Supporting Information

Copper Catalyzed Aerobic Oxidative Cyclization and Ketonization: One Pot Synthesis of Benzoimidazo[1,2-a]imidazolones

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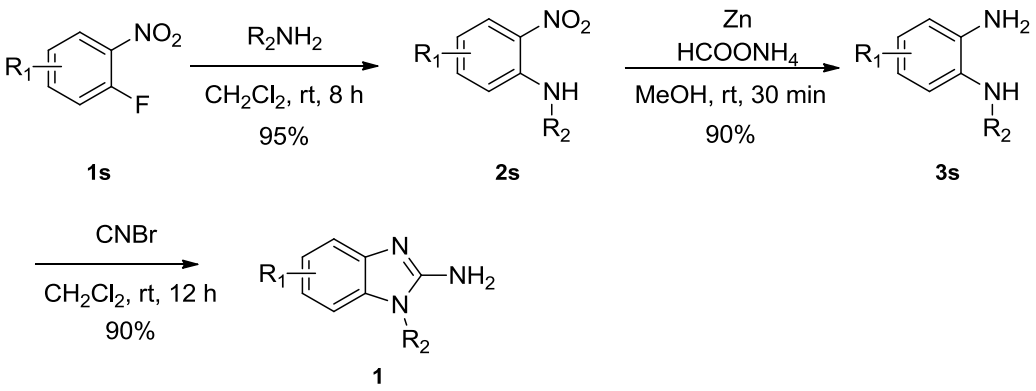
General Remarks:

Methanol and acetone were distilled before use. All reactions were performed under an inert atmosphere with unpurified reagents and dry solvents. Analytical thin-layer chromatography (TLC) was performed using 0.25mm silica gel coated plates. Flash chromatography was performed using the indicated solvent and silica gel 60 (230-400 mesh). ^{1}H NMR (300 MHz) and ^{13}C NMR (75 MHz) spectra were recorded on a 300 MHz spectrometer. Chemical shifts are reported in parts per million (ppm) on the scale from an internal standard.

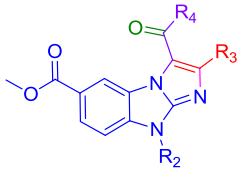
Preparation of 2-aminobenzimidazoles 1.

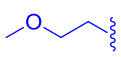
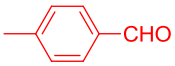
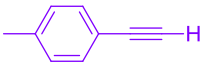
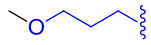
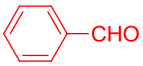
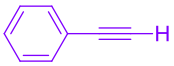
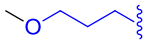
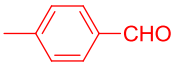
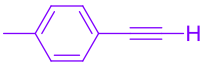
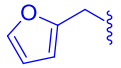
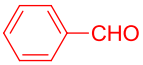
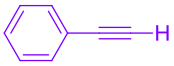
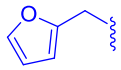
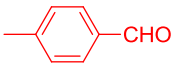
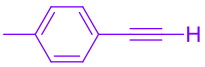
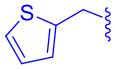
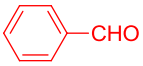
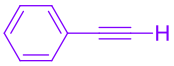
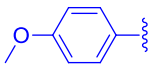
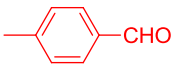
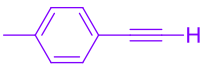
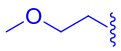
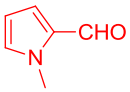
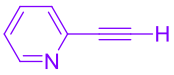
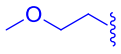
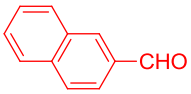
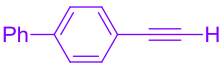
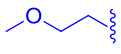
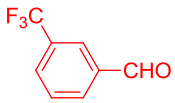
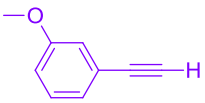
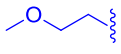
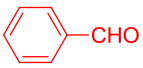
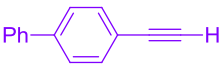
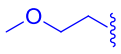
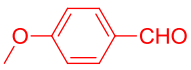
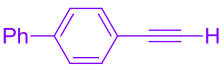
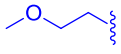
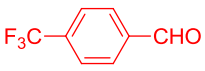
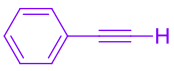
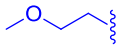
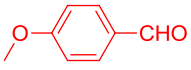
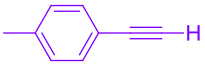
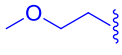
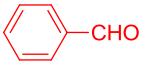
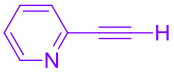
The preparation of 2-aminobenzimidazoles 1 is accomplished by following literature methods.[15] The synthesis of 2-aminobenzimidazoles **1** from 1-fluoro-2-nitrobenzene **1s** involves a sequential three steps as shown in Scheme 6. Reaction of 1-fluoro-2-nitrobenzene **1s** with primary amines furnished ortho nitro anilines **2s**. Subsequent steps involved a nitro group reduction to **3s** followed by ring closure with cyanogen bromide to deliver 2-aminobenzimidazole **1**.



Scheme 6. Preparation of 2-aminobenzimidazoles **1**

Table 2(continued). Three component synthesis of benzoimidazo [1,2-a]imidazolones



Entry	R_2	R_3—CHO	R_4—≡—H	Yield (%)[b]
5l				77
5m				70
5n				75
5o				55
5p				50
5q				51
5r				62
5s				55
5t				57
5u				61
5v				60
5w				51
5x				53
5y				62
5z				62

[b] Isolated Yields

Experimental Procedure for the synthesis of methyl 3-benzoyl-9-isopropyl-2-phenyl-9H-benzo[d]imidazo[1,2-a] imidazole-6-carboxylate (5a)

A solution of methyl 2-amino-1-isopropyl-1H-benzo[d]imidazole-5-carboxylate **1a** (0.12 g, 0.52 mmol) in toluene (10 mL) was added benzaldehyde (0.065 g, 0.62 mmol), phenyl acetylene (0.063 g, 0.62 mmol), Cs_2CO_3 (0.25 g, 0.78 mmol) followed by CuI (0.0098 g, 10 mol %) and the resulting reaction mixture was allowed to reflux at 110 ℃ under oxygen atmosphere. Upon completion (8-10 h) of the reaction, the mixture was filtered through a pad of celite and washed with ethyl acetate (25 mL x 2). The filtrate was concentrated under reduced pressure to give the crude mixture, which was purified by column chromatography on silica gel to afford compound **5a** (0.18 g, 77 %).

Spectral Data of compounds 5 and 6:

Methyl3-benzoyl-9-isopropyl-2-phenyl-9H-benzo[d]imidazo[1,2-a] imidazole-6-carboxylate (5a): ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.28 (s, 1H), 8.15 (d, *J* = 8.6 Hz, 1H), 7.57 (d, *J* = 8.2 Hz, 2H), 7.49 (d, *J* = 8.6 Hz, 1H), 7.28-7.26 (m, 3H), 7.08-6.99 (m, 5H), 4.99 (m, 1H), 3.95 (s, 3H), 1.80 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.5, 167.0, 154.9, 150.0, 138.5, 137.5, 134.4, 131.4, 130.1, 129.5, 128.0, 127.7, 127.6, 125.9, 125.4, 122.8, 117.6, 109.7, 52.2, 48.3, 20.7; MS (ESI-MS) *m/z*: 460 $(M+Na)^+$; HRMS calcd for $C_{27}H_{23}N_3O_3(M+Na)^+$: 460.1637; Found 460.1635; IR (cm^{-1}, neat): 3063, 2984, 2937, 1716, 1618, 1568.

Methyl 3-benzoyl-9-pentyl-2-phenyl-9H-benzo[d]imidazo[1,2-a] imidazole -6-carboxylate (5b): ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.27 (s, 1H), 8.16 (d, *J* = 7.8 Hz, 1H), 7.55-7.50 (m, 2H), 7.45 (m, 1H), 7.27- 7.23 (m, 3H), 7.14-7.03 (m, 5H), 4.35 (t, *J* = 7.3 Hz, 2H), 3.96 (s, 3H), 2.04-2.02 (m, 2H), 1.42-1.39 (m, 4H), 0.91 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.5, 167.0, 155.0, 150.6, 138.4, 134.3, 131.4, 130.1, 129.5, 128.1, 127.6, 126.1, 125.4, 123.0, 121.9, 117.6, 109.1, 52.2, 43.6, 28.9, 28.4, 22.3, 13.9; MS (ESI-MS) *m/z*: 488 $(M+Na)^+$; HRMS (ESI) calcd for $C_{29}H_{27}N_3O_3(M+Na)^+$: 488.1950; Found 488.1952; IR (cm^{-1}, neat): 3052, 2940, 2843, 1717, 1618, 1588.

Methyl 3-(4-methylbenzoyl)-9-pentyl-2-(p-tolyl)-9H-benzo[d]imidazo[1,2-a] imidazole-6-carboxylate (5c): ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.19 (s, 1H), 8.15 (d, *J* = 8.3 Hz, 1H), 7.45 (d, *J* = 8.3 Hz, 2H), 7.39 (d, *J* = 8.6 Hz, 1H), 7.18 (d, *J* = 7.8 Hz, 2H), 6.90-6.87(m, *J* = 7.3 Hz, 4H), 4.34 (t, *J* = 7.1 Hz, 2H), 3.95 (s, 3H), 2.26 (s, 3H), 2.24 (s, 3H), 1.96 -1.94 (m, 2H), 1.68- 1.65 (m, 2H), 1.41 (m, 2H), 0.90 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.4, 167.1, 154.6, 150.5, 142.0, 138.4, 137.8, 135.7, 131.5, 129.9, 129.7, 128.3, 125.9, 125.4, 122.9, 121.7, 117.4, 109.0, 76.6, 52.2, 43.6, 28.9, 28.4, 22.3, 21.4, 21.1, 13.9; MS (ESI-MS) *m/z*: 494.4 $(M+H)^+$; HRMS (ESI) calcd for $C_{31}H_{31}N_3O_3(M+H)^+$: 494.2438; Found 494.2451; IR (cm^{-1}, neat): 2954, 2926, 2855, 1717,1621, 1605, 1583.

Methyl 3-benzoyl-2-phenyl-9-propyl-9H-benzo[d]imidazo[1,2-a]imidazole -6-carboxylate (5d): ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.28 (d, *J* = 1.6 Hz, 1H), 8.18 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.61 – 7.52 (m, 2H), 7.43 (d, *J* = 8.6 Hz, 1H), 7.32 – 7.27 (m, 2H), 7.24 (t, *J* = 8.6 Hz, 1H), 7.16 – 7.03 (m, 5H), 4.34 (t, *J* = 7.4 Hz, 2H), 3.97 (s, 3H), 2.05 (sextet, *J* = 7.4 Hz, 2H), 1.07 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 186.0, 167.5, 155.5, 151.1, 138.9, 138.8, 134.8, 131.9, 130.6, 129.9, 128.5, 128.1, 126.6, 125.9, 123.5, 122.4, 118.1, 109.6, 52.7, 45.6, 22.6, 11.8; MS (ESI-MS) *m/z*: 437.5 $(M+H)^+$; HRMS (ESI) calcd for $C_{27}H_{23}N_3O_3$ $(M+H)^+$; 437.1734; Found 437.2538; IR (cm^{-1}, neat): 2973, 2934, 2867, 1714, 1620, 1584.

Methyl 9-isopropyl-3-(4-methylbenzoyl)-2-(p-tolyl)-9H-benzo[d]imidazo [1,2-a]imidazole-6-carboxylate (5e): ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.19 (d, *J* = 1.4 Hz, 1H), 8.13 (dd, *J* = 8.6, 1.4 Hz, 1H), 7.47-7.44 (m, 3H), 7.18 (dd, *J* = 8.0, 1.4 Hz, 2H), 6.92-6.86 (m, 4H), 4.97 (m, 1H), 3.95 (s, 3H), 2.26 (s, 3H), 2.24 (s, 3H), 1.78 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.4, 167.1, 154.5, 149.9, 142.0, 137.8, 137.5, 135.8, 131.6, 130.0, 129.7, 128.3, 125.7, 125.4, 122.6, 121.3, 117.4, 109.6, 52.1, 48.2, 21.4, 21.1, 20.7; MS (ESI-MS) *m/z*: 466.3 $(M+H)^+$; HRMS (ESI) calcd for $C_{29}H_{27}N_3O_3(M+H)^+$: 466.2125; Found 466.2132; IR (cm^{-1}, neat): 3025, 2979, 2947, 1717, 1619, 1604, 1571.

Methyl 9-isopropyl-3-(4-methoxybenzoyl)-2-(4-methoxyphenyl)-9H-benzo [d]imidazo[1,2-a]imidazole-6-carboxylate (5f): ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.14 (s, 1H), 8.13 (dd, *J* = 8.7, 1.7 Hz, 1H), 7.63 (d, *J* = 8.5 Hz, 2H), 7.46 (d, *J* = 8.5 Hz,

1H), 7.30-7.26 (m, 2H), 6.68-6.63 (m, 4H), 4.99 (m, 1H), 3.96 (s, 3H), 3.76 (s, 3H), 3.74 (s, 3H), 1.79 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (150 MHz,$CDCl_3$) δ 184.9, 167.5, 162.9, 159.9, 154.1, 150.3, 138.0, 132.3, 131.9, 131.5, 127.7, 126.1, 125.9, 123.1, 121.3, 117.7, 113.8, 113.6, 110.1, 55.8, 55.7, 52.6, 48.6, 21.2; MS (ESI-MS) *m/z*: 498.4 $(M+H)^+$; HRMS (ESI) calcd for $C_{29}H_{27}N_3O_5$ $(M+H)^+$:b498.2023; Found 498.2018; IR (cm^{-1}, neat): 2952, 2931, 2839, 1716, 1599, 1571.

Methylbenzoyl-9-cyclopentyl-2-phenyl-9H-benzo[d]imidazo[1,2-a] imidazole-6-carboxylate (5g): ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.28 (s, 1H), 8.15 (d, *J* = 8.6 Hz, 1H), 7.55-7.48 (m, 3H), 7.28-7.23 (m, 3H), 7.12-7.05 (m, 5H), 5.08 (m, 1H), 3.96 (s, 3H), 2.47- 2.40 (m, 2H), 2.26-2.20 (m, 2H), 2.10-2.06 (m, 2H), 1.89-1.80 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.5, 167.0, 154.8, 150.2, 138.5, 137.8, 134.4, 131.4, 130.2, 129.5, 128.0, 127.7, 127.6, 125.8, 125.4, 122.8, 121.5, 117.6, 109.8, 56.6, 52.2, 29.9, 24.6; MS (ESI-MS) *m/z*: 486 $(M+Na)^+$; HRMS calcd for $C_{29}H_{25}N_3O_3$ $(M+Na)^+$; *m/z*: 486.1797; Found 486.1794; IR (cm^{-1}, neat): 3066, 2948, 2872, 1715, 1617, 1569.

Methyl 9-cyclopentyl-3-(4-methylbenzoyl)-2-(p-tolyl)-9H-benzo] imidazo[1,2-a]imidazole-6-carboxylate (5h): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.17 (d, *J* = 1.4 Hz, 1H), 8.14-8.12 (m, 1H), 7.48-7.44 (m, 3H), 7.21 (d, *J* = 6.6 Hz, 2H), 5.08 (m, 1H), 6.91-6.88 (m, 4H), 3.95 (s, 3H), 2.44-2.38 (m, 3H), 2.26 (s, 3H), 2.24 (s, 3H), 2.10 (m, 3H), 1.82 (m, 2H); ^{13}C NMR (150 MHz,$CDCl_3$) δ 185.1, 166.5, 143.0, 140.3, 139.0, 136.8, 134.7, 131.5, 130.1, 129.7, 129.6, 128.9, 128.6, 128.6, 126.3, 125.4, 123.8, 117.8, 110.8, 57.5, 52.3, 29.9, 24.8, 21.5, 21.2; MS (ESI-MS) *m/z*: 492.2 $(M+H)^+$; HRMS (ESI) calcd for $C_{31}H_{29}N_3O_3$ $(M+H)^+$; *m/z*: 492.2282; Found 492.2282; IR (cm^{-1}, neat): 3025, 2952, 2922, 2871, 1718, 1620, 1605, 1573.

Methyl 9-cyclopentyl-3-(4-methoxybenzoyl)-2-(4-methoxyphenyl)-9H-benzo[d] imidazo[1,2-a]imidazole-6-carboxylate (5i): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.12 (s, 1H), 8.11 (d, *J* = 8.5 Hz, 1H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.41 (m, 1H), 7.28-7.25 (m, 2H), 6.64 (d, *J* = 8.2 Hz, 4H), 5.08 (s, 1H), 3.95 (s, 3H), 3.75 (s, 3H), 3.73 (s, 3H), 2.47-2.43 (m, 2H), 2.24-2.20 (m, 2H), 2.11-2.08 (m, 2H), 1.85-1.81 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 184.3, 166.9, 162.5, 159.5, 137.5, 131.8, 130.8, 125.7, 125.4, 125.4, 122.8, 117.2, 113.3, 113.1, 109.9, 109.8, 56.7, 55.3, 55.2, 52.1, 29.9, 29.1, 25.2, 24.6; MS (ESI-MS) *m/z*: 524.2 $(M+H)^+$; HRMS (ESI) calcd for

$C_{31}H_{29}N_3O_3$ $(M+H)^+$; *m/z*: 524.2180; Found 524.2177; IR (cm^{-1}, neat): 3010, 2958, 2873, 1719, 1604.

Methyl3-benzoyl-9-[2-(cyclohex-1-en-1-yl)ethyl]-2-phenyl-9H-benzo-[d]imidazo[1,2-a]imidazole-6-carboxylate (5j): ^1H NMR (400 MHz, $CDCl_3$) δ 9.26 (d, *J* = 1.6 Hz, 1H), 8.16 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.55-7.50 (m, 2H), 7.40 (d, *J* = 8.6 Hz, 1H), 7.27-7.23 (m, 3H), 7.12-7.04 (m, 5H), 5.30 (s, 1H), 4.46 (t, *J* = 7.1 Hz, 2H), 3.96 (s, 3H), 2.58 (t, *J* = 7.0 Hz, 2H), 2.09-2.05 (m, 2H), 1.81- 1.76 (m, 2H), 1.60-1.57 (m, 2H), 1.49-1.45 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 185.8, 166.8, 138.4, 137.5, 133.6, 133.1, 131.9, 130.8, 130.0, 128.6, 127.5, 125.8, 125.6, 125.1, 120.8, 118.5, 111.0, 52.9, 44.4, 37.1, 28.8, 25.7, 23.2, 22.4; MS (ESI-MS) *m/z*: 504.4 $(M+H)^+$; HRMS (ESI) calcd for $C_{32}H_{29}N_3O_3$ $(M+H)^+$; *m/z*: 504.2282; Found 504.2276; IR (cm^{-1}, neat): 3063, 3022, 2929, 2852, 1717, 1676, 1622.

Methyl9-(2-methoxyethyl)-3-(3-methylbenzoyl)-2-phenyl-9H-benzo-[d]imidazo[1,2-a]imidazole-6-carboxylate (5k): ^1H NMR (300 MHz, $CDCl_3$) δ 9.17 (d, *J* = 1.6 Hz, 1H), 8.14 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.56-7.46 (m, 3H), 7.30-7.25 (m, 2H), 7.14-7.11 (m, 3H), 6.90 (t, *J* = 8.6 Hz, 2H), 4.53 (t, *J* = 5.2 Hz, 2H), 3.95 (s, 3H), 3.89 (t, *J* = 5.2 Hz, 2H), 3.34 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.6, 167.0, 155.0, 154.2, 150.4, 139.1, 138.4, 138.0, 135.5, 134.4, 131.3, 130.1, 129.9, 129.7, 129.5, 128.3, 127.9, 127.6, 126.0, 125.4, 125.3, 70.5, 59.0, 52.2, 43.7, 21.4; MS (ESI-MS) *m/z*: 468.4 $(M+H)^+$; HRMS (ESI) calcd for $C_{28}H_{25}N_3O_4$ $(M+H)^+$; *m/z*: 468.1918; Found 468.1933; IR (cm^{-1}, neat): 2990, 2949, 2902, 2852, 1715, 1620, 1584.

Methyl 9-(2-methoxyethyl)-3-(4-methylbenzoyl)-2-(p-tolyl)-9H-benzo-[d]imidazo[1,2-a]imidazole-6-carboxylate (5l): ^1H NMR (300 MHz, $CDCl_3$) δ 9.16 (s, 1H), 8.15 (d, *J* = 8.7 Hz, 1H), 7.517.47 (m, 3H), 7.18 (d, *J* = 8.0 Hz, 2H), 6.93-6.87 (m, 4H), 4.53 (t, *J* = 5.4 Hz, 2H), 3.96 (s, 3H), 3.90 (t, *J* = 5.4 Hz, 2H), 3.35 (s, 3H), 2.26 (d, *J* = 6.2 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.3, 166.9, 154.2, 150.2, 142.0, 139.0, 137.8, 135.6, 131.4, 129.9, 129.6, 128.3, 125.9, 125.3, 122.9, 121.7, 117.1, 110.0, 70.4, 59.0, 52.1, 43.6, 21.4, 21.1; MS (ESI-MS) *m/z*: 482.3 $(M+H)^+$; HRMS (ESI) calcd for $C_{29}H_{27}N_3O_4$ $(M+H)^+$; *m/z*: 482.2074; Found 482.2089; IR (cm^{-1}, neat): 3034, 2984, 2948, 1717, 1678, 1621, 1605, 1584.

Methyl 3-benzoyl-9-(3-methoxypropyl)-2phenyl-9H-benzo[d]imidazo-[1,2-a]imidazole-6-carboxylate (5m): ^1H NMR (300 MHz, $CDCl_3$) δ 9.26 (s, 1H),

8.17 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 7.5 Hz, 2H), 7.50 (d, *J* = 8.5 Hz, 1H), 7.27 (t, *J* = 8.4 Hz, 3H), 7.24-7.05 (m, 5H), 4.49 (t, *J* = 6.2 Hz, 2H), 3.97 (s, 3H), 3.43-3.40 (m, 2H), 3.34 (s, 3H), 2.28 (t, *J* = 6.2 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.5, 167.0, 154.9, 150.4, 138.8, 138.3, 134.3, 131.5, 130.1, 129.5, 128.1, 127.7, 126.1, 125.2, 123.0, 121.9, 117.5, 109.2, 68.7, 58.7, 52.2, 40.4, 28.8; MS (ESI-MS) *m/z*: 468.1 $(M+H)^+$; HRMS (ESI) calcd for $C_{28}H_{25}N_3O_4$ $(M+H)^+$; *m/z*: 468.1918; Found 468.1922; IR (cm^{-1}, neat): 3056, 3010, 2975, 2952, 2923, 2857, 1715, 1657, 1619, 1584.

Methyl 9-(3-methoxypropyl)-3-(4-methylbenzoyl)-2-(p-tolyl)-9H-benzo-[d]imidazo[1,2-a]imidazole-6-carboxylate (5n): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.17 (s, 1H), 8.15 (d, *J* = 8.5 Hz, 1H), 7.48 (d, *J* = 8.2 Hz, 3H), 7.18 (d, *J* = 8.0 Hz, 2H), 6.92-6.87 (m, 4H), 4.47 (t, *J* = 6.7 Hz, 2H), 3.96 (s, 3H), 3.40 (m, 2H), 3.33 (s, 3H), 2.28-2.16, m, 8H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.4, 167.0, 154.5, 150.3, 142.1, 137.9, 135.6, 129.9, 129.7, 128.3, 126.0, 125.3, 122.9, 121.7, 117.3, 109.1, 68.7, 58.6, 52.2, 40.3, 28.8, 21.4, 21.1; MS (ESI-MS) *m/z*: 496.3 $(M+H)^+$; HRMS (ESI) calcd for $C_{30}H_{29}N_3O_4$ $(M+H)^+$; *m/z*: 496.2231; Found 496.2229; IR (cm^{-1}, neat): 3022, 2984, 2946, 2923, 2863,2807, 1716, 1620, 1605, 1583.

Methyl 3-benzoyl-9-(furan-2-ylmethyl)-2-phenyl-9H-benzo[d]imidazo [1,2-a]imidazole-6-carboxylate (5o): ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.23 (s, 1H), 8.14 (d, *J* = 8.5 Hz, 1H), 7.54-7.50 (m, 3H), 7.38 (s, 1H), 7.27-7.23 (m, 3H), 7.09-7.04 (m, 5H), 6.51 (d, *J* = 7.2 Hz, 1H), 6.36 (d, *J* = 7.2 Hz, 1H), 5.53 (s, 2H), 3.95 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.6, 166.9, 154.8, 150.2, 148.0, 143.1, 138.3, 138.1, 134.2, 131.5, 130.1, 129.5, 128.1, 127.7, 126.2, 125.6, 123.5, 122.1, 117.5, 110.7, 109.8, 109.7, 52.2, 40.0; MS (ESI-MS) *m/z*: 476.3 $(M+H)^+$; HRMS (ESI) calcd for $C_{29}H_{21}N_3O_4$ $(M+H)^+$; *m/z*: 476.1605; Found 476.1610 IR (cm^{-1}, neat): 3122, 3060, 2951, 1717, 1620, 1585.

Methyl 9-(furan-2-ylmethyl)-3-(4-methylbenzoyl)-2-(p-tolyl)-9H-benzo [d]imidazo[1,2-a]imidazole-6-carboxylate (5p): ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.14 (s, 1H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 3H), 7.37 (m, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 6.90 (t, *J* = 7.2 Hz, 4H), 6.50 (d, *J* = 7.2 Hz, 1H), 6.34 (m, 1H), 5.52 (s, 2H), 3.94 (s, 3H), 2.26 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.5, 166.9, 154.4, 150.1, 148.1, 143.1, 142.1, 138.1, 137.9, 135.6, 131.4, 129.9, 129.7, 128.3, 126.1, 125.6, 123.4, 121.9, 117.3, 110.7, 109.7, 109.6, 52.2, 40.0, 21.4, 21.2;

MS (ESI-MS) *m/z*: 504.3 $(M+H)^+$; HRMS (ESI) calcd for $C_{31}H_{25}N_3O_4$ $(M+H)^+$; *m/z*: 504.1918; Found 504.1922; IR (cm^{-1}, neat): 3034, 2952, 2922, 2852, 1717, 1621, 1605, 1585.

Methyl 3-benzoyl-2-phenyl-9-(thiophen-2-ylmethyl)-9H-benzo[d]imidazo-[1,2-a]imidazole-6-carboxylate (5q): ^1H NMR (300 MHz, $CDCl_3$) δ 9.23 (d, *J* = 1.6 Hz, 1H), 8.14 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.59-7.53 (m, 2H), 7.45 (d, *J* = 8.6 Hz, 1H), 7.32-7.27 (m, 4H), 7.27-7.23 (m, 2H), 7.18-7.10 (m, 4H), 6.98 (m, 1H), 5.72 (s, 2H), 3.95 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 186.2, 167.0, 146.5, 141.8, 136.8, 136.5, 133.4, 132.8, 131.2, 130.1, 129.5, 128.3, 125.6, 123.5, 121.9, 110.4, 52.0, 32.1; MS (ESI-MS) *m/z*: 492.4 $(M+H)^+$; HRMS (ESI) calcd for $C_{29}H_{21}N_3O_3S$ $(M+H)^+$; *m/z* : 492.1376; Found 492.1369; IR (cm^{-1}, neat) :3060, 2949, 2852, 1716, 1621, 1586.

Methyl 9-(4-methoxyphenyl)-3-(4-methylbenzoyl)-2-(p-tolyl)-9H-benzo [d]imidazo[1,2-a]imidazole-6-carboxylate (5r): ^1H NMR (300 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.09 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.66 (d, *J* = 8.9 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 8.6 Hz, 1H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 8.9 Hz, 2H), 6.92 (d, *J* = 8.1 Hz, 2H), 6.85 (d, *J* = 8.1 Hz, 2H), 3.95 (s, 3H), 3.89 (s, 3H), 2.26 (s, 3H), 2.21(s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.5, 166.9, 159.5, 154.4, 149.9, 142.2, 138.6, 137.9, 135.6, 131.4, 130.0, 129.7, 128.4, 128.2, 126.7, 126.6, 126.2, 125.4, 123.7, 121.6, 117.4, 115.3, 110.0, 55.6, 52.2, 21.4, 21.1; MS (ESI-MS) *m/z*: 530.3 $(M+H)^+$; HRMS (ESI) calcd for $C_{33}H_{27}N_3O_4$ $(M+H)^+$; *m/z*: 530.2074; Found 530.2092; IR (cm^{-1}, neat): 3031, 3005, 2949, 2839, 1717, 1620, 1564.

Methyl9-(2-methoxyethyl)-2-(1-methyl-1H-pyrrol-2-yl)-3-picolinoyl-9H-benzo[d] imidazo[1,2-a]imidazole-6-carboxylate (5s): ^1H NMR (400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 8.26 (d, *J* = 8.6 Hz, 1H), 8.14 (d, *J* = 8.6 Hz, 1H), 7.67 – 7.63 (m, 2H), 7.50 (d, *J* = 8.6 Hz, 1H), 7.15 (m, 1H), 6.45 (m, 1H), 5.75-5.68 (m, 2H), 4.49 (t, *J* = 6.2 Hz, 2H), 3.94 (s, 3H), 3.86 (t, *J* = 6.2 Hz, 2H), 3.74 (s, 3H), 3.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.6, 167.0, 148.1, 138.9, 136.1, 126.2, 125.4, 124.9, 123.8, 123.5, 123.3, 117.5, 114.0, 110.0, 107.8, 70.3, 59.0, 52.2, 43.7; MS (ESI) : *m/z* 458.3 $[M+H]^+$; HRMS (ESI) calcd for $C_{25}H_{23}N_5O_4$ $(M+H)^+$; 458.1823; Found 458.1815.

Methyl3-([1,1'-biphenyl]-4-carbonyl)-9-(2-methoxyethyl)-2-(naphthalen-2-yl)-9H -benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5t): ^1H NMR (400 MHz, DMSO-d_6) δ 10.15 (d, *J* = 7.2, 1H), 8.70 (d, *J* = 7.2 Hz, 1H), 8.28 – 8.05 (m, 3H),

7.92 – 7.83 (m, 2H), 7.78 – 7.59 (m, 6H), 7.44 – 7.33 (m, 2H), 7.26 (d, *J* = 7.4 Hz, 1H), 7.09 (m, 1H), 6.94 – 6.82 (m, 2H), 4.51 (t, *J* = 6.2 Hz, 2H), 3.90 (t, *J* = 6.2 Hz, 2H), 3.71 (s, 3H), 3.28 (t, *J* = 6.2 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 166.3, 152.0, 149.3, 148.8, 140.0, 137.5, 133.6, 133.3, 128.3, 127.9, 127.6, 126.6, 126.0, 124.9, 124.8, 124.3, 123.6, 121.3, 121.3, 121.1, 118.2, 117.8, 112.9, 110.8, 102.8, 69.7, 58.6, 52.4; MS (ESI): *m/z* 580.3 $[M+H]^+$; HRMS (ESI) calcd for $C_{37}H_{29}N_3O_4$ $(M+H)^+$; 580.2231; Found 580.2221

Methyl3-(3-methoxybenzoyl)-9-(2-methoxyethyl)-2-(3-(trifluoromethyl)phenyl)-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5u): ^{1}H NMR (400 MHz, Acetone-d_6) δ 9.26 (s, 1H), 8.14 (m, 1H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.42 (m, 1H), 7.32 – 7.23 (m, 2H), 7.08 – 6.96 (m, 3H), 6.77 (m, 1H), 4.59 (t, *J* = 6.2 Hz, 2H), 3.93 (t, *J* = 6.2 Hz, 2H), 3.85 (s, 3H), 3.68 (s, 3H), 3.29 (s, 3H); ^{13}C NMR (100 MHz, Acetone-d_6) δ 184.2, 166.2, 158.9, 151.8, 150.3, 140.2, 139.2, 133.7, 130.8, 128.6, 128.5, 126.0, 125.9, 125.7, 125.2, 123.4, 122.7, 121.1, 117.2, 117.1, 113.5, 110.6, 69.4, 57.9, 54.6, 51.5, 43.4; MS (ESI): *m/z* 552.2 $[M+H]^+$; HRMS (ESI) calcd for $C_{29}H_{24}F_3N_3O_5$ $(M+H)^+$; 552.1741; Found 552.1744.

Methyl3-([1,1'-biphenyl]-4-carbonyl)-9-(2-methoxyethyl)-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5v): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.22 (s, 1H), 8.17 (m, 1H), 7.62 – 7.20 (m, 12H), 7.07 – 7.01 (m, 3H), 4.51 (t, *J* = 6.2, 2H), 3.91 (s, 3H), 3.88 (t, *J* = 6.2, 2H), 3.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.1, 179.6, 161.6, 145.1, 138.8, 135.3, 135.1, 134.8, 133.8, 133.1, 131.7, 129.0, 127.9, 126.1, 125.2, 124.8, 124.2, 123.6, 123.5, 122.7, 122.2, 121.8, 121.6, 121.0, 120.7, 117.7, 116.7, 112.0, 104.9, 65.1, 53.3, 46.9, 38.4; MS (ESI): *m/z* 530.3 $[M+H]^+$; HRMS (ESI) calcd for $C_{33}H_{27}N_3O_4$ $(M+H)^+$; 530.2074; Found; 530.2074.

Methyl3-([1,1'-biphenyl]-4-carbonyl)-9-(2-methoxyethyl)-2-(4-methoxyphenyl)-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5w): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (s, 1H), 8.07 (d, *J* = 7.0 Hz, 1H), 7.58 (t, *J* = 7.0 Hz, 2H), 7.42 – 7.15 (m, 5H), 7.33 – 7.15 (m, 5H), 6.55 (t, *J* = 6.6 Hz, 2H), 4.48 (t, *J* = 6.2 Hz, 2H), 3.91 (s, 3H), 3.85 (t, 6.2 Hz, 2H), 3.57 (s, 3H), 3.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.5, 167.0, 162.6, 153.3, 150.4, 140.6, 140.6, 139.1, 133.5, 131.8, 130.9, 130.5, 128.7, 127.4, 126.9, 126.4, 126.0, 125.3, 123.1, 121.8, 117.1, 113.1, 110.0, 77.2, 70.5,

59.0, 55.3, 52.2, 43.7; MS (ESI): *m/z* 560.4 $[M+H]^+$; HRMS (ESI): calcd for $C_{34}H_{29}N_3O_5[M+H]^+$; 560.2180, Found; 560.2175

Methyl3-benzoyl-9-(2-methoxyethyl)-2-(4-(trifluoromethyl)phenyl)-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5x): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.24 (d, *J* = 1.6 Hz, 1H), 8.19 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.61 – 7.52 (m, 3H), 7.42 (d, *J* = 8.1 Hz, 2H), 7.38 – 7.31 (m, 3H), 7.14 (t, *J* = 7.6 Hz, 2H), 4.57 (t, *J* = 6.2 Hz, 2H), 3.99 (s, 3H), 3.93 (t, *J* = 6.2 Hz, 2H), 3.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.4, 167.0, 152.8, 150.6, 139.2, 138.2, 138.1, 131.9, 130.4, 130.1, 129.5, 129.5, 128.0, 127.9, 126.4, 125.3, 124.6, 124.5, 124.5, 123.4, 122.5, 117.6, 110.3, 77.3, 70.5, 59.2, 52.3, 43.9; MS (ESI): *m/z* 522.2 $[M+H]^+$; HRMS (ESI): calcd for $C_{28}H_{23}N_3O_4[M+H]^+$; 522.1635, Found; 522.1633.

Methyl9-(2-methoxyethyl)-2-(4-methoxyphenyl)-3-(4-methylbenzoyl)-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5y): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.24 (d, *J* = 7.5 Hz, 1H), 8.22 (d, *J* = 8.3 Hz, 1H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.87 (d, *J* = 7.8 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 1H), 7.54 (t, *J* = 7.1 Hz, 2H), 7.27 (m, 1H), 7.09 (d, *J* = 7.8 Hz, 1H), 6.89 (d, *J* = 8.4 Hz, 1H), 6.80 (d, *J* = 8.4 Hz, 1H), 4.56 (t, *J* = 6.2 Hz, 2H), 3.92 (s, 3H), 3.86 (t, *J* = 6.2 Hz, 2H), 3.75 (s, 3H), 3.32 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.8, 166.3, 166.6, 162.3, 162.0, 161.1, 158.3, 148.1, 144.1, 140.2, 135.6, 131.8, 130.7, 130.0, 129.5, 128.9, 128.4, 125.1, 125.0, 118.2, 118.1, 114.2, 113.7, 113.6, 109.7, 70.2, 59.0, 55.4, 43.0; MS (ESI): *m/z* 498.3 $[M+H]^+$. HRMS (ESI): calcd for $C_{29}H_{27}N_3O_5$ $[M+H]^+$; 498.2023, Found; 498.2026.

Methyl9-(2-methoxyethyl)-2-phenyl-3-picolinoyl-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5z): ^{1}H NMR (400 MHz, Acetone-d_6) δ 9.26 (s, 1H), 8.10 – 8.03 (m, 2H), 7.83 – 7.71 (m, 3H), 7.31 – 7.18 (m, 3H), 7.13 – 7.05 (m, 3H), 4.61 (t, *J* = 6.4 Hz, 2H), 3.95 – 3.92 (m, 5H), 3.30 (s, 3H); ^{13}C NMR (100 MHz, Acetone-d_6) δ 183.7, 166.3, 156.3, 150.7, 148.1, 136.3, 135.5, 129.6, 127.5, 127.3, 125.5, 125.3, 123.7, 122.7, 116.9, 110.6, 69.7, 57.9, 51.5, 43.4; MS (ESI) : *m/z* 455.3 $[M+H]^+$; HRMS (ESI): calcd for $C_{26}H_{22}N_4O_4$ $[M+H]^+$; 455.1714, Found; 455.1719

(9-(2-methoxyethyl)-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazol-3-yl)(phenyl)methanone (5aa): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 8.2, 1H), 7.58 – 7.52 (m, 2H), 7.47 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.37 (dt, *J* = 8.2, 1.2 Hz, 1H), 7.31 – 7.20 (m, 4H), 7.11 – 7.00 (m, 5H), 4.49 (t, *J* = 6.2 Hz, 2H), 3.88 (t, *J* = 6.2 Hz, 2H), 3.34 (s,

3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.3, 154.9, 150.1, 138.6, 135.8, 134.7, 131.3, 130.1, 129.6, 127.9, 127.6, 125.8, 124.0, 121.1, 115.9, 110.3, 70.5, 59.0, 43.4; MS (ESI): *m/z* 396.3 $[M+H]^+$; HRMS (ESI): calcd for $C_{25}H_{21}N_3O_2$ $[M+H]^+$: 396.1707; Found: 396.1717.

(7-chloro-9-(2-methoxyethyl)-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazol-3-yl)(phenyl)methanone (5ba): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 8.0 Hz, 1H), 7.55 – 7.48 (m, 3H), 7.27 – 7.19 (m, 4H), 7.12 – 7.00 (m, 5H), 4.45 (t, *J* = 6.6 Hz, 2H), 3.86 (t, *J* = 6.6 Hz, 2H), 3.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.5, 154.8, 150.2, 138.3, 136.6, 134.4, 131.4, 130.1, 129.8, 129.5, 128.0, 127.6, 124.4, 121.7, 121.4, 116.8, 110.7, 70.5, 59.1, 43.7; MS (ESI): *m/z* 430.2 $[M+H]^+$; HRMS (ESI): calcd for $C_{25}H_{20}ClN_3O_2$ $[M+H]^+$; *m/z* 430.1321, found 430.1317.

3-benzoyl-9-(2-methoxyethyl)-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazole-6-carbonitrile (5ca): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 (s, 1H), 7.64 (d, *J* = 8.5 Hz, 1H), 7.57 (d, *J* = 8.5 Hz, 1H), 7.55 – 7.49 (m, 2H), 7.28 – 7.22 (m, 4H), 7.01 – 7.22 (m, 5H), 4.52 (t, *J* = 6.4 Hz, 2H), 3.91 (t, *J* = 6.4 Hz, 2H), 3.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.6, 155.0, 150.2, 138.7, 137.9, 134.0, 131.7, 130.1, 129.5, 128.3, 128.0, 127.7, 125.4, 120.0, 119.2, 111.4, 104.2, 70.6, 59.1, 44.0; MS (ESI): *m/z* 421.1 $[M+H]^+$; HRMS (ESI): calcd for $C_{26}H_{21}N_4O_2$ $[M+H]^+$; 421.1659, found; 421.1664.

2-methoxyethyl 3-benzoyl-9-(2-methoxyethyl)-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5da): ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.24 (s, *J* = 1.6 Hz, 1H), 8.17 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.55 (dd, *J* = 9.3, 7.9 Hz, 3H), 7.29 (m, 2H), 7.24 (d, *J* = 1.3 Hz, 1H), 7.09 (m, 5H), 4.54 (m, 4H), 3.90 (t, *J* = 5.2 Hz, 2H), 3.78-3.70 (m, 2H), 3.46 (s, 3H), 3.35 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.4, 166.4, 154.6, 139.2, 138.3, 134.3, 131.5, 130.1, 129.5, 128.1, 127.7, 126.2, 125.4, 123.1, 122.0, 117.6, 110.0, 70.6, 70.5, 64.0, 59.1, 59.0, 43.7; MS (ESI-MS) *m/z*: 498.4 $(M+H)^+$; HRMS (ESI) calcd for $C_{29}H_{27}N_3O_5$ $(M+H)^+$; 498.2023, found 498.2016; IR (cm^{-1}, neat): 3061, 2926, 2854, 1713, 1620, 1584.

(9-(2-methoxyethyl)-6-methyl-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazol-3-yl)(phenyl)methanone (5ea): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.57 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.34 (d, *J* = 8.3 Hz, 1H), 7.25 – 7.20 (m, 3H), 7.20 (m, 1H), 7.04 (m, 6H), 4.45 (t, *J* = 6.2 Hz, 2H), 3.85 (t, *J* = 6.2 Hz, 2H), 3.33 (s, 3H), 2.50 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.4, 154.9, 138.7, 134.7, 133.8, 131.3, 131.1, 130.1,

129.6, 127.9, 127.6, 125.9, 125.0, 116.1, 109.9, 70.6, 59.0, 43.3, 21.6; MS (ESI): *m/z* 410.3 $[M+H]^+$; HRMS (ESI): calcd for $C_{26}H_{24}N_3O_2[M+H]^+$; 410.1863, Found; 410.1859.

(9-(2-methoxyethyl)-6-nitro-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazol-3-yl)(phenyl)methanone (5fa): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.49 (d, *J* = 2.2 Hz, 1H), 8.31 (dd, *J* = 9.0, 2.2 Hz, 1H), 7.61 – 7.49 (m, 3H), 7.26 (m, 3H), 7.08 (m, 5H), 4.55 (t, *J* = 6.2 Hz, 2H), 3.89 (t, *J* = 6.2 Hz, 2H), 3.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.5, 154.8, 141.8, 140.2, 137.9, 133.9, 131.7, 130.1, 129.5, 128.4, 127.8, 127.7, 125.0, 120.1, 112.4, 110.4, 70.6, 59.1, 44.2; MS (ESI): *m/z* 441.1 $[M+H]^+$; HRMS (ESI): calcd for $C_{25}H_{20}N_4O_4$ $M+H]^+$; 441.1557, Found 441.1566.

(6-methoxy-9-(2-methoxyethyl)-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazol-3-yl)(phenyl)methanone (5ga): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 2.2 Hz, 1H), 7.56 – 7.49 (m, 2H), 7.37 (d, *J* = 8.9 Hz, 1H), 7.24 – 7.18 (m, 3H), 7.10 – 7.03 (m, 4H), 7.03 – 6.95 (m, 2H), 4.46 (t, *J* = 6.2 Hz, 2H), 3.92 (s, 3H), 3.86 (t, *J* = 6.2 Hz, 2H), 3.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.4, 155.4, 154.9, 150.6, 138.8, 134.7, 131.2, 130.1, 129.9, 129.5, 127.9, 127.6, 127.5, 126.2, 121.4, 112.9, 110.9, 100.2, 70.7, 59.0, 56.1, 43.4; MS (ESI): *m/z* 426.3 $[M+H]^+$; HRMS (ESI): calcd for $C_{26}H_{23}N_3O_3$ $[M+H]^+$; 426.1816, found 426.1812.

9-(2-methoxyethyl)-2-phenyl-6-(trifluoromethyl)-9H-benzo[d]imidazo[1,2-a]imidazol-3-yl)(phenyl)methanone (5ha): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (s, 1H), 7.65 (d, *J* = 8.6 Hz, 1H), 7.57 (d, *J* = 8.6 Hz, 1H), 7.55 – 7.50 (m, 2H), 7.28 – 7.20 (m, 3H), 7.13 – 7.01 (m, 5H), 4.52 (t, *J* = 6.4 Hz, 2H), 3.87 (t, *J* = 6.4 Hz, 2H), 3.32 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 185.6, 155.1, 150.4, 138.2, 138.0, 134.2, 131.6, 130.1, 129.5, 128.2, 127.7, 125.4, 121.9, 121.2, 121.1, 113.7, 113.6, 110.7, 70.6, 59.1, 43.8; MS (ESI): *m/z* 464.2 $[M+H]^+$; HRMS (ESI): calcd for $C_{26}H_{20}F_3N_3O_2$ $[M+H]^+$; 464.1580, found 464.1585.

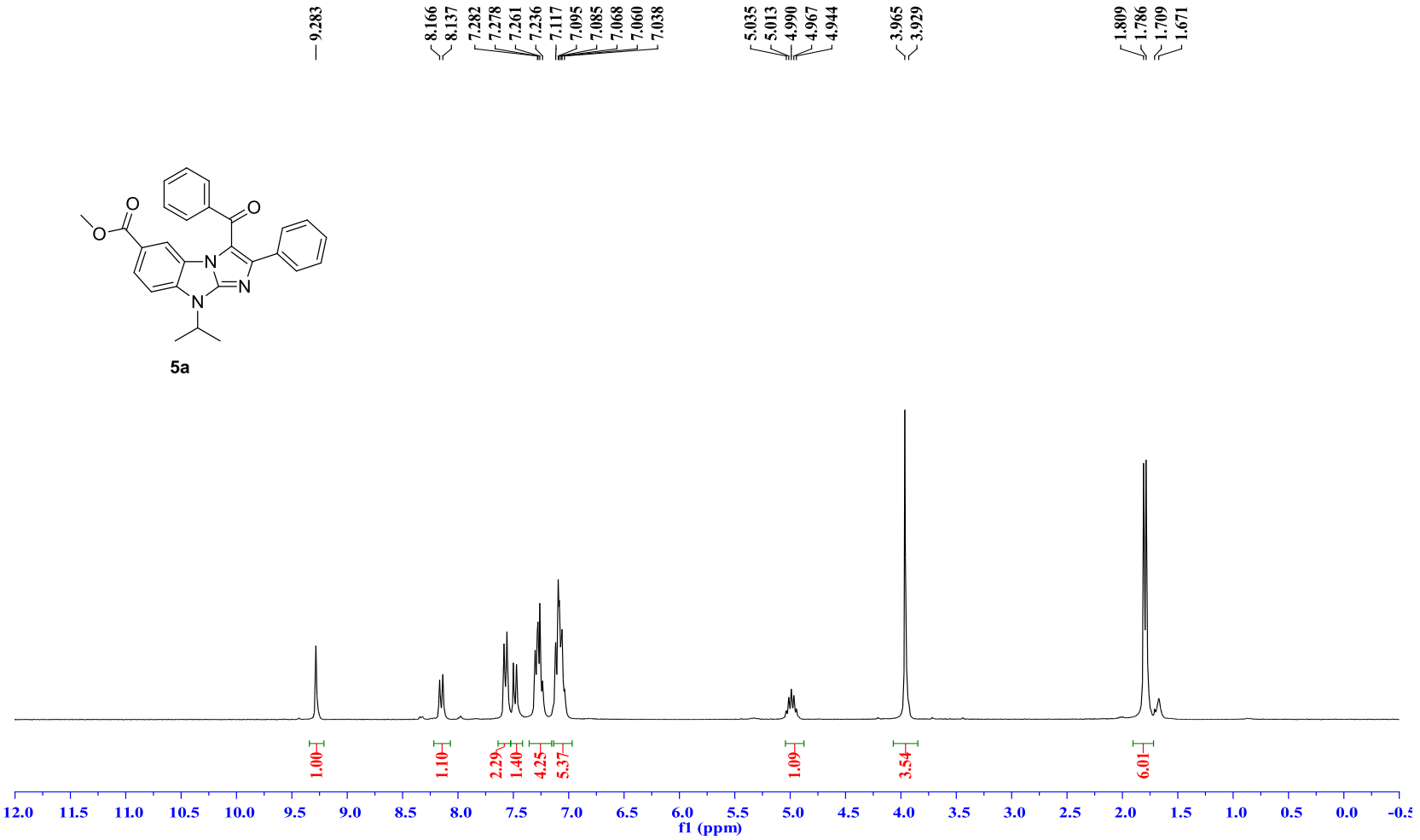
Methyl 3-benzoyl-9-(2-methoxyethyl)-2-phenyl-9H-benzo[d]imidazo-[1,2-a]imidazole-6-carboxylate (5ia): ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.24 (s, 1H), 8.15 (dd, *J* = 8.6, 1.4 Hz, 1H), 7.55 (t, *J* = 7.9 Hz, 3H), 7.26 (t, *J* = 8.1 Hz, 3H), 7.08 (m, 5H), 4.53 (t, *J* = 6.2 Hz, 2H), 3.96 (s, 3H), 3.90 (t, *J* = 6.2 Hz, 2H), 3.34 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.5, 167.0, 154.8, 150.4, 150.4, 139.1, 138.3, 134.3, 131.5, 130.1, 129.5, 128.1, 127.7, 126.1, 125.4, 123.2, 122.0, 117.4, 110.1, 70.5, 59.0,

52.2, 43.7; MS (ESI-MS) *m/z*: 476 $(M+Na)^+$; HRMS calcd for $C_{27}H_{23}N_3O_4$ $(M+Na)^+$; 476.1586, found 476.1588; IR (cm^{-1}, neat): 3066, 2925, 2851, 1711, 1623, 1586.

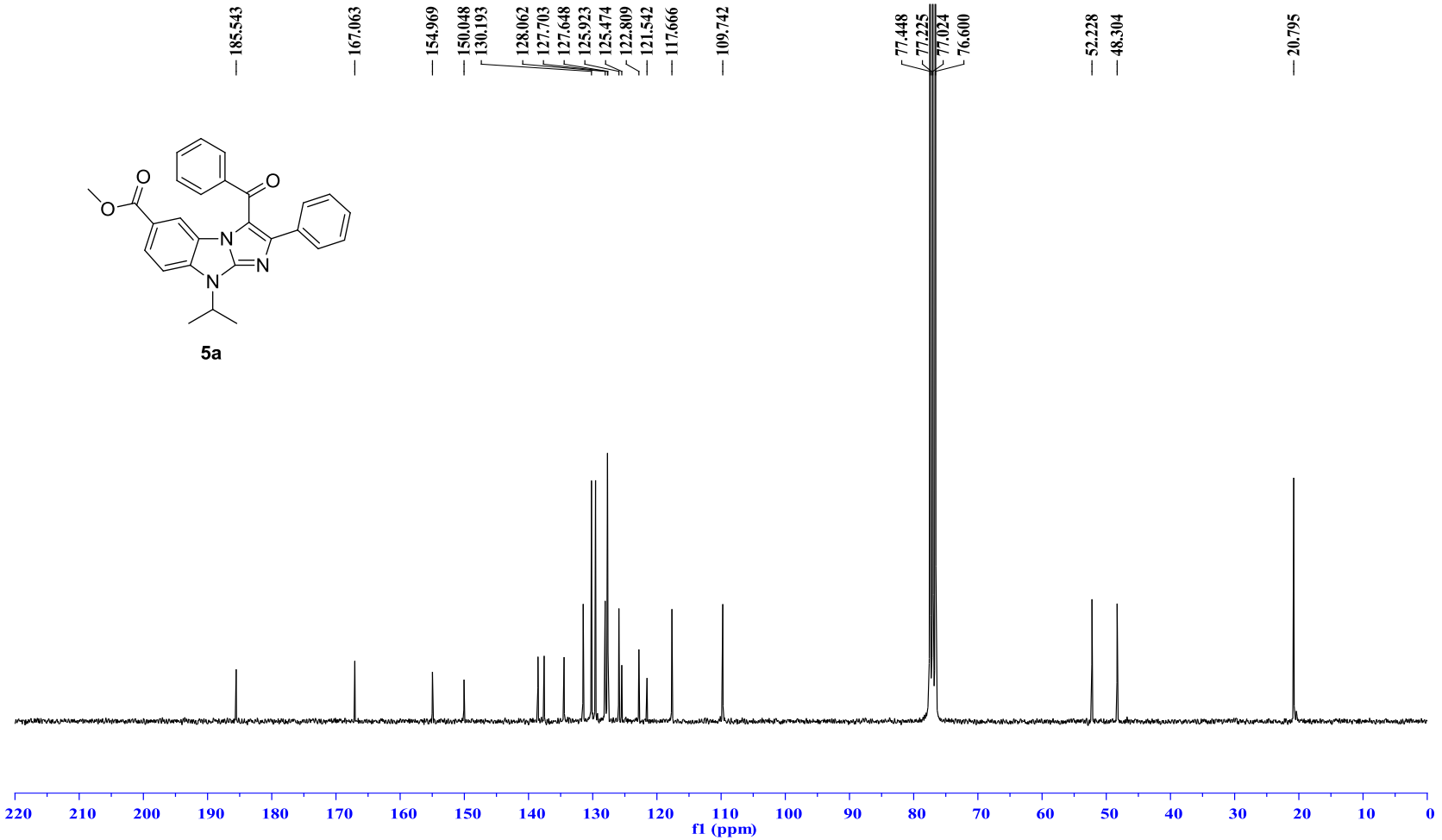
Phenyl(2-phenylimidazo[1,2-a]pyridin-3-yl)methanone (6a): ^1H NMR (400 MHz, Acetone-d_6) δ 9.46 (d, 1.2 Hz, 1H), 7.79 (dd, *J* = 9.0, 1.2 Hz, 1H), 7.65 (dd, *J* = 9.0, 1.2 Hz, 1H), 7.56 – 7.51 (m, 2H), 7.39 – 7.34 (m, 2H), 7.33 – 7.23 (m, 2H), 7.18 – 7.06 (m, 5H); ^{13}C NMR (100 MHz, Acetone-d_6) δ 186.7, 154.1, 147.2, 134.5, 131.5, 130.2, 129.5, 129.1, 128.0, 127.9, 127.7, 127.5, 117.3, 114.5; MS (ESI): *m/z* 299.3 $[M+H]^+$; HRMS (ESI): calcd for $C_{20}H_{14}N_2O$ $[M+H]^+$; 299.1179, found, 299.1181.

(2-(4-nitrophenyl)imidazo[1,2-a]pyrazin-3-yl)(phenyl)methanone (6b): ^1H NMR (400 MHz, Acetone-d_6) δ 9.33 (d, *J* = 1.5 Hz, 1H), 9.23 (dd, *J* = 7.2, 1.5 Hz, 1H), 8.28 (d, *J* = 7.2 Hz, 1H), 8.07 – 8.04 (m, 2H), 7.74 (d, *J* = 7.4, 2H), 7.64 (d, *J* = 7.4, 2H), 7.42 (m, 1H), 7.27 – 7.23 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.0, 162.5, 1513, 147.7, 144.3, 139.5, 137.4, 133.4, 132.6, 131.0, 129.6, 128.5, 123.2, 121.0, 120.2; MS (ESI): *m/z* 325.2 $[M+H]^+$; HRMS (ESI): calcd for $C_{19}H_{12}N_4O_3$ $[M+H]^+$; 345.0982, found 345.0984.

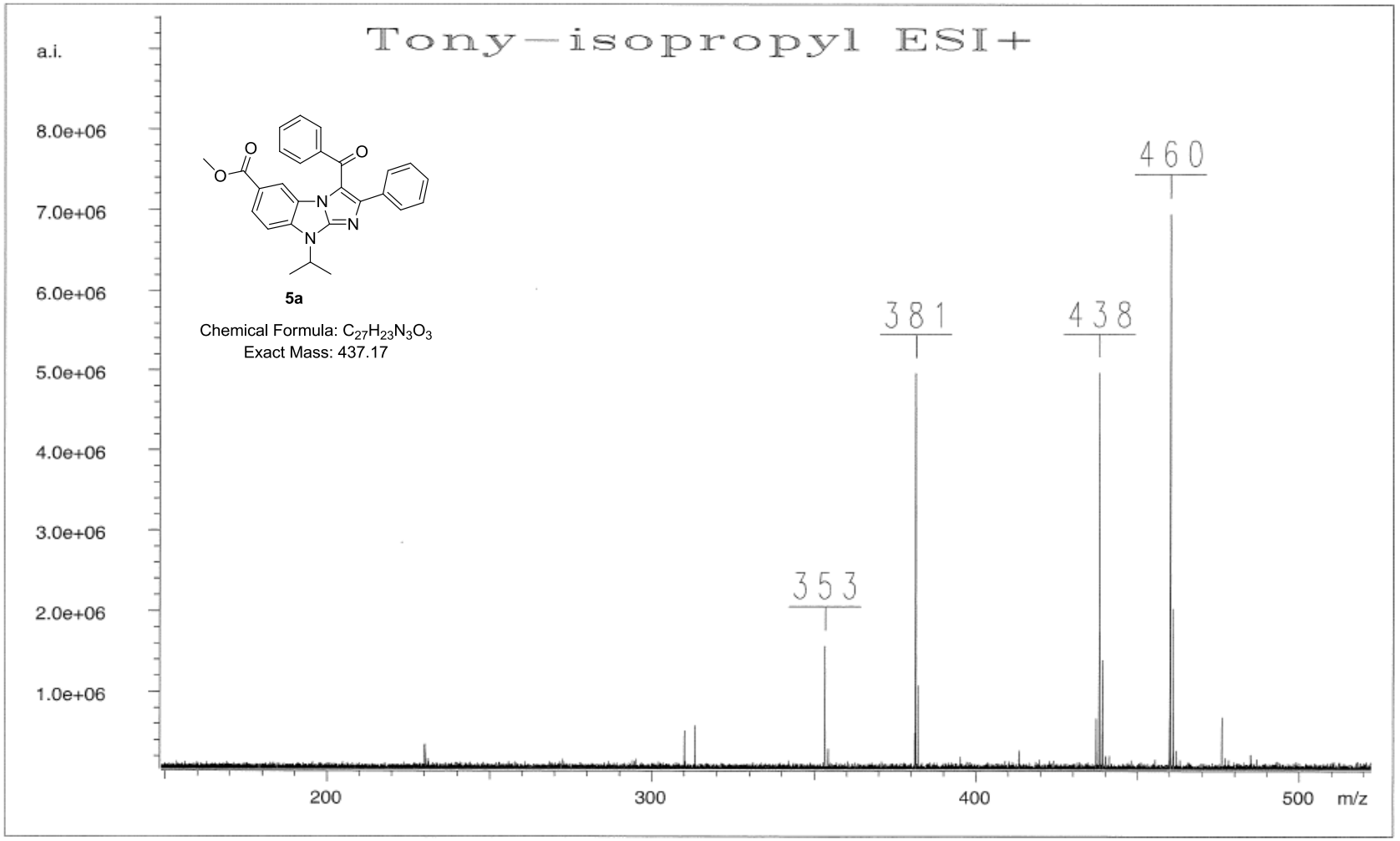
Phenyl(2-phenylimidazo[1,2-a]pyrazin-3-yl)methanone (6c): ^1H NMR (400 MHz, Acetone-d_6) δ 9.24 (s, 1H), 9.18 (dd, J = 7.4, 1.5 Hz, 1H), 8.21 (d, J = 7.4 Hz, 1H), 7.65 – 7.56 (m, 2H), 7.47 – 7.30 (m, 3H), 7.27 – 7.10 (m, 5H); ^{13}C NMR (100 MHz, Acetone-d_6) δ 187.2, 153.4, 143.6, 141.3, 137.9, 133.7, 132.3, 131.7, 130.2, 129.5, 128.5, 127.9, 127.7, 120.3, 120.1. MS (ESI): *m/z* 300.2 $[M+H]^+$; HRMS (ESI): calcd for $C_{19}H_{14}N_3O_3[M+H]^+$; 300.1131, found 300.1132



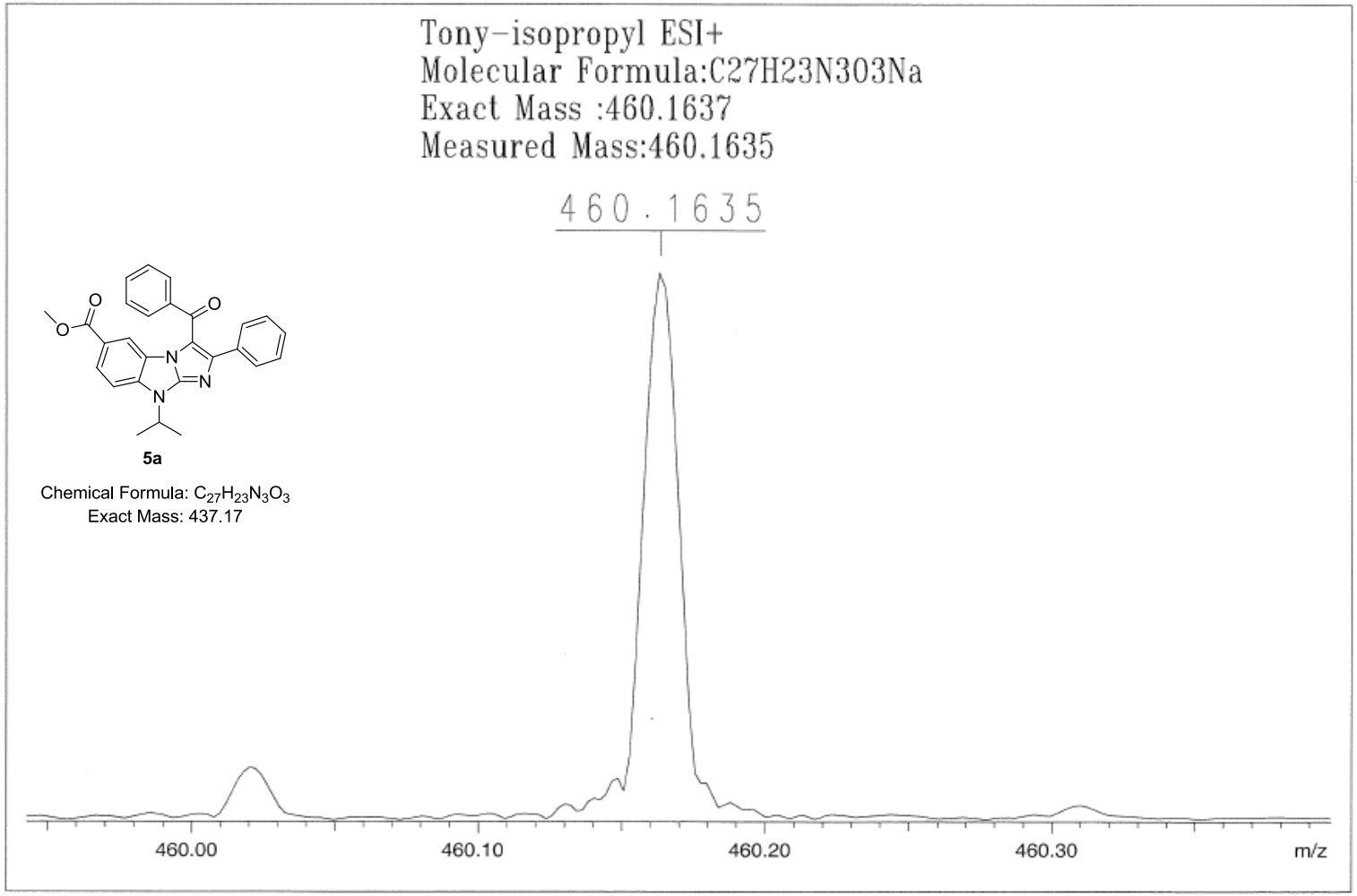
^{1}H NMR spectrum (300MHz) of compound **5a** in $CDCl_3$



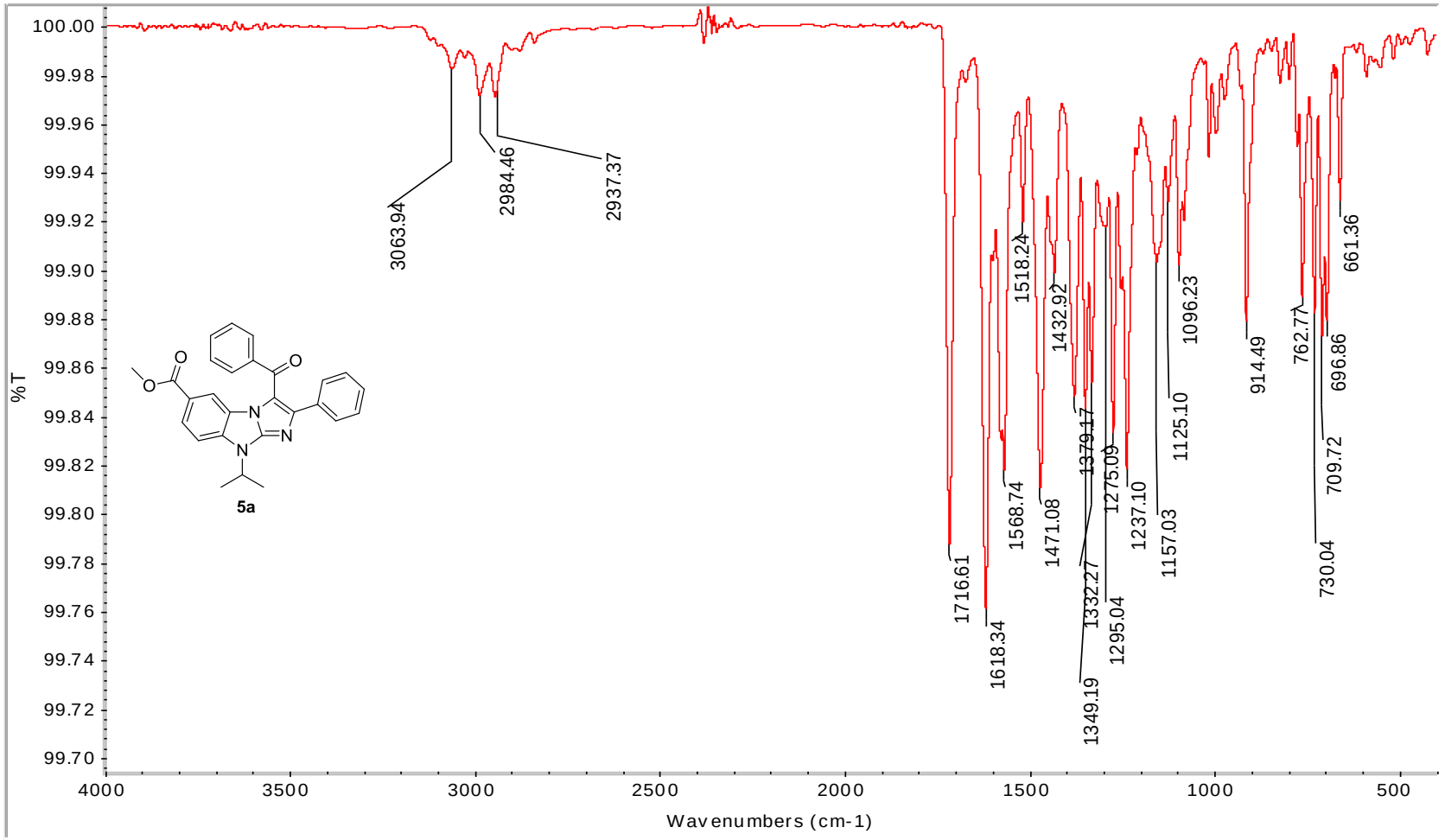
^{13}C NMR spectrum (75MHz) of compound **5a in CDCl3**



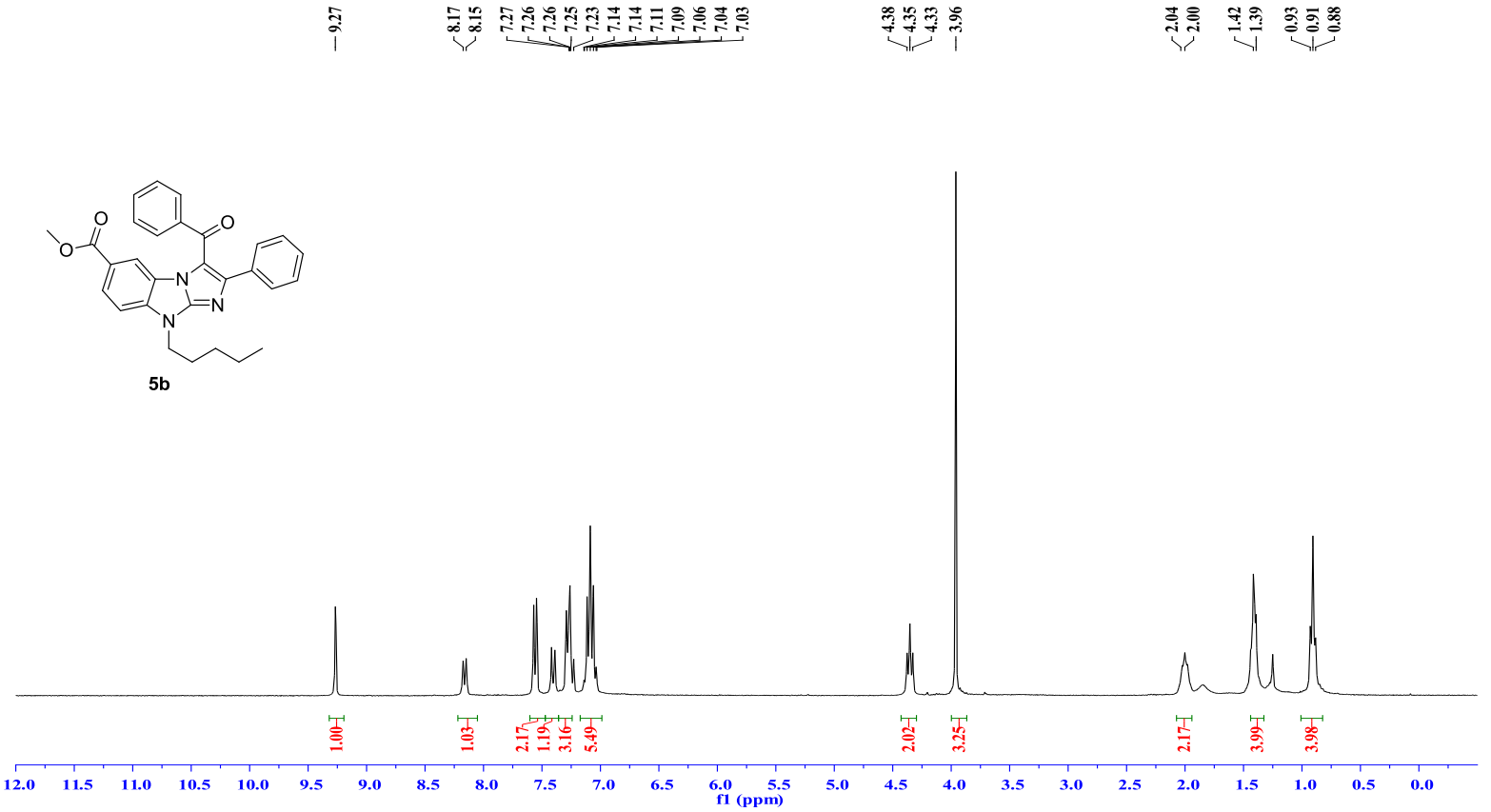
ESI$^+$ Mass spectrum of compound **5a**



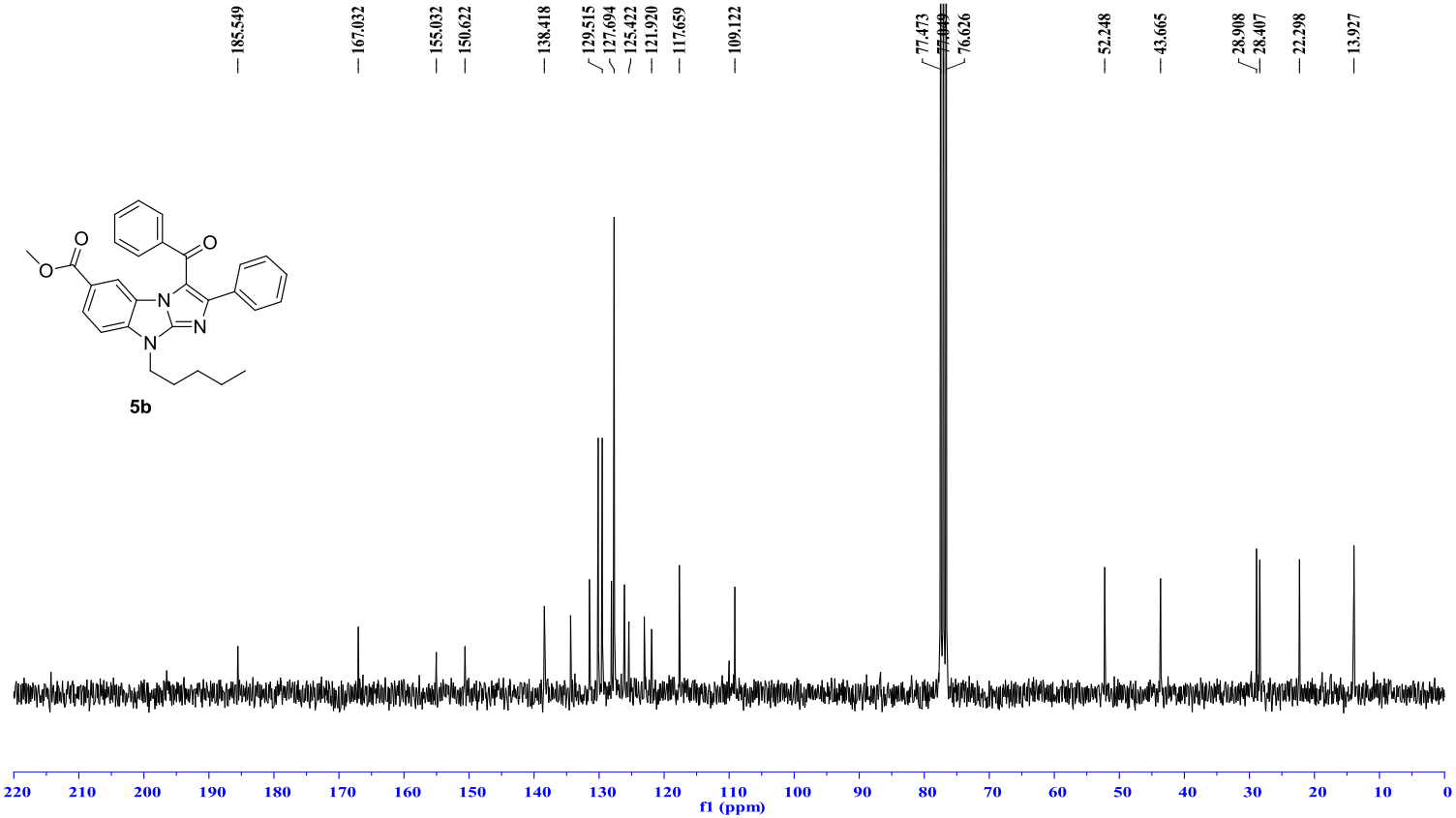
High resolution mass (ESI^+) spectrum of compound **5a**



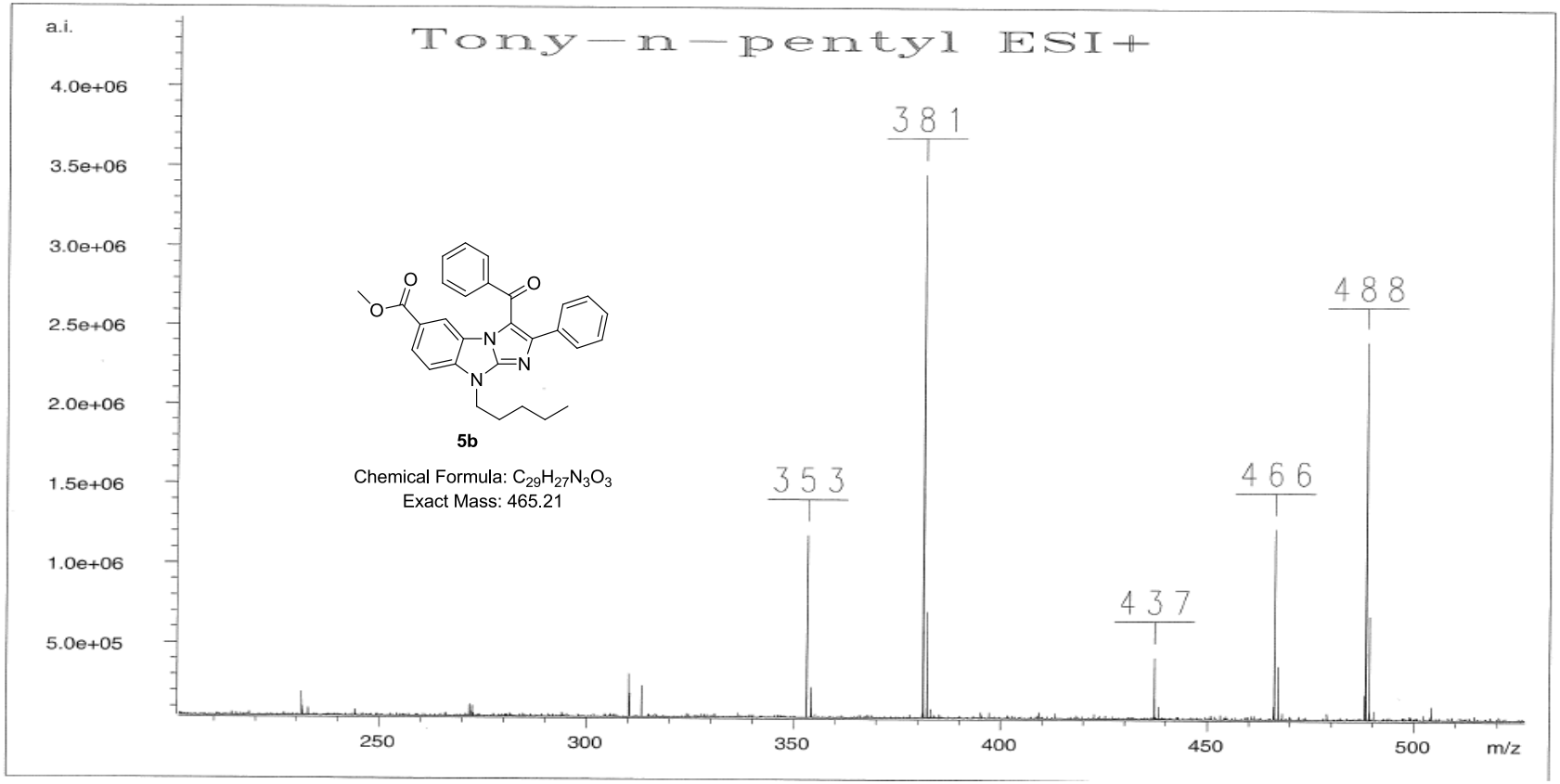
IR spectrum of compound **5a**



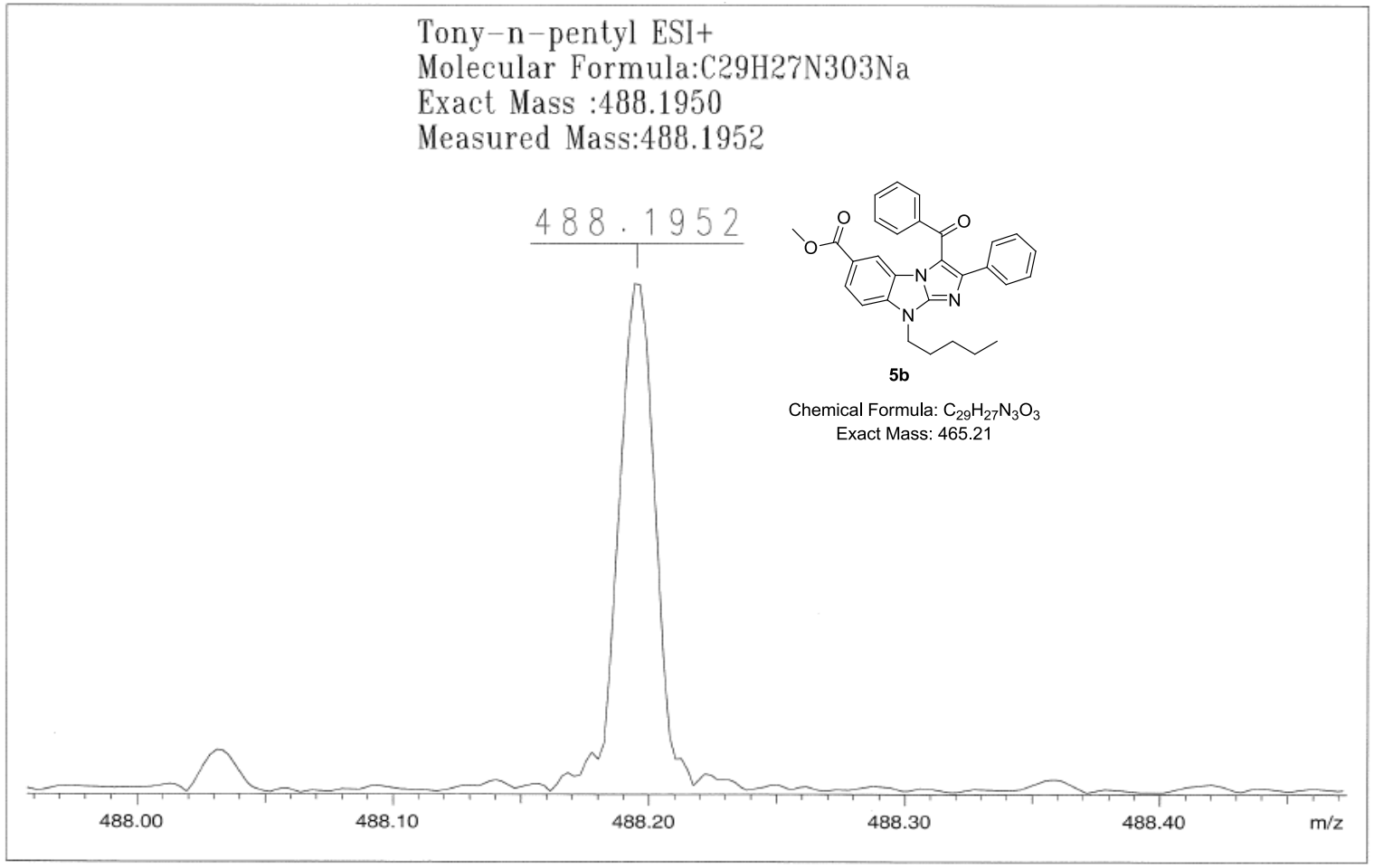
^{1}H NMR spectrum (300MHz) of compound **5b** in $CDCl_3$



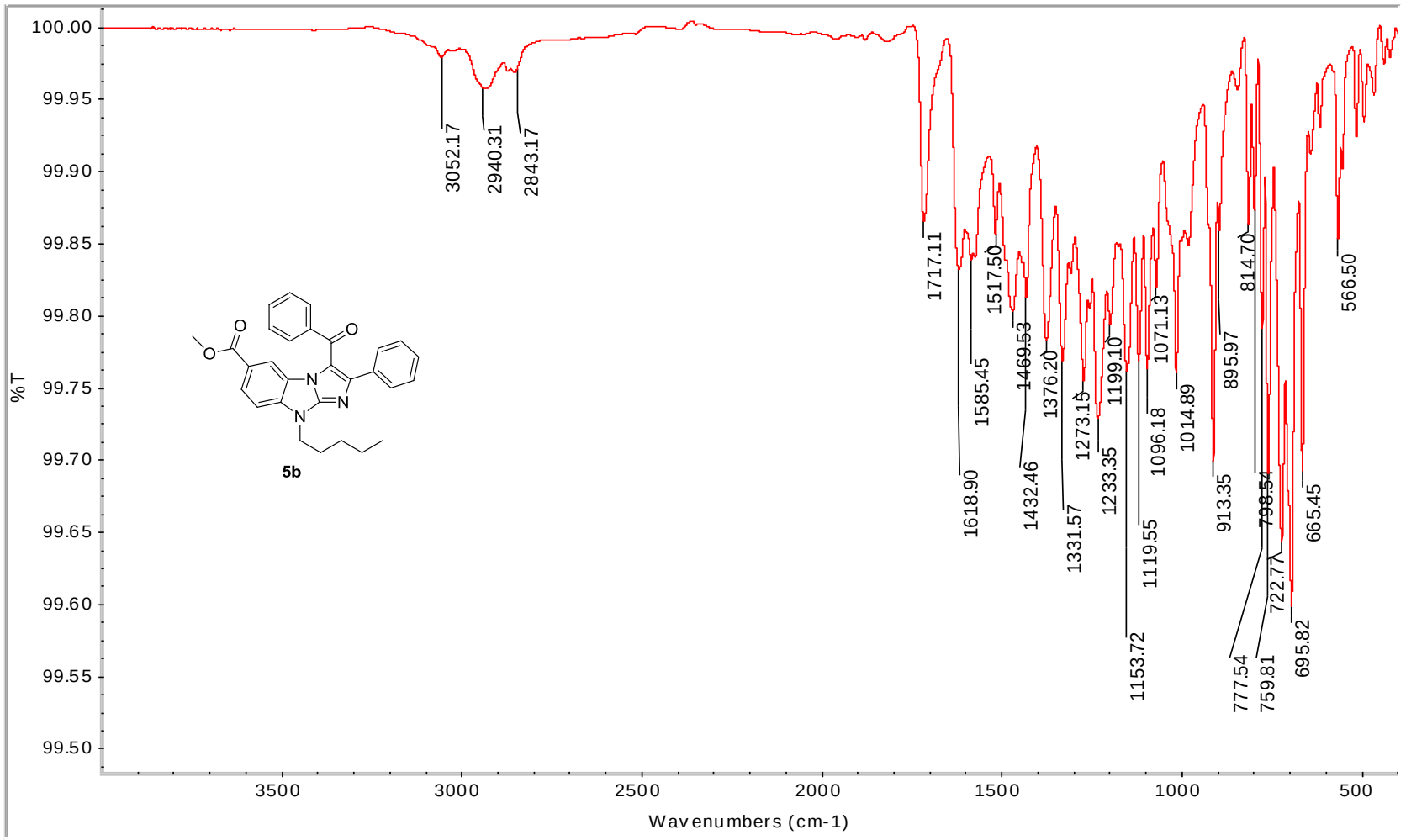
^{13}C NMR spectrum (75MHz) of compound **5b** in $CDCl_3$



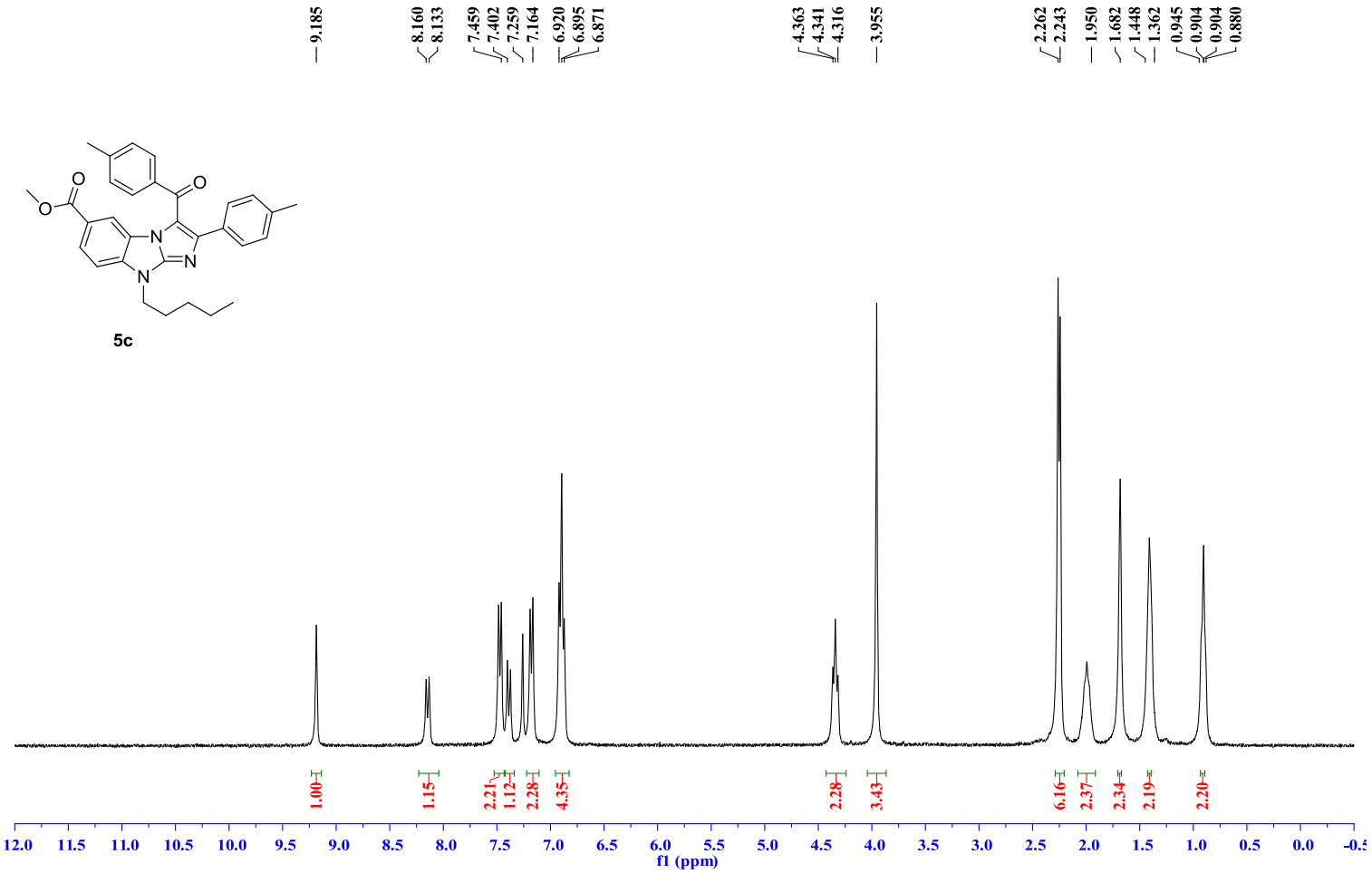
ESI$^+$ Mass spectrum of compound **5b**



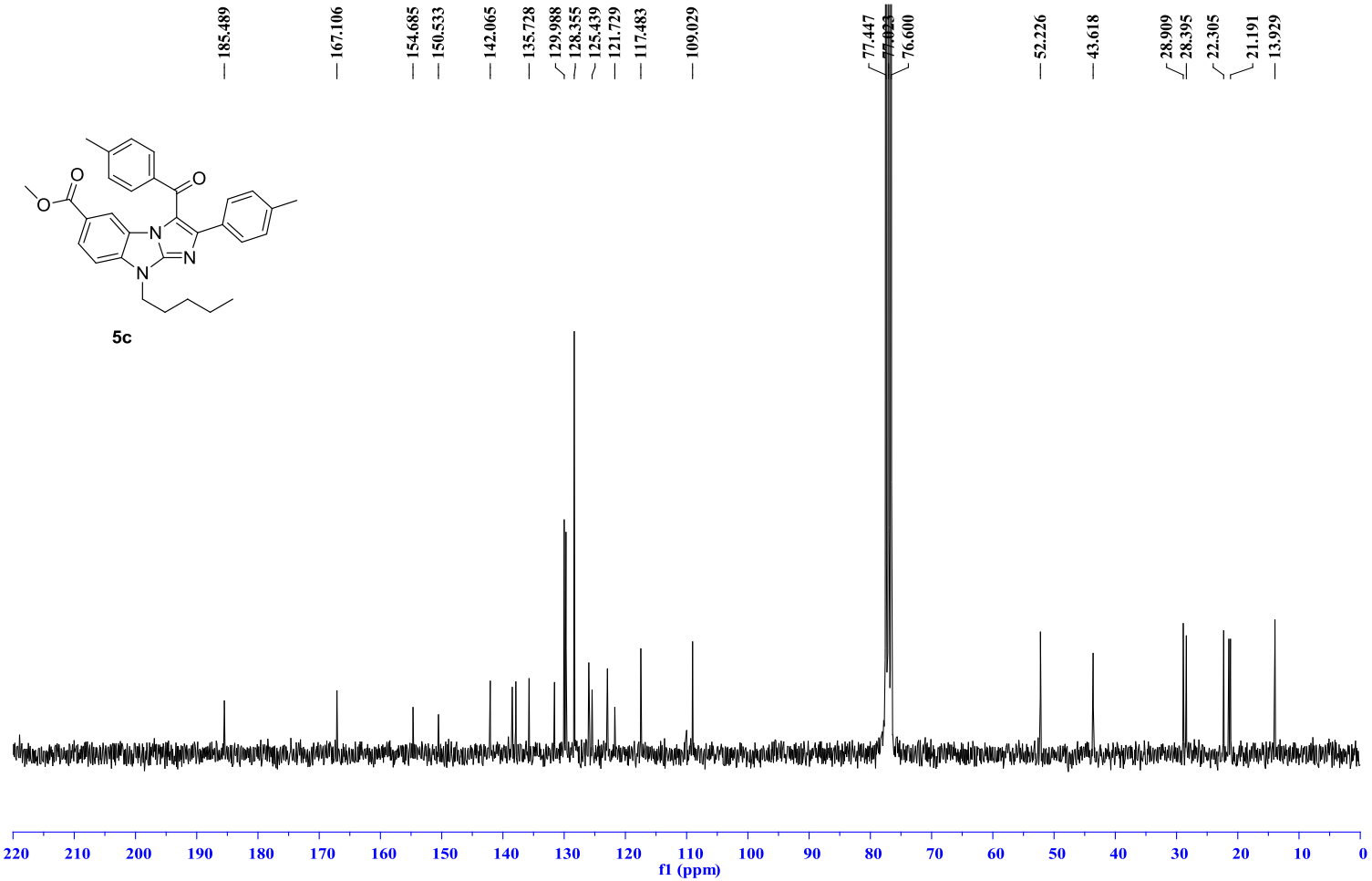
High resolution mass (ESI^+) spectrum of compound **5b**



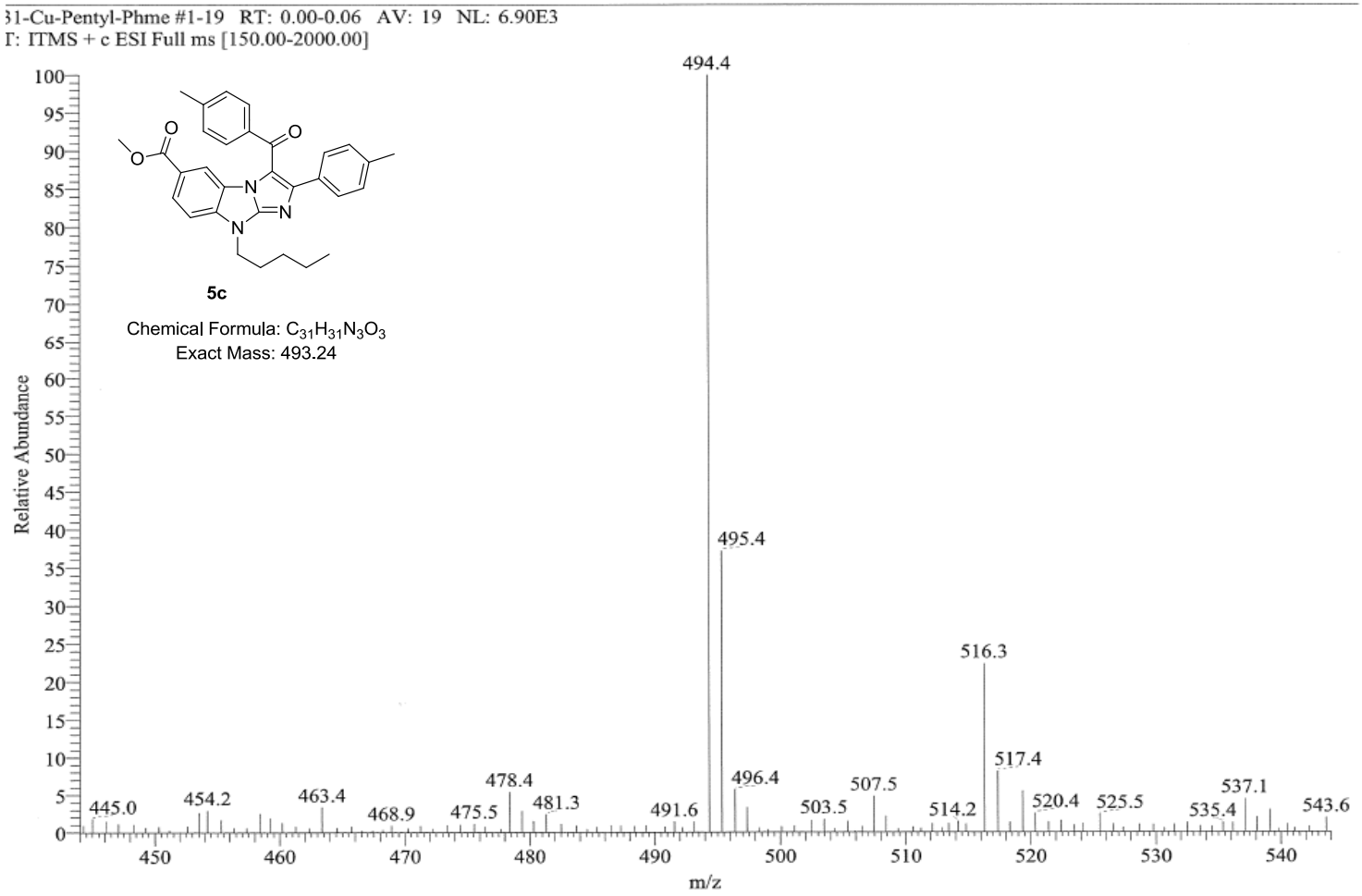
IR spectrum of compound **5b**



^{1}H NMR spectrum (300MHz) of compound **5c** in $CDCl_3$



^{13}C NMR spectrum (75MHz) of compound **5c** in $CDCl_3$



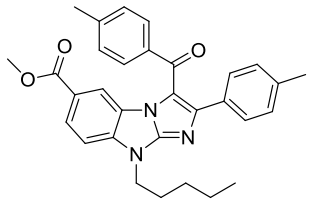
ESI^{+} Mass spectrum of compound **5c**

