

Copper-Mediated Synthesis of Pyrazolo[1, 5-a]pyridines Through Oxidative Linkage of C-C/N-N Bonds

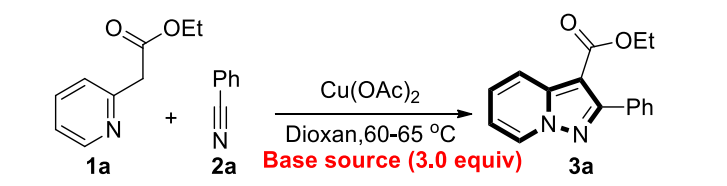
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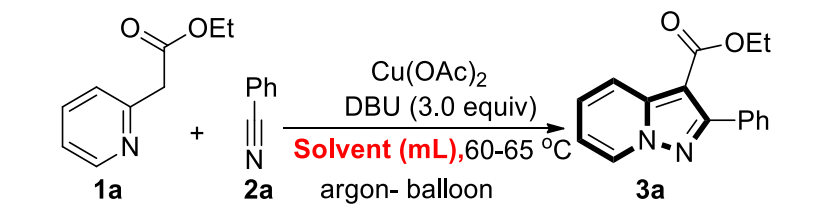
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Table S1. Screening of Bases^a


Entry	Base source	Yield(%) ^(b)
1	DBU	19
2	DBN	17
3	Pyridine	00
4	DABCO	trace
5	Et ₃ N	00
6	CsCO ₃	00
7	KOAc	trace
8	AgCO ₃	trace
9	KOtBu	16
10	-	trace

^aReaction conditions: **1a** (0.3 mmol), **2a** (1.5 mmol), catalyst (0.45 mmol), solvent (1 mL), in an oil bath under nitrogen atmosphere, 6 h. [b] Isolated yield. [nr = no reaction].

Table S2. Screening of Solvents^a


Entry	Solvent (mL)	Yield(%) ^(b)
1	THF(1.0)	22
2	CH ₃ NO ₂ (1.0)	--
3	EDC(1.0)	29
4	1,2 DCB(1.0)	17
5	toluene(1.0)	12
6	CIPh(1.0)	20
7	EtOH(1.0)	19
8	DMF(1.0)	23
9	DMSO(1.0)	30
11	DMSO(0.25)	33
12	DMSO(0.5)	39
13	1,3 DCB(0.5)	35

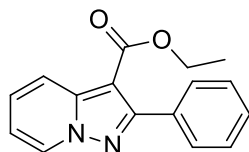
^aReaction conditions: **1a** (0.3 mmol), **2a** (1.5 mmol), catalyst (0.3 mmol), Base and solvent , in an oil bath under nitrogen atmosphere, 6 h. [b] Isolated yield. [nr = no reaction].

General Experimental Section: All commercially available chemicals and reagents were used without any further purification unless otherwise indicated. ^1H and ^{13}C NMR spectra were recorded at 500, and 125 MHz, respectively. The spectra were recorded in CDCl_3 as solvent. Multiplicity was indicated as follows: s (singlet); d (doublet); t (triplet); m (multiplet); dd (doublet of doublets), etc. and coupling constants (J) was given in Hz. Chemical shifts are reported in ppm relative to TMS as an internal standard. The peaks around delta values of ^1H NMR (7.2), and ^{13}C NMR (77.0) are correspond to deuterated solvent chloroform respectively. Mass spectra were obtained using electron impact (EI) ionization method. Progress of the reactions was monitored by thin layer chromatography (TLC). All products were purified through column chromatography using silica gel 100-200 mesh size with hexane/ethyl acetate as eluent unless otherwise indicated.

Typical procedure for the synthesis of Ethyl 2-phenylpyrazolo [1,5-a]pyridine-3-carboxylate (3a): 49.5 mg (0.3 mmol) of ethyl 2-(pyridin-2-yl)acetate **1a**, 463.5 mg (4.5 mmol) of Benzonitrile (**2a**), $\text{Cu}(\text{OAc})_2$ (0.3 mmol), CuBr (0.3 mmol), DBU (0.9 mmol) and DMSO (0.5 mL) were placed in a 25-mL double-necked round-bottomed flask. The mixture was heated in an oil bath at 60-65 °C for 6 h under an argon atmosphere (balloon). After completion of the reaction, it was allowed to attain room temperature and then the mixture was purified through column chromatography using silica gel (5 % EtOAc/hexane) to afford **3a**; yield: 49.5 mg (62%).

