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Supporting Information

Regioselective Synthesis of Imidazo[1,5-*a*]quinoxalines and Methyl *N*-Phenylbenzimidats on Ionic Liquid Support

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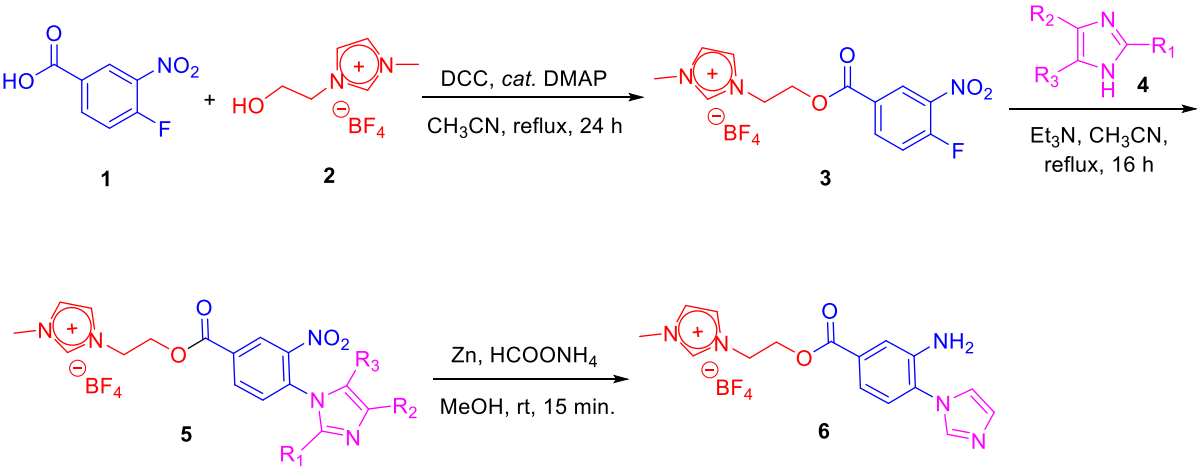
1. General Methods

Chemical shifts are reported in parts per million (ppm) on the δ scale from an internal standard (TMS) and coupling constants are reported in Hertz. Analytical thin-layer chromatography (TLC) was performed using 0.25 mm silica gel-coated Kiselgel 60 F_{254} plates. Compound purification was carried out by flash chromatography using the indicated solvent and silica gel 60 (Merck, 230-400 mesh). Microwave irradiation experiments were carried out in 5 mL glass vials sealed with Teflon® cap in a CEM-Discover microwave instrument using irradiation power from 0 to 100 W. High-resolution mass spectra (HRMS) were recorded in ESI mode using a magnetic sector mass analyzer and TOF mass spectrometer. IR spectra were obtained using FT-IR spectrometer. All reagents were purchased from commercial sources and used without further purification.

2. Experimental procedures

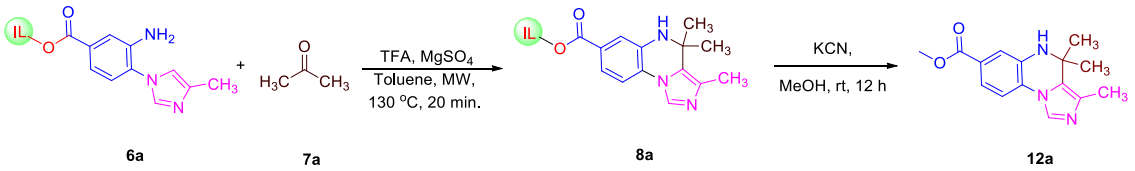
General procedure for the synthesis of IL-attached amine 6



To the stirred solution of 4-fluoro-3-nitrobenzoic acid **1** (1.12 mmol, 1.2 equiv) in acetonitrile was added DCC (1.12 mmol, 1.2 equiv), DMAP (0.04 mmol, 0.05 equiv), and 1-(2-hydroxyethyl)-3-methylimidazolium tetrafluoroborate ([hydemim] [BF_4]) **2** (0.93 mmol, 1 equiv). The reaction mixture was refluxed for 24 h. After completion of the reaction, dicyclohexylurea was filtered off, and the filtrate was concentrated. The crude residue was washed with cold diethyl ether (50 mL × 3) and dried *in vacuo* to afford **3** in 96% yield. A mixture of **3** (1.41 mmol, 1 equiv), triethyl amine (7.05 mmol, 5 equiv) and imidazole **4** (1.7 mmol, 1.2 equiv) in acetonitrile was refluxed for 16 h. After completion of the reaction, the solvent was evaporated under reduced pressure. The reaction mixture was precipitated and washed with cold diethyl ether (50 mL × 3). The precipitate was dried to give **5** in 90% yield. To a stirred solution of **5** in methanol were added zinc (8.96 mmol, 7 equiv) and ammonium formate (19.2

mmol, 15 equiv), and the reaction mixture was stirred at room temperature for 15 min. After completion of the reaction, the reaction mixture was filtered through a Celite bed to remove zinc, and the filtrate was concentrated. Dichloromethane (30 mL) was added to the crude residue to precipitate ammonium formate, and the mixture was again passed through a Celite bed. The filtrate was concentrated to yield **6** in 88% yield.

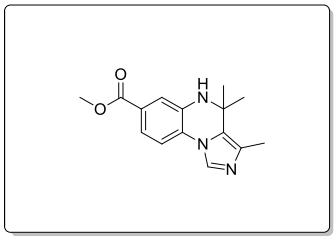
General experimental procedure for the synthesis of methyl 4,4-dimethyl-4,5-dihydroimidazo[1,5-*a*]quinoxaline-7-carboxylate (12a)



To a stirred solution of acetone **7a** (0.055 g, 0.96 mmol) in toluene (10 mL) was added trifluoroacetic acid (0.01 mL), amine **6a** (0.1 g 0.32 mmol) and $MgSO_4$ (0.1 g, w/w) at room temperature. The resulting reaction mixture was irradiated in microwave for 20 min at 130 °C (250 W). The progress of the reaction was monitored by regular proton NMR. After completion of the reaction, reaction mixture was filtered to remove $MgSO_4$. The solvent was evaporated under reduced pressure. The residue of **8a** was washed with excess of cold ether (25 mL x 3) and dried *in vacuo*. The crude product obtained was used as it is for methanolysis reaction. To a stirred solution of **8a** (0.1 g, 0.227 mmol) in methanol (20 mL) was added potassium cyanide (0.103 g, 1.59 mmol) and the

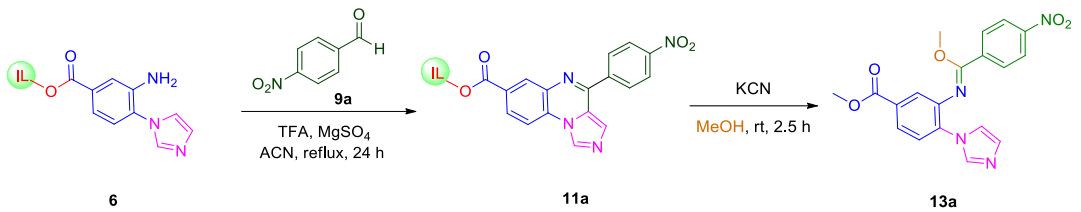
reaction mixture was stirred at room temperature for 2 h. The solvent was removed under reduced pressure and the reaction mixture was precipitated and washed with diethyl ether (50 mL). The combined organic layers were concentrated under vacuum. The crude product was purified by flash chromatography (eluent: 20 % EA in hexanes) to obtain the corresponding imidazo[1,5-*a*]quinoxaline **12a** (0.051 g, 89 %). This procedure was used for the synthesis of all the rest derivatives of **12**.

Methyl 4,5-dihydro-3,4,4-trimethylimidazo[1,5-*a*]quinoxaline-7-carboxylate (12a)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.54 (dd, J = 8.3, 1.7 Hz, 1H), 7.47 (d, J = 1.7 Hz, 1H), 7.41 (d, J = 8.3 Hz, 1H), 3.91 (s, 3H), 3.88 (s, NH), 2.36 (s, 3H), 1.58 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.9, 135.2, 131.6, 129.5, 128.1, 127.1, 125.9, 120.9, 117.3, 114.9, 52.6, 52.2, 29.6, 14.8; MS (ESI, *m/z*): 272 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{15}H_{18}N_3O_2$ $[M+H]^+$ 272.1399, found 272.1397; IR (cm^{-1}, neat): 3349, 2956, 2923, 1710.

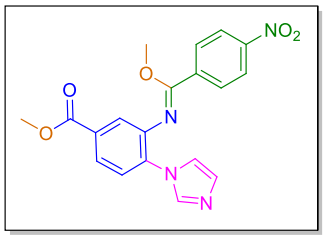
General experimental procedure for the synthesis of (Z)-methyl 4-(1H-imidazol-1-yl)-3-((methoxy(4-nitrophenyl)methylene)amino)benzoate (13a)



6 11a 13a

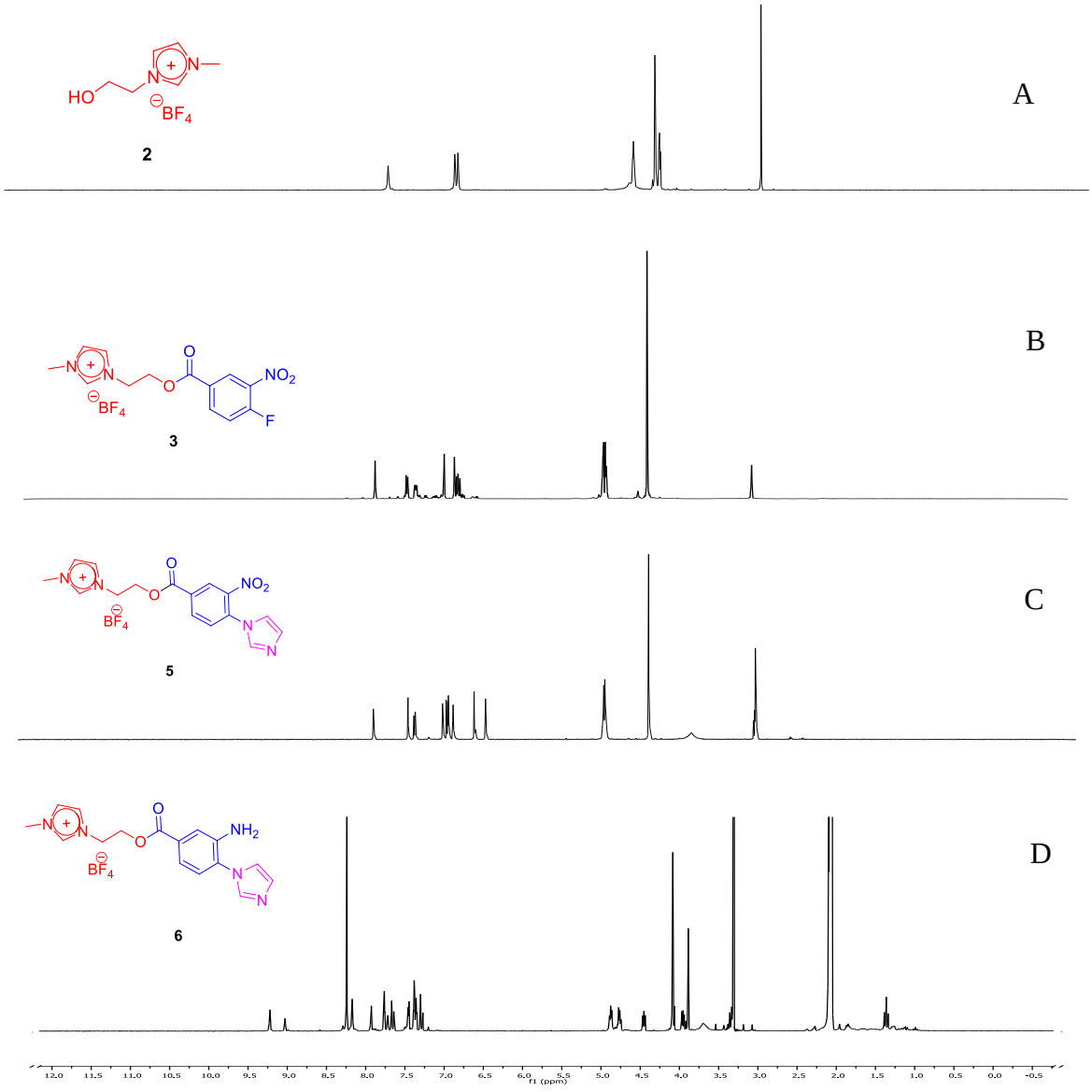
To a stirred solution of 4-nitrobenzaldehyde **9a** (0.11 g, 0.75 mmol) in acetonitrile (10 mL) was added trifluoroacetic acid (0.01 mL), amine **6** (0.1 g 0.25 mmol) and $MgSO_4$ (0.1 g, w/w) at room temperature. The reaction mixture was refluxed for 24 h. Progress of the reaction was directly monitored by proton NMR with ionic liquid support attached. After completion of the reaction, $MgSO_4$ was removed by filtration and the filtrate was evaporated under reduced pressure. The crude product **11a** was washed with excess of cold diethyl ether (25 mL x 3) and dried *in vacuo*. The obtained crude product was used as it is for the next step. To a stirred solution of **11a** (0.1 g, 0.18 mmol) in methanol (20 mL) was added potassium cyanide (0.085 g, 1.32 mmol) and the reaction mixture was stirred at room temperature for 2.5 h. The solvent was evaporated under reduced pressure. To the crude residue of **13a**, cold diethyl ether (10 mL) was added to precipitate ionic liquid support. The precipitated ionic liquid support was filtered and washed with excess of cold diethyl ether (10 mL × 3). The filtrate was concentrated under vacuum. The crude product was purified by flash chromatography (eluent: 55 % EA in hexanes) to afford (*Z*)-methyl 4-(1H-imidazol-1-yl)-3-((methoxy(4-nitrophenyl) methylene) amino) benzoate **13a** (0.061 g, 85 %). This procedure was used for the synthesis of the rest all derivatives of **13**.

(Z)-methyl 4-(1H-imidazol-1-yl)-3-((methoxy(4-nitrophenyl)methylene)amino)benzoate (13a)



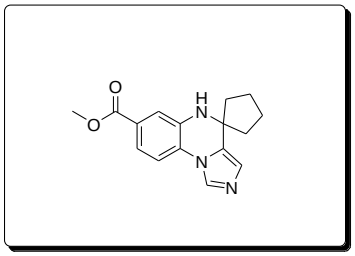
Pale yellow solid, 147-149 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (d, J = 8.7 Hz, 2H), 7.77 (dd, J = 8.2, 1.8 Hz, 1H), 7.58 (d, J = 1.7 Hz, 1H), 7.48 (s, 1H), 7.23 (d, J = 8.2 Hz, 1H), 7.18 (d, J = 8.7 Hz, 2H), 7.10 (s, 1H), 6.95 (s, 1H), 3.99 (s, 3H), 3.87 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.1, 159.5, 148.9, 142.0, 137.1, 136.2, 132.1, 130.8, 129.9, 129.6, 126.0, 125.8, 125.2, 123.7, 119.5, 55.4, 52.8; MS (ESI, *m/z*): 381.4 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{19}H_{17}N_4O_5$ $[M+H]^+$ 381.1199, found 381.1195; IR(cm^{-1}, neat): 3448, 3087, 2996, 2950, 1722.

3. Stepwise proton NMR monitoring of the synthesis of 6



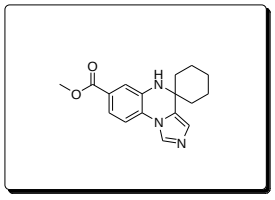
4. Characterization Data for Compound 12b-12s

Methyl 5'*H*-spiro[cyclopentane-1,4'-imidazo[1,5-*a*]quinoxaline]-7'-carboxylate (12b)



^{1}H NMR (300 MHz, DMSO-d_6) δ 8.40, (s, 1H), 7.77 (d, J = 7.9 Hz, 1H), 7.57 (s, 1H), 7.32 (d, J = 7.9 Hz, 1H), 6.89 (s, 1H), 6.58 (s, NH), 3.82 (s, 3H), 1.90-1.71 (m, 8H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 166.8, 137.2, 133.2, 132.8, 127.9, 125.9, 122.5, 119.5, 117.2, 116.4, 61.1, 52.9, 40.2, 23.8; MS (ESI, *m/z*): 284 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{16}H_{18}N_3O_2$ $[M+H]^+$ 284.1399, found 284.1402; IR (cm^{-1}, neat): 3365, 3093, 2927, 2859, 1704.

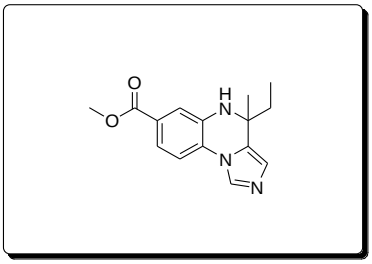
Methyl 5'*H*-spiro[cyclohexane-1,4'-imidazo[1,5-*a*]quinoxaline]-7'-carboxylate (12c)



^{1}H NMR (300 MHz, DMSO-d_6) δ 8.39 (s, 1H), 7.77 (d, J = 8.2 Hz, 1H), 7.76 (d, J = 1.8 Hz, 1H), 7.33 (dd, J = 8.2, 1.8 Hz, 1H), 6.93 (s, 1H), 6.59 (s, NH), 3.83 (s, 3H), 1.70-1.67 (m, 6H), 1.53-1.50 (m, 4H); ^{13}C NMR (75 MHz, DMSO-d_6) δ

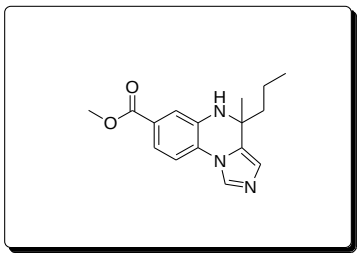
166.2, 136.5, 133.8, 132.7, 128.0, 125.9, 123.0, 119.5, 117.7, 116.3, 52.9, 52.5, 37.0, 25.7, 21.3; MS (ESI, *m/z*): 298 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{17}H_{20}N_3O_2$ $[M+H]^+$ 298.1555, found 298.1558; IR (cm^{-1}, neat): 3187, 2950, 2865, 1708.

Methyl 4-ethyl-4,5-dihydro-4-methylimidazo[1,5-*a*]quinoxaline-7-Carboxylate (12d)



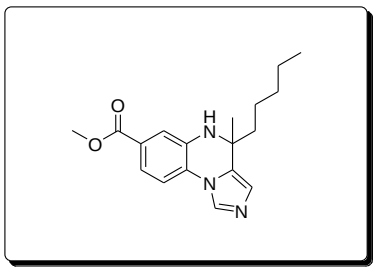
^1H NMR (300 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.56 (dd, J = 8.1, 1.8 Hz, 1H), 7.52 (d, J = 1.8 Hz, 1H), 7.50 (d, J = 8.1 Hz, 1H), 6.91 (s, 1H), 3.98 (s, NH), 3.92 (s, 3H), 1.78 (m, 2H), 1.55 (s, 3H), 0.91 (t, J = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166,9, 135.9, 132.2, 131.4, 128.4, 125.5, 123.6, 120.5, 117.3, 115.2, 54.2, 52.6, 35.0, 26.8, 8.9; MS (ESI, *m/z*): 272 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{15}H_{18}N_3O_2$ $[M+H]^+$ 272.1399, found 272.1397; IR(cm^{-1}, neat): 3222, 2971, 2994, 2921, 1704.

Methyl 4,5-dihydro-4-methyl-4-propylimidazo[1,5-*a*]quinoxaline-7-Carboxylate (12e)



^{1}H NMR (300 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.53 (dd, J = 8.2, 1.7 Hz, 1H), 7.48 (d, J = 1.7 Hz, 1H), 7.43 (d, J = 8.2 Hz, 1H), 6.90 (s, 1H), 4.01 (s, NH), 3.92 (s, 3H), 1.74-1.66 (m, 2H), 1.56 (s, 3H), 1.29-1.10 (m, 2H), 0.86 (t, J = 7.3 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.9, 135.8, 132.3, 131.4, 128.5, 125.5, 123.6, 120.6, 117.2, 115.2, 53.9, 52.6, 44.9, 27.6, 17.9, 14.6; MS (ESI, *m/z*): 286 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{16}H_{20}N_3O_2$ $[M+H]^+$ 286.1555, found 286.1557; IR (cm^{-1}, neat): 3349, 2952, 2931, 2865, 1708.

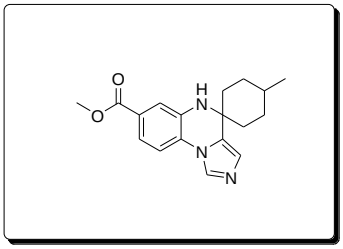
Methyl 4,5-dihydro-4-methyl-4-pentylimidazo[1,5-*a*]quinoxaline-7-Carboxylate (12f)



^{1}H NMR (300 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.53 (dd, J = 8.2, 1.7 Hz, 1H), 7.48 (d, J = 1.7 Hz, 1H), 7.43 (d, J = 8.2 Hz, 1H), 6.90 (s, 1H), 4.00 (s, NH), 3.92 (s, 3H), 1.75-1.67 (m, 2H), 1.55 (s, 3H), 1.36-1.17 (m, 6H), 0.84 (t, J = 6.9 Hz, 3H);

^{13}C NMR (75 MHz, $CDCl_3$) δ 166.9, 136.7, 132.4, 131.4, 128.5, 125.5, 123.5, 120.6, 117.3, 115.2, 53.9, 52.6, 42.4, 32.2, 27.5, 24.3, 22.9, 14.4; MS (ESI, *m/z*): 314 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{18}H_{24}N_3O_2$ $[M+H]^+$ 314.1868, found 314.1865; IR(cm^{-1}, neat): 3355, 2952, 2931, 2857, 1716.

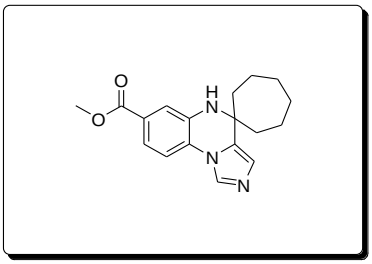
Methyl 4-methyl-5'*H*-spiro[cyclohexane-1,4'-imidazo[1,5-*a*]quinoxaline]-7'-carboxylate (12g)



^{1}H NMR (300 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.55 (d, *J* = 1.7 Hz, 1H), 7.52 (dd, *J* = 7.4, 1.7 Hz, 1H), 7.43 (d, *J* = 7.4 Hz, 1H), 6.91 (s, 1H), 4.60 (s, NH), 3.92 (s, 3H), 2.05-2.00 (m, 2H), 1.81-1.70 (m, 4H), 1.53-1.48 (m, 1H), 1.29-1.15 (m, 2H), 1.00 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.8, 134.9, 134.3, 131.5, 128.5, 126.3, 122.6, 121.2, 117.8, 115.4, 52.6, 51.9, 35.9, 31.9, 30.1, 22.7; MS (ESI, *m/z*): 312 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{18}H_{22}N_3O_2$ $[M+H]^+$ 312.1712, found 312.1713; IR (cm^{-1}, neat): 3363, 3089, 2937, 2913, 2863, 1704.

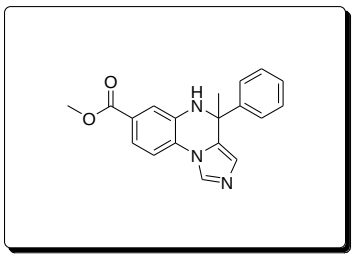
Methyl 5'*H*-spiro[cycloheptane-1,4'-imidazo[1,5-*a*]quinoxaline]-7'-

carboxylate (12h)



^{1}H NMR (300 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.54 (dd, J = 8.1, 1.7 Hz, 1H), 7.52 (d, J = 1.7 Hz, 1H), 7.42 (d, J = 8.1 Hz, 1H), 6.97 (s, 1H), 4.31 (s, NH), 3.92 (s, 3H), 2.12-2.04 (m, 2H), 1.96-1.88 (m, 2H), 1.66-1.53 (m, 8H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.9, 135.4, 134.7, 131.4, 128.5, 126.2, 122.9, 120.9, 117.8, 115.2, 56.7, 52.5, 40.7, 30.3, 22.8; MS (ESI, *m/z*): 312 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{18}H_{22}N_3O_2$ $[M+H]^+$ 312.1712, found 312.1710; IR(cm^{-1}, neat): 3349, 3330, 3093, 2931, 1704.

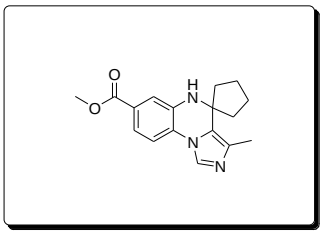
Methyl 4,5-dihydro-4-methyl-4-phenylimidazo[1,5-*a*]quinoxaline-7-carboxylate (12i)



^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.64 (d, J = 1.6 Hz, 1H), 7.49 (dd, J = 8.3, 1.6 Hz, H), 7.38 (d, J = 8.3 Hz, 1H), 7.39-7.10 (m, 5H), 7.02 (s, 1H), 5.14 (s, NH), 3.88 (s, 3H), 1.93 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.9, 145.2 ,135.7, 132.3, 131.9, 128.9, 128.6, 127.8, 126.2, 125.9, 124.6, 121.2,

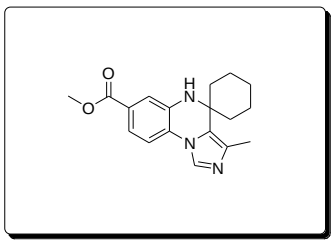
117.8, 115.5, 56.7, 52.6, 29.6; MS (ESI, *m/z*): 320 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{19}H_{18}N_3O_2$ $[M+H]^+$ 320.1399, found 320.1397; IR(cm^{-1}, neat): 3357, 2981, 2944, 1714.

Methyl 3'-methyl-5'*H*-spiro[cyclopentane-1,4'-imidazo[1,5-*a*]quinoxaline]-7'-carboxylate (12j)



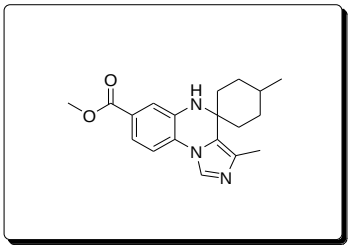
^1H NMR (300 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.55 (dd, J = 8.3, 1.7 Hz, 1H), 7.46 (d, J = 1.7 Hz, 1H), 7.41 (d, J = 8.3 Hz, 1H), 4.10 (s, NH), 3.91 (s, 3H), 2.34 (s, 3H), 2.48-2.16 (m, 2H), 1.95-1.74 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.9, 135.3, 131.2, 129.7, 127.9, 127.0, 126.5, 121.0, 117.4, 115.0, 62.5, 52.6, 39.7, 24.2, 14.7; MS (ESI, *m/z*): 298 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{17}H_{20}N_3O_2$ $[M+H]^+$ 298.1555, found 298.1553; IR(cm^{-1}, neat): 3291, 3124, 2950, 1702.

Methyl 3'-methyl-5'*H*-spiro[cyclohexane-1,4'-imidazo[1,5-*a*]quinoxaline]-7'-carboxylate (12k)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.53-7.50 (m, 2H), 7.38 (d, J = 8.8 Hz, 1H), 4.66 (s, NH), 3.91 (s, 3H), 2.39 (s, 3H), 1.94-1.72 (m, 8H), 1.58-1.21 (m, 2H);^{13}C NMR (75 MHz, $CDCl_3$) δ 166.9, 134.6, 131.5, 129.4, 128.1, 127.8, 126.3, 120.9, 117.5, 114.9, 53.6, 52.6, 35.2, 25.3, 21.3, 15.5; MS (ESI, *m/z*): 312 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{18}H_{22}N_3O_2$ $[M+H]^+$ 312.1712, found 312.1710; IR(cm^{-1}, neat): 3372, 3116, 2919, 2850, 1706.

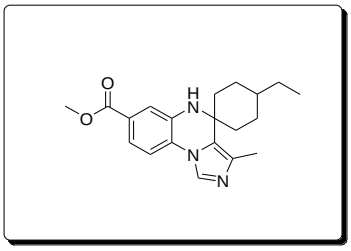
Methyl 3',4-dimethyl-5'*H*-spiro[cyclohexane-1,4'-imidazo[1,5-*a*]quinoxaline] -7'-carboxylate (12l)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.51 (d, J = 1.4 Hz, 1H), 7.48 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.36 (d, *J* = 8.3 Hz, 1H), 4.66 (s, NH), 3.88 (s, 3H), 2.36 (s, 3H), 1.93-1.84 (m, 3H), 1.70-1.66 (m, 2H), 1.49-1.43 (m, 1H), 1.27-1.03 (m, 3H), 0.98 (d, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.9, 134.6, 131.5, 129.5, 128.1, 127.5, 126.4, 120.9, 117.5, 114.9, 53.1, 52.5, 35.2, 32.1, 30.0, 22.7, 15.5; MS (ESI, *m/z*): 326 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{19}H_{24}N_3O_2$

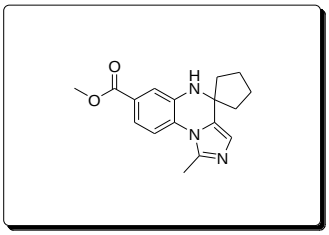
[M+H]$^+$ 326.1868, found 326.1869; IR(cm^{-1}, neat): 3363, 3093, 2915, 2859, 1702.

Methyl 4-ethyl-3'-methyl-5'*H*-spiro[cyclohexane-1,4'-imidazo[1,5-*a*]-quinoxaline]-7'-carboxylate (12m)



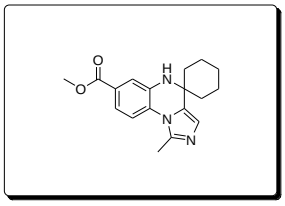
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.52 (d, *J* = 1.6 Hz, 1H), 7.51 (dd, *J* = 8.7, 1.6 Hz, 1H), 7.39 (d, *J* = 8.7 Hz, 1H), 4.60 (s, NH), 3.92 (s, 3H), 2.38 (s, 3H), 2.01-1.65 (m, 8H), 1.39-1.09 (m, 3H), 0.95 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.9, 134.6, 131.5, 129.5, 128.1, 127.6, 126.4, 120.9, 117.5, 114.9, 53.6, 52.5, 38.7, 35.2, 30.1, 27.7, 15.4, 11.8; MS (ESI, *m/z*): 340 (M+H)$^+$; HRMS (ESI, *m/z*) calcd for $C_{20}H_{26}N_3O_2$ [M+H]$^+$ 340.2025, found 340.2024; IR (cm^{-1}, neat): 3305, 3118, 2948, 2856, 1704.

Methyl 1'-methyl-5'*H*-spiro[cyclopentane-1,4'-imidazo[1,5-*a*]quinoxaline]-7'-carboxylate (12n)



^{1}H NMR (300 MHz, DMSO-d_6) δ 7.65 (d, J = 8.4 Hz, 1H), 7.62 (d, J = 1.7 Hz, 1H), 7.37 (dd, J = 8.4, 1.7 Hz, 1H), 6.69 (s, 1H), 6.50 (s, NH), 3.83 (s, 3H), 2.50 (s, 3H), 1.87-1.66 (m, 8H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 166.8, 142.5, 138.9, 135.2, 127.9, 127.5, 119.8, 119.7, 118.2, 117.5, 61.2, 52.9, 39.1, 23.7, 15.0; MS (ESI, *m/z*): 298 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{17}H_{20}N_3O_2$ $[M+H]^+$ 298.1555, found 298.1556; IR(cm^{-1}, neat): 3345, 2950, 2871, 1718.

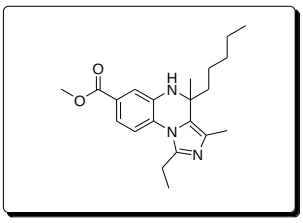
Methyl 1'-methyl-5'*H*-spiro[cyclohexane-1,4'-imidazo[1,5-*a*]quinoxaline]-7'-carboxylate (12o)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 (s, 1H), 7.51-7.46 (m, 2H), 6.75 (s, 1H), 4.65 (s, NH), 3.86 (s, 3H), 2.68 (s, 3H), 1.76-1.67 (m, 2H), 1.60-1.34 (m, 8H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.9, 142.6, 136.6, 135.6, 128.3, 127.9, 121.0, 120.2, 118.0, 117.5, 52.6, 52.6, 35.8, 25.4, 21.9, 17.7; MS (ESI, *m/z*): 312 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{18}H_{22}N_3O_2$ $[M+H]^+$ 312.1712, found 312.1709; IR(cm^{-1}, neat): 3369, 2929, 2852, 1716.

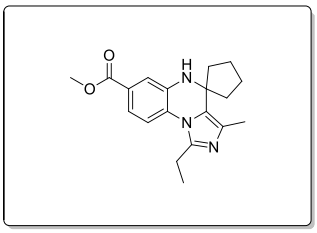
Methyl 1-ethyl-3,4-dimethyl-4-pentyl-4,5-dihydroimidazo[1,5-*a*]-quinoxalin

e-7-carboxylate (12p)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 (dd, J = 8.7, 1.6 Hz, 1H), 7.47 (d, J = 1.5 Hz, 1H), 7.46 (d, J = 8.7 Hz, 1H), 3.83 (s, 3H), 3.02 (q, J = 7.4 Hz, 2H), 2.30 (s, 3H), 1.55 (s, 3H), 1.42 (t, J = 7.4 Hz, 3H), 1.32-1.16 (m, 8H), 0.82 (t, J = 6.8 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.0, 145.9, 136.9, 129.0, 127.9, 127.8, 127.6, 120.8, 117.5, 117.4, 55.1, 52.6, 41.2, 32.3, 26.9, 24.2, 24.2, 22.9, 14.8, 14.4, 12.4; MS (ESI, *m/z*): 356 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{21}H_{30}N_3O_2$ $[M+H]^+$ 356.2338, found 356.2340; IR(cm^{-1}, neat): 3349, 2954, 2931, 2857, 1720.

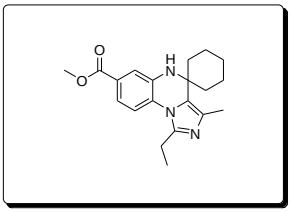
Methyl 1'-ethyl-3'-methyl-5'*H*-spiro[cyclopentane-1,4'-imidazo[1,5-*a*]-quinoxaline]-7'-carboxylate (12q)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 (dd, J = 8.4, 1.8 Hz, 1H), 7.49 (d, J = 1.8 Hz, 1H), 7.46 (d, J = 8.4 Hz, 1H), 4.12 (s, NH), 3.90(s, 3H), 3.02 (q, J = 7.4 Hz, 2H), 2.31 (s, 3H), 2.19-2.15 (m, 2H), 1.83-1.80 (m, 6H), 1.41 (t, J = 7.4 Hz, 3H); ^{13}C

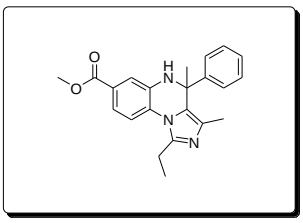
NMR (75 MHz, $CDCl_3$) δ 166.9, 145.9, 137.3, 128.9, 128.7, 128.0, 127.5, 121.3, 121.3, 117.8, 117.7, 62.9, 52.6, 38.6, 24.0, 14.6, 12.5; MS (ESI, *m/z*): 326 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{19}H_{24}N_3O_2$ $[M+H]^+$ 326.1868, found 326.1870; IR(cm^{-1}, neat): 3351, 2950, 2871, 1718.

Methyl 1'-ethyl-3'-methyl-5'*H*-spiro[cyclohexane-1,4'-imidazo[1,5-*a*]-quinoxaline]-7'-carboxylate (12r)



^1H NMR (300 MHz, $CDCl_3$) δ 7.53-7.50 (m, 2H), 7.41 (d, *J* = 8.2 Hz, 1H), 4.67 (s, NH), 3.87 (s, 3H), 2.97 (q, *J* = 7.4 Hz, 2H), 2.32 (s, 3H), 2.01-1.68 (m, 10H), 1.37 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.9, 145.6, 136.3, 129.6, 128.6, 128.2, 127.6, 121.2, 117.8, 117.6, 53.7, 52.5, 34.3, 25.3, 23.9, 21.3, 14.6, 12.5; MS (ESI, *m/z*): 340 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{20}H_{26}N_3O_2$ $[M+H]^+$ 340.2025, found 340.2026; IR(cm^{-1}, neat): 3378, 2927, 2856, 1718.

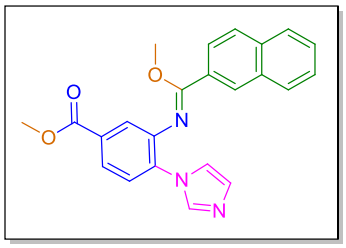
1-Ethyl-3,4-dimethyl-4-phenyl-4,5-dihydroimidazo[1,5-*a*]quinoxalin-7-yl acetate (12s)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.54-7.50 (m, 2H), 7.45 (d, J = 8.8 Hz, 1H), 7.39-7.36 (m, 2H), 7.32-7.21 (m, 3H), 4.52 (s, NH), 3.89 (s, 3H), 3.04 (q, J = 7.4 Hz, 2H), 1.99 (s, 3H), 1.88 (s, 3H), 1.45 (t, J = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.9, 146.0, 144.8, 136.9, 129.9, 128.8, 128.5, 128.1, 127.8, 126.8, 126.8, 121.2, 117.8, 117.8, 57.7, 52.6, 28.2, 24.0, 14.0, 12.4; MS (ESI, *m/z*): 362 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{22}H_{24}N_3O_2$ $[M+H]^+$ 362.1868, found 362.1866; IR(cm^{-1}, neat): 3372, 2977, 2933, 1718.

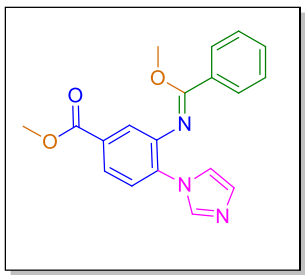
5. Characterization Data for Compound 13b-i

(Z)-methyl 4-(1H-imidazol-1-yl)-3-((methoxy (naphthalen-2-yl) methylene) amino)benzoate (13b)



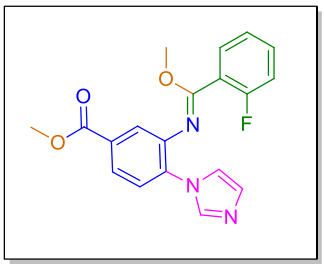
Yellow oil; ^{1}H NMR (300 MHz, Acetone-d_6) δ 7.83 (dd, J = 8.3, 1.7, Hz, 2H), 7.77 (s, 1H), 7.75 – 7.69 (m, 3H), 7.60 – 7.49 (m, 3H), 7.46 (d, J = 8.3 Hz, 1H), 7.33 (s, 1H), 7.20 (dd, J = 8.5, 1.7 Hz, 1H), 7.08 (s, 1H), 4.04 (s, 1H), 3.79 (s, 1H); ^{13}C NMR (75 MHz, Acetone-d_6) δ 165.4, 161.2, 142.7, 137.0, 133.8, 132.8, 132.4, 129.8, 129.1, 128.6, 127.9, 127.8, 127.7, 127.6, 126.7, 125.3, 124.6, 124.4, 119.5, 54.2, 51.6; MS (ESI, *m/z*): 386.3 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{23}H_{20}N_3O_3$ $[M+H]^+$ 386.1505, found 386.1500.

(Z)-methyl 4-(1H-imidazol-1-yl)-3-((methoxy (phenyl) methylene) amino) benzoate (13c)



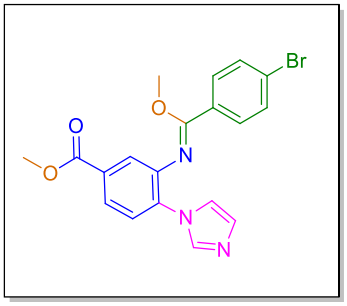
Yellow solid; 159-161 °C; ^{1}H NMR (300 MHz, Acetone-d_6) δ 7.74 (dd, J= 8.4, 1.7 Hz, 1H), 7.66 (s, 1H), 7.49 – 7.44 (m, 2H), 7.41 – 7.33 (m, 1H), 7.33 – 7.22 (m, 3H), 7.18 – 7.10 (m, 2H), 7.05 (s, 1H), 3.99 (s, 3H), 3.85 (s, 3H); ^{13}C NMR (75 MHz, Acetone-d_6) δ 165.4, 161.2, 142.7, 136.9, 132.6, 130.4, 129.9, 129.0, 128.9, 128.2, 128.1, 127.1, 125.3, 124.5, 124.4, 119.5, 54.0, 51.6; MS (ESI, *m/z*): 336.2 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{19}H_{18}N_3O_3$ $[M+H]^+$ 386.1348, found 386.1344.

(Z)-methyl 3-(((2-fluorophenyl) (methoxy) methylene) amino)-4-(1H-imidazol-1-yl)benzoate (13d)



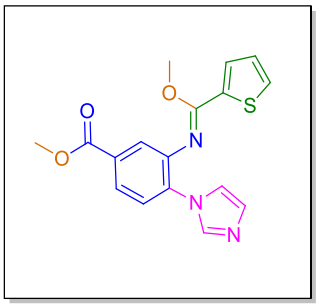
Brown oil; ^{1}H NMR (300 MHz, Acetone-d_6) δ 7.82 (s, 1H), 7.73 (dd, *J* = 8.3, 1.9 Hz, 1H), 7.51 – 7.38 (m, 3H), 7.36 (d, *J* = 1.8 Hz, 1H), 7.23 – 7.13 (m, 2H), 7.11 (s, 1H), 7.01 (t, *J* = 8.5 Hz, 1H), 4.01 (s, 3H), 3.82 (s, 3H); ^{13}C NMR (75 MHz, Acetone-d_6) δ 165.3, 160.0, 158.7, 156.7, 141.5, 137.2, 133.4, 132.6, 132.4, 130.0, 129.3, 129.0, 125.1, 124.9, 124.5, 123.7, 119.7, 119.6, 115.7, 115.5, 54.4, 51.5; MS (ESI, *m/z*): 354.2 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{19}H_{17}FN_3O_3$ $[M+H]^+$ 354.1254, found 354.1252.

(Z)-methyl 3-(((4-bromophenyl)(methoxy) methylene) amino)-4-(1H-imidazol-1-yl)benzoate (13e)



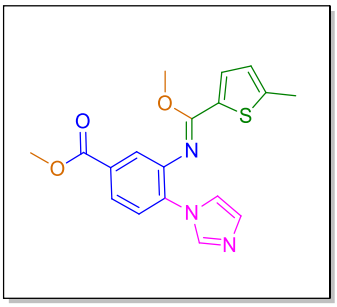
Yellow solid; 114-116 °C; ^{1}H NMR (300 MHz, MeOD) δ 7.79 (dd, J = 8.3, 1.9 Hz, 1H), 7.63 (s, 1H), 7.57 (d, J = 1.8 Hz, 1H), 7.44 – 7.36 (m, 3H), 7.26 – 7.21 (m, 1H), 7.10 – 7.06 (m, 1H), 7.01 – 6.93 (m, 2H), 3.97 (s, 3H), 3.90 (s, 3H); ^{13}C NMR (75 MHz, MeOD) δ 165.92, 160.59, 142.58, 137.02, 131.85, 131.23, 130.45, 129.69, 129.14, 127.86, 125.58, 124.75, 124.57, 119.87, 53.86, 51.50; MS (ESI, *m/z*): 414 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{19}H_{17}BrN_3O_3$ $[M+H]^+$ 414.0453, found 414.0450.

(Z)-methyl 4-(1H-imidazol-1-yl)-3-((methoxy (thiophen-2-yl) methylene) amino)benzoate (13f)



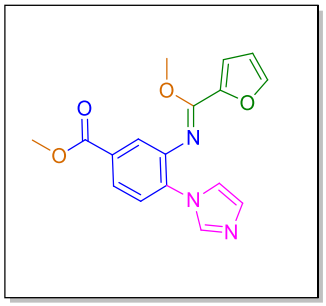
Yellow oil; ^{1}H NMR (300 MHz, Acetone-d_6) δ 7.90 (dd, J = 8.3, 2.0 Hz, 1H), 7.68 (s, 1H), 7.66 – 7.58 (m, 3H), 7.26 (s, 1H), 7.10 (dd, J = 3.8, 1.2 Hz, 1H), 7.04 – 6.95 (m, 2H), 3.94 (s, 3H), 3.89 (s, 3H); ^{13}C NMR (75 MHz, Acetone-d_6) δ 165.4, 154.0, 142.8, 136.9, 132.6, 131.9, 131.2, 130.7, 130.5, 129.0, 127.2, 126.0, 125.1, 123.9, 119.6, 53.9, 51.7; MS (ESI, *m/z*): 342.2 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{17}H_{16}N_3O_3S$ $[M+H]^+$ 342.0912, found 342.0906.

(Z)-methyl 4-(1H-imidazol-1-yl)-3-((methoxy (5-methylthiophen-2-yl) methylene) amino)benzoate (13g)



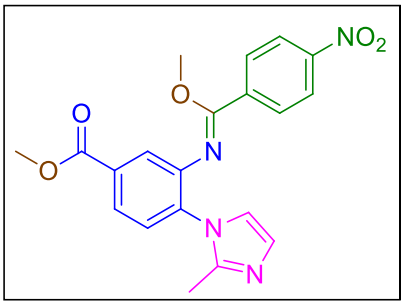
Pale yellow solid; 119-121 °C; ^{1}H NMR (300 MHz, Acetone-d_6) δ 7.89 (dd, J = 8.2, 1.9 Hz, 1H), 7.70 (s, 1H), 7.65 – 7.57 (m, 2H), 7.27 (s, 1H), 7.01 (s, 1H), 6.92 (d, J = 3.8 Hz, 1H), 6.70 – 6.64 (m, 1H), 3.91 (s, 3H), 3.90 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (75 MHz, Acetone-d_6) δ 165.4, 154.0, 146.2, 142.9, 137.0, 132.6, 132.4, 130.5, 128.9, 128.2, 126.0, 125.8, 125.0, 123.9, 119.6, 53.7, 51.7, 14.2; MS (ESI, *m/z*): 356.1 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{18}H_{18}N_3O_3S$ $[M+H]^+$ 356.1069, found 356.1068.

(Z)-methyl 3-((furan-2-yl(methoxy)methylene)amino)-4-(1H-imidazol-1-yl)benzoate (13h)



Brown solid; 89-91 °C; ^{1}H NMR (300 MHz, Acetone-d_6) δ 7.85 (dd, J = 8.2, 1.9 Hz, 1H), 7.67 (s, 1H), 7.62 – 7.51 (m, 3H), 7.24 (d, J = 1.0 Hz, 1H), 7.00 (s, 1H), 6.54 (dd, J = 3.6, 0.7 Hz, 1H), 6.46 (dd, J = 3.5, 1.8 Hz, 1H), 3.91 (s, 3H), 3.89 (s, 3H); ^{13}C NMR (75 MHz, Acetone-d_6) δ 165.5, 150.7, 145.6, 143.5, 143.0, 137.0, 132.4, 130.2, 128.9, 125.7, 124.6, 123.3, 119.6, 116.3, 111.5, 53.5, 51.6; MS (ESI, *m/z*): 326.1 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{17}H_{16}N_3O_4$ $[M+H]^+$ 326.1141, found 326.1133.

(Z)-methyl 3-((methoxy(4-nitrophenyl)methylene)amino)-4-(2-methyl-1H-imidazol-1-yl)benzoate (13i)

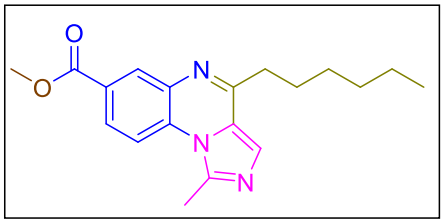


Yellow solid; 163-165 °C; ^{1}H NMR (300 MHz, Acetone-d_6) δ 8.17 (s, 1H), 8.15 (s, 1H), 7.78 (dd, J = 8.2, 1.9 Hz, 1H), 7.68 (d, J = 1.9 Hz, 1H), 7.43-7.36 (m,

3H), 6.85 (dd, J = 7.4, 1.4 Hz, 2H), 3.96 (s, 3H), 3.89 (s, 3H), 1.94 (s, 3H); ^{13}C NMR (75 MHz, Acetone-d_6) δ 165.4, 158.6, 148.8, 144.2, 143.7, 136.2, 132.4, 131.0, 129.8, 128.1, 127.6, 124.7, 124.2, 123.3, 120.1, 54.3, 51.7, 12.4; MS (ESI, *m/z*): 395.3 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{20}H_{19}N_4O_5$ $[M+H]^+$ 395.1355, found 395.1349.

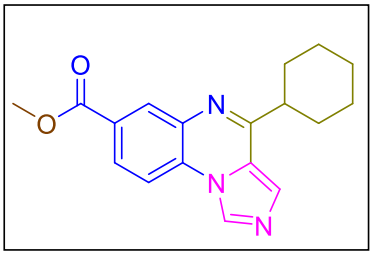
6. Characteristic Data for Compound 14b-c

Methyl 4-hexyl-1-methylimidazo[1,5-a]quinoxaline-7-carboxylate (14a)



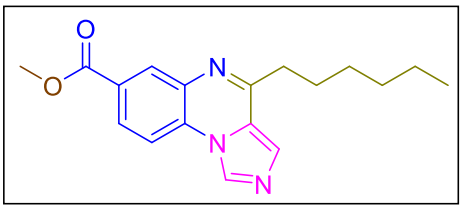
Off white solid; 81-83 °C; ^{1}H NMR (400 MHz, acetone) δ 8.40 (d, *J* = 2.0 Hz, 1H), 8.36 (d, *J* = 8.7 Hz, 1H), 8.09 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.80 (s, 1H), 3.95 (s, 3H), 3.06 (s, 3H), 3.01 – 2.96 (m, 2H), 1.90 (dt, *J* = 15.3, 7.5 Hz, 2H), 1.52 – 1.42 (m, 2H), 1.41-1.32 (m, 4H), 0.89 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, acetone-d_6) *δ* 165.5, 158.1, 136.8, 130.3, 127.4, 125.1, 116.2, 51.6, 34.5, 31.5, 27.1, 22.3, 17.7, 13.4; MS (ESI, *m/z*): 326.2 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{19}H_{24}N_3O_2$ $[M+H]^+$ 326.1869, found 326.1863.

Methyl 4-cyclohexylimidazo[1,5-a]quinoxaline-7-carboxylate (14b)



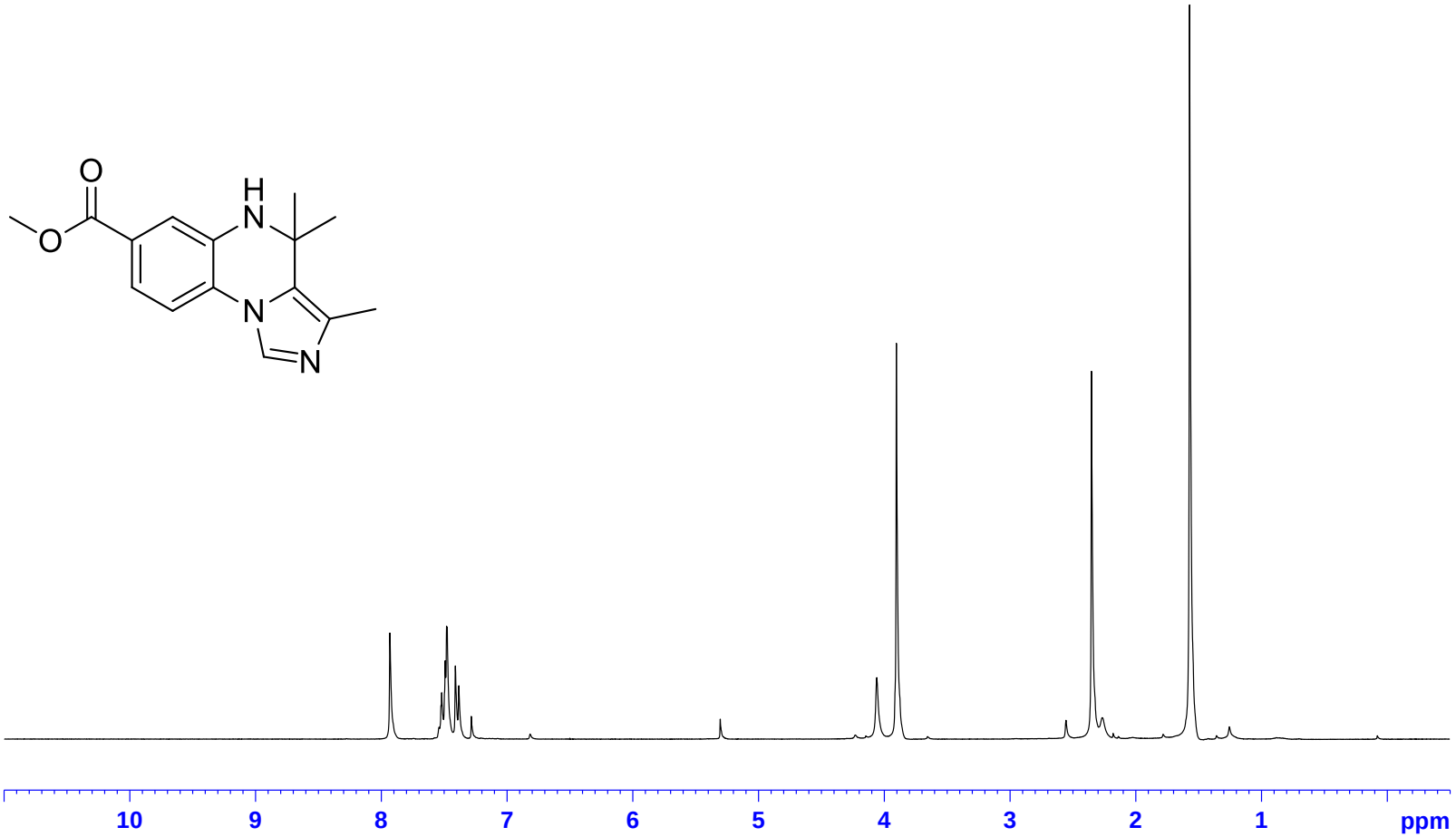
Off-white solid; 171-173 °C; ^{1}H NMR (400 MHz, acetone-d_6) *δ* 9.11 (s, 1H), 8.47 (d, *J* = 1.7 Hz, 1H), 8.36 (d, *J* = 8.4 Hz, 1H), 8.14 (dd, *J* = 8.6, 1.9 Hz, 1H), 8.00 (s, 1H), 3.96 (s, 3H), 3.22 (tt, *J* = 11.5, 3.5 Hz, 1H), 1.98 – 1.86 (m, 3H), 1.85 – 1.75 (m, 3H), 1.61 – 1.47 (m, 3H), 1.42 – 1.31 (m, 1H); ^{13}C NMR (101 MHz, acetone-d_6) *δ* 165.2, 161.7, 135.8, 130.7, 128.3, 128.0, 126.5, 115.1, 51.7, 43.2, 31.0, 25.9, 25.9; MS (ESI, *m/z*): 310.3 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{18}H_{20}N_3O_2$ $[M+H]^+$ 310.1556, found 310.1551.

Methyl 4-hexylimidazo[1,5-a]quinoxaline-7-carboxylate (14c)

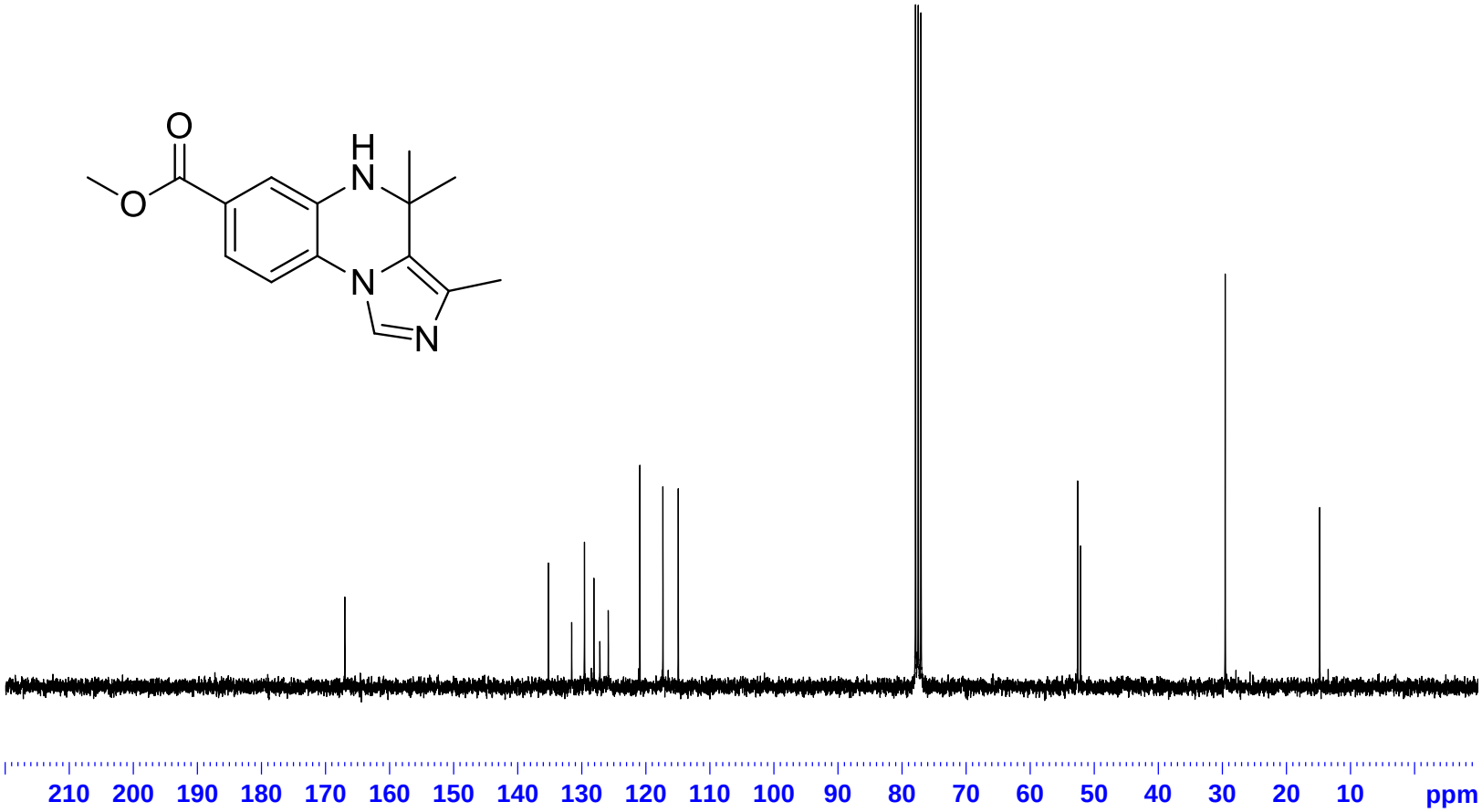


Off-white solid; 175-177 °C; ^{1}H NMR (400 MHz, acetone-d_6) δ 9.12 (s, 1H), 8.47 (d, J = 1.9 Hz, 1H), 8.38 (d, J = 8.5 Hz, 1H), 8.16 (dd, J = 8.5, 1.9 Hz, 1H), 7.97 (s, 1H), 3.96 (s, 3H), 3.11 – 3.03 (m, 2H), 1.93 (dt, J = 15.3, 7.5 Hz, 2H), 1.54 – 1.44 (m, 2H), 1.41 – 1.30 (m, 4H), 0.89 (t, J = 7.1 Hz, 3H); MS (ESI, *m/z*): 312.3 $(M+H)^+$; HRMS (ESI, *m/z*) calcd for $C_{18}H_{22}N_3O_2$ $[M+H]^+$ 312.1712, found 312.1706.

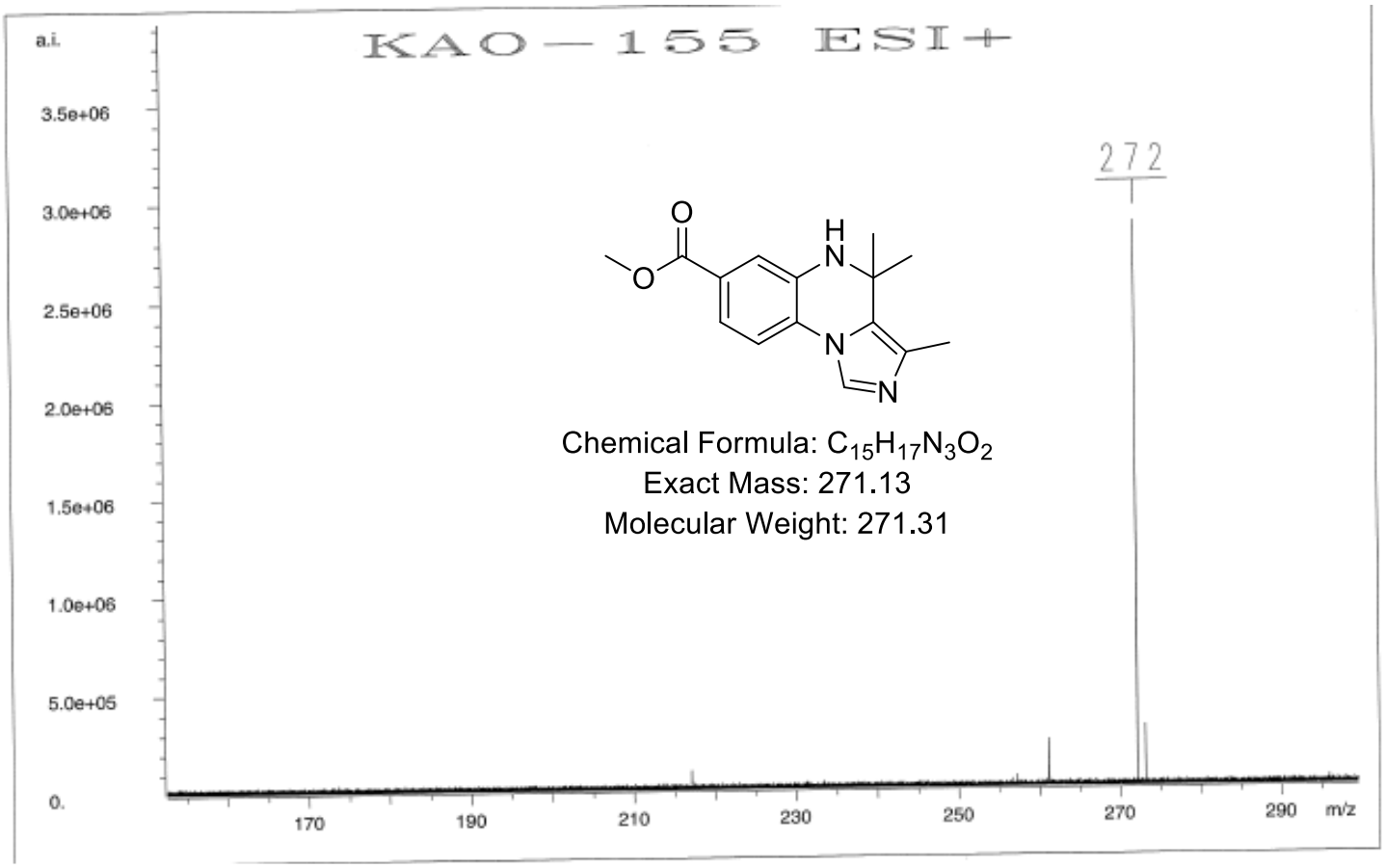
7. ^{1}H NMR, ^{13}C NMR, LRMS, HRMS and IR spectra of Compound 12a-s



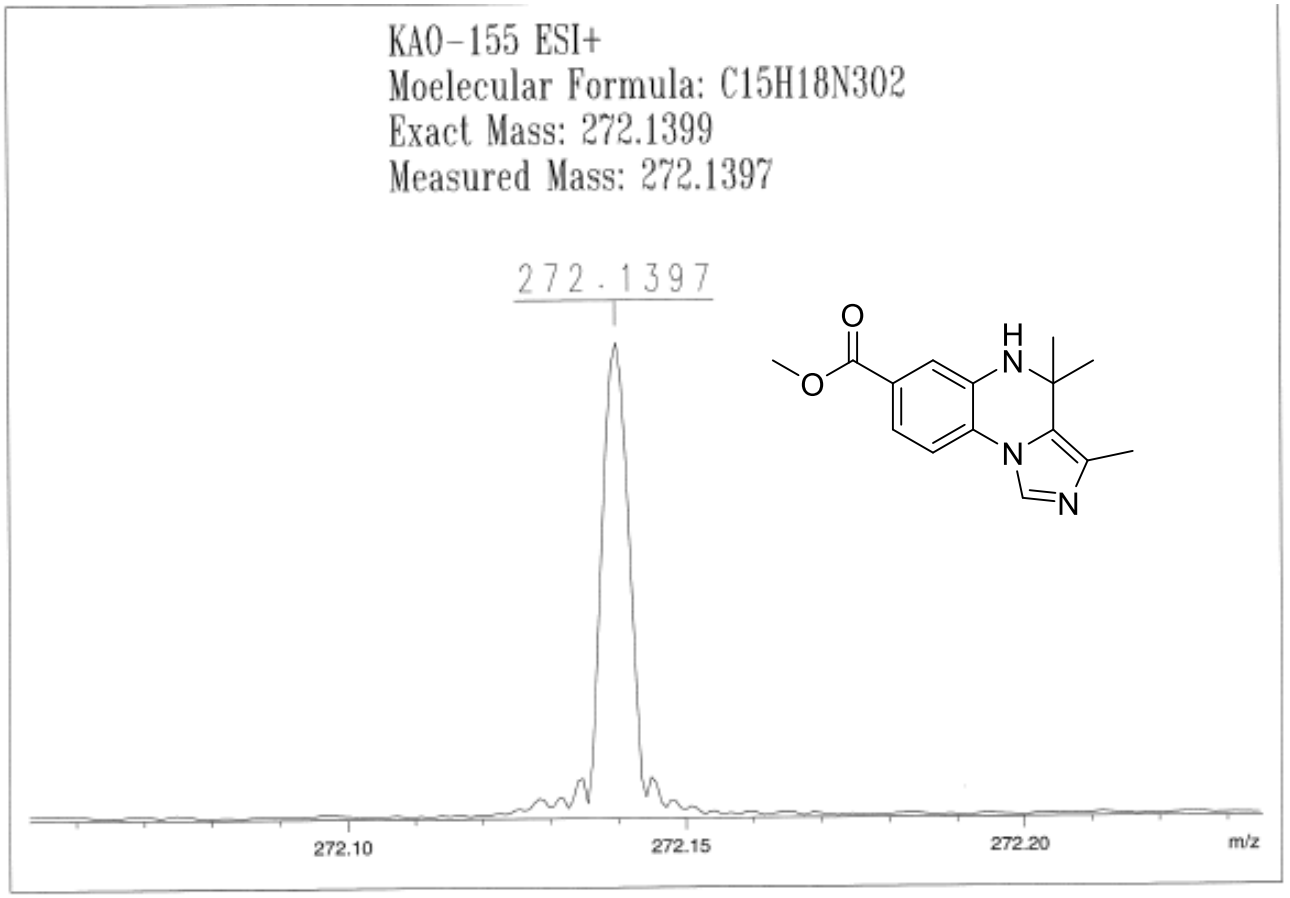
^{1}H NMR spectrum (300 MHz) of compound **12a** in $CDCl_3$



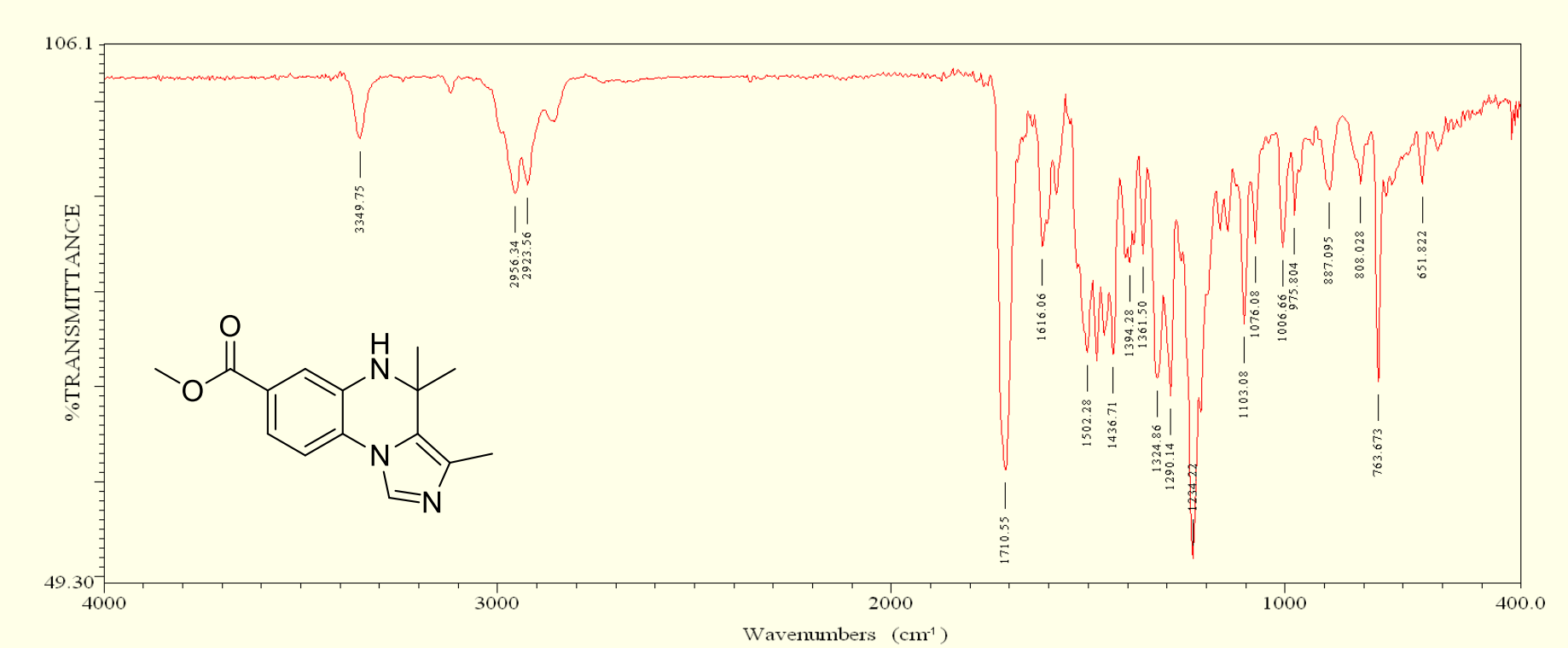
^{13}C NMR spectrum (75 MHz) of compound **12a** in $CDCl_3$