27-Cu-Pentyl-Phme-H#1-20 RT: 0.00-0.28 AV: 20
T: FTMS + p ESI Full ms [150.00-2000.00]
m/z= 479.6690-514.0850

Isotope	Min	Max
N-14	0	3
C-12	0	35
H-1	0	35
O-16	0	3

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

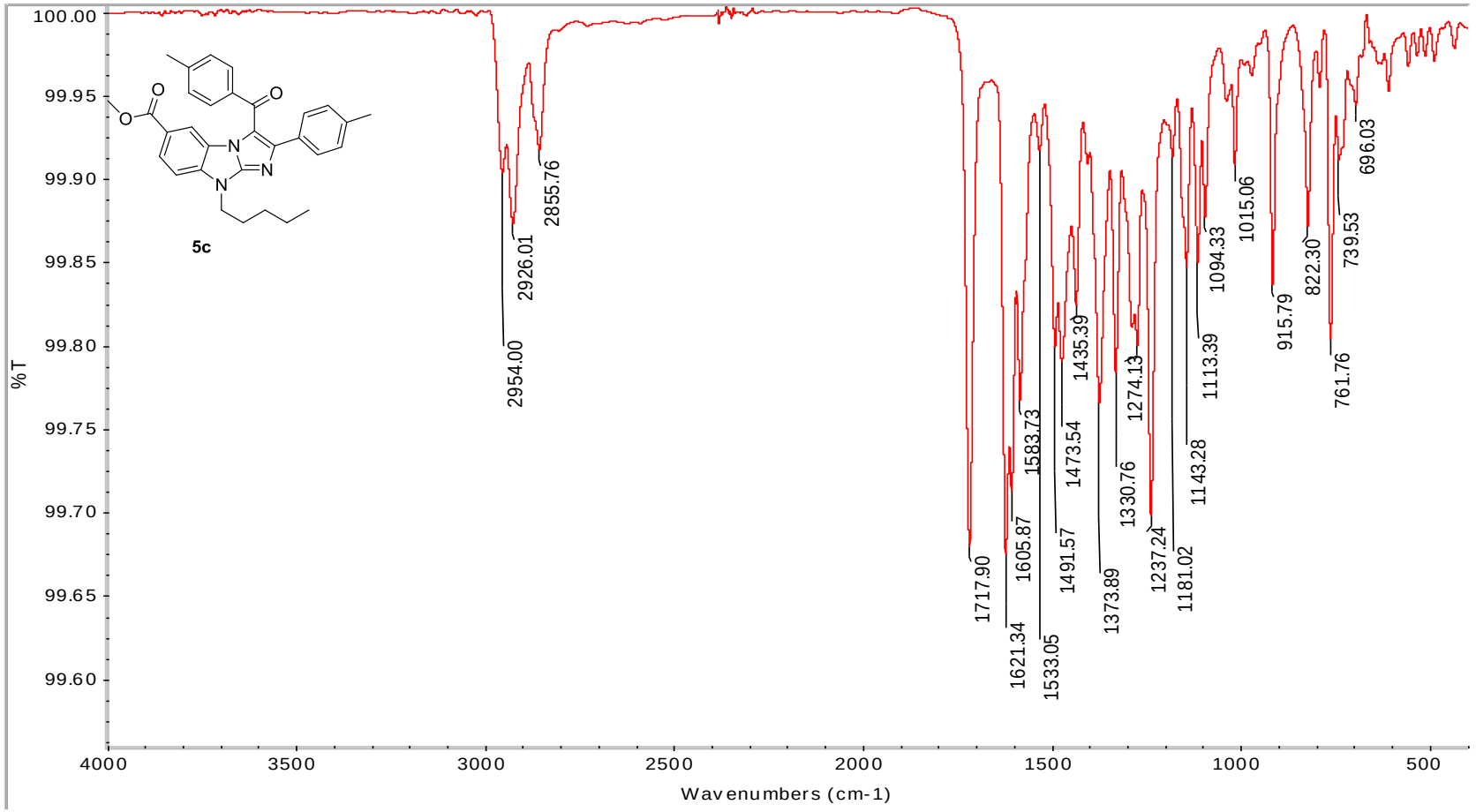
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
494.2451	2235576.8	100.00	494.2438	2.53	$C_{31}H_{32}O_3N_3$



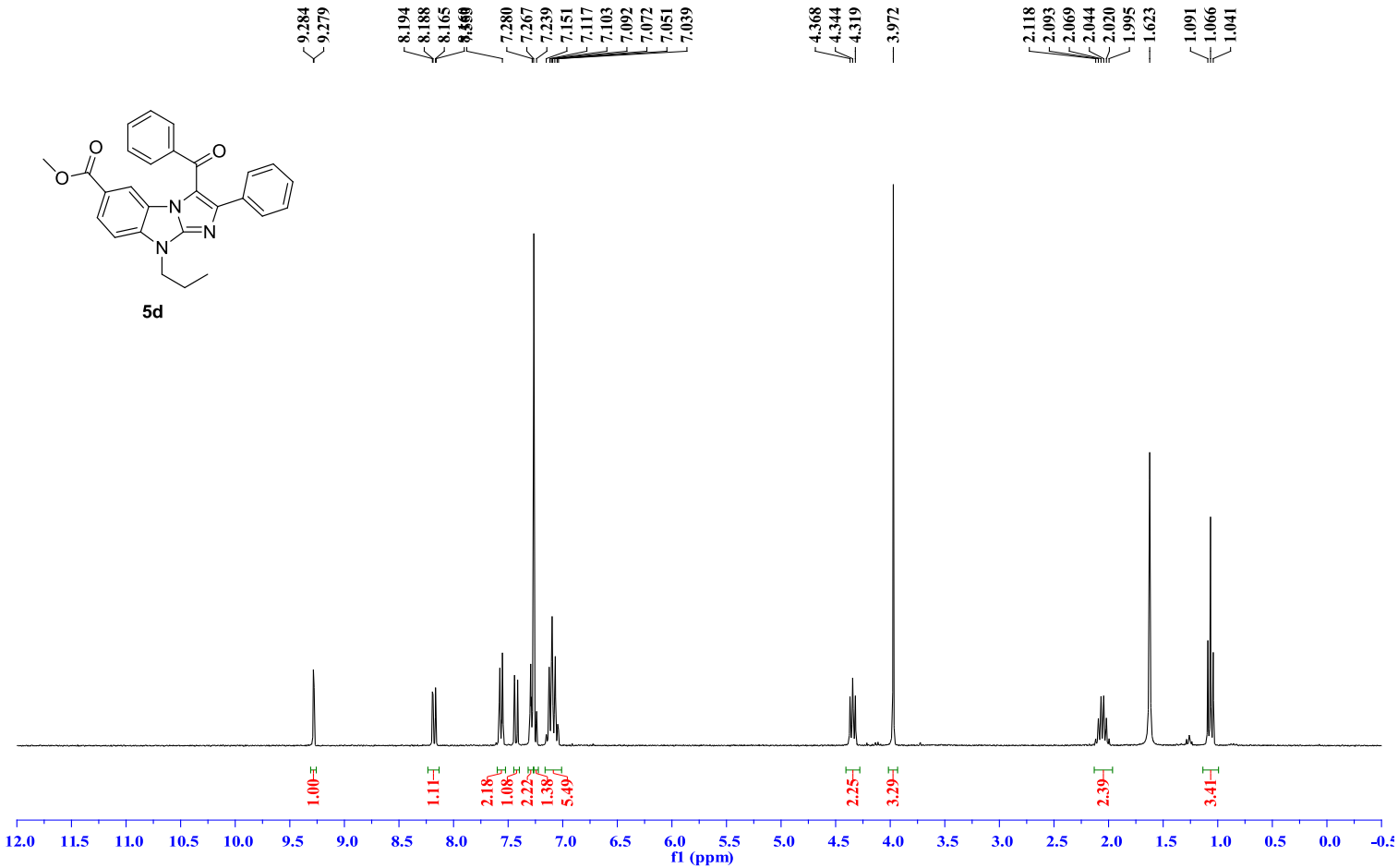
5c

Chemical Formula: $C_{31}H_{31}N_3O_3$
Exact Mass: 493.24

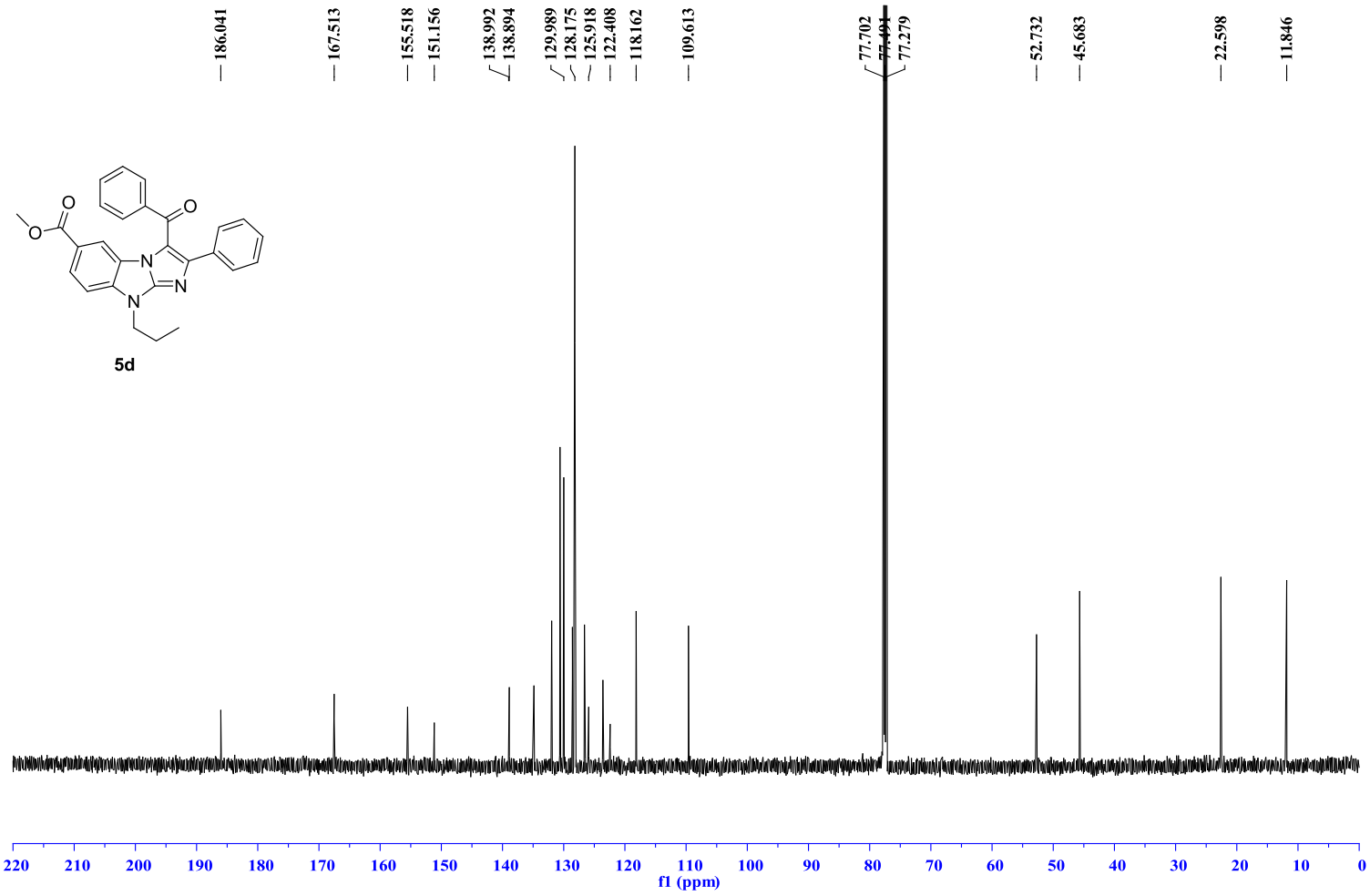
High resolution mass (ESI^+) spectrum of compound **5c**



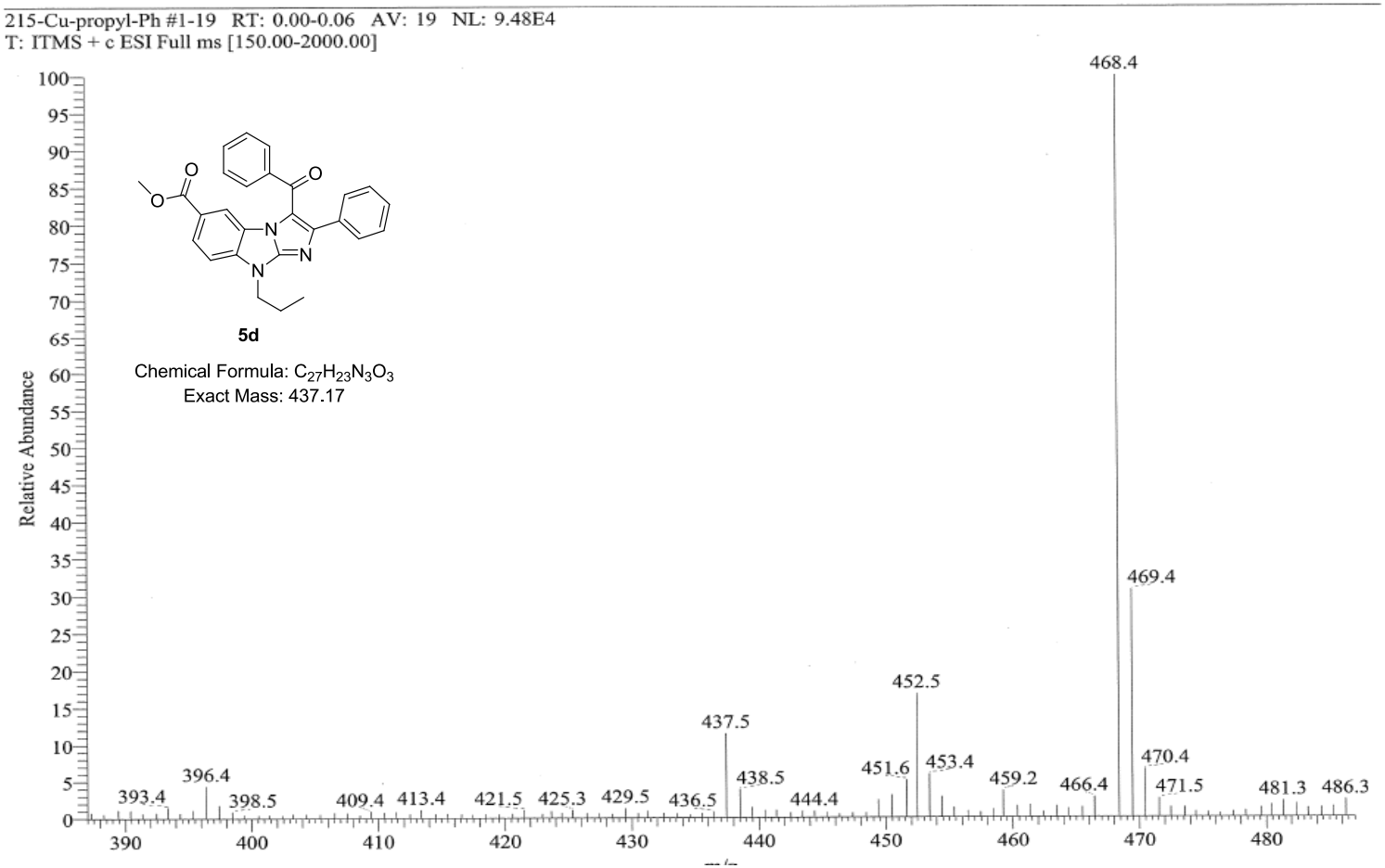
IR spectrum of compound **5c**



1H NMR spectrum (300MHz) of compound **5d** in CDCl3



^{13}C NMR spectrum (150MHz) of compound **5d** in CDCl3



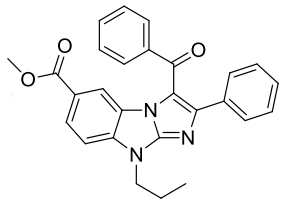
ESI$^+$ Mass spectrum of compound **5d**

216-Cu-propyl-Ph-H#1-20 RT: 0.01-0.28 AV: 20
T: FTMS + p ESI Full ms [150.00-2000.00]
m/z= 434.1664-441.2478

Isotope	Min	Max
C-12	0	27
H-1	0	30
O-16	0	3
N-14	0	3

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

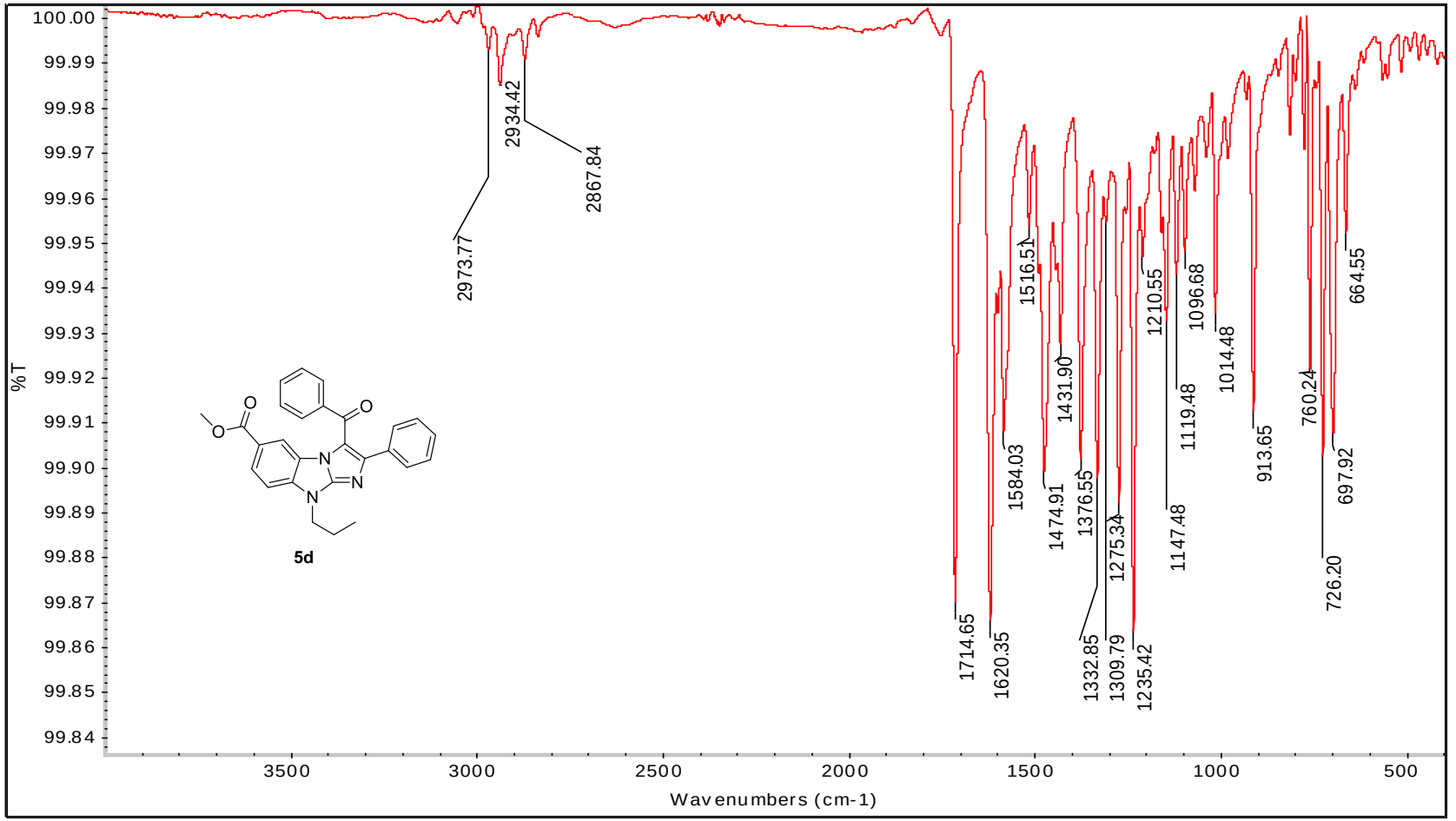
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
437.2538	115639.1	100.00	437.1734	183.84	$C_{27}H_{23}O_3N_3$



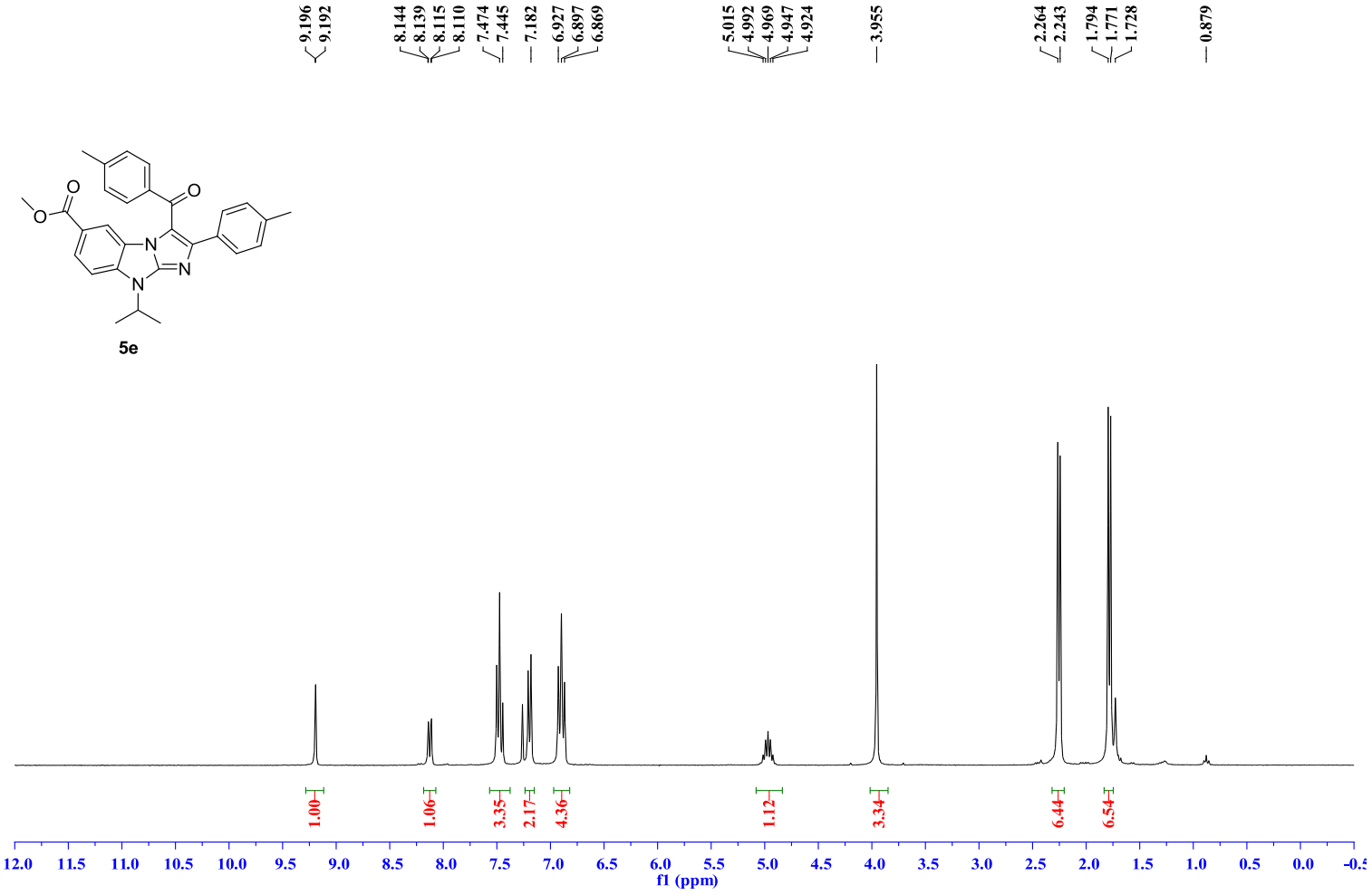
5d

Chemical Formula: $C_{27}H_{23}N_3O_3$
Exact Mass: 437.17

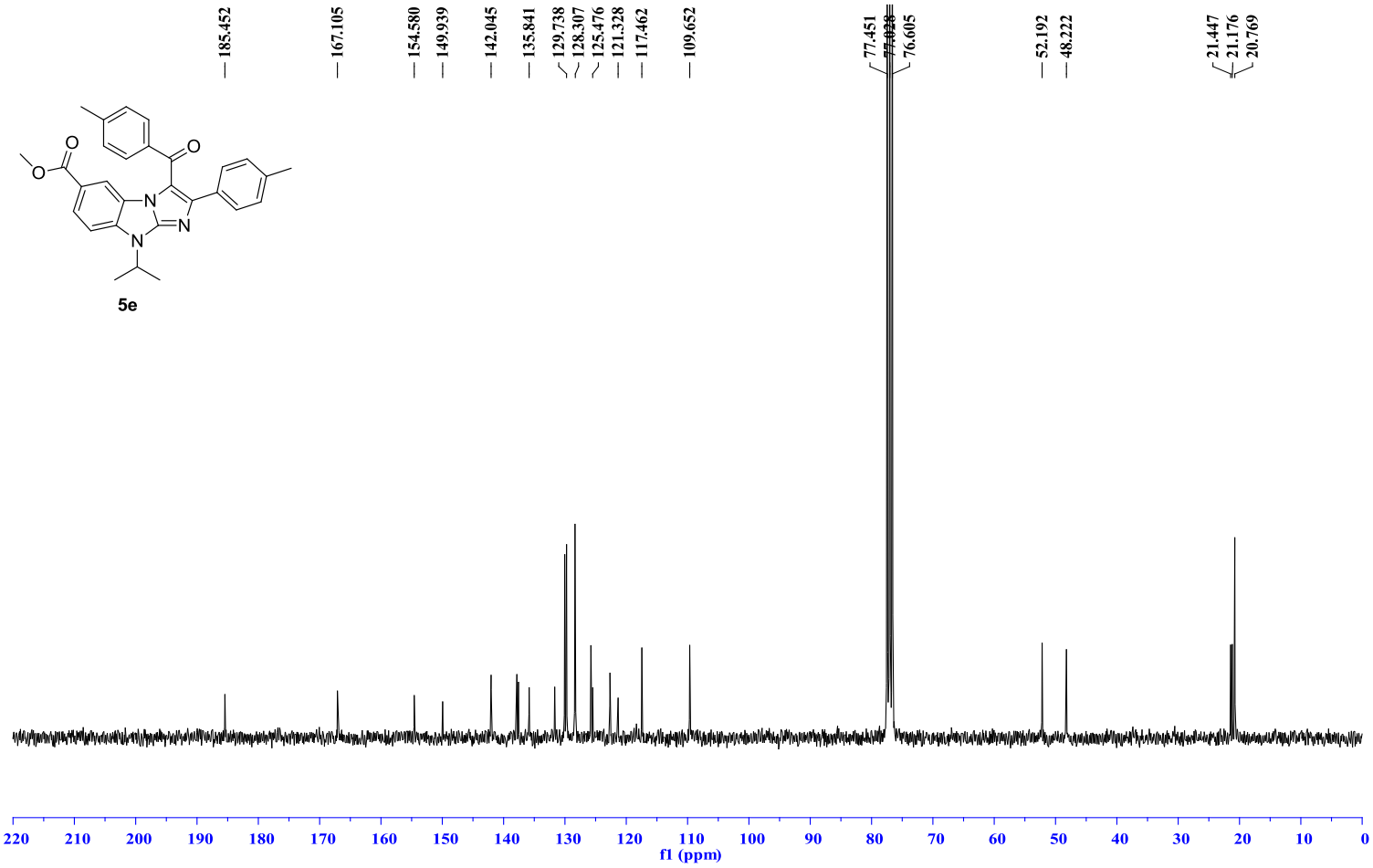
High resolution mass (ESI^+) spectrum of compound **5d**



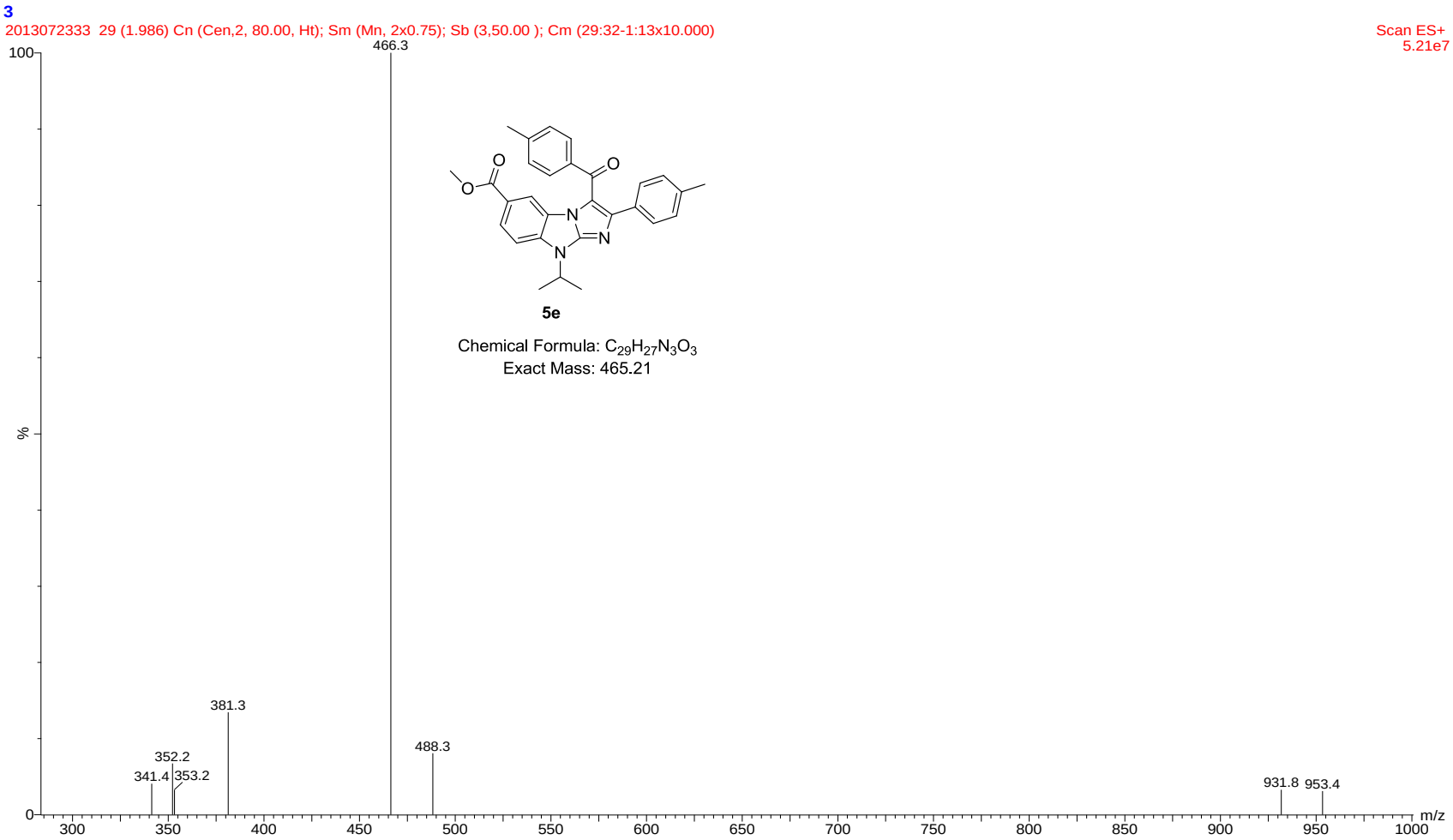
IR spectrum of compound **5d**



^{1}H NMR spectrum (300MHz) of compound **5e** in $CDCl_3$



^{13}C NMR spectrum (75MHz) of compound **5e** in $CDCl_3$



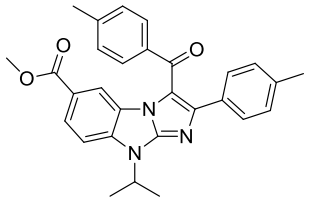
ESI^{+} Mass spectrum of compound **5e**

114-Tony-isopropyl-phem-phem-H#1-20 RT: 0.01-0.28 AV: 20
T: FTMS + p ESI Full ms [460.00-500.00]
m/z= 465.0159-468.8548

Isotope	Min	Max
C-12	0	30
H-1	0	30
O-16	0	3
N-14	0	3

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

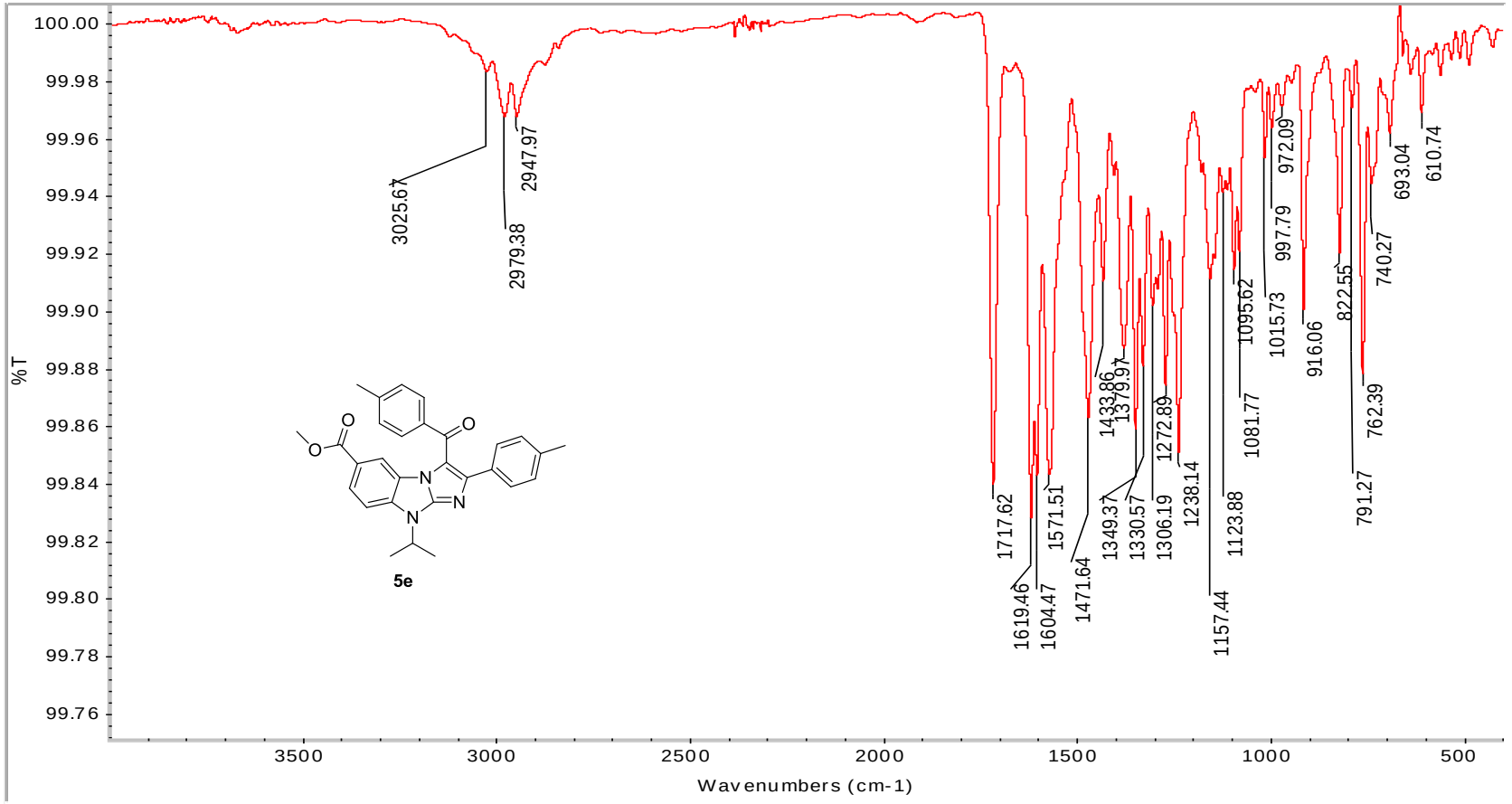
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
466.2132	560122.9	100.00	466.2125	1.52	$C_{29}H_{28}O_3N_3$



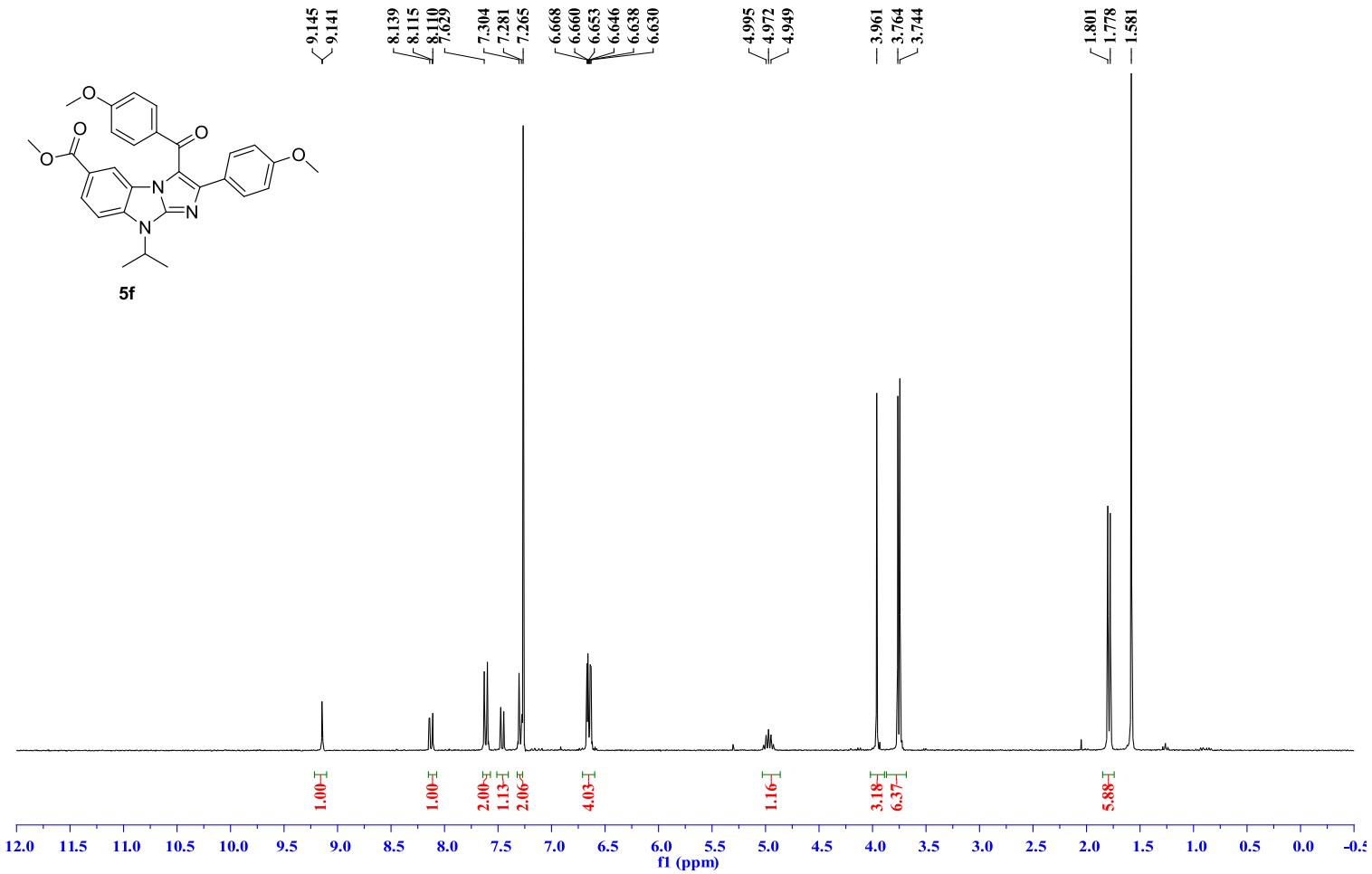
5e

Chemical Formula: $C_{29}H_{27}N_3O_3$
Exact Mass: 465.21

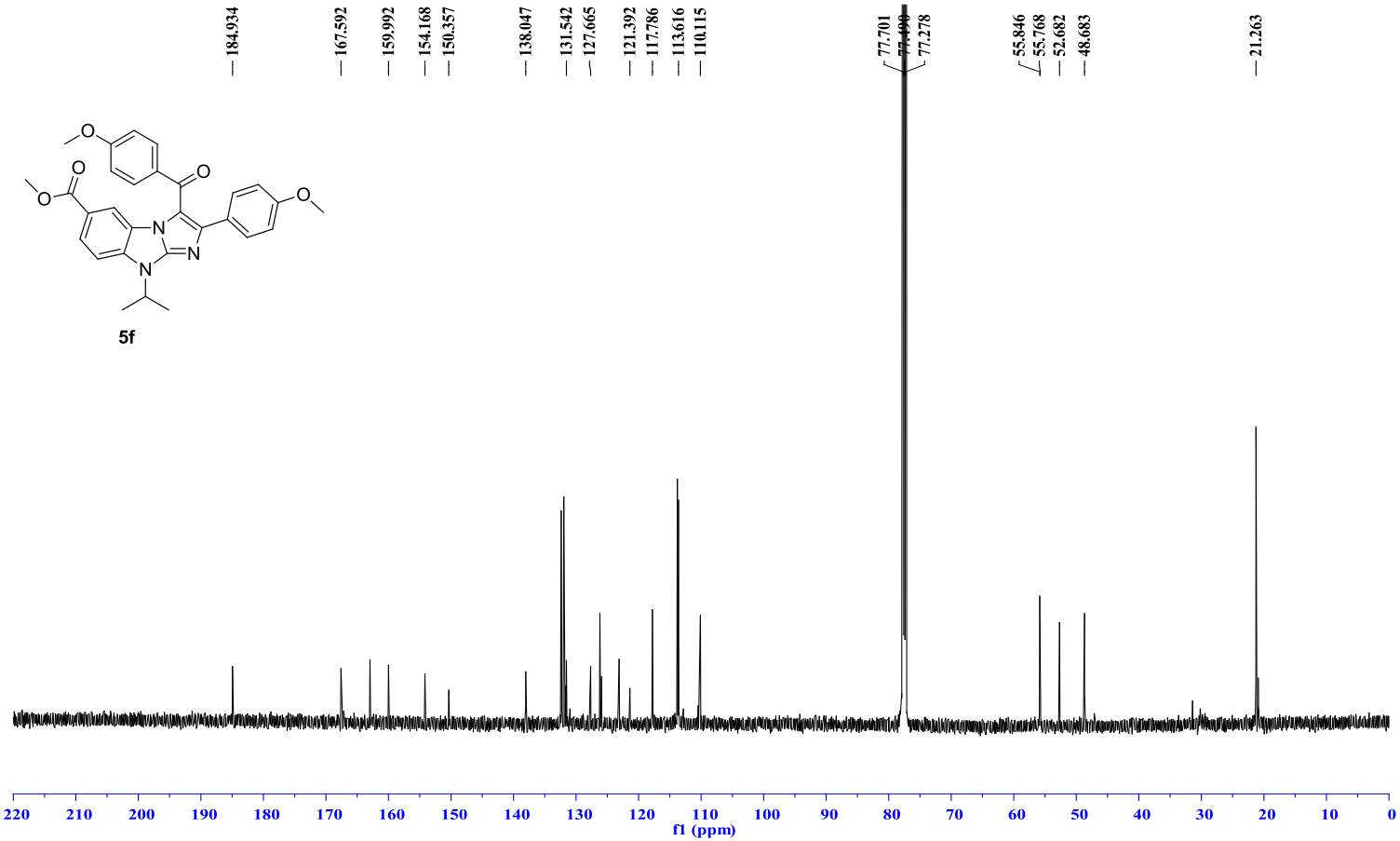
High resolution mass (ESI^+) spectrum of compound **5e**



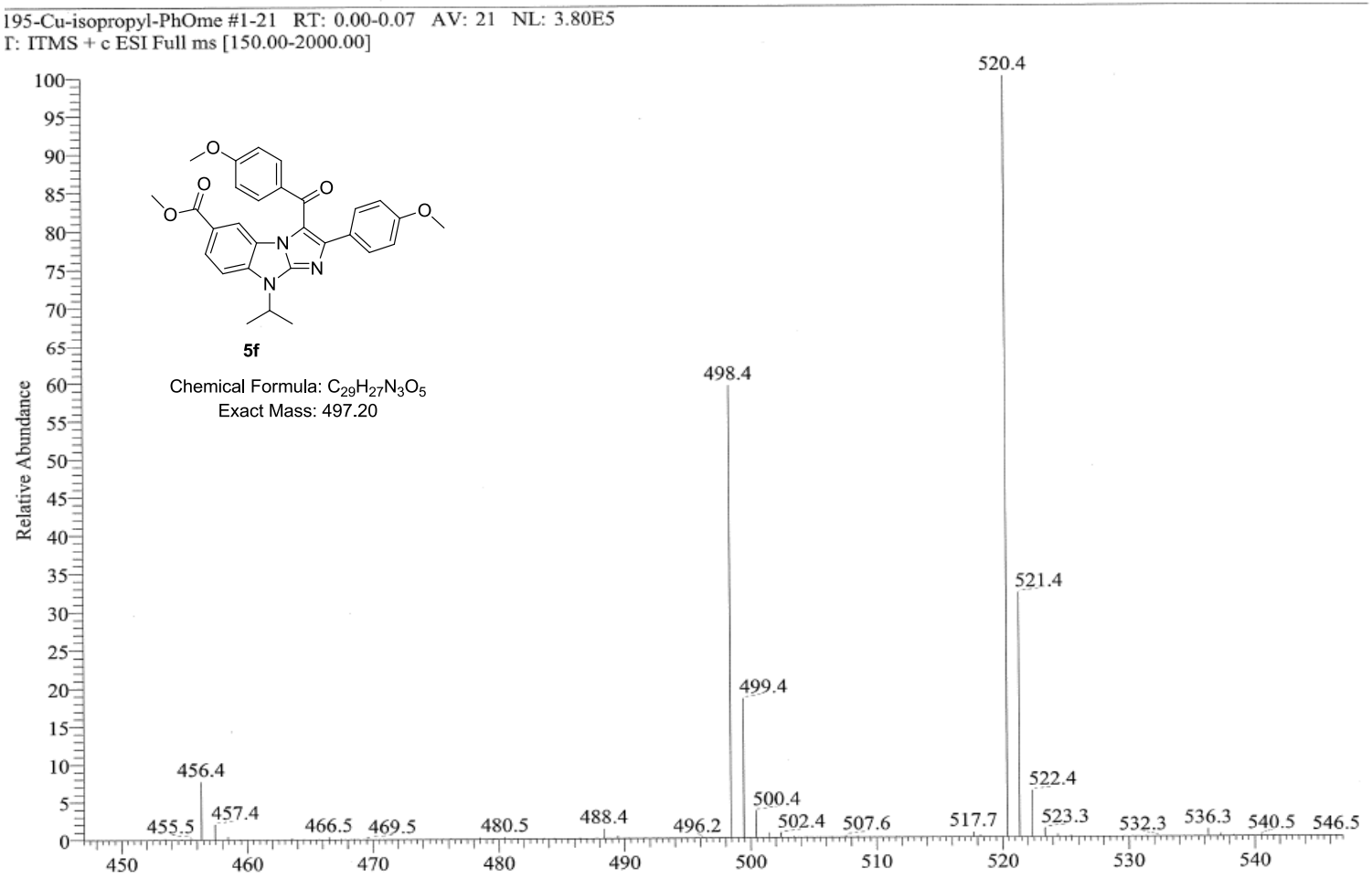
IR spectrum of compound **5e**



^{1}H NMR spectrum (300MHz) of compound **5f** in $CDCl_3$



^{13}C NMR spectrum (150MHz) of compound **5f** in $CDCl_3$

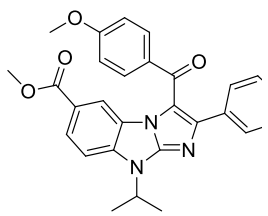


ESI$^+$ Mass spectrum of compound **5f**

194-Cu-isopropyl-PhOme-H#1-20 RT: 0.00-0.27 AV: 20
T: FTMS + p ESI Full ms [150.00-2000.00]
m/z= 470.6126-512.2741

Isotope	Min	Max
C-12	0	30
H-1	0	30
O-16	0	5
N-14	0	5

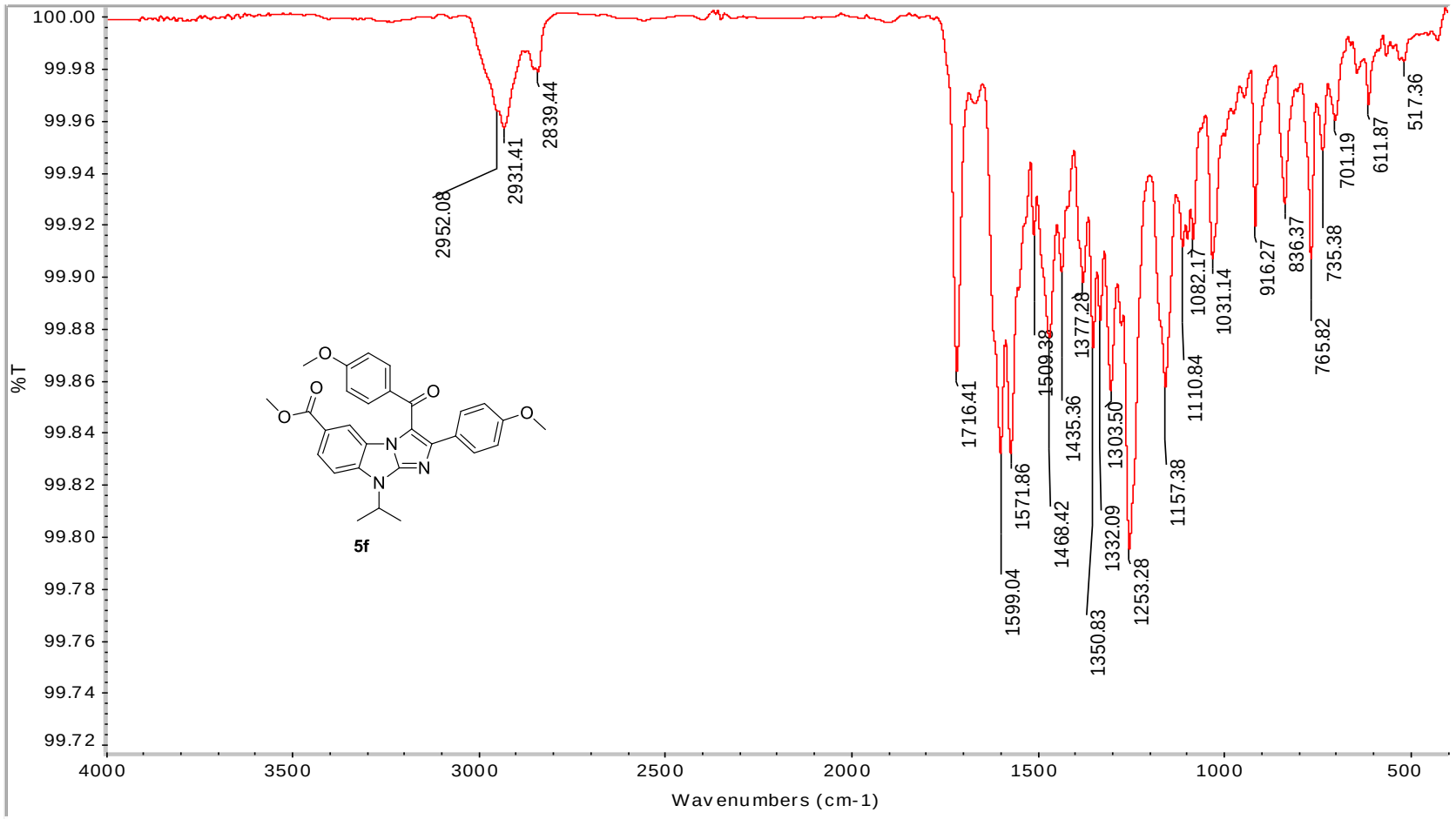
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1



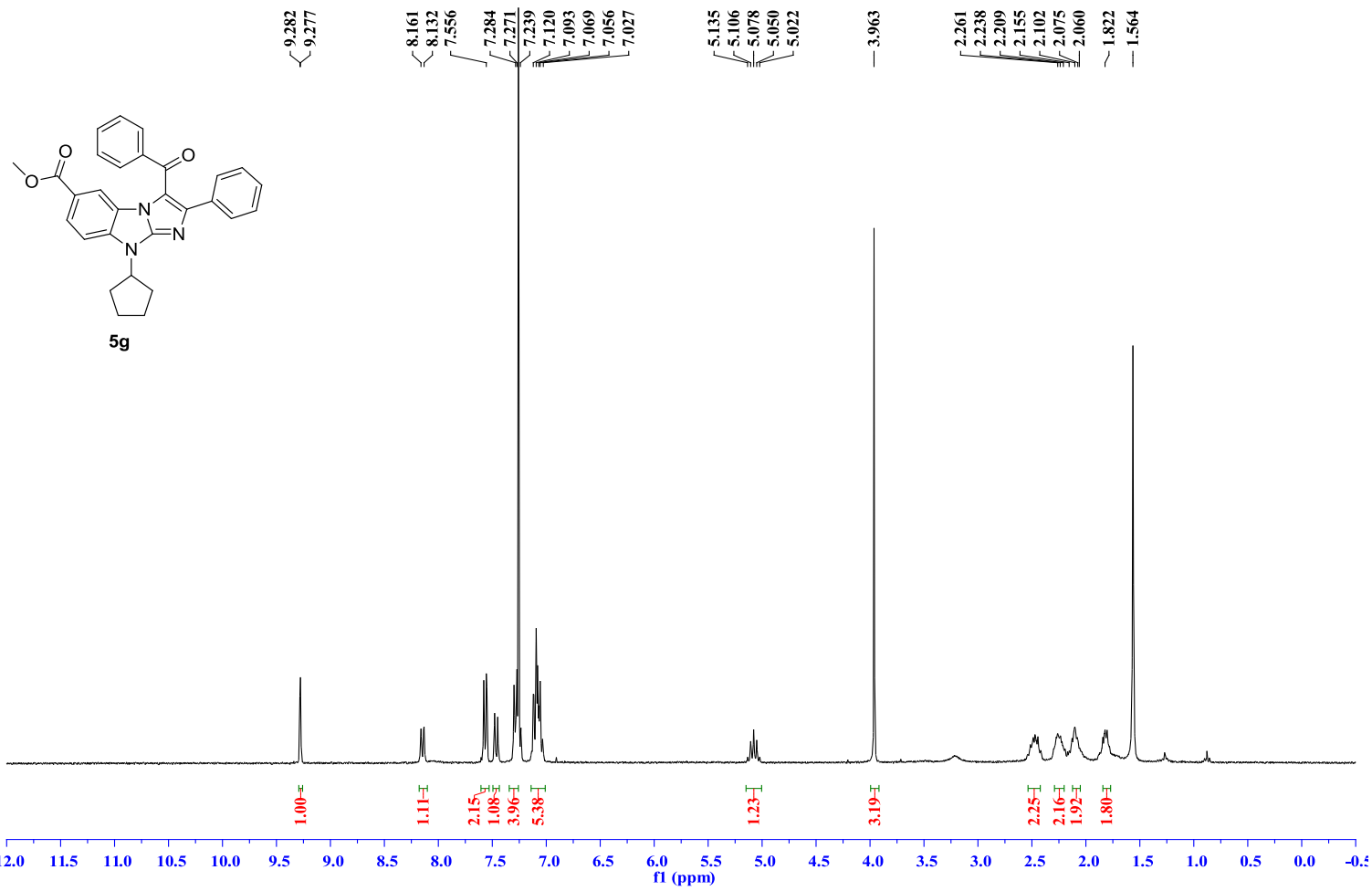
5f

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
498.2018	4095549.3	100.00	498.2023	-1.20	$C_{29}H_{28}O_5N_3$

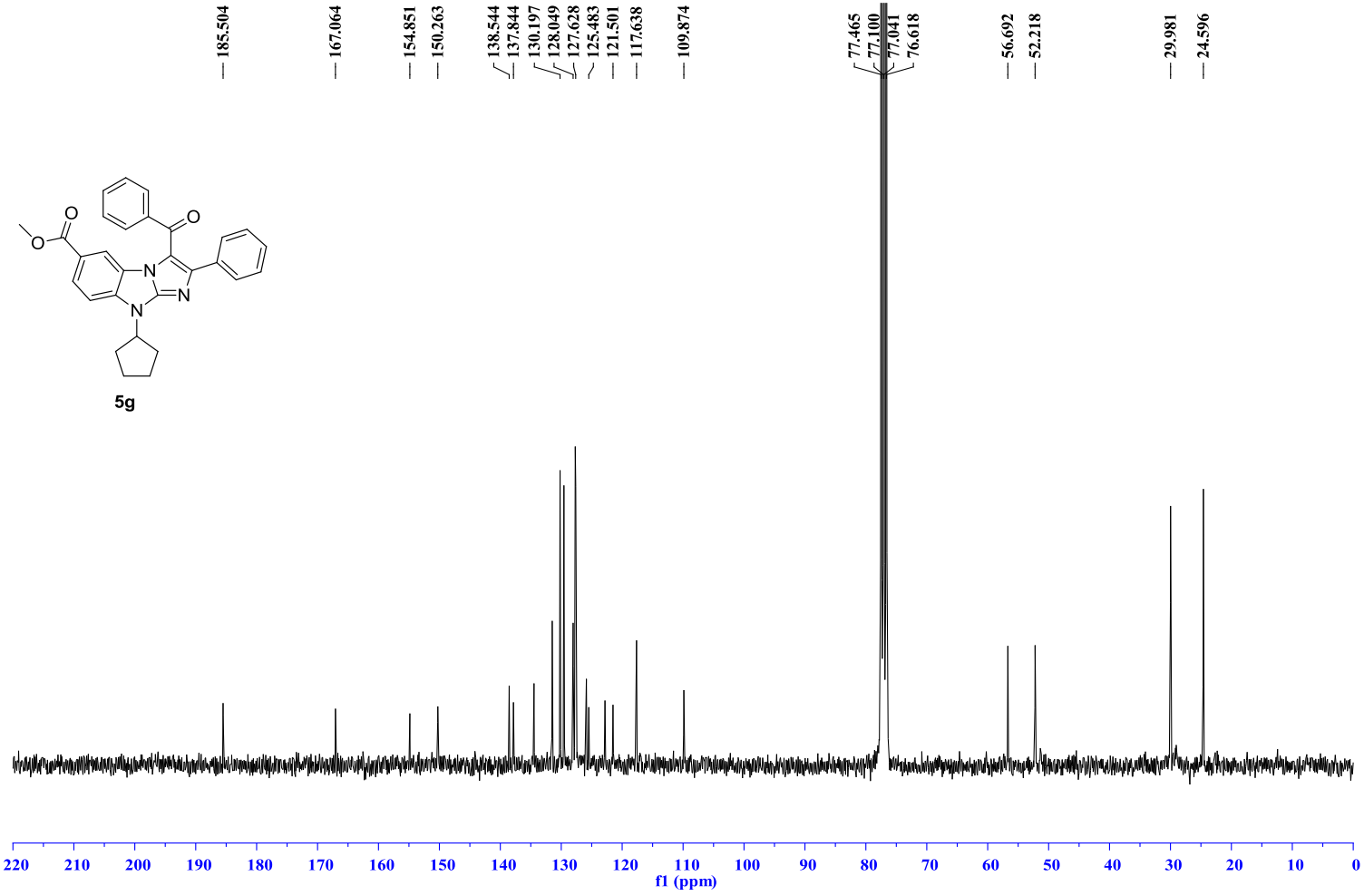
High resolution mass (ESI^+) spectrum of compound **5f**



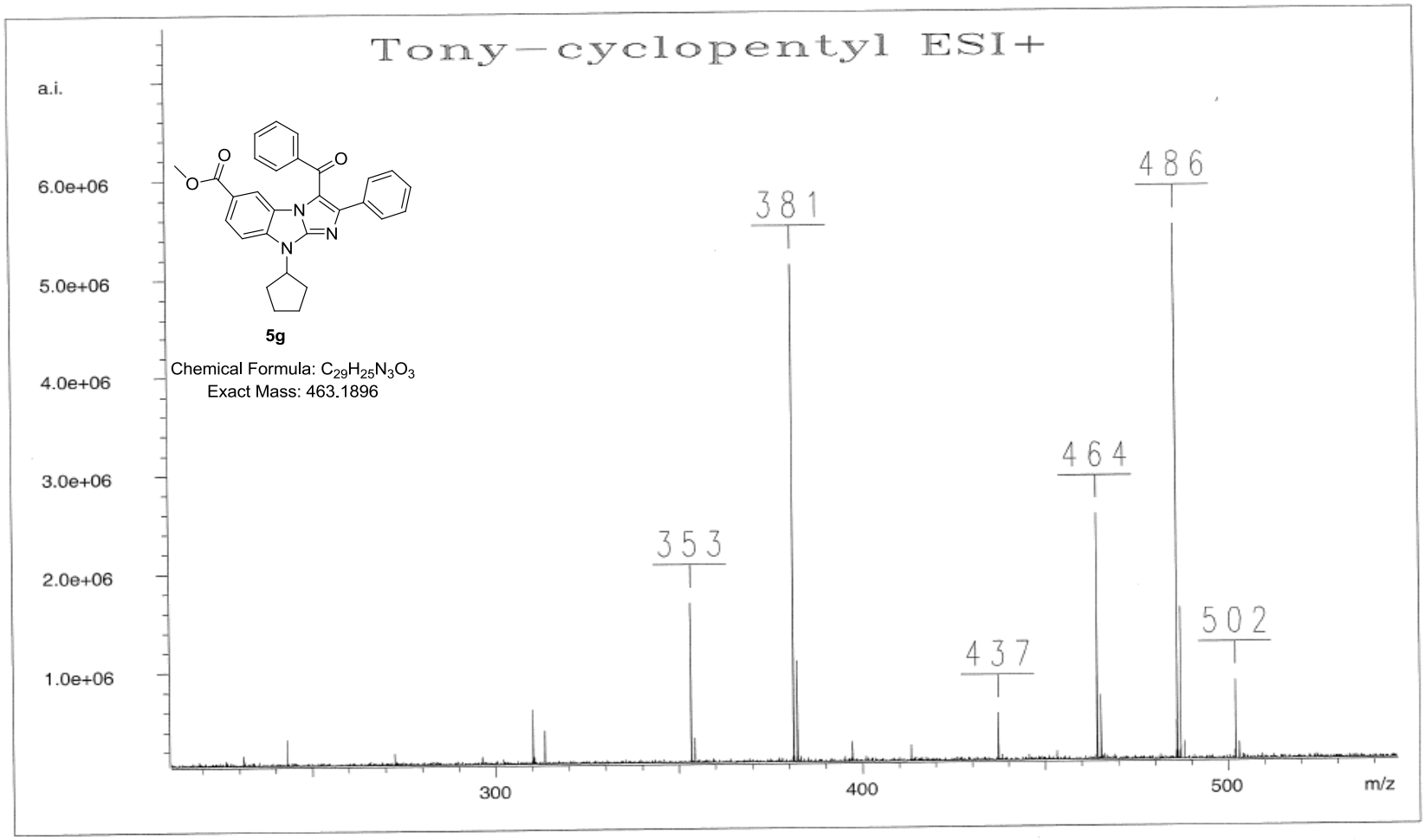
IR spectrum of compound **5f**



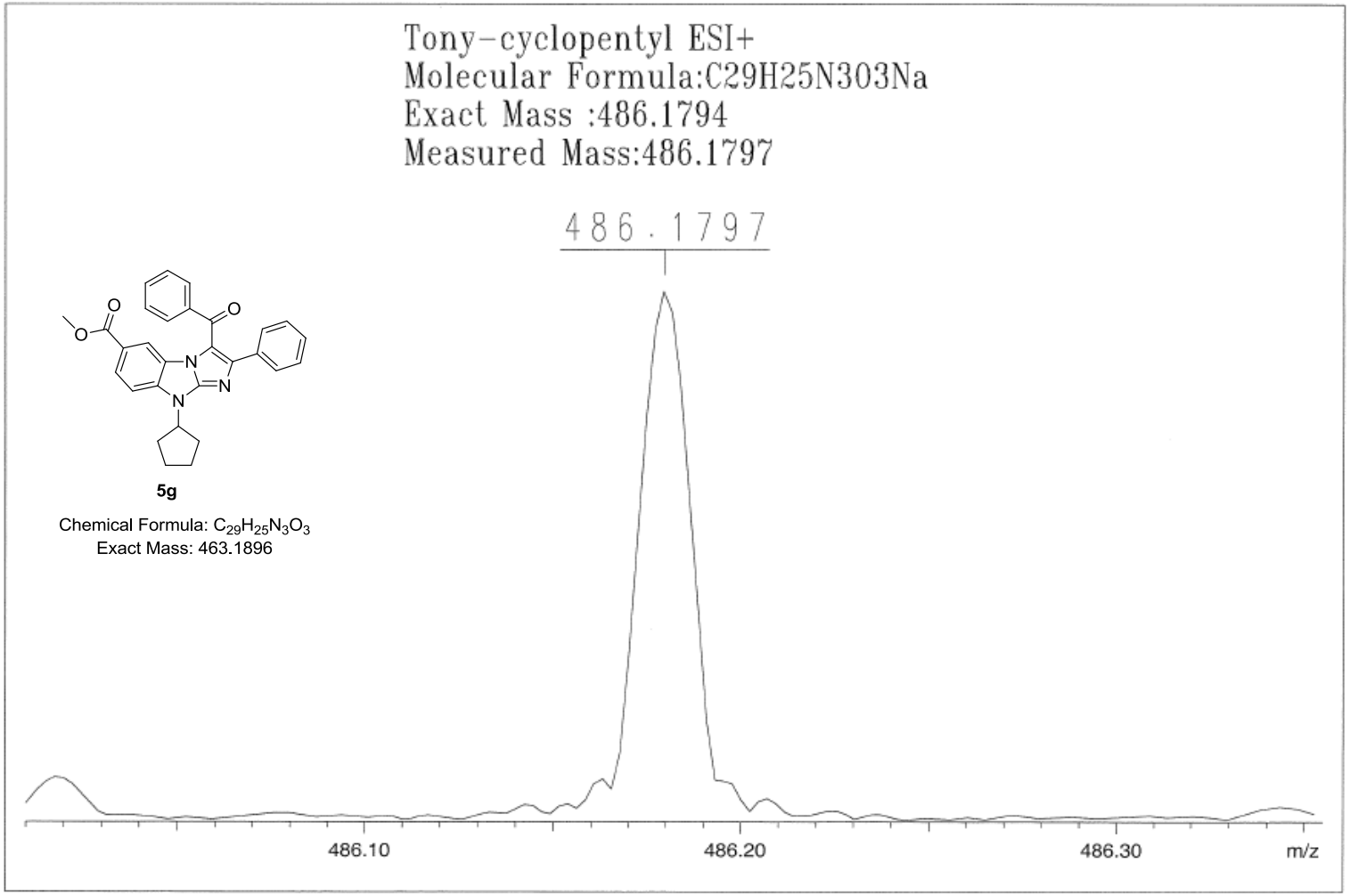
^{1}H NMR spectrum (300MHz) of compound **5g** in $CDCl_3$



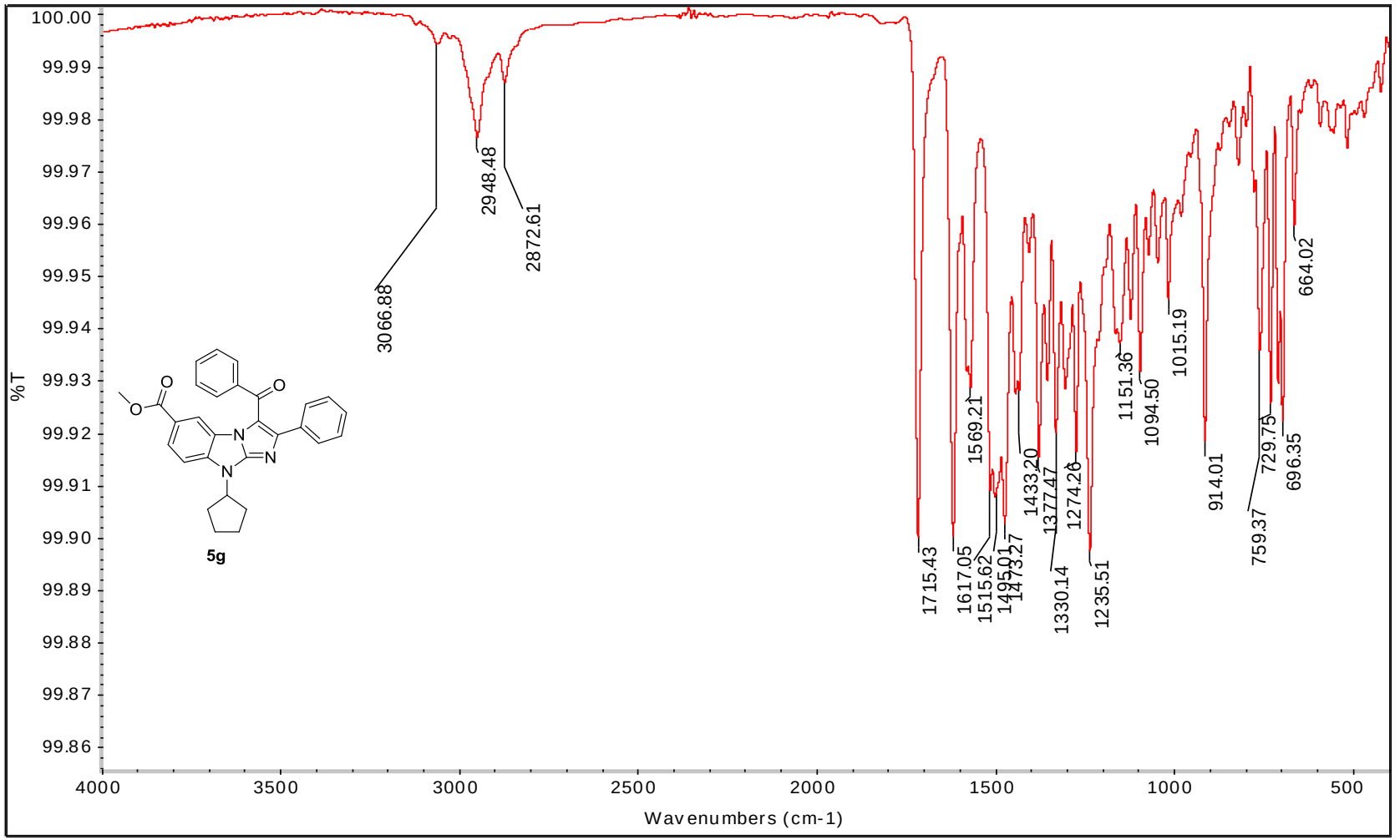
^{13}C NMR spectrum (75MHz) of compound **5g** in $CDCl_3$



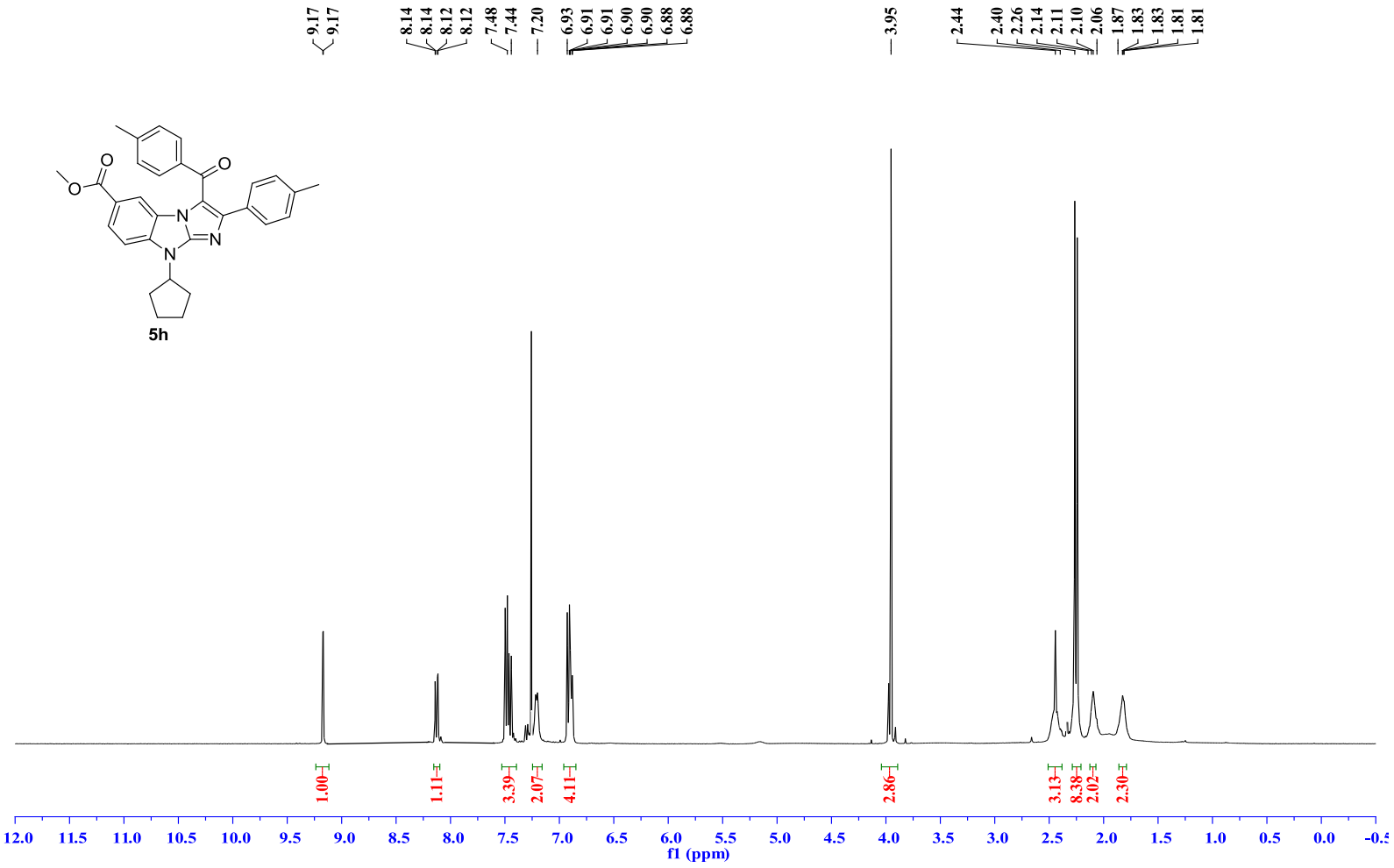
ESI^{+} Mass spectrum of compound **5g**



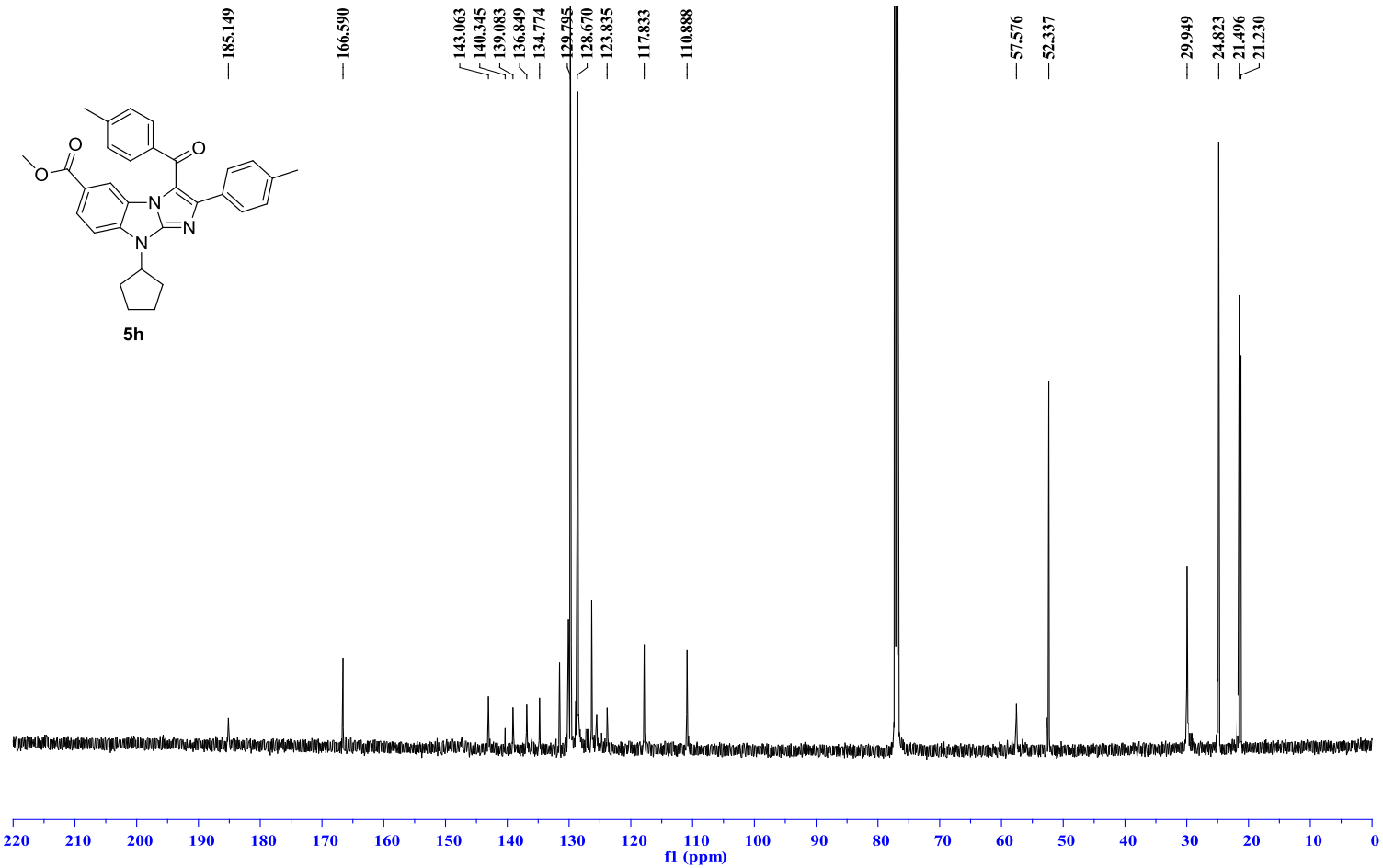
High resolution mass (ESI^+) spectrum of compound **5g**



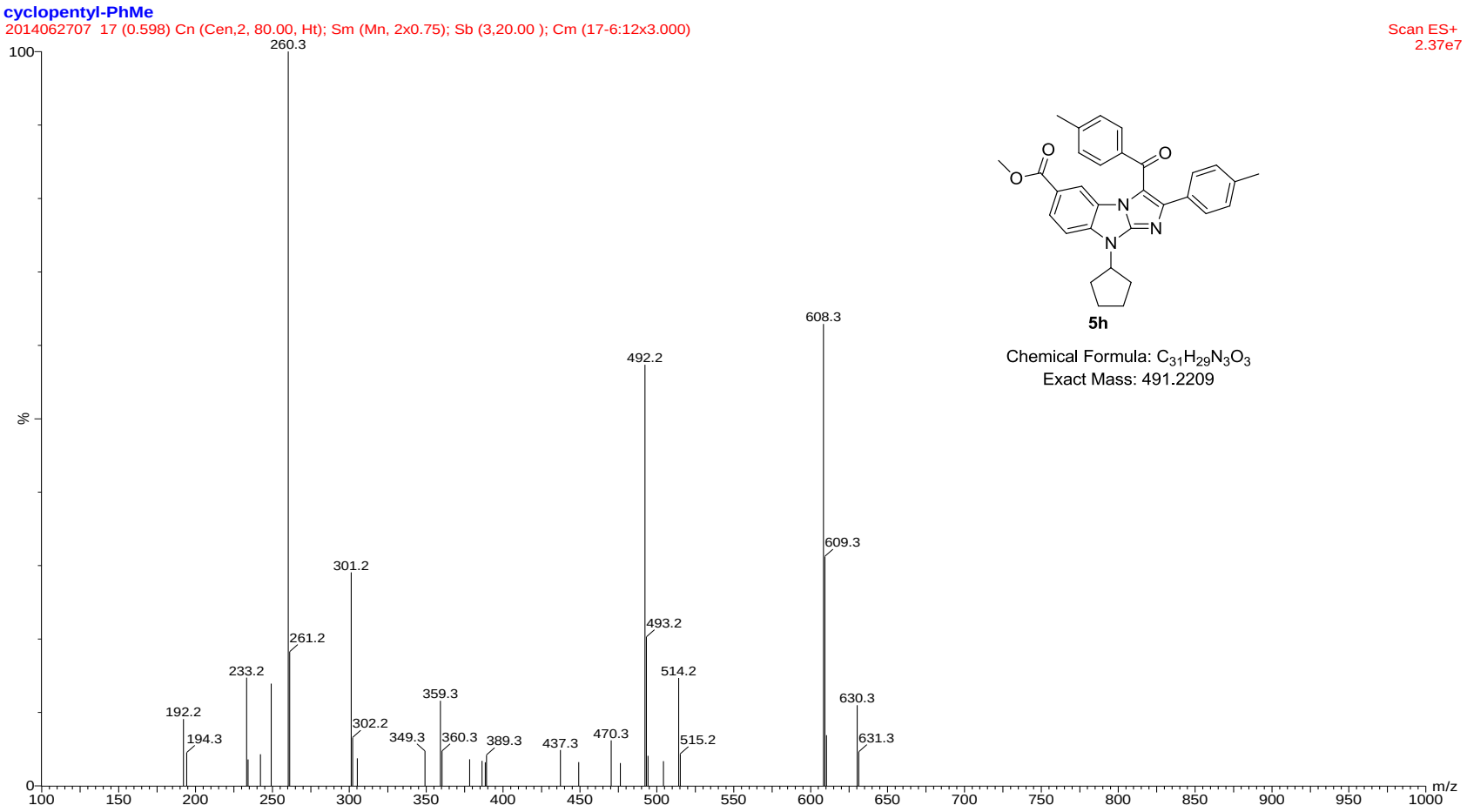
IR spectrum of compound **5g**



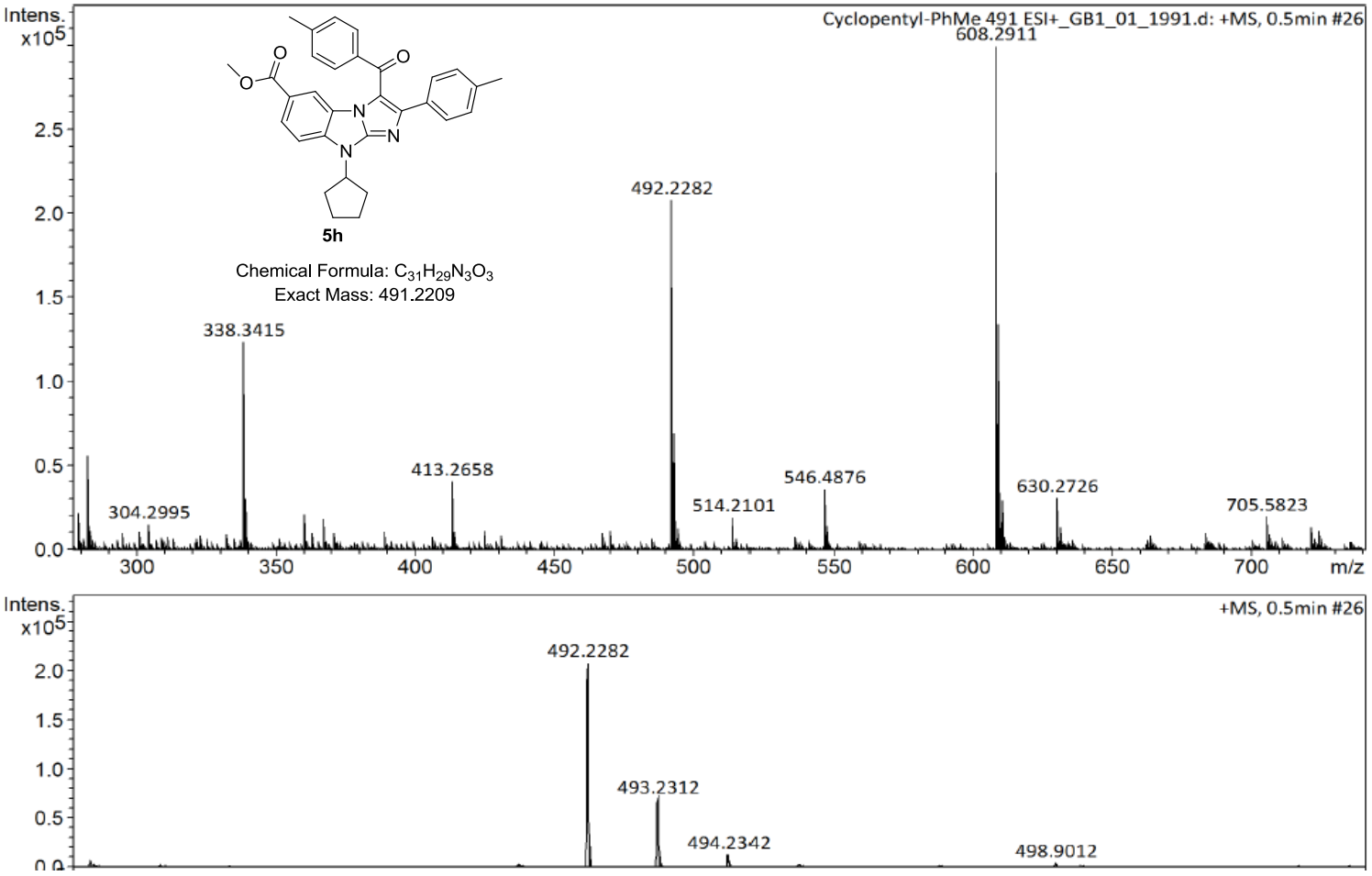
^{1}H NMR spectrum (300MHz) of compound **5h** in $CDCl_3$



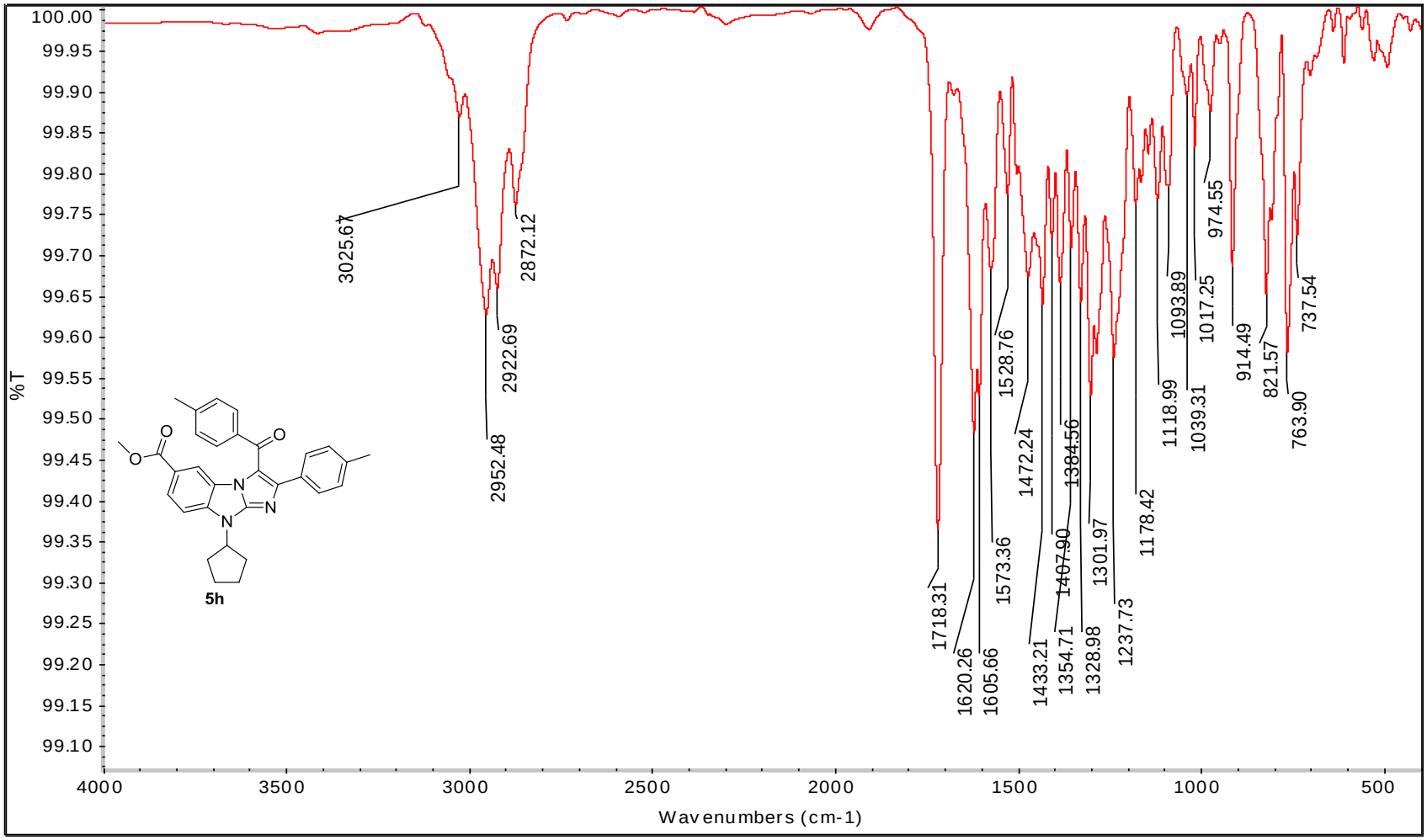
^{13}C NMR spectrum (150MHz) of compound **5h** in $CDCl_3$



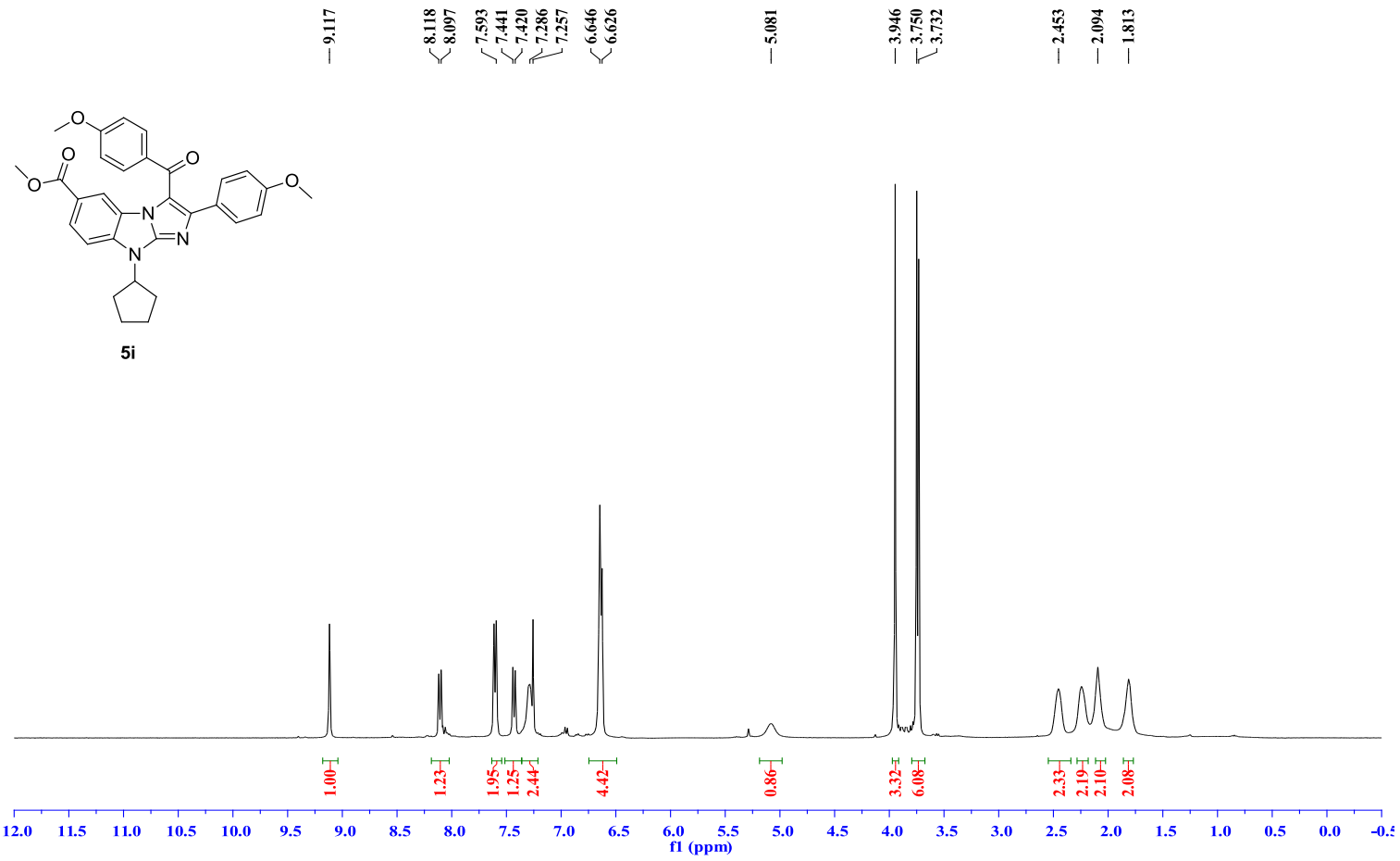
ESI$^+$ Mass spectrum of compound **5h**



