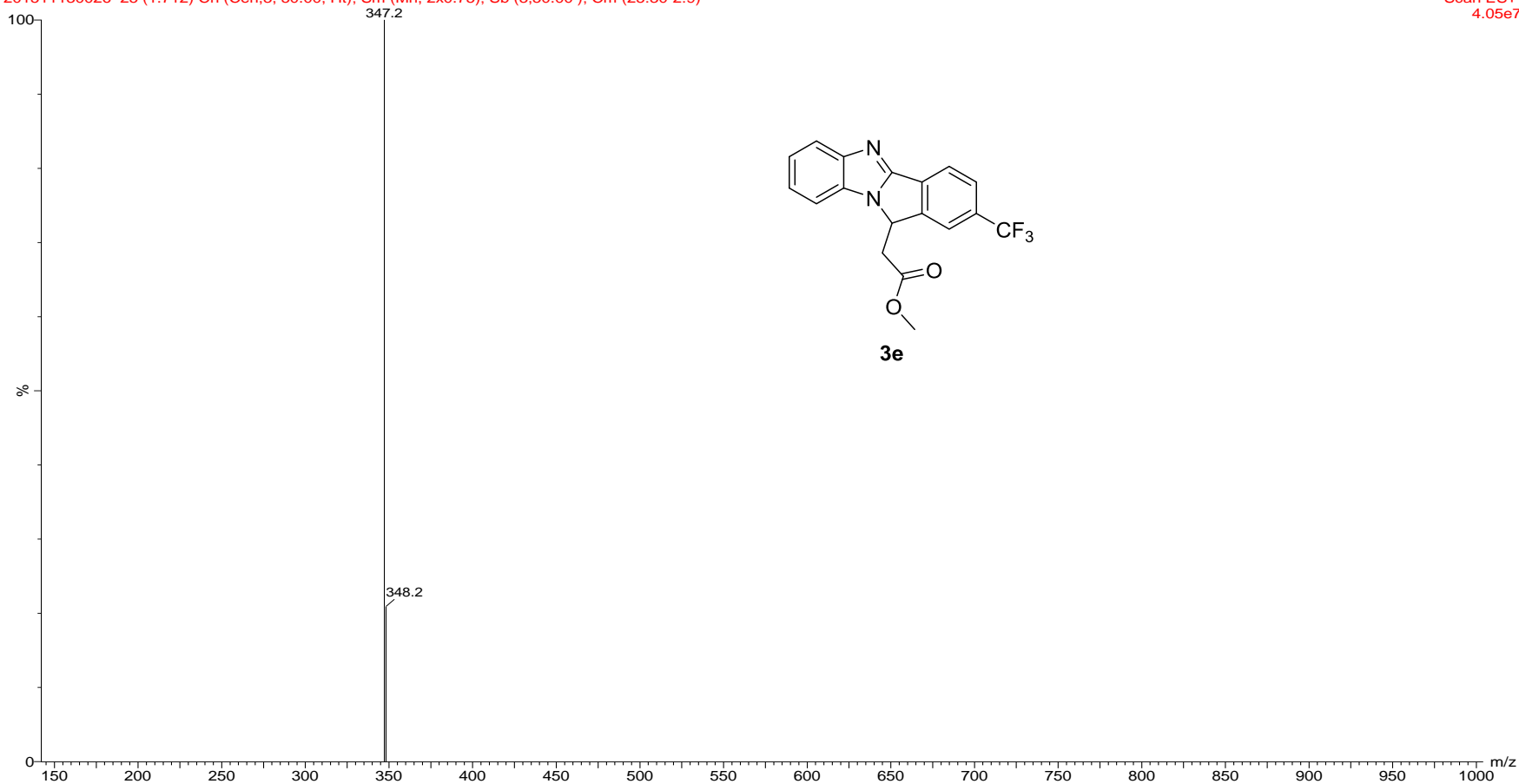


<sup>13</sup>C NMR Spectrum (100 MHz) of compound **3e** CDCl<sub>3</sub>

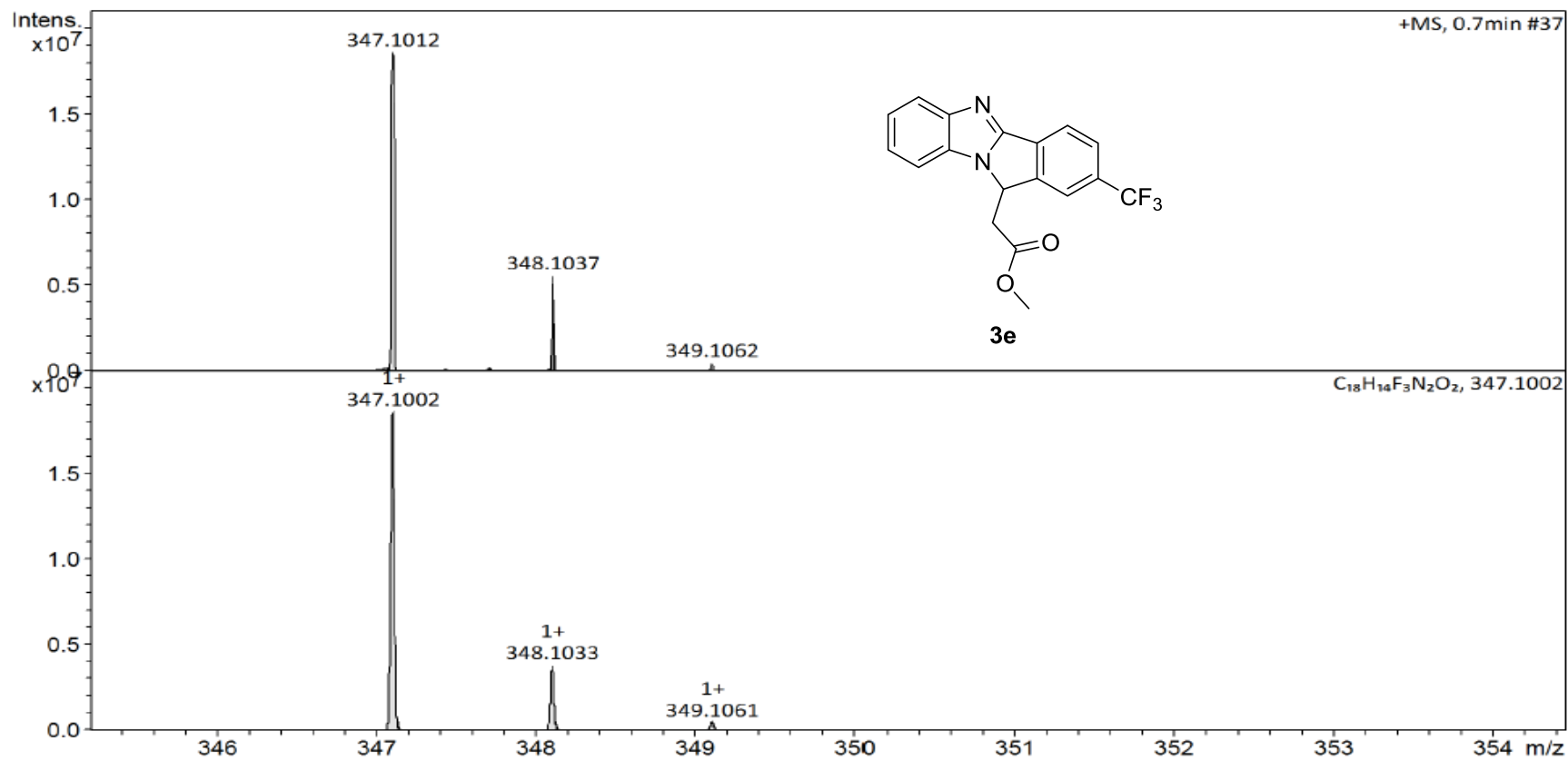
1109-CF3-Ru-6-8

201511130026 25 (1.712) Cn (Cen,3, 50.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00); Cm (25:30-2:9)

Scan ES+  
4.05e7



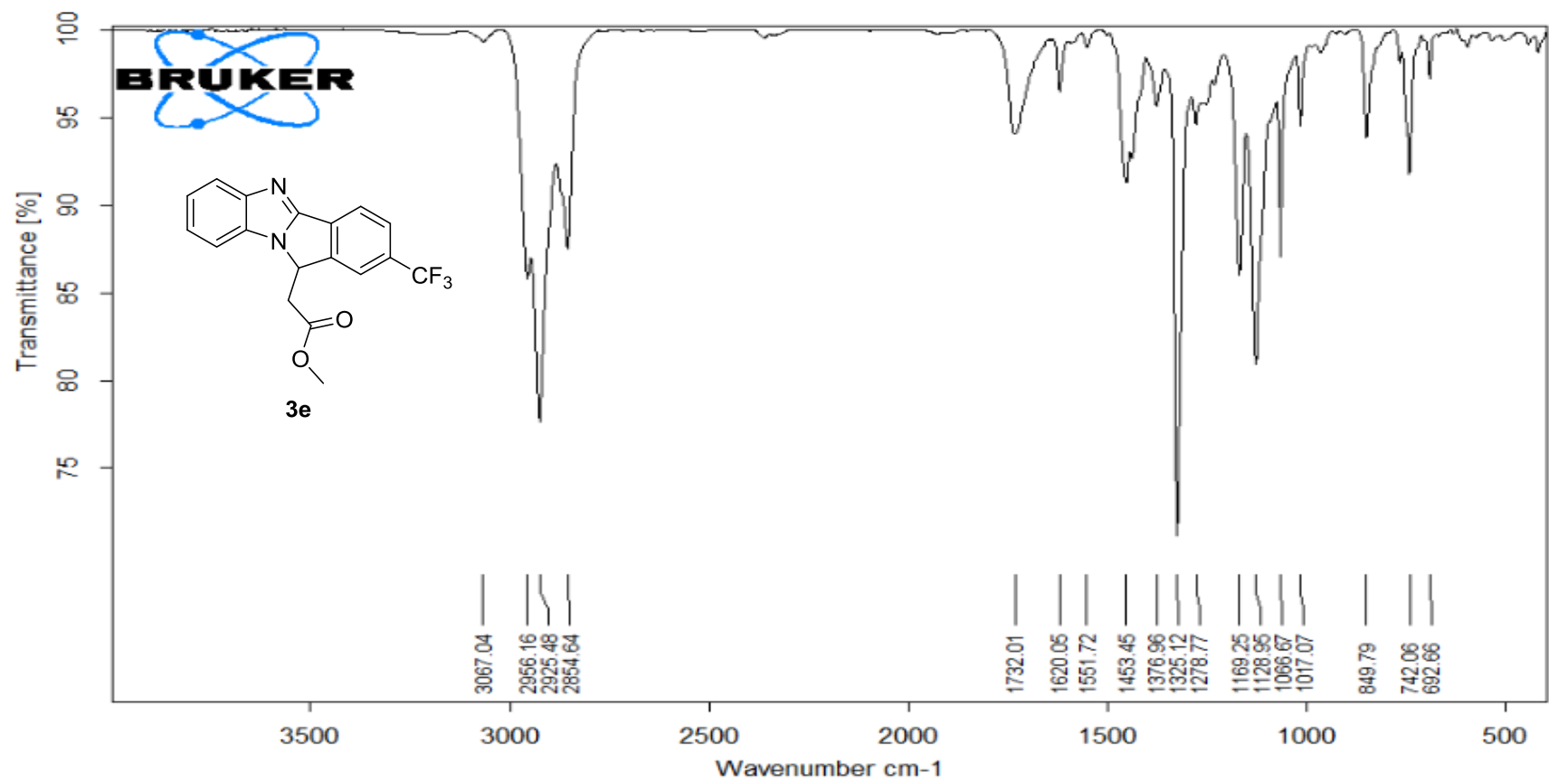
ESI<sup>+</sup> Mass spectrum of compound **3e**



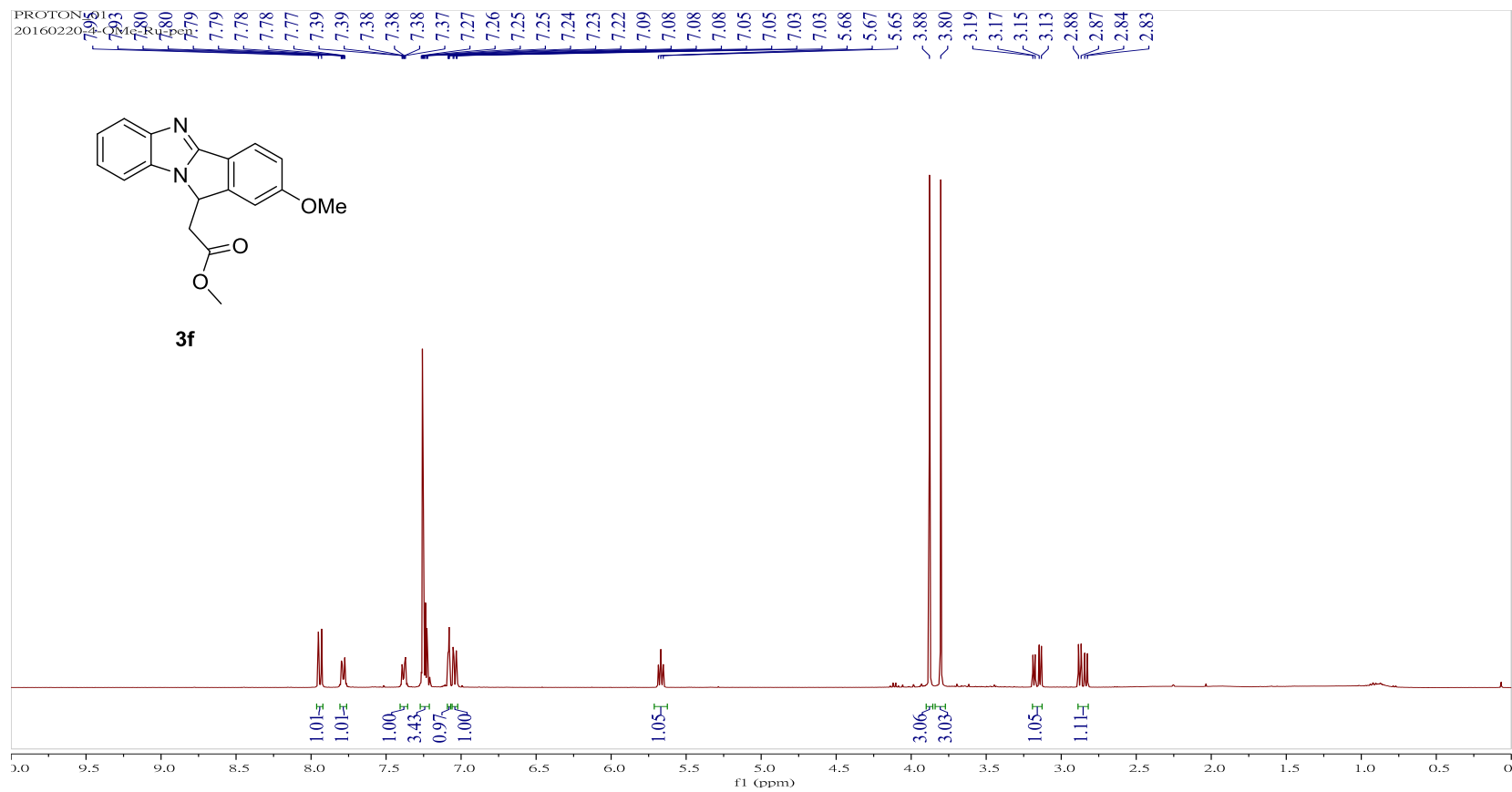
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
347.1012	1	C <sub>18</sub> H <sub>14</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>	347.1002	2.9	54.6	1	100.00	11.5	even	ok	M+H

High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3e**

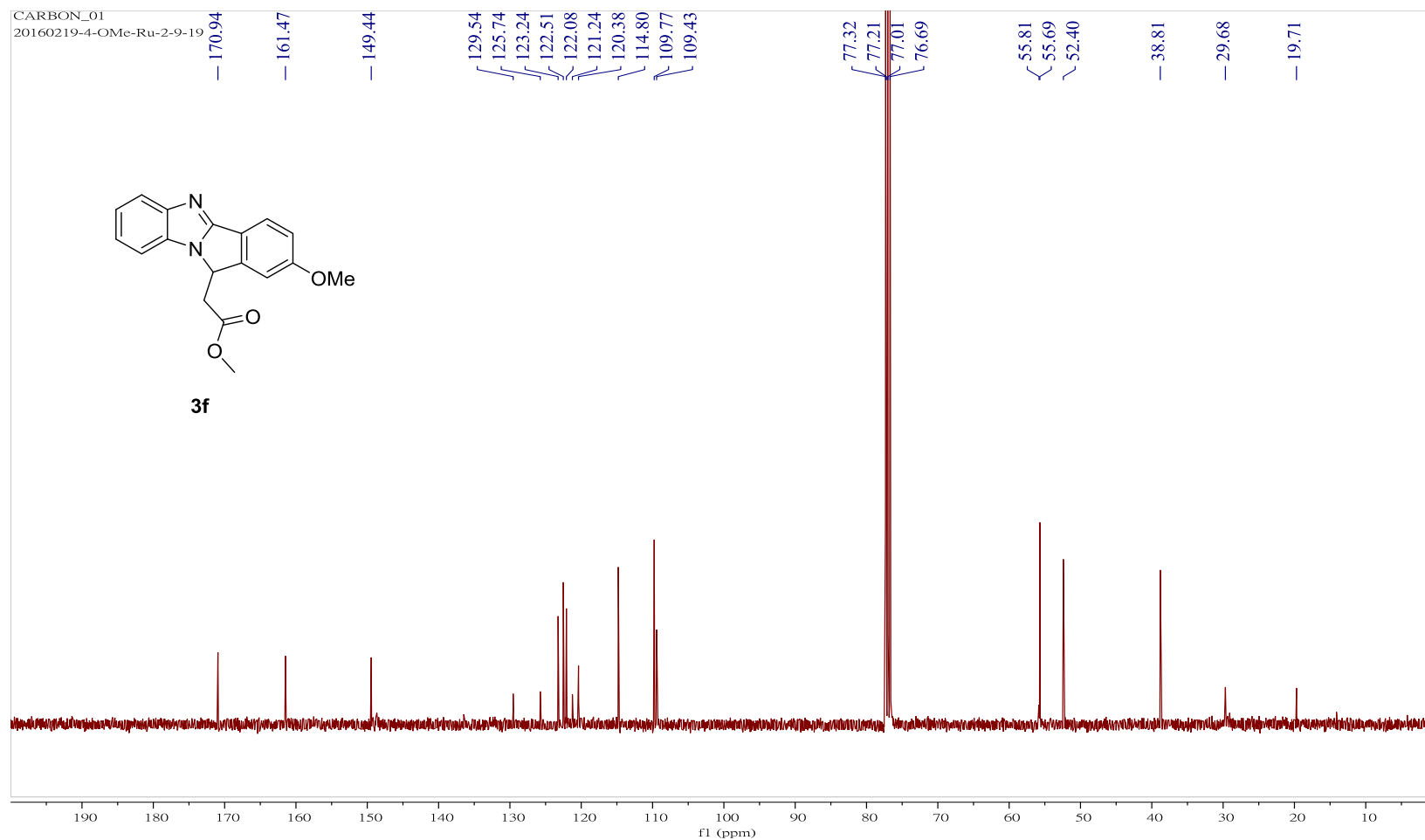




IR spectrum of compound of 3e



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **3f** in CDCl<sub>3</sub>

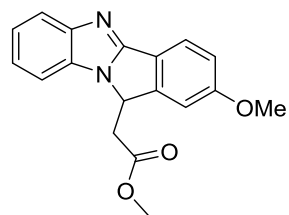
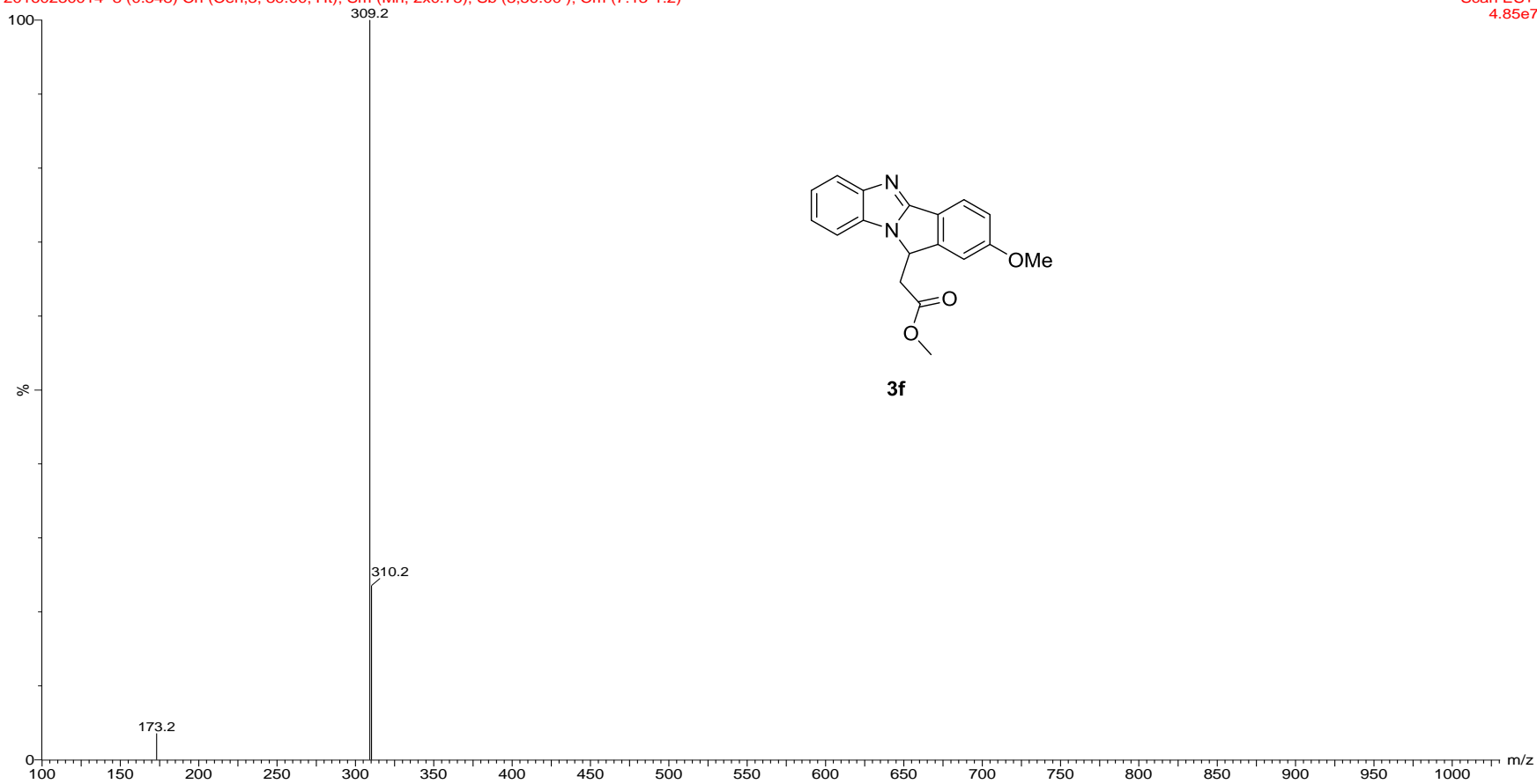


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3f** in  $\text{CDCl}_3$

4-OMe-Ru

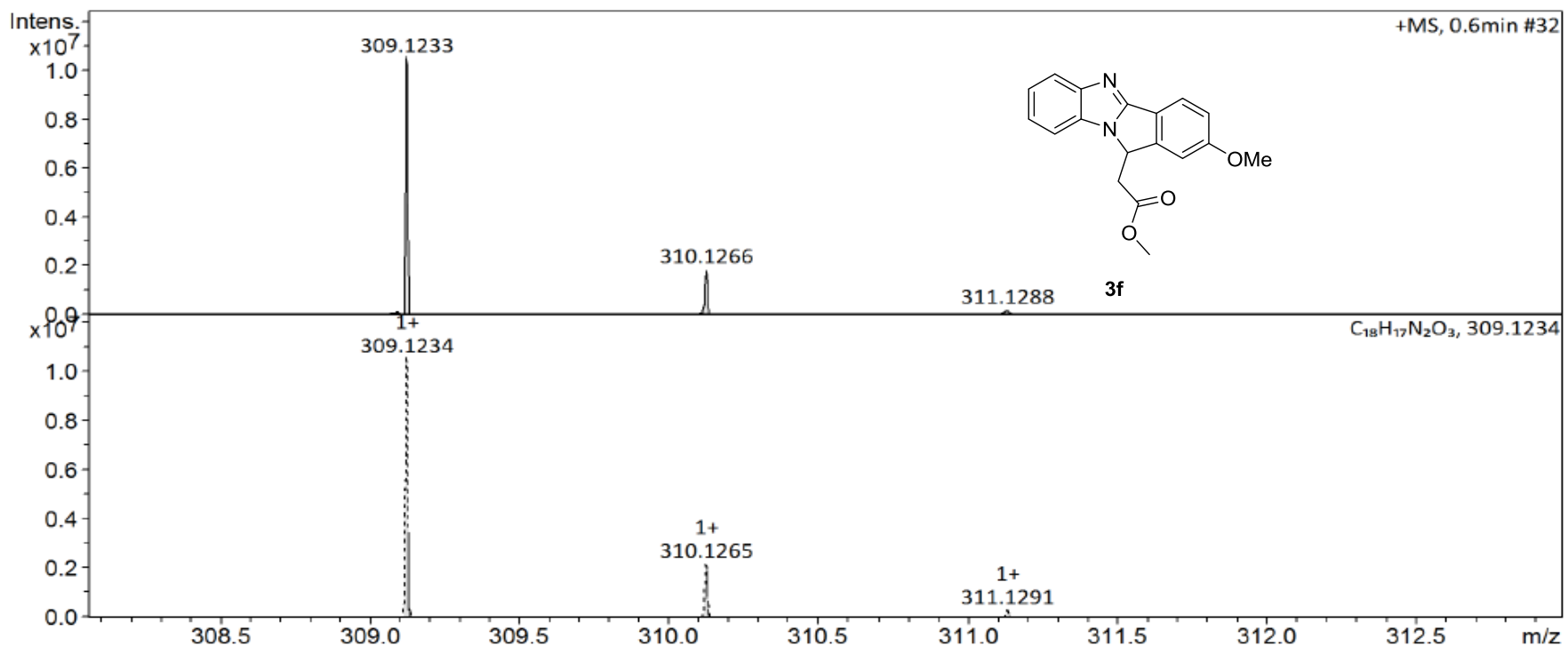
20160230014 8 (0.548) Cn (Cen,3, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00 ); Cm (7:13-1:2)

Scan ES+  
4.85e7



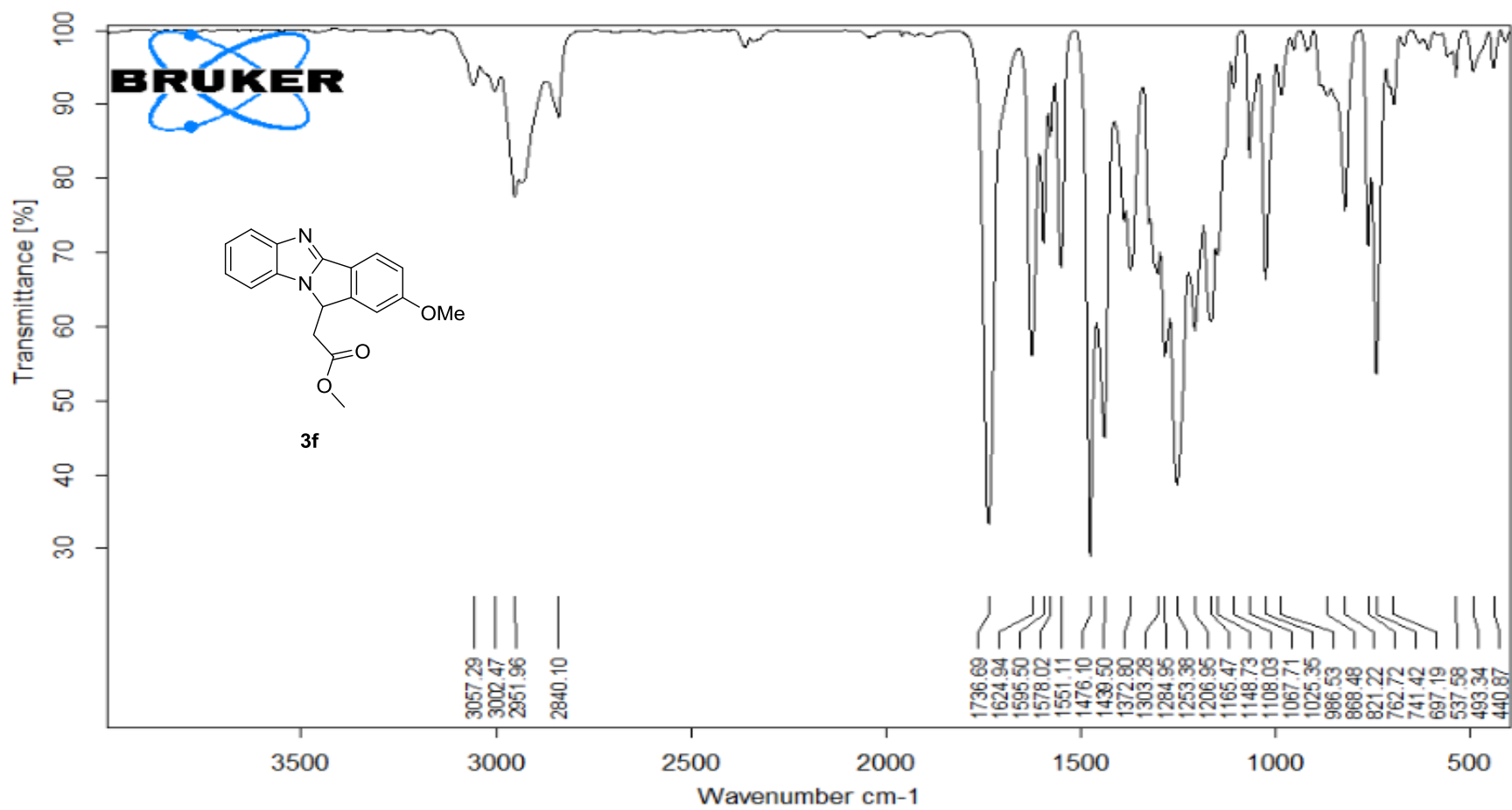
3f

ESI<sup>+</sup> Mass spectrum of compound 3f

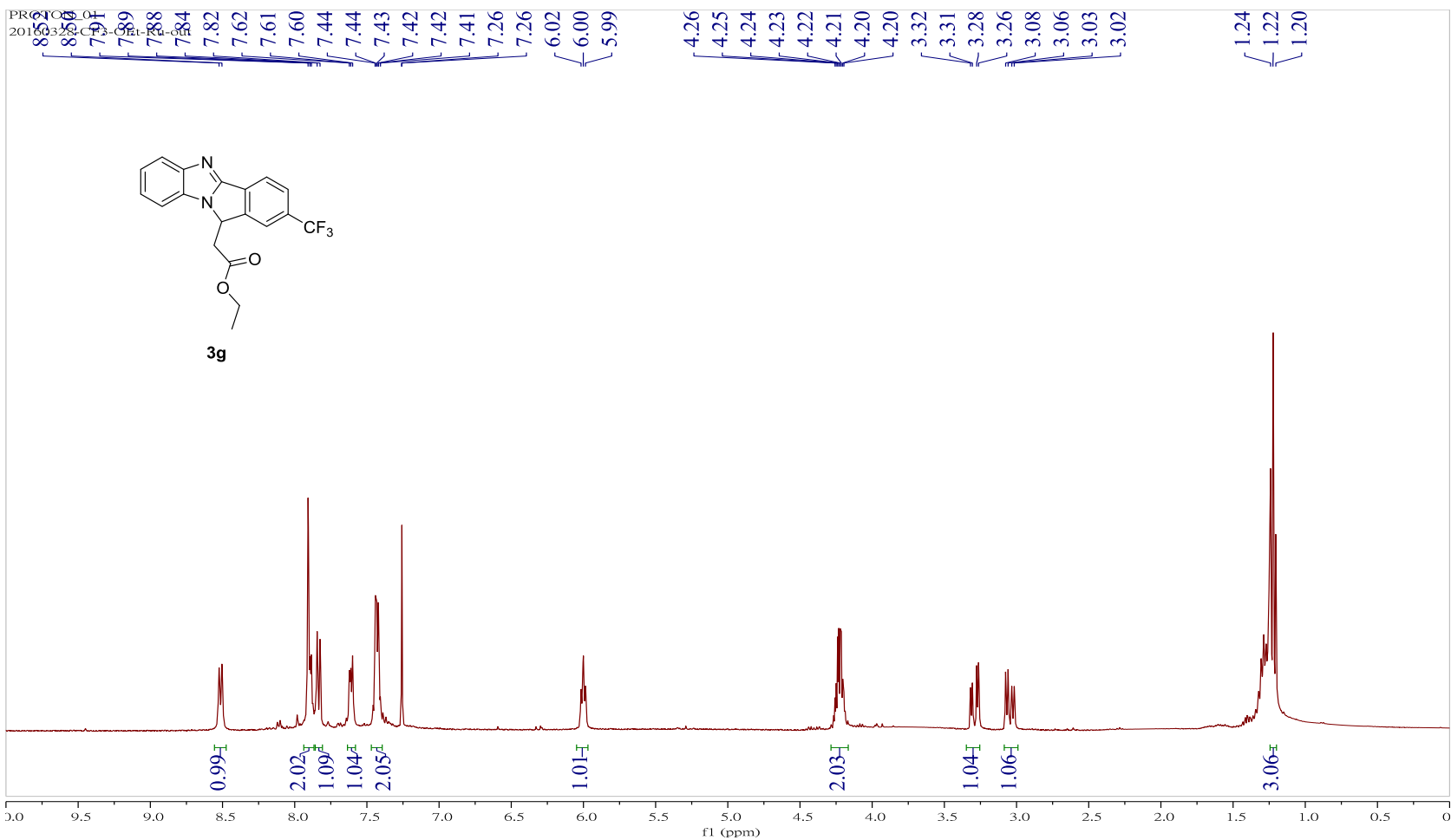


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
309.1233	1	C <sub>18</sub> H <sub>17</sub> N <sub>2</sub> O <sub>3</sub>	309.1234	-0.3	17.5	1	100.00	11.5	even	ok	M+H

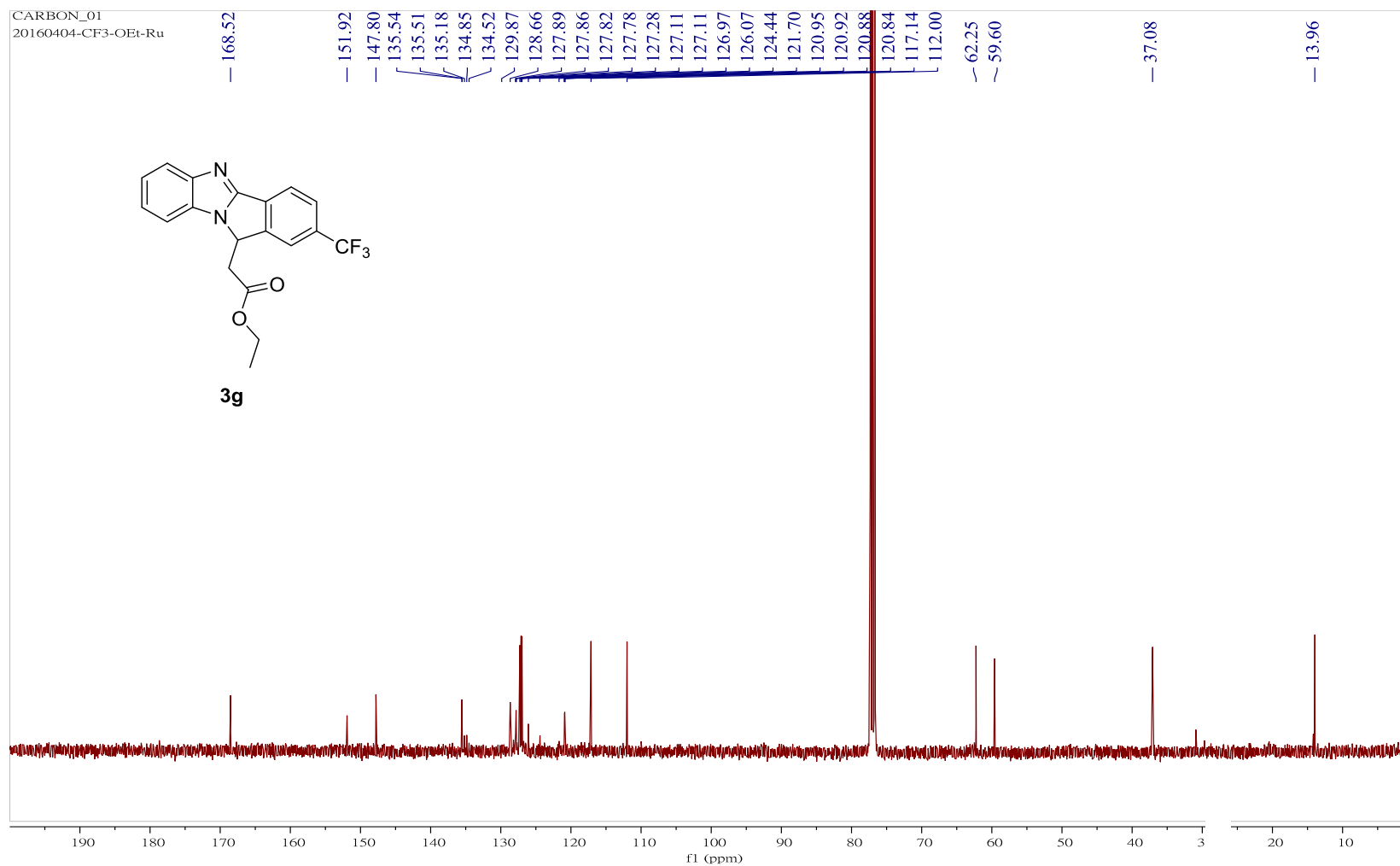
High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3f**



IR spectrum of compound of 3f



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **3g** in CDCl<sub>3</sub>



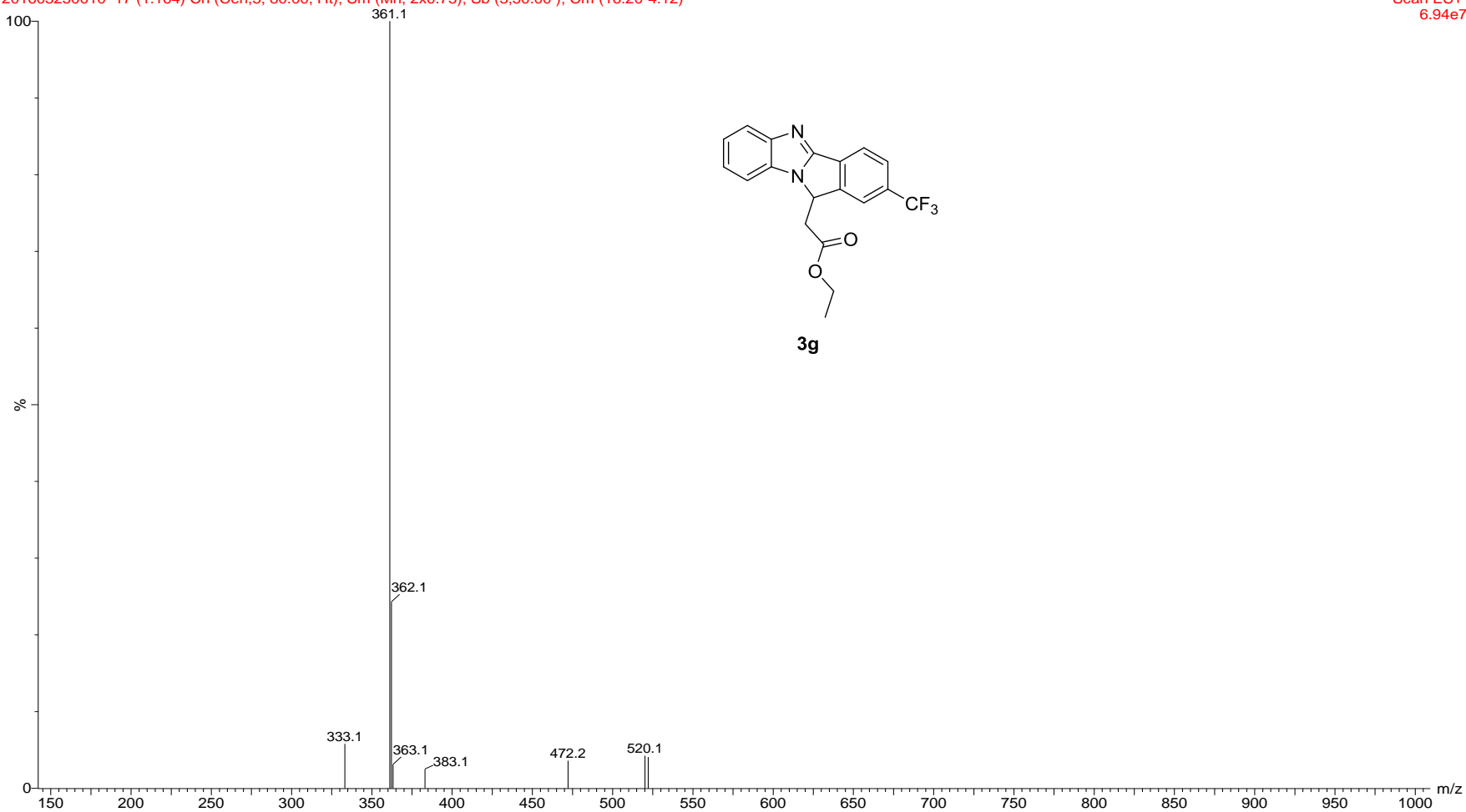
$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3g** in  $\text{CDCl}_3$



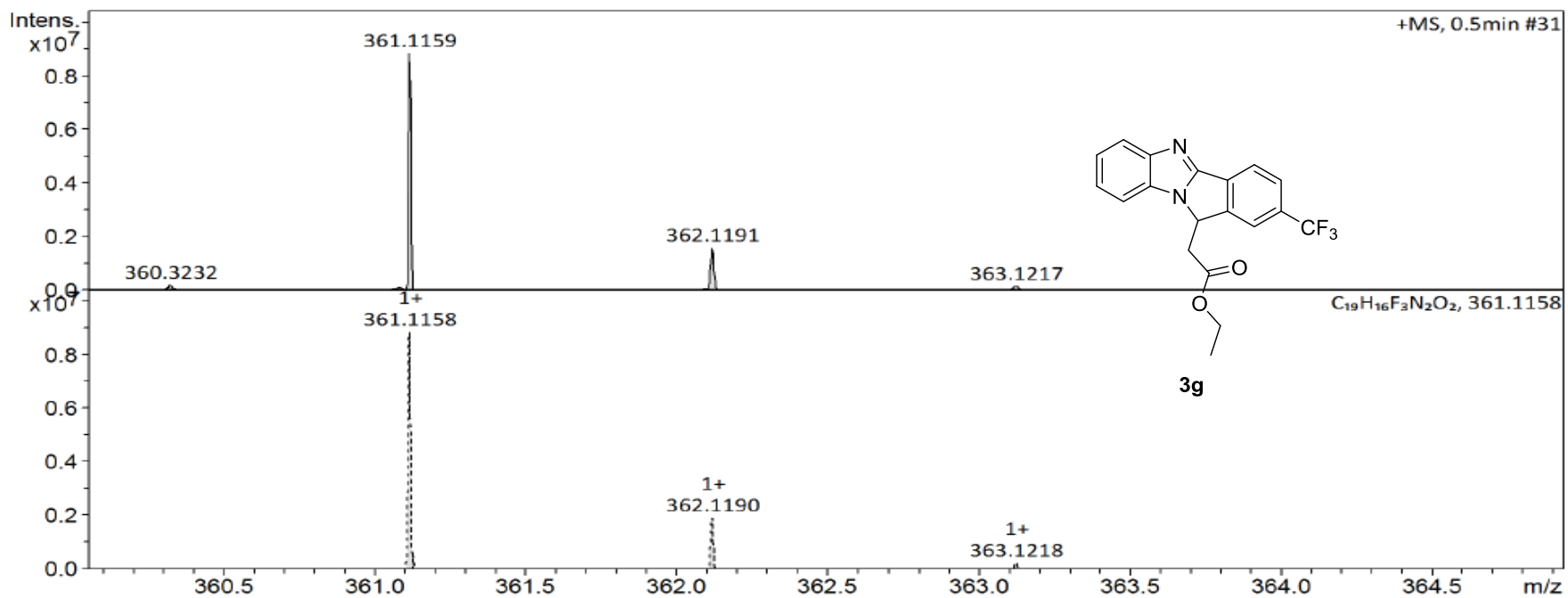
CF3-OEt-Ru

201603250010 17 (1.164) Cn (Cen,3, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00 ); Cm (16:20-4:12)