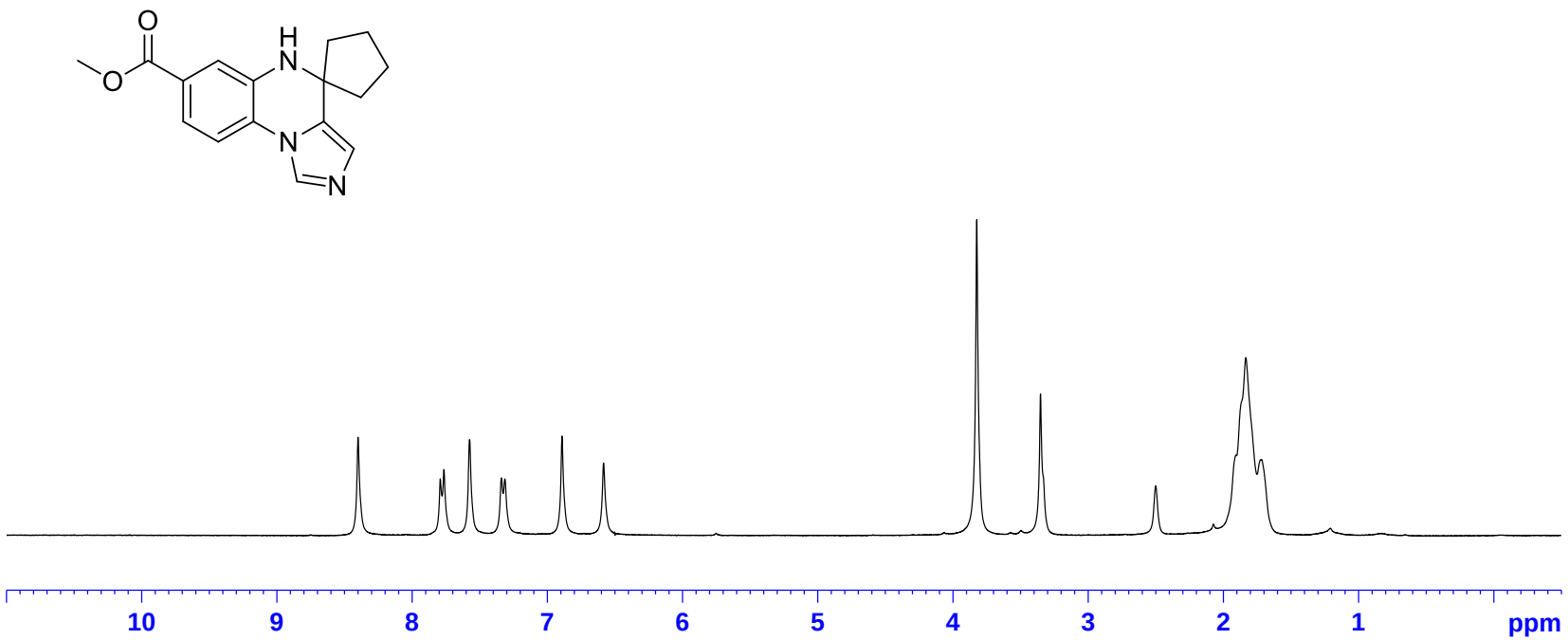
ESI-LRMS of compound **12a**



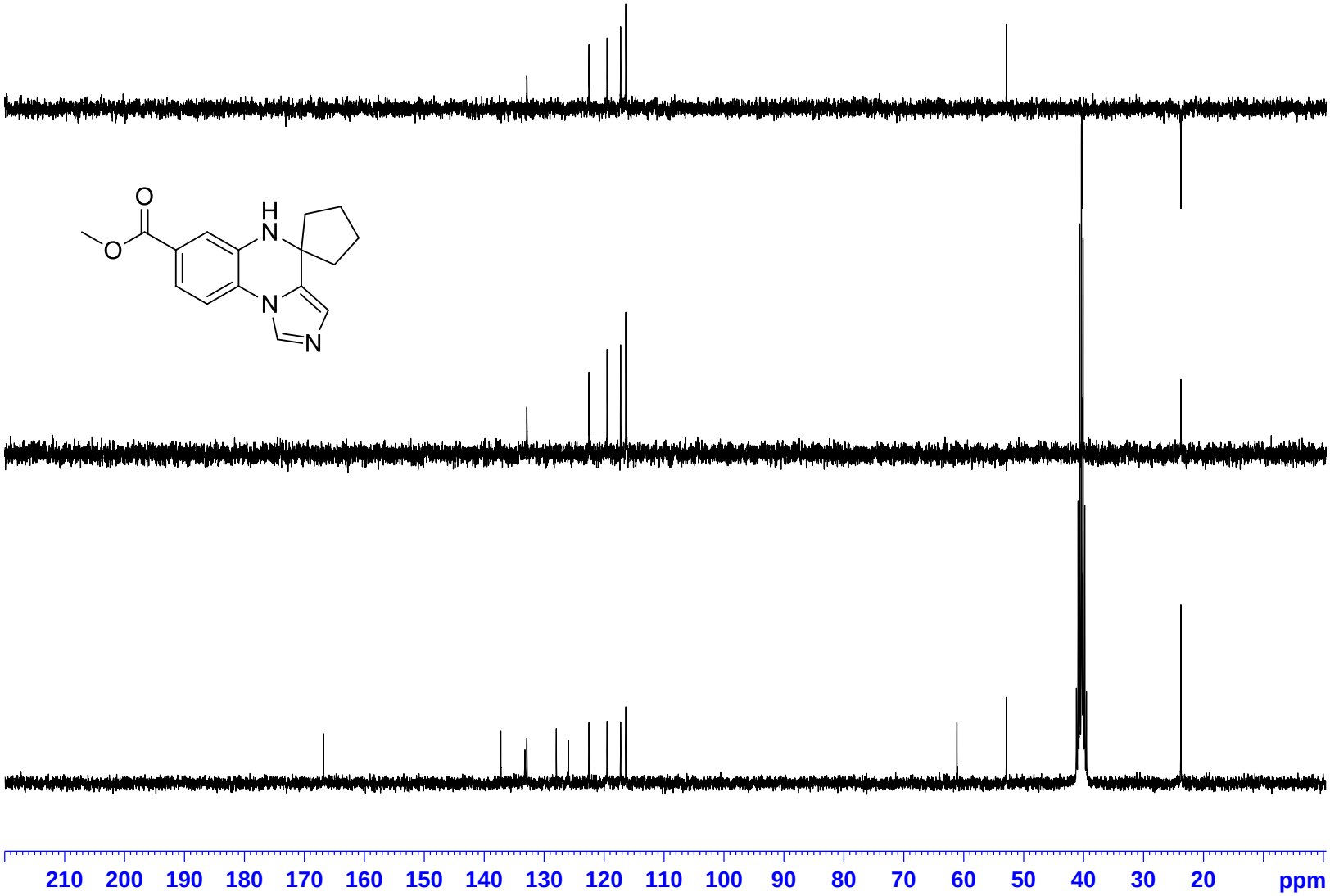
ESI-HRMS of compound **12a**



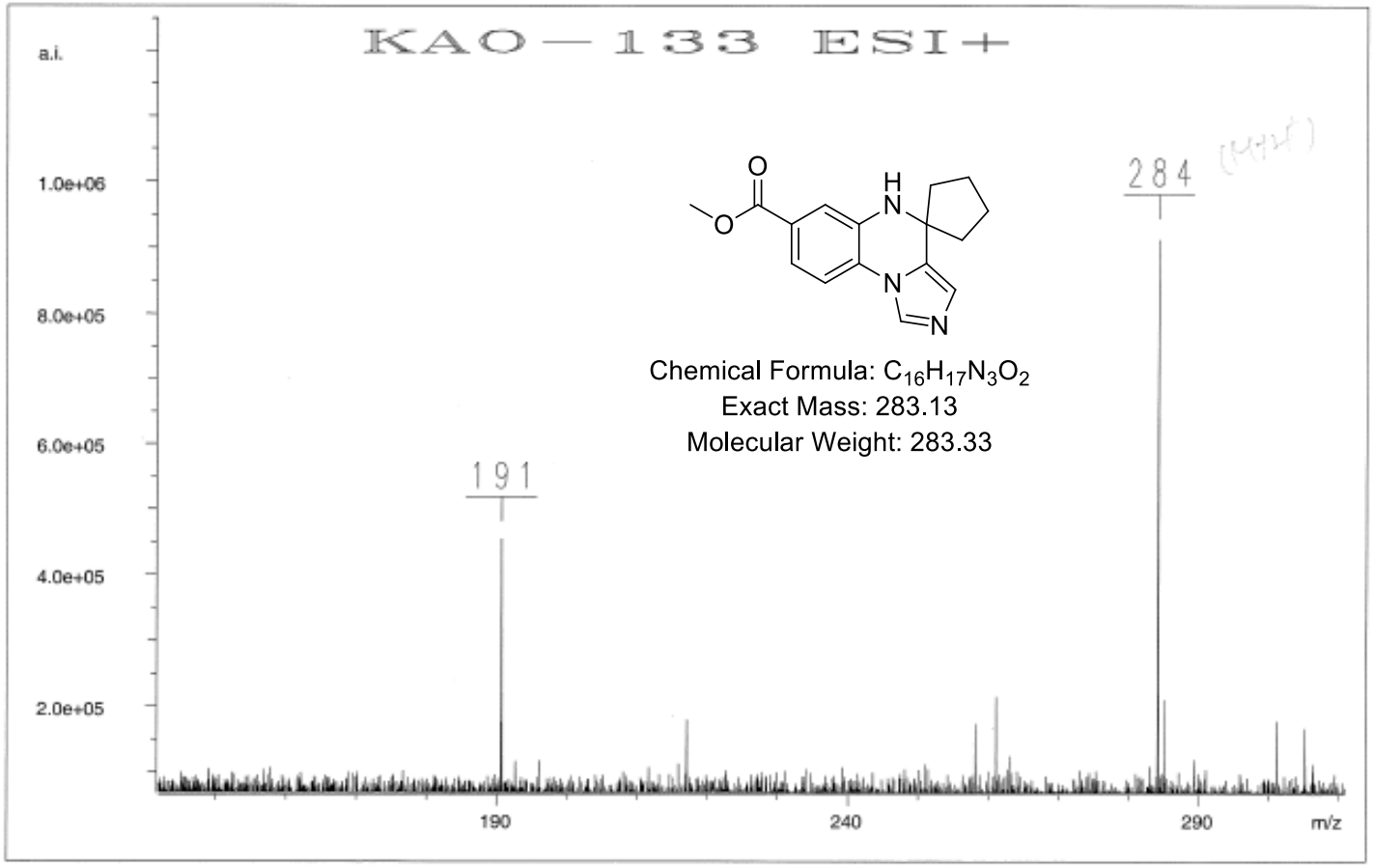
IR spectrum of compound **12a**



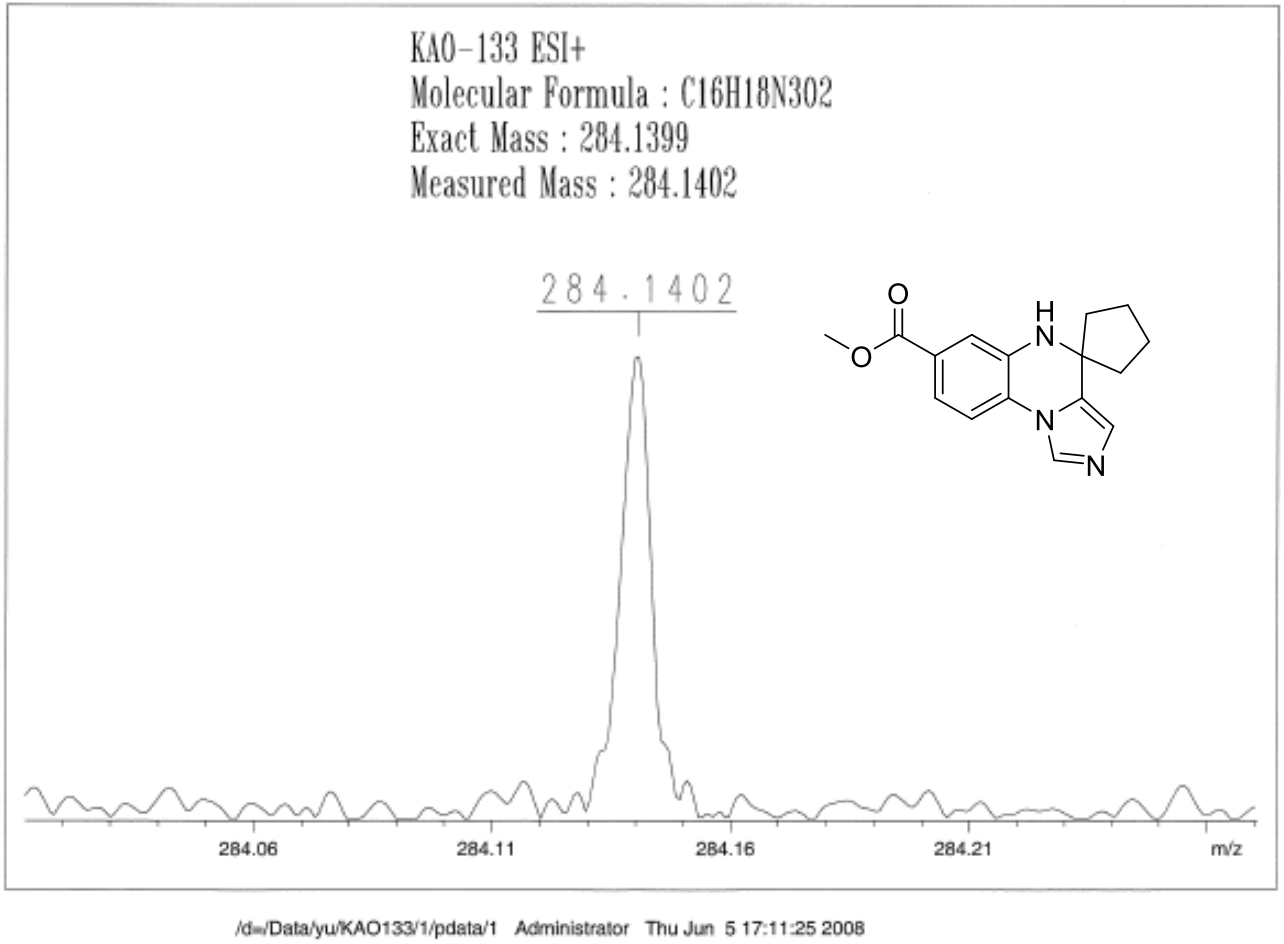
^{1}H NMR spectrum (300 MHz) of compound **12b** in DMSO-d_6



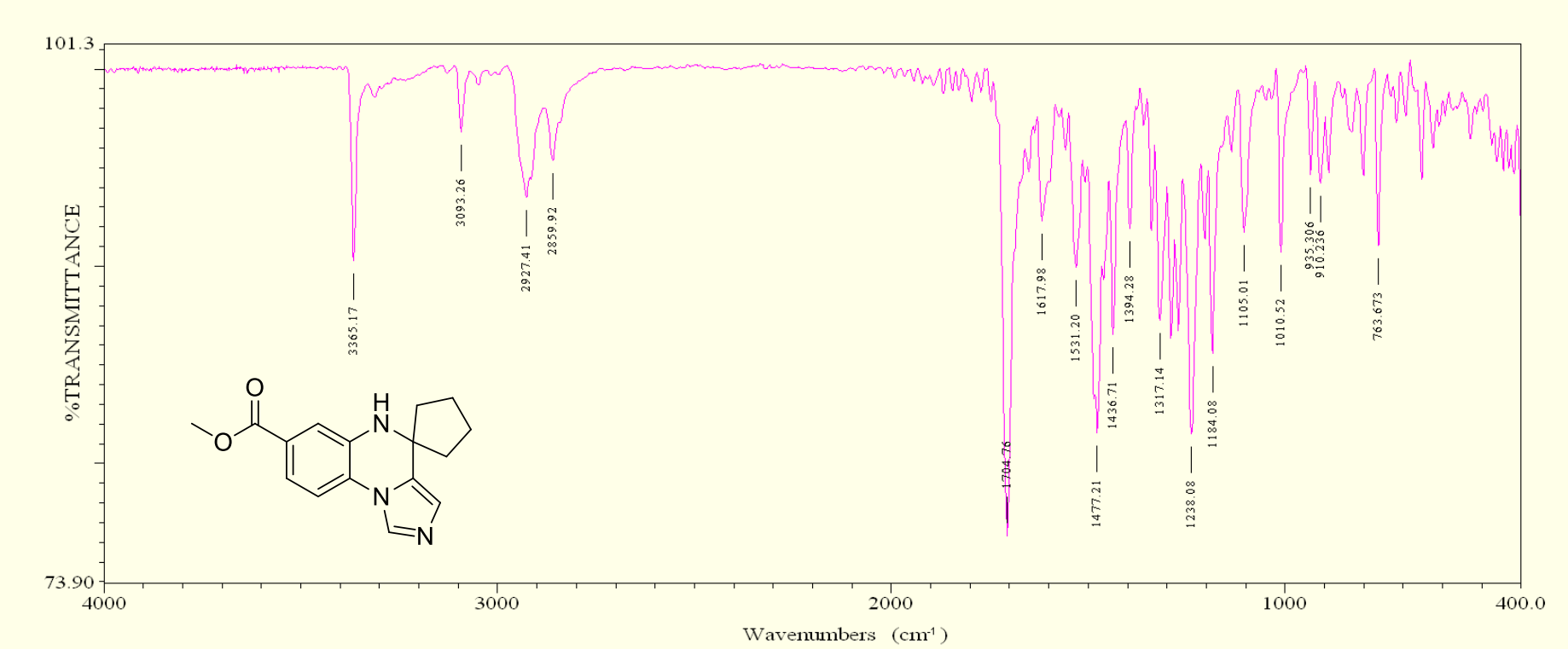
DEPT ^{13}C NMR spectrum (75 MHz) of compound **12b** in DMSO-d_6



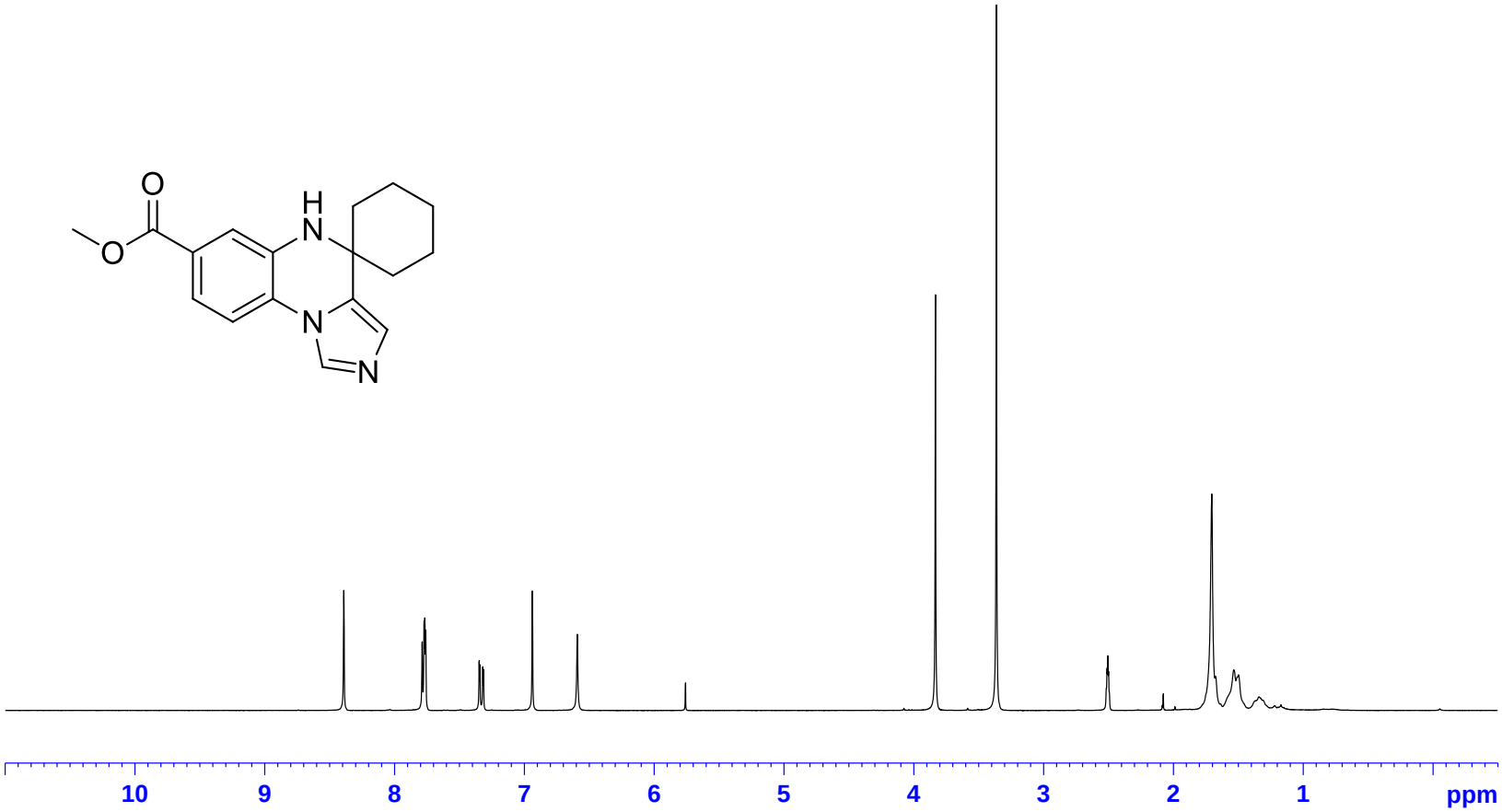
ESI-LRMS of compound **12b**



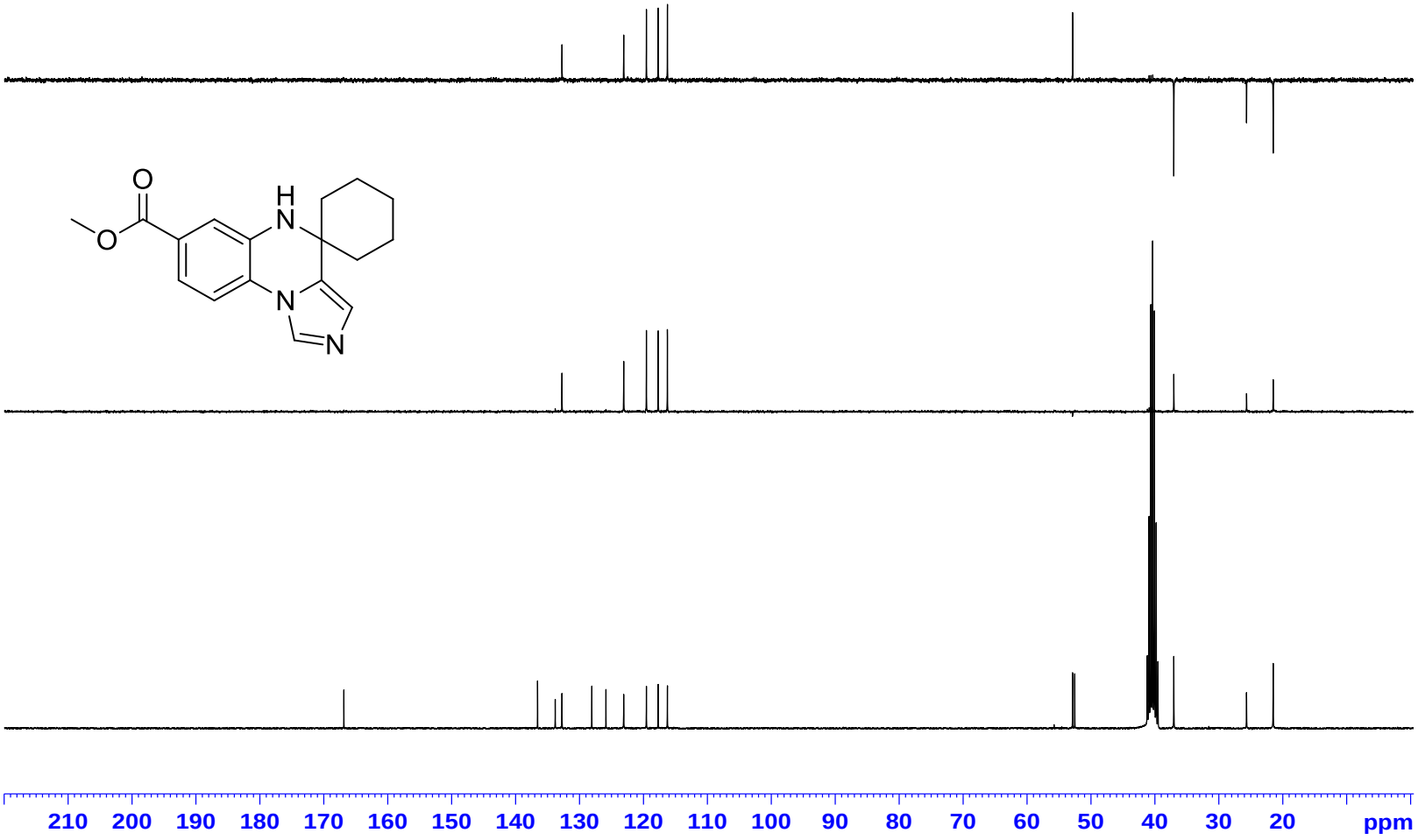
ESI-HRMS of compound **12b**



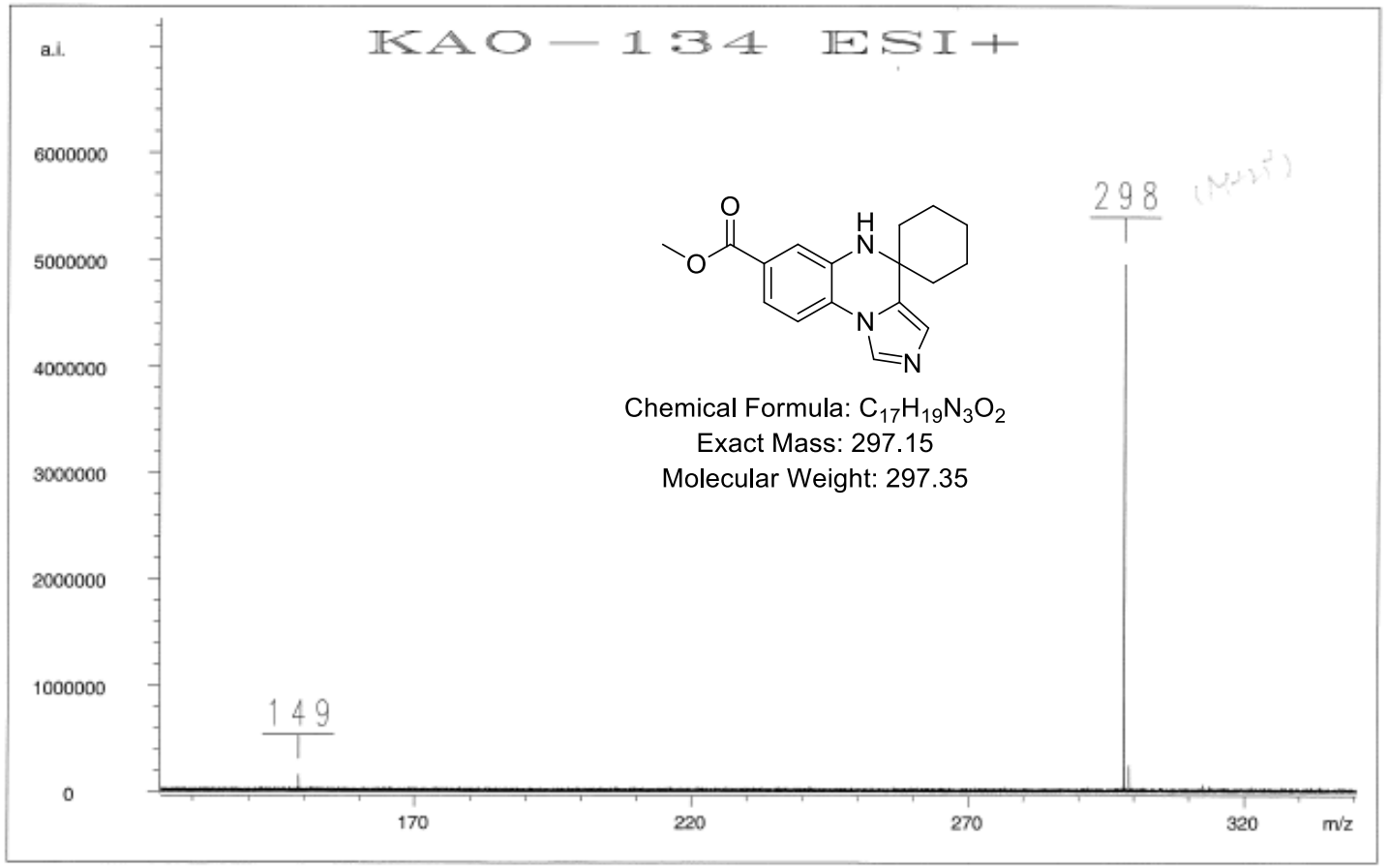
IR spectrum of compound **12b**



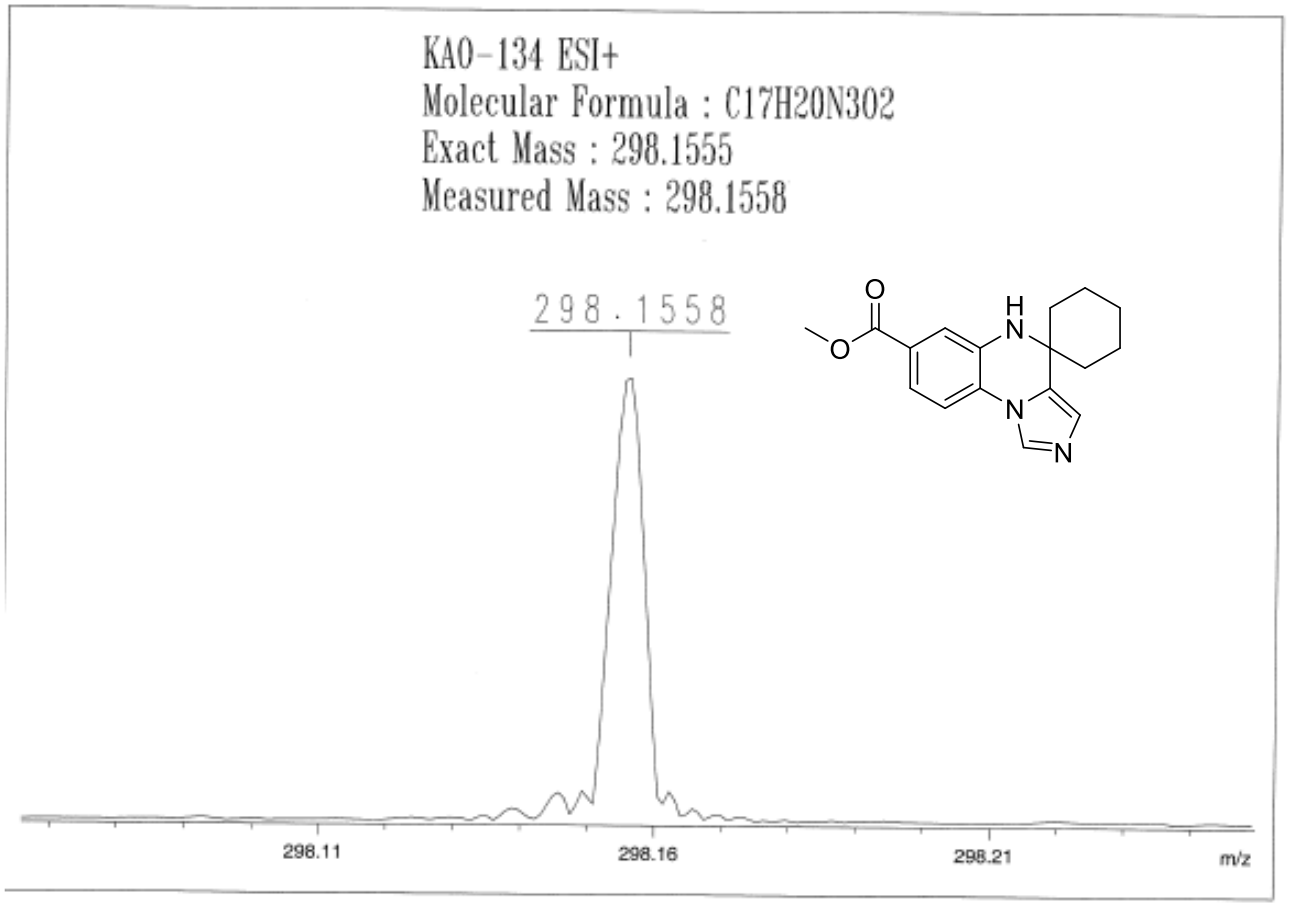
^{1}H NMR spectrum (300 MHz) of compound **12c** in DMSO-d_6



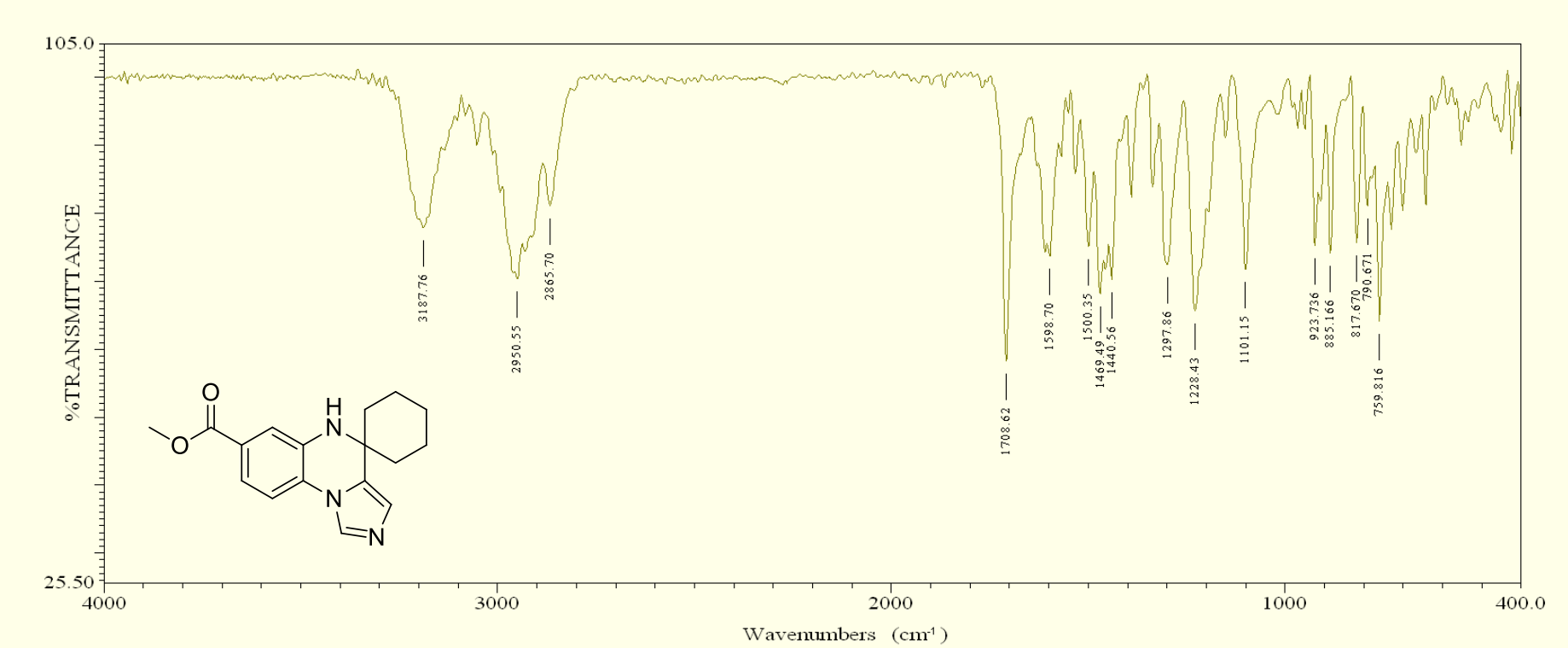
DEPT ^{13}C NMR spectrum (75 MHz) of compound **12c** in DMSO-d_6



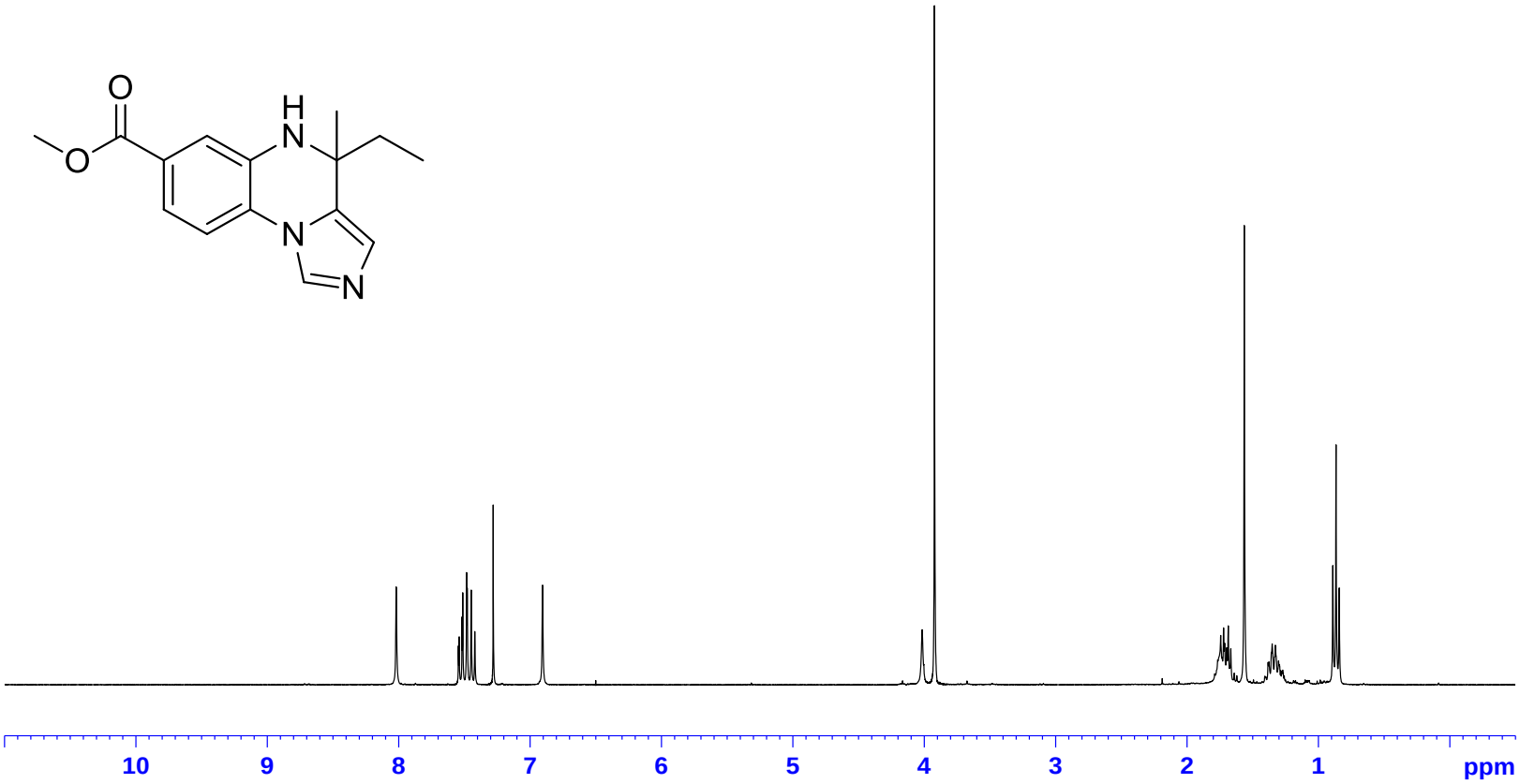
ESI-LRMS of compound **12c**



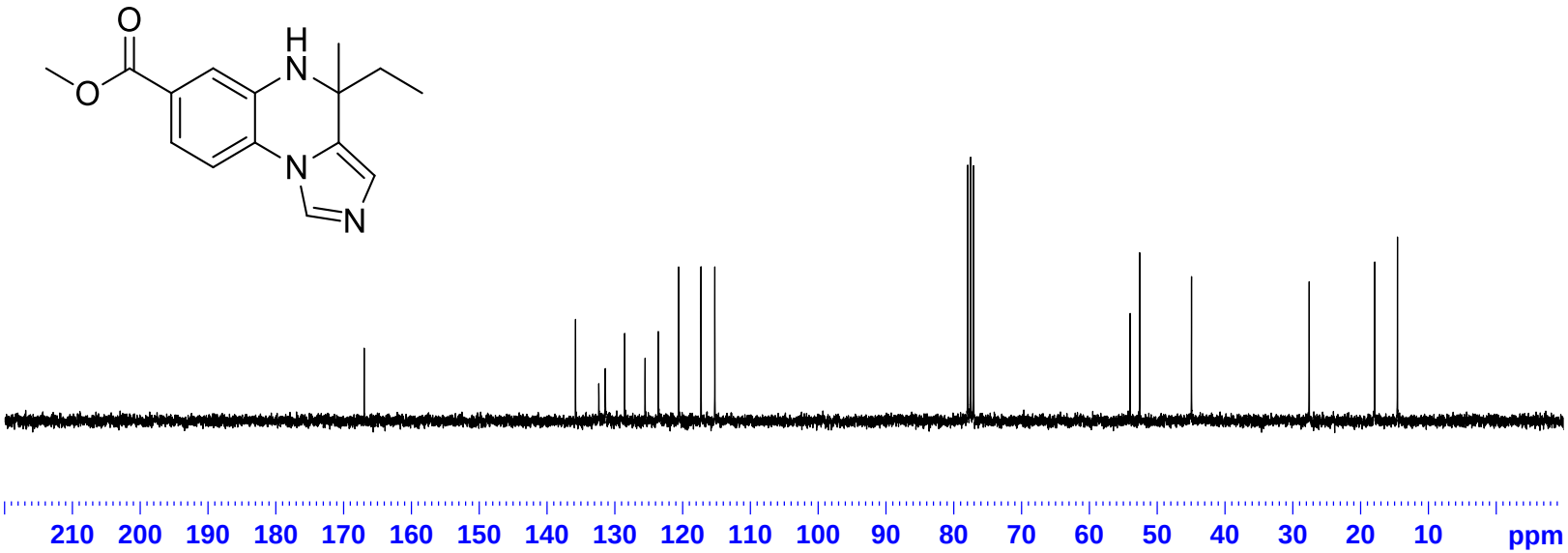
ESI-HRMS of compound **12c**



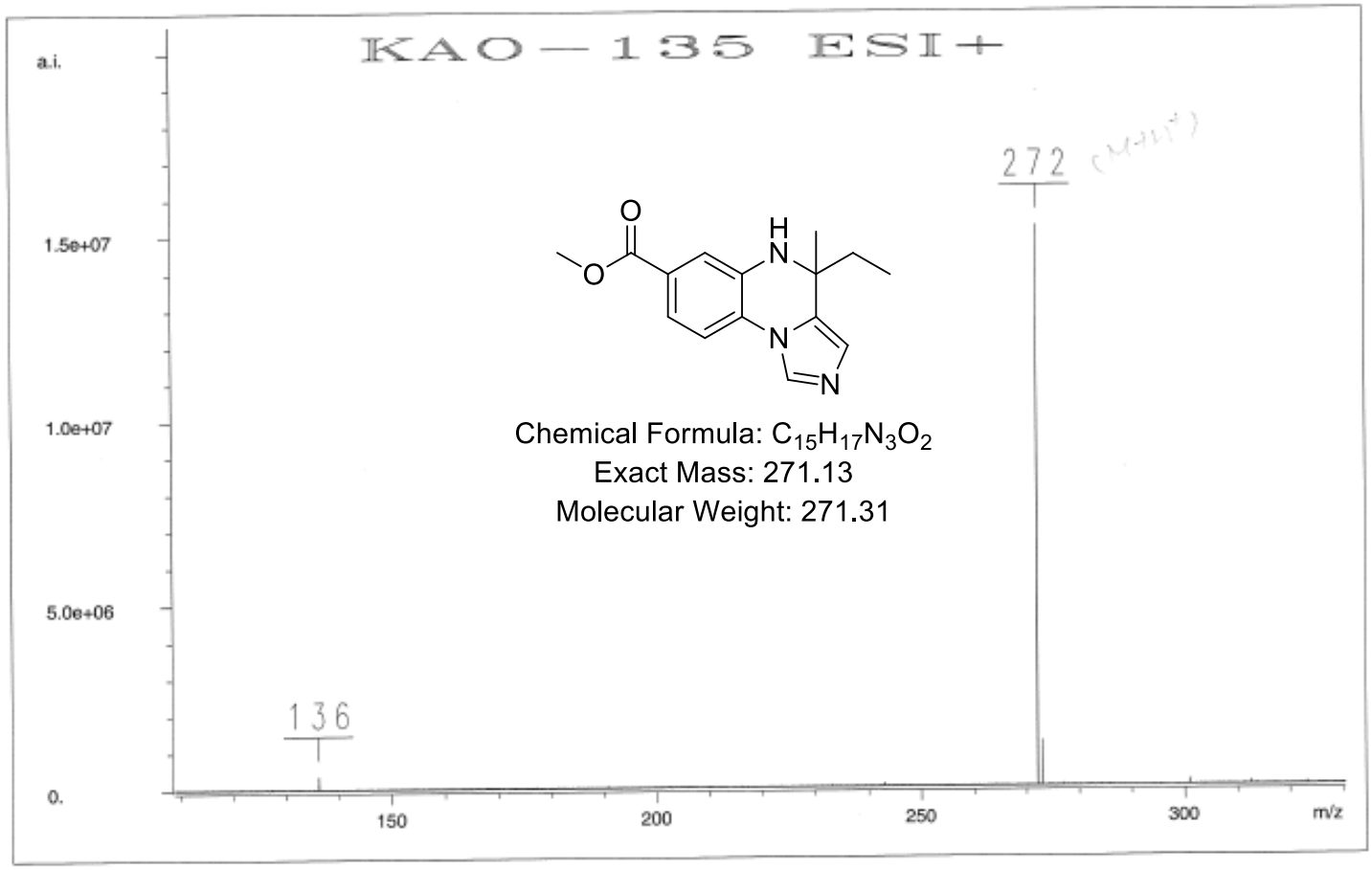
IR spectrum of compound **12c**



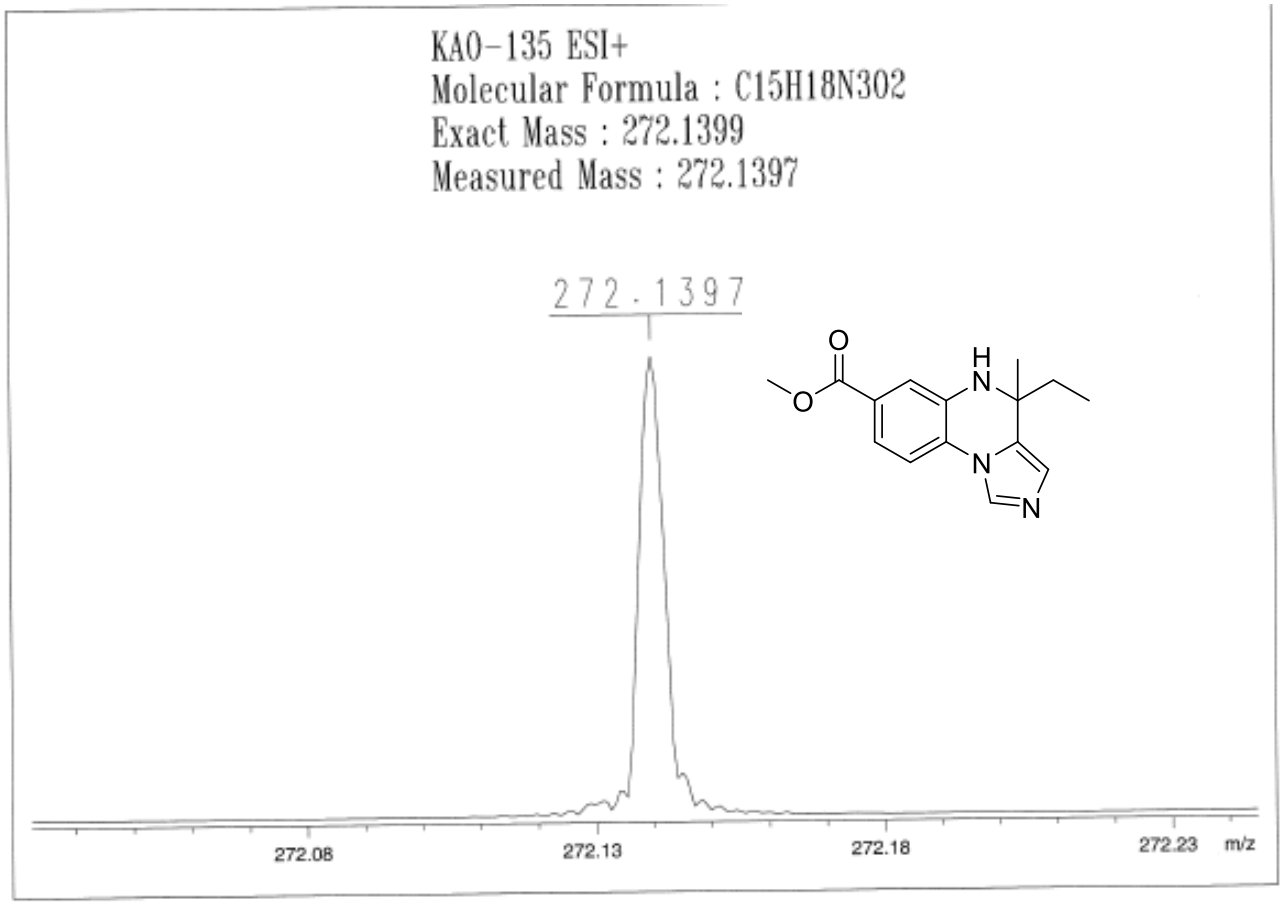
^{1}H NMR spectrum (300 MHz) of compound **12d** in $CDCl_3$



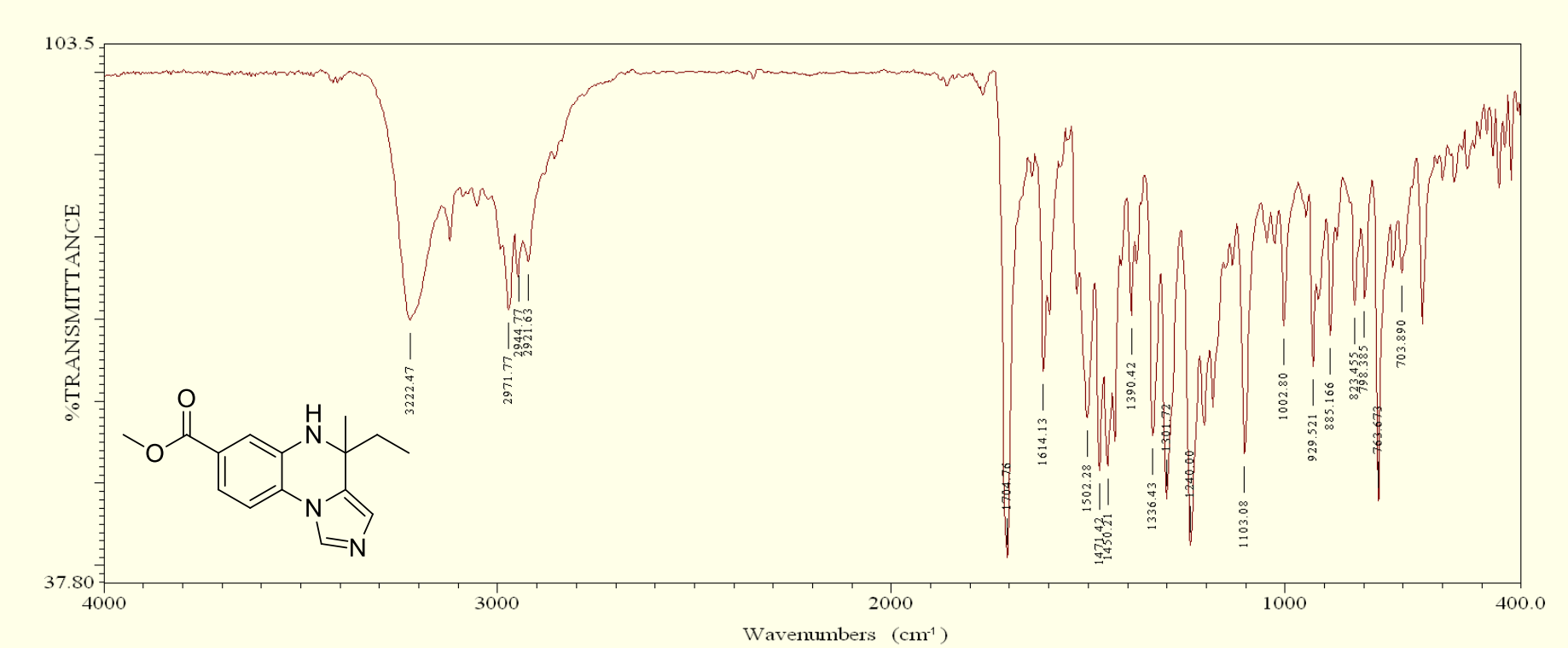
^{13}C NMR spectrum (75 MHz) of compound **12d** in $CDCl_3$



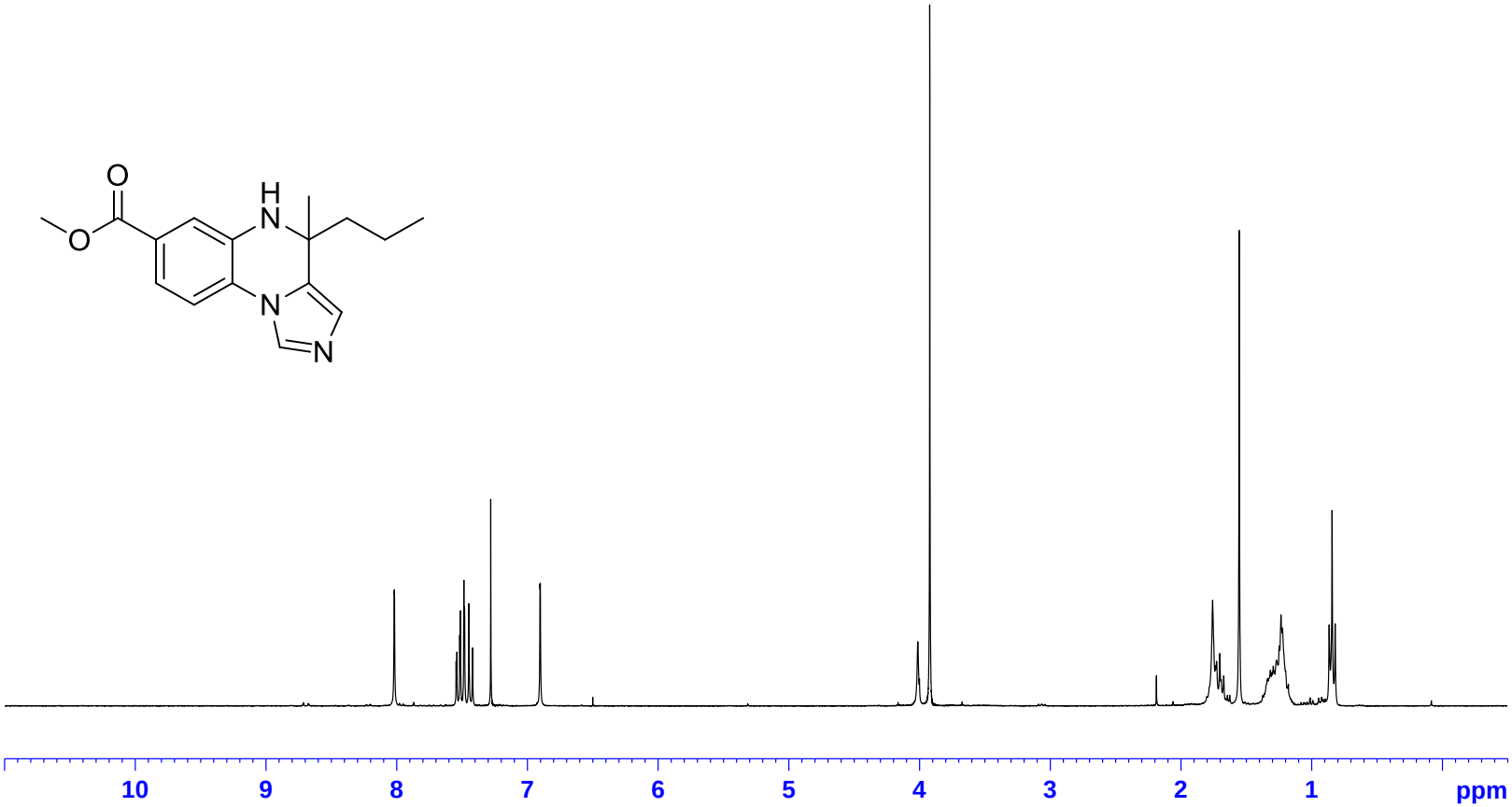
ESI-LRMS of compound **12d**



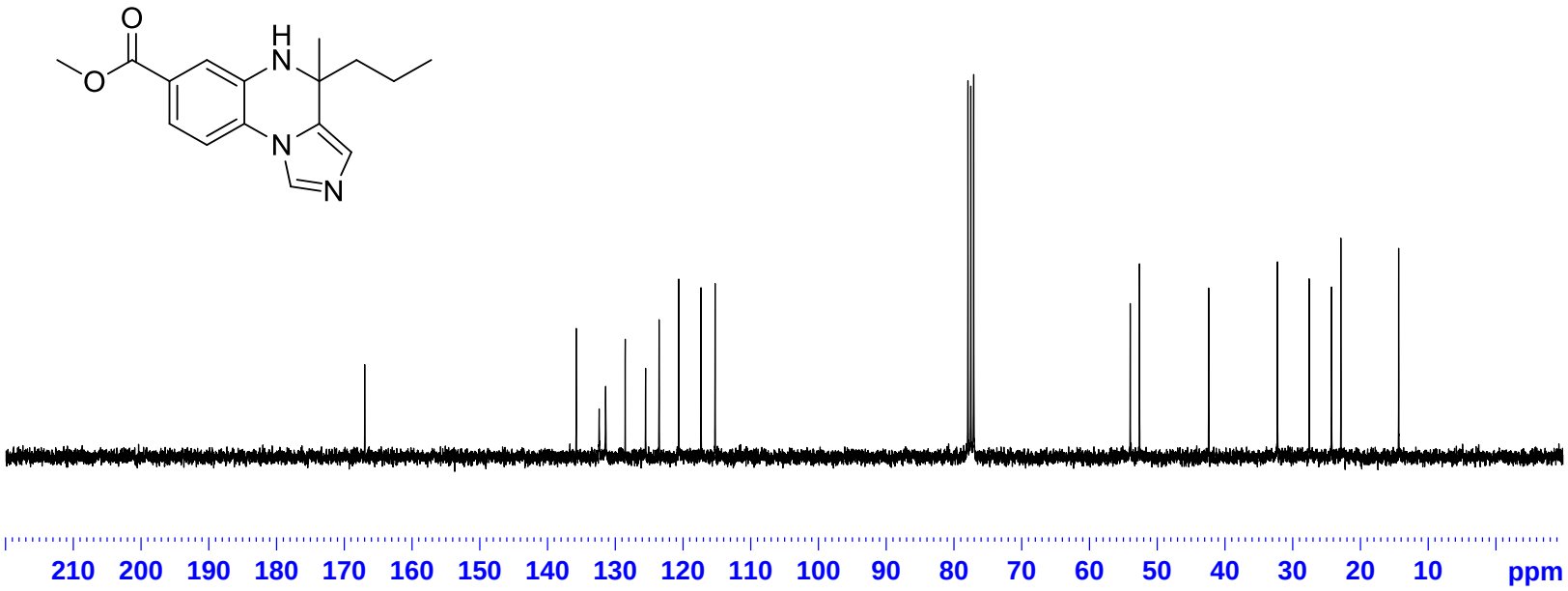
ESI-HRMS of compound **12d**



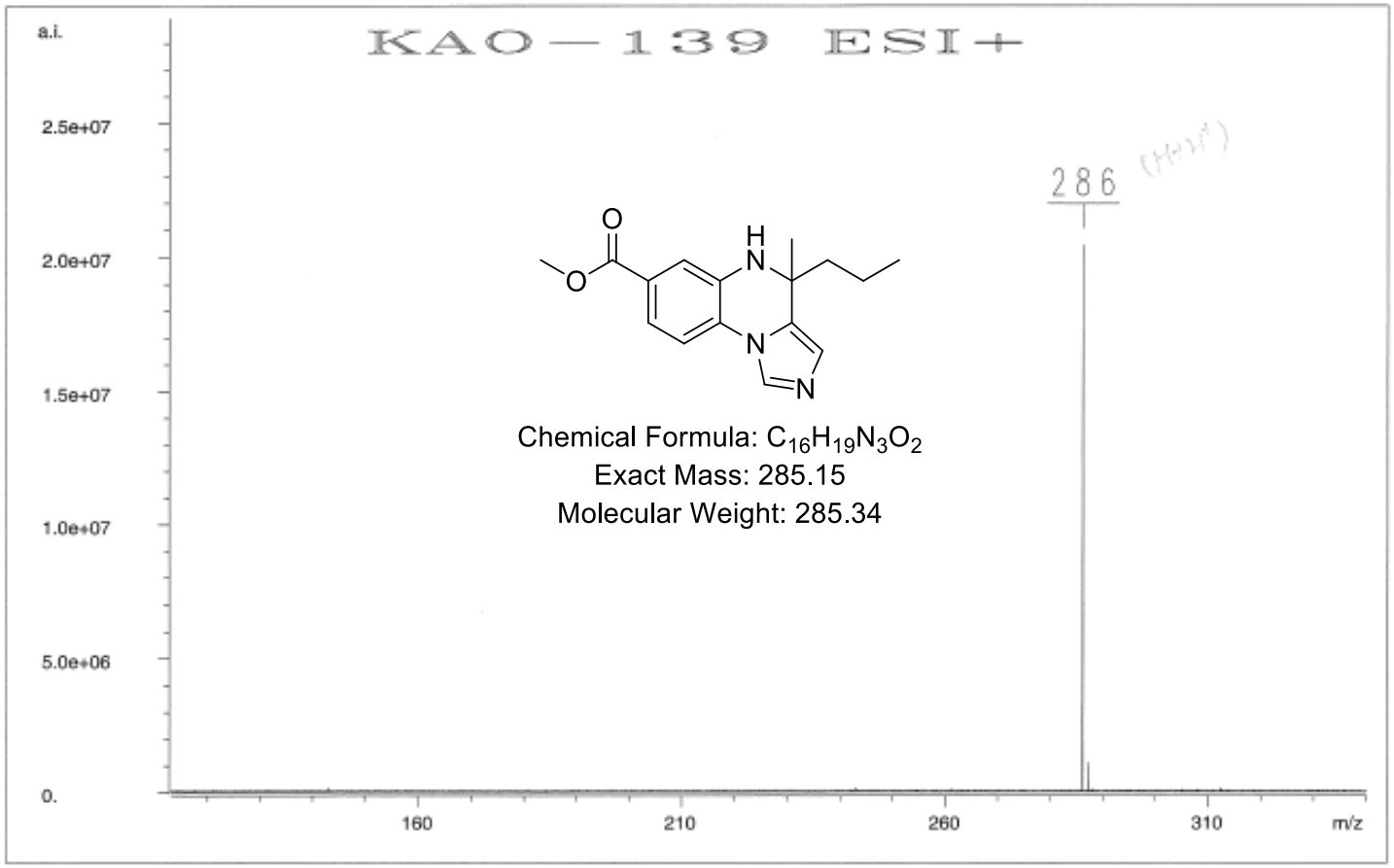
IR spectrum of compound **12d**



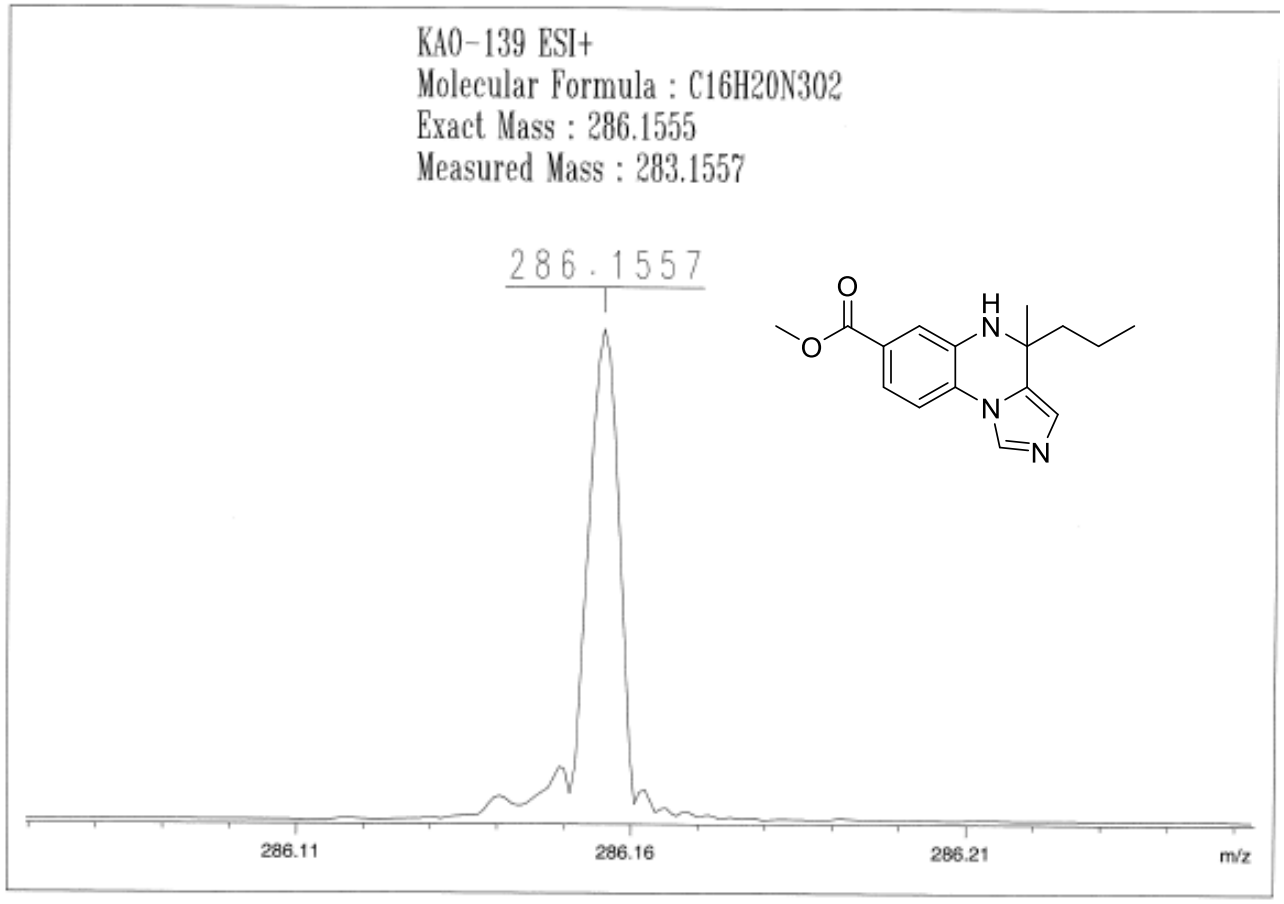
^{1}H NMR spectrum (300 MHz) of compound **12e** in $CDCl_3$



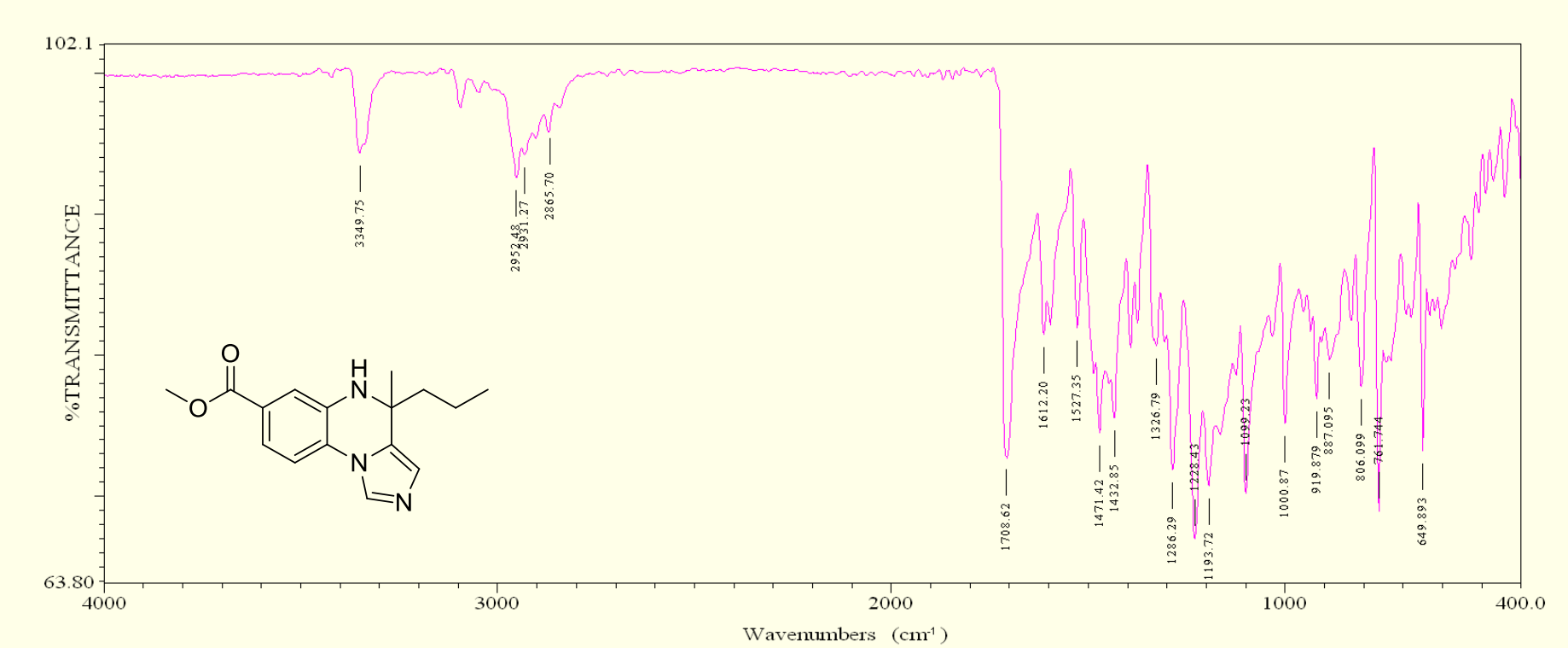
^{13}C NMR spectrum (75 MHz) of compound **12e** in $CDCl_3$