High resolution mass (ESI^+) spectrum of compound **5h**

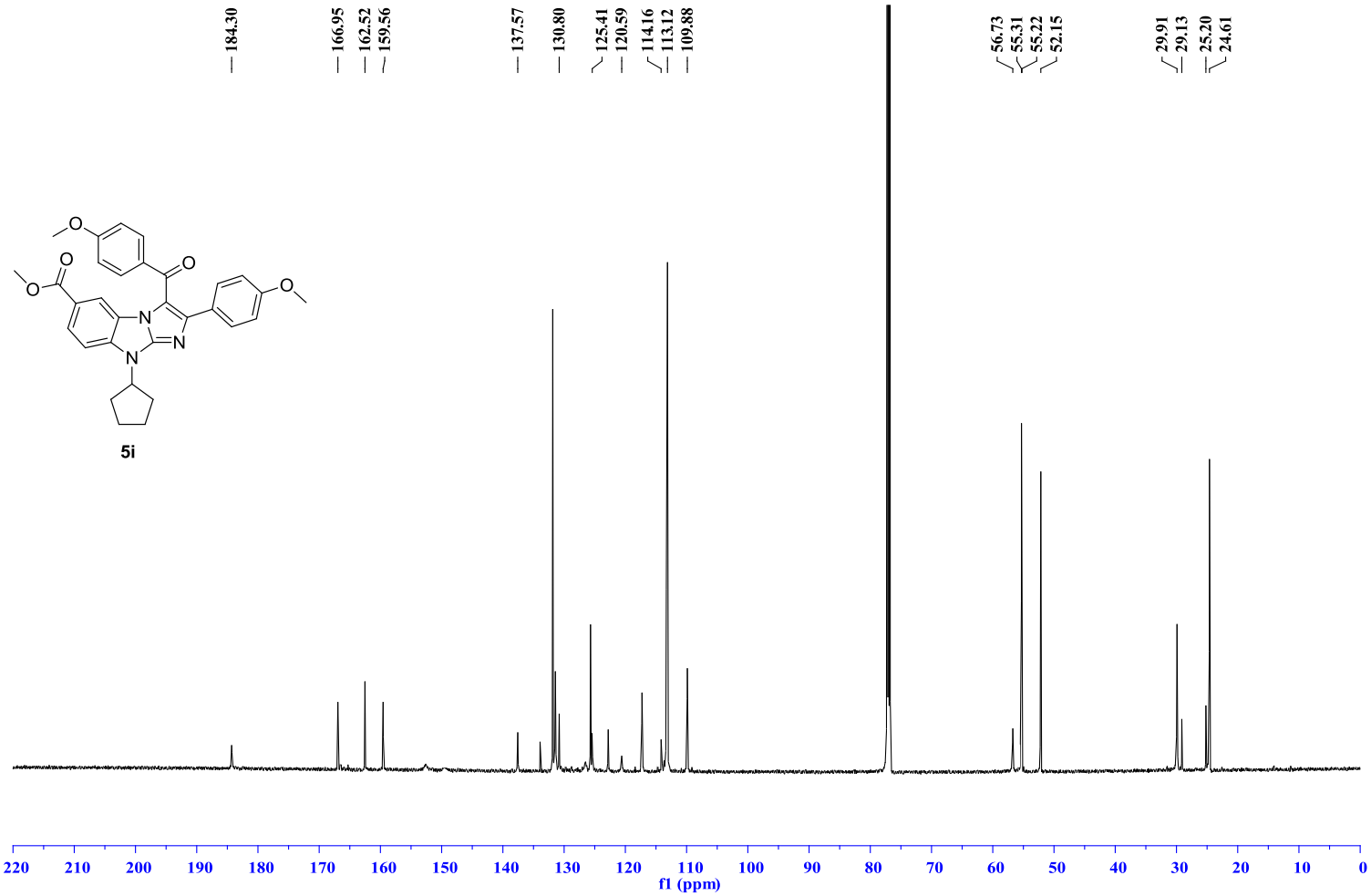


IR spectrum of compound **5h**

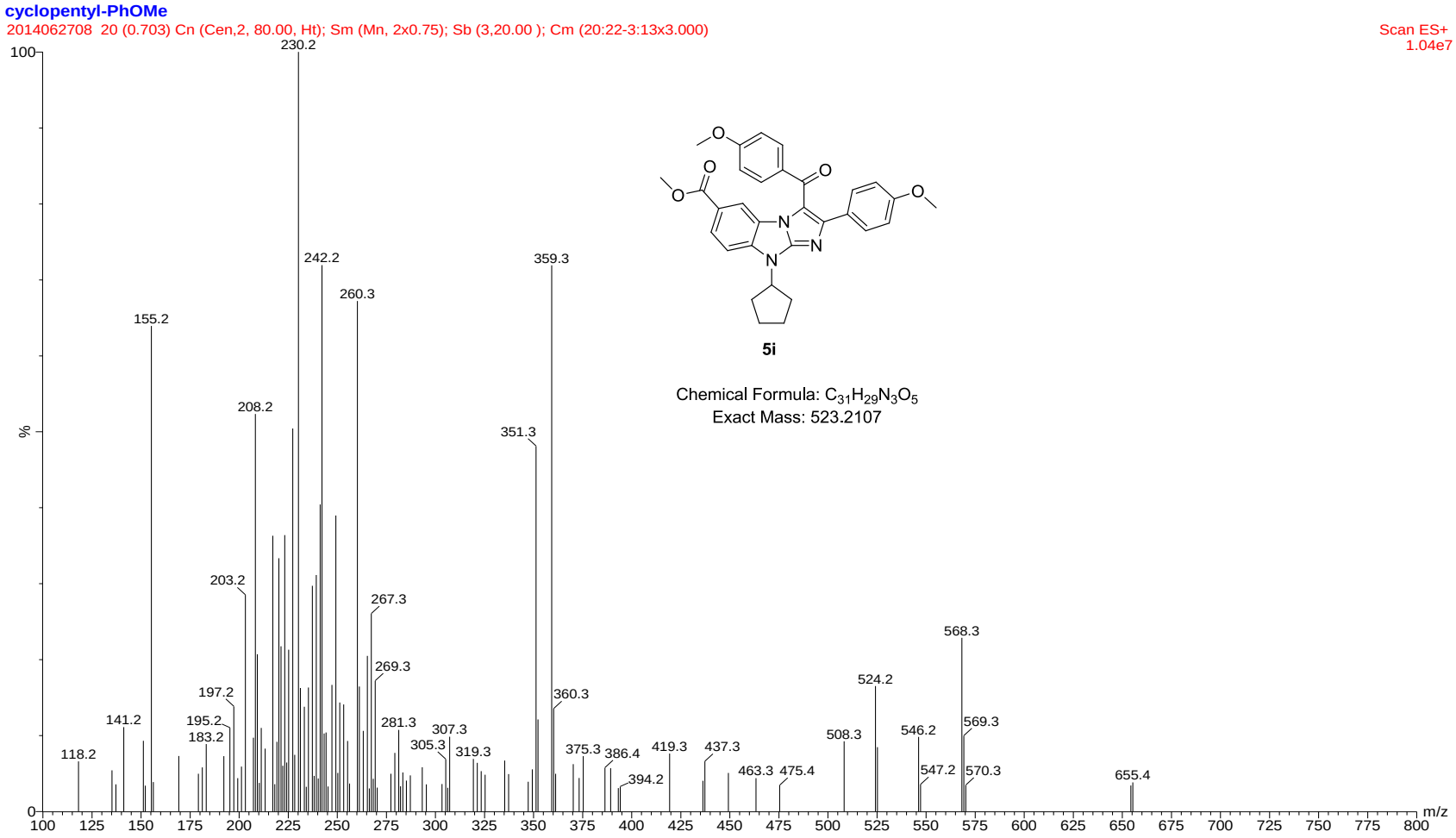


5i

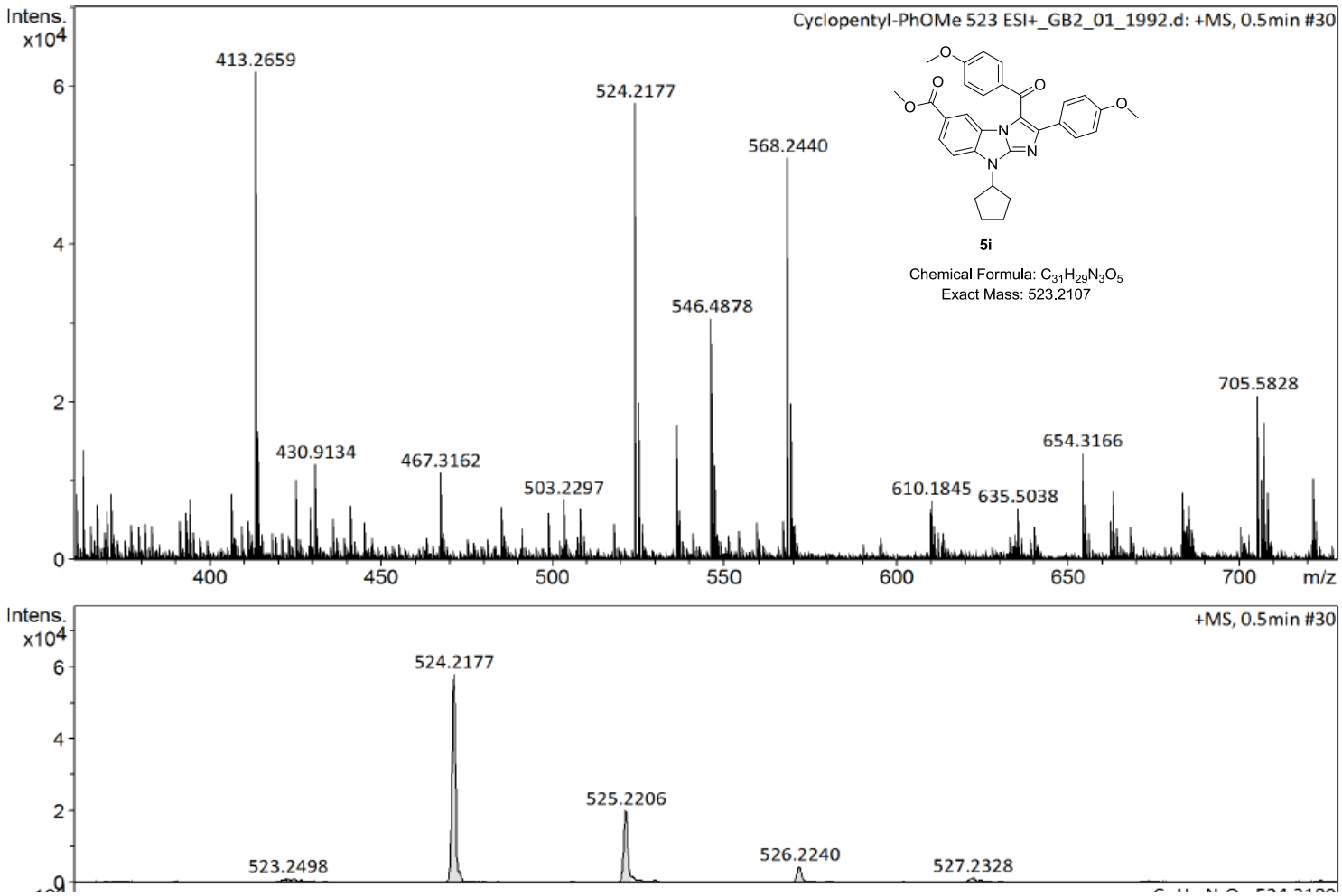
^{1}H NMR spectrum (400MHz) of compound **5i** in $CDCl_3$



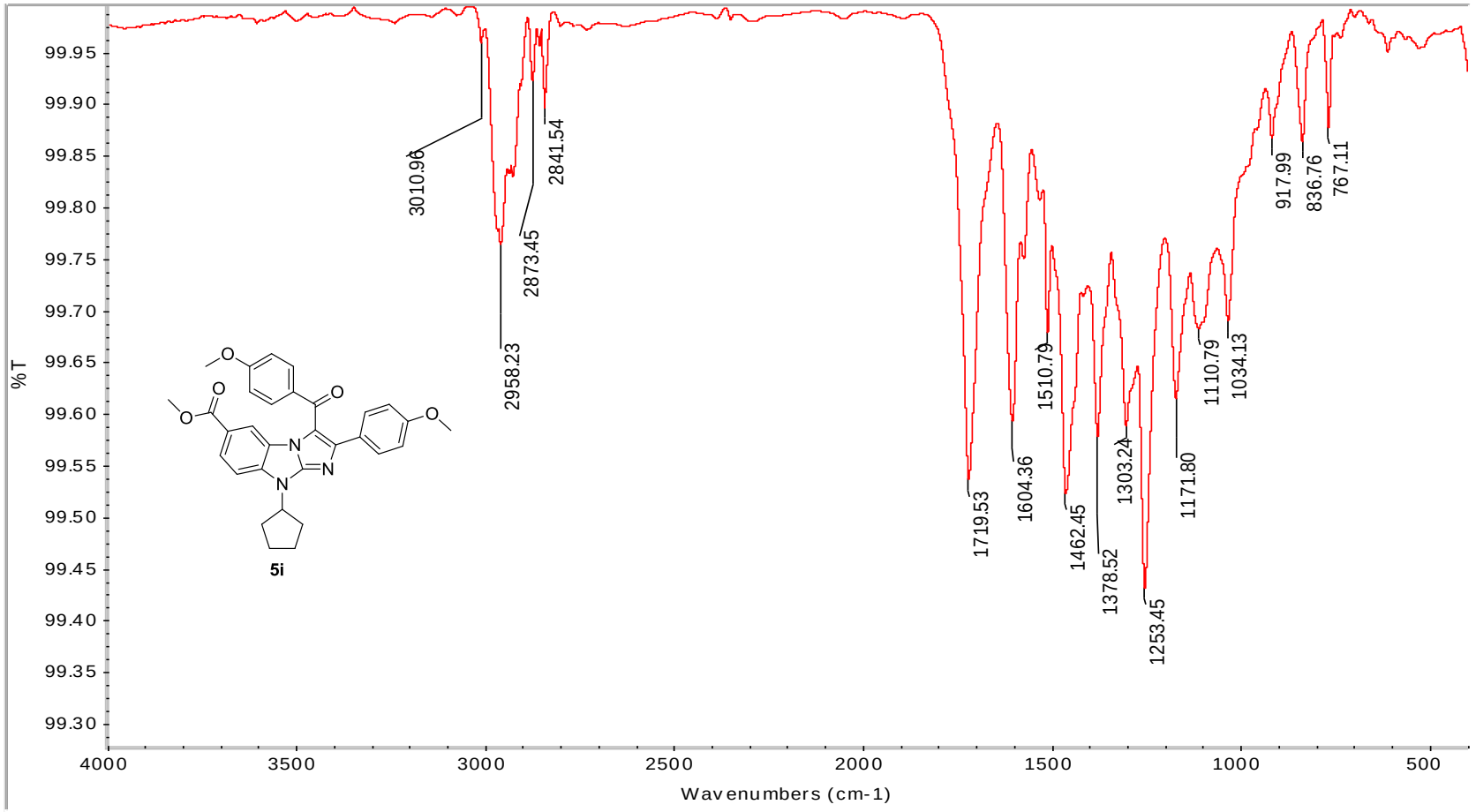
^{13}C NMR spectrum (150MHz) of compound **5i** in $CDCl_3$



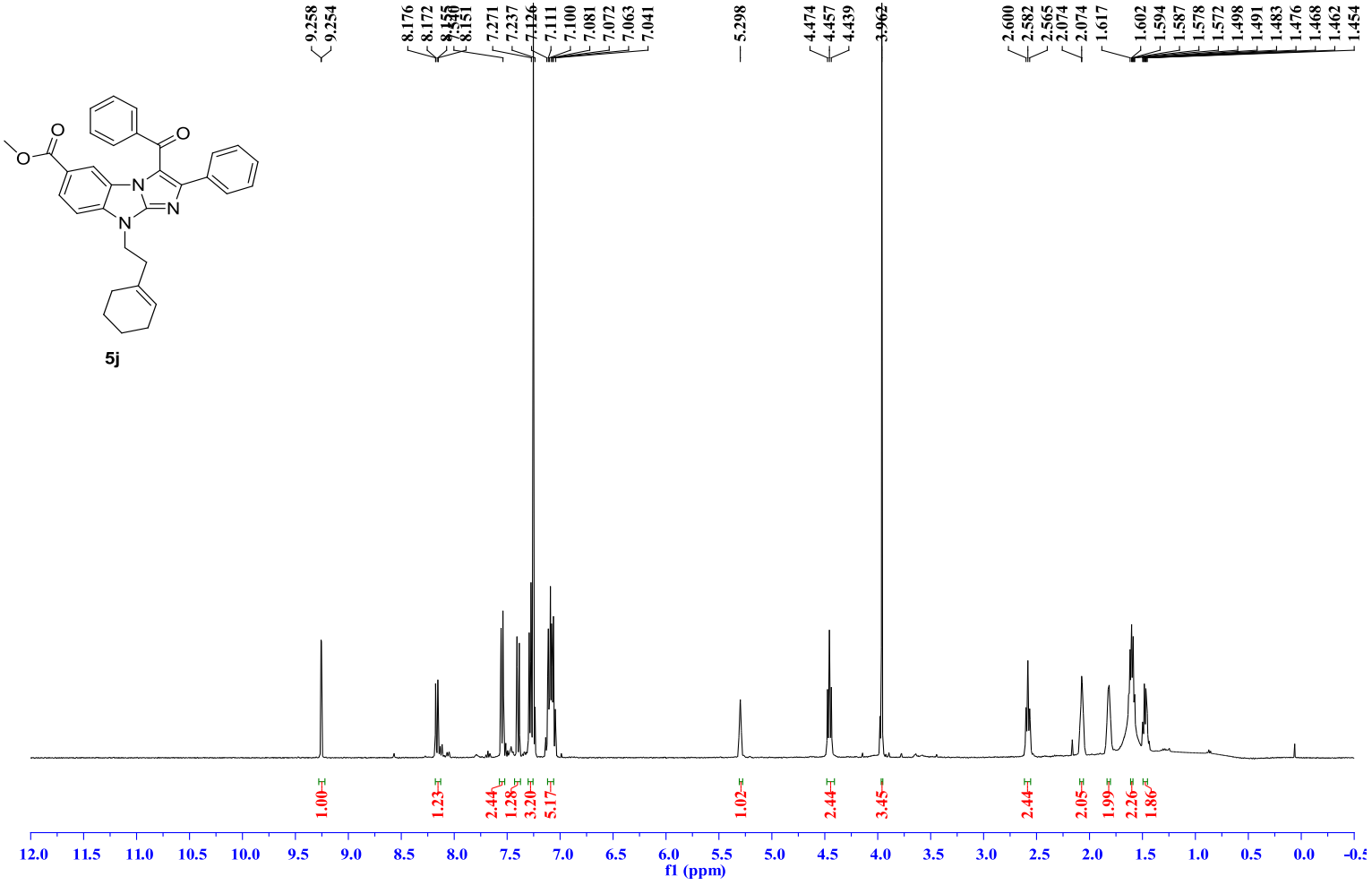
ESI$^+$ Mass spectrum of compound **5i**



High resolution mass (ESI^+) spectrum of compound **5i**

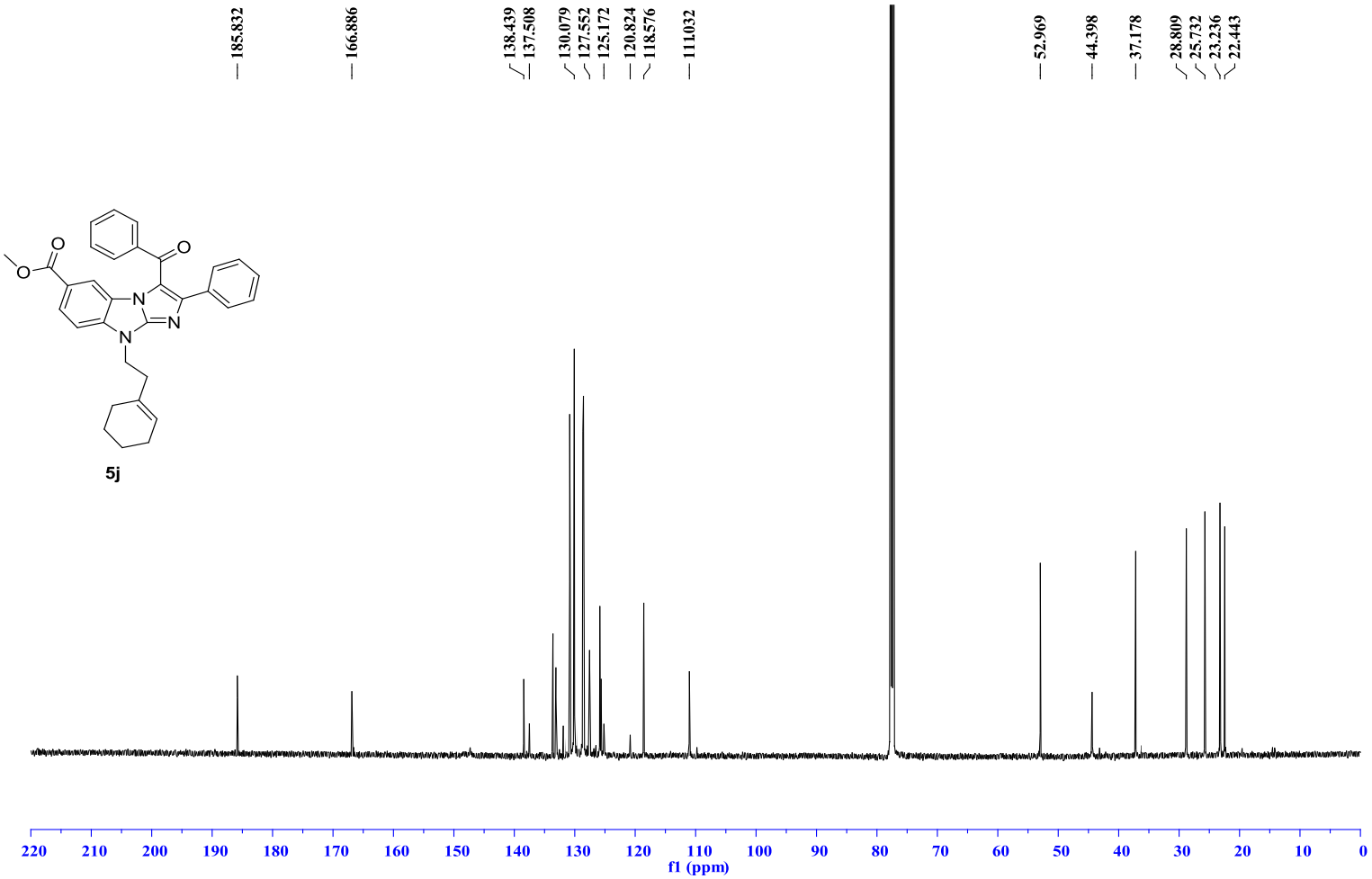


IR spectrum of compound **5i**

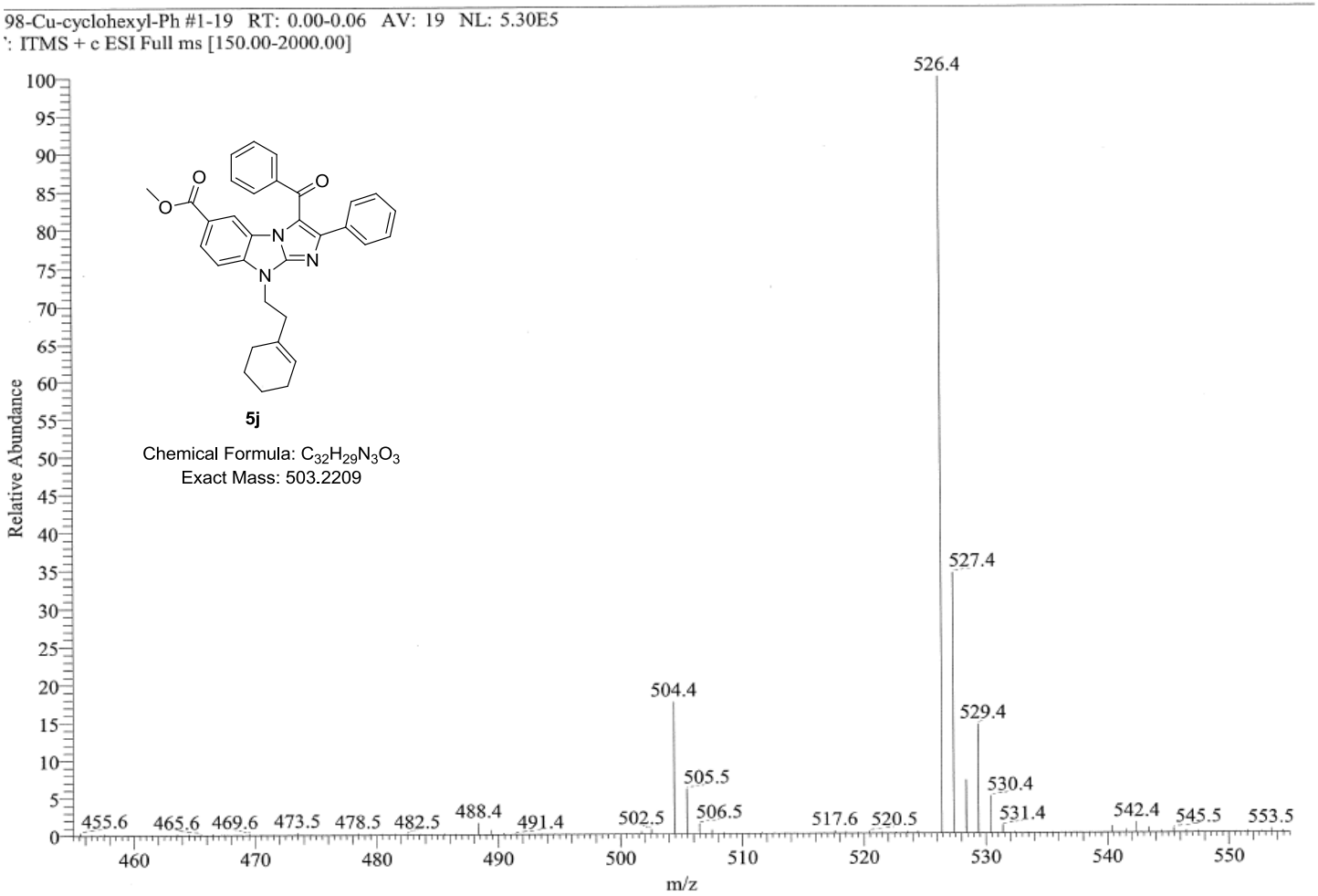


5j

^{1}H NMR spectrum (400MHz) of compound **5j** in $CDCl_3$



^{13}C NMR spectrum (150MHz) of compound **5j** in $CDCl_3$



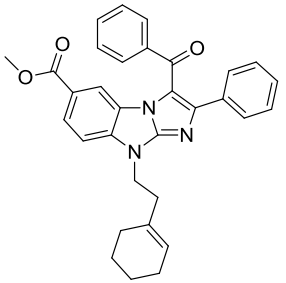
ESI$^+$ Mass spectrum of compound **5j**

200-Cu-cyclohexyl-Ph-H#1-20 RT: 0.01-0.28 AV: 20
T: FTMS + p ESI Full ms [150.00-2000.00]
m/z= 472.4239-517.7081

Isotope	Min	Max
C-12	0	33
H-1	0	30
O-16	0	3
N-14	0	3

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

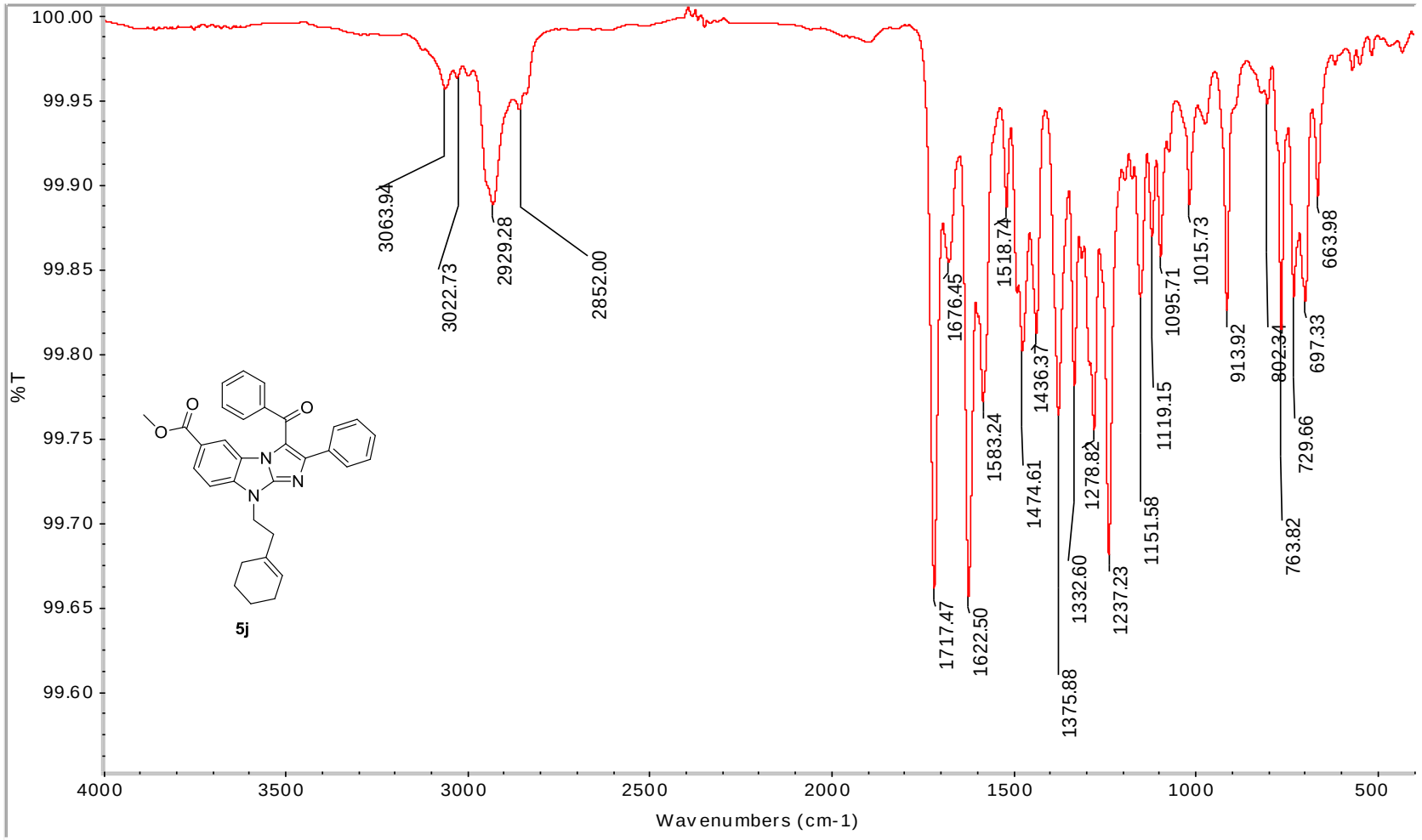
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
504.2276	1354612.3	100.00	504.2282	-1.04	$C_{32}H_{30}O_3N_3$



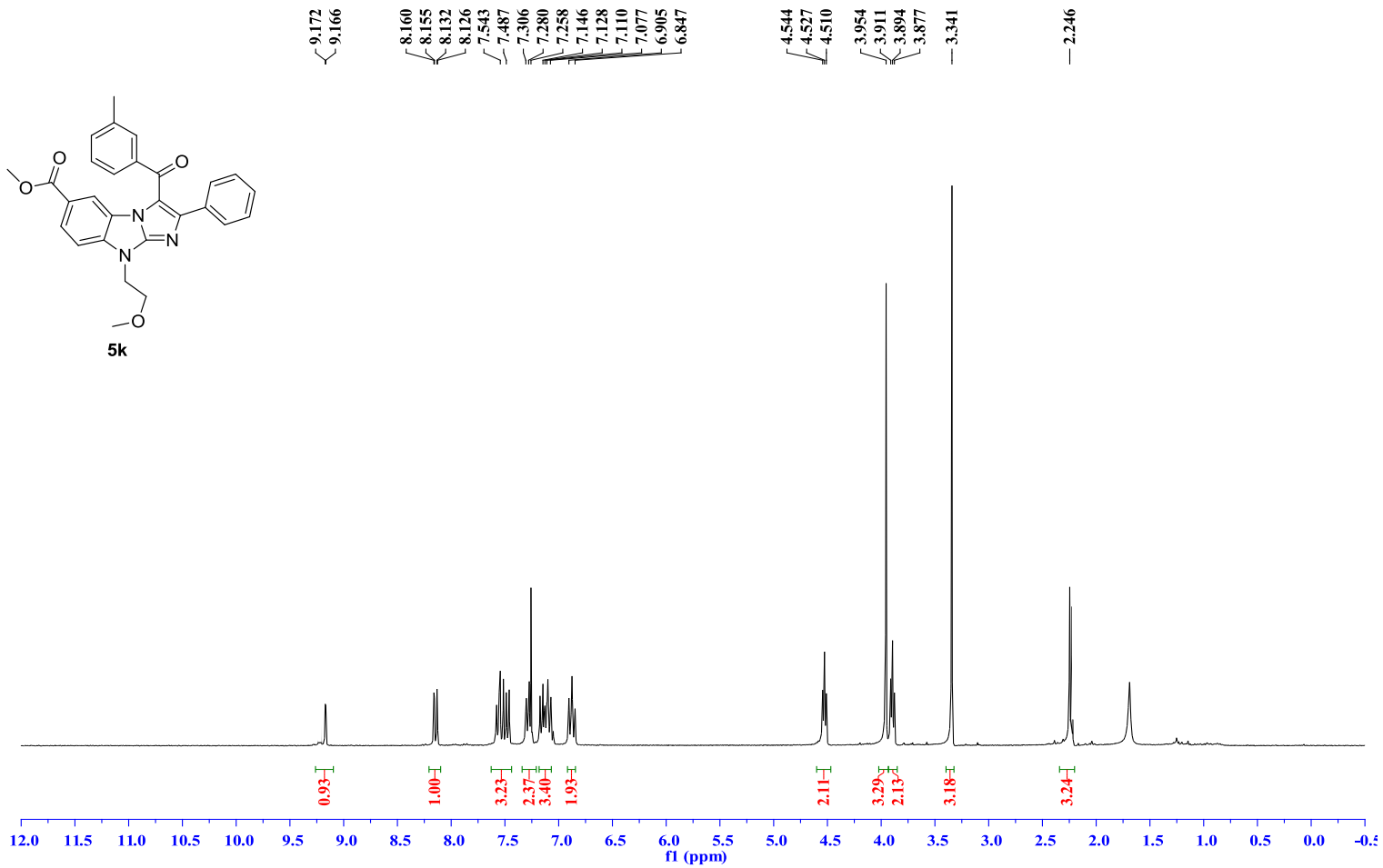
5j

Chemical Formula: $C_{32}H_{29}N_3O_3$
Exact Mass: 503.2209

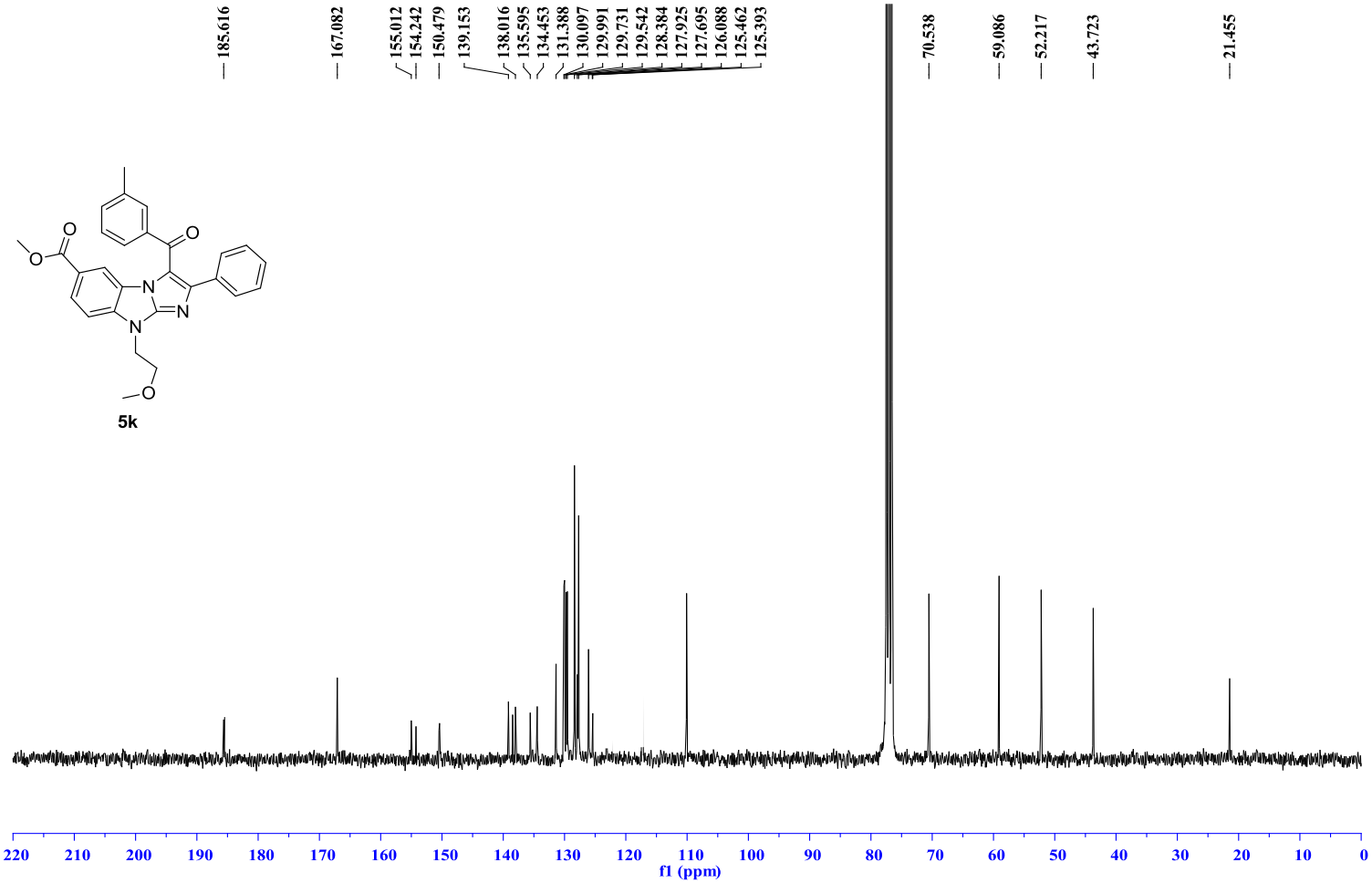
High resolution mass (ESI^+) spectrum of compound **5j**



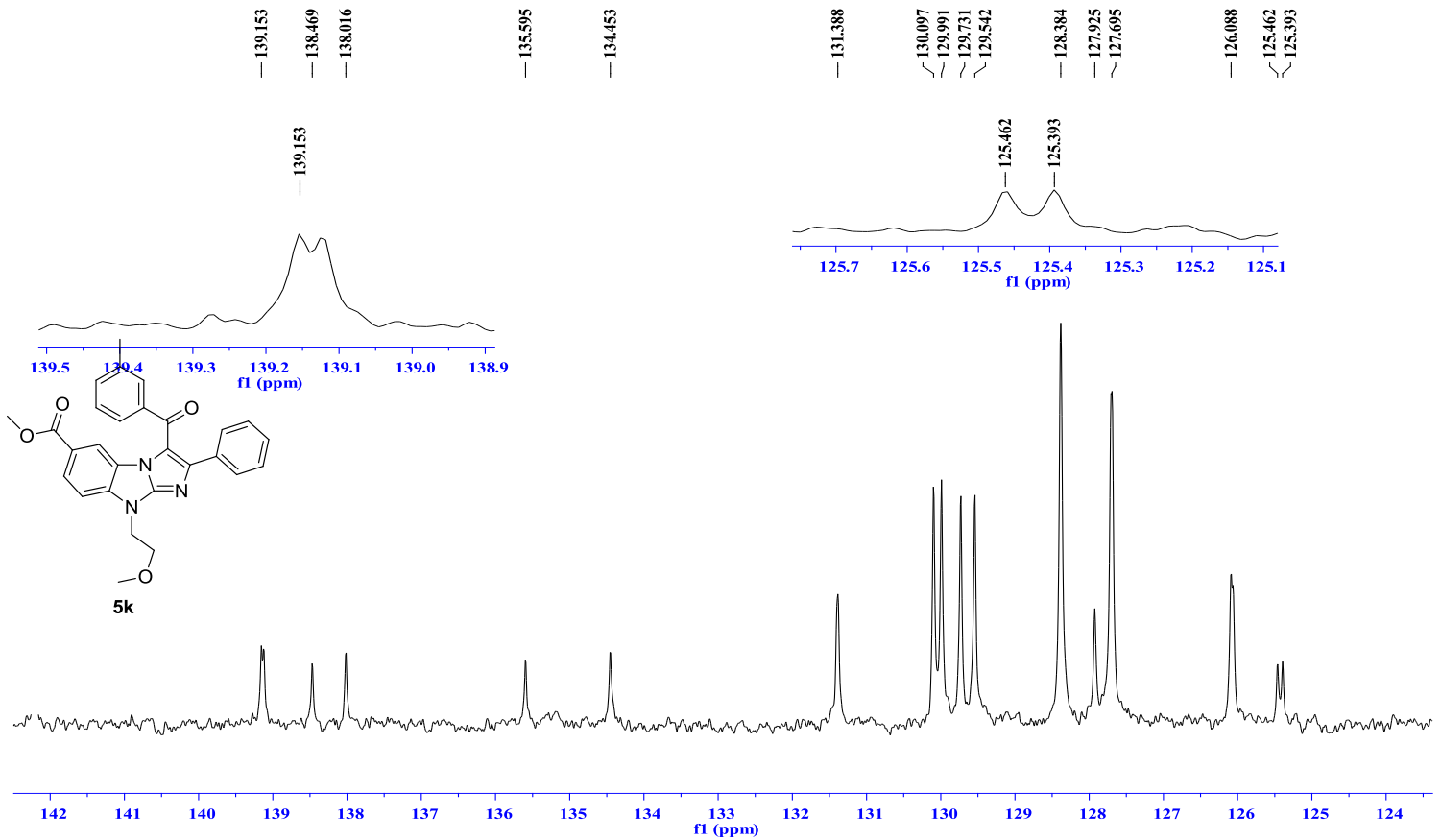
IR spectrum of compound **5j**



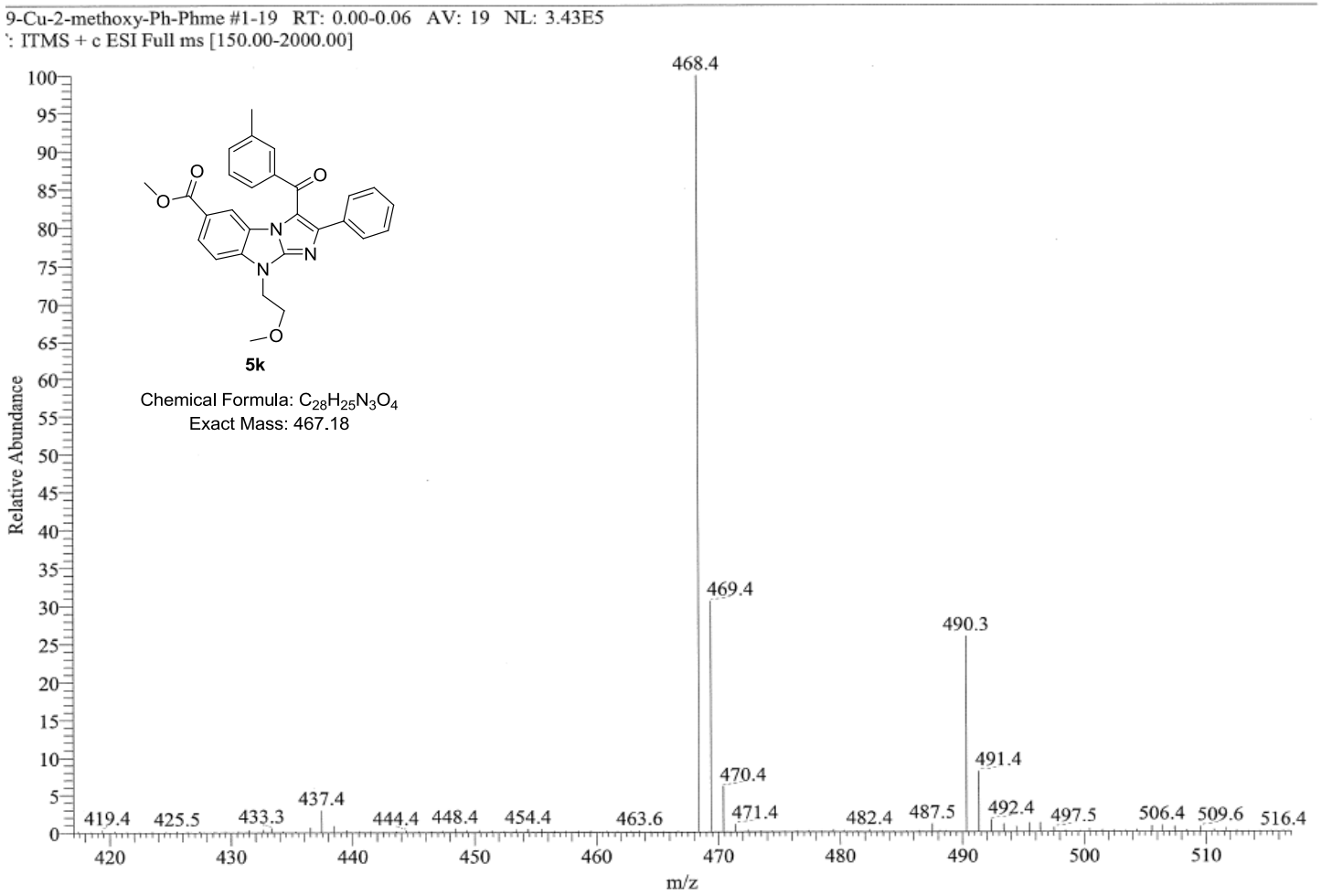
^{1}H NMR spectrum (300MHz) of compound **5k** in $CDCl_3$



^{13}C NMR spectrum (75MHz) of compound **5k** in $CDCl_3$



Expanding ^{13}C NMR spectrum (75MHz) of compound **5k** in $CDCl_3$



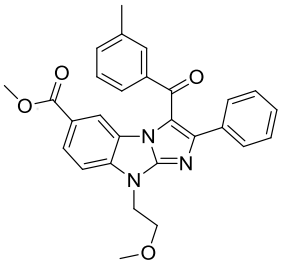
ESI$^+$ Mass spectrum of compound **5k**

77-Cu-2-methoxy-Ph-Phme-H#1-20 RT: 0.01-0.37 AV: 20
T: FTMS + p ESI Full ms [150.00-2000.00]
m/z= 459.7440-477.8576

Isotope	Min	Max
C-12	0	28
H-1	0	150
O-16	0	10
N-14	0	4

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

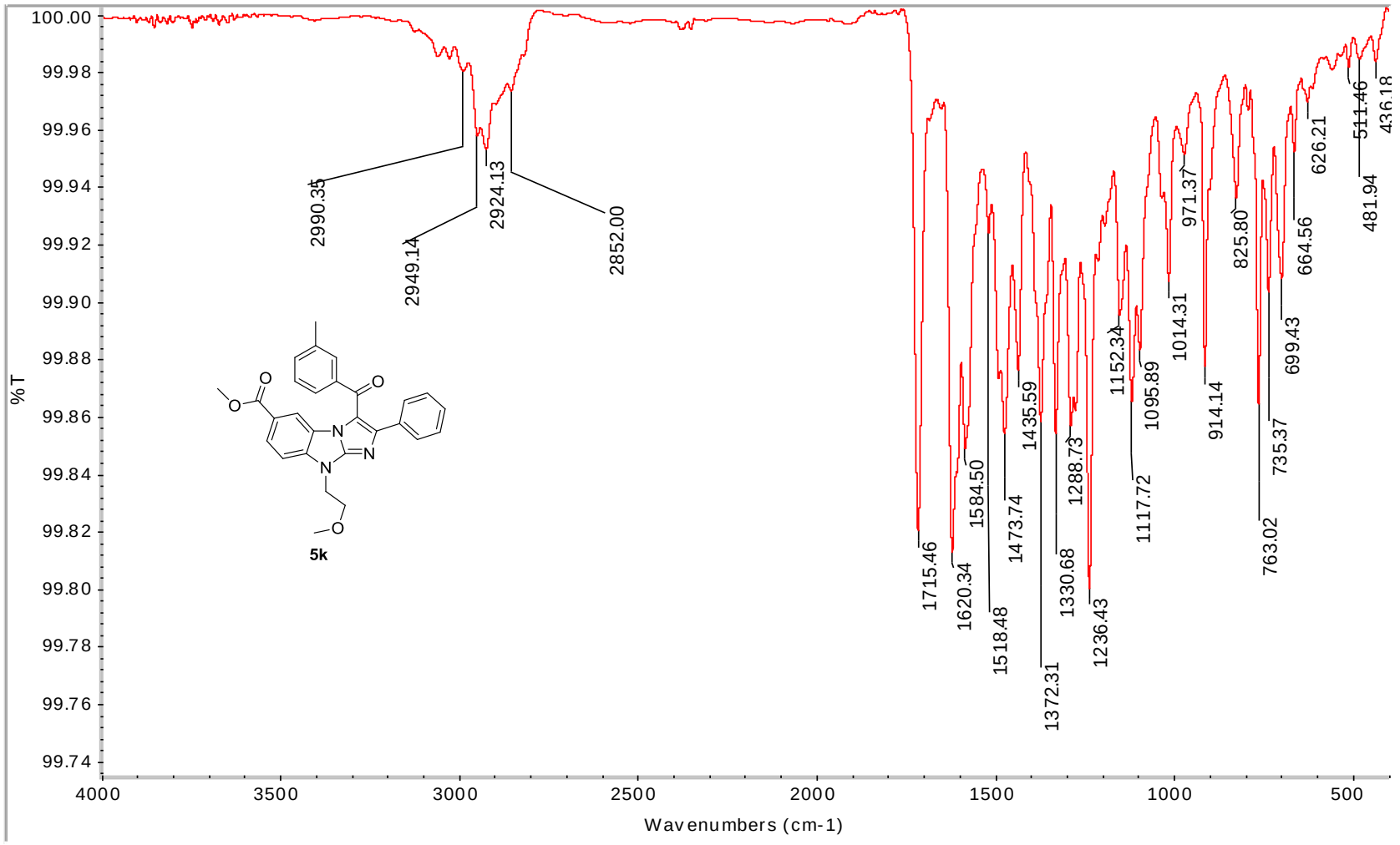
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
468.1933	1262440.8	100.00	468.1918	3.15	$C_{28}H_{26}O_4N_3$



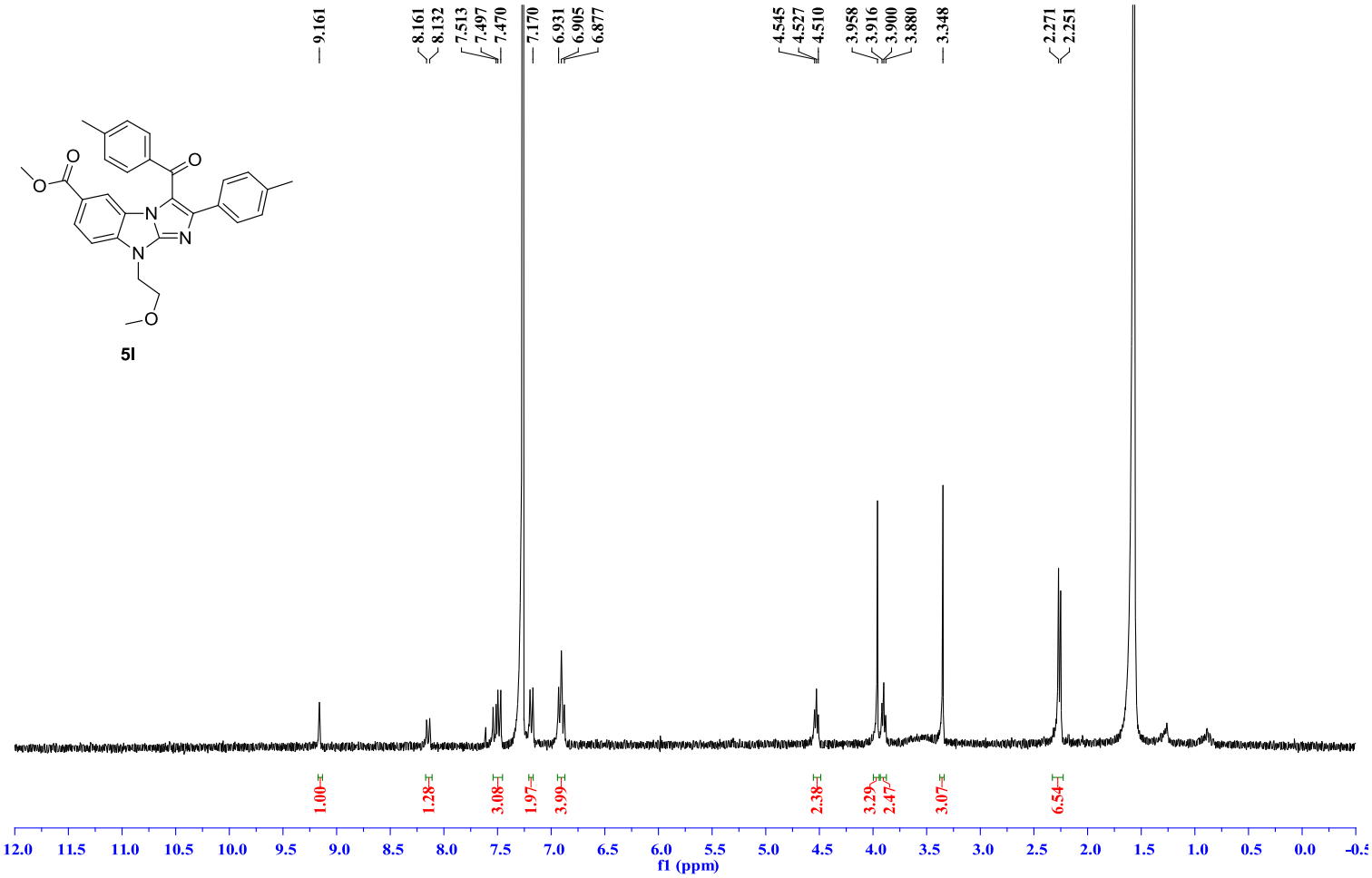
5k

Chemical Formula: $C_{28}H_{25}N_3O_4$
Exact Mass: 467.18

High resolution mass (ESI^+) spectrum of compound **5k**

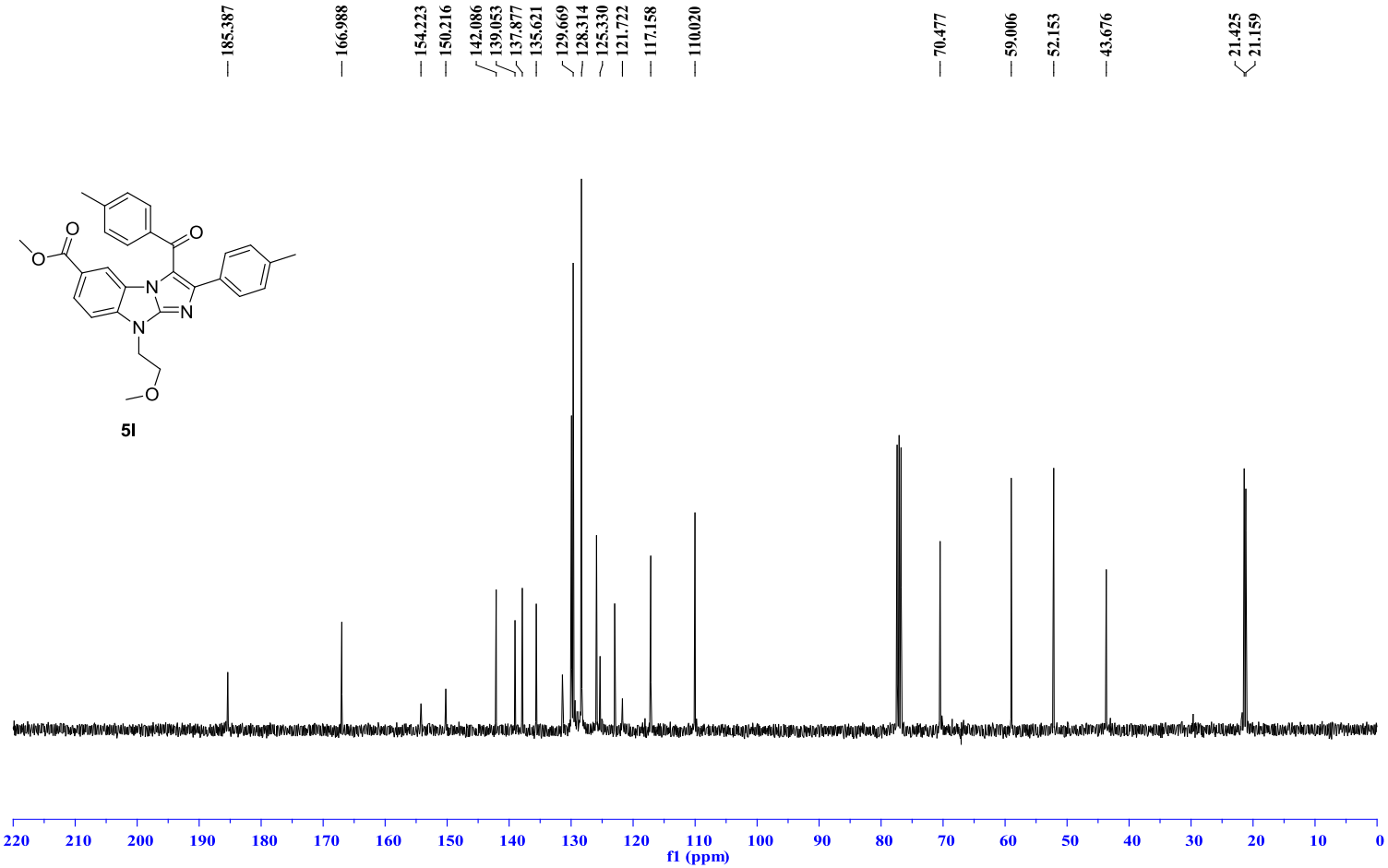


IR spectrum of compound **5k**

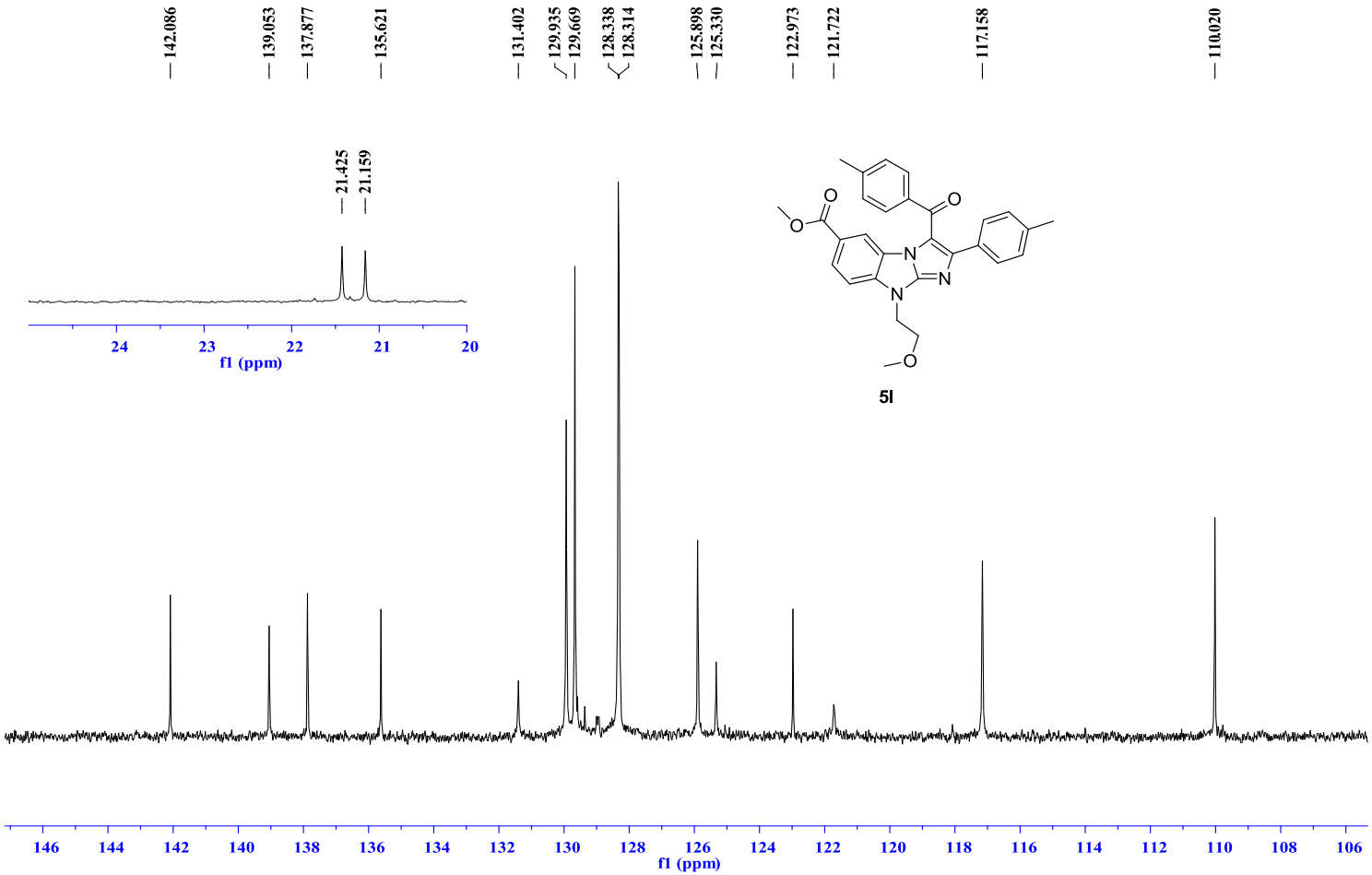


5l

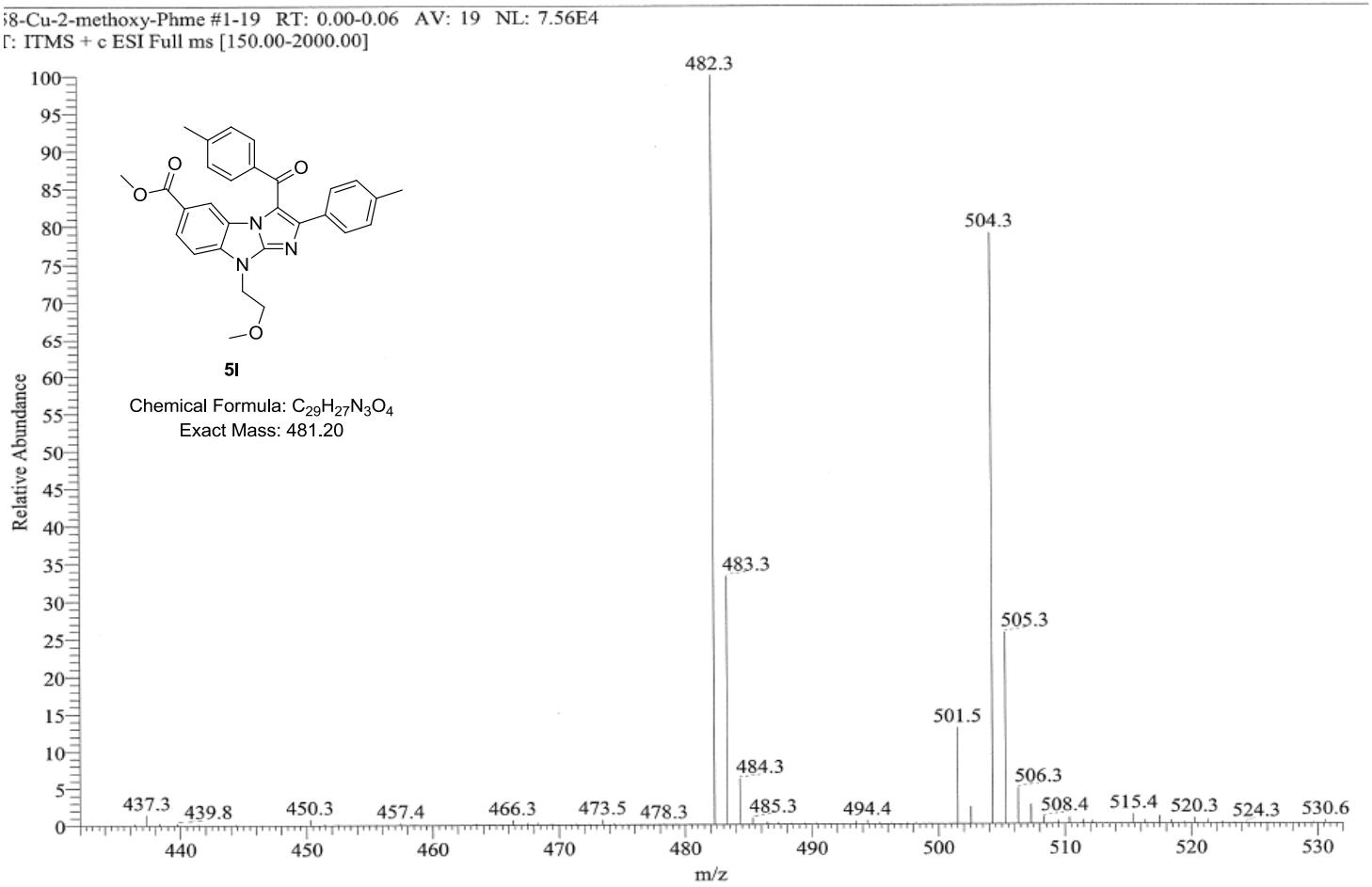
^{1}H NMR spectrum (300MHz) of compound **5l** in $CDCl_3$



^{13}C NMR spectrum (75 MHz) of compound **5l** in $CDCl_3$



Expanding ^{13}C NMR spectrum (75MHz) of compound **5l** in $CDCl_3$



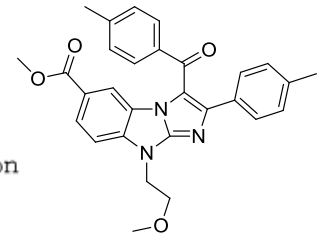
ESI$^+$ Mass spectrum of compound **5l**

60-Cu-2-methoxy-Phme-H#1-20 RT: 0.01-0.43 AV: 20
T: FTMS + p ESI Full ms [150.00-700.00]
m/z= 445.7723-498.4735

Isotope	Min	Max
C-12	0	29
H-1	0	80
O-16	0	9
N-14	0	4

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

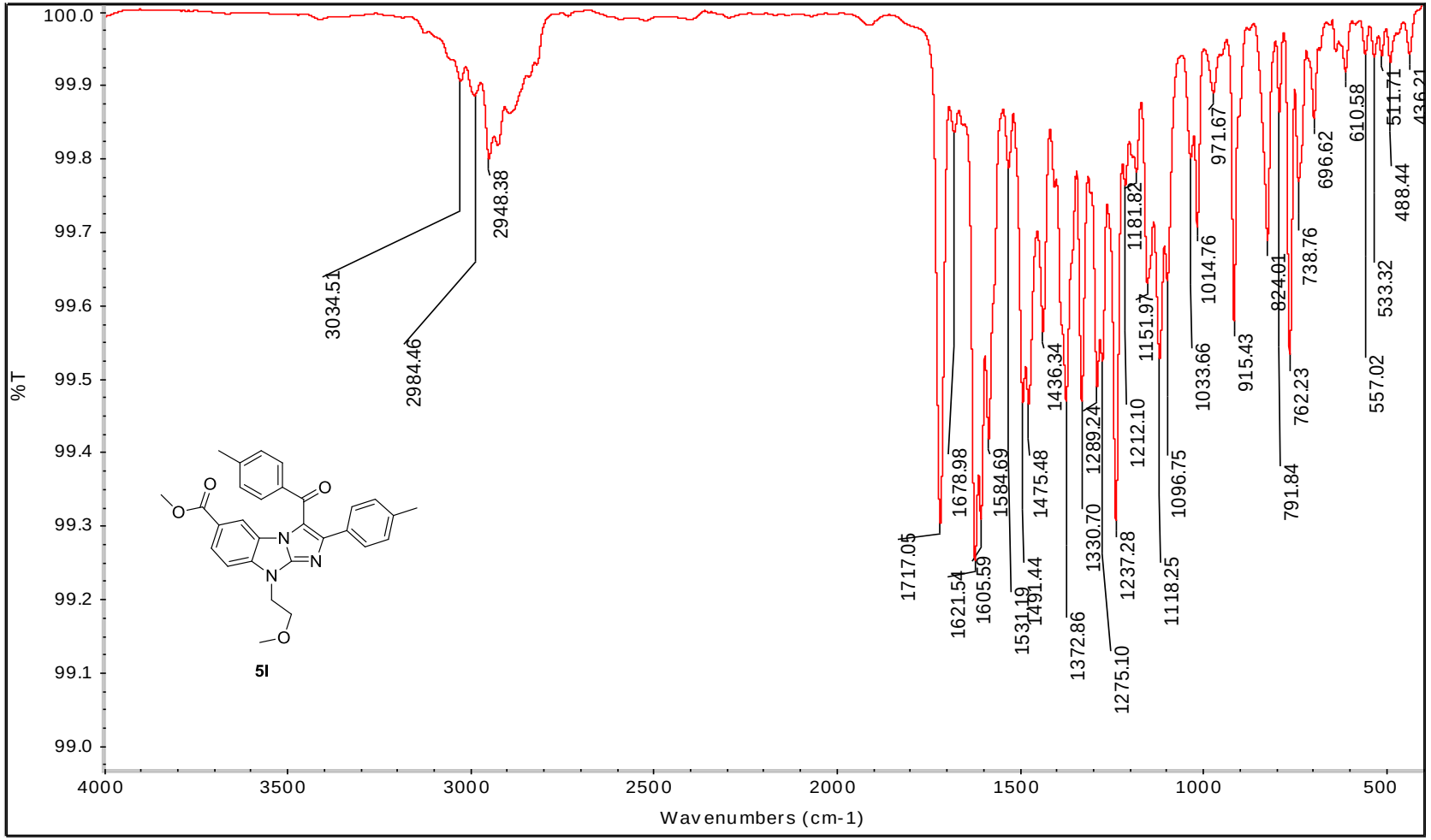
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
482.2089	991545.9	100.00	482.2074	3.10	$C_{29}H_{28}O_4N_3$



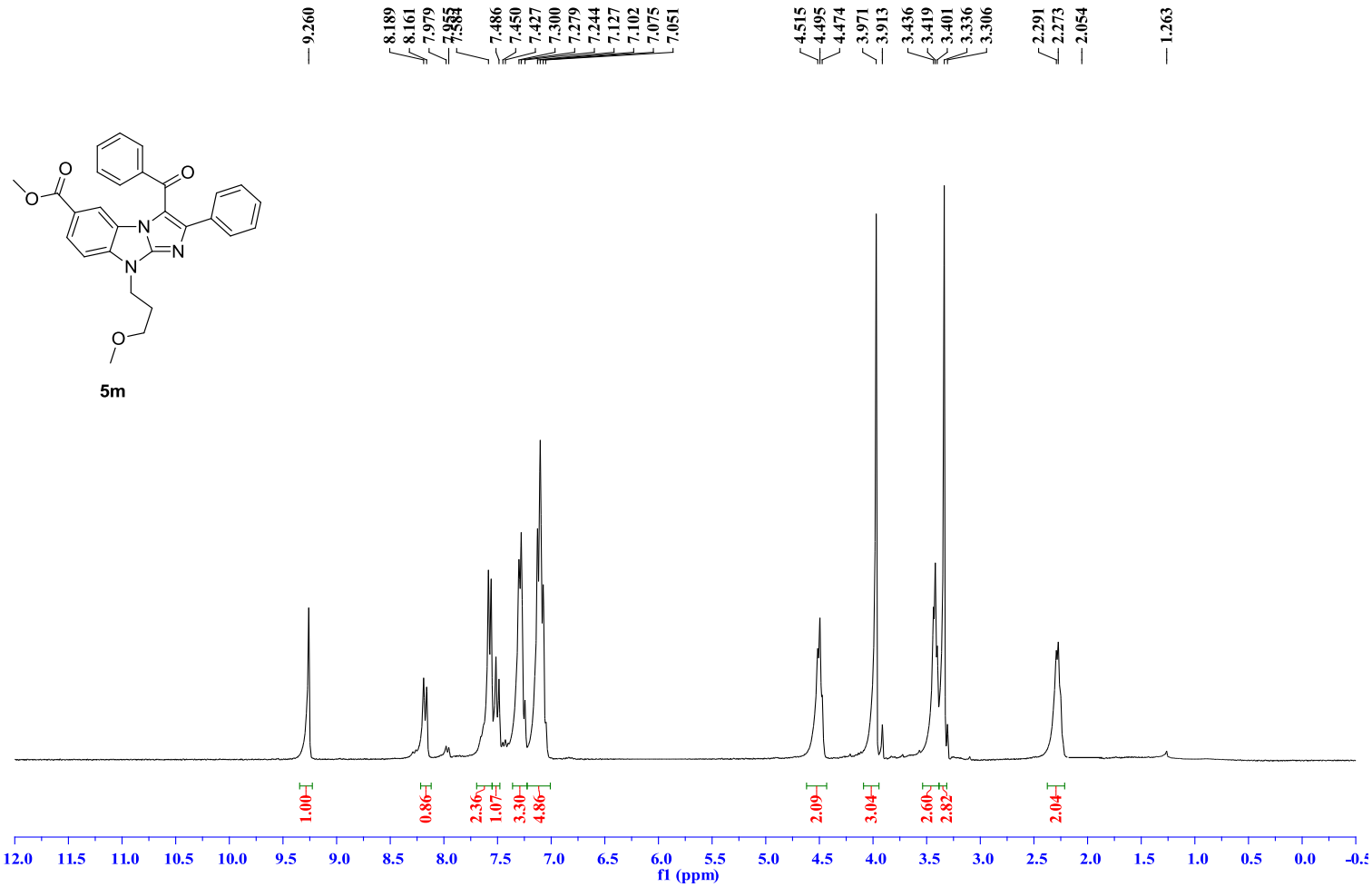
5l

Chemical Formula: $C_{29}H_{27}N_3O_4$
Exact Mass: 481.20

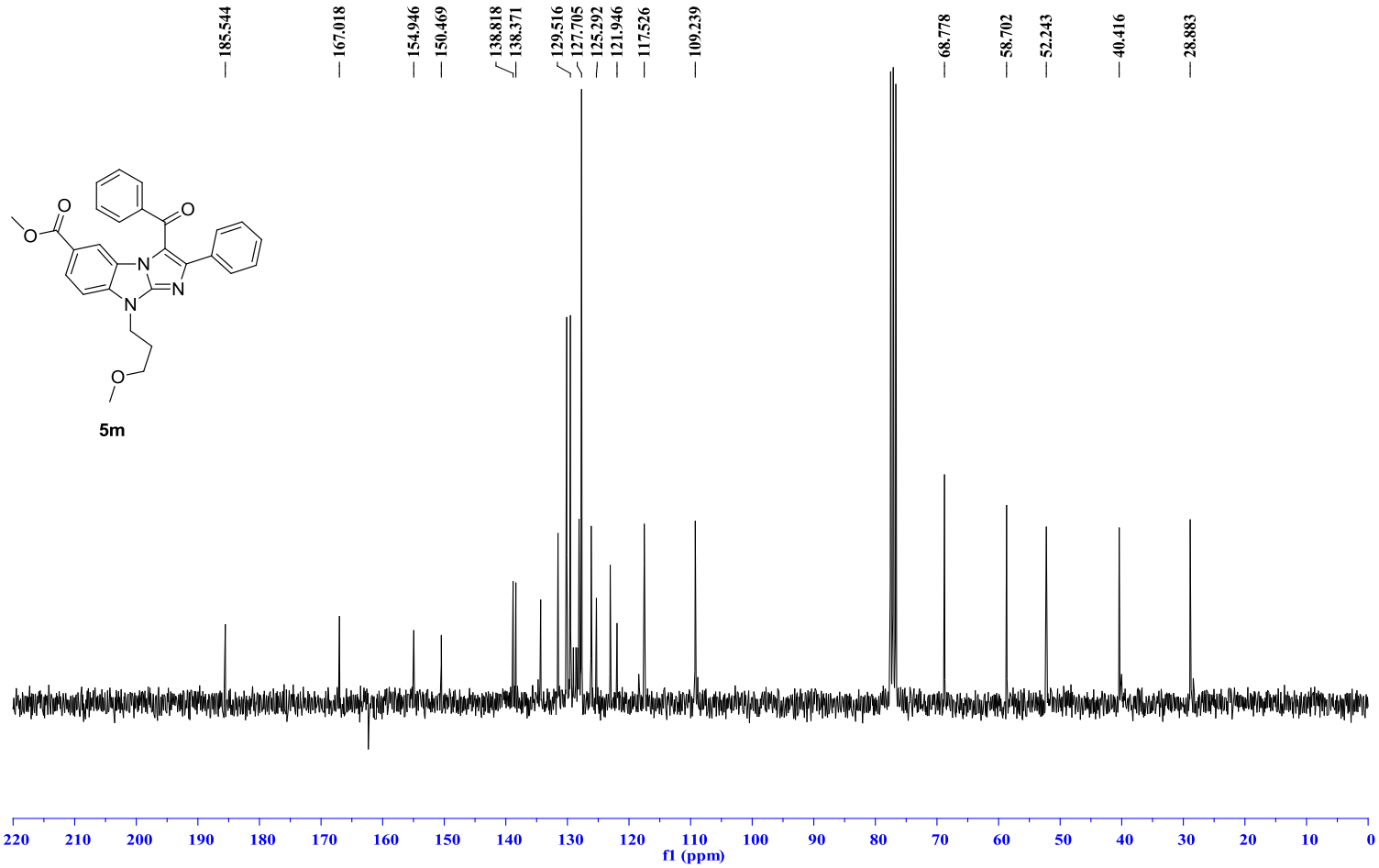
High resolution mass (ESI^+) spectrum of compound **5l**



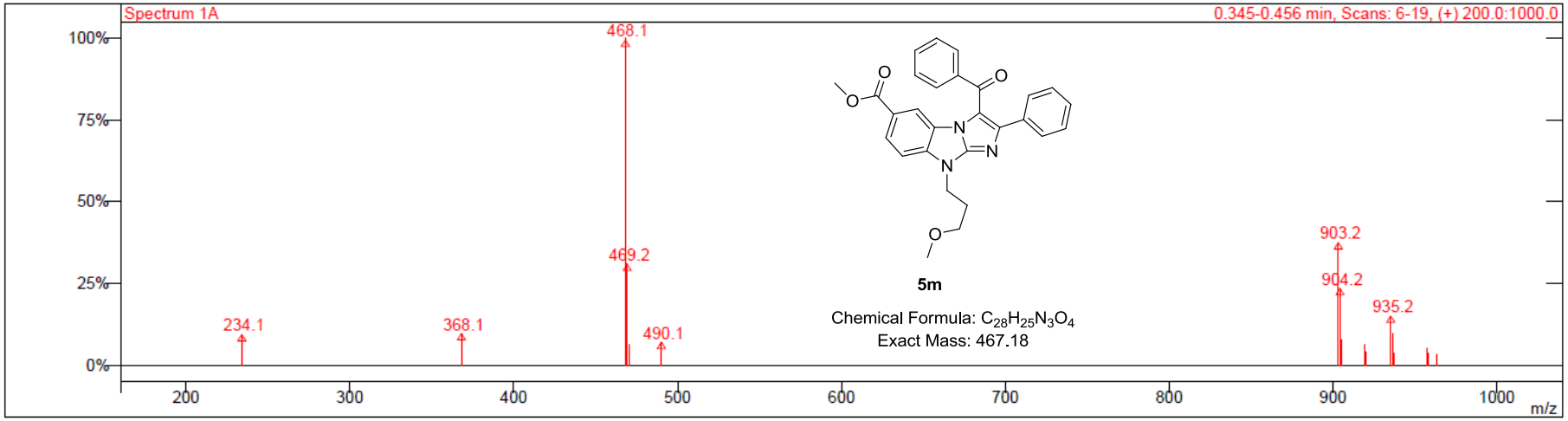
IR spectrum of compound **5l**



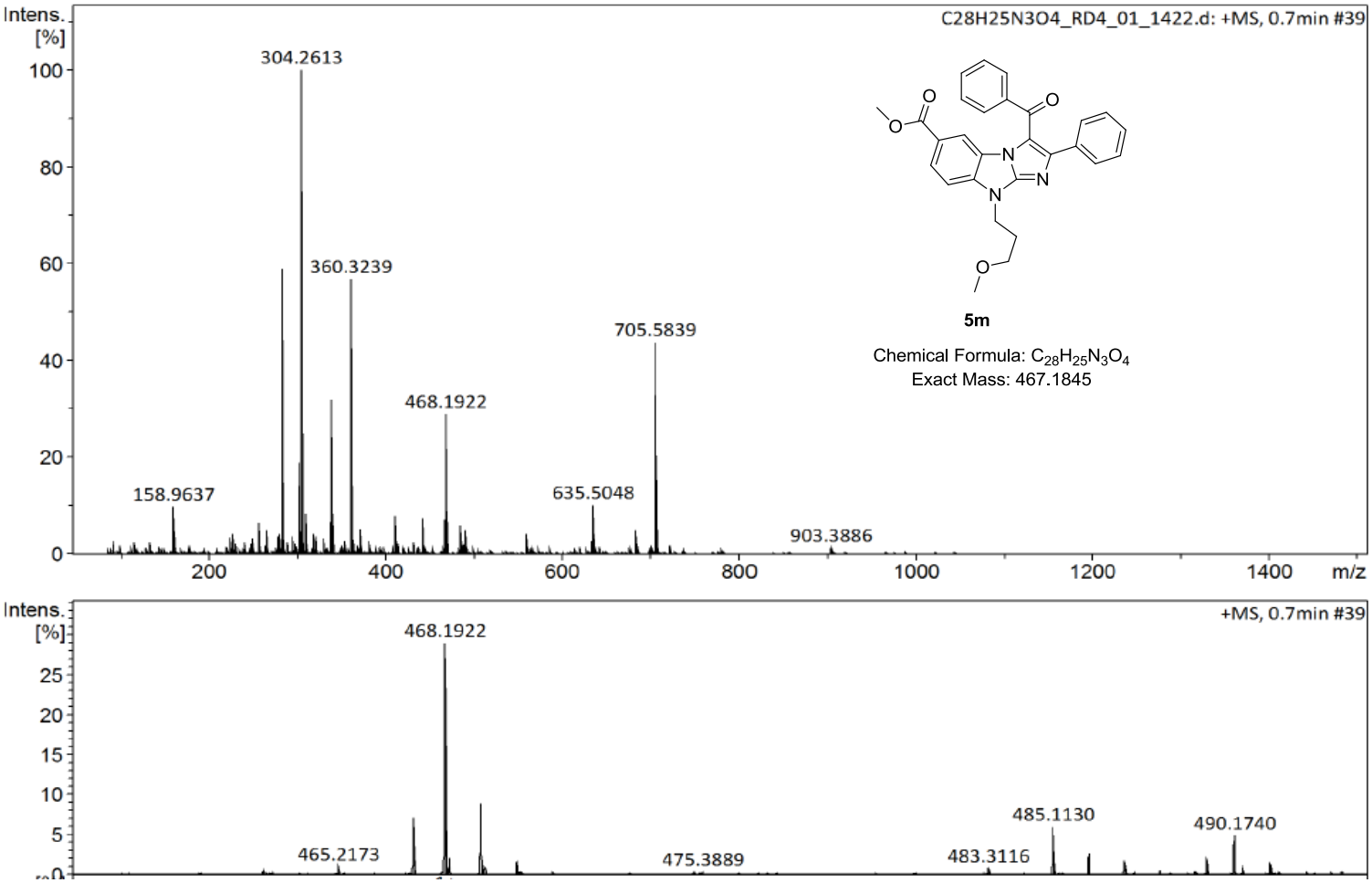
^{1}H NMR spectrum (300MHz) of compound **5m** in $CDCl_3$



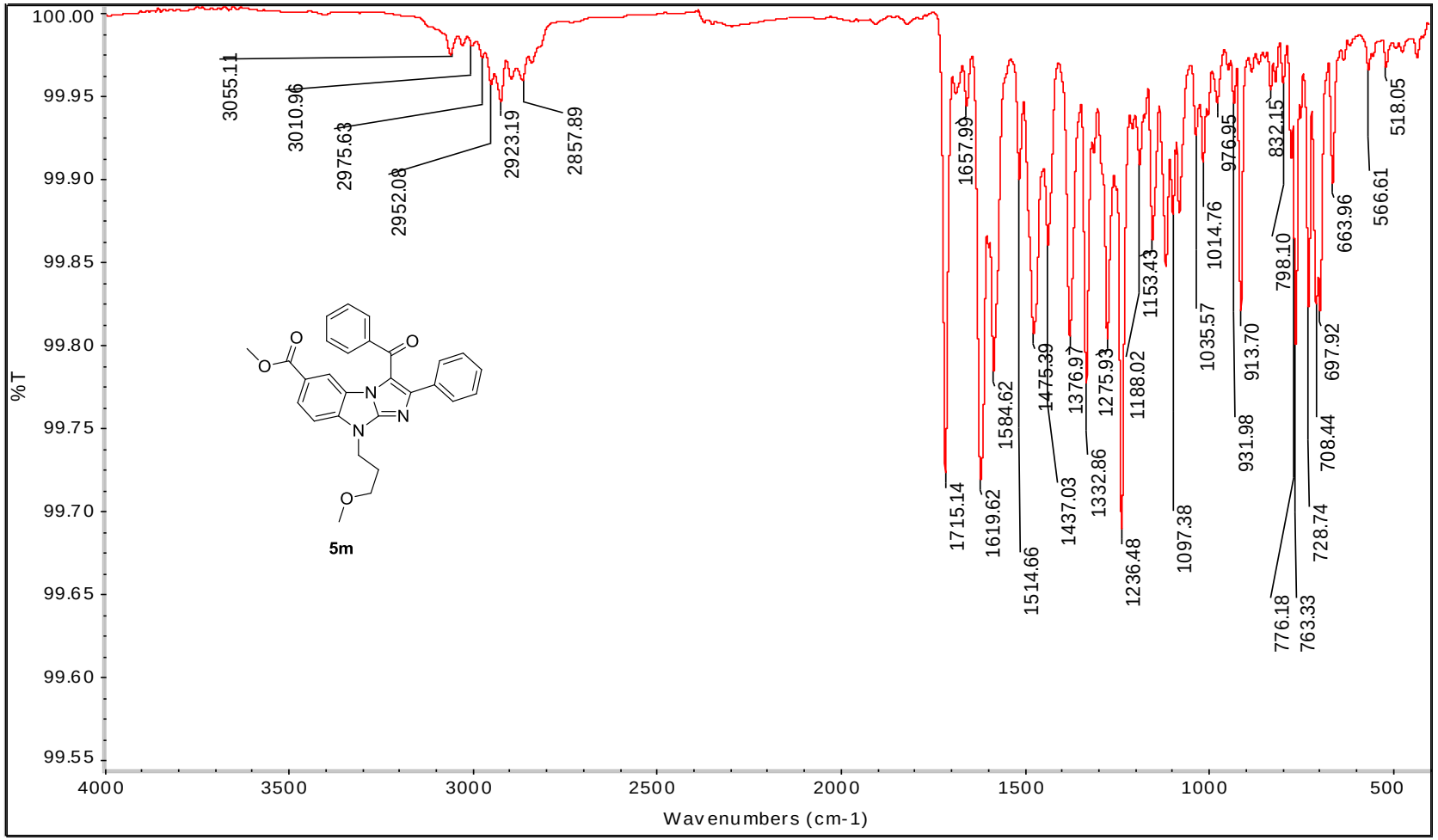
^{13}C NMR spectrum (75MHz) of compound **5m** in $CDCl_3$



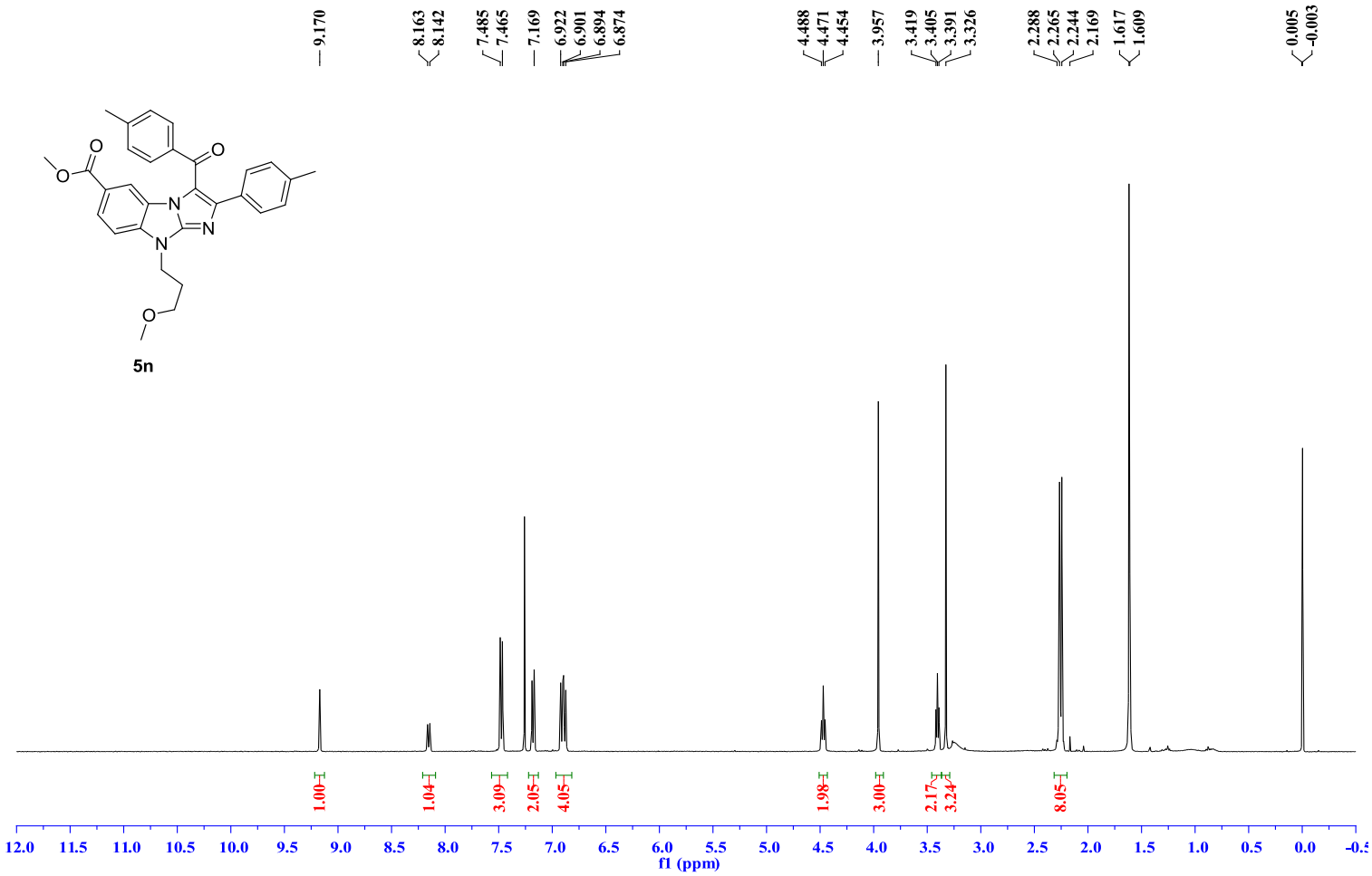
ESI$^+$ Mass spectrum of compound **5m**



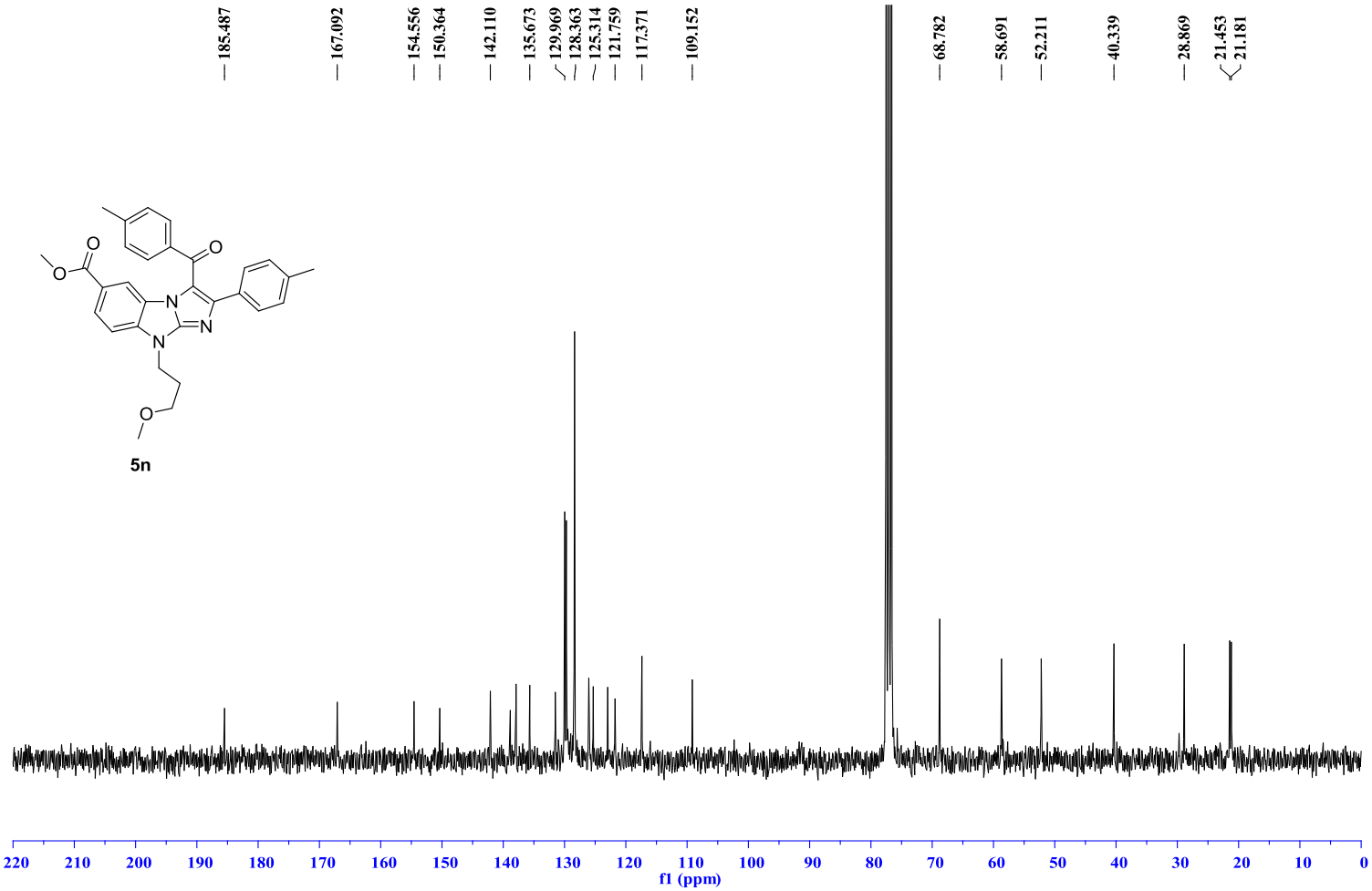
High resolution mass (ESI^+) spectrum of compound **5m**



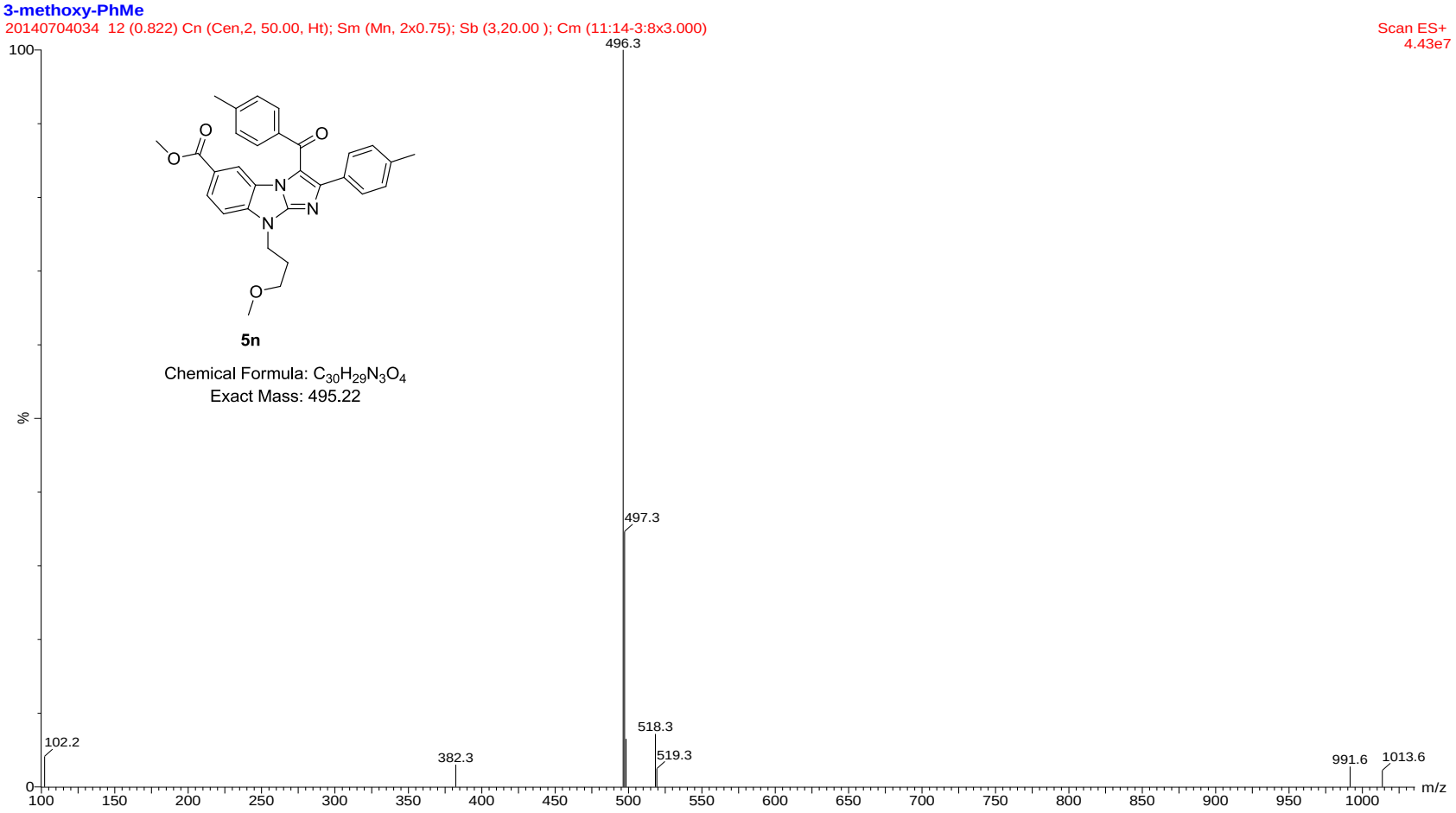
IR spectrum of compound **5m**



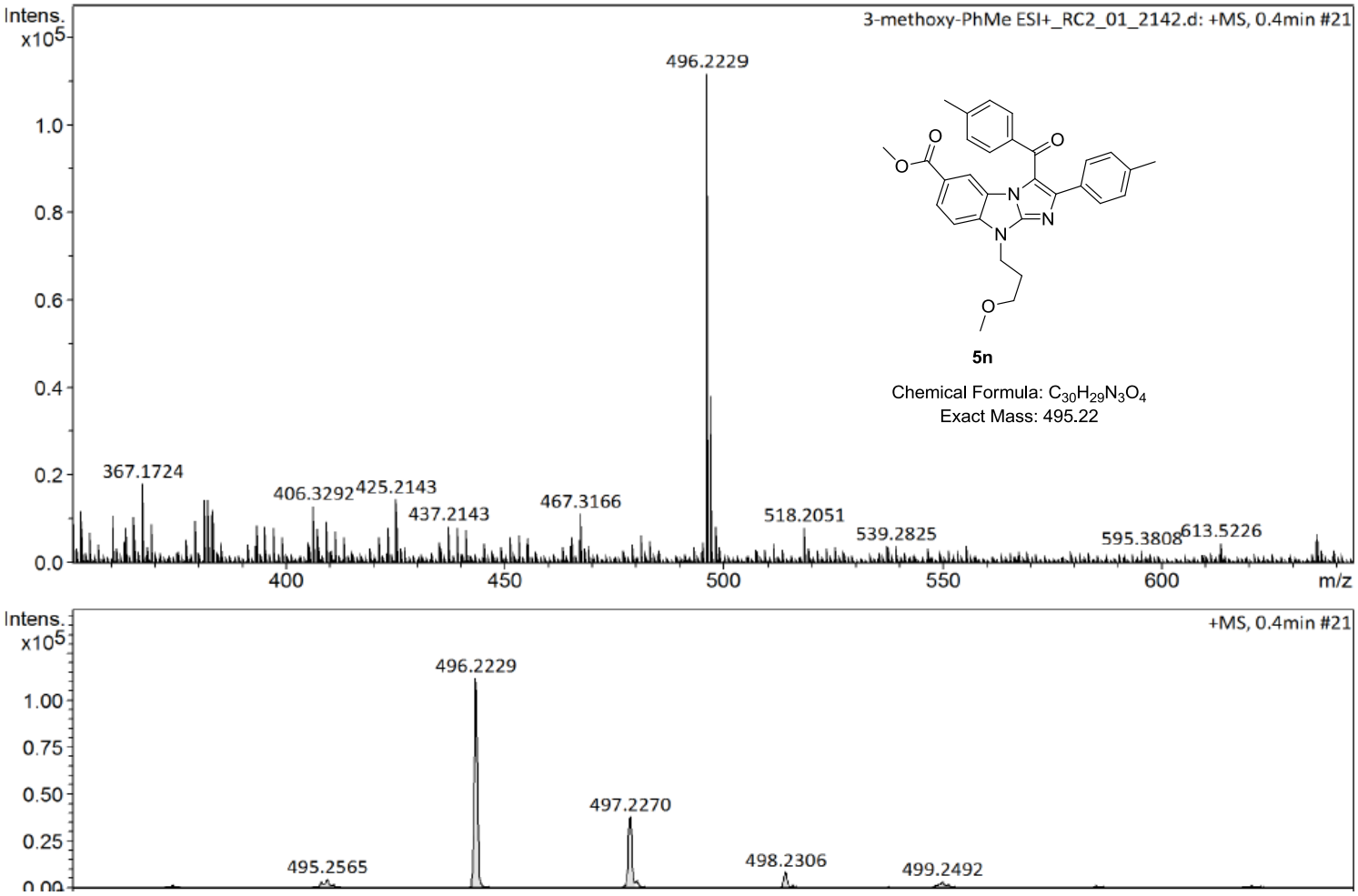
^{1}H NMR spectrum (400MHz) of compound **5n** in $CDCl_3$