Scan ES+  
6.94e7

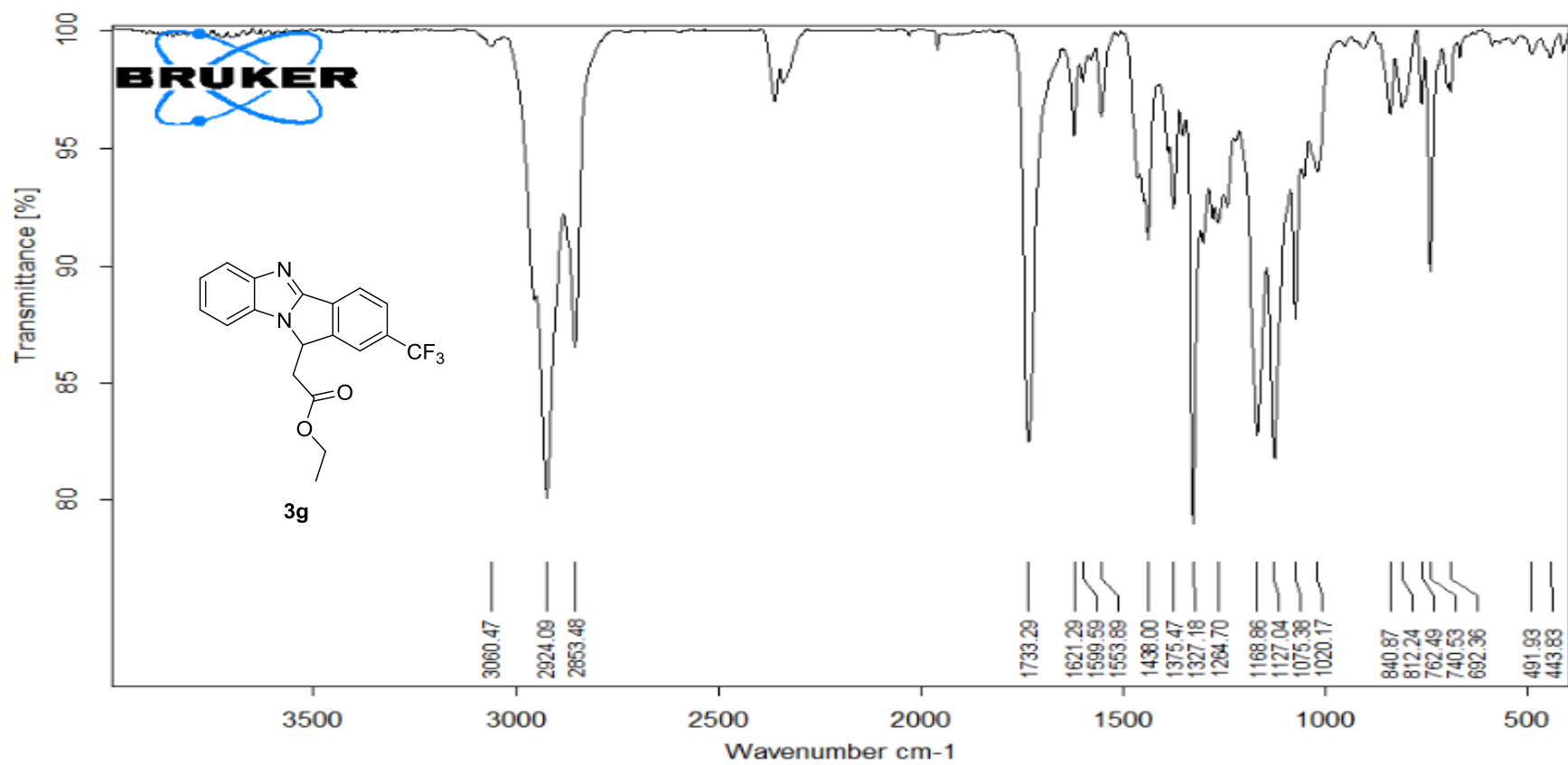


ESI<sup>+</sup> Mass spectrum of compound **3g**

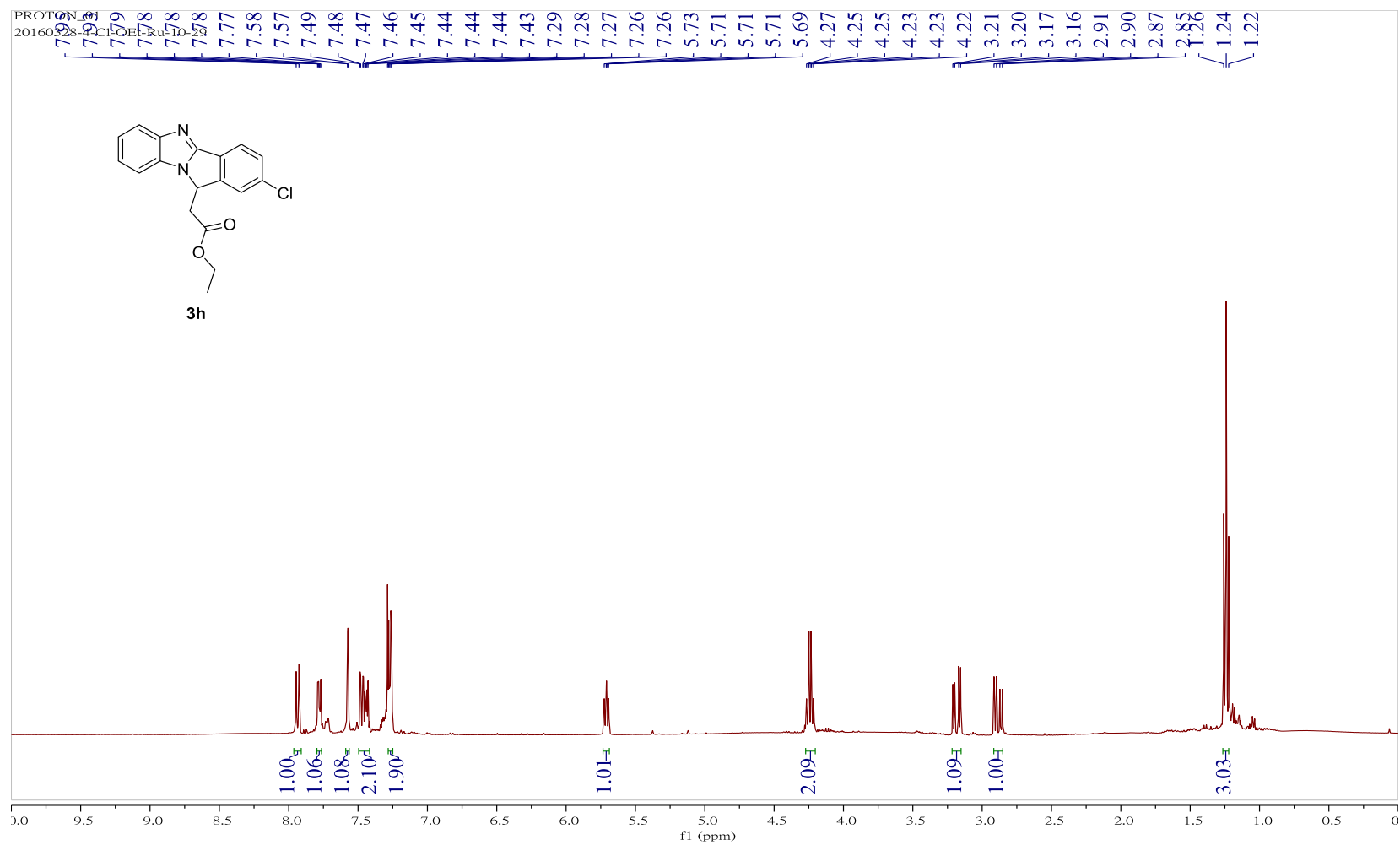


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
361.1159	1	C <sub>19</sub> H <sub>16</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>	361.1158	0.3	20.4	1	100.00	11.5	even	ok	M+H

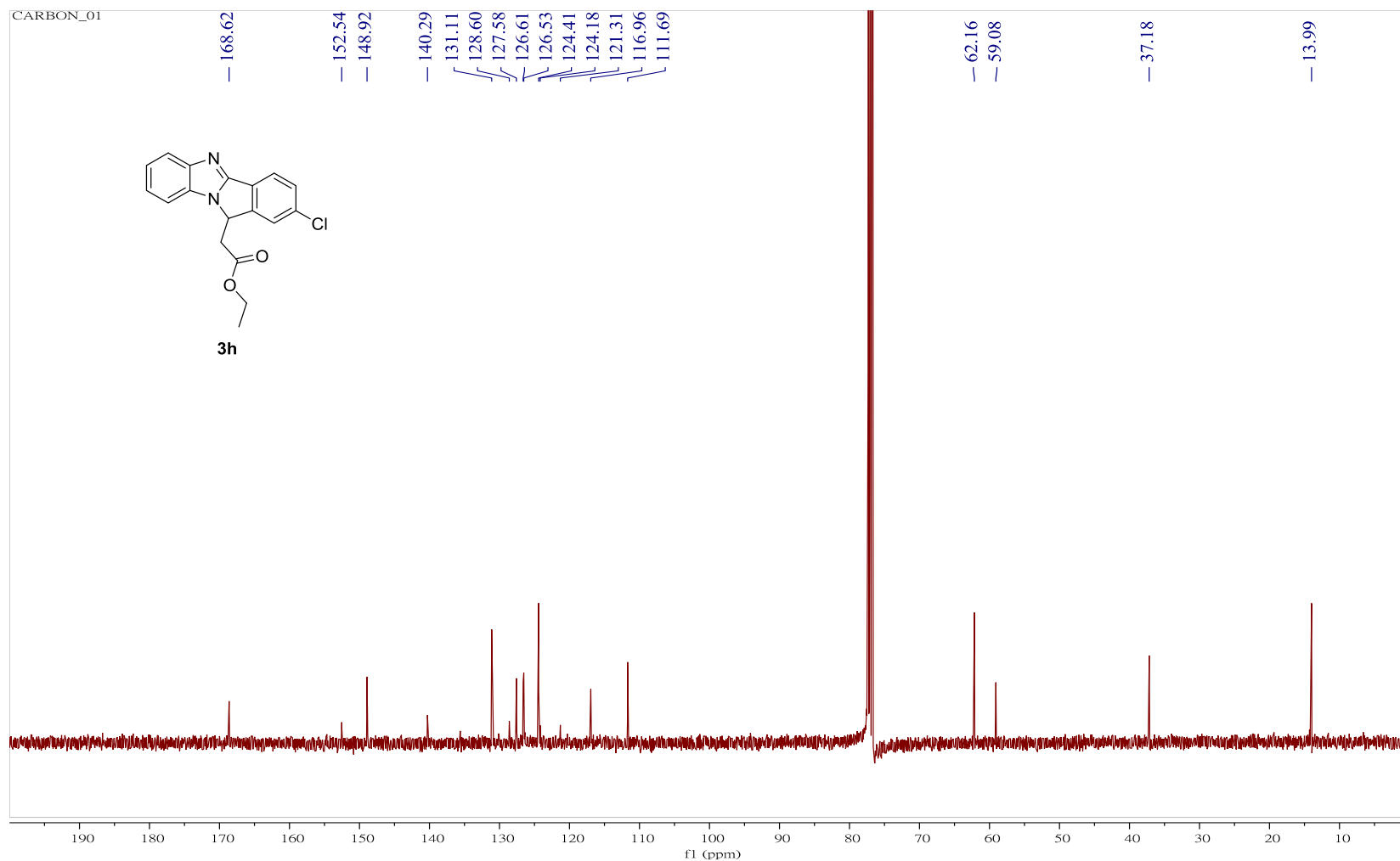
High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3g**



IR spectrum of compound of **3g**



$^1\text{H}$  NMR Spectrum (400 MHz) of compound **3h** in  $\text{CDCl}_3$

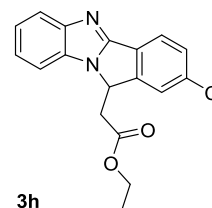
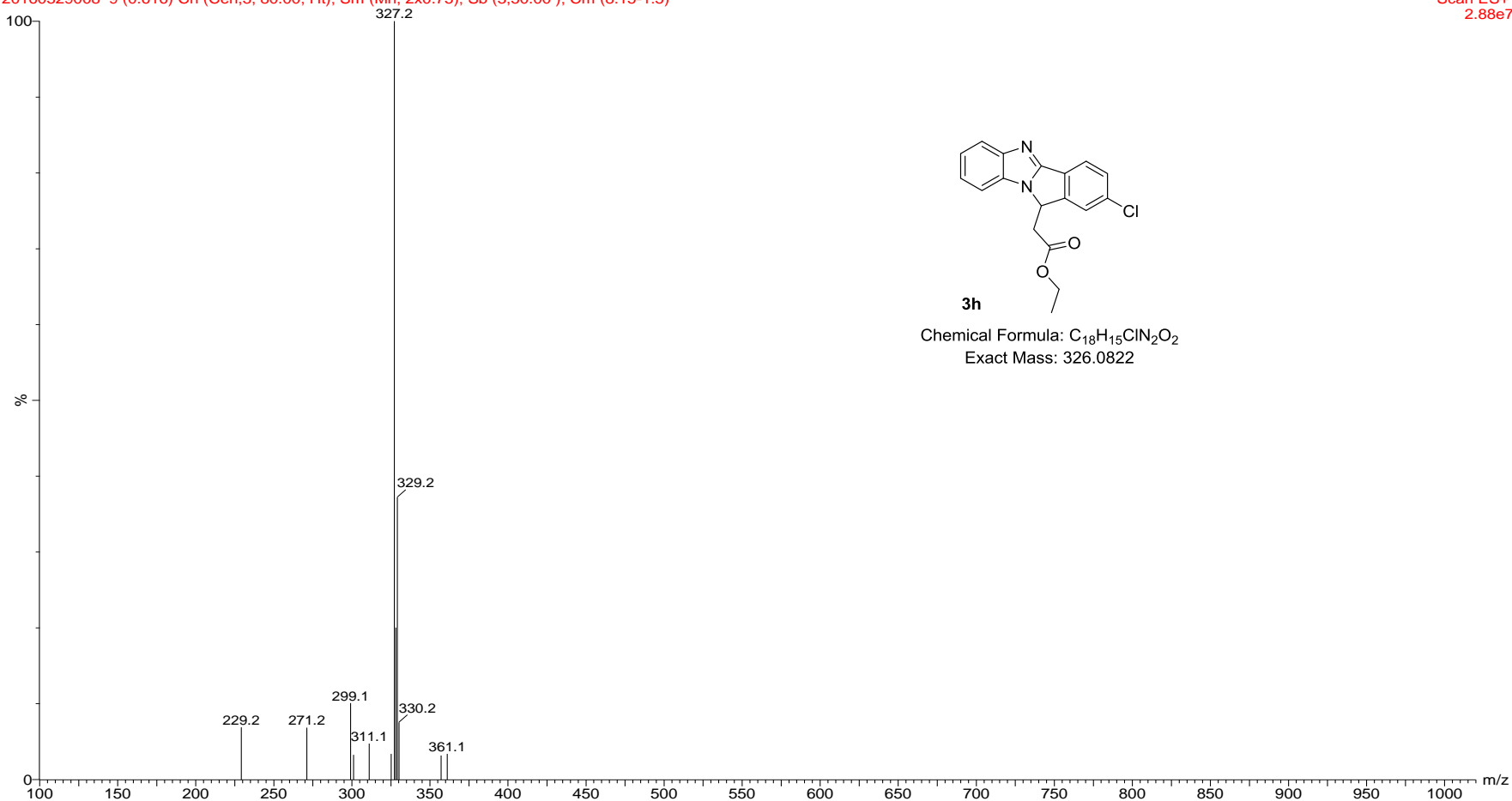


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3h** in  $\text{CDCl}_3$

**4-Cl-OEt-Ru**

20160329008 9 (0.616) Cn (Cen,3, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00 ); Cm (8:15-1:5)

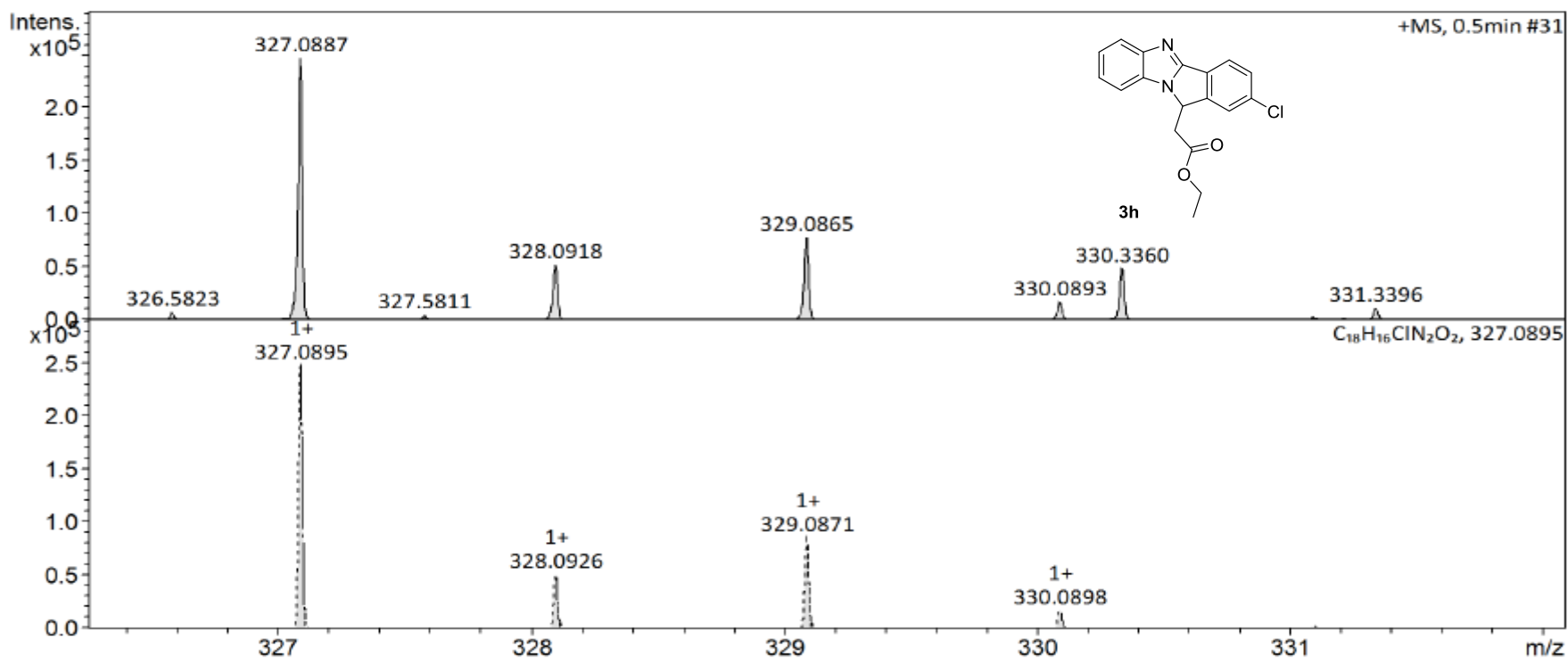
Scan ES+  
2.88e7



Chemical Formula: C<sub>18</sub>H<sub>15</sub>ClN<sub>2</sub>O<sub>2</sub>

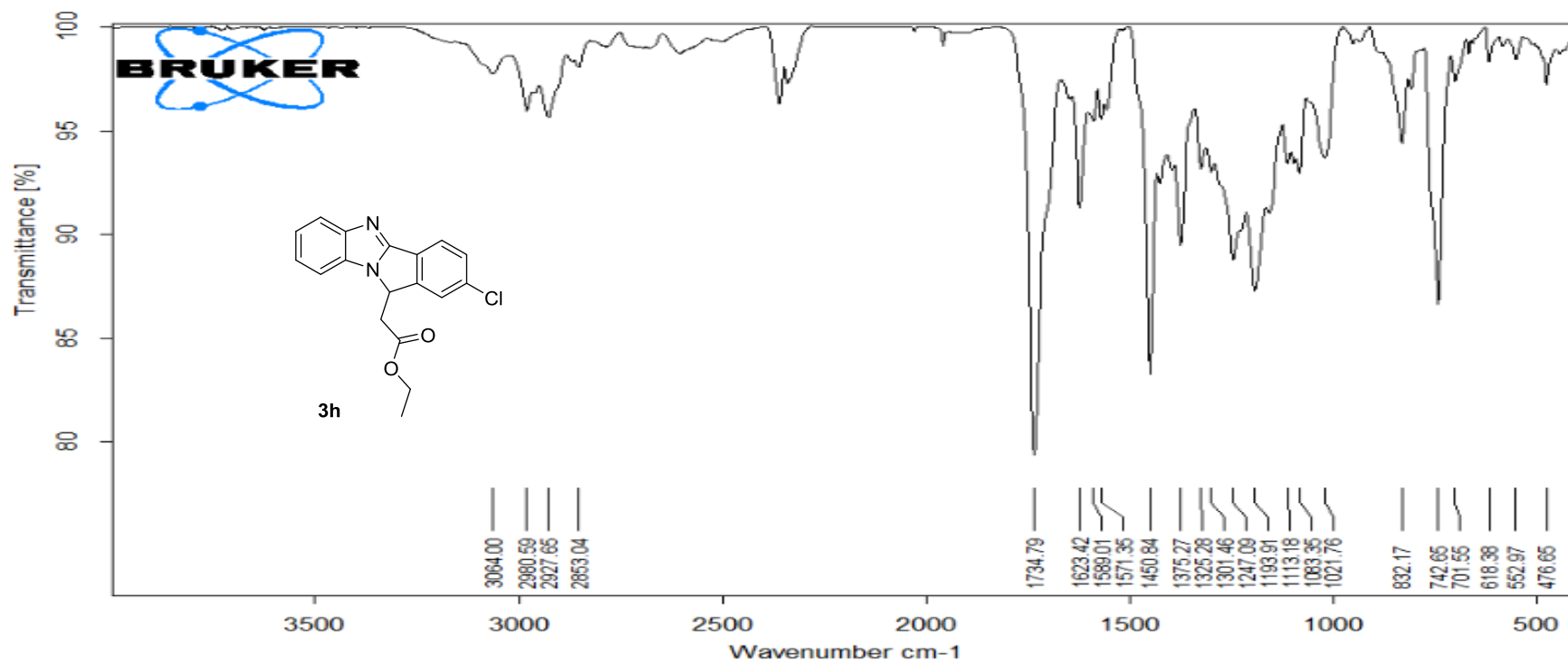
Exact Mass: 326.0822

ESI<sup>+</sup> Mass spectrum of compound **3h**



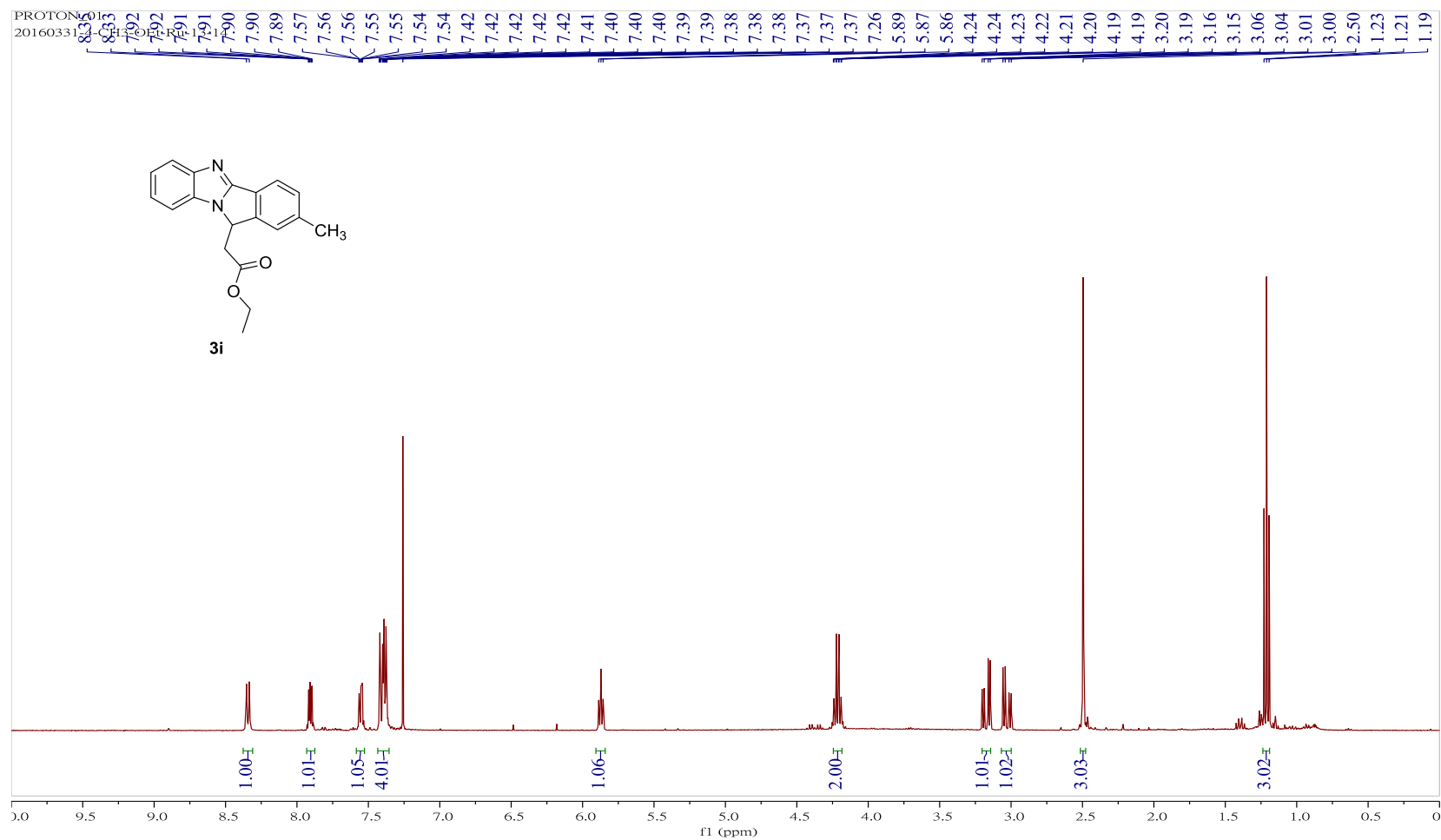
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
327.0887	1	C <sub>18</sub> H <sub>16</sub> ClN <sub>2</sub> O <sub>2</sub>	327.0895	2.3	14.1	1	100.00	11.5	even	ok	M+H

High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3h**

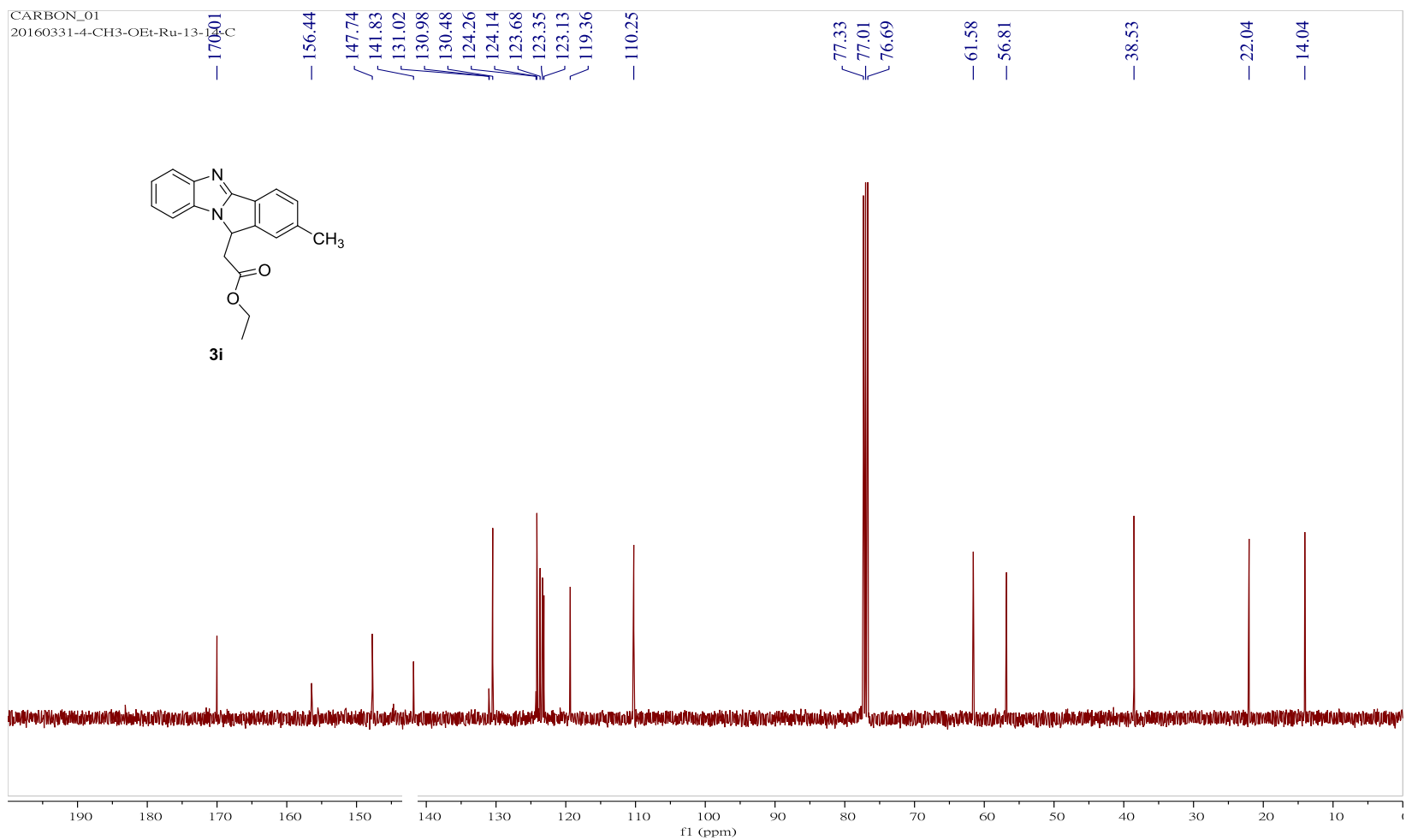


IR spectrum of compound of **3h**





$^1\text{H}$  NMR Spectrum (400 MHz) of compound **3i** in  $\text{CDCl}_3$

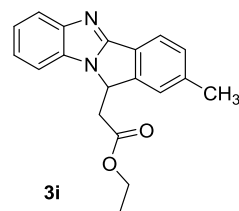
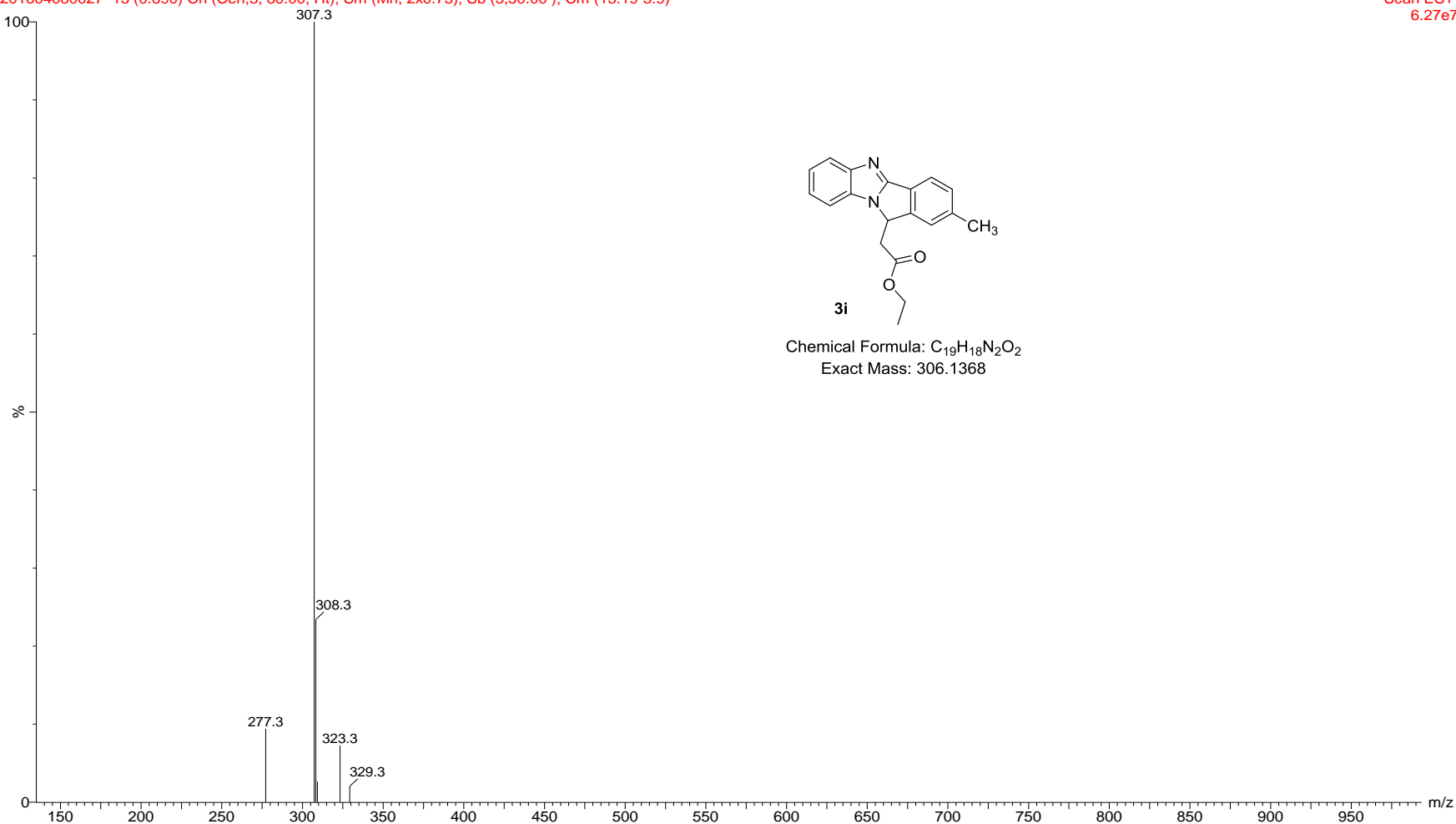


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3i** in  $\text{CDCl}_3$

4-CH3-OEt-Ru

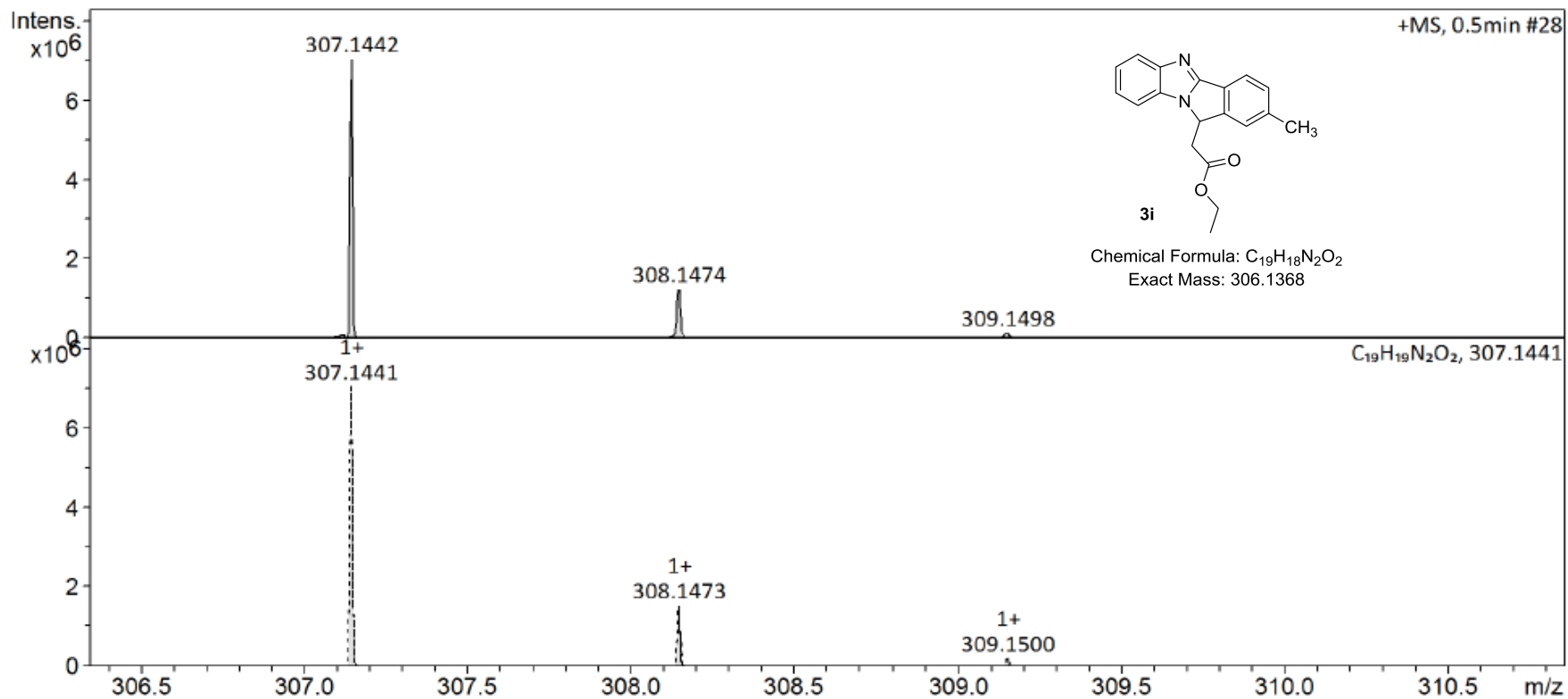
201604080027 13 (0.890) Cn (Cen,3, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00); Cm (13:19-3:9)

Scan ES+  
6.27e7



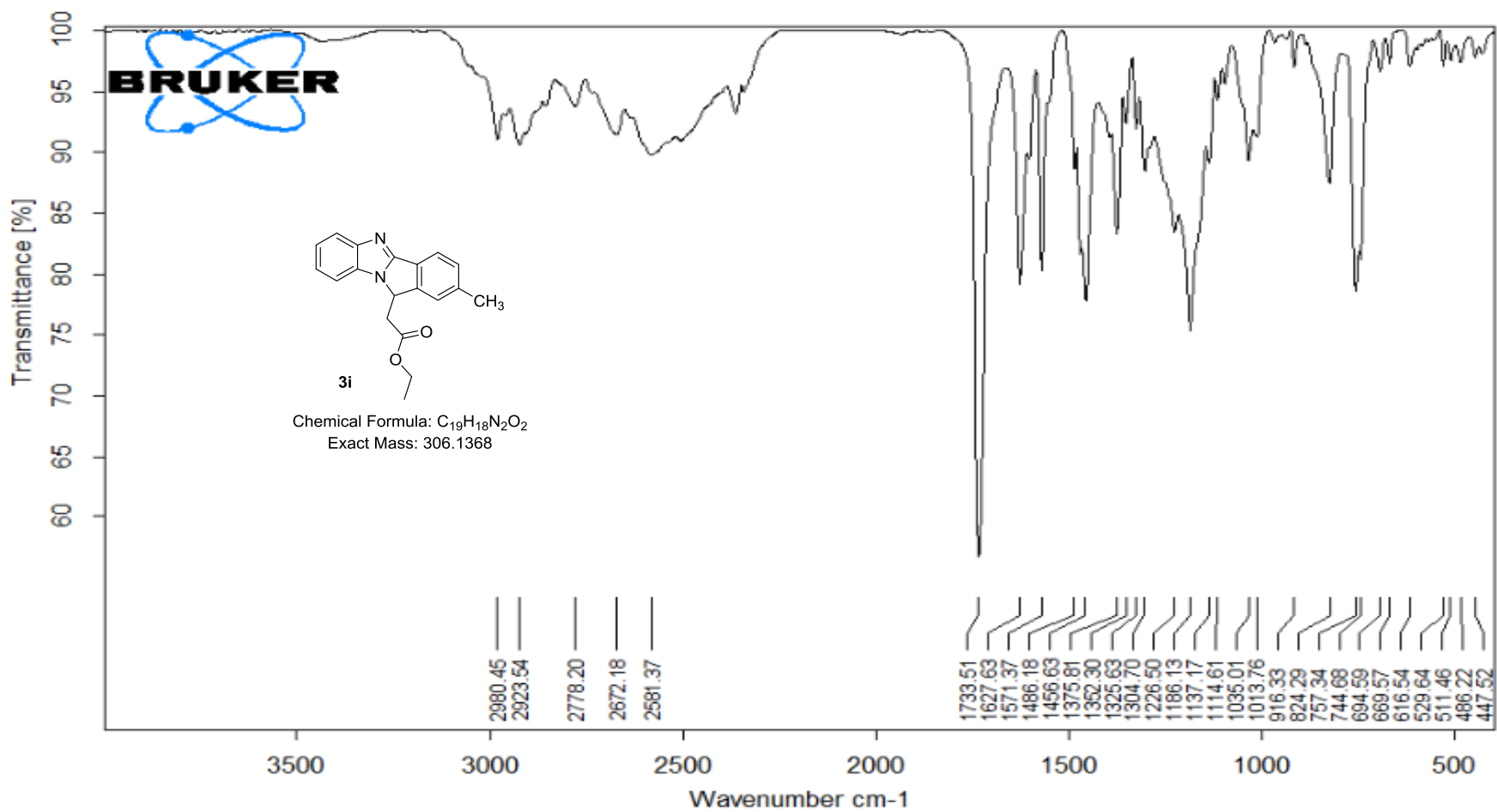
Chemical Formula: C<sub>19</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>  
Exact Mass: 306.1368

ESI<sup>+</sup> Mass spectrum of compound **3i**

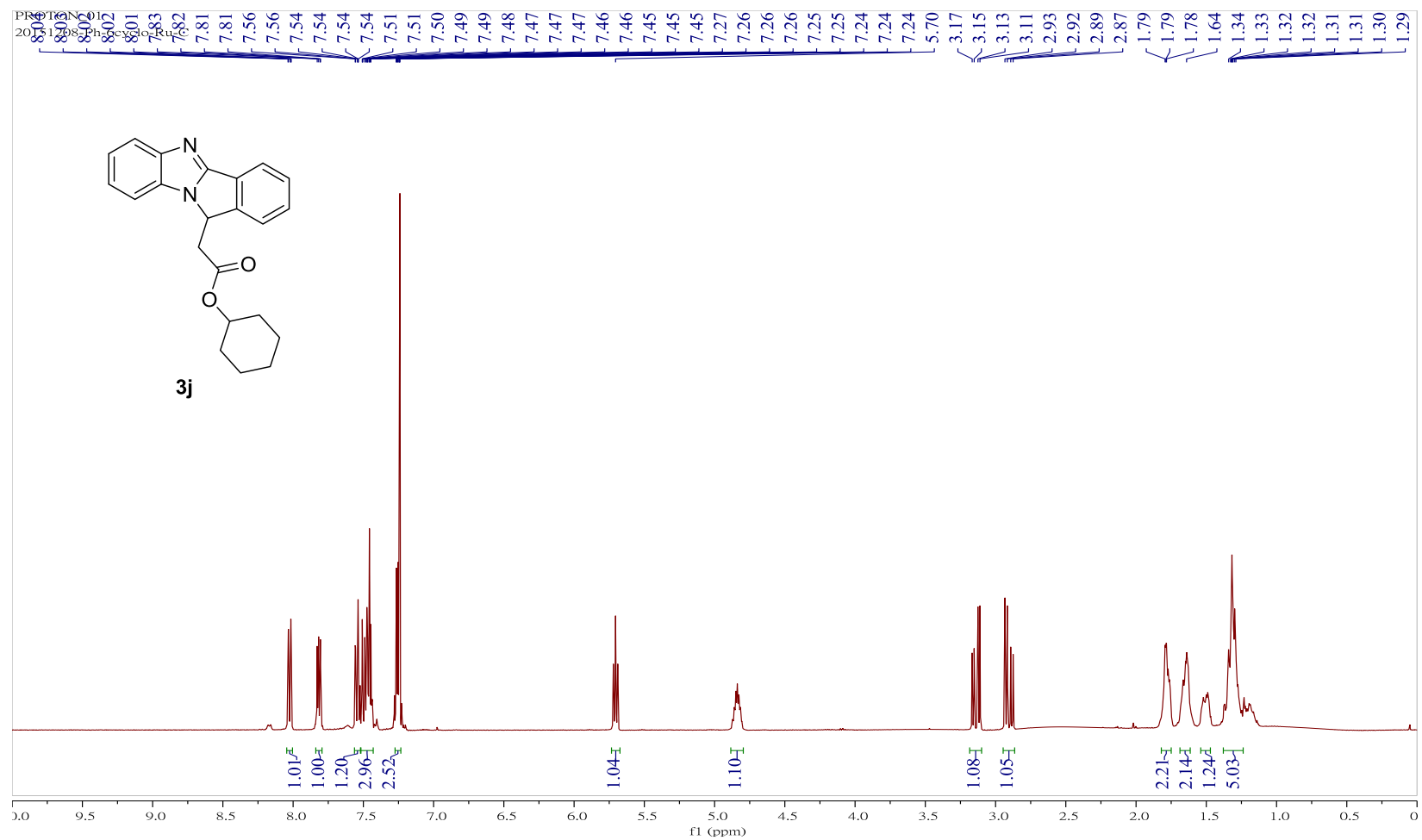


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
307.1442	1	C <sub>19</sub> H <sub>19</sub> N <sub>2</sub> O <sub>2</sub>	307.1441	0.4	24.5	1	100.00	11.5	even	ok	M+H