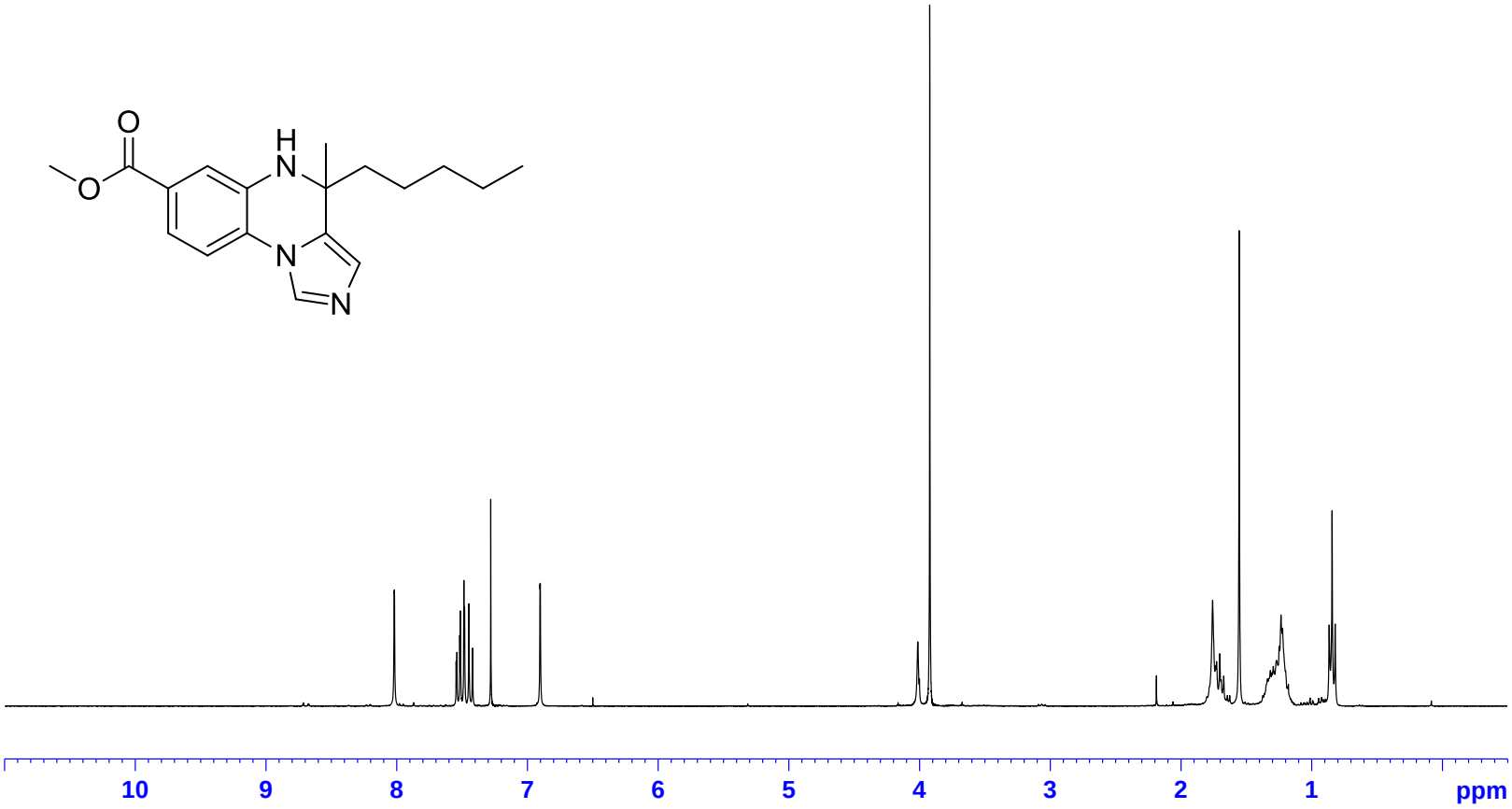
ESI-LRMS of compound **12e**



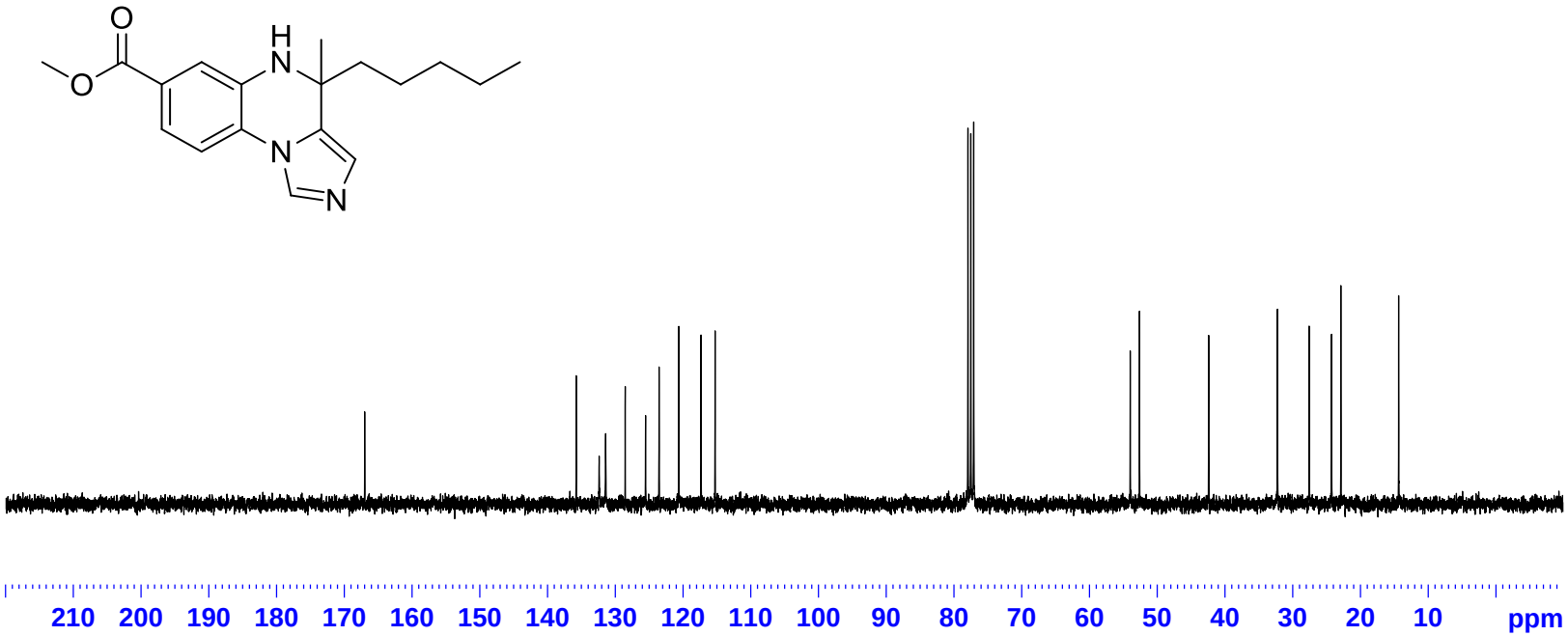
ESI-HRMS of compound **12e**



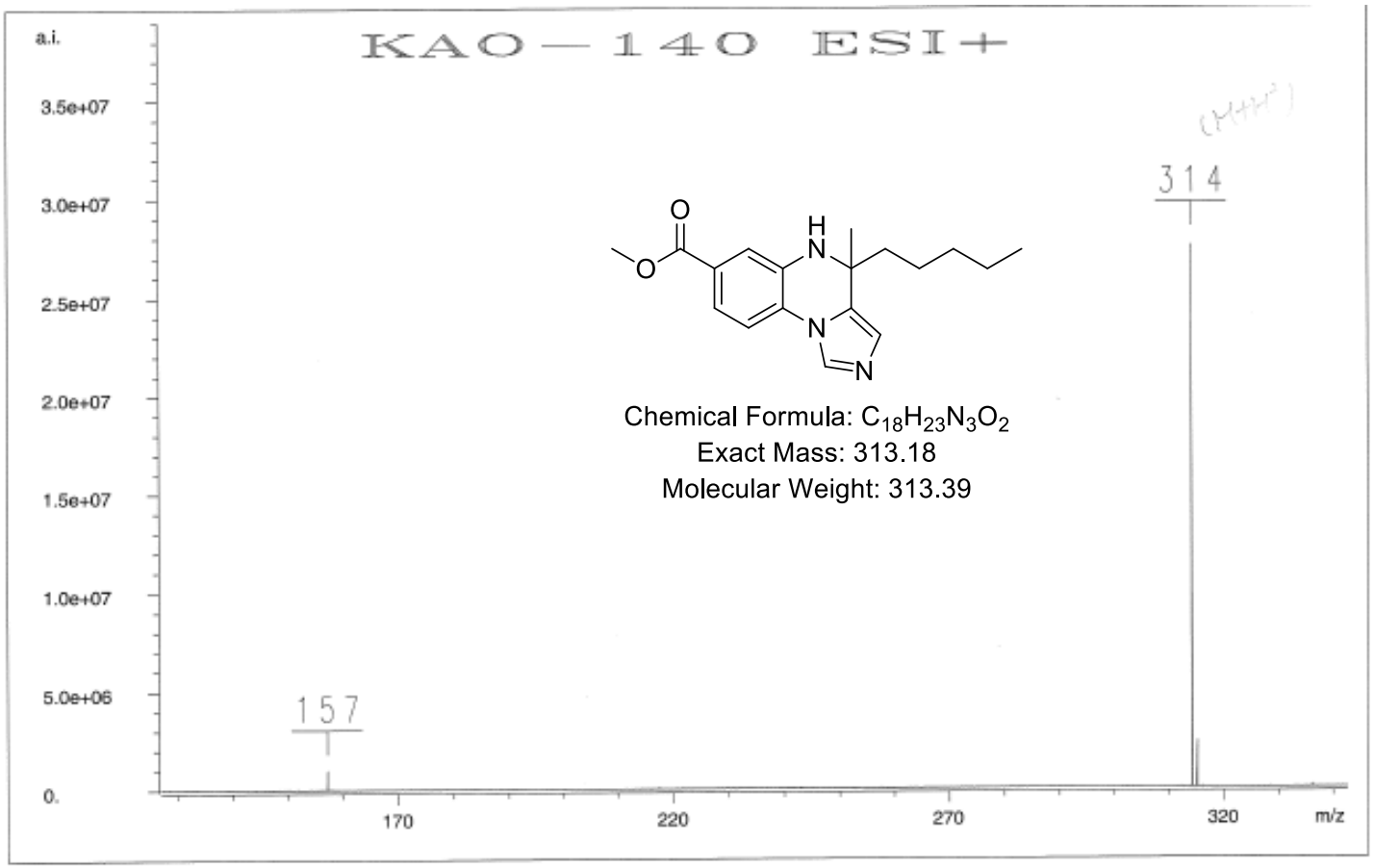
IR spectrum of compound **12e**



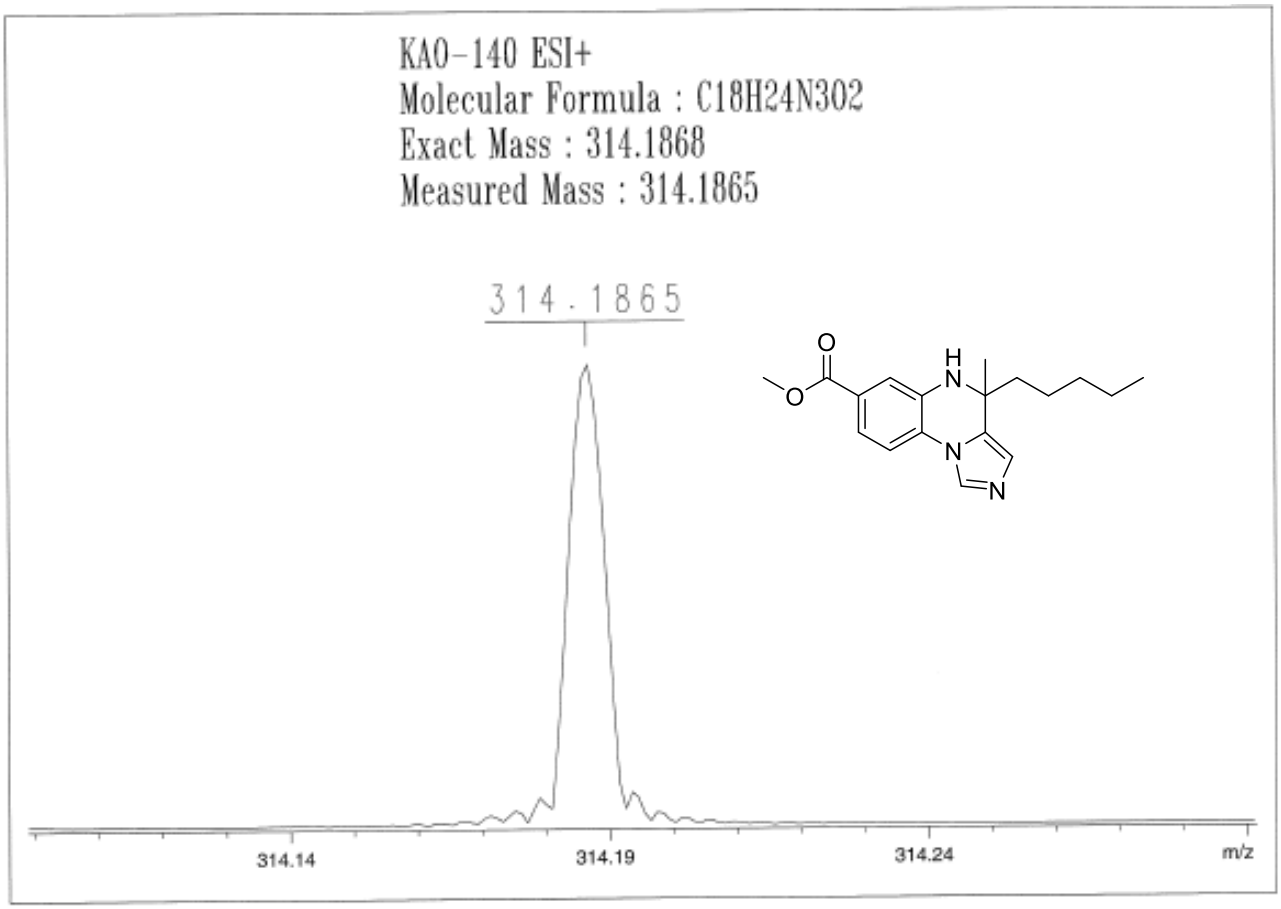
^{1}H NMR spectrum (300 MHz) of compound **12f** in $CDCl_3$



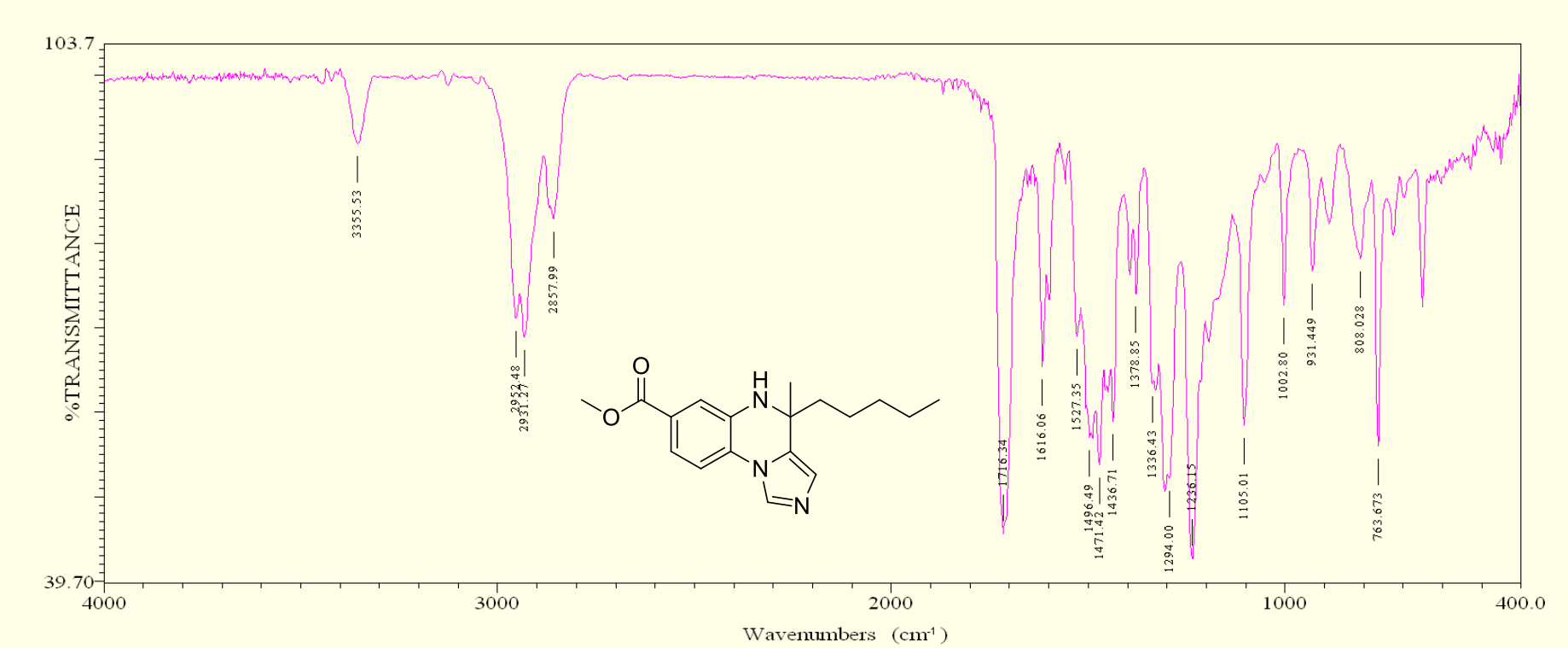
^{13}C NMR spectrum (75 MHz) of compound **12f** in $CDCl_3$



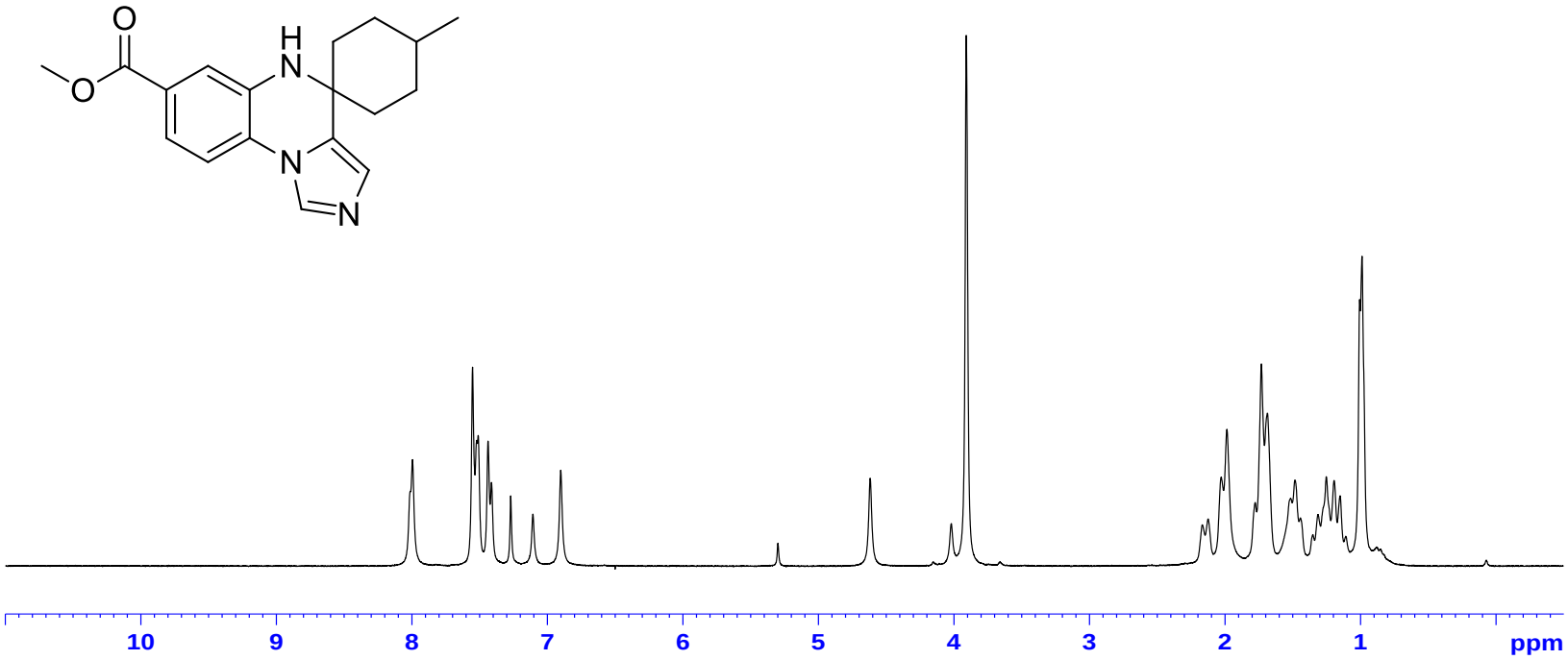
ESI-LRMS of compound **12f**



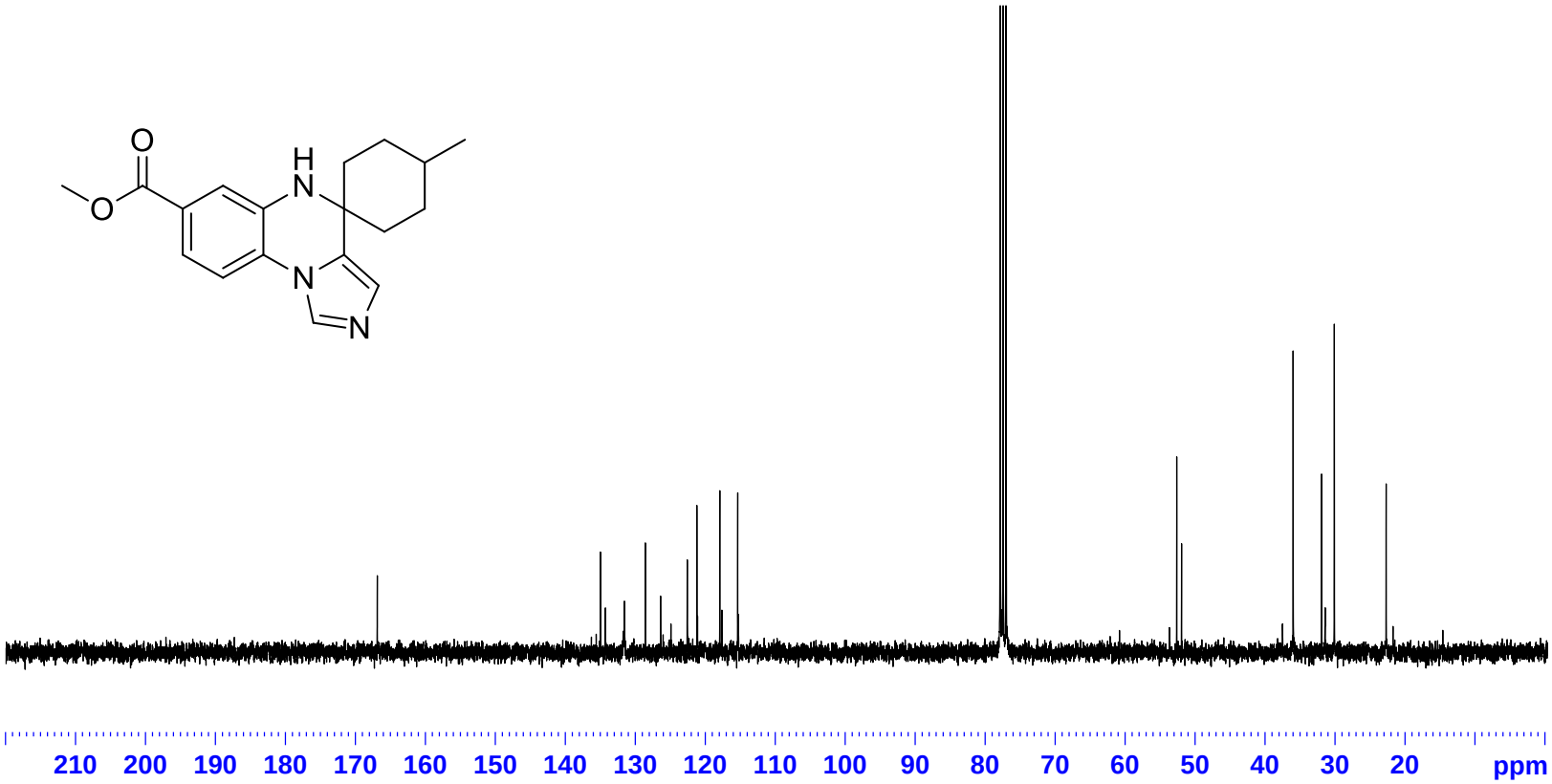
ESI-HRMS of compound **12f**



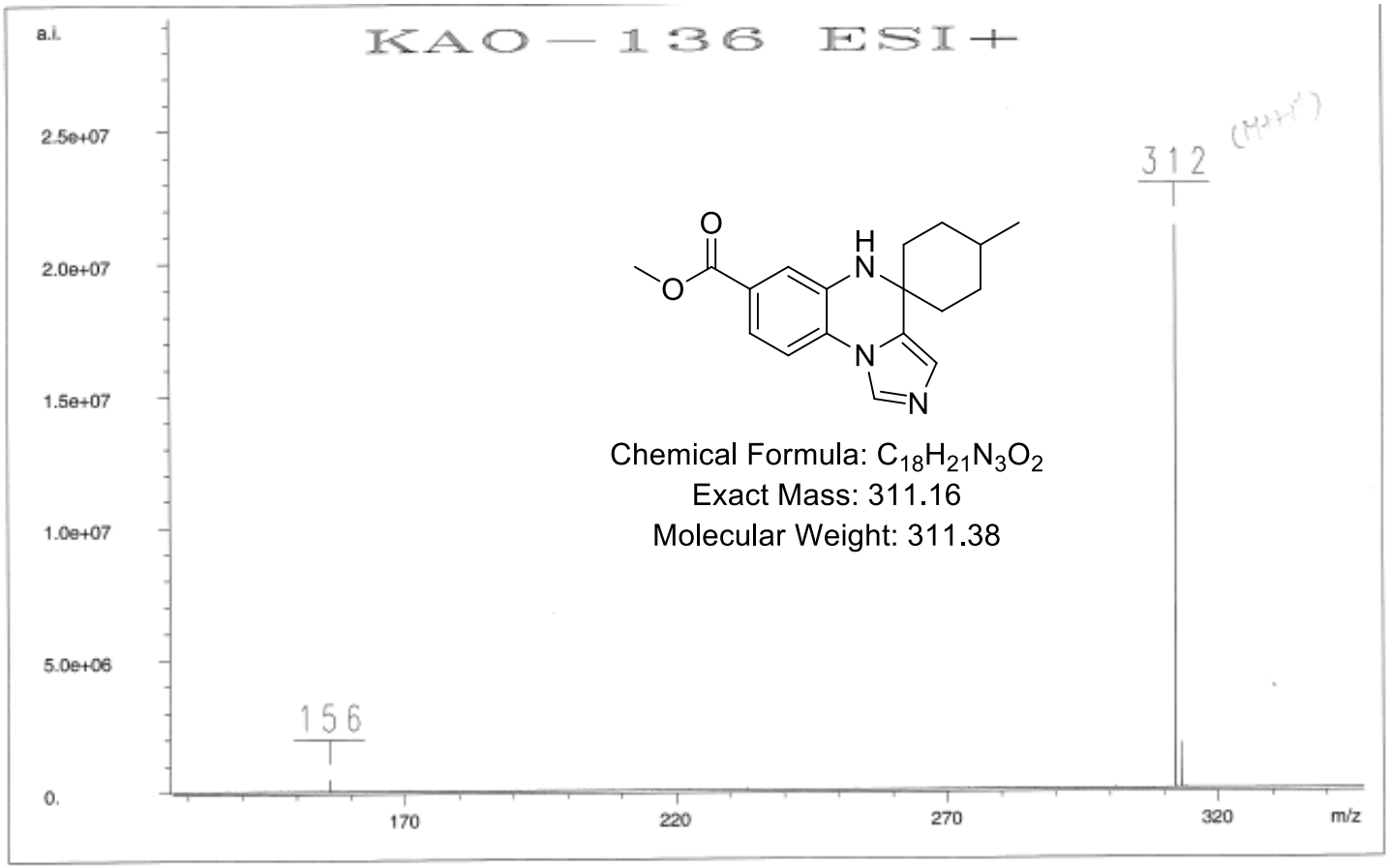
IR spectrum of compound **12f**



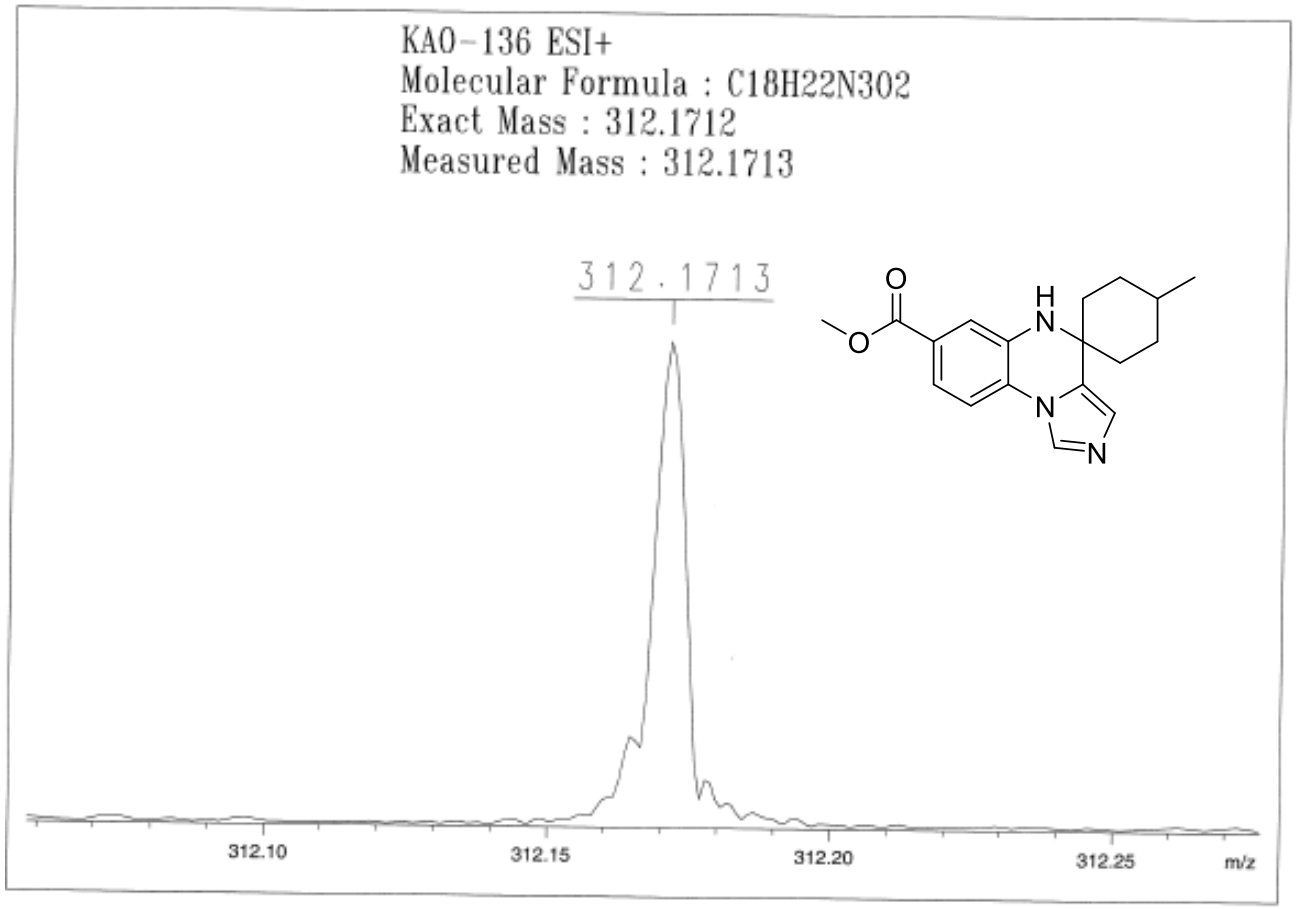
^{1}H NMR spectrum (300 MHz) of compound **12g** in $CDCl_3$



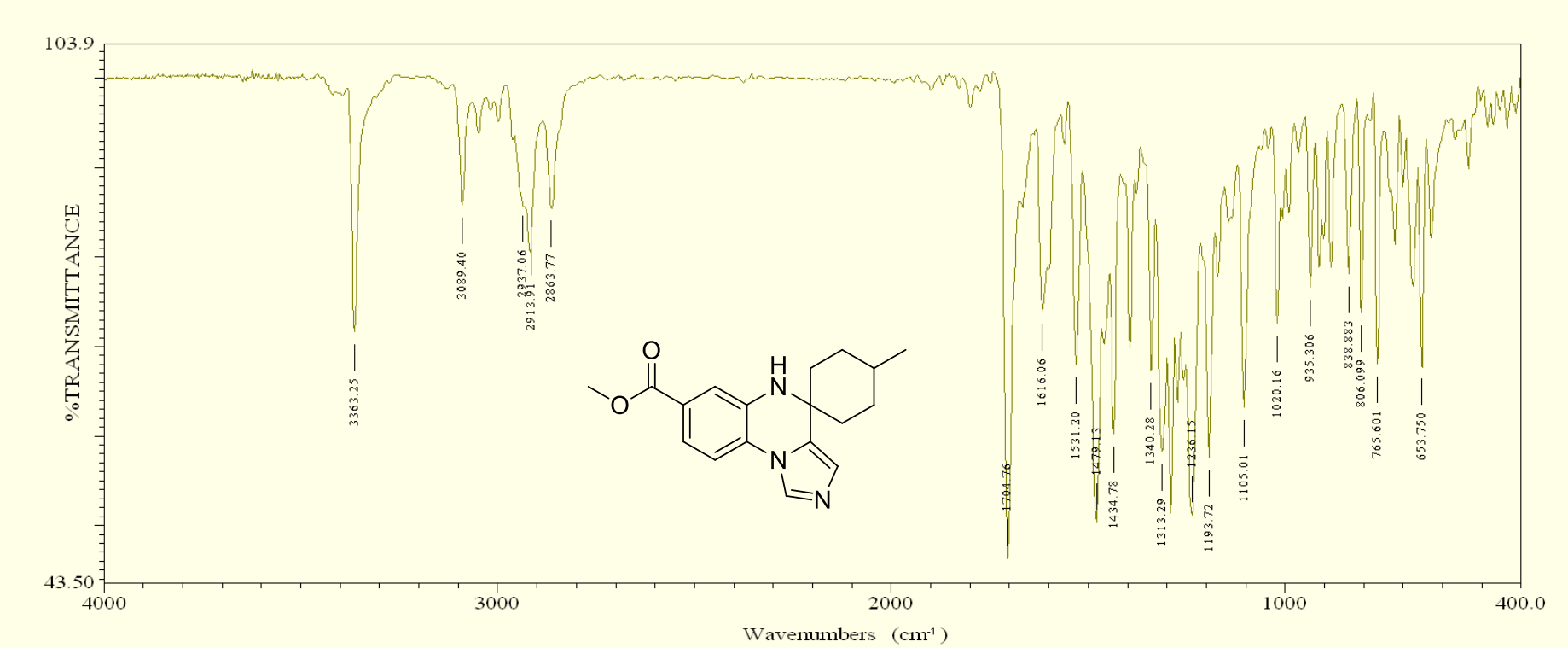
^{13}C NMR spectrum (75 MHz) of compound **12g** in $CDCl_3$



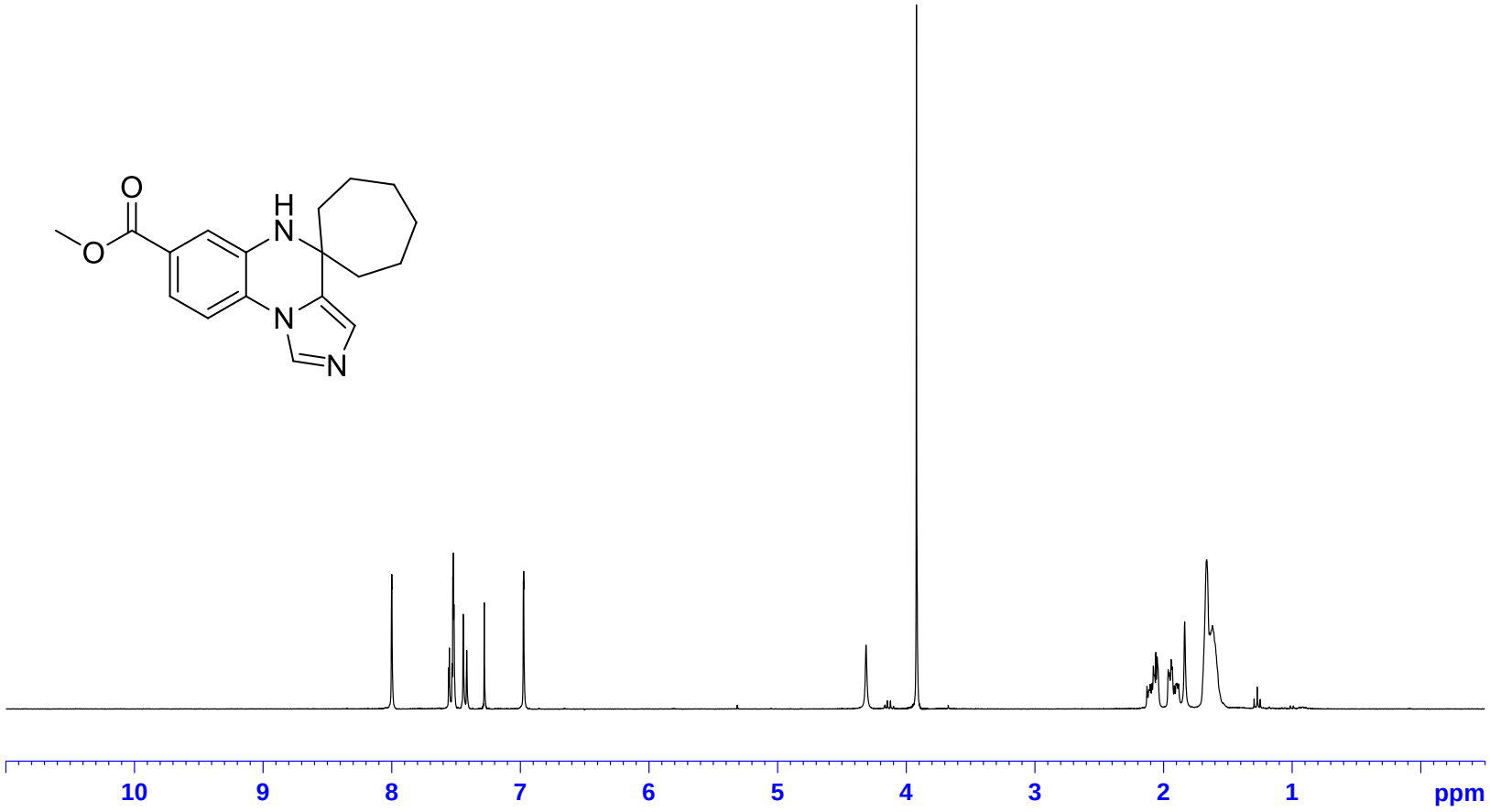
ESI-LRMS of compound **12g**



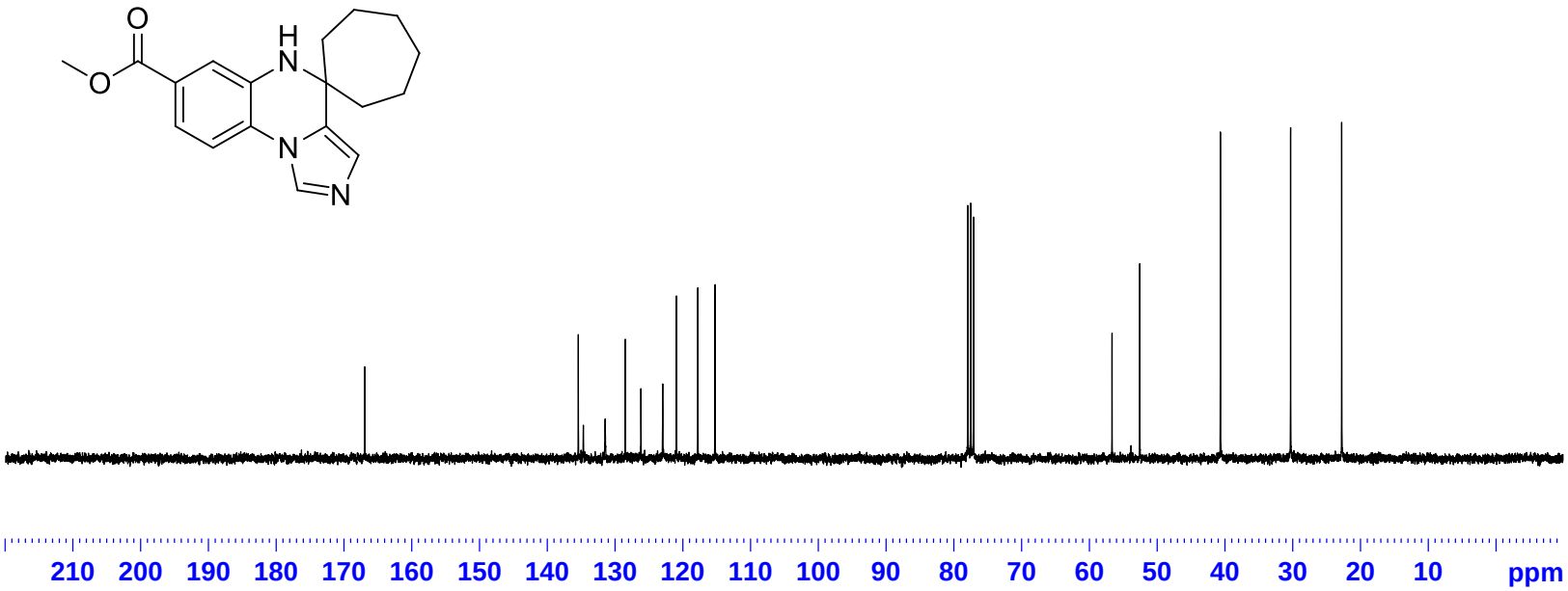
ESI-HRMS of compound **12g**



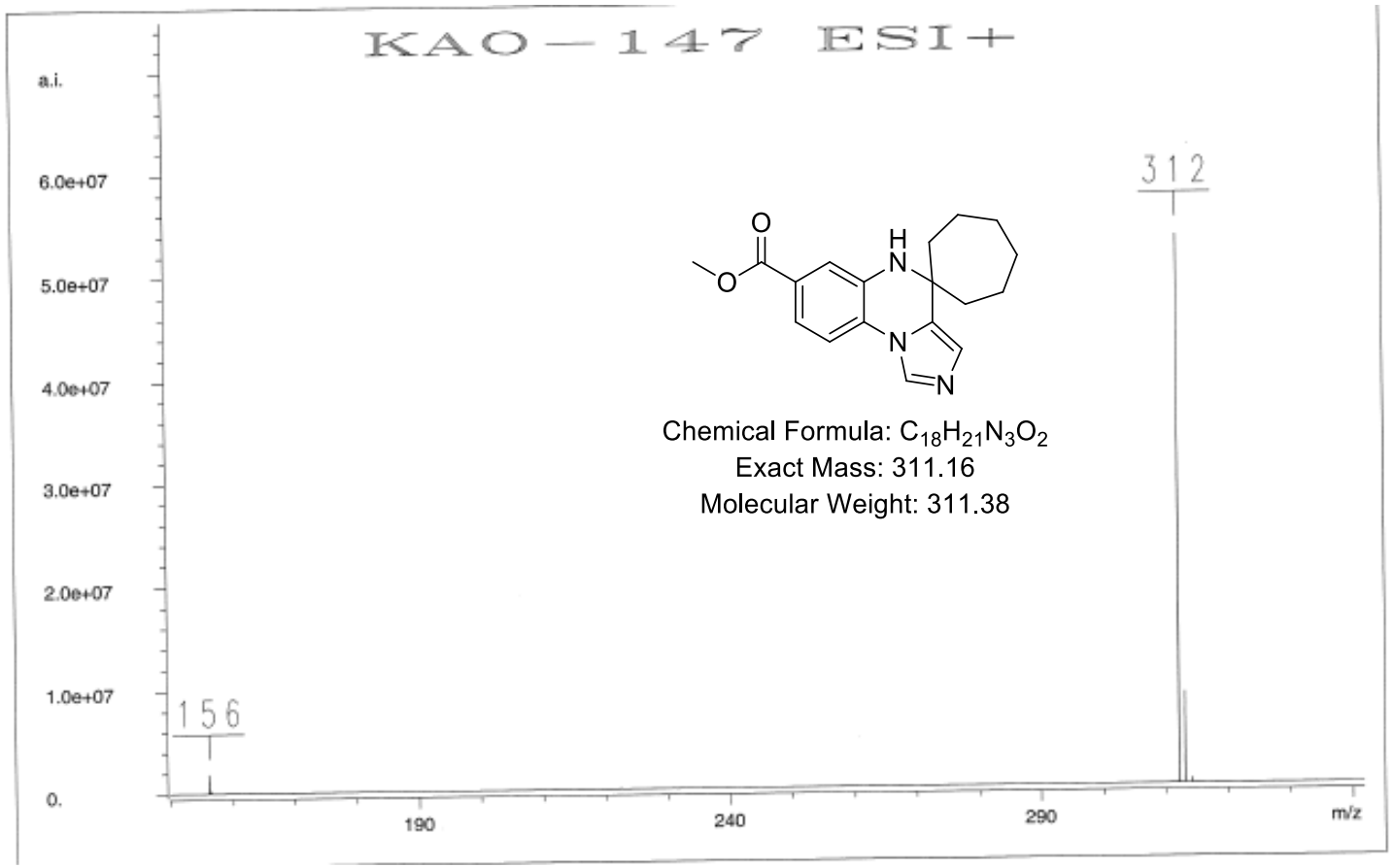
IR spectrum of compound **12g**



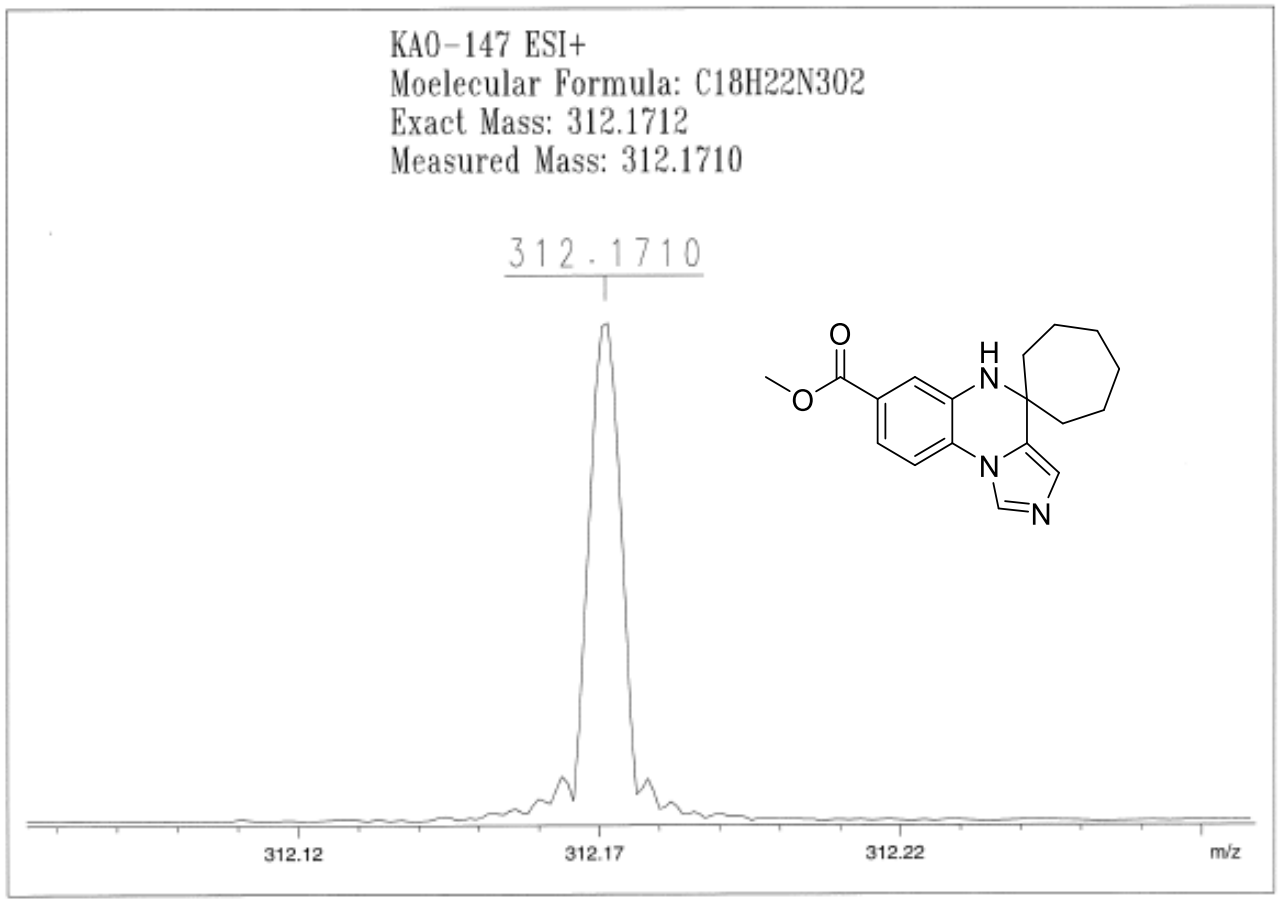
^{1}H NMR spectrum (300 MHz) of compound **12h** in $CDCl_3$



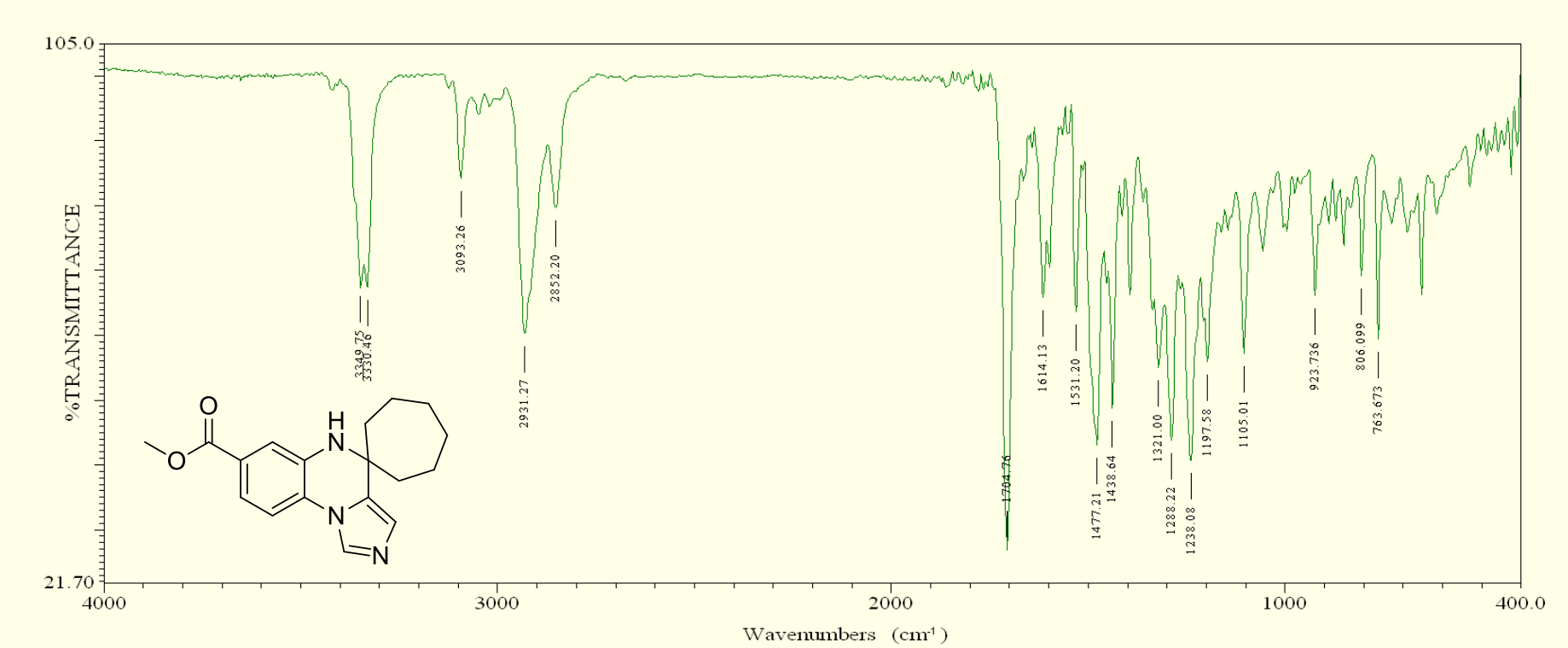
^{13}C NMR spectrum (75 MHz) of compound **12h** in $CDCl_3$



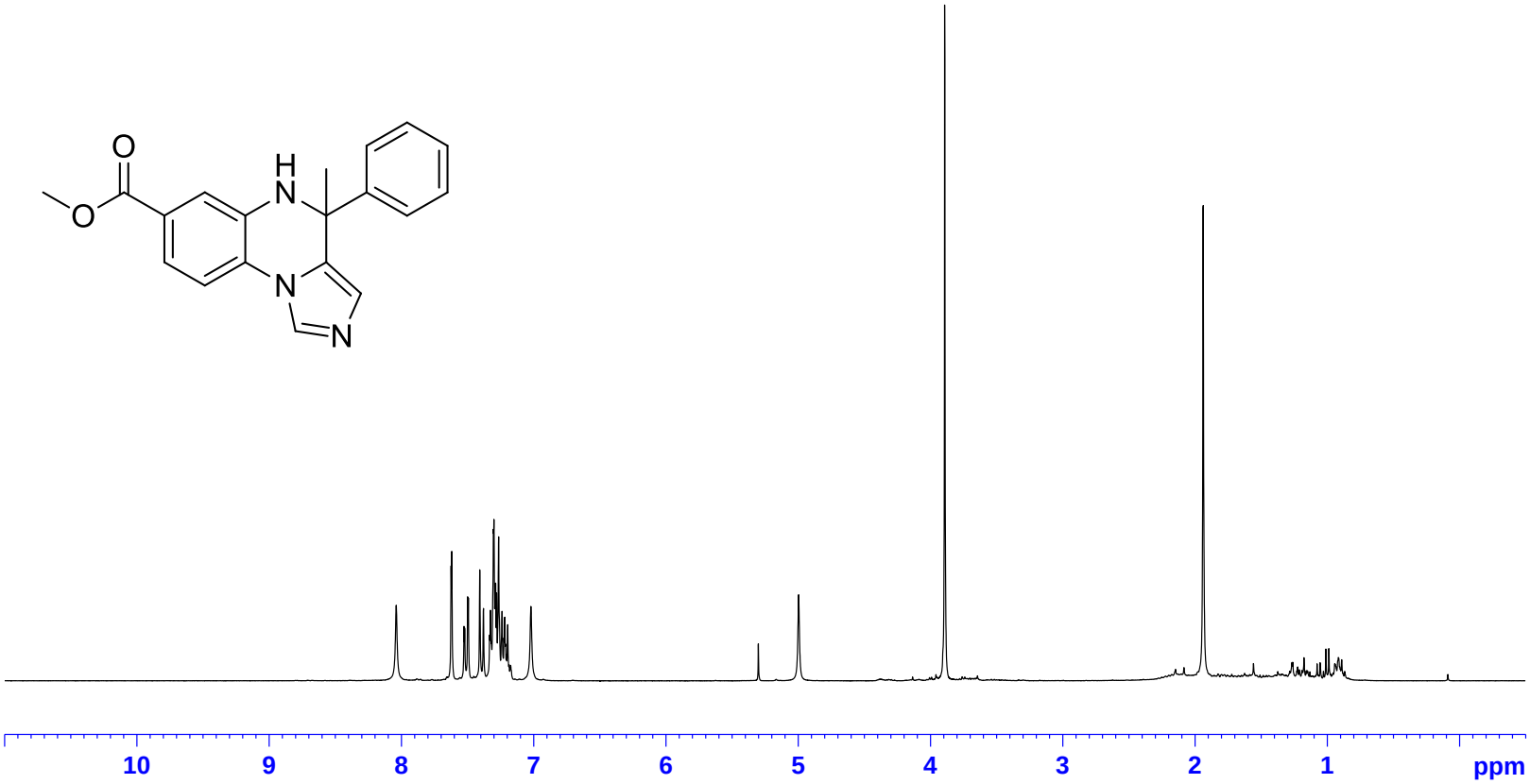
ESI-LRMS of compound **12h**



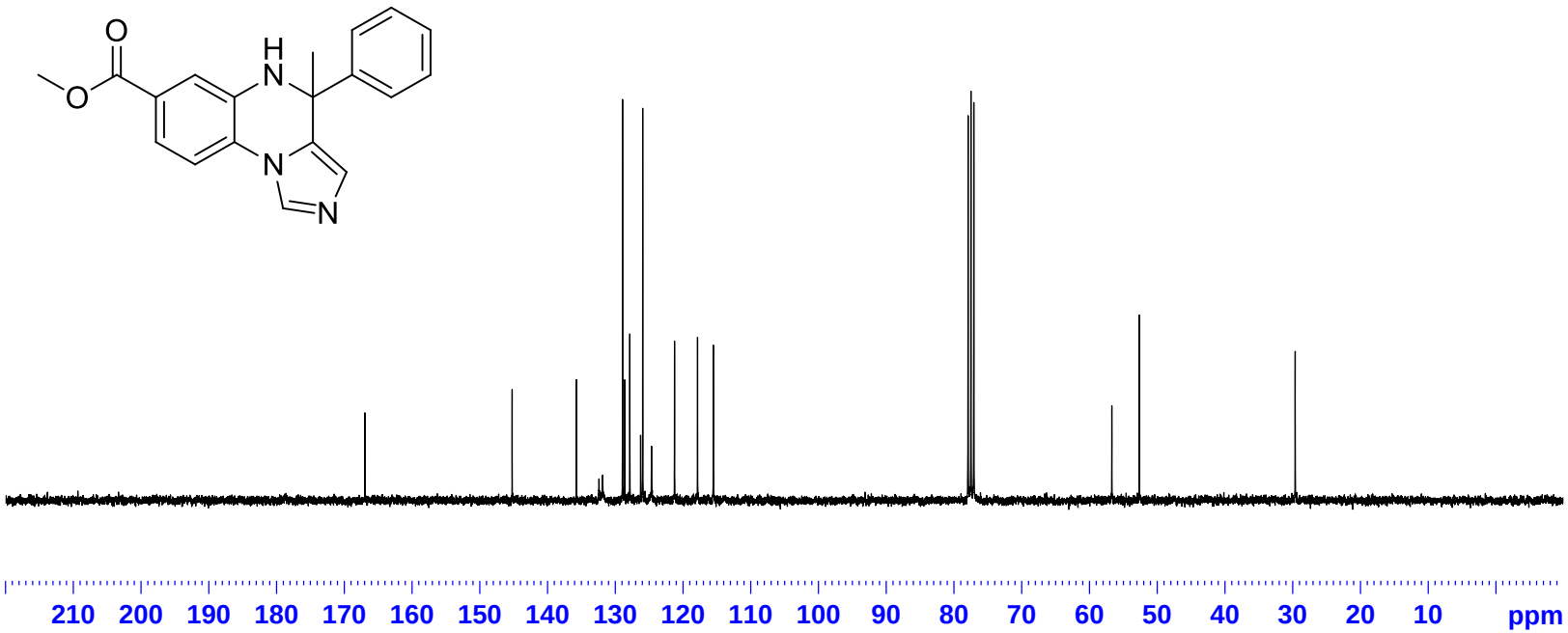
ESI-HRMS of compound **12h**



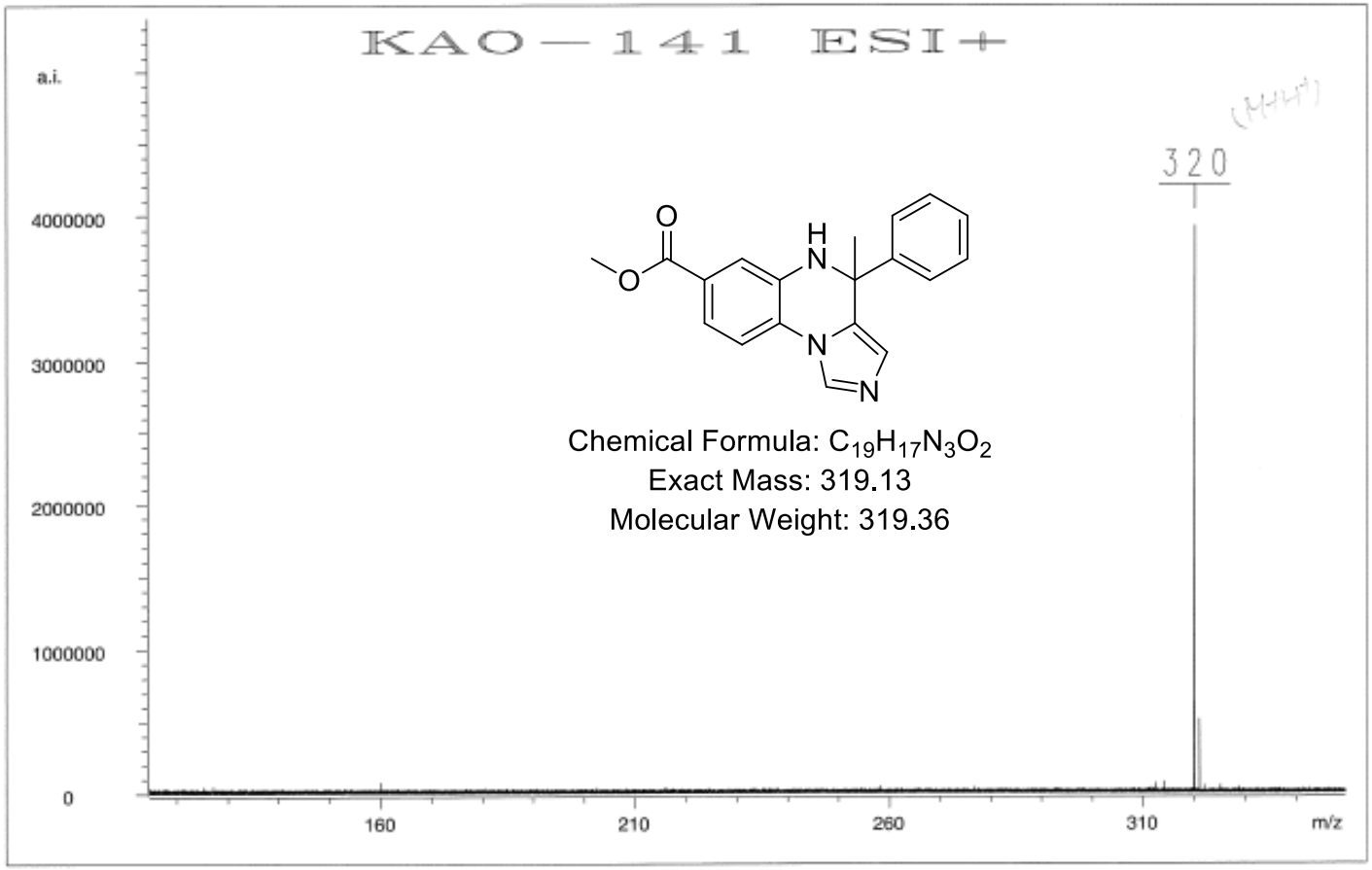
IR spectrum of compound **12h**



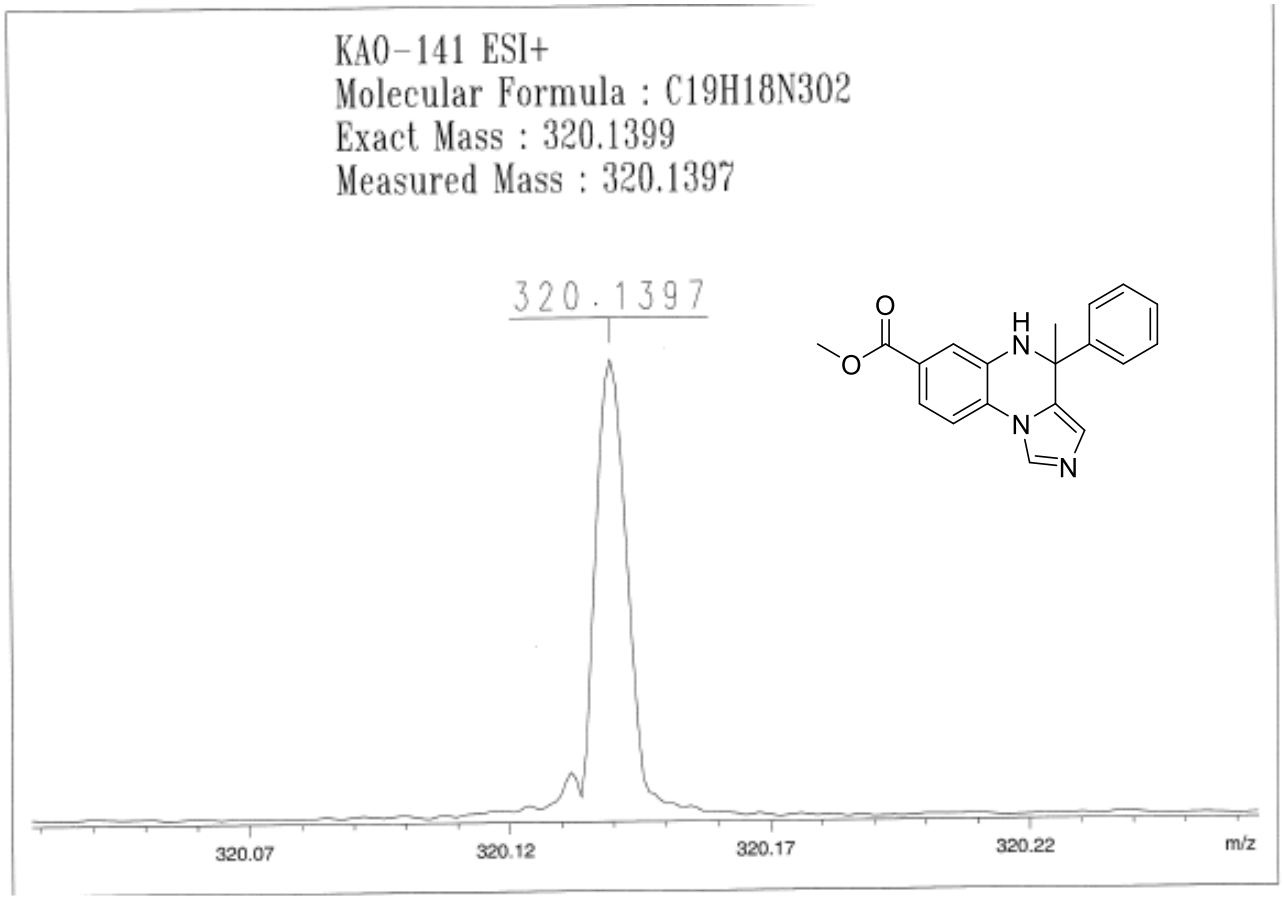
^{1}H NMR spectrum (300 MHz) of compound **12i** in $CDCl_3$



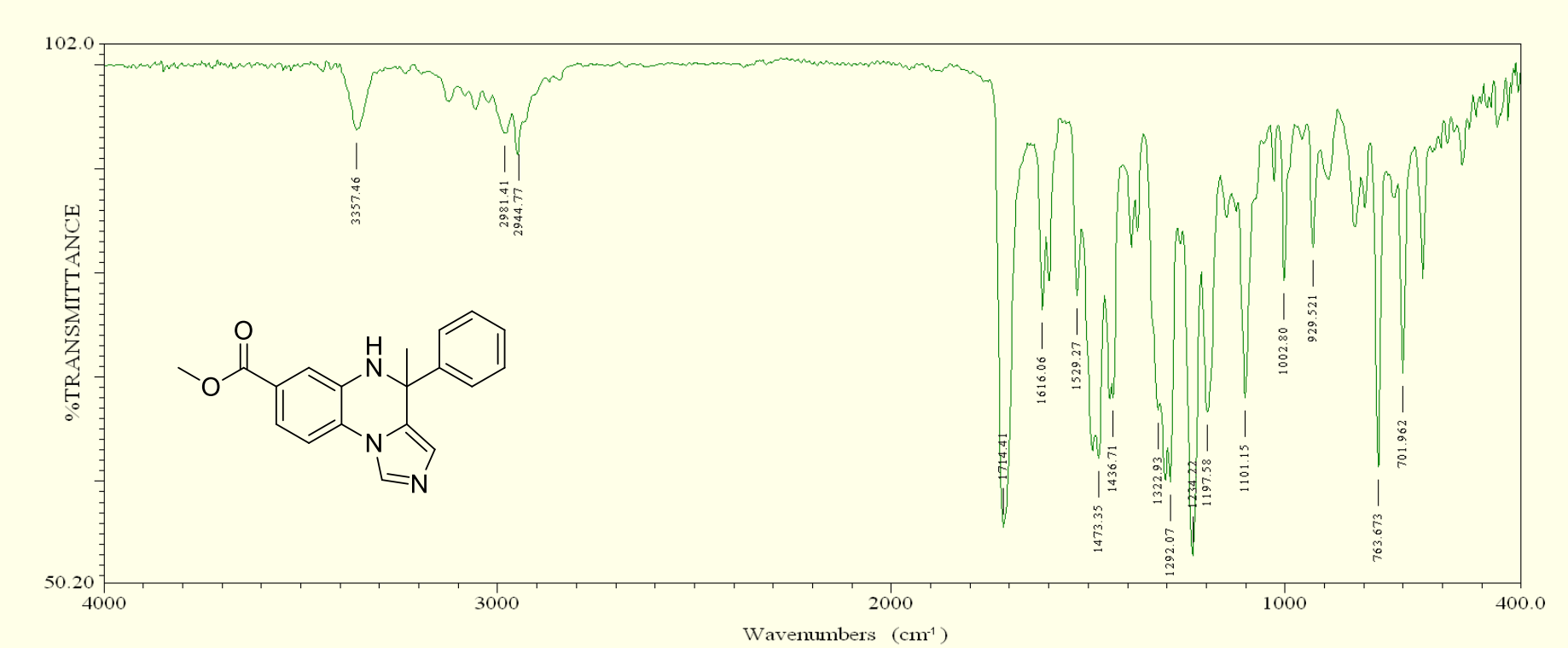
^{13}C NMR spectrum (75 MHz) of compound **12i** in $CDCl_3$