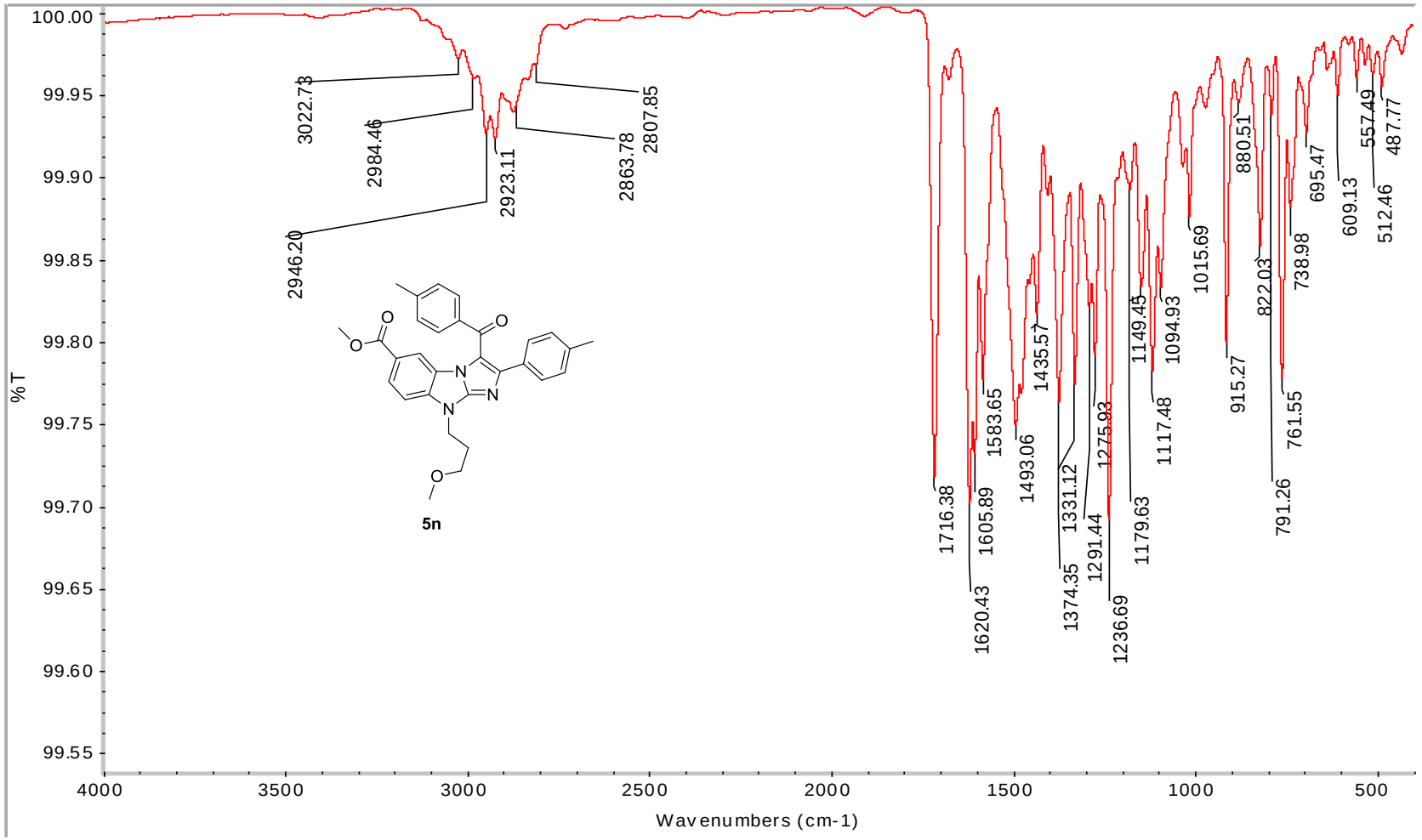
^{13}C NMR spectrum (75MHz) of compound **5n** in $CDCl_3$



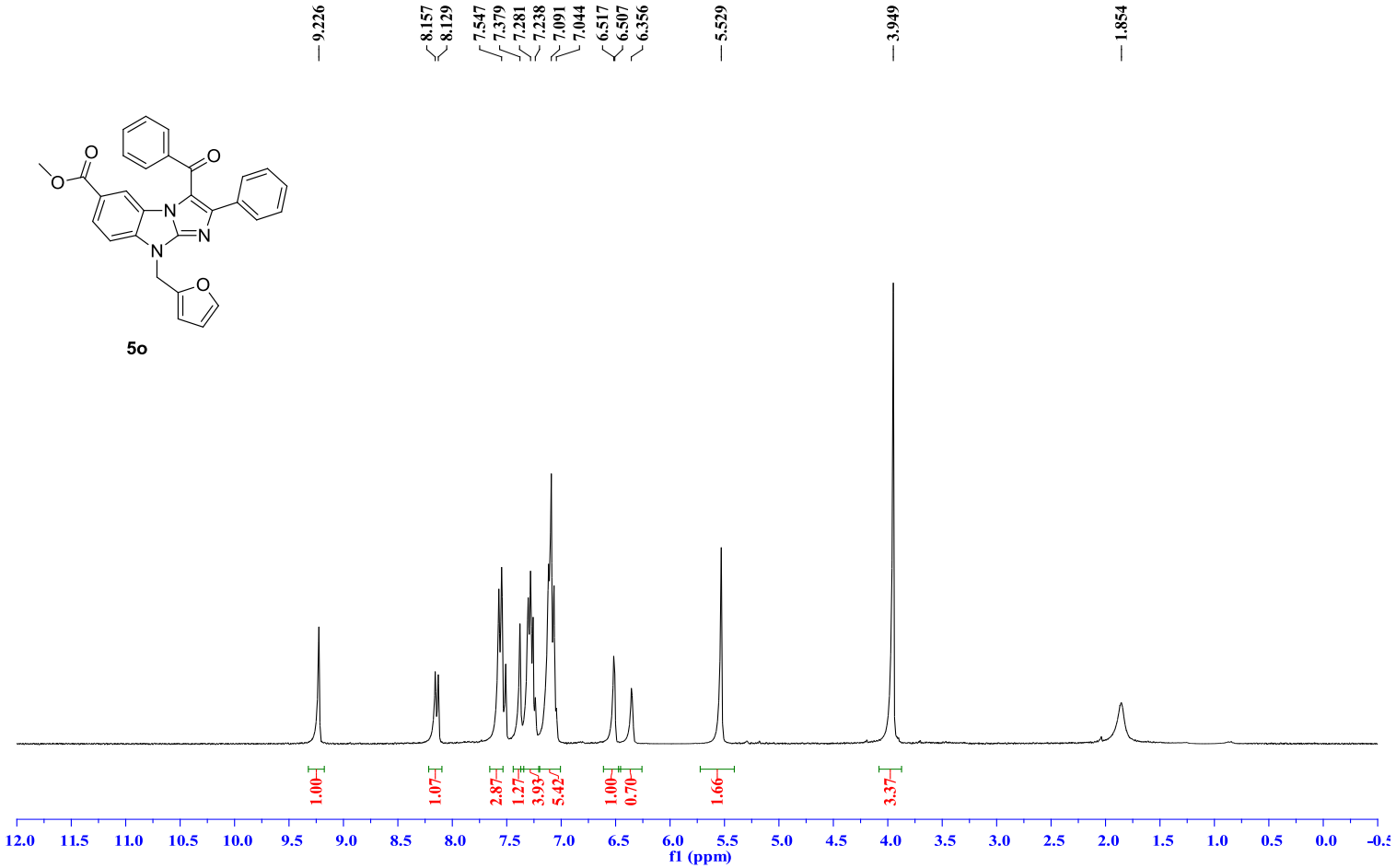
ESI$^+$ Mass spectrum of compound **5n**



High resolution mass (ESI^+) spectrum of compound **5n**

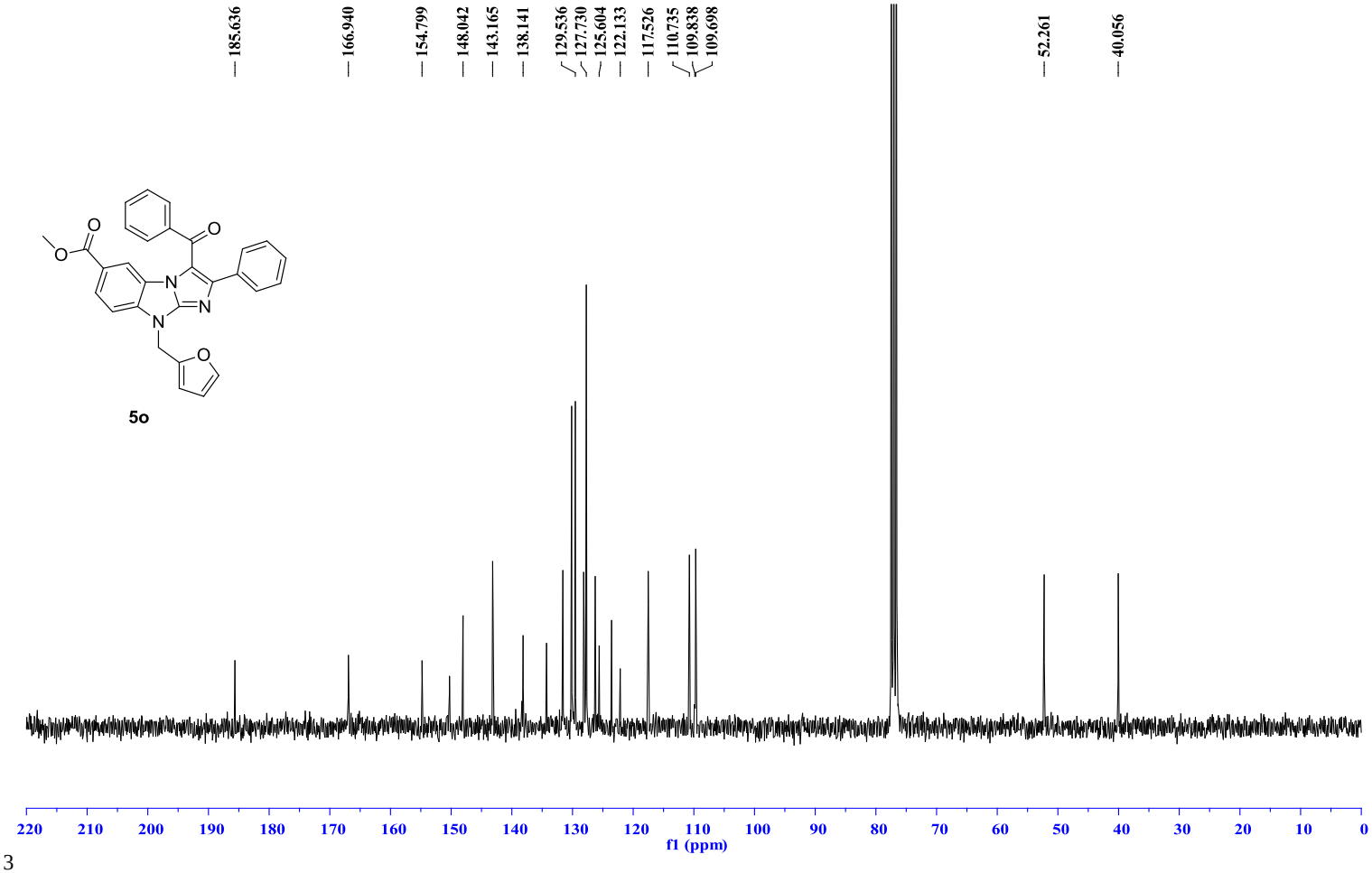


IR spectrum of compound **5n**



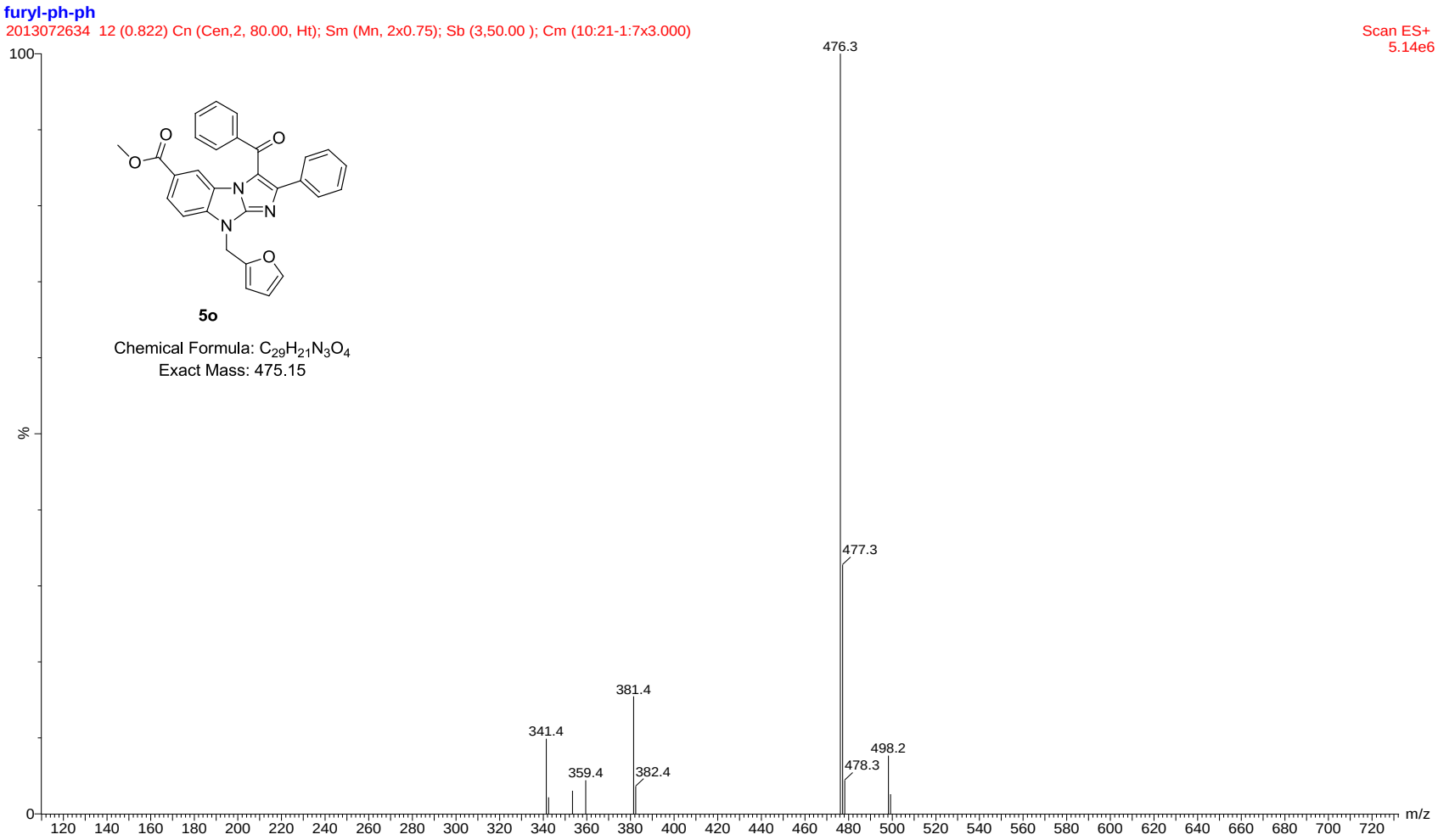
5o

^{1}H NMR spectrum (300MHz) of compound **5o** in $CDCl_3$



3

^{13}C NMR spectrum (75MHz) of compound **5o** in $CDCl_3$



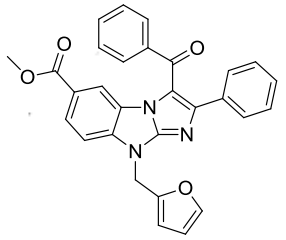
ESI$^+$ Mass spectrum of compound **5o**

111-Tony-furul-ph-ph-H#1-20 RT: 0.01-0.28 AV: 20
T: FTMS + p ESI Full ms [460.00-500.00]

Isotope	Min	Max
C-12	0	32
H-1	0	30
O-16	0	5
N-14	0	4

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00

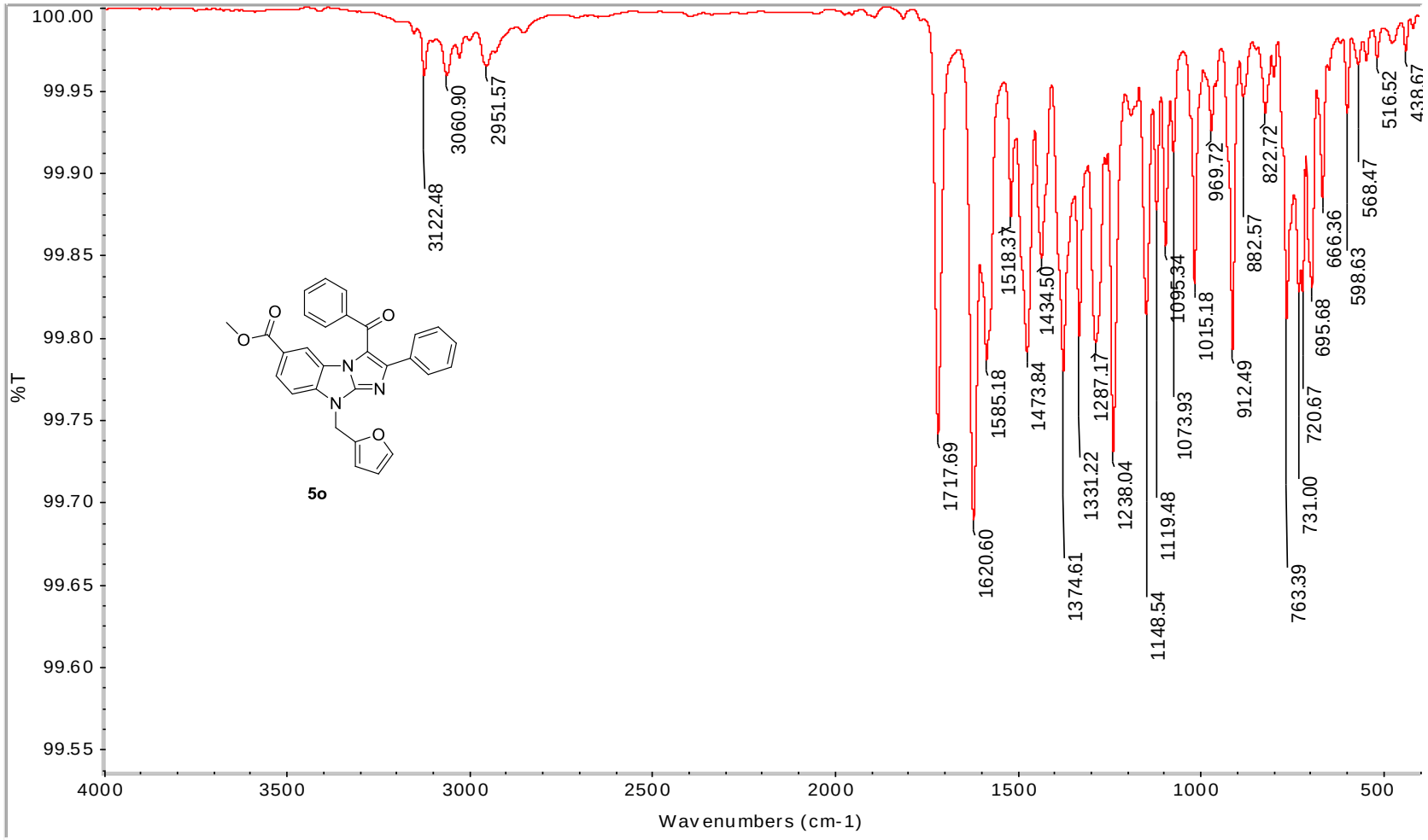
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
476.1610	549746.7	100.00	476.1605	1.08	$C_{29}H_{22}O_4N_3$



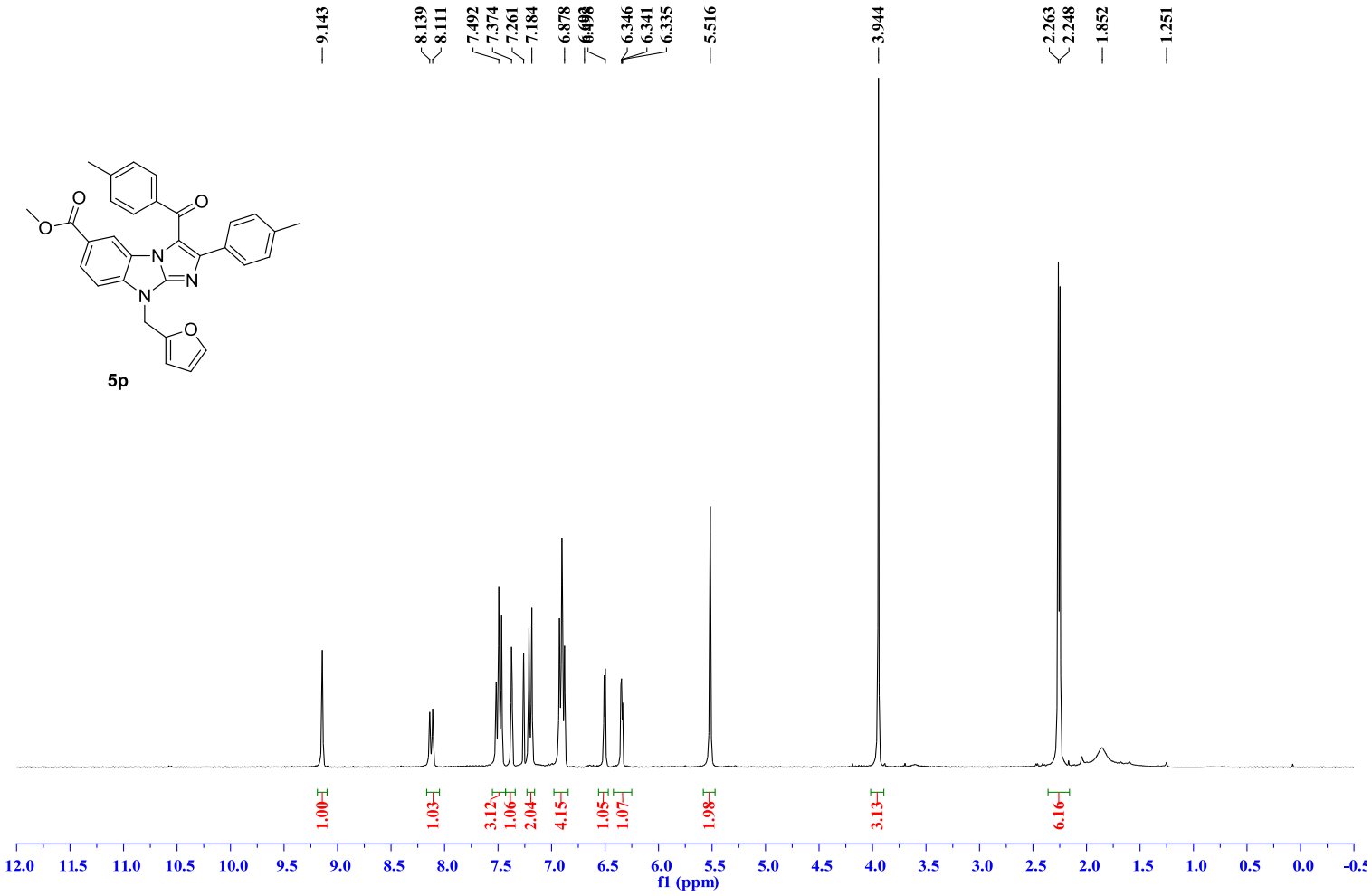
5o

Chemical Formula: $C_{29}H_{21}N_3O_4$
Exact Mass: 475.15

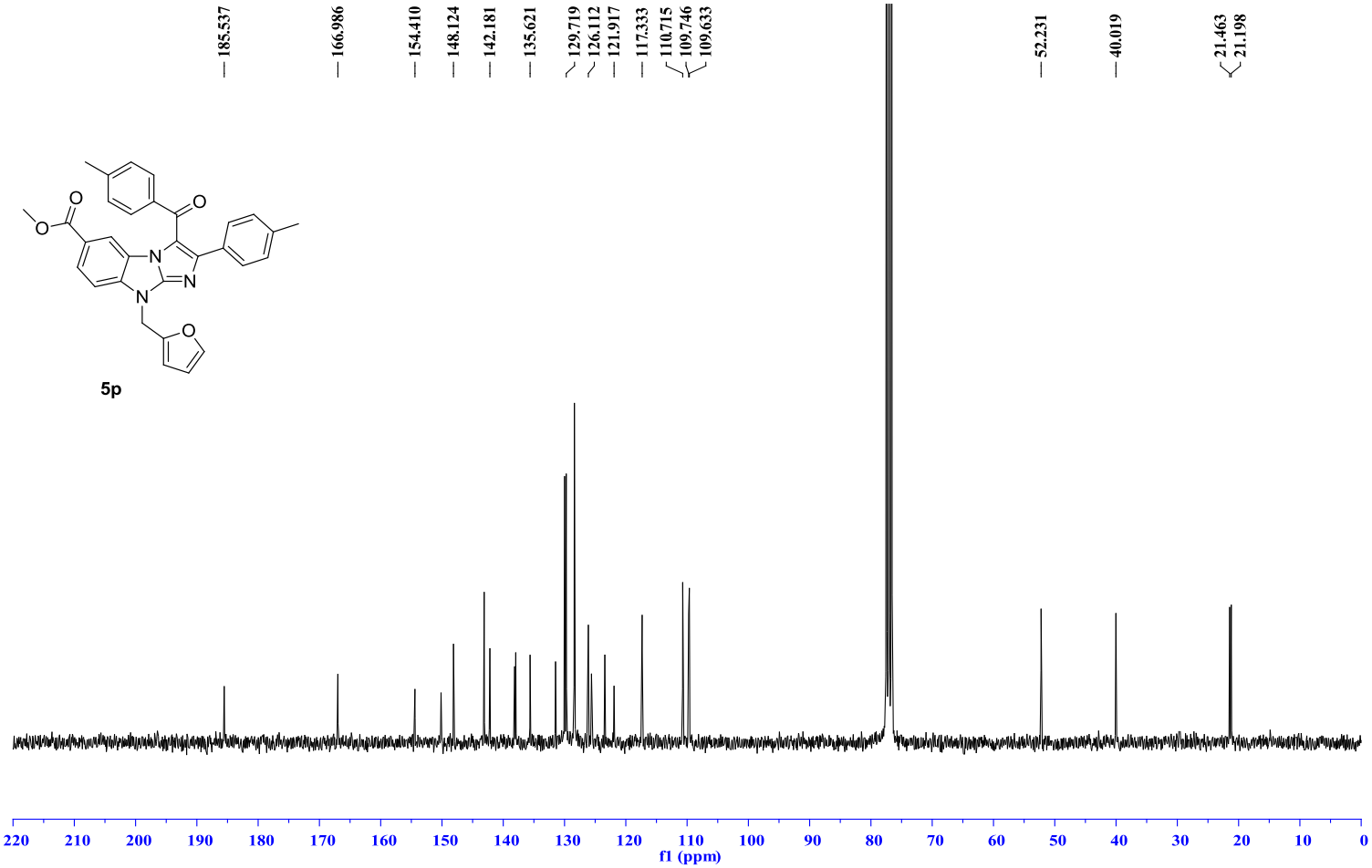
High resolution mass (ESI^+) spectrum of compound **5o**



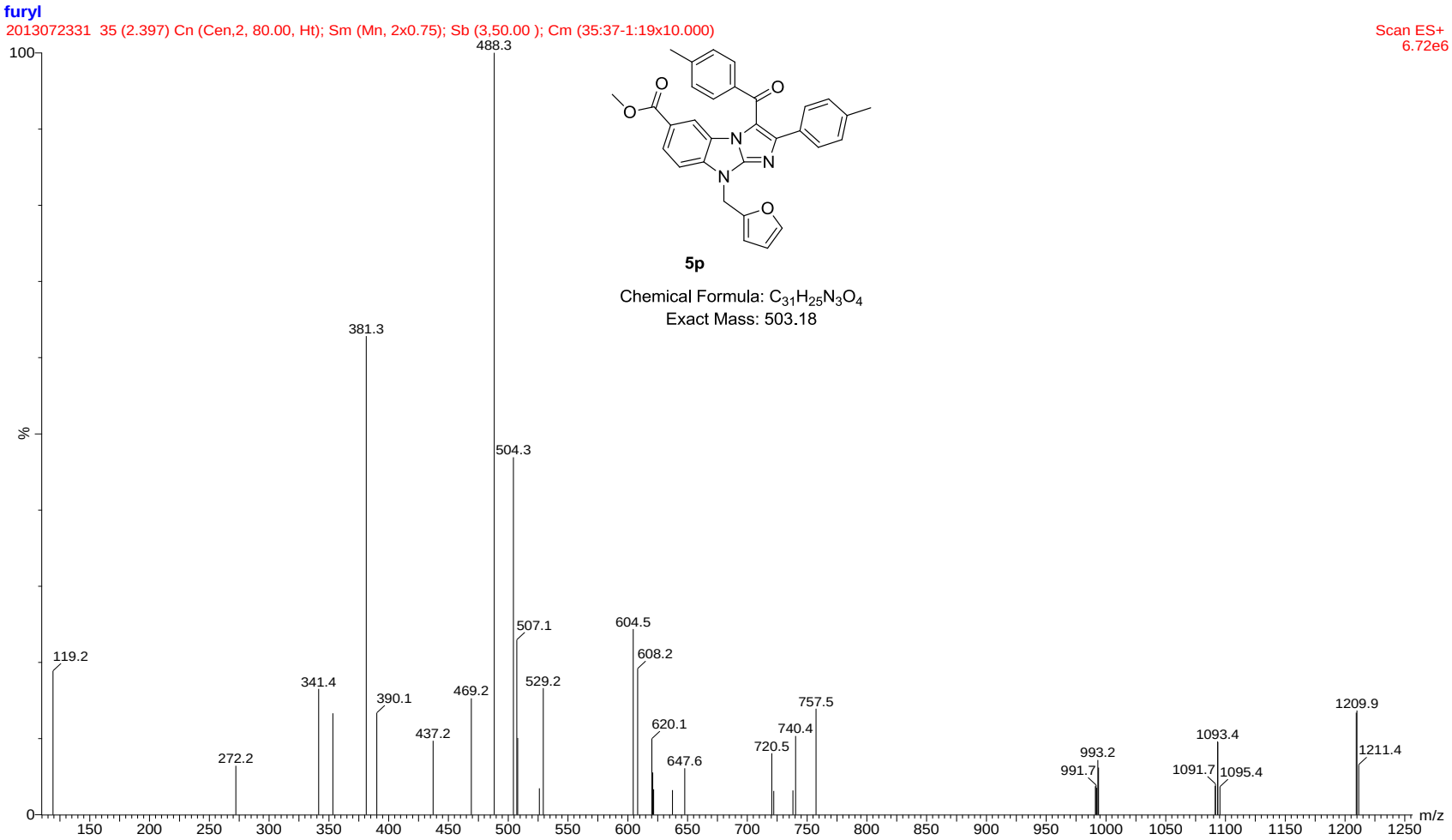
IR spectrum of compound **5o**



^{1}H NMR spectrum (300MHz) of compound **5p** in $CDCl_3$



^{13}C NMR spectrum (75MHz) of compound **5p** in $CDCl_3$



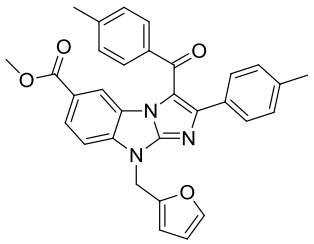
ESI$^+$ Mass spectrum of compound **5p**

109-Tony-furul-phem-phem-H#1-20 RT: 0.01-0.28 AV: 20
T: FTMS + p ESI Full ms [500.00-510.00]

Isotope	Min	Max
C-12	0	32
H-1	0	30
O-16	0	5
N-14	0	4

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00

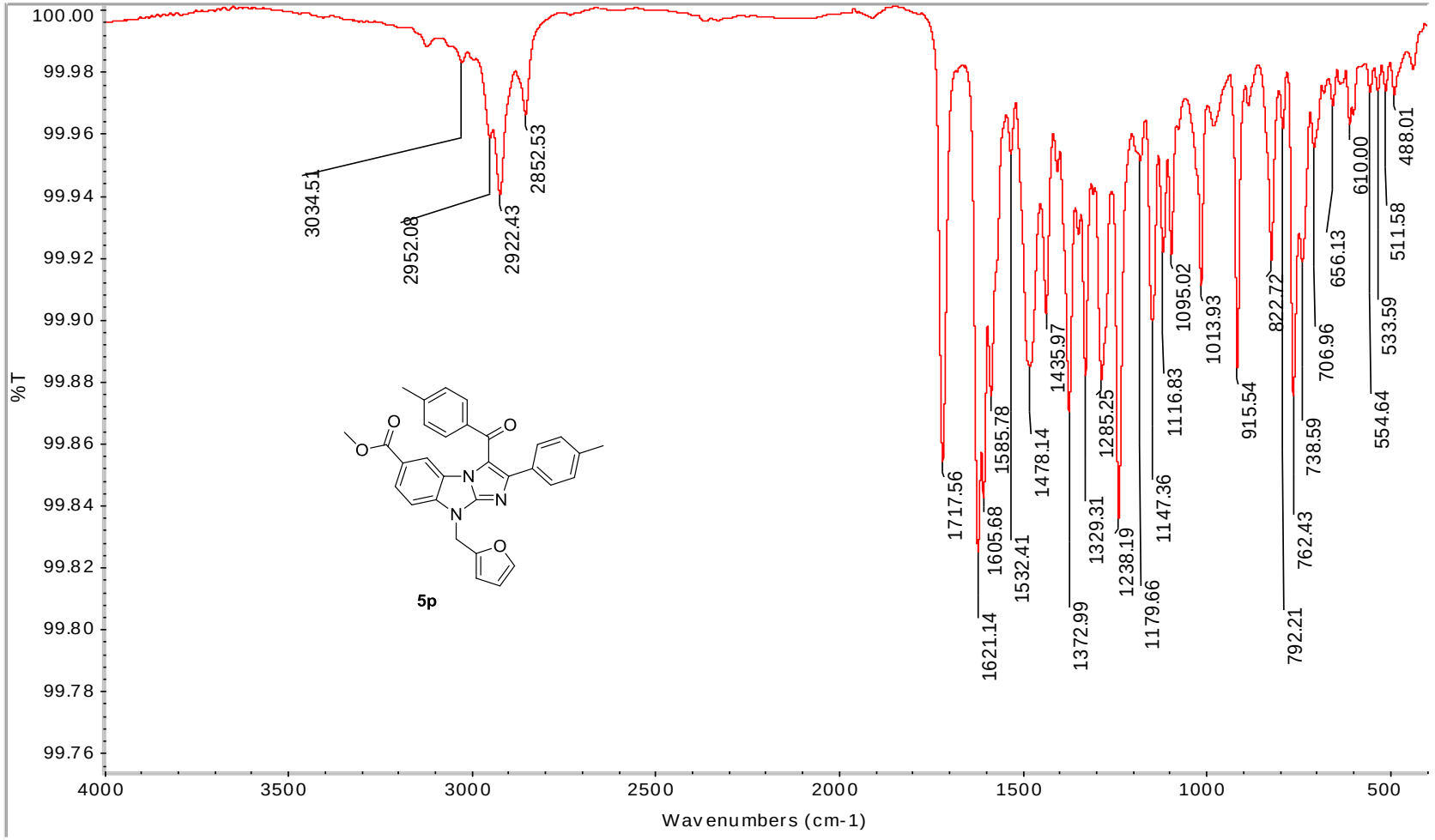
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
504.1922	215573.9	100.00	504.1918	0.75	$C_{31}H_{26}O_4N_3$



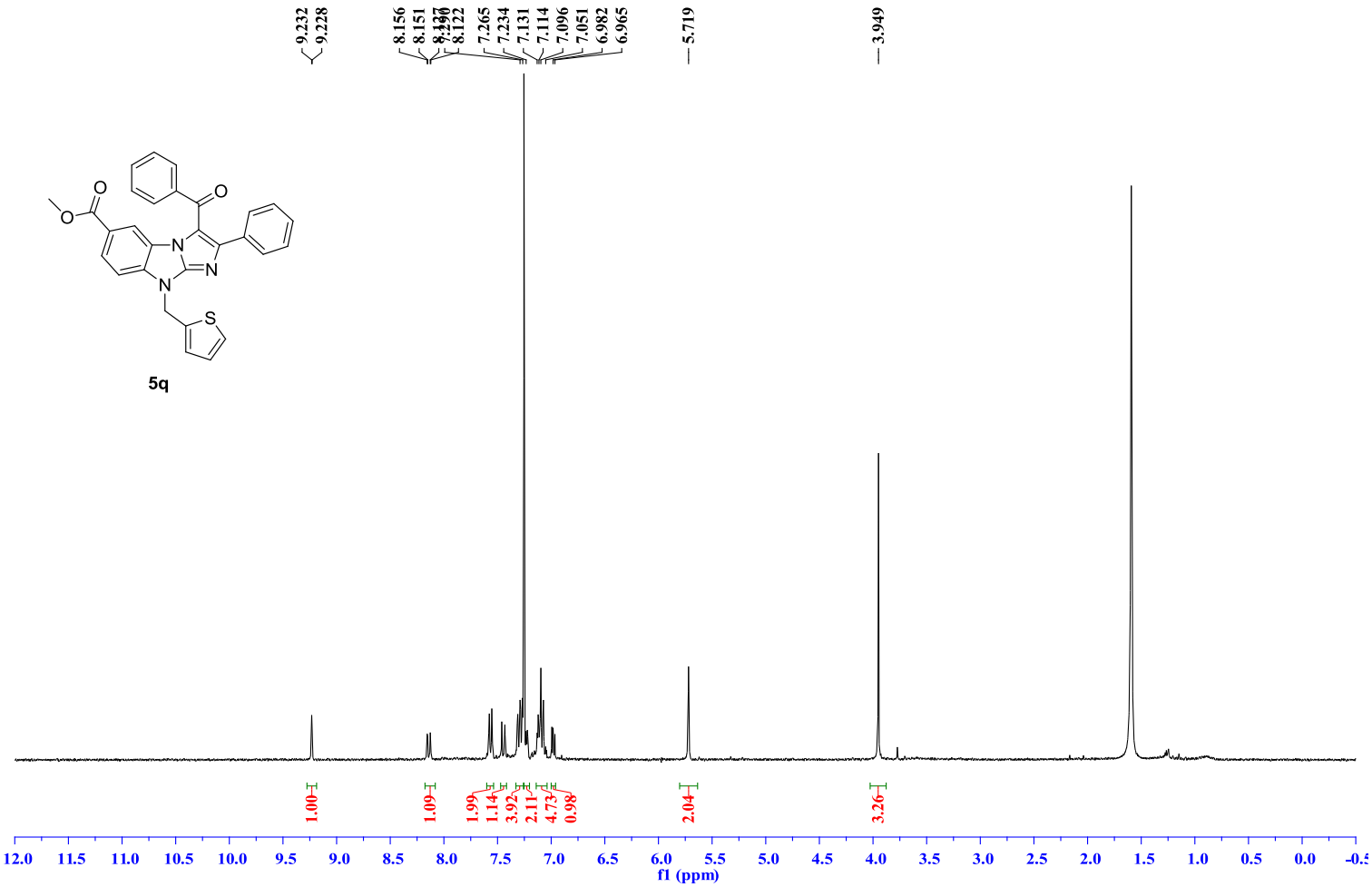
5p

Chemical Formula: $C_{31}H_{25}N_3O_4$
Exact Mass: 503.18

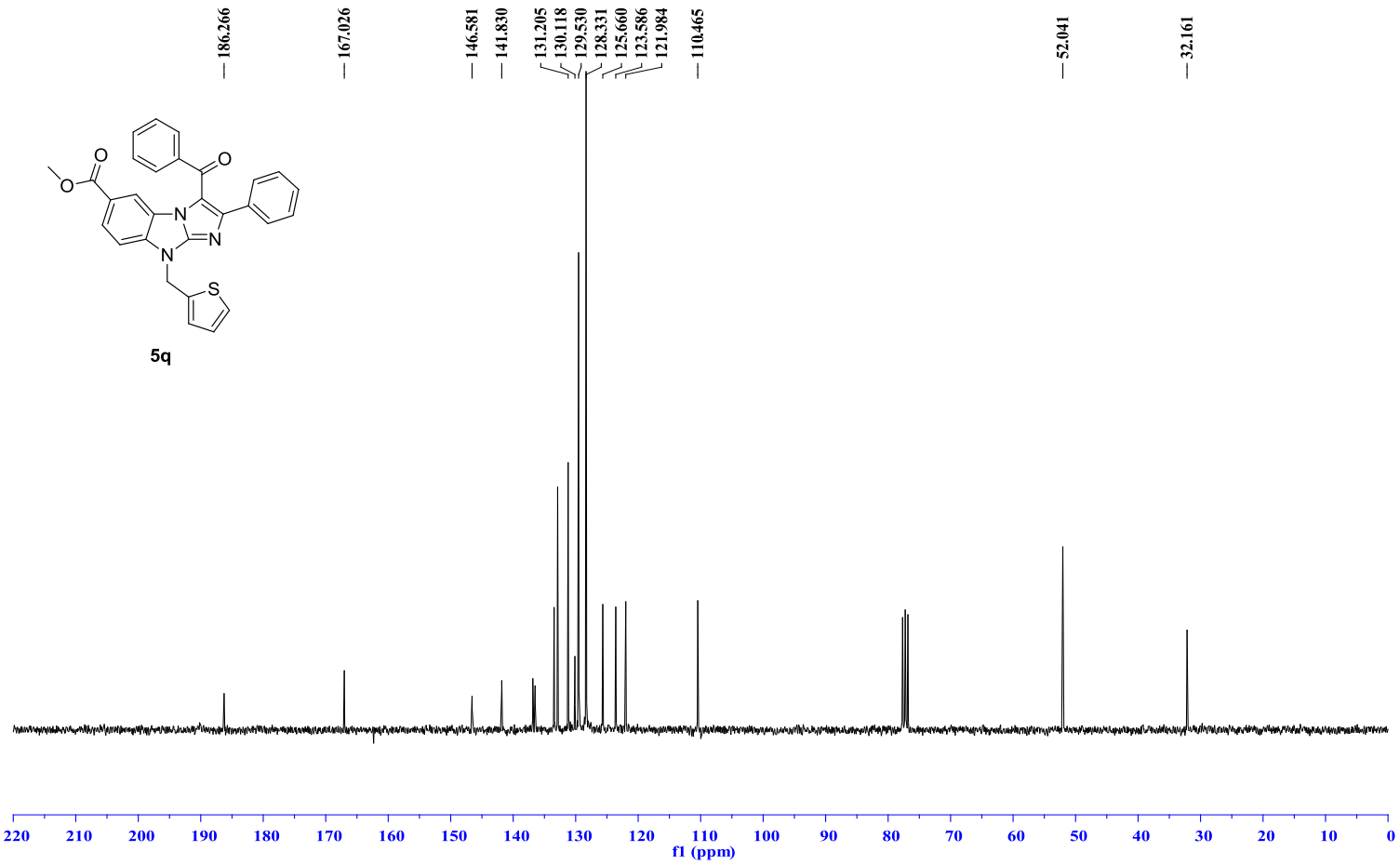
High resolution mass (ESI^+) spectrum of compound **5p**



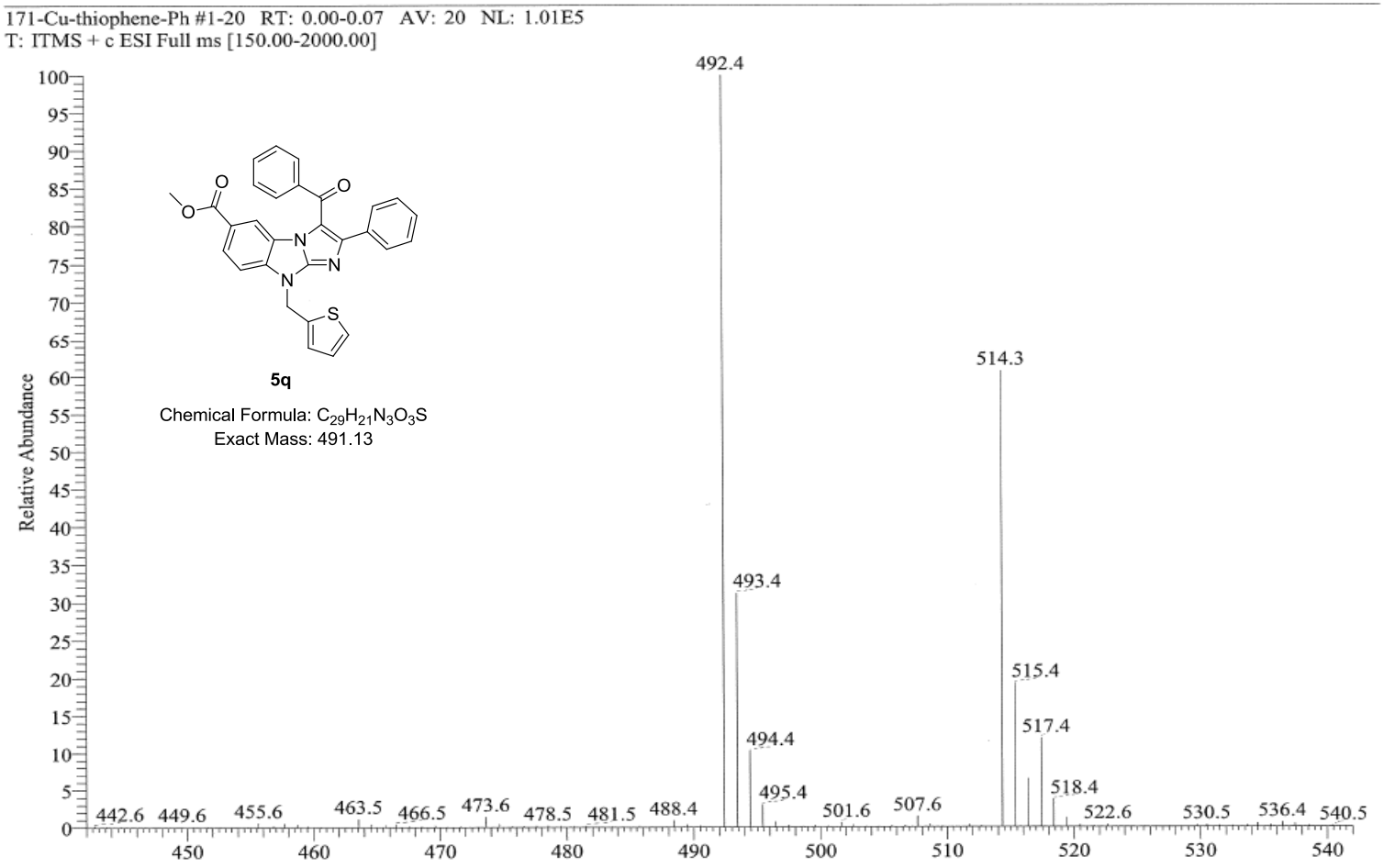
IR spectrum of compound **5p**



^{1}H NMR spectrum (300MHz) of compound **5q** in $CDCl_3$



^{13}C NMR spectrum (75MHz) of compound **5q** in $CDCl_3$



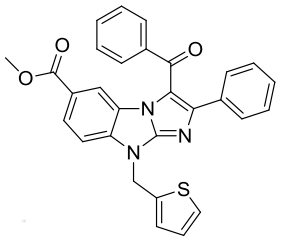
ESI$^+$ Mass spectrum of compound **5q**

173-Cu-thiophene-Ph-H#1-20 RT: 0.00-0.28 AV: 20
T: FTMS + p ESI Full ms [150.00-2000.00]
m/z= 465.1785-497.7831

Isotope	Min	Max
C-12	0	30
H-1	0	30
O-16	0	4
N-14	0	4
S-32	0	1

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

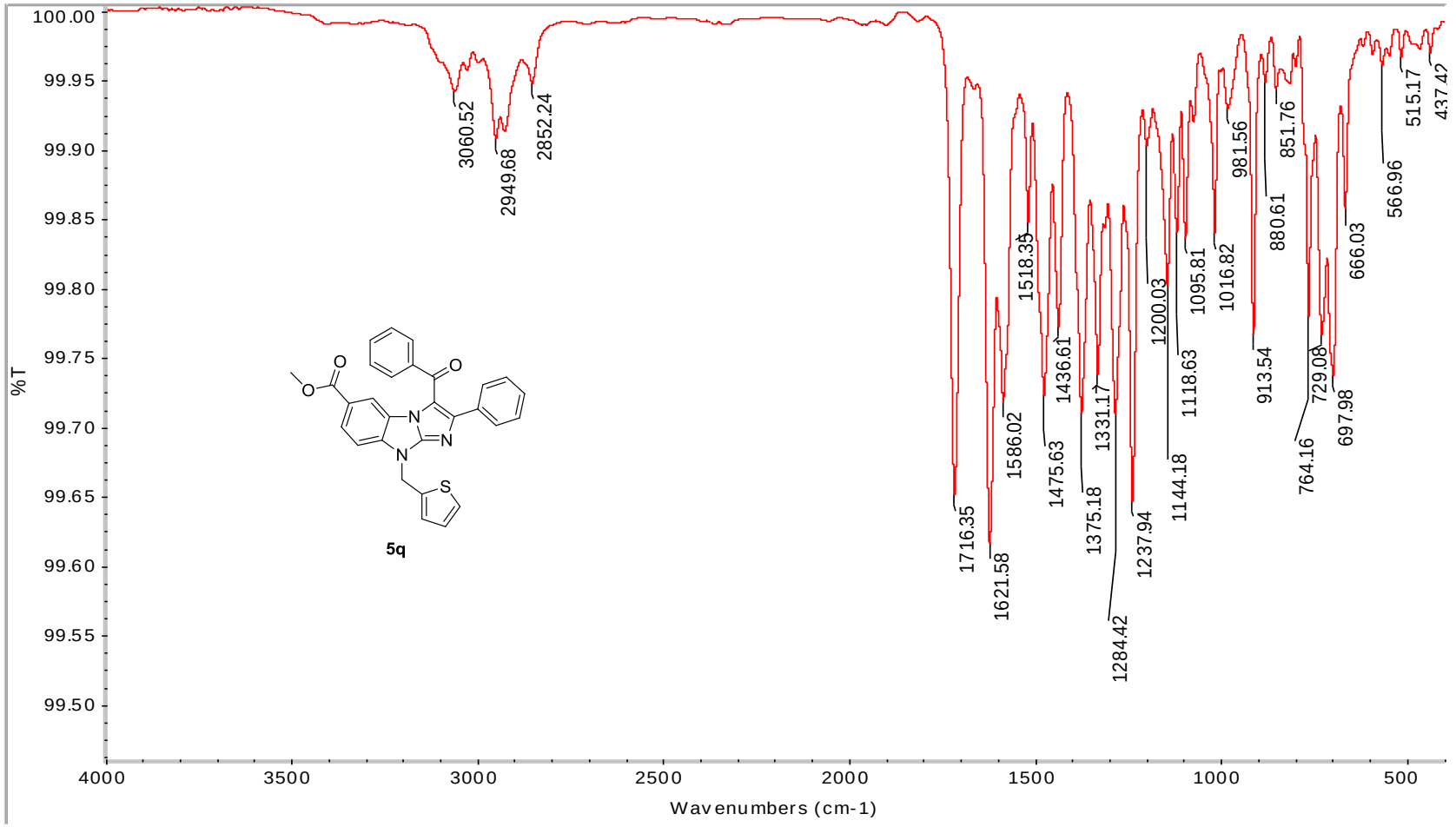
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
492.1369	2048909.3	100.00	492.1376	-1.47	$C_{29}H_{22}O_3N_3S$



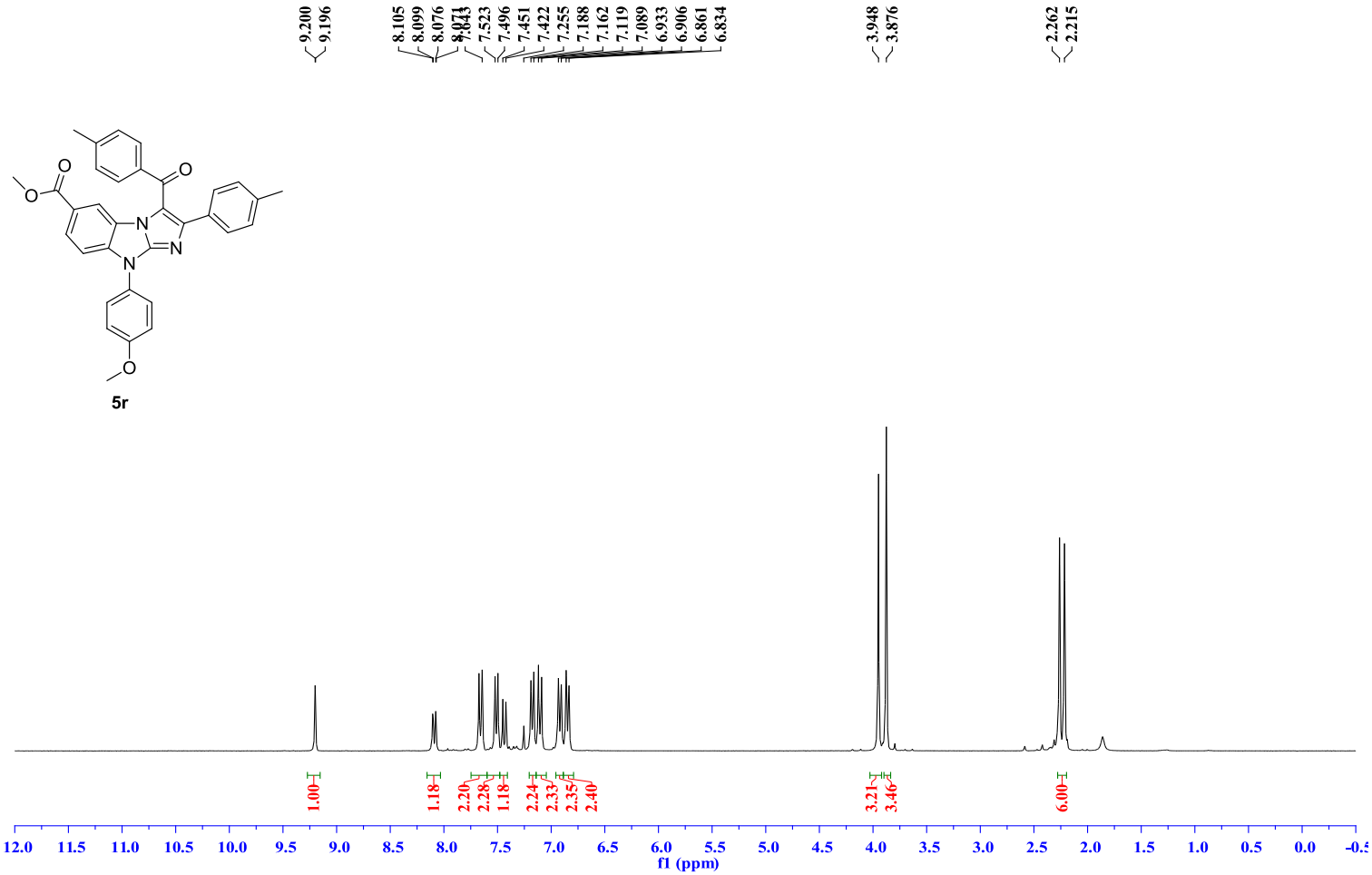
5q

Chemical Formula: $C_{29}H_{21}N_3O_3S$
Exact Mass: 491.13

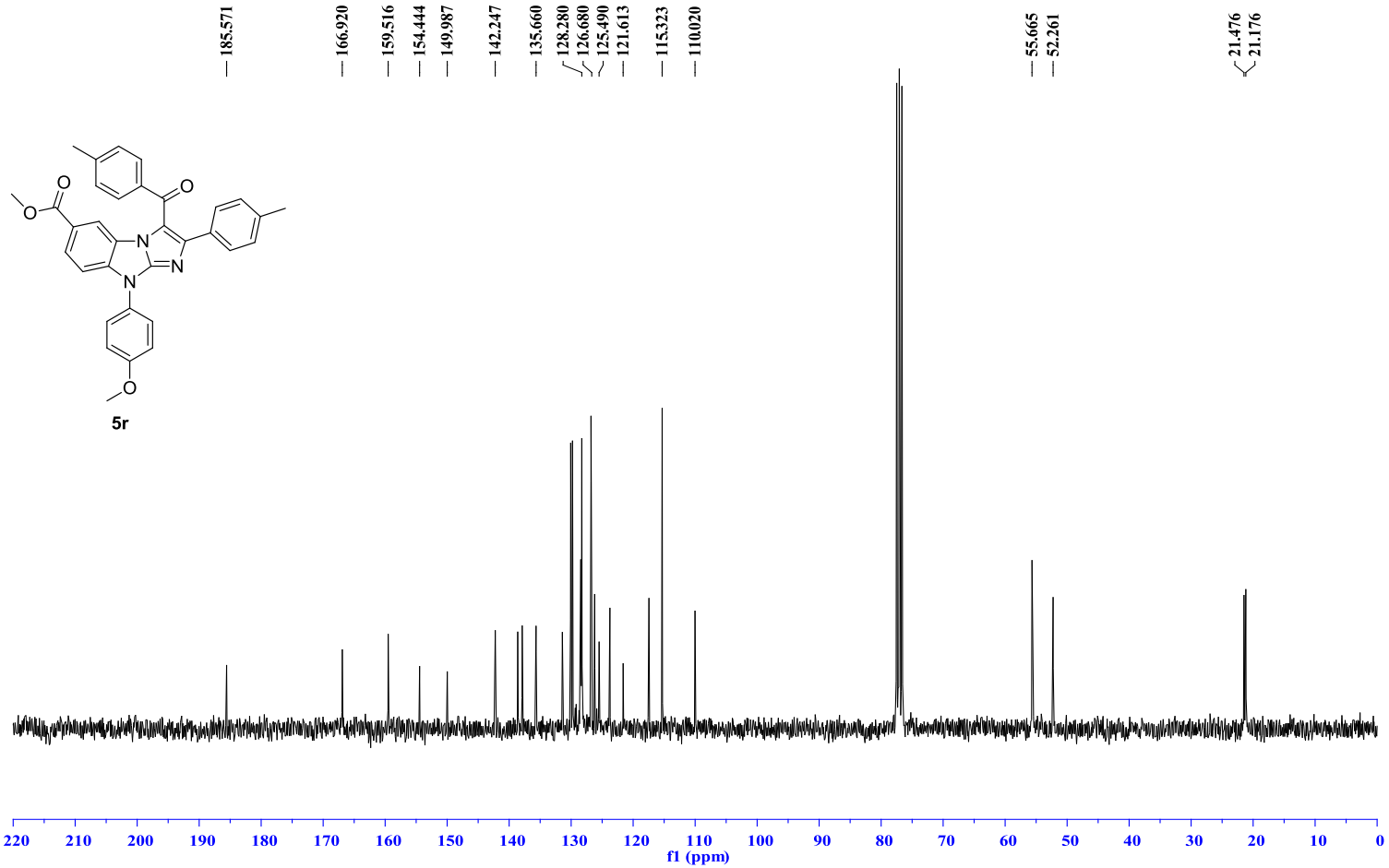
High resolution mass (ESI^+) spectrum of compound **5q**



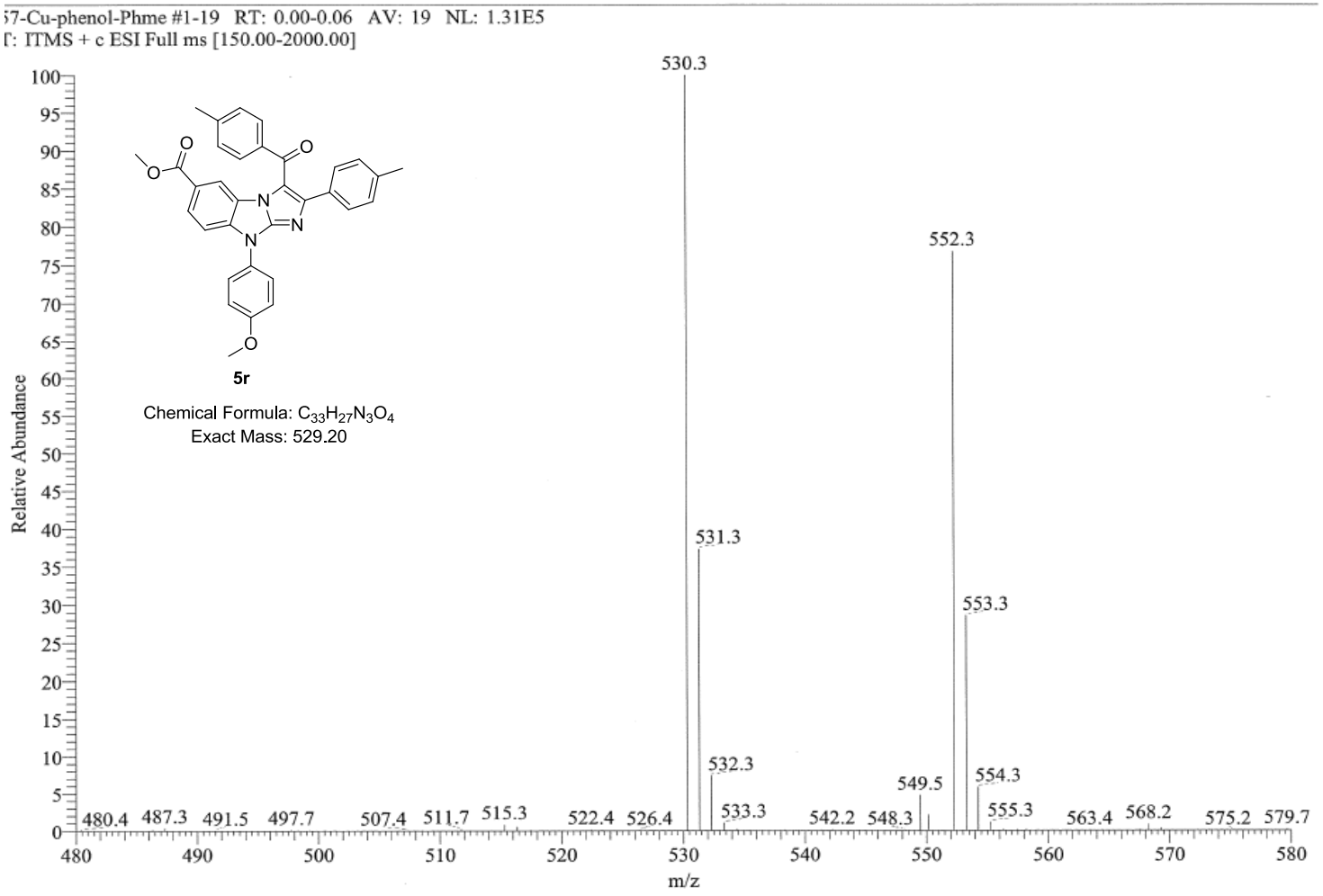
IR spectrum of compound **5q**



^{1}H NMR spectrum (300MHz) of compound **5r** in $CDCl_3$



^{13}C NMR spectrum (75MHz) of compound **5r** in $CDCl_3$



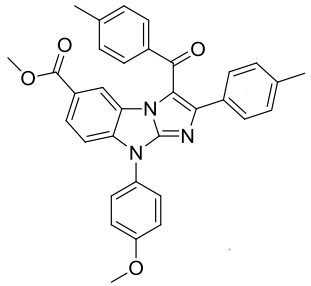
ESI$^+$ Mass spectrum of compound **5r**

54-Cu-phenol-Phme-H#1-20 RT: 0.01-0.44 AV: 20
T: FTMS + p ESI Full ms [150.00-2000.00]
m/z= 527.4008-533.7494

Isotope	Min	Max
C-12	0	33
H-1	0	80
O-16	0	9
N-14	0	4

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

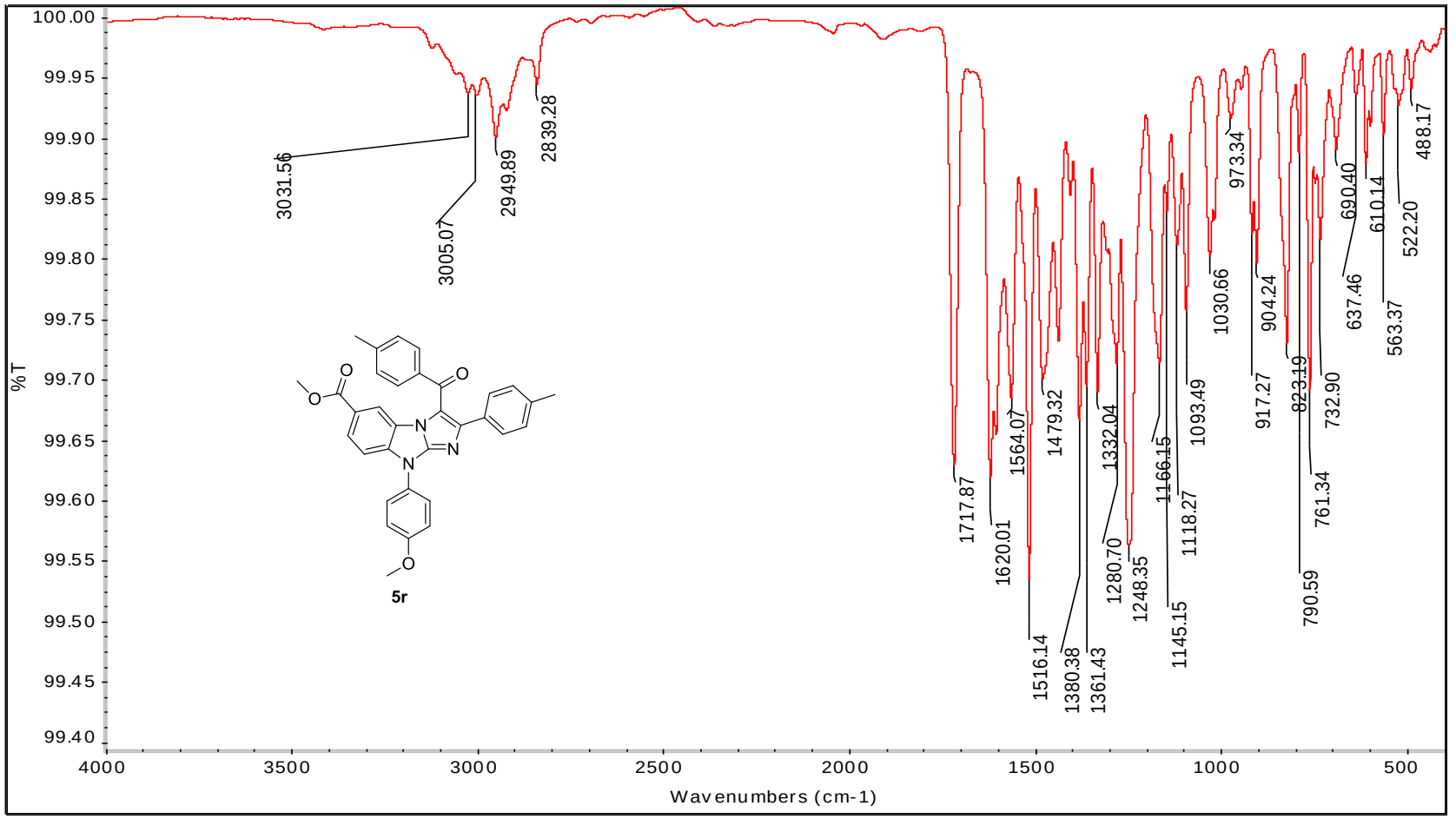
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
530.2092	812383.4	100.00	530.2074	3.33	$C_{33}H_{28}O_4N_3$



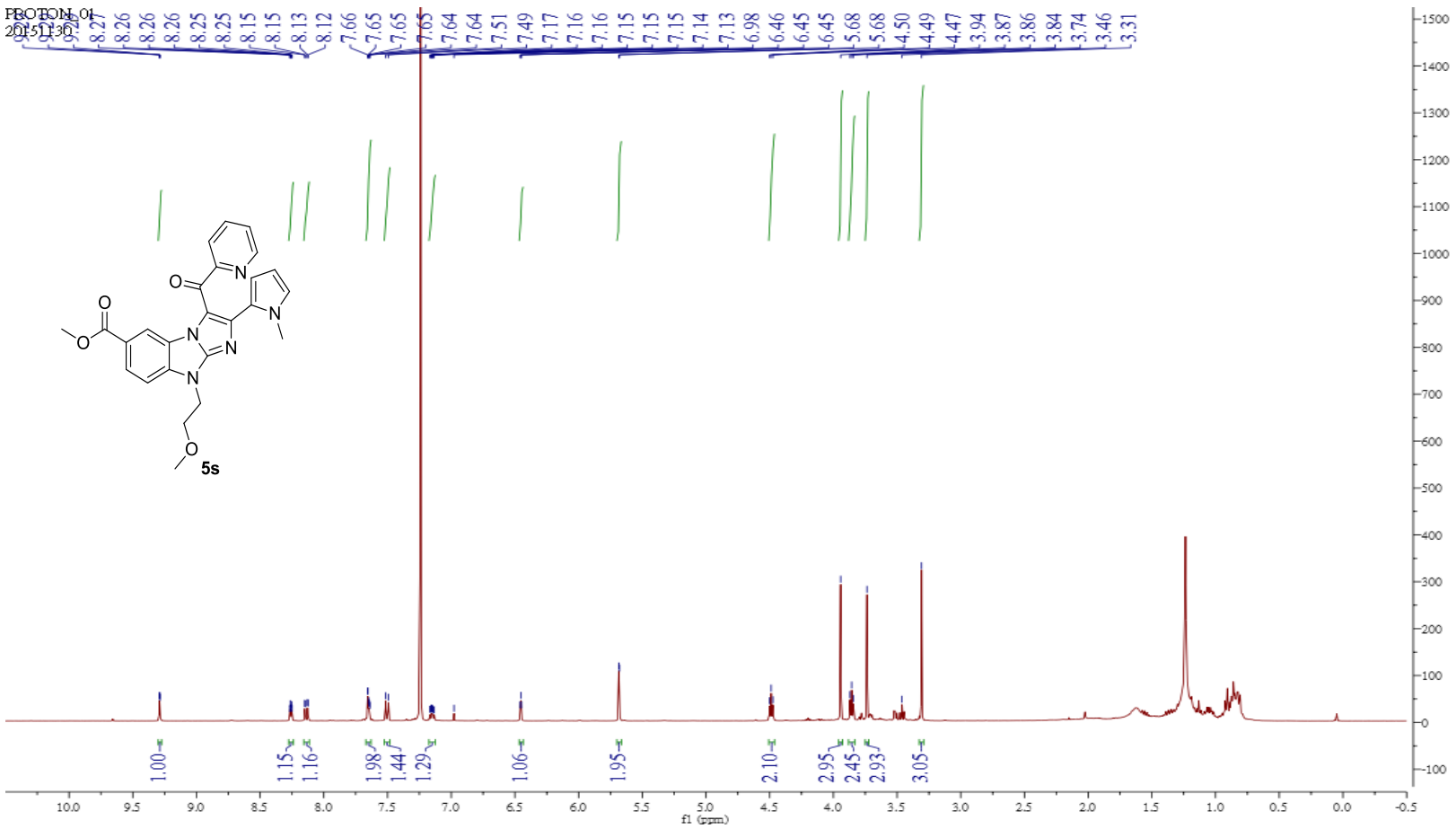
5r

Chemical Formula: $C_{33}H_{27}N_3O_4$
Exact Mass: 529.20

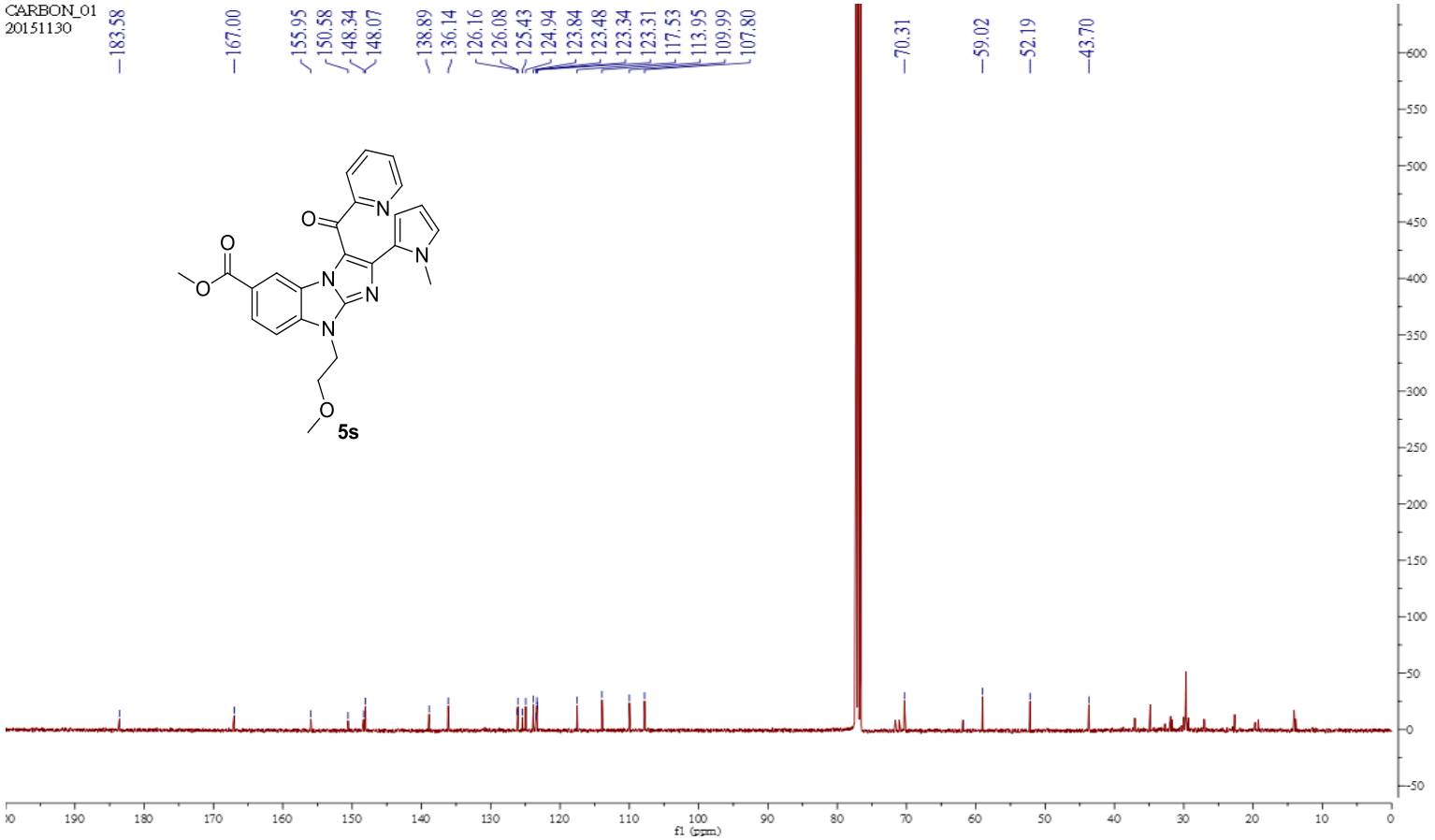
High resolution mass (ESI^+) spectrum of compound **5r**



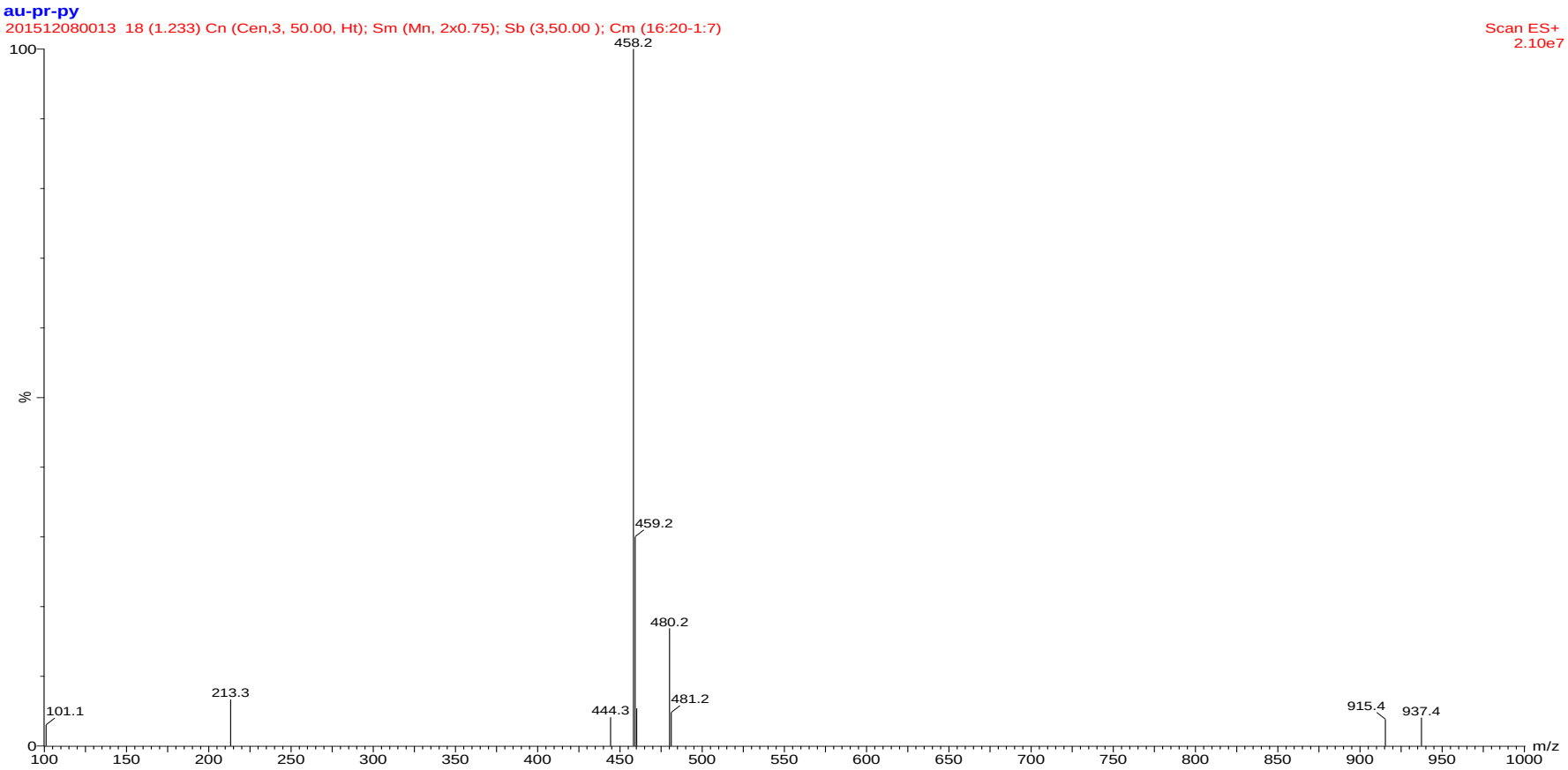
IR spectrum of compound **5r**



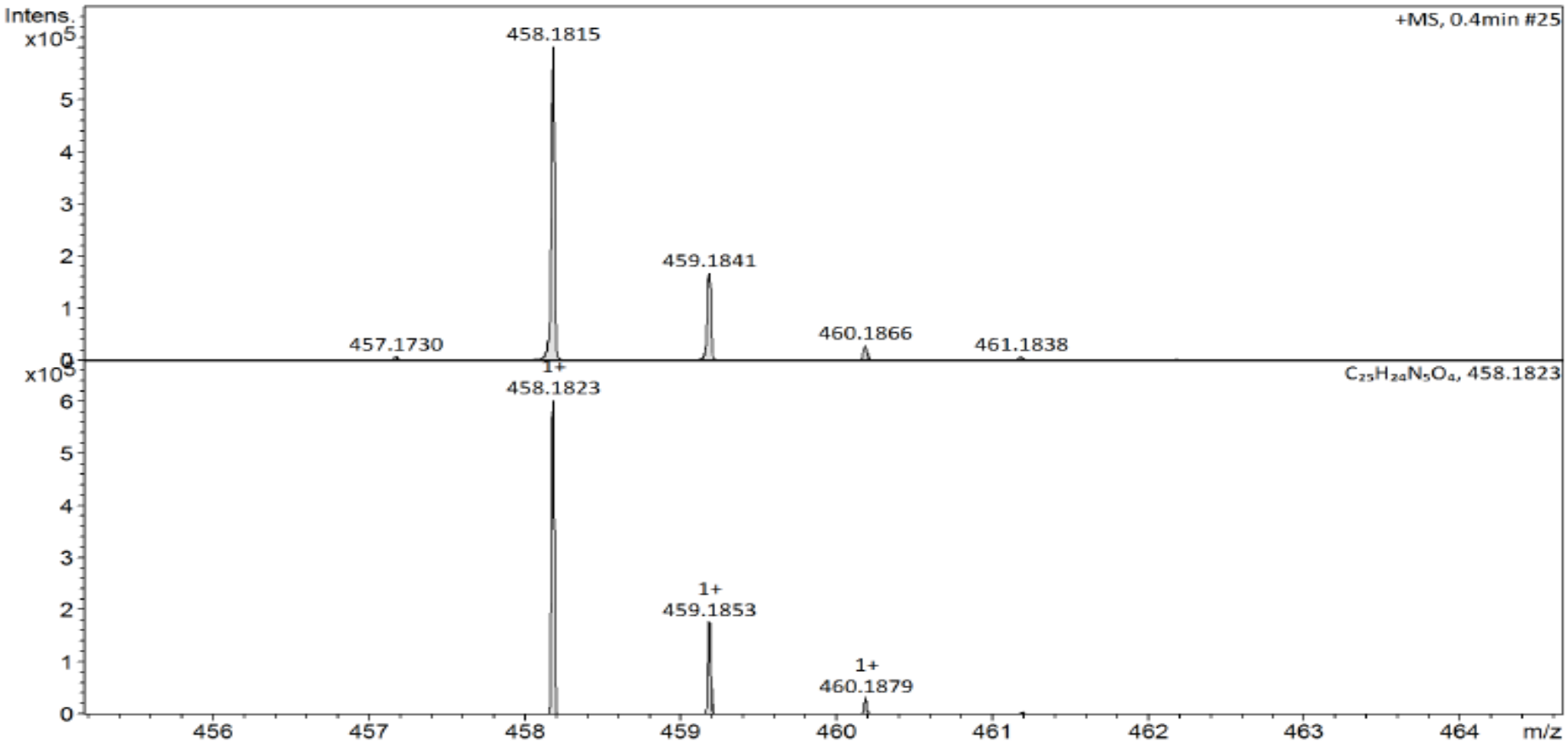
^{1}H NMR spectrum (400MHz) of compound **5s** in $CDCl_3$



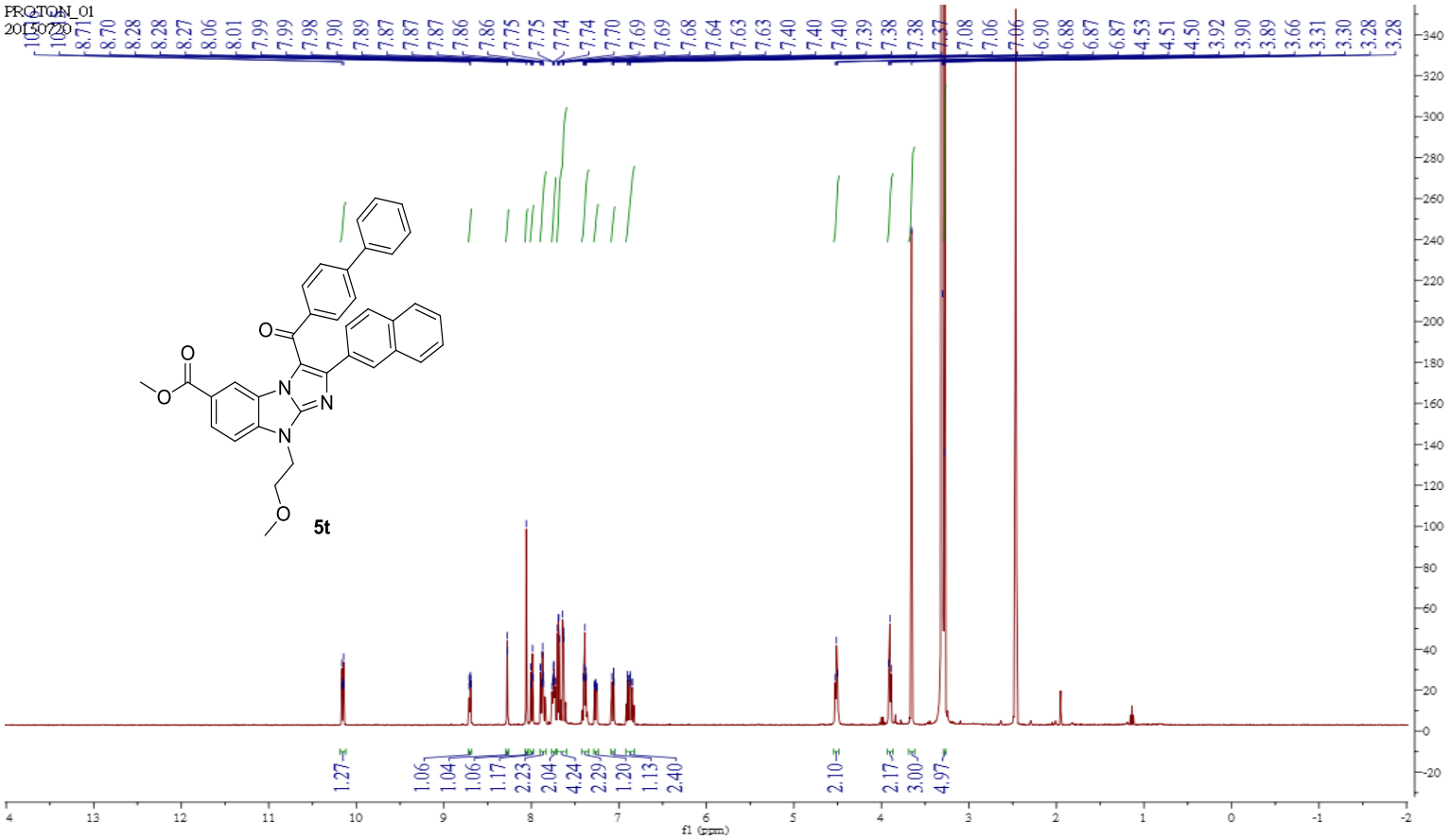
^{13}C NMR spectrum (100MHz) of compound **5s** in $CDCl_3$



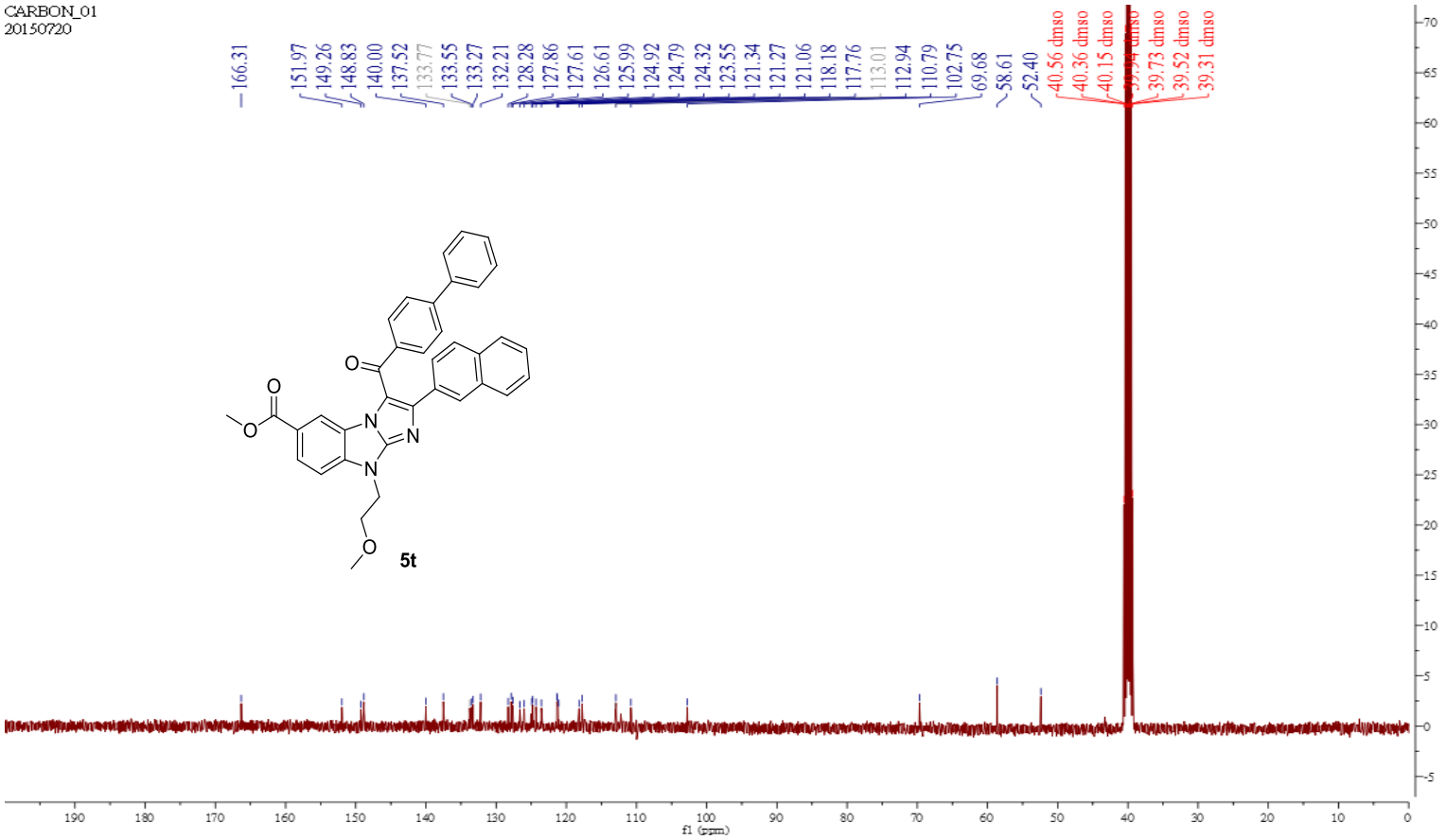
ESI^{+} Mass spectrum of compound **5s**



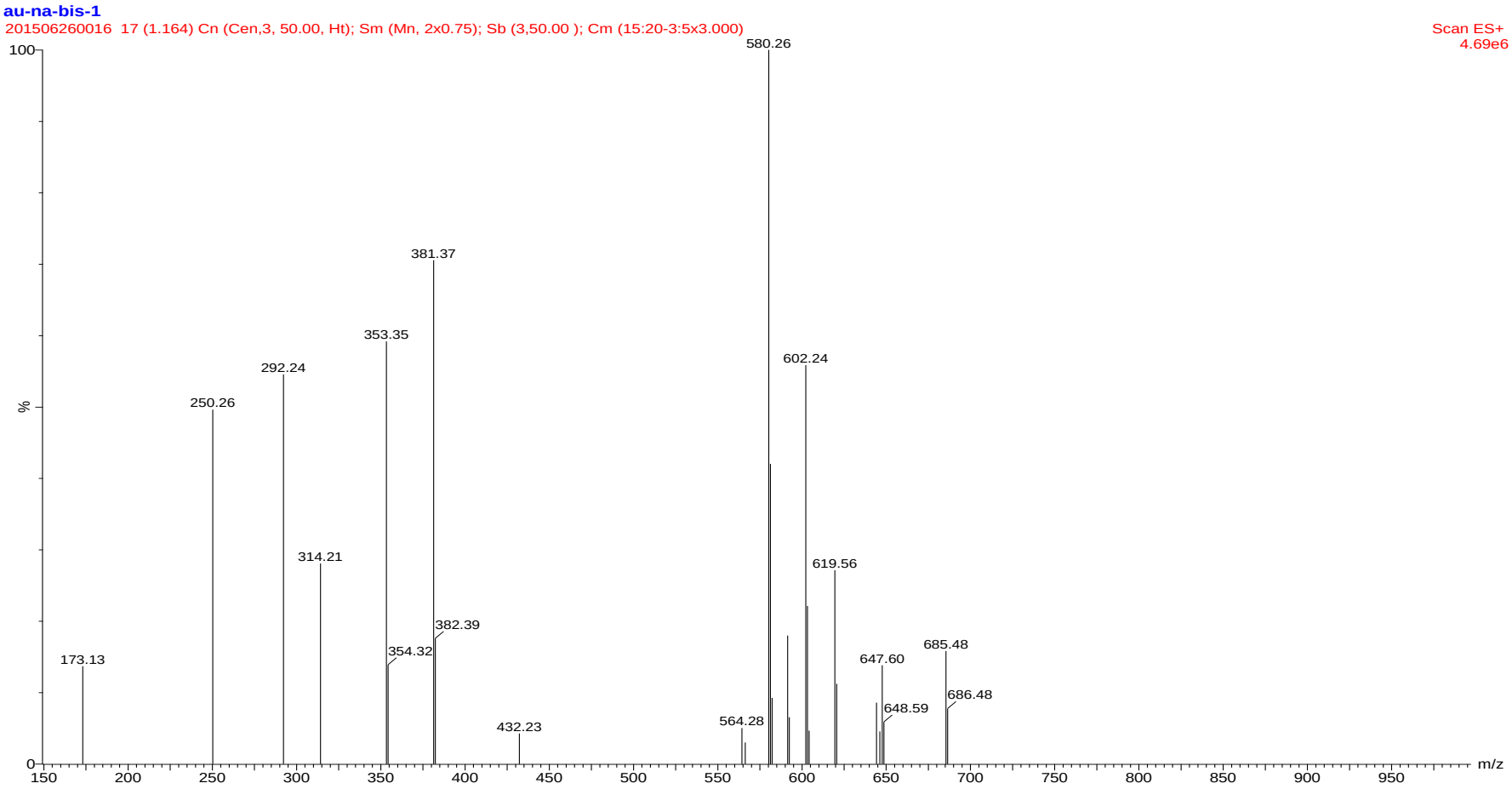
High resolution mass (ESI^+) spectrum of compound **5s**



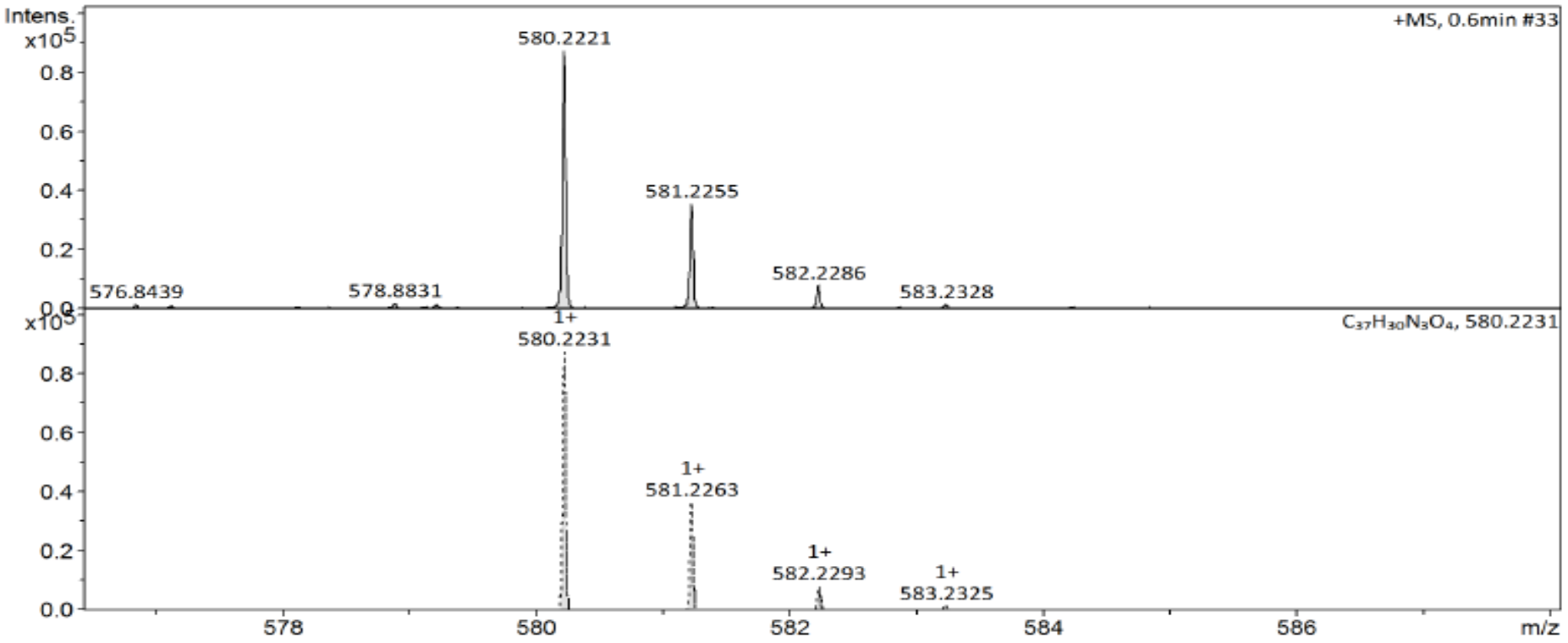
^{1}H NMR spectrum (400MHz) of compound **5t** in DMSO-d_6