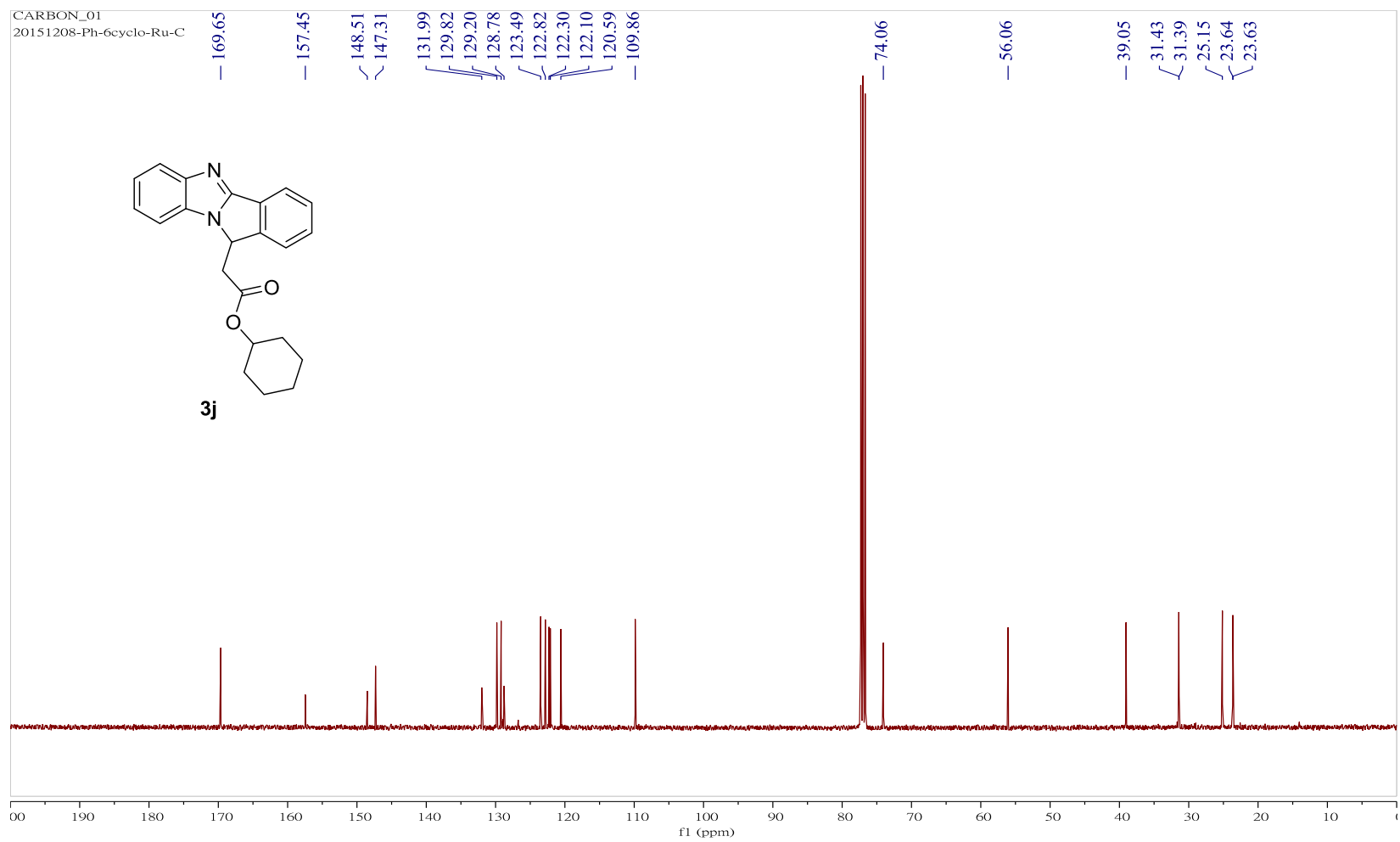
High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3i**



IR spectrum of compound of **3i**



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **3j** in CDCl<sub>3</sub>

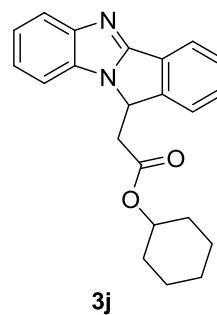
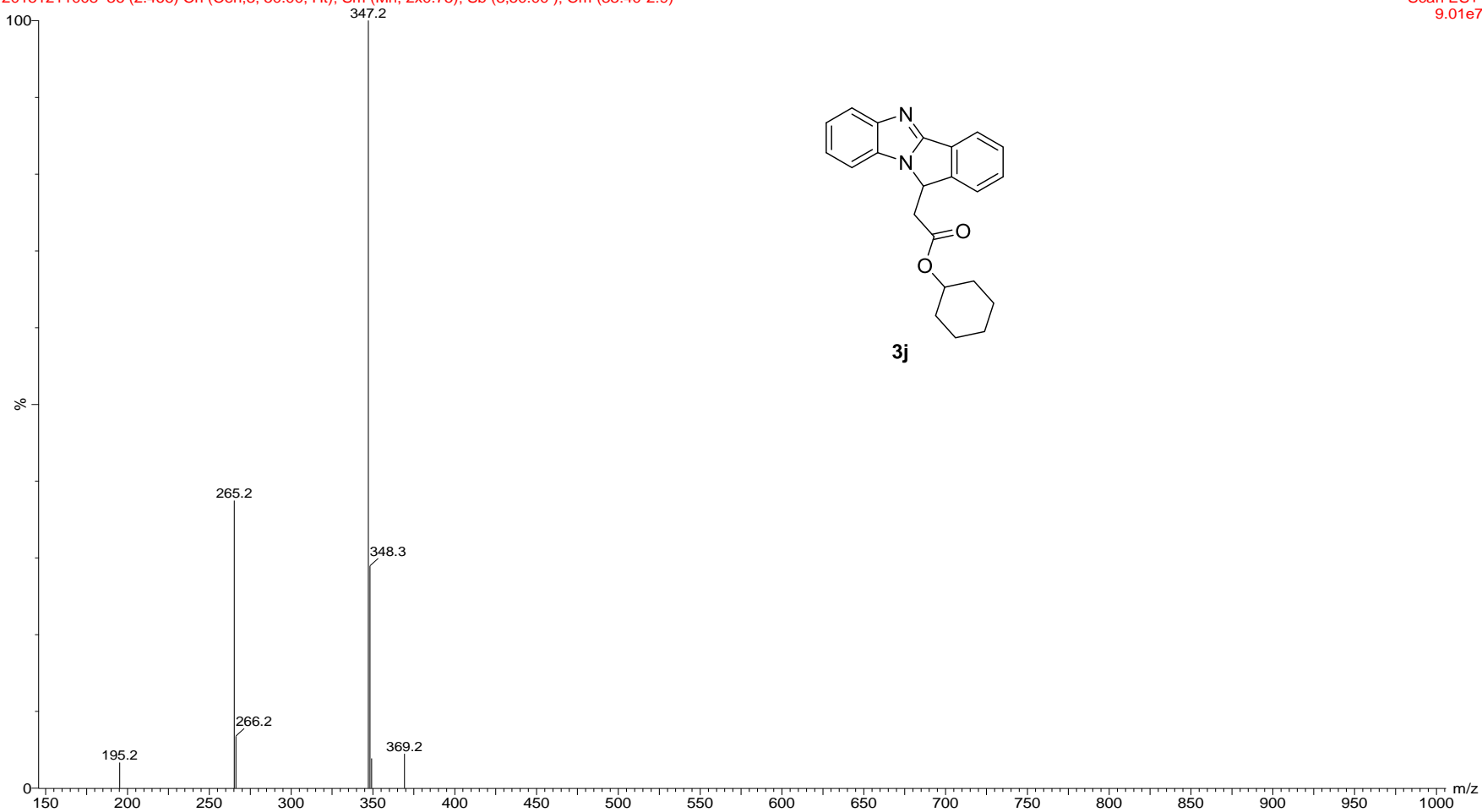


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3j** in  $\text{CDCl}_3$

**Ph-6cyclo-Ru**

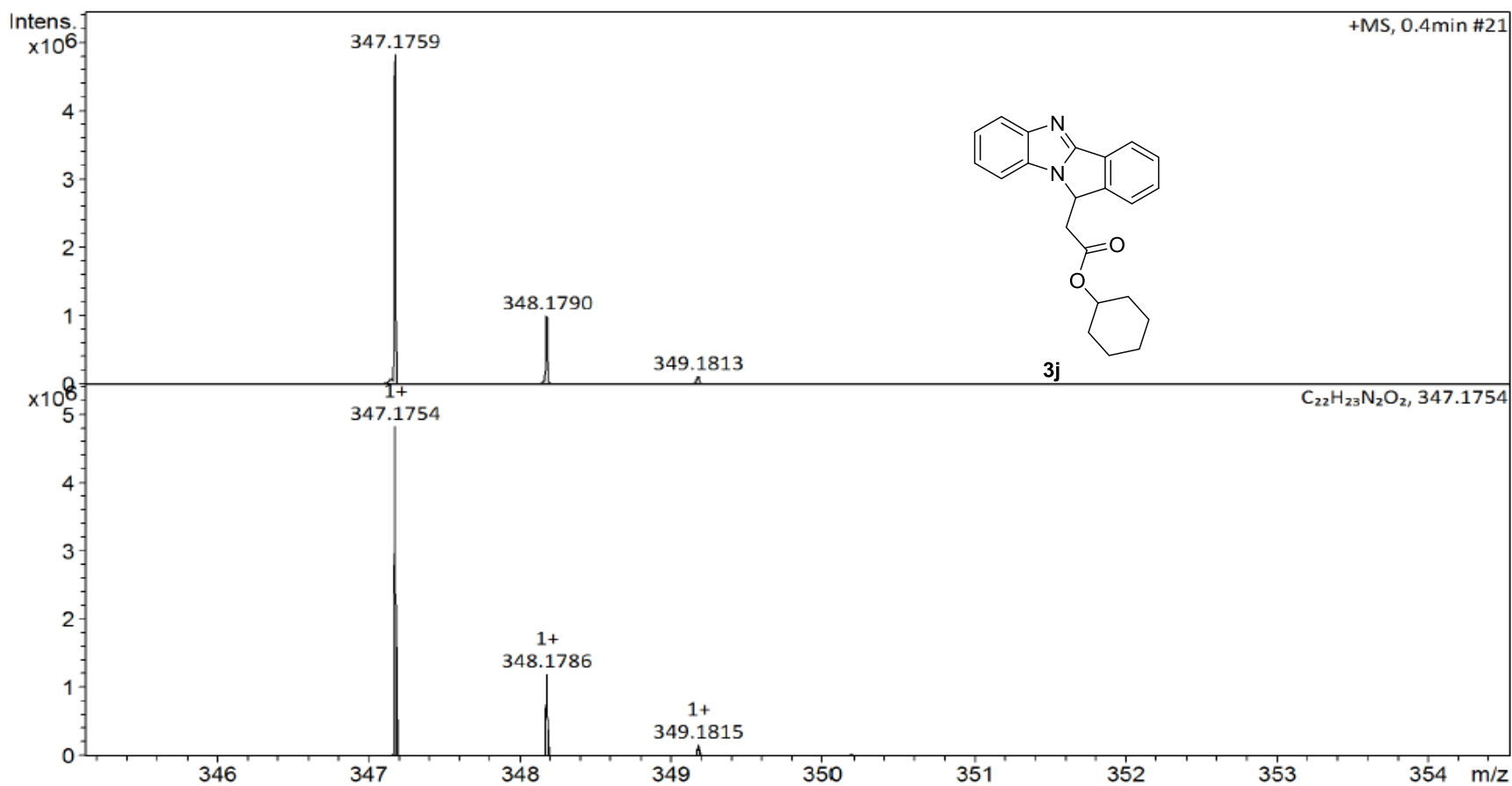
20151211008 36 (2.466) Cn (Cen,3, 50.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00 ); Cm (33:40-2:9)

Scan ES+  
9.01e7



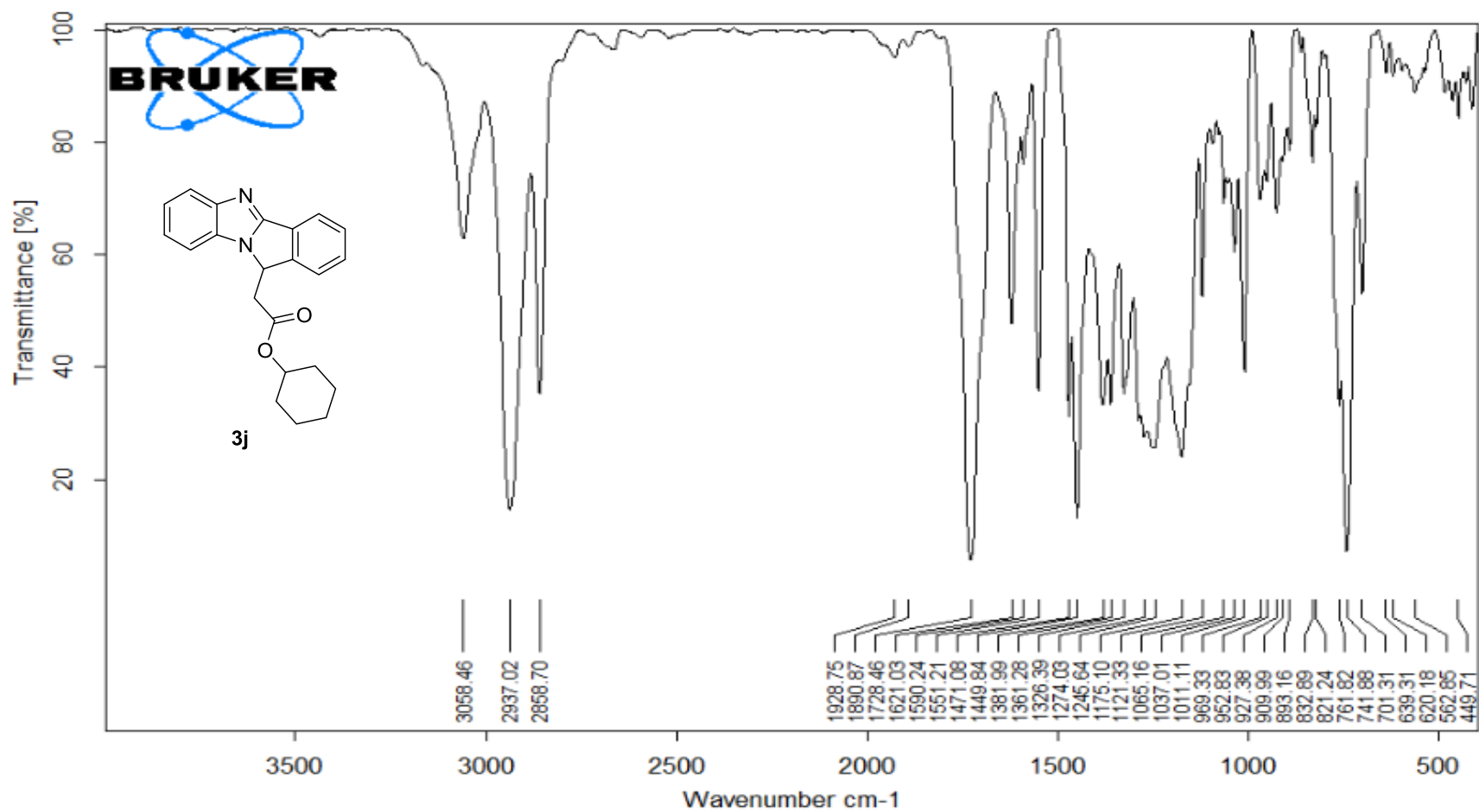
ESI<sup>+</sup> Mass spectrum of compound **3j**



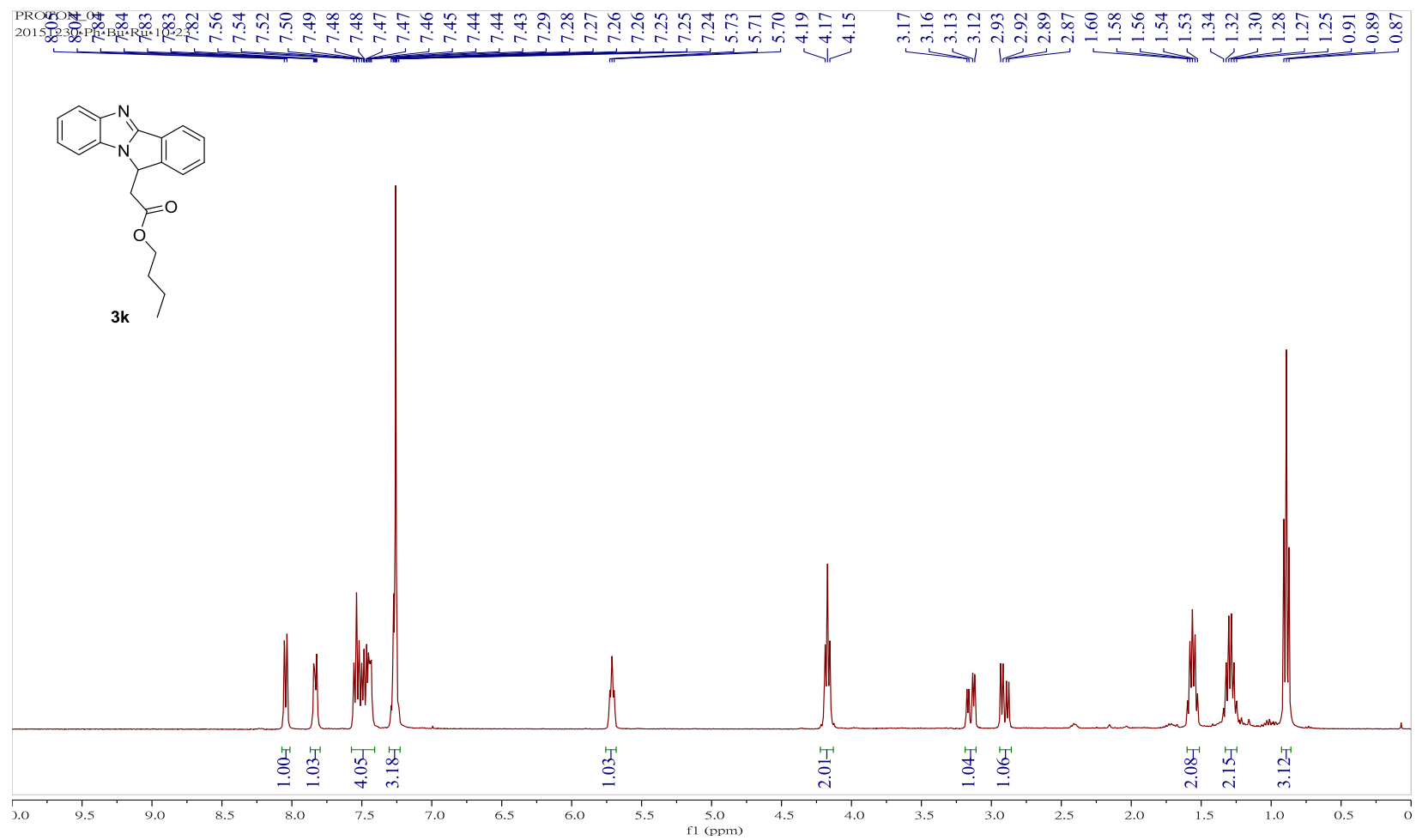


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
347.1759	1	C <sub>22</sub> H <sub>23</sub> N <sub>2</sub> O <sub>2</sub>	347.1754	1.5	24.5	1	100.00	12.5	even	ok	M+H

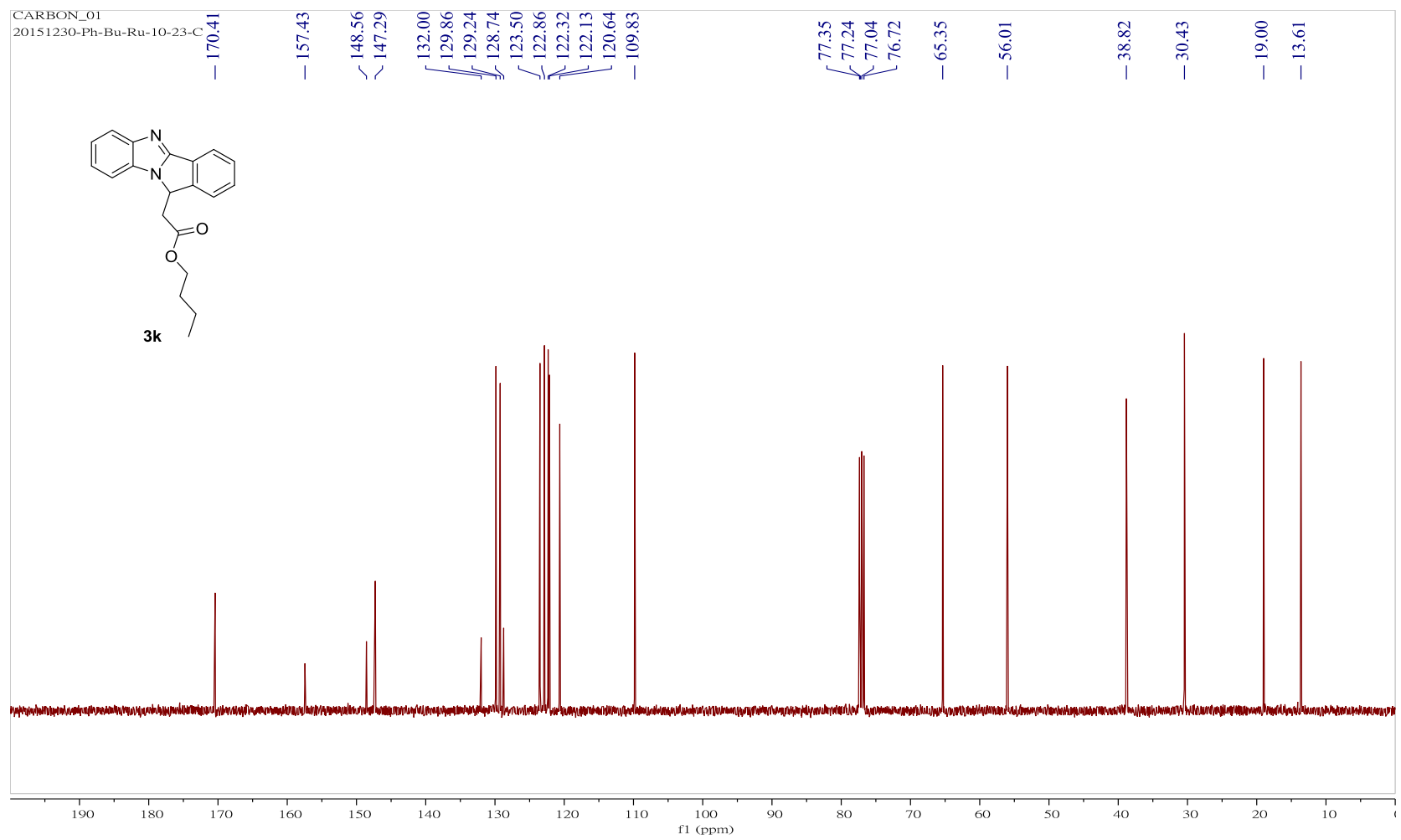
High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3j**



IR spectrum of compound of 3j



$^1\text{H}$  NMR Spectrum (400 MHz) of compound **3k** in  $\text{CDCl}_3$

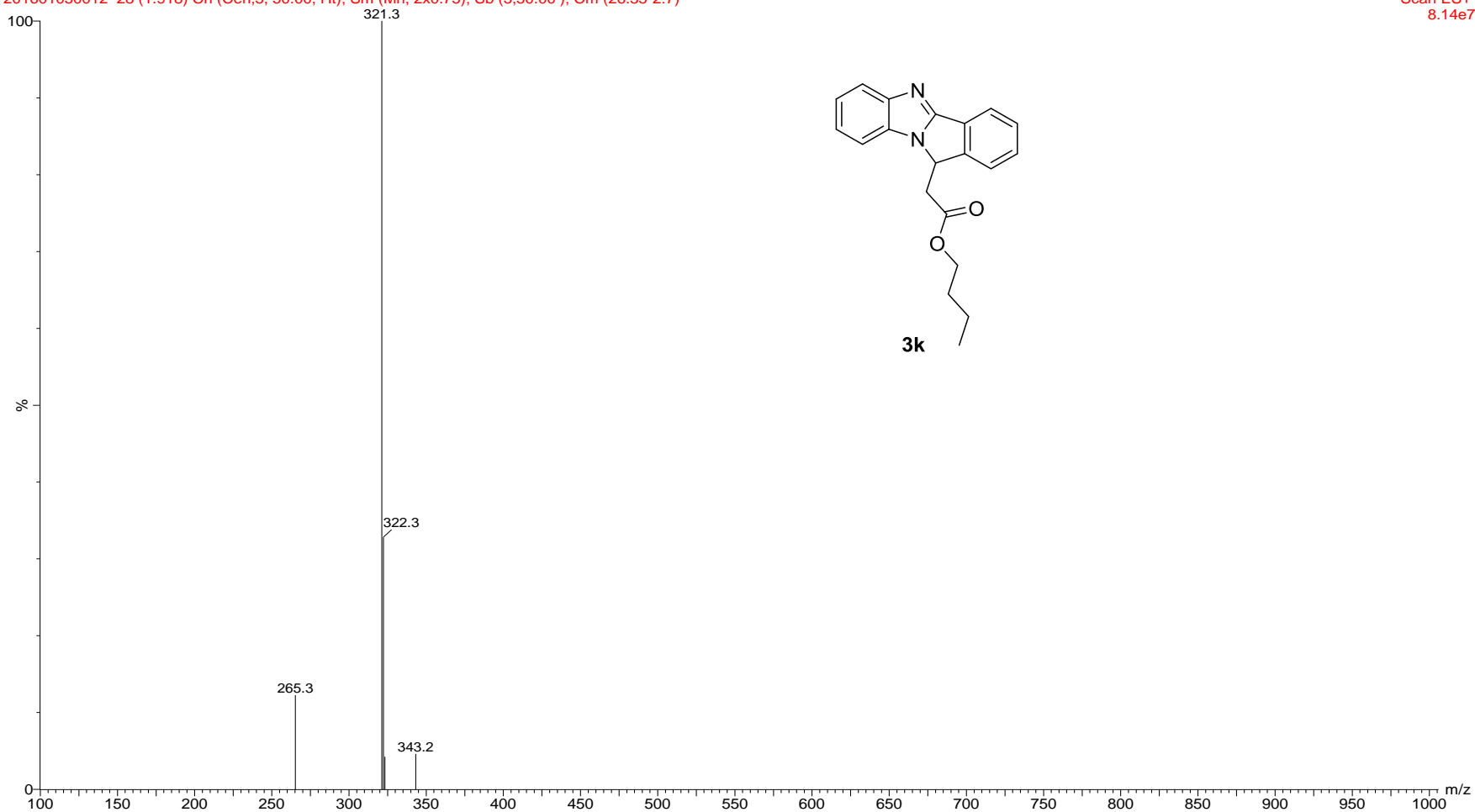


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3k** in  $\text{CDCl}_3$

**Ph-Bu-Ru**

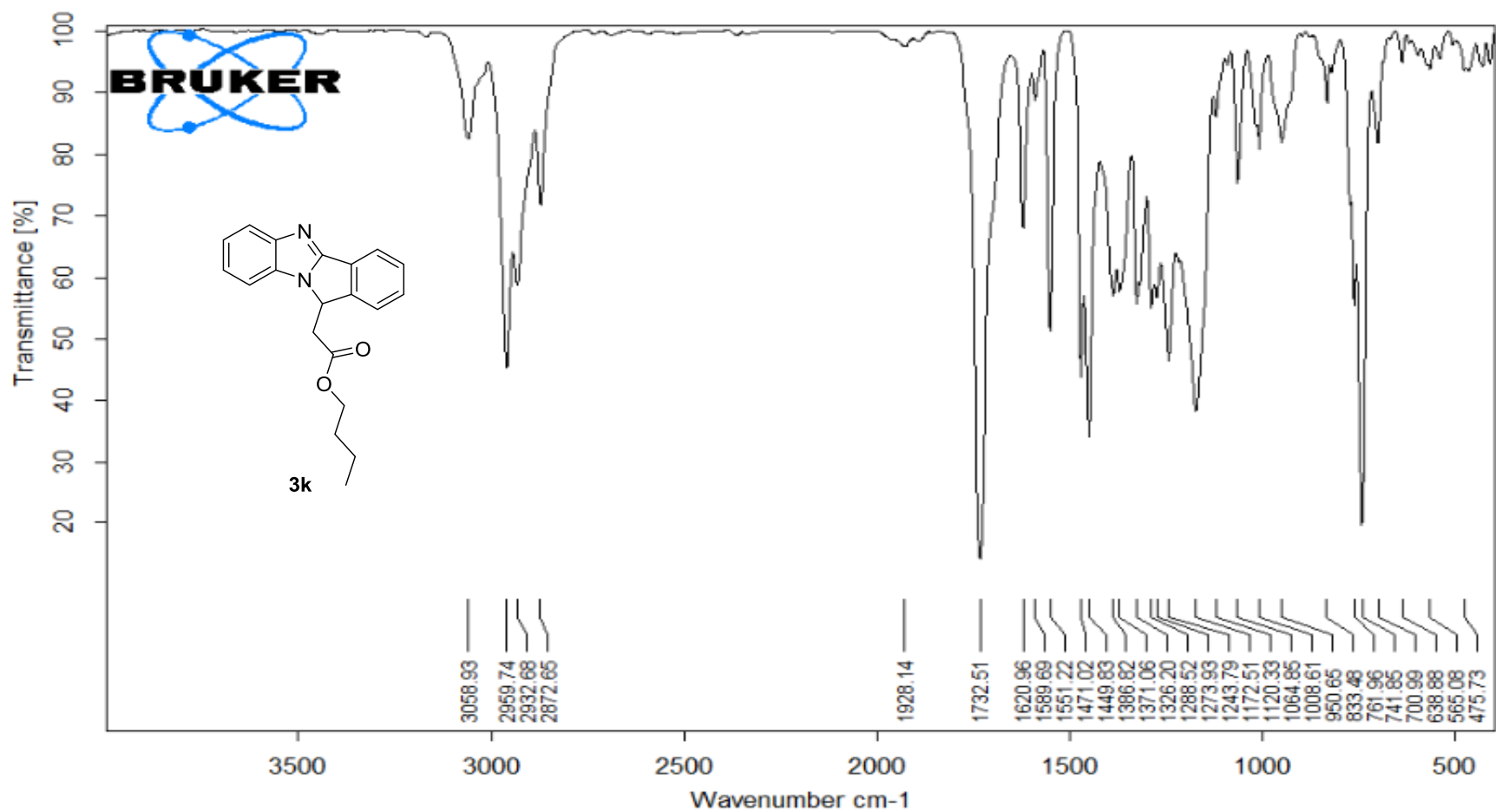
201601050012 28 (1.918) Cn (Cen,3, 50.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00); Cm (26:35-2:7)

Scan ES+  
8.14e7

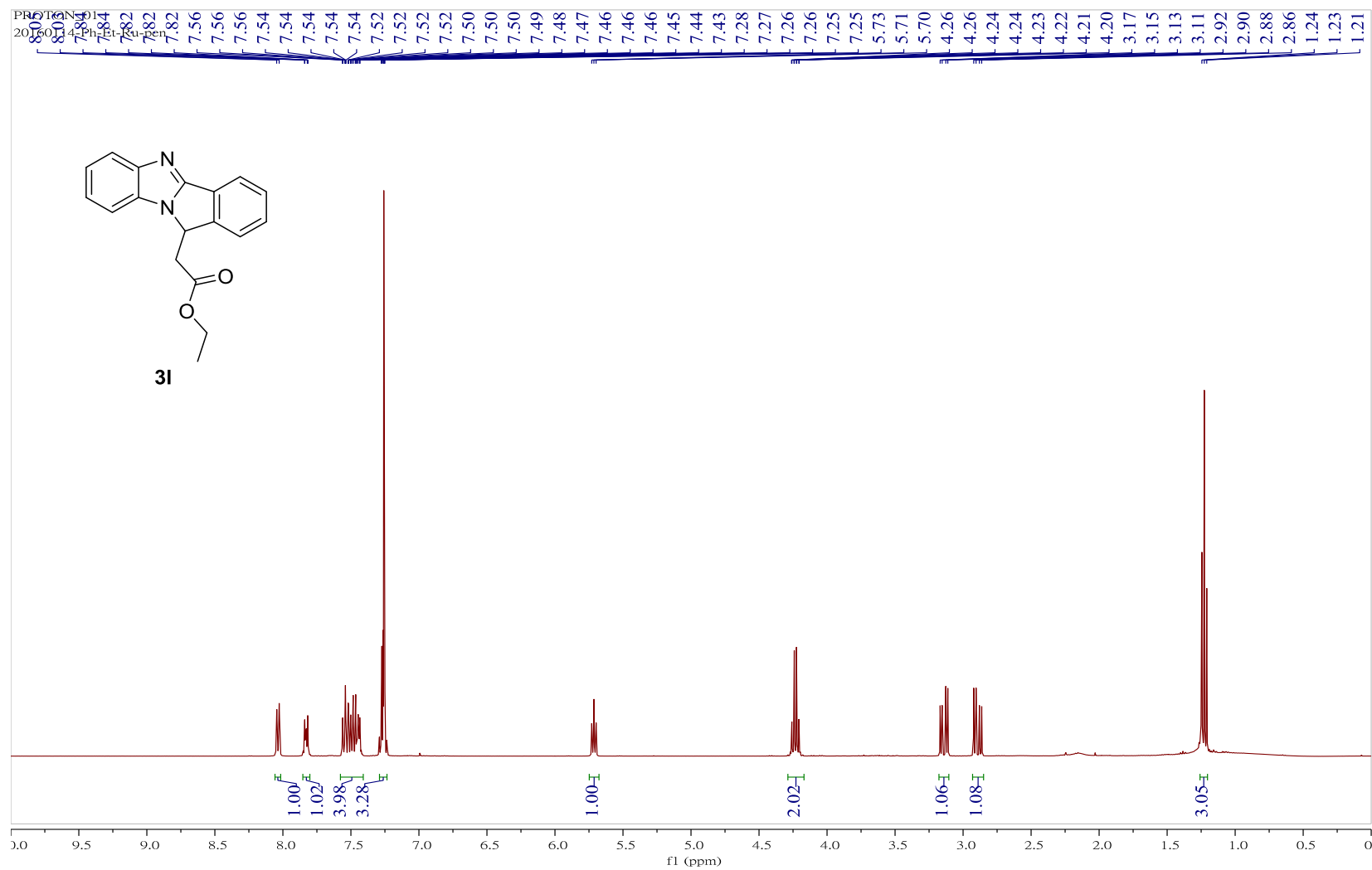


ESI<sup>+</sup> Mass spectrum of compound **3k**



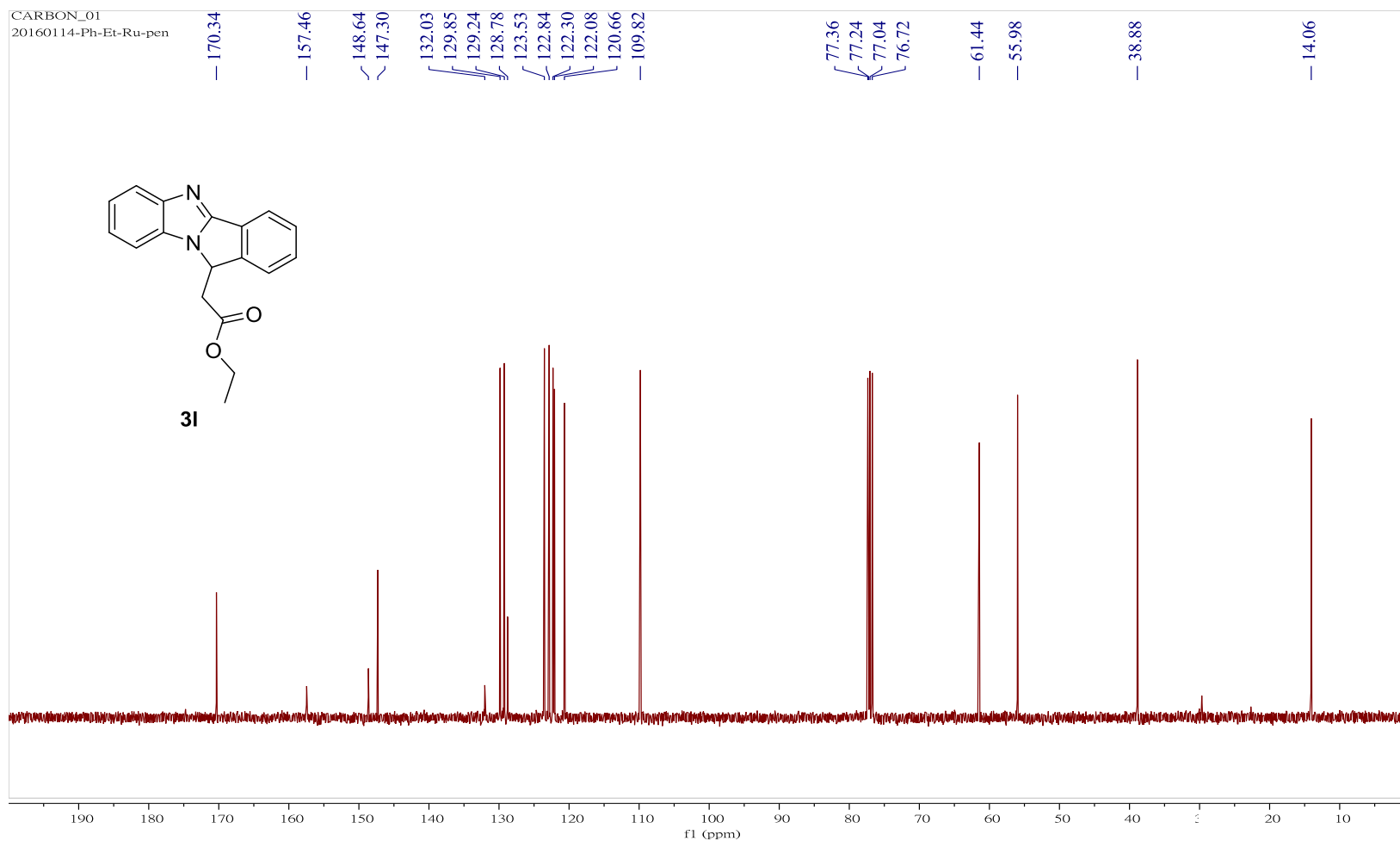


IR spectrum of compound of **3k**



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **31** in CDCl<sub>3</sub>



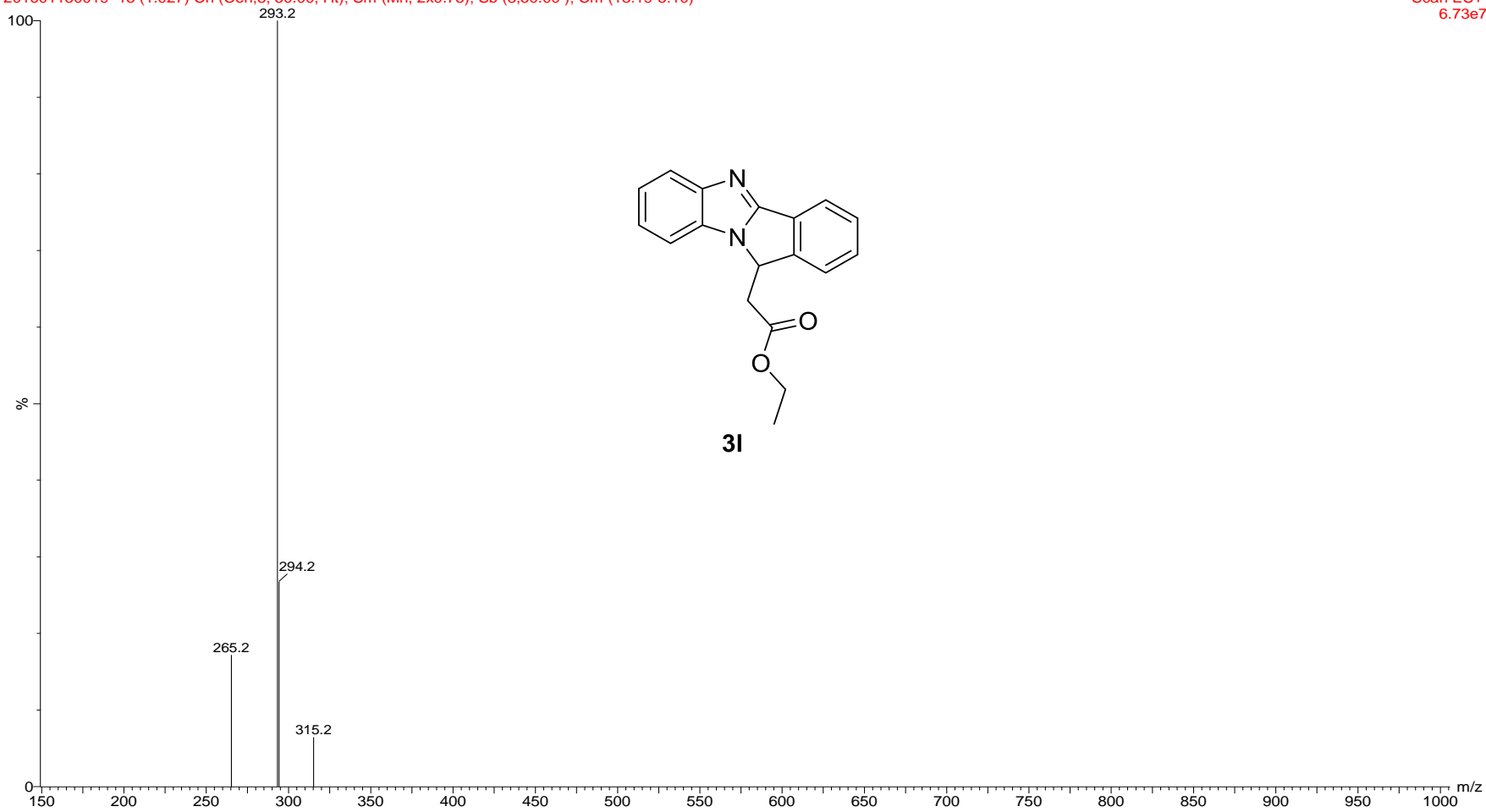


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **31** in  $\text{CDCl}_3$

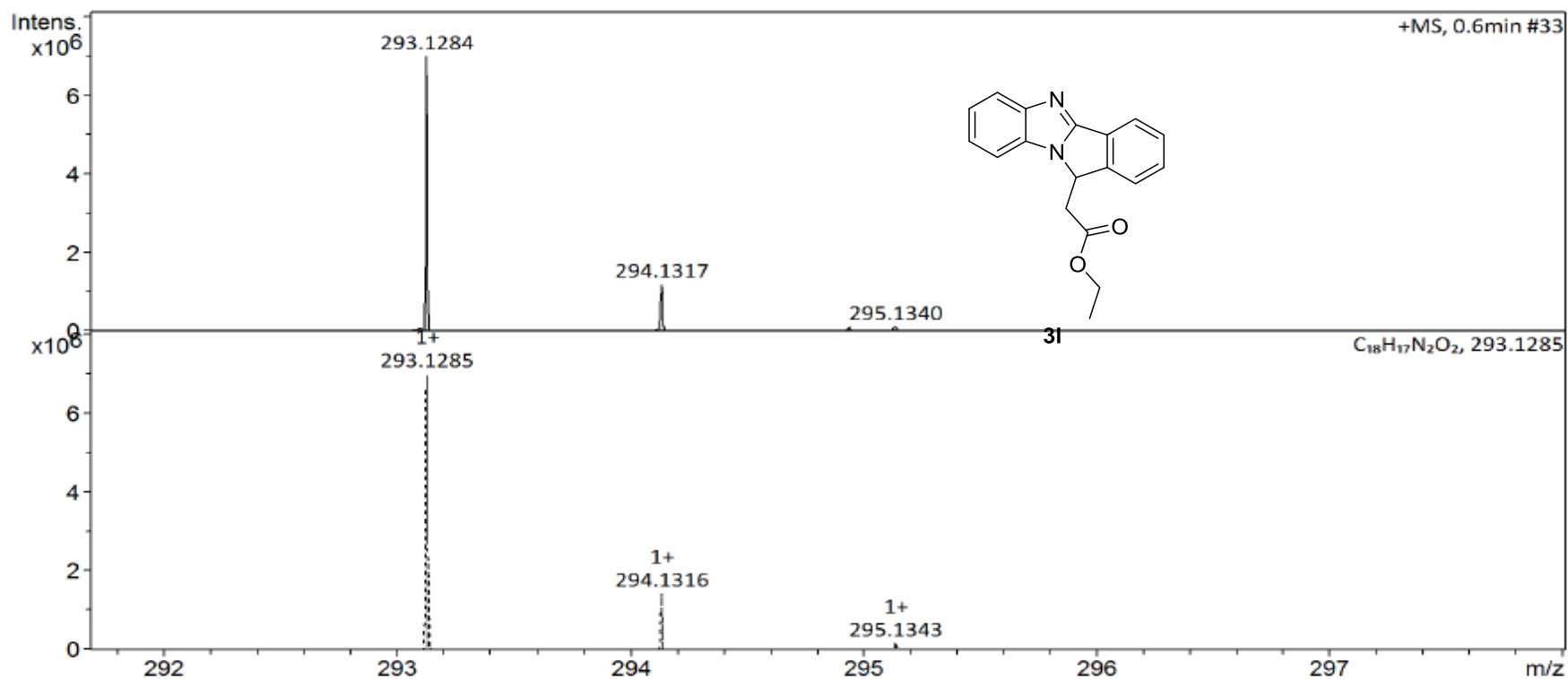
Ph-Et-Ru

201601150019 15 (1.027) Cn (Cen,3, 50.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00); Cm (13:19-5:10)