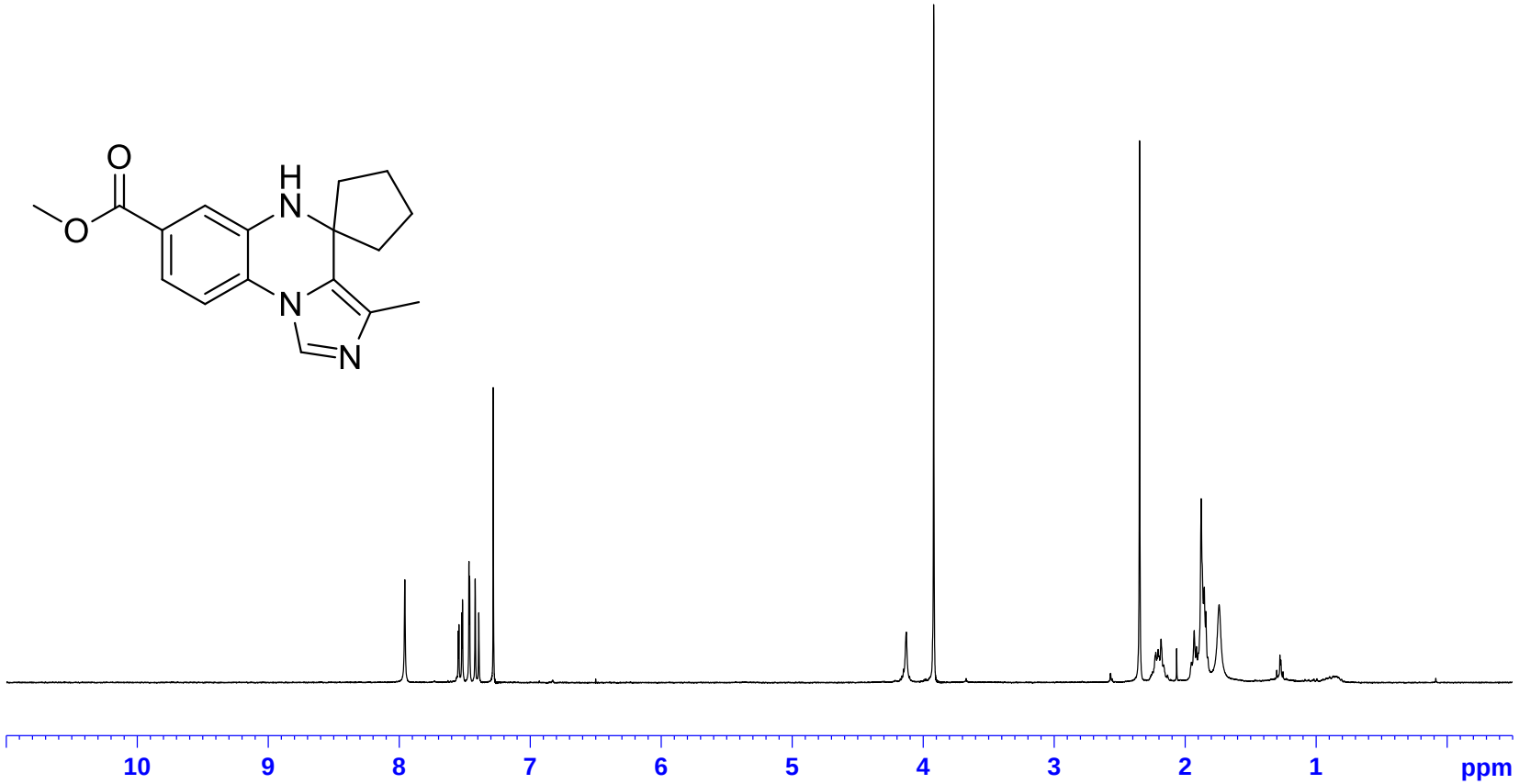
ESI-LRMS of compound **12i**



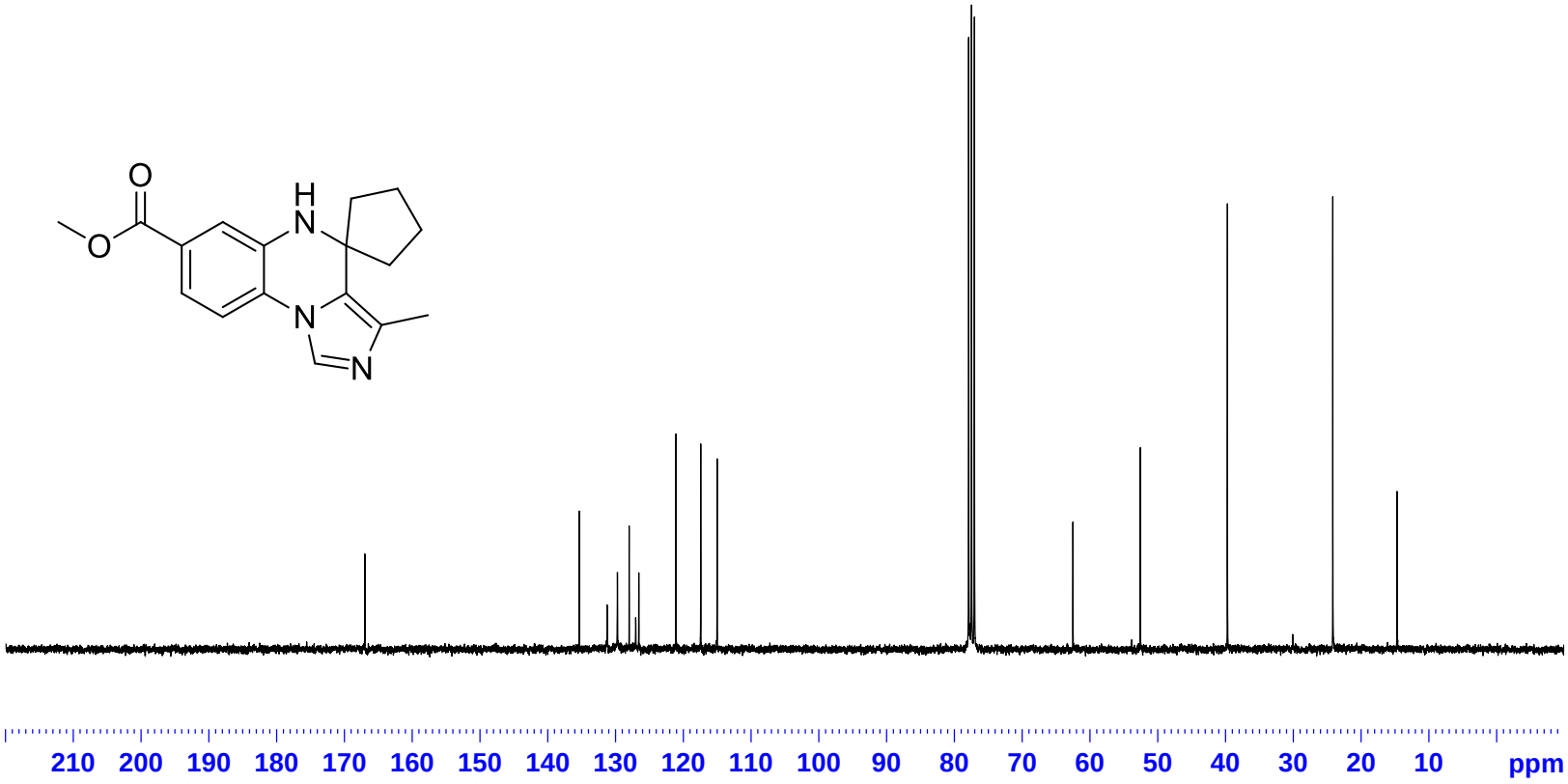
ESI-HRMS of compound **12i**



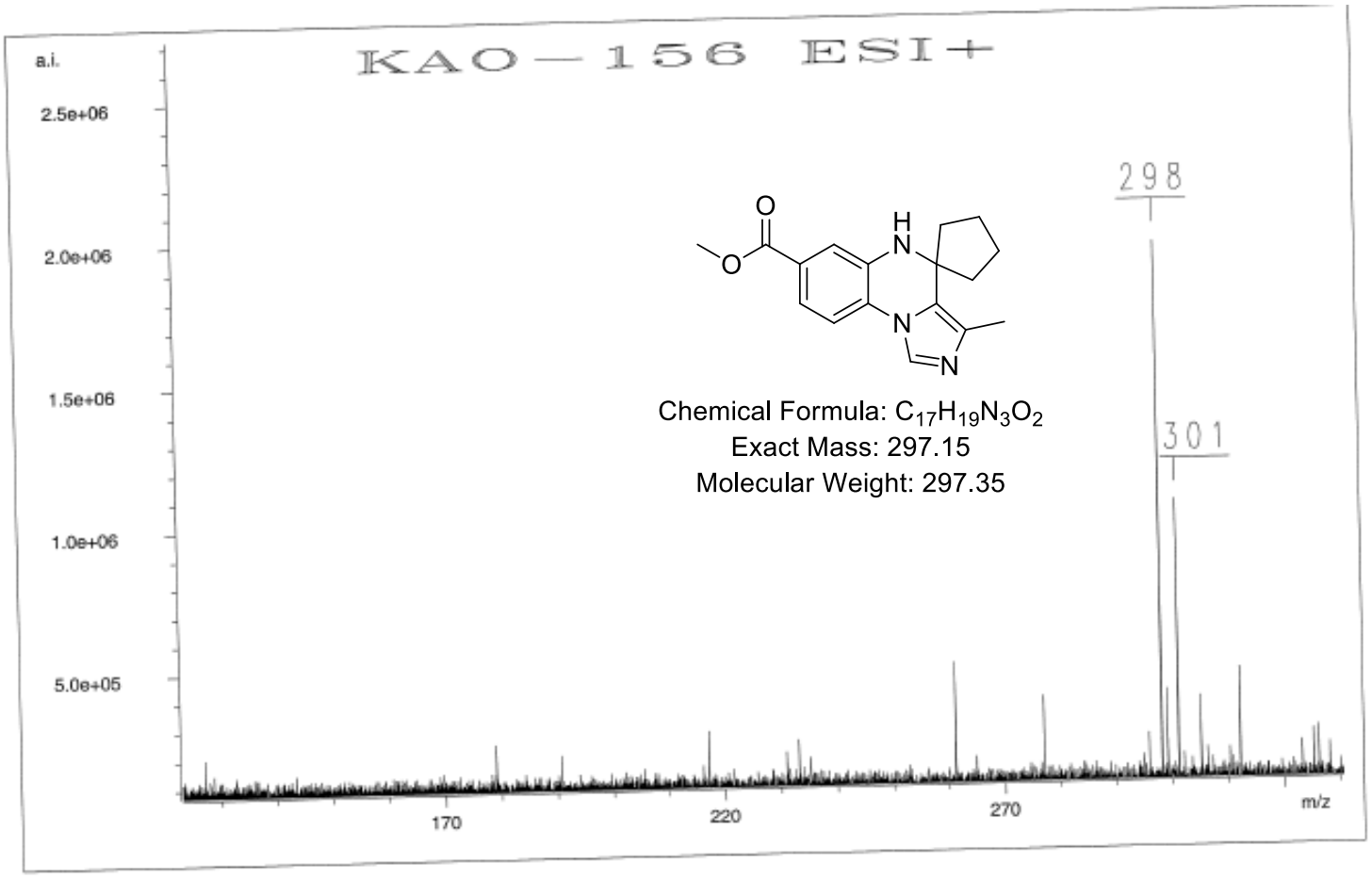
IR spectrum of compound **12i**



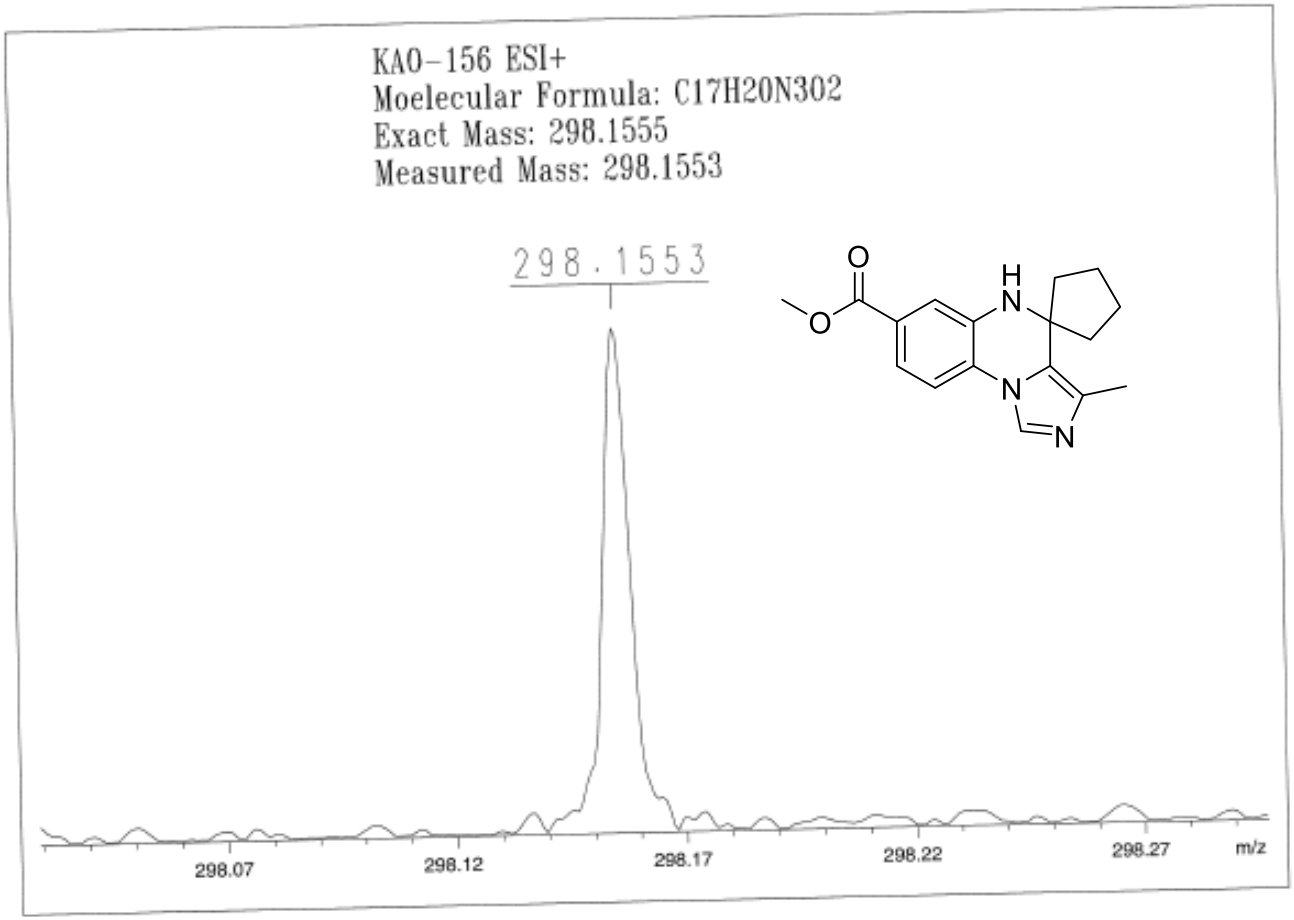
^{1}H NMR spectrum (300 MHz) of compound **12j** in $CDCl_3$



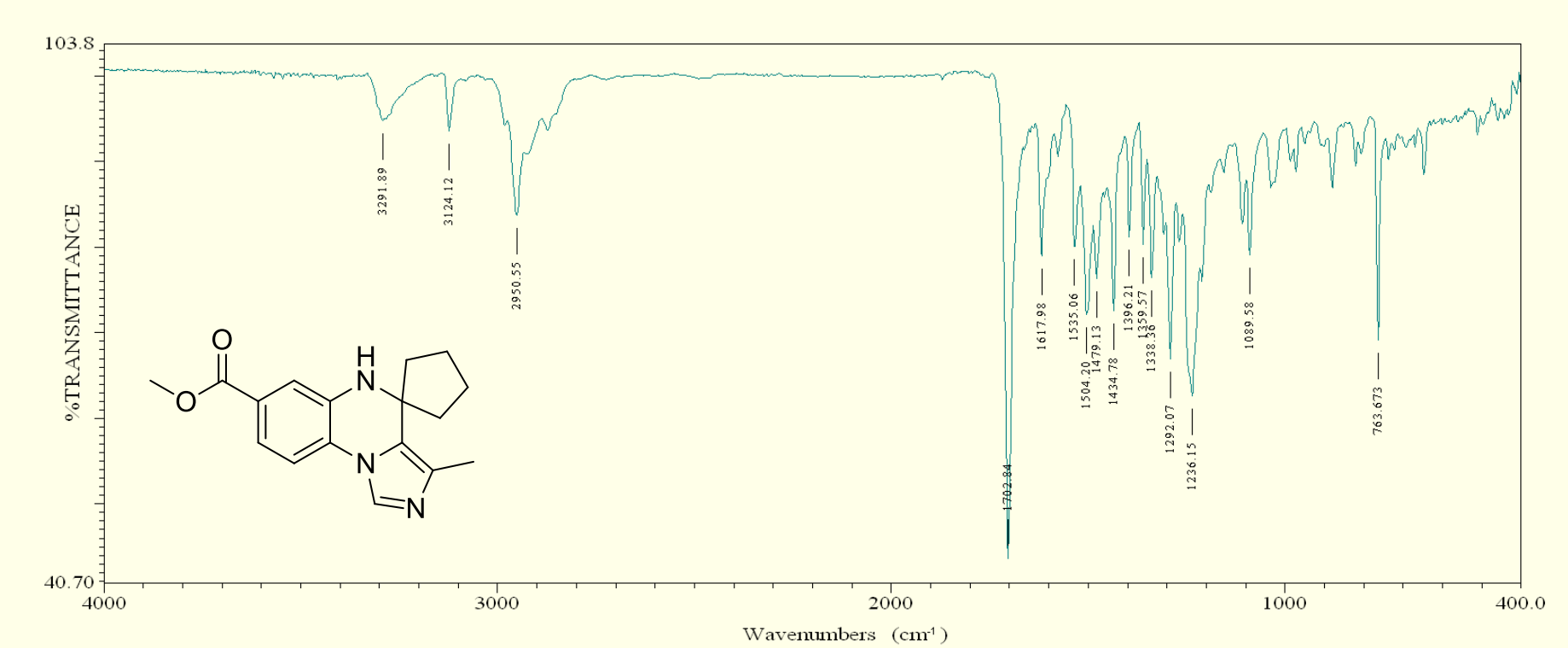
^{13}C NMR spectrum (75 MHz) of compound **12j** in $CDCl_3$



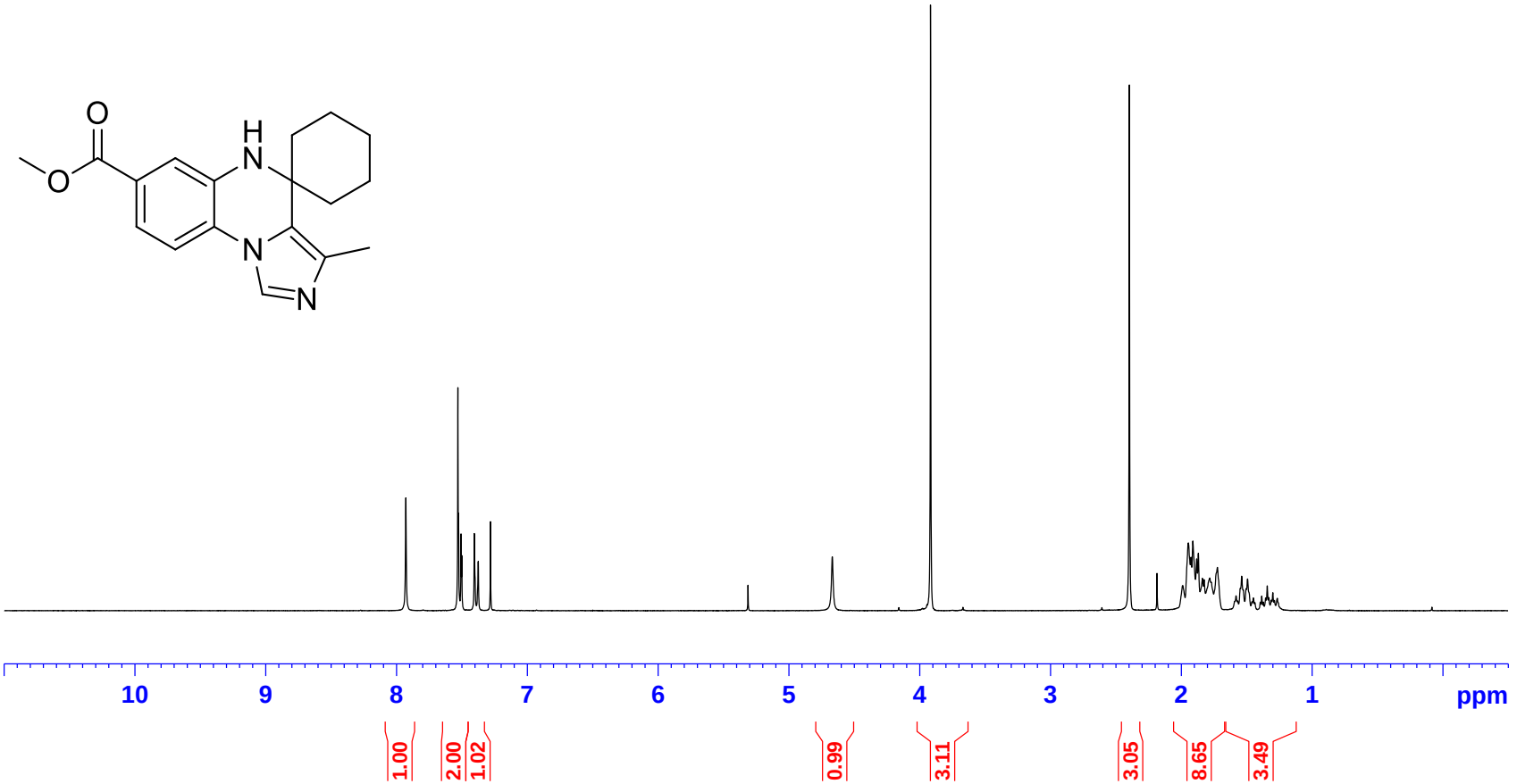
ESI-LRMS of compound **12j**



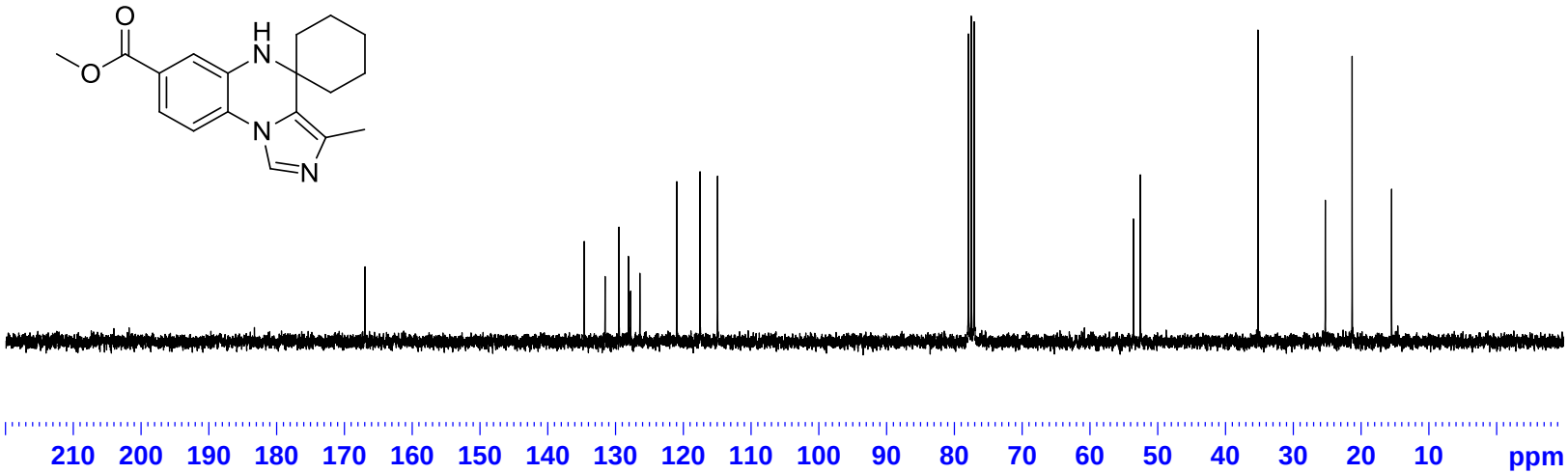
ESI-HRMS of compound **12j**



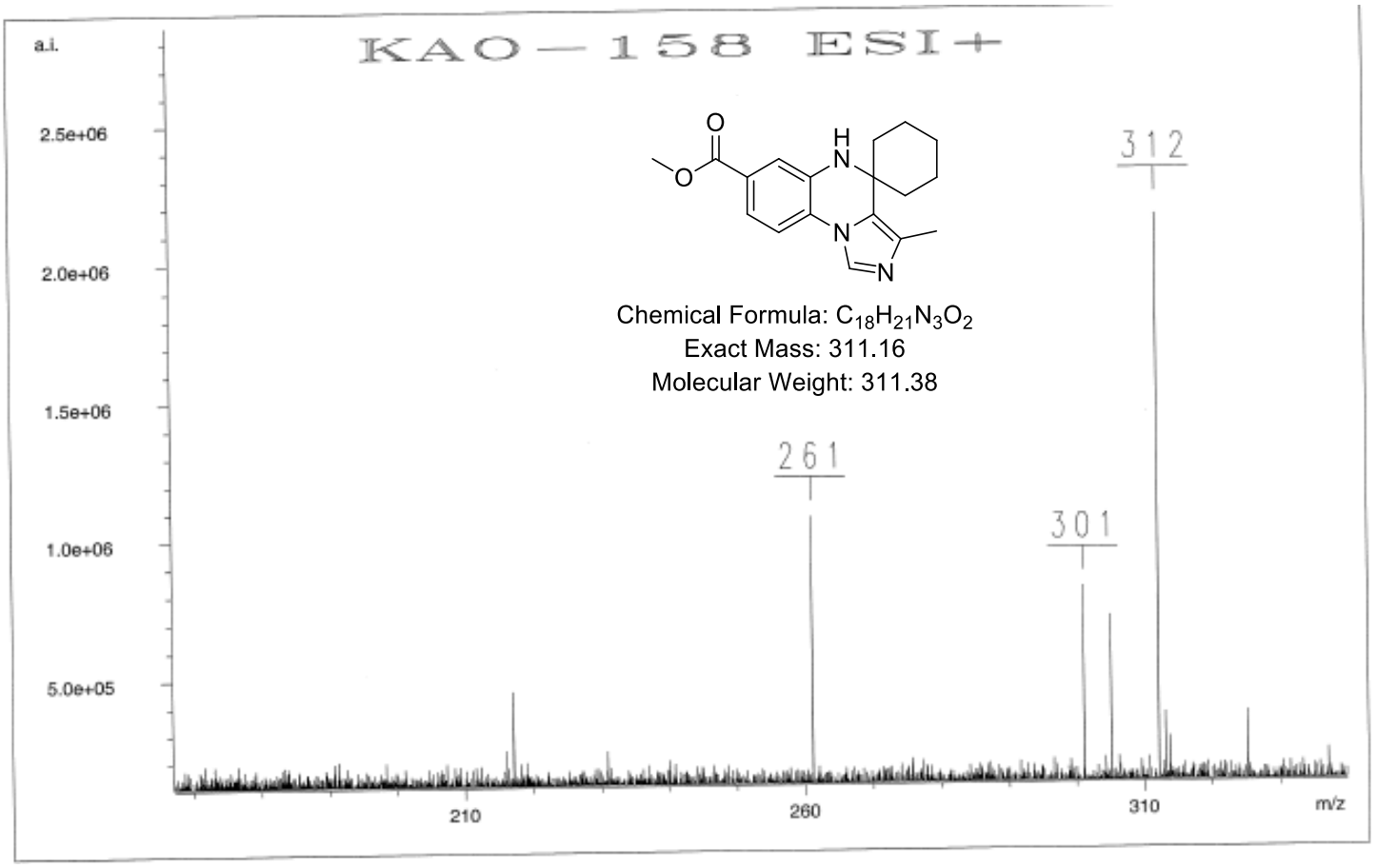
IR spectrum of compound **12j**



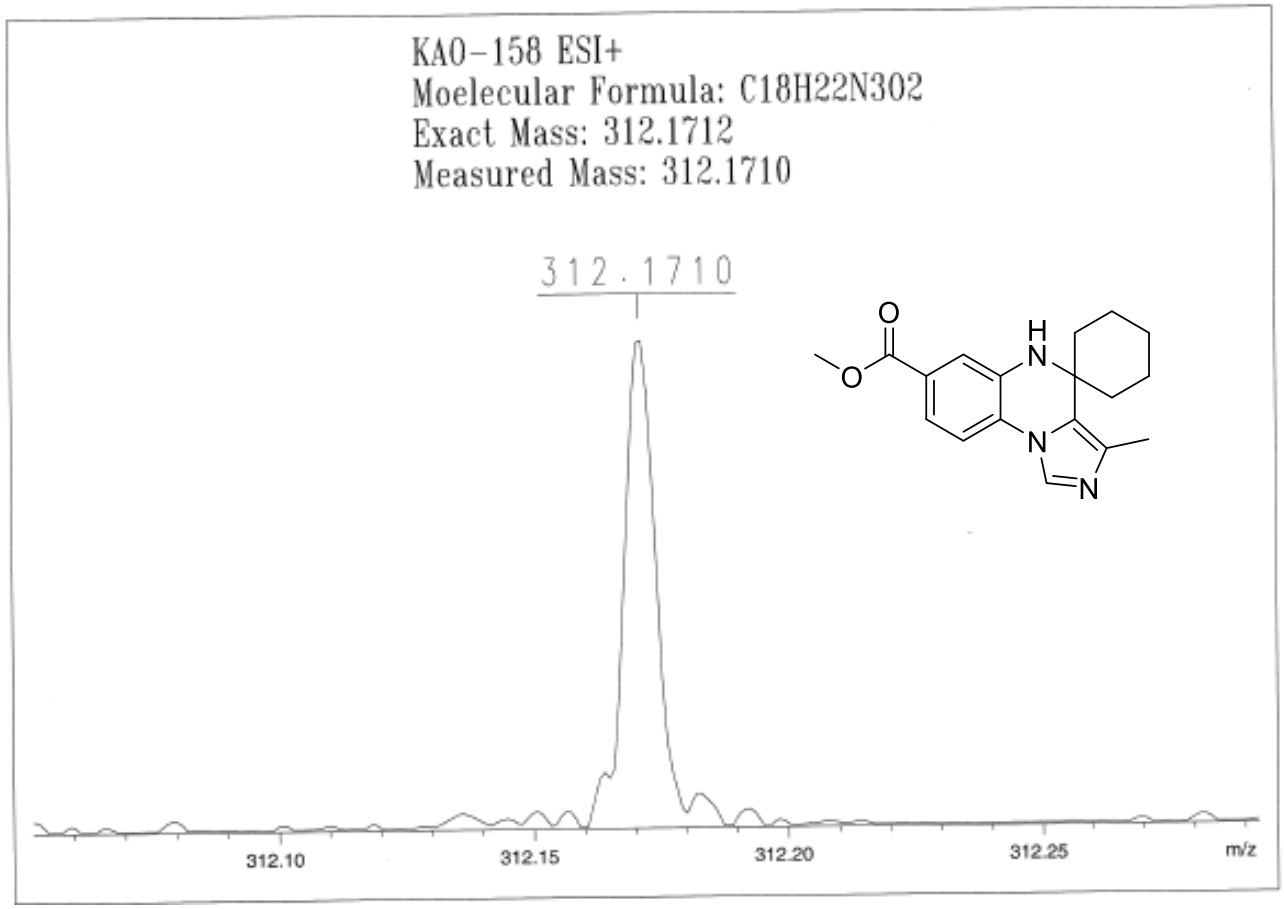
^{1}H NMR spectrum (300 MHz) of compound **12k** in $CDCl_3$



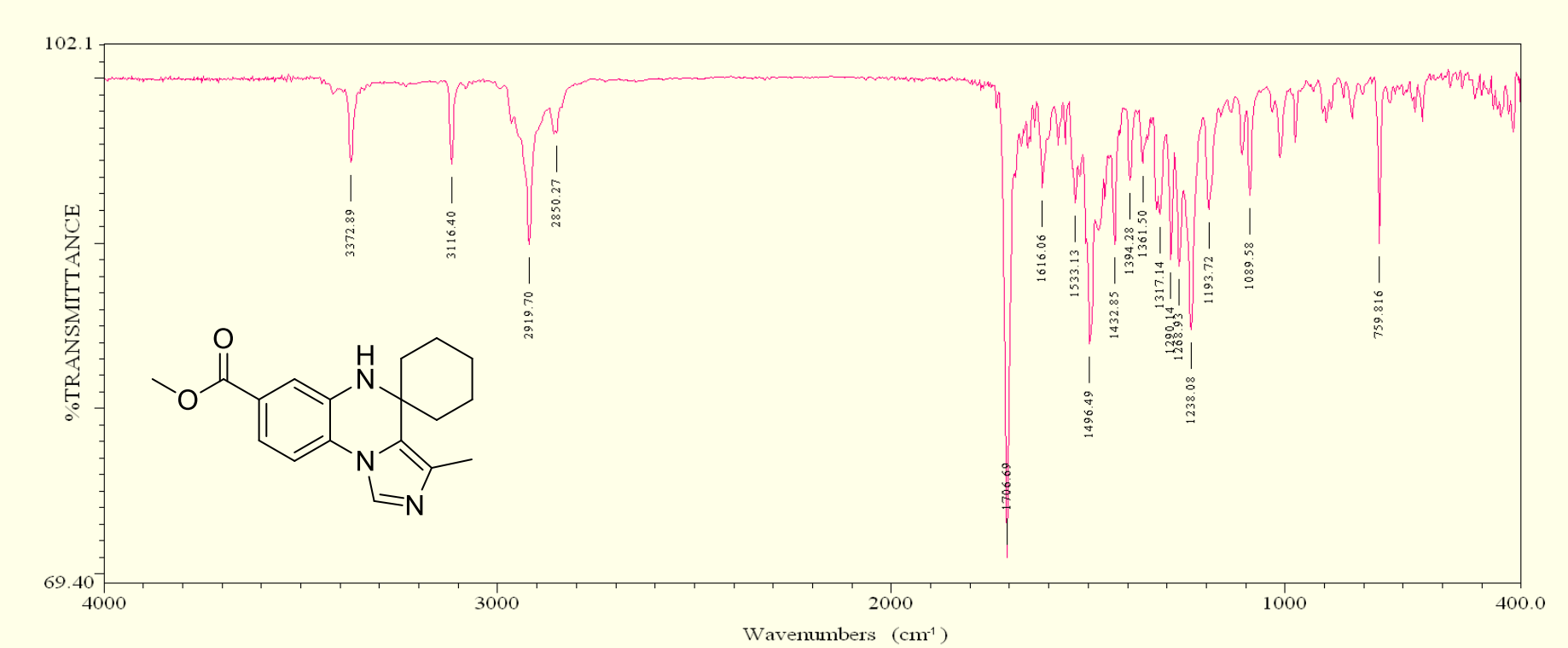
^{13}C NMR spectrum (75 MHz) of compound **12k** in $CDCl_3$



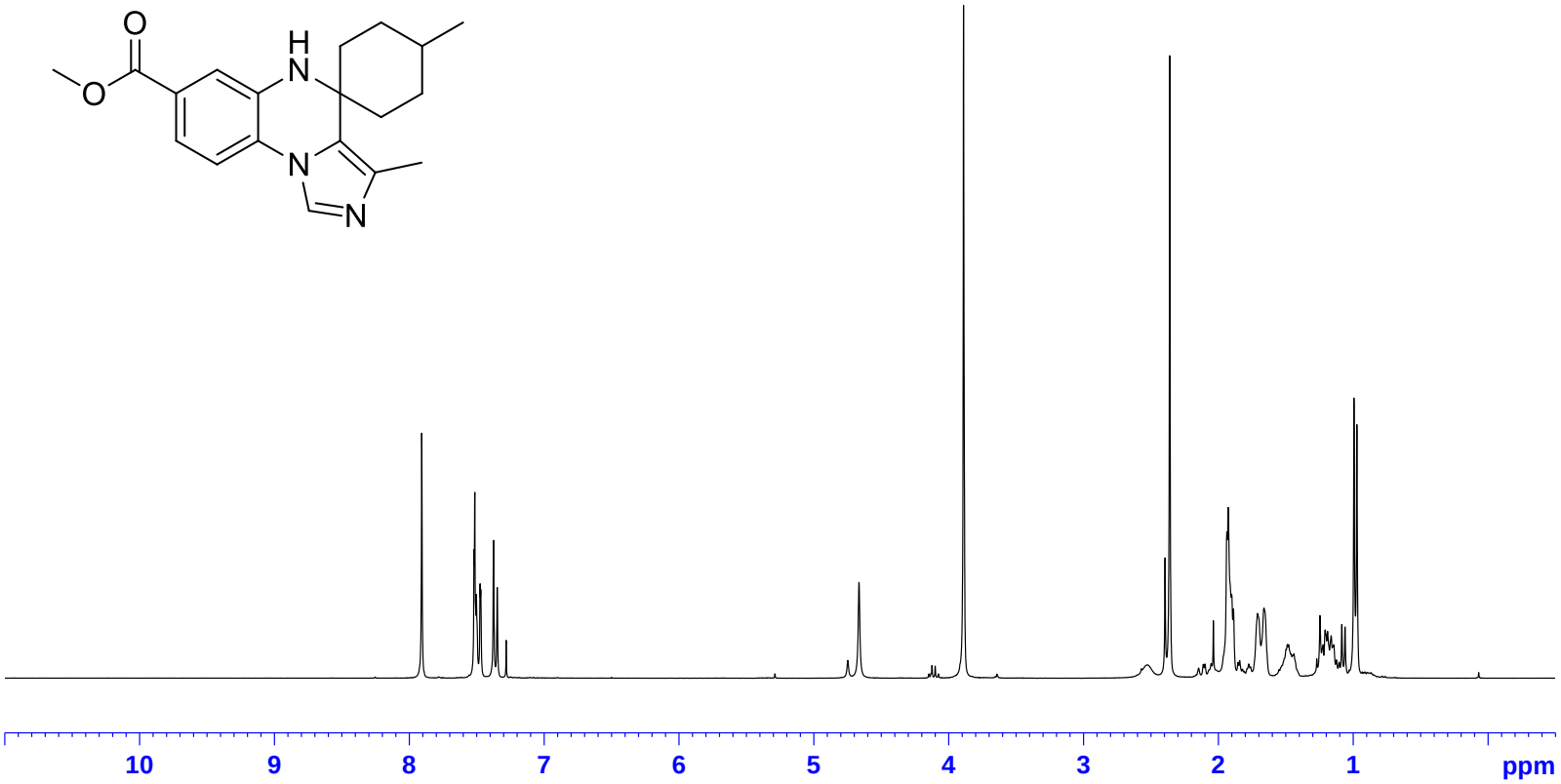
ESI-LRMS of compound **12k**



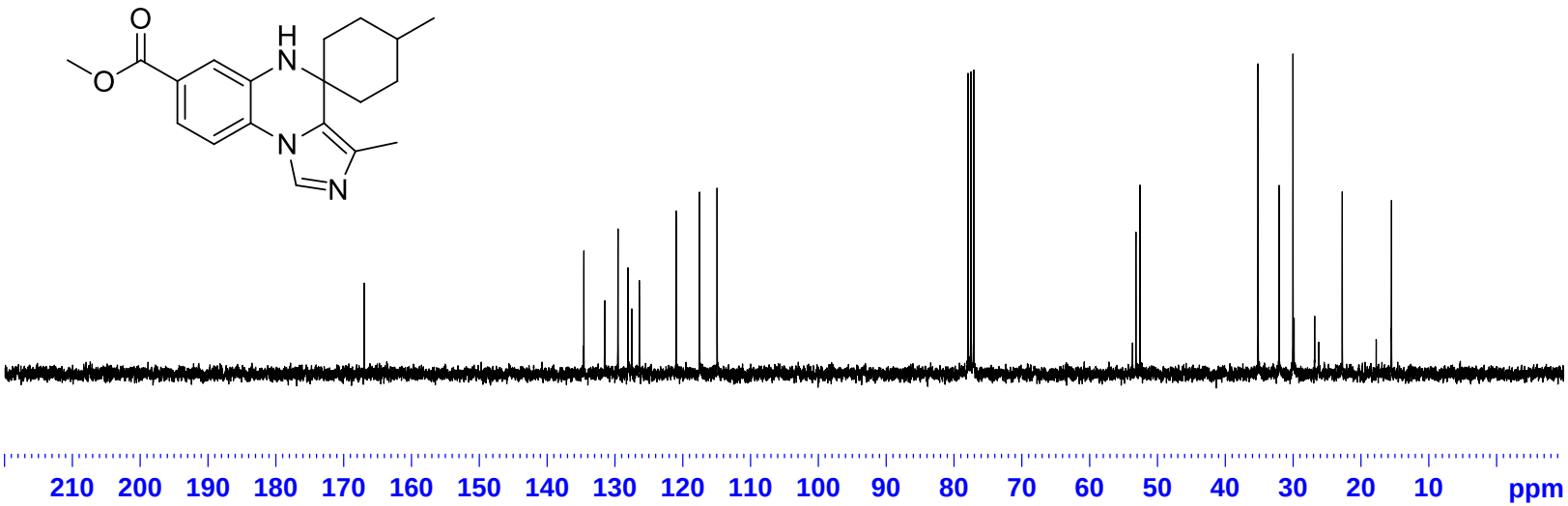
ESI-HRMS of compound **12k**



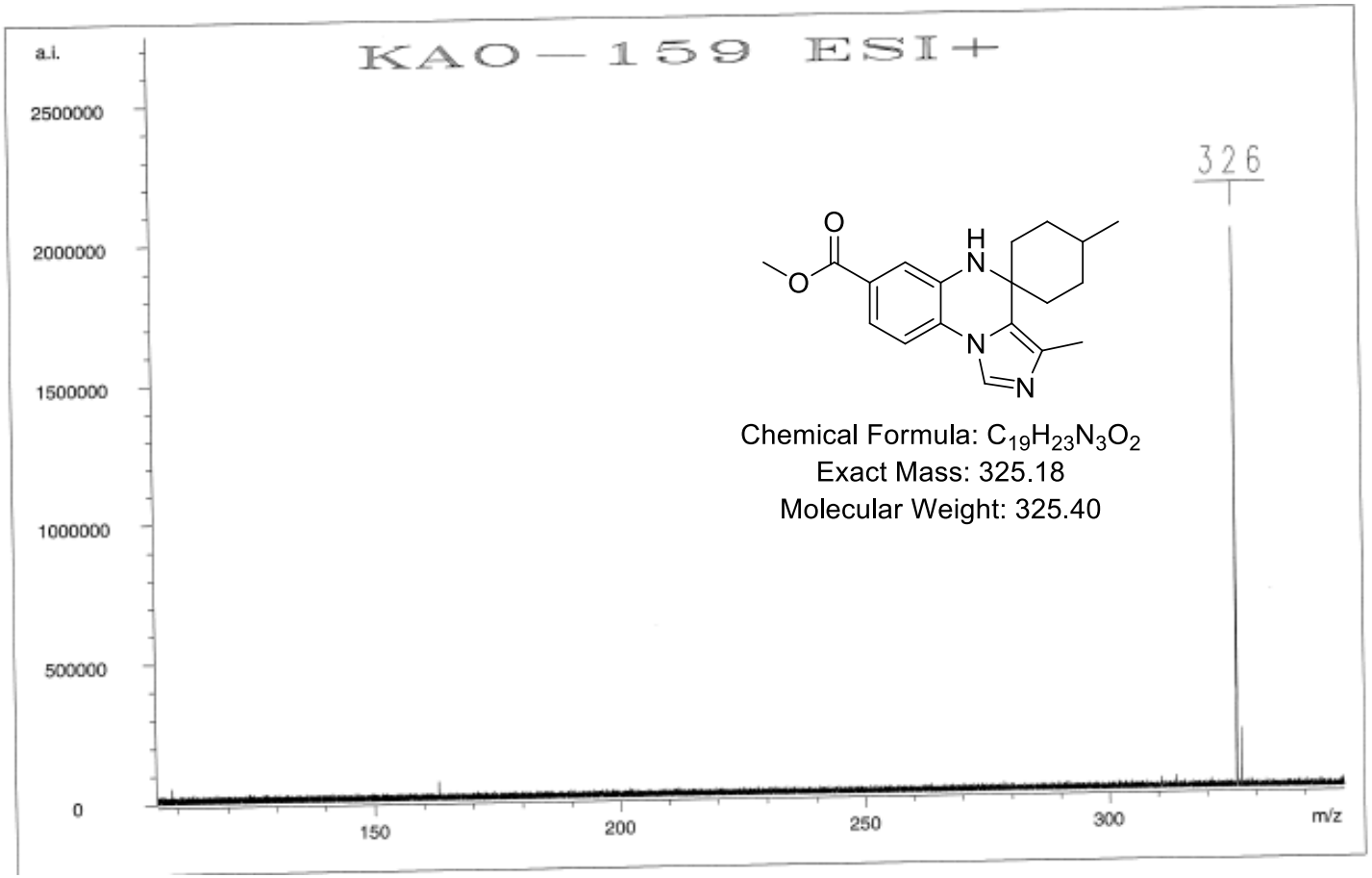
IR spectrum of compound **12k**



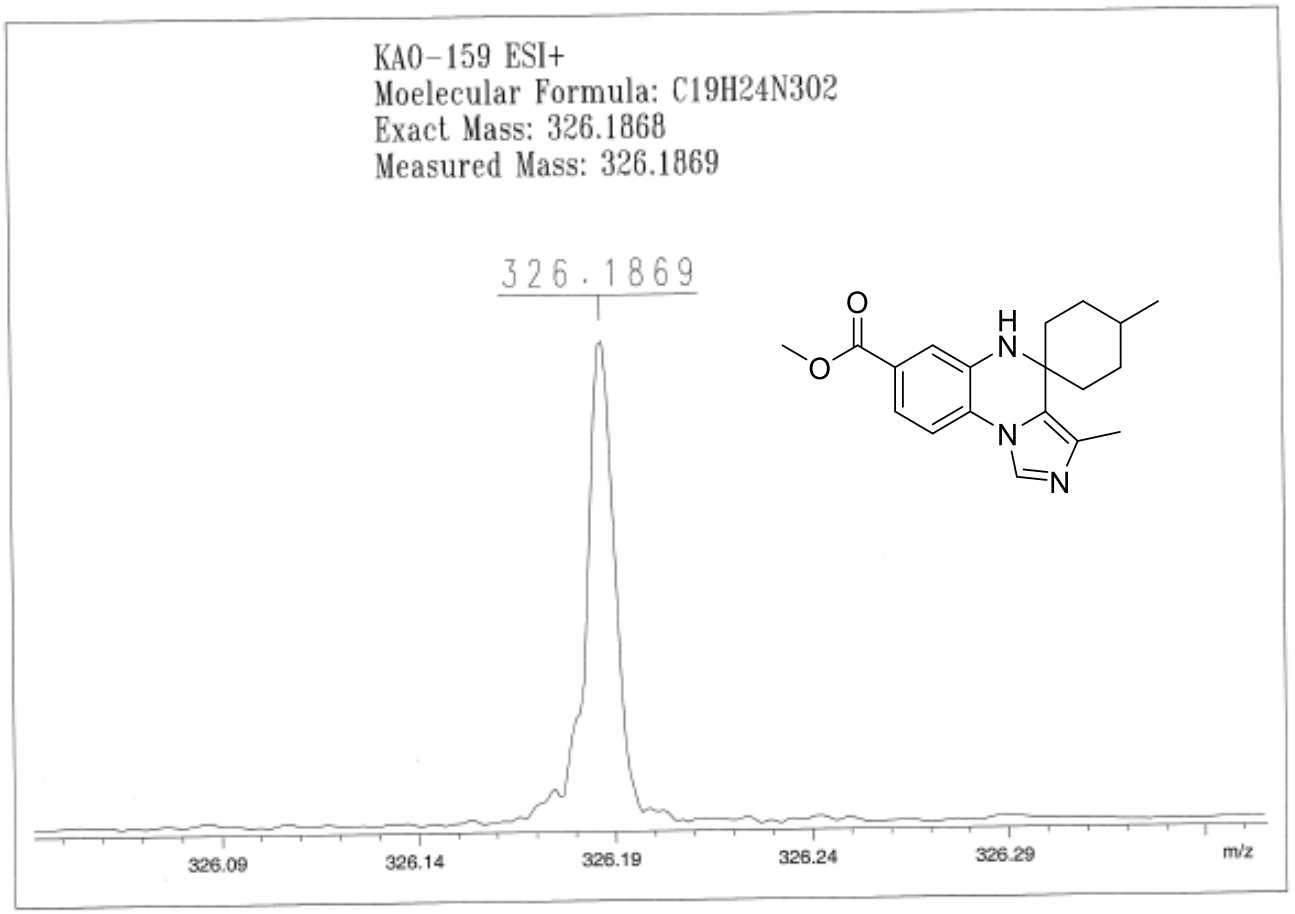
^{1}H NMR spectrum (300 MHz) of compound **12l** in $CDCl_3$



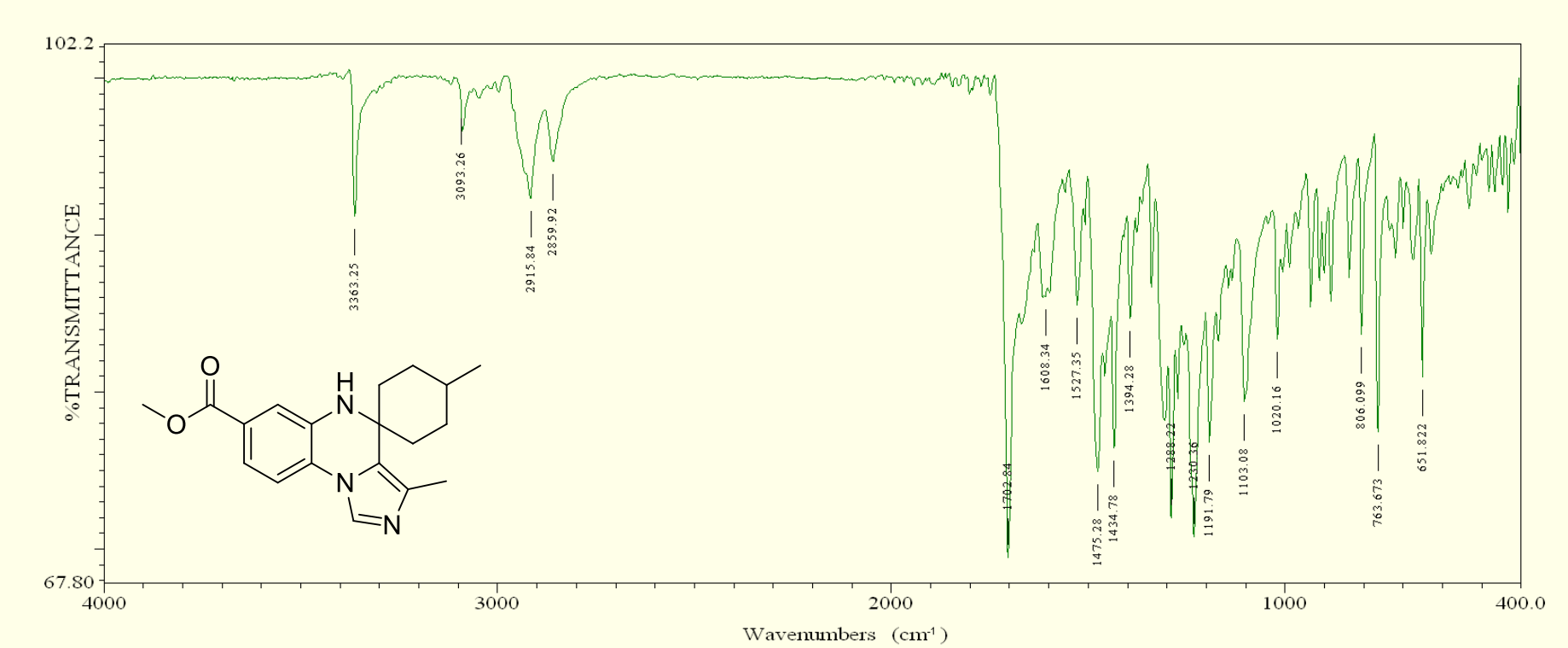
^{13}C NMR spectrum (75 MHz) of compound **12l** in $CDCl_3$



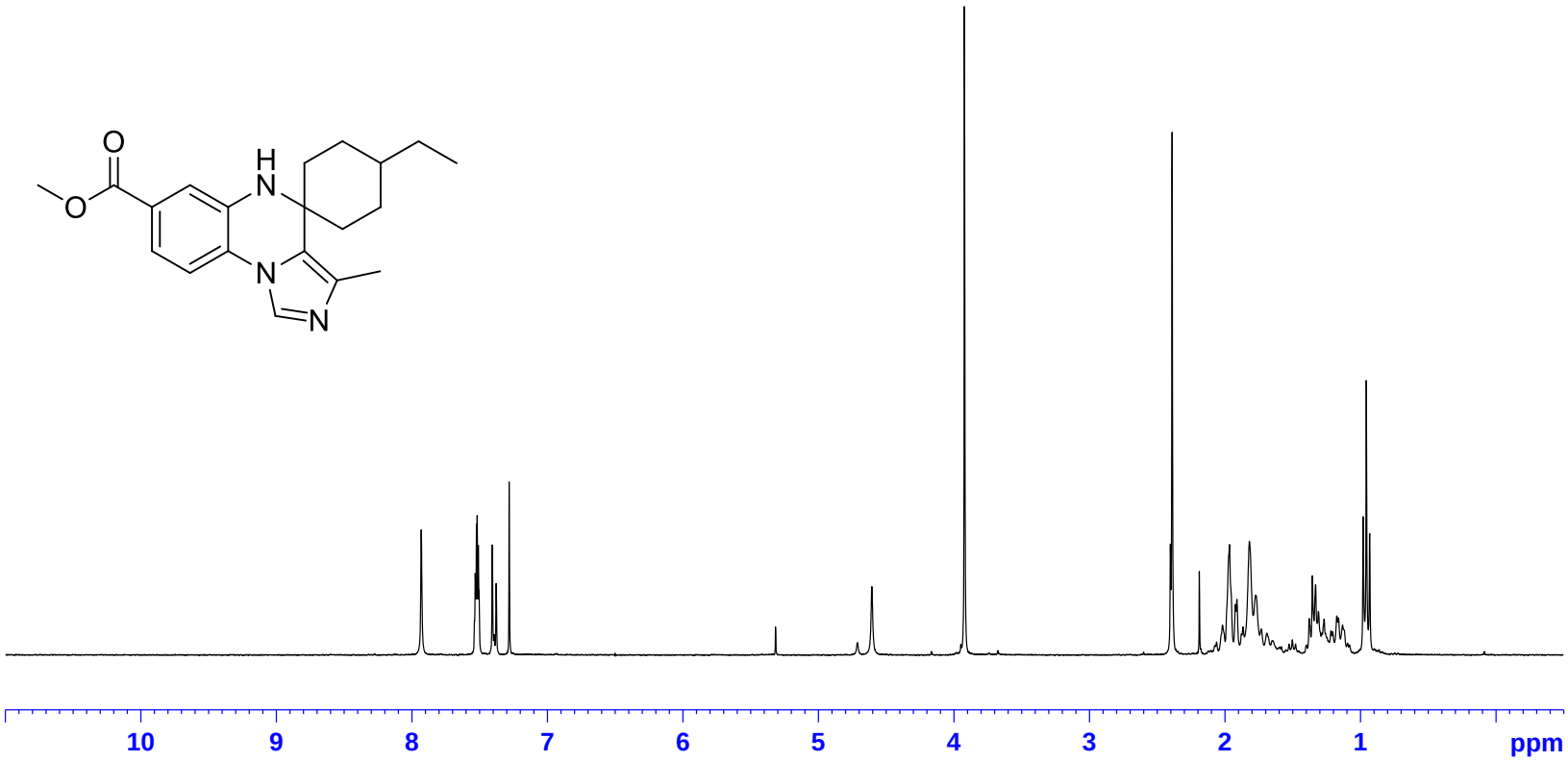
ESI-LRMS of compound **12l**



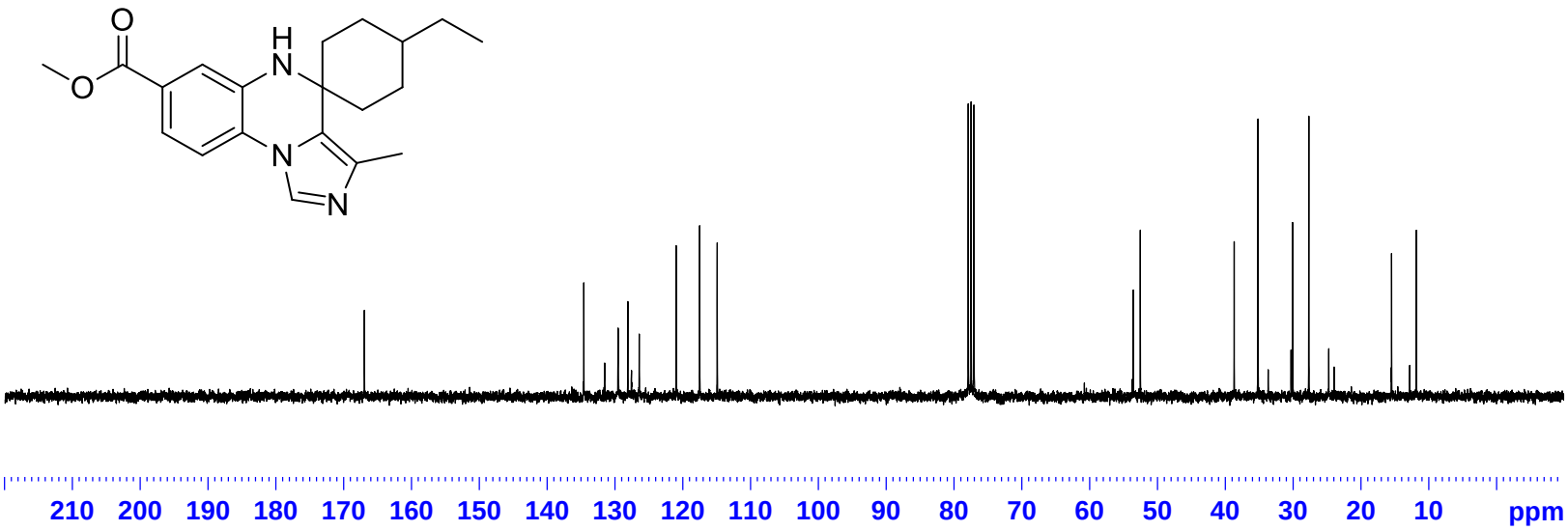
ESI-HRMS of compound **12l**



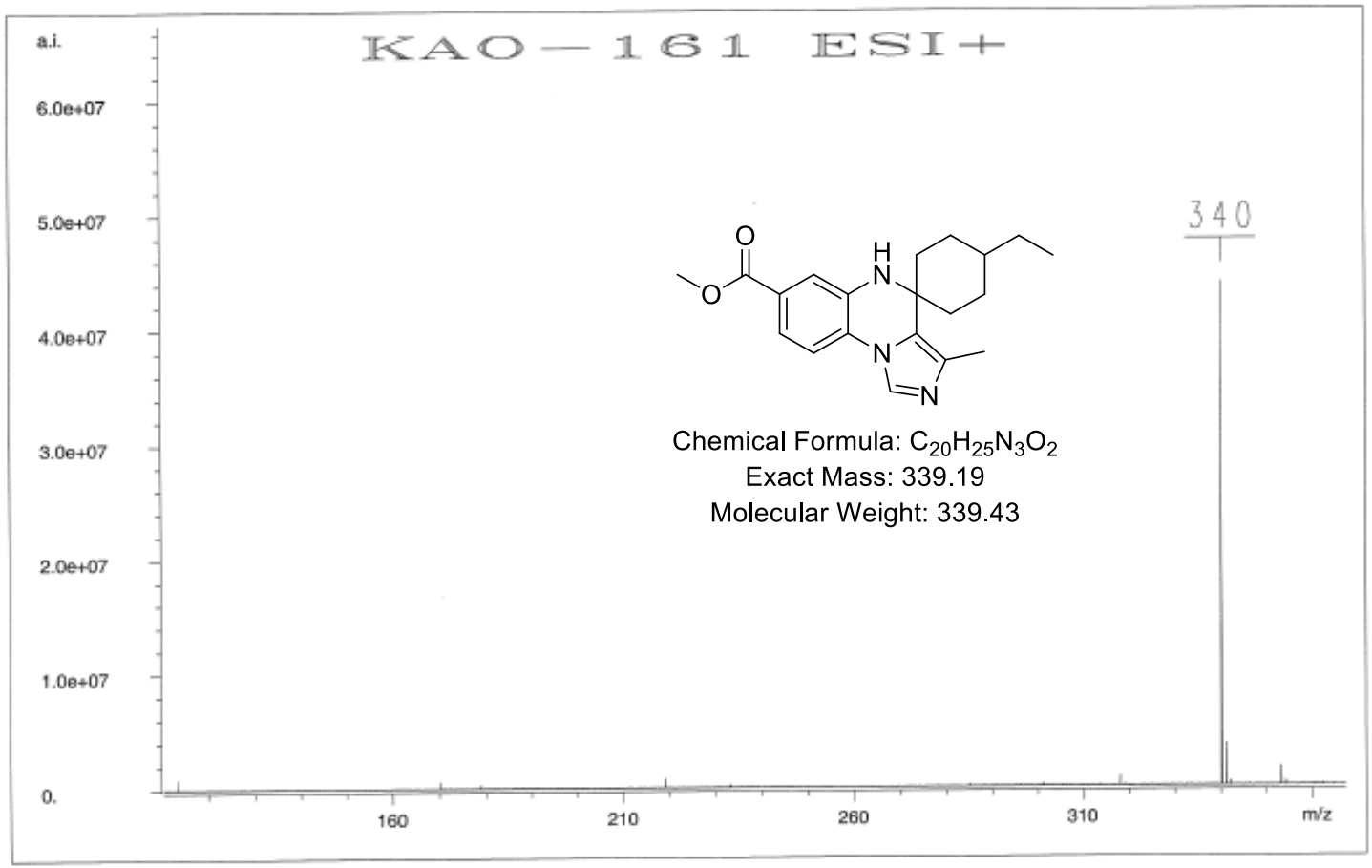
IR spectrum of compound **12l**



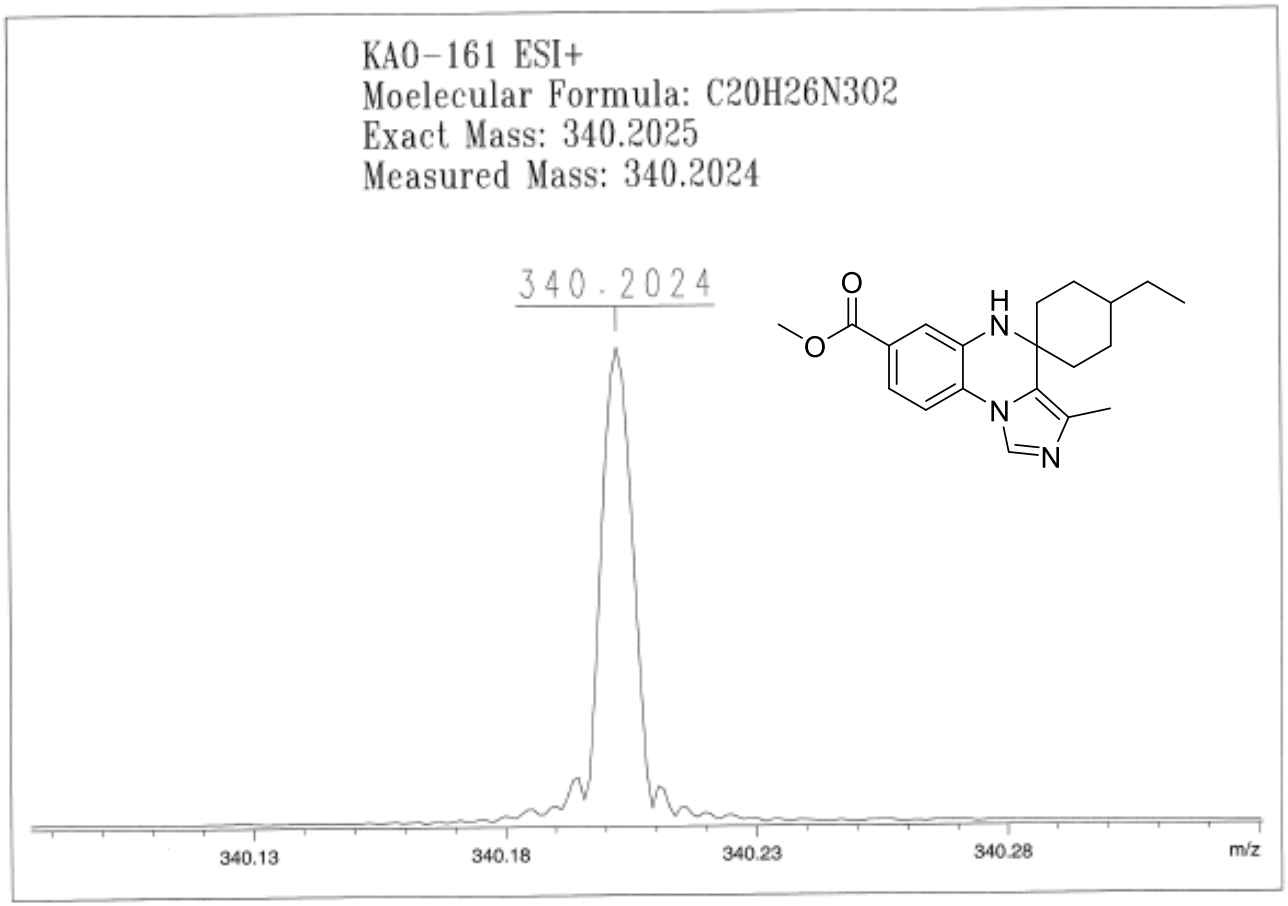
^{1}H NMR spectrum (300 MHz) of compound **12m** in $CDCl_3$



^{13}C NMR spectrum (75 MHz) of compound **12m** in $CDCl_3$



ESI-LRMS of compound **12m**



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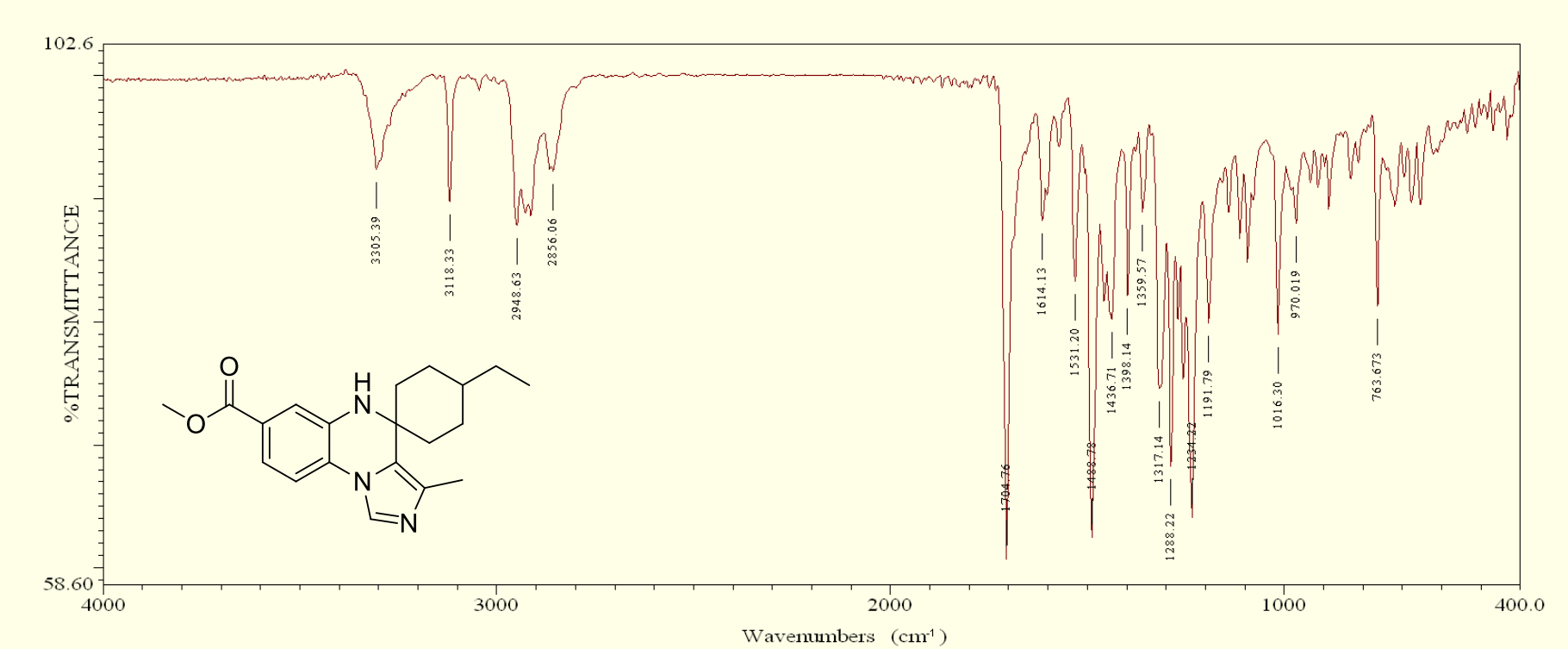
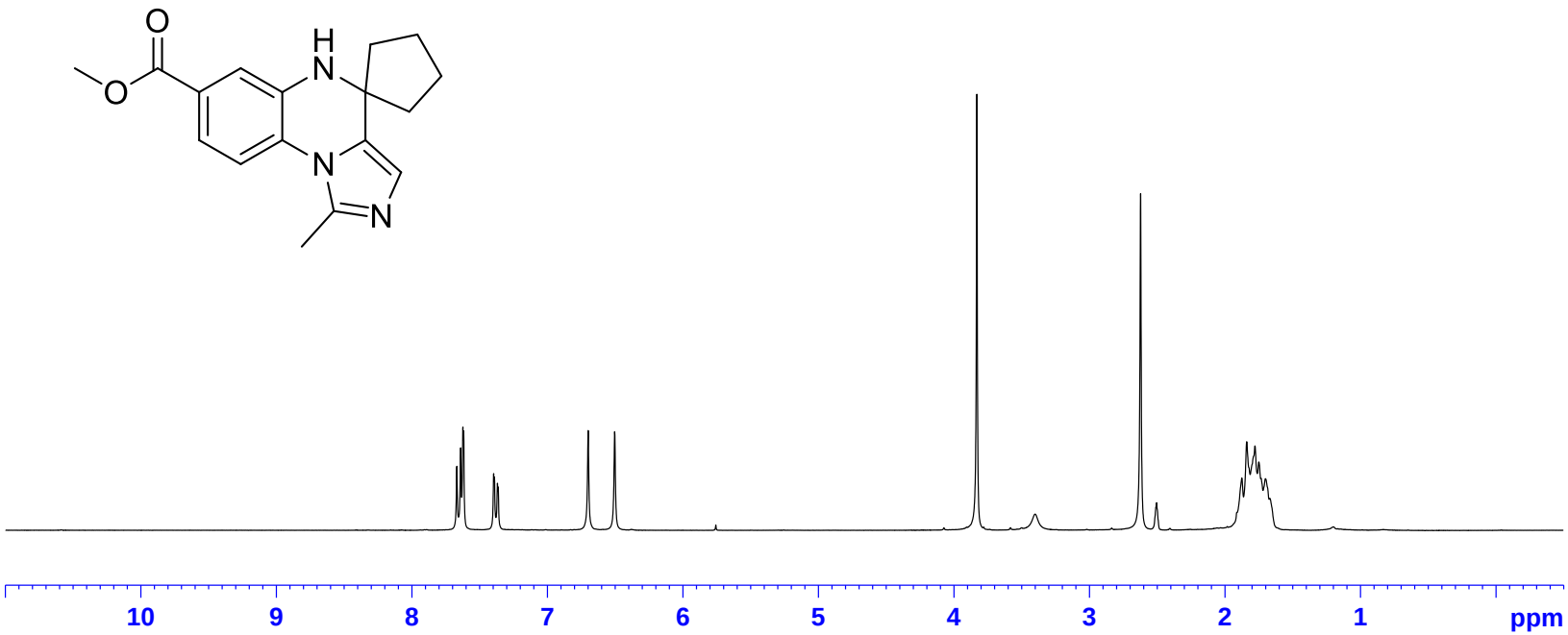
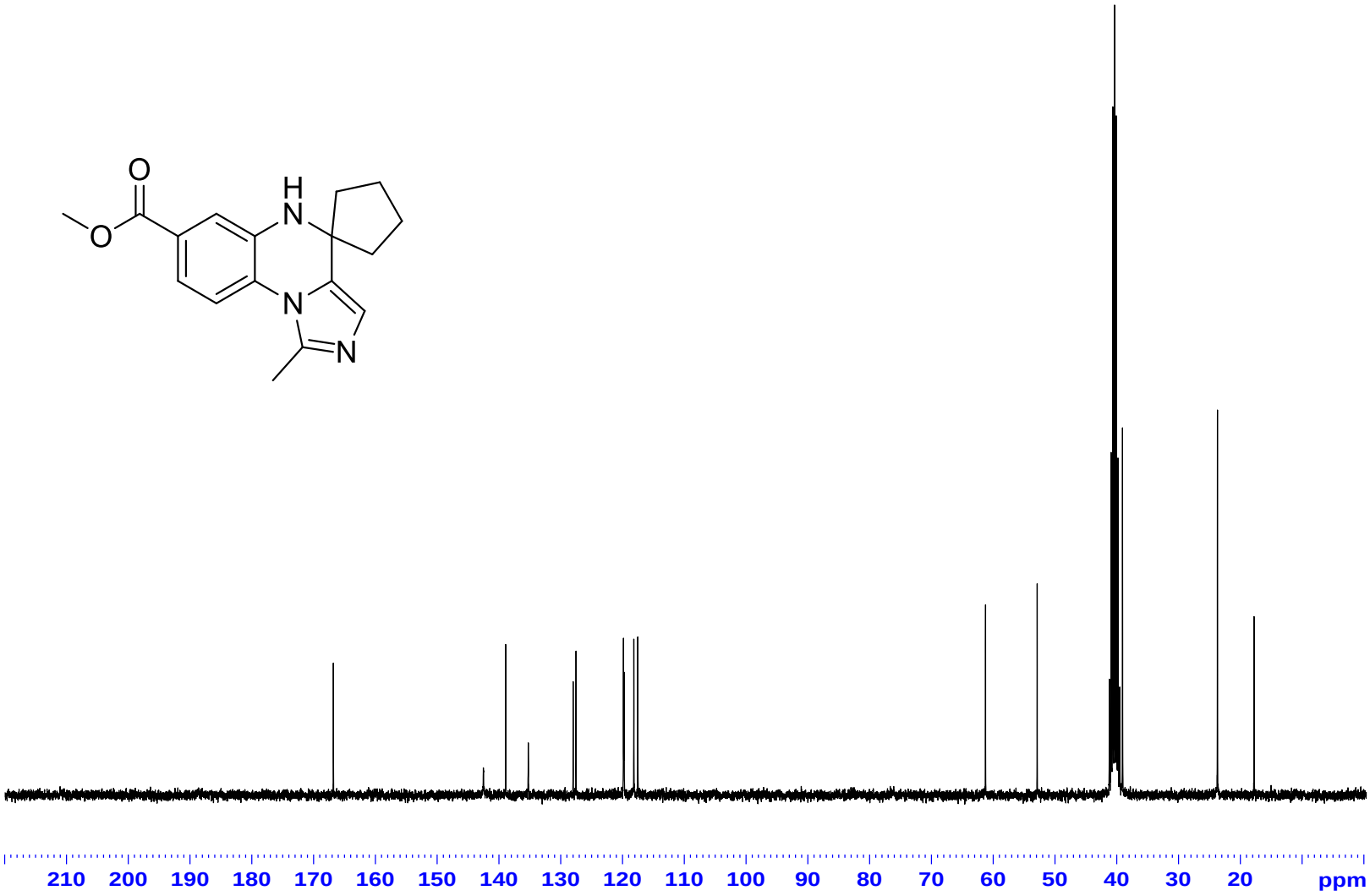


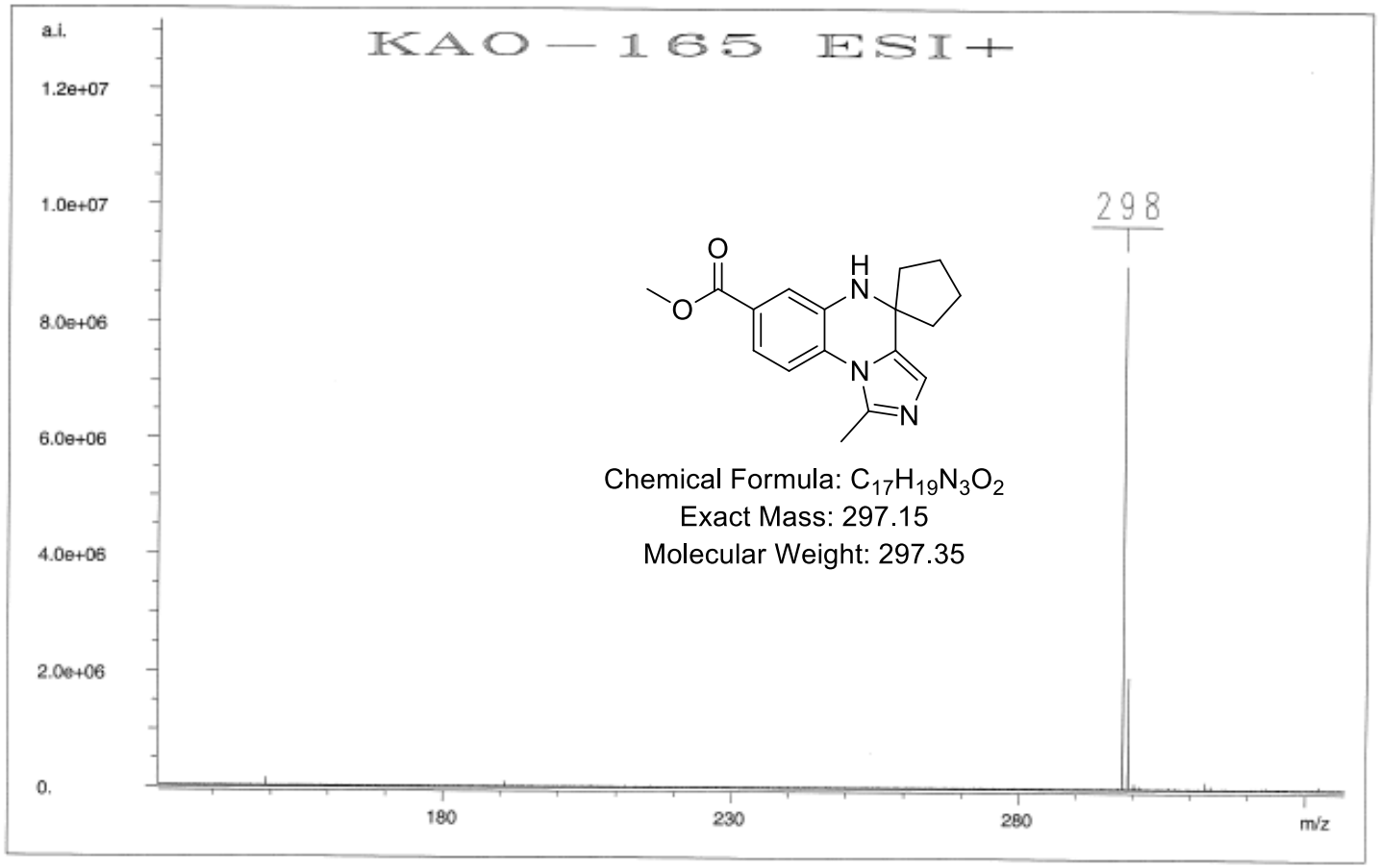
IR spectrum of compound **12m**



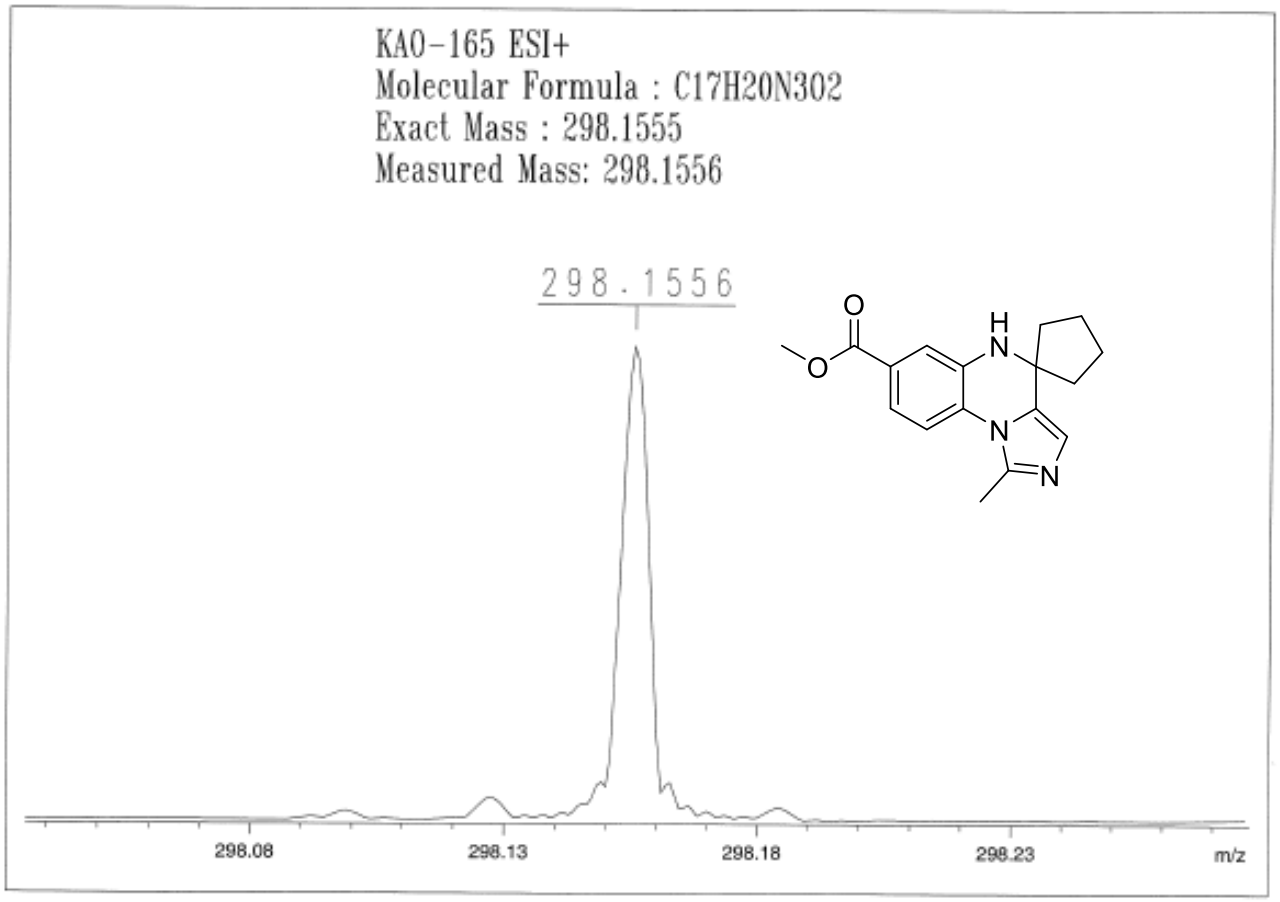
^{1}H NMR spectrum (300 MHz) of compound **12n** in $CDCl_3$