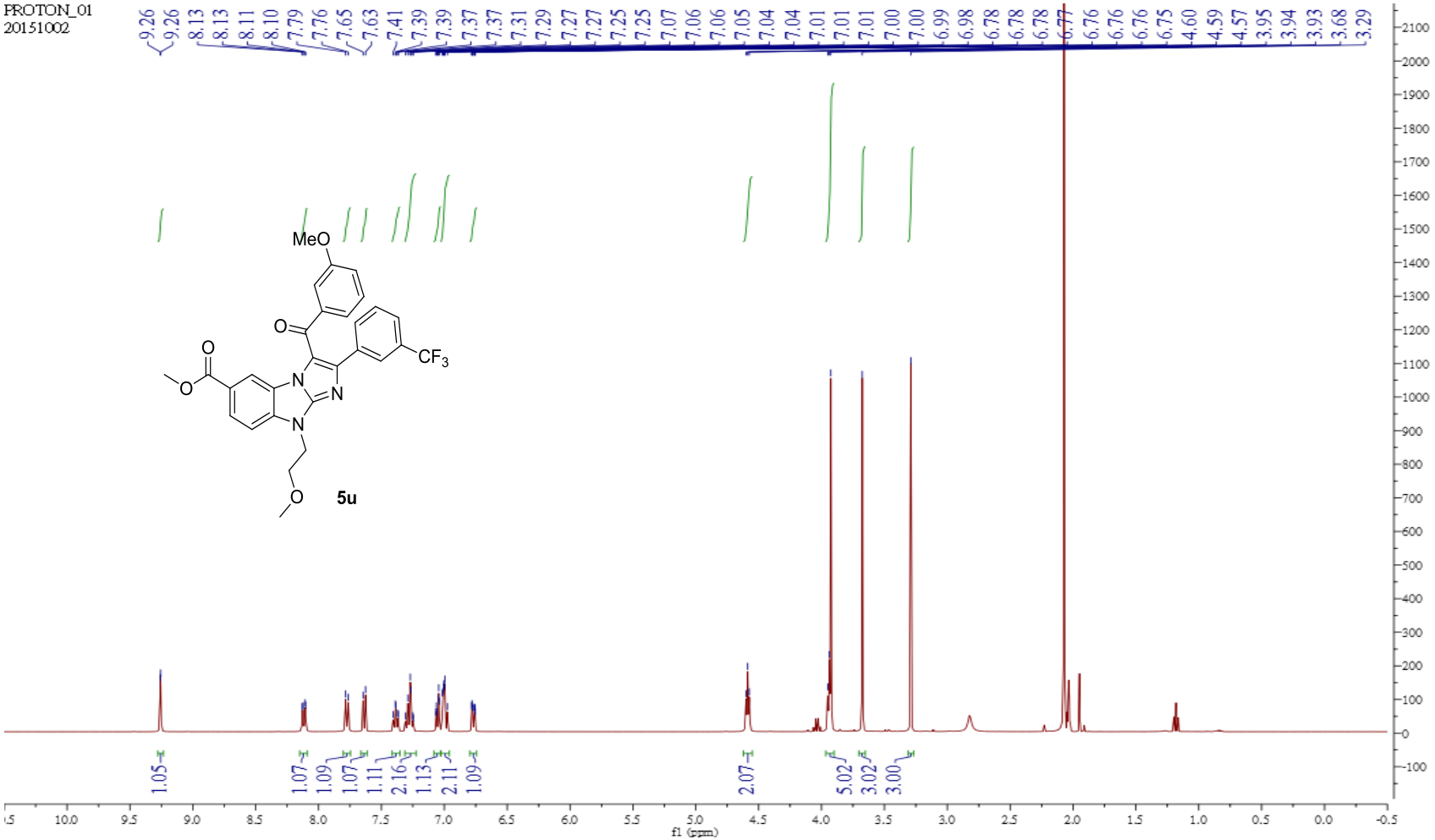
^{13}C NMR spectrum (75MHz) of compound **5t** in DMSO-d_6



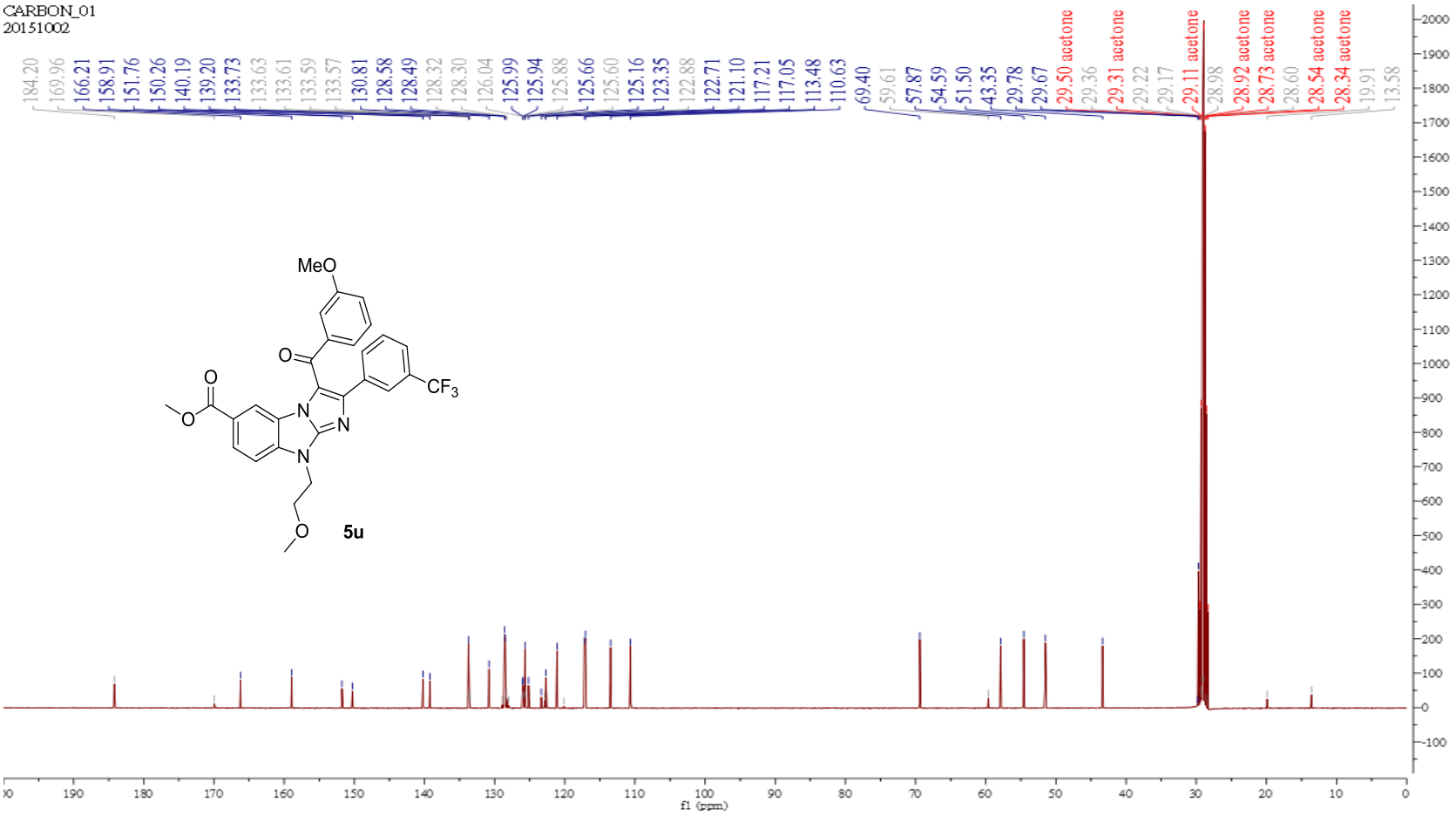
ESI$^+$ Mass spectrum of compound **5t**



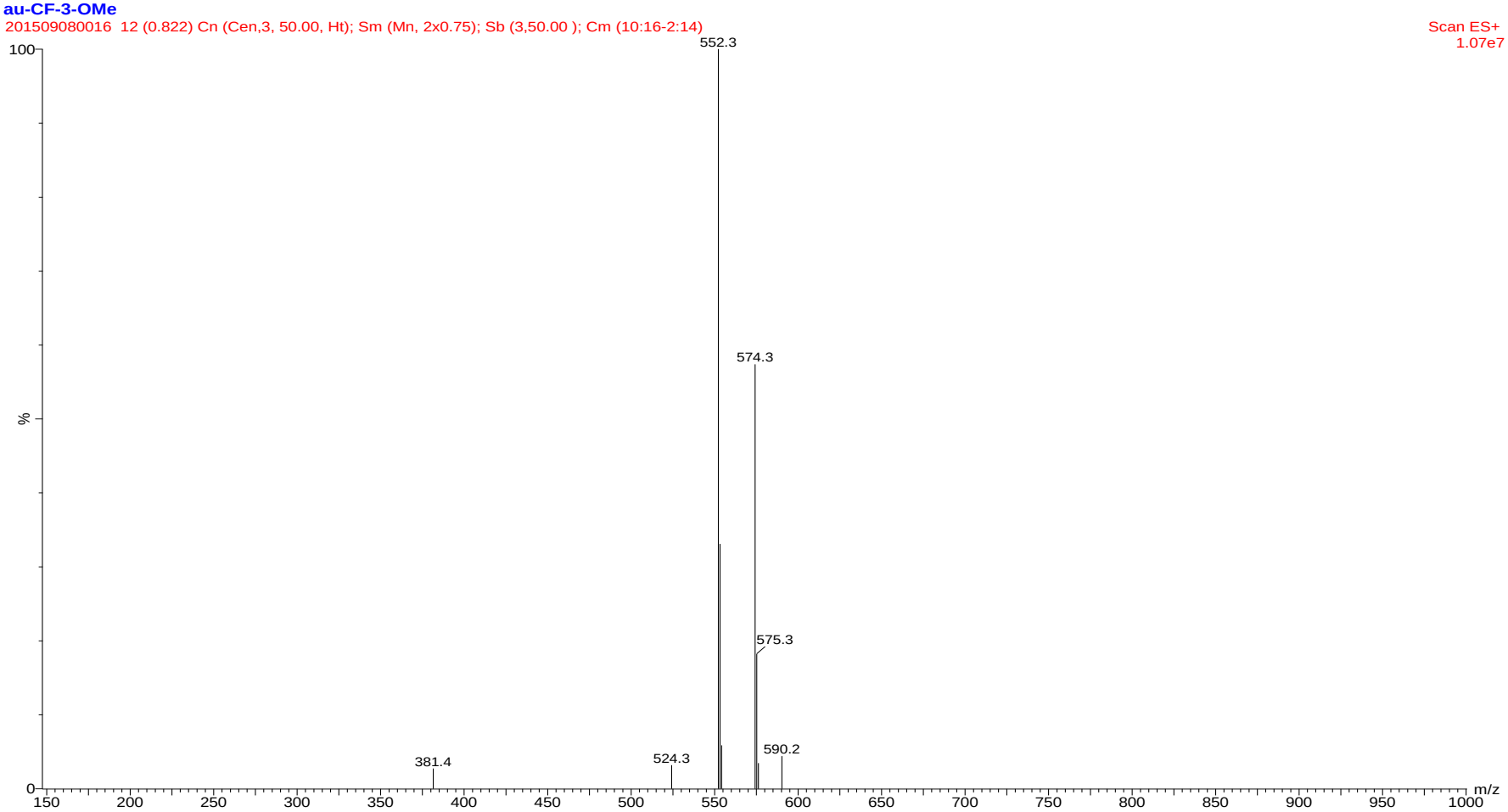
High resolution mass (ESI^+) spectrum of compound **5t**



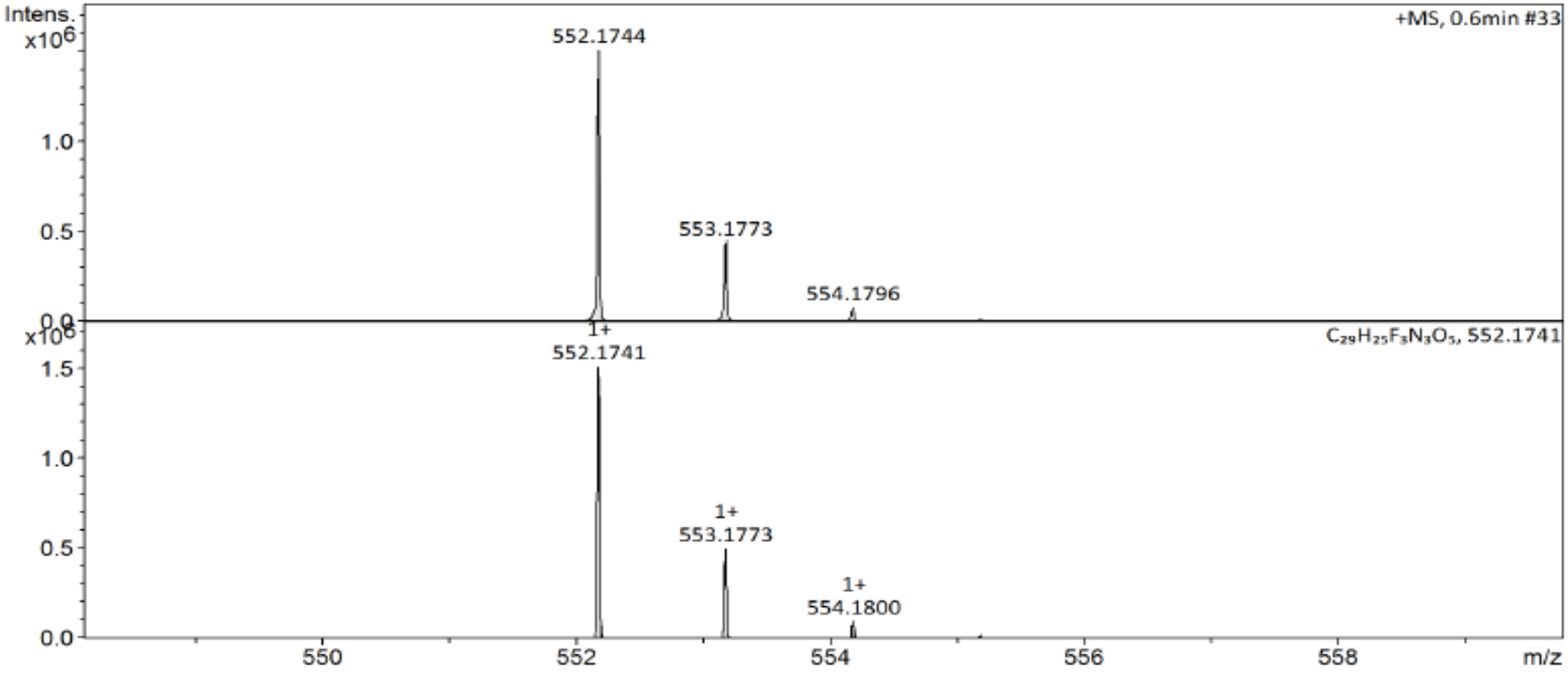
^{1}H NMR spectrum (400MHz) of compound **5u** in Acetone-d_6



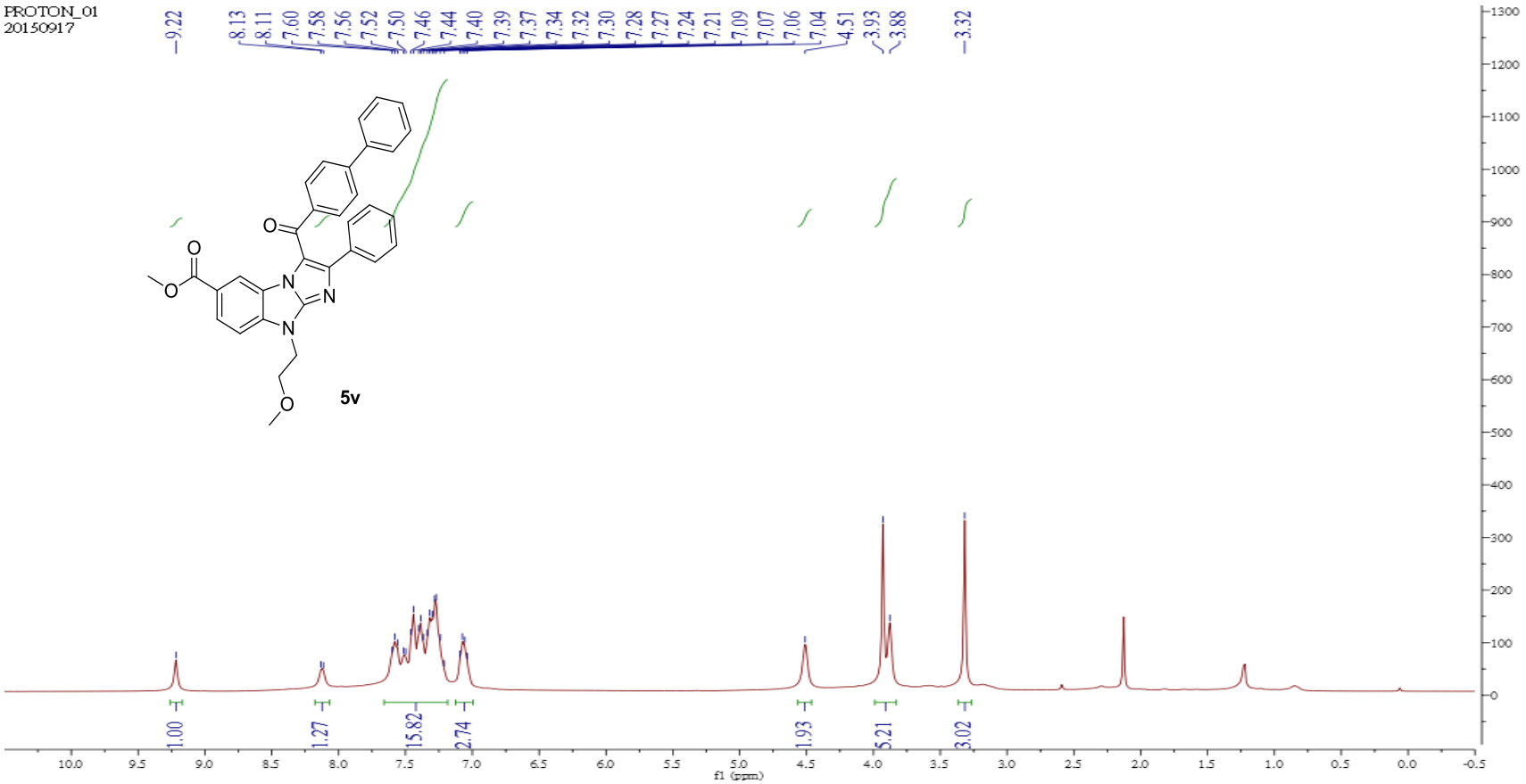
^{13}C NMR spectrum (100MHz) of compound **5u** in Acetone-d_6



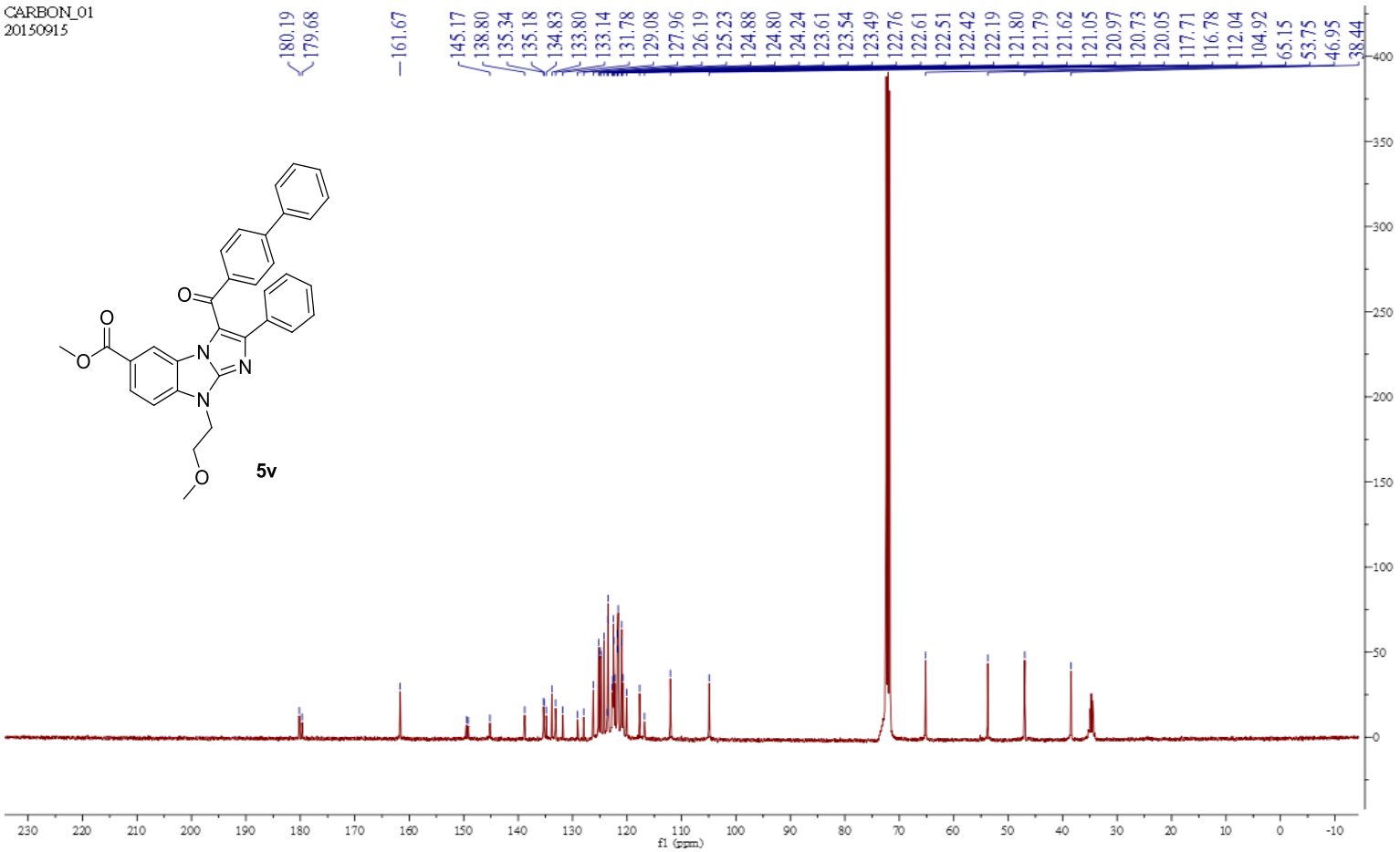
ESI$^+$ Mass spectrum of compound **5u**



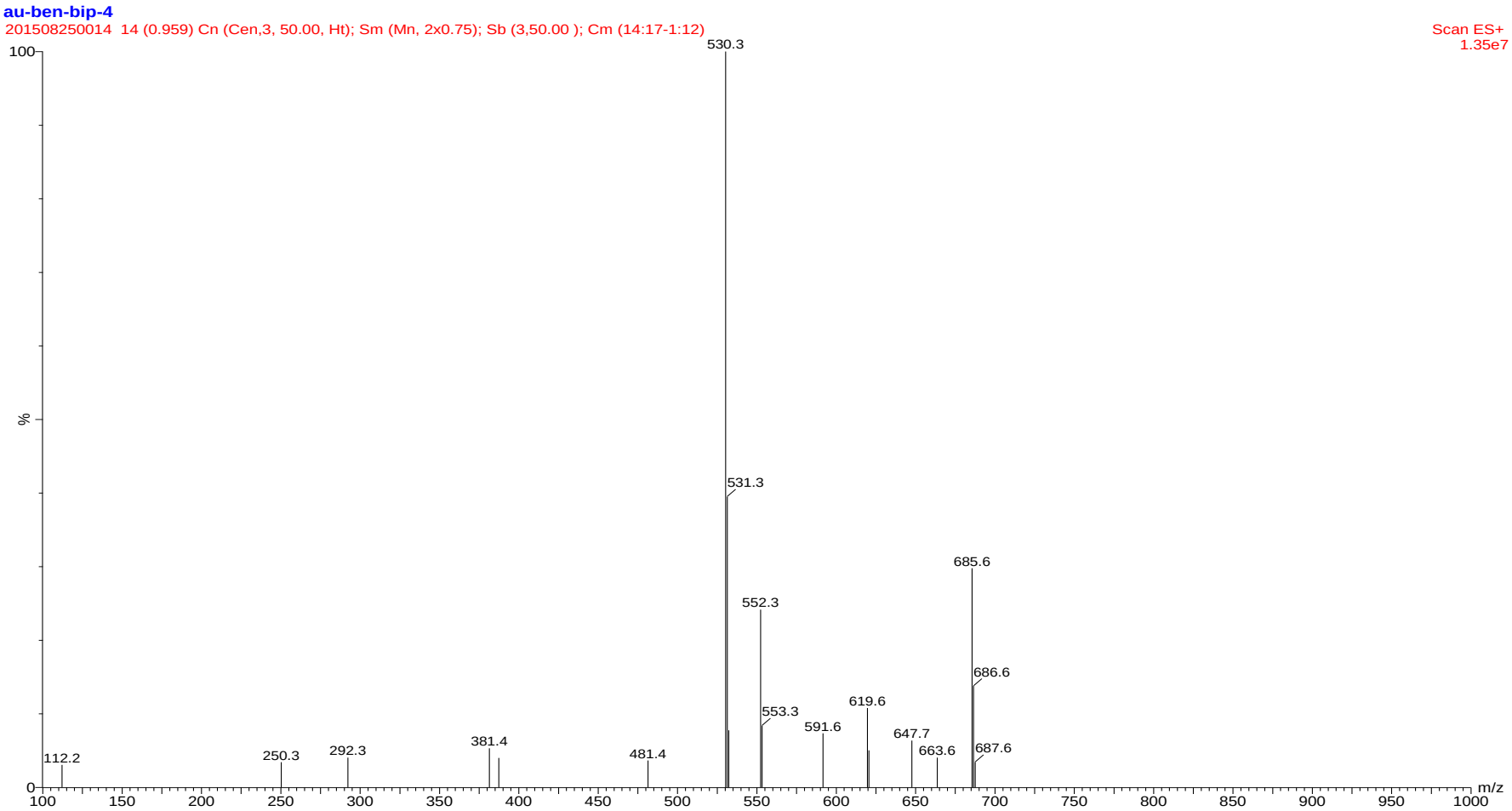
High resolution mass (ESI^+) spectrum of compound **5u**



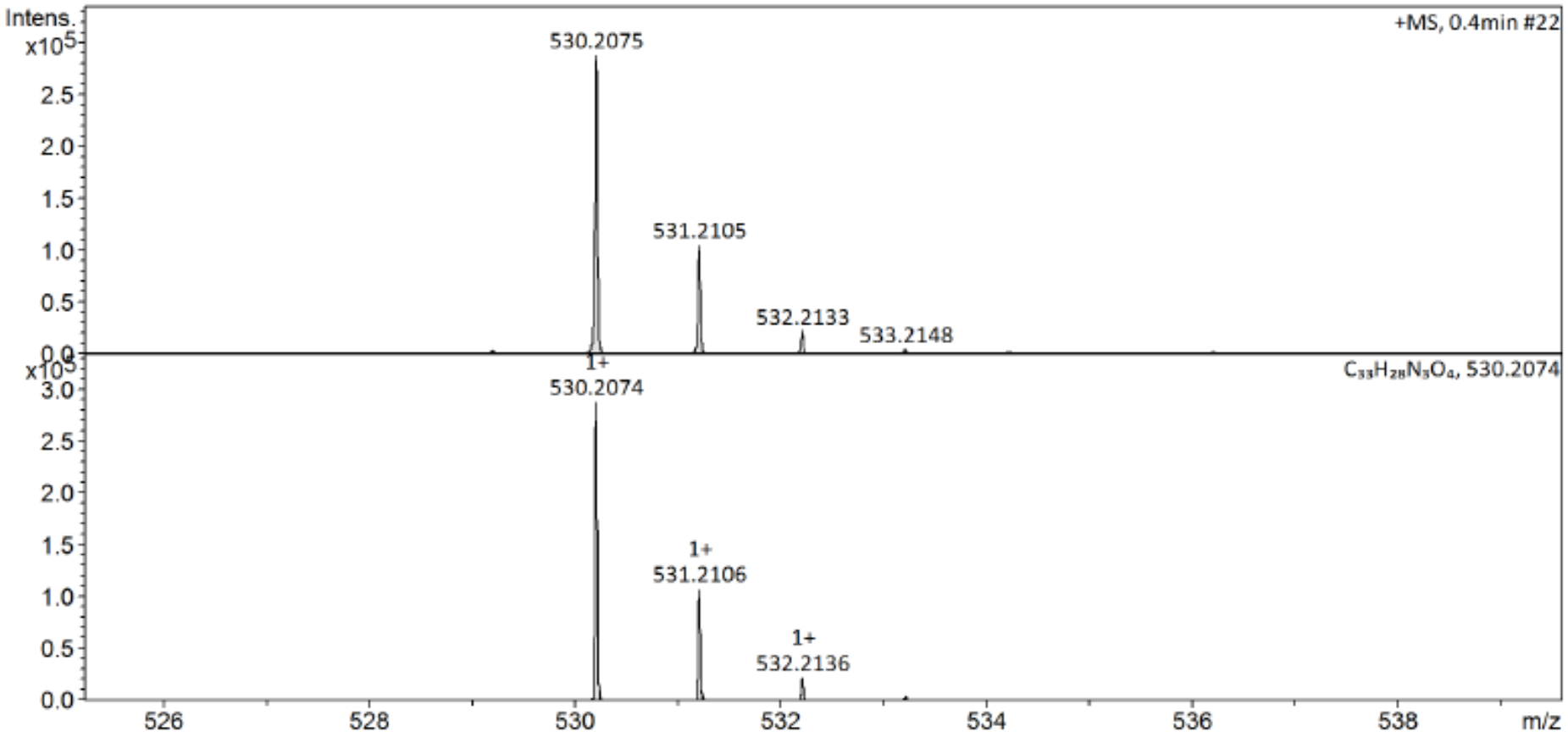
^{1}H NMR spectrum (400MHz) of compound **5v** in $CDCl_3$



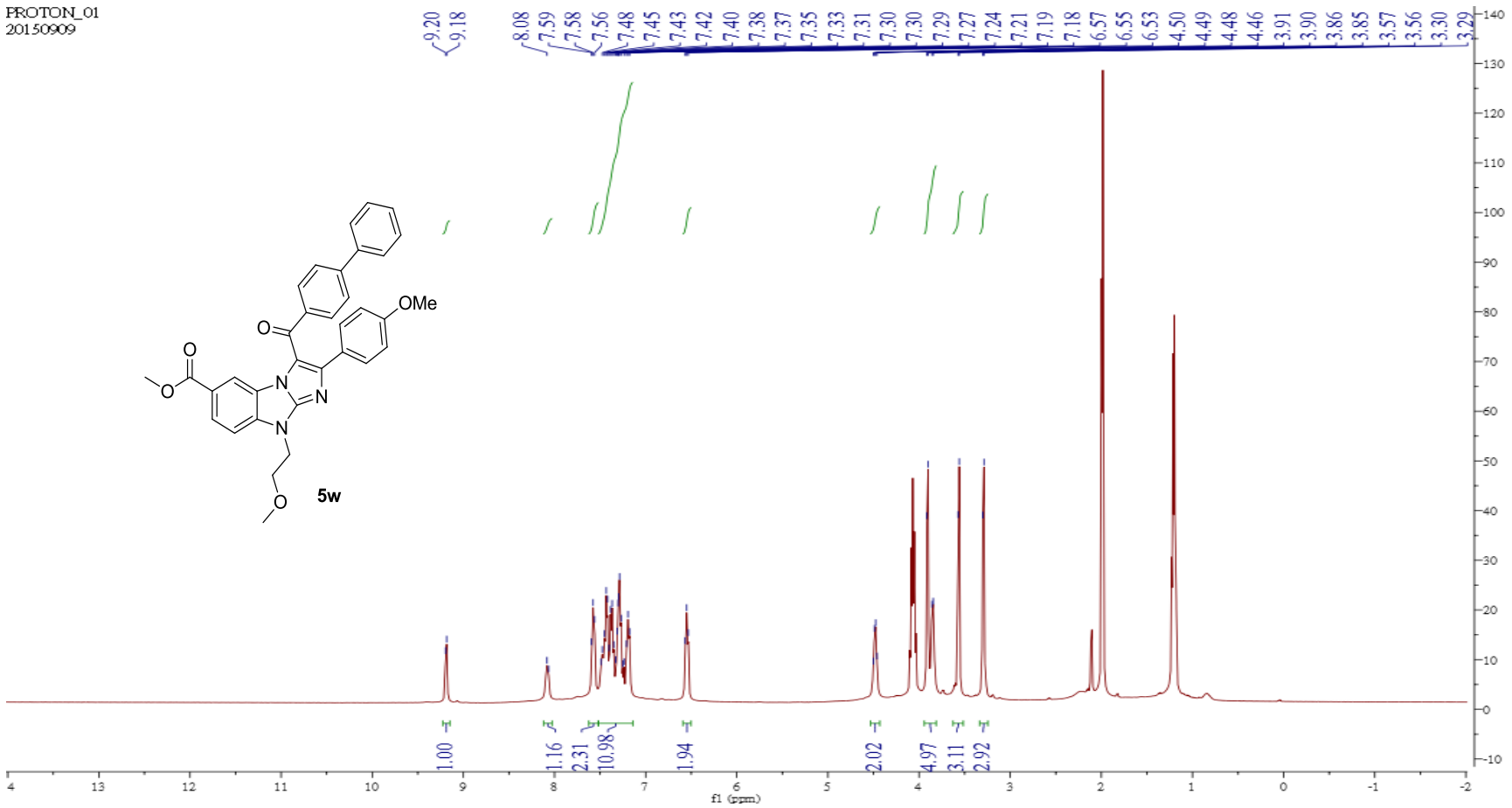
^{13}C NMR spectrum (100MHz) of compound **5v** in $CDCl_3$



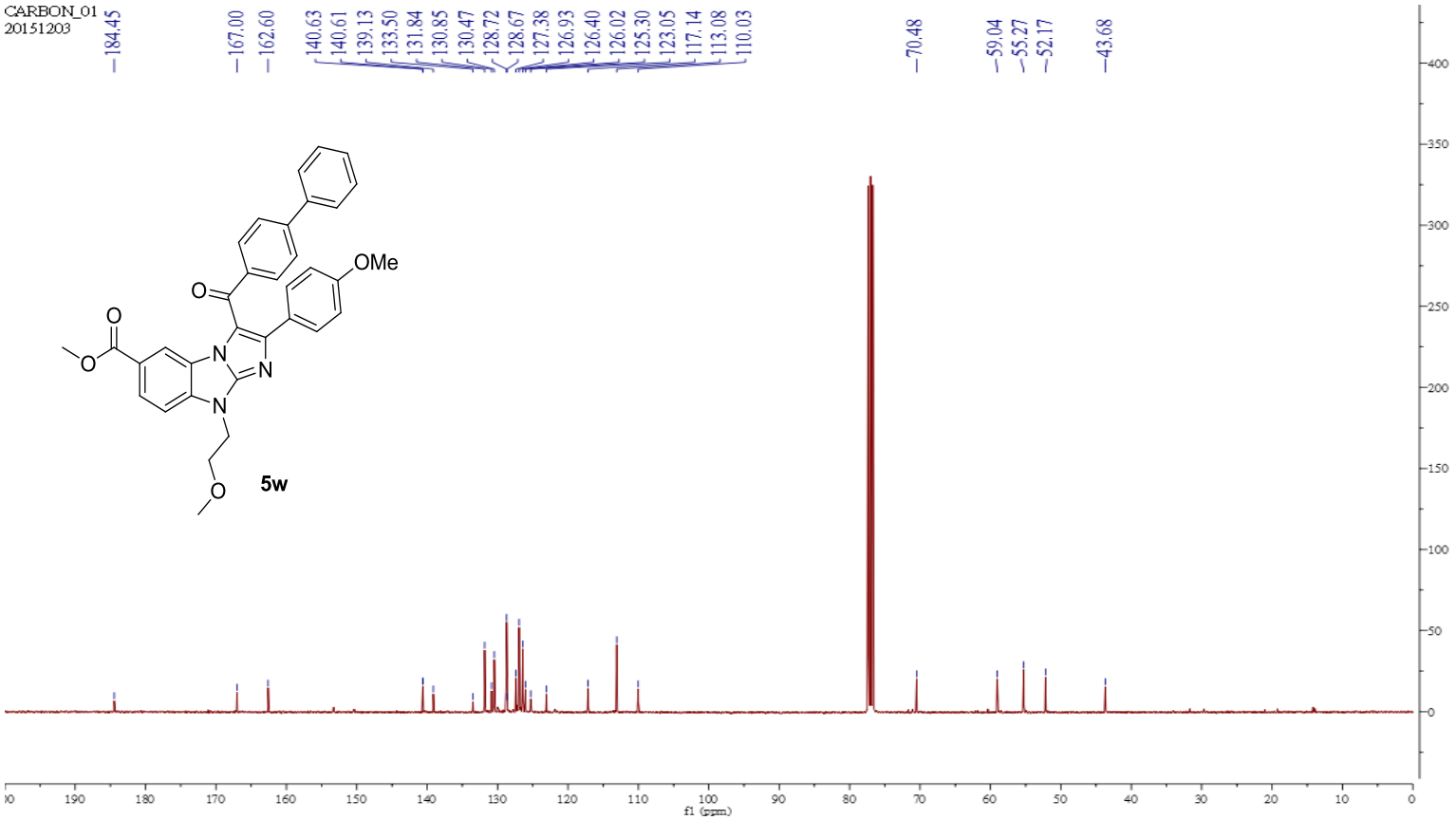
ESI^{+} Mass spectrum of compound **5v**



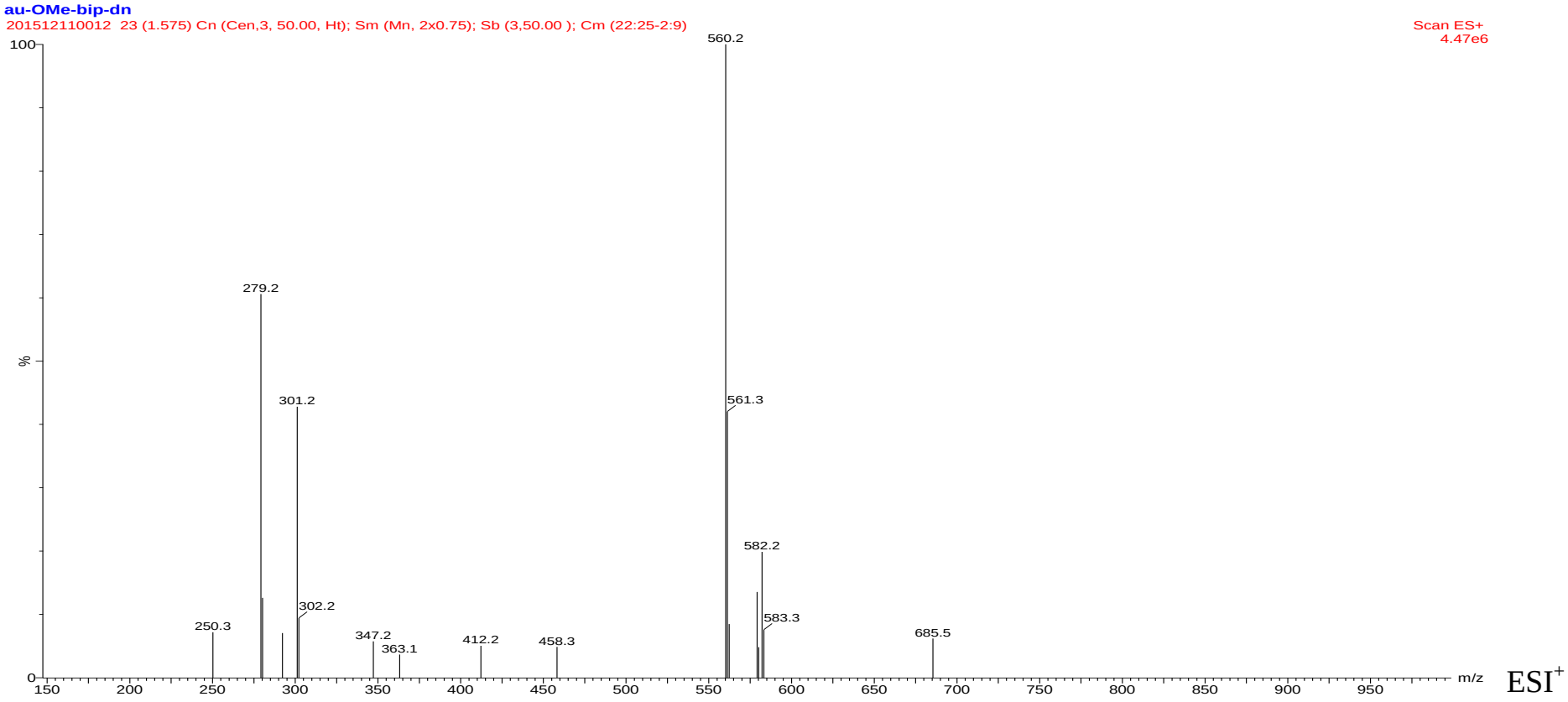
High resolution mass (ESI$^+$) spectrum of compound **5v**



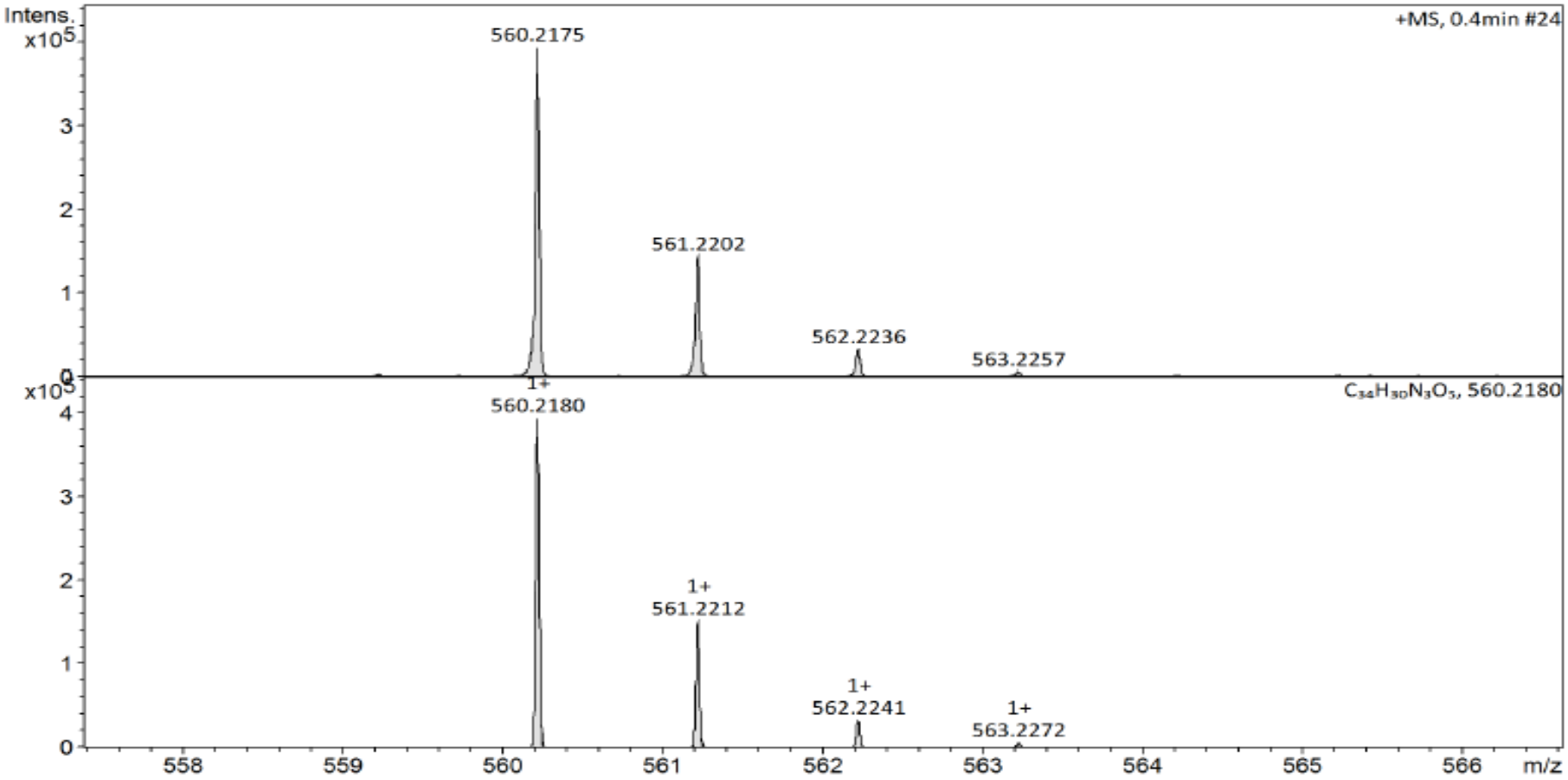
^{1}H NMR spectrum (400MHz) of compound **5w** in $CDCl_3$



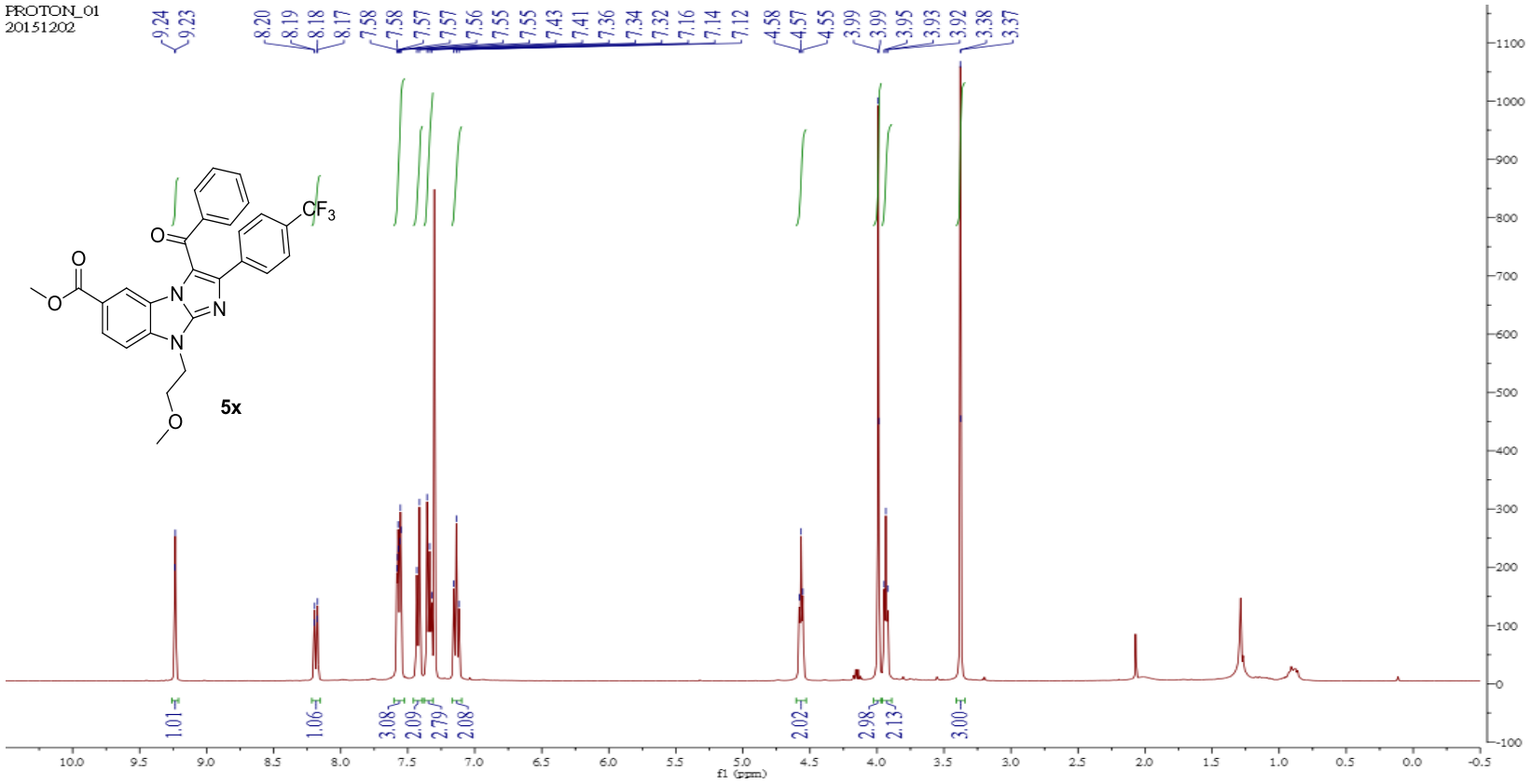
^{13}C NMR spectrum (100MHz) of compound **5w** in $CDCl_3$



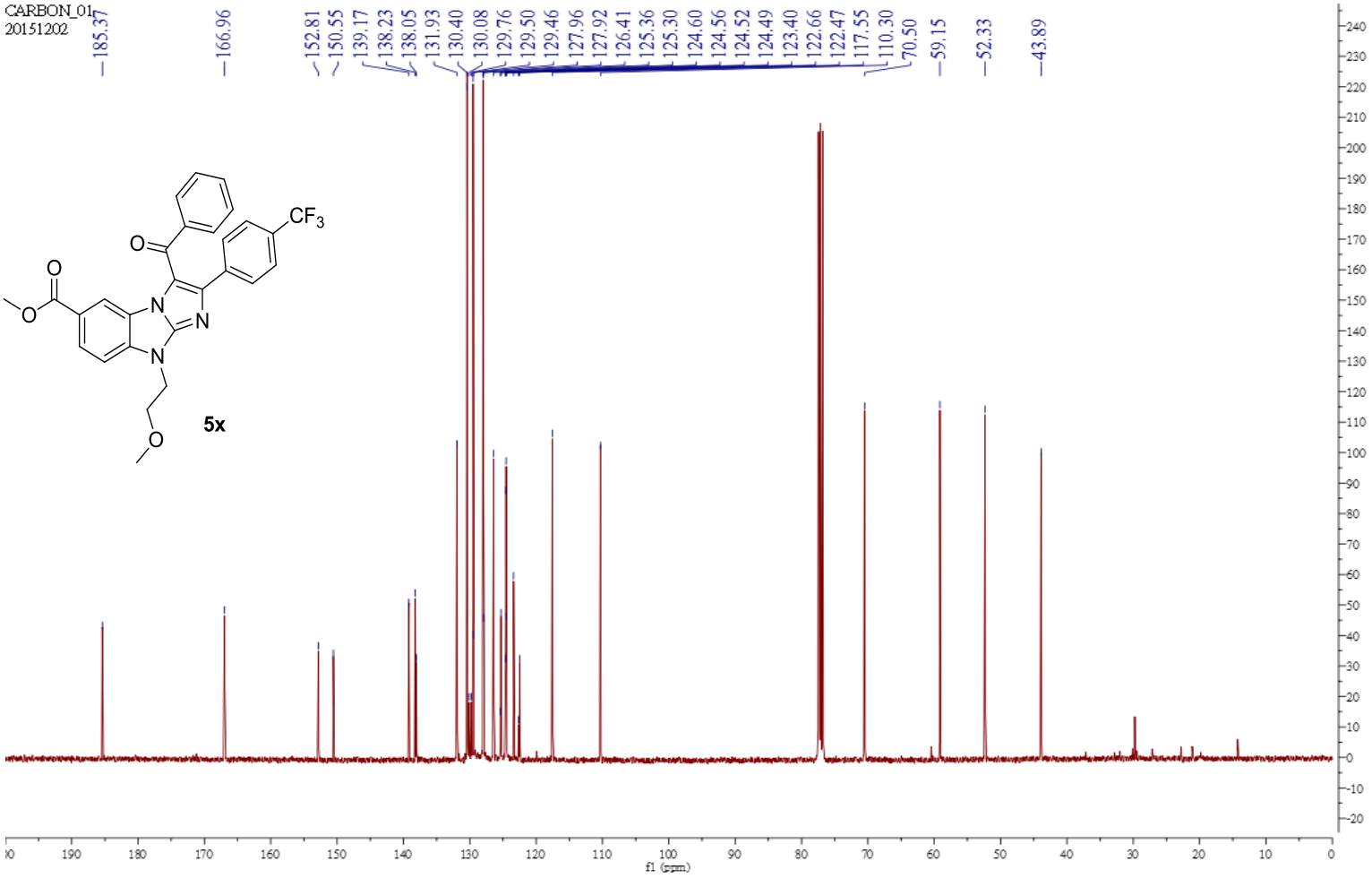
Mass spectrum of compound **5w**



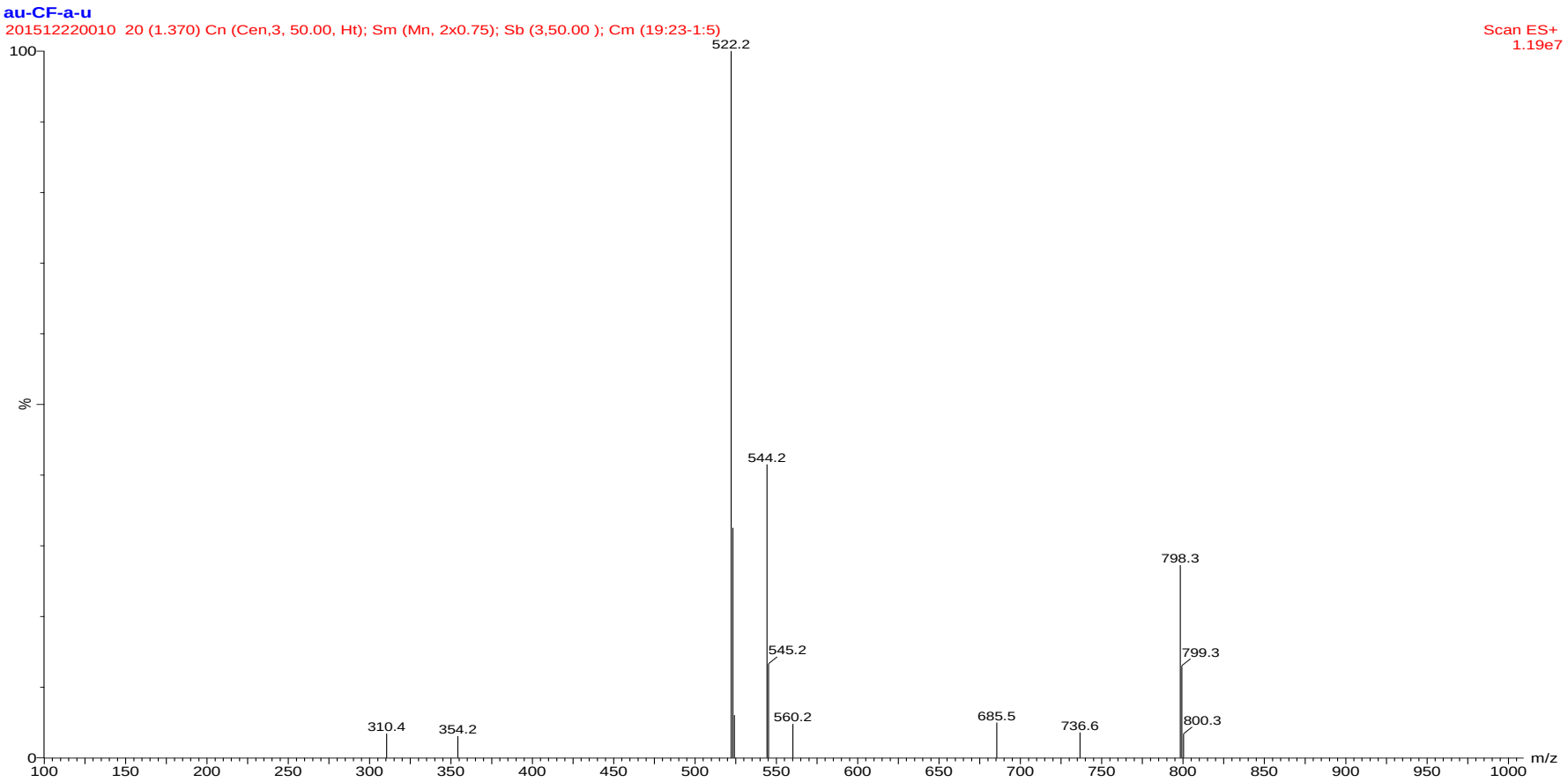
High resolution mass (ESI^+) spectrum of compound **5w**



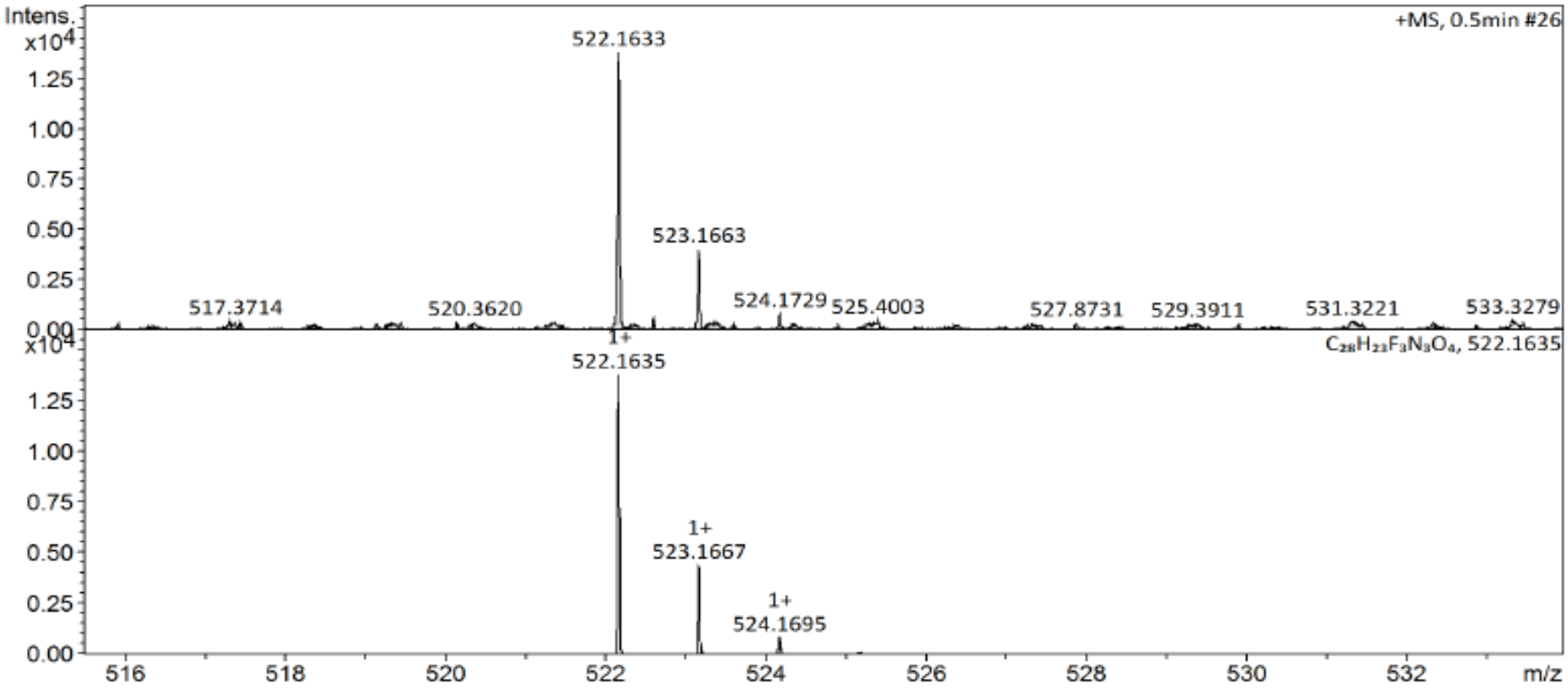
^{1}H NMR spectrum (400MHz) of compound **5x** in $CDCl_3$



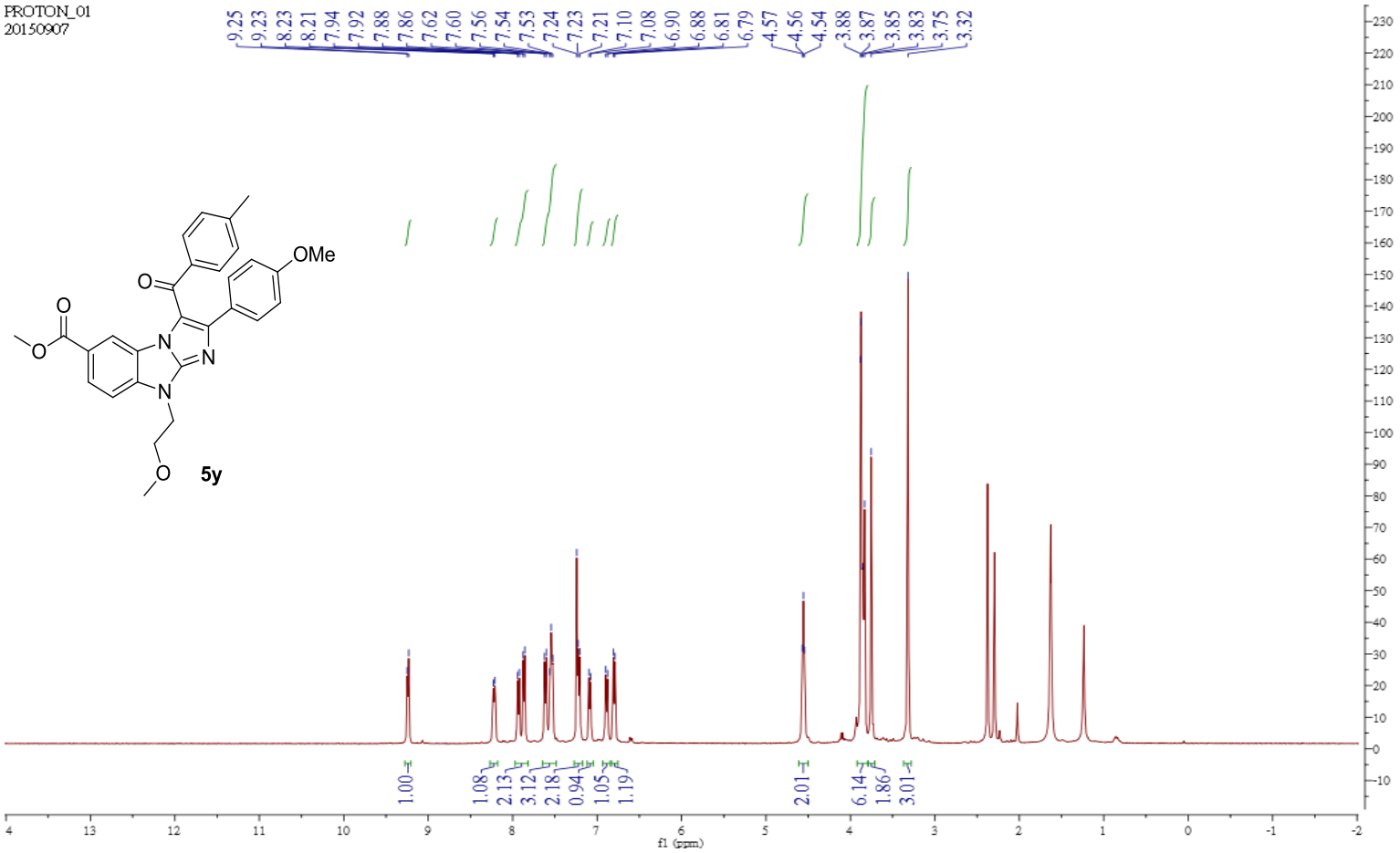
^{13}C NMR spectrum (100MHz) of compound **5x** in $CDCl_3$



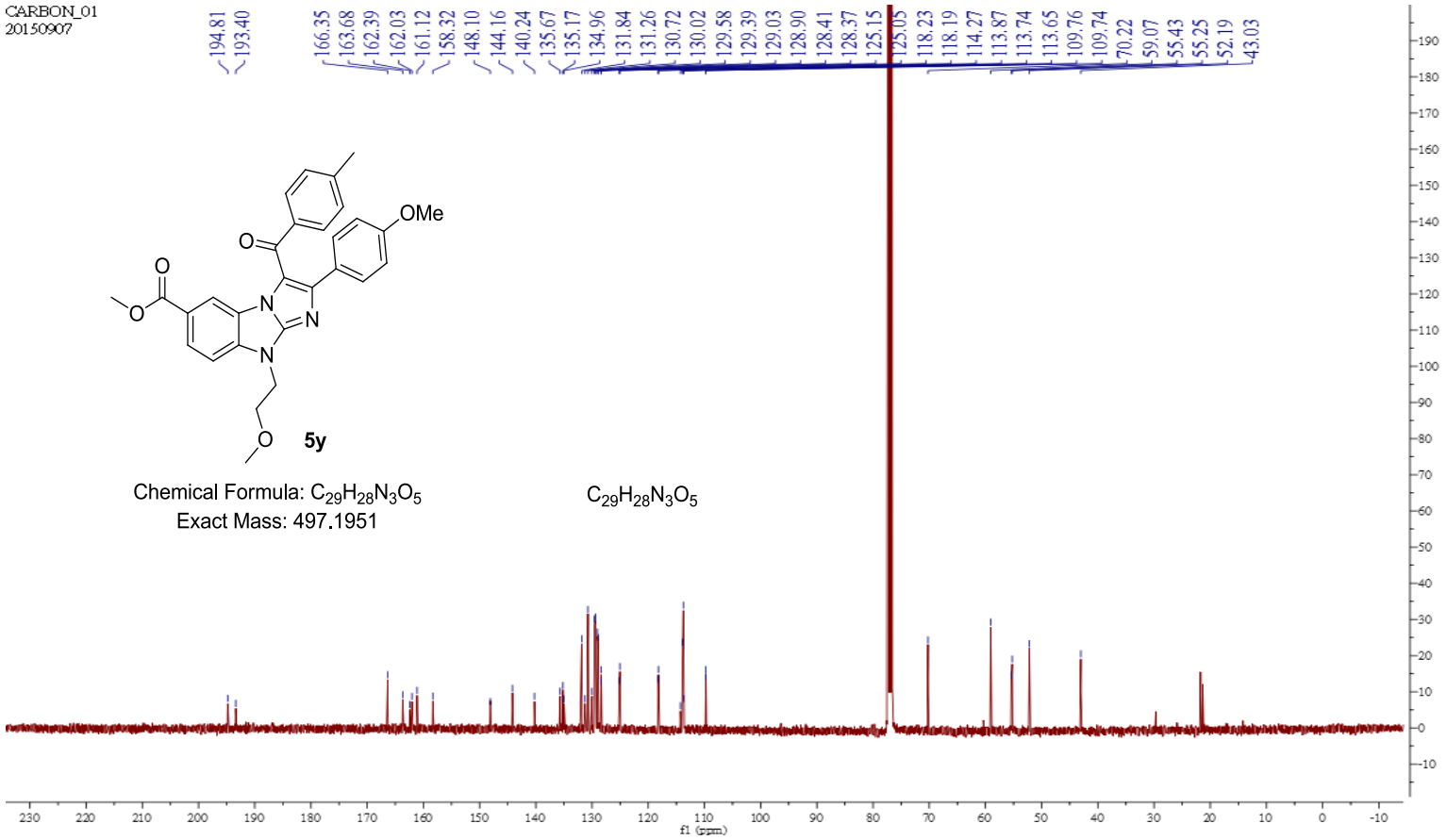
ESI^{+} Mass spectrum of compound **5x**



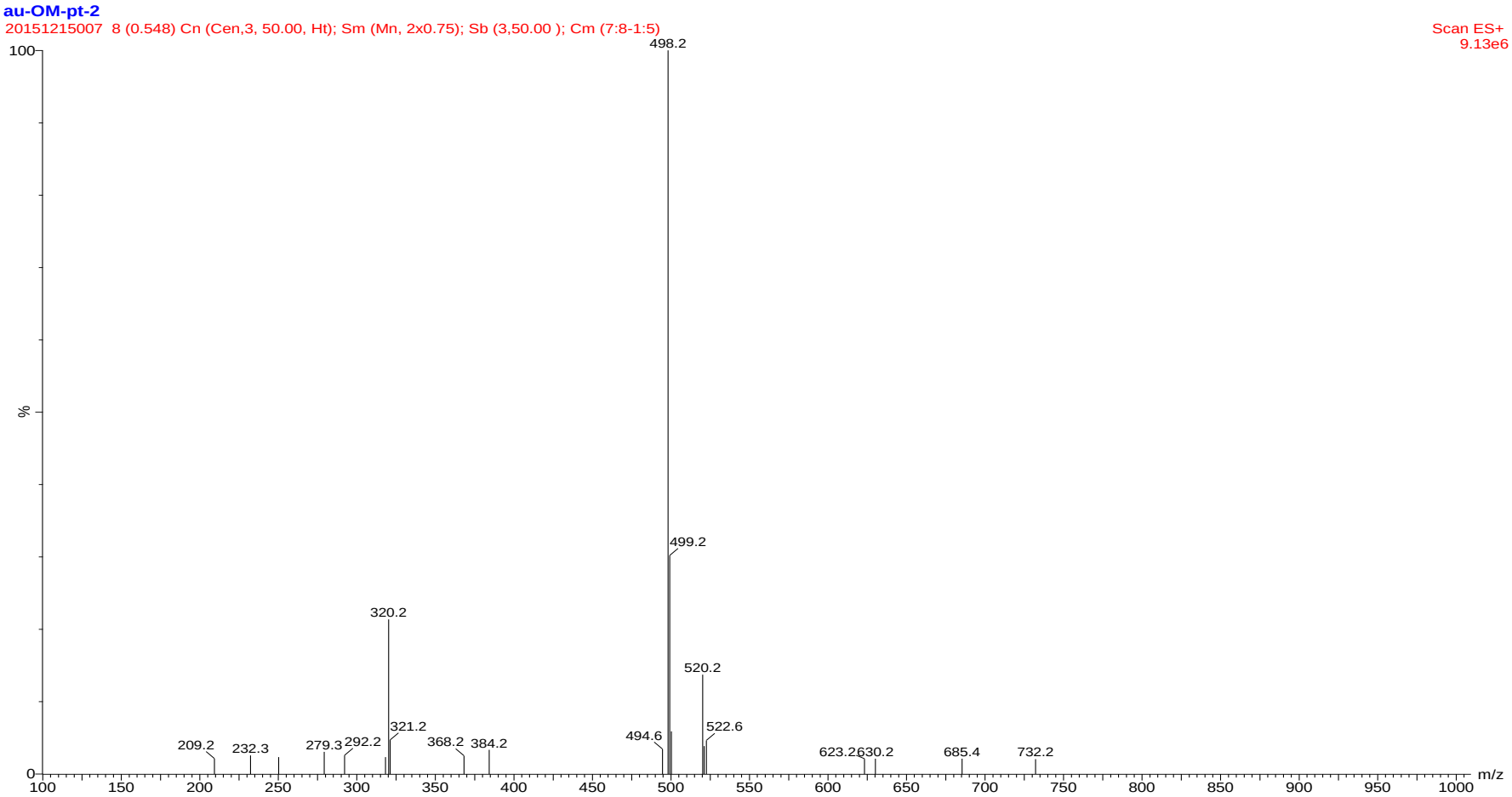
High resolution mass (ESI^+) spectrum of compound **5x**



^{1}H NMR spectrum (400MHz) of compound **5y** in $CDCl_3$



^{13}C NMR spectrum (100MHz) of compound **5y** in $CDCl_3$



ESI^{+} Mass spectrum of compound **5y**

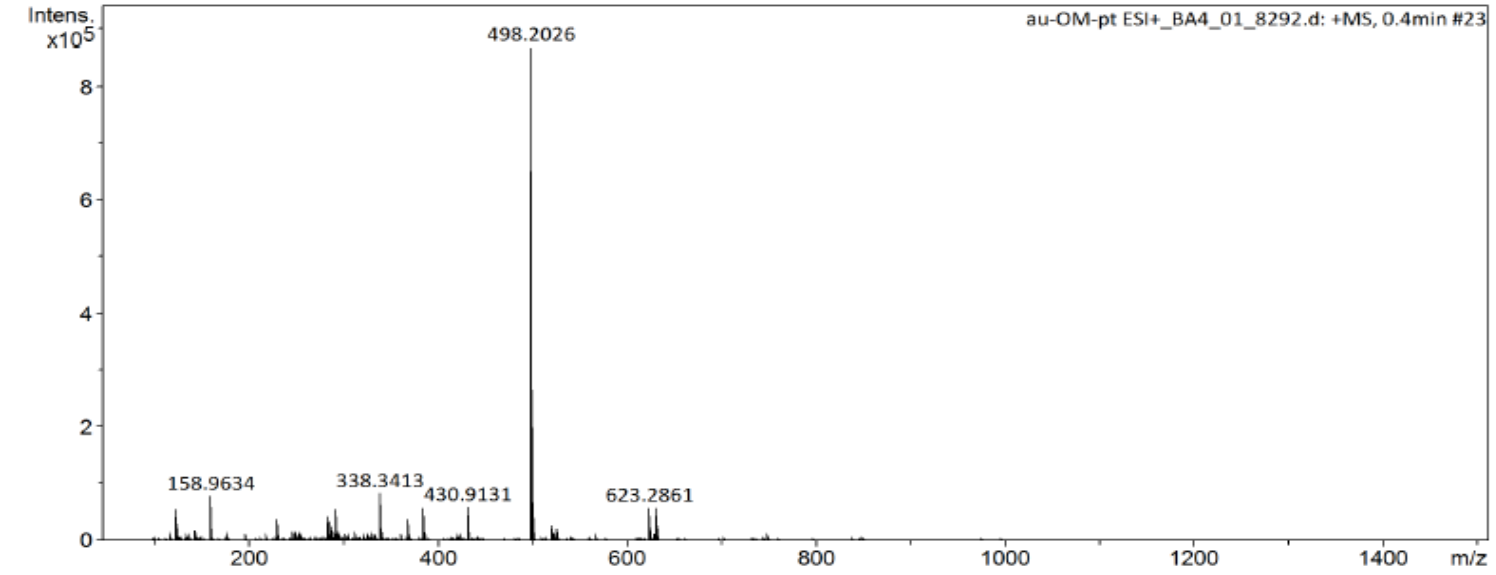
Display Report

Analysis Info

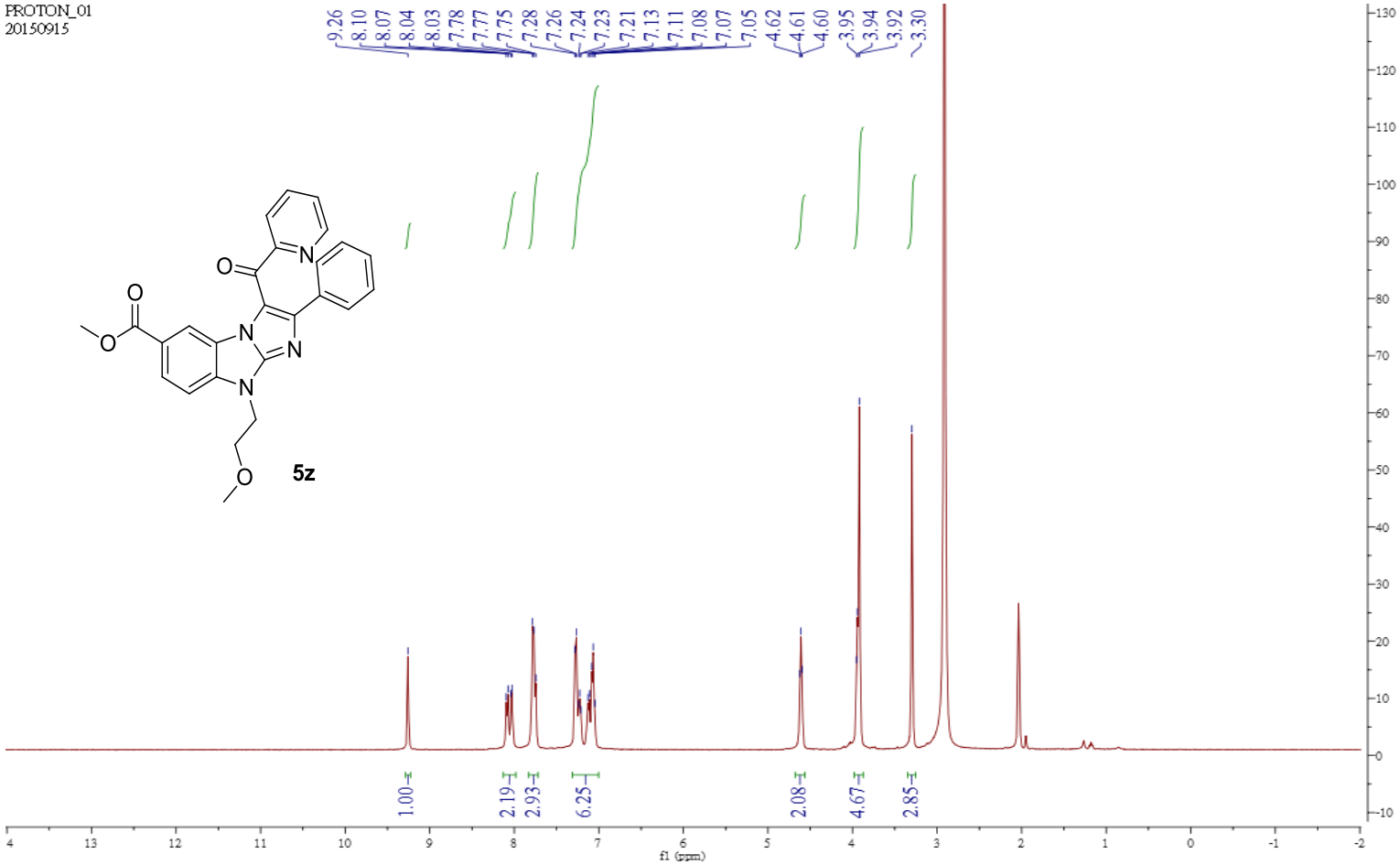
Analysis Name	D:\Data\nctu service\data\2015\20151222\au-OM-pt ESI+_BA4_01_8292.d	Acquisition Date	12/22/2015 12:34:12 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	au-OM-pt ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

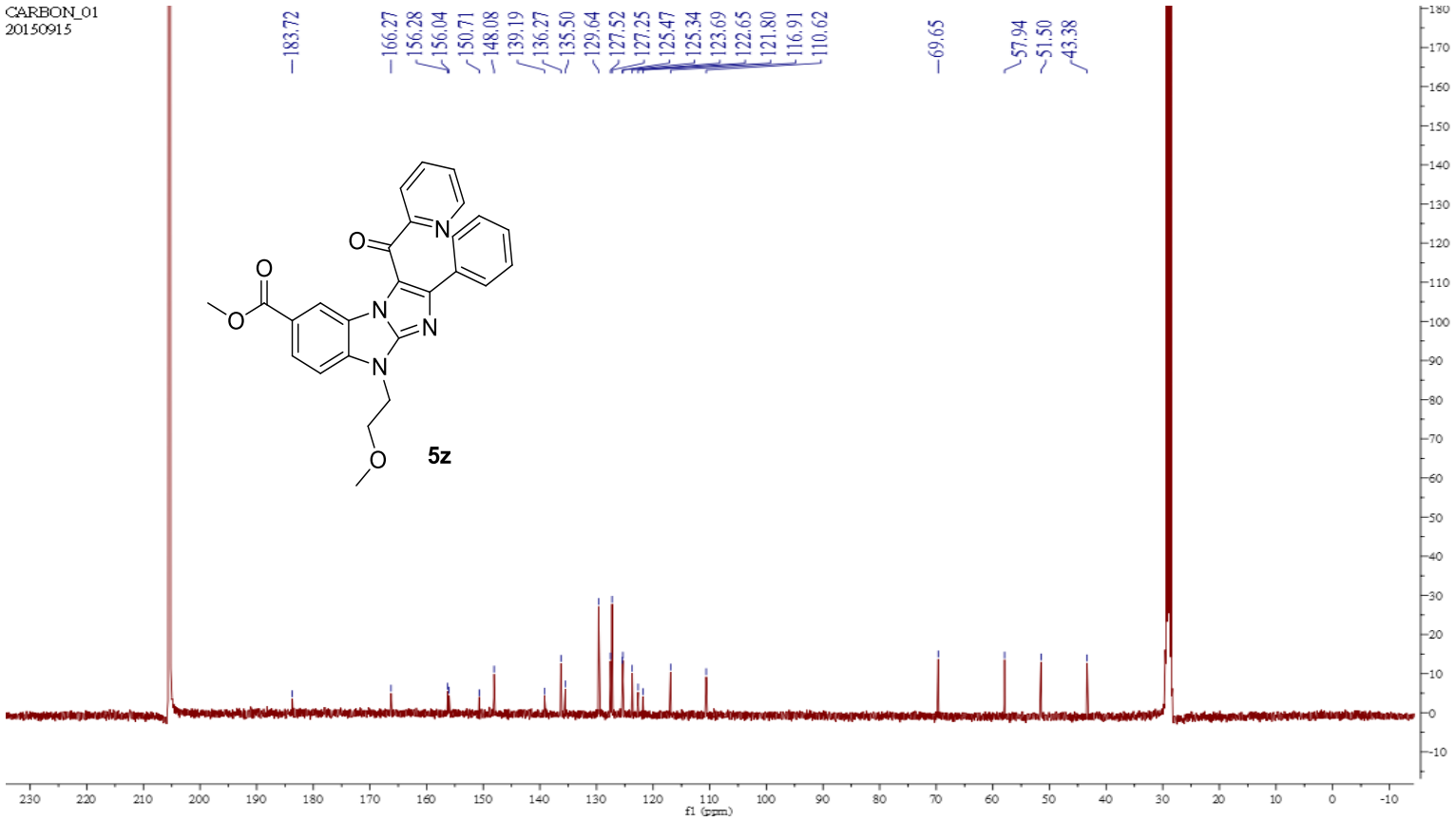
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



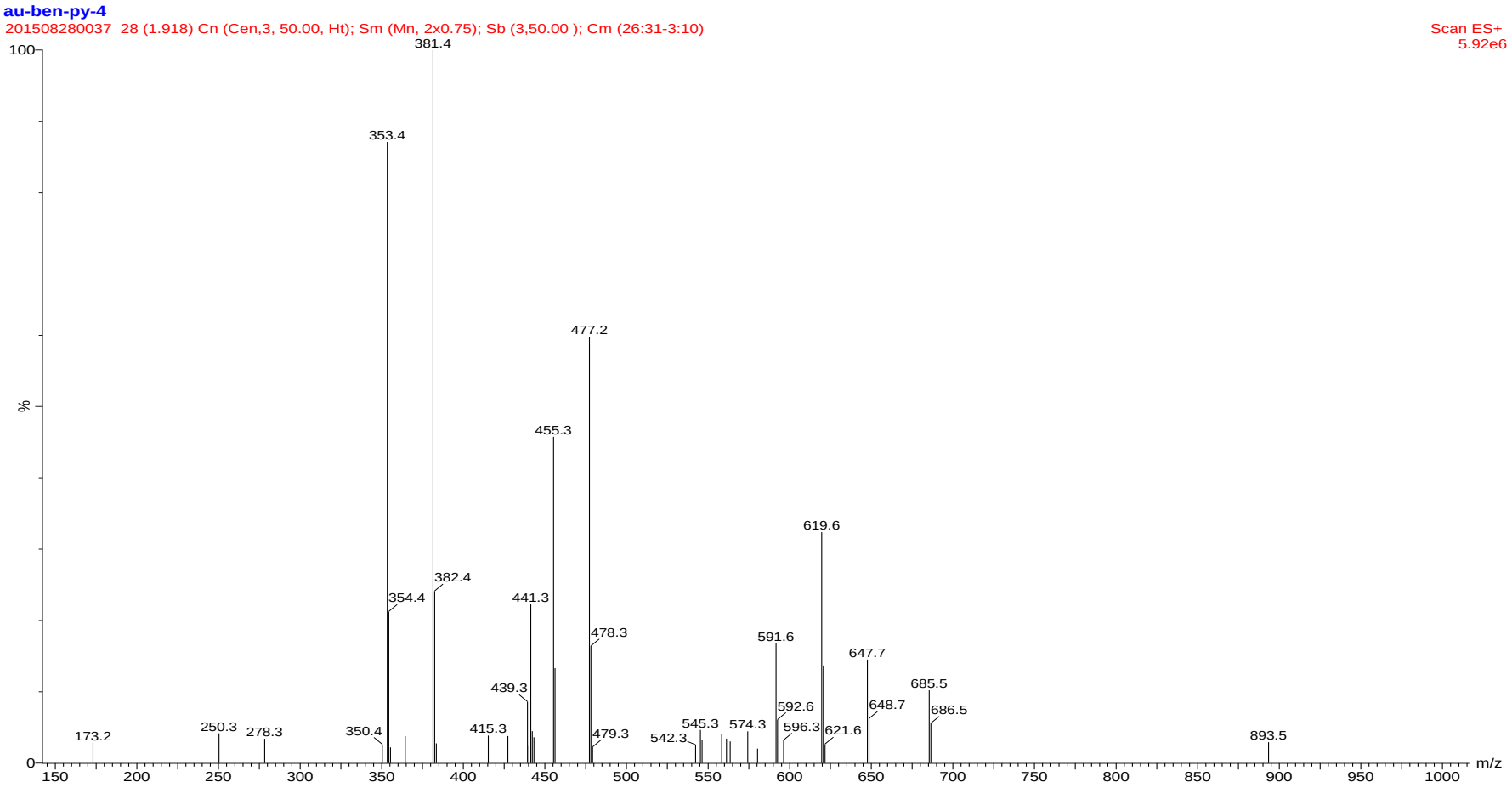
High resolution mass (ESI^+) spectrum of compound **5y**



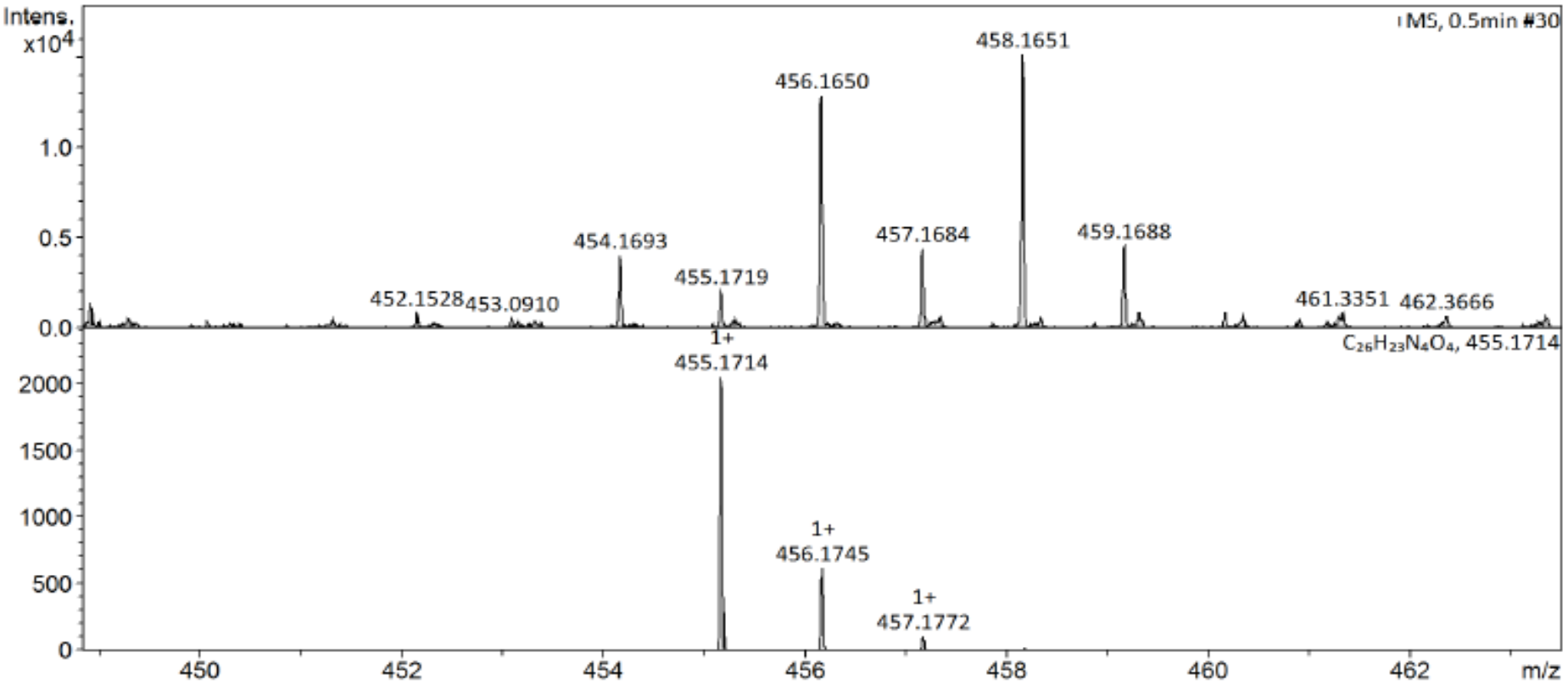
^{1}H NMR spectrum (400MHz) of compound **5z** in Acetone-d_6



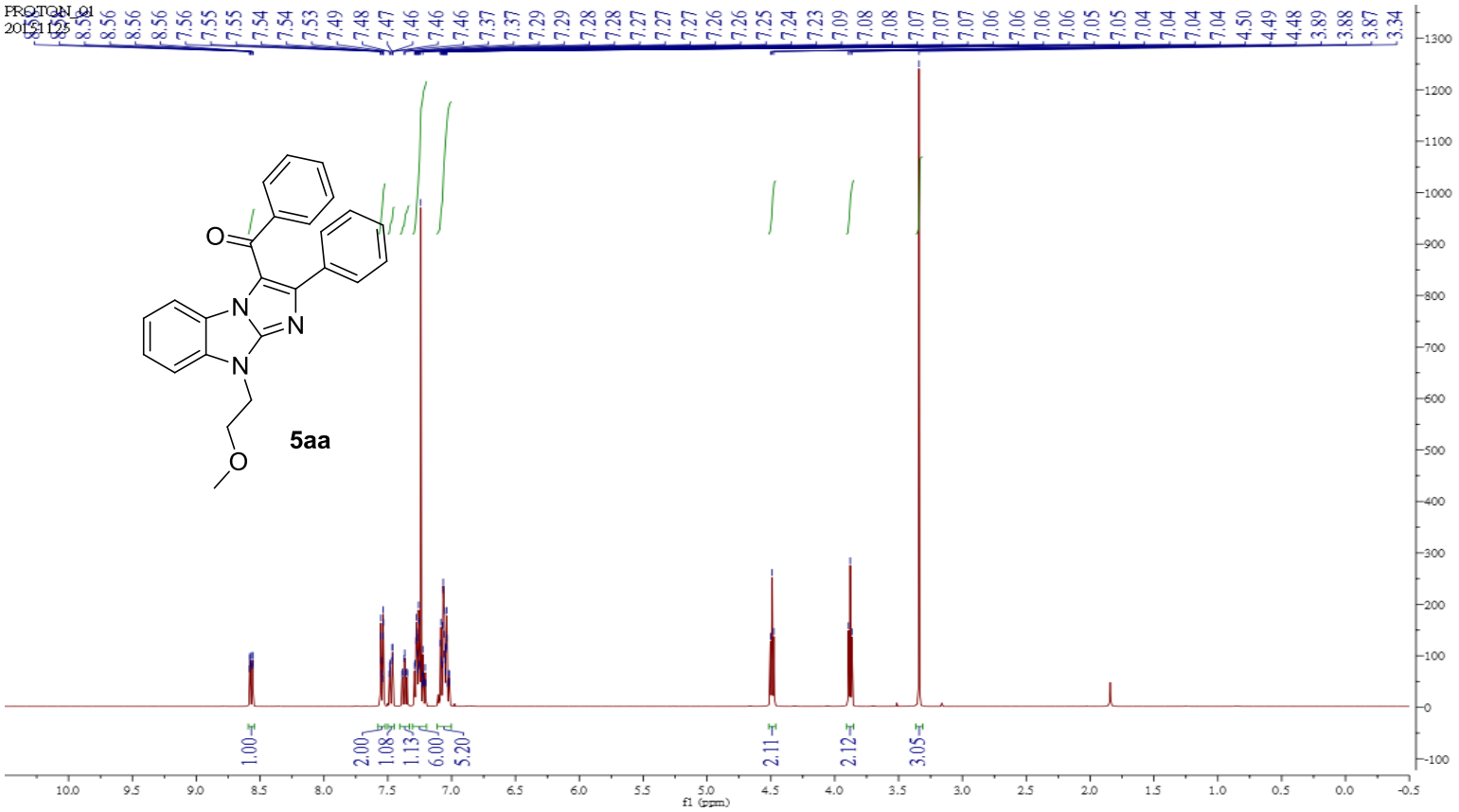
^{13}C NMR spectrum (100MHz) of compound **5z** in Acetone-d_6



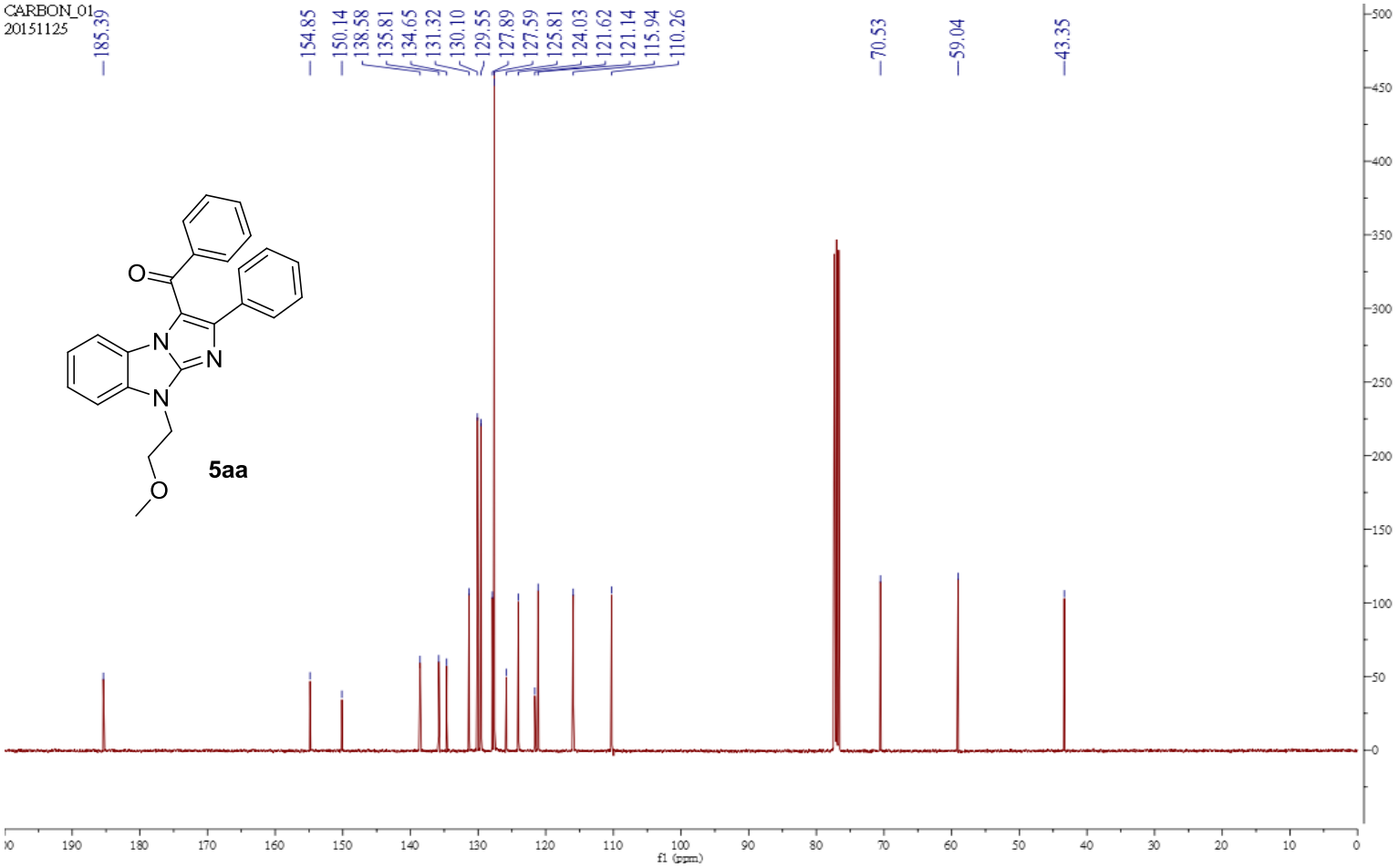
ESI$^+$ Mass spectrum of compound **5z**



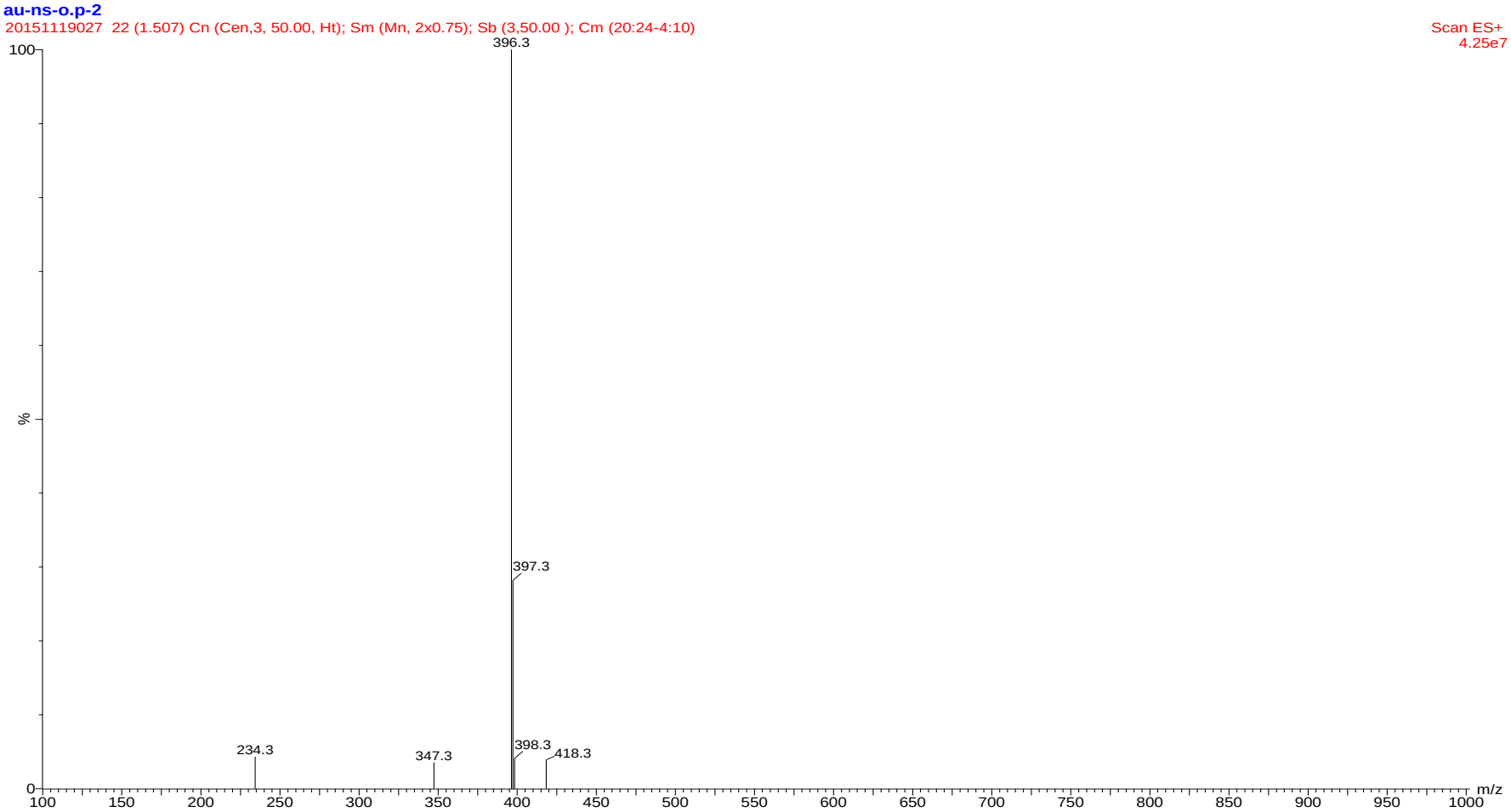
High resolution mass (ESI$^+$) spectrum of compound **5z**