Scan ES+  
6.73e7

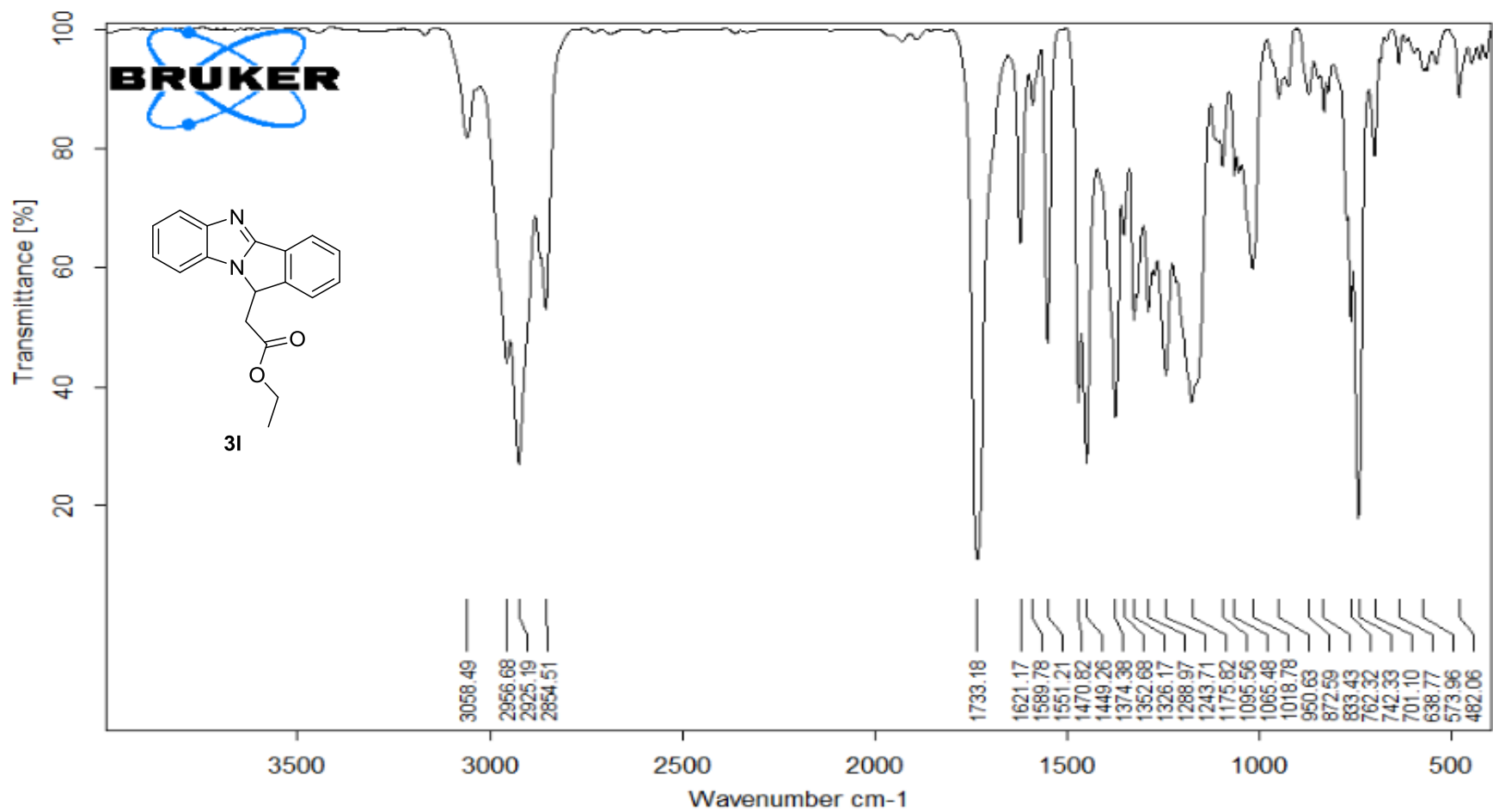


ESI<sup>+</sup> Mass spectrum of compound **31**

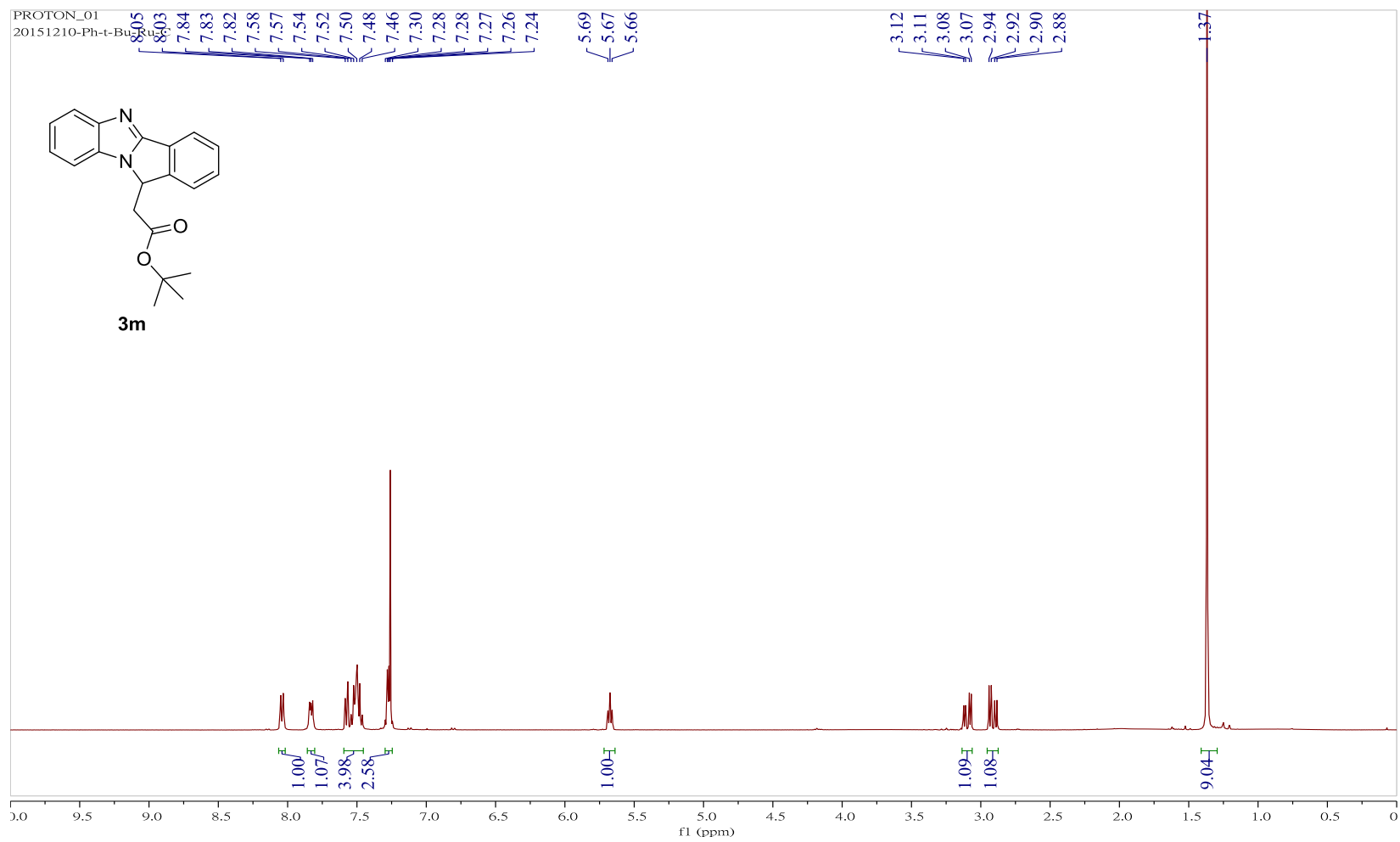


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
293.1284	1	C <sub>18</sub> H <sub>17</sub> N <sub>2</sub> O <sub>2</sub>	293.1285	0.2	20.0	1	100.00	11.5	even	ok	M+H

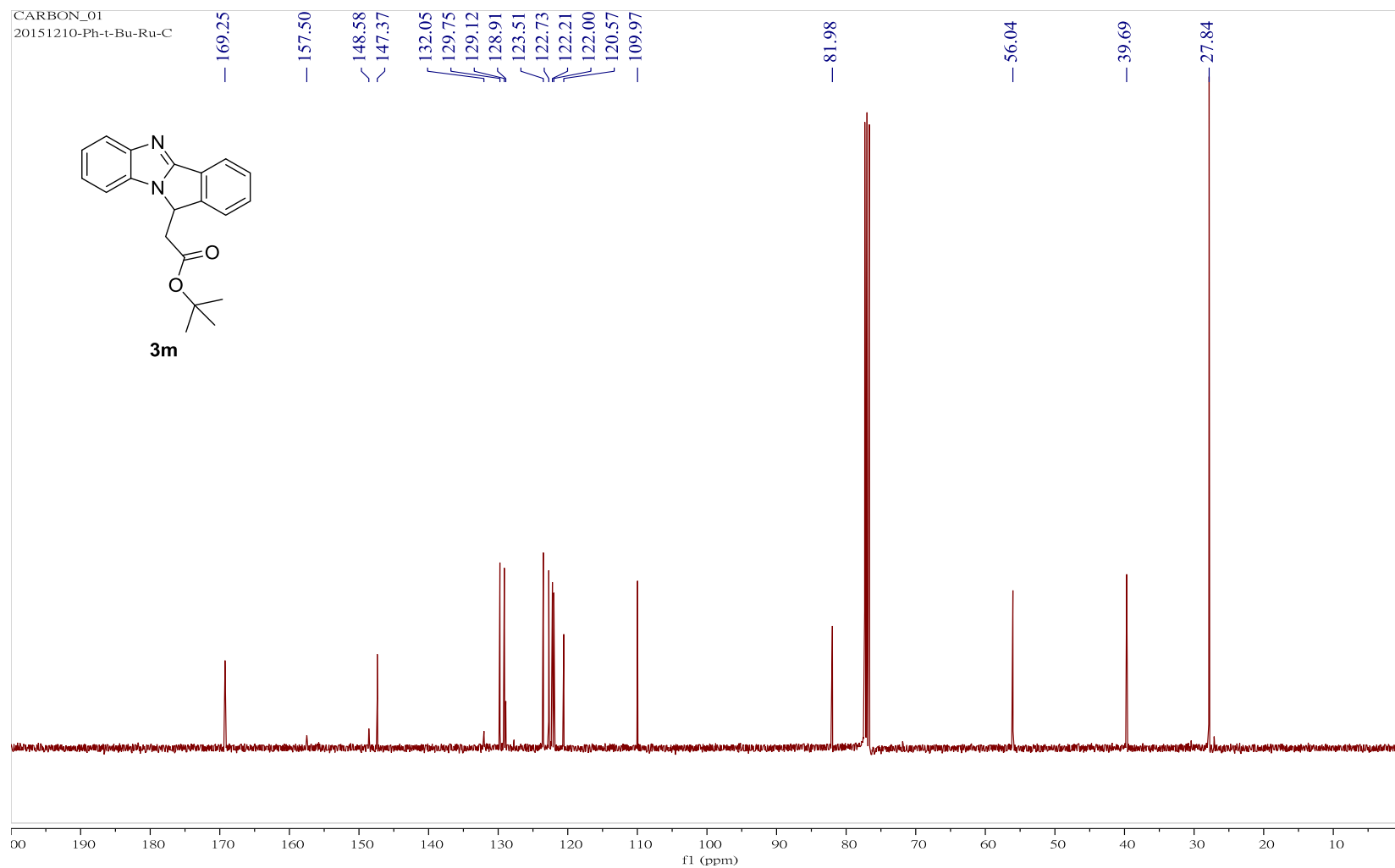
High resolution mass (ESI)<sup>+</sup> spectrum of compound of **31**



IR spectrum of compound of **31**



$^1\text{H}$  NMR Spectrum (400 MHz) of compound **3m** in  $\text{CDCl}_3$

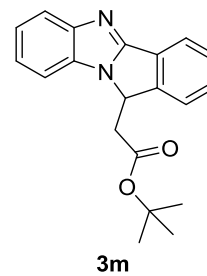
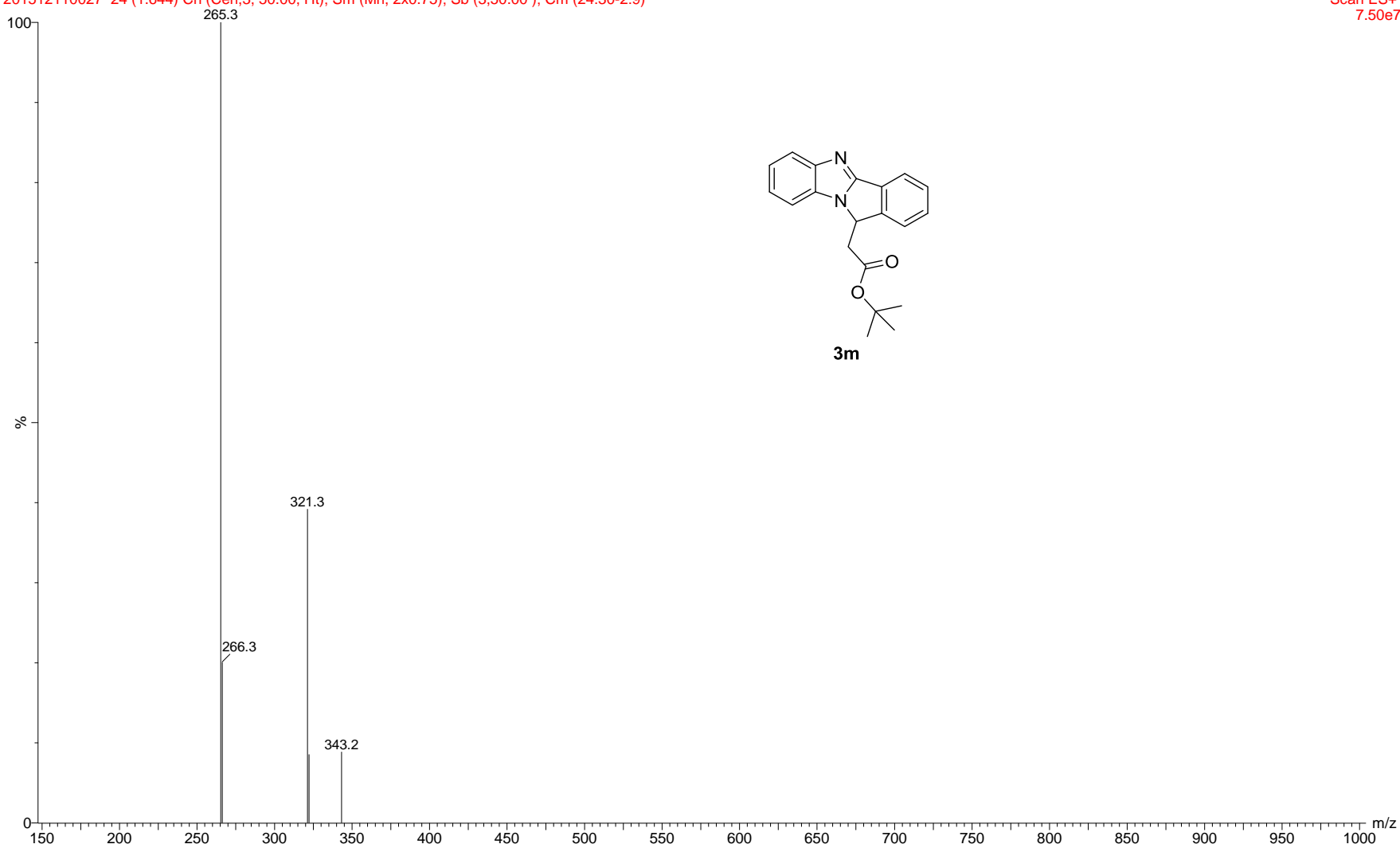


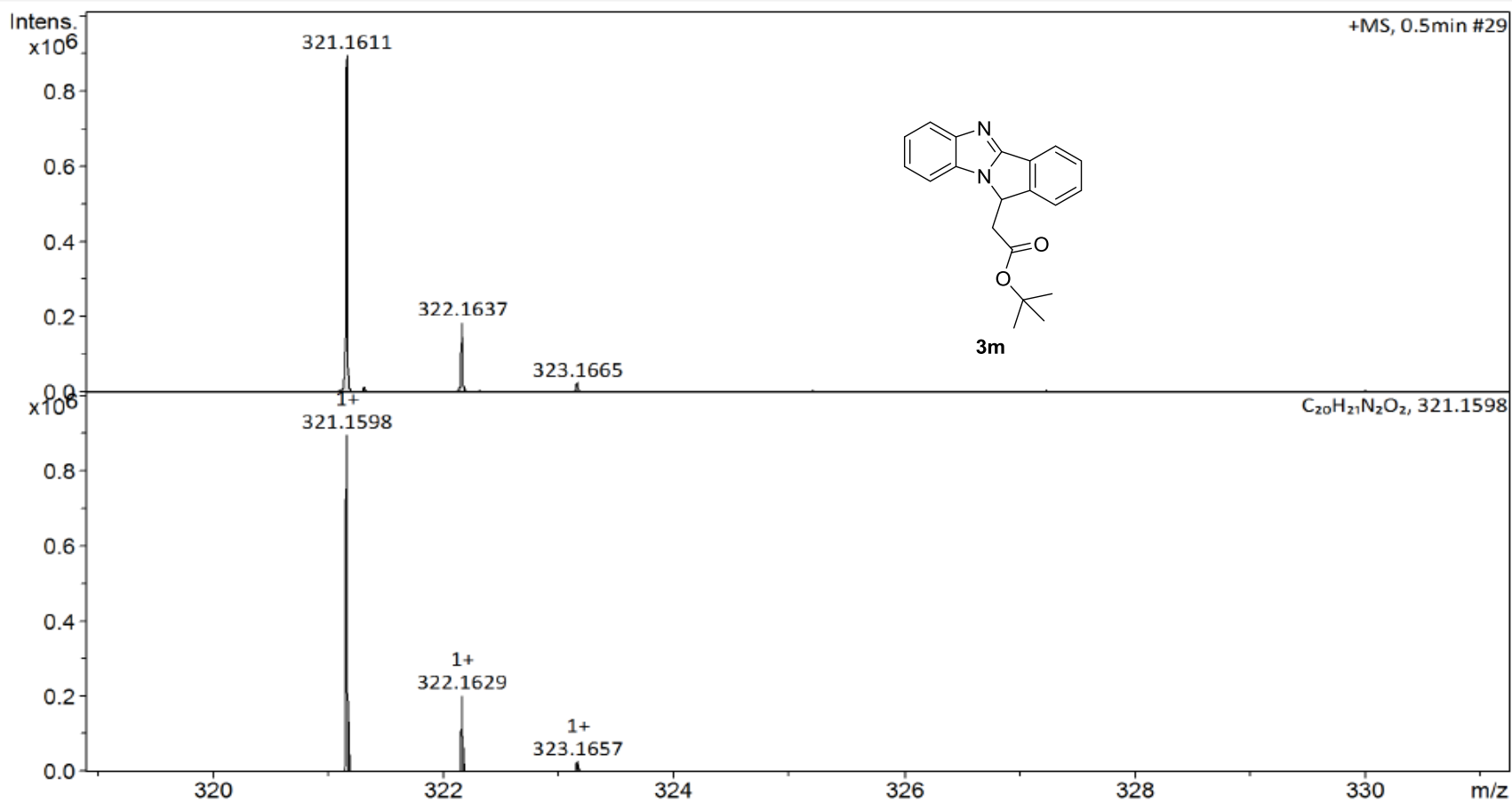
$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3m** in  $\text{CDCl}_3$

Ph-t-Bu-Ru

201512110027 24 (1.644) Cn (Cen,3, 50.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00); Cm (24:30-2:9)

Scan ES+  
7.50e7

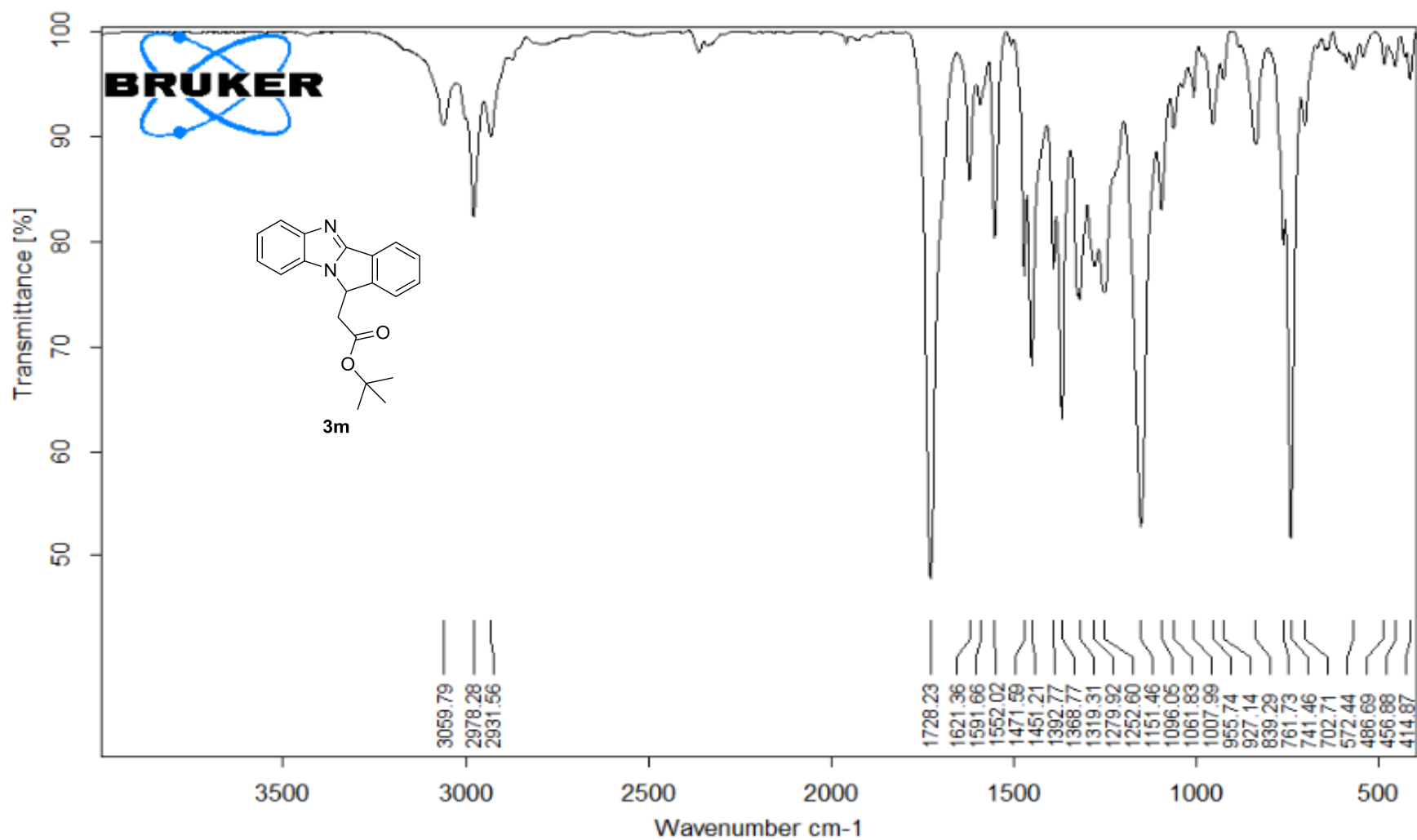




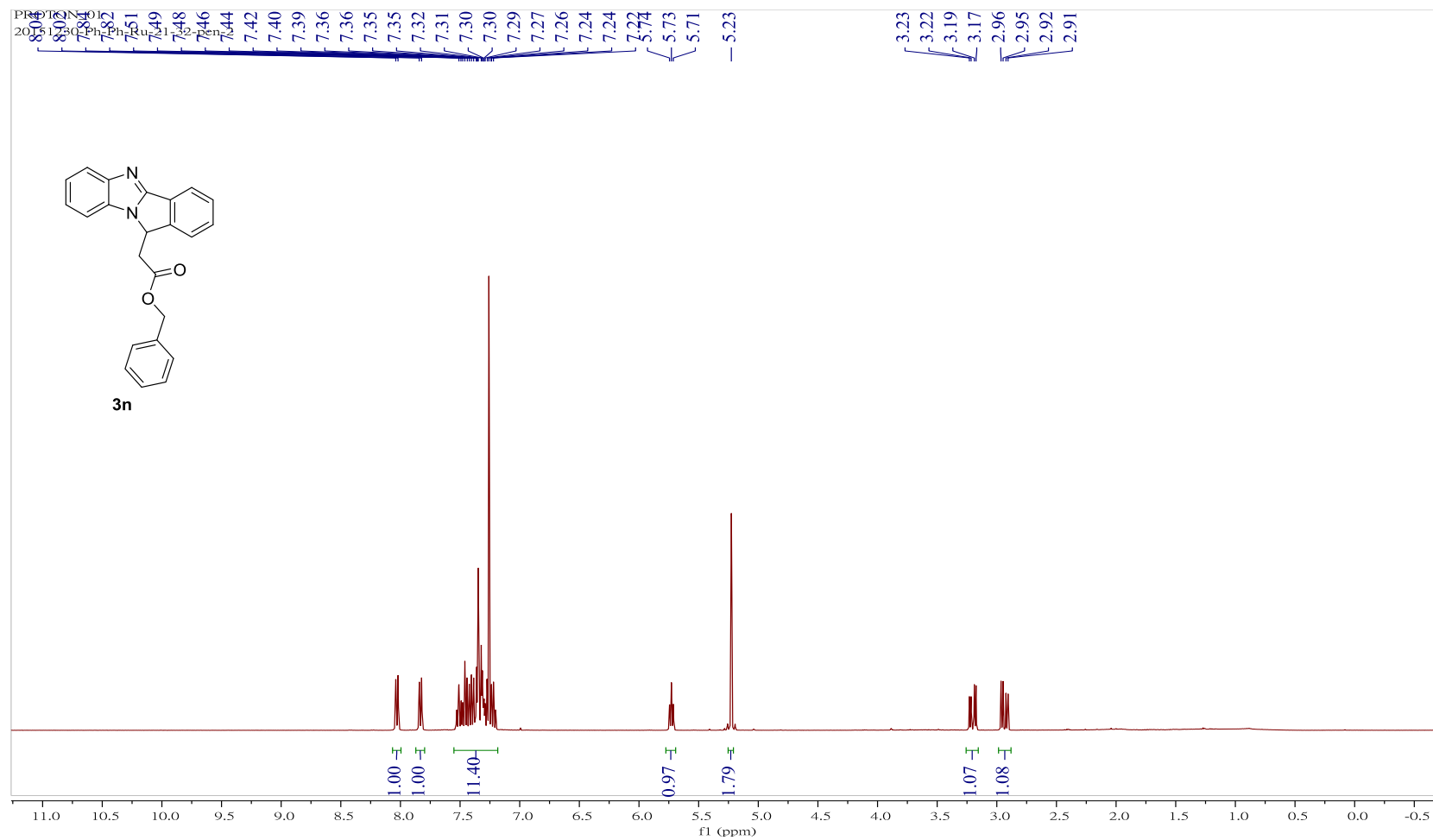
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
321.1611	1	C <sub>20</sub> H <sub>21</sub> N <sub>2</sub> O <sub>2</sub>	321.1598	4.1	11.7	1	100.00	11.5	even	ok	M+H

High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3m**

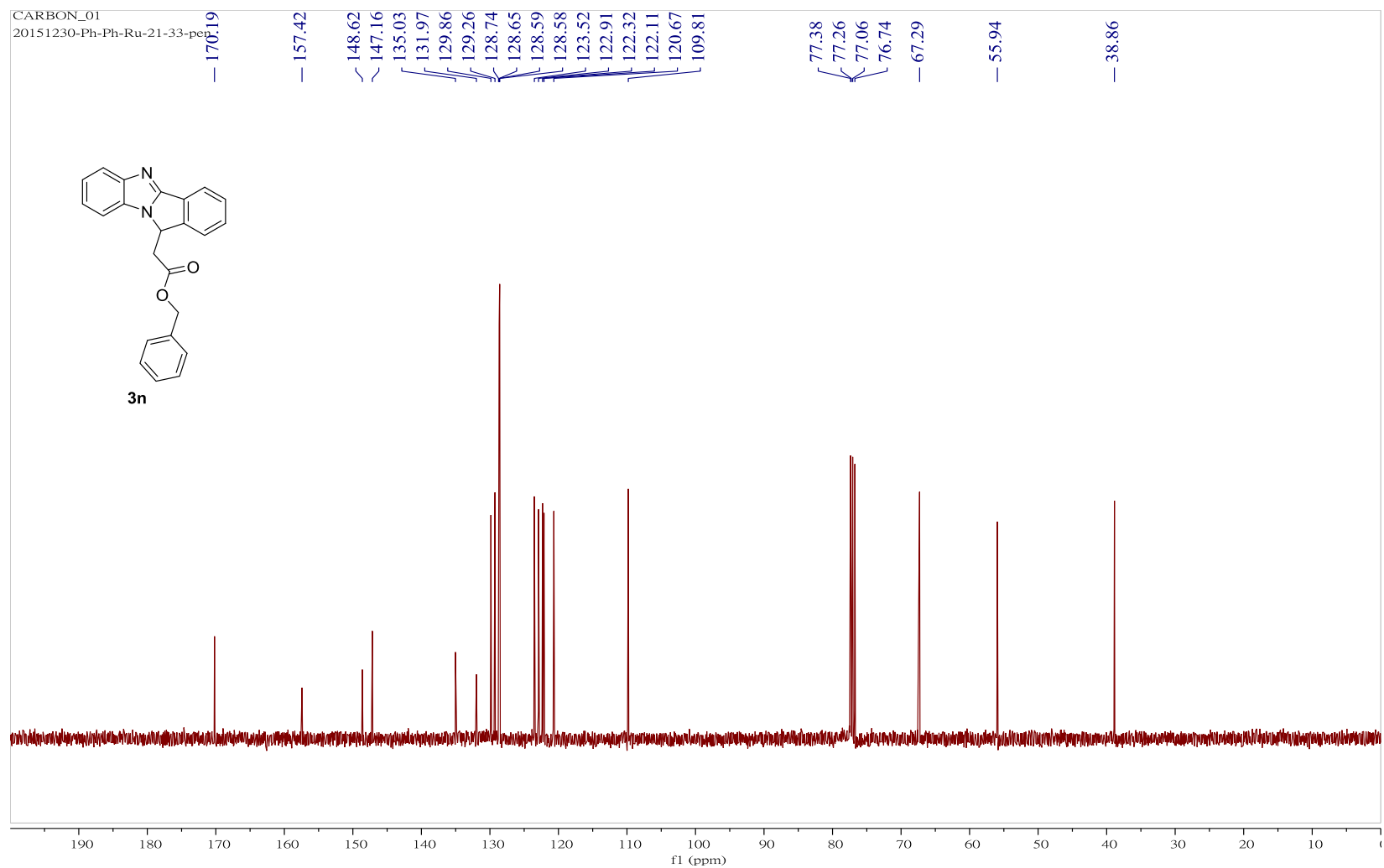




IR spectrum of compound of **3m**



**<sup>1</sup>H NMR Spectrum (400 MHz) of compound 3n in CDCl<sub>3</sub>**

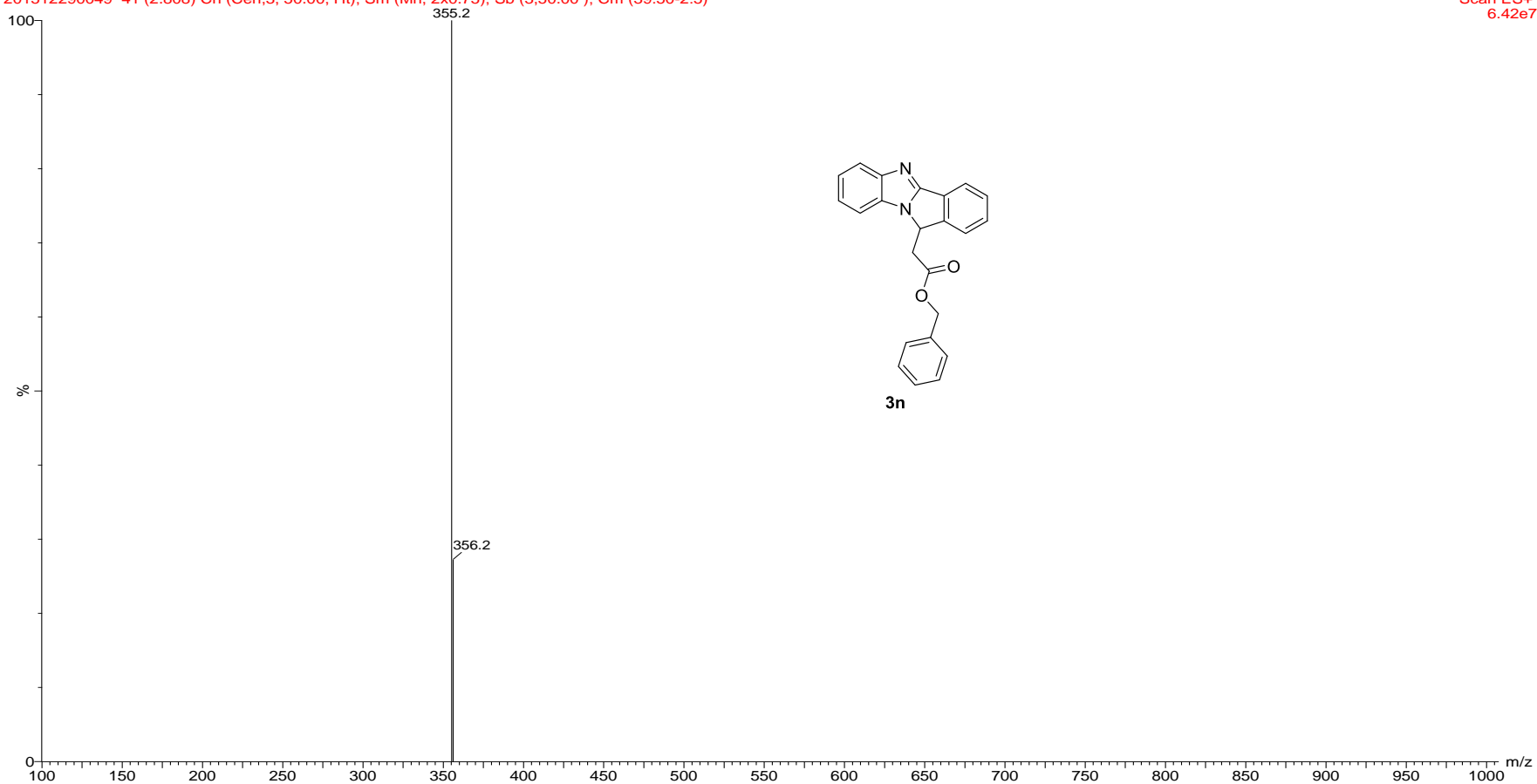


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3n** in  $\text{CDCl}_3$

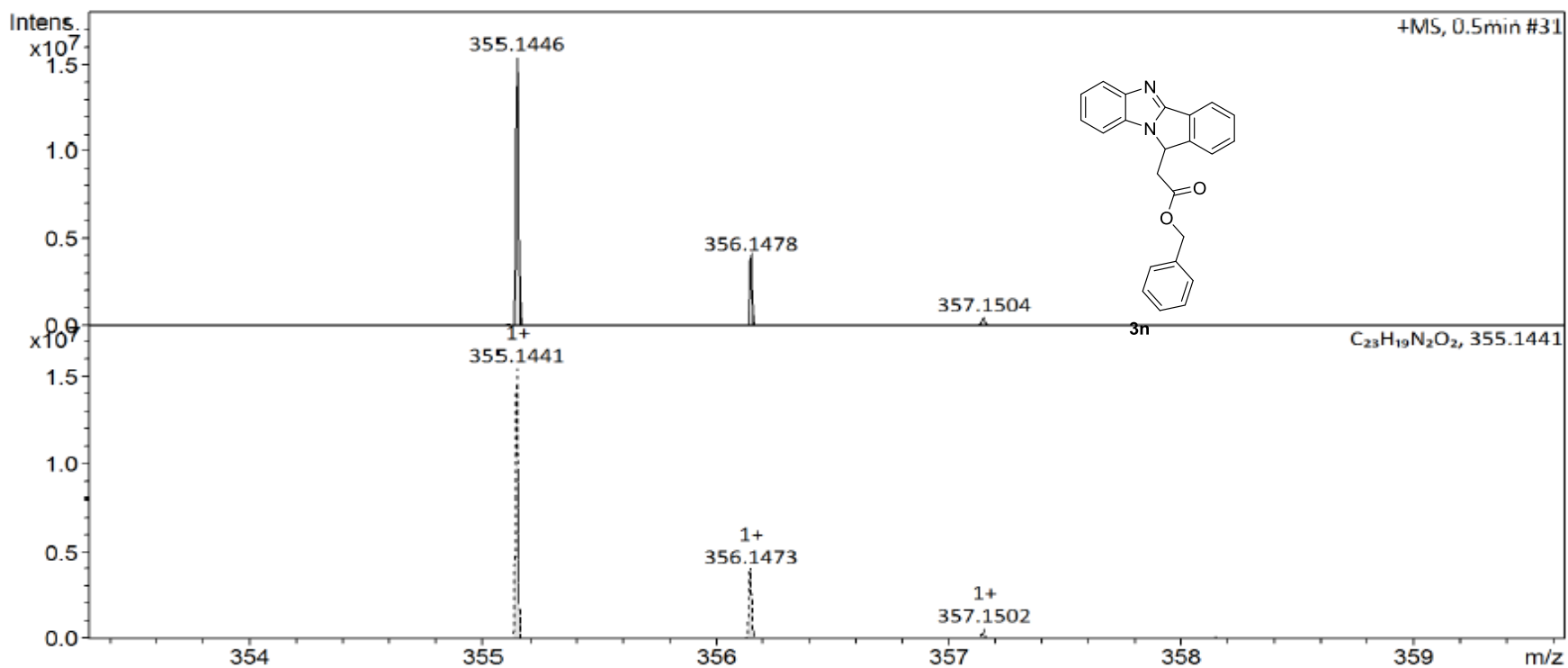
ph-ph-Ru-2-21-32

201512290049 41 (2.808) Cn (Cen,3, 50.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00 ); Cm (39:50-2:5)

Scan ES+  
6.42e7

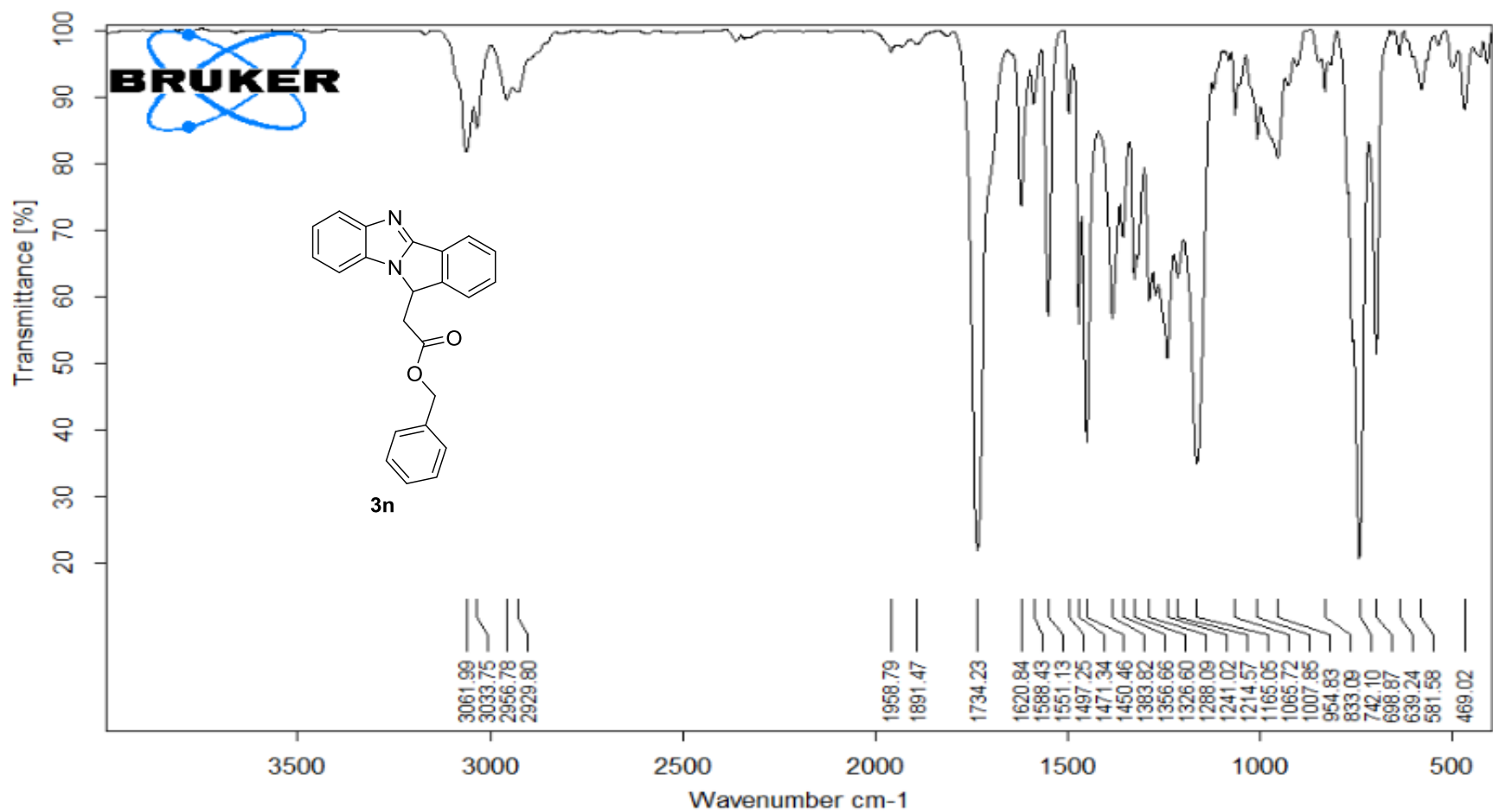


ESI<sup>+</sup> Mass spectrum of compound **3n**

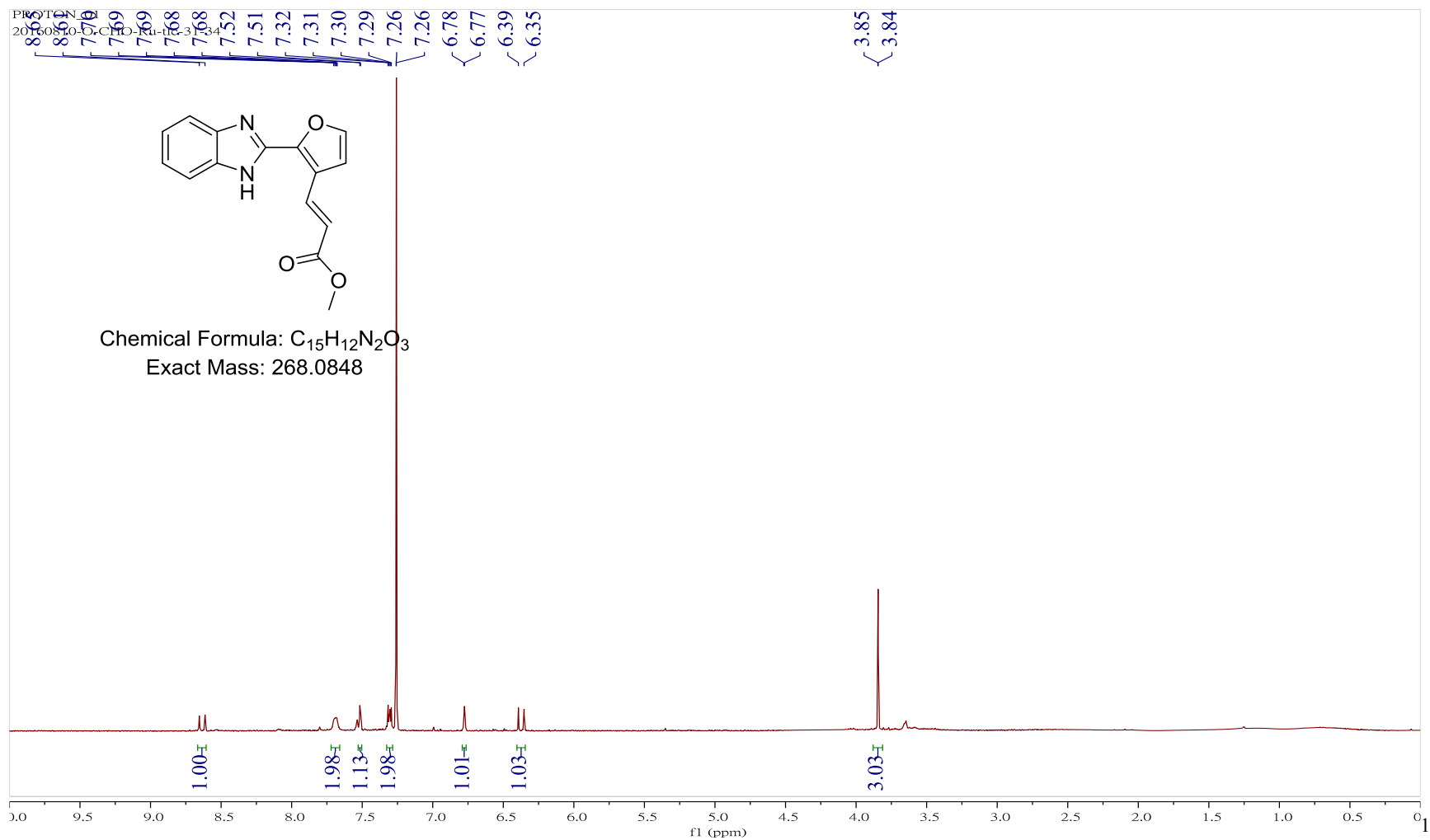


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
355.1446	1	C <sub>23</sub> H <sub>19</sub> N <sub>2</sub> O <sub>2</sub>	355.1441	1.4	4.2	1	100.00	15.5	even	ok	M+H