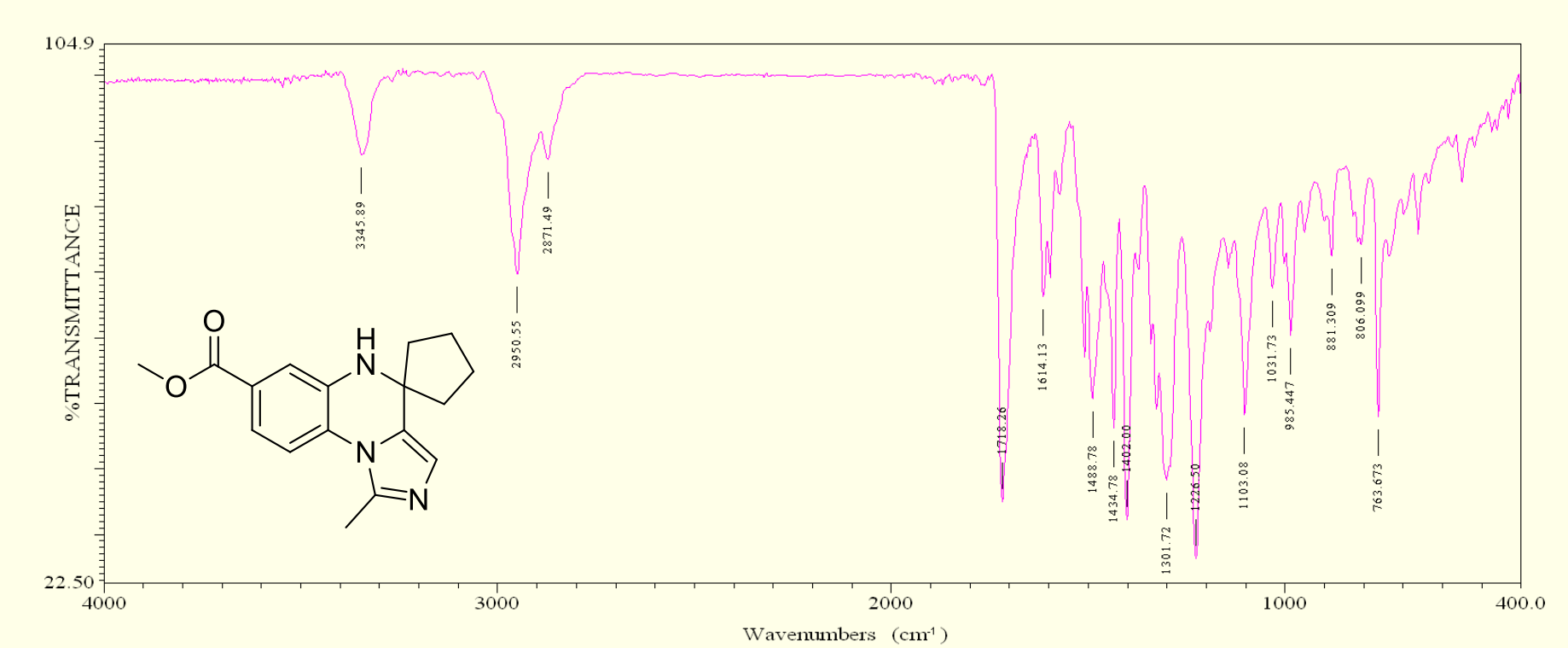
^{13}C NMR spectrum (75 MHz) of compound **12n** in $CDCl_3$



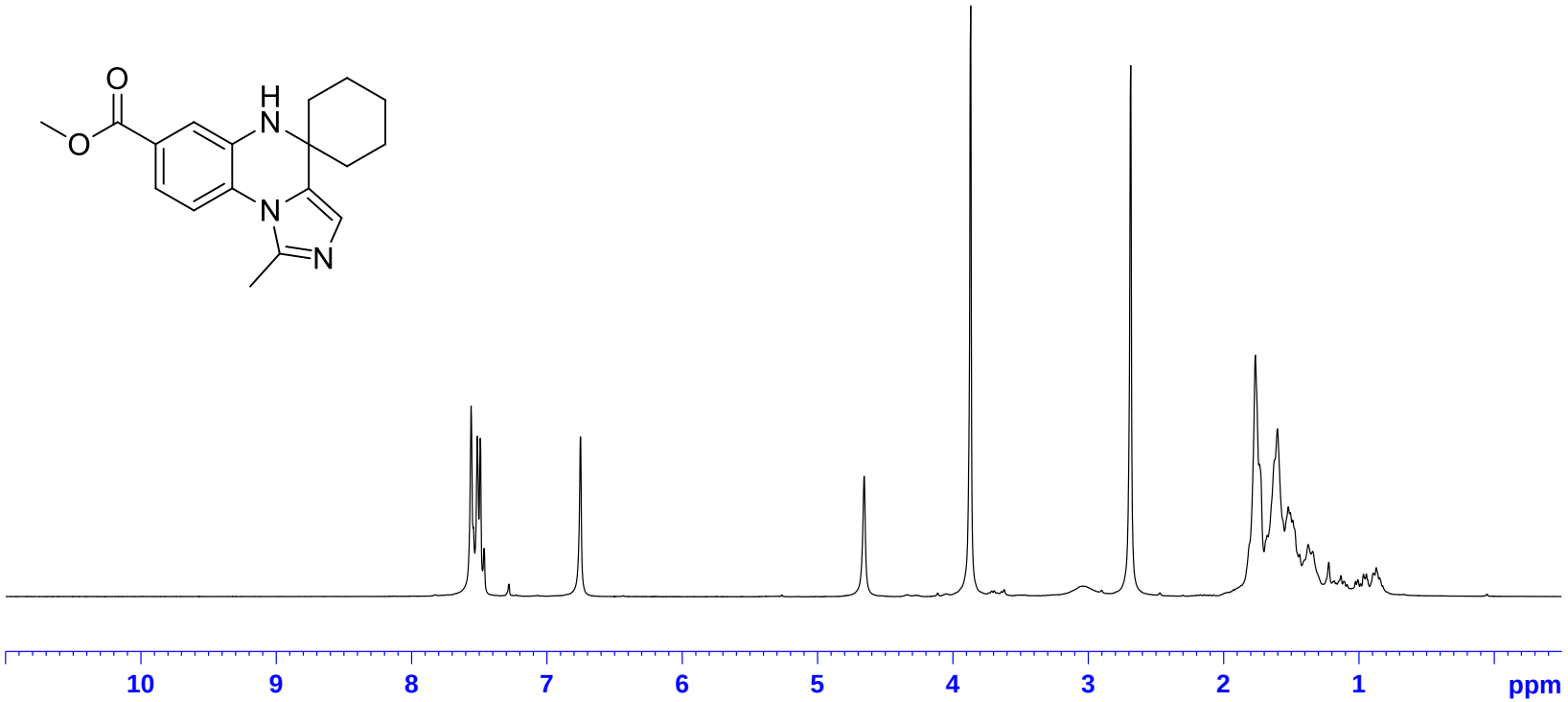
ESI-LRMS of compound **12n**



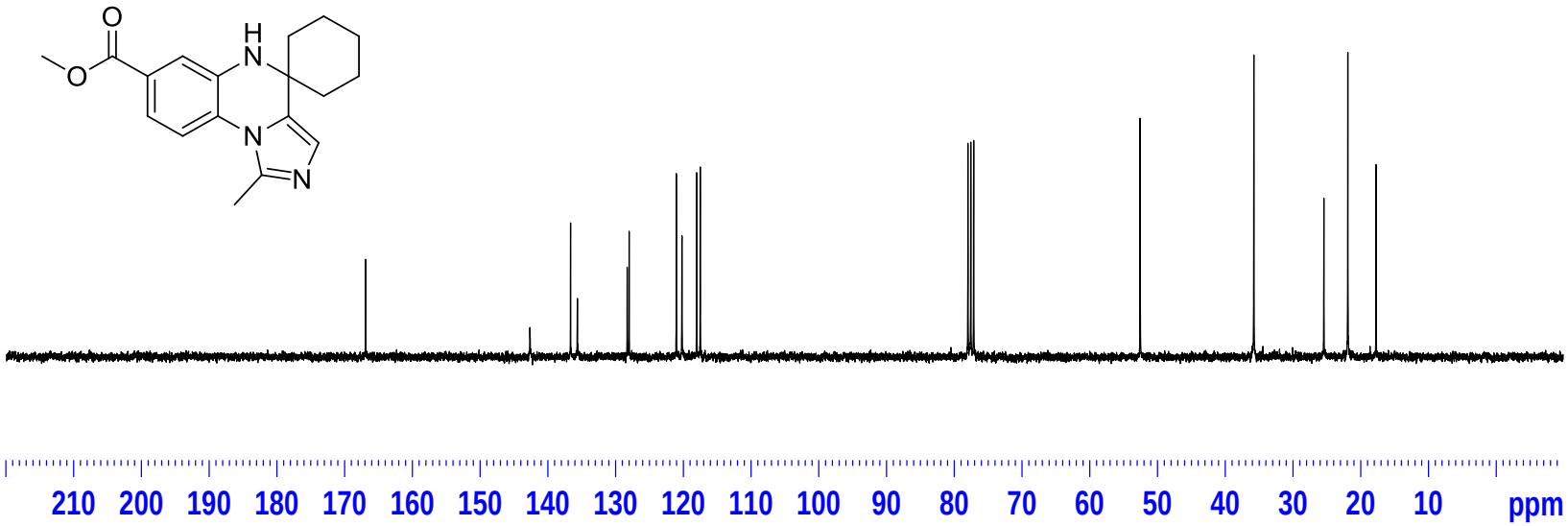
ESI-HRMS of compound **12n**



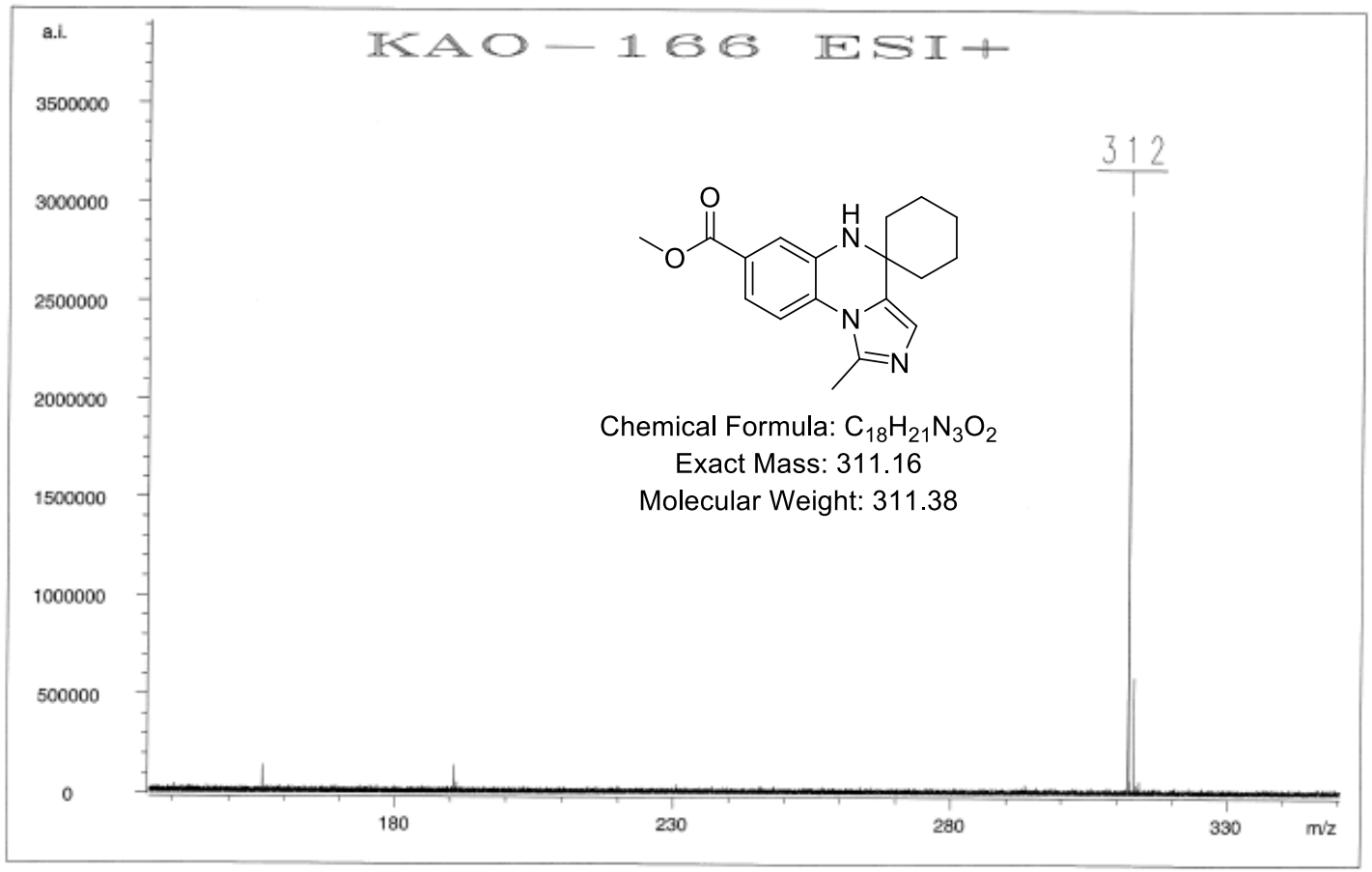
IR spectrum of compound **12n**



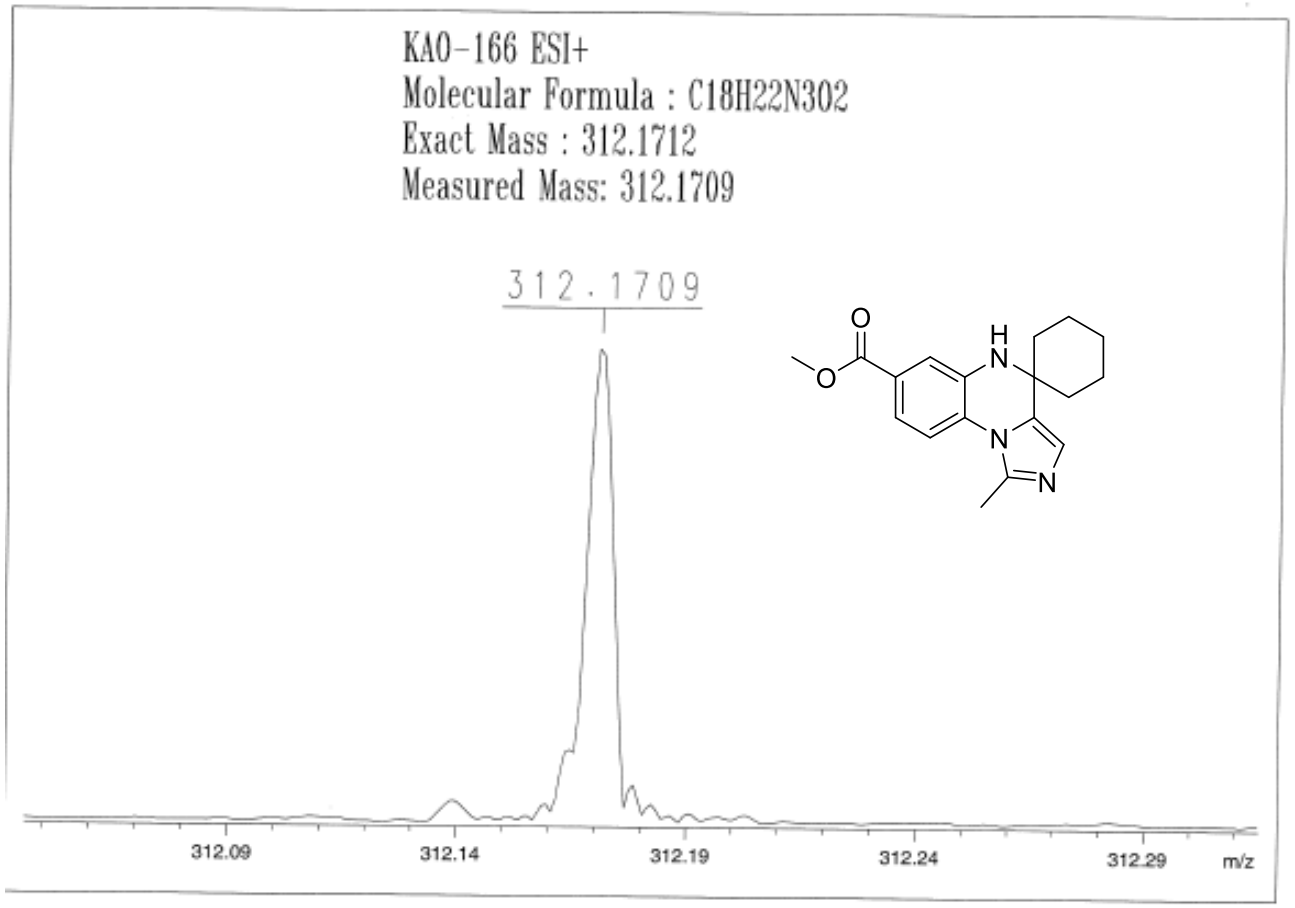
^{1}H NMR spectrum (300 MHz) of compound **12o** in $CDCl_3$



^{13}C NMR spectrum (75 MHz) of compound **12o** in $CDCl_3$



ESI-LRMS of compound **12o**



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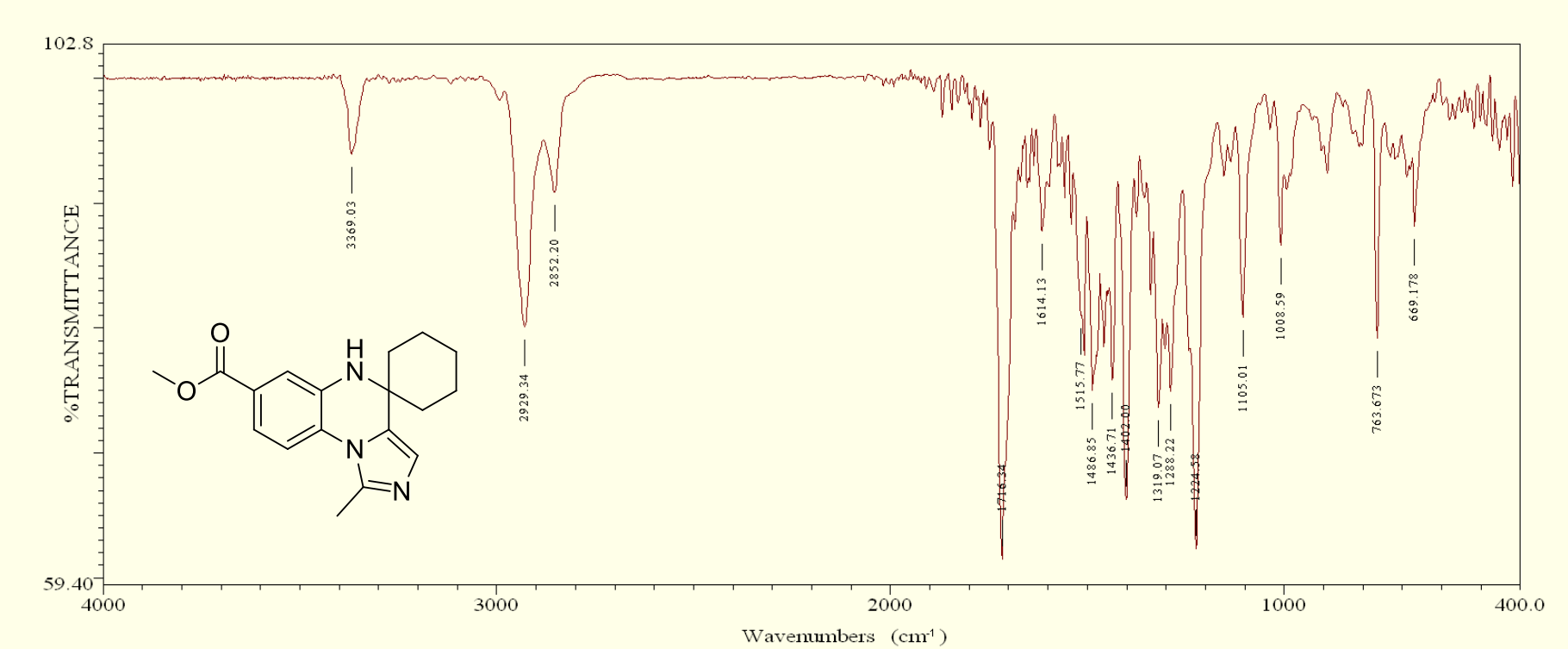
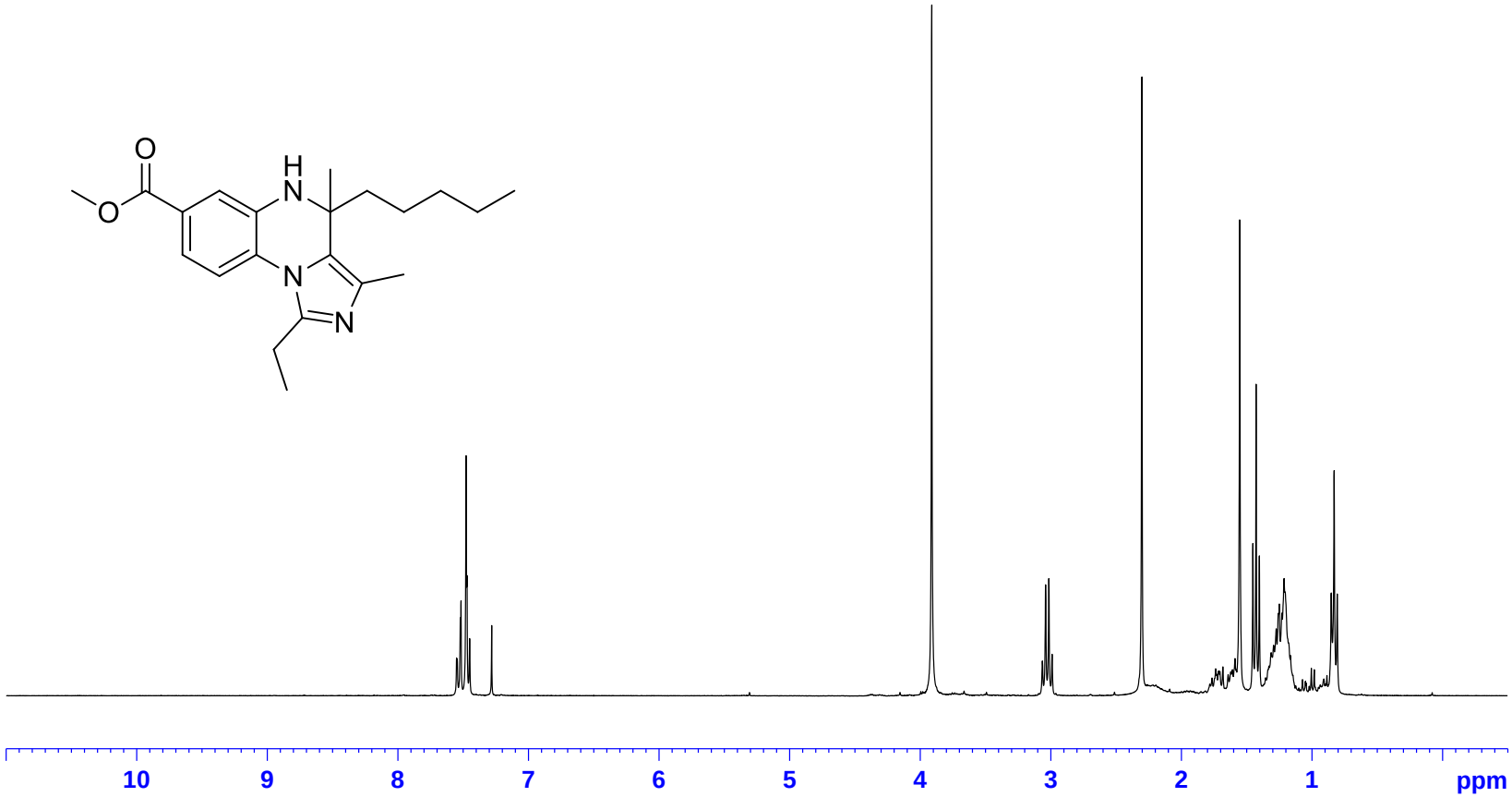
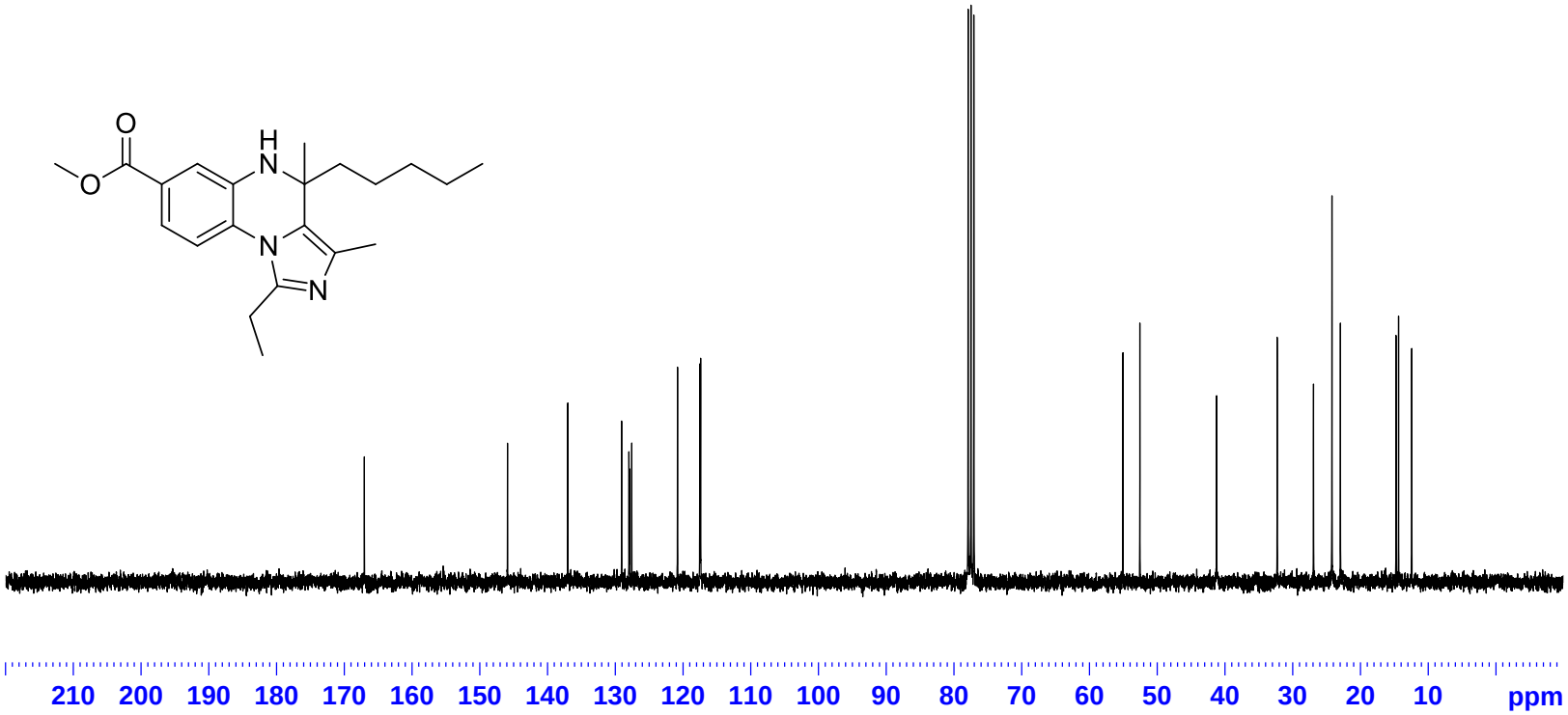


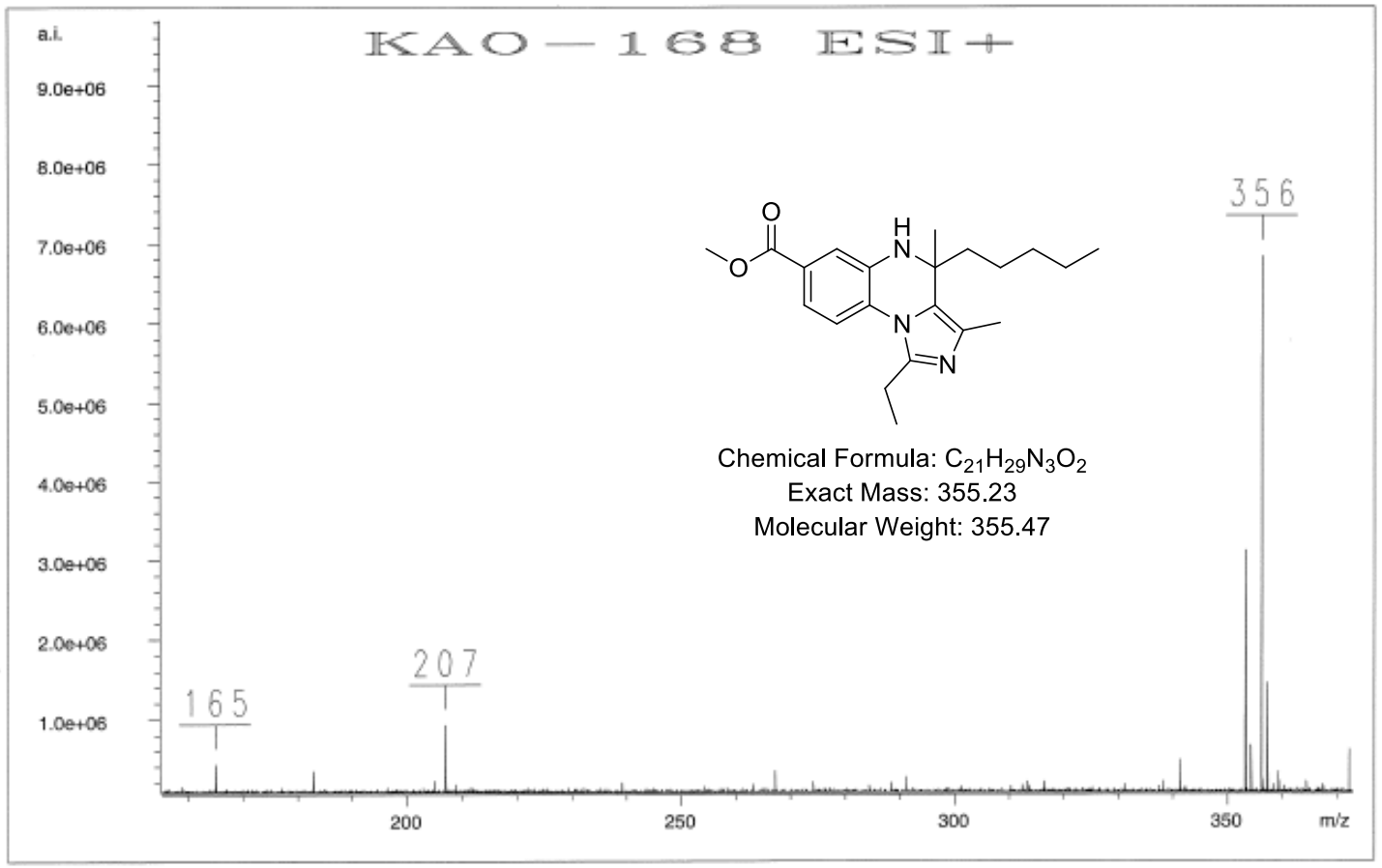
IR spectrum of compound **12o**



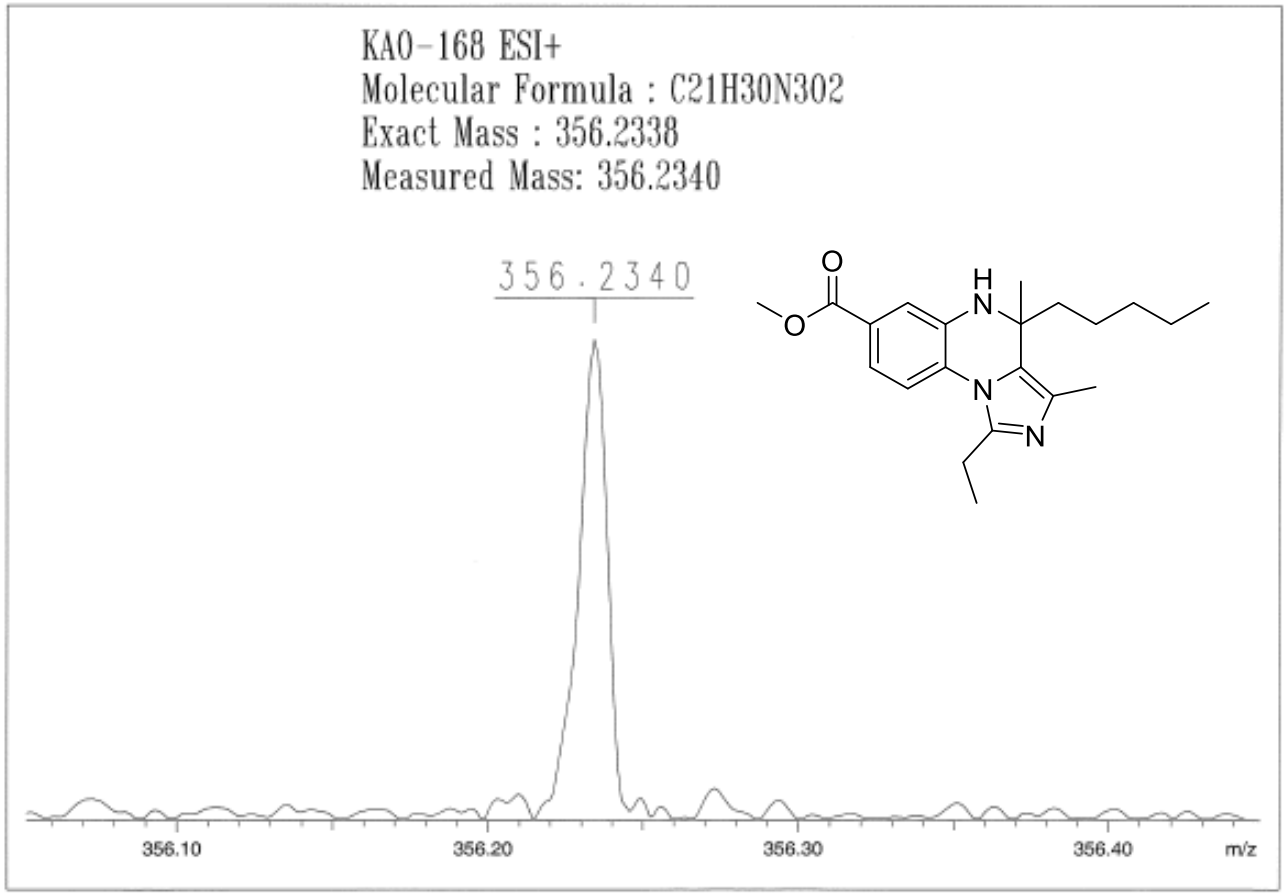
^{1}H NMR spectrum (300 MHz) of compound **12p** in $CDCl_3$



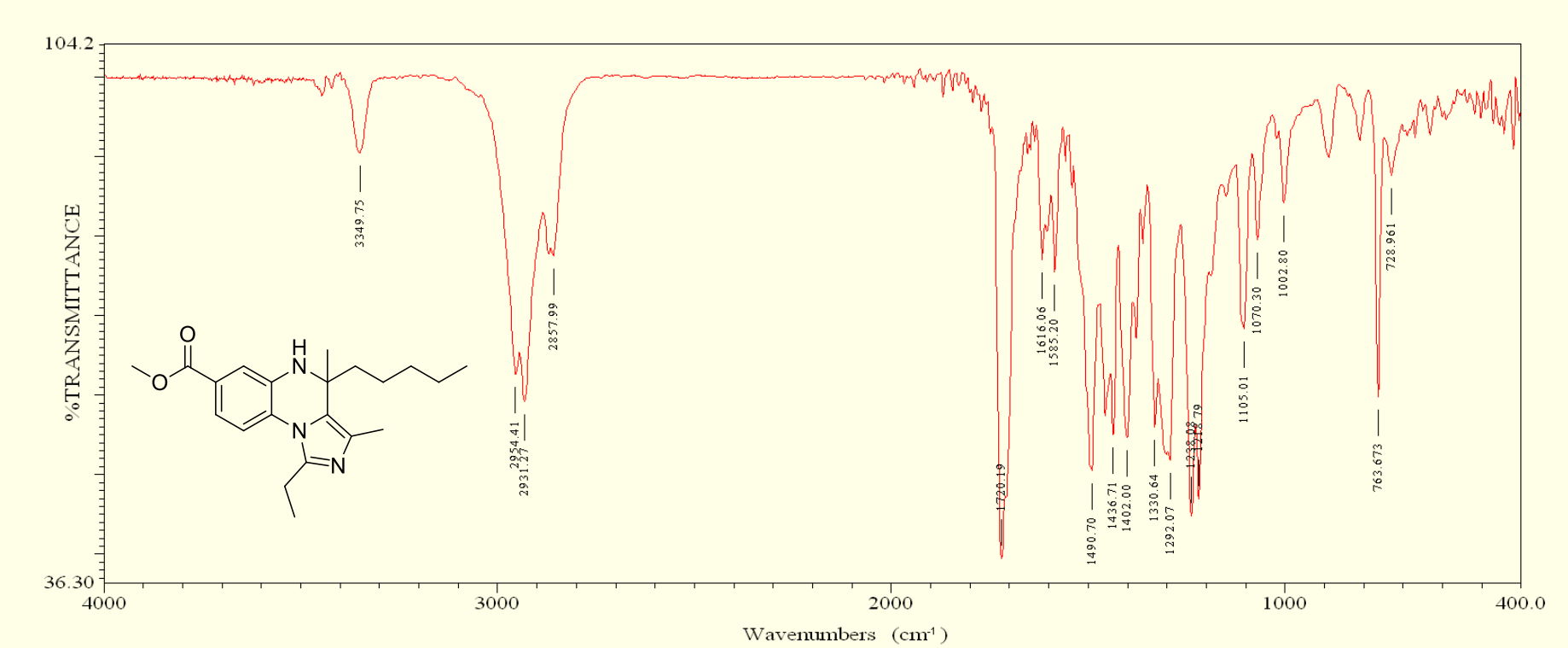
^{13}C NMR spectrum (75 MHz) of compound **12p** in $CDCl_3$



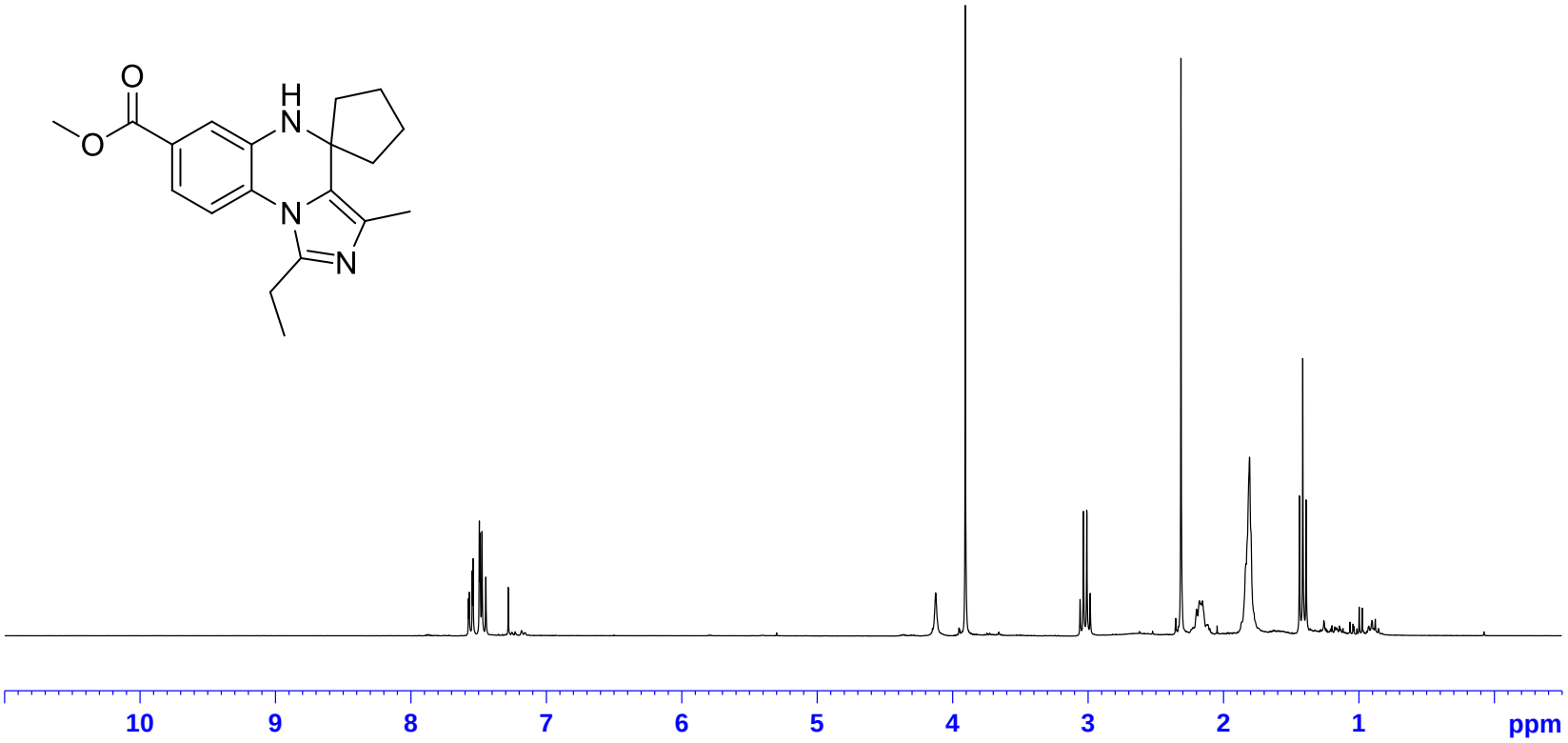
ESI-LRMS of compound **12p**



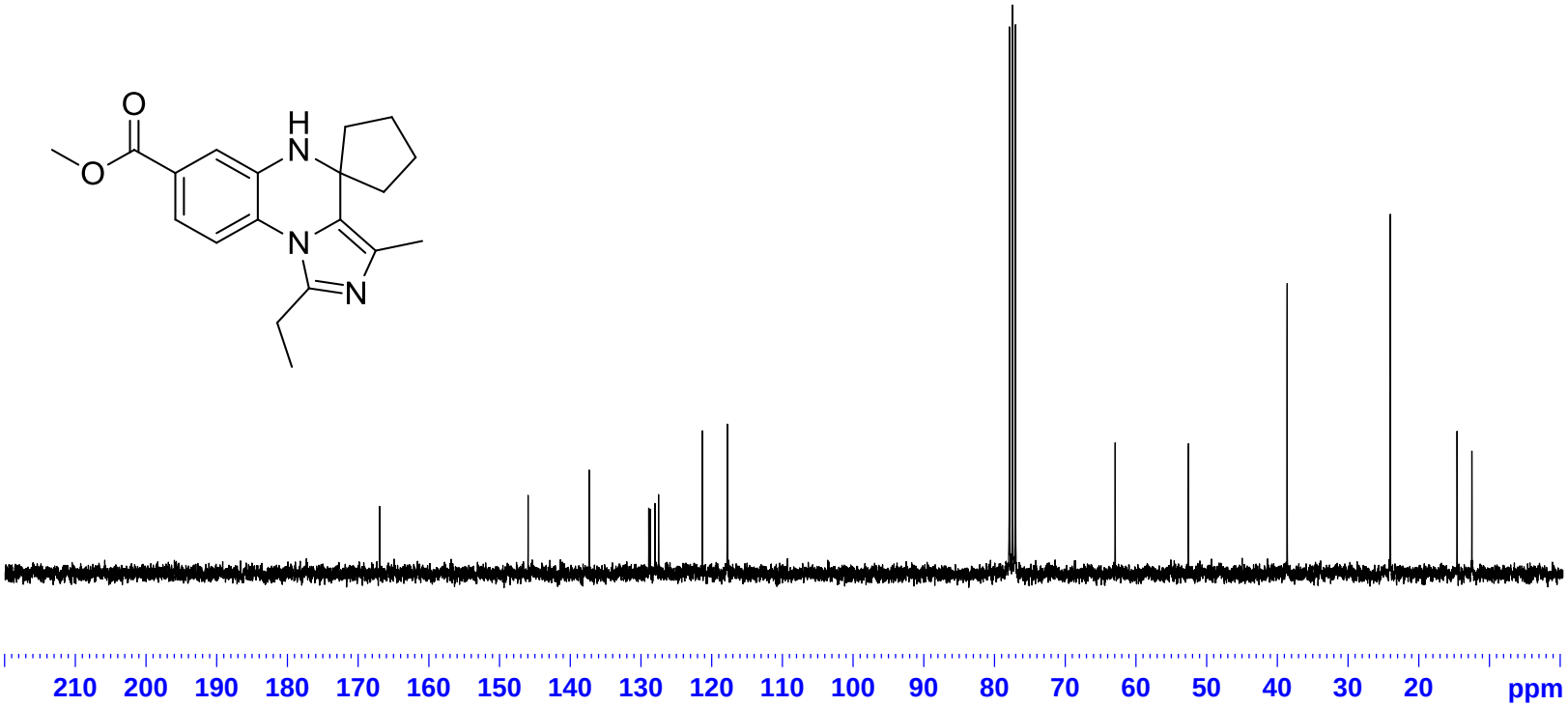
ESI-HRMS of compound **12p**



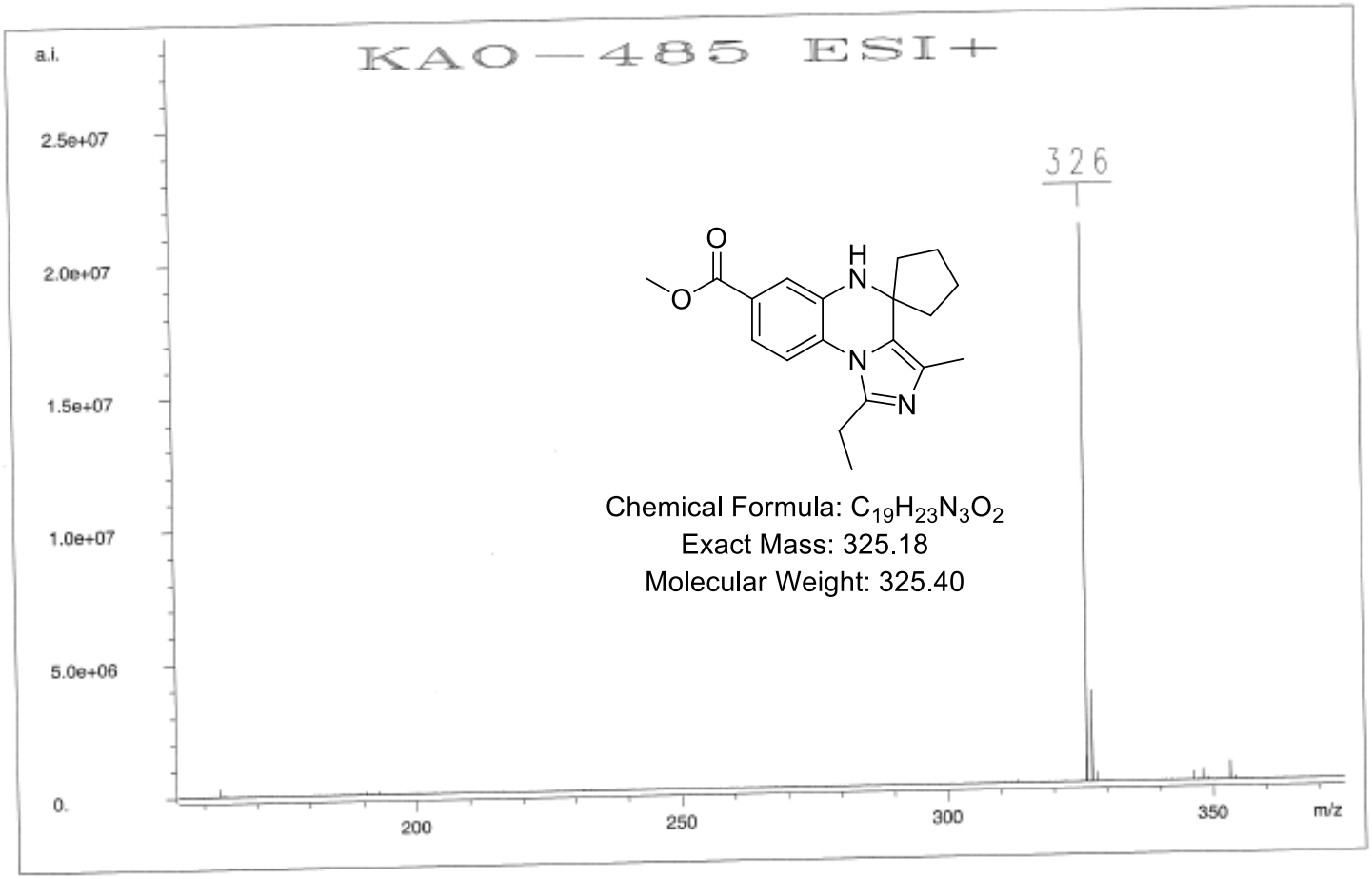
IR spectrum of compound **12p**



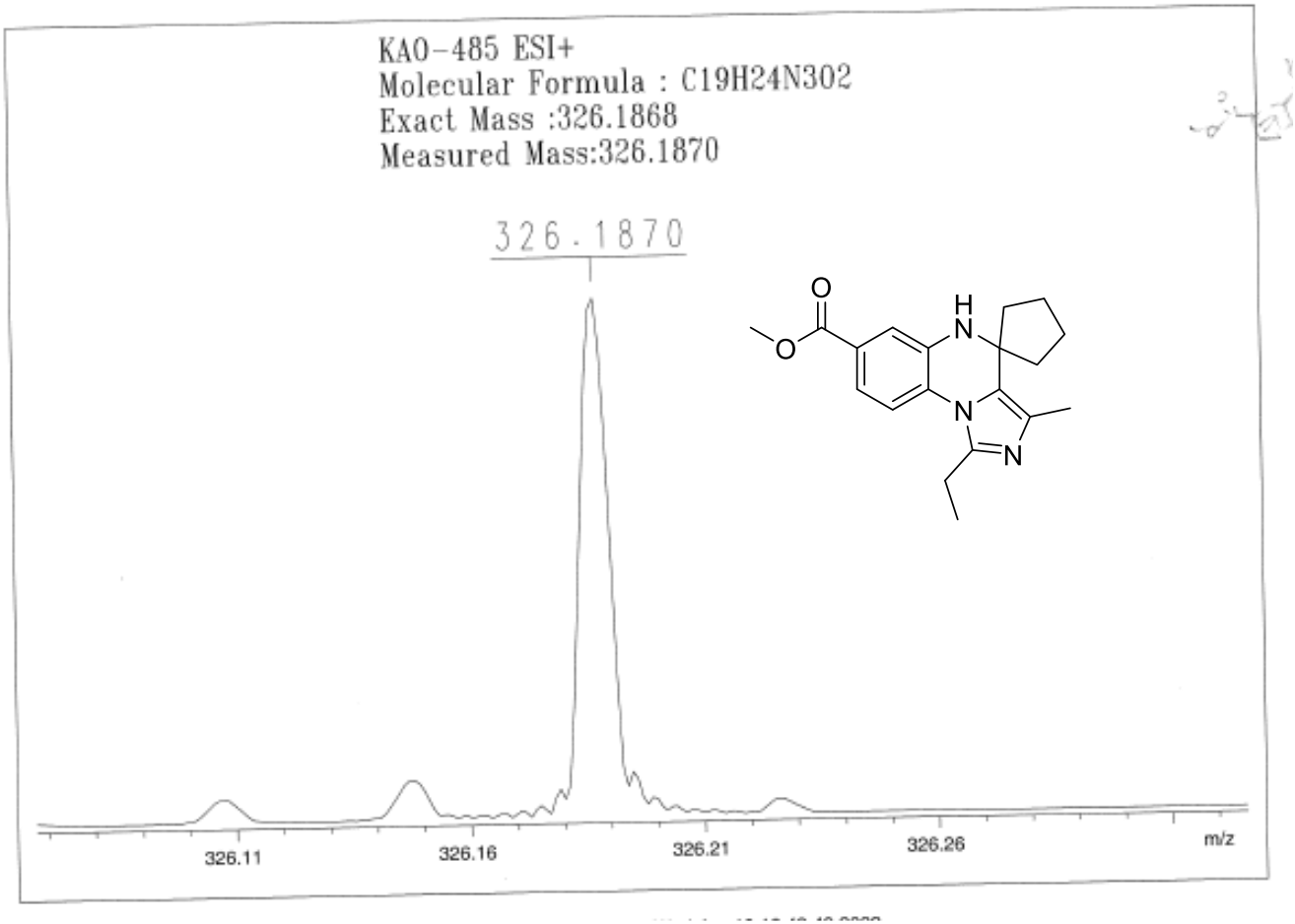
^{1}H NMR spectrum (300 MHz) of compound **12q** in $CDCl_3$



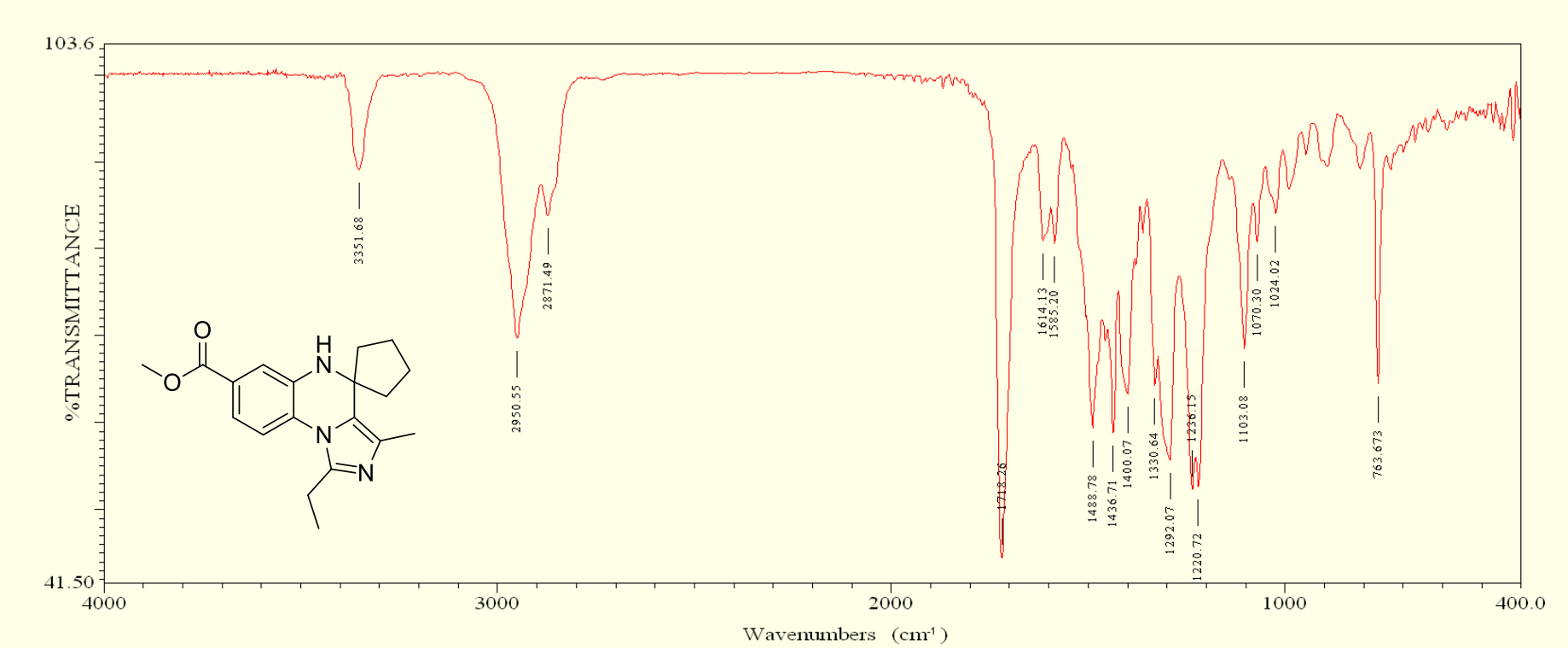
^{13}C NMR spectrum (75 MHz) of compound **12q** in $CDCl_3$



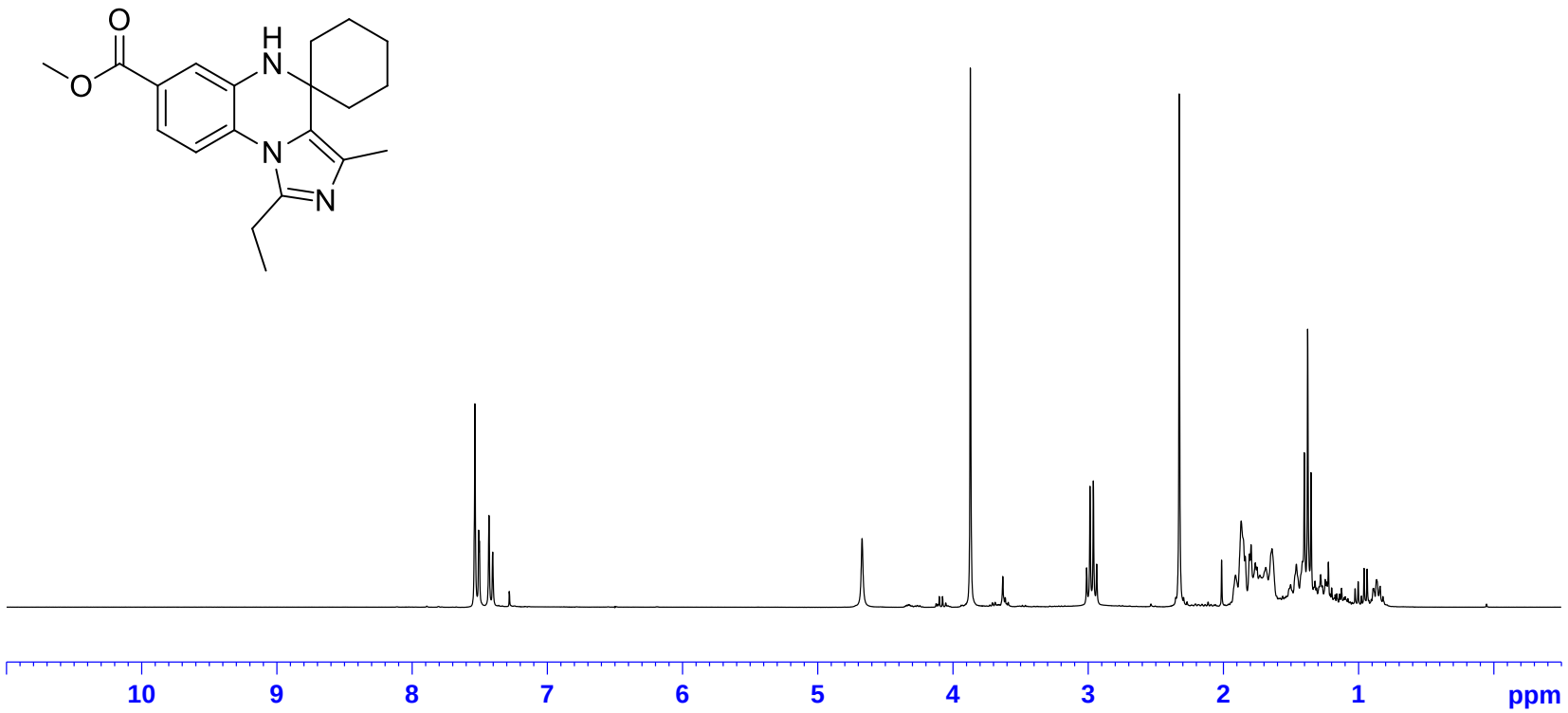
ESI-LRMS of compound **12q**



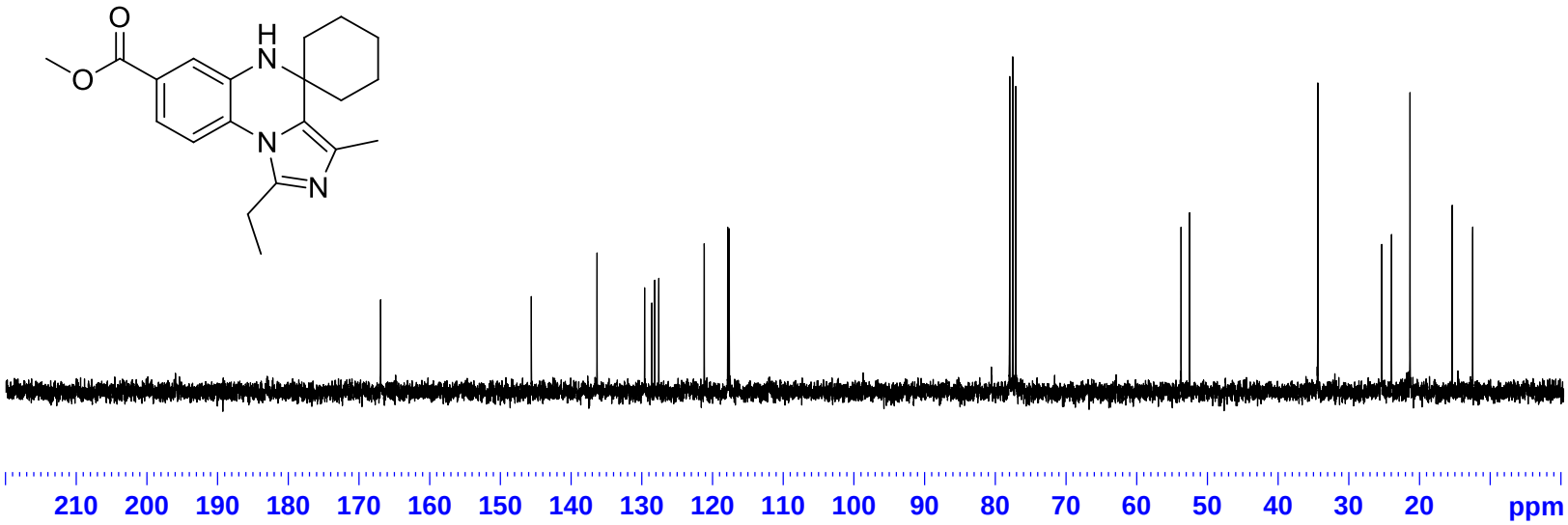
ESI-HRMS of compound **12q**



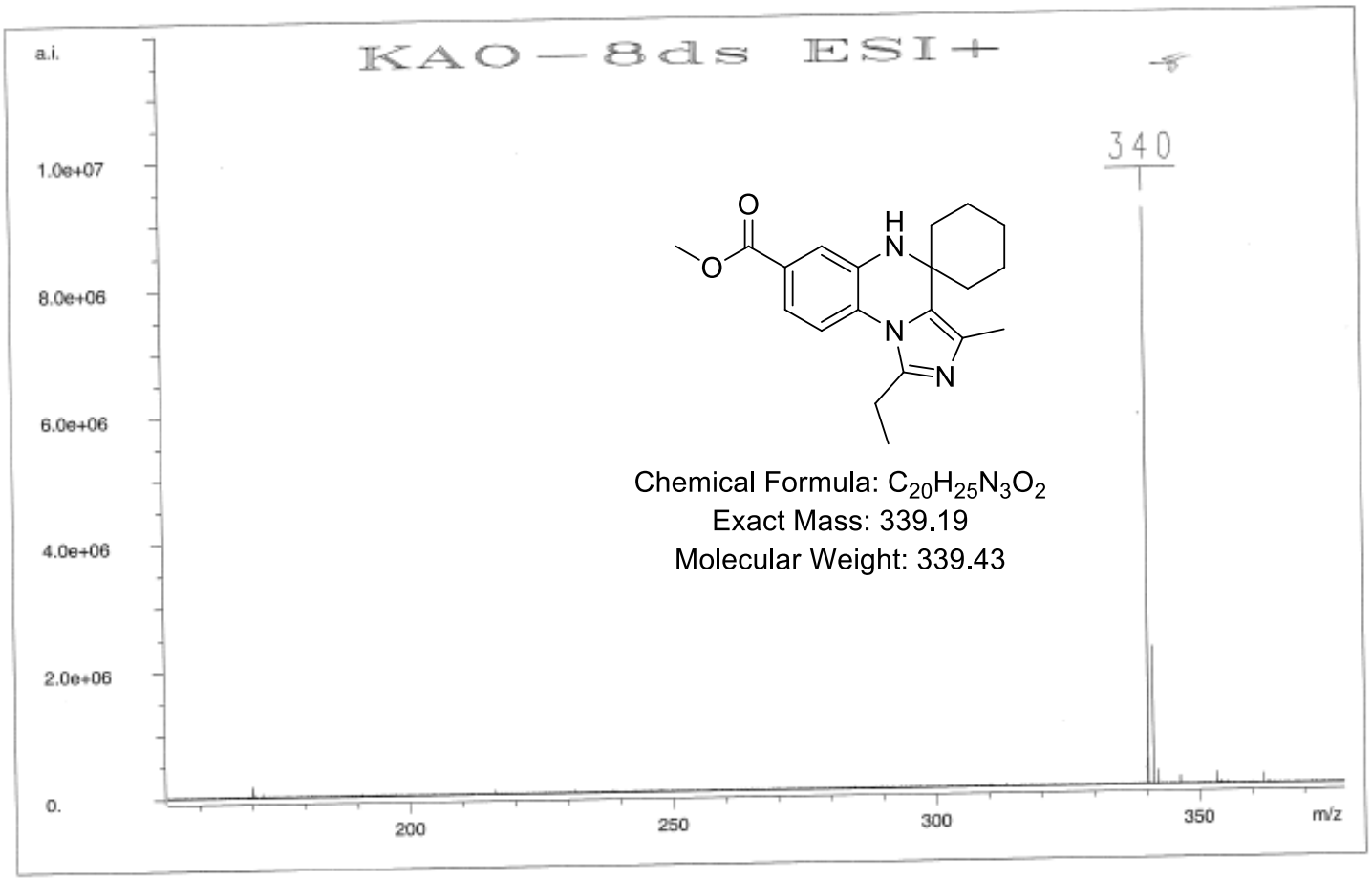
IR spectrum of compound **12q**



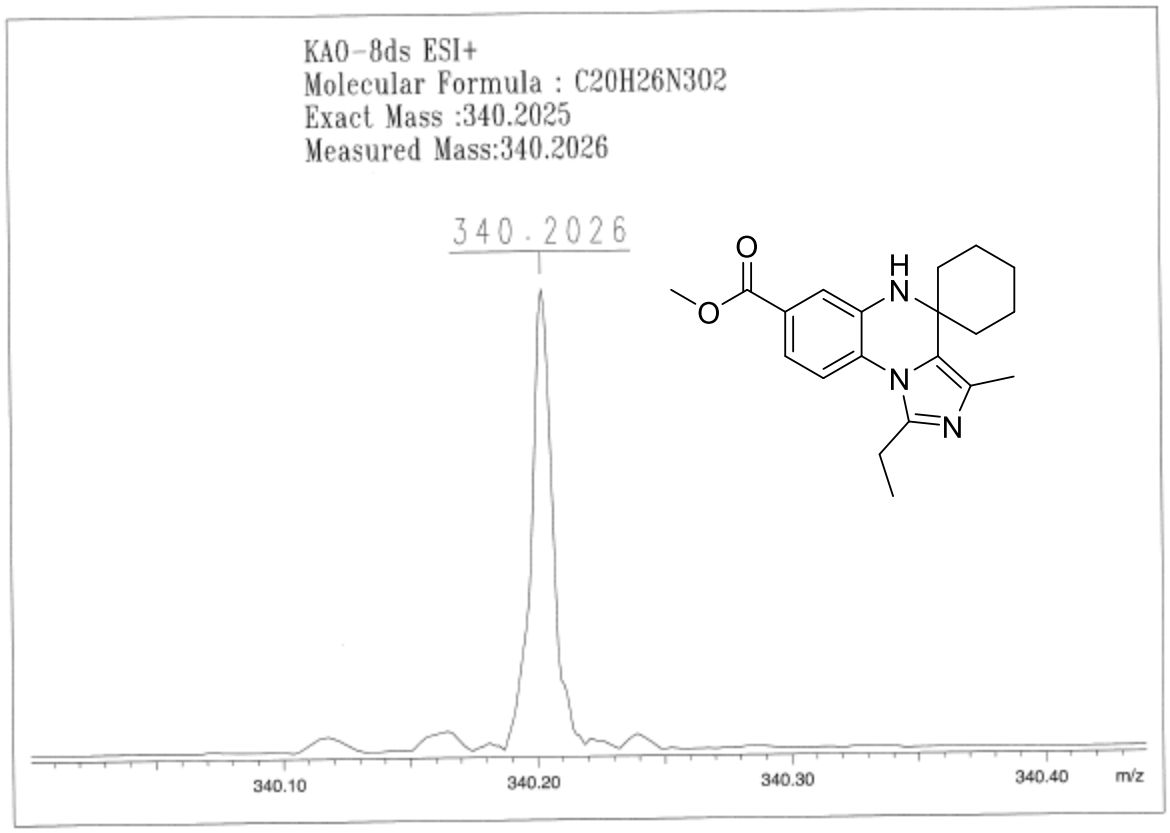
^{1}H NMR spectrum (300 MHz) of compound **12r** in $CDCl_3$