^{1}H NMR spectrum (400MHz) of compound **5aa** in $CDCl_3$



^{13}C NMR spectrum (100MHz) of compound **5aa** in $CDCl_3$



ESI^{+} Mass spectrum of compound **5aa**

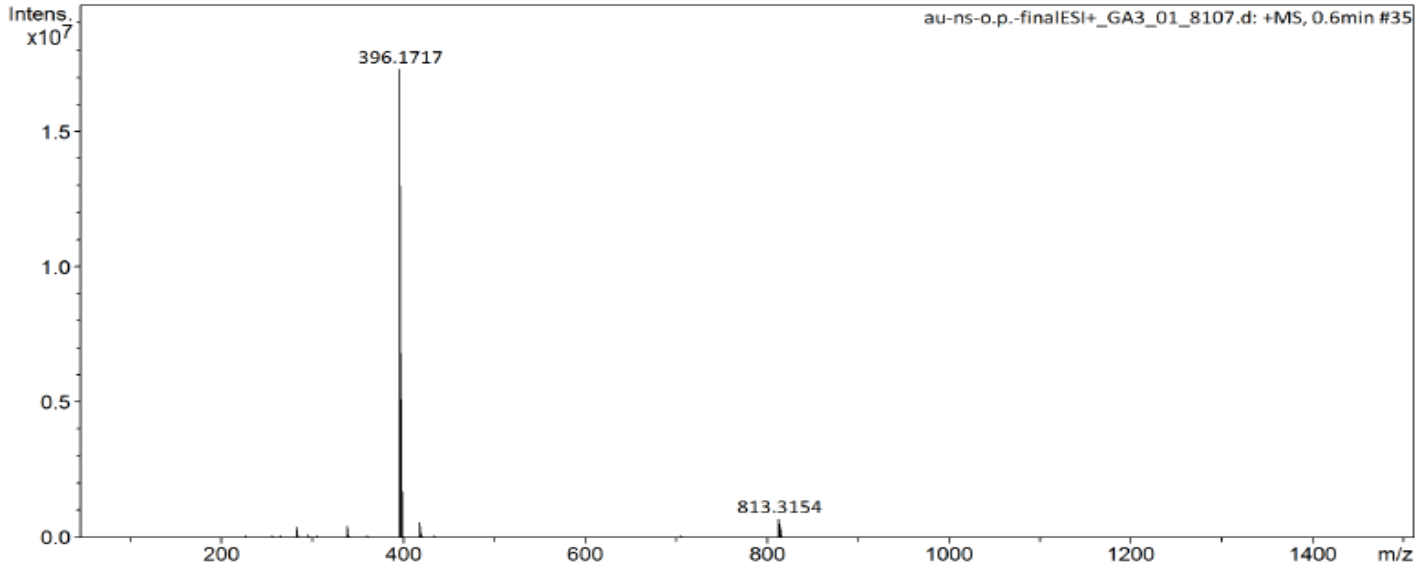
Display Report

Analysis Info

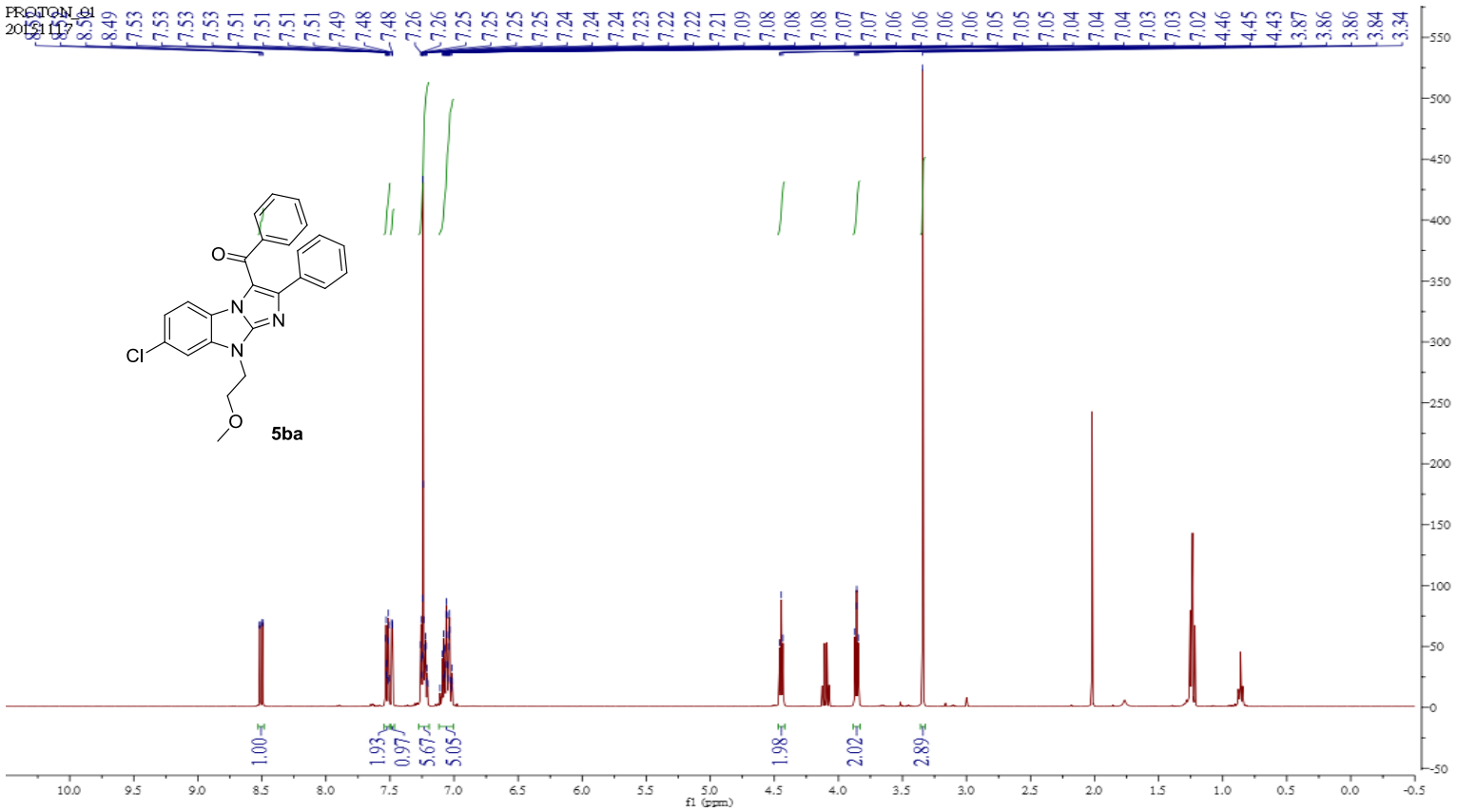
Analysis Name	D:\Data\nctu service\data\2015\20150108\20151127\au-ns-o.p.-finalESI+_GA3_01_8107.d	Acquisition Date	11/27/2015 2:02:23 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	au-ns-o.p.-finalESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

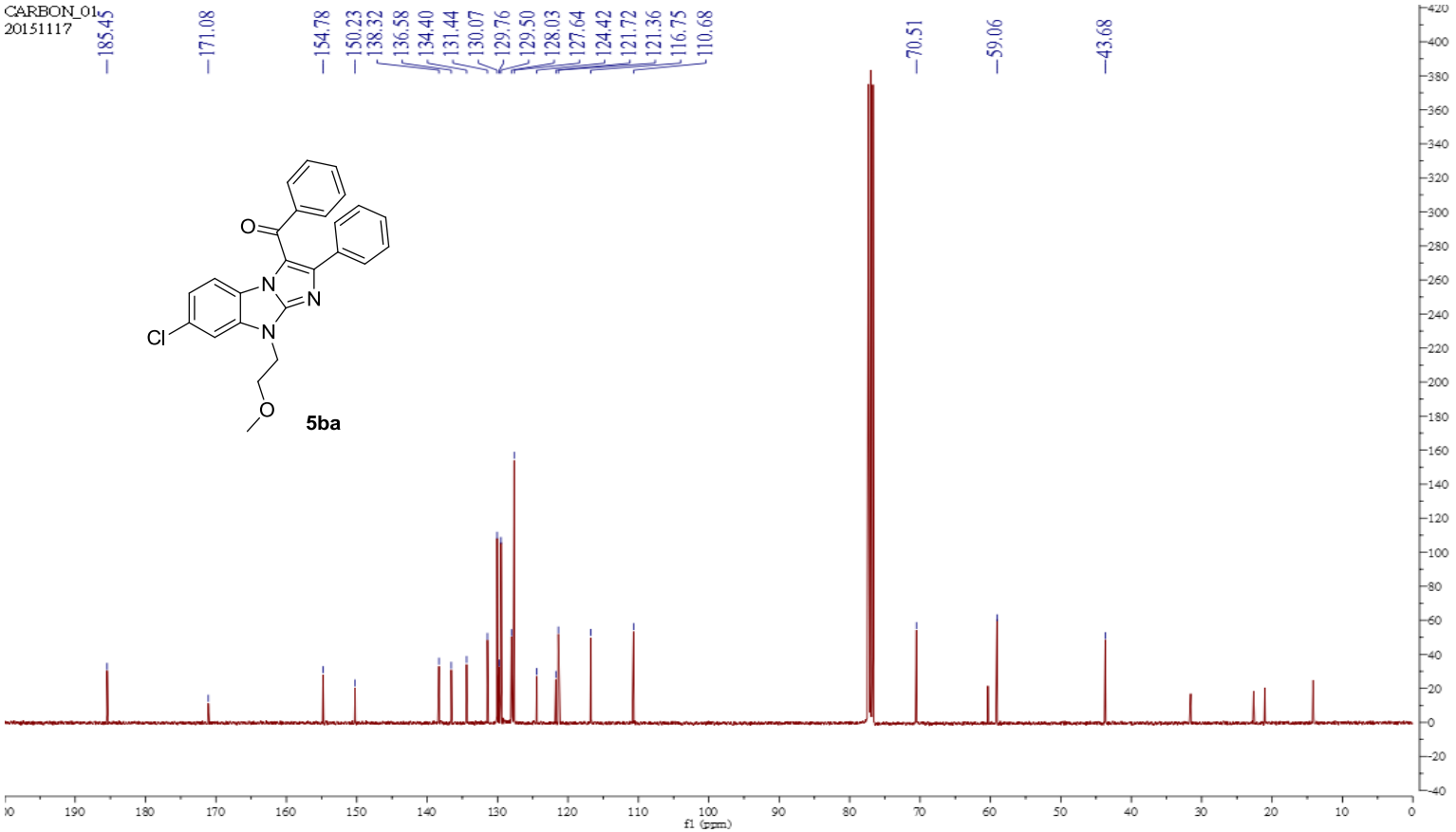
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



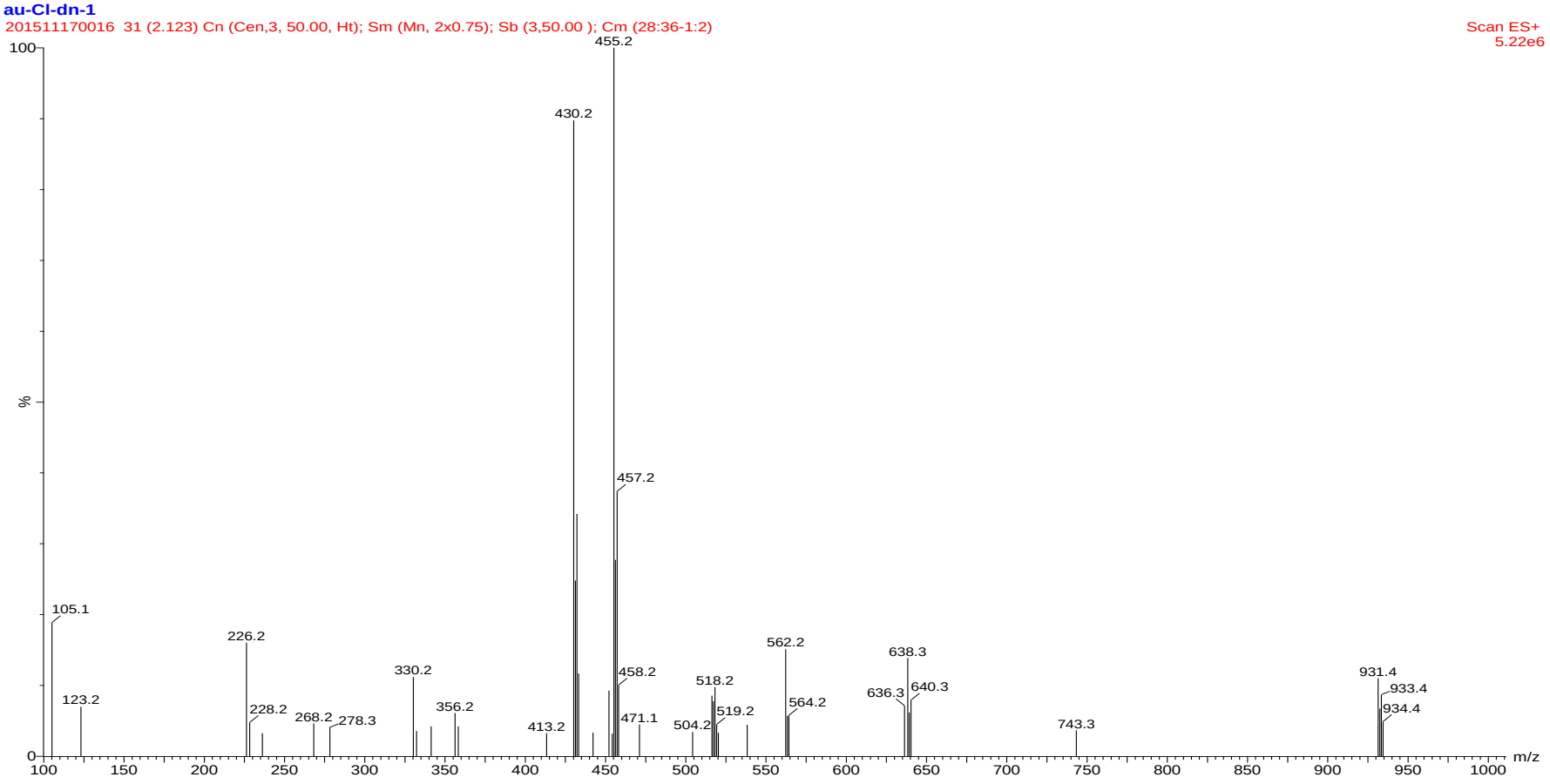
High resolution mass (ESI^+) spectrum of compound **5aa**



^{1}H NMR spectrum (400MHz) of compound **5ba** in $CDCl_3$



^{13}C NMR spectrum (100MHz) of compound **5ba** in $CDCl_3$



ESI^{+} Mass spectrum of compound **5ba**

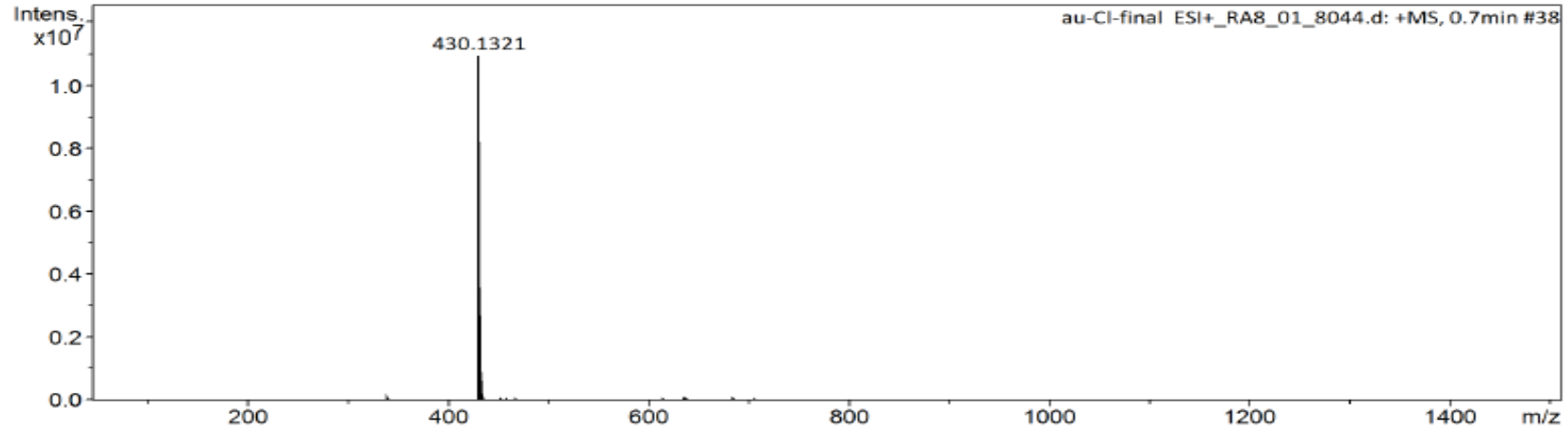
Display Report

Analysis Info

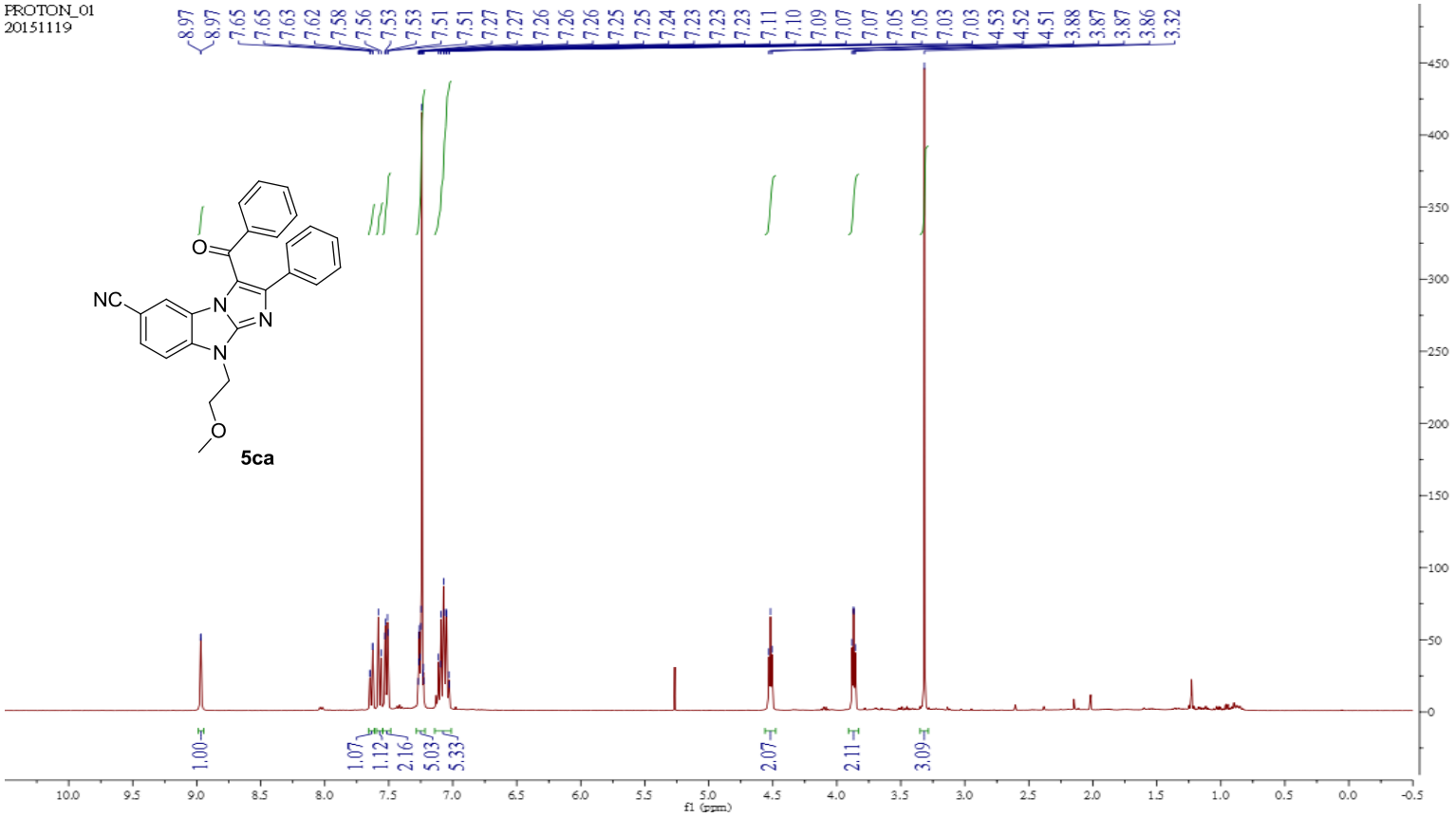
Analysis Name	D:\Data\nctu service\data\2015\20151119\au-Cl-final ESI+_RA8_01_8044.d	Acquisition Date	11/19/2015 4:05:42 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	au-Cl-final ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

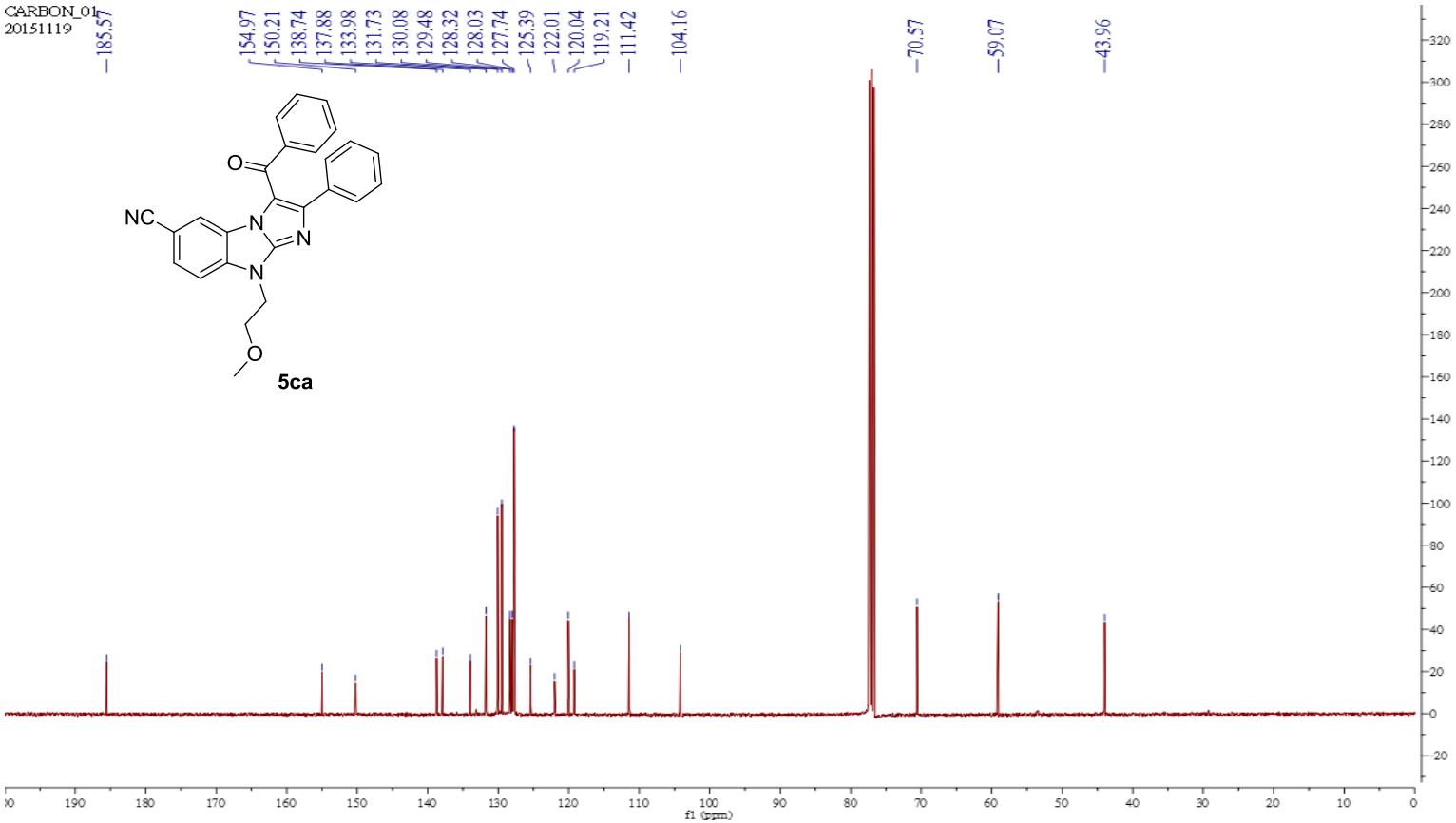
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



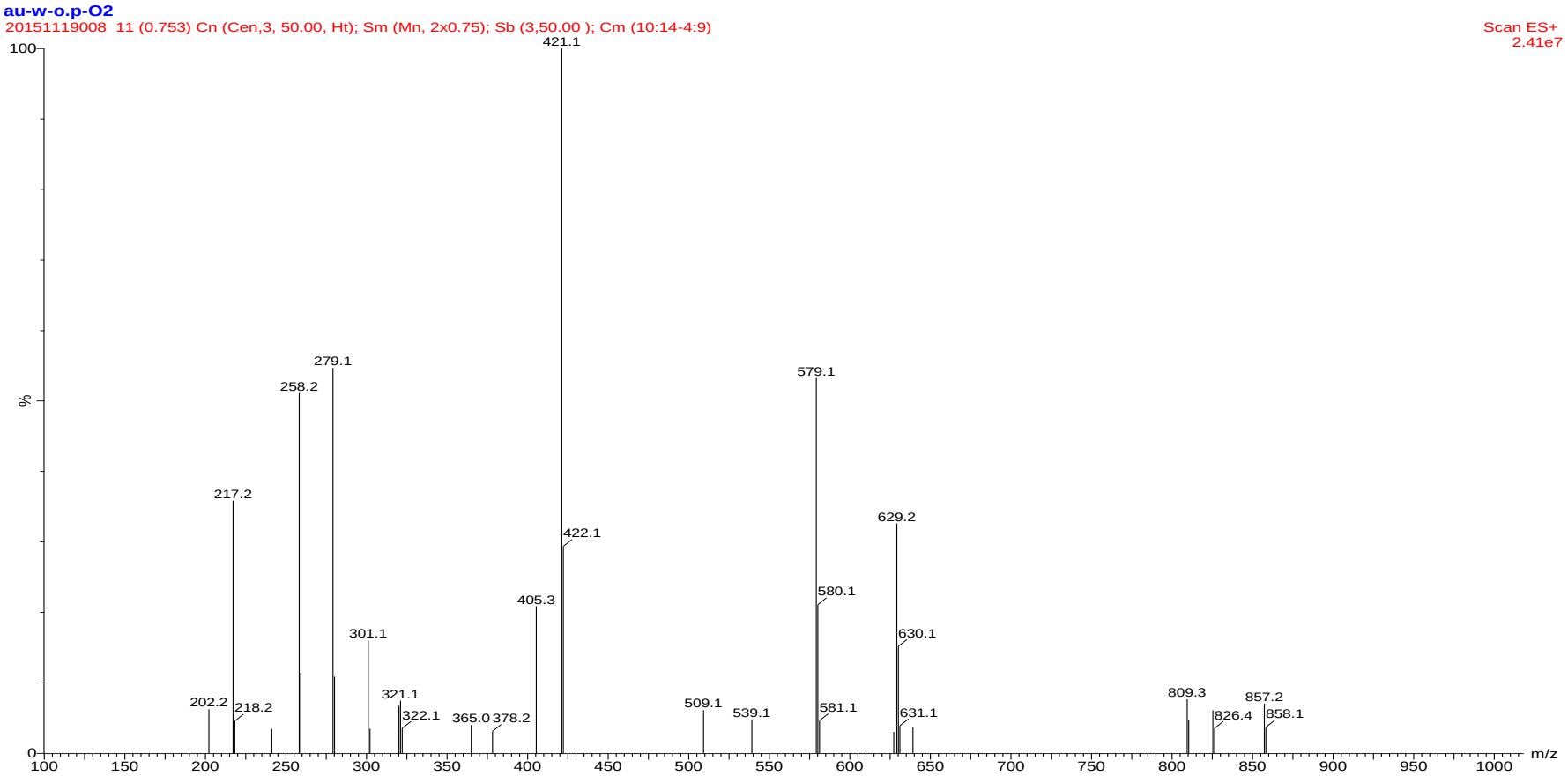
High resolution mass (ESI^+) spectrum of compound **5ba**



^{1}H NMR spectrum (400MHz) of compound **5ca** in $CDCl_3$



^{13}C NMR spectrum (100MHz) of compound **5ca** in $CDCl_3$



ESI^{+} Mass spectrum of compound **5ca**

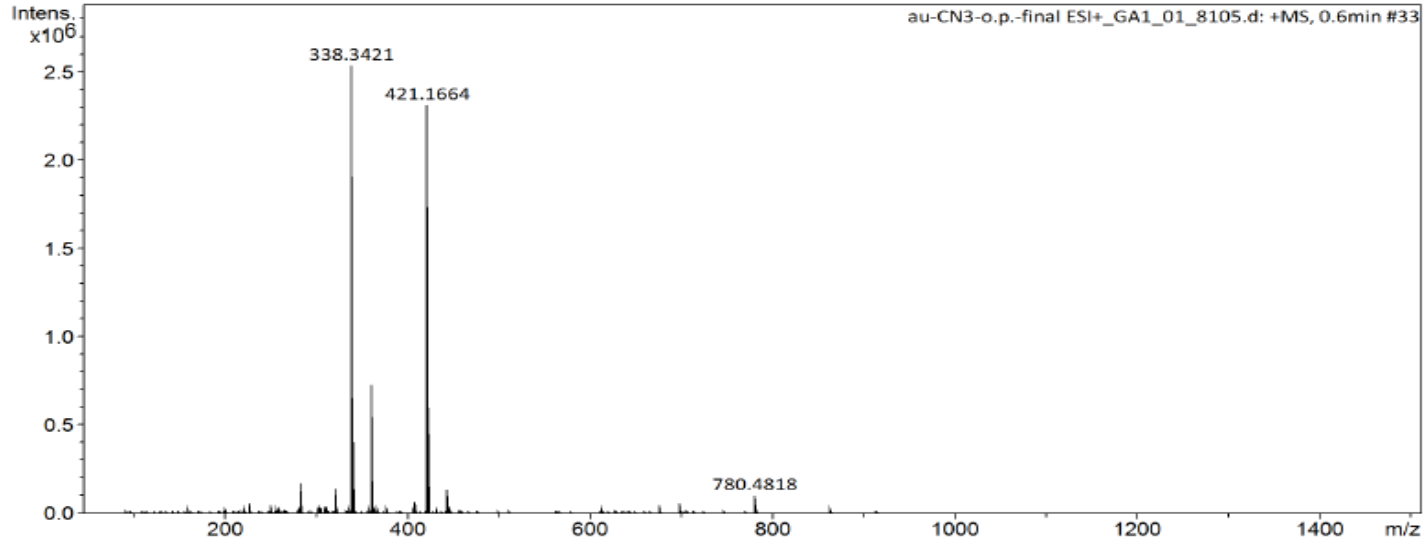
Display Report

Analysis Info

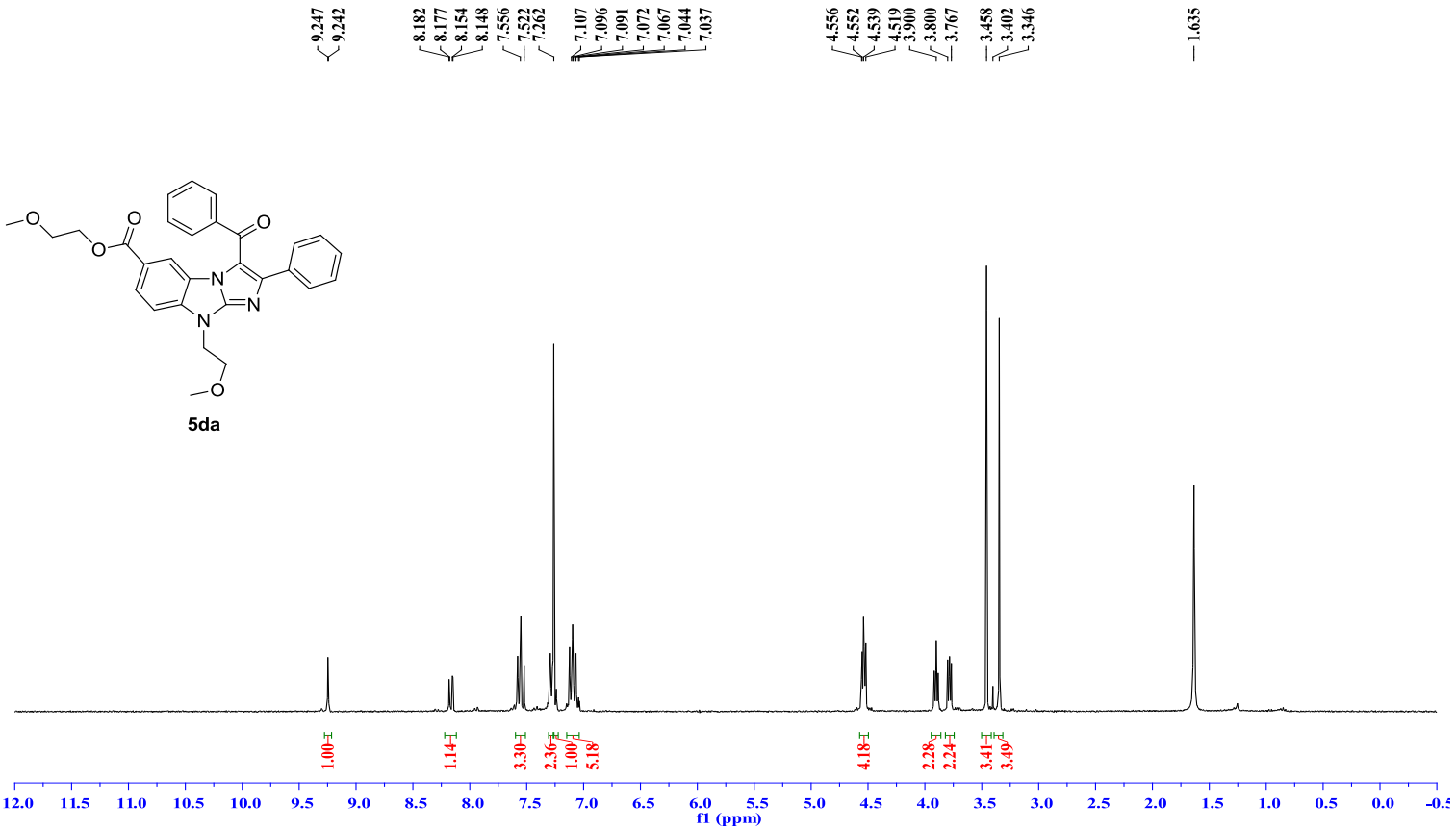
Analysis Name	D:\Data\nctu service\data\2015\20150108\20151127\au-CN3-o.p.-final ESI+_GA1_01_8105.d	Acquisition Date	11/27/2015 1:53:47 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	au-CN3-o.p.-final ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

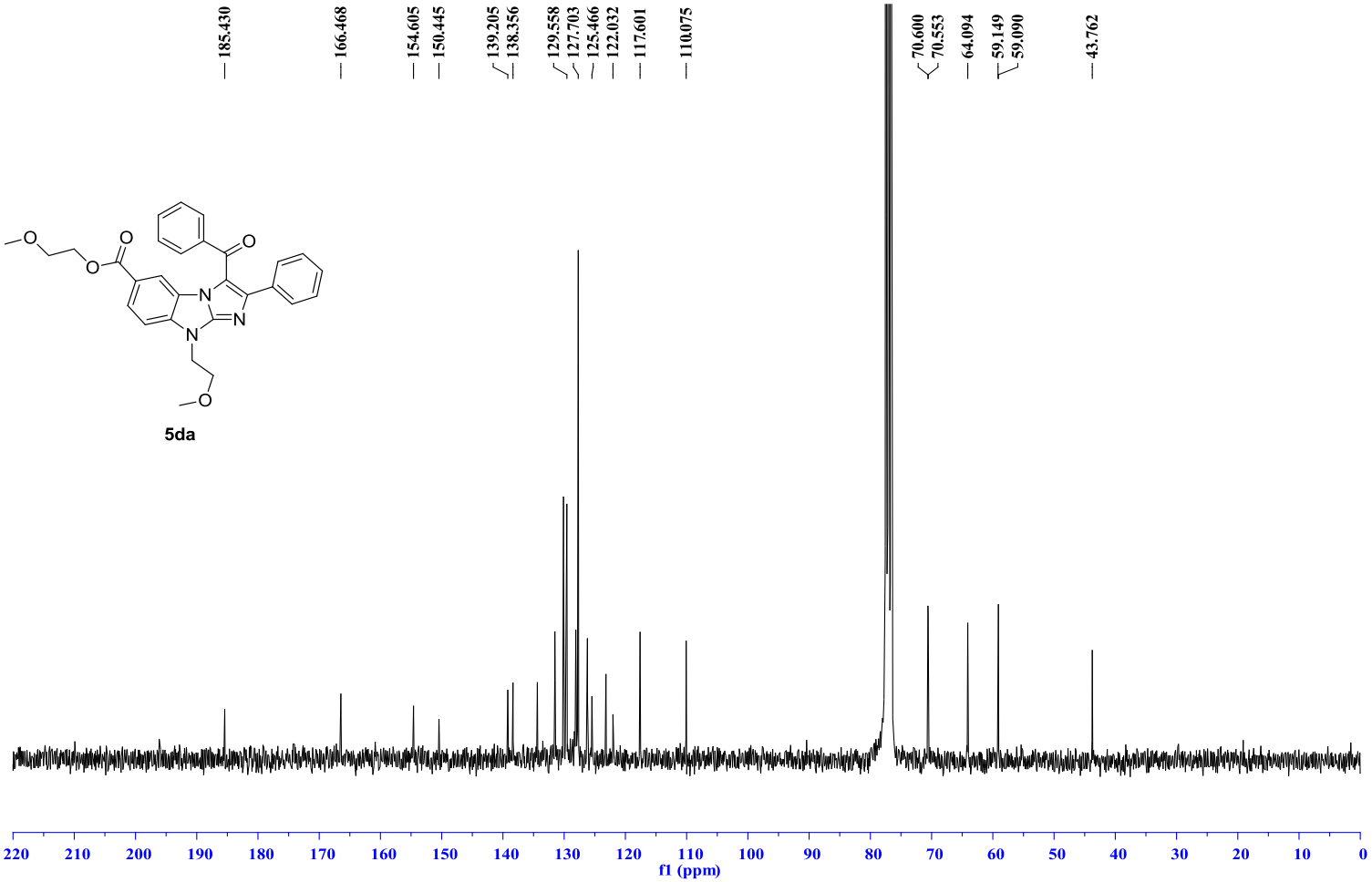
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



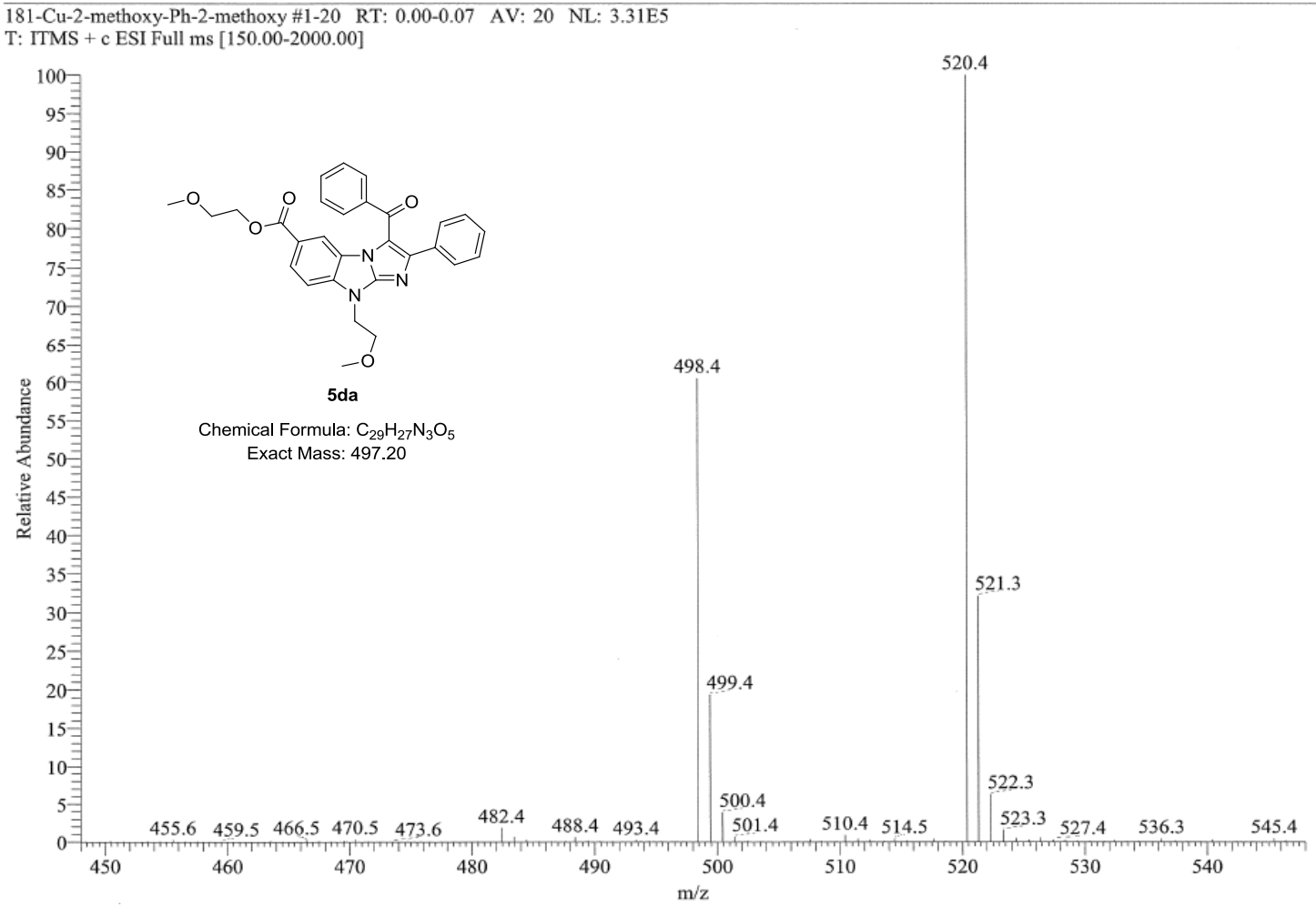
High resolution mass (ESI^+) spectrum of compound **5ca**



^{1}H NMR spectrum (300MHz) of compound **5da** in $CDCl_3$



^{13}C NMR spectrum (75MHz) of compound **5da** in $CDCl_3$

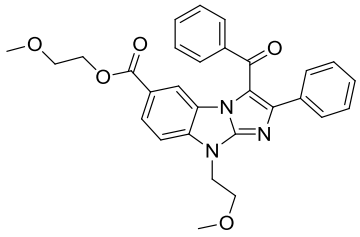


ESI$^+$ Mass spectrum of compound **5da**

180-Cu-2-methoxy-Ph-2-methoxy-H#1-20 RT: 0.00-0.28 AV: 20
T: FTMS + p ESI Full ms [150.00-2000.00]
m/z= 486.9149-508.6513

Isotope	Min	Max
C-12	0	30
H-1	0	30
O-16	0	5
N-14	0	4

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

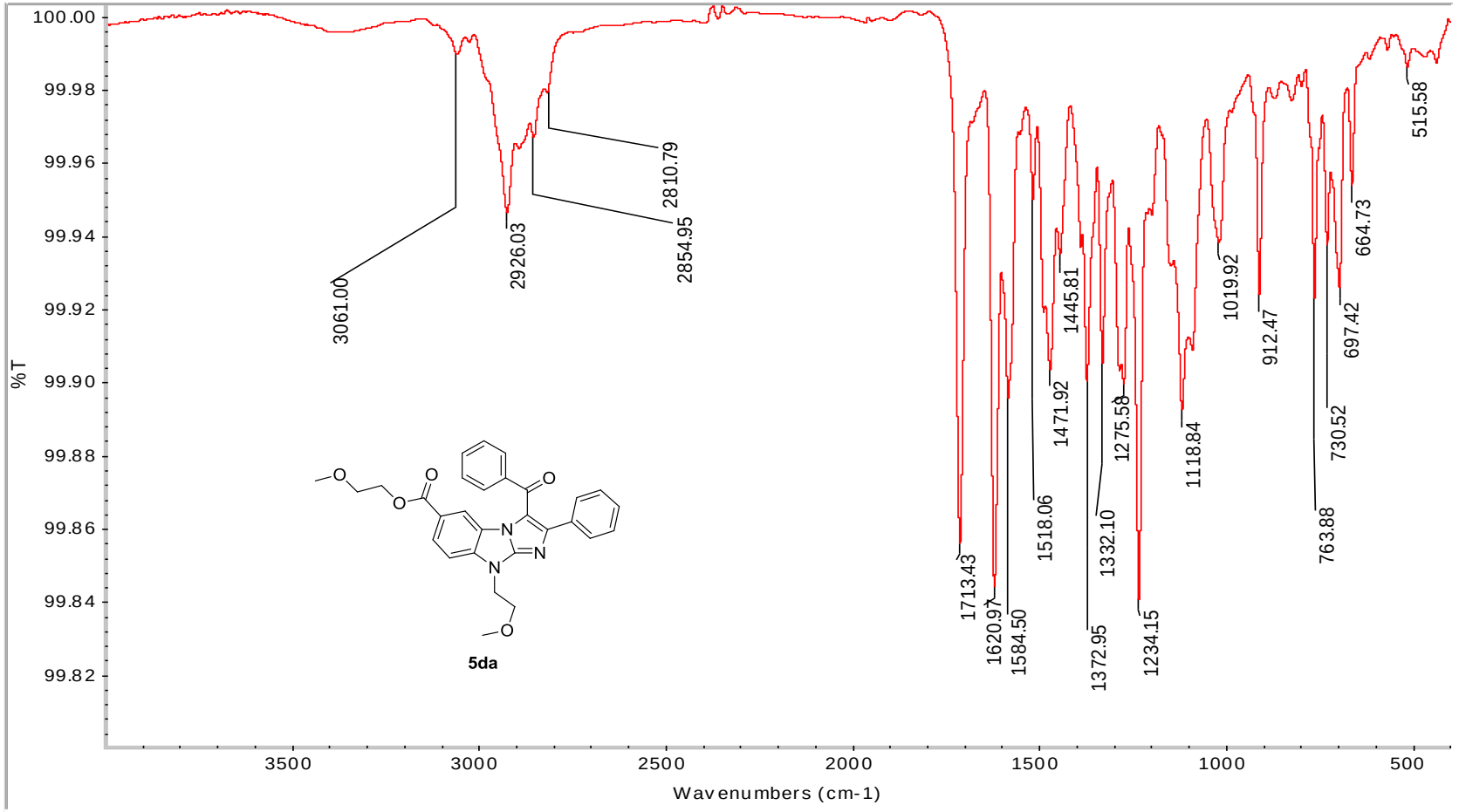


5da

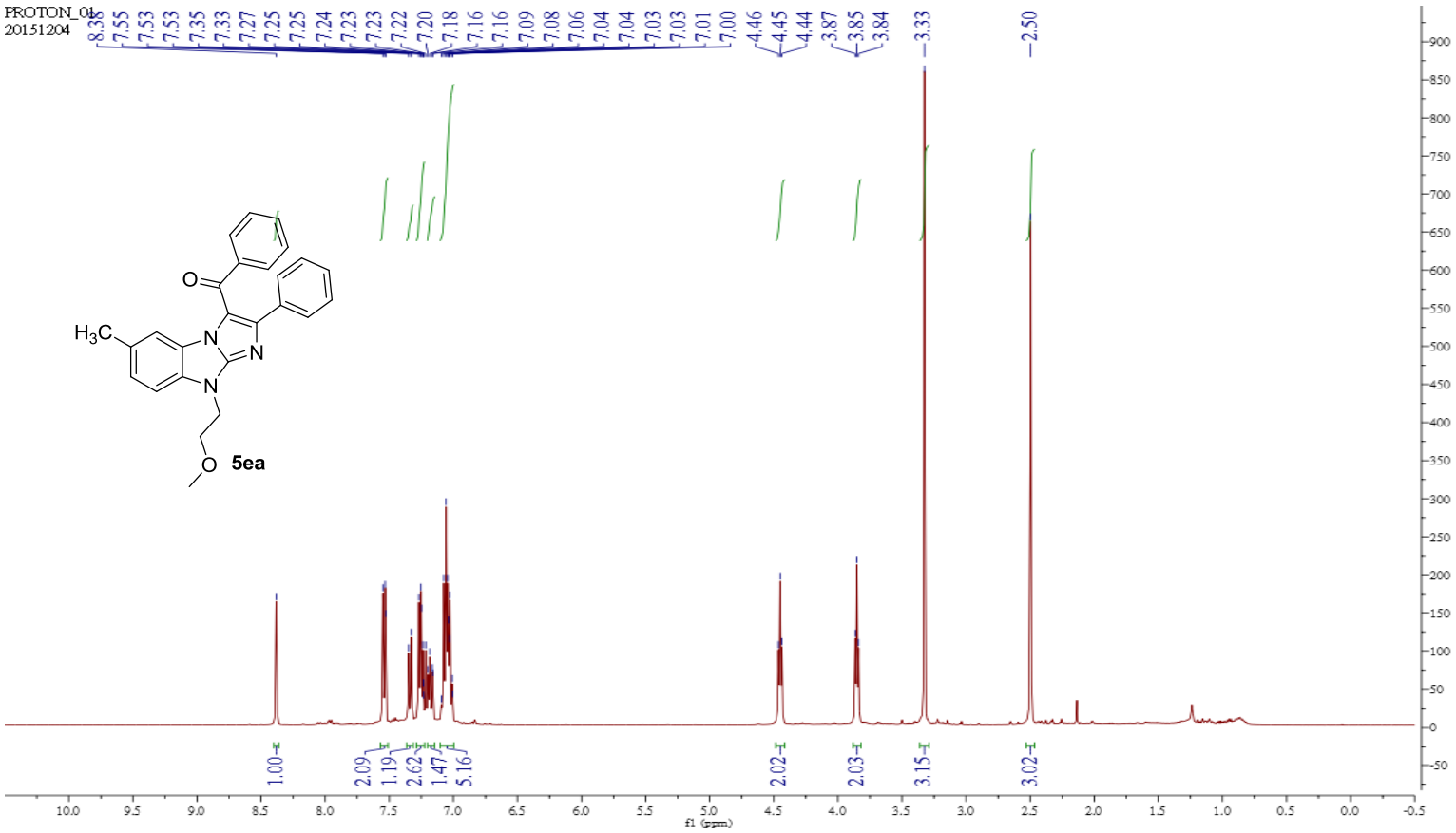
Chemical Formula: $C_{29}H_{27}N_3O_5$
Exact Mass: 497.20

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
498.2016	3386090.8	100.00	498.2023	-1.49	$C_{29}H_{28}O_5N_3$

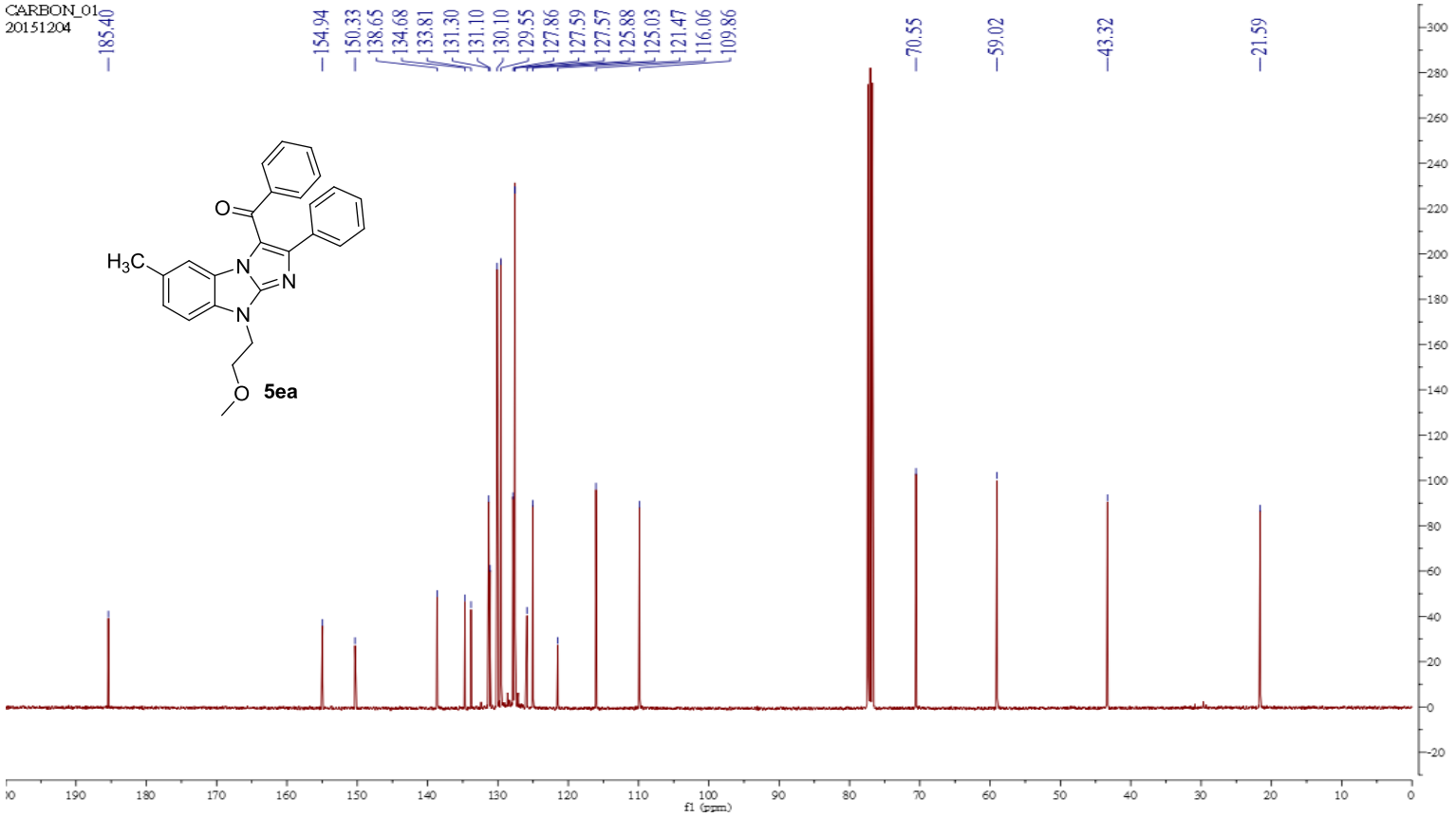
High resolution mass (ESI^+) spectrum of compound **5da**



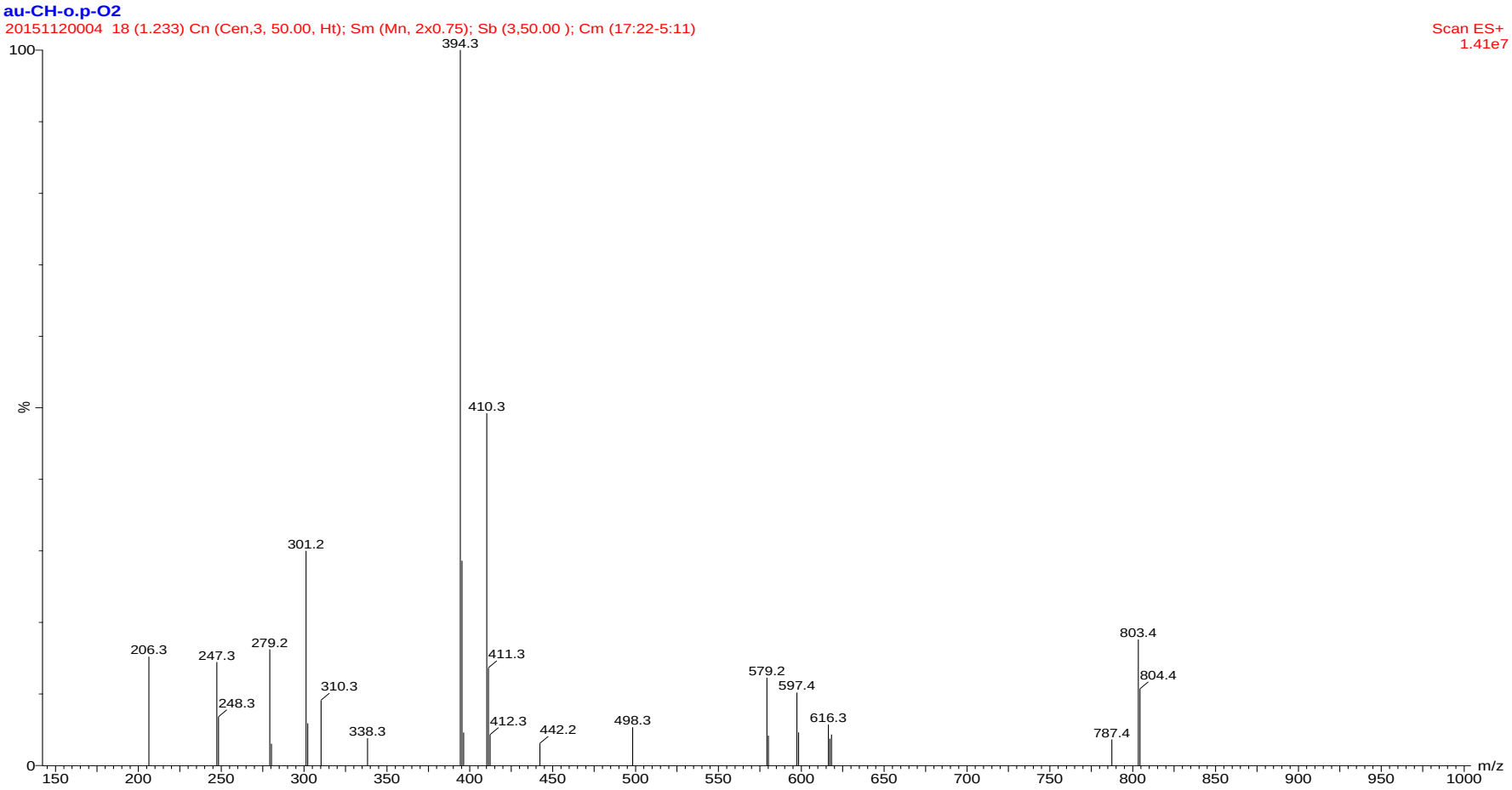
IR spectrum of compound **5da**



^{1}H NMR spectrum (400MHz) of compound **5ea** in $CDCl_3$



^{13}C NMR spectrum (100MHz) of compound **5ea** in $CDCl_3$



ESI^{+} Mass spectrum of compound **5ea**

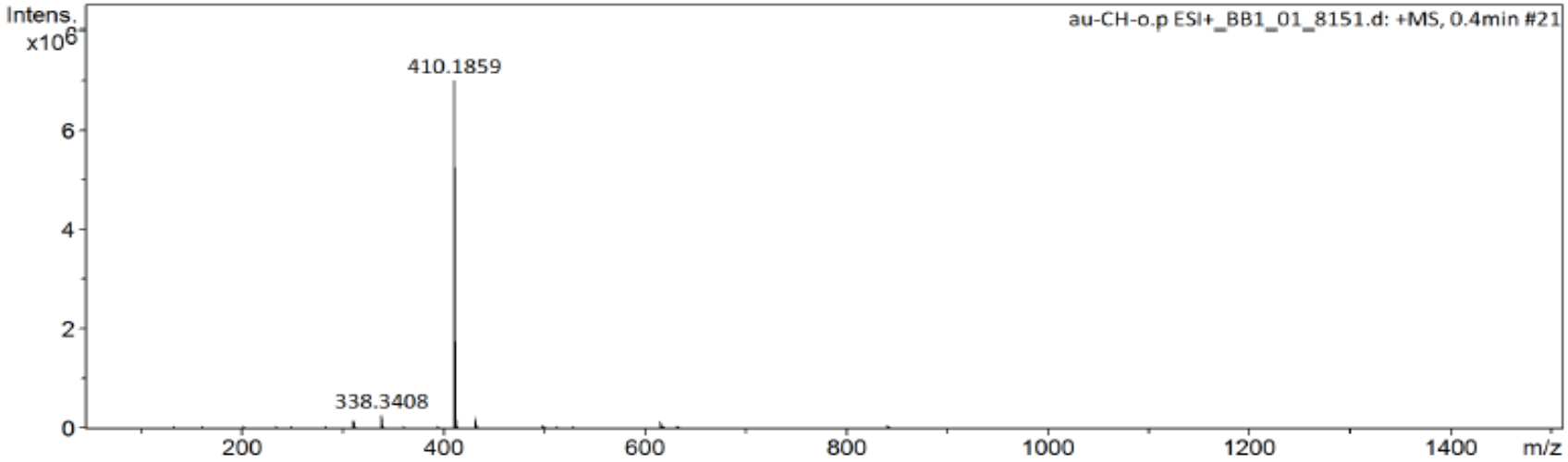
Display Report

Analysis Info

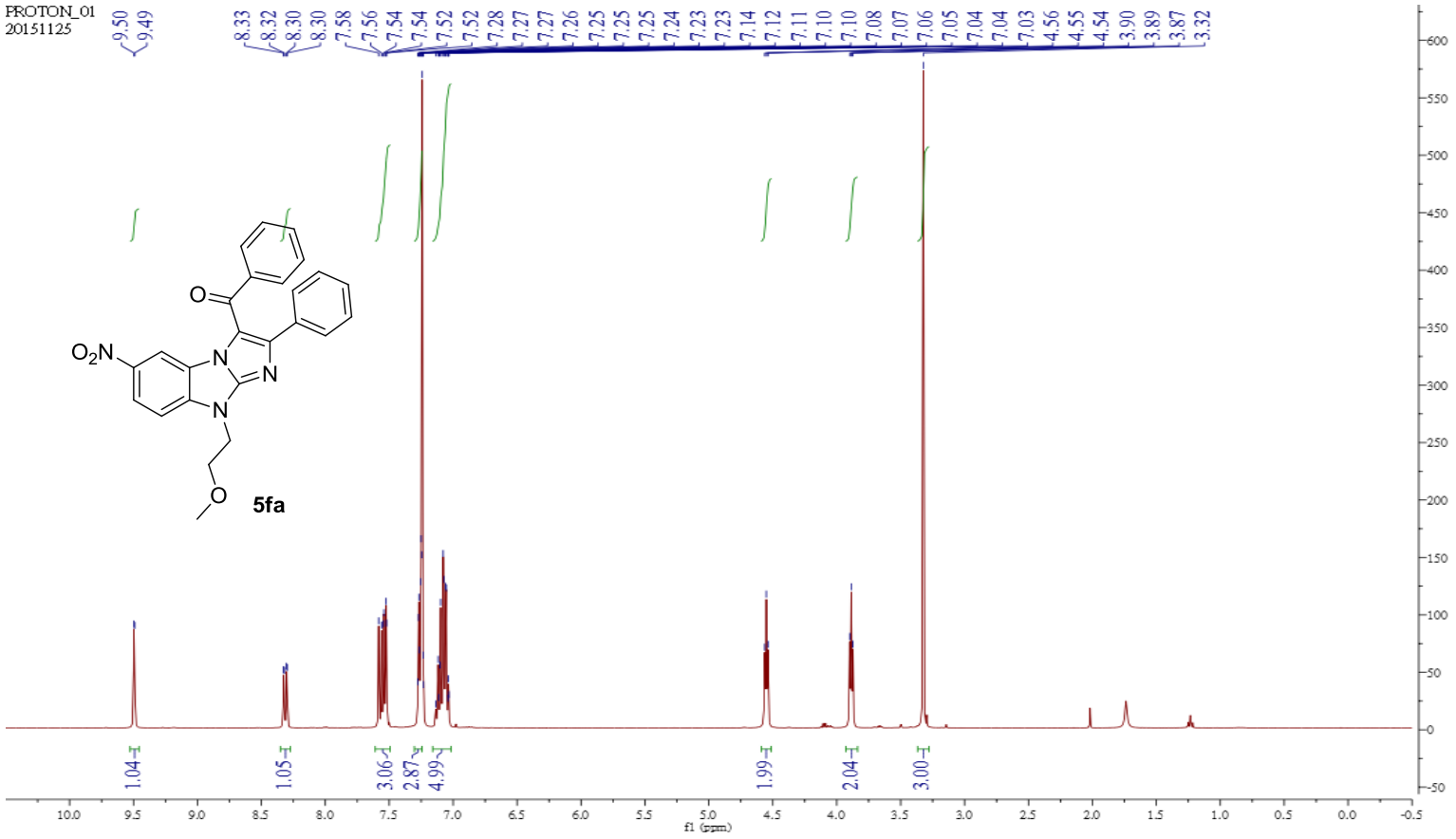
Analysis Name	D:\Data\nctu service\data\2015\20151208\au-CH-o.p ESI+_BB1_01_8151.d	Acquisition Date	12/8/2015 1:33:55 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	au-CH-o.p ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

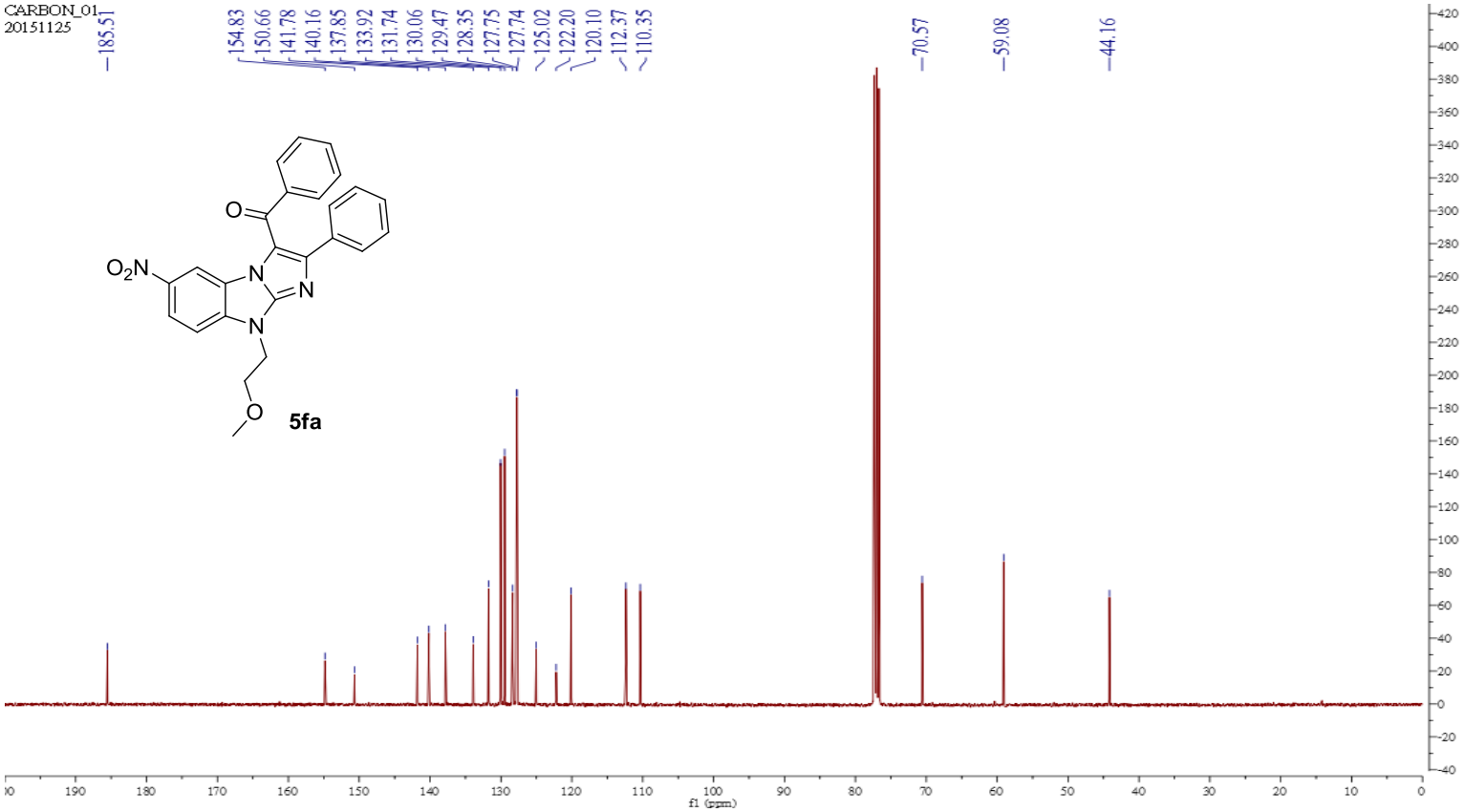
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



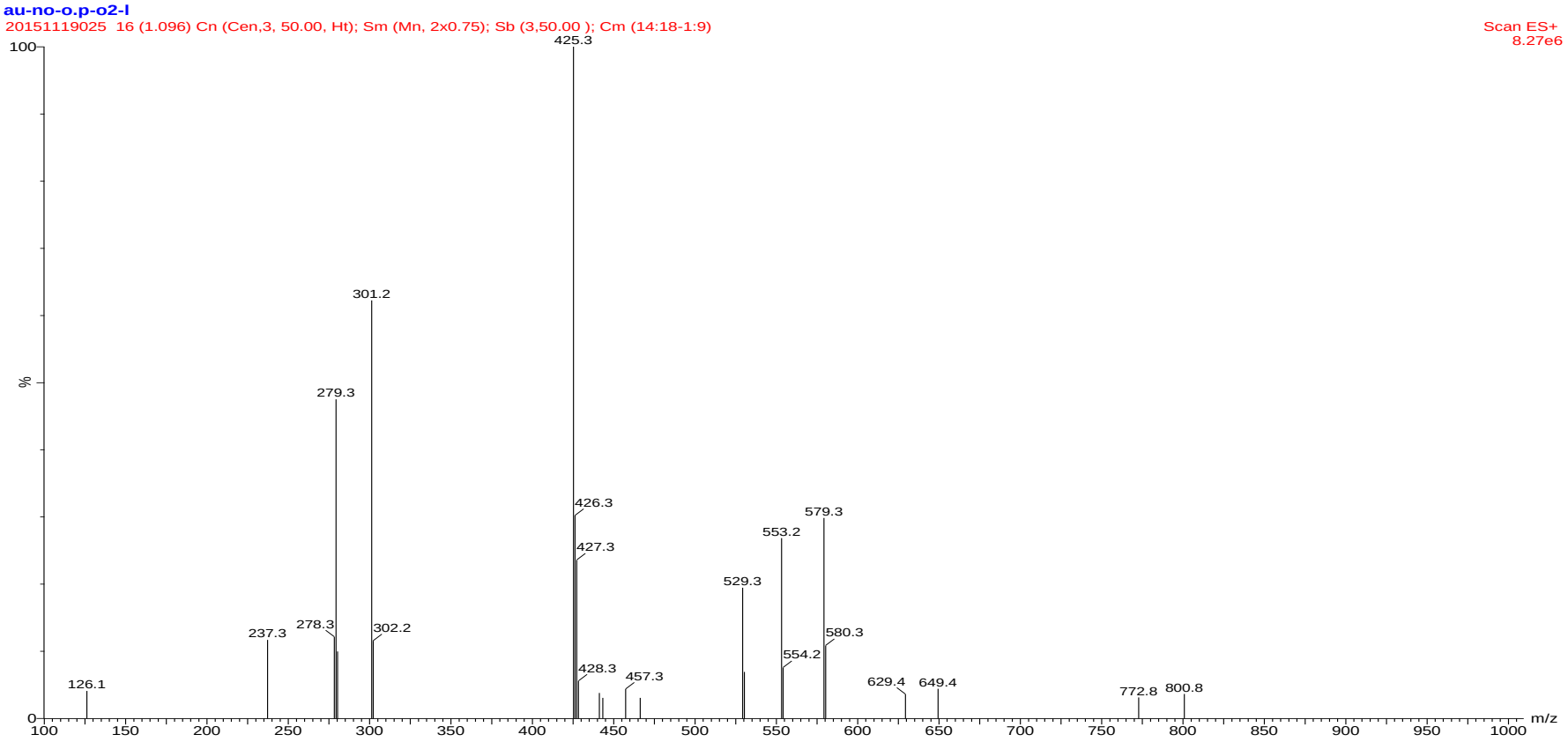
High resolution mass (ESI^+) spectrum of compound **5ea**



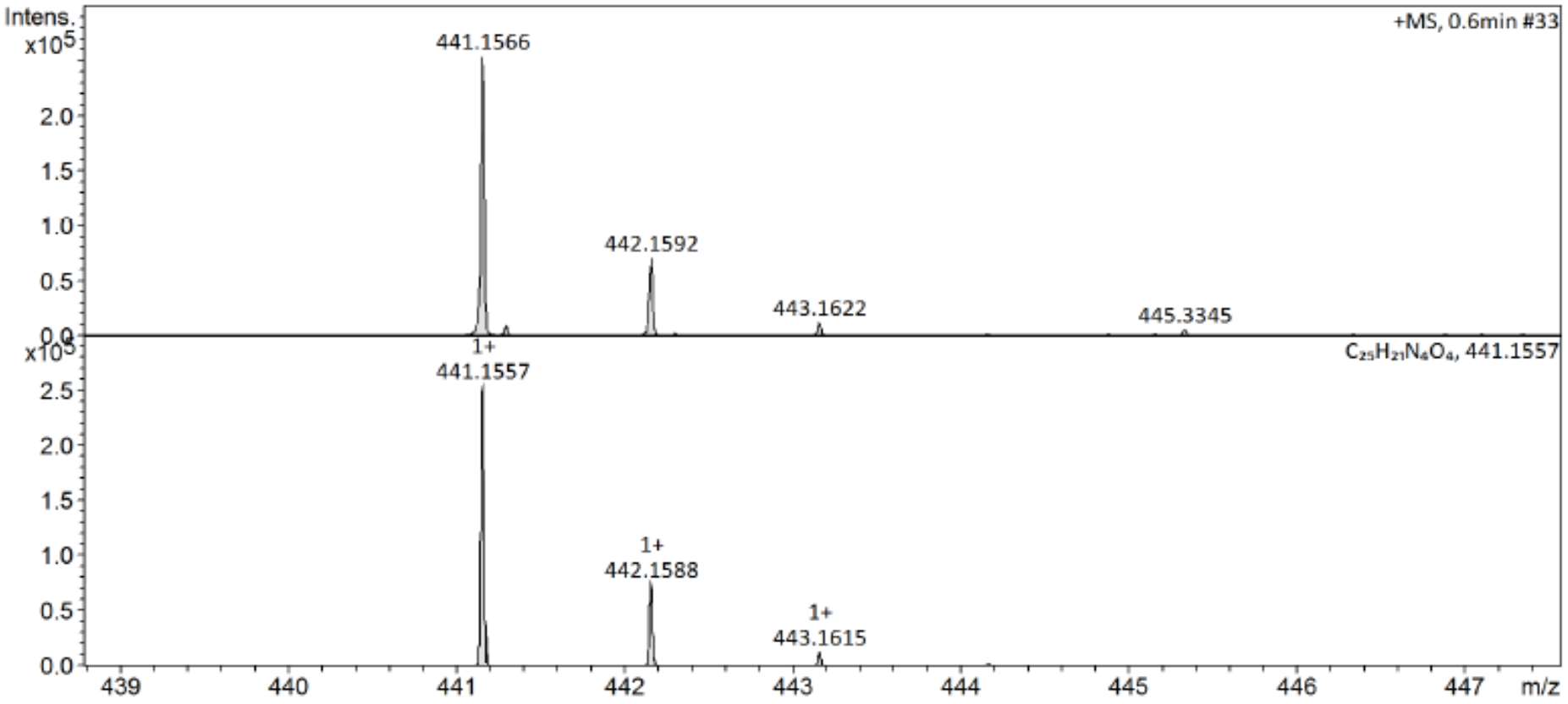
^{1}H NMR spectrum (400MHz) of compound **5fa** in $CDCl_3$



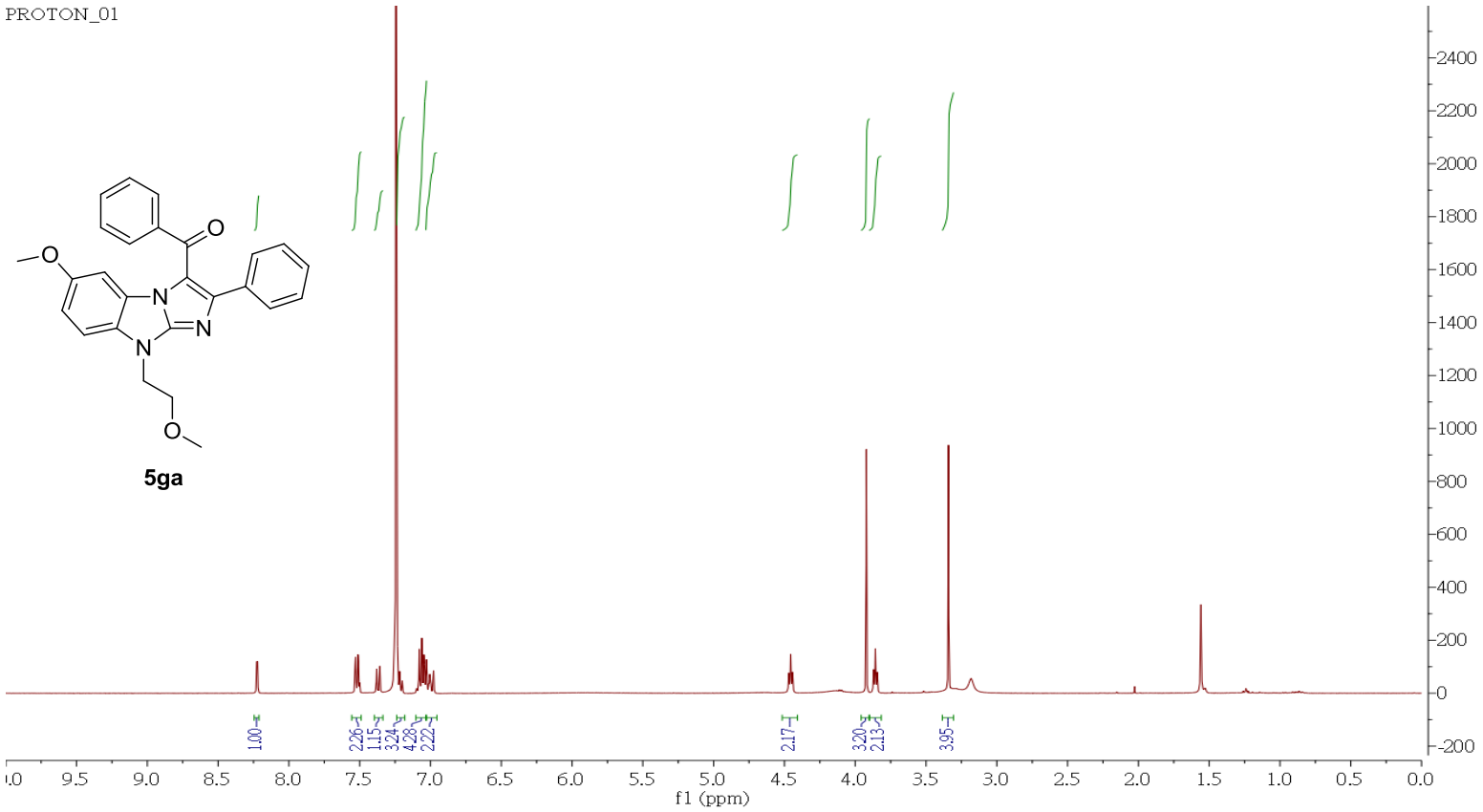
^{13} C NMR spectrum (100MHz) of compound **5fa** in $CDCl_3$



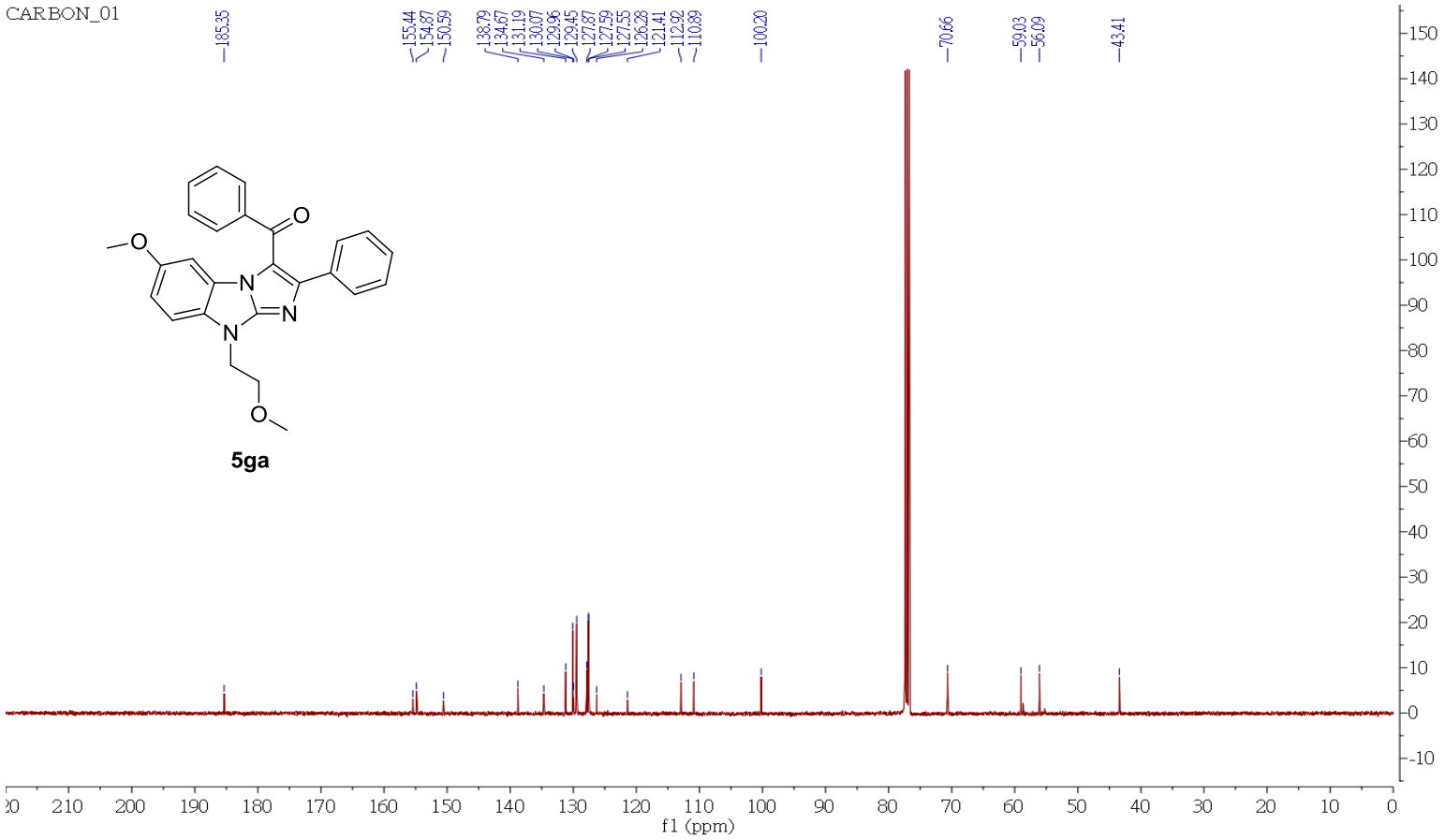
ESI^{+} Mass spectrum of compound **5fa**



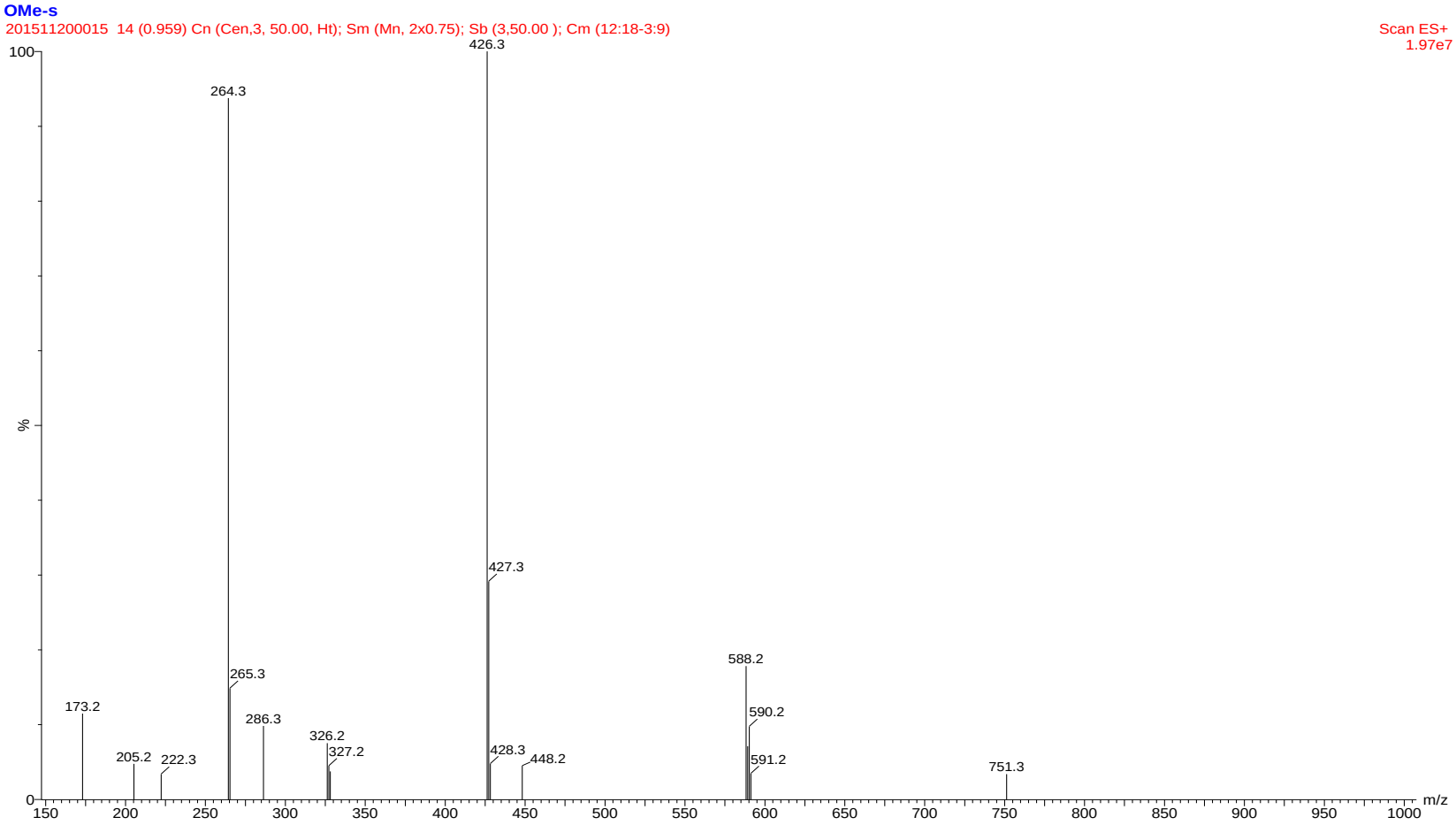
High resolution mass (ESI^+) spectrum of compound **5fa**



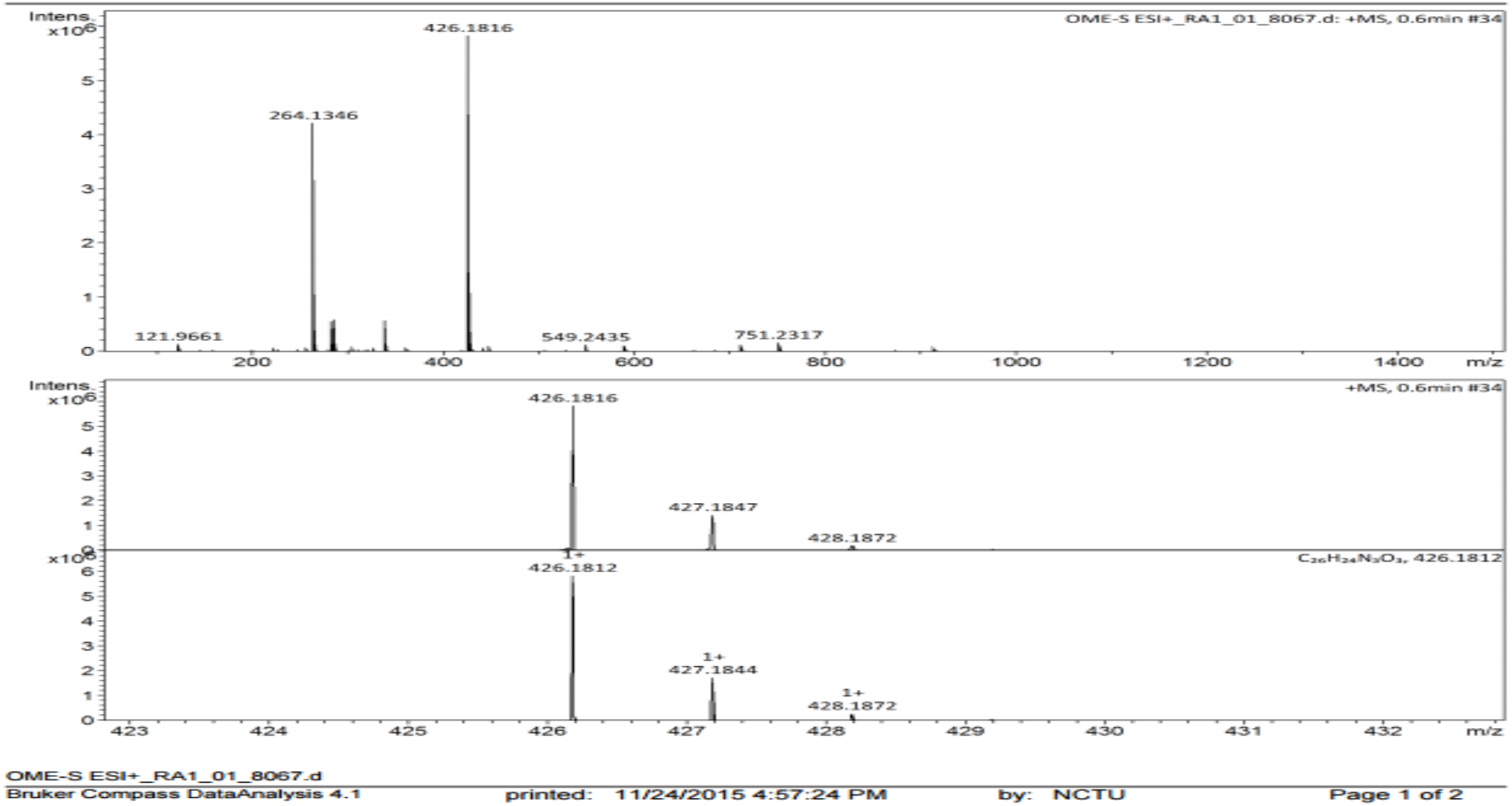
^{1}H NMR spectrum (400MHz) of compound **5ga** in $CDCl_3$



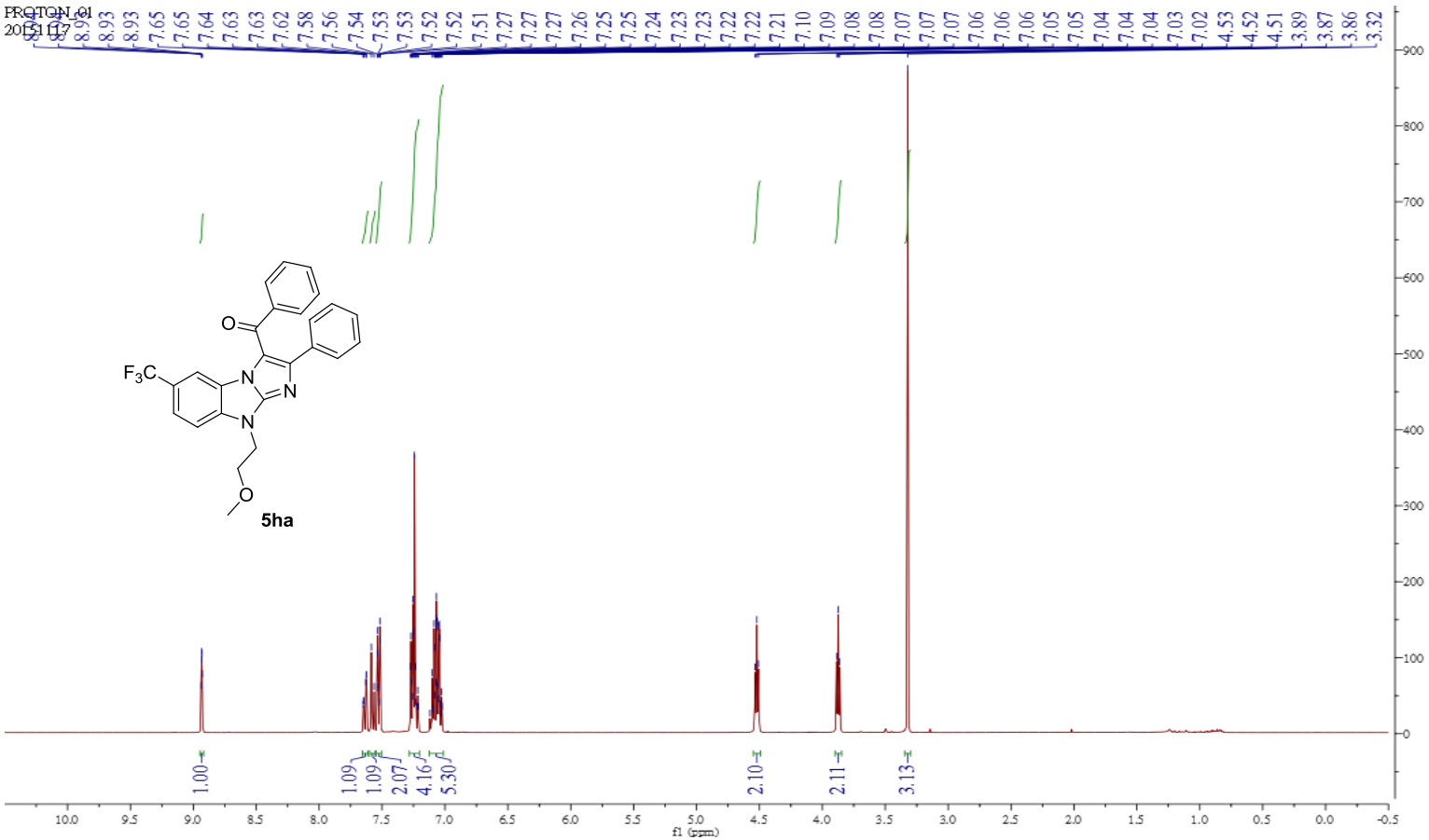
^{13}C NMR spectrum (100MHz) of compound **5ga** in $CDCl_3$



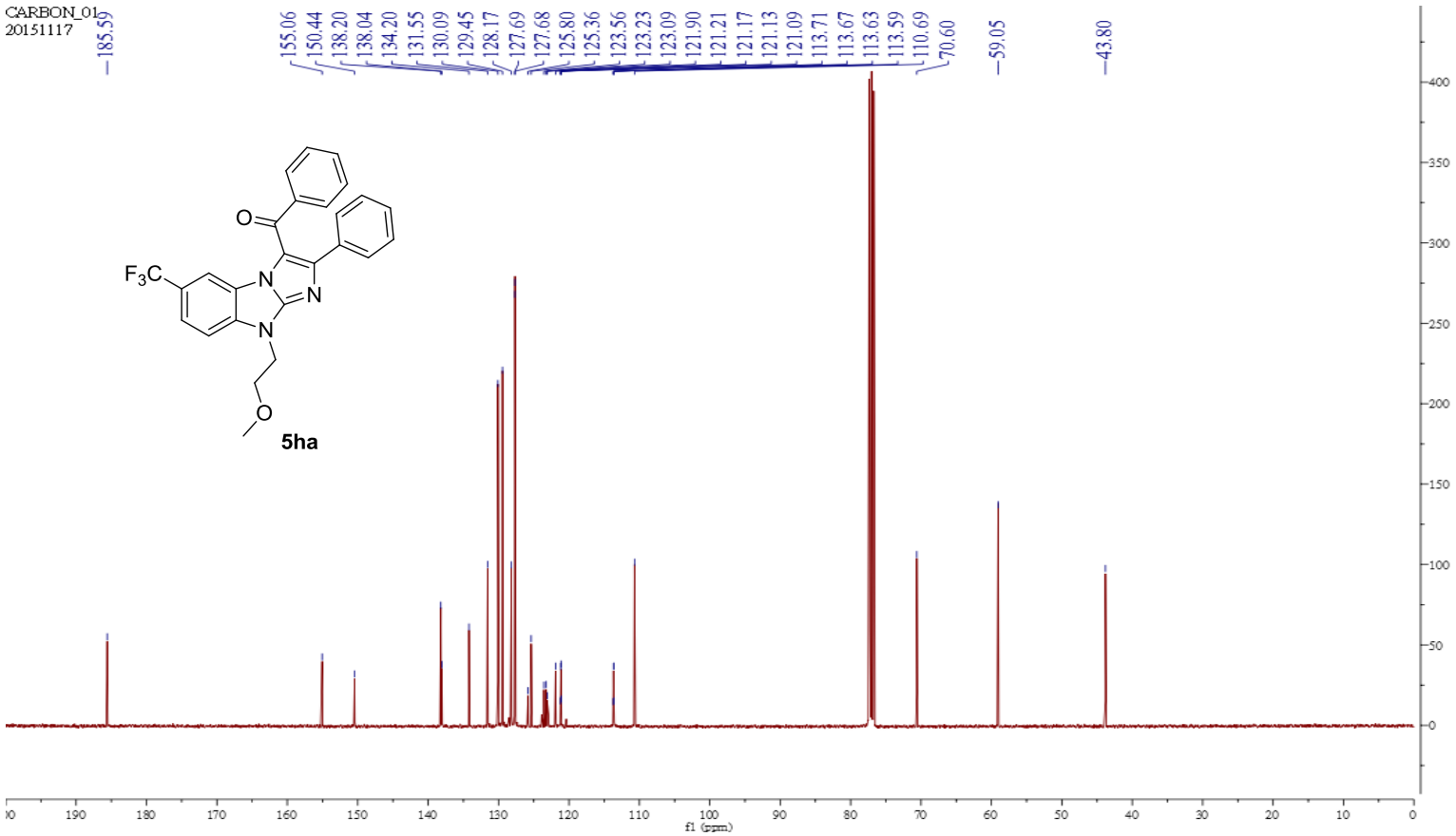
ESI$^+$ Mass spectrum of compound **5ga**