High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3n**



IR spectrum of compound of **3n**

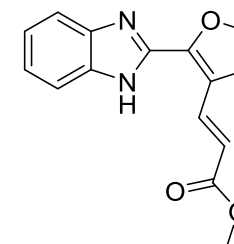


$^1H$  NMR Spectrum (400 MHz) of compound **4b** in  $CDCl_3$

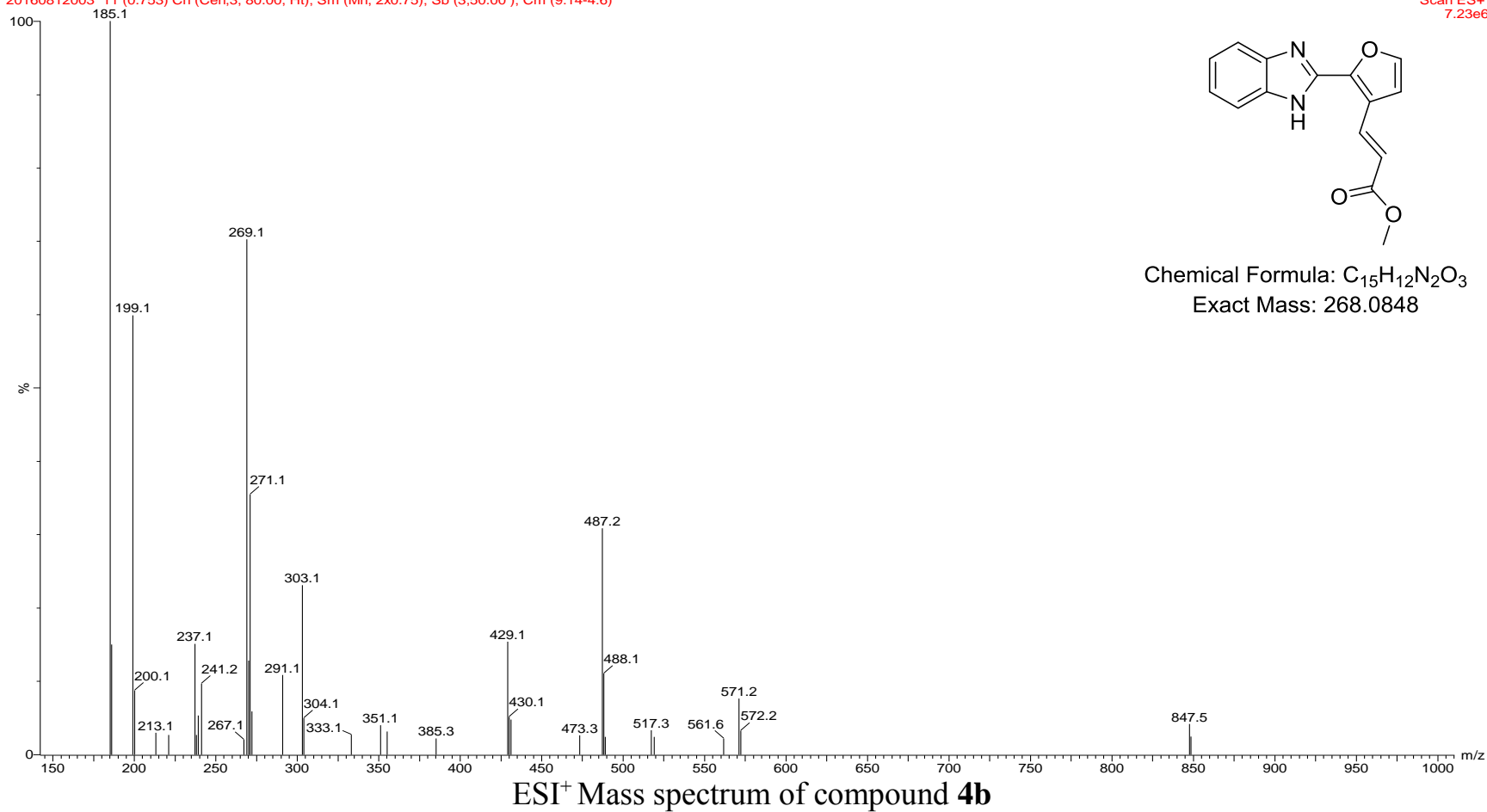
**O-CHO-Ru-2**

20160812003\_11 (0.753) Cn (Cen,3, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00); Cm (9:14-4:6)

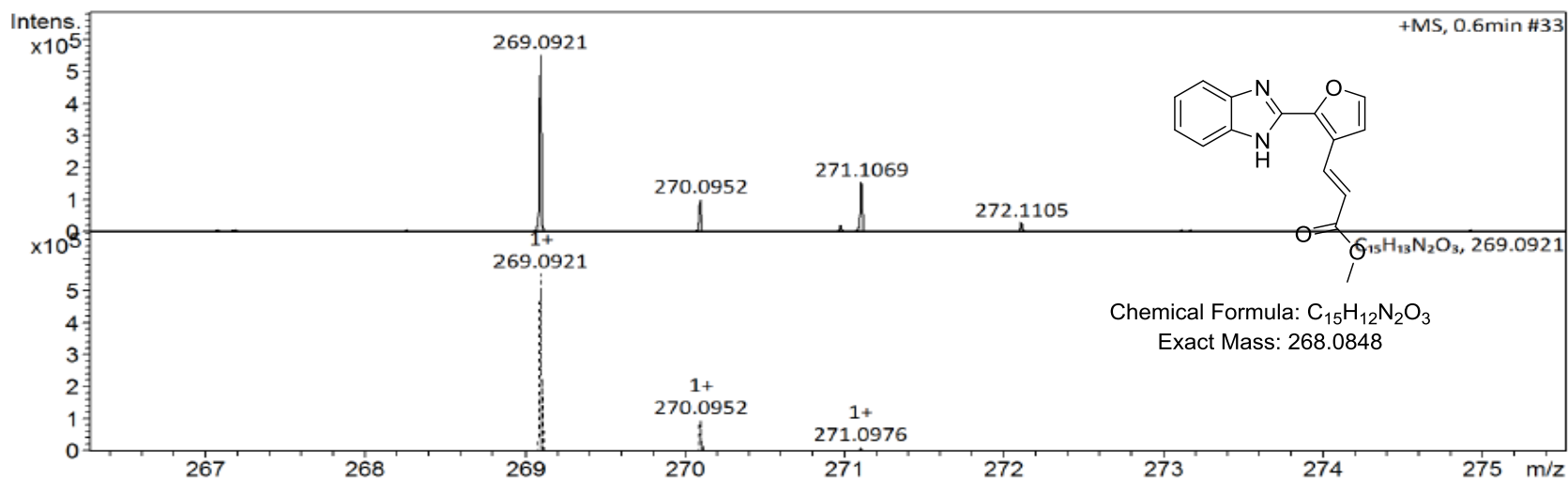
Scan ES+  
7.23e6



Chemical Formula: C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>O<sub>3</sub>  
Exact Mass: 268.0848

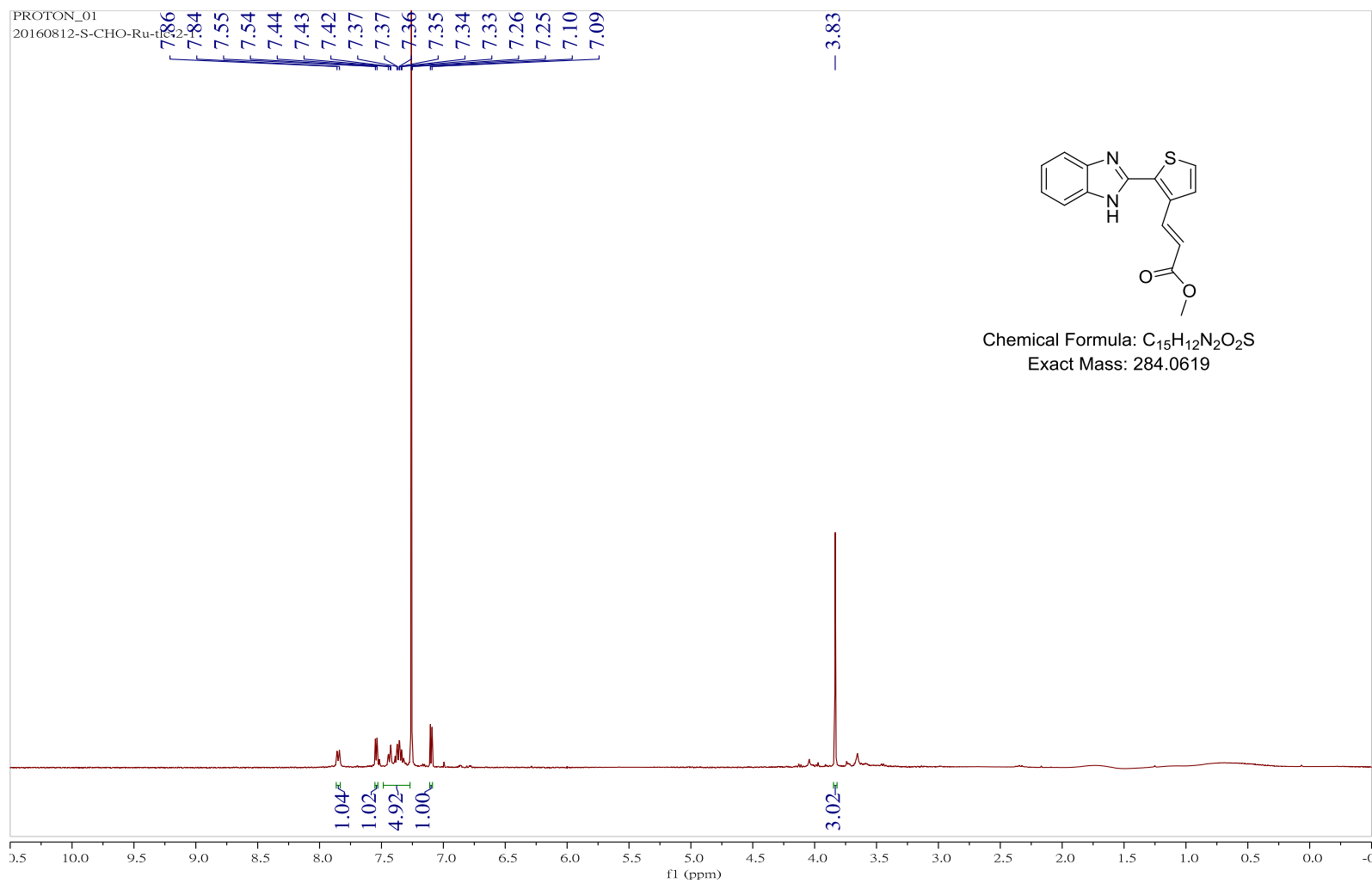






Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
269.0921	1	C <sub>15</sub> H <sub>13</sub> N <sub>2</sub> O <sub>3</sub>	269.0921	-0.3	12.8	1	100.00	10.5	even	ok	M+H

High resolution mass (ESI)<sup>+</sup> spectrum of compound of **4b**

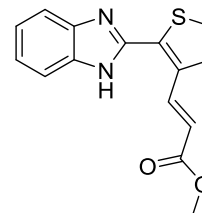
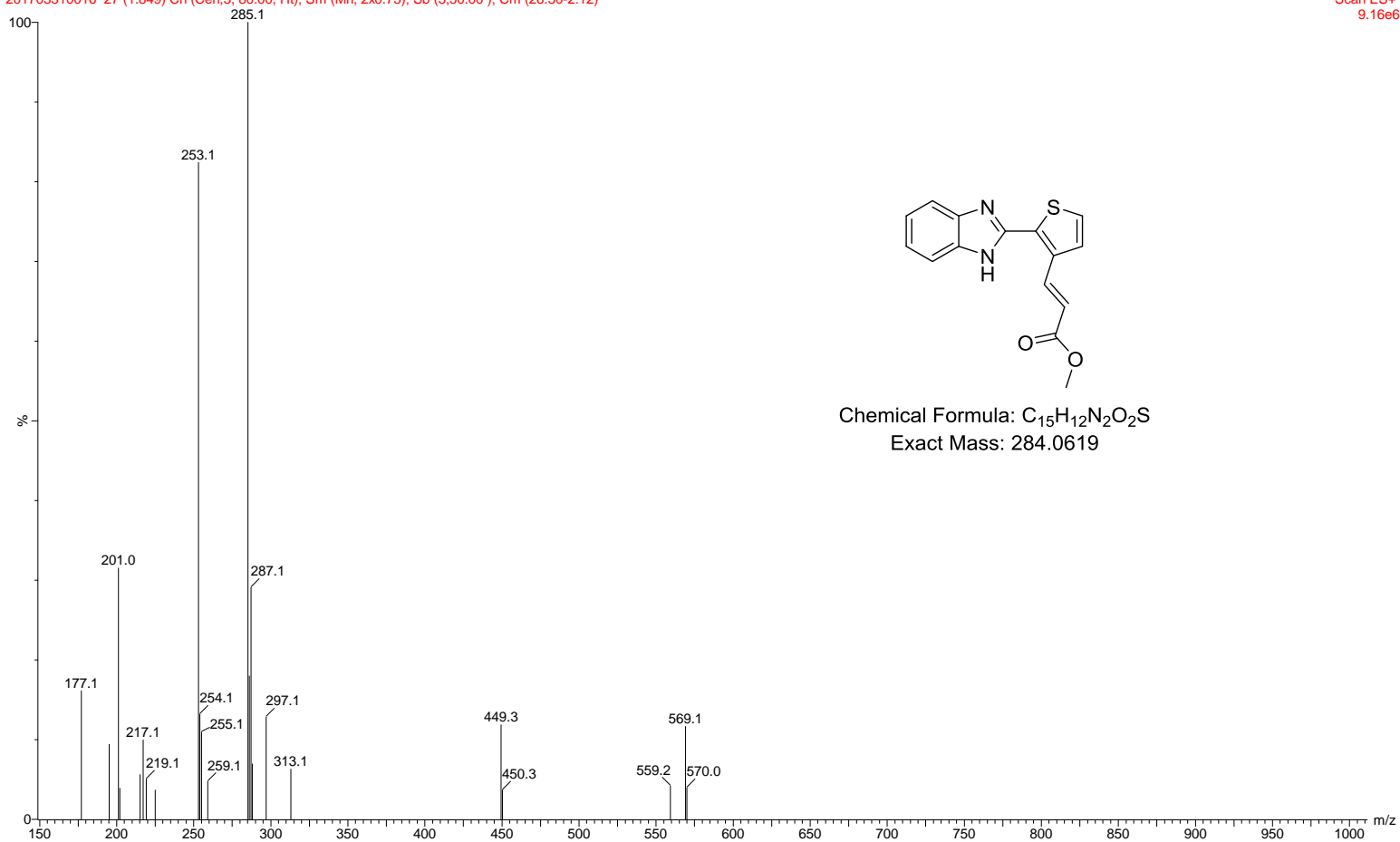


<sup>1</sup>H NMR Spectrum (400 MHz) of compound **4c** in CDCl<sub>3</sub>

SD-N7-03-I

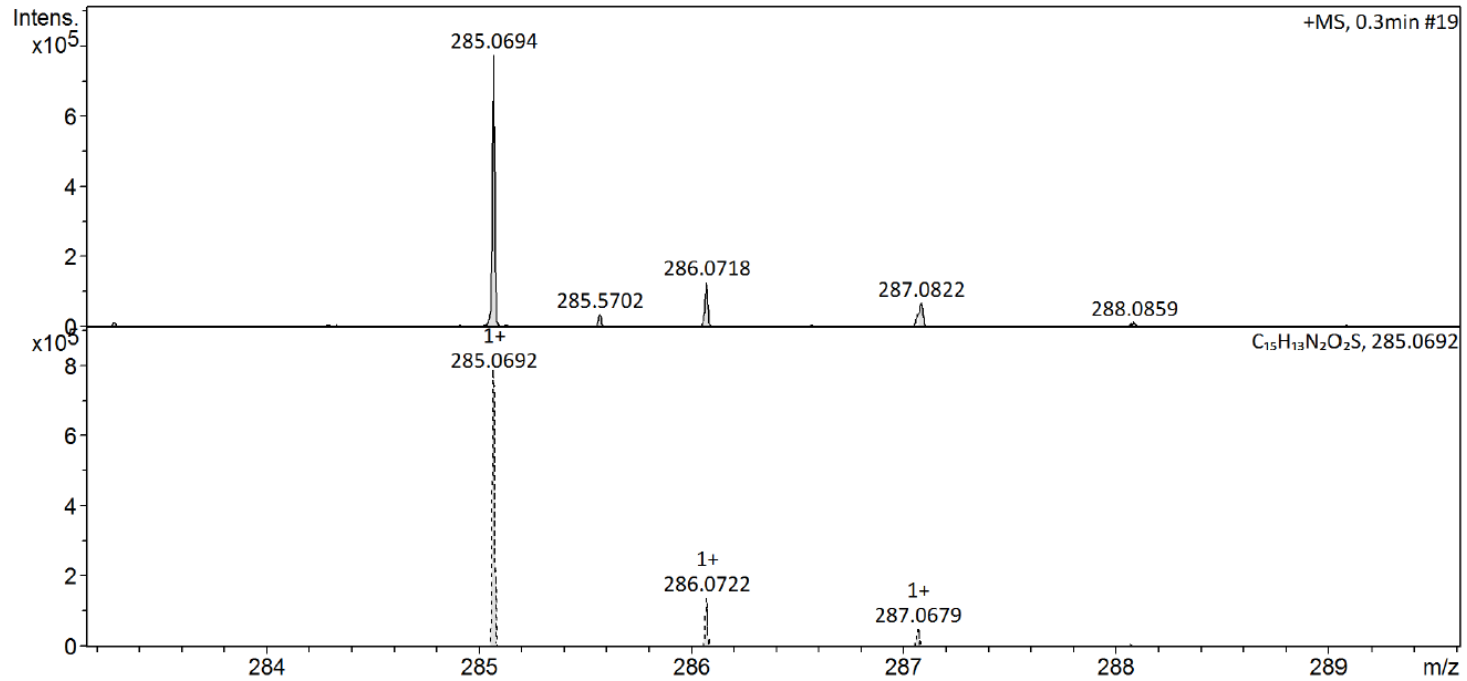
201703310016 27 (1.849) Cn (Cen,3, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00); Cm (26:30-2:12)

Scan ES+  
9.16e6



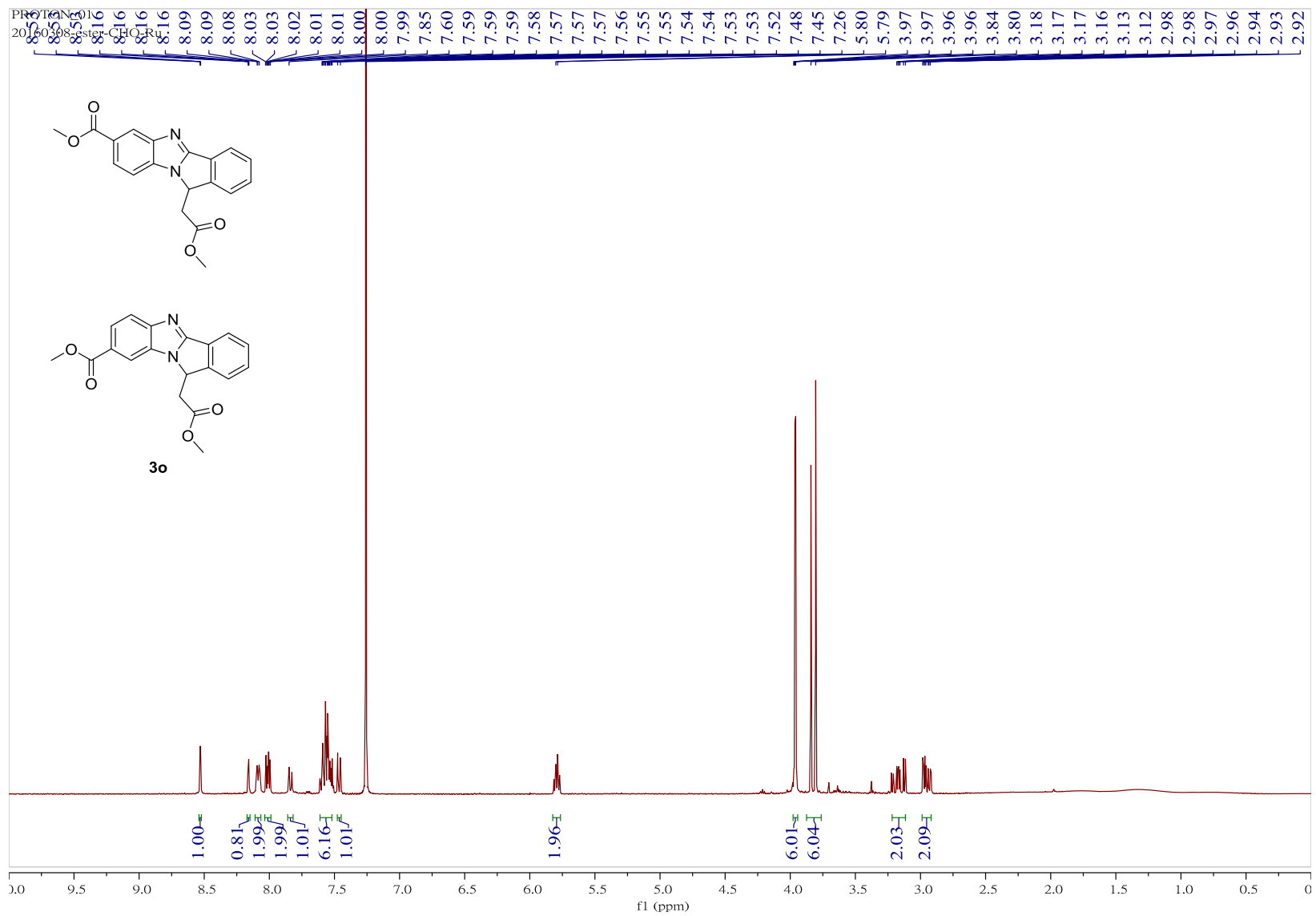
Chemical Formula: C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>S  
Exact Mass: 284.0619

ESI<sup>+</sup> Mass spectrum of compound **4c**

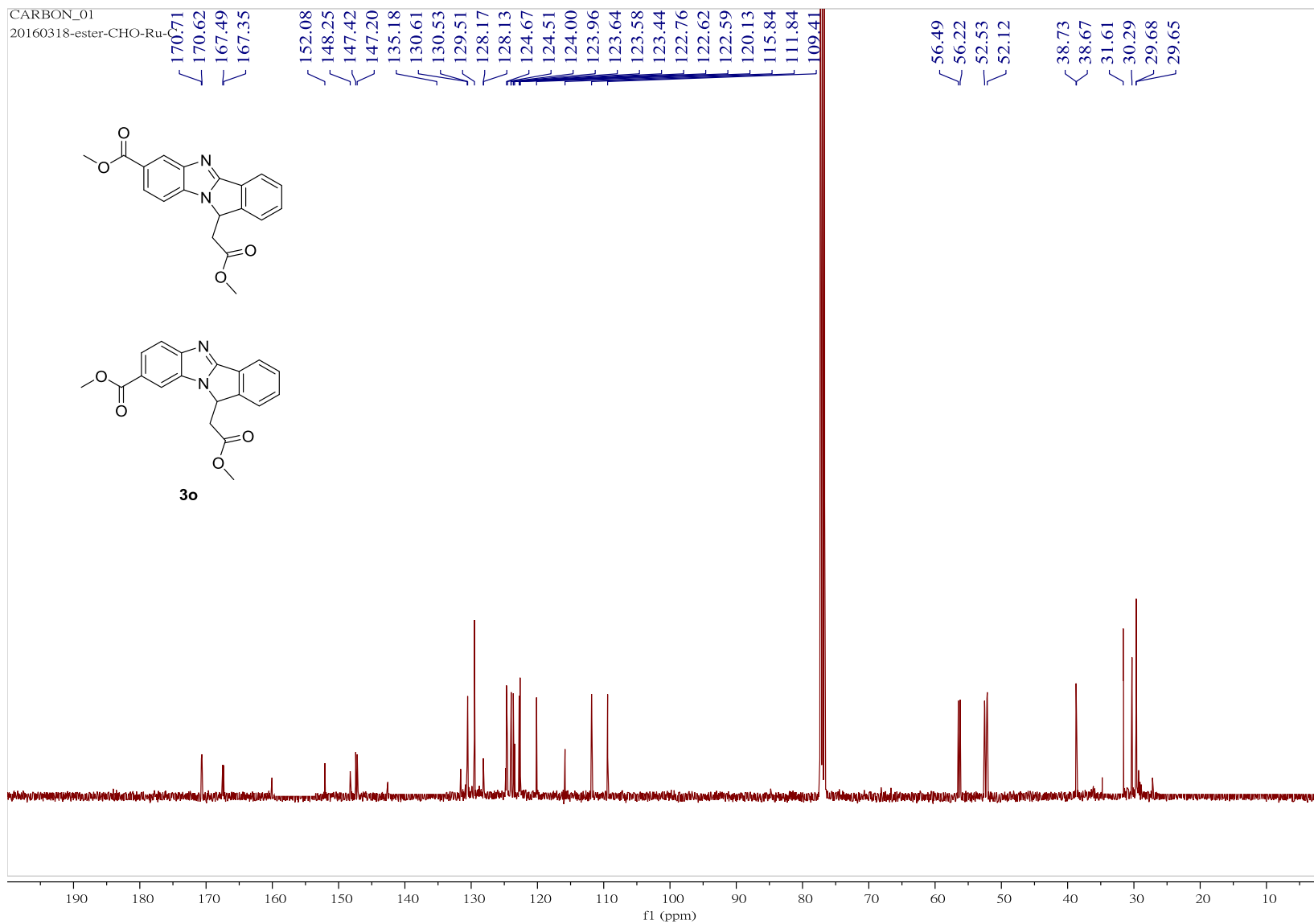


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
285.0694	1	C <sub>15</sub> H <sub>13</sub> N <sub>2</sub> O <sub>2</sub> S	285.0692	0.8	33.0	1	100.00	10.5	even	ok	M+H

High resolution mass (ESI)<sup>+</sup> spectrum of compound of **4c**



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **3o** in CDCl<sub>3</sub>

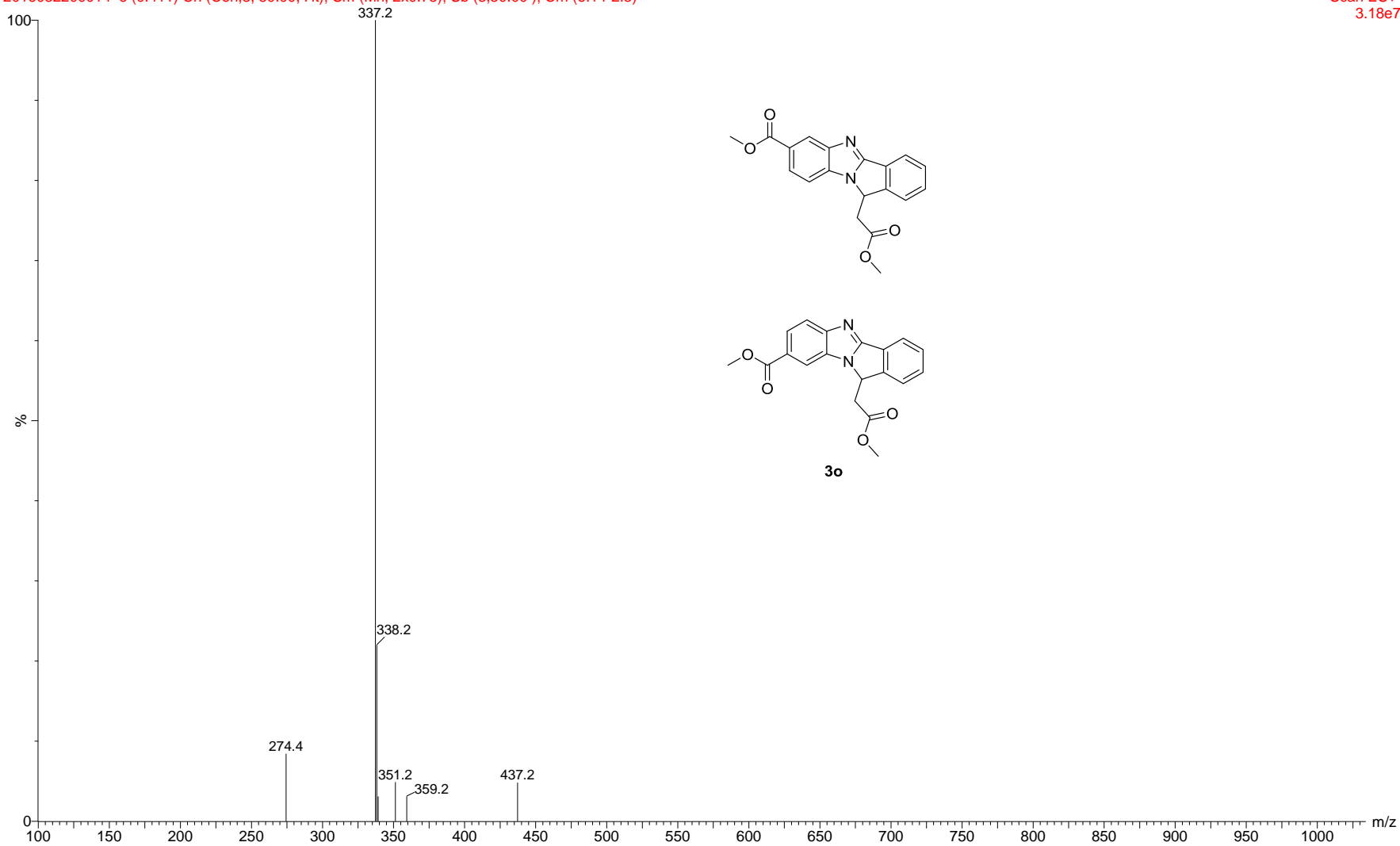


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3o** in  $\text{CDCl}_3$

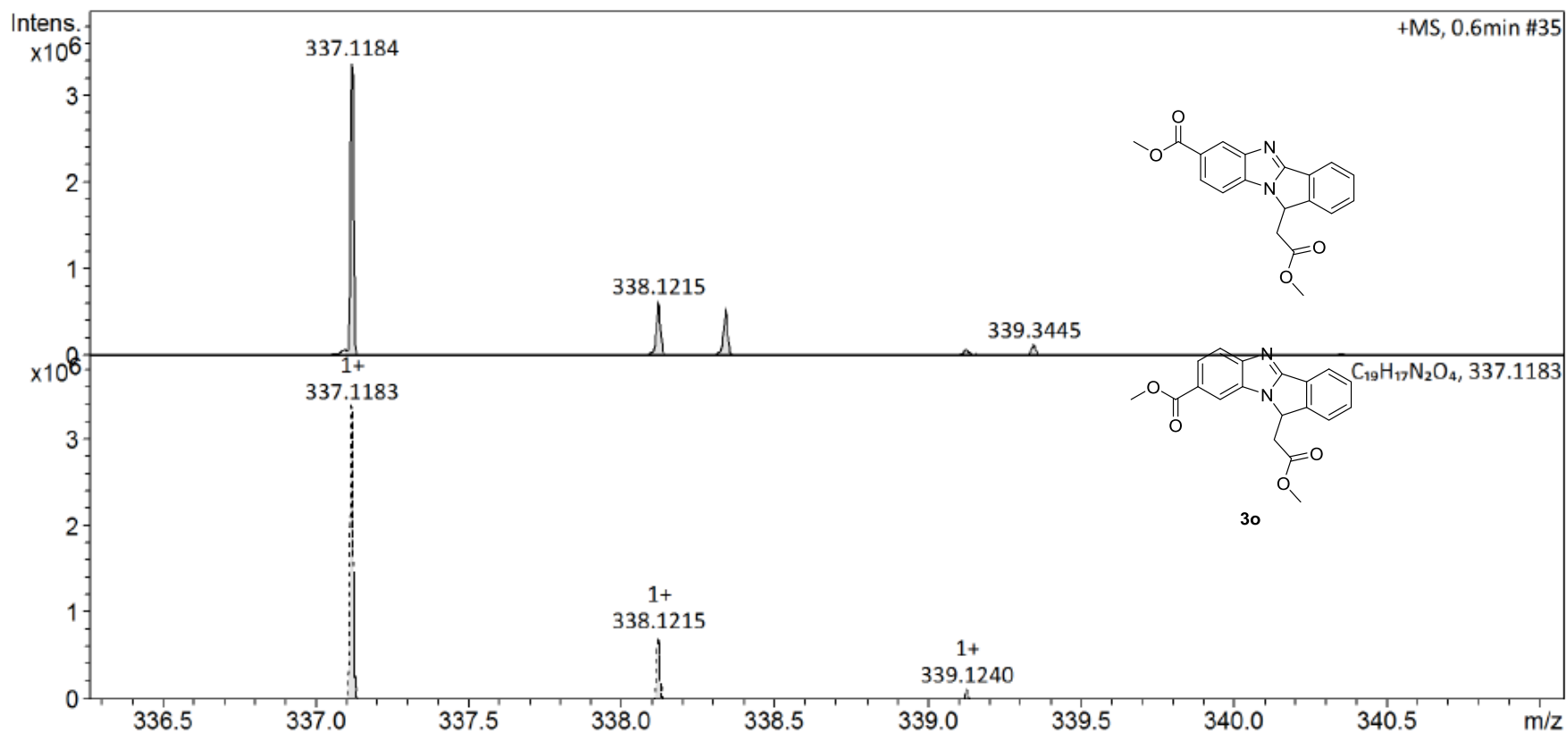
ester-CHO-Ru

2016032200014 6 (0.411) Cn (Cen,3, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00); Cm (6:14-2:3)

Scan ES+  
3.18e7

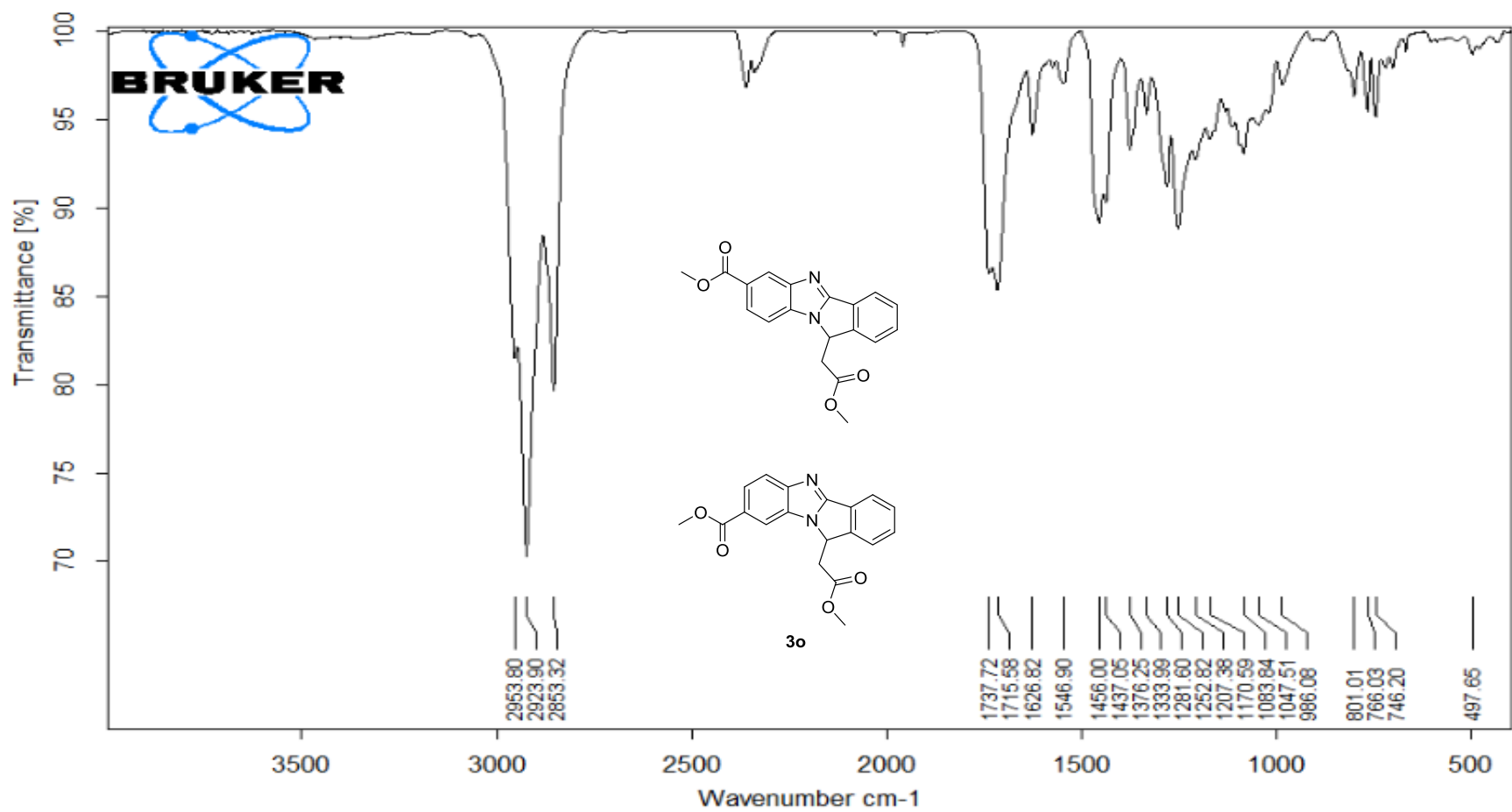


ESI<sup>+</sup> Mass spectrum of compound **3o**

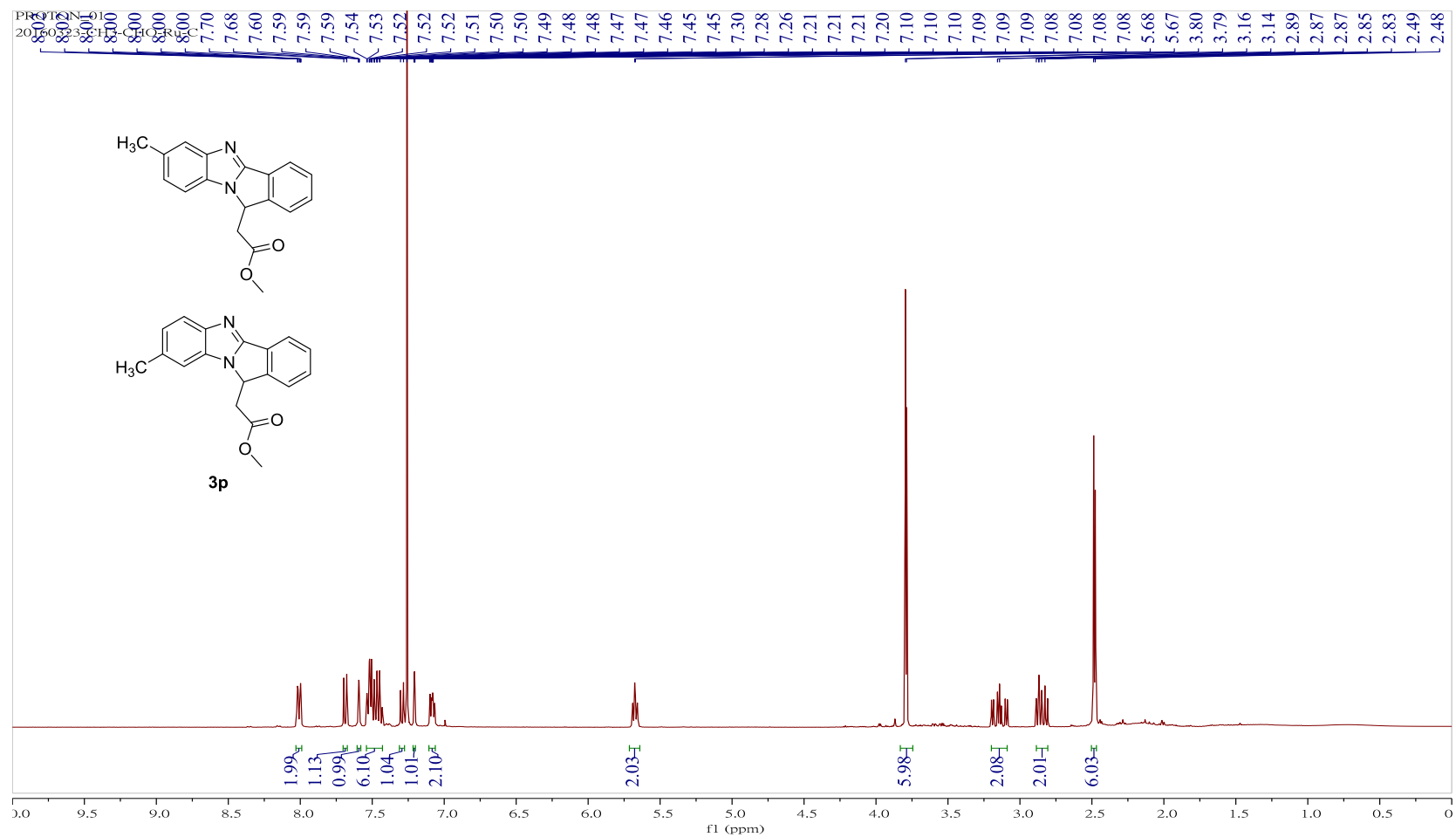


High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3o**

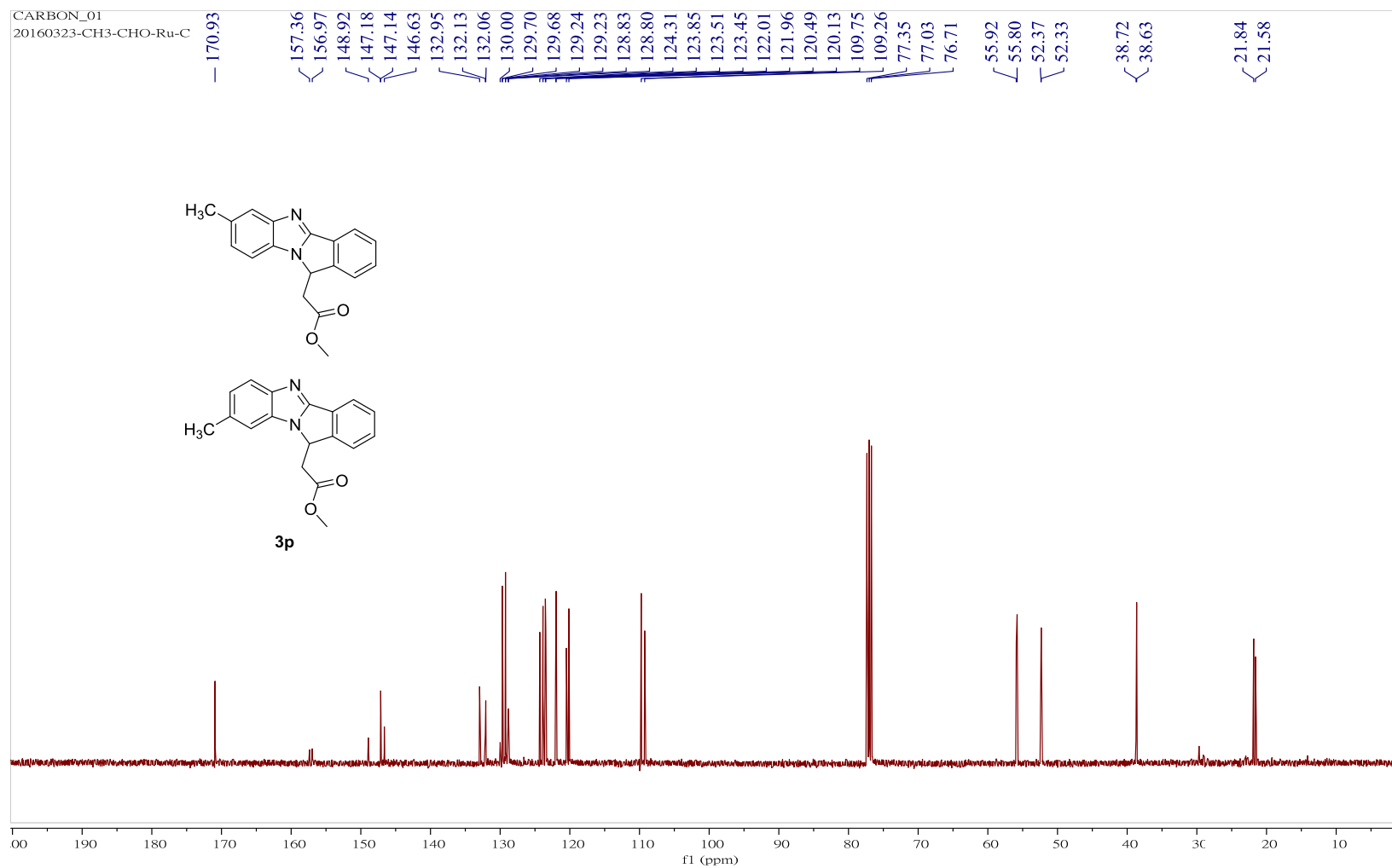




IR spectrum of compound of **3o**



$^1\text{H}$  NMR Spectrum (400 MHz) of compound **3p** in  $\text{CDCl}_3$

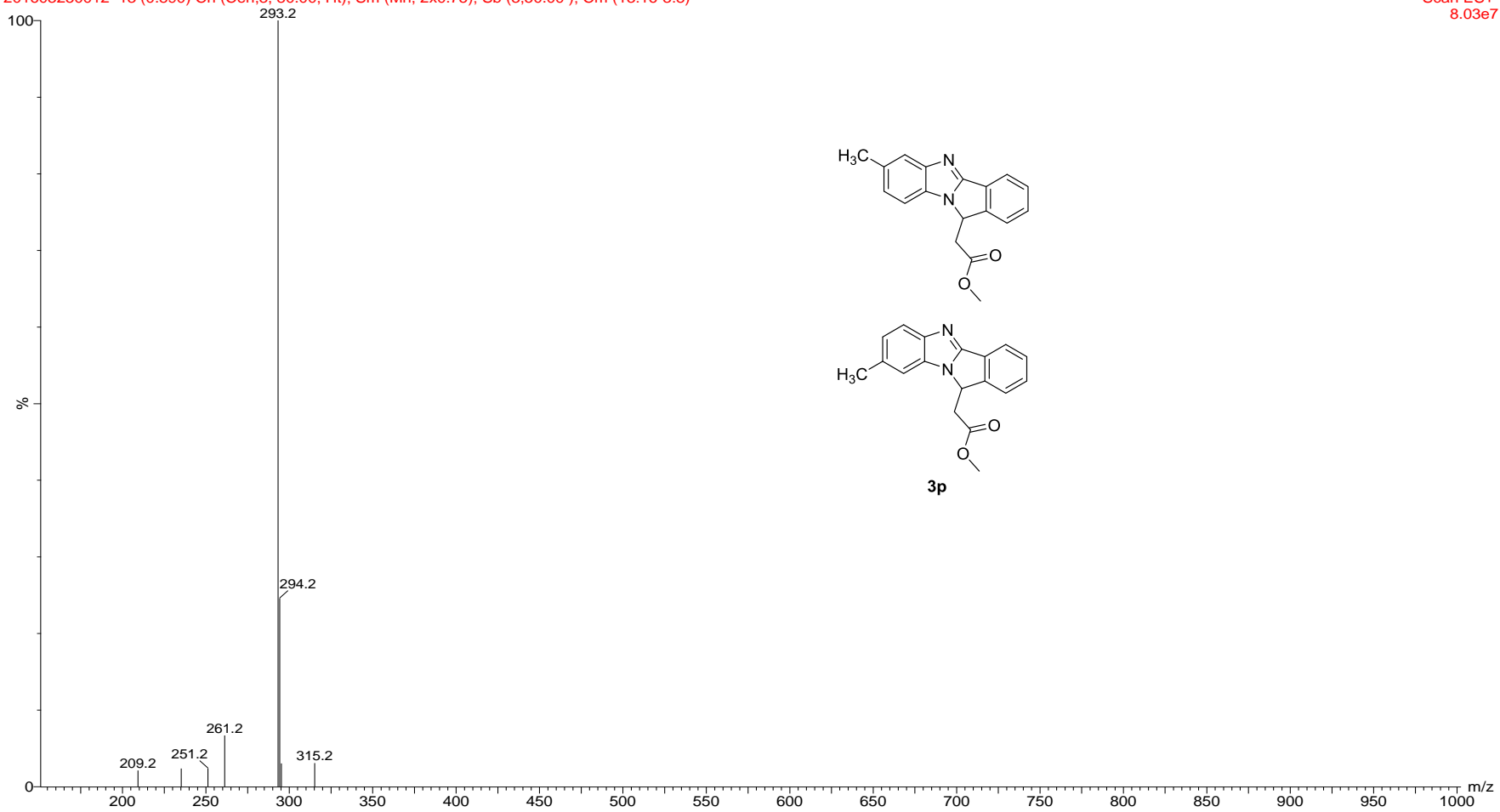


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3p** in  $\text{CDCl}_3$

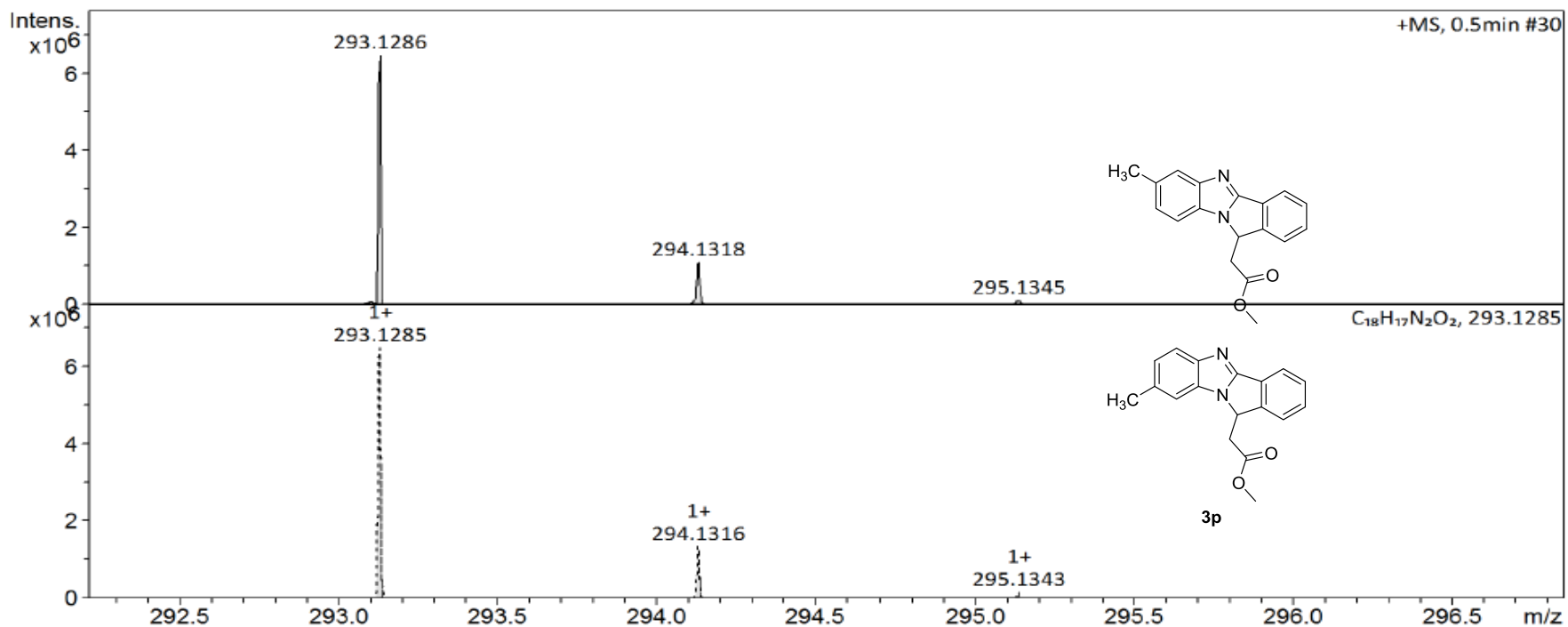
**CH3-CHO-Ru**

201603250012 13 (0.890) Cn (Cen,3, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00 ); Cm (13:16-3:8)