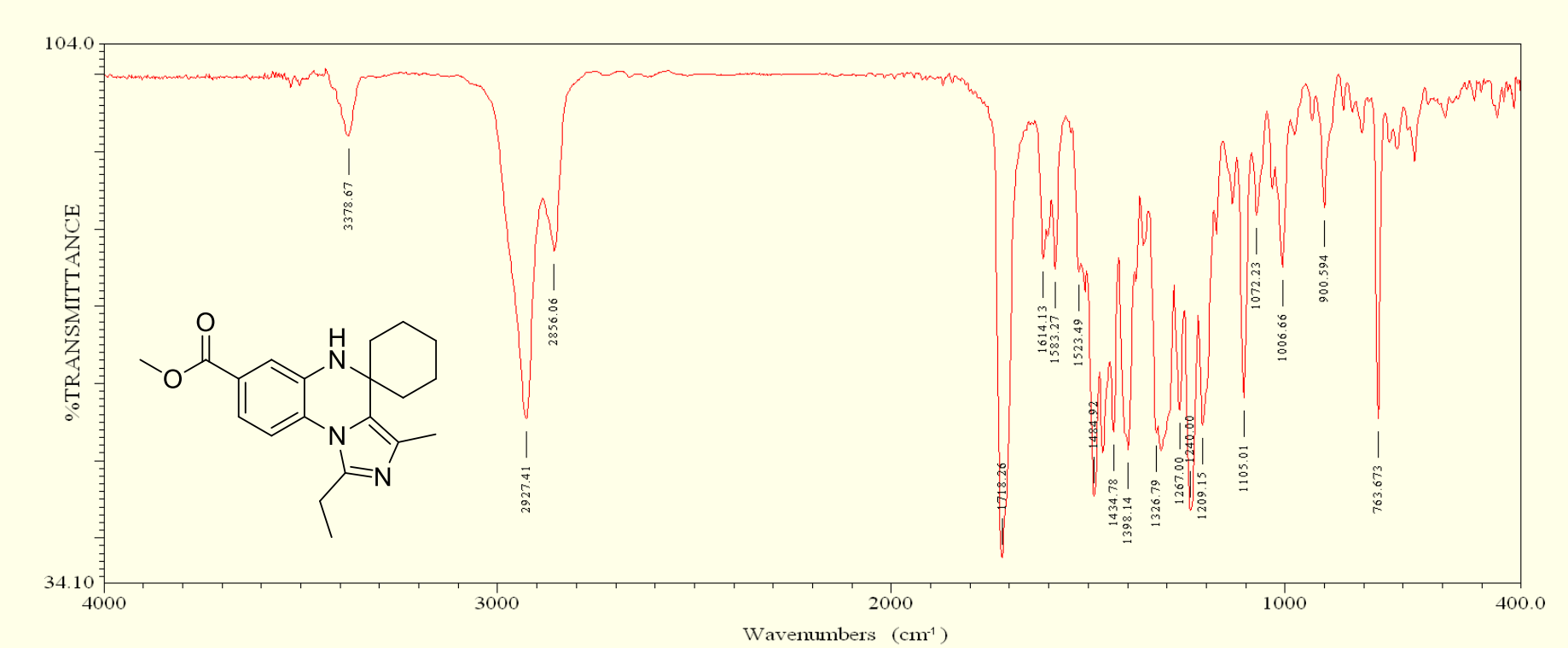
^{13}C NMR spectrum (75 MHz) of compound **12r** in $CDCl_3$



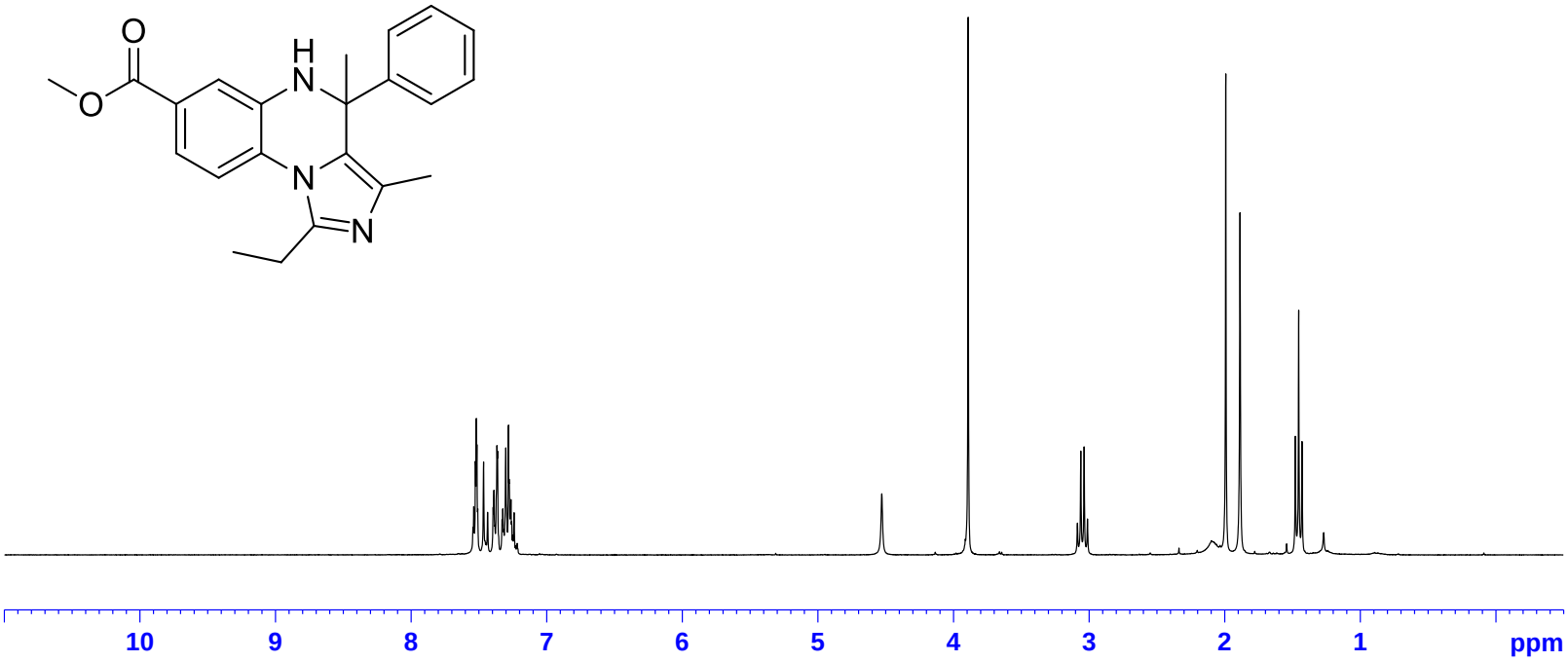
ESI-LRMS of compound **12r**



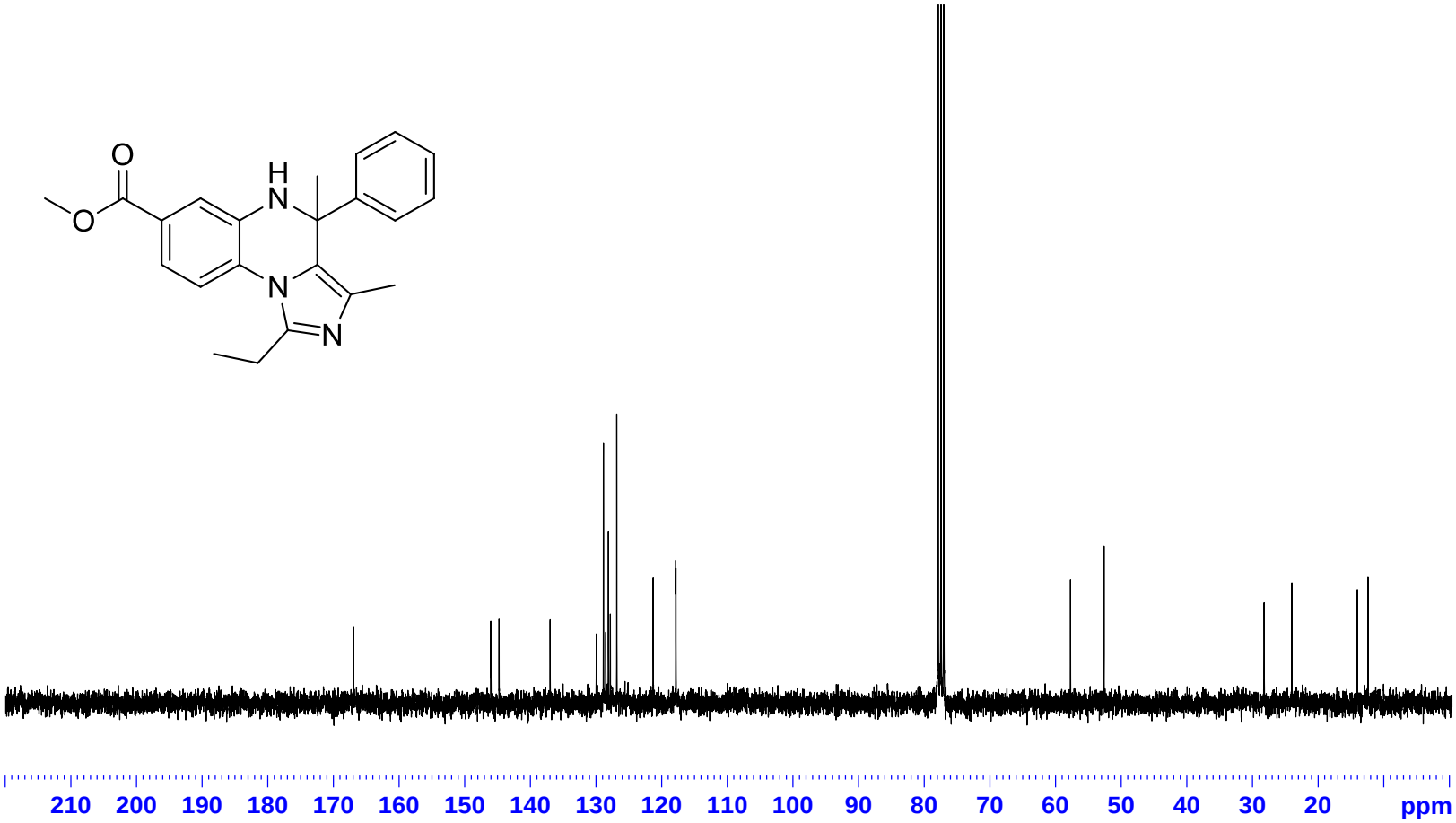
ESI-HRMS of compound **12r**



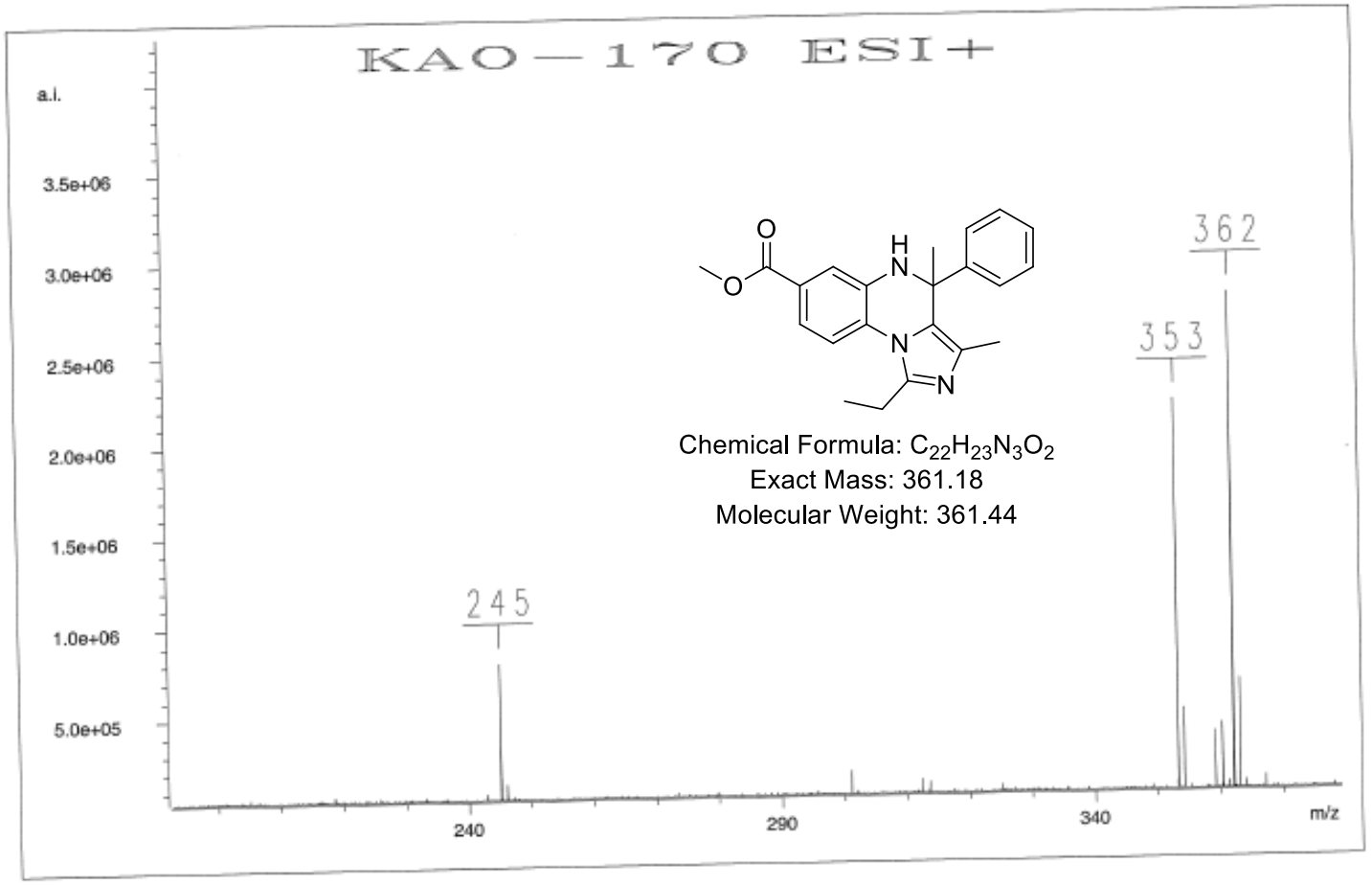
IR spectrum of compound **12r**



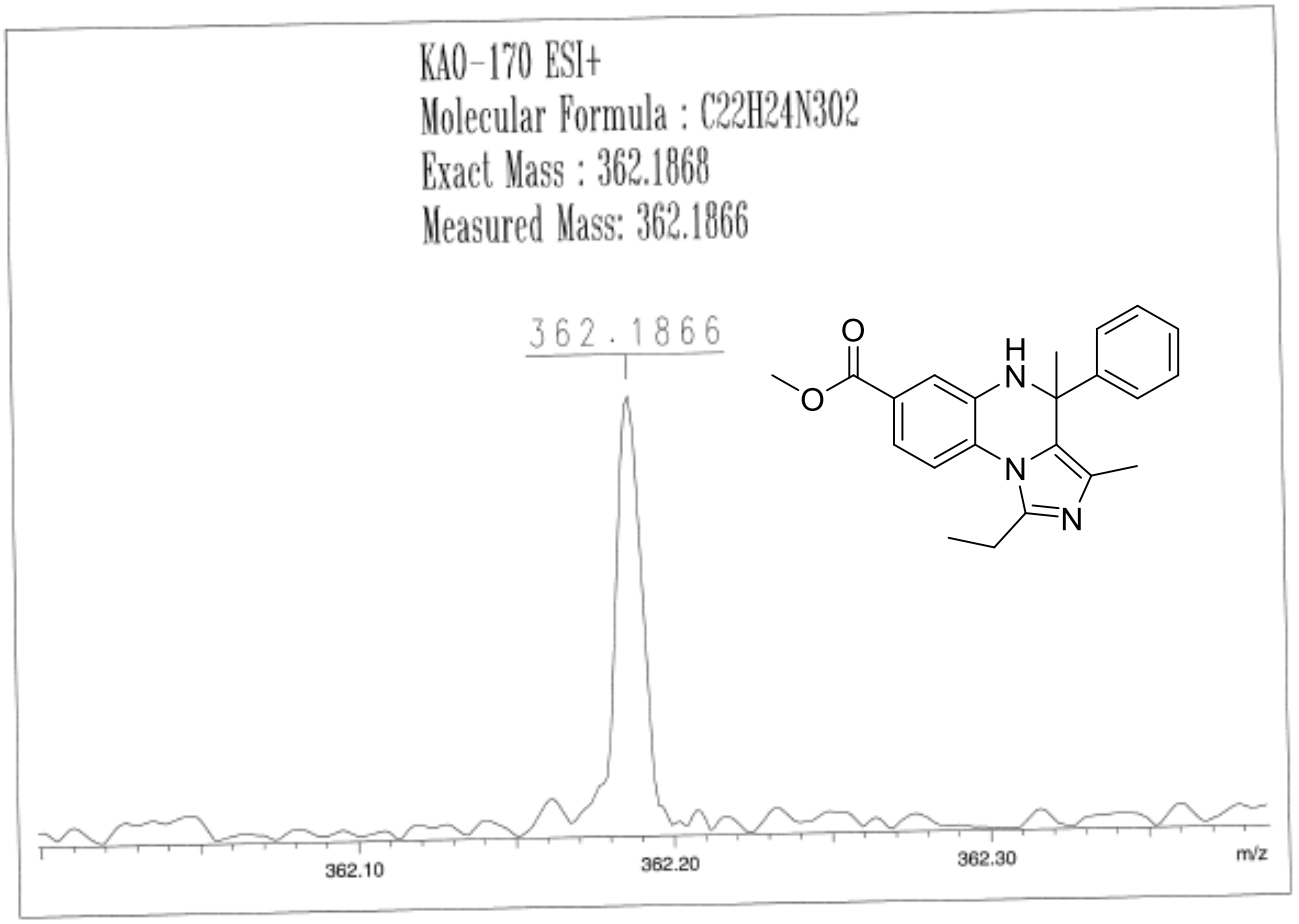
^{1}H NMR spectrum (300 MHz) of compound **12s** in $CDCl_3$



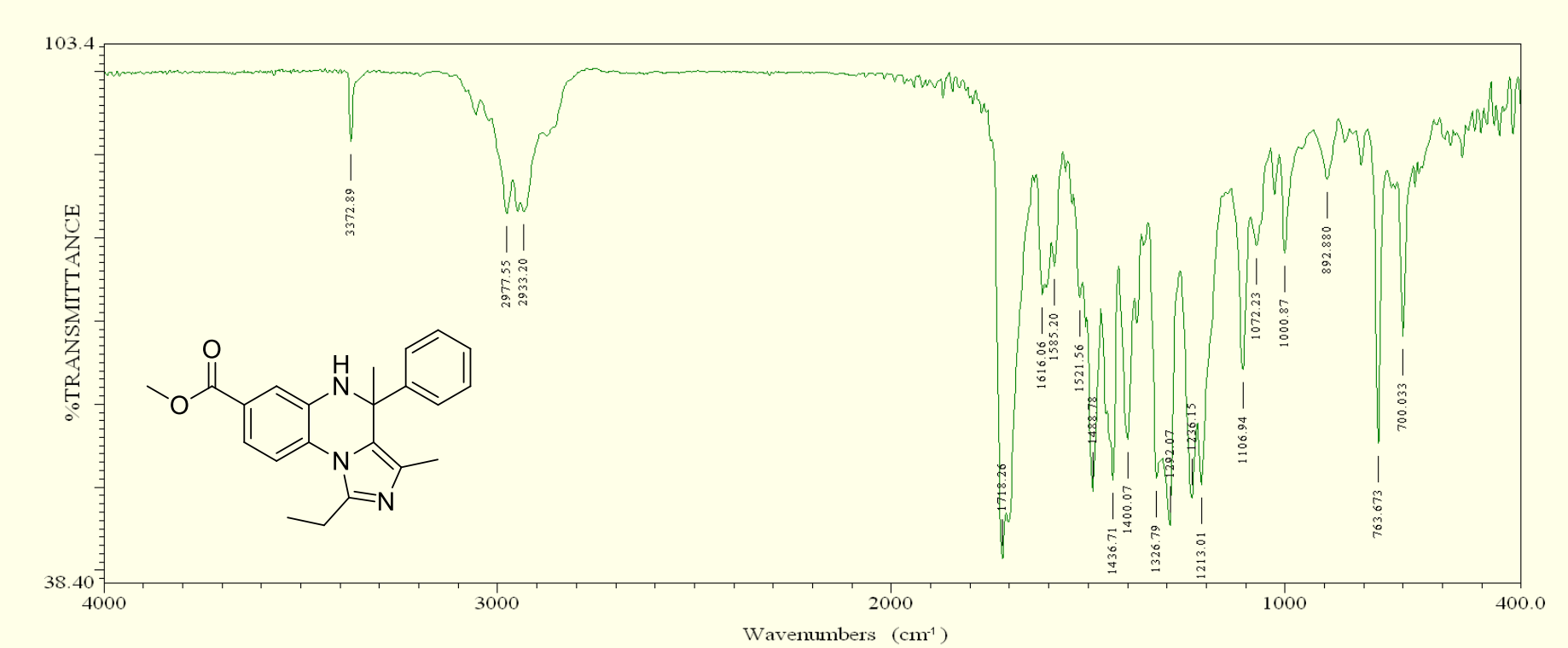
^{13}C NMR spectrum (75 MHz) of compound **12s** in $CDCl_3$



ESI-LRMS of compound **12s**

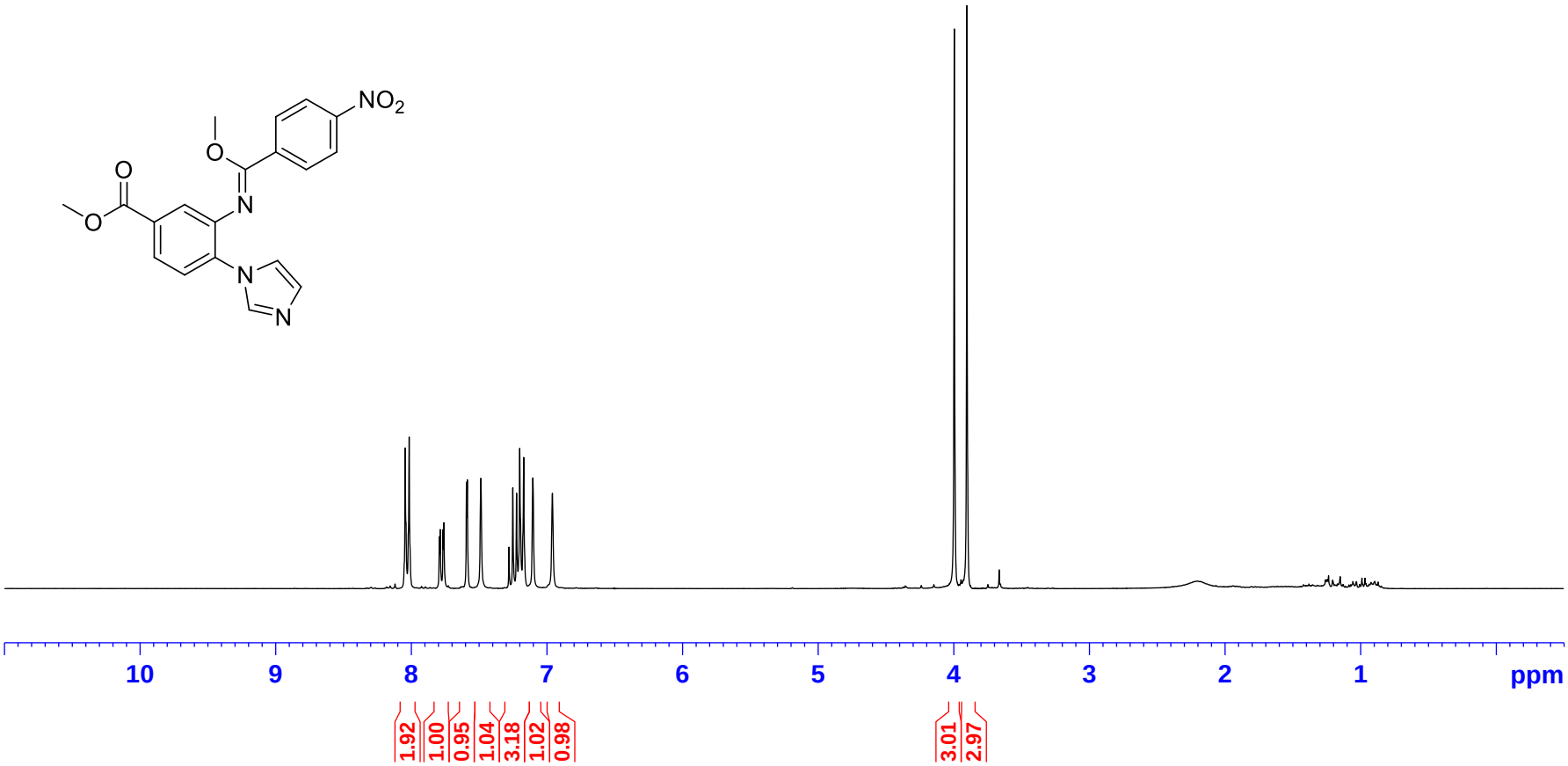


ESI-HRMS of compound **12s**

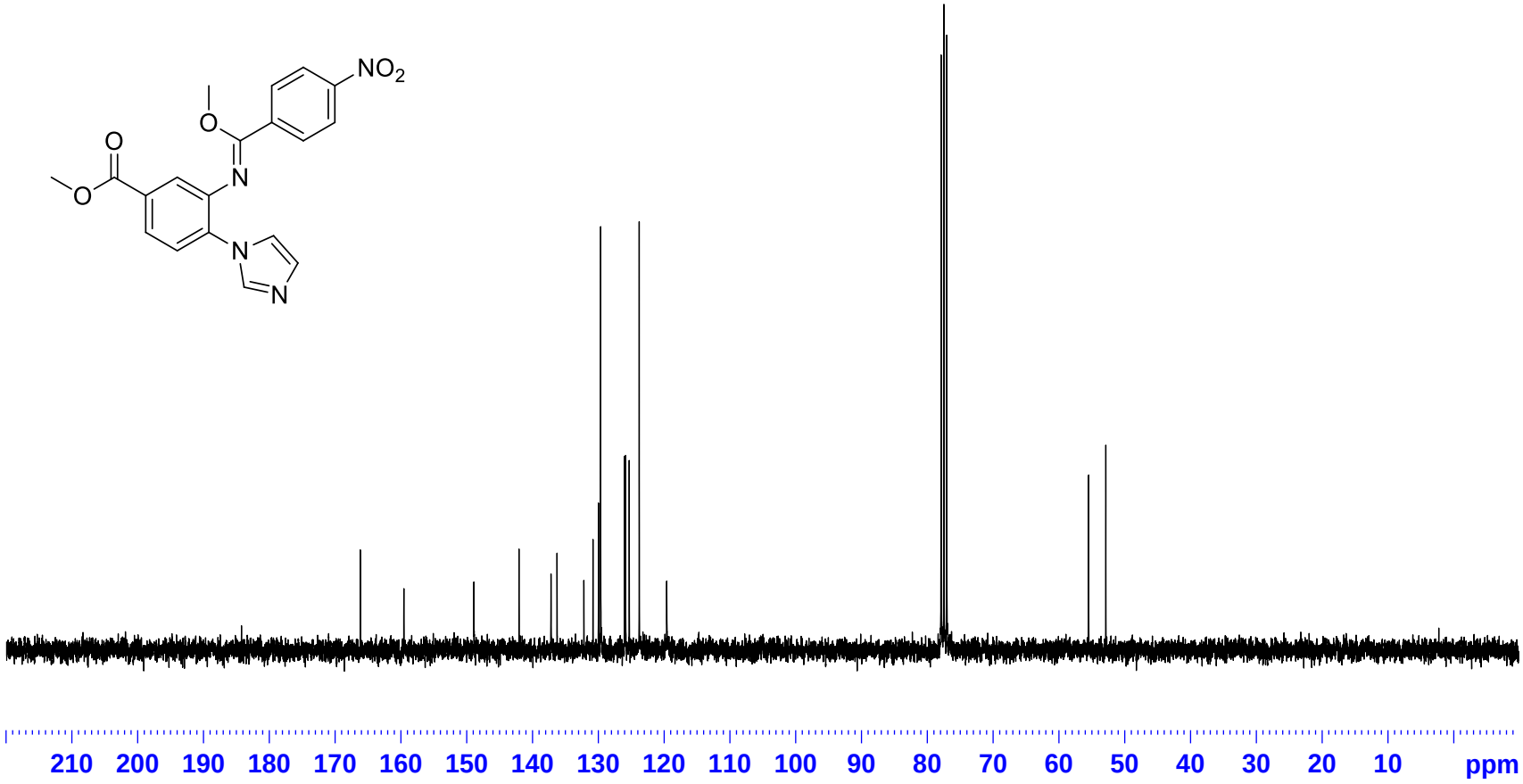


IR spectrum of compound **12s**

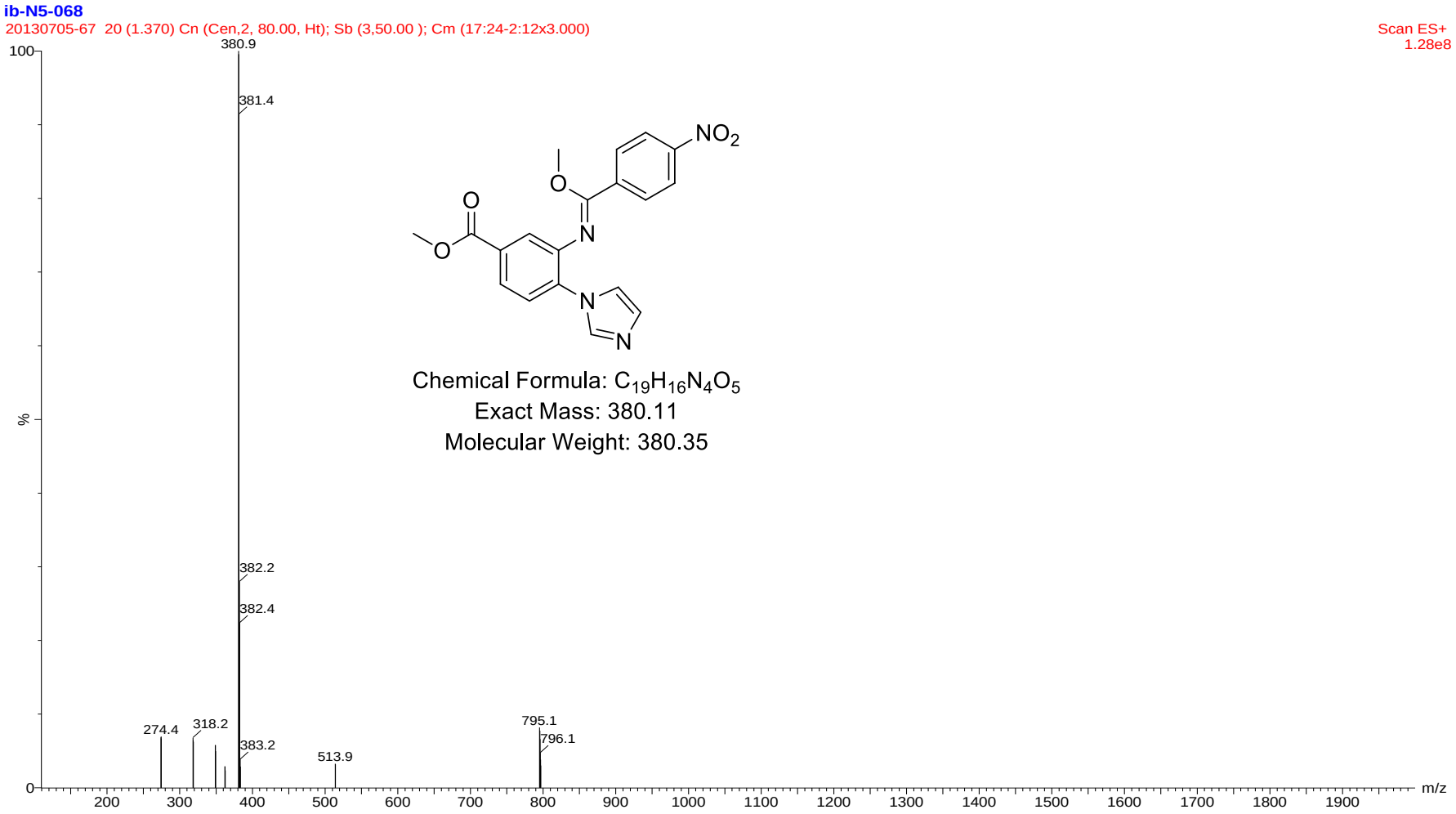
8. ^{1}H NMR, ^{13}C NMR, LRMS and HRMS of Compound 13a-i



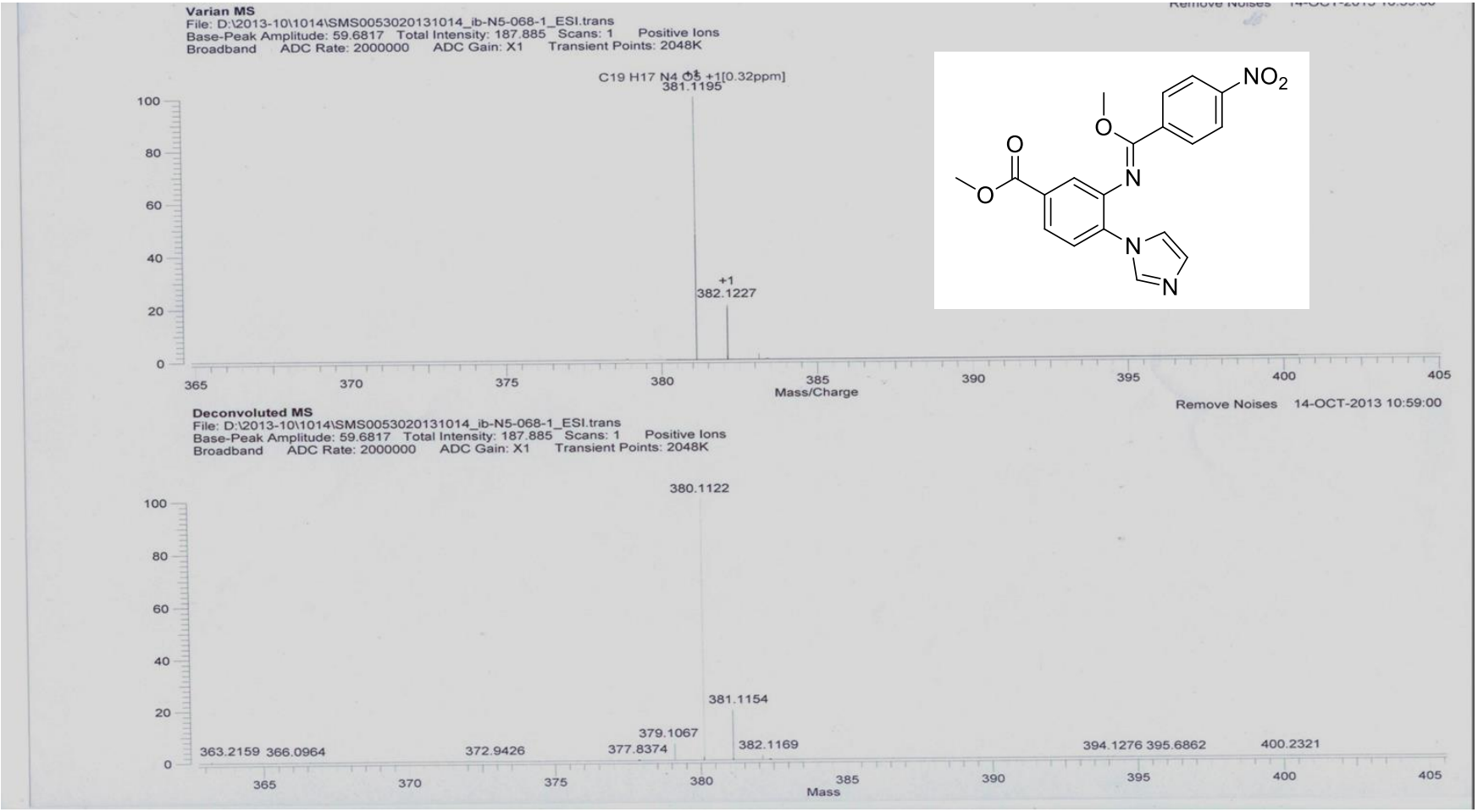
^{1}H NMR spectrum (300 MHz) of compound **13a** in $CDCl_3$



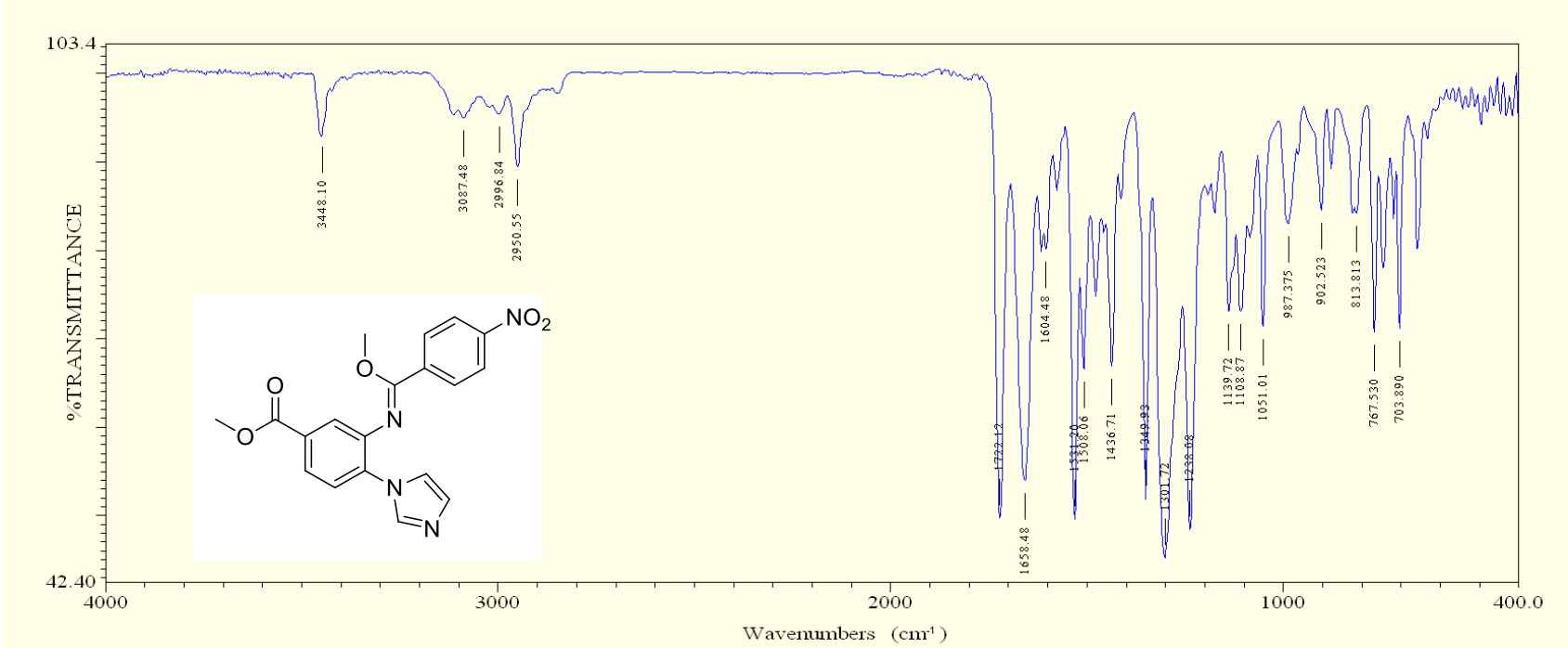
^{13}C NMR spectrum (75 MHz) of compound **13a** in $CDCl_3$



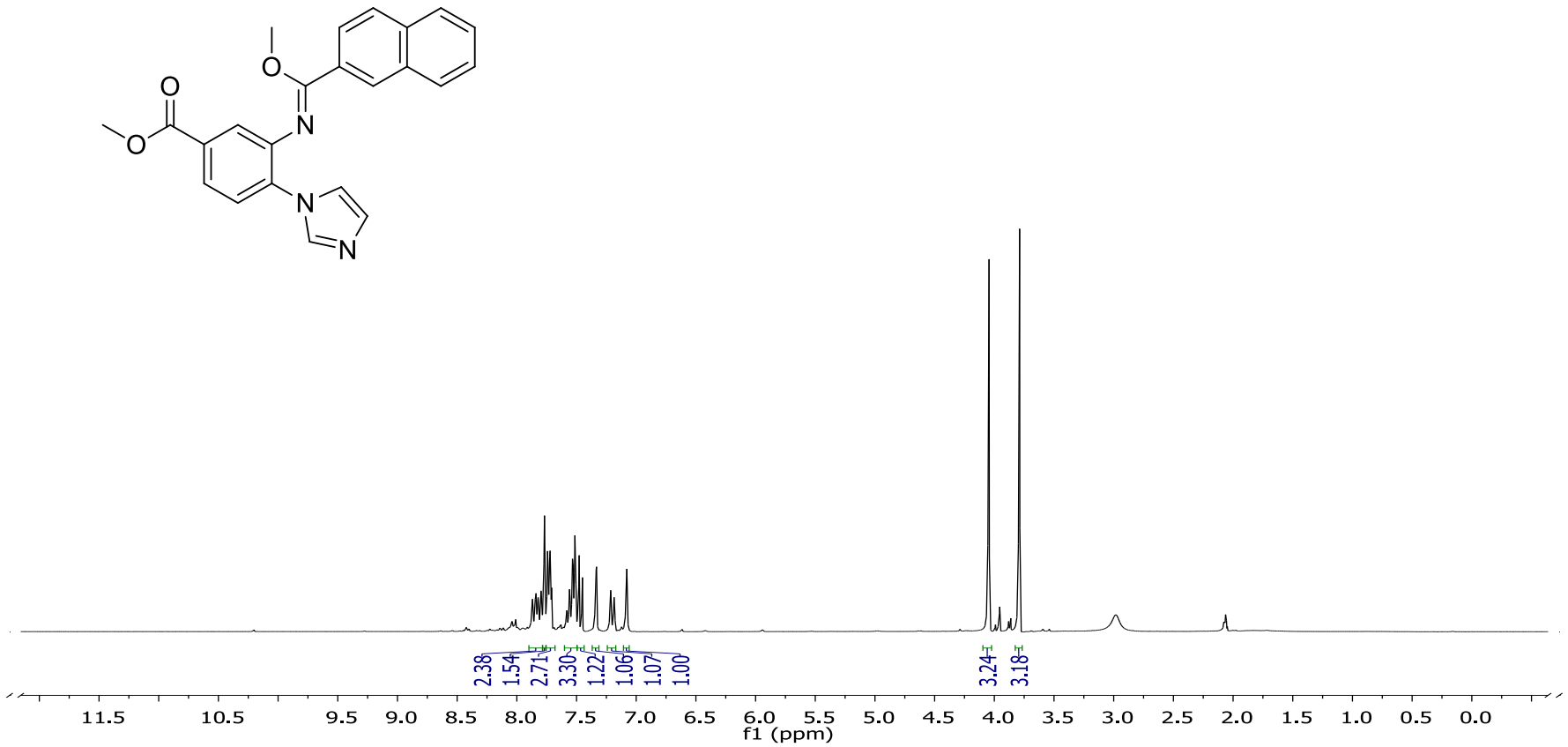
ESI-LRMS of compound **13a**



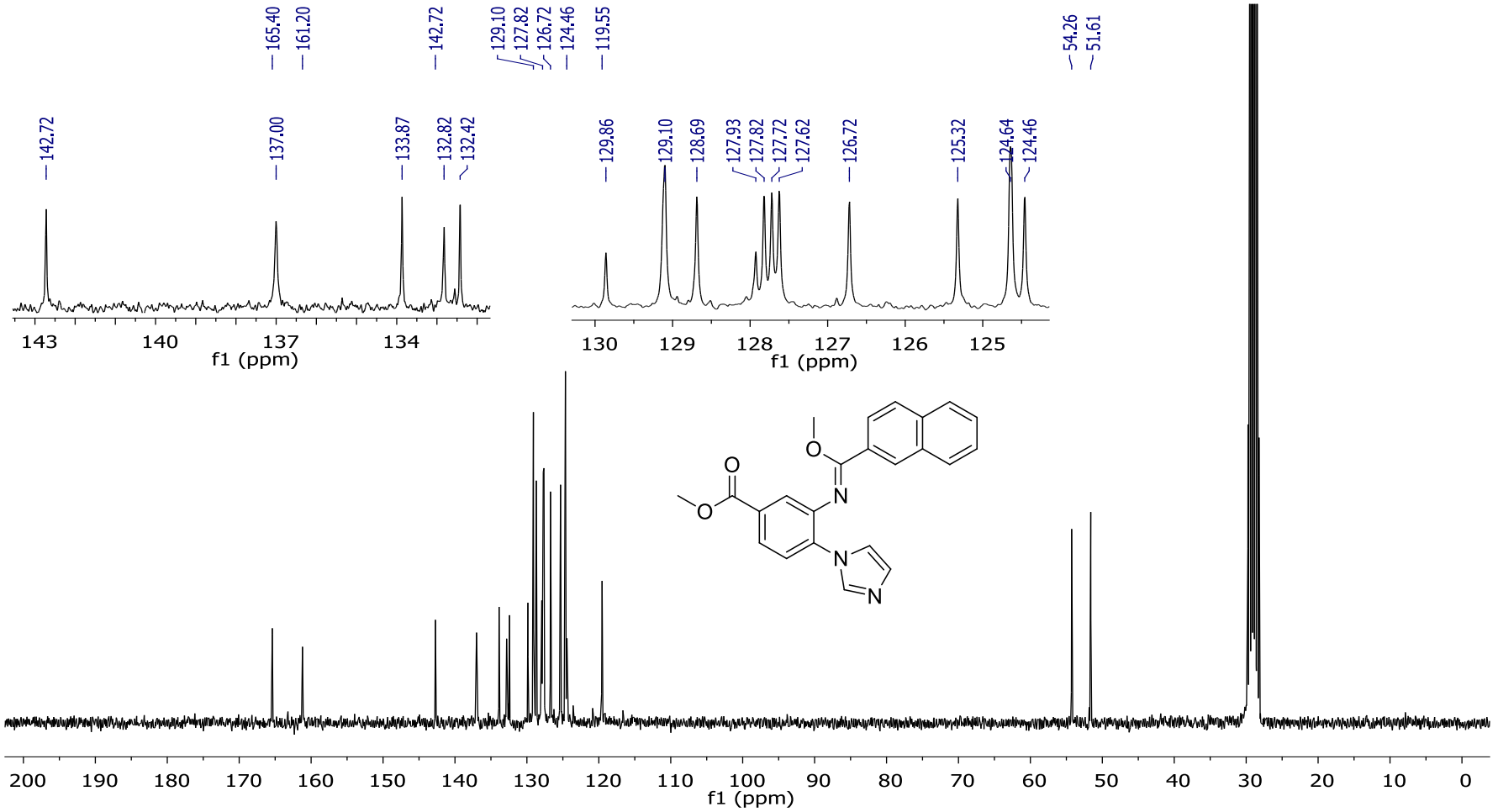
ESI-HRMS of compound **13a**



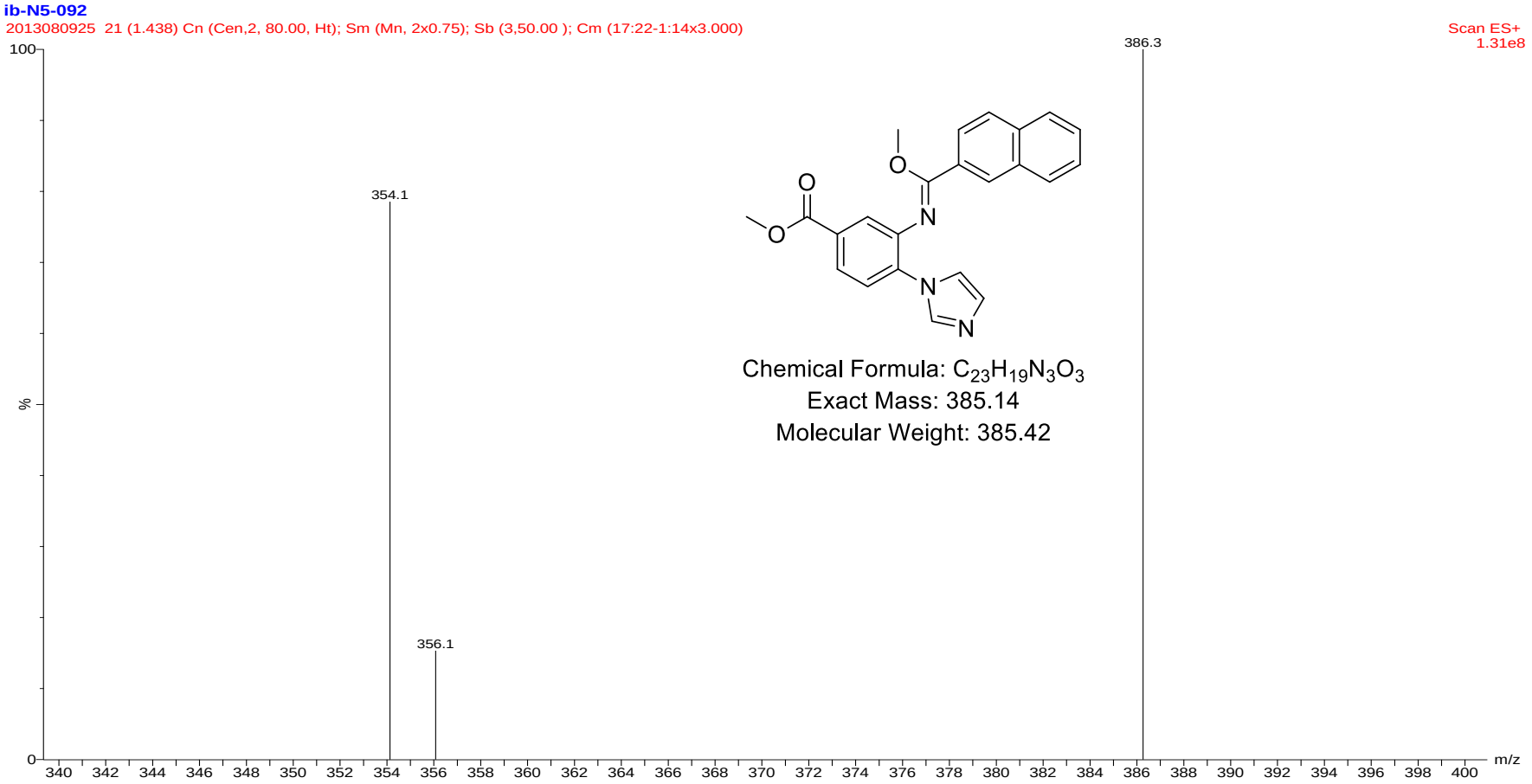
IR spectrum of compound **13a**



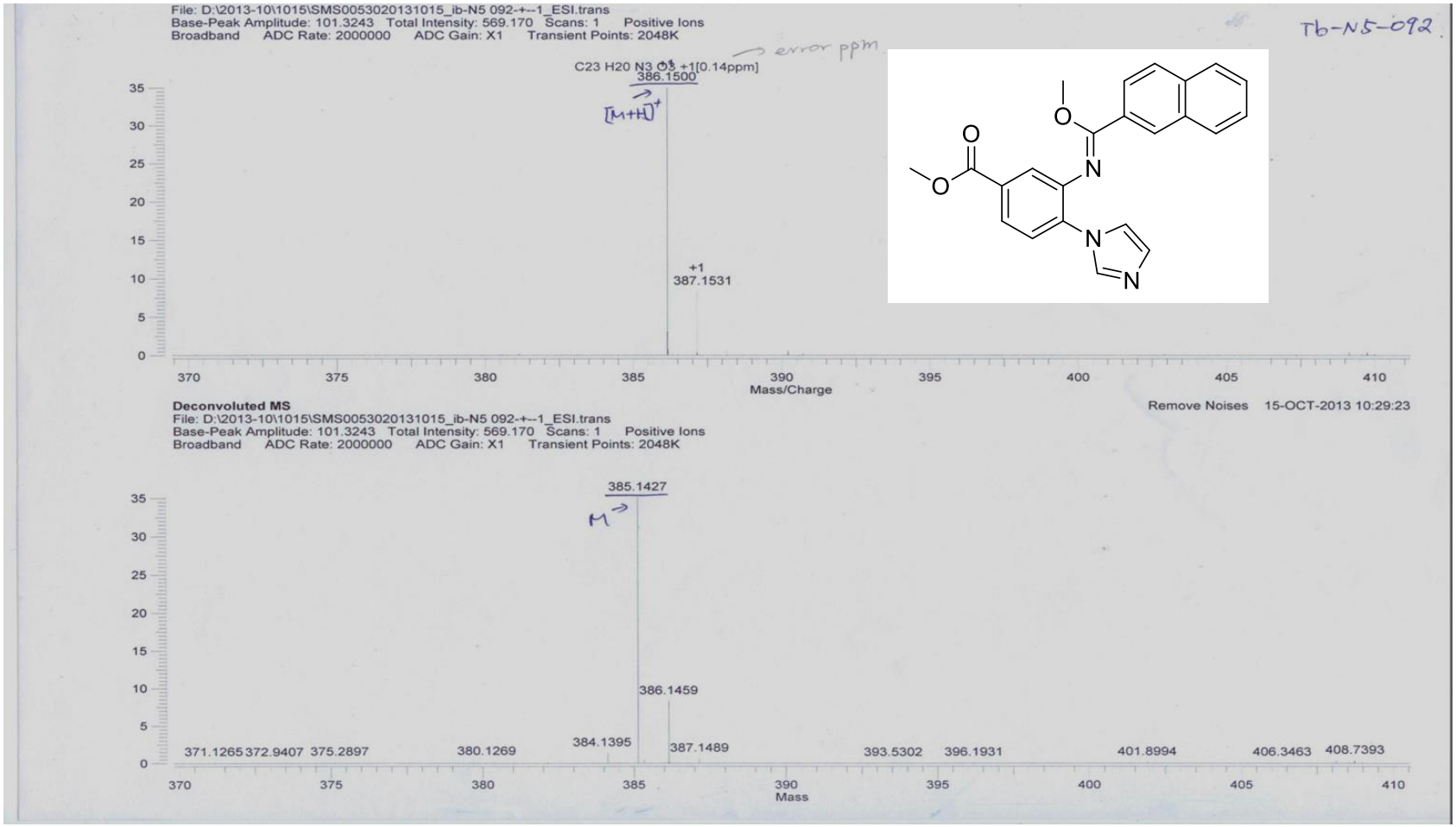
^{1}H NMR spectrum (400 MHz) of compound **13b** in Acetone-d_6



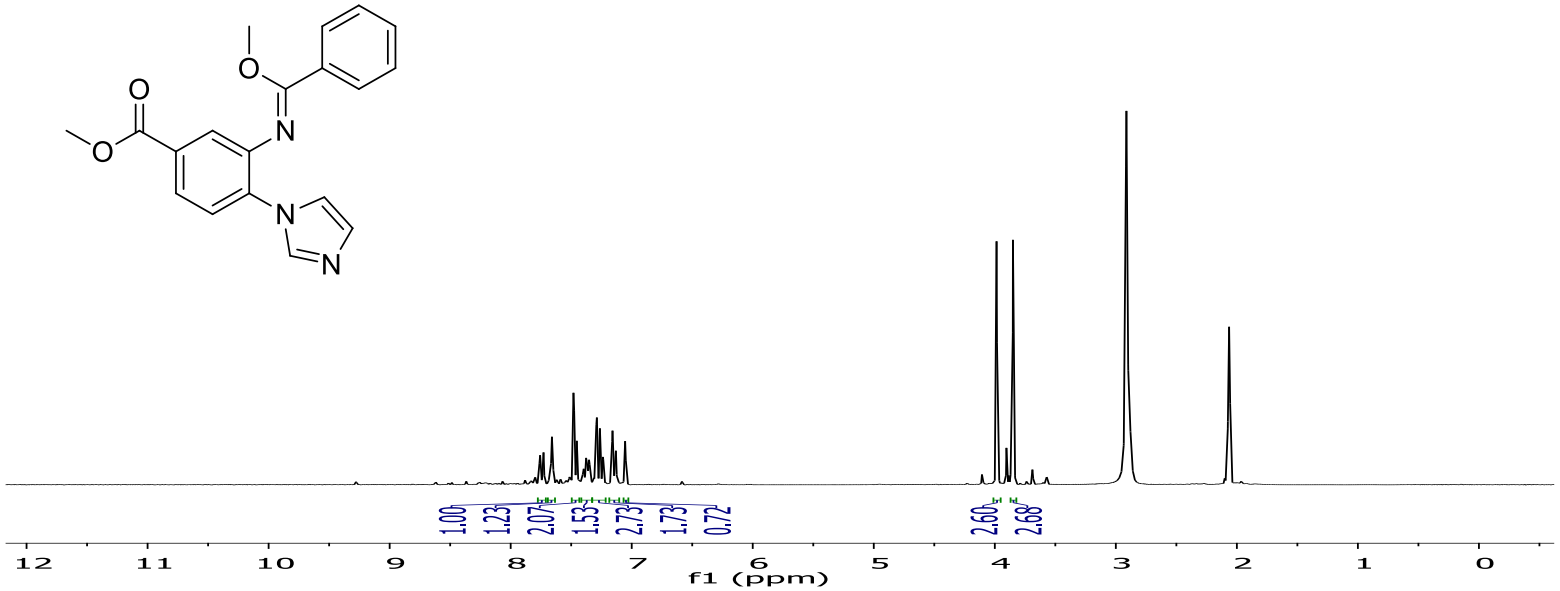
^{13}C NMR spectrum (101 MHz) of compound **13b** in Acetone-d_6



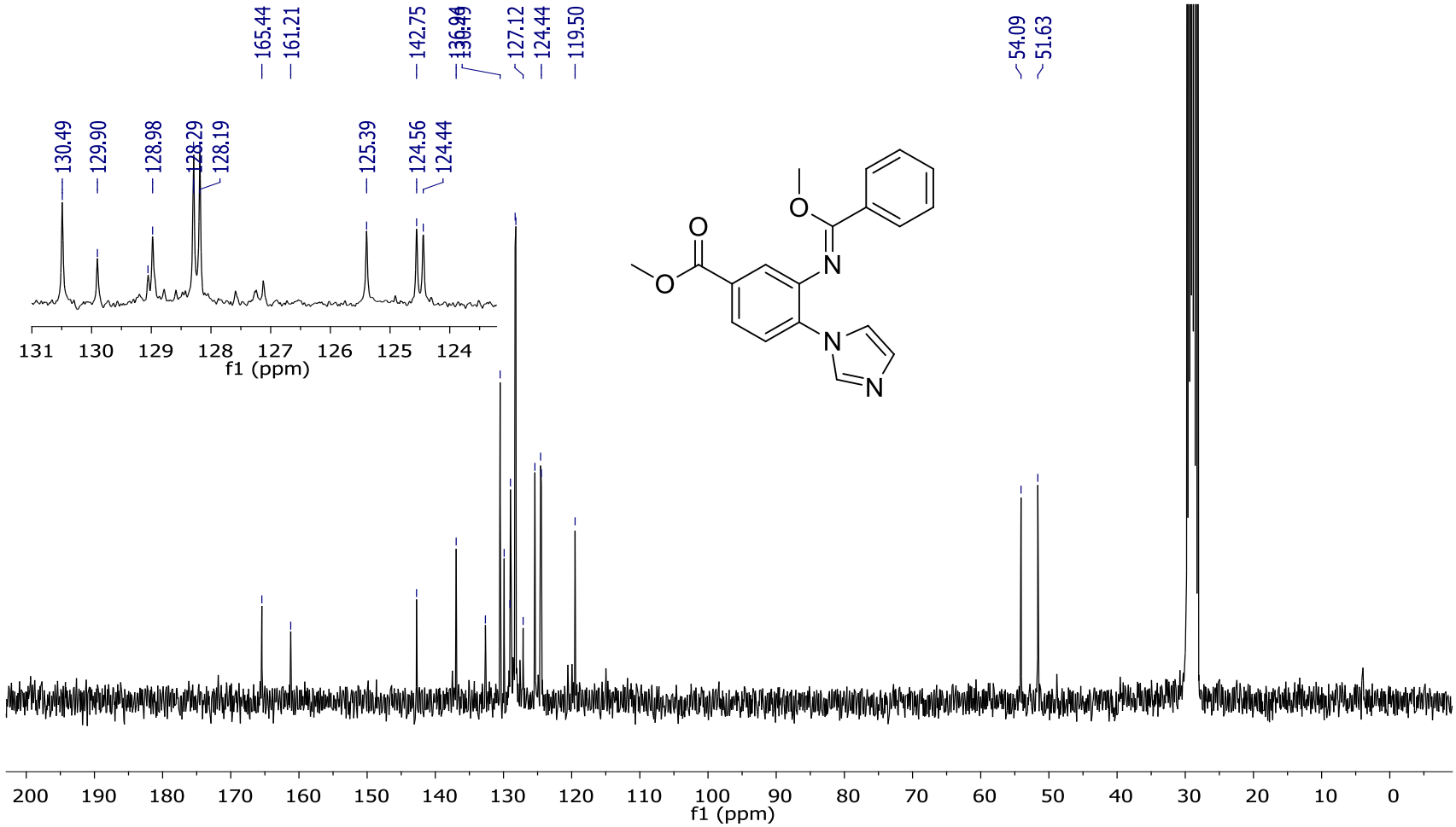
ESI-LRMS of compound **13b**



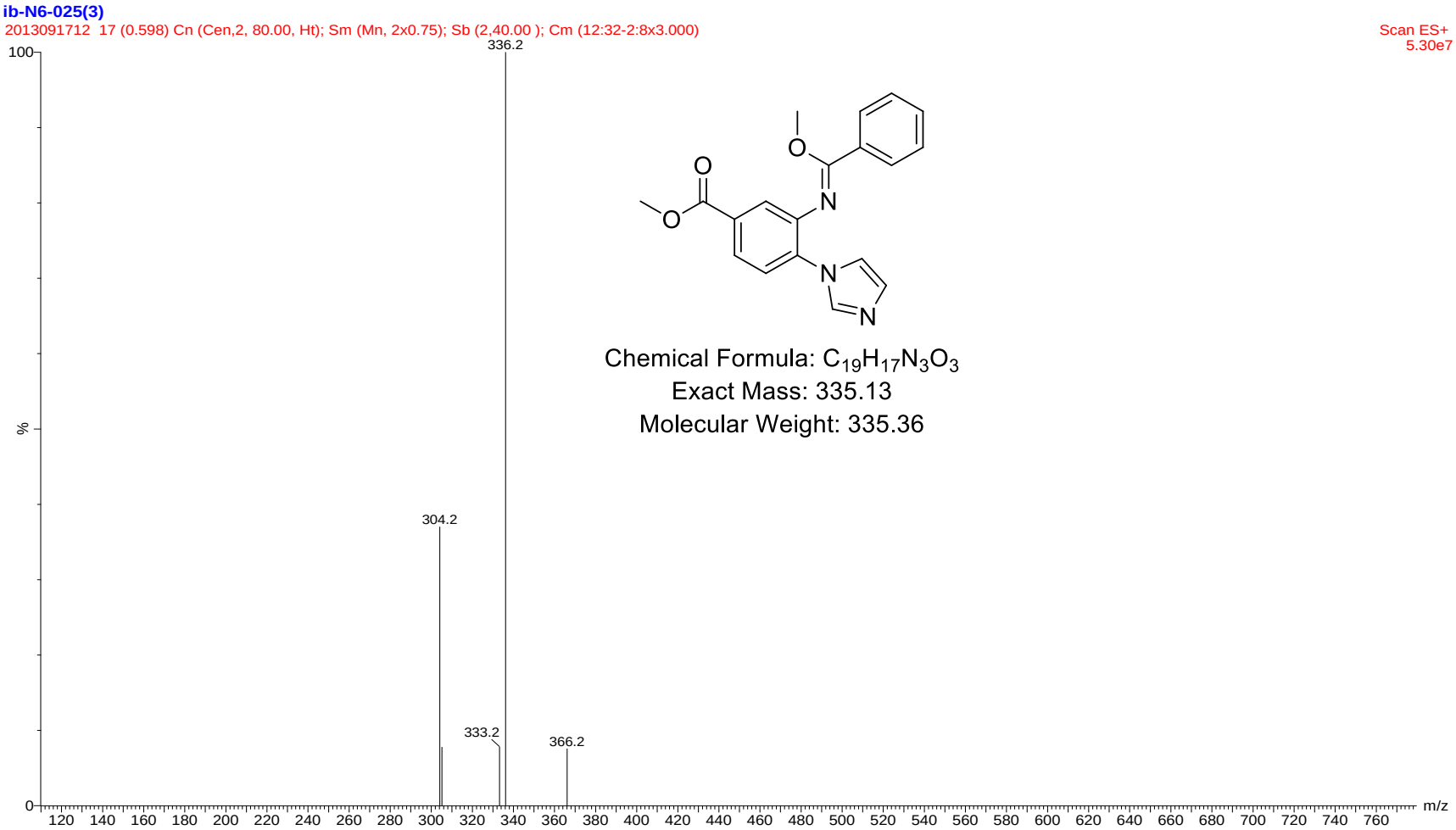
ESI-HRMS of compound **13b**



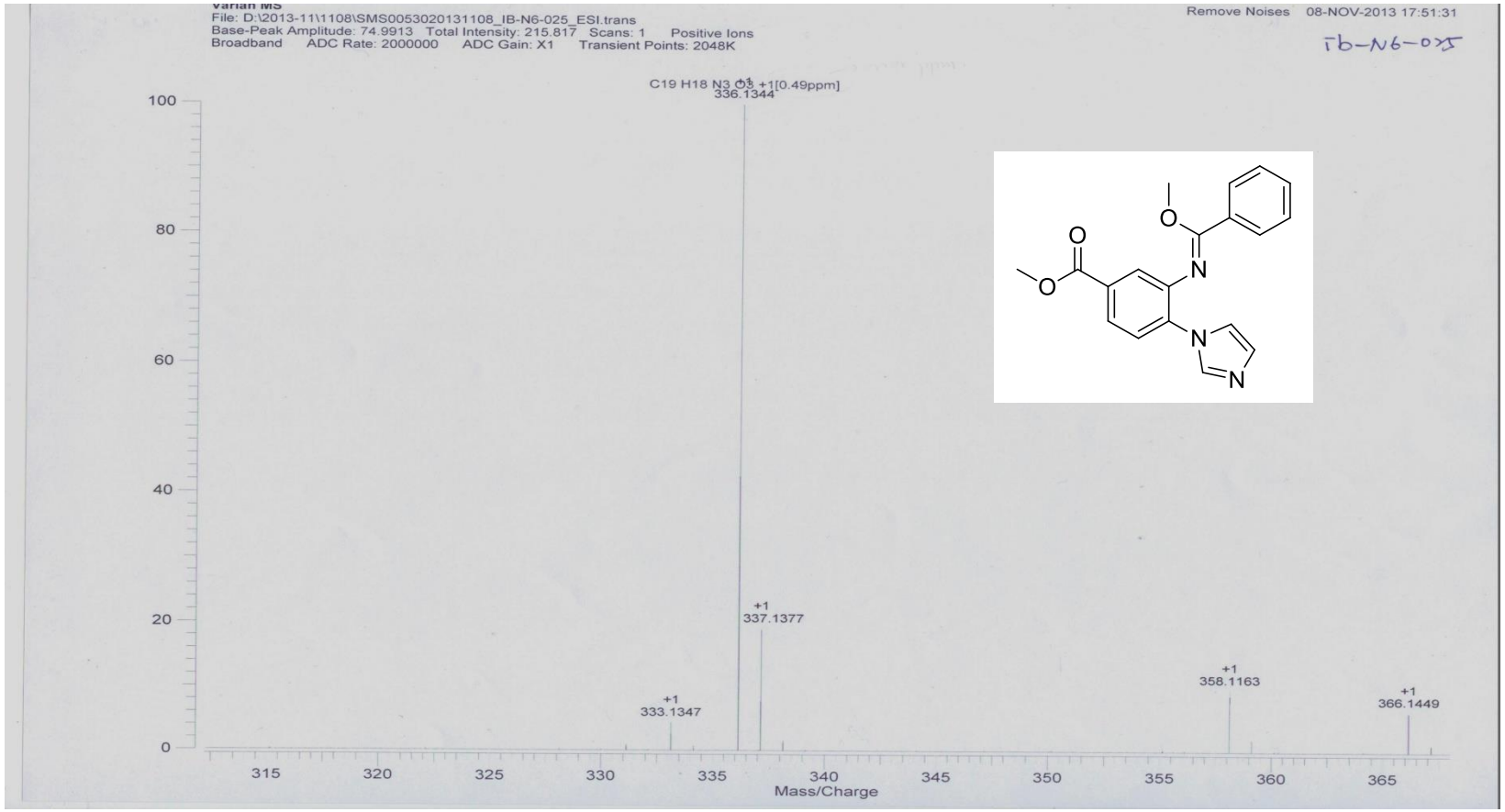
^{1}H NMR spectrum (400 MHz) of compound **13c** in Acetone-d_6



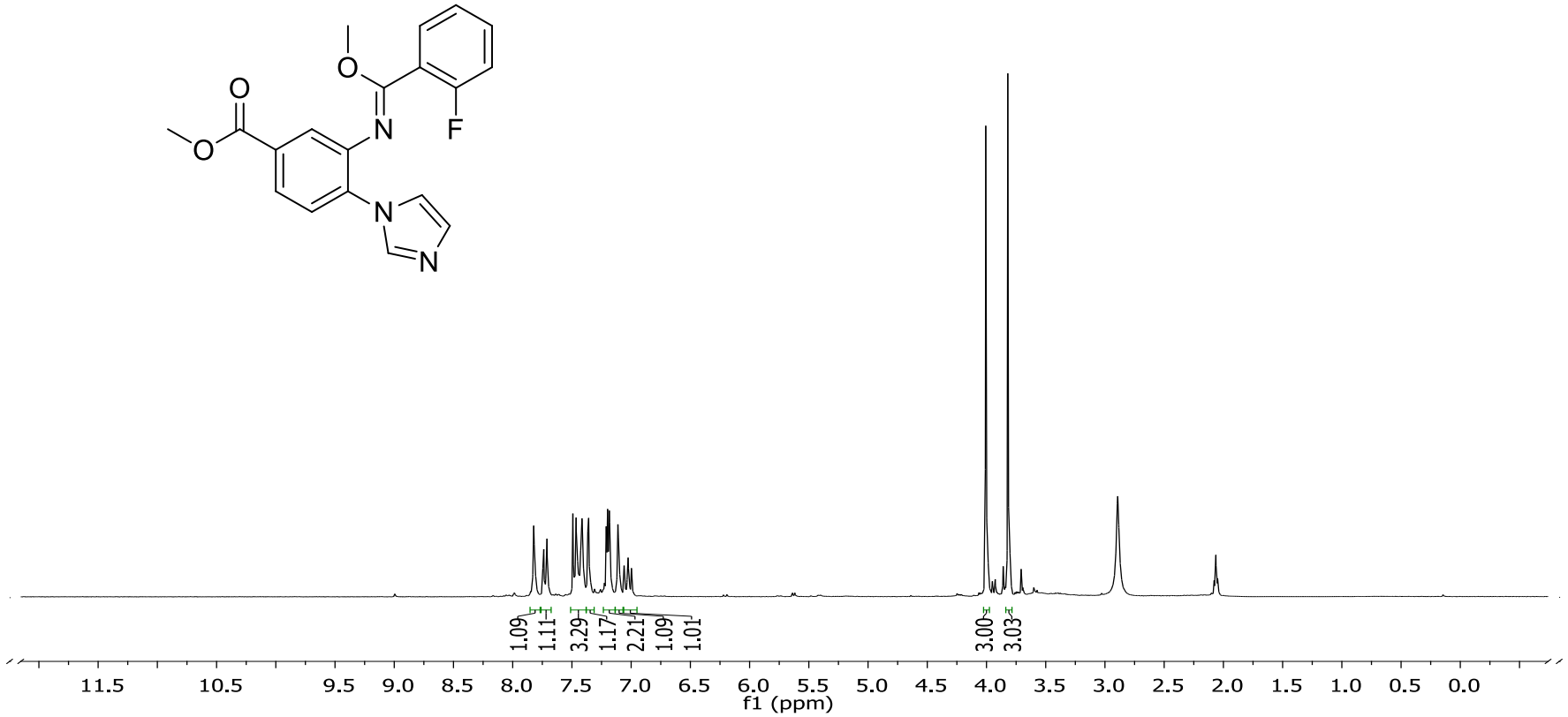
^{13}C NMR spectrum (101 MHz) of compound **13c** in Acetone-d_6