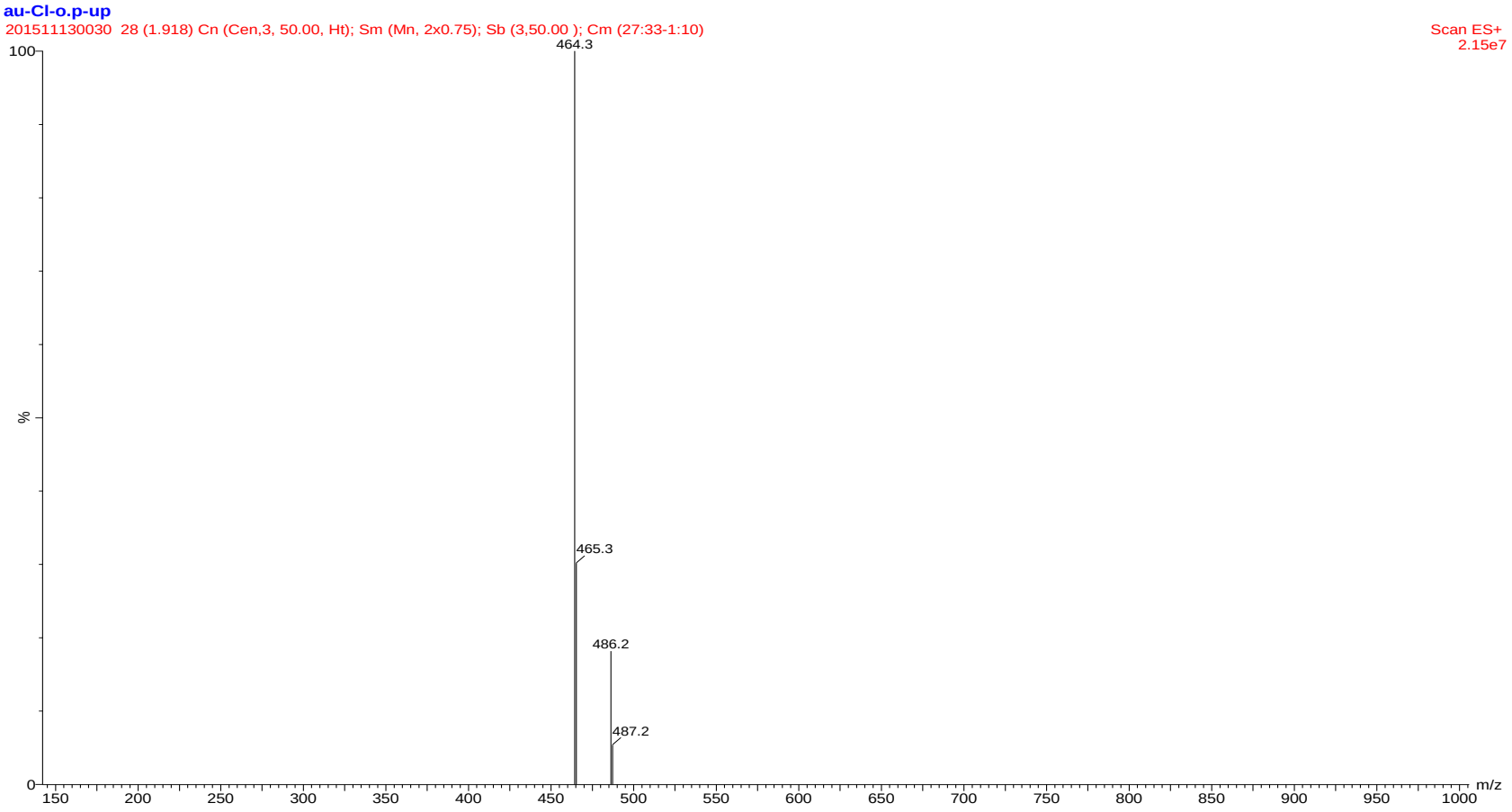
High resolution mass (ESI^+) spectrum of compound **5ga**



^{1}H NMR spectrum (400MHz) of compound **5ha** in $CDCl_3$



^{1}H NMR spectrum (100MHz) of compound **5ha** in $CDCl_3$



ESI$^+$ Mass spectrum of compound **5ha**

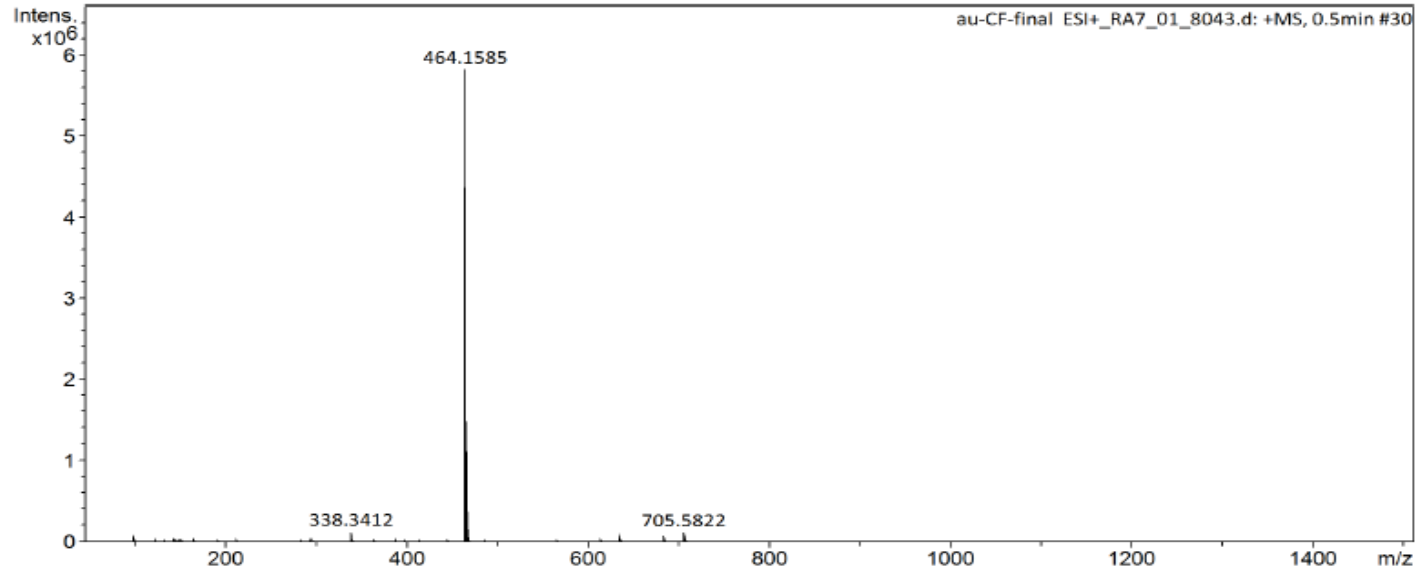
Display Report

Analysis Info

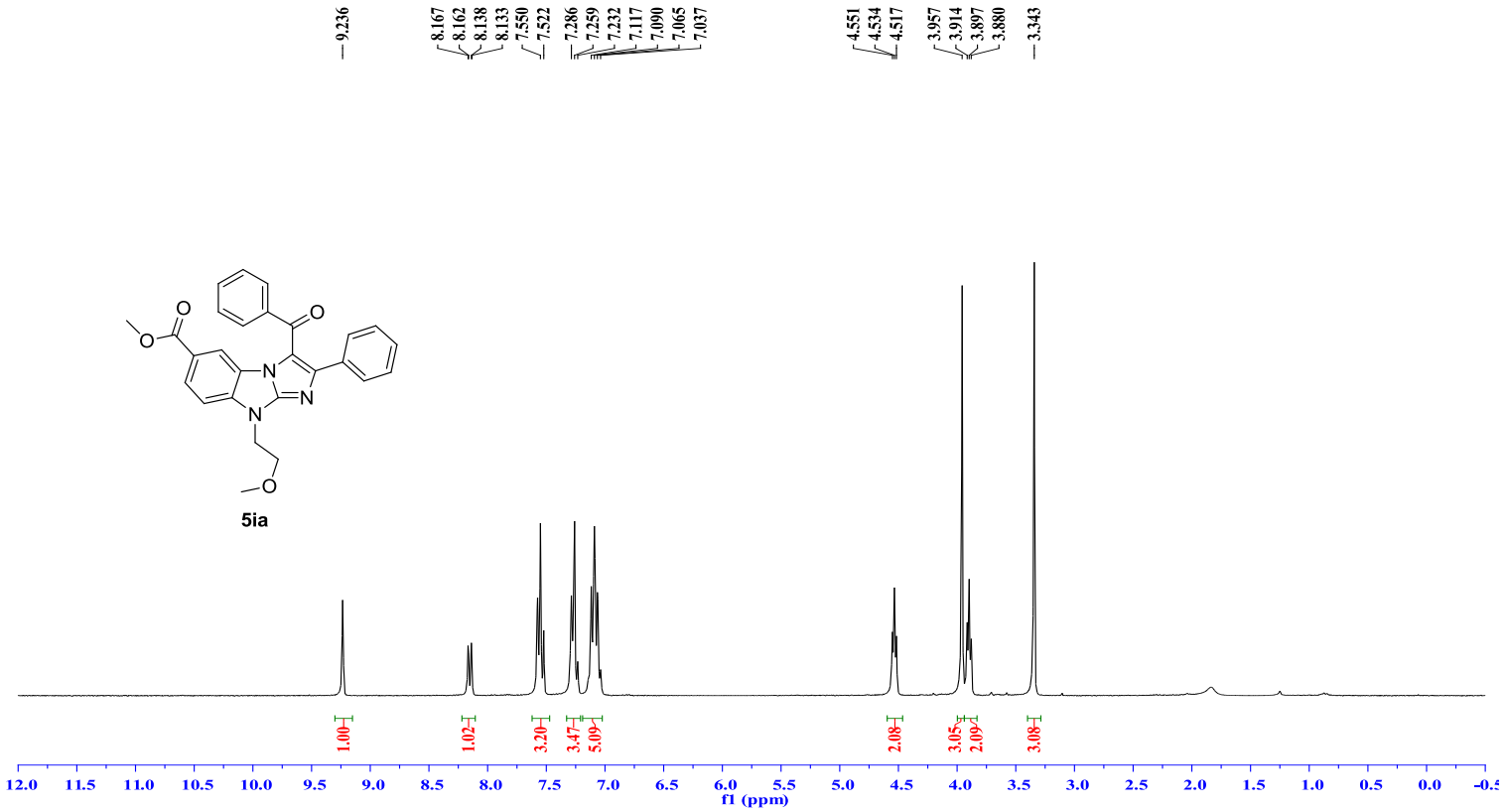
Analysis Name	D:\Data\nctu service\data\2015\20151119\au-CF-final ESI+_RA7_01_8043.d	Acquisition Date	11/19/2015 4:01:28 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	au-CF-final ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

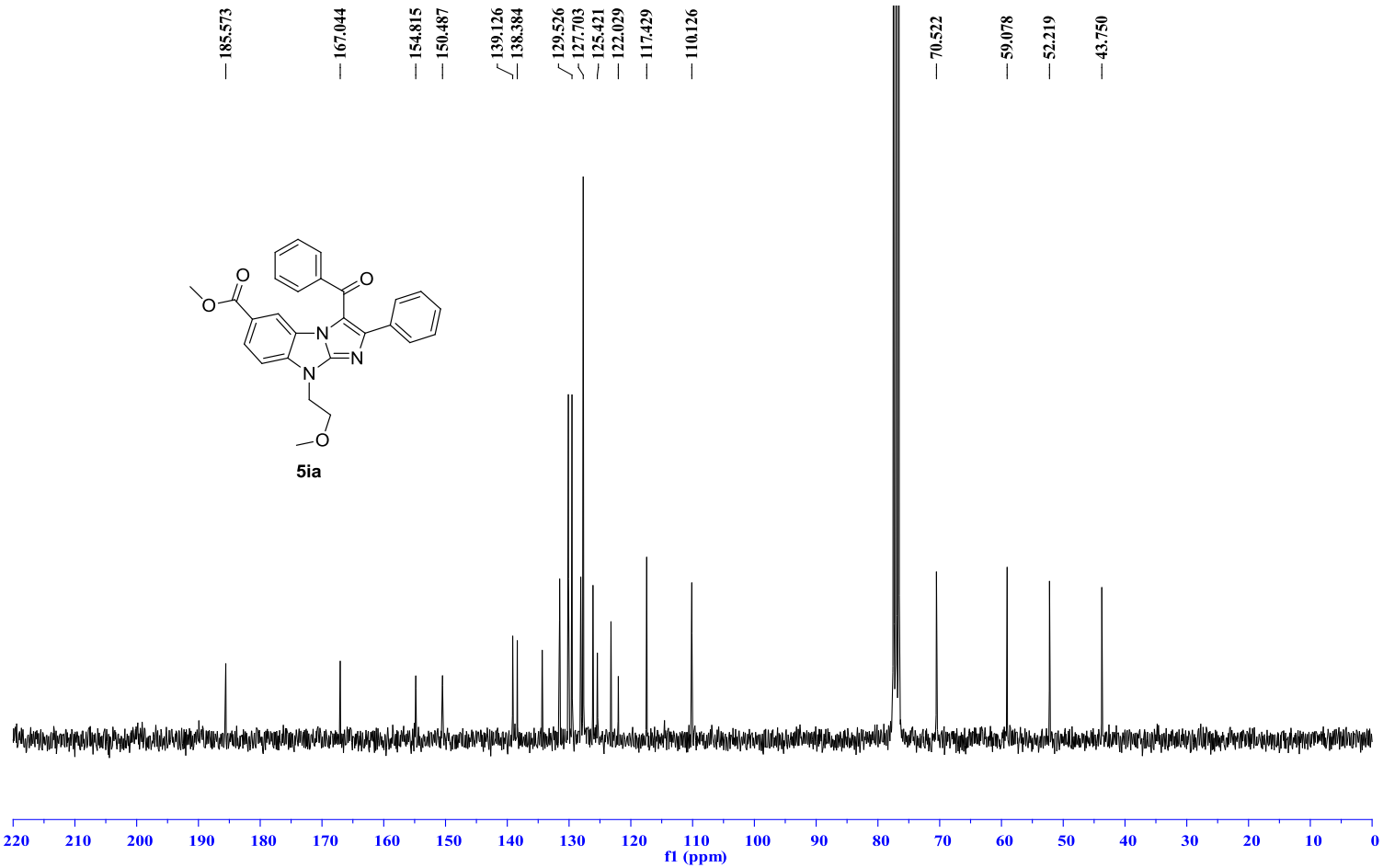
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



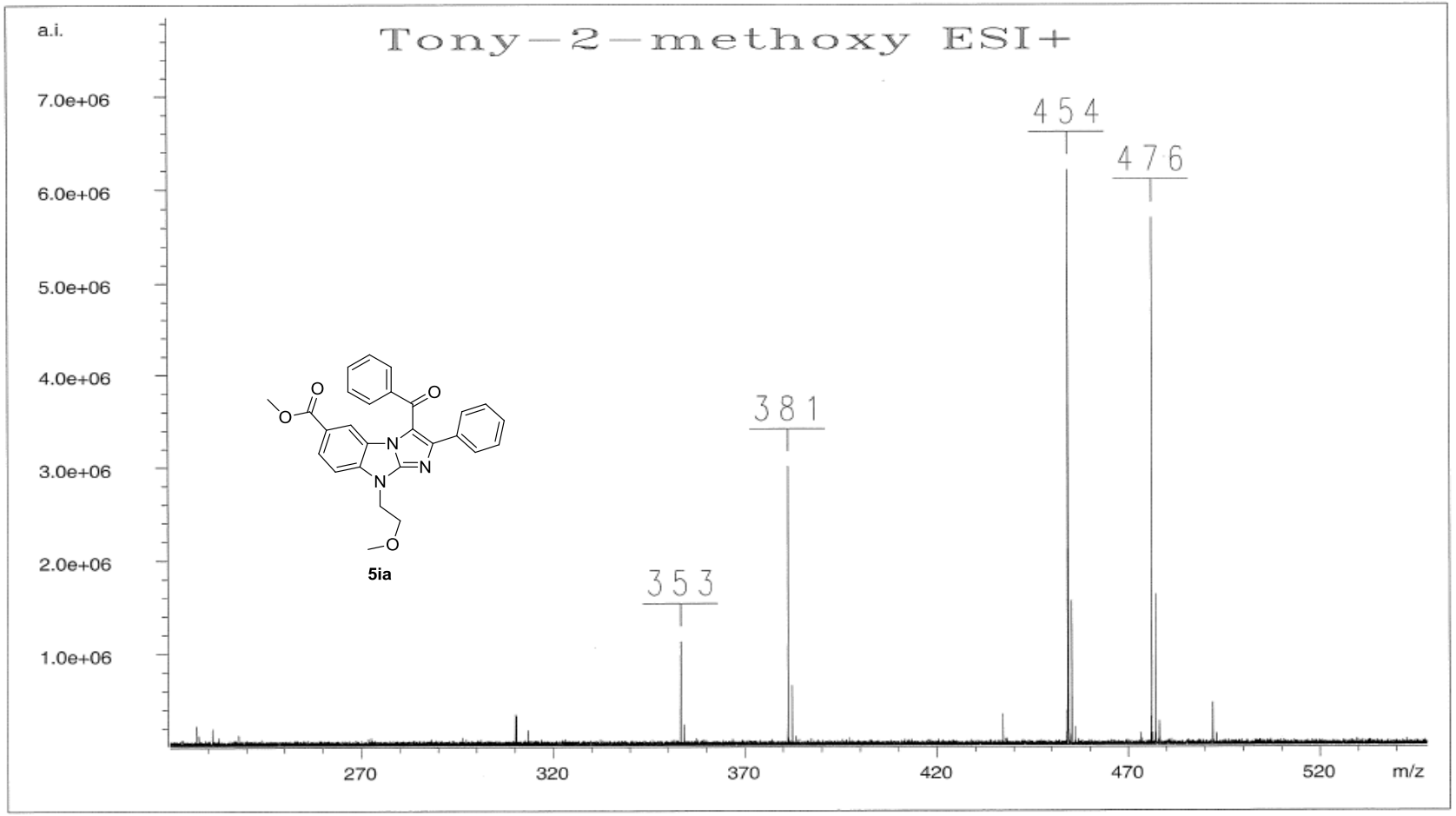
High resolution mass (ESI^+) spectrum of compound **5ha**



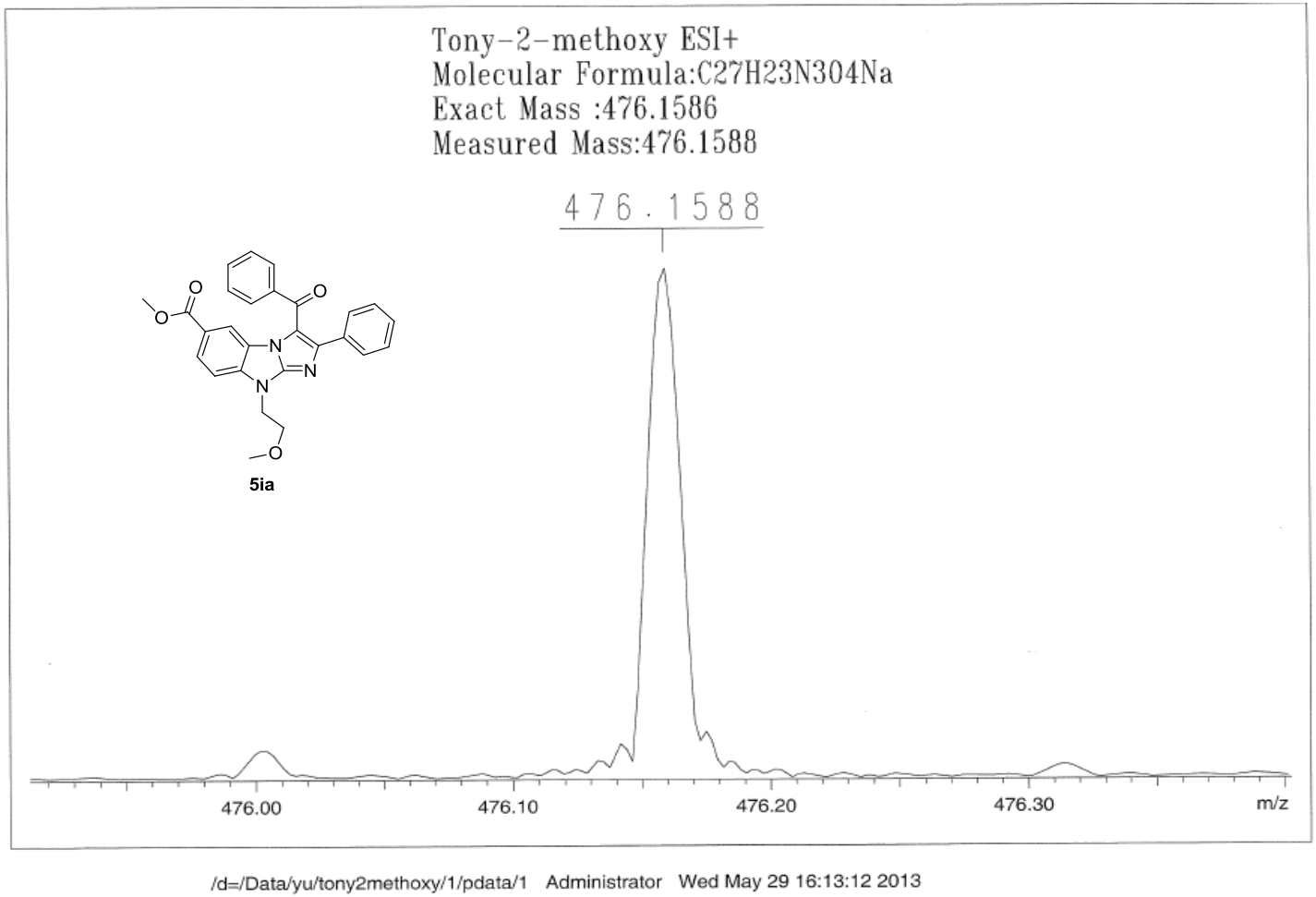
^{1}H NMR spectrum (300MHz) of compound **5ia** in $CDCl_3$



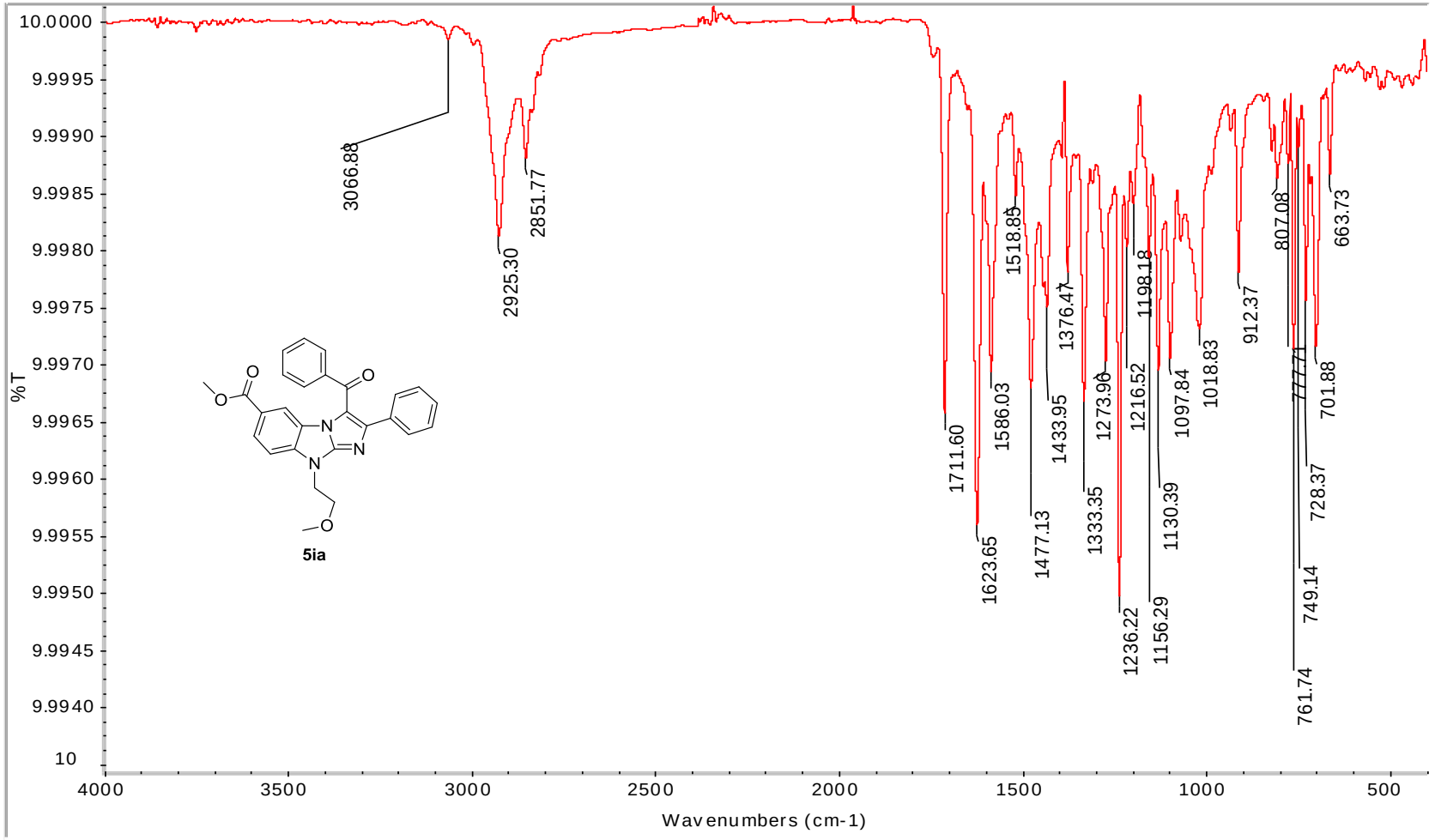
^{13}C NMR spectrum (75MHz) of compound **5ia** in $CDCl_3$



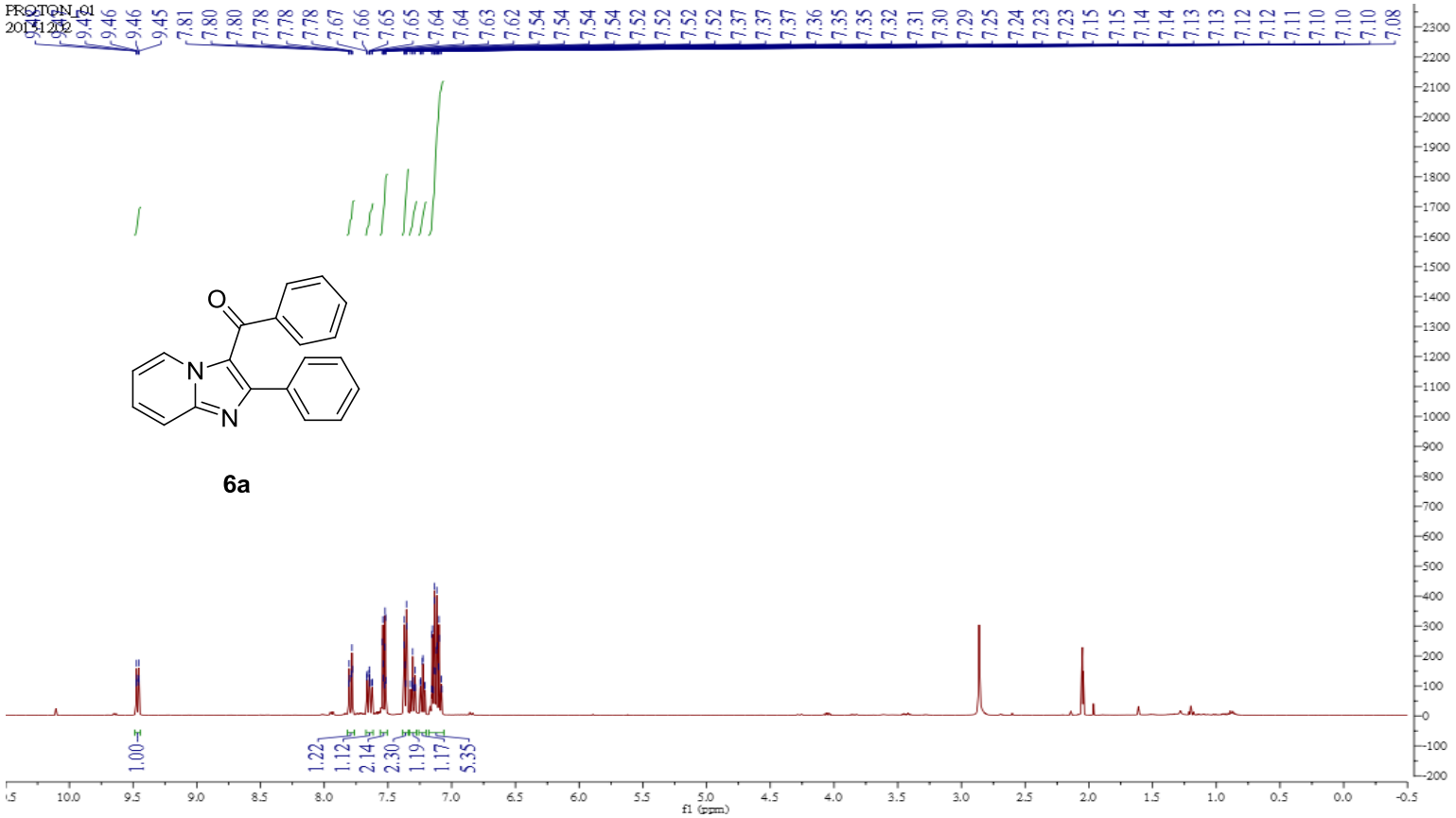
ESI^{+} Mass spectrum of compound **5ia**



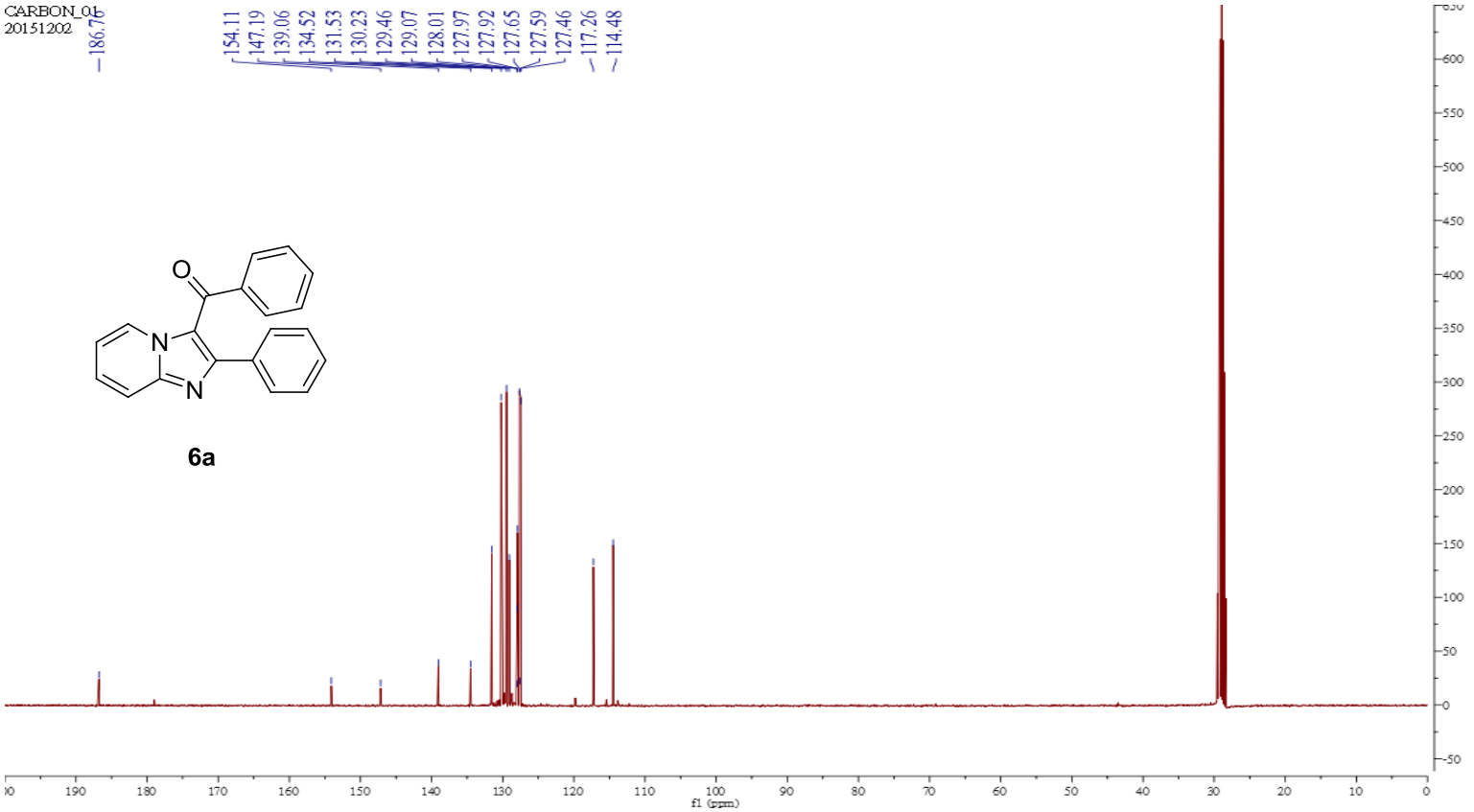
High resolution mass (ESI^+) spectrum of compound **5ia**



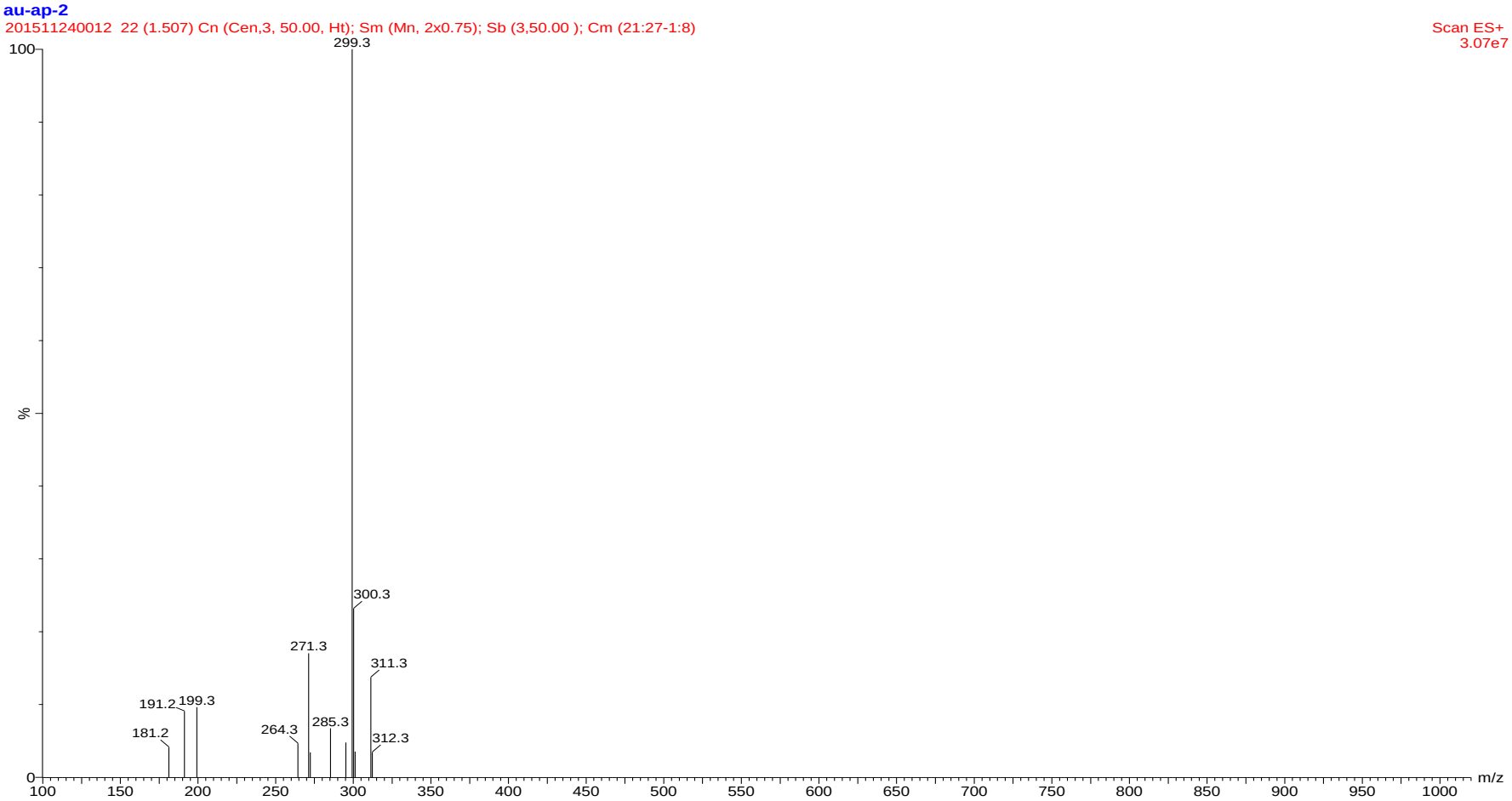
IR spectrum of compound **5ia**



^{1}H NMR spectrum (400MHz) of compound **6a** in Acetone-d_6



^{13}C NMR spectrum (100MHz) of compound **6a** in Acetone-d_6



ESI$^+$ Mass spectrum of compound **6a**

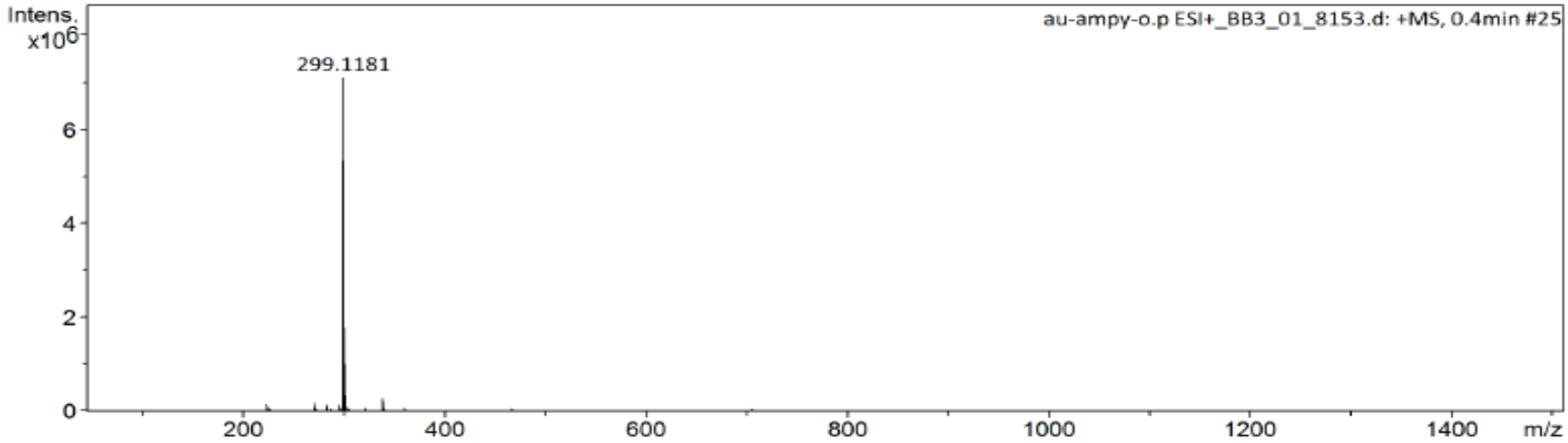
Display Report

Analysis Info

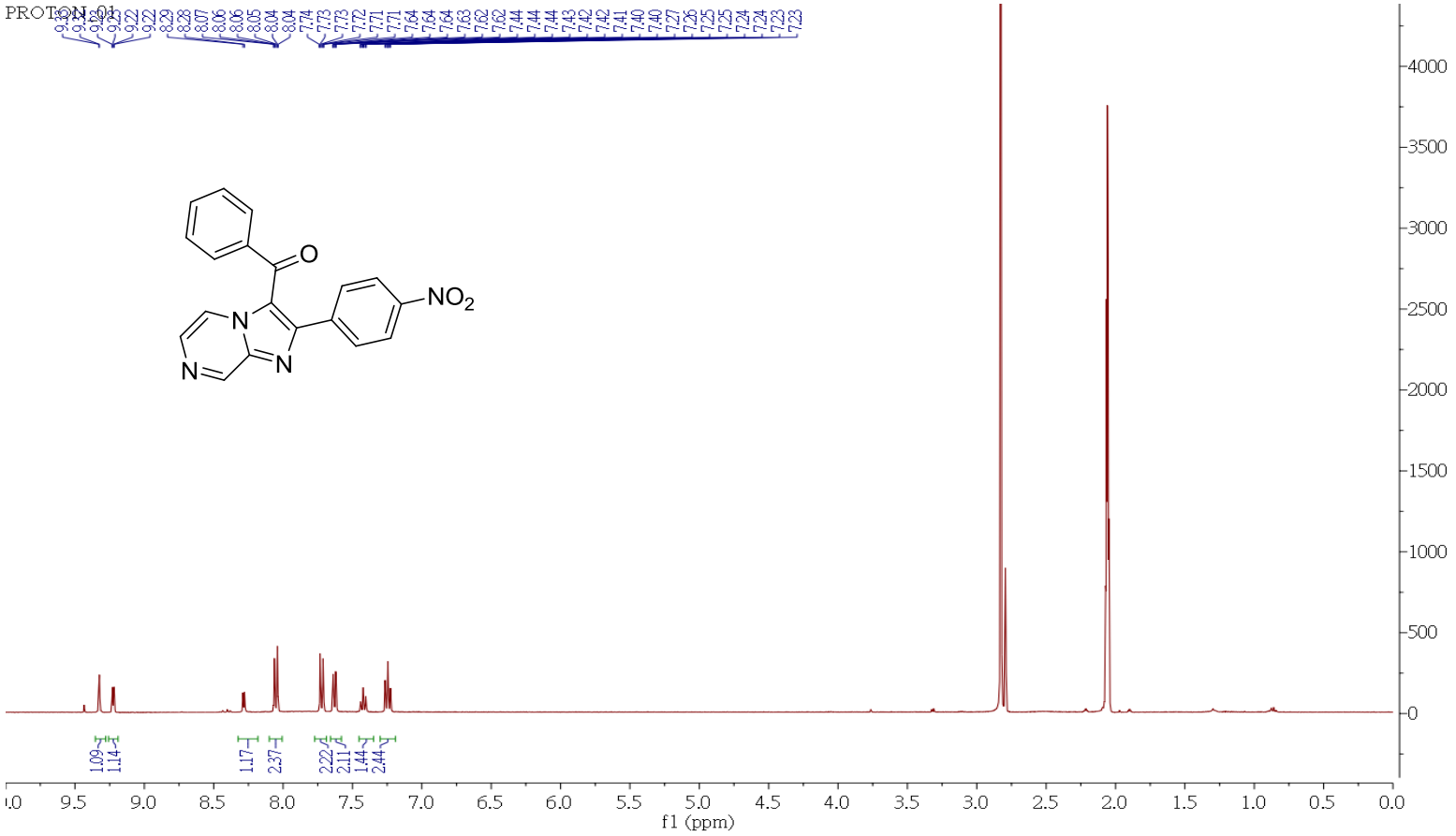
Analysis Name	D:\Data\nctu service\data\2015\20151208\au-ampy-o.p ESI+_BB3_01_8153.d	Acquisition Date	12/8/2015 1:42:30 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	au-ampy-o.p ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

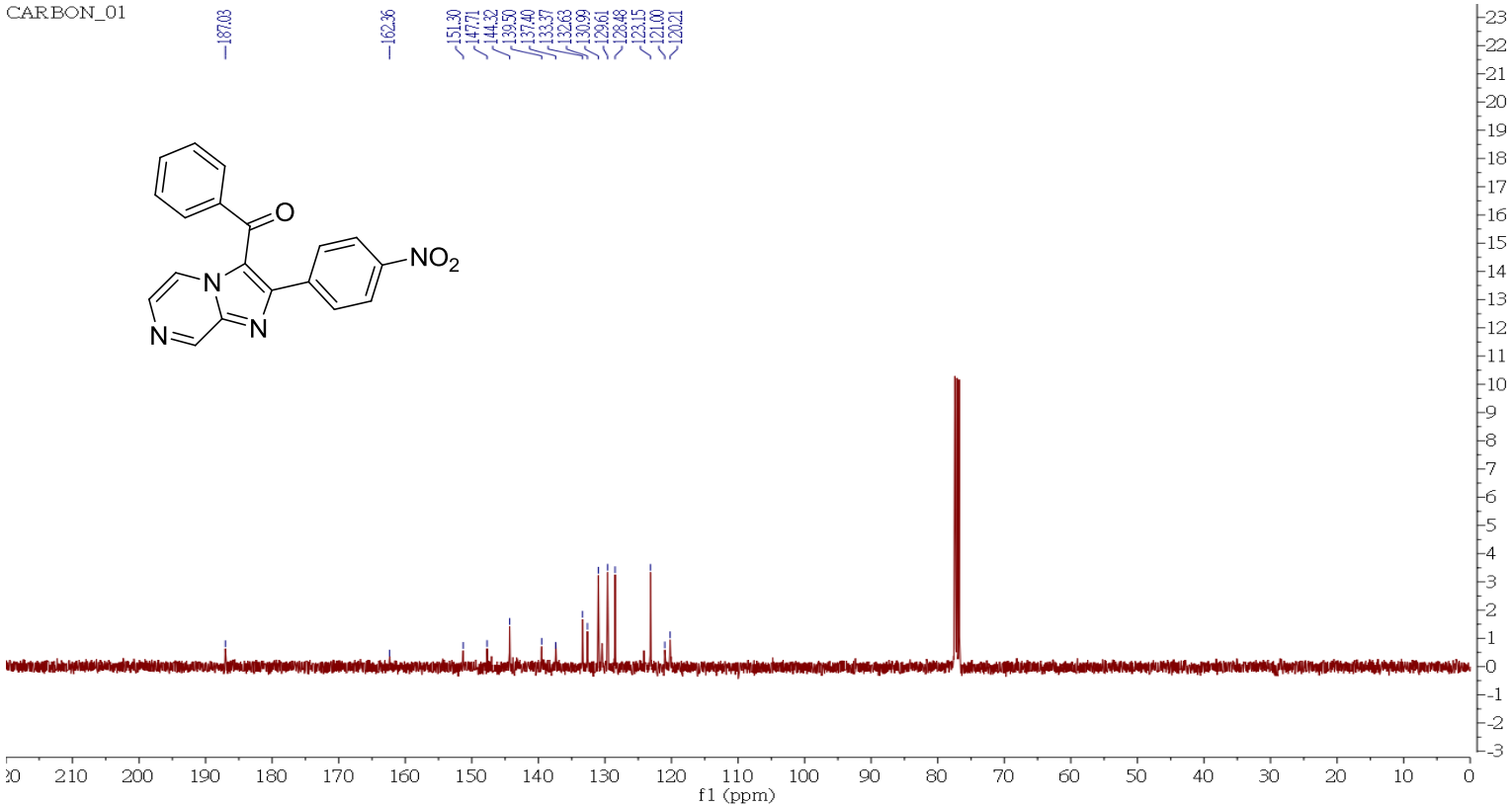
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



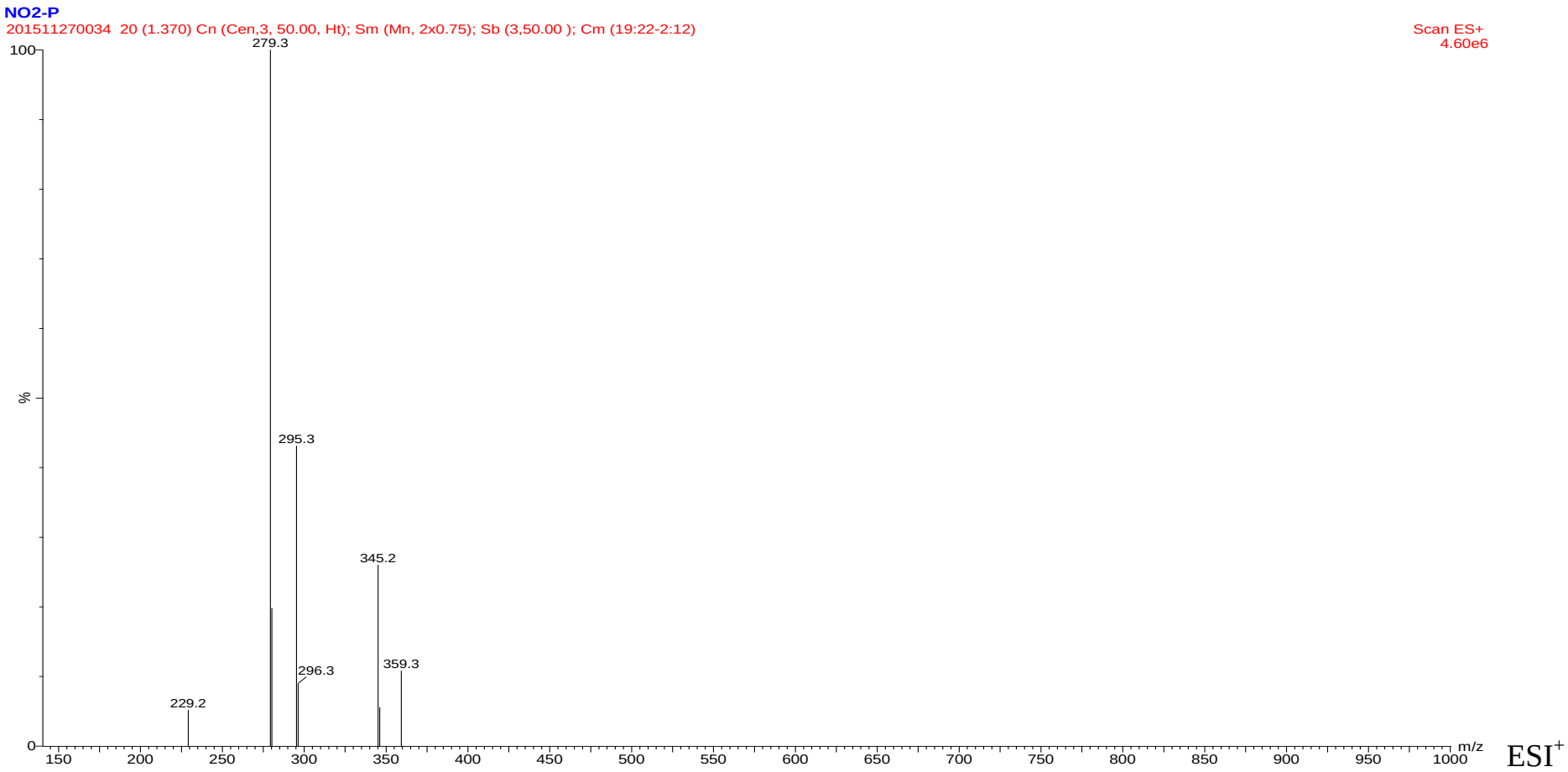
High resolution mass (ESI^+) spectrum of compound **6a**



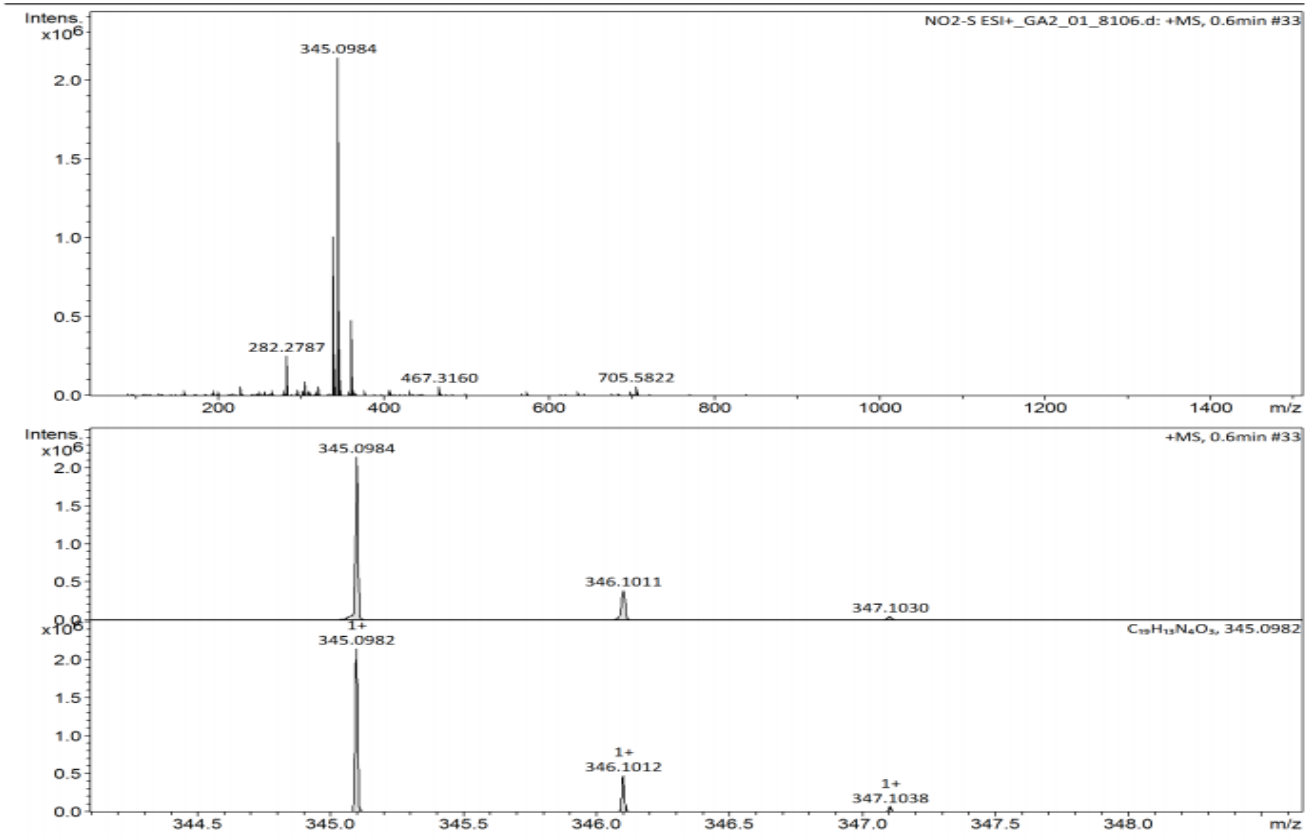
^{1}H NMR spectrum (400MHz) of compound **6b** in Acetone-d_6



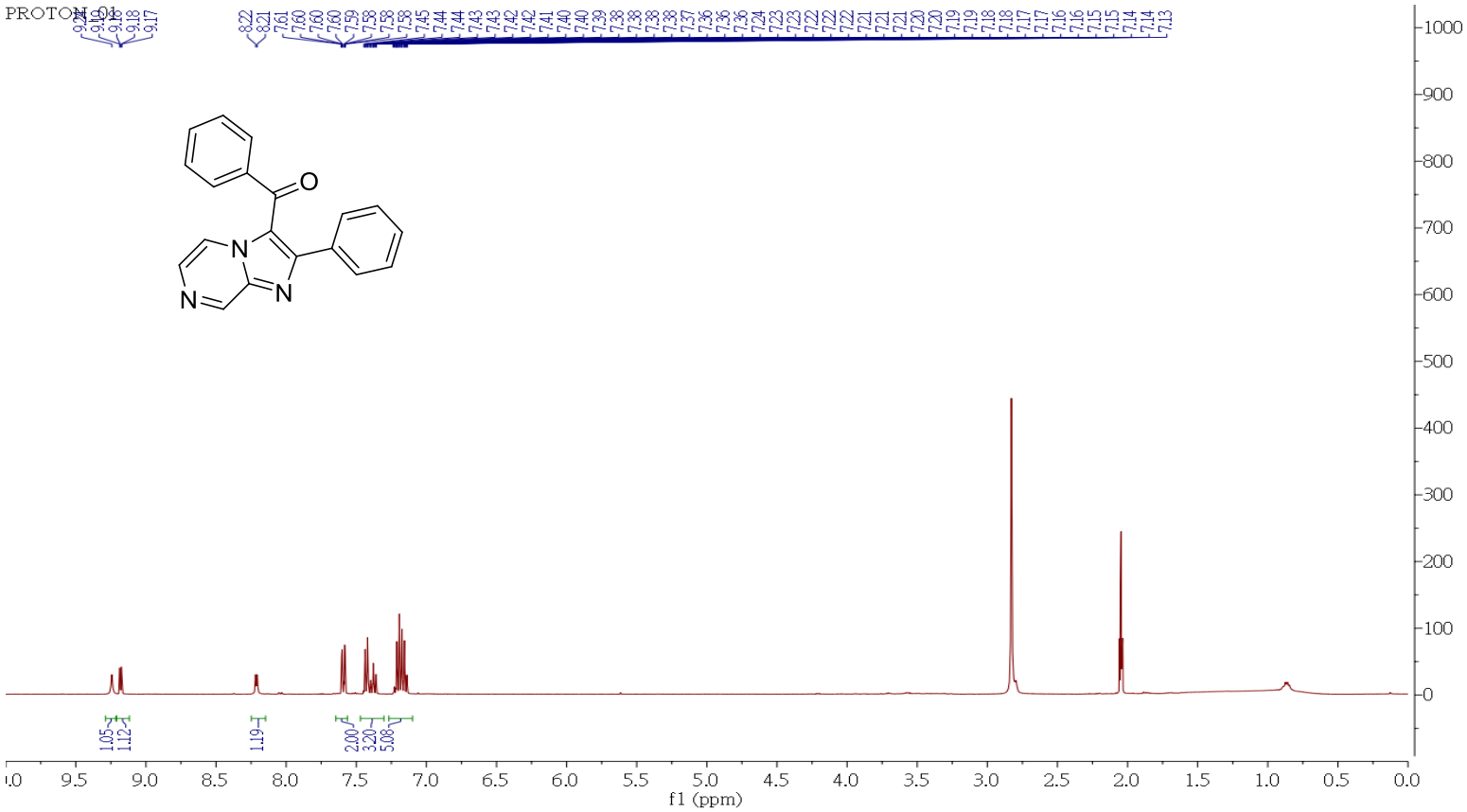
^{13}C NMR spectrum (100MHz) of compound **6b** in Acetone-d_6



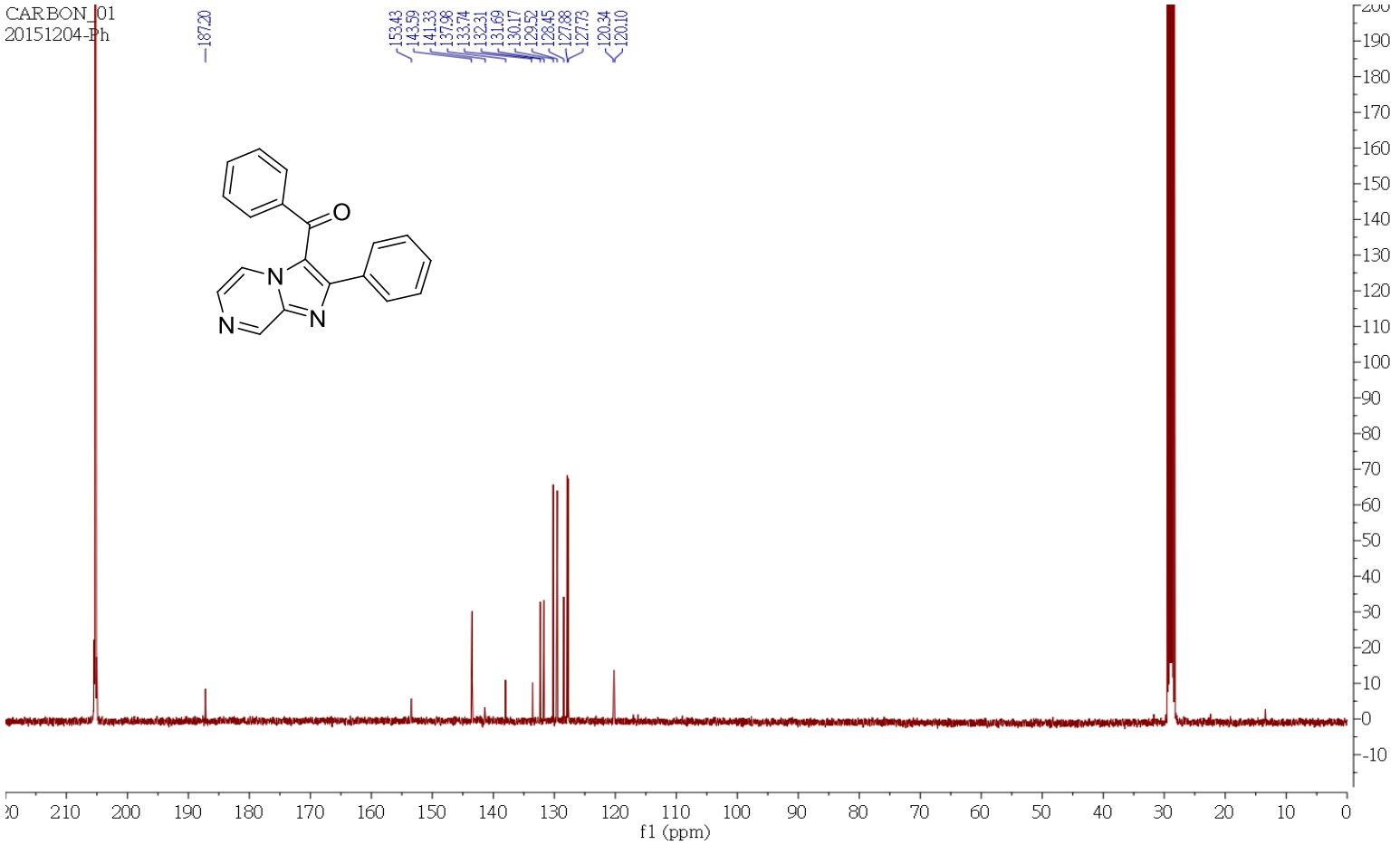
Mass spectrum of compound **6b**



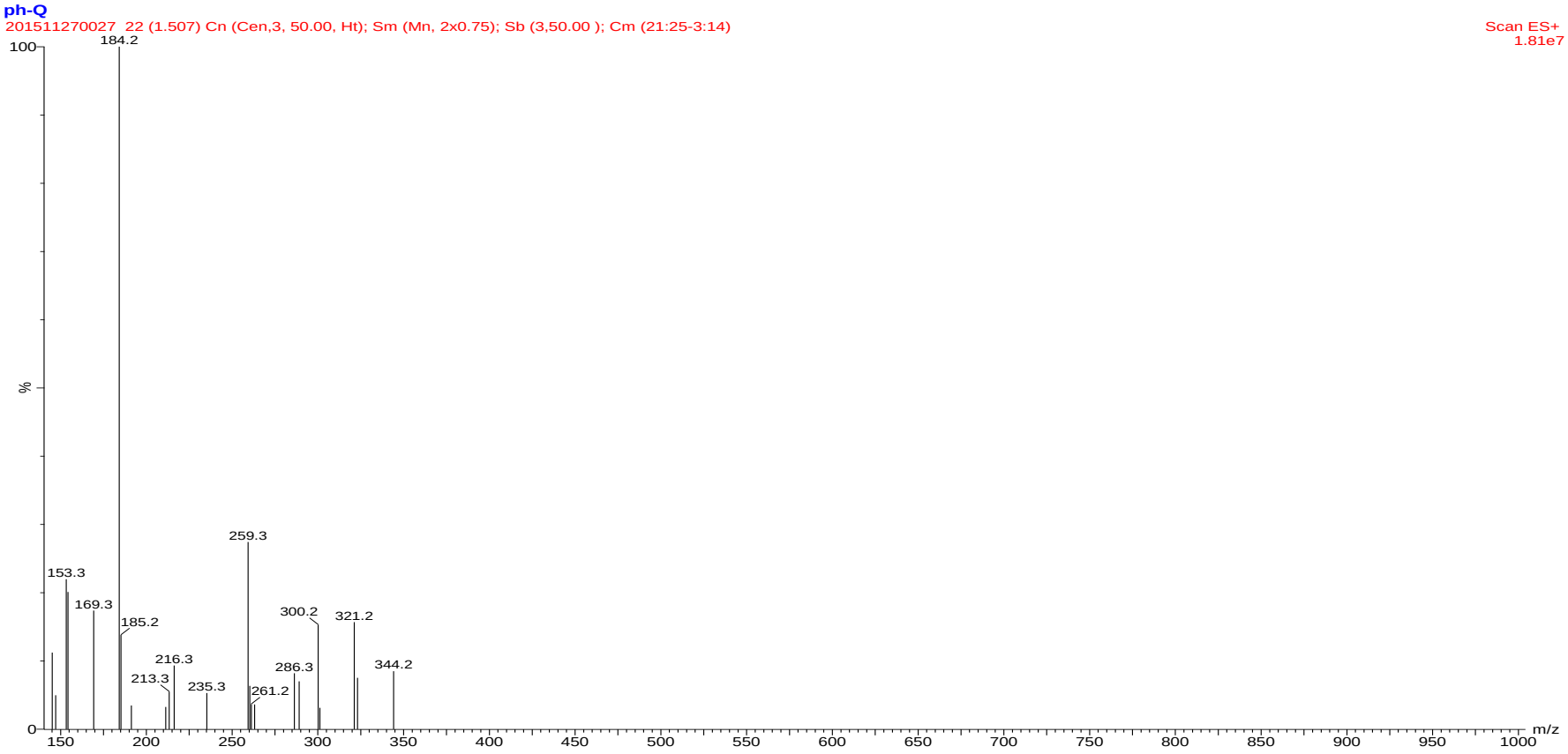
High resolution mass (ESI^+) spectrum of compound **6b**



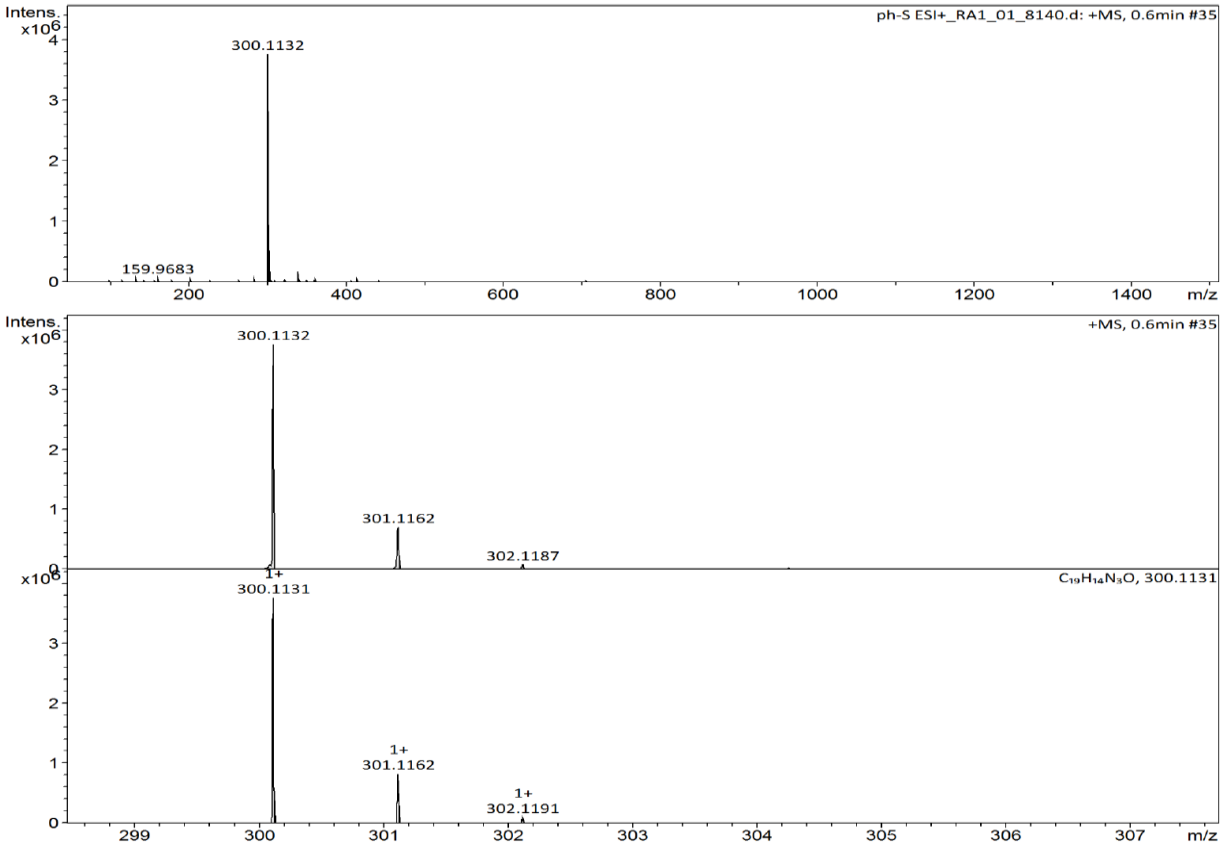
^{1}H NMR spectrum (400MHz) of compound **6c** in Acetone-d_6



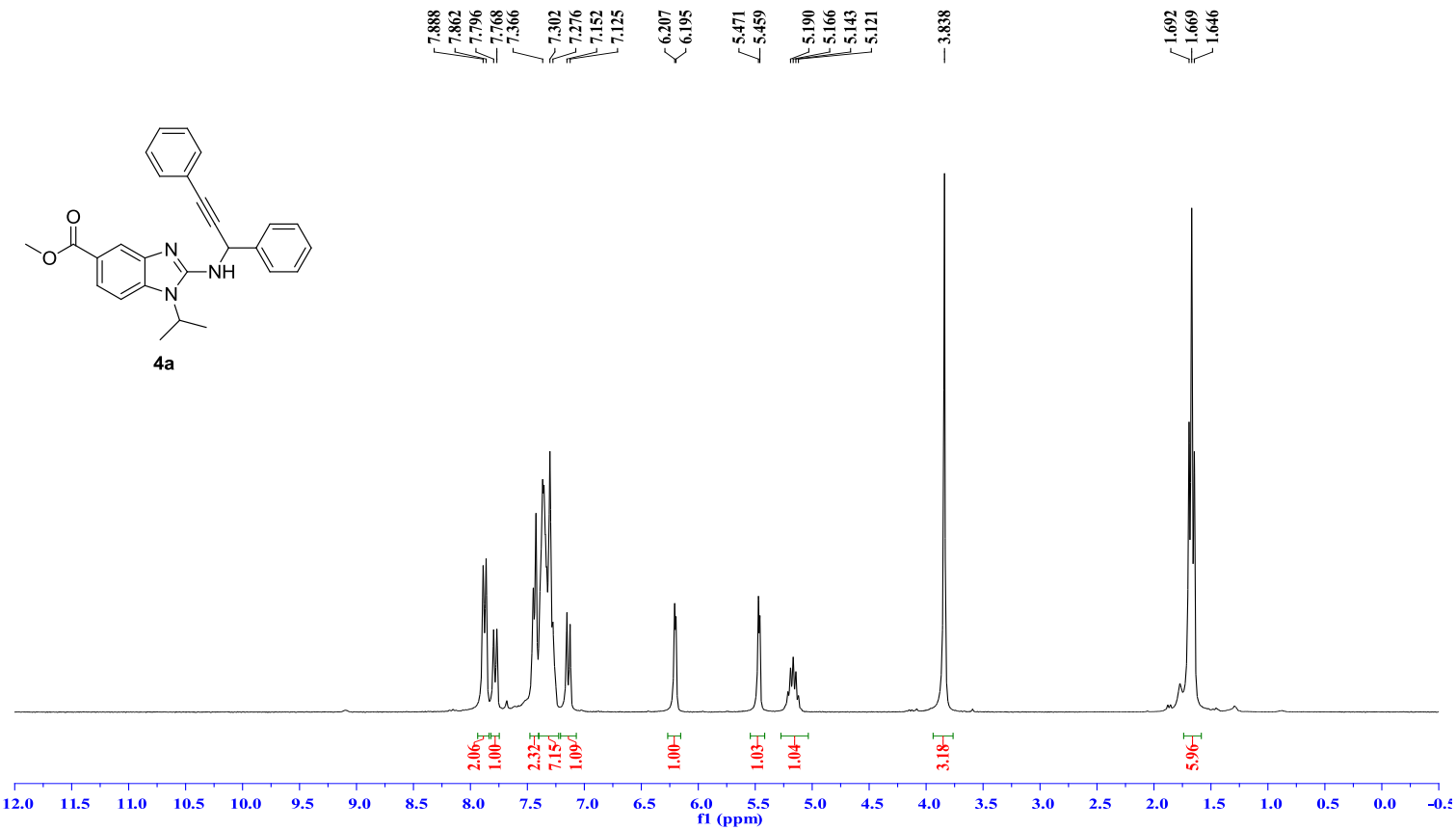
^{13}C NMR spectrum (100MHz) of compound **6c** in Acetone-d_6



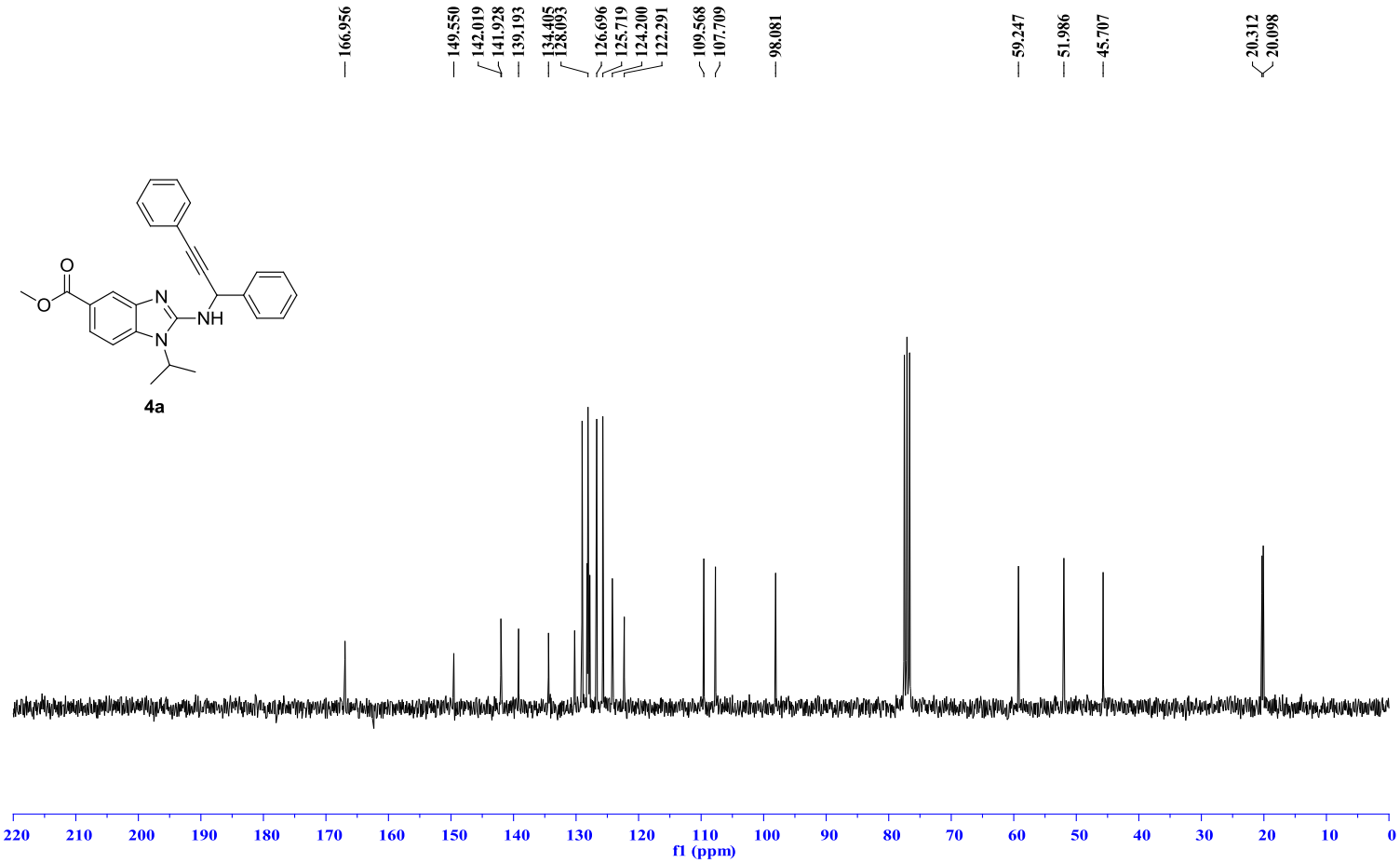
ESI^{+} Mass spectrum of compound **6c**



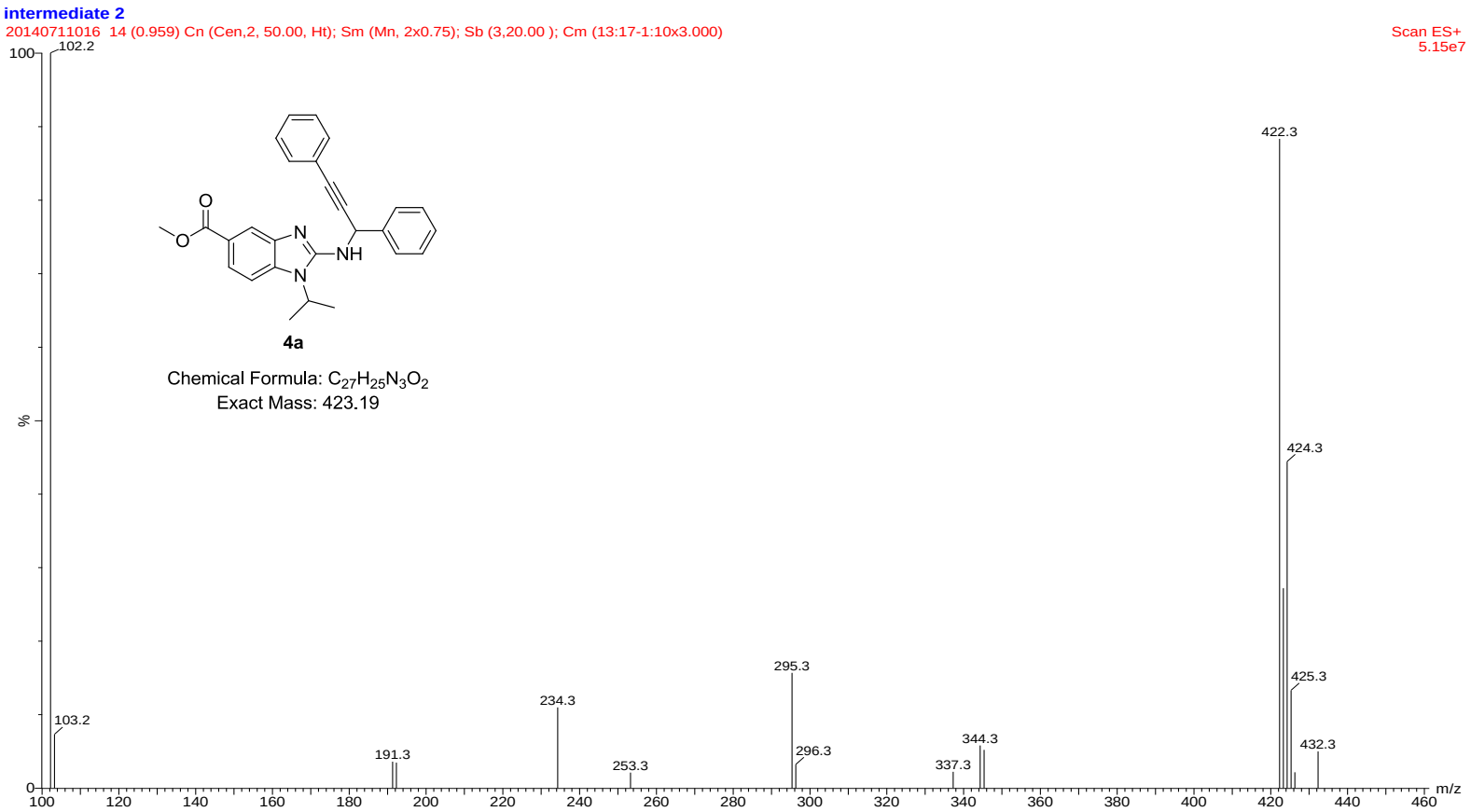
High resolution mass (ESI^+) spectrum of compound **5r**



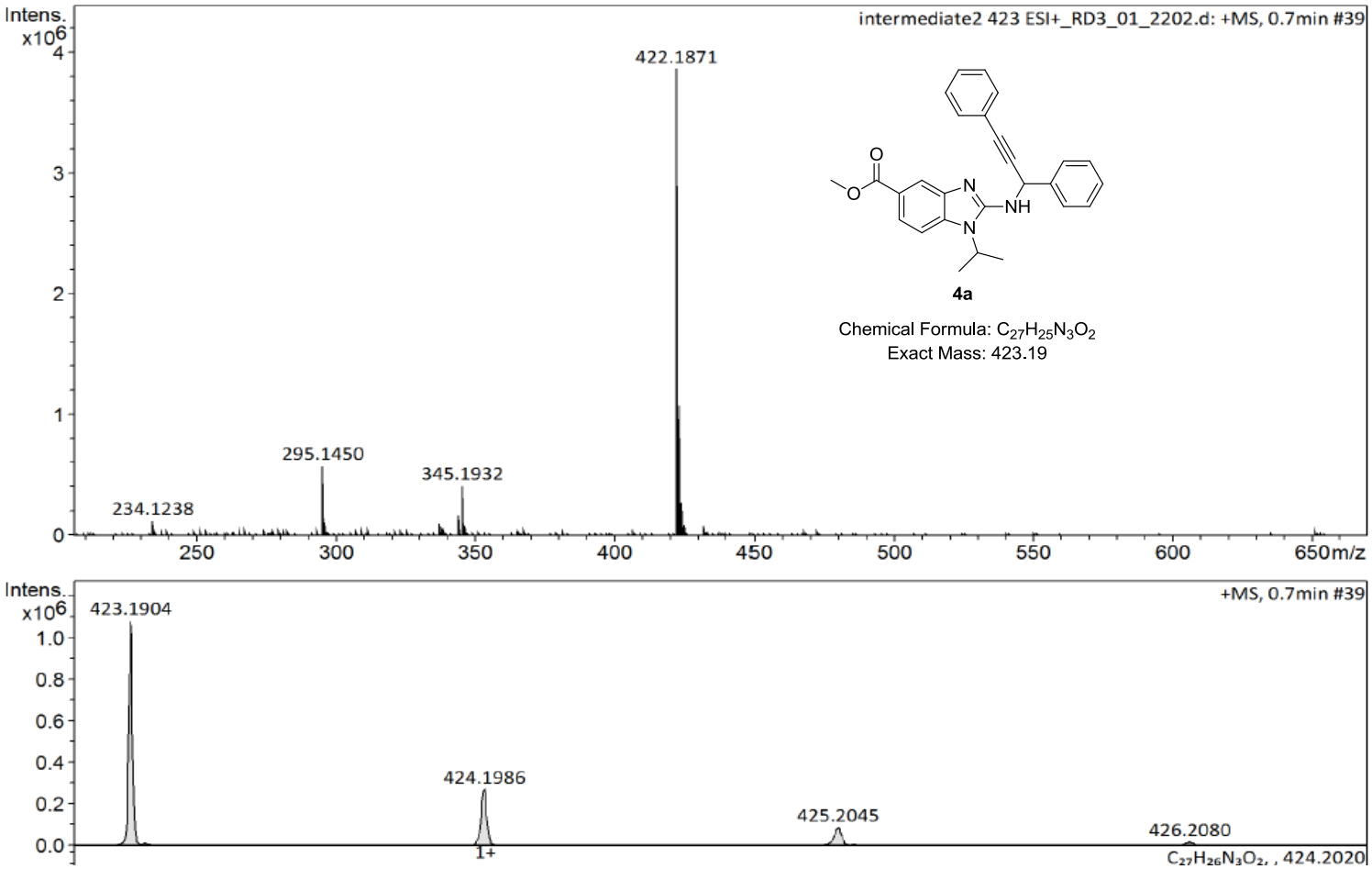
^{1}H NMR spectrum (300MHz) of compound **4a** in $CDCl_3$



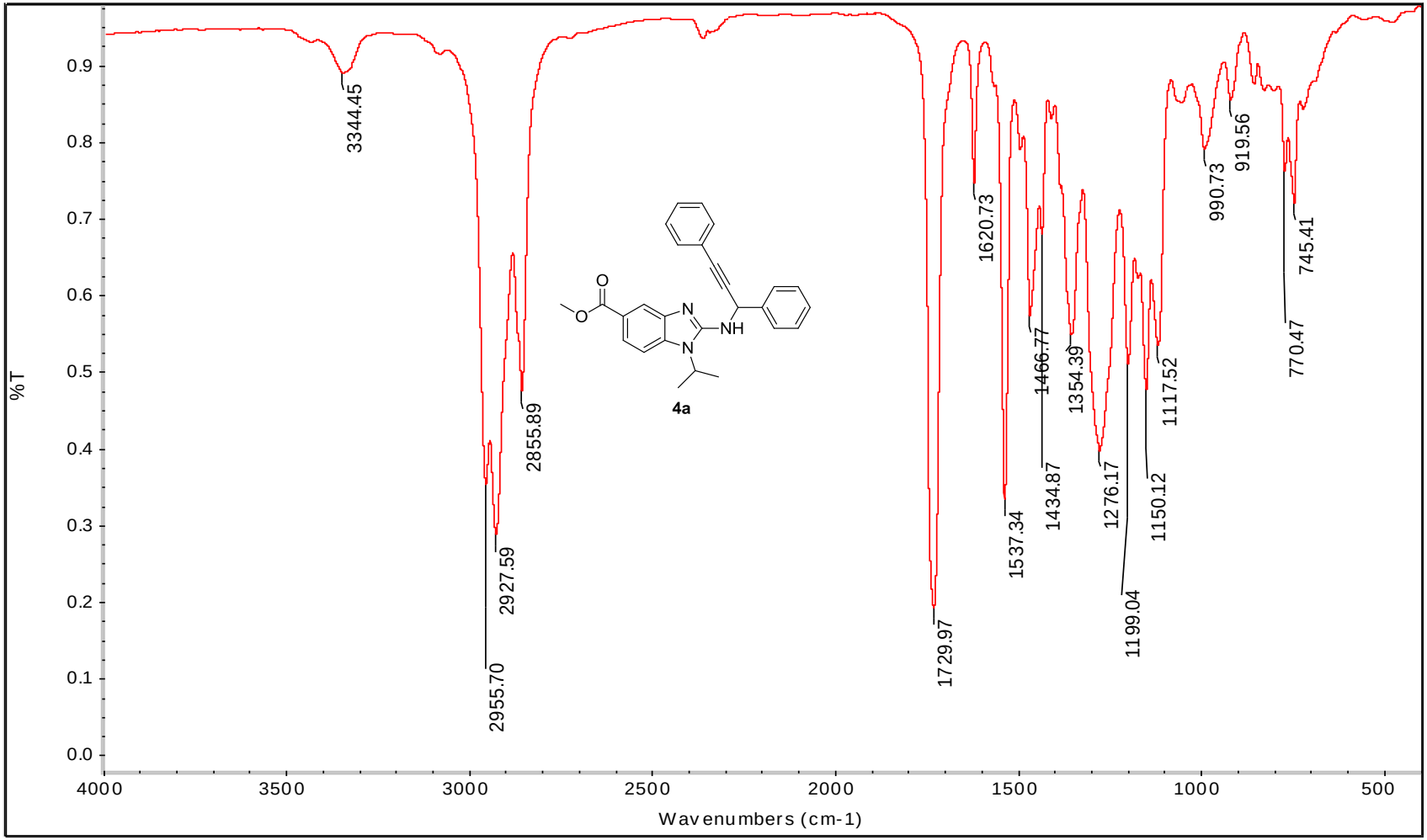
^{13}C NMR spectrum (75MHz) of compound **4a** in $CDCl_3$



ESI^{+} Mass spectrum of compound **4a**

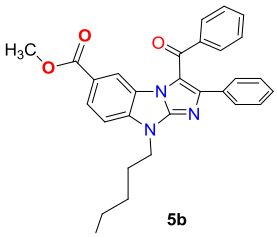


High resolution mass (ESI^+) spectrum of compound **4a**



IR spectrum of compound **4a**

ORTEP diagram of compound **5b**



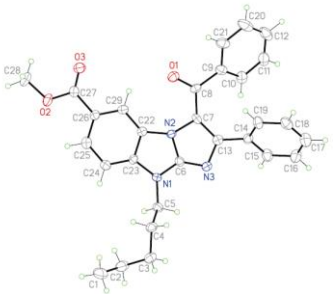


Table 1. Crystal data and structure refinement for 121122LT_0m.

Identification code	121122lt_0m	
Empirical formula	C29 H27 N3 O3	
Formula weight	465.54	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 17.181(2) Å	α= 90°.
	b = 26.757(3) Å	β= 96.526(4)°.
	c = 21.323(3) Å	γ = 90°.
Volume	9739(2) Å^3	
Z	16	
Density (calculated)	1.270 Mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
F(000)	3936	
Crystal size	0.15 x 0.03 x 0.03 mm^3	
Theta range for data collection	1.23 to 26.32°.	
Index ranges	-21<=h<=21, -33<=k<=22, -26<=l<=26	
Reflections collected	78830	
Independent reflections	19771 [R(int) = 0.1268]	
Completeness to theta = 26.32°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9486 and 0.8604	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	19771 / 0 / 1270	
Goodness-of-fit on F^2	0.979	

Final R indices [I>2sigma(I)]	R1 = 0.0937, wR2 = 0.2148
R indices (all data)	R1 = 0.2285, wR2 = 0.3196
Extinction coefficient	0.0107(7)
Largest diff. peak and hole	1.705 and -1.228 e.Å $^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for 121122LT_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	6226(2)	6777(1)	11067(2)	27(1)
O(2)	2642(2)	7138(1)	11142(2)	29(1)
O(3)	3827(2)	7043(1)	11705(2)	30(1)
O(4)	6765(2)	9183(2)	10749(2)	33(1)
O(5)	3557(2)	9632(1)	11807(2)	28(1)
O(6)	4835(2)	9429(1)	12040(2)	30(1)
O(7)	2707(2)	8512(1)	-584(2)	33(1)
O(8)	5872(2)	7906(1)	-1525(2)	31(1)
O(9)	4578(2)	8029(1)	-1792(2)	30(1)
O(10)	5609(2)	5430(1)	-1463(2)	29(1)
O(11)	6778(2)	5429(1)	-870(2)	28(1)
O(12)	3122(2)	5725(1)	-885(2)	32(1)
N(1)	4711(2)	6803(2)	8918(2)	21(1)
N(2)	5553(2)	6803(1)	9800(2)	19(1)
N(3)	6146(3)	6708(2)	8912(2)	21(1)
N(4)	5606(2)	9271(1)	9684(2)	19(1)
N(5)	4477(2)	9343(2)	9054(2)	26(1)
N(6)	5737(2)	9123(2)	8653(2)	23(1)
N(7)	3742(2)	8303(1)	522(2)	20(1)
N(8)	4844(3)	8232(2)	1193(2)	24(1)
N(9)	3532(3)	8430(2)	1538(2)	25(1)
N(10)	4626(2)	5821(2)	1283(2)	20(1)
N(11)	3796(2)	5746(2)	400(2)	21(1)
N(12)	3181(3)	5904(2)	1268(2)	21(1)
C(1)	2430(4)	6003(2)	7338(3)	47(2)
C(2)	2948(3)	6451(2)	7243(3)	37(2)
C(3)	3806(3)	6310(2)	7313(3)	30(1)

C(4)	4177(3)	6278(2)	7997(2)	27(1)
C(5)	4421(3)	6796(2)	8247(2)	23(1)
C(6)	5481(3)	6760(2)	9157(2)	21(1)
C(7)	6370(3)	6807(2)	9993(2)	22(1)
C(8)	6653(3)	6879(2)	10653(2)	21(1)
C(9)	7454(3)	7094(2)	10858(3)	26(1)
C(10)	7821(3)	7423(2)	10479(3)	29(1)
C(11)	8533(4)	7635(2)	10703(3)	38(2)
C(12)	8891(4)	7513(2)	11289(3)	44(2)
C(13)	6708(3)	6740(2)	9427(2)	22(1)
C(14)	7523(3)	6651(2)	9315(2)	24(1)
C(15)	7790(3)	6855(2)	8780(3)	32(1)
C(16)	8541(4)	6758(2)	8627(3)	40(2)
C(17)	9043(4)	6460(2)	9021(3)	43(2)
C(18)	8779(3)	6256(2)	9554(3)	34(2)
C(19)	8030(3)	6353(2)	9701(3)	29(1)
C(20)	8530(4)	7194(2)	11682(3)	45(2)
C(21)	7807(3)	6992(2)	11469(3)	32(1)
C(22)	4802(3)	6885(2)	9991(2)	20(1)
C(23)	4283(3)	6878(2)	9424(2)	20(1)
C(24)	3484(3)	6953(2)	9432(2)	23(1)
C(25)	3213(3)	7026(2)	10010(3)	25(1)
C(26)	3726(3)	7020(2)	10578(2)	20(1)
C(27)	3429(3)	7067(2)	11204(3)	23(1)
C(28)	2291(4)	7132(2)	11728(3)	35(2)
C(29)	4527(3)	6954(2)	10564(2)	21(1)
C(30)	9438(3)	9258(2)	10056(3)	32(1)
C(31)	9144(3)	8978(2)	10528(3)	31(1)
C(32)	8346(3)	8962(2)	10570(3)	25(1)
C(33)	7830(3)	9217(2)	10141(2)	21(1)
C(34)	6969(3)	9188(2)	10214(2)	22(1)
C(35)	6408(3)	9166(2)	9664(2)	19(1)
C(36)	5258(3)	9246(2)	9078(2)	23(1)
C(37)	3891(4)	9247(3)	8486(3)	49(2)
C(38)	3652(4)	9715(2)	8175(3)	54(2)
C(39)	3082(4)	9580(3)	7560(3)	65(2)
C(40)	3483(4)	9323(2)	7053(3)	37(2)

C(41)	2962(4)	9302(2)	6434(3)	49(2)
C(42)	8923(3)	9522(2)	9630(3)	34(2)
C(43)	8125(3)	9502(2)	9671(2)	26(1)
C(44)	5020(3)	9381(2)	10077(2)	19(1)
C(45)	5021(3)	9420(2)	10723(2)	21(1)
C(46)	4298(3)	9517(2)	10954(2)	23(1)
C(47)	4276(3)	9524(2)	11649(3)	25(1)
C(48)	3454(4)	9575(2)	12464(3)	38(2)
C(49)	3601(3)	9574(2)	10541(3)	23(1)
C(50)	3599(3)	9530(2)	9892(3)	24(1)
C(51)	4317(3)	9428(2)	9669(2)	22(1)
C(52)	6449(3)	9064(2)	9021(2)	21(1)
C(53)	7120(3)	8870(2)	8716(2)	23(1)
C(54)	7300(3)	9074(2)	8144(3)	30(1)
C(55)	7914(3)	8882(2)	7850(3)	37(2)
C(56)	8349(3)	8480(2)	8109(3)	33(1)
C(57)	8165(3)	8271(2)	8675(3)	30(1)
C(58)	7562(3)	8470(2)	8975(2)	25(1)
C(59)	77(4)	7865(2)	-312(3)	47(2)
C(60)	342(4)	8186(2)	-749(3)	45(2)
C(61)	1095(3)	8367(2)	-660(3)	33(1)
C(62)	1593(3)	8240(2)	-129(2)	22(1)
C(63)	2430(3)	8401(2)	-94(2)	20(1)
C(64)	2931(3)	8398(2)	509(2)	23(1)
C(65)	4048(3)	8324(2)	1138(2)	22(1)
C(66)	5369(3)	8235(2)	1777(2)	24(1)
C(67)	5545(3)	7712(2)	2039(3)	30(1)
C(68)	6124(4)	7712(2)	2633(3)	40(2)
C(69)	5754(6)	7926(4)	3191(4)	102(4)
C(70)	6328(6)	7938(4)	3805(5)	121(4)
C(71)	573(3)	7733(2)	222(3)	33(1)
C(72)	1325(3)	7916(2)	318(2)	24(1)
C(73)	5037(3)	8150(2)	585(2)	20(1)
C(74)	4353(3)	8192(2)	144(2)	21(1)
C(75)	4376(3)	8136(2)	-492(2)	20(1)
C(76)	5107(3)	8035(2)	-704(3)	22(1)
C(77)	5134(3)	7992(2)	-1394(3)	24(1)

C(78)	5979(4)	7905(2)	-2187(3)	40(2)
C(79)	5780(3)	7995(2)	-260(3)	27(1)
C(80)	5766(3)	8051(2)	380(3)	24(1)
C(81)	2840(3)	8484(2)	1145(2)	23(1)
C(82)	2145(3)	8673(2)	1427(2)	20(1)
C(83)	2014(3)	8515(2)	2037(3)	27(1)
C(84)	1395(3)	8704(2)	2322(3)	30(1)
C(85)	899(3)	9055(2)	2014(3)	33(1)
C(86)	1019(3)	9217(2)	1408(3)	31(1)
C(87)	1639(3)	9025(2)	1117(3)	27(1)
C(88)	6457(5)	5321(3)	3925(4)	87(3)
C(89)	5963(5)	5202(2)	3352(3)	76(3)
C(90)	5580(4)	5642(2)	2973(3)	46(2)
C(91)	5186(3)	5493(2)	2325(3)	32(1)
C(92)	4928(3)	5951(2)	1925(2)	23(1)
C(93)	3860(3)	5832(2)	1039(2)	20(1)
C(94)	2977(3)	5753(2)	196(2)	20(1)
C(95)	2692(3)	5675(2)	-464(3)	24(1)
C(96)	1848(3)	5516(2)	-638(3)	26(1)
C(97)	1450(3)	5702(2)	-1200(3)	31(1)
C(98)	686(4)	5543(2)	-1393(3)	43(2)
C(99)	335(4)	5193(2)	-1030(3)	45(2)
C(100)	2637(3)	5866(2)	755(2)	21(1)
C(101)	4554(3)	5678(2)	217(2)	20(1)
C(102)	4845(3)	5589(2)	-356(2)	19(1)
C(103)	5656(3)	5540(2)	-342(2)	21(1)
C(104)	5980(3)	5465(2)	-954(3)	22(1)
C(105)	7153(3)	5392(2)	-1436(3)	32(1)
C(106)	6152(3)	5573(2)	232(3)	24(1)
C(107)	5861(3)	5657(2)	798(3)	23(1)
C(108)	5061(3)	5717(2)	779(2)	22(1)
C(109)	1479(3)	5168(2)	-279(3)	31(1)
C(110)	728(4)	5009(2)	-484(3)	40(2)
C(111)	1806(3)	5971(2)	851(3)	23(1)
C(112)	1534(3)	5820(2)	1413(3)	26(1)
C(113)	784(3)	5949(2)	1545(3)	36(2)
C(114)	304(4)	6236(2)	1118(3)	35(2)

C(115)	571(3)	6387(2)	561(3)	32(1)
C(116)	1320(3)	6263(2)	424(3)	27(1)

Table 3. Bond lengths [Å] and angles [°] for 121122LT_0m.