Scan ES+  
8.03e7

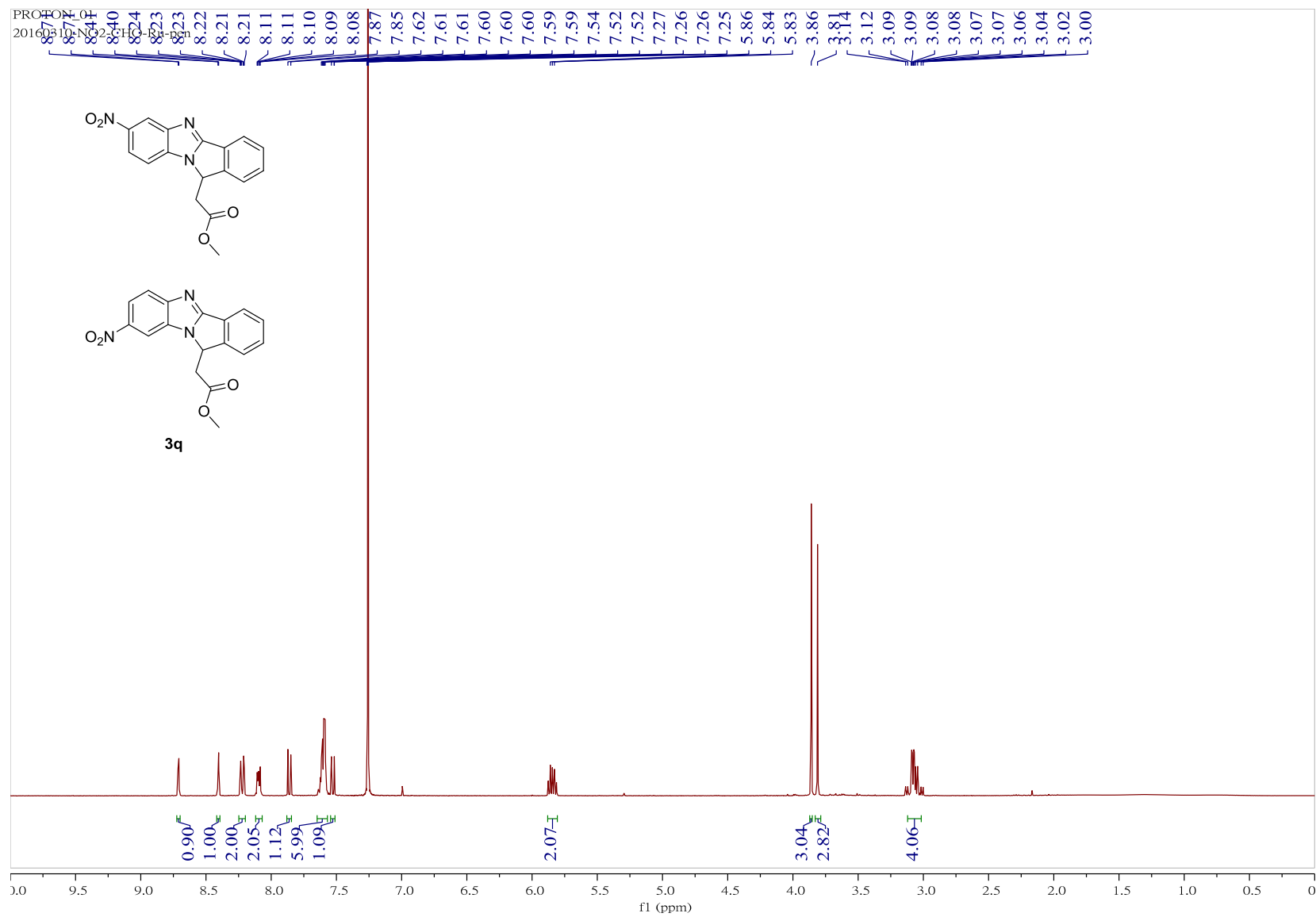


ESI<sup>+</sup> Mass spectrum of compound **3p**

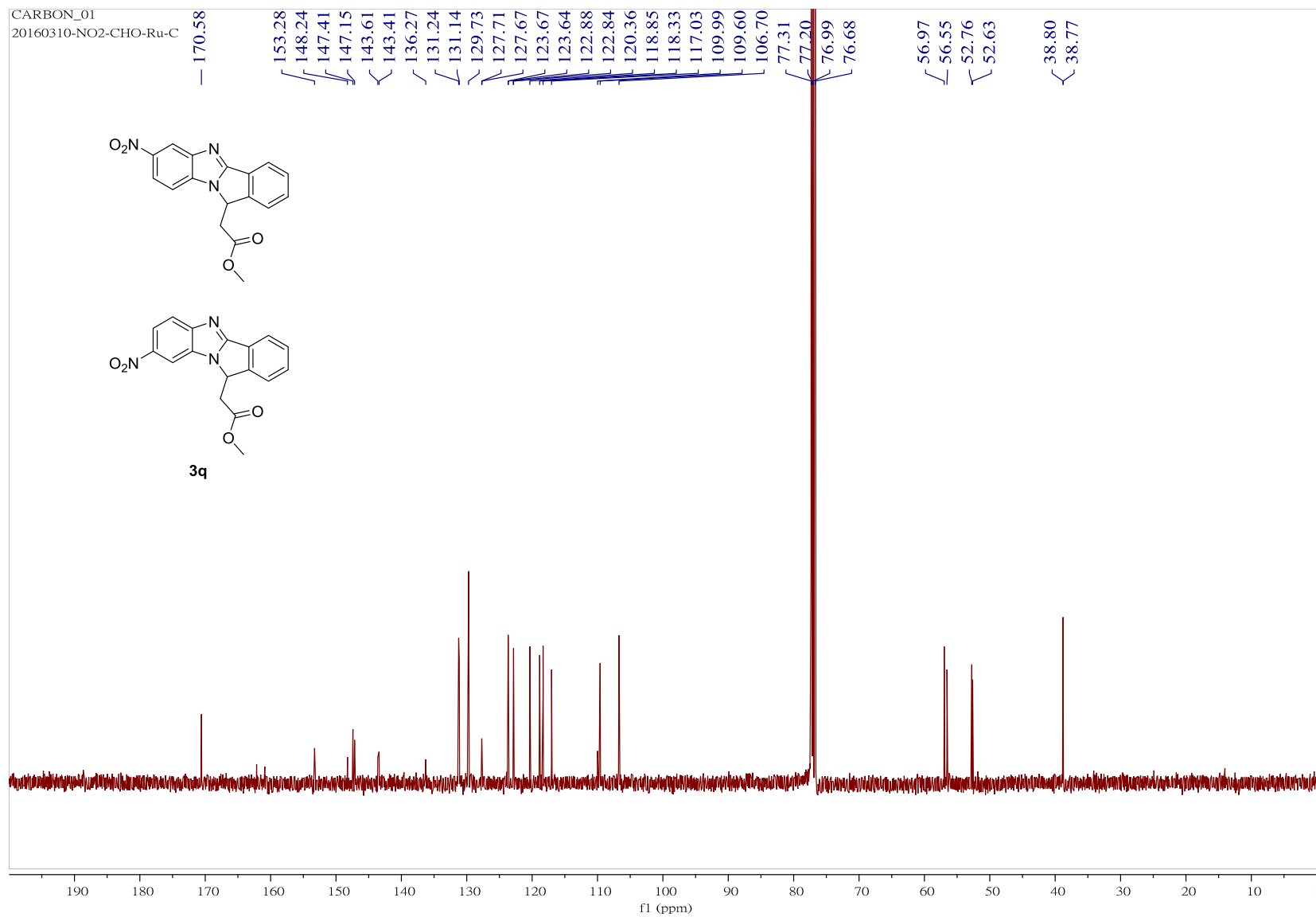


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
293.1286	1	C <sub>18</sub> H <sub>17</sub> N <sub>2</sub> O <sub>2</sub>	293.1285	0.5	20.9	1	100.00	11.5	even	ok	M+H

High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3p**



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **3q** in CDCl<sub>3</sub>

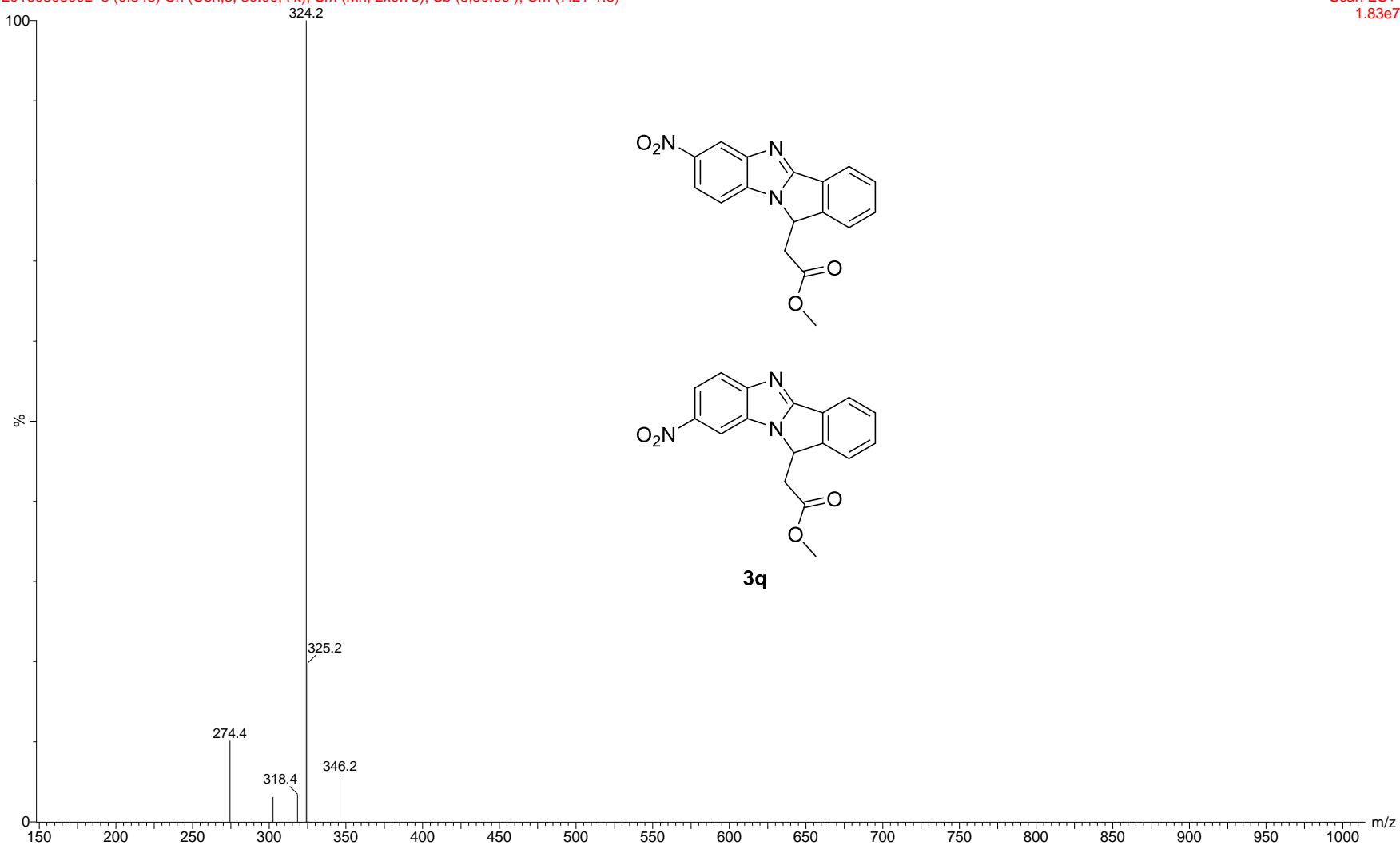


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3q** in  $\text{CDCl}_3$

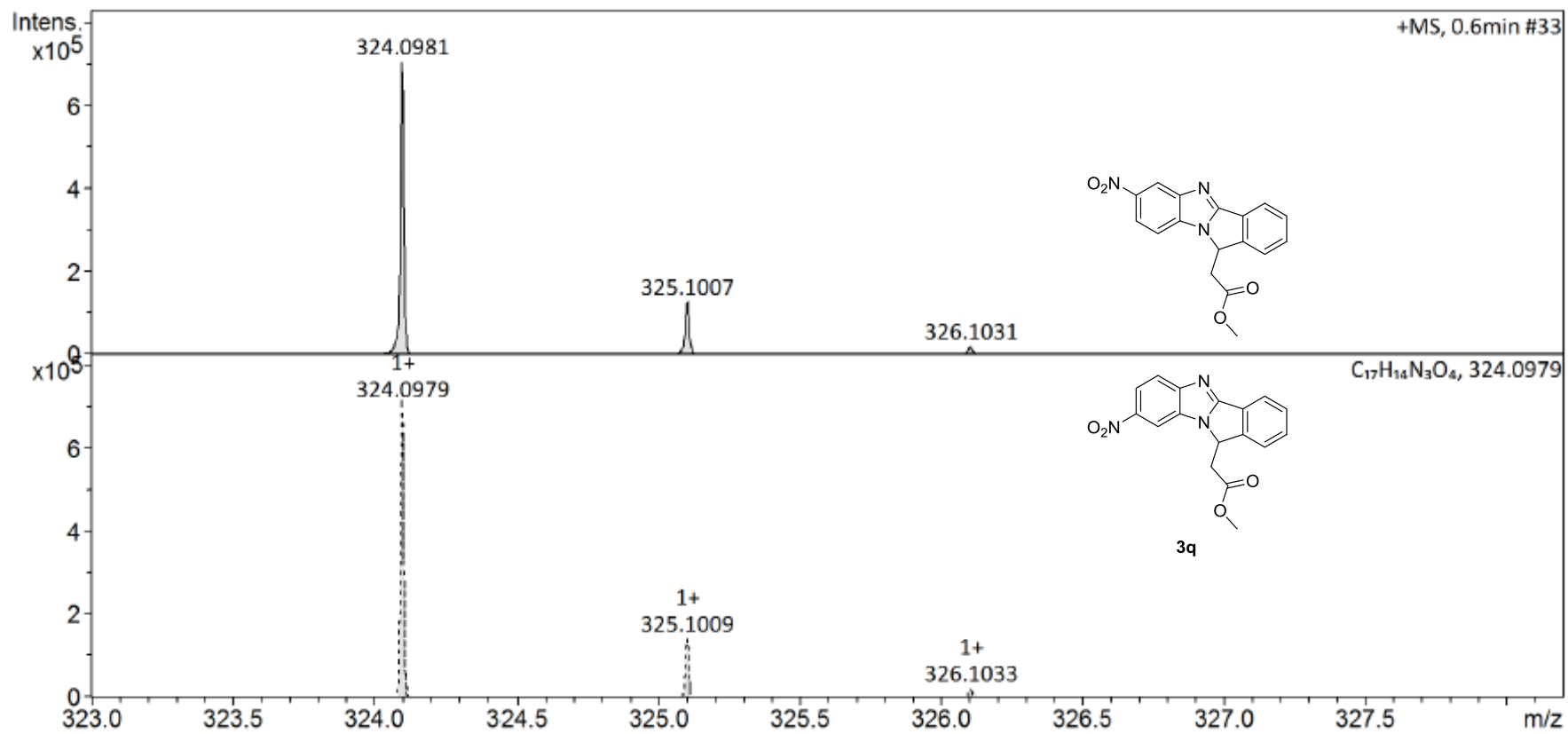
**NO2-CHO-Ru**

20160308002 8 (0.548) Cn (Cen,3, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00); Cm (7:21-1:3)

Scan ES+  
1.83e7

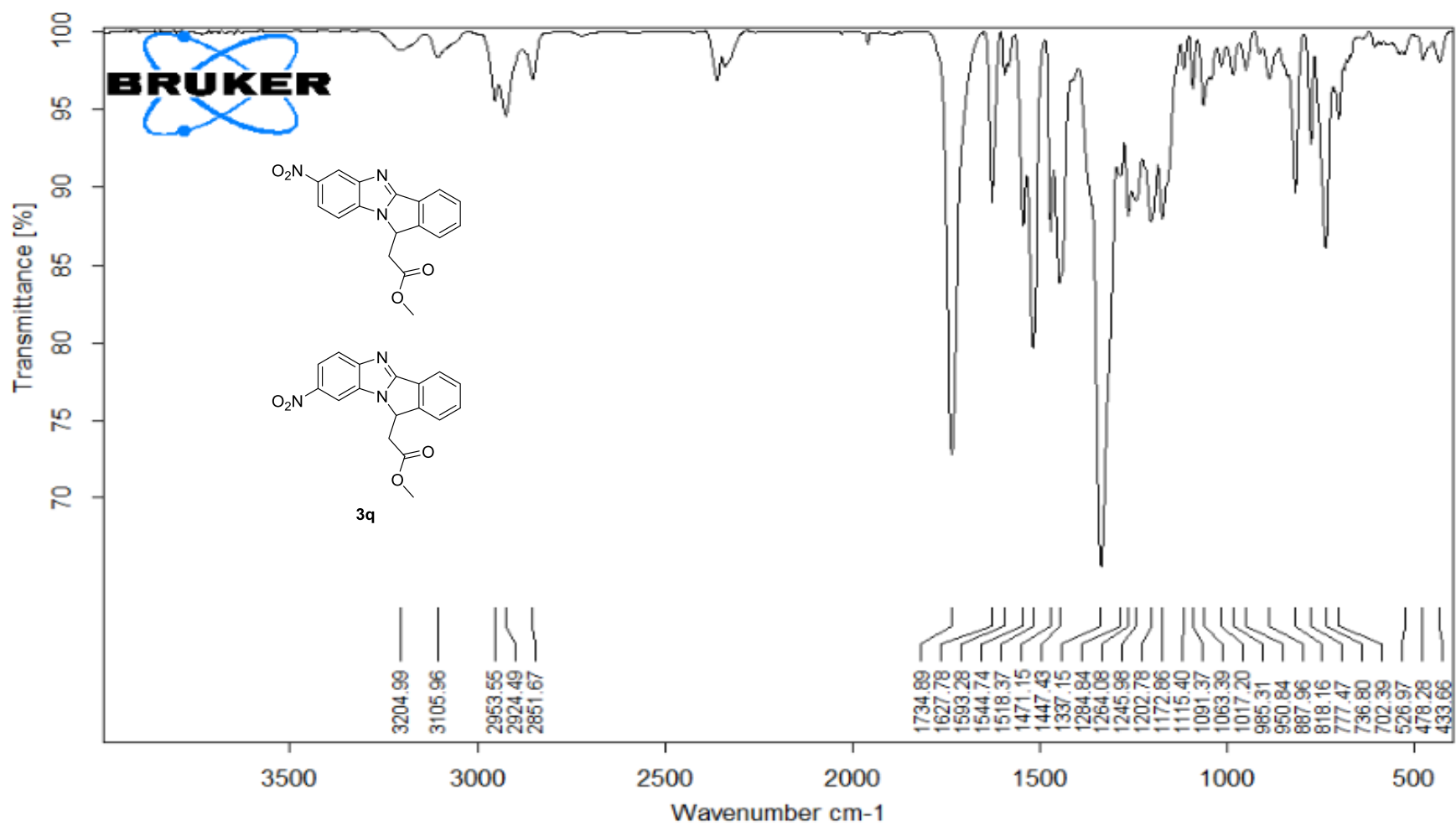




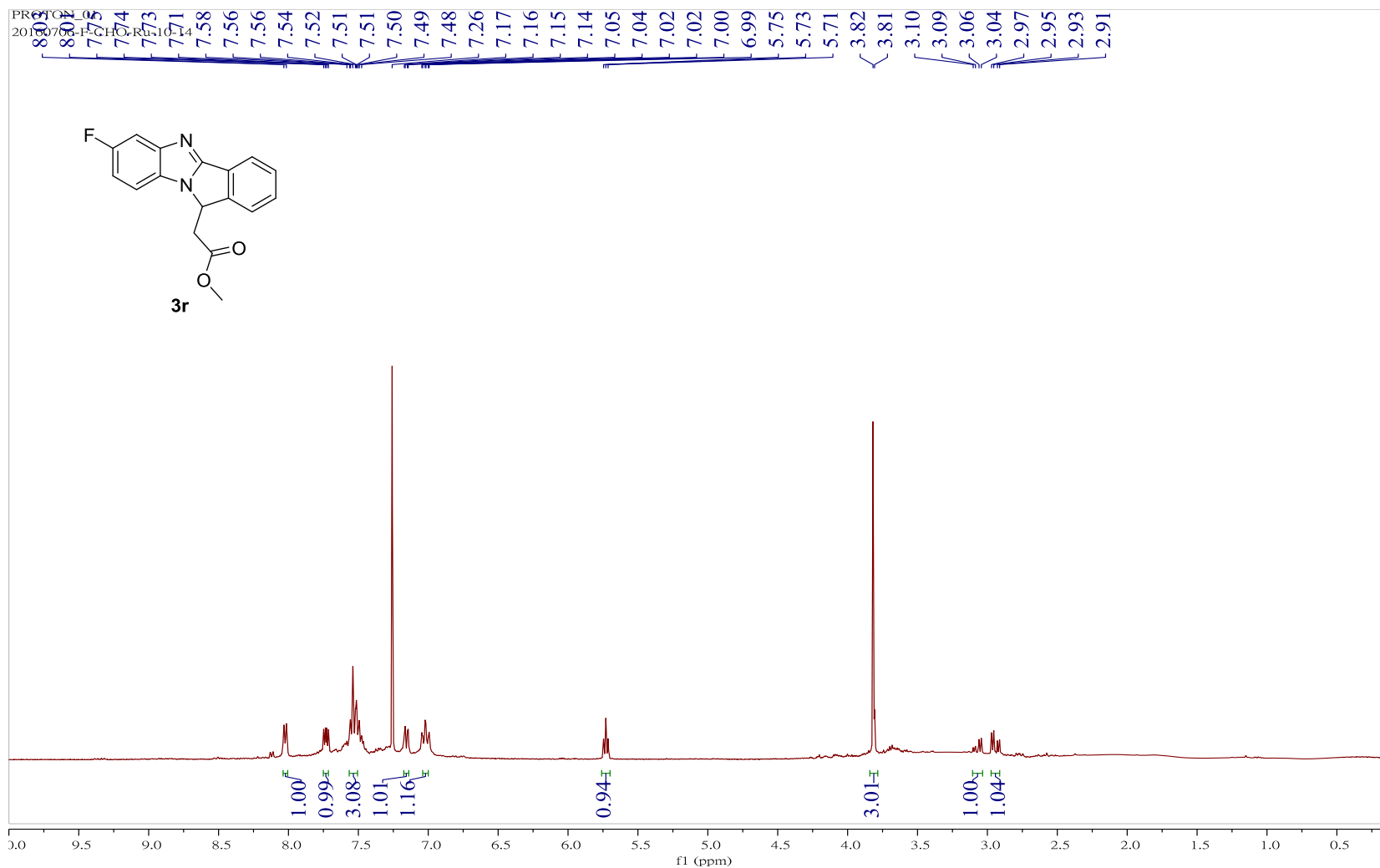


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
324.0981	1	C <sub>17</sub> H <sub>14</sub> N <sub>3</sub> O <sub>4</sub>	324.0979	0.5	12.5	1	100.00	12.5	even	ok	M+H

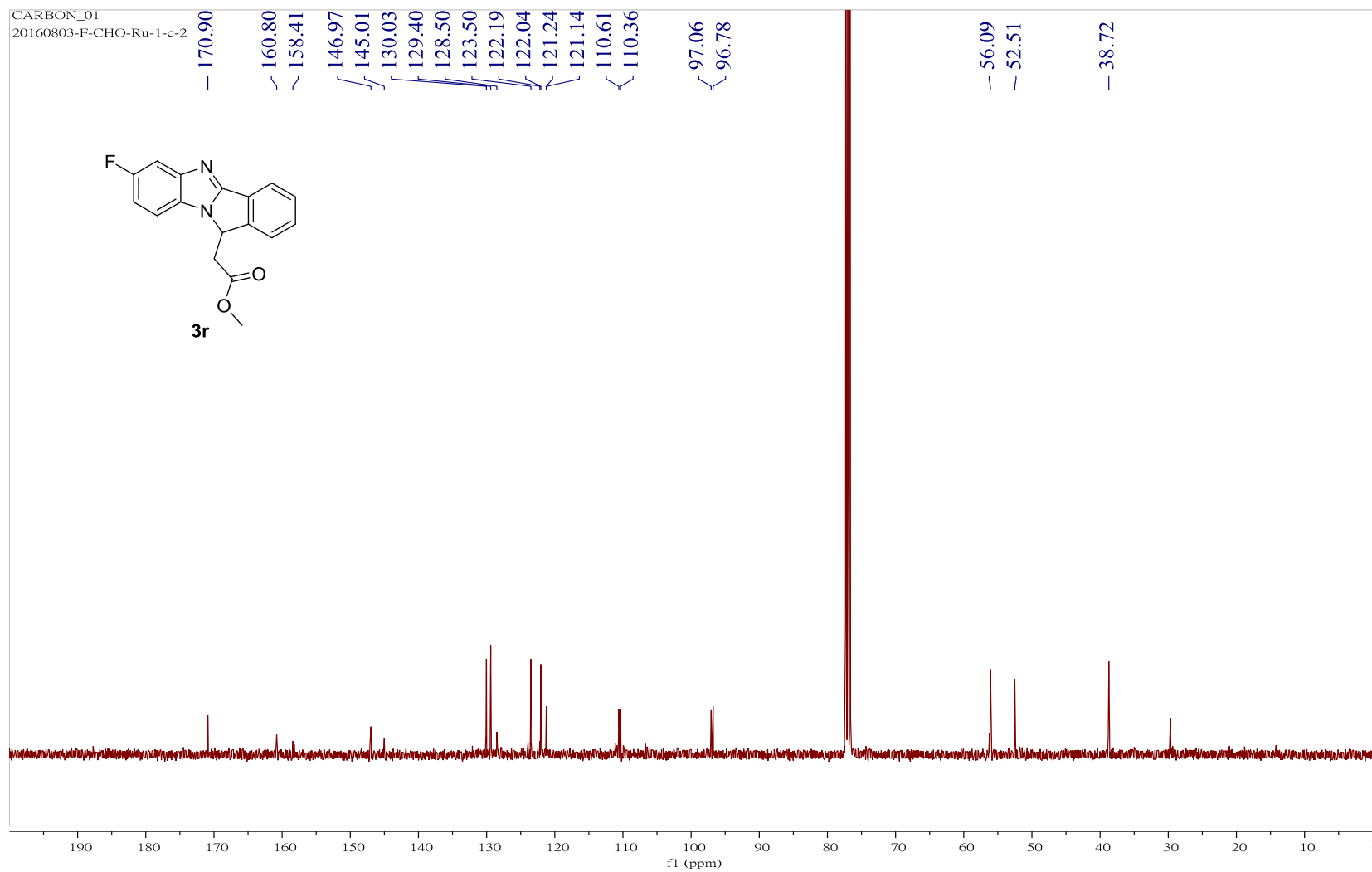
High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3q**



IR spectrum of compound of **3q**



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **3r** in CDCl<sub>3</sub>

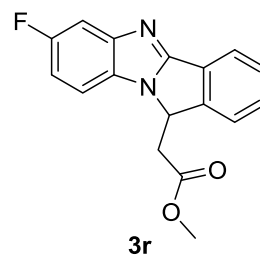
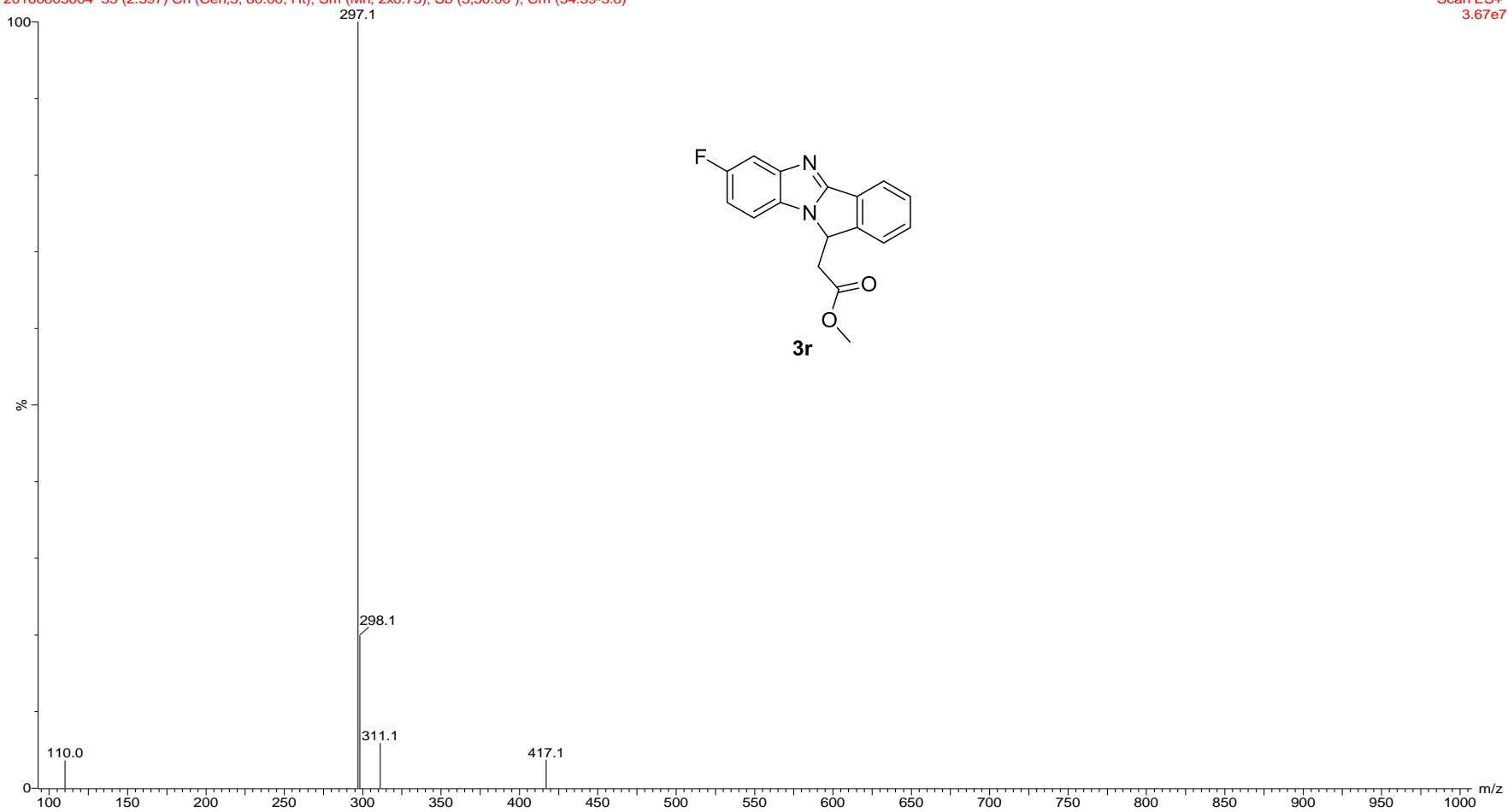


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3r** in  $\text{CDCl}_3$

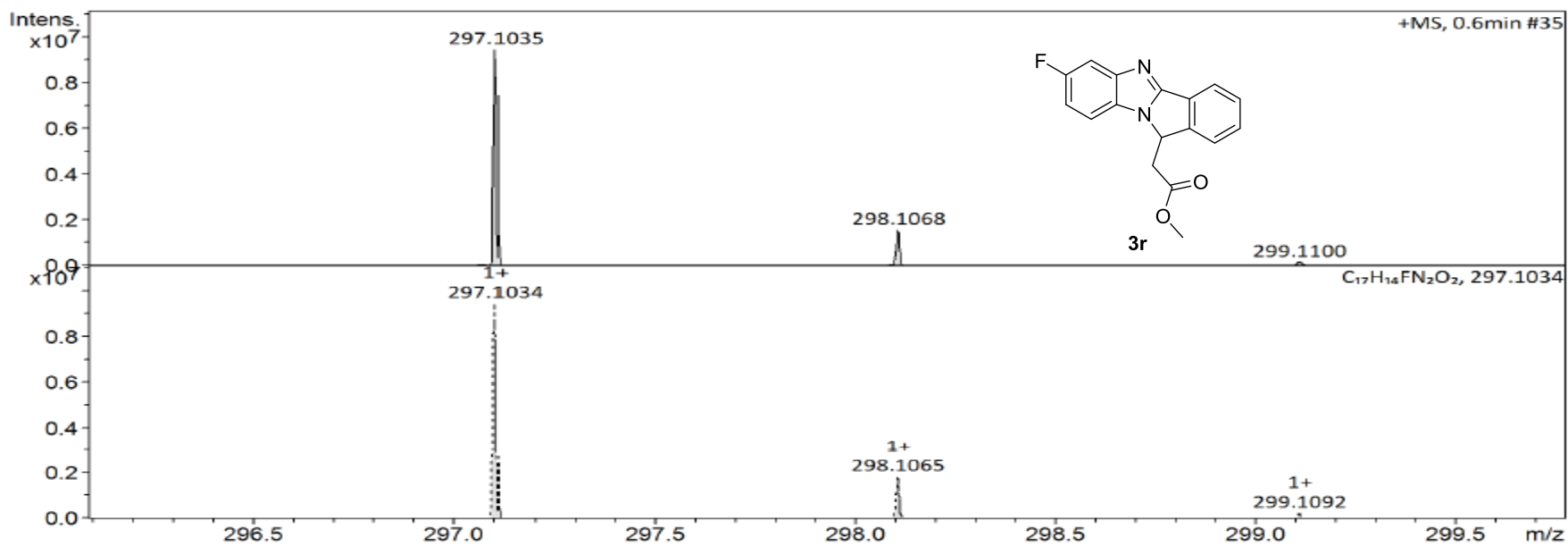
**F-CHO-Ru**

20160805004 35 (2.397) Cn (Cen,3, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00); Cm (34:39-3:8)

Scan ES+  
3.67e7

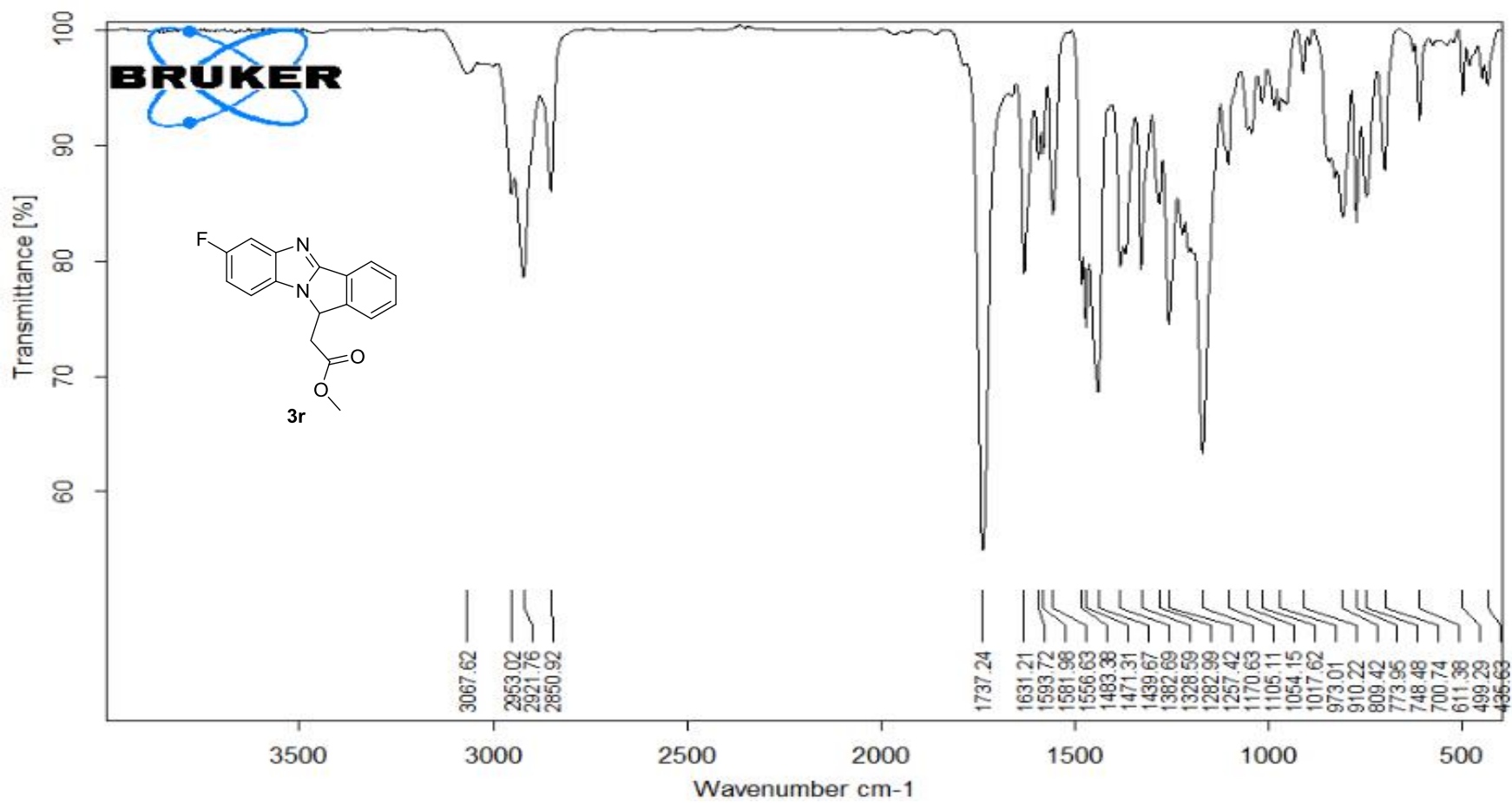


ESI<sup>+</sup> Mass spectrum of compound **3r**

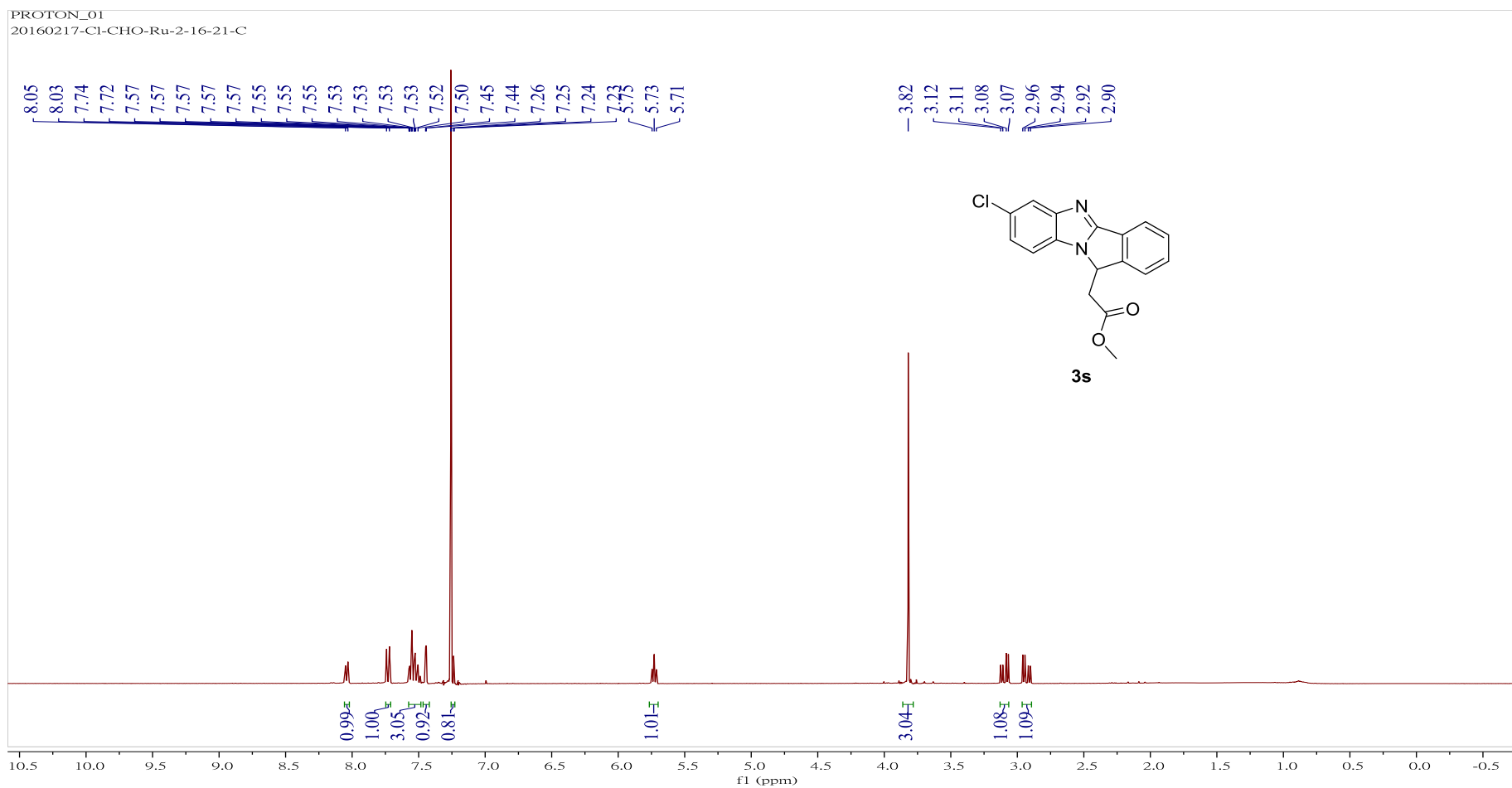


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
297.1035	1	C <sub>17</sub> H <sub>14</sub> FN <sub>2</sub> O <sub>2</sub>	297.1034	-0.2	17.2	1	100.00	11.5	even	ok	M+H