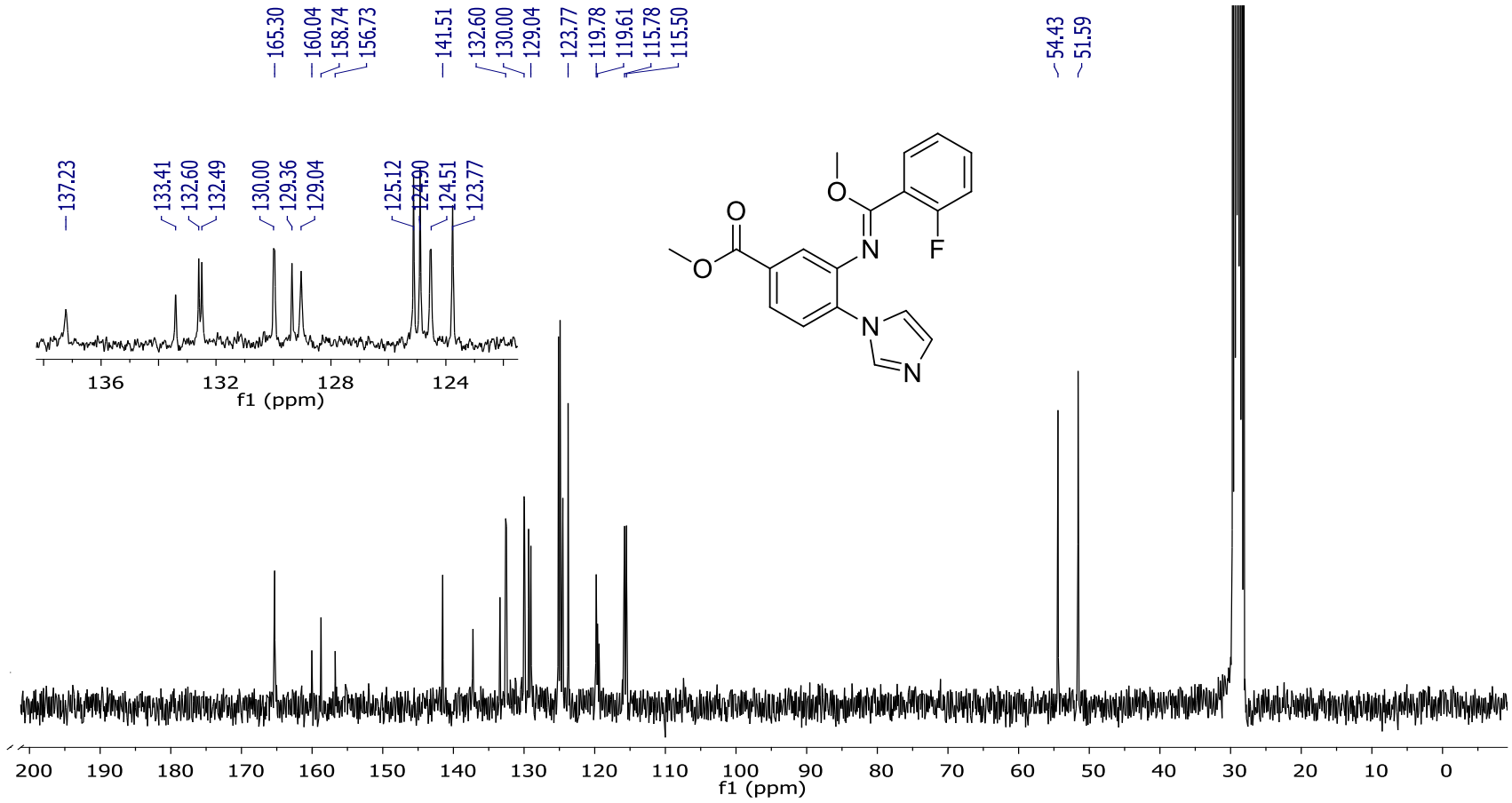
ESI-LRMS of compound **13c**



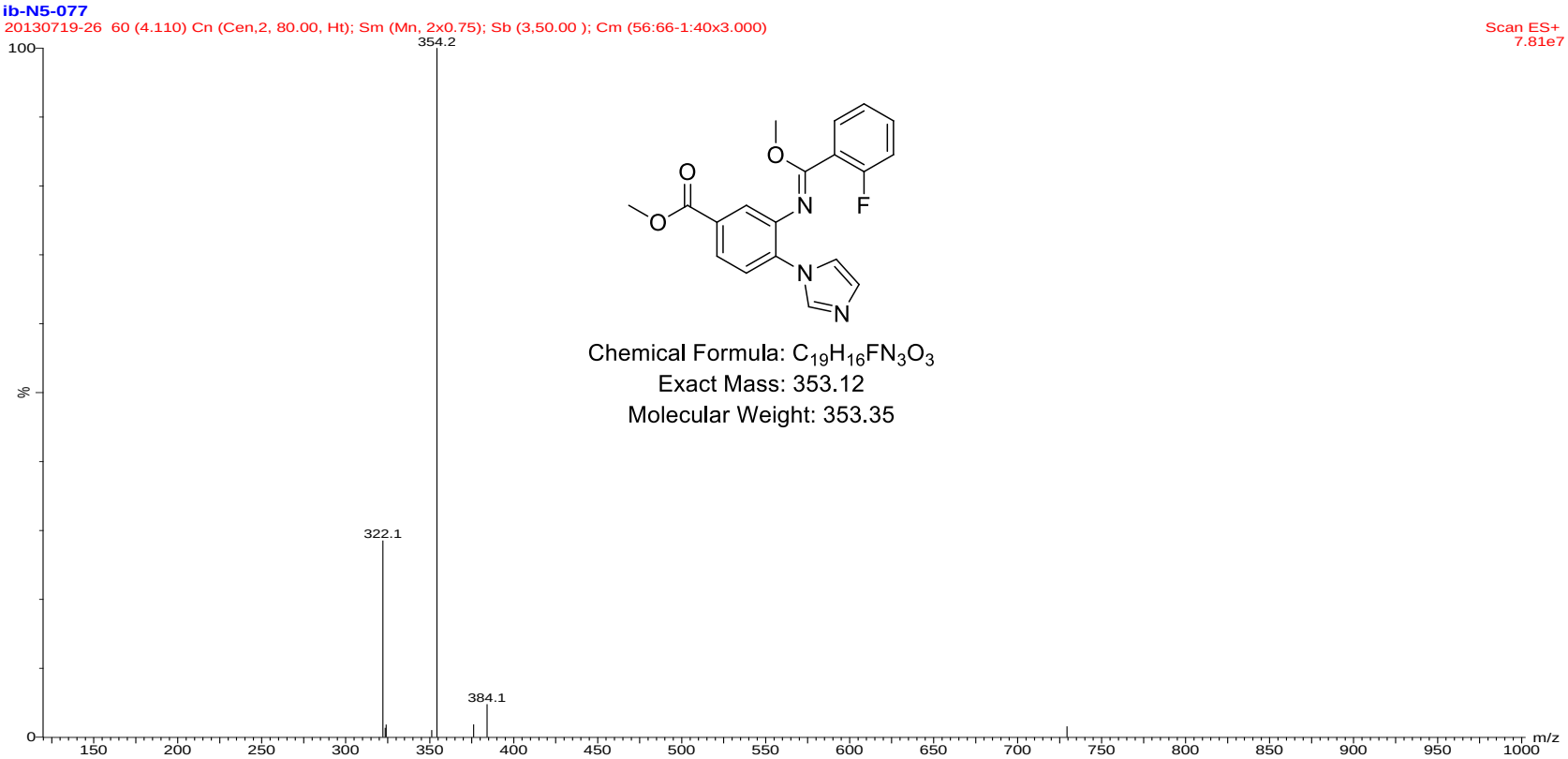
ESI-HRMS of compound **13c**



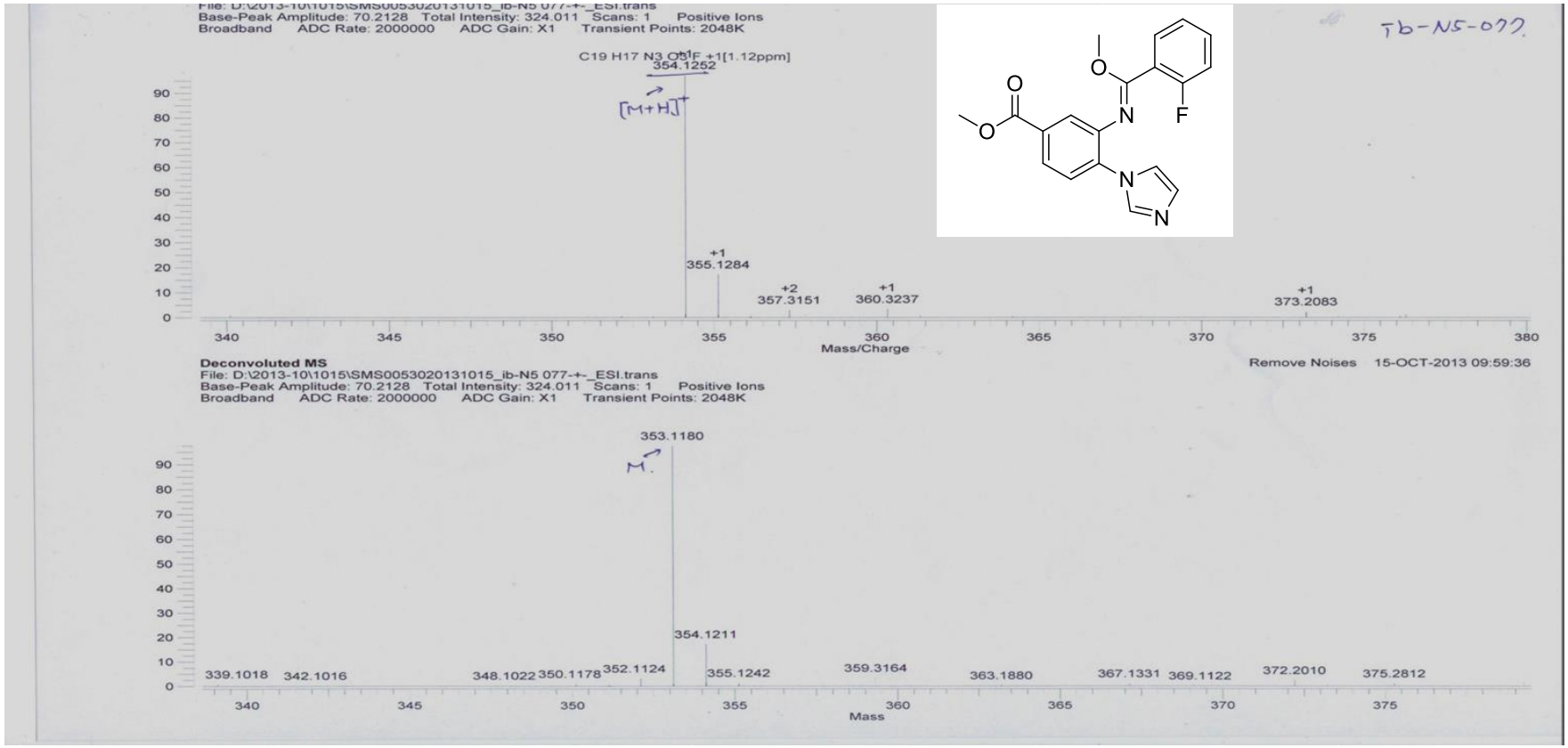
^{1}H NMR spectrum (400 MHz) of compound **13d** in Acetone-d_6



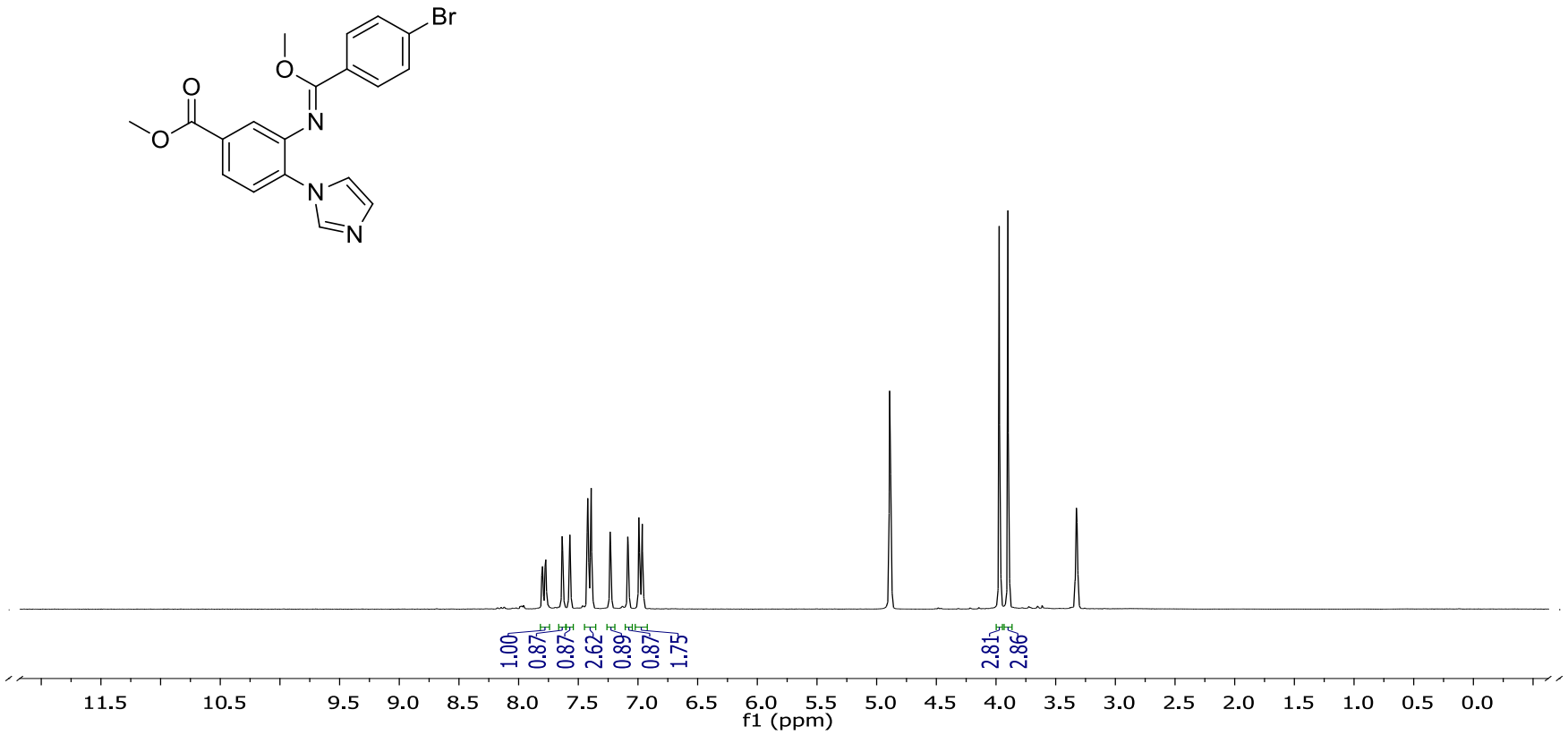
^{13}C NMR spectrum (101 MHz) of compound **13d** in Acetone-d_6



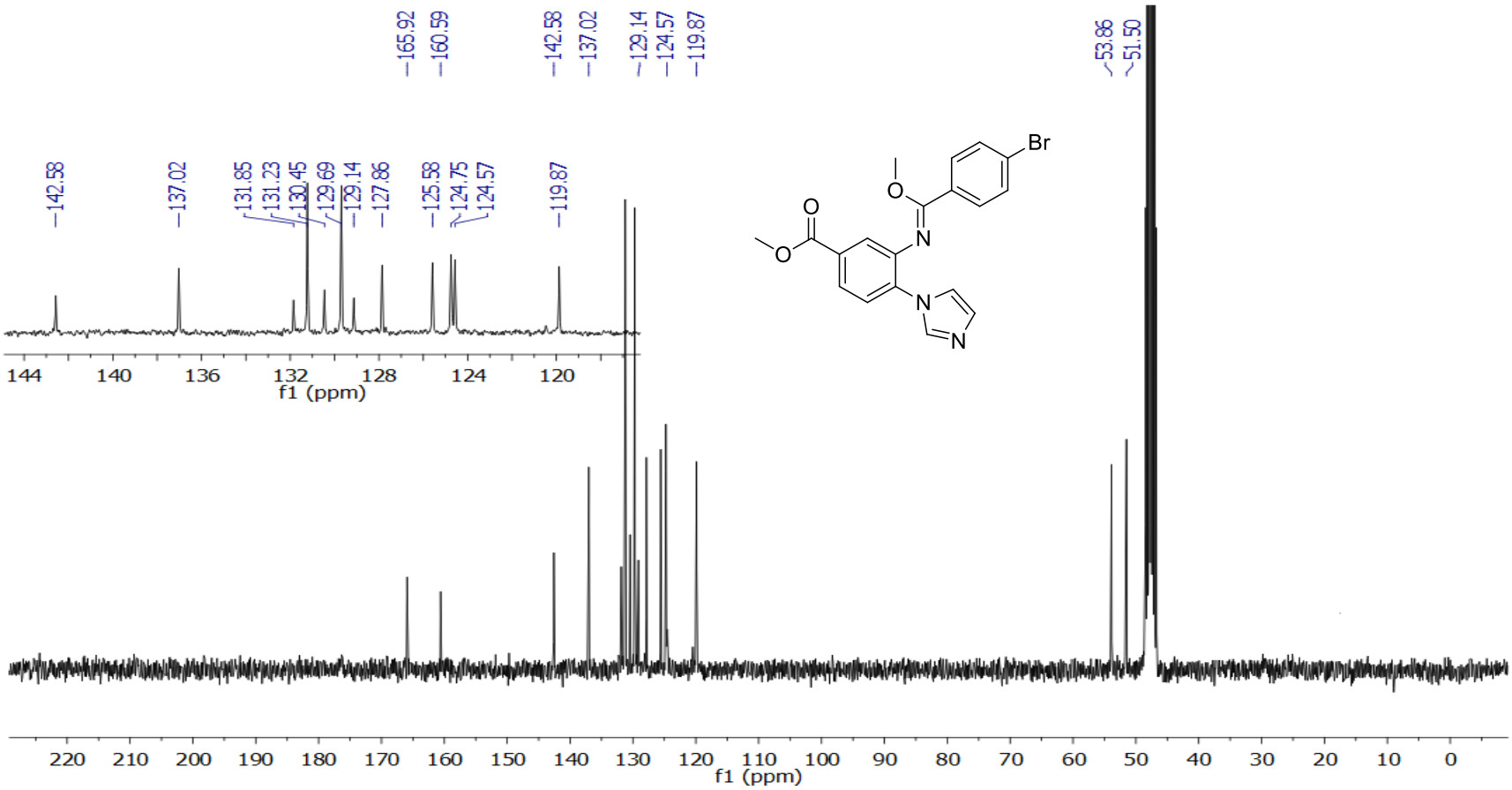
ESI-LRMS of compound **13d**



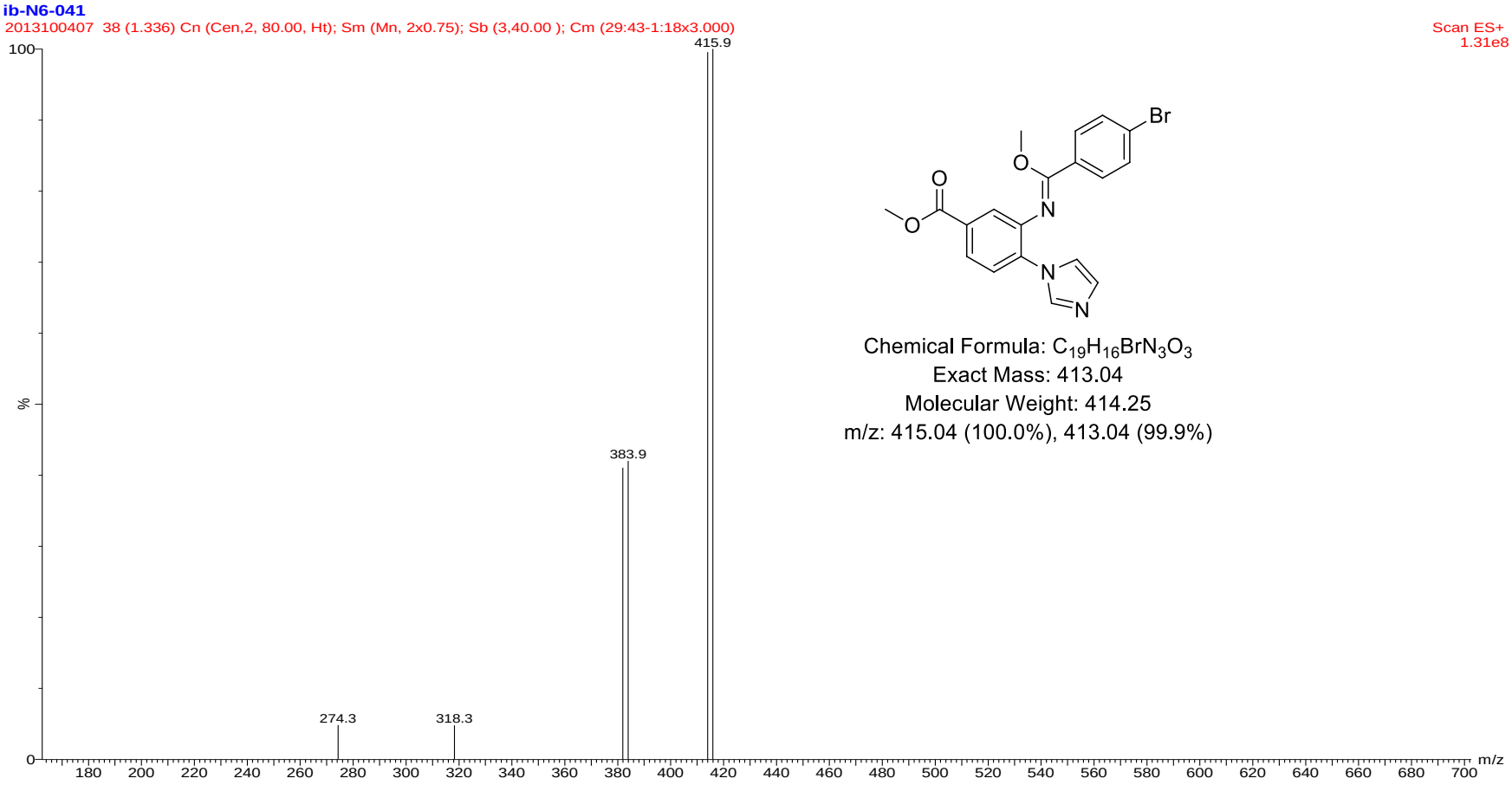
ESI-HRMS of compound **13d**



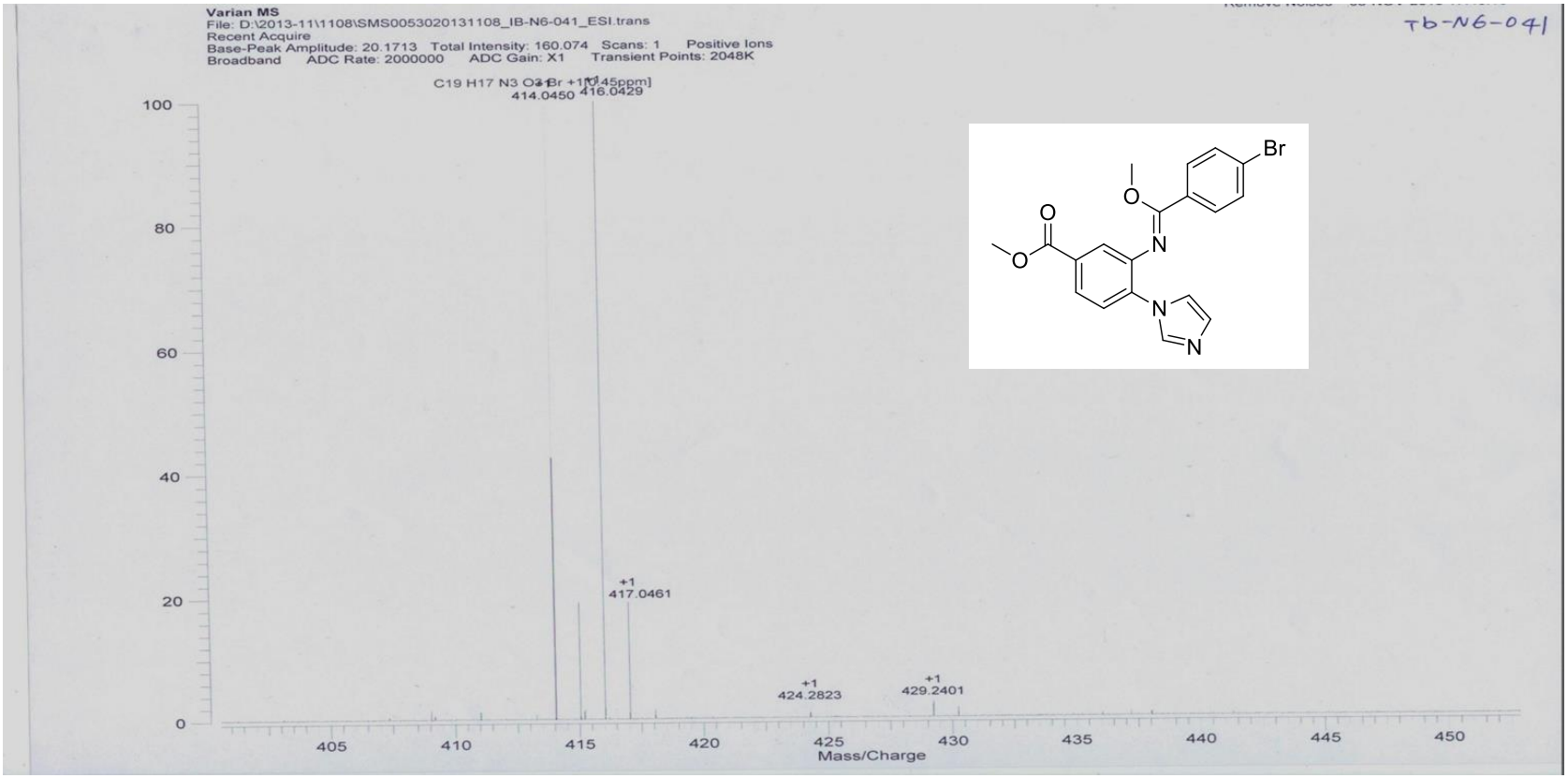
^{1}H NMR spectrum (400 MHz) of compound **13e** in Acetone-d_6



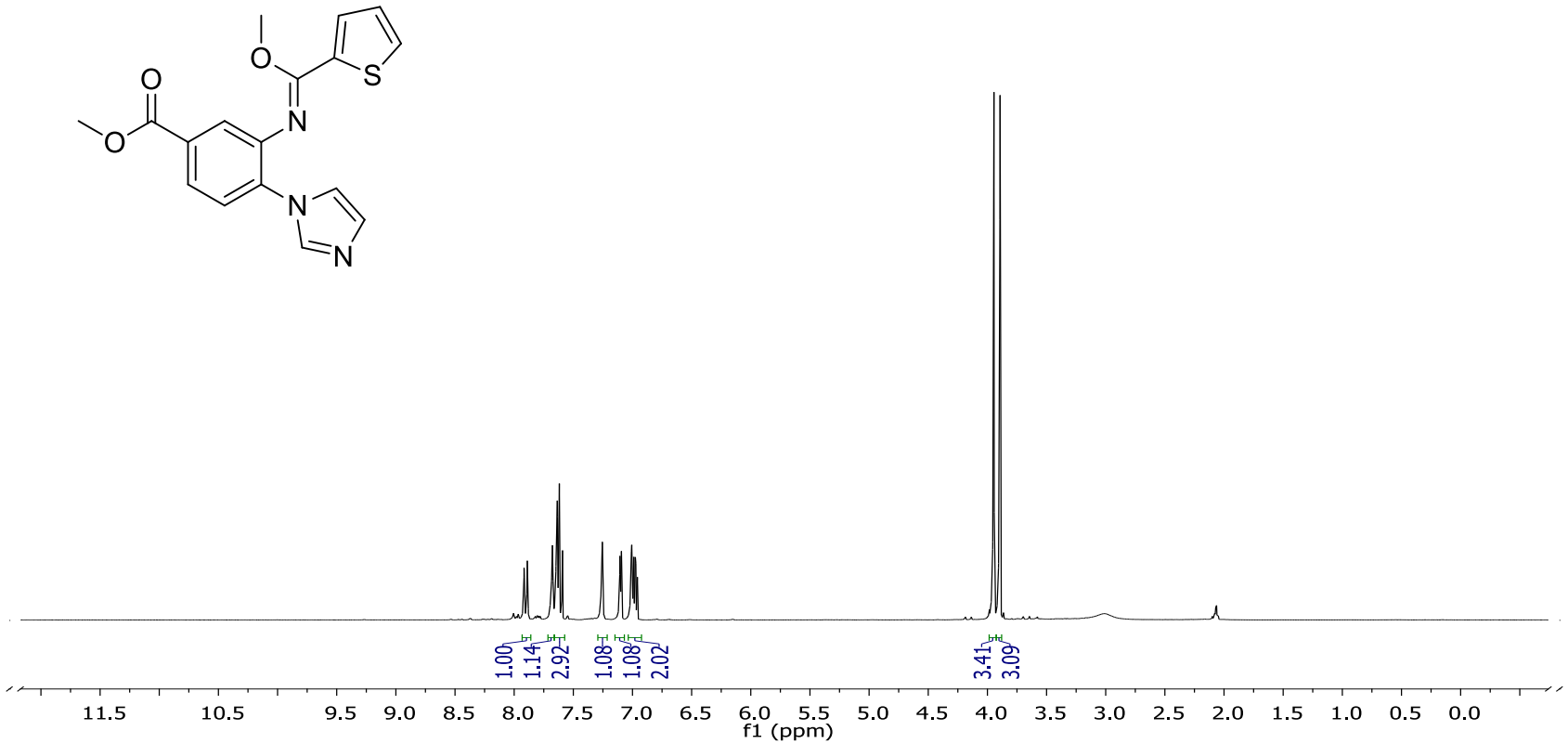
^{13}C NMR spectrum (101 MHz) of compound **13e** in Acetone-d_6



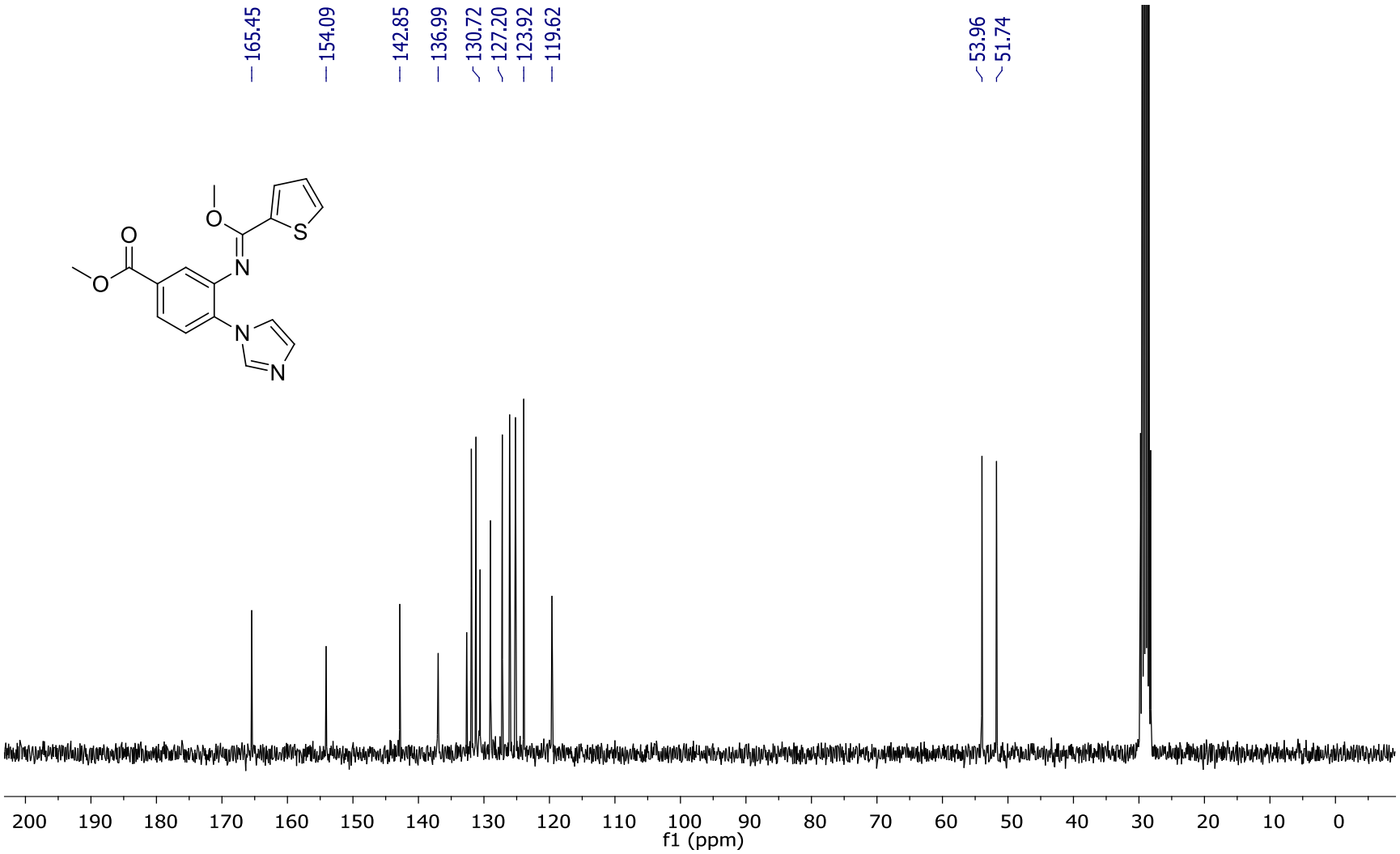
ESI-LRMS of compound **13e**



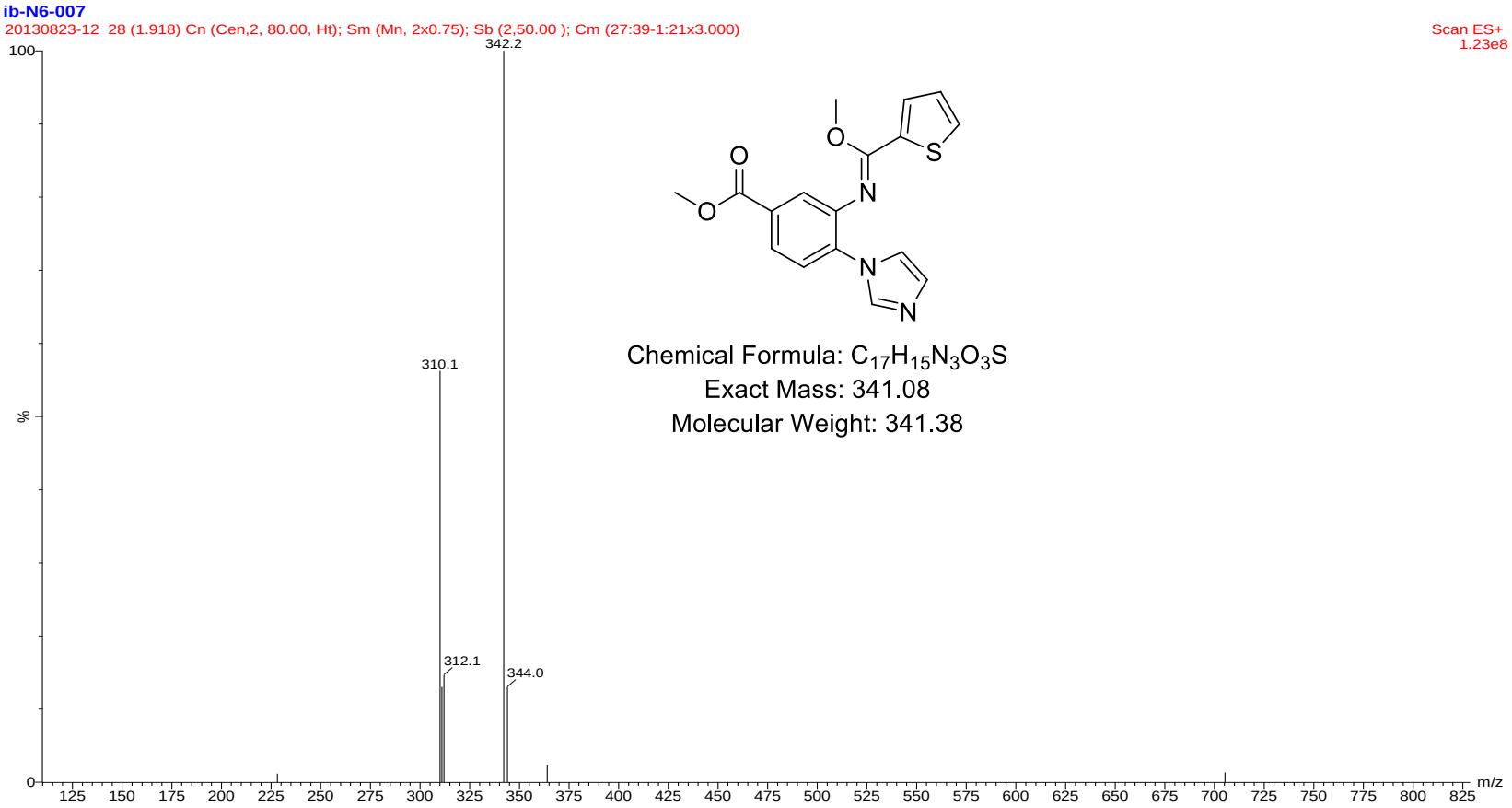
ESI-HRMS of compound **13e**



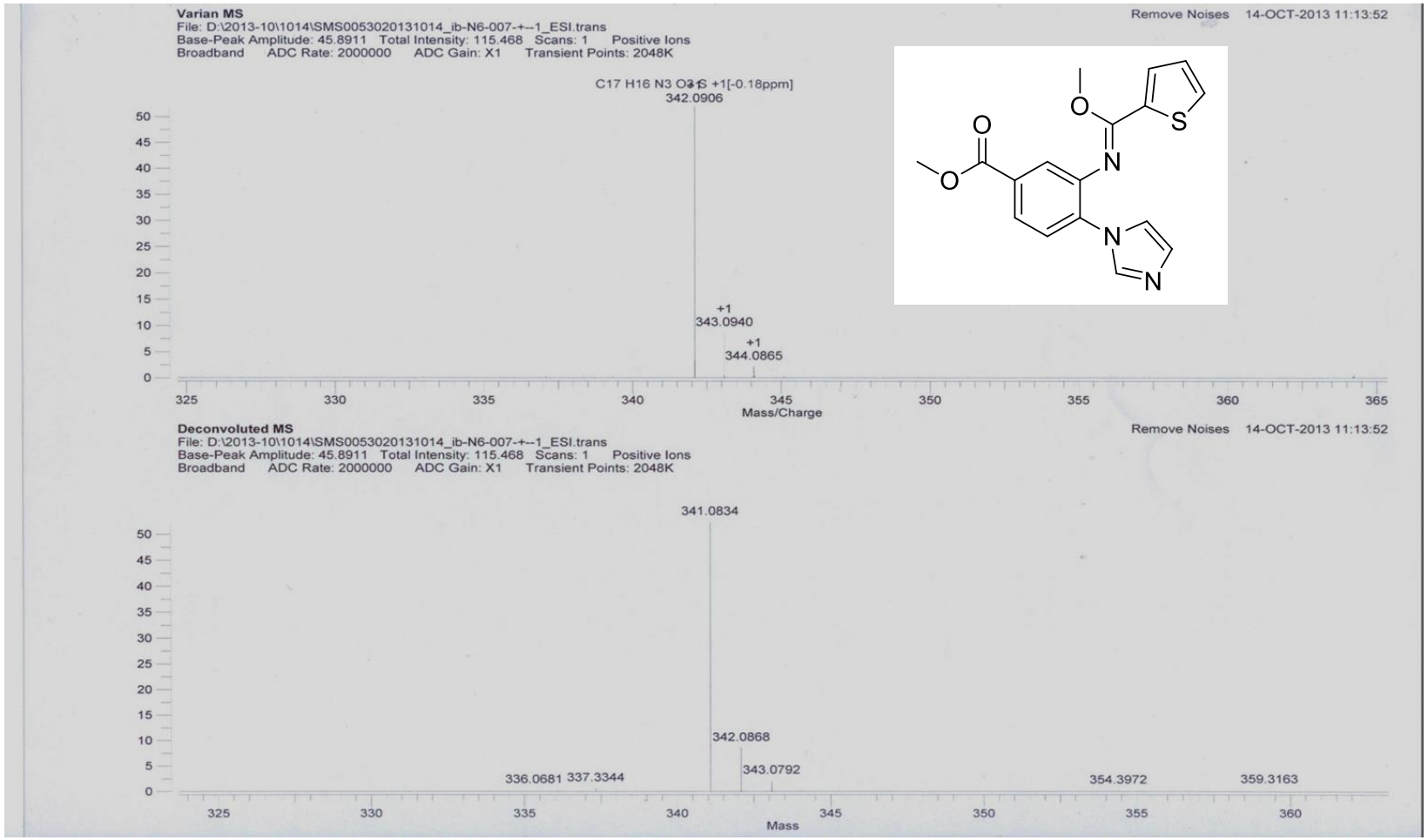
^{1}H NMR spectrum (400 MHz) of compound **13f** in Acetone-d_6



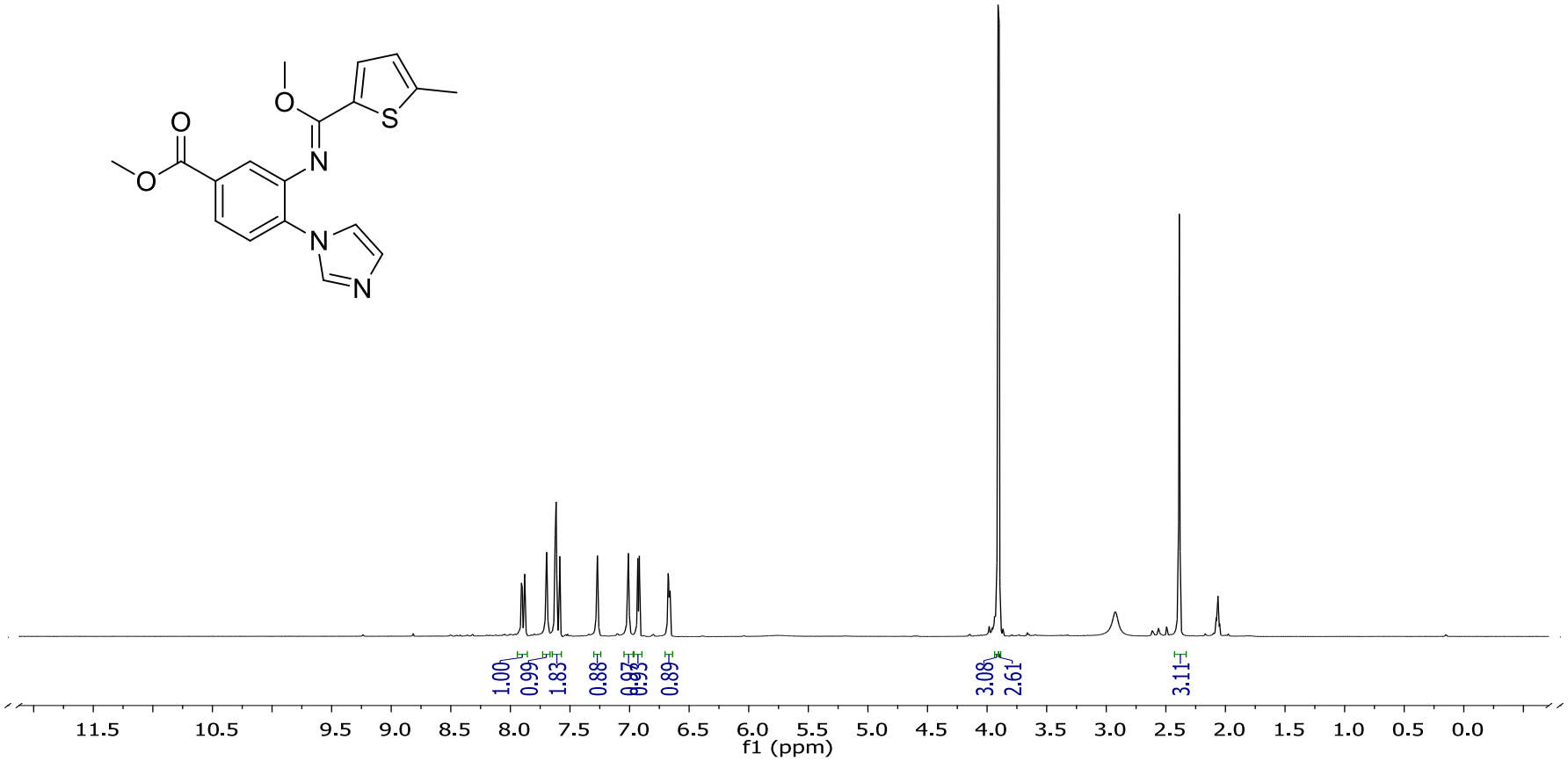
^{13}C NMR spectrum (101 MHz) of compound **13f** in Acetone-d_6



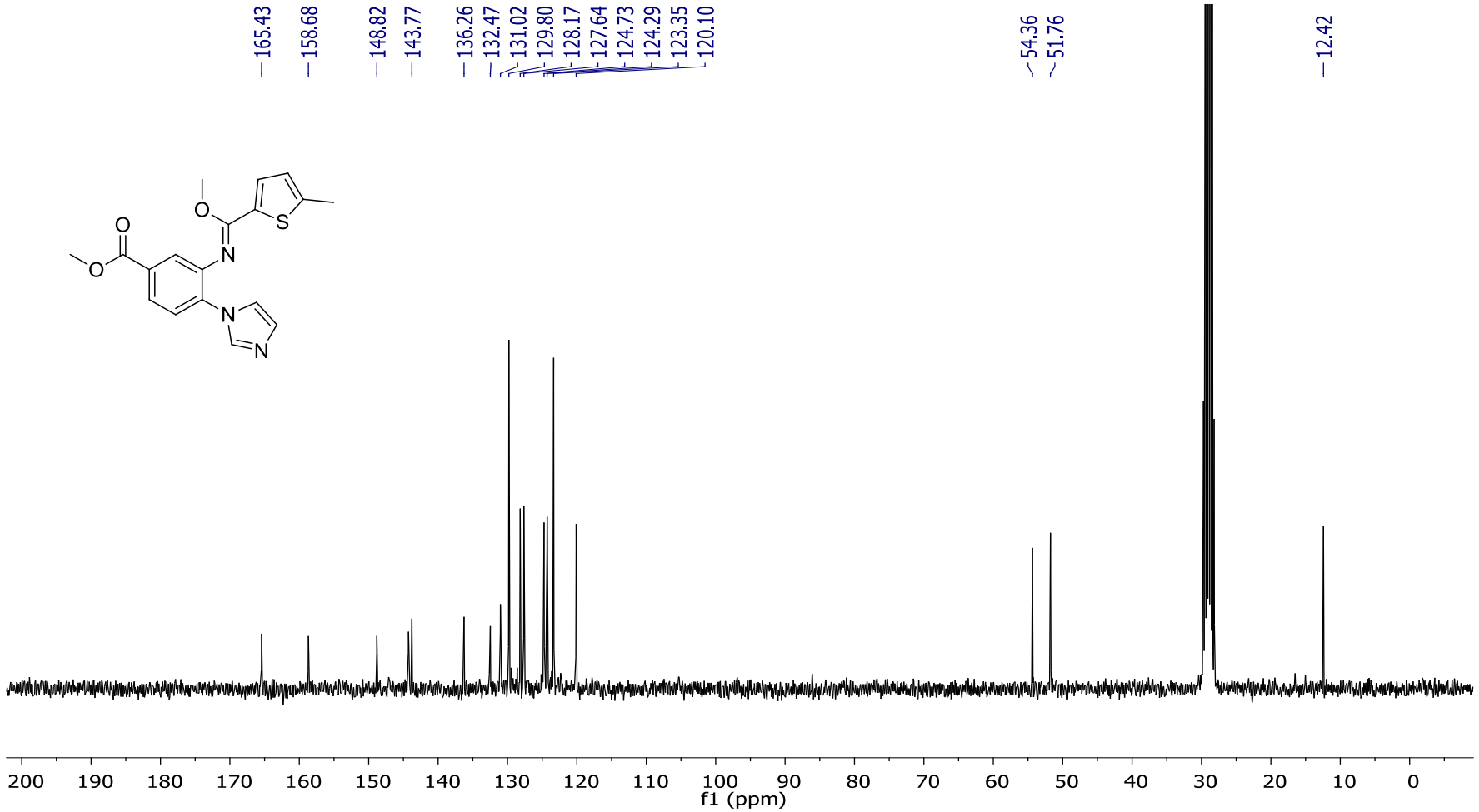
ESI-LRMS of compound **13f**



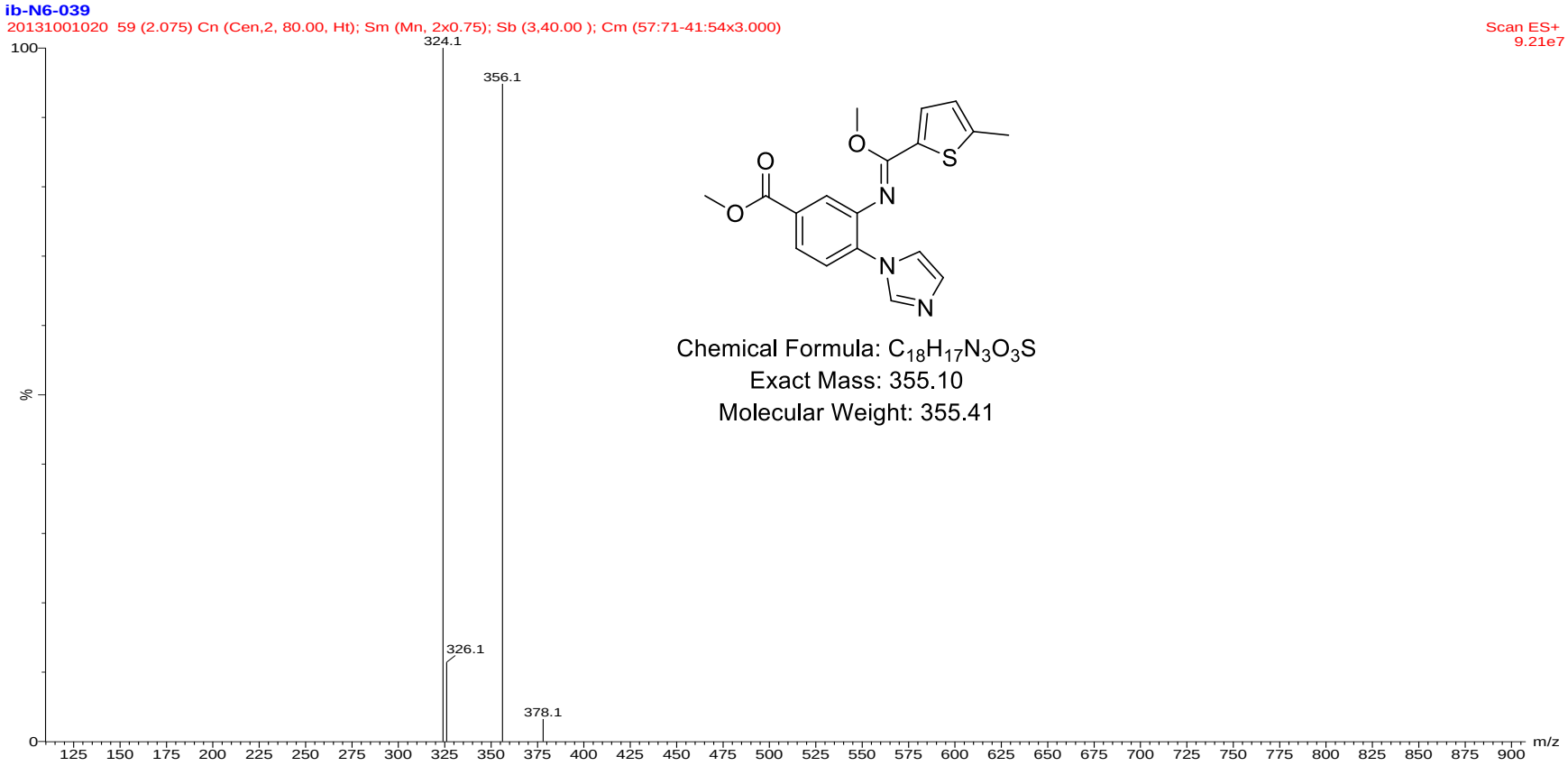
ESI-HRMS of compound **13f**



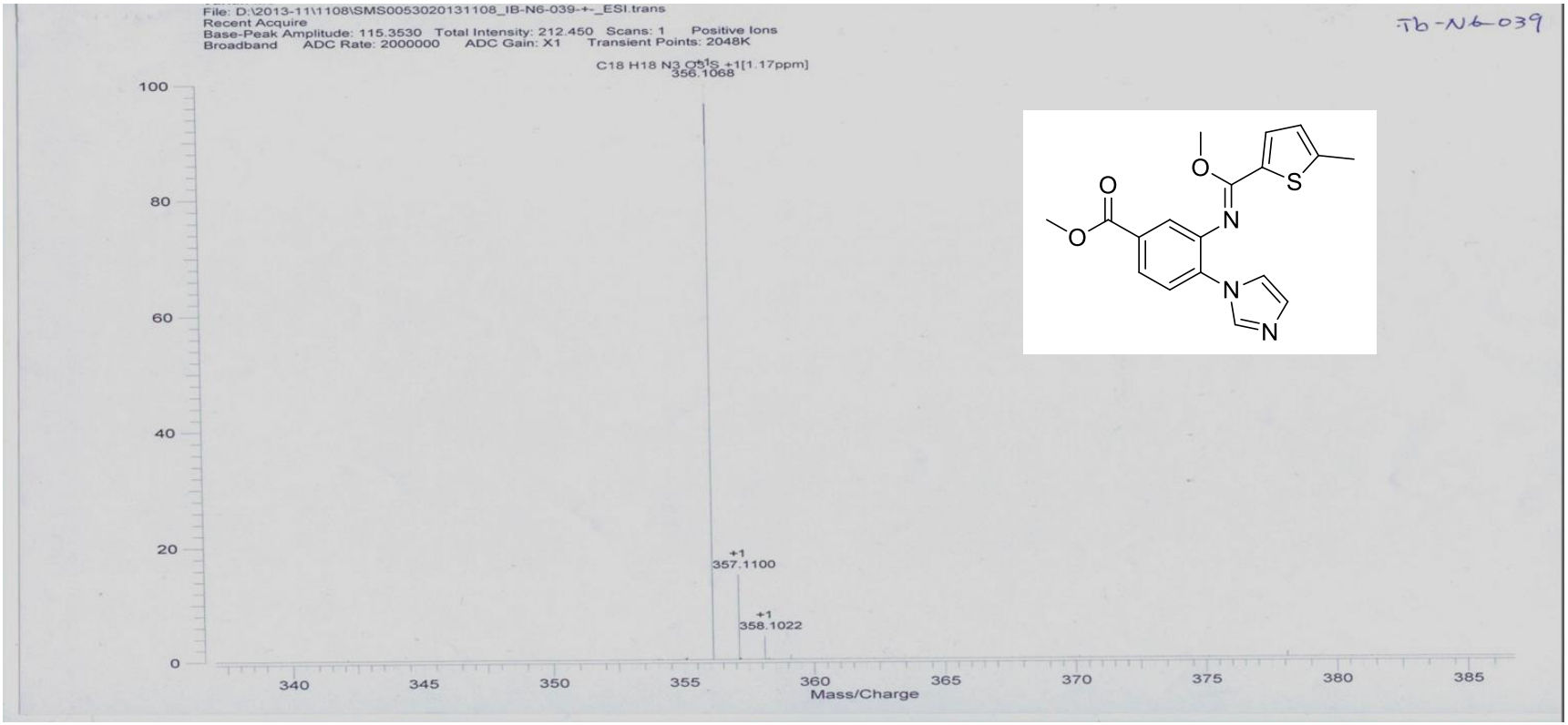
^{1}H NMR spectrum (400 MHz) of compound **13g** in Acetone-d_6



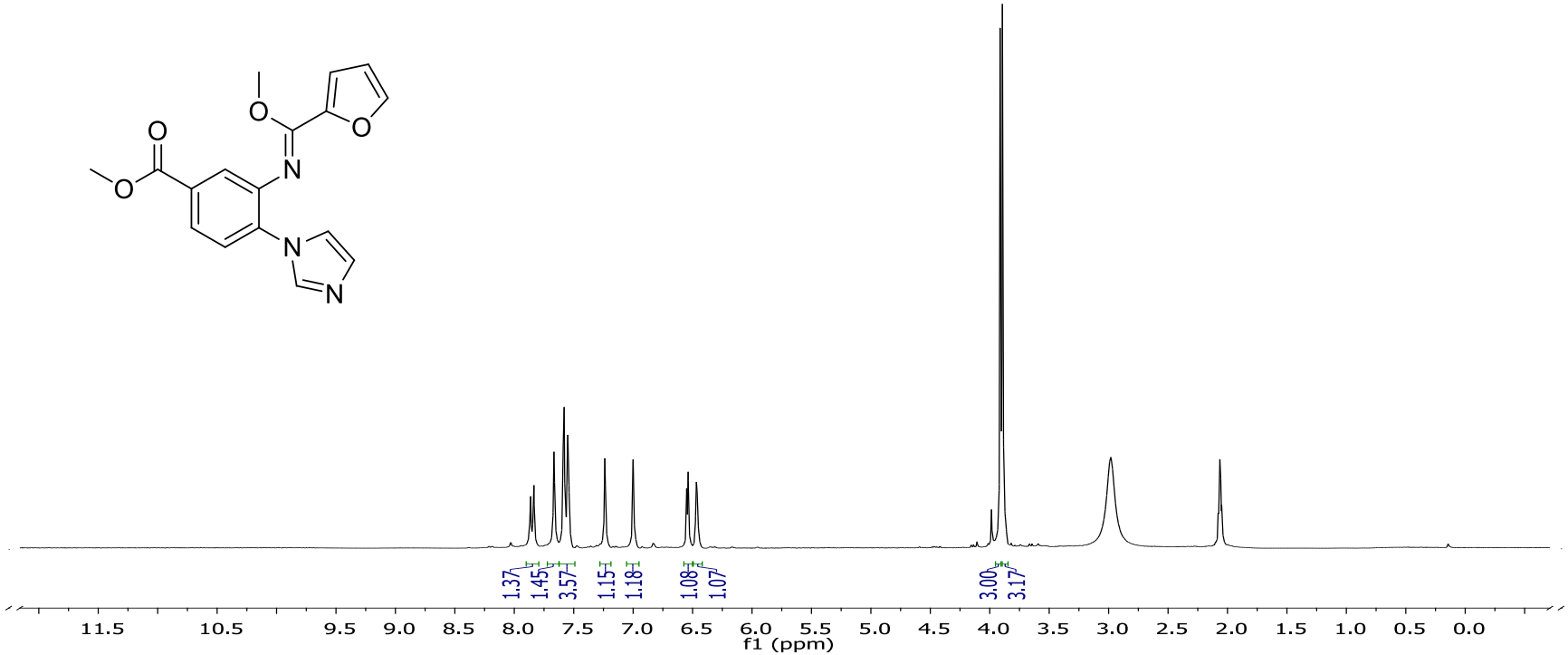
^{13}C NMR spectrum (101 MHz) of compound **13g** in Acetone-d_6



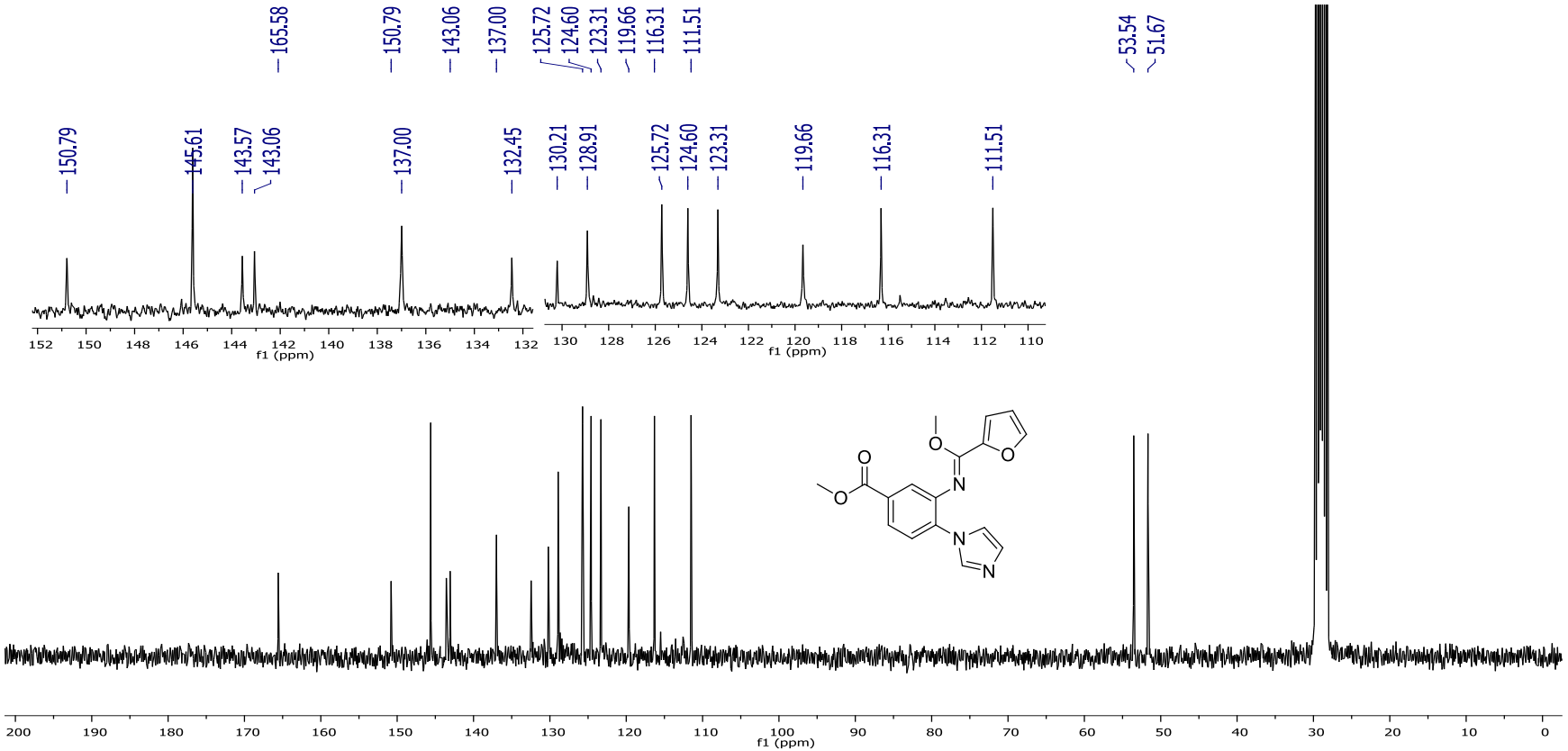
ESI-LRMS of compound **13g**



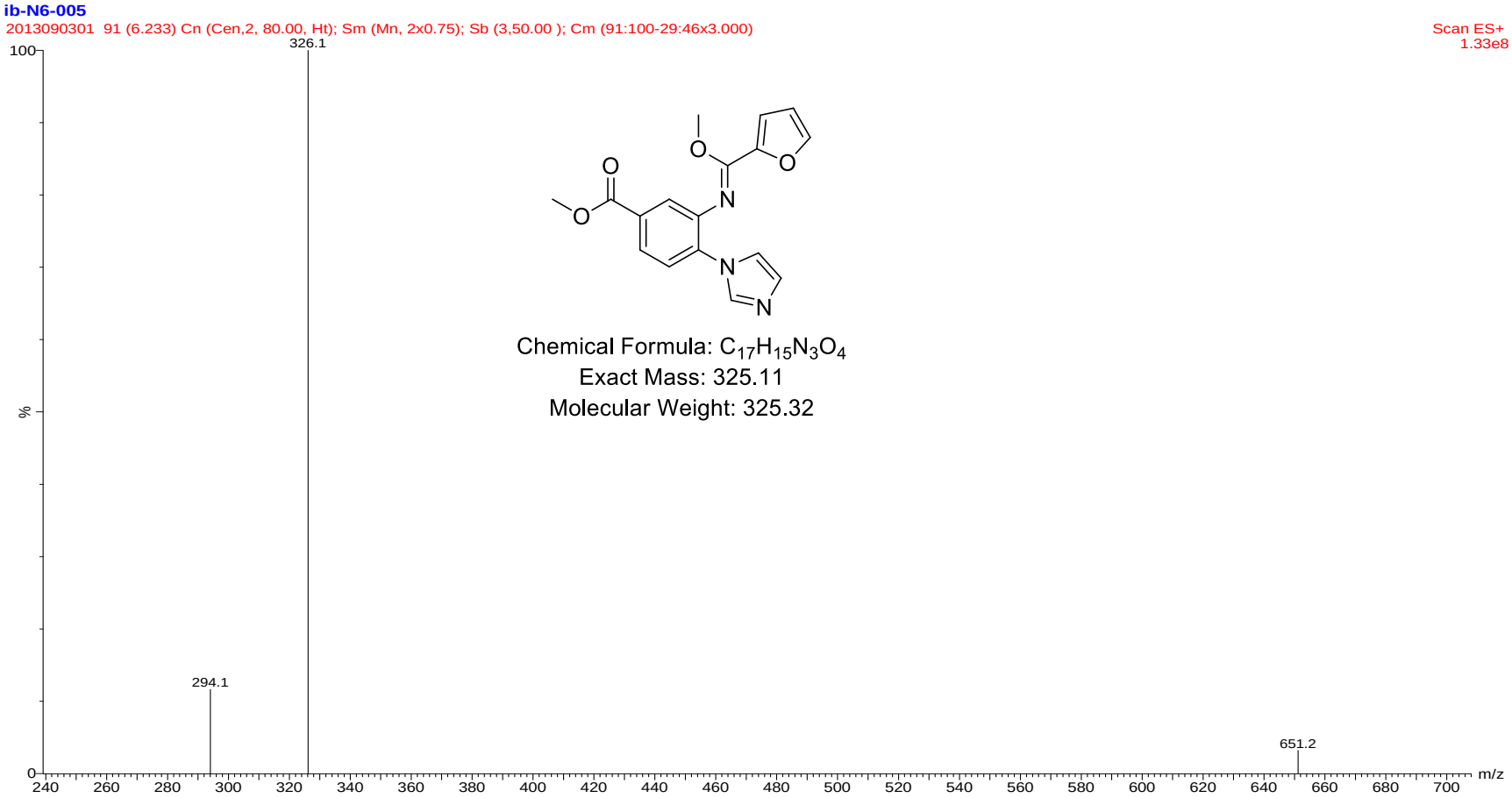
ESI-HRMS of compound **13g**



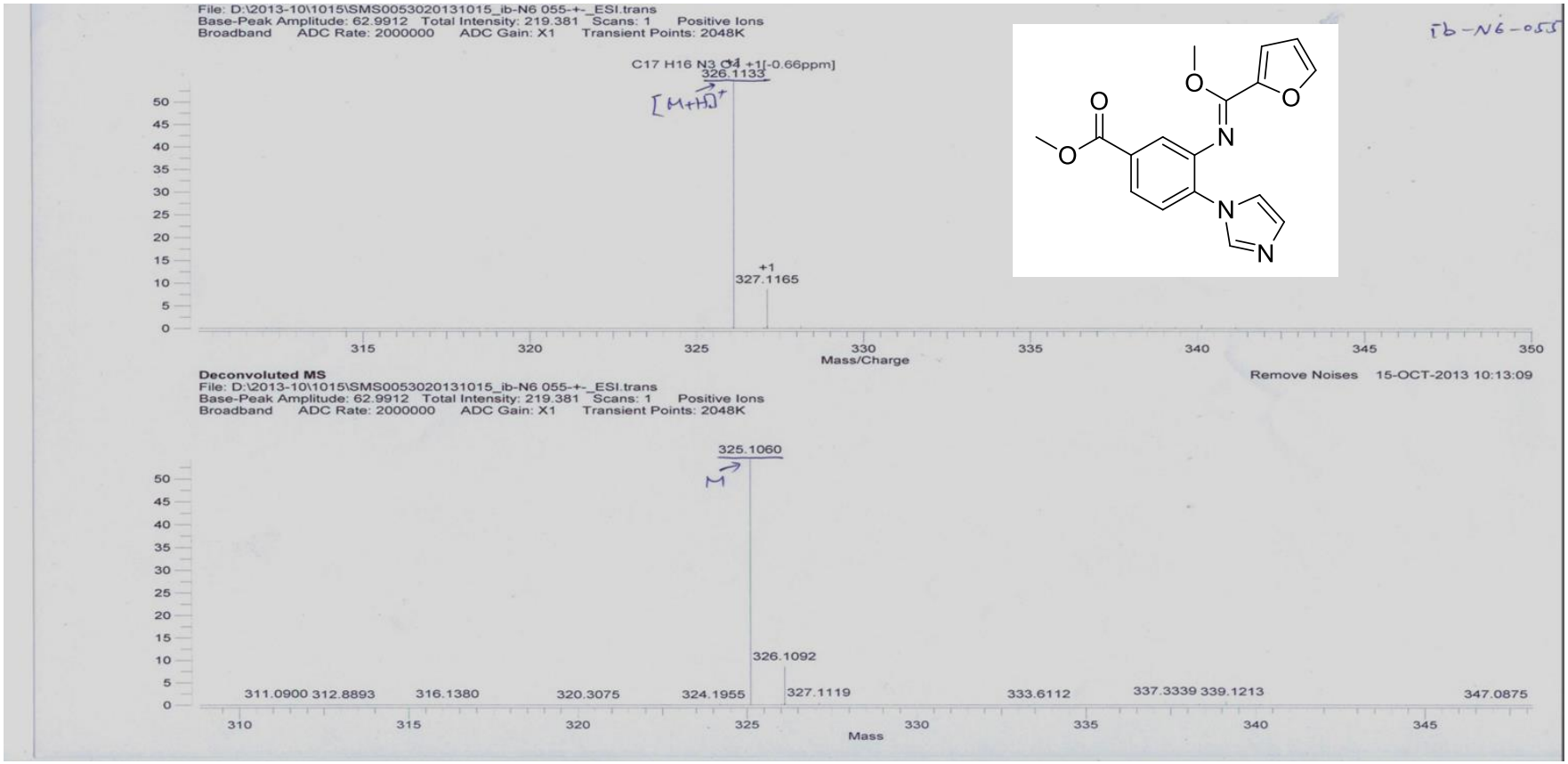
^{1}H NMR spectrum (400 MHz) of compound **13h** in Acetone-d_6



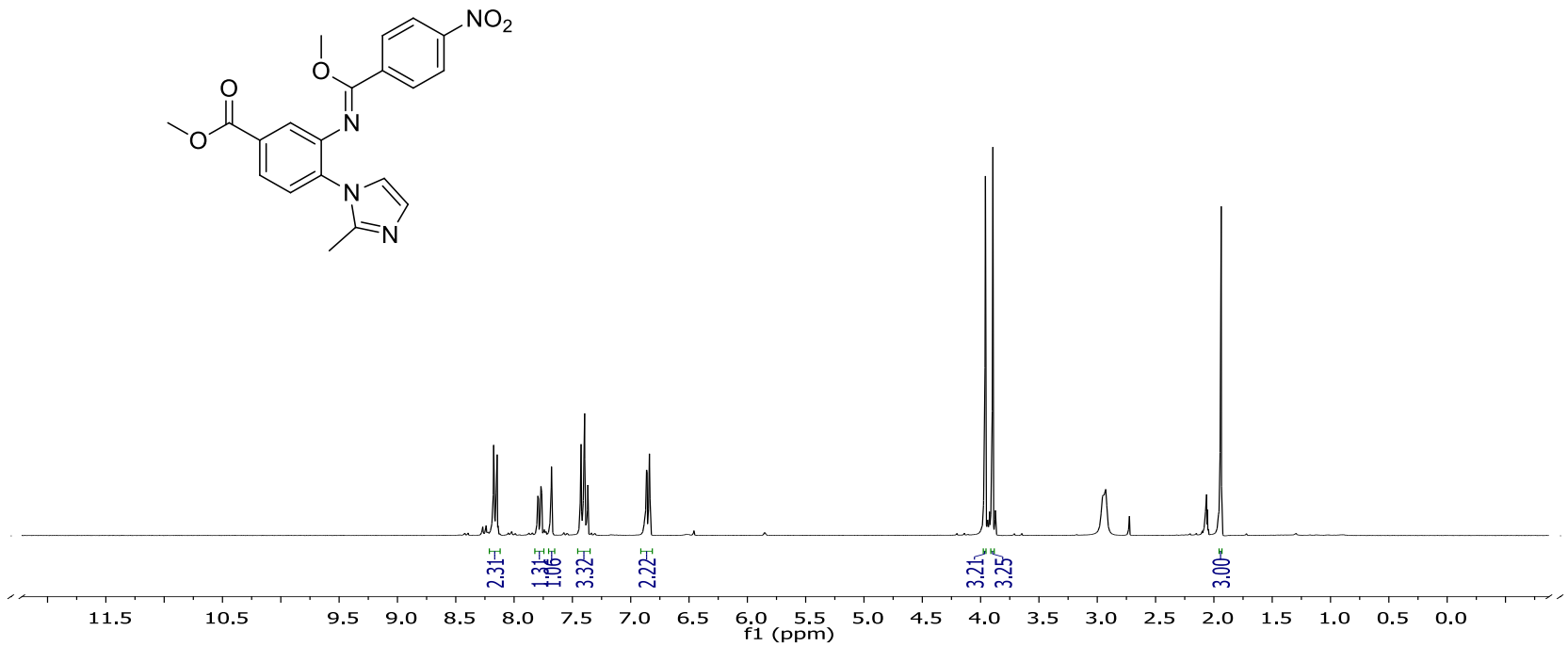
^{13}C NMR spectrum (101 MHz) of compound **13h** in Acetone-d_6