O(1)-C(8)	1.240(6)
O(2)-C(27)	1.357(6)
O(2)-C(28)	1.447(6)
O(3)-C(27)	1.203(6)
O(4)-C(34)	1.232(6)
O(5)-C(47)	1.348(6)
O(5)-C(48)	1.441(6)
O(6)-C(47)	1.223(6)
O(7)-C(63)	1.233(6)
O(8)-C(77)	1.348(6)
O(8)-C(78)	1.443(6)
O(9)-C(77)	1.208(6)
O(10)-C(104)	1.199(6)
O(11)-C(104)	1.365(6)
O(11)-C(105)	1.435(6)
O(12)-C(95)	1.233(6)
N(1)-C(6)	1.367(6)
N(1)-C(23)	1.388(6)
N(1)-C(5)	1.462(6)
N(2)-C(6)	1.366(6)
N(2)-C(22)	1.415(6)
N(2)-C(7)	1.417(6)
N(3)-C(6)	1.317(6)
N(3)-C(13)	1.379(6)
N(4)-C(36)	1.363(6)
N(4)-C(35)	1.411(6)
N(4)-C(44)	1.412(6)
N(5)-C(36)	1.362(6)
N(5)-C(51)	1.388(6)
N(5)-C(37)	1.508(8)
N(6)-C(36)	1.331(6)
N(6)-C(52)	1.385(6)

N(7)-C(65)	1.360(6)
N(7)-C(64)	1.414(6)
N(7)-C(74)	1.425(6)
N(8)-C(65)	1.381(7)
N(8)-C(73)	1.391(6)
N(8)-C(66)	1.454(6)
N(9)-C(65)	1.328(7)
N(9)-C(81)	1.383(7)
N(10)-C(93)	1.359(6)
N(10)-C(108)	1.405(6)
N(10)-C(92)	1.449(6)
N(11)-C(93)	1.374(6)
N(11)-C(101)	1.412(6)
N(11)-C(94)	1.425(6)
N(12)-C(93)	1.329(6)
N(12)-C(100)	1.359(6)
C(1)-C(2)	1.519(8)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-C(3)	1.513(8)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.528(7)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.527(7)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(7)-C(13)	1.410(7)
C(7)-C(8)	1.449(7)
C(8)-C(9)	1.511(7)
C(9)-C(10)	1.390(8)
C(9)-C(21)	1.402(8)
C(10)-C(11)	1.383(8)

C(10)-H(10)	0.9500
C(11)-C(12)	1.369(9)
C(11)-H(11)	0.9500
C(12)-C(20)	1.390(9)
C(12)-H(12)	0.9500
C(13)-C(14)	1.466(7)
C(14)-C(19)	1.381(7)
C(14)-C(15)	1.389(7)
C(15)-C(16)	1.390(8)
C(15)-H(15)	0.9500
C(16)-C(17)	1.385(9)
C(16)-H(16)	0.9500
C(17)-C(18)	1.383(8)
C(17)-H(17)	0.9500
C(18)-C(19)	1.383(8)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
C(20)-C(21)	1.383(8)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(29)	1.370(7)
C(22)-C(23)	1.419(7)
C(23)-C(24)	1.388(7)
C(24)-C(25)	1.382(7)
C(24)-H(24)	0.9500
C(25)-C(26)	1.413(7)
C(25)-H(25)	0.9500
C(26)-C(29)	1.392(7)
C(26)-C(27)	1.487(7)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29)	0.9500
C(30)-C(42)	1.387(8)
C(30)-C(31)	1.393(8)
C(30)-H(30)	0.9500
C(31)-C(32)	1.384(7)

C(31)-H(31)	0.9500
C(32)-C(33)	1.380(7)
C(32)-H(32)	0.9500
C(33)-C(43)	1.398(7)
C(33)-C(34)	1.507(7)
C(34)-C(35)	1.432(7)
C(35)-C(52)	1.406(7)
C(37)-C(38)	1.455(9)
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(38)-C(39)	1.588(9)
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(39)-C(40)	1.511(9)
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900
C(40)-C(41)	1.509(8)
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-C(43)	1.386(8)
C(42)-H(42)	0.9500
C(43)-H(43)	0.9500
C(44)-C(45)	1.383(7)
C(44)-C(51)	1.412(7)
C(45)-C(46)	1.412(7)
C(45)-H(45)	0.9500
C(46)-C(49)	1.413(7)
C(46)-C(47)	1.486(7)
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-C(50)	1.389(7)
C(49)-H(49)	0.9500
C(50)-C(51)	1.398(7)

C(50)-H(50)	0.9500
C(52)-C(53)	1.482(7)
C(53)-C(58)	1.389(7)
C(53)-C(54)	1.403(7)
C(54)-C(55)	1.387(8)
C(54)-H(54)	0.9500
C(55)-C(56)	1.387(8)
C(55)-H(55)	0.9500
C(56)-C(57)	1.399(8)
C(56)-H(56)	0.9500
C(57)-C(58)	1.385(7)
C(57)-H(57)	0.9500
C(58)-H(58)	0.9500
C(59)-C(60)	1.382(9)
C(59)-C(71)	1.388(8)
C(59)-H(59)	0.9500
C(60)-C(61)	1.373(8)
C(60)-H(60)	0.9500
C(61)-C(62)	1.382(7)
C(61)-H(61)	0.9500
C(62)-C(72)	1.403(7)
C(62)-C(63)	1.496(7)
C(63)-C(64)	1.463(7)
C(64)-C(81)	1.402(7)
C(66)-C(67)	1.525(7)
C(66)-H(66A)	0.9900
C(66)-H(66B)	0.9900
C(67)-C(68)	1.518(8)
C(67)-H(67A)	0.9900
C(67)-H(67B)	0.9900
C(68)-C(69)	1.523(11)
C(68)-H(68A)	0.9900
C(68)-H(68B)	0.9900
C(69)-C(70)	1.546(12)
C(69)-H(69A)	0.9900
C(69)-H(69B)	0.9900
C(70)-H(70A)	0.9800

C(70)-H(70B)	0.9800
C(70)-H(70C)	0.9800
C(71)-C(72)	1.375(7)
C(71)-H(71)	0.9500
C(72)-H(72)	0.9500
C(73)-C(80)	1.399(7)
C(73)-C(74)	1.424(7)
C(74)-C(75)	1.369(7)
C(75)-C(76)	1.409(7)
C(75)-H(75)	0.9500
C(76)-C(79)	1.412(7)
C(76)-C(77)	1.483(7)
C(78)-H(78A)	0.9800
C(78)-H(78B)	0.9800
C(78)-H(78C)	0.9800
C(79)-C(80)	1.376(7)
C(79)-H(79)	0.9500
C(80)-H(80)	0.9500
C(81)-C(82)	1.486(7)
C(82)-C(87)	1.396(7)
C(82)-C(83)	1.409(7)
C(83)-C(84)	1.381(8)
C(83)-H(83)	0.9500
C(84)-C(85)	1.383(8)
C(84)-H(84)	0.9500
C(85)-C(86)	1.399(8)
C(85)-H(85)	0.9500
C(86)-C(87)	1.391(7)
C(86)-H(86)	0.9500
C(87)-H(87)	0.9500
C(88)-C(89)	1.441(10)
C(88)-H(88A)	0.9800
C(88)-H(88B)	0.9800
C(88)-H(88C)	0.9800
C(89)-C(90)	1.534(8)
C(89)-H(89A)	0.9900
C(89)-H(89B)	0.9900

C(90)-C(91)	1.521(8)
C(90)-H(90A)	0.9900
C(90)-H(90B)	0.9900
C(91)-C(92)	1.530(7)
C(91)-H(91A)	0.9900
C(91)-H(91B)	0.9900
C(92)-H(92A)	0.9900
C(92)-H(92B)	0.9900
C(94)-C(100)	1.419(7)
C(94)-C(95)	1.452(7)
C(95)-C(96)	1.516(7)
C(96)-C(97)	1.400(8)
C(96)-C(109)	1.402(8)
C(97)-C(98)	1.396(8)
C(97)-H(97)	0.9500
C(98)-C(99)	1.395(9)
C(98)-H(98)	0.9500
C(99)-C(110)	1.370(9)
C(99)-H(99)	0.9500
C(100)-C(111)	1.491(7)
C(101)-C(102)	1.392(7)
C(101)-C(108)	1.404(7)
C(102)-C(103)	1.396(7)
C(102)-H(102)	0.9500
C(103)-C(106)	1.413(7)
C(103)-C(104)	1.490(7)
C(105)-H(10A)	0.9800
C(105)-H(10B)	0.9800
C(105)-H(10C)	0.9800
C(106)-C(107)	1.377(7)
C(106)-H(106)	0.9500
C(107)-C(108)	1.379(7)
C(107)-H(107)	0.9500
C(109)-C(110)	1.382(8)
C(109)-H(109)	0.9500
C(110)-H(110)	0.9500
C(111)-C(112)	1.395(7)

C(111)-C(116)	1.402(7)
C(112)-C(113)	1.393(8)
C(112)-H(112)	0.9500
C(113)-C(114)	1.389(8)
C(113)-H(113)	0.9500
C(114)-C(115)	1.380(8)
C(114)-H(114)	0.9500
C(115)-C(116)	1.391(8)
C(115)-H(115)	0.9500
C(116)-H(116)	0.9500

C(27)-O(2)-C(28)	115.0(4)
C(47)-O(5)-C(48)	116.0(4)
C(77)-O(8)-C(78)	115.4(4)
C(104)-O(11)-C(105)	115.8(4)
C(6)-N(1)-C(23)	107.3(4)
C(6)-N(1)-C(5)	124.8(4)
C(23)-N(1)-C(5)	127.7(4)
C(6)-N(2)-C(22)	108.7(4)
C(6)-N(2)-C(7)	105.5(4)
C(22)-N(2)-C(7)	145.1(4)
C(6)-N(3)-C(13)	103.9(4)
C(36)-N(4)-C(35)	106.6(4)
C(36)-N(4)-C(44)	107.9(4)
C(35)-N(4)-C(44)	145.5(4)
C(36)-N(5)-C(51)	107.3(4)
C(36)-N(5)-C(37)	124.2(4)
C(51)-N(5)-C(37)	126.9(5)
C(36)-N(6)-C(52)	102.5(4)
C(65)-N(7)-C(64)	106.5(4)
C(65)-N(7)-C(74)	109.1(4)
C(64)-N(7)-C(74)	144.4(4)
C(65)-N(8)-C(73)	106.7(4)
C(65)-N(8)-C(66)	125.7(4)
C(73)-N(8)-C(66)	127.5(4)
C(65)-N(9)-C(81)	102.9(4)
C(93)-N(10)-C(108)	106.7(4)

C(93)-N(10)-C(92)	125.7(4)
C(108)-N(10)-C(92)	127.2(4)
C(93)-N(11)-C(101)	108.9(4)
C(93)-N(11)-C(94)	105.4(4)
C(101)-N(11)-C(94)	145.7(4)
C(93)-N(12)-C(100)	104.2(4)
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(3)-C(2)-C(1)	111.7(5)
C(3)-C(2)-H(2A)	109.3
C(1)-C(2)-H(2A)	109.3
C(3)-C(2)-H(2B)	109.3
C(1)-C(2)-H(2B)	109.3
H(2A)-C(2)-H(2B)	107.9
C(2)-C(3)-C(4)	113.8(5)
C(2)-C(3)-H(3A)	108.8
C(4)-C(3)-H(3A)	108.8
C(2)-C(3)-H(3B)	108.8
C(4)-C(3)-H(3B)	108.8
H(3A)-C(3)-H(3B)	107.7
C(5)-C(4)-C(3)	110.4(4)
C(5)-C(4)-H(4A)	109.6
C(3)-C(4)-H(4A)	109.6
C(5)-C(4)-H(4B)	109.6
C(3)-C(4)-H(4B)	109.6
H(4A)-C(4)-H(4B)	108.1
N(1)-C(5)-C(4)	113.6(4)
N(1)-C(5)-H(5A)	108.8
C(4)-C(5)-H(5A)	108.8
N(1)-C(5)-H(5B)	108.8
C(4)-C(5)-H(5B)	108.8
H(5A)-C(5)-H(5B)	107.7
N(3)-C(6)-N(2)	114.9(5)

N(3)-C(6)-N(1)	135.1(5)
N(2)-C(6)-N(1)	109.9(4)
C(13)-C(7)-N(2)	103.9(4)
C(13)-C(7)-C(8)	136.4(5)
N(2)-C(7)-C(8)	119.7(5)
O(1)-C(8)-C(7)	120.2(5)
O(1)-C(8)-C(9)	118.2(5)
C(7)-C(8)-C(9)	121.6(5)
C(10)-C(9)-C(21)	119.1(5)
C(10)-C(9)-C(8)	122.1(5)
C(21)-C(9)-C(8)	118.5(5)
C(11)-C(10)-C(9)	120.1(6)
C(11)-C(10)-H(10)	120.0
C(9)-C(10)-H(10)	120.0
C(12)-C(11)-C(10)	120.3(6)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9
C(11)-C(12)-C(20)	120.8(6)
C(11)-C(12)-H(12)	119.6
C(20)-C(12)-H(12)	119.6
N(3)-C(13)-C(7)	111.7(5)
N(3)-C(13)-C(14)	117.2(5)
C(7)-C(13)-C(14)	130.8(5)
C(19)-C(14)-C(15)	118.1(5)
C(19)-C(14)-C(13)	123.1(5)
C(15)-C(14)-C(13)	118.7(5)
C(14)-C(15)-C(16)	121.5(5)
C(14)-C(15)-H(15)	119.3
C(16)-C(15)-H(15)	119.3
C(17)-C(16)-C(15)	119.6(6)
C(17)-C(16)-H(16)	120.2
C(15)-C(16)-H(16)	120.2
C(18)-C(17)-C(16)	119.1(6)
C(18)-C(17)-H(17)	120.5
C(16)-C(17)-H(17)	120.5
C(17)-C(18)-C(19)	120.7(6)
C(17)-C(18)-H(18)	119.6

C(19)-C(18)-H(18)	119.6
C(14)-C(19)-C(18)	120.9(6)
C(14)-C(19)-H(19)	119.5
C(18)-C(19)-H(19)	119.5
C(21)-C(20)-C(12)	119.2(6)
C(21)-C(20)-H(20)	120.4
C(12)-C(20)-H(20)	120.4
C(20)-C(21)-C(9)	120.4(6)
C(20)-C(21)-H(21)	119.8
C(9)-C(21)-H(21)	119.8
C(29)-C(22)-N(2)	134.2(5)
C(29)-C(22)-C(23)	120.9(5)
N(2)-C(22)-C(23)	104.9(4)
N(1)-C(23)-C(24)	129.9(5)
N(1)-C(23)-C(22)	109.1(4)
C(24)-C(23)-C(22)	121.0(5)
C(25)-C(24)-C(23)	117.7(5)
C(25)-C(24)-H(24)	121.2
C(23)-C(24)-H(24)	121.2
C(24)-C(25)-C(26)	121.5(5)
C(24)-C(25)-H(25)	119.2
C(26)-C(25)-H(25)	119.2
C(29)-C(26)-C(25)	120.3(5)
C(29)-C(26)-C(27)	118.1(5)
C(25)-C(26)-C(27)	121.6(5)
O(3)-C(27)-O(2)	123.6(5)
O(3)-C(27)-C(26)	125.0(5)
O(2)-C(27)-C(26)	111.4(5)
O(2)-C(28)-H(28A)	109.5
O(2)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
O(2)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(22)-C(29)-C(26)	118.6(5)
C(22)-C(29)-H(29)	120.7
C(26)-C(29)-H(29)	120.7

C(42)-C(30)-C(31)	119.3(5)
C(42)-C(30)-H(30)	120.3
C(31)-C(30)-H(30)	120.3
C(32)-C(31)-C(30)	120.4(5)
C(32)-C(31)-H(31)	119.8
C(30)-C(31)-H(31)	119.8
C(33)-C(32)-C(31)	120.5(5)
C(33)-C(32)-H(32)	119.7
C(31)-C(32)-H(32)	119.7
C(32)-C(33)-C(43)	119.1(5)
C(32)-C(33)-C(34)	118.1(5)
C(43)-C(33)-C(34)	122.8(5)
O(4)-C(34)-C(35)	121.5(5)
O(4)-C(34)-C(33)	118.9(5)
C(35)-C(34)-C(33)	119.7(5)
C(52)-C(35)-N(4)	103.0(4)
C(52)-C(35)-C(34)	134.6(5)
N(4)-C(35)-C(34)	122.4(4)
N(6)-C(36)-N(5)	134.8(5)
N(6)-C(36)-N(4)	114.8(5)
N(5)-C(36)-N(4)	110.4(4)
C(38)-C(37)-N(5)	110.3(6)
C(38)-C(37)-H(37A)	109.6
N(5)-C(37)-H(37A)	109.6
C(38)-C(37)-H(37B)	109.6
N(5)-C(37)-H(37B)	109.6
H(37A)-C(37)-H(37B)	108.1
C(37)-C(38)-C(39)	107.1(6)
C(37)-C(38)-H(38A)	110.3
C(39)-C(38)-H(38A)	110.3
C(37)-C(38)-H(38B)	110.3
C(39)-C(38)-H(38B)	110.3
H(38A)-C(38)-H(38B)	108.5
C(40)-C(39)-C(38)	114.0(6)
C(40)-C(39)-H(39A)	108.8
C(38)-C(39)-H(39A)	108.8
C(40)-C(39)-H(39B)	108.8

C(38)-C(39)-H(39B)	108.8
H(39A)-C(39)-H(39B)	107.7
C(41)-C(40)-C(39)	111.6(6)
C(41)-C(40)-H(40A)	109.3
C(39)-C(40)-H(40A)	109.3
C(41)-C(40)-H(40B)	109.3
C(39)-C(40)-H(40B)	109.3
H(40A)-C(40)-H(40B)	108.0
C(40)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(43)-C(42)-C(30)	120.1(5)
C(43)-C(42)-H(42)	120.0
C(30)-C(42)-H(42)	120.0
C(42)-C(43)-C(33)	120.5(5)
C(42)-C(43)-H(43)	119.7
C(33)-C(43)-H(43)	119.7
C(45)-C(44)-C(51)	120.8(5)
C(45)-C(44)-N(4)	133.4(5)
C(51)-C(44)-N(4)	105.8(4)
C(44)-C(45)-C(46)	117.4(5)
C(44)-C(45)-H(45)	121.3
C(46)-C(45)-H(45)	121.3
C(45)-C(46)-C(49)	121.3(5)
C(45)-C(46)-C(47)	118.2(5)
C(49)-C(46)-C(47)	120.4(5)
O(6)-C(47)-O(5)	123.0(5)
O(6)-C(47)-C(46)	124.7(5)
O(5)-C(47)-C(46)	112.3(5)
O(5)-C(48)-H(48A)	109.5
O(5)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
O(5)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5

H(48B)-C(48)-H(48C)	109.5
C(50)-C(49)-C(46)	121.3(5)
C(50)-C(49)-H(49)	119.4
C(46)-C(49)-H(49)	119.4
C(49)-C(50)-C(51)	117.0(5)
C(49)-C(50)-H(50)	121.5
C(51)-C(50)-H(50)	121.5
N(5)-C(51)-C(50)	129.1(5)
N(5)-C(51)-C(44)	108.6(5)
C(50)-C(51)-C(44)	122.3(5)
N(6)-C(52)-C(35)	113.1(5)
N(6)-C(52)-C(53)	118.1(4)
C(35)-C(52)-C(53)	128.6(5)
C(58)-C(53)-C(54)	118.8(5)
C(58)-C(53)-C(52)	120.9(5)
C(54)-C(53)-C(52)	120.3(5)
C(55)-C(54)-C(53)	120.1(5)
C(55)-C(54)-H(54)	119.9
C(53)-C(54)-H(54)	119.9
C(54)-C(55)-C(56)	120.7(5)
C(54)-C(55)-H(55)	119.6
C(56)-C(55)-H(55)	119.6
C(55)-C(56)-C(57)	119.3(5)
C(55)-C(56)-H(56)	120.3
C(57)-C(56)-H(56)	120.3
C(58)-C(57)-C(56)	119.9(5)
C(58)-C(57)-H(57)	120.0
C(56)-C(57)-H(57)	120.0
C(57)-C(58)-C(53)	121.1(5)
C(57)-C(58)-H(58)	119.5
C(53)-C(58)-H(58)	119.5
C(60)-C(59)-C(71)	119.5(6)
C(60)-C(59)-H(59)	120.3
C(71)-C(59)-H(59)	120.3
C(61)-C(60)-C(59)	120.2(6)
C(61)-C(60)-H(60)	119.9
C(59)-C(60)-H(60)	119.9

C(60)-C(61)-C(62)	120.8(6)
C(60)-C(61)-H(61)	119.6
C(62)-C(61)-H(61)	119.6
C(61)-C(62)-C(72)	119.2(5)
C(61)-C(62)-C(63)	118.2(5)
C(72)-C(62)-C(63)	122.2(5)
O(7)-C(63)-C(64)	120.1(5)
O(7)-C(63)-C(62)	119.3(5)
C(64)-C(63)-C(62)	120.5(5)
C(81)-C(64)-N(7)	103.2(4)
C(81)-C(64)-C(63)	136.9(5)
N(7)-C(64)-C(63)	119.9(5)
N(9)-C(65)-N(7)	114.7(5)
N(9)-C(65)-N(8)	135.2(5)
N(7)-C(65)-N(8)	110.1(4)
N(8)-C(66)-C(67)	112.8(4)
N(8)-C(66)-H(66A)	109.0
C(67)-C(66)-H(66A)	109.0
N(8)-C(66)-H(66B)	109.0
C(67)-C(66)-H(66B)	109.0
H(66A)-C(66)-H(66B)	107.8
C(68)-C(67)-C(66)	112.9(4)
C(68)-C(67)-H(67A)	109.0
C(66)-C(67)-H(67A)	109.0
C(68)-C(67)-H(67B)	109.0
C(66)-C(67)-H(67B)	109.0
H(67A)-C(67)-H(67B)	107.8
C(67)-C(68)-C(69)	111.1(6)
C(67)-C(68)-H(68A)	109.4
C(69)-C(68)-H(68A)	109.4
C(67)-C(68)-H(68B)	109.4
C(69)-C(68)-H(68B)	109.4
H(68A)-C(68)-H(68B)	108.0
C(68)-C(69)-C(70)	112.7(8)
C(68)-C(69)-H(69A)	109.0
C(70)-C(69)-H(69A)	109.0
C(68)-C(69)-H(69B)	109.0

C(70)-C(69)-H(69B)	109.0
H(69A)-C(69)-H(69B)	107.8
C(69)-C(70)-H(70A)	109.5
C(69)-C(70)-H(70B)	109.5
H(70A)-C(70)-H(70B)	109.5
C(69)-C(70)-H(70C)	109.5
H(70A)-C(70)-H(70C)	109.5
H(70B)-C(70)-H(70C)	109.5
C(72)-C(71)-C(59)	120.7(6)
C(72)-C(71)-H(71)	119.7
C(59)-C(71)-H(71)	119.7
C(71)-C(72)-C(62)	119.6(5)
C(71)-C(72)-H(72)	120.2
C(62)-C(72)-H(72)	120.2
N(8)-C(73)-C(80)	129.6(5)
N(8)-C(73)-C(74)	109.7(4)
C(80)-C(73)-C(74)	120.7(5)
C(75)-C(74)-C(73)	122.0(5)
C(75)-C(74)-N(7)	133.6(5)
C(73)-C(74)-N(7)	104.4(4)
C(74)-C(75)-C(76)	117.8(5)
C(74)-C(75)-H(75)	121.1
C(76)-C(75)-H(75)	121.1
C(75)-C(76)-C(79)	119.4(5)
C(75)-C(76)-C(77)	117.6(5)
C(79)-C(76)-C(77)	123.0(5)
O(9)-C(77)-O(8)	123.8(5)
O(9)-C(77)-C(76)	125.4(5)
O(8)-C(77)-C(76)	110.8(5)
O(8)-C(78)-H(78A)	109.5
O(8)-C(78)-H(78B)	109.5
H(78A)-C(78)-H(78B)	109.5
O(8)-C(78)-H(78C)	109.5
H(78A)-C(78)-H(78C)	109.5
H(78B)-C(78)-H(78C)	109.5
C(80)-C(79)-C(76)	123.5(5)
C(80)-C(79)-H(79)	118.2

C(76)-C(79)-H(79)	118.2
C(79)-C(80)-C(73)	116.5(5)
C(79)-C(80)-H(80)	121.7
C(73)-C(80)-H(80)	121.7
N(9)-C(81)-C(64)	112.8(5)
N(9)-C(81)-C(82)	117.7(5)
C(64)-C(81)-C(82)	129.1(5)
C(87)-C(82)-C(83)	119.0(5)
C(87)-C(82)-C(81)	121.5(5)
C(83)-C(82)-C(81)	119.4(5)
C(84)-C(83)-C(82)	120.5(5)
C(84)-C(83)-H(83)	119.7
C(82)-C(83)-H(83)	119.7
C(83)-C(84)-C(85)	120.2(5)
C(83)-C(84)-H(84)	119.9
C(85)-C(84)-H(84)	119.9
C(84)-C(85)-C(86)	120.1(5)
C(84)-C(85)-H(85)	120.0
C(86)-C(85)-H(85)	120.0
C(87)-C(86)-C(85)	119.9(5)
C(87)-C(86)-H(86)	120.0
C(85)-C(86)-H(86)	120.0
C(86)-C(87)-C(82)	120.3(5)
C(86)-C(87)-H(87)	119.9
C(82)-C(87)-H(87)	119.9
C(89)-C(88)-H(88A)	109.5
C(89)-C(88)-H(88B)	109.5
H(88A)-C(88)-H(88B)	109.5
C(89)-C(88)-H(88C)	109.5
H(88A)-C(88)-H(88C)	109.5
H(88B)-C(88)-H(88C)	109.5
C(88)-C(89)-C(90)	117.0(6)
C(88)-C(89)-H(89A)	108.1
C(90)-C(89)-H(89A)	108.1
C(88)-C(89)-H(89B)	108.1
C(90)-C(89)-H(89B)	108.1
H(89A)-C(89)-H(89B)	107.3

C(91)-C(90)-C(89)	113.5(5)
C(91)-C(90)-H(90A)	108.9
C(89)-C(90)-H(90A)	108.9
C(91)-C(90)-H(90B)	108.9
C(89)-C(90)-H(90B)	108.9
H(90A)-C(90)-H(90B)	107.7
C(90)-C(91)-C(92)	111.6(4)
C(90)-C(91)-H(91A)	109.3
C(92)-C(91)-H(91A)	109.3
C(90)-C(91)-H(91B)	109.3
C(92)-C(91)-H(91B)	109.3
H(91A)-C(91)-H(91B)	108.0
N(10)-C(92)-C(91)	112.7(4)
N(10)-C(92)-H(92A)	109.1
C(91)-C(92)-H(92A)	109.1
N(10)-C(92)-H(92B)	109.1
C(91)-C(92)-H(92B)	109.1
H(92A)-C(92)-H(92B)	107.8
N(12)-C(93)-N(10)	135.6(5)
N(12)-C(93)-N(11)	114.5(5)
N(10)-C(93)-N(11)	109.9(4)
C(100)-C(94)-N(11)	103.5(4)
C(100)-C(94)-C(95)	136.0(5)
N(11)-C(94)-C(95)	120.5(5)
O(12)-C(95)-C(94)	121.7(5)
O(12)-C(95)-C(96)	119.2(5)
C(94)-C(95)-C(96)	119.0(5)
C(97)-C(96)-C(109)	119.7(5)
C(97)-C(96)-C(95)	118.0(5)
C(109)-C(96)-C(95)	122.1(5)
C(98)-C(97)-C(96)	119.7(6)
C(98)-C(97)-H(97)	120.1
C(96)-C(97)-H(97)	120.1
C(99)-C(98)-C(97)	119.5(6)
C(99)-C(98)-H(98)	120.3
C(97)-C(98)-H(98)	120.3
C(110)-C(99)-C(98)	120.7(6)

C(110)-C(99)-H(99)	119.7
C(98)-C(99)-H(99)	119.7
N(12)-C(100)-C(94)	112.4(5)
N(12)-C(100)-C(111)	117.2(5)
C(94)-C(100)-C(111)	130.3(5)
C(102)-C(101)-C(108)	120.8(5)
C(102)-C(101)-N(11)	134.3(5)
C(108)-C(101)-N(11)	104.9(4)
C(101)-C(102)-C(103)	117.0(5)
C(101)-C(102)-H(102)	121.5
C(103)-C(102)-H(102)	121.5
C(102)-C(103)-C(106)	121.1(5)
C(102)-C(103)-C(104)	117.7(5)
C(106)-C(103)-C(104)	121.2(5)
O(10)-C(104)-O(11)	122.5(5)
O(10)-C(104)-C(103)	126.2(5)
O(11)-C(104)-C(103)	111.3(5)
O(11)-C(105)-H(10A)	109.5
O(11)-C(105)-H(10B)	109.5
H(10A)-C(105)-H(10B)	109.5
O(11)-C(105)-H(10C)	109.5
H(10A)-C(105)-H(10C)	109.5
H(10B)-C(105)-H(10C)	109.5
C(107)-C(106)-C(103)	121.7(5)
C(107)-C(106)-H(106)	119.1
C(103)-C(106)-H(106)	119.1
C(106)-C(107)-C(108)	117.0(5)
C(106)-C(107)-H(107)	121.5
C(108)-C(107)-H(107)	121.5
C(107)-C(108)-C(101)	122.5(5)
C(107)-C(108)-N(10)	128.0(5)
C(101)-C(108)-N(10)	109.6(5)
C(110)-C(109)-C(96)	119.7(6)
C(110)-C(109)-H(109)	120.2
C(96)-C(109)-H(109)	120.2
C(99)-C(110)-C(109)	120.7(6)
C(99)-C(110)-H(110)	119.6

C(109)-C(110)-H(110)	119.6
C(112)-C(111)-C(116)	119.1(5)
C(112)-C(111)-C(100)	118.9(5)
C(116)-C(111)-C(100)	121.7(5)
C(113)-C(112)-C(111)	120.7(5)
C(113)-C(112)-H(112)	119.7
C(111)-C(112)-H(112)	119.7
C(114)-C(113)-C(112)	119.9(6)
C(114)-C(113)-H(113)	120.1
C(112)-C(113)-H(113)	120.1
C(115)-C(114)-C(113)	119.6(6)
C(115)-C(114)-H(114)	120.2
C(113)-C(114)-H(114)	120.2
C(114)-C(115)-C(116)	121.1(5)
C(114)-C(115)-H(115)	119.4
C(116)-C(115)-H(115)	119.4
C(115)-C(116)-C(111)	119.5(5)
C(115)-C(116)-H(116)	120.2
C(111)-C(116)-H(116)	120.2

Symmetry transformations used to generate equivalent atoms: Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for 121122LT_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)	30(2)	28(2)	25(2)	-2(2)	5(2)	3(2)
O(2)	28(2)	33(2)	27(2)	8(2)	12(2)	5(2)
O(3)	33(2)	31(2)	25(2)	-2(2)	3(2)	-2(2)
O(4)	28(2)	56(3)	16(2)	1(2)	4(2)	3(2)
O(5)	28(2)	31(2)	29(2)	-5(2)	14(2)	3(2)
O(6)	33(2)	33(2)	23(2)	-2(2)	4(2)	-2(2)
O(7)	30(2)	44(2)	23(2)	9(2)	4(2)	-1(2)
O(8)	32(2)	34(2)	28(2)	5(2)	13(2)	2(2)
O(9)	35(3)	34(2)	22(2)	-2(2)	4(2)	-2(2)
O(10)	37(2)	35(2)	17(2)	-3(2)	4(2)	2(2)
O(11)	28(2)	30(2)	28(2)	0(2)	12(2)	3(2)

O(12)	29(2)	47(2)	20(2)	1(2)	5(2)	-3(2)
N(1)	20(3)	24(2)	17(2)	-3(2)	0(2)	-2(2)
N(2)	21(3)	21(2)	15(2)	-2(2)	3(2)	-2(2)
N(3)	23(3)	22(2)	18(2)	0(2)	3(2)	1(2)
N(4)	19(2)	18(2)	21(3)	-1(2)	4(2)	2(2)
N(5)	19(3)	36(3)	23(3)	-2(2)	1(2)	0(2)
N(6)	23(3)	29(3)	18(3)	-2(2)	3(2)	2(2)
N(7)	23(3)	19(2)	18(2)	1(2)	4(2)	0(2)
N(8)	24(3)	23(2)	23(3)	3(2)	-1(2)	2(2)
N(9)	29(3)	23(2)	22(3)	-1(2)	0(2)	2(2)
N(10)	20(3)	22(2)	18(2)	1(2)	-1(2)	-3(2)
N(11)	20(3)	20(2)	22(3)	0(2)	1(2)	-2(2)
N(12)	25(3)	22(2)	17(2)	0(2)	1(2)	-1(2)
C(1)	45(4)	66(5)	29(4)	5(3)	-7(3)	-8(3)
C(2)	44(4)	44(4)	24(3)	-3(3)	2(3)	8(3)
C(3)	36(4)	29(3)	25(3)	-2(2)	6(3)	6(3)
C(4)	30(3)	31(3)	19(3)	3(2)	3(3)	5(2)
C(5)	23(3)	24(3)	23(3)	0(2)	0(2)	-3(2)
C(6)	19(3)	20(3)	24(3)	-4(2)	2(2)	-1(2)
C(7)	16(3)	22(3)	26(3)	2(2)	-2(2)	-2(2)
C(8)	30(3)	15(3)	18(3)	-2(2)	5(3)	2(2)
C(9)	28(3)	21(3)	28(3)	-8(2)	-1(3)	5(2)
C(10)	29(3)	19(3)	39(4)	-6(2)	7(3)	-1(2)
C(11)	30(4)	33(4)	52(4)	-17(3)	14(3)	-7(3)
C(12)	30(4)	39(4)	62(5)	-26(3)	-3(4)	-5(3)
C(13)	27(3)	18(3)	22(3)	1(2)	3(3)	3(2)
C(14)	23(3)	23(3)	25(3)	-3(2)	5(3)	0(2)
C(15)	25(3)	33(3)	35(4)	4(3)	1(3)	5(3)
C(16)	35(4)	48(4)	38(4)	-3(3)	13(3)	-5(3)
C(17)	28(4)	53(4)	47(4)	-4(3)	7(3)	1(3)
C(18)	27(4)	29(3)	44(4)	-4(3)	-4(3)	3(3)
C(19)	23(3)	28(3)	38(4)	1(3)	4(3)	3(2)
C(20)	41(4)	39(4)	50(4)	-17(3)	-14(3)	2(3)
C(21)	38(4)	27(3)	31(4)	-8(3)	-4(3)	3(3)
C(22)	24(3)	16(3)	20(3)	1(2)	3(2)	-1(2)
C(23)	23(3)	17(3)	19(3)	1(2)	5(2)	-2(2)
C(24)	25(3)	22(3)	23(3)	3(2)	0(2)	-1(2)

C(25)	25(3)	18(3)	32(3)	5(2)	5(3)	2(2)
C(26)	24(3)	18(3)	20(3)	3(2)	4(2)	-2(2)
C(27)	23(3)	18(3)	30(4)	-2(2)	6(3)	-1(2)
C(28)	39(4)	35(3)	33(4)	4(3)	20(3)	4(3)
C(29)	29(3)	15(3)	17(3)	1(2)	2(2)	-6(2)
C(30)	24(3)	37(3)	36(4)	5(3)	8(3)	-1(3)
C(31)	22(3)	35(3)	36(4)	1(3)	-2(3)	3(2)
C(32)	27(3)	26(3)	23(3)	0(2)	3(3)	-2(2)
C(33)	22(3)	26(3)	14(3)	-1(2)	-2(2)	2(2)
C(34)	25(3)	23(3)	18(3)	-1(2)	-2(2)	3(2)
C(35)	16(3)	18(3)	24(3)	4(2)	6(2)	0(2)
C(36)	24(3)	26(3)	18(3)	3(2)	2(2)	-2(2)
C(37)	44(4)	76(5)	28(4)	7(3)	11(3)	25(4)
C(38)	68(5)	41(4)	57(5)	-11(3)	20(4)	-9(3)
C(39)	55(5)	97(6)	38(4)	5(4)	-12(4)	22(4)
C(40)	43(4)	45(4)	22(3)	6(3)	-3(3)	-6(3)
C(41)	66(5)	48(4)	31(4)	3(3)	-5(3)	-6(3)
C(42)	35(4)	33(3)	36(4)	3(3)	3(3)	-7(3)
C(43)	25(3)	31(3)	21(3)	1(2)	-3(2)	-1(2)
C(44)	24(3)	16(3)	19(3)	2(2)	6(2)	-2(2)
C(45)	22(3)	17(3)	22(3)	0(2)	-2(2)	-4(2)
C(46)	28(3)	17(3)	25(3)	-2(2)	9(3)	-5(2)
C(47)	32(4)	15(3)	28(3)	-4(2)	3(3)	-3(2)
C(48)	39(4)	50(4)	26(4)	-4(3)	18(3)	0(3)
C(49)	24(3)	14(3)	34(3)	0(2)	7(3)	-1(2)
C(50)	24(3)	22(3)	28(3)	1(2)	5(3)	1(2)
C(51)	25(3)	23(3)	16(3)	2(2)	2(2)	-1(2)
C(52)	24(3)	22(3)	16(3)	3(2)	-2(2)	-1(2)
C(53)	22(3)	26(3)	22(3)	-6(2)	3(2)	-2(2)
C(54)	29(4)	37(3)	22(3)	6(3)	2(3)	2(3)
C(55)	30(4)	61(4)	21(3)	5(3)	5(3)	-1(3)
C(56)	24(3)	47(4)	29(4)	-7(3)	6(3)	4(3)
C(57)	31(4)	33(3)	27(3)	-4(3)	3(3)	0(3)
C(58)	27(3)	30(3)	19(3)	-4(2)	6(3)	1(2)
C(59)	25(4)	66(5)	47(4)	-4(4)	-1(3)	-12(3)
C(60)	30(4)	65(5)	38(4)	10(3)	-8(3)	-9(3)
C(61)	25(4)	44(4)	30(4)	11(3)	2(3)	0(3)

C(62)	20(3)	27(3)	19(3)	-2(2)	2(2)	1(2)
C(63)	23(3)	19(3)	16(3)	2(2)	-3(2)	2(2)
C(64)	22(3)	25(3)	23(3)	4(2)	6(2)	4(2)
C(65)	29(3)	16(3)	21(3)	-2(2)	2(3)	2(2)
C(66)	25(3)	22(3)	24(3)	-5(2)	-5(2)	2(2)
C(67)	31(4)	26(3)	32(3)	-2(2)	-2(3)	1(2)
C(68)	45(4)	38(4)	33(4)	2(3)	-17(3)	2(3)
C(69)	114(9)	94(7)	84(7)	-4(6)	-47(7)	-1(6)
C(70)	123(10)	112(9)	117(10)	-10(7)	-38(8)	-11(7)
C(71)	34(4)	31(3)	33(4)	3(3)	0(3)	-12(3)
C(72)	27(3)	22(3)	23(3)	0(2)	-2(2)	-1(2)
C(73)	27(3)	13(3)	19(3)	1(2)	2(2)	-3(2)
C(74)	23(3)	19(3)	22(3)	3(2)	4(2)	0(2)
C(75)	24(3)	16(3)	17(3)	2(2)	0(2)	0(2)
C(76)	23(3)	18(3)	28(3)	2(2)	9(3)	-1(2)
C(77)	33(4)	16(3)	25(3)	0(2)	9(3)	-2(2)
C(78)	44(4)	51(4)	27(4)	1(3)	16(3)	-5(3)
C(79)	24(3)	21(3)	36(4)	7(2)	10(3)	2(2)
C(80)	16(3)	26(3)	29(3)	5(2)	-2(2)	1(2)
C(81)	25(3)	20(3)	23(3)	4(2)	4(3)	-4(2)
C(82)	22(3)	19(3)	20(3)	-3(2)	4(2)	-6(2)
C(83)	32(3)	25(3)	25(3)	0(2)	3(3)	-4(2)
C(84)	33(4)	39(4)	22(3)	-1(3)	11(3)	-3(3)
C(85)	30(4)	42(4)	31(4)	-9(3)	11(3)	-3(3)
C(86)	26(3)	31(3)	38(4)	-2(3)	7(3)	2(2)
C(87)	26(3)	31(3)	26(3)	2(2)	7(3)	-3(2)
C(88)	91(7)	52(5)	107(8)	31(5)	-42(6)	-11(4)
C(89)	133(8)	27(4)	56(5)	21(3)	-35(5)	-26(4)
C(90)	66(5)	31(4)	35(4)	6(3)	-21(3)	-9(3)
C(91)	38(4)	30(3)	26(3)	4(2)	-3(3)	-6(3)
C(92)	26(3)	28(3)	14(3)	-4(2)	0(2)	-4(2)
C(93)	28(3)	17(3)	15(3)	0(2)	2(2)	-4(2)
C(94)	24(3)	14(3)	23(3)	0(2)	3(2)	1(2)
C(95)	27(3)	23(3)	22(3)	3(2)	6(3)	2(2)
C(96)	29(3)	25(3)	23(3)	-14(2)	-3(3)	0(2)
C(97)	32(4)	35(3)	27(3)	-8(3)	1(3)	-2(3)
C(98)	39(4)	47(4)	40(4)	-14(3)	-8(3)	9(3)

C(99)	24(4)	42(4)	67(5)	-17(4)	-4(4)	-3(3)
C(100)	28(3)	14(3)	22(3)	3(2)	3(3)	-2(2)
C(101)	21(3)	18(3)	21(3)	2(2)	0(2)	-1(2)
C(102)	23(3)	15(3)	18(3)	1(2)	1(2)	1(2)
C(103)	25(3)	17(3)	23(3)	0(2)	6(2)	-2(2)
C(104)	23(3)	16(3)	27(3)	3(2)	9(3)	-1(2)
C(105)	31(4)	38(3)	29(3)	4(3)	15(3)	11(3)
C(106)	28(3)	14(3)	30(3)	-1(2)	2(3)	-2(2)
C(107)	24(3)	23(3)	22(3)	-2(2)	0(2)	2(2)
C(108)	28(3)	16(3)	22(3)	0(2)	8(3)	-4(2)
C(109)	33(4)	26(3)	33(4)	-2(3)	3(3)	-3(3)
C(110)	29(4)	31(3)	60(5)	-10(3)	11(3)	-3(3)
C(111)	25(3)	18(3)	27(3)	-7(2)	1(3)	-5(2)
C(112)	28(3)	27(3)	25(3)	-3(2)	6(3)	-5(2)
C(113)	31(4)	32(3)	46(4)	-7(3)	15(3)	-8(3)
C(114)	27(4)	32(4)	47(4)	-9(3)	7(3)	-2(3)
C(115)	32(4)	25(3)	40(4)	-4(3)	-3(3)	3(2)
C(116)	31(4)	24(3)	26(3)	-4(2)	0(3)	1(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10 ^{3}) for 121122LT_0m.

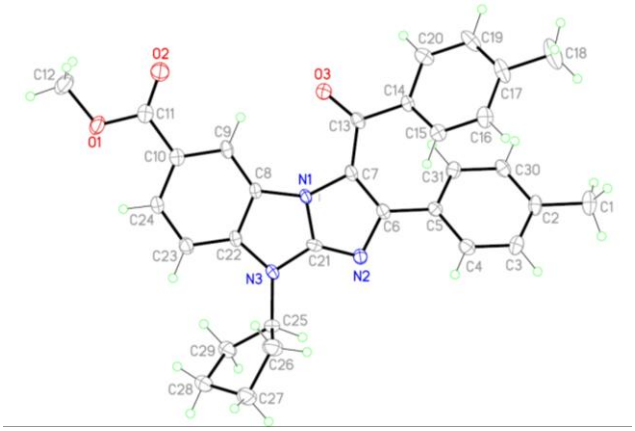
	x	y	z	U(eq)
H(1A)	2459	5764	6994	71
H(1B)	1887	6115	7341	71
H(1C)	2610	5842	7742	71
H(2A)	2800	6591	6816	45
H(2B)	2860	6712	7556	45
H(3A)	4096	6561	7088	36
H(3B)	3864	5983	7107	36
H(4A)	3796	6131	8261	32
H(4B)	4641	6057	8024	32
H(5A)	4836	6926	8004	28
H(5B)	3966	7024	8173	28
H(10)	7582	7501	10067	34

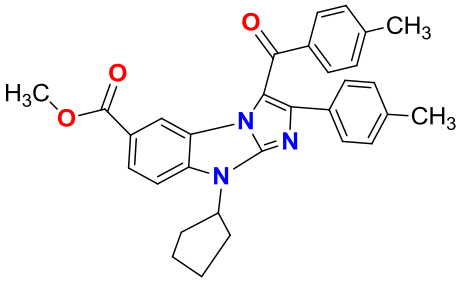
H(11)	8774	7866	10448	45
H(12)	9393	7647	11429	53
H(15)	7452	7064	8512	38
H(16)	8709	6896	8255	47
H(17)	9561	6398	8927	51
H(18)	9116	6046	9822	41
H(19)	7861	6213	10072	35
H(20)	8776	7116	12092	54
H(21)	7548	6782	11740	39
H(24)	3136	6954	9052	28
H(25)	2670	7083	10027	30
H(28A)	2330	6795	11908	52
H(28B)	1738	7228	11646	52
H(28C)	2567	7368	12026	52
H(29)	4876	6958	10943	25
H(30)	9985	9267	10027	38
H(31)	9493	8798	10823	37
H(32)	8152	8774	10896	30
H(37A)	4127	9026	8186	58
H(37B)	3426	9075	8619	58
H(38A)	4115	9899	8060	65
H(38B)	3378	9928	8460	65
H(39A)	2661	9359	7680	78
H(39B)	2833	9891	7383	78
H(40A)	3970	9506	6992	45
H(40B)	3629	8979	7191	45
H(41A)	2499	9099	6485	74
H(41B)	3251	9152	6111	74
H(41C)	2798	9641	6305	74
H(42)	9119	9717	9311	41
H(43)	7775	9682	9377	31
H(45)	5490	9384	11001	25
H(48A)	3588	9232	12599	56
H(48B)	2907	9644	12524	56
H(48C)	3797	9810	12717	56
H(49)	3124	9644	10710	28
H(50)	3131	9567	9612	29

H(54)	7000	9345	7957	35
H(55)	8038	9027	7467	45
H(56)	8766	8349	7904	40
H(57)	8455	7993	8854	36
H(58)	7448	8331	9364	30
H(59)	-440	7734	-377	56
H(60)	2	8283	-1111	55
H(61)	1275	8581	-968	40
H(66A)	5130	8436	2096	29
H(66B)	5867	8399	1701	29
H(67A)	5050	7555	2134	36
H(67B)	5760	7507	1713	36
H(68A)	6588	7914	2561	48
H(68B)	6301	7366	2731	48
H(69A)	5292	7721	3263	122
H(69B)	5569	8269	3087	122
H(70A)	6567	7608	3880	182
H(70B)	6042	8029	4161	182
H(70C)	6738	8186	3762	182
H(71)	391	7515	525	40
H(72)	1661	7824	684	29
H(75)	3914	8164	-781	23
H(78A)	5692	7623	-2396	59
H(78B)	6538	7871	-2233	59
H(78C)	5781	8219	-2380	59
H(79)	6267	7925	-411	32
H(80)	6228	8023	668	29
H(83)	2355	8276	2253	33
H(84)	1310	8594	2732	37
H(85)	476	9186	2213	40
H(86)	678	9457	1196	38
H(87)	1718	9133	704	33
H(88A)	6869	5553	3828	131
H(88B)	6696	5014	4109	131
H(88C)	6142	5478	4226	131
H(89A)	5541	4977	3463	91
H(89B)	6279	5012	3074	91

H(90A)	5185	5797	3215	55
H(90B)	5985	5896	2920	55
H(91A)	4723	5283	2375	38
H(91B)	5555	5292	2104	38
H(92A)	4518	6132	2124	27
H(92B)	5380	6179	1916	27
H(97)	1698	5935	-1448	38
H(98)	408	5672	-1769	51
H(99)	-183	5082	-1163	54
H(102)	4507	5563	-740	23
H(10A)	6930	5111	-1690	47
H(10B)	7716	5337	-1325	47
H(10C)	7070	5702	-1678	47
H(106)	6702	5537	228	29
H(107)	6195	5674	1184	28
H(109)	1744	5042	104	37
H(110)	482	4769	-244	48
H(112)	1863	5627	1709	32
H(113)	602	5841	1927	43
H(114)	-206	6328	1208	42
H(115)	238	6578	266	39
H(116)	1501	6377	44	32

ORTEP diagram of 5h





Compound Name: **5h**

Formula: $C_{31}H_{29}N_3O_3$

Unit Cell Parameters: a 15.4841(5) b 28.1687(10) c 17.1022(5) P21/c

Table 1. Crystal data and structure refinement for 140616LT_0M.

Identification code	140616LT_0m	
Empirical formula	C31 H29 N3 O3	
Formula weight	491.57	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 15.4841(5) Å	α= 90°.
	b = 28.1687(10) Å	β= 98.999(2)°.
	c = 17.1022(5) Å	γ = 90°.
Volume	7367.6(4) $Å^3$	
Z	12	
Density (calculated)	1.330 Mg/m^3	
Absorption coefficient	0.086 mm^{-1}	
F(000)	3120	
Crystal size	0.30 x 0.25 x 0.03 mm^3	
Theta range for data collection	1.331 to 26.411°.	
Index ranges	-19<=h<=13, -28<=k<=35, -21<=l<=19	
Reflections collected	59484	
Independent reflections	15029 [R(int) = 0.0510]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8258	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15029 / 0 / 1009	
Goodness-of-fit on F^2	1.041	
Final R indices [I>2sigma(I)]	R1 = 0.0789, wR2 = 0.2033	
R indices (all data)	R1 = 0.1260, wR2 = 0.2424	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.072 and -0.417 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3)
for 140616LT_0M. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	6531(1)	4008(1)	3811(1)	25(1)
O(2)	6438(2)	4768(1)	4171(1)	35(1)
O(3)	6978(1)	6150(1)	2881(1)	25(1)
O(4)	7286(1)	5131(1)	-1022(1)	35(1)
O(5)	6956(2)	5910(1)	-1080(1)	44(1)
O(6)	6327(1)	3867(1)	237(1)	29(1)
O(7)	10101(1)	5918(1)	2647(1)	28(1)
O(8)	10509(1)	5158(1)	2584(1)	27(1)
O(9)	9681(1)	3824(1)	3806(1)	22(1)
N(1)	7858(1)	5562(1)	1858(1)	15(1)
N(2)	8455(1)	5809(1)	802(1)	17(1)
N(3)	8352(1)	4966(1)	1179(1)	18(1)
N(4)	5616(2)	4532(1)	1245(1)	22(1)
N(5)	5010(2)	4363(1)	2333(1)	25(1)
N(6)	5243(2)	5184(1)	1851(1)	26(1)
N(7)	8837(1)	4450(1)	4810(1)	13(1)
N(8)	8326(1)	5068(1)	5414(1)	18(1)
N(9)	8215(1)	4238(1)	5872(1)	17(1)
C(1)	8504(2)	8066(1)	-116(2)	29(1)
C(2)	8398(2)	7577(1)	207(2)	20(1)
C(3)	9016(2)	7226(1)	151(2)	23(1)
C(4)	8936(2)	6779(1)	467(2)	21(1)
C(5)	8232(2)	6667(1)	848(1)	16(1)
C(6)	8178(2)	6194(1)	1195(2)	16(1)
C(7)	7828(2)	6060(1)	1872(2)	16(1)
C(8)	7683(2)	5140(1)	2241(2)	15(1)
C(9)	7262(2)	5051(1)	2882(2)	17(1)
C(10)	7180(2)	4577(1)	3093(2)	18(1)
C(11)	6688(2)	4475(1)	3745(2)	20(1)
C(12)	5983(2)	3885(1)	4380(2)	32(1)
C(13)	7514(2)	6324(1)	2505(2)	17(1)

C(14)	7881(2)	6809(1)	2691(1)	16(1)
C(15)	8726(2)	6929(1)	2590(1)	19(1)
C(16)	9034(2)	7385(1)	2729(2)	24(1)
C(17)	8507(2)	7737(1)	2990(2)	27(1)
C(18)	8850(2)	8236(1)	3143(2)	42(1)
C(19)	7675(2)	7614(1)	3114(2)	28(1)
C(20)	7360(2)	7156(1)	2970(2)	23(1)
C(21)	8252(2)	5446(1)	1227(1)	16(1)
C(22)	8013(2)	4771(1)	1812(1)	15(1)
C(23)	7955(2)	4303(1)	2049(2)	20(1)
C(24)	7528(2)	4210(1)	2682(2)	18(1)
C(25)	8832(2)	4742(1)	601(2)	19(1)
C(26)	9767(2)	4614(1)	965(2)	28(1)
C(27)	9988(2)	4192(1)	482(2)	28(1)
C(28)	9140(2)	3905(1)	384(2)	27(1)
C(29)	8423(2)	4284(1)	219(2)	23(1)
C(30)	7685(2)	7458(1)	569(2)	20(1)
C(31)	7596(2)	7010(1)	878(2)	18(1)
C(32)	4744(2)	2124(1)	3437(2)	34(1)
C(33)	4879(2)	2601(1)	3082(2)	25(1)
C(34)	5630(2)	2702(1)	2758(2)	23(1)
C(35)	5755(2)	3137(1)	2420(2)	22(1)
C(36)	5115(2)	3489(1)	2369(2)	22(1)
C(37)	5220(2)	3946(1)	1978(2)	23(1)
C(38)	5577(2)	4032(1)	1290(2)	21(1)
C(39)	5870(2)	4922(1)	809(2)	24(1)
C(40)	6287(2)	4965(1)	157(2)	24(1)
C(41)	6456(2)	5423(1)	-97(2)	30(1)
C(42)	6910(2)	5521(1)	-773(2)	33(1)
C(43)	7751(2)	5204(1)	-1704(2)	49(1)
C(44)	5833(2)	3728(1)	686(2)	21(1)
C(45)	5459(2)	3234(1)	611(1)	18(1)
C(46)	4609(2)	3131(1)	726(1)	19(1)
C(47)	4304(2)	2670(1)	668(2)	19(1)
C(48)	4840(2)	2296(1)	506(2)	24(1)
C(49)	4495(2)	1795(1)	474(2)	41(1)
C(50)	5679(2)	2401(1)	372(2)	26(1)

C(51)	5989(2)	2864(1)	412(2)	22(1)
C(52)	5251(2)	4698(1)	1867(2)	25(1)
C(53)	5621(2)	5326(1)	1215(2)	26(1)
C(54)	5794(2)	5781(1)	953(2)	30(1)
C(55)	6209(2)	5822(1)	307(2)	30(1)
C(56)	4914(2)	5516(1)	2396(2)	31(1)
C(57)	4617(3)	5288(1)	3104(2)	50(1)
C(58)	4099(2)	5670(1)	3431(2)	49(1)
C(59)	3718(3)	5975(1)	2725(2)	51(1)
C(60)	4086(2)	5777(1)	2014(2)	41(1)
C(61)	4255(2)	2964(1)	3053(2)	30(1)
C(62)	4366(2)	3398(1)	2697(2)	28(1)
C(63)	10672(2)	6029(1)	2095(2)	39(1)
C(64)	10106(2)	5463(1)	2877(2)	21(1)
C(65)	9584(2)	5386(1)	3517(1)	18(1)
C(66)	9486(2)	4921(1)	3769(1)	15(1)
C(67)	9037(2)	4855(1)	4397(1)	14(1)
C(68)	8863(2)	3952(1)	4835(1)	14(1)
C(69)	9154(2)	3668(1)	4212(1)	14(1)
C(70)	8756(2)	3186(1)	4056(1)	14(1)
C(71)	7899(2)	3090(1)	4158(1)	17(1)
C(72)	7557(2)	2638(1)	4038(1)	18(1)
C(73)	8059(2)	2268(1)	3817(2)	21(1)
C(74)	7675(2)	1777(1)	3706(2)	30(1)
C(75)	9216(2)	5766(1)	3877(2)	20(1)
C(76)	8767(2)	5698(1)	4508(2)	21(1)
C(77)	8697(2)	5240(1)	4779(2)	16(1)
C(78)	7809(2)	5318(1)	5938(2)	22(1)
C(79)	6956(2)	5530(1)	5512(2)	36(1)
C(80)	6710(2)	5871(1)	6113(2)	30(1)
C(81)	7574(2)	6096(1)	6482(2)	38(1)
C(82)	8288(2)	5732(1)	6403(2)	21(1)
C(83)	8424(2)	4585(1)	5420(1)	16(1)
C(84)	8498(2)	3840(1)	5512(1)	14(1)
C(85)	8425(2)	3373(1)	5882(1)	15(1)
C(86)	7719(2)	3277(1)	6269(2)	19(1)
C(87)	7625(2)	2835(1)	6598(2)	20(1)

C(88)	8228(2)	2474(1)	6545(1)	18(1)
C(89)	8939(2)	2576(1)	6169(1)	18(1)
C(90)	9046(2)	3019(1)	5855(1)	17(1)
C(91)	8106(2)	1989(1)	6879(2)	25(1)
C(92)	8910(2)	2368(1)	3696(2)	22(1)
C(93)	9253(2)	2821(1)	3804(2)	18(1)

Table 3. Bond lengths [Å] and angles [°] for 140616LT_0M.

O(1)-C(11)	1.345(3)
O(1)-C(12)	1.430(3)
O(2)-C(11)	1.204(3)
O(3)-C(13)	1.228(3)
O(4)-C(42)	1.343(4)
O(4)-C(43)	1.477(4)
O(5)-C(42)	1.223(4)
O(6)-C(44)	1.230(3)
O(7)-C(64)	1.342(3)
O(7)-C(63)	1.424(4)
O(8)-C(64)	1.216(3)
O(9)-C(69)	1.231(3)
N(1)-C(21)	1.359(3)
N(1)-C(8)	1.403(3)
N(1)-C(7)	1.404(3)
N(2)-C(21)	1.319(3)
N(2)-C(6)	1.380(3)
N(3)-C(21)	1.367(3)
N(3)-C(22)	1.389(3)
N(3)-C(25)	1.468(3)
N(4)-C(52)	1.363(4)
N(4)-C(38)	1.411(4)
N(4)-C(39)	1.418(4)
N(5)-C(52)	1.327(4)
N(5)-C(37)	1.385(3)
N(6)-C(52)	1.370(4)
N(6)-C(53)	1.372(4)
N(6)-C(56)	1.466(4)

N(7)-C(83)	1.361(3)
N(7)-C(67)	1.401(3)
N(7)-C(68)	1.403(3)
N(8)-C(83)	1.368(3)
N(8)-C(77)	1.393(3)
N(8)-C(78)	1.472(3)
N(9)-C(83)	1.317(3)
N(9)-C(84)	1.382(3)
C(1)-C(2)	1.504(4)
C(1)-H(24)	0.9800
C(1)-H(1)	0.9800
C(1)-H(25)	0.9800
C(2)-C(30)	1.387(4)
C(2)-C(3)	1.390(4)
C(3)-C(4)	1.383(4)
C(3)-H(26)	0.9500
C(4)-C(5)	1.390(4)
C(4)-H(27)	0.9500
C(5)-C(31)	1.388(4)
C(5)-C(6)	1.467(4)
C(6)-C(7)	1.404(4)
C(7)-C(13)	1.459(4)
C(8)-C(9)	1.383(4)
C(8)-C(22)	1.413(4)
C(9)-C(10)	1.393(4)
C(9)-H(28)	0.9500
C(10)-C(24)	1.404(4)
C(10)-C(11)	1.474(4)
C(12)-H(29)	0.9800
C(12)-H(3)	0.9800
C(12)-H(2)	0.9800
C(13)-C(14)	1.495(4)
C(14)-C(15)	1.387(4)
C(14)-C(20)	1.400(4)
C(15)-C(16)	1.378(4)
C(15)-H(4)	0.9500
C(16)-C(17)	1.401(4)

C(16)-H(5)	0.9500
C(17)-C(19)	1.383(4)
C(17)-C(18)	1.510(4)
C(18)-H(8)	0.9800
C(18)-H(6)	0.9800
C(18)-H(7)	0.9800
C(19)-C(20)	1.387(4)
C(19)-H(9)	0.9500
C(20)-H(10)	0.9500
C(22)-C(23)	1.386(4)
C(23)-C(24)	1.379(4)
C(23)-H(12)	0.9500
C(24)-H(11)	0.9500
C(25)-C(26)	1.527(4)
C(25)-C(29)	1.539(4)
C(25)-H(13)	1.0000
C(26)-C(27)	1.516(4)
C(26)-H(14)	0.9900
C(26)-H(15)	0.9900
C(27)-C(28)	1.529(4)
C(27)-H(17)	0.9900
C(27)-H(16)	0.9900
C(28)-C(29)	1.533(4)
C(28)-H(18)	0.9900
C(28)-H(19)	0.9900
C(29)-H(21)	0.9900
C(29)-H(20)	0.9900
C(30)-C(31)	1.383(4)
C(30)-H(23)	0.9500
C(31)-H(22)	0.9500
C(32)-C(33)	1.505(4)
C(32)-H(54)	0.9800
C(32)-H(30)	0.9800
C(32)-H(53)	0.9800
C(33)-C(34)	1.393(4)
C(33)-C(61)	1.404(4)
C(34)-C(35)	1.380(4)

C(34)-H(55)	0.9500
C(35)-C(36)	1.397(4)
C(35)-H(56)	0.9500
C(36)-C(62)	1.388(4)
C(36)-C(37)	1.470(4)
C(37)-C(38)	1.397(4)
C(38)-C(44)	1.444(4)
C(39)-C(40)	1.378(4)
C(39)-C(53)	1.417(4)
C(40)-C(41)	1.401(4)
C(40)-H(57)	0.9500
C(41)-C(55)	1.403(4)
C(41)-C(42)	1.469(5)
C(43)-H(58)	0.9800
C(43)-H(31)	0.9800
C(43)-H(32)	0.9800
C(44)-C(45)	1.505(4)
C(45)-C(46)	1.391(4)
C(45)-C(51)	1.403(4)
C(46)-C(47)	1.381(4)
C(46)-H(39)	0.9500
C(47)-C(48)	1.395(4)
C(47)-H(38)	0.9500
C(48)-C(50)	1.386(4)
C(48)-C(49)	1.508(4)
C(49)-H(34)	0.9800
C(49)-H(35)	0.9800
C(49)-H(33)	0.9800
C(50)-C(51)	1.388(4)
C(50)-H(37)	0.9500
C(51)-H(36)	0.9500
C(53)-C(54)	1.397(4)
C(54)-C(55)	1.366(4)
C(54)-H(40)	0.9500
C(55)-H(41)	0.9500
C(56)-C(57)	1.505(5)
C(56)-C(60)	1.534(4)

C(56)-H(42)	1.0000
C(57)-C(58)	1.501(5)
C(57)-H(50)	0.9900
C(57)-H(49)	0.9900
C(58)-C(59)	1.525(5)
C(58)-H(48)	0.9900
C(58)-H(47)	0.9900
C(59)-C(60)	1.528(4)
C(59)-H(46)	0.9900
C(59)-H(45)	0.9900
C(60)-H(44)	0.9900
C(60)-H(43)	0.9900
C(61)-C(62)	1.389(4)
C(61)-H(52)	0.9500
C(62)-H(51)	0.9500
C(63)-H(59)	0.9800
C(63)-H(87)	0.9800
C(63)-H(61)	0.9800
C(64)-C(65)	1.473(4)
C(65)-C(66)	1.396(4)
C(65)-C(75)	1.400(4)
C(66)-C(67)	1.379(4)
C(66)-H(73)	0.9500
C(67)-C(77)	1.410(4)
C(68)-C(84)	1.401(4)
C(68)-C(69)	1.460(3)
C(69)-C(70)	1.498(4)
C(70)-C(71)	1.391(4)
C(70)-C(93)	1.392(4)
C(71)-C(72)	1.381(4)
C(71)-H(81)	0.9500
C(72)-C(73)	1.388(4)
C(72)-H(86)	0.9500
C(73)-C(92)	1.394(4)
C(73)-C(74)	1.506(4)
C(74)-H(60)	0.9800
C(74)-H(84)	0.9800

C(74)-H(85)	0.9800
C(75)-C(76)	1.385(4)
C(75)-H(62)	0.9500
C(76)-C(77)	1.383(4)
C(76)-H(63)	0.9500
C(78)-C(79)	1.526(4)
C(78)-C(82)	1.536(4)
C(78)-H(72)	1.0000
C(79)-C(80)	1.500(4)
C(79)-H(70)	0.9900
C(79)-H(71)	0.9900
C(80)-C(81)	1.525(4)
C(80)-H(69)	0.9900
C(80)-H(68)	0.9900
C(81)-C(82)	1.529(4)
C(81)-H(67)	0.9900
C(81)-H(66)	0.9900
C(82)-H(64)	0.9900
C(82)-H(65)	0.9900
C(84)-C(85)	1.472(4)
C(85)-C(86)	1.390(4)
C(85)-C(90)	1.392(4)
C(86)-C(87)	1.383(4)
C(86)-H(80)	0.9500
C(87)-C(88)	1.392(4)
C(87)-H(79)	0.9500
C(88)-C(89)	1.389(4)
C(88)-C(91)	1.504(4)
C(89)-C(90)	1.379(4)
C(89)-H(75)	0.9500
C(90)-H(74)	0.9500
C(91)-H(77)	0.9800
C(91)-H(78)	0.9800
C(91)-H(76)	0.9800
C(92)-C(93)	1.383(4)
C(92)-H(82)	0.9500
C(93)-H(83)	0.9500

C(11)-O(1)-C(12)	115.4(2)
C(42)-O(4)-C(43)	115.2(3)
C(64)-O(7)-C(63)	115.3(2)
C(21)-N(1)-C(8)	108.2(2)
C(21)-N(1)-C(7)	105.8(2)
C(8)-N(1)-C(7)	146.0(2)
C(21)-N(2)-C(6)	102.7(2)
C(21)-N(3)-C(22)	106.5(2)
C(21)-N(3)-C(25)	122.6(2)
C(22)-N(3)-C(25)	130.5(2)
C(52)-N(4)-C(38)	105.8(2)
C(52)-N(4)-C(39)	109.1(2)
C(38)-N(4)-C(39)	145.1(2)
C(52)-N(5)-C(37)	103.5(2)
C(52)-N(6)-C(53)	107.6(2)
C(52)-N(6)-C(56)	128.9(3)
C(53)-N(6)-C(56)	123.5(3)
C(83)-N(7)-C(67)	109.1(2)
C(83)-N(7)-C(68)	105.7(2)
C(67)-N(7)-C(68)	145.2(2)
C(83)-N(8)-C(77)	107.0(2)
C(83)-N(8)-C(78)	122.8(2)
C(77)-N(8)-C(78)	129.7(2)
C(83)-N(9)-C(84)	102.5(2)
C(2)-C(1)-H(24)	109.5
C(2)-C(1)-H(1)	109.5
H(24)-C(1)-H(1)	109.5
C(2)-C(1)-H(25)	109.5
H(24)-C(1)-H(25)	109.5
H(1)-C(1)-H(25)	109.5
C(30)-C(2)-C(3)	117.6(3)
C(30)-C(2)-C(1)	121.8(3)
C(3)-C(2)-C(1)	120.7(3)
C(4)-C(3)-C(2)	121.0(3)
C(4)-C(3)-H(26)	119.5
C(2)-C(3)-H(26)	119.5

C(3)-C(4)-C(5)	120.9(3)
C(3)-C(4)-H(27)	119.5
C(5)-C(4)-H(27)	119.5
C(31)-C(5)-C(4)	118.2(3)
C(31)-C(5)-C(6)	122.1(2)
C(4)-C(5)-C(6)	119.7(2)
N(2)-C(6)-C(7)	112.3(2)
N(2)-C(6)-C(5)	118.3(2)
C(7)-C(6)-C(5)	129.2(2)
C(6)-C(7)-N(1)	103.7(2)
C(6)-C(7)-C(13)	133.8(2)
N(1)-C(7)-C(13)	122.5(2)
C(9)-C(8)-N(1)	132.3(2)
C(9)-C(8)-C(22)	122.0(2)
N(1)-C(8)-C(22)	105.6(2)
C(8)-C(9)-C(10)	116.9(3)
C(8)-C(9)-H(28)	121.5
C(10)-C(9)-H(28)	121.5
C(9)-C(10)-C(24)	121.2(3)
C(9)-C(10)-C(11)	117.6(3)
C(24)-C(10)-C(11)	121.2(3)
O(2)-C(11)-O(1)	122.7(3)
O(2)-C(11)-C(10)	125.2(3)
O(1)-C(11)-C(10)	112.1(2)
O(1)-C(12)-H(29)	109.5
O(1)-C(12)-H(3)	109.5
H(29)-C(12)-H(3)	109.5
O(1)-C(12)-H(2)	109.5
H(29)-C(12)-H(2)	109.5
H(3)-C(12)-H(2)	109.5
O(3)-C(13)-C(7)	121.1(2)
O(3)-C(13)-C(14)	121.3(2)
C(7)-C(13)-C(14)	117.6(2)
C(15)-C(14)-C(20)	118.5(3)
C(15)-C(14)-C(13)	122.1(2)
C(20)-C(14)-C(13)	119.4(2)
C(16)-C(15)-C(14)	121.0(3)

C(16)-C(15)-H(4)	119.5
C(14)-C(15)-H(4)	119.5
C(15)-C(16)-C(17)	120.8(3)
C(15)-C(16)-H(5)	119.6
C(17)-C(16)-H(5)	119.6
C(19)-C(17)-C(16)	118.3(3)
C(19)-C(17)-C(18)	121.2(3)
C(16)-C(17)-C(18)	120.5(3)
C(17)-C(18)-H(8)	109.5
C(17)-C(18)-H(6)	109.5
H(8)-C(18)-H(6)	109.5
C(17)-C(18)-H(7)	109.5
H(8)-C(18)-H(7)	109.5
H(6)-C(18)-H(7)	109.5
C(17)-C(19)-C(20)	121.1(3)
C(17)-C(19)-H(9)	119.4
C(20)-C(19)-H(9)	119.4
C(19)-C(20)-C(14)	120.3(3)
C(19)-C(20)-H(10)	119.9
C(14)-C(20)-H(10)	119.9
N(2)-C(21)-N(1)	115.4(2)
N(2)-C(21)-N(3)	133.9(2)
N(1)-C(21)-N(3)	110.7(2)
C(23)-C(22)-N(3)	130.8(3)
C(23)-C(22)-C(8)	120.3(3)
N(3)-C(22)-C(8)	108.9(2)
C(24)-C(23)-C(22)	118.0(3)
C(24)-C(23)-H(12)	121.0
C(22)-C(23)-H(12)	121.0
C(23)-C(24)-C(10)	121.5(3)
C(23)-C(24)-H(11)	119.3
C(10)-C(24)-H(11)	119.3
N(3)-C(25)-C(26)	112.0(2)
N(3)-C(25)-C(29)	115.3(2)
C(26)-C(25)-C(29)	105.9(2)
N(3)-C(25)-H(13)	107.8
C(26)-C(25)-H(13)	107.8

C(29)-C(25)-H(13)	107.8
C(27)-C(26)-C(25)	104.2(2)
C(27)-C(26)-H(14)	110.9
C(25)-C(26)-H(14)	110.9
C(27)-C(26)-H(15)	110.9
C(25)-C(26)-H(15)	110.9
H(14)-C(26)-H(15)	108.9
C(26)-C(27)-C(28)	102.1(2)
C(26)-C(27)-H(17)	111.3
C(28)-C(27)-H(17)	111.3
C(26)-C(27)-H(16)	111.3
C(28)-C(27)-H(16)	111.3
H(17)-C(27)-H(16)	109.2
C(27)-C(28)-C(29)	103.7(2)
C(27)-C(28)-H(18)	111.0
C(29)-C(28)-H(18)	111.0
C(27)-C(28)-H(19)	111.0
C(29)-C(28)-H(19)	111.0
H(18)-C(28)-H(19)	109.0
C(28)-C(29)-C(25)	105.5(2)
C(28)-C(29)-H(21)	110.6
C(25)-C(29)-H(21)	110.6
C(28)-C(29)-H(20)	110.6
C(25)-C(29)-H(20)	110.6
H(21)-C(29)-H(20)	108.8
C(31)-C(30)-C(2)	121.7(3)
C(31)-C(30)-H(23)	119.1
C(2)-C(30)-H(23)	119.1
C(30)-C(31)-C(5)	120.4(3)
C(30)-C(31)-H(22)	119.8
C(5)-C(31)-H(22)	119.8
C(33)-C(32)-H(54)	109.5
C(33)-C(32)-H(30)	109.5
H(54)-C(32)-H(30)	109.5
C(33)-C(32)-H(53)	109.5
H(54)-C(32)-H(53)	109.5
H(30)-C(32)-H(53)	109.5

C(34)-C(33)-C(61)	116.8(3)
C(34)-C(33)-C(32)	121.4(3)
C(61)-C(33)-C(32)	121.8(3)
C(35)-C(34)-C(33)	121.8(3)
C(35)-C(34)-H(55)	119.1
C(33)-C(34)-H(55)	119.1
C(34)-C(35)-C(36)	120.8(3)
C(34)-C(35)-H(56)	119.6
C(36)-C(35)-H(56)	119.6
C(62)-C(36)-C(35)	118.3(3)
C(62)-C(36)-C(37)	120.2(3)
C(35)-C(36)-C(37)	121.5(3)
N(5)-C(37)-C(38)	111.8(3)
N(5)-C(37)-C(36)	119.5(3)
C(38)-C(37)-C(36)	128.5(3)
C(37)-C(38)-N(4)	104.3(2)
C(37)-C(38)-C(44)	133.4(3)
N(4)-C(38)-C(44)	122.2(3)
C(40)-C(39)-C(53)	121.7(3)
C(40)-C(39)-N(4)	134.1(3)
C(53)-C(39)-N(4)	104.2(3)
C(39)-C(40)-C(41)	117.7(3)
C(39)-C(40)-H(57)	121.1
C(41)-C(40)-H(57)	121.1
C(40)-C(41)-C(55)	120.4(3)
C(40)-C(41)-C(42)	123.5(3)
C(55)-C(41)-C(42)	116.1(3)
O(5)-C(42)-O(4)	122.7(3)
O(5)-C(42)-C(41)	124.9(3)
O(4)-C(42)-C(41)	112.4(3)
O(4)-C(43)-H(58)	109.5
O(4)-C(43)-H(31)	109.5
H(58)-C(43)-H(31)	109.5
O(4)-C(43)-H(32)	109.5
H(58)-C(43)-H(32)	109.5
H(31)-C(43)-H(32)	109.5
O(6)-C(44)-C(38)	121.7(3)

O(6)-C(44)-C(45)	120.6(2)
C(38)-C(44)-C(45)	117.7(3)
C(46)-C(45)-C(51)	118.8(3)
C(46)-C(45)-C(44)	122.8(2)
C(51)-C(45)-C(44)	118.4(3)
C(47)-C(46)-C(45)	120.5(3)
C(47)-C(46)-H(39)	119.8
C(45)-C(46)-H(39)	119.8
C(46)-C(47)-C(48)	121.1(3)
C(46)-C(47)-H(38)	119.4
C(48)-C(47)-H(38)	119.4
C(50)-C(48)-C(47)	118.3(3)
C(50)-C(48)-C(49)	122.0(3)
C(47)-C(48)-C(49)	119.7(3)
C(48)-C(49)-H(34)	109.5
C(48)-C(49)-H(35)	109.5
H(34)-C(49)-H(35)	109.5
C(48)-C(49)-H(33)	109.5
H(34)-C(49)-H(33)	109.5
H(35)-C(49)-H(33)	109.5
C(48)-C(50)-C(51)	121.2(3)
C(48)-C(50)-H(37)	119.4
C(51)-C(50)-H(37)	119.4
C(50)-C(51)-C(45)	120.0(3)
C(50)-C(51)-H(36)	120.0
C(45)-C(51)-H(36)	120.0
N(5)-C(52)-N(4)	114.5(3)
N(5)-C(52)-N(6)	136.1(3)
N(4)-C(52)-N(6)	109.4(3)
N(6)-C(53)-C(54)	130.4(3)
N(6)-C(53)-C(39)	109.8(3)
C(54)-C(53)-C(39)	119.8(3)
C(55)-C(54)-C(53)	118.4(3)
C(55)-C(54)-H(40)	120.8
C(53)-C(54)-H(40)	120.8
C(54)-C(55)-C(41)	122.0(3)
C(54)-C(55)-H(41)	119.0

C(41)-C(55)-H(41)	119.0
N(6)-C(56)-C(57)	114.9(3)
N(6)-C(56)-C(60)	112.7(2)
C(57)-C(56)-C(60)	102.0(3)
N(6)-C(56)-H(42)	109.0
C(57)-C(56)-H(42)	109.0
C(60)-C(56)-H(42)	109.0
C(58)-C(57)-C(56)	104.1(3)
C(58)-C(57)-H(50)	110.9
C(56)-C(57)-H(50)	110.9
C(58)-C(57)-H(49)	110.9
C(56)-C(57)-H(49)	110.9
H(50)-C(57)-H(49)	109.0
C(57)-C(58)-C(59)	105.8(3)
C(57)-C(58)-H(48)	110.6
C(59)-C(58)-H(48)	110.6
C(57)-C(58)-H(47)	110.6
C(59)-C(58)-H(47)	110.6
H(48)-C(58)-H(47)	108.7
C(58)-C(59)-C(60)	106.2(3)
C(58)-C(59)-H(46)	110.5
C(60)-C(59)-H(46)	110.5
C(58)-C(59)-H(45)	110.5
C(60)-C(59)-H(45)	110.5
H(46)-C(59)-H(45)	108.7
C(59)-C(60)-C(56)	103.1(2)
C(59)-C(60)-H(44)	111.1
C(56)-C(60)-H(44)	111.1
C(59)-C(60)-H(43)	111.1
C(56)-C(60)-H(43)	111.1
H(44)-C(60)-H(43)	109.1
C(62)-C(61)-C(33)	121.7(3)
C(62)-C(61)-H(52)	119.2
C(33)-C(61)-H(52)	119.2
C(36)-C(62)-C(61)	120.5(3)
C(36)-C(62)-H(51)	119.7
C(61)-C(62)-H(51)	119.7

O(7)-C(63)-H(59)	109.5
O(7)-C(63)-H(87)	109.5
H(59)-C(63)-H(87)	109.5
O(7)-C(63)-H(61)	109.5
H(59)-C(63)-H(61)	109.5
H(87)-C(63)-H(61)	109.5
O(8)-C(64)-O(7)	122.3(3)
O(8)-C(64)-C(65)	125.4(3)
O(7)-C(64)-C(65)	112.3(2)
C(66)-C(65)-C(75)	120.7(3)
C(66)-C(65)-C(64)	117.8(2)
C(75)-C(65)-C(64)	121.5(3)
C(67)-C(66)-C(65)	117.4(2)
C(67)-C(66)-H(73)	121.3
C(65)-C(66)-H(73)	121.3
C(66)-C(67)-N(7)	132.9(2)
C(66)-C(67)-C(77)	121.8(2)
N(7)-C(67)-C(77)	105.3(2)
C(84)-C(68)-N(7)	103.8(2)
C(84)-C(68)-C(69)	133.6(2)
N(7)-C(68)-C(69)	122.5(2)
O(9)-C(69)-C(68)	121.6(2)
O(9)-C(69)-C(70)	120.8(2)
C(68)-C(69)-C(70)	117.5(2)
C(71)-C(70)-C(93)	118.6(2)
C(71)-C(70)-C(69)	121.9(2)
C(93)-C(70)-C(69)	119.5(2)
C(72)-C(71)-C(70)	120.8(3)
C(72)-C(71)-H(81)	119.6
C(70)-C(71)-H(81)	119.6
C(71)-C(72)-C(73)	121.0(3)
C(71)-C(72)-H(86)	119.5
C(73)-C(72)-H(86)	119.5
C(72)-C(73)-C(92)	118.0(3)
C(72)-C(73)-C(74)	119.9(3)
C(92)-C(73)-C(74)	122.1(3)
C(73)-C(74)-H(60)	109.5

C(73)-C(74)-H(84)	109.5
H(60)-C(74)-H(84)	109.5
C(73)-C(74)-H(85)	109.5
H(60)-C(74)-H(85)	109.5
H(84)-C(74)-H(85)	109.5
C(76)-C(75)-C(65)	121.7(3)
C(76)-C(75)-H(62)	119.1
C(65)-C(75)-H(62)	119.1
C(77)-C(76)-C(75)	117.7(3)
C(77)-C(76)-H(63)	121.2
C(75)-C(76)-H(63)	121.2
C(76)-C(77)-N(8)	130.5(3)
C(76)-C(77)-C(67)	120.6(3)
N(8)-C(77)-C(67)	108.9(2)
N(8)-C(78)-C(79)	114.1(2)
N(8)-C(78)-C(82)	114.5(2)
C(79)-C(78)-C(82)	105.2(2)
N(8)-C(78)-H(72)	107.6
C(79)-C(78)-H(72)	107.6
C(82)-C(78)-H(72)	107.6
C(80)-C(79)-C(78)	102.6(2)
C(80)-C(79)-H(70)	111.3
C(78)-C(79)-H(70)	111.3
C(80)-C(79)-H(71)	111.3
C(78)-C(79)-H(71)	111.3
H(70)-C(79)-H(71)	109.2
C(79)-C(80)-C(81)	104.4(2)
C(79)-C(80)-H(69)	110.9
C(81)-C(80)-H(69)	110.9
C(79)-C(80)-H(68)	110.9
C(81)-C(80)-H(68)	110.9
H(69)-C(80)-H(68)	108.9
C(80)-C(81)-C(82)	106.6(2)
C(80)-C(81)-H(67)	110.4
C(82)-C(81)-H(67)	110.4
C(80)-C(81)-H(66)	110.4
C(82)-C(81)-H(66)	110.4

H(67)-C(81)-H(66)	108.6
C(81)-C(82)-C(78)	104.9(2)
C(81)-C(82)-H(64)	110.8
C(78)-C(82)-H(64)	110.8
C(81)-C(82)-H(65)	110.8
C(78)-C(82)-H(65)	110.8
H(64)-C(82)-H(65)	108.8
N(9)-C(83)-N(7)	115.5(2)
N(9)-C(83)-N(8)	134.9(2)
N(7)-C(83)-N(8)	109.7(2)
N(9)-C(84)-C(68)	112.4(2)
N(9)-C(84)-C(85)	118.8(2)
C(68)-C(84)-C(85)	128.7(2)
C(86)-C(85)-C(90)	118.4(2)
C(86)-C(85)-C(84)	119.9(2)
C(90)-C(85)-C(84)	121.7(2)
C(87)-C(86)-C(85)	120.6(3)
C(87)-C(86)-H(80)	119.7
C(85)-C(86)-H(80)	119.7
C(86)-C(87)-C(88)	121.1(3)
C(86)-C(87)-H(79)	119.5
C(88)-C(87)-H(79)	119.5
C(89)-C(88)-C(87)	117.9(2)
C(89)-C(88)-C(91)	121.2(3)
C(87)-C(88)-C(91)	120.9(3)
C(90)-C(89)-C(88)	121.2(3)
C(90)-C(89)-H(75)	119.4
C(88)-C(89)-H(75)	119.4
C(89)-C(90)-C(85)	120.6(3)
C(89)-C(90)-H(74)	119.7
C(85)-C(90)-H(74)	119.7
C(88)-C(91)-H(77)	109.5
C(88)-C(91)-H(78)	109.5
H(77)-C(91)-H(78)	109.5
C(88)-C(91)-H(76)	109.5
H(77)-C(91)-H(76)	109.5
H(78)-C(91)-H(76)	109.5

C(93)-C(92)-C(73)	121.3(3)
C(93)-C(92)-H(82)	119.4
C(73)-C(92)-H(82)	119.4
C(92)-C(93)-C(70)	120.2(3)
C(92)-C(93)-H(83)	119.9
C(70)-C(93)-H(83)	119.9

Symmetry transformations used to generate equivalent atoms: Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for 140616LT_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)	27(1)	22(1)	29(1)	9(1)	11(1)	1(1)
O(2)	56(2)	27(1)	25(1)	-7(1)	17(1)	-11(1)
O(3)	26(1)	18(1)	33(1)	-1(1)	14(1)	-2(1)
O(4)	33(1)	33(1)	38(1)	10(1)	7(1)	2(1)
O(5)	49(2)	29(1)	49(1)	10(1)	-6(1)	3(1)
O(6)	25(1)	23(1)	40(1)	-7(1)	14(1)	-2(1)
O(7)	28(1)	21(1)	39(1)	16(1)	13(1)	4(1)
O(8)	39(1)	20(1)	22(1)	1(1)	10(1)	-1(1)
O(9)	25(1)	16(1)	28(1)	-3(1)	14(1)	-2(1)
N(1)	17(1)	9(1)	19(1)	1(1)	3(1)	1(1)
N(2)	17(1)	14(1)	21(1)	1(1)	4(1)	-1(1)
N(3)	21(1)	10(1)	23(1)	0(1)	7(1)	2(1)
N(4)	18(1)	20(1)	28(1)	-9(1)	-2(1)	6(1)
N(5)	18(1)	28(2)	29(1)	-15(1)	-1(1)	6(1)
N(6)	25(1)	20(1)	31(1)	-12(1)	-4(1)	11(1)
N(7)	16(1)	9(1)	15(1)	-1(1)	4(1)	1(1)
N(8)	22(1)	10(1)	22(1)	-3(1)	6(1)	4(1)
N(9)	18(1)	13(1)	19(1)	-2(1)	4(1)	0(1)
C(1)	32(2)	21(2)	31(2)	8(1)	-2(1)	-7(1)
C(2)	21(2)	18(2)	19(1)	4(1)	-4(1)	-6(1)
C(3)	22(2)	22(2)	25(2)	3(1)	4(1)	-6(1)
C(4)	21(2)	18(2)	23(1)	-2(1)	4(1)	2(1)
C(5)	16(1)	15(2)	16(1)	-1(1)	1(1)	1(1)
C(6)	15(1)	13(1)	21(1)	-1(1)	1(1)	0(1)

C(7)	15(1)	11(1)	23(1)	0(1)	1(1)	1(1)
C(8)	14(1)	11(1)	18(1)	1(1)	1(1)	-2(1)
C(9)	16(1)	12(1)	21(1)	0(1)	-3(1)	-3(1)
C(10)	16(1)	18(2)	17(1)	1(1)	-2(1)	-2(1)
C(11)	21(2)	22(2)	16(1)	2(1)	-3(1)	-4(1)
C(12)	34(2)	34(2)	32(2)	13(1)	15(1)	3(2)
C(13)	16(2)	12(1)	22(1)	1(1)	-1(1)	3(1)
C(14)	18(2)	12(1)	18(1)	1(1)	0(1)	0(1)
C(15)	17(2)	20(2)	17(1)	0(1)	-2(1)	0(1)
C(16)	22(2)	23(2)	24(1)	1(1)	-5(1)	-5(1)
C(17)	31(2)	14(2)	29(2)	1(1)	-12(1)	-1(1)
C(18)	46(2)	19(2)	52(2)	0(2)	-18(2)	-5(2)
C(19)	31(2)	16(2)	33(2)	-6(1)	-7(1)	7(1)
C(20)	21(2)	22(2)	25(2)	-5(1)	-1(1)	4(1)
C(21)	14(1)	16(2)	17(1)	-4(1)	3(1)	3(1)
C(22)	15(1)	12(1)	18(1)	0(1)	0(1)	-2(1)
C(23)	20(2)	16(2)	25(1)	1(1)	4(1)	1(1)
C(24)	18(2)	13(1)	22(1)	2(1)	0(1)	-1(1)
C(25)	22(2)	17(2)	20(1)	-2(1)	10(1)	1(1)
C(26)	23(2)	29(2)	34(2)	-8(1)	6(1)	0(1)
C(27)	29(2)	25(2)	31(2)	0(1)	7(1)	7(1)
C(28)	29(2)	21(2)	34(2)	-5(1)	11(1)	1(1)
C(29)	26(2)	21(2)	22(1)	-3(1)	4(1)	1(1)
C(30)	20(2)	15(2)	22(1)	0(1)	-2(1)	3(1)
C(31)	17(1)	19(2)	19(1)	1(1)	1(1)	-3(1)
C(32)	25(2)	46(2)	31(2)	2(2)	1(1)	-8(2)
C(33)	21(2)	33(2)	21(1)	-7(1)	1(1)	-1(1)
C(34)	19(2)	35(2)	15(1)	-4(1)	0(1)	5(1)
C(35)	14(2)	36(2)	17(1)	-7(1)	2(1)	2(1)
C(36)	17(2)	33(2)	15(1)	-13(1)	1(1)	-3(1)
C(37)	14(1)	25(2)	30(2)	-13(1)	-2(1)	3(1)
C(38)	15(1)	18(2)	28(2)	-6(1)	-2(1)	4(1)
C(39)	18(2)	15(2)	34(2)	-4(1)	-14(1)	4(1)
C(40)	20(2)	22(2)	27(2)	-4(1)	-6(1)	4(1)
C(41)	21(2)	25(2)	36(2)	-1(1)	-16(1)	2(1)
C(42)	22(2)	38(2)	34(2)	-1(2)	-7(1)	2(2)
C(43)	51(2)	66(3)	36(2)	10(2)	23(2)	-6(2)

C(44)	17(2)	20(2)	26(2)	-6(1)	-1(1)	4(1)
C(45)	21(2)	15(2)	15(1)	-3(1)	0(1)	4(1)
C(46)	17(2)	21(2)	17(1)	-2(1)	-2(1)	5(1)
C(47)	20(2)	19(2)	17(1)	-1(1)	0(1)	0(1)
C(48)	29(2)	20(2)	23(1)	-5(1)	-1(1)	2(1)
C(49)	50(2)	20(2)	54(2)	-6(2)	7(2)	-2(2)
C(50)	29(2)	20(2)	28(2)	-9(1)	3(1)	10(1)
C(51)	20(2)	24(2)	20(1)	-6(1)	2(1)	4(1)
C(52)	20(2)	26(2)	28(2)	-7(1)	-1(1)	8(1)
C(53)	24(2)	25(2)	26(2)	-3(1)	-6(1)	5(1)
C(54)	28(2)	18(2)	40(2)	-5(1)	-9(1)	7(1)
C(55)	32(2)	23(2)	31(2)	5(1)	-9(1)	2(1)
C(56)	32(2)	28(2)	32(2)	-10(1)	5(1)	5(1)
C(57)	65(3)	39(2)	48(2)	0(2)	18(2)	21(2)
C(58)	54(2)	52(3)	46(2)	-5(2)	20(2)	4(2)
C(59)	64(3)	47(2)	44(2)	-2(2)	16(2)	28(2)
C(60)	43(2)	39(2)	41(2)	1(2)	10(2)	14(2)
C(61)	20(2)	45(2)	25(2)	-15(1)	10(1)	-6(2)
C(62)	22(2)	31(2)	32(2)	-15(1)	7(1)	1(1)
C(63)	40(2)	35(2)	46(2)	21(2)	22(2)	5(2)
C(64)	22(2)	18(2)	19(1)	4(1)	-5(1)	-1(1)
C(65)	17(2)	17(2)	17(1)	2(1)	-4(1)	0(1)
C(66)	14(1)	12(1)	18(1)	1(1)	-2(1)	-2(1)
C(67)	15(1)	10(1)	16(1)	0(1)	0(1)	-1(1)
C(68)	14(1)	10(1)	16(1)	-1(1)	1(1)	-1(1)
C(69)	15(1)	11(1)	16(1)	-1(1)	0(1)	3(1)
C(70)	16(1)	13(1)	12(1)	-1(1)	0(1)	1(1)
C(71)	22(2)	16(2)	14(1)	-1(1)	-1(1)	2(1)
C(72)	16(1)	19(2)	18(1)	0(1)	0(1)	-1(1)
C(73)	26(2)	14(2)	19(1)	-2(1)	-2(1)	-3(1)
C(74)	32(2)	17(2)	40(2)	-6(1)	0(1)	-6(1)
C(75)	22(2)	12(2)	24(1)	3(1)	-2(1)	1(1)
C(76)	22(2)	14(2)	25(1)	-2(1)	2(1)	4(1)
C(77)	14(1)	12(1)	20(1)	-1(1)	0(1)	0(1)
C(78)	26(2)	17(2)	25(2)	-4(1)	11(1)	2(1)
C(79)	26(2)	42(2)	38(2)	-18(2)	2(1)	7(2)
C(80)	28(2)	30(2)	31(2)	-5(1)	5(1)	8(1)

C(81)	31(2)	26(2)	58(2)	-13(2)	11(2)	2(2)
C(82)	24(2)	19(2)	20(1)	-1(1)	5(1)	2(1)
C(83)	15(1)	14(2)	18(1)	-3(1)	1(1)	2(1)
C(84)	13(1)	10(1)	19(1)	-3(1)	0(1)	0(1)
C(85)	13(1)	16(2)	14(1)	-3(1)	0(1)	-2(1)
C(86)	19(2)	18(2)	21(1)	-3(1)	6(1)	1(1)
C(87)	19(2)	21(2)	22(1)	0(1)	10(1)	-2(1)
C(88)	23(2)	15(2)	14(1)	1(1)	-1(1)	-2(1)
C(89)	18(2)	18(2)	18(1)	1(1)	1(1)	2(1)
C(90)	16(1)	20(2)	15(1)	1(1)	3(1)	-1(1)
C(91)	27(2)	22(2)	25(2)	3(1)	4(1)	-7(1)
C(92)	22(2)	15(2)	29(2)	-8(1)	2(1)	4(1)
C(93)	14(1)	17(2)	24(1)	-4(1)	2(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10^3) for 140616LT_0M.

	x	y	z	U(eq)
H(24)	7929	8215	-256	43
H(1)	8788	8044	-588	43
H(25)	8866	8259	286	43
H(26)	9501	7294	-108	28
H(27)	9368	6545	423	25
H(28)	7040	5301	3165	20
H(29)	6295	3946	4914	49
H(3)	5829	3548	4327	49
H(2)	5449	4077	4288	49
H(4)	9097	6693	2424	22
H(5)	9610	7461	2646	29
H(8)	8377	8442	3261	63
H(6)	9071	8355	2673	63
H(7)	9325	8234	3595	63
H(9)	7313	7847	3301	34
H(10)	6787	7078	3062	28
H(12)	8201	4053	1783	24
H(11)	7468	3891	2844	21
H(13)	8864	4977	168	23
H(14)	10171	4882	921	34
H(15)	9800	4527	1530	34
H(17)	10484	4008	768	34
H(16)	10131	4294	-37	34
H(18)	9088	3726	873	33
H(19)	9110	3680	-63	33
H(21)	7904	4192	457	28
H(20)	8243	4327	-358	28
H(23)	7248	7690	605	24
H(22)	7095	6937	1113	22
H(54)	4351	1933	3057	51
H(30)	4485	2166	3920	51

H(53)	5308	1961	3567	51
H(55)	6069	2465	2771	28
H(56)	6283	3197	2220	27
H(57)	6454	4692	-111	29
H(58)	7343	5330	-2152	74
H(31)	7989	4901	-1853	74
H(32)	8230	5430	-1558	74
H(39)	4236	3380	844	22
H(38)	3720	2606	741	23
H(34)	4157	1733	-50	62
H(35)	4118	1753	879	62
H(33)	4986	1572	573	62
H(37)	6049	2151	251	31
H(36)	6561	2930	304	26
H(40)	5627	6055	1216	36
H(41)	6333	6130	127	36
H(42)	5379	5754	2582	37
H(50)	4249	5006	2946	59
H(49)	5124	5191	3499	59
H(48)	4480	5862	3830	59
H(47)	3626	5529	3684	59
H(46)	3893	6311	2818	61
H(45)	3071	5957	2635	61
H(44)	4228	6036	1663	49
H(43)	3667	5557	1704	49
H(52)	3743	2912	3284	35
H(51)	3926	3635	2676	34
H(59)	11268	5929	2310	58
H(87)	10663	6372	1998	58
H(61)	10477	5861	1596	58
H(73)	9719	4660	3519	18
H(81)	7546	3338	4312	21
H(86)	6970	2580	4107	21
H(60)	7383	1697	4158	45
H(84)	8142	1547	3670	45
H(85)	7248	1767	3218	45
H(62)	9276	6079	3684	24

H(63)	8515	5958	4746	25
H(72)	7655	5083	6332	26
H(70)	7048	5697	5022	43
H(71)	6504	5282	5379	43
H(69)	6434	5703	6518	36
H(68)	6299	6115	5858	36
H(67)	7566	6171	7046	45
H(66)	7678	6393	6201	45
H(64)	8578	5625	6931	25
H(65)	8735	5869	6113	25
H(80)	7297	3517	6307	23
H(79)	7141	2777	6864	24
H(75)	9360	2335	6128	22
H(74)	9549	3083	5618	20
H(77)	7725	1799	6486	37
H(78)	7837	2019	7359	37
H(76)	8675	1832	7009	37
H(82)	9261	2121	3536	27
H(83)	9830	2883	3707	22