High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3r**

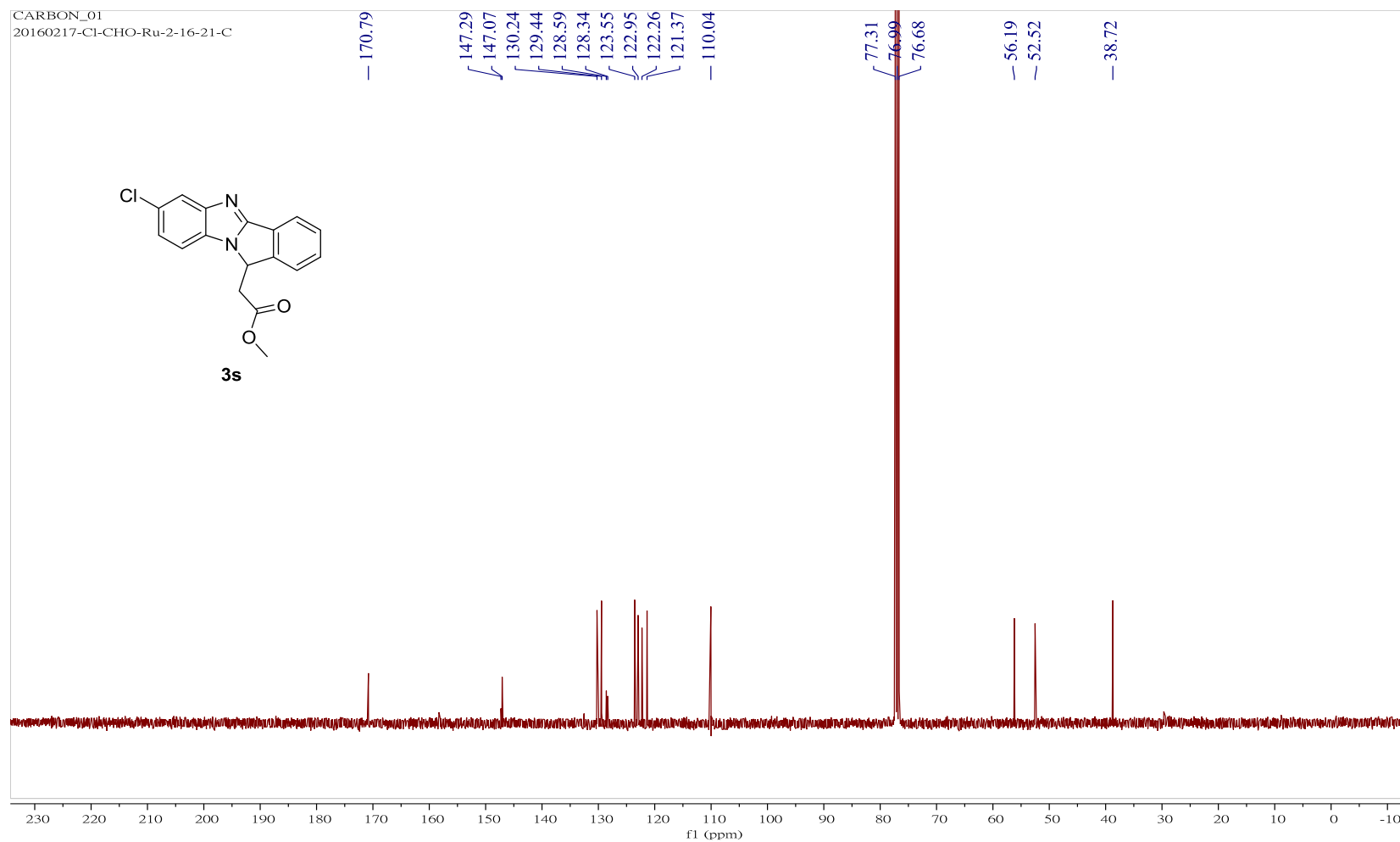


IR spectrum of compound of **3r**



$^1\text{H}$  NMR Spectrum (400 MHz) of compound **3s** in  $\text{CDCl}_3$



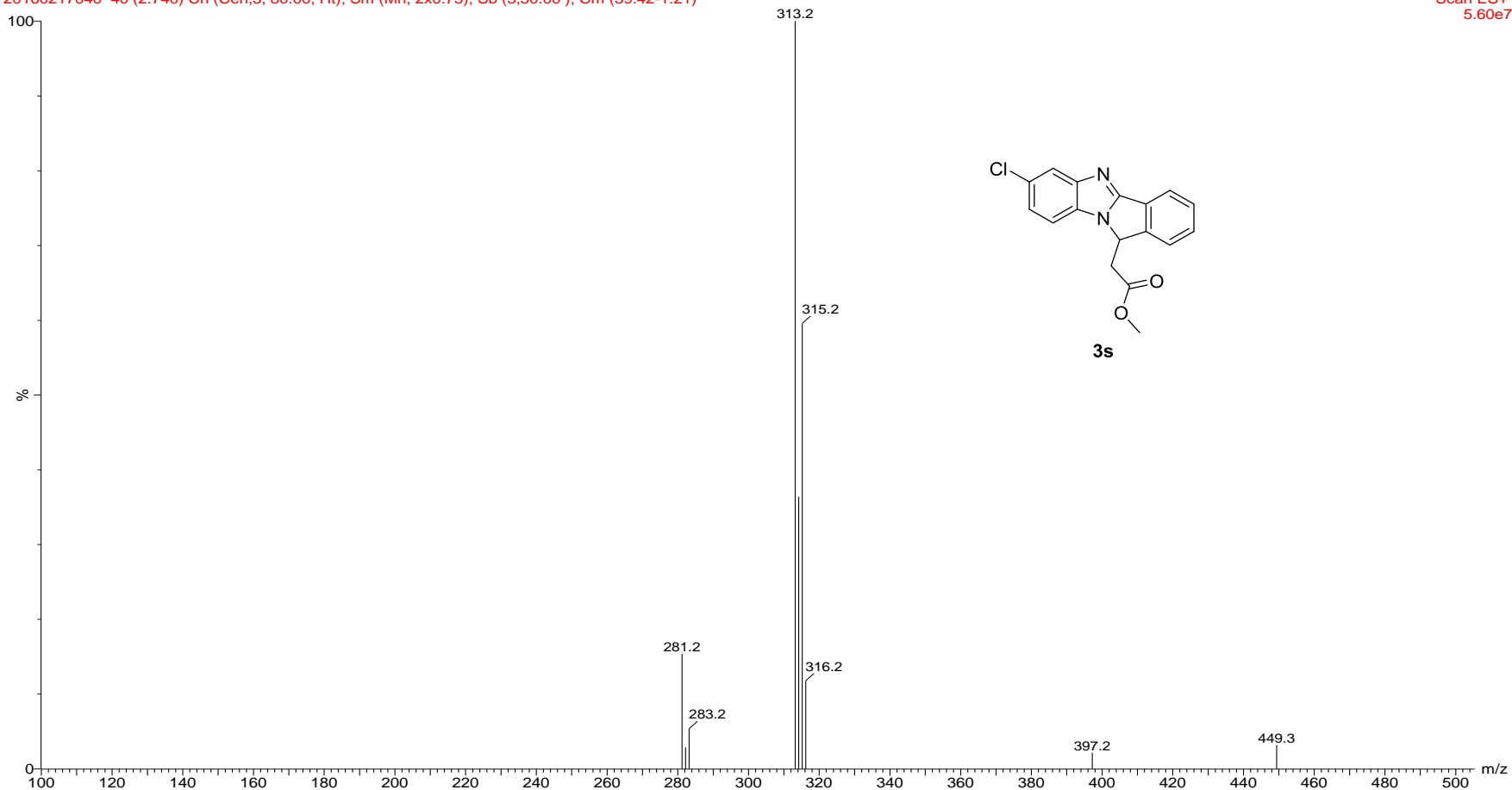


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3s** in  $\text{CDCl}_3$

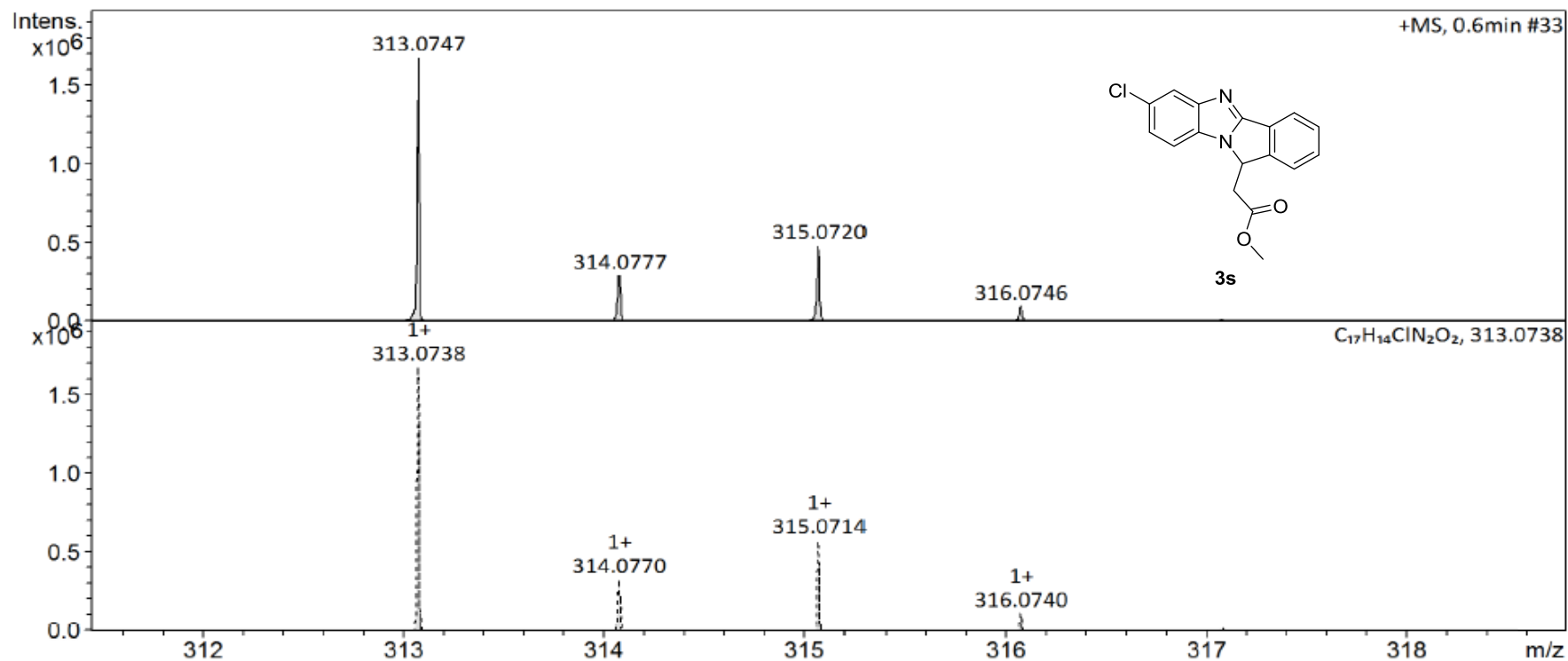
**Cl-CHO-Ru-2-16-F**

20160217040 40 (2.740) Cn (Cen,3, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00 ); Cm (39:42-1:21)

Scan ES+  
5.60e7

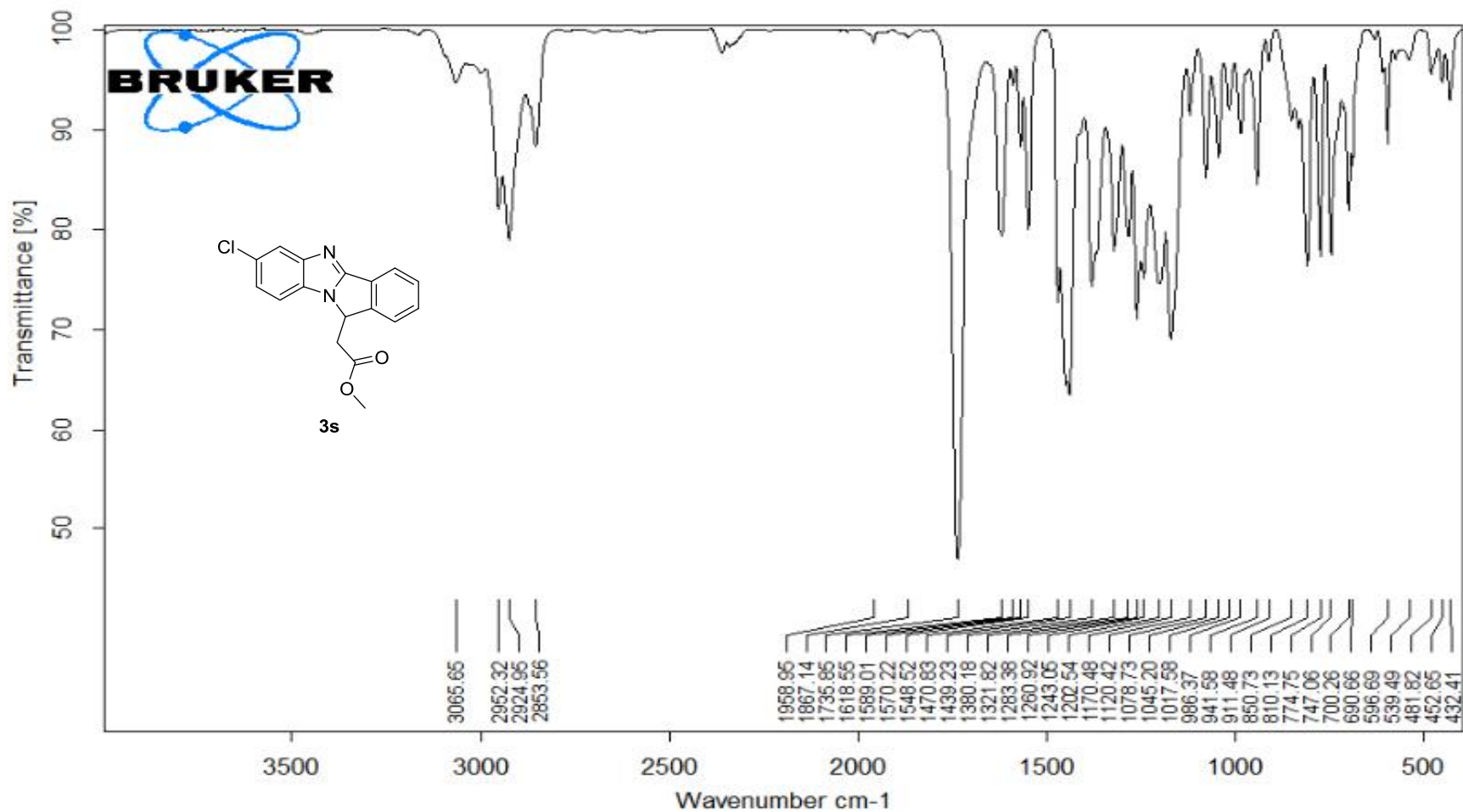


ESI<sup>+</sup> Mass spectrum of compound **3s**

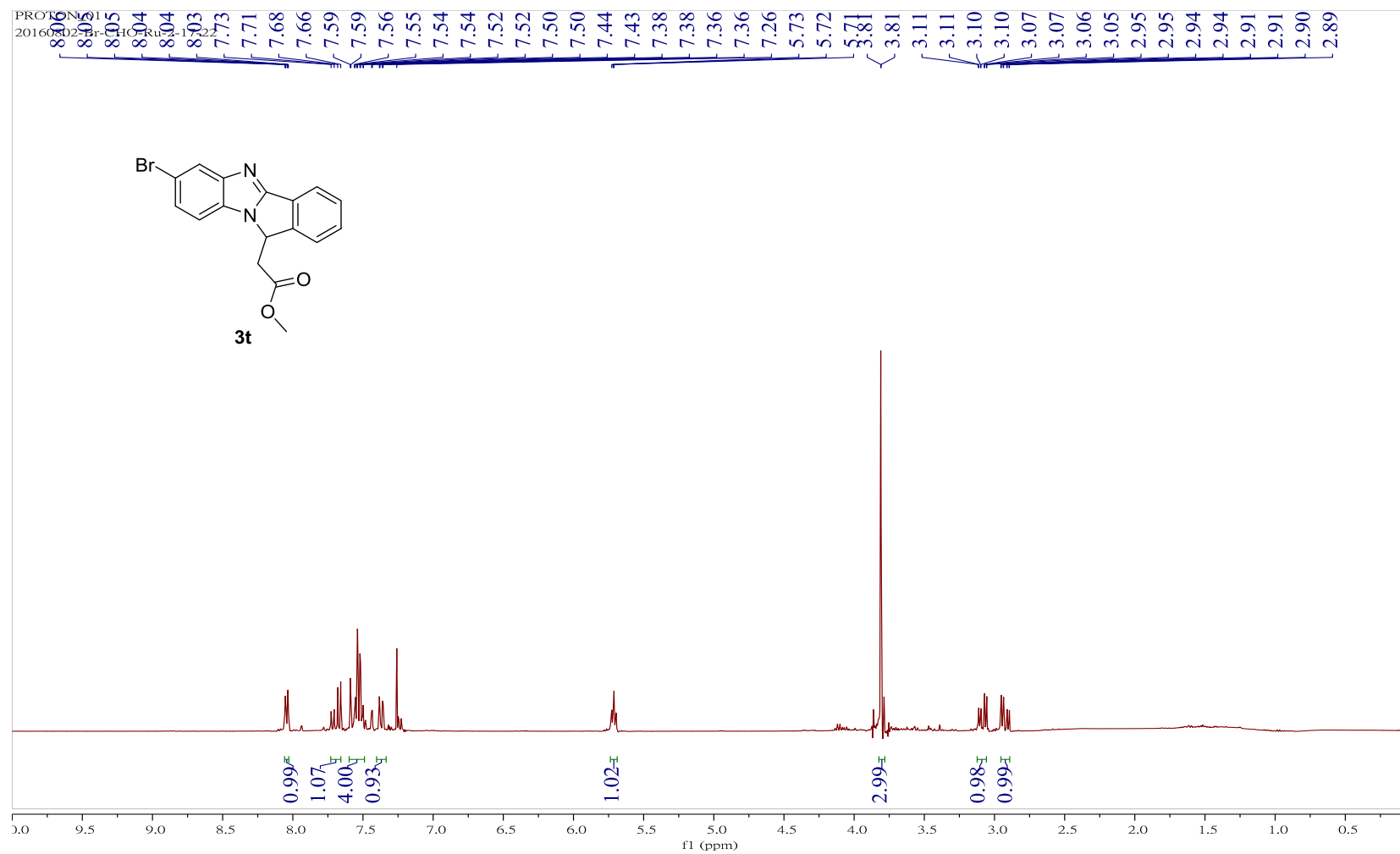


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
313.0747	1	C <sub>17</sub> H <sub>14</sub> ClN <sub>2</sub> O <sub>2</sub>	313.0738	-2.8	27.1	1	100.00	11.5	even	ok	M+H

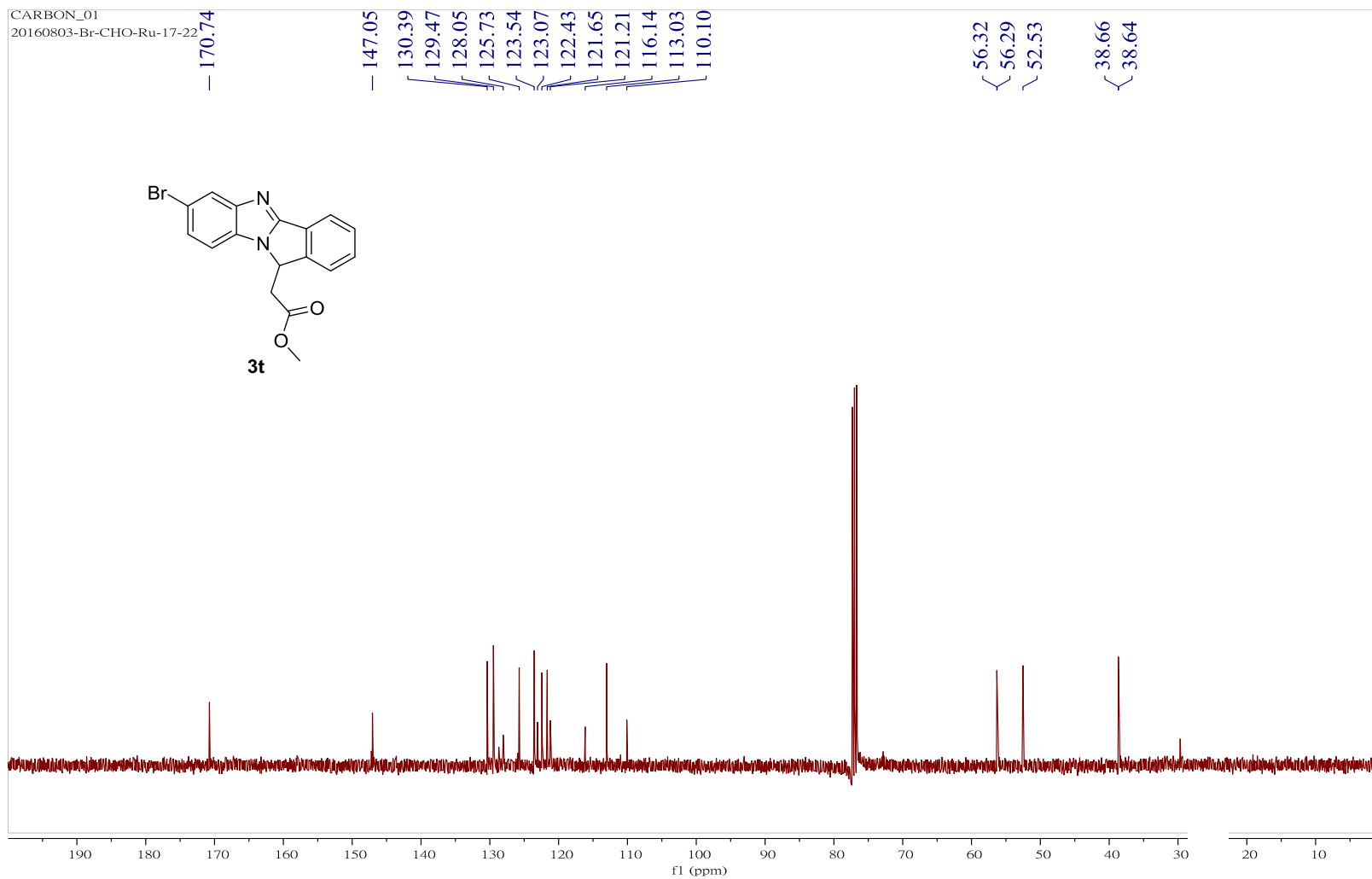
High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3s**



IR spectrum of compound of 3s



$^1\text{H}$  NMR Spectrum (400 MHz) of compound **3t** in  $\text{CDCl}_3$

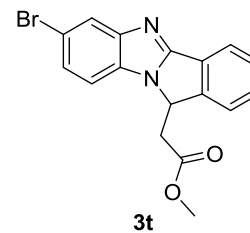
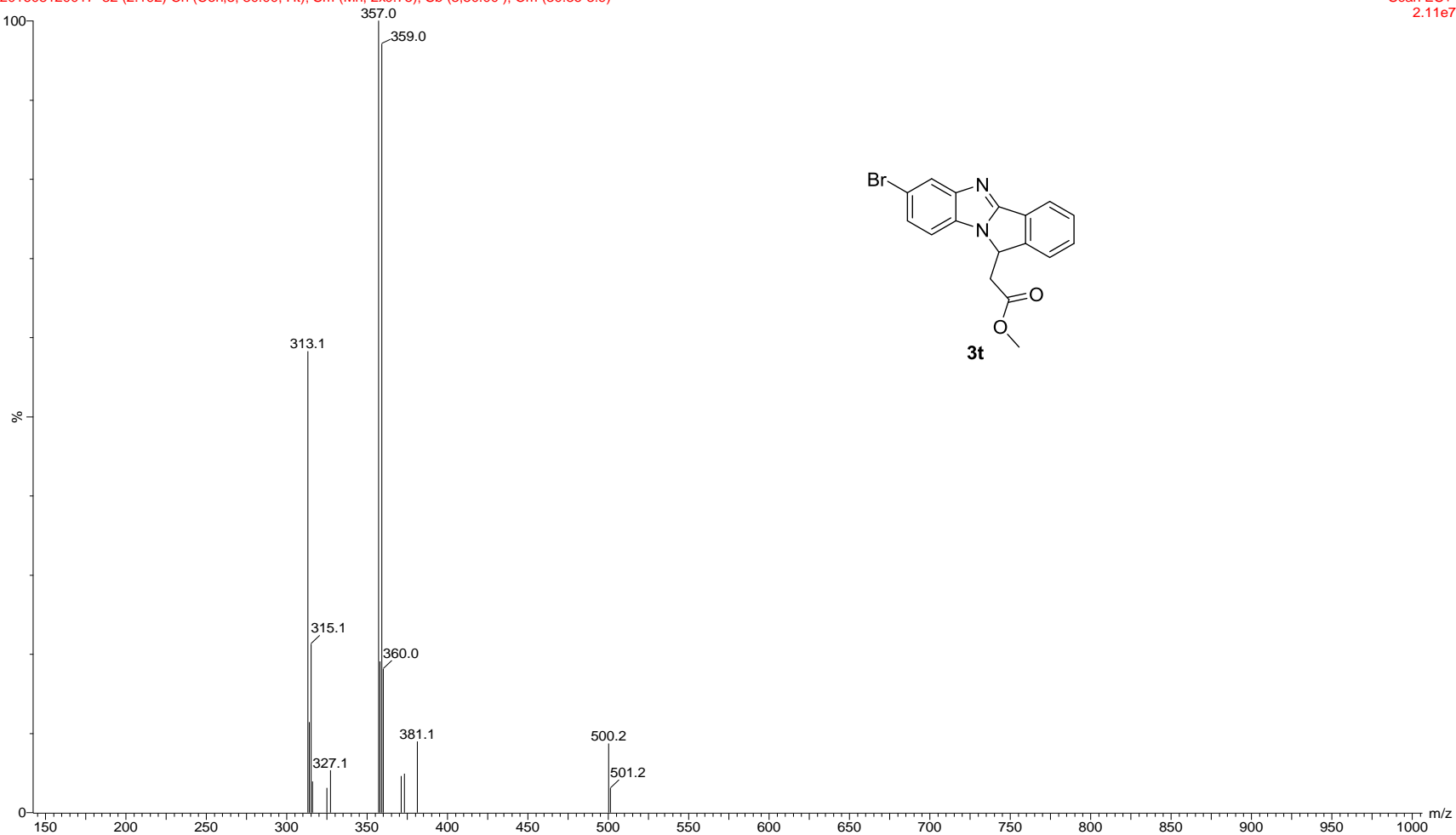


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **3t** in  $\text{CDCl}_3$

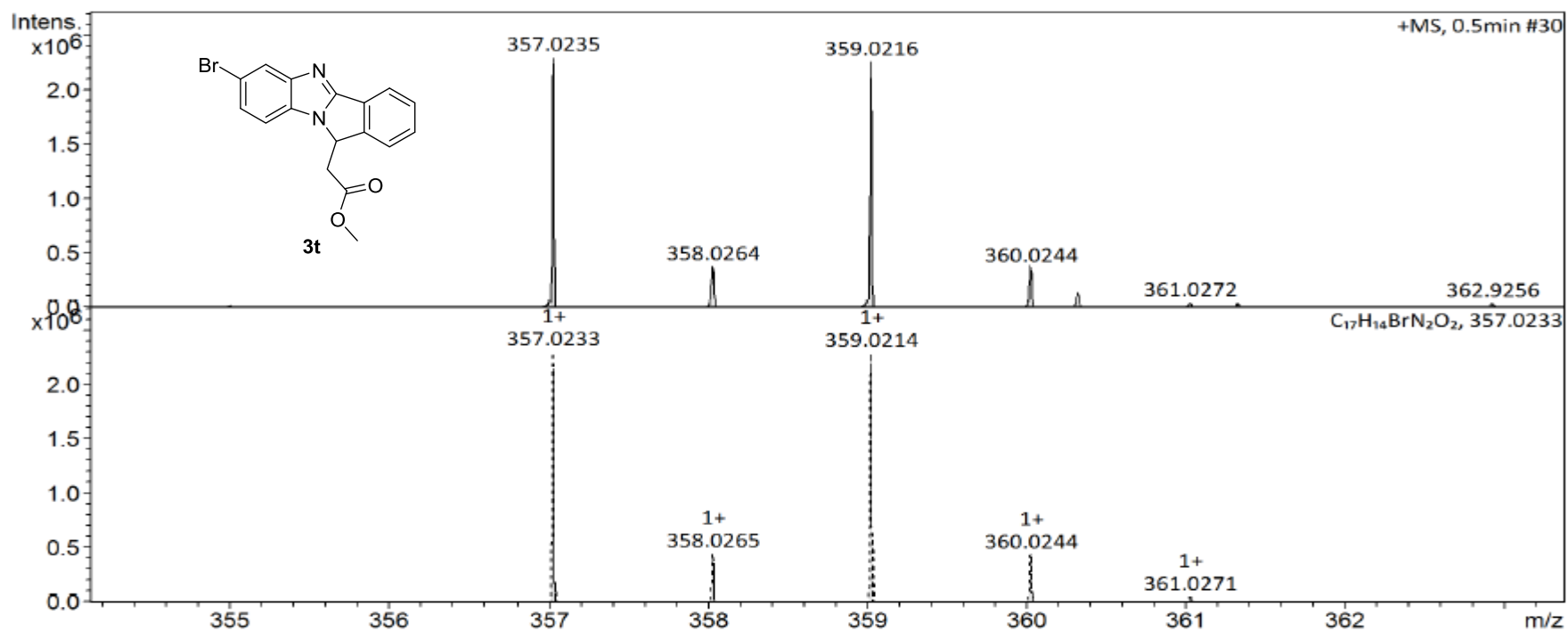
**Br-CHO-Ru**

201608120017 32 (2.192) Cn (Cen,3, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00); Cm (30:36-3:9)

Scan ES+  
2.11e7



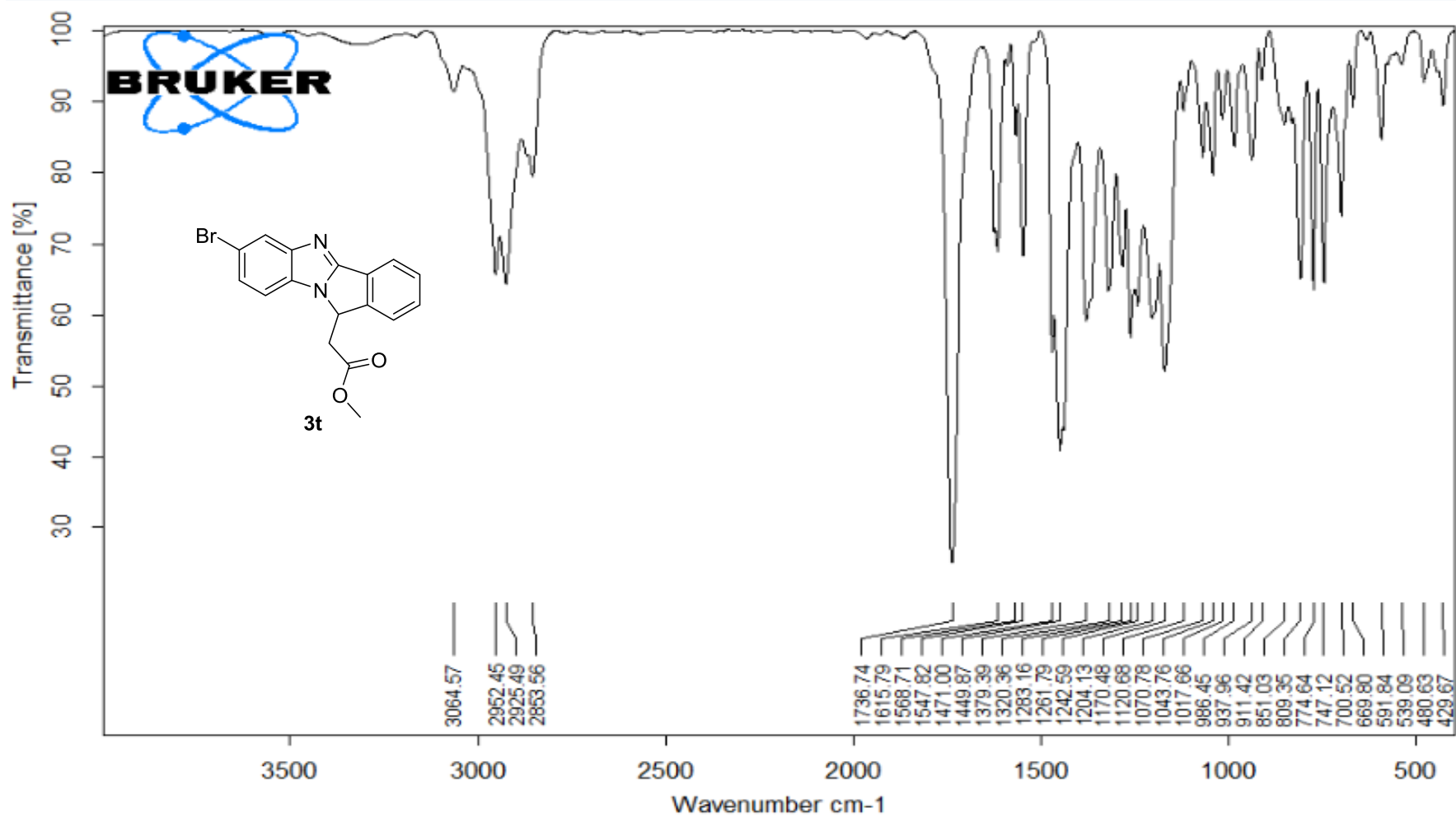
ESI<sup>+</sup> Mass spectrum of compound **3t**



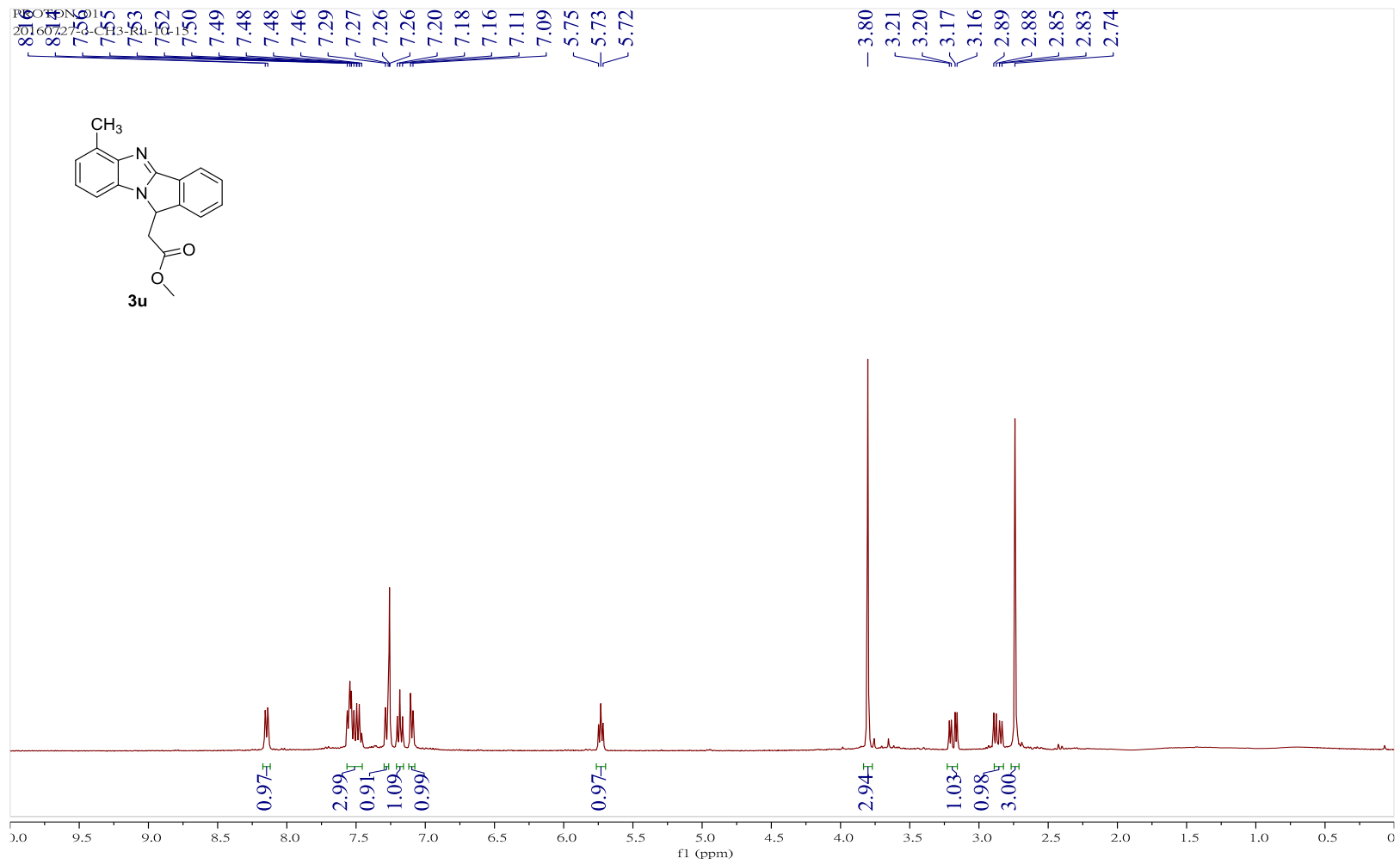
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
357.0235	1	C <sub>17</sub> H <sub>14</sub> BrN <sub>2</sub> O <sub>2</sub>	357.0233	-0.4	21.4	1	100.00	11.5	even	ok	M+H

High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3t**

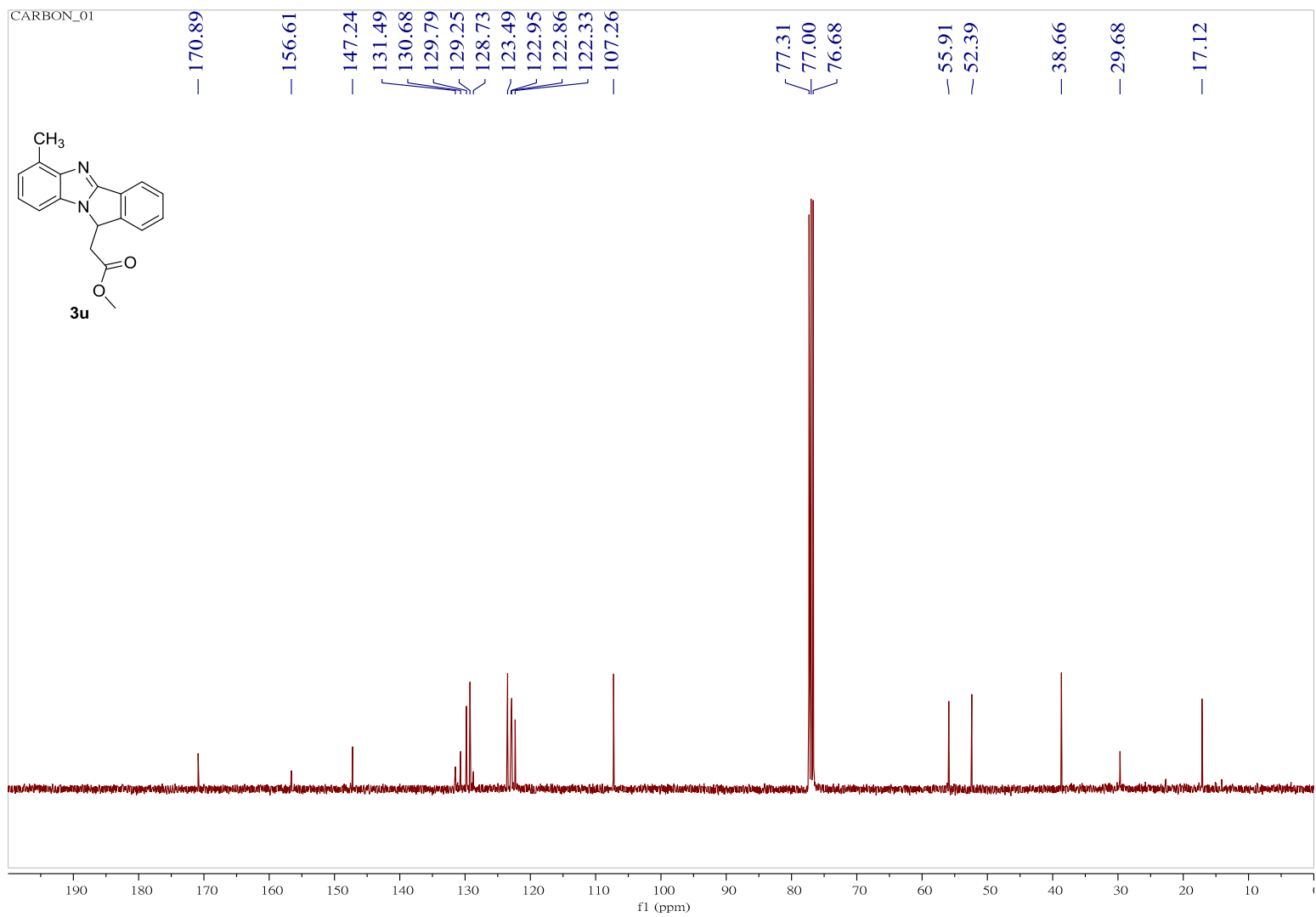




IR spectrum of compound of 3t



$^1\text{H}$  NMR Spectrum (400 MHz) of compound **3u** in  $\text{CDCl}_3$

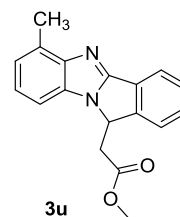
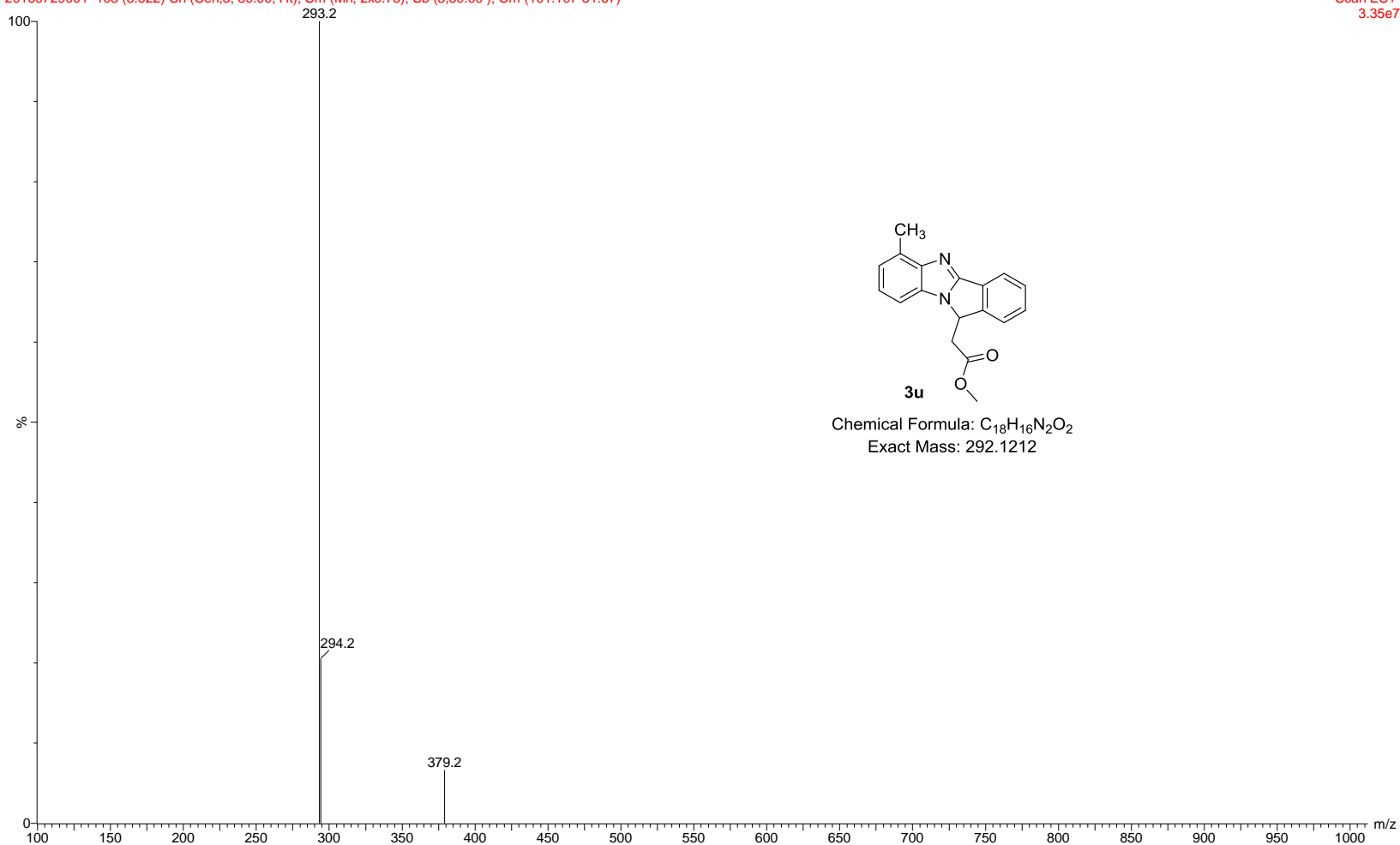