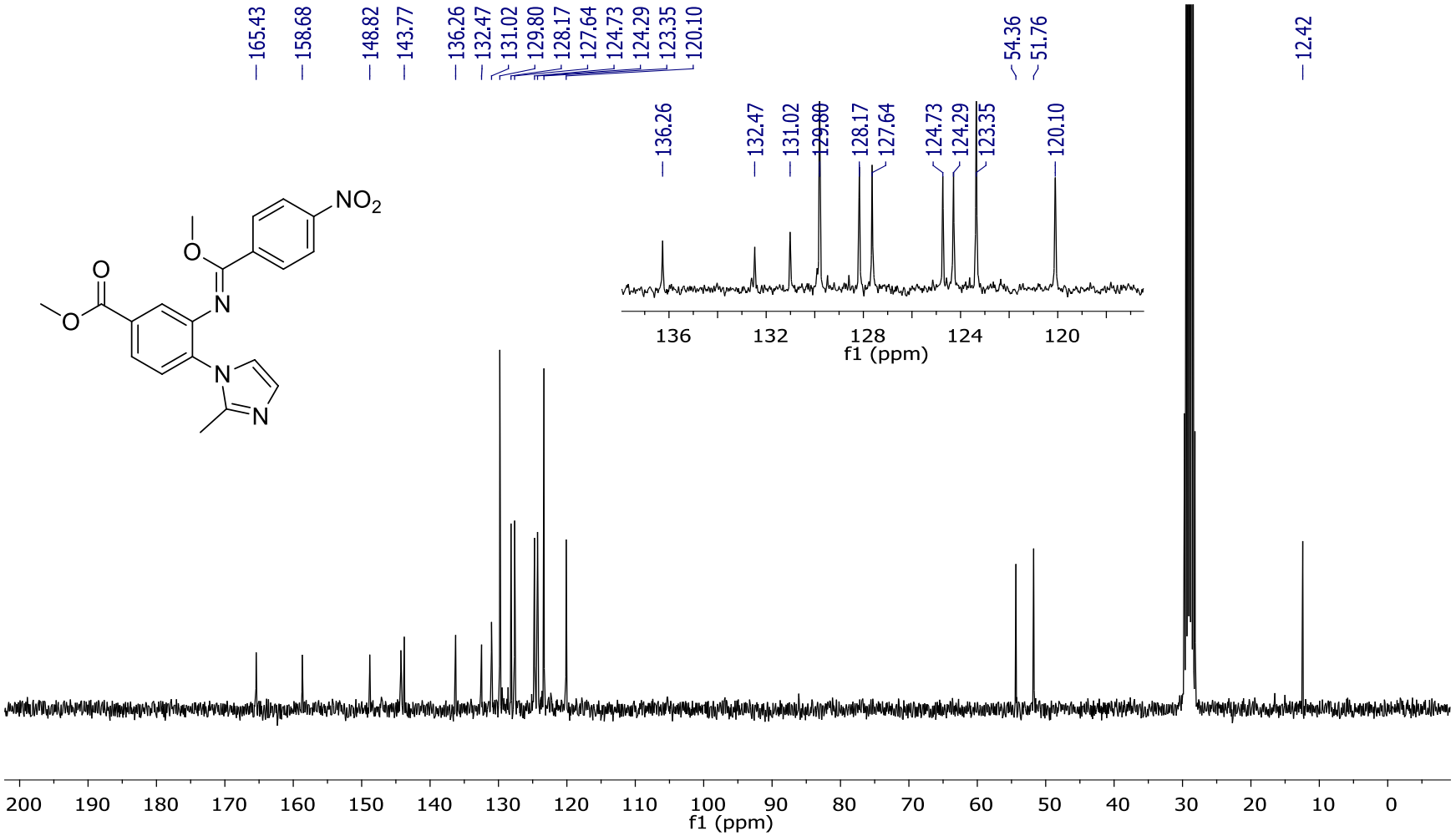
ESI-LRMS of compound **13h**



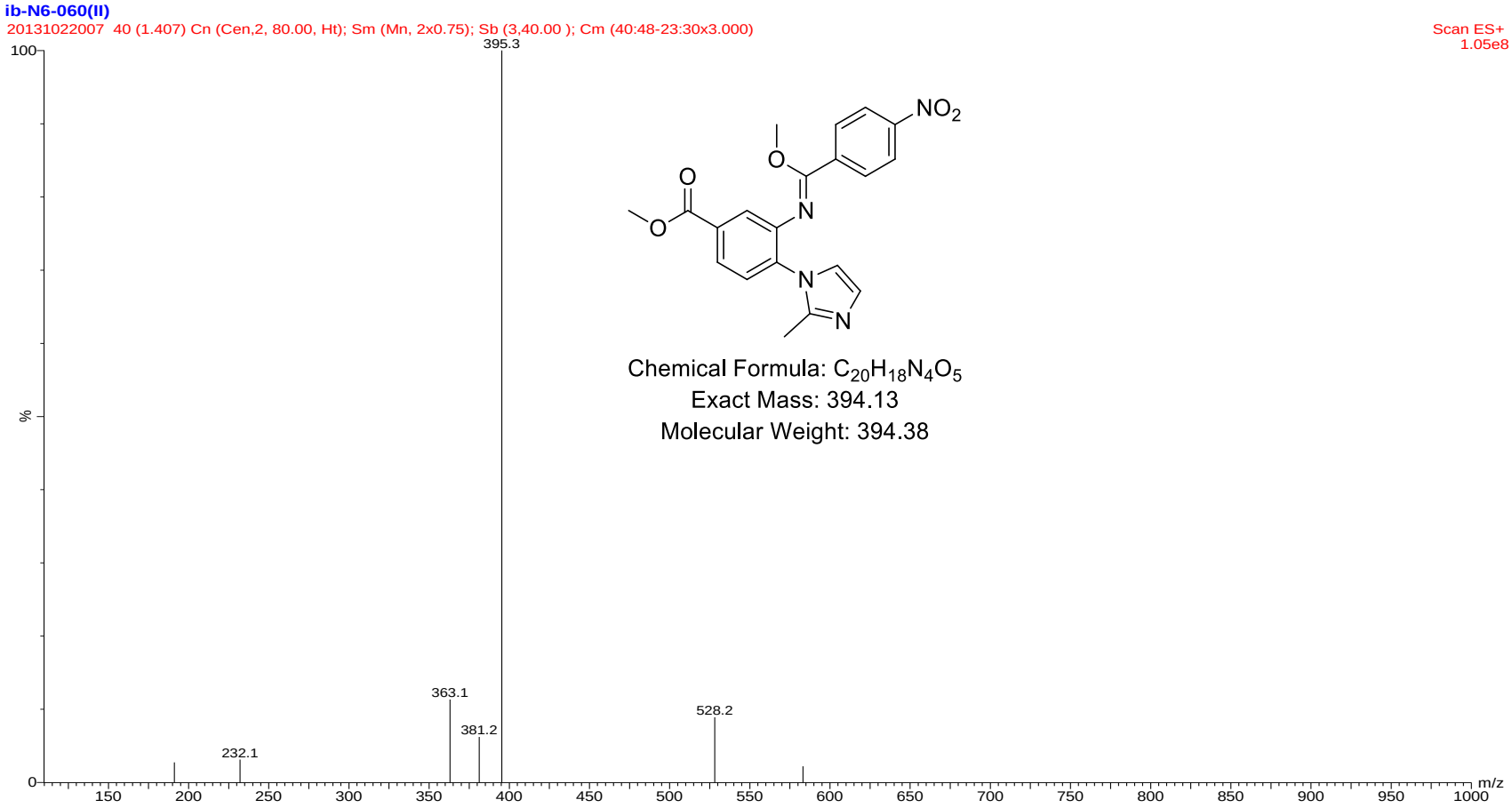
ESI-HRMS of compound **13h**



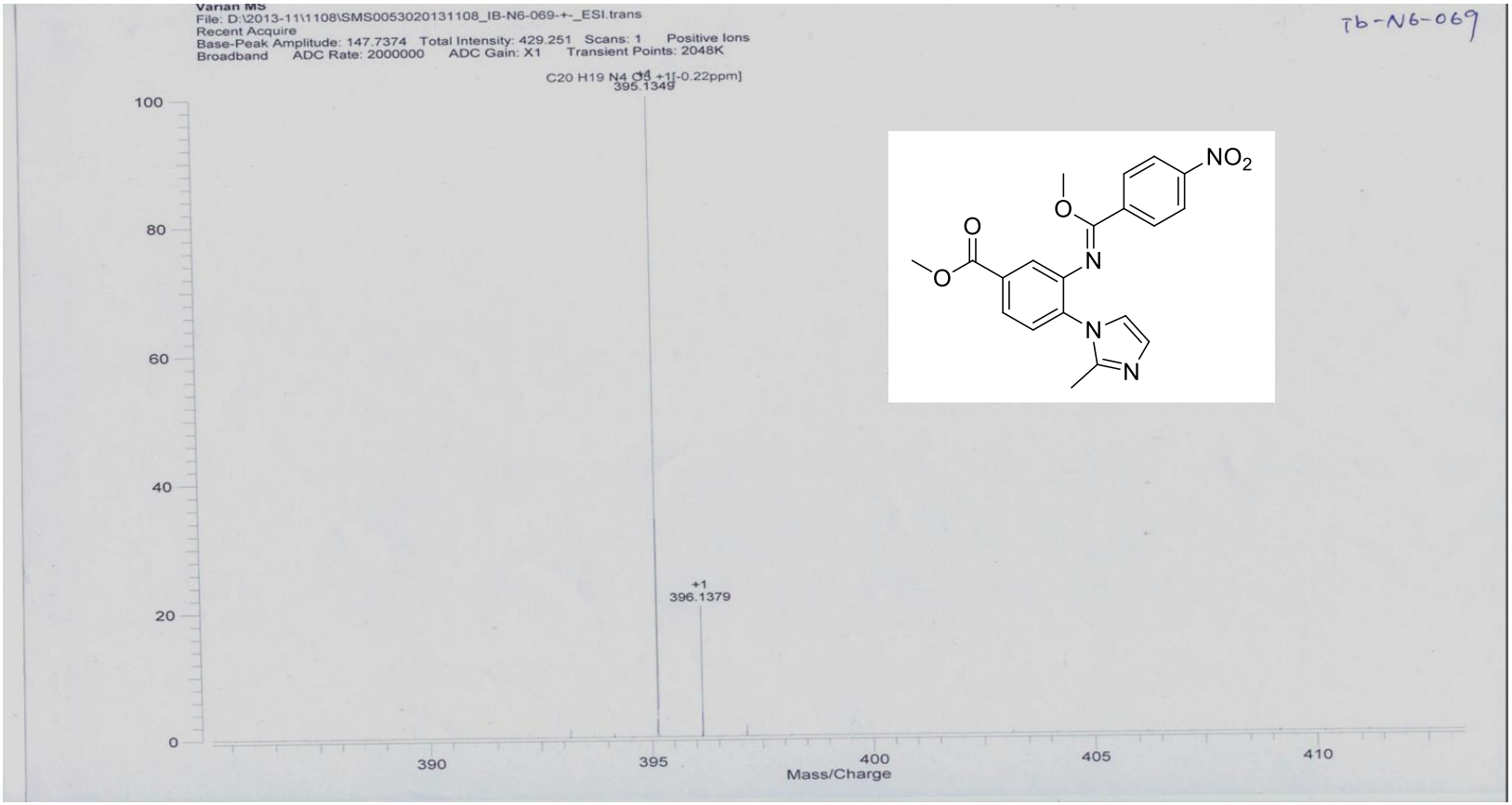
^{1}H NMR spectrum (400 MHz) of compound **13i** in Acetone-d_6



^{13}C NMR spectrum (101 MHz) of compound **13i** in Acetone-d_6

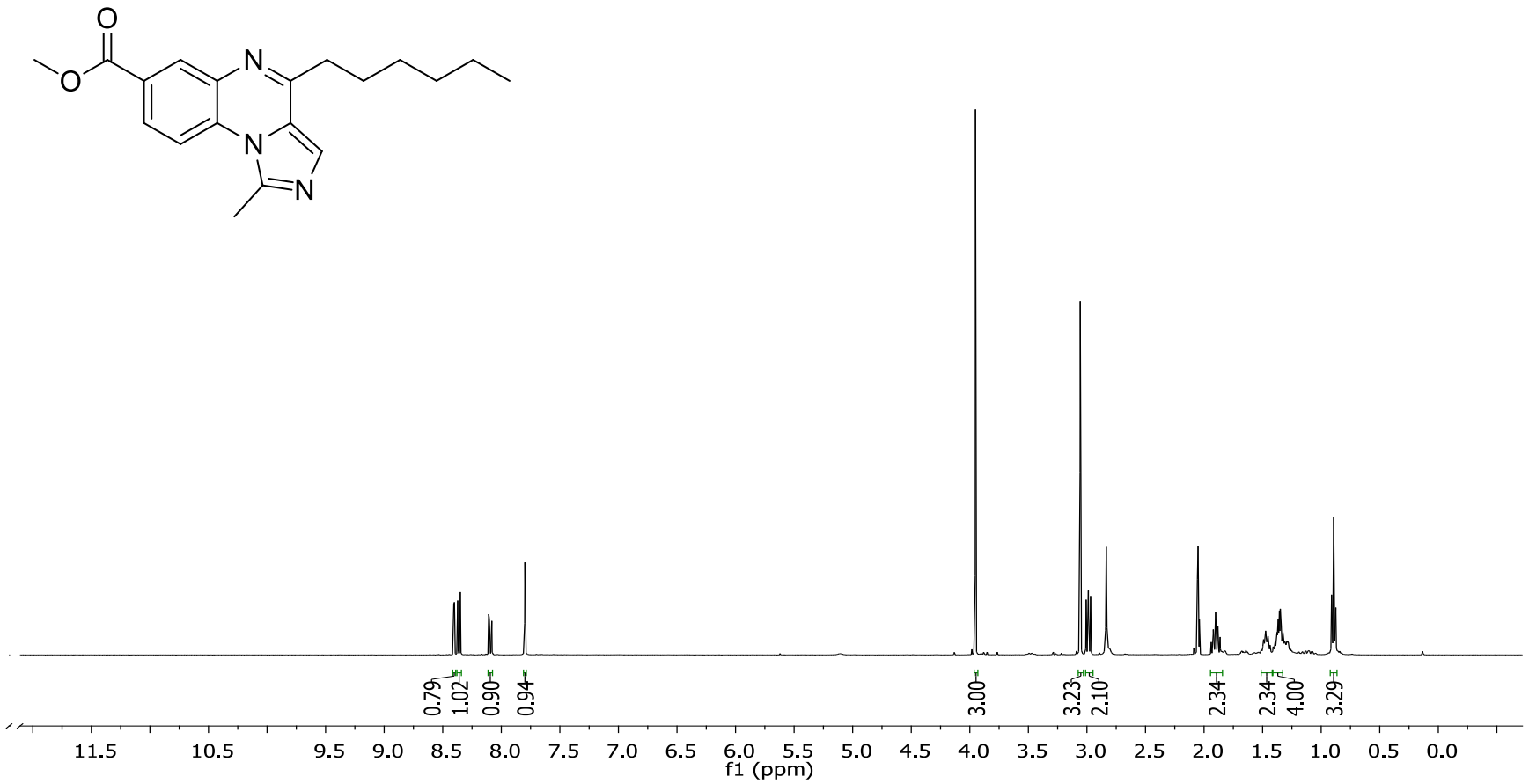


ESI-LRMS of compound **13i**

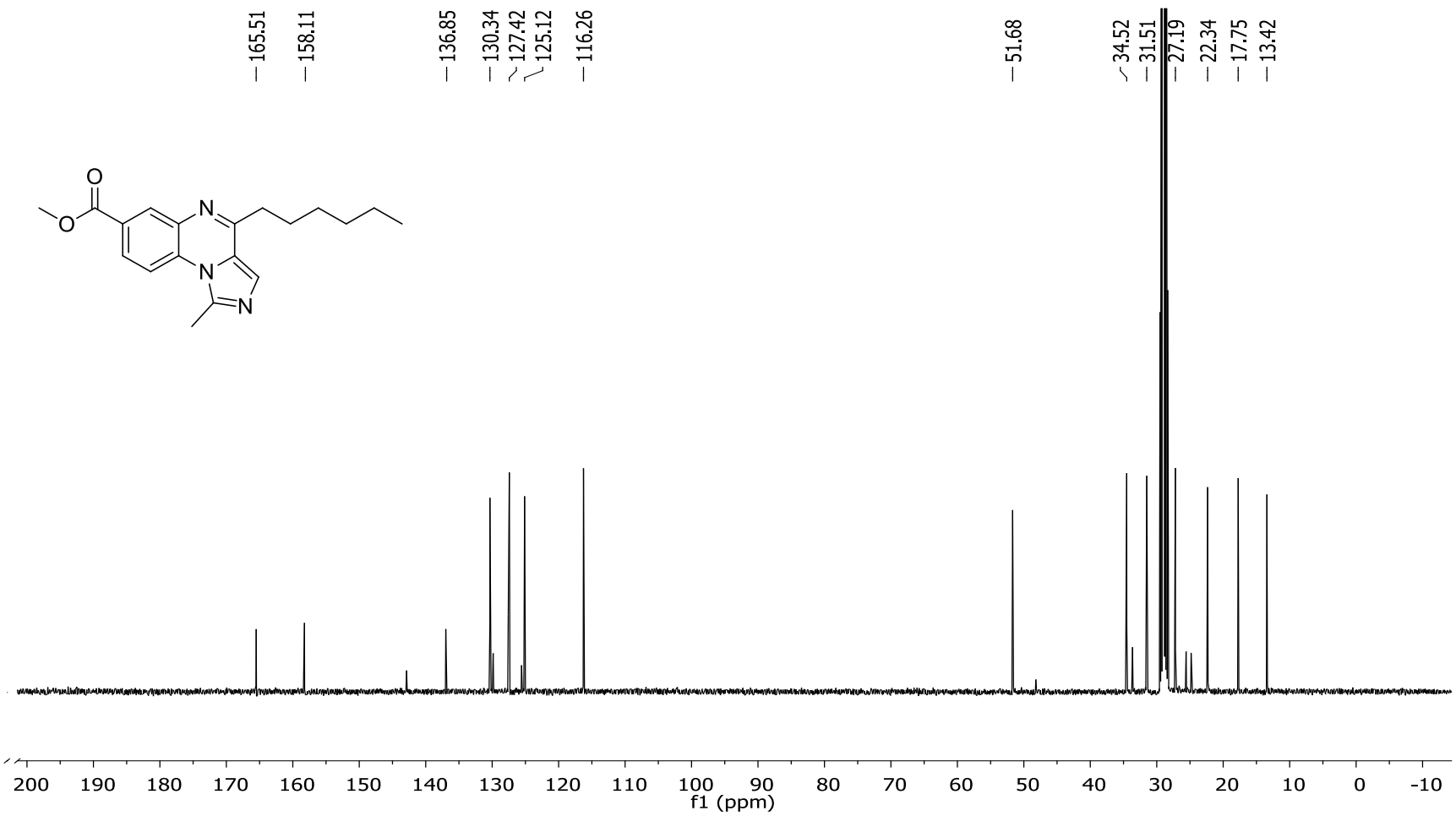


ESI-HRMS of compound **13i**

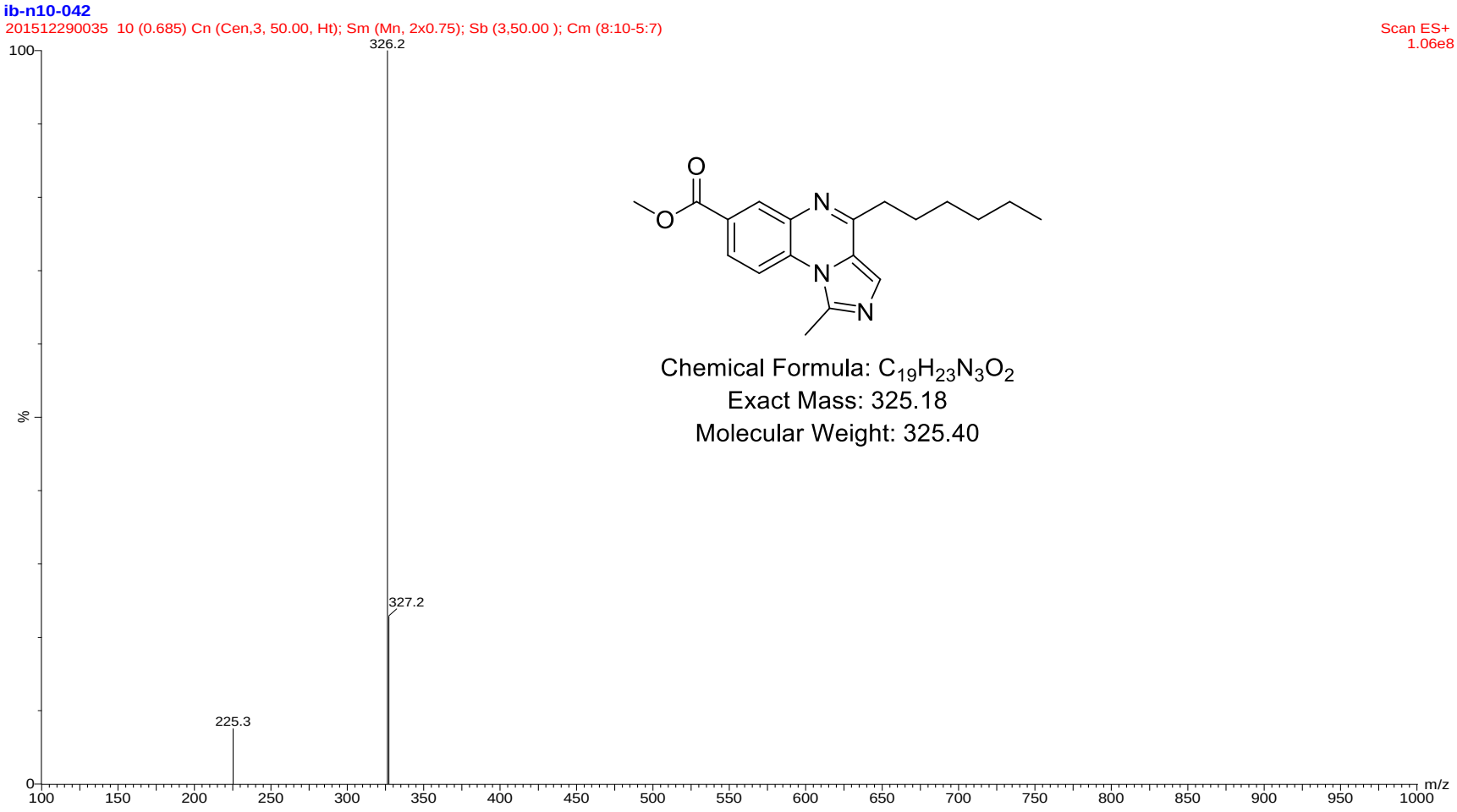
9. ^{1}H NMR, ^{13}C NMR, LRMS and HRMS of Compound 14a-c



^{1}H NMR spectrum (400 MHz) of compound **14a** in Acetone-d_6



^{13}C NMR spectrum (101 MHz) of compound **14a** in Acetone-d_6



ESI-LRMS of compound **14a**

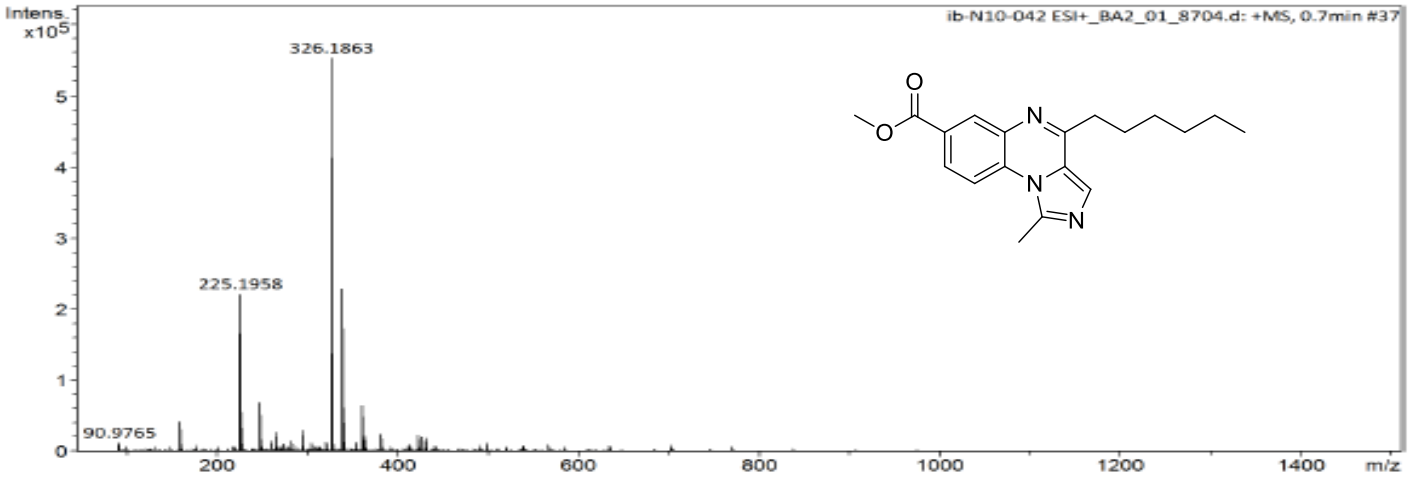
Display Report

Analysis Info

Analysis Name	D:\Data\nctu service\data\2016\20160202\ib-N10-042 ESI+_BA2_01_8704.d	Acquisition Date	2/2/2016 12:29:43 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	ib-N10-042 ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

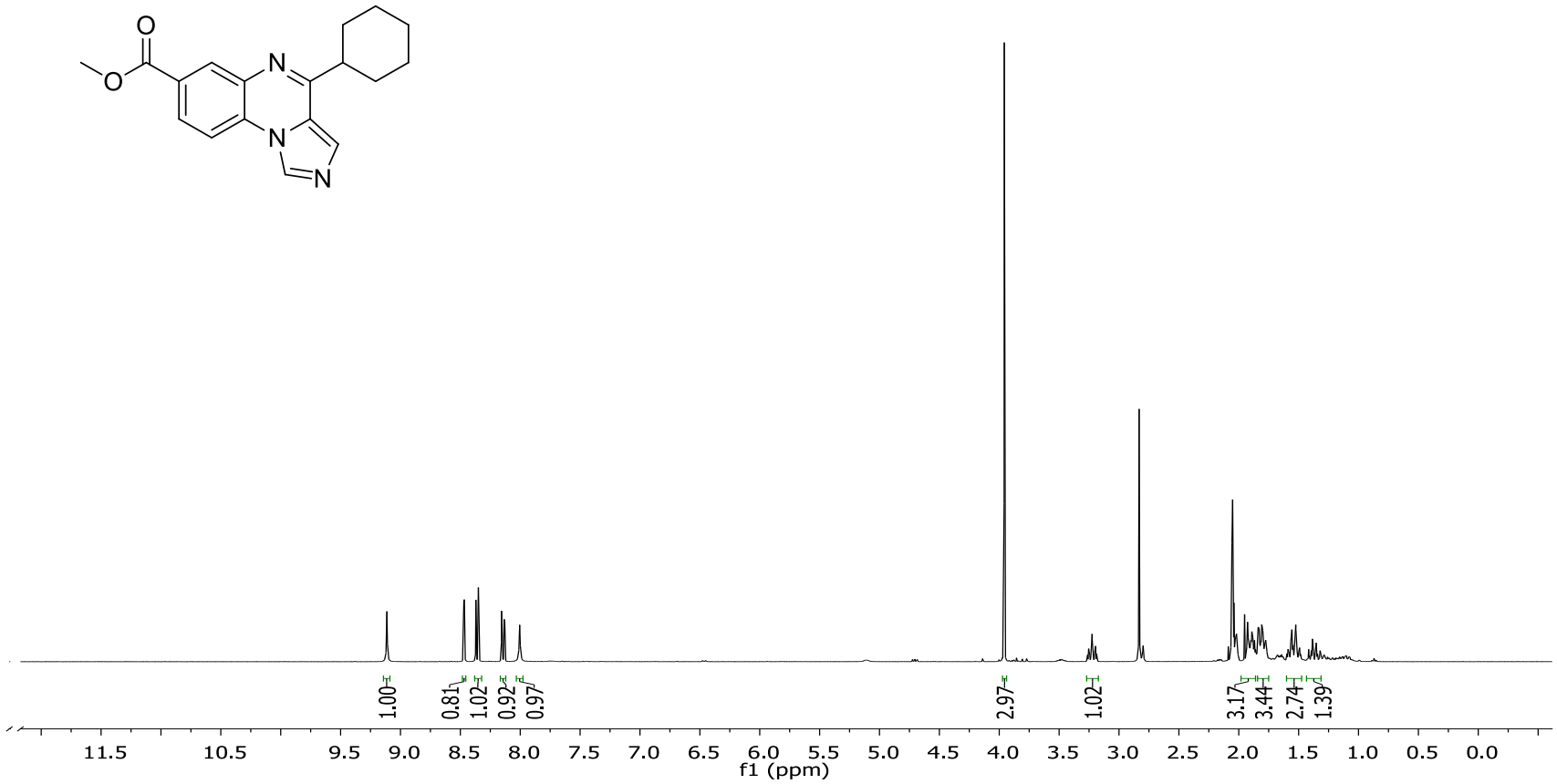
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



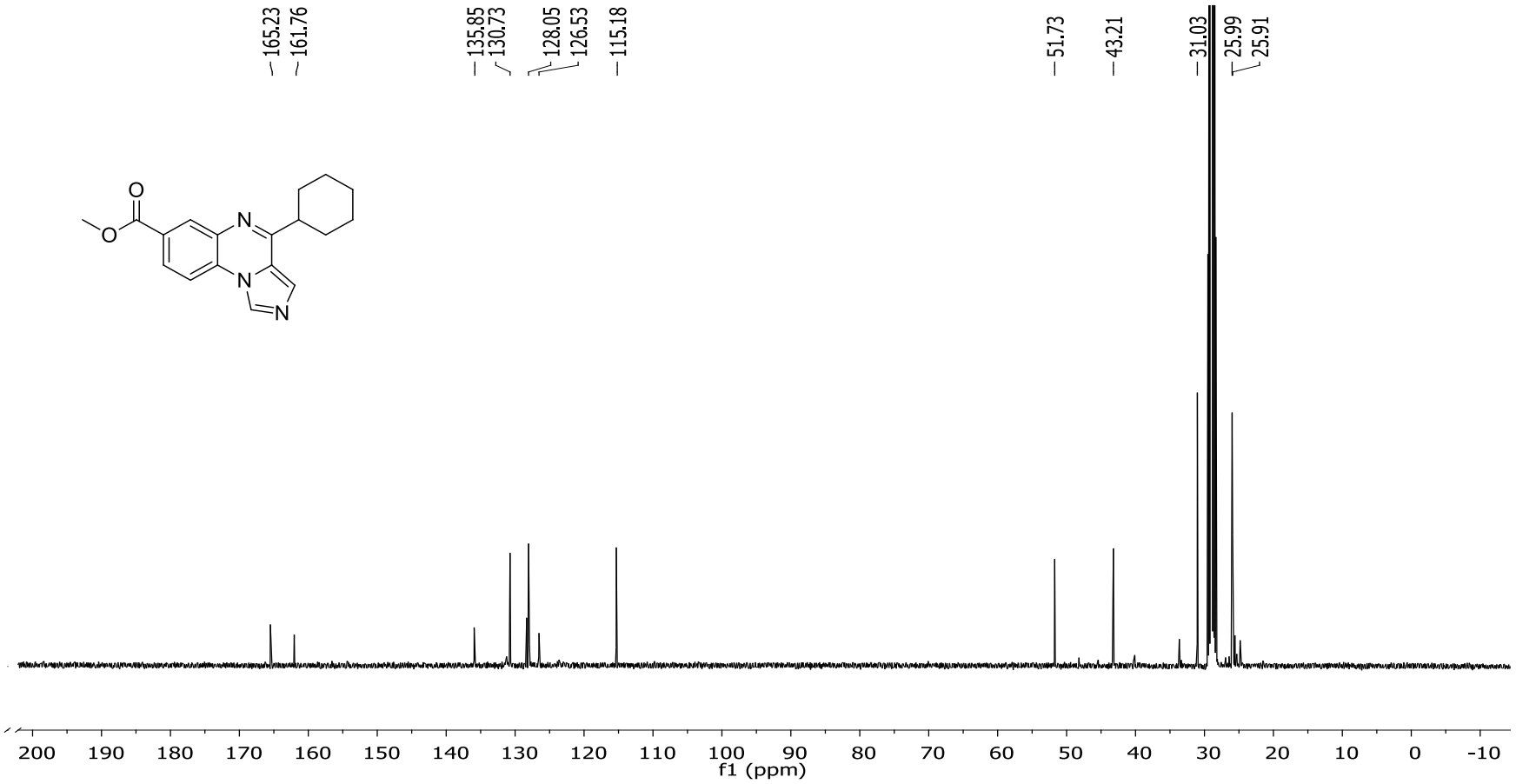
Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule	Adduct
326.1863	1	C19H24N3O2	326.1863	-0.0	10.8	1	100.00	9.5	even	ok	M

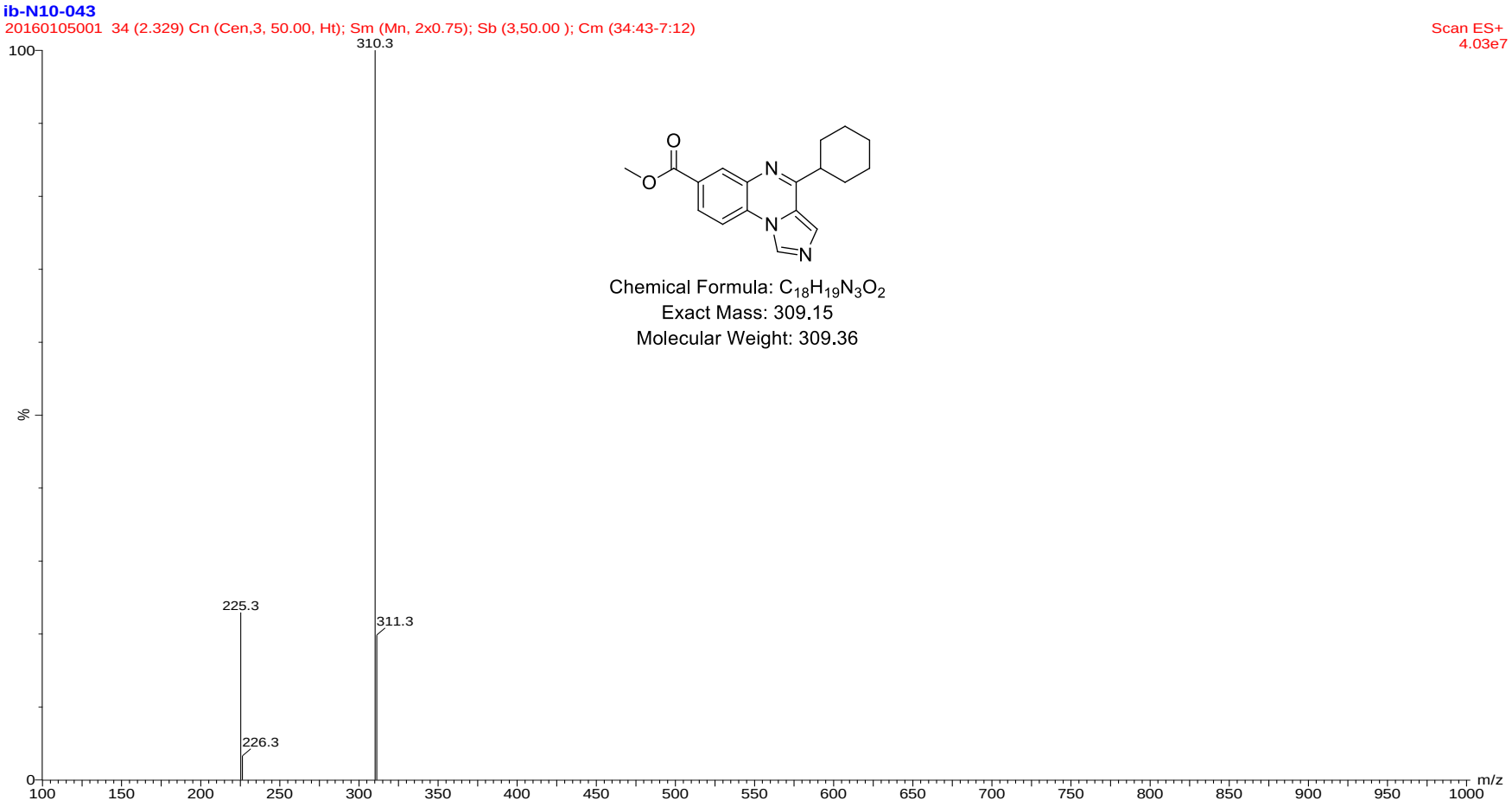
ESI-HRMS of compound **14a**



^{1}H NMR spectrum (400 MHz) of compound **14b** in Acetone-d_6



^{13}C NMR spectrum (101 MHz) of compound **14b** in Acetone-d_6



ESI-LRMS of compound **14b**

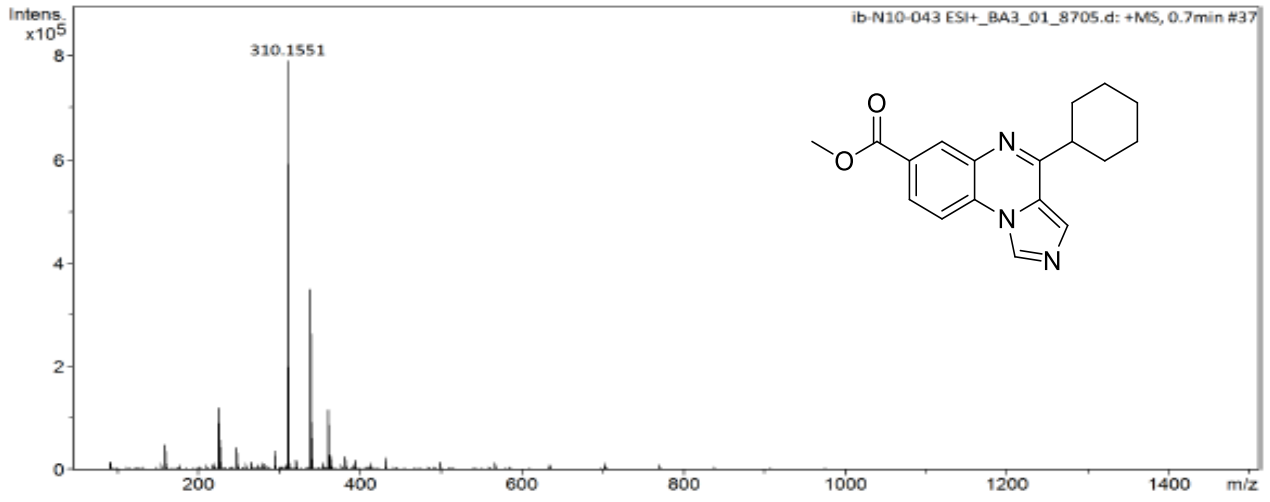
Display Report

Analysis Info

Analysis Name	D:\Data\nctu service\data\2016\20160202\ib-N10-043 ESI+_BA3_01_8705.d	Acquisition Date	2/2/2016 12:34:01 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	ib-N10-043 ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

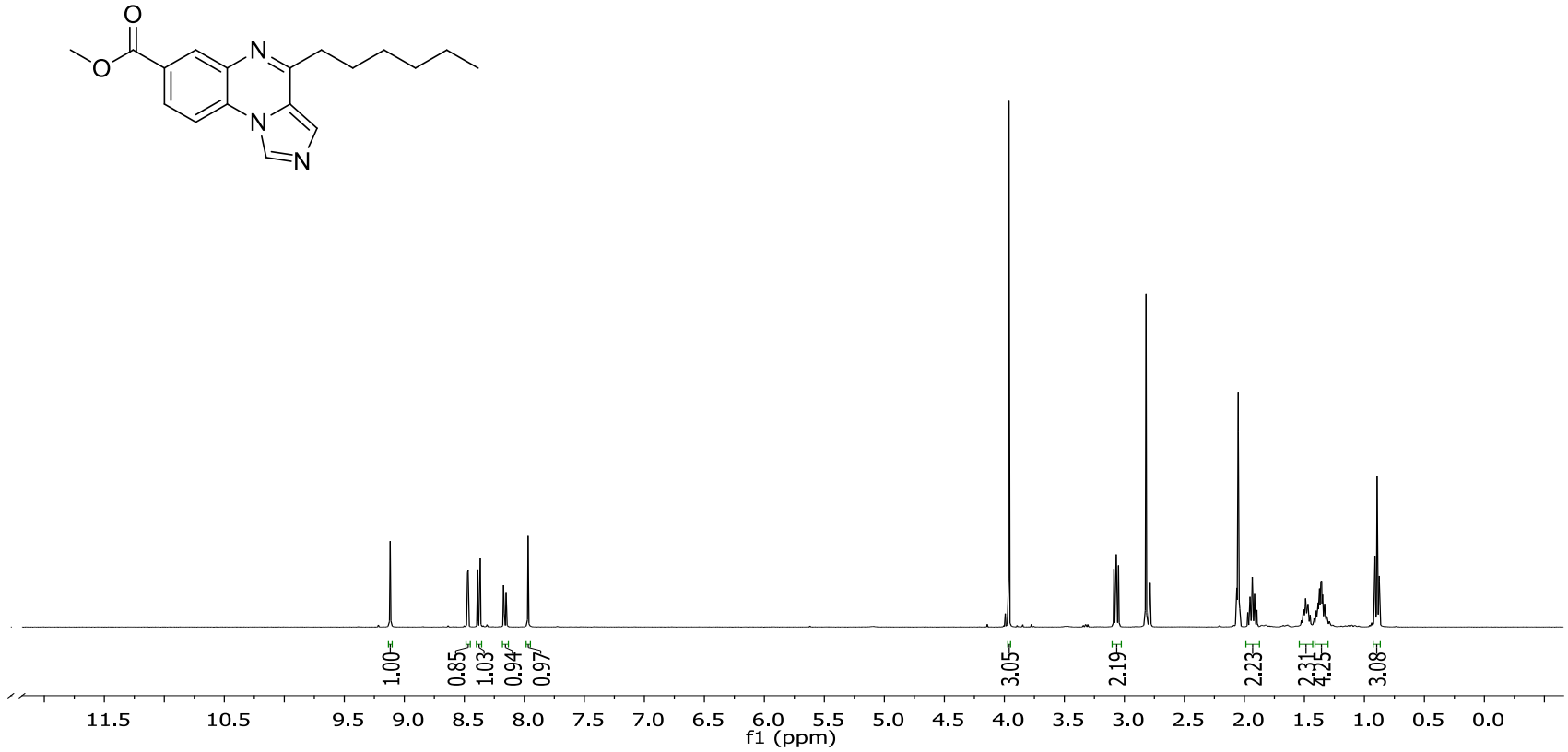
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



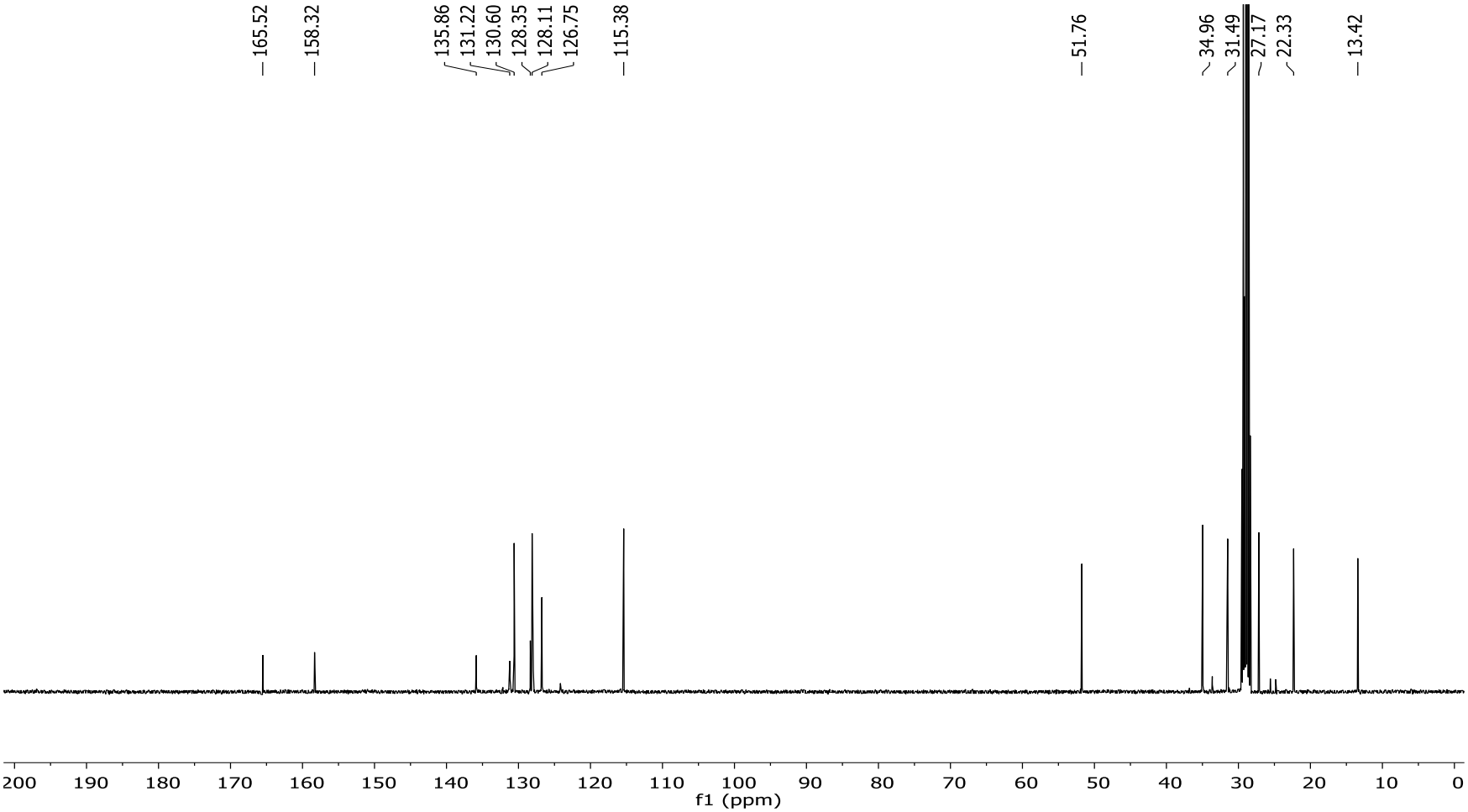
Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule	Adduct
310.1551	1	C18H20N3O2	310.1550	-0.2	14.0	1	100.00	10.5	even	ok	M

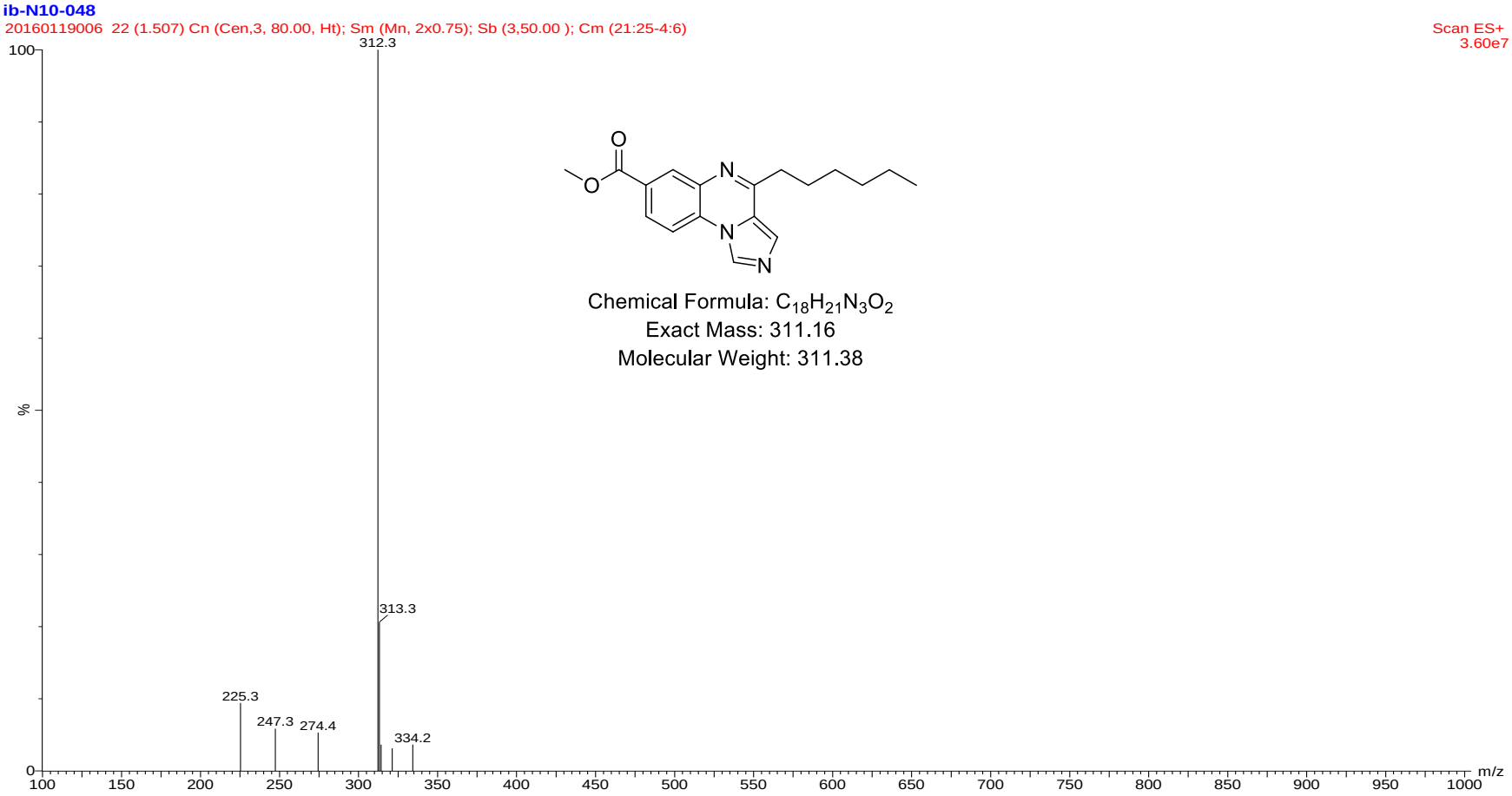
ESI-HRMS of compound **14b**



^{1}H NMR spectrum (400 MHz) of compound **14c** in Acetone-d_6



^{13}C NMR spectrum (101 MHz) of compound **14c** in Acetone-d_6



ESI-LRMS of compound **14c**

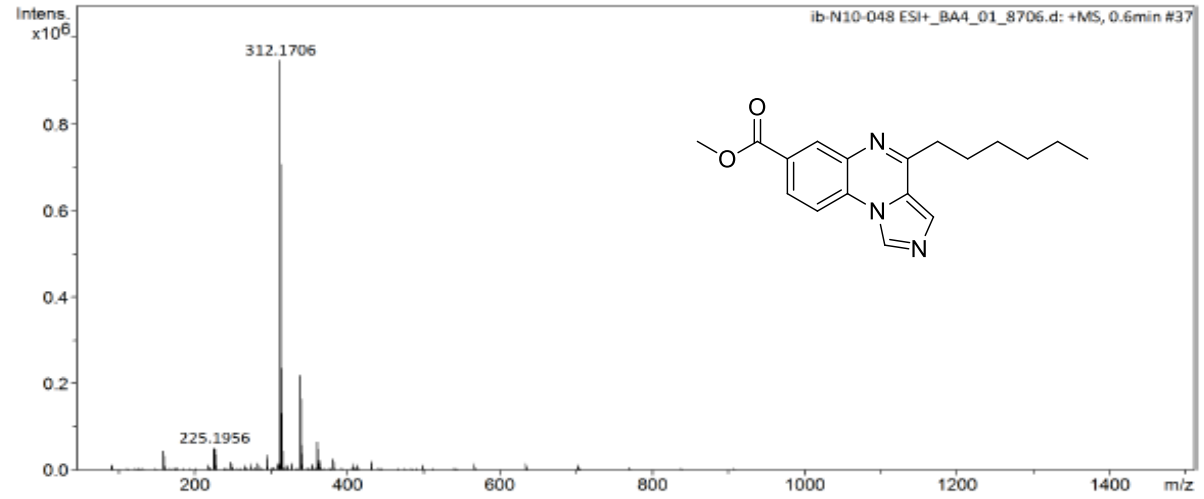
Display Report

Analysis Info

Analysis Name	D:\Data\nctu service\data\2016\20160202\ib-N10-048 ESI+_BA4_01_8706.d	Acquisition Date	2/2/2016 12:38:24 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	ib-N10-048 ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

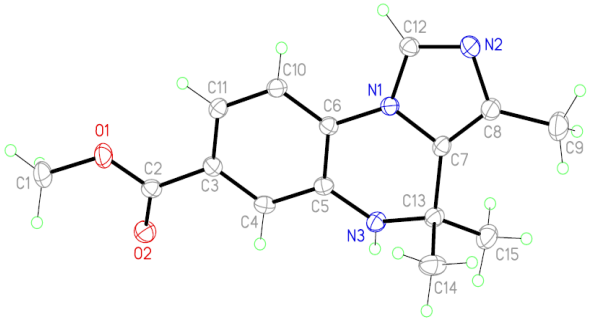


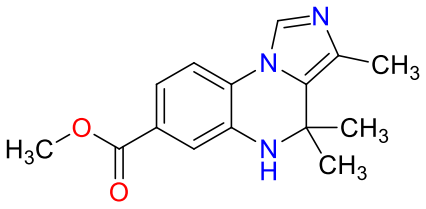
Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule	Adduct
312.1706	1	C18H22N3O2	312.1707	0.1	13.0	1	100.00	9.5	even	ok	M

ESI-HRMS of compound **14c**

10. X-ray crystal data of compound 12a





12a

ORTEP diagram of compound 12a. Atomic displacement ellipsoids are drawn at the 50% probability level

CCDC no. of **12a**: 891457

Table 1. Crystal data and structure refinement for mo_120560lt_0m.

Identification code	mo_120560lt_0m	
Empirical formula	C15 H17 N3 O2	
Formula weight	271.32	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 8.2166(6) Å	α= 90°.
	b = 15.0686(10) Å	β= 90°.
	c = 22.6298(15) Å	γ = 90°.
Volume	2801.9(3) $Å^3$	
Z	8	
Density (calculated)	1.286 Mg/m^3	
Absorption coefficient	0.088 mm^{-1}	
F(000)	1152	
Crystal size	0.25 x 0.20 x 0.20 mm^3	

Theta range for data collection	1.80 to 26.48°.
Index ranges	-10<=h<=10, -18<=k<=18, -28<=l<=26
Reflections collected	19670
Independent reflections	2893 [R(int) = 0.0454]
Completeness to theta = 26.48°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9486 and 0.7938
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2893 / 0 / 185
Goodness-of-fit on F^2	1.033
Final R indices [I>2sigma(I)]	R1 = 0.0438, wR2 = 0.1096
R indices (all data)	R1 = 0.0585, wR2 = 0.1185
Largest diff. peak and hole	0.585 and -0.581 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_120560lt_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	8716(1)	6133(1)	5076(1)	22(1)
O(2)	7931(1)	7130(1)	4397(1)	24(1)
N(1)	3548(2)	3811(1)	3686(1)	16(1)
N(2)	2430(2)	2549(1)	3395(1)	21(1)
N(3)	3238(2)	5547(1)	3361(1)	17(1)
C(1)	9864(2)	6781(1)	5293(1)	25(1)
C(2)	7814(2)	6399(1)	4615(1)	18(1)
C(3)	6678(2)	5703(1)	4404(1)	16(1)
C(4)	5486(2)	5949(1)	4000(1)	16(1)
C(5)	4396(2)	5323(1)	3775(1)	16(1)
C(6)	4600(2)	4436(1)	3952(1)	16(1)
C(7)	2223(2)	4038(1)	3338(1)	17(1)
C(8)	1538(2)	3255(1)	3168(1)	20(1)
C(9)	48(2)	3070(1)	2805(1)	34(1)
C(10)	5779(2)	4189(1)	4358(1)	18(1)
C(11)	6815(2)	4824(1)	4591(1)	18(1)
C(12)	3620(2)	2909(1)	3700(1)	18(1)
C(13)	1779(2)	5005(1)	3259(1)	18(1)
C(14)	430(2)	5265(1)	3695(1)	27(1)
C(15)	1232(2)	5198(1)	2625(1)	26(1)

Table 3. Bond lengths [Å] and angles [°] for mo_120560lt_0m.

O(1)-C(2)	1.340(2)
O(1)-C(1)	1.4434(19)
O(2)-C(2)	1.2113(19)
N(1)-C(12)	1.361(2)
N(1)-C(7)	1.386(2)
N(1)-C(6)	1.414(2)
N(2)-C(12)	1.314(2)
N(2)-C(8)	1.389(2)
N(3)-C(5)	1.377(2)
N(3)-C(13)	1.469(2)
N(3)-H(3)	0.8800
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-C(3)	1.483(2)
C(3)-C(4)	1.391(2)
C(3)-C(11)	1.394(2)
C(4)-C(5)	1.396(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.406(2)
C(6)-C(10)	1.386(2)
C(7)-C(8)	1.363(2)
C(7)-C(13)	1.513(2)
C(8)-C(9)	1.499(2)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(11)	1.385(2)
C(10)-H(10)	0.9500
C(11)-H(11)	0.9500

C(12)-H(12)	0.9500
C(13)-C(15)	1.531(2)
C(13)-C(14)	1.535(2)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(2)-O(1)-C(1)	115.12(13)
C(12)-N(1)-C(7)	107.12(13)
C(12)-N(1)-C(6)	128.98(14)
C(7)-N(1)-C(6)	123.89(13)
C(12)-N(2)-C(8)	105.78(13)
C(5)-N(3)-C(13)	122.34(13)
C(5)-N(3)-H(3)	118.8
C(13)-N(3)-H(3)	118.8
O(1)-C(1)-H(1A)	109.5
O(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
O(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
O(2)-C(2)-O(1)	122.94(15)
O(2)-C(2)-C(3)	124.27(15)
O(1)-C(2)-C(3)	112.79(13)
C(4)-C(3)-C(11)	120.69(14)
C(4)-C(3)-C(2)	117.76(14)
C(11)-C(3)-C(2)	121.52(14)
C(3)-C(4)-C(5)	120.69(14)
C(3)-C(4)-H(4)	119.7
C(5)-C(4)-H(4)	119.7

N(3)-C(5)-C(4)	121.69(14)
N(3)-C(5)-C(6)	120.59(14)
C(4)-C(5)-C(6)	117.54(14)
C(10)-C(6)-C(5)	121.86(14)
C(10)-C(6)-N(1)	122.06(14)
C(5)-C(6)-N(1)	116.08(14)
C(8)-C(7)-N(1)	105.74(14)
C(8)-C(7)-C(13)	134.47(14)
N(1)-C(7)-C(13)	119.65(14)
C(7)-C(8)-N(2)	109.85(14)
C(7)-C(8)-C(9)	130.77(15)
N(2)-C(8)-C(9)	119.36(15)
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(11)-C(10)-C(6)	119.72(15)
C(11)-C(10)-H(10)	120.1
C(6)-C(10)-H(10)	120.1
C(10)-C(11)-C(3)	119.39(15)
C(10)-C(11)-H(11)	120.3
C(3)-C(11)-H(11)	120.3
N(2)-C(12)-N(1)	111.51(14)
N(2)-C(12)-H(12)	124.2
N(1)-C(12)-H(12)	124.2
N(3)-C(13)-C(7)	108.64(12)
N(3)-C(13)-C(15)	106.36(13)
C(7)-C(13)-C(15)	111.35(14)
N(3)-C(13)-C(14)	110.25(13)
C(7)-C(13)-C(14)	110.08(13)

C(15)-C(13)-C(14)	110.09(14)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5

Symmetry transformations used to generate equivalent atoms:

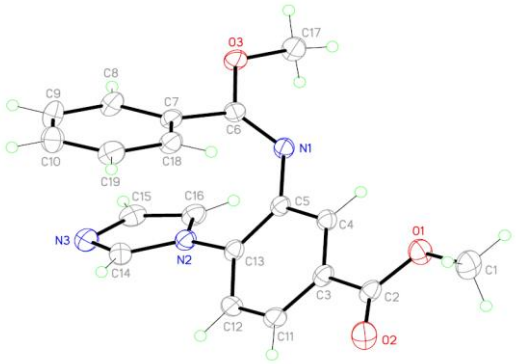
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_120560lt_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

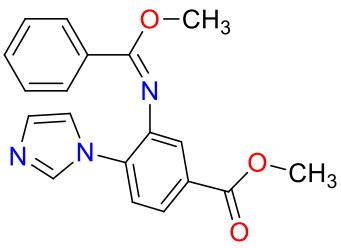
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	22(1)	20(1)	25(1)	0(1)	-5(1)	-5(1)
O(2)	21(1)	16(1)	33(1)	1(1)	-2(1)	-3(1)
N(1)	15(1)	14(1)	19(1)	0(1)	0(1)	1(1)
N(2)	21(1)	18(1)	23(1)	0(1)	-2(1)	-2(1)
N(3)	17(1)	15(1)	20(1)	4(1)	-1(1)	-1(1)
C(1)	23(1)	23(1)	29(1)	-3(1)	-5(1)	-6(1)
C(2)	14(1)	18(1)	21(1)	-2(1)	4(1)	2(1)
C(3)	13(1)	17(1)	19(1)	-2(1)	4(1)	-1(1)
C(4)	17(1)	13(1)	20(1)	1(1)	4(1)	1(1)
C(5)	15(1)	17(1)	15(1)	-1(1)	3(1)	2(1)
C(6)	13(1)	15(1)	18(1)	-1(1)	2(1)	0(1)
C(7)	14(1)	20(1)	16(1)	0(1)	0(1)	1(1)
C(8)	19(1)	20(1)	23(1)	2(1)	-2(1)	-1(1)
C(9)	32(1)	27(1)	42(1)	1(1)	-16(1)	-6(1)
C(10)	17(1)	15(1)	22(1)	1(1)	0(1)	2(1)
C(11)	14(1)	19(1)	21(1)	0(1)	-1(1)	1(1)
C(12)	18(1)	14(1)	22(1)	1(1)	0(1)	0(1)
C(13)	15(1)	17(1)	22(1)	1(1)	0(1)	0(1)
C(14)	22(1)	22(1)	38(1)	0(1)	7(1)	4(1)
C(15)	26(1)	24(1)	30(1)	5(1)	-9(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_120560lt_0m.

	x	y	z	U(eq)
H(3)	3378	6032	3150	21
H(1A)	10675	6906	4986	38
H(1B)	10409	6548	5645	38
H(1C)	9287	7329	5394	38
H(4)	5412	6550	3875	20
H(9A)	-876	3401	2967	51
H(9B)	-193	2433	2816	51
H(9C)	240	3253	2396	51
H(10)	5876	3586	4477	22
H(11)	7611	4663	4876	22
H(12)	4429	2580	3905	22
H(14A)	803	5156	4100	40
H(14B)	-544	4909	3617	40
H(14C)	171	5896	3648	40
H(15A)	1091	5839	2573	40
H(15B)	198	4896	2547	40
H(15C)	2059	4981	2348	40

11. X-ray crystal data of compound 13c





13c

ORTEP diagram of compound 13c. Atomic displacement ellipsoids are drawn at the 50% probability level

CCDC no. of **13c**: 891458

Table 1. Crystal data and structure refinement for mo_120626lt_0m.

Identification code	mo_120626lt_0m	
Empirical formula	C19 H17 N3 O3	
Formula weight	335.36	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 11.587(2) Å	α= 90°.
	b = 10.3387(17) Å	β= 101.378(4)°.
	c = 14.091(2) Å	γ = 90°.
Volume	1654.9(5) $Å^3$	
Z	4	
Density (calculated)	1.346 Mg/m^3	
Absorption coefficient	0.093 mm^{-1}	

F(000)	704
Crystal size	0.30 x 0.25 x 0.25 mm^3
Theta range for data collection	2.08 to 26.52°.
Index ranges	-14<=h<=14, -11<=k<=12, -17<=l<=17
Reflections collected	11817
Independent reflections	3378 [R(int) = 0.0555]
Completeness to theta = 26.52°	98.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9486 and 0.6285
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3378 / 0 / 228
Goodness-of-fit on F^2	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0434, wR2 = 0.1087
R indices (all data)	R1 = 0.0618, wR2 = 0.1192
Largest diff. peak and hole	0.348 and -0.319 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_120626lt_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4818(1)	1691(1)	5636(1)	30(1)
O(2)	4337(1)	164(1)	6622(1)	33(1)
O(3)	10928(1)	2340(1)	6042(1)	24(1)
N(1)	9185(1)	2274(1)	6556(1)	21(1)
N(2)	9824(1)	930(1)	8421(1)	21(1)
N(3)	11452(1)	79(1)	9299(1)	29(1)
C(1)	3602(1)	1705(2)	5120(1)	35(1)
C(2)	5065(1)	868(2)	6382(1)	23(1)
C(3)	6323(1)	923(2)	6886(1)	21(1)
C(4)	7169(1)	1614(2)	6512(1)	21(1)
C(5)	8349(1)	1605(1)	6984(1)	20(1)
C(6)	10071(1)	1677(2)	6350(1)	20(1)
C(7)	10334(1)	268(2)	6418(1)	21(1)
C(8)	11475(1)	-159(2)	6790(1)	26(1)
C(9)	11698(2)	-1467(2)	6918(1)	32(1)
C(10)	10799(2)	-2363(2)	6667(1)	32(1)
C(11)	6641(1)	250(2)	7750(1)	24(1)
C(12)	7788(1)	304(2)	8258(1)	24(1)
C(13)	8642(1)	973(2)	7880(1)	20(1)
C(14)	10371(1)	-146(2)	8845(1)	26(1)
C(15)	11610(1)	1384(2)	9163(1)	27(1)
C(16)	10627(1)	1930(2)	8625(1)	24(1)
C(17)	10791(1)	3726(2)	5974(1)	29(1)
C(18)	9437(1)	-639(2)	6149(1)	24(1)
C(19)	9669(1)	-1945(2)	6274(1)	29(1)

Table 3. Bond lengths [Å] and angles [°] for mo_120626lt_0m.

O(1)-C(2)	1.339(2)
O(1)-C(1)	1.4525(18)
O(2)-C(2)	1.2115(19)
O(3)-C(6)	1.3472(18)
O(3)-C(17)	1.4424(19)
N(1)-C(6)	1.2796(19)
N(1)-C(5)	1.4178(19)
N(2)-C(14)	1.360(2)
N(2)-C(16)	1.383(2)
N(2)-C(13)	1.4306(18)
N(3)-C(14)	1.310(2)
N(3)-C(15)	1.380(2)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-C(3)	1.492(2)
C(3)-C(11)	1.386(2)
C(3)-C(4)	1.398(2)
C(4)-C(5)	1.398(2)
C(4)-H(4)	0.9500
C(5)-C(13)	1.402(2)
C(6)-C(7)	1.488(2)
C(7)-C(8)	1.394(2)
C(7)-C(18)	1.396(2)
C(8)-C(9)	1.382(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.386(2)
C(9)-H(9)	0.9500
C(10)-C(19)	1.386(2)
C(10)-H(10)	0.9500
C(11)-C(12)	1.381(2)
C(11)-H(11)	0.9500

C(12)-C(13)	1.396(2)
C(12)-H(12)	0.9500
C(14)-H(14)	0.9500
C(15)-C(16)	1.360(2)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(19)	1.381(2)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
C(2)-O(1)-C(1)	115.81(12)
C(6)-O(3)-C(17)	116.64(12)
C(6)-N(1)-C(5)	120.42(13)
C(14)-N(2)-C(16)	106.52(13)
C(14)-N(2)-C(13)	125.05(13)
C(16)-N(2)-C(13)	128.44(13)
C(14)-N(3)-C(15)	104.23(13)
O(1)-C(1)-H(1A)	109.5
O(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
O(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
O(2)-C(2)-O(1)	123.23(15)
O(2)-C(2)-C(3)	123.95(15)
O(1)-C(2)-C(3)	112.81(13)
C(11)-C(3)-C(4)	120.20(14)
C(11)-C(3)-C(2)	117.68(13)
C(4)-C(3)-C(2)	122.12(14)
C(5)-C(4)-C(3)	120.64(15)

C(5)-C(4)-H(4)	119.7
C(3)-C(4)-H(4)	119.7
C(4)-C(5)-C(13)	118.16(13)
C(4)-C(5)-N(1)	118.69(14)
C(13)-C(5)-N(1)	123.11(13)
N(1)-C(6)-O(3)	120.18(14)
N(1)-C(6)-C(7)	128.49(14)
O(3)-C(6)-C(7)	111.32(12)
C(8)-C(7)-C(18)	119.35(15)
C(8)-C(7)-C(6)	120.10(14)
C(18)-C(7)-C(6)	120.49(13)
C(9)-C(8)-C(7)	119.86(15)
C(9)-C(8)-H(8)	120.1
C(7)-C(8)-H(8)	120.1
C(8)-C(9)-C(10)	120.58(15)
C(8)-C(9)-H(9)	119.7
C(10)-C(9)-H(9)	119.7
C(19)-C(10)-C(9)	119.76(16)
C(19)-C(10)-H(10)	120.1
C(9)-C(10)-H(10)	120.1
C(12)-C(11)-C(3)	119.79(14)
C(12)-C(11)-H(11)	120.1
C(3)-C(11)-H(11)	120.1
C(11)-C(12)-C(13)	120.27(15)
C(11)-C(12)-H(12)	119.9
C(13)-C(12)-H(12)	119.9
C(12)-C(13)-C(5)	120.71(14)
C(12)-C(13)-N(2)	117.19(14)
C(5)-C(13)-N(2)	122.04(13)
N(3)-C(14)-N(2)	112.79(15)
N(3)-C(14)-H(14)	123.6
N(2)-C(14)-H(14)	123.6
C(16)-C(15)-N(3)	111.33(15)

C(16)-C(15)-H(15)	124.3
N(3)-C(15)-H(15)	124.3
C(15)-C(16)-N(2)	105.12(15)
C(15)-C(16)-H(16)	127.4
N(2)-C(16)-H(16)	127.4
O(3)-C(17)-H(17A)	109.5
O(3)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
O(3)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(19)-C(18)-C(7)	120.35(15)
C(19)-C(18)-H(18)	119.8
C(7)-C(18)-H(18)	119.8
C(18)-C(19)-C(10)	120.07(15)
C(18)-C(19)-H(19)	120.0
C(10)-C(19)-H(19)	120.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_120626lt_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	17(1)	31(1)	39(1)	8(1)	2(1)	-1(1)
O(2)	21(1)	25(1)	54(1)	8(1)	8(1)	-5(1)
O(3)	20(1)	19(1)	34(1)	2(1)	11(1)	-3(1)
N(1)	18(1)	17(1)	28(1)	2(1)	6(1)	0(1)
N(2)	19(1)	19(1)	26(1)	0(1)	6(1)	0(1)
N(3)	23(1)	34(1)	30(1)	4(1)	6(1)	4(1)
C(1)	19(1)	39(1)	44(1)	4(1)	-1(1)	0(1)
C(2)	20(1)	17(1)	33(1)	-4(1)	9(1)	0(1)
C(3)	19(1)	15(1)	32(1)	-2(1)	8(1)	0(1)
C(4)	21(1)	16(1)	28(1)	2(1)	7(1)	2(1)
C(5)	20(1)	12(1)	29(1)	0(1)	9(1)	0(1)
C(6)	17(1)	21(1)	23(1)	1(1)	4(1)	-2(1)
C(7)	21(1)	19(1)	24(1)	-2(1)	8(1)	0(1)
C(8)	20(1)	25(1)	33(1)	-4(1)	6(1)	1(1)
C(9)	28(1)	26(1)	40(1)	-2(1)	5(1)	9(1)
C(10)	40(1)	18(1)	39(1)	0(1)	12(1)	6(1)
C(11)	22(1)	18(1)	34(1)	2(1)	12(1)	-2(1)
C(12)	26(1)	19(1)	28(1)	4(1)	10(1)	1(1)
C(13)	19(1)	15(1)	27(1)	-2(1)	6(1)	1(1)
C(14)	25(1)	25(1)	29(1)	4(1)	7(1)	2(1)
C(15)	23(1)	32(1)	27(1)	-3(1)	7(1)	-2(1)
C(16)	22(1)	23(1)	30(1)	-3(1)	8(1)	-2(1)
C(17)	26(1)	18(1)	46(1)	4(1)	14(1)	-3(1)
C(18)	22(1)	22(1)	30(1)	-2(1)	8(1)	0(1)
C(19)	32(1)	20(1)	37(1)	-5(1)	12(1)	-4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_120626lt_0m.

	x	y	z	U(eq)
H(1A)	3405	865	4807	53
H(1B)	3498	2386	4627	53
H(1C)	3083	1873	5577	53
H(4)	6940	2095	5931	25
H(8)	12097	448	6957	31
H(9)	12474	-1755	7179	38
H(10)	10957	-3260	6764	38
H(11)	6071	-245	7991	29
H(12)	7997	-116	8867	29
H(14)	10009	-974	8815	31
H(15)	12315	1843	9413	32
H(16)	10516	2809	8430	29
H(17A)	10064	3936	5514	44
H(17B)	11464	4103	5749	44
H(17C)	10750	4078	6612	44
H(18)	8661	-356	5879	29
H(19)	9054	-2557	6091	35