<sup>13</sup>C NMR Spectrum (100 MHz) of compound **3u** in CDCl<sub>3</sub>

O-CH3-Ru-10-15

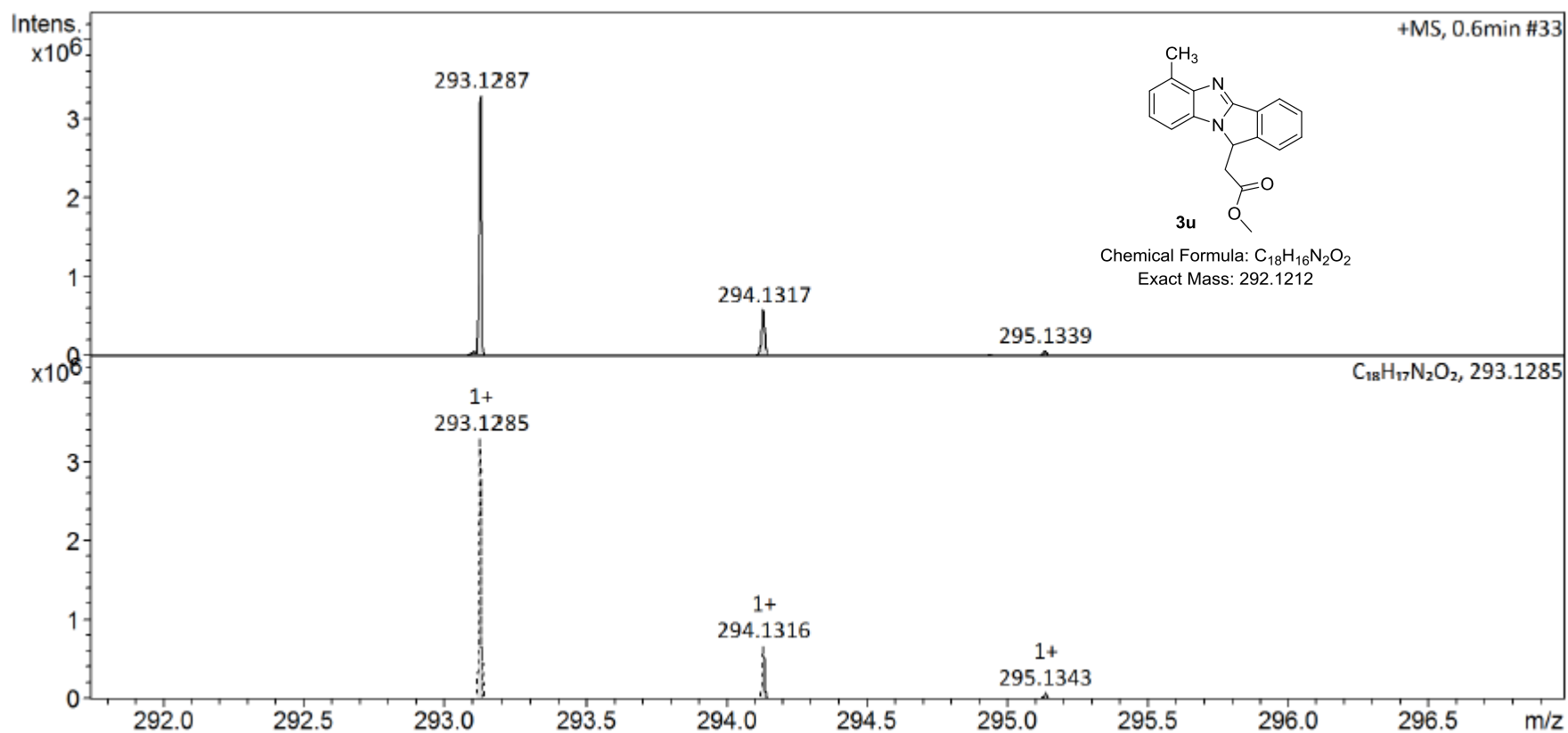
20160729001 103 (3.622) Cn (Cen,3, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00 ); Cm (101:107-51:67)

Scan ES+  
3.35e7



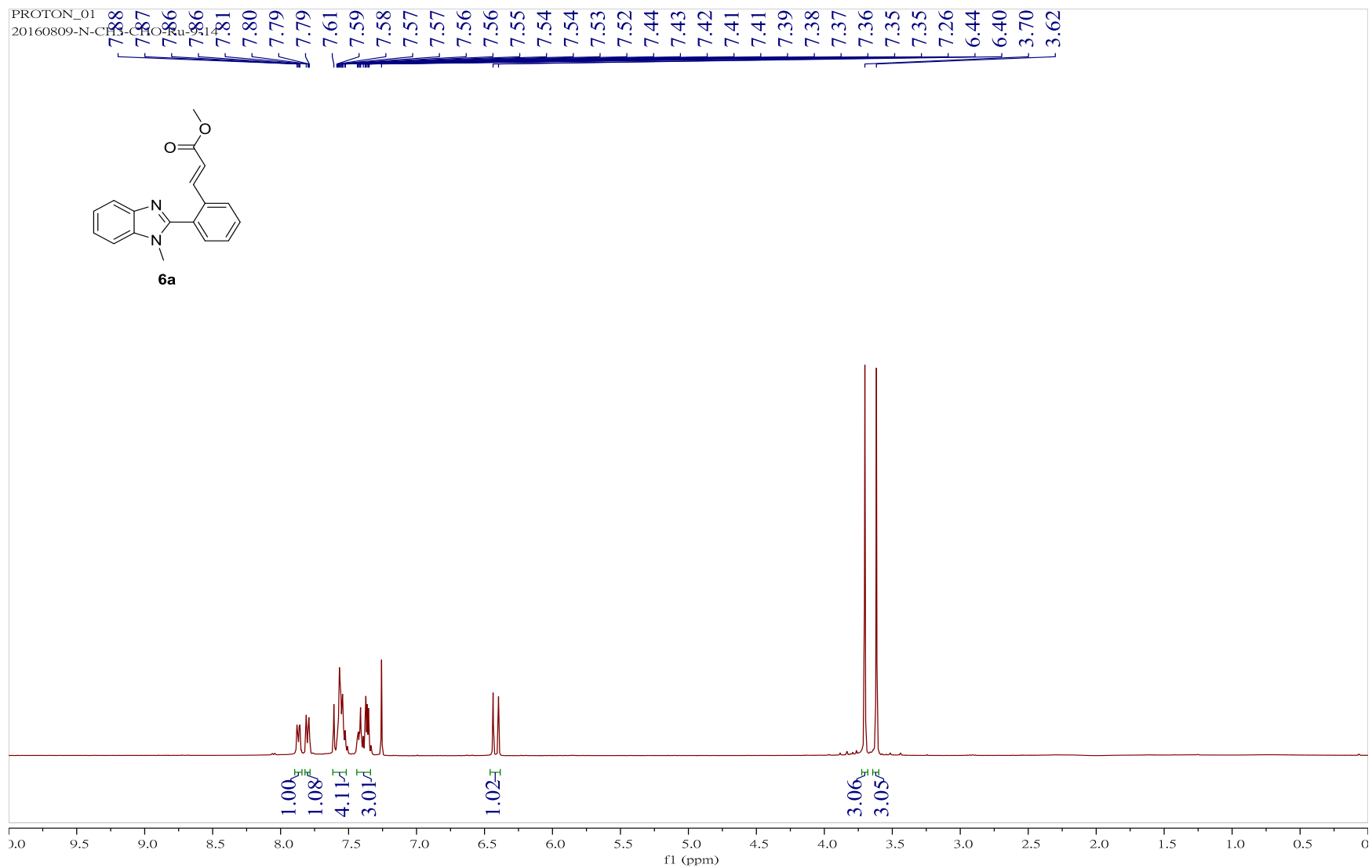
Chemical Formula: C<sub>18</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>  
Exact Mass: 292.1212

ESI<sup>+</sup> Mass spectrum of compound **3u**

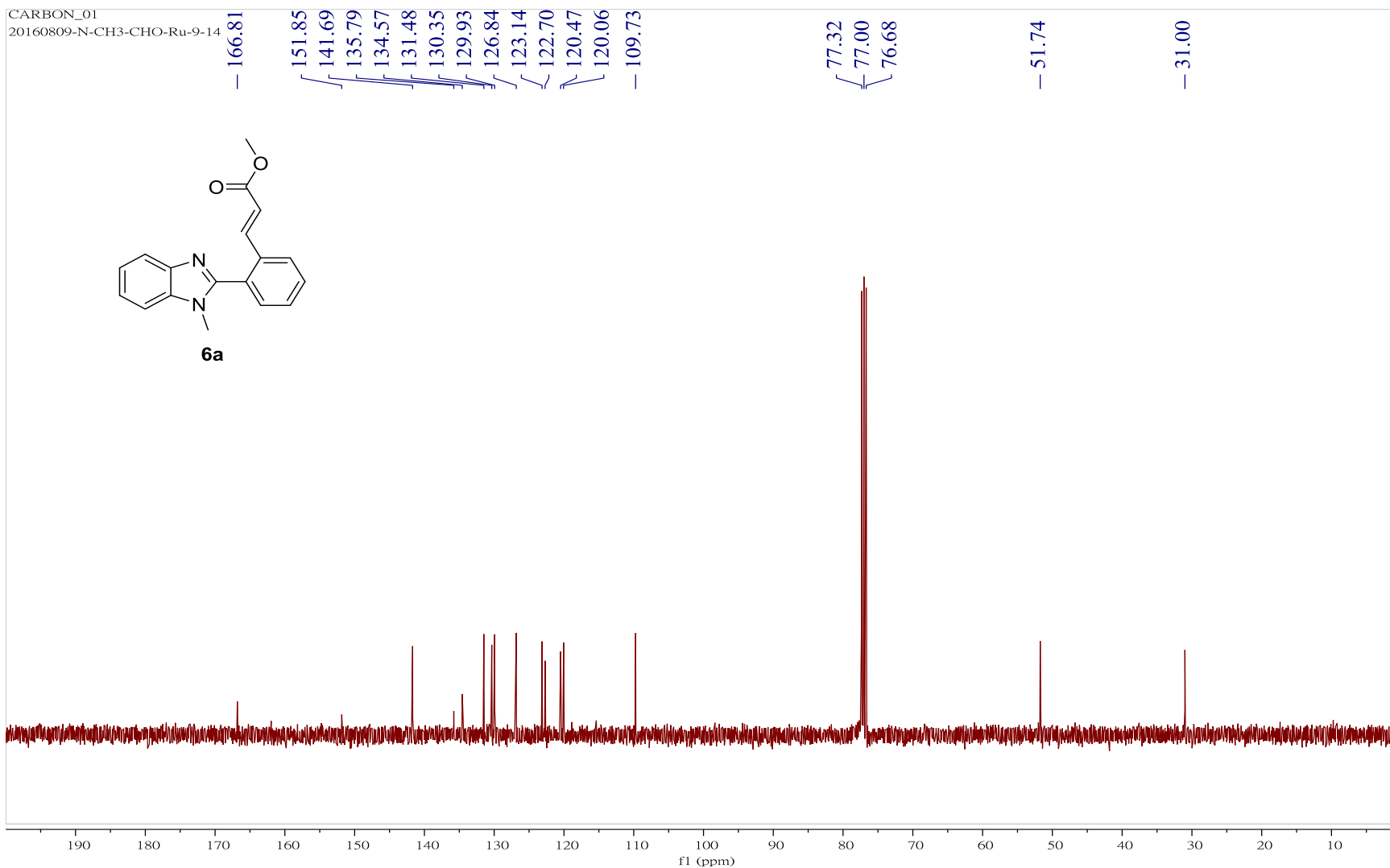


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
293.1287	1	C <sub>18</sub> H <sub>17</sub> N <sub>2</sub> O <sub>2</sub>	293.1285	0.7	17.1	1	100.00	11.5	even	ok	M+H

High resolution mass (ESI)<sup>+</sup> spectrum of compound of **3u**



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **6a** in CDCl<sub>3</sub>

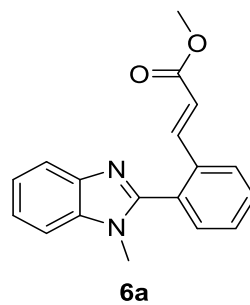
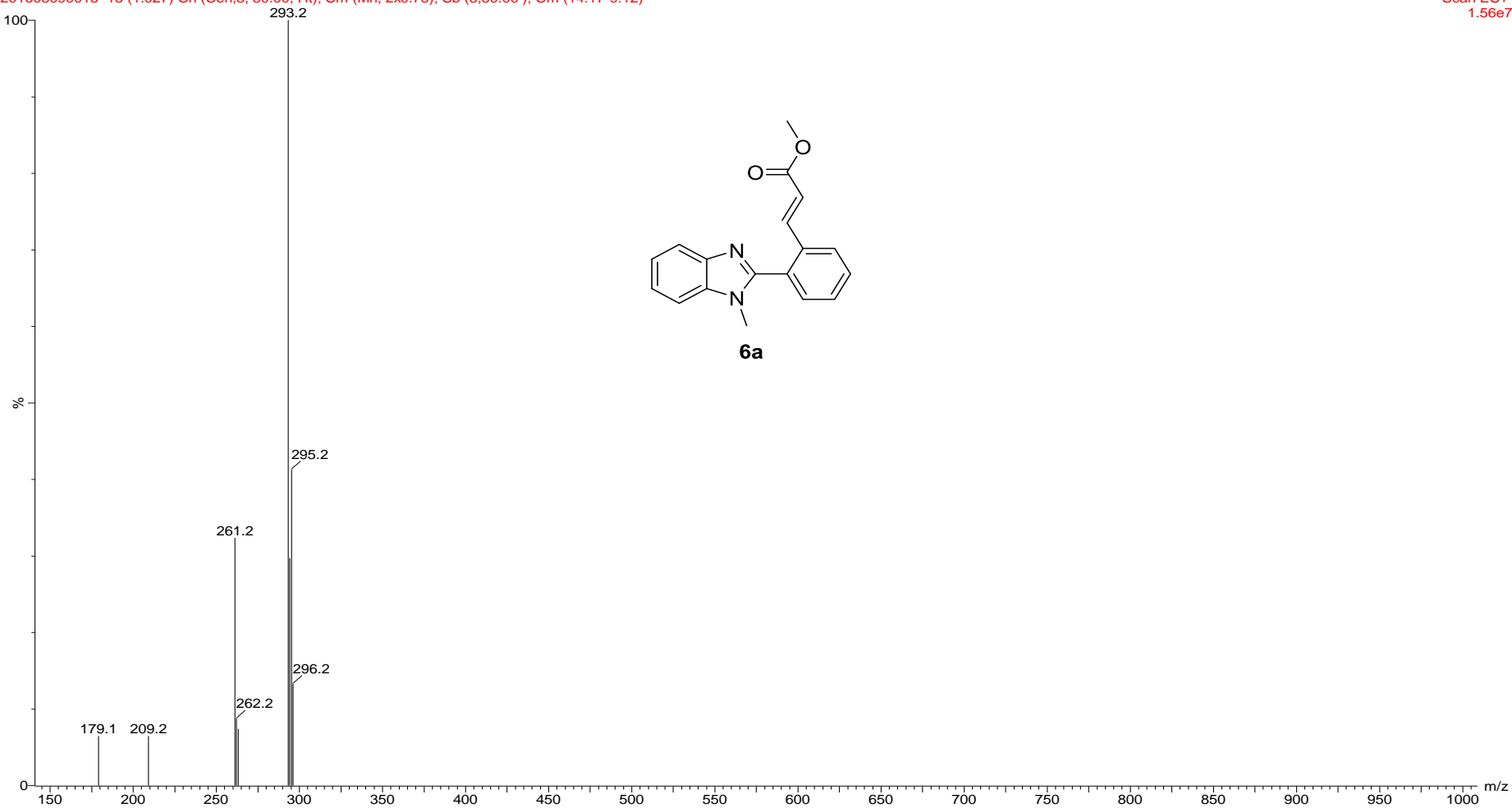


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **6a** in  $\text{CDCl}_3$

**N-CH3-Ru-3**

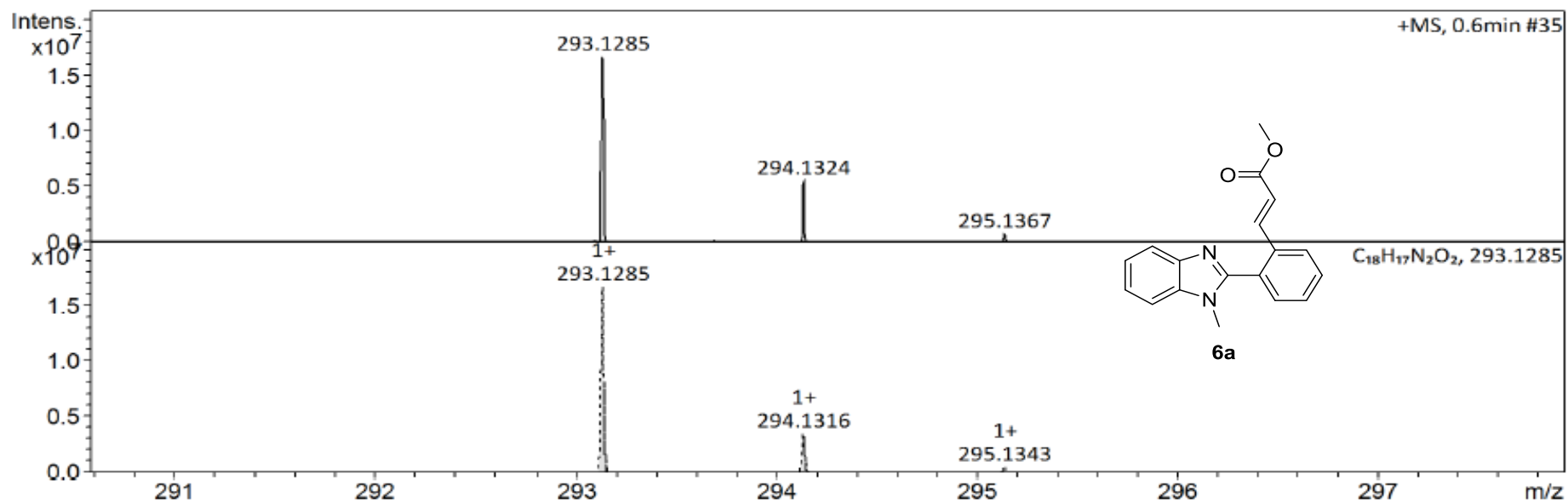
201608090015 15 (1.027) Cn (Cen,3, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00 ); Cm (14:17-9:12)

Scan ES+  
1.56e7



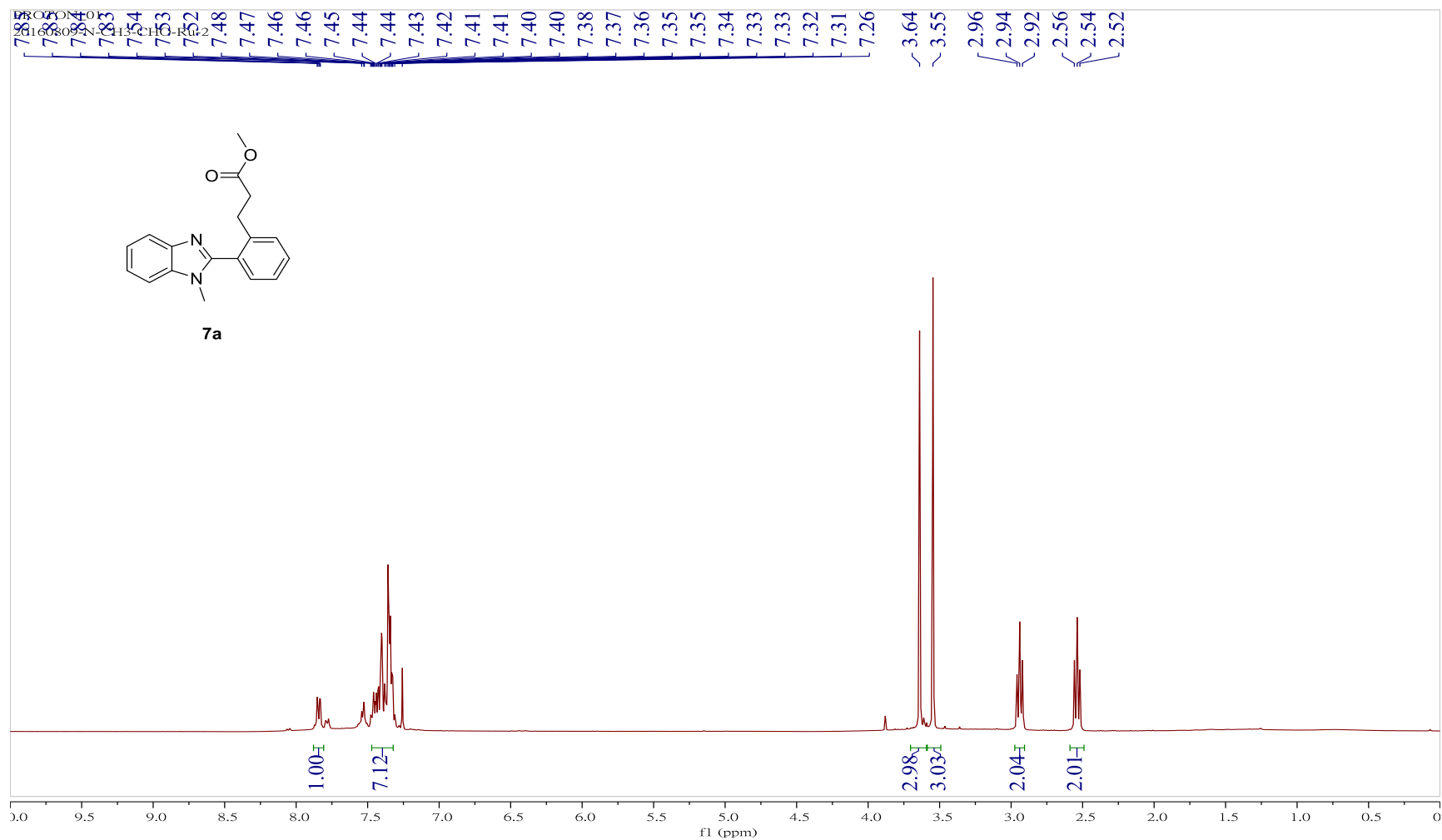
ESI mass spectrum of compound **6a**



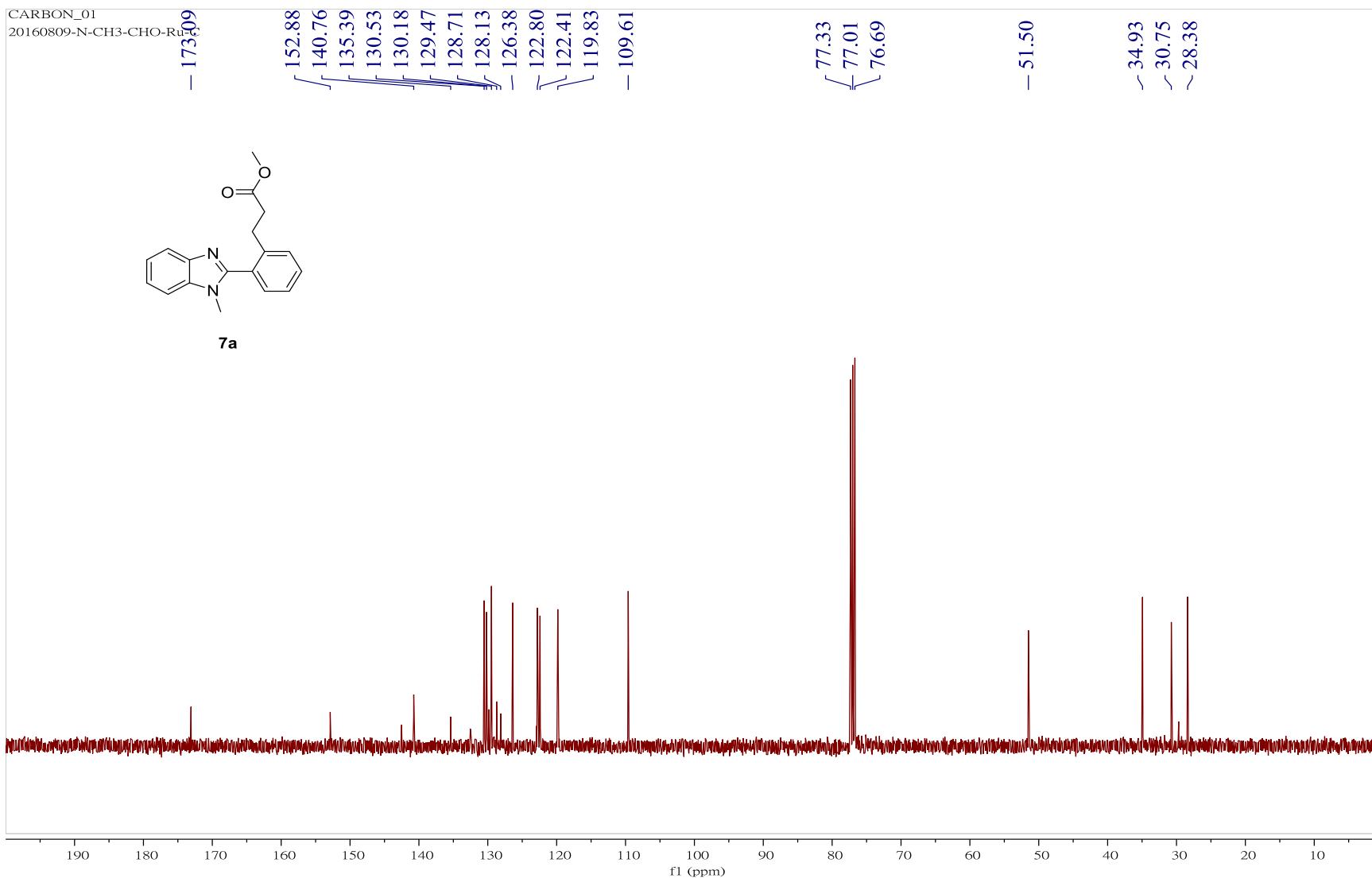


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	Adduct
293.1285	1	C <sub>18</sub> H <sub>17</sub> N <sub>2</sub> O <sub>2</sub>	293.1285	-0.1	72.0	1	100.00	11.5	even	ok	M+H

HRMS Spectrum of compound **6a**



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **7a** in CDCl<sub>3</sub>

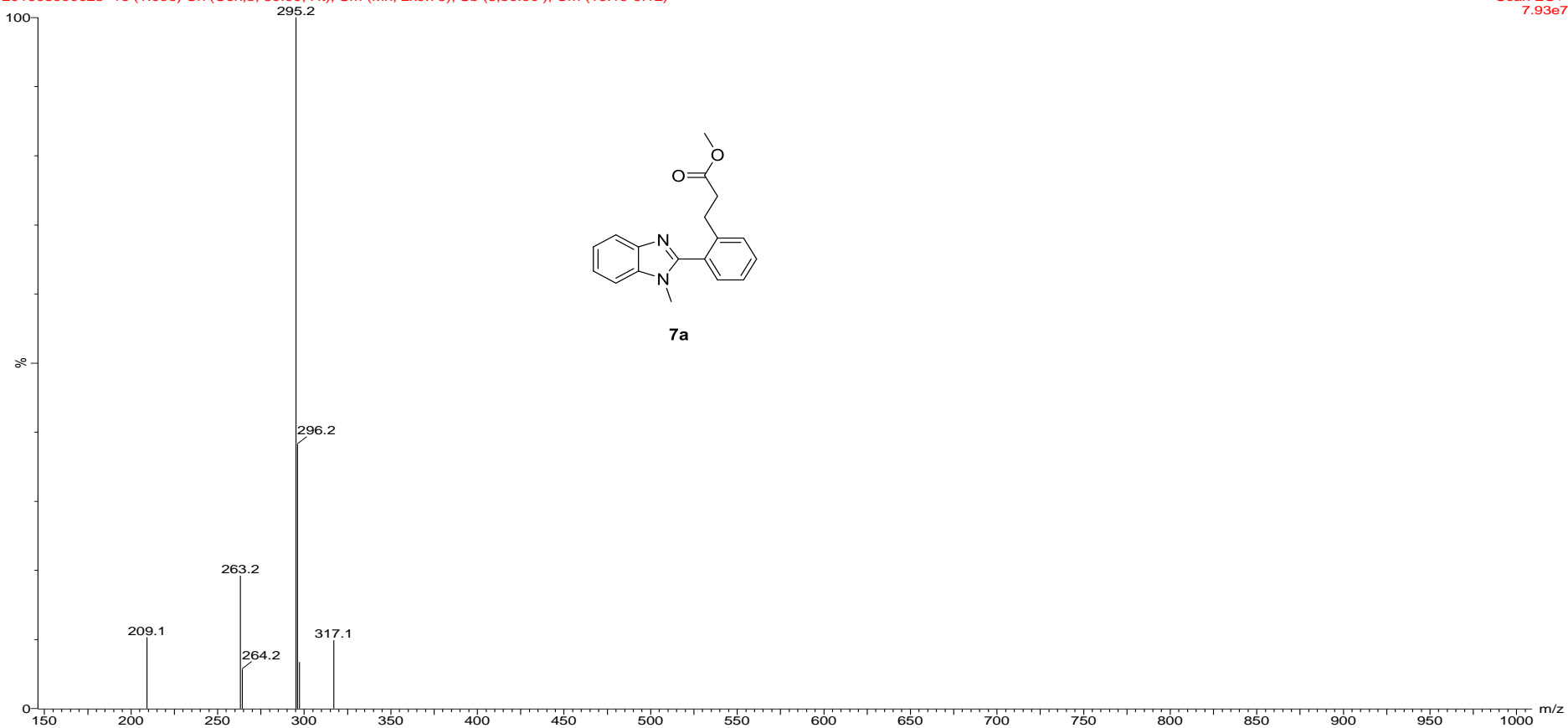


$^{13}\text{C}$  NMR Spectrum (100 MHz) of compound **7a** in  $\text{CDCl}_3$

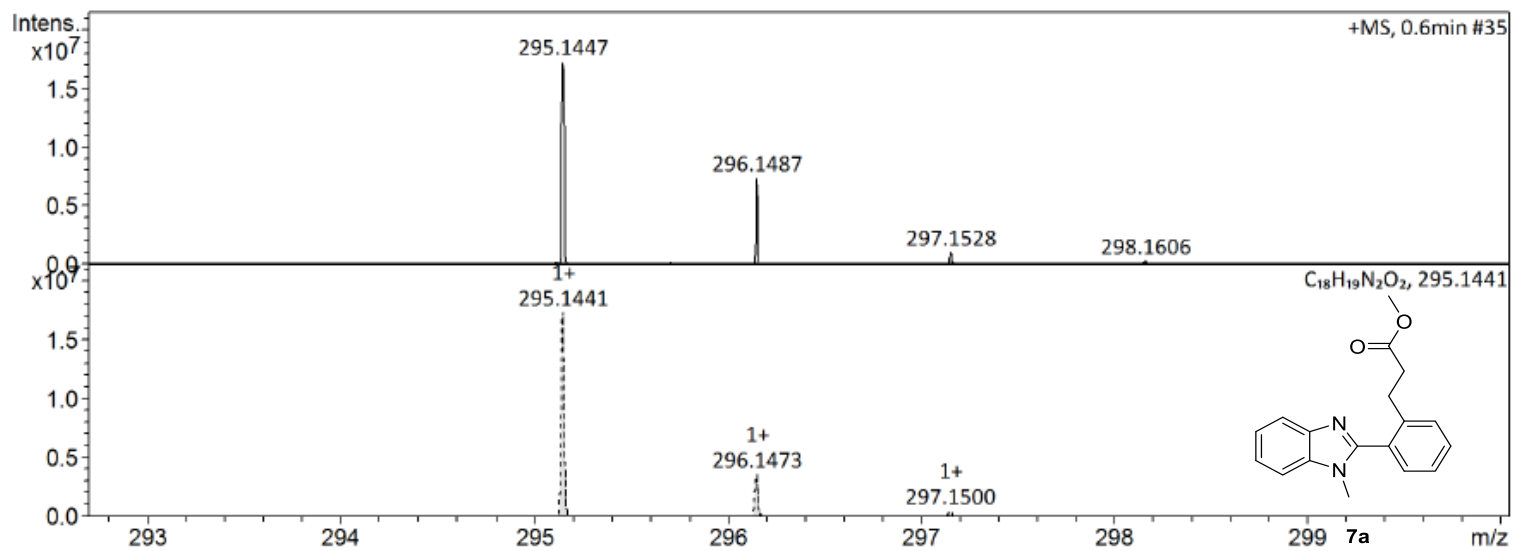
**N-CH3-Ru-2**

201608090023 16 (1.096) Cn (Cen,3, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00 ); Cm (16:19-9:12)

Scan ES+  
7.93e7



ESI<sup>+</sup> Mass spectrum of compound 7a



HRMS Spectrum of compound **7a**

## X-ray crystallography data of compound **3b**

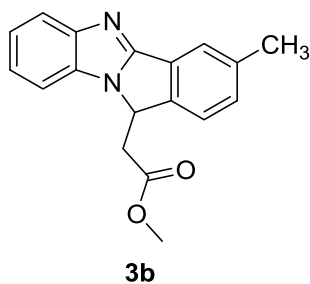
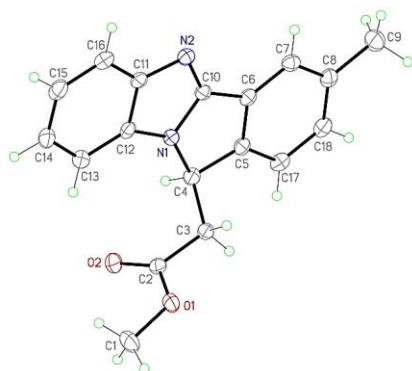


Table 1. Crystal data and structure refinement for mo\_160318lt\_0m.

Identification code	mo_160318LT_0m	
Empirical formula	C <sub>18</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	
Formula weight	292.33	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 12.4244(9) Å	α = 90°.
	b = 8.0614(6) Å	β = 100.607(2)°.
	c = 14.7164(10) Å	γ = 90°.
Volume	1448.78(18) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.340 Mg/m <sup>3</sup>	
Absorption coefficient	0.089 mm <sup>-1</sup>	
F(000)	616	
Crystal size	0.25 x 0.20 x 0.20 mm <sup>3</sup>	
Theta range for data collection	2.816 to 26.379°.	
Index ranges	-15 ≤ h ≤ 15, -10 ≤ k ≤ 5, -18 ≤ l ≤ 18	
Reflections collected	11617	
Independent reflections	2954 [R(int) = 0.0265]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.9082	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	2954 / 0 / 201	
Goodness-of-fit on F <sup>2</sup>	1.030	

Final R indices [I>2sigma(I)]	R1 = 0.0376, wR2 = 0.0917
R indices (all data)	R1 = 0.0463, wR2 = 0.0982
Extinction coefficient	n/a
Largest diff. peak and hole	0.241 and -0.197 e.Å <sup>-3</sup>

Table 2. Atomic coordinates (x 10<sup>4</sup>) and equivalent isotropic displacement parameters (Å<sup>2</sup>x 10<sup>3</sup>) for mo\_160318lt\_0m. U(eq) is defined as one third of the trace of the orthogonalized U<sup>ij</sup> tensor.

	x	y	z	U(eq)
O(1)	1865(1)	318(1)	2540(1)	28(1)
O(2)	1451(1)	2566(1)	3309(1)	28(1)
N(1)	3651(1)	1886(1)	5090(1)	18(1)
N(2)	4607(1)	825(1)	6419(1)	19(1)
C(1)	715(1)	101(2)	2169(1)	40(1)
C(2)	2122(1)	1645(2)	3089(1)	20(1)
C(3)	3343(1)	1808(2)	3356(1)	18(1)
C(4)	3731(1)	2802(2)	4238(1)	19(1)
C(5)	4961(1)	3120(2)	4401(1)	18(1)
C(6)	5484(1)	2433(2)	5235(1)	18(1)
C(7)	6605(1)	2559(2)	5531(1)	20(1)
C(8)	7225(1)	3407(2)	4981(1)	22(1)
C(9)	8442(1)	3621(2)	5300(1)	30(1)
C(10)	4644(1)	1653(2)	5658(1)	16(1)
C(11)	3494(1)	486(2)	6350(1)	18(1)
C(12)	2874(1)	1179(2)	5534(1)	18(1)
C(13)	1735(1)	1083(2)	5341(1)	24(1)
C(14)	1242(1)	232(2)	5972(1)	27(1)
C(15)	1850(1)	-509(2)	6765(1)	26(1)
C(16)	2976(1)	-392(2)	6963(1)	22(1)
C(17)	5571(1)	3946(2)	3842(1)	21(1)
C(18)	6696(1)	4083(2)	4143(1)	23(1)

Table 3. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for mo\_160318lt\_0m.

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O(1)-C(2)	1.3432(16)
O(1)-C(1)	1.4432(16)
O(2)-C(2)	1.2044(16)
N(1)-C(10)	1.3702(16)
N(1)-C(12)	1.3848(16)
N(1)-C(4)	1.4735(16)
N(2)-C(10)	1.3118(16)
N(2)-C(11)	1.3952(16)
C(1)-H(16)	0.9800
C(1)-H(3)	0.9800
C(1)-H(1)	0.9800
C(2)-C(3)	1.5009(17)
C(3)-C(4)	1.5254(17)
C(3)-H(14)	0.9900
C(3)-H(15)	0.9900
C(4)-C(5)	1.5252(17)
C(4)-H(13)	1.0000
C(5)-C(17)	1.3868(18)
C(5)-C(6)	1.3936(18)
C(6)-C(7)	1.3847(18)
C(6)-C(10)	1.4525(17)
C(7)-C(8)	1.3953(19)
C(7)-H(8)	0.9500
C(8)-C(18)	1.3967(19)
C(8)-C(9)	1.5080(18)
C(9)-H(9)	0.9800
C(9)-H(2)	0.9800
C(9)-H(10)	0.9800
C(11)-C(16)	1.3937(18)
C(11)-C(12)	1.4165(18)
C(12)-C(13)	1.3936(18)
C(13)-C(14)	1.384(2)



C(13)-H(7)	0.9500
C(14)-C(15)	1.402(2)
C(14)-H(6)	0.9500
C(15)-C(16)	1.3782(19)
C(15)-H(5)	0.9500
C(16)-H(4)	0.9500
C(17)-C(18)	1.3905(19)
C(17)-H(12)	0.9500
C(18)-H(11)	0.9500
C(2)-O(1)-C(1)	115.67(11)
C(10)-N(1)-C(12)	106.42(10)
C(10)-N(1)-C(4)	113.19(10)
C(12)-N(1)-C(4)	140.37(11)
C(10)-N(2)-C(11)	103.13(10)
O(1)-C(1)-H(16)	109.5
O(1)-C(1)-H(3)	109.5
H(16)-C(1)-H(3)	109.5
O(1)-C(1)-H(1)	109.5
H(16)-C(1)-H(1)	109.5
H(3)-C(1)-H(1)	109.5
O(2)-C(2)-O(1)	123.61(12)
O(2)-C(2)-C(3)	126.25(12)
O(1)-C(2)-C(3)	110.13(10)
C(2)-C(3)-C(4)	114.52(10)
C(2)-C(3)-H(14)	108.6
C(4)-C(3)-H(14)	108.6
C(2)-C(3)-H(15)	108.6
C(4)-C(3)-H(15)	108.6
H(14)-C(3)-H(15)	107.6
N(1)-C(4)-C(5)	99.95(9)
N(1)-C(4)-C(3)	113.57(10)
C(5)-C(4)-C(3)	111.90(10)

N(1)-C(4)-H(13)	110.3
C(5)-C(4)-H(13)	110.3
C(3)-C(4)-H(13)	110.3
C(17)-C(5)-C(6)	119.76(12)
C(17)-C(5)-C(4)	128.95(12)
C(6)-C(5)-C(4)	111.29(11)
C(7)-C(6)-C(5)	121.77(12)
C(7)-C(6)-C(10)	131.13(12)
C(5)-C(6)-C(10)	107.10(11)
C(6)-C(7)-C(8)	118.97(12)
C(6)-C(7)-H(8)	120.5
C(8)-C(7)-H(8)	120.5
C(7)-C(8)-C(18)	118.90(12)
C(7)-C(8)-C(9)	120.31(12)
C(18)-C(8)-C(9)	120.78(12)
C(8)-C(9)-H(9)	109.5
C(8)-C(9)-H(2)	109.5
H(9)-C(9)-H(2)	109.5
C(8)-C(9)-H(10)	109.5
H(9)-C(9)-H(10)	109.5
H(2)-C(9)-H(10)	109.5
N(2)-C(10)-N(1)	114.98(11)
N(2)-C(10)-C(6)	136.56(12)
N(1)-C(10)-C(6)	108.46(11)
C(16)-C(11)-N(2)	128.47(12)
C(16)-C(11)-C(12)	120.32(12)
N(2)-C(11)-C(12)	111.21(11)
N(1)-C(12)-C(13)	134.14(12)
N(1)-C(12)-C(11)	104.19(11)
C(13)-C(12)-C(11)	121.66(12)
C(14)-C(13)-C(12)	116.63(13)
C(14)-C(13)-H(7)	121.7
C(12)-C(13)-H(7)	121.7

C(13)-C(14)-C(15)	122.16(13)
C(13)-C(14)-H(6)	118.9
C(15)-C(14)-H(6)	118.9
C(16)-C(15)-C(14)	121.19(13)
C(16)-C(15)-H(5)	119.4
C(14)-C(15)-H(5)	119.4
C(15)-C(16)-C(11)	117.97(12)
C(15)-C(16)-H(4)	121.0
C(11)-C(16)-H(4)	121.0
C(5)-C(17)-C(18)	118.45(12)
C(5)-C(17)-H(12)	120.8
C(18)-C(17)-H(12)	120.8
C(17)-C(18)-C(8)	122.14(12)
C(17)-C(18)-H(11)	118.9
C(8)-C(18)-H(11)	118.9

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for mo\_160318lt\_0m. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
O(1)	16(1)	39(1)	28(1)	-11(1)	3(1)	0(1)
O(2)	23(1)	35(1)	26(1)	-1(1)	4(1)	11(1)
N(1)	18(1)	19(1)	16(1)	0(1)	3(1)	1(1)
N(2)	20(1)	19(1)	18(1)	-1(1)	4(1)	0(1)
C(1)	17(1)	63(1)	40(1)	-18(1)	0(1)	-3(1)
C(2)	21(1)	26(1)	14(1)	2(1)	3(1)	4(1)
C(3)	19(1)	20(1)	16(1)	2(1)	3(1)	4(1)
C(4)	21(1)	18(1)	18(1)	3(1)	5(1)	3(1)
C(5)	21(1)	15(1)	19(1)	-3(1)	5(1)	2(1)
C(6)	22(1)	14(1)	18(1)	-3(1)	5(1)	1(1)

C(7)	23(1)	18(1)	18(1)	-3(1)	2(1)	0(1)
C(8)	22(1)	20(1)	24(1)	-9(1)	6(1)	-3(1)
C(9)	24(1)	34(1)	32(1)	-5(1)	6(1)	-7(1)
C(10)	18(1)	15(1)	16(1)	-4(1)	2(1)	1(1)
C(11)	21(1)	18(1)	17(1)	-5(1)	4(1)	1(1)
C(12)	22(1)	18(1)	17(1)	-4(1)	7(1)	0(1)
C(13)	21(1)	31(1)	22(1)	-4(1)	4(1)	1(1)
C(14)	20(1)	37(1)	26(1)	-6(1)	8(1)	-3(1)
C(15)	28(1)	30(1)	23(1)	-3(1)	12(1)	-5(1)
C(16)	28(1)	22(1)	18(1)	-2(1)	6(1)	-1(1)
C(17)	28(1)	19(1)	18(1)	0(1)	6(1)	0(1)
C(18)	27(1)	21(1)	22(1)	-4(1)	10(1)	-4(1)

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for mo\_160318lt\_0m.

	x	y	z	U(eq)
H(16)	321	-121	2675	61
H(3)	619	-837	1737	61
H(1)	425	1111	1843	61
H(14)	3624	2345	2842	22
H(15)	3666	683	3439	22
H(13)	3322	3874	4216	23
H(8)	6947	2075	6100	24
H(9)	8590	4724	5574	45
H(2)	8813	3507	4770	45
H(10)	8714	2771	5761	45
H(7)	1317	1576	4803	29
H(6)	466	147	5864	33
H(5)	1480	-1103	7172	31
H(4)	3386	-893	7501	27
H(12)	5229	4406	3267	26
H(11)	7119	4655	3766	27