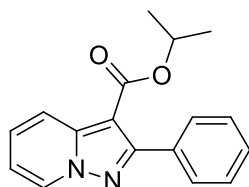
Characterization data

Ethyl 2-phenylpyrazolo [1,5-a]pyridine-3-carboxylate (3a):



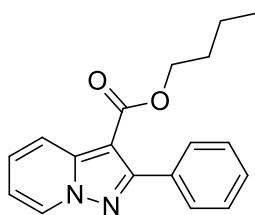
White solid; M.p.68-73°C; ¹H NMR (500 MHz, CDCl₃) δ 8.45 (d, *J* = 9.0 Hz, 1H), 8.15 (d, *J* = 9.0 Hz, 1H), 7.71-7.70 (m, 2H), 7.39-7.31 (m, 4H), 6.88 (t, *J* = 7.0 Hz, 1H). 4.28 (q, *J* = 7.0 Hz, 2H), 1.23 (t, *J* = 7.0 Hz, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 163.5, 156.9, 142.6, 132.5, 129.9, 128.8, 127.7, 127.2, 119.7, 113.8, 100.7, 59.8, 14.2. HRMS calcd for C₁₆H₁₄N₂NaO₂: 289.0953. Found: 289.0940.

Isopropyl 2-phenylpyrazolo[1,5-a]pyridine-3-carboxylate (3b)



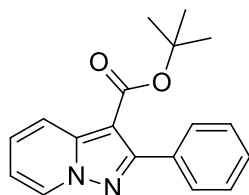
(Eluent: 5% EtOAc/hexane); 53% yield (45 mg); colour less liquid; ¹H NMR (500 MHz, CDCl₃) δ 8.53 (t, *J* = 7.0 Hz, 1H), 8.22 (d, *J* = 9.0 Hz, 1H), 7.78-7.77 (m, 2H), 7.47-7.38 (m, 4H), 6.94 (t, *J* = 6.5 Hz, 1H), 5.29 (sept, *J* = 6.5 Hz, 1H), 1.29 (d, *J* = 6.0 Hz, 6H). ¹³C NMR (125 MHz, CDCl₃) δ 163.1, 156.9, 142.6, 132.6, 130.0, 128.7, 127.6, 127.0, 119.7, 113.7, 101.1, 67.3, 22.0. HRMS calcd for C₁₇ H₁₆ O₂ N₂ Na: 303.1109. Found: 303.1097.

Butyl 2-phenylpyrazolo[1,5-a]pyridine-3-carboxylate (3c)



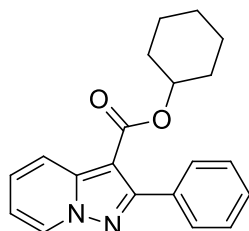
Eluent: 5% EtOAc/hexane); 52% yield (46 mg); White solid; M.p.62-67 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.53 (d, $J = 6.5$ Hz, 1H), 8.22 (d, $J = 9.0$ Hz, 1H), 7.77-7.75 (m, 2H), 7.47-7.39 (m, 4H), 6.95 (t, $J = 7.0$ Hz, 1H), 4.25 (t, $J = 7.0$ Hz, 2H), 1.63 (quin, $J = 7.0$ Hz, 2H), 1.30 (quin, $J = 7.5$ Hz, 2H), 0.89 (t, $J = 7.5$ Hz, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 163.7, 156.9, 142.7, 132.6, 129.9, 128.8, 128.7, 127.7, 127.2, 119.6, 113.8, 100.8, 63.8, 30.7, 19.2, 13.6. HRMS calcd for $\text{C}_{18}\text{H}_{19}\text{O}_2\text{N}_2$: 295.1447. Found: 295.1451.

Tert-butyl-2-phenylpyrazolo[1,5-a]pyridine-3-carboxylate (3d)



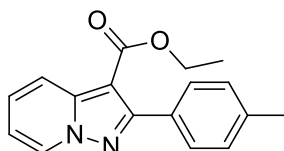
(Eluent: 5% EtOAc/hexane); 62% yield (54.6 mg); White solid; M.p.88-93°C; ^1H NMR (500 MHz, CDCl_3) δ 8.50 (d, $J = 6.5$ Hz, 1H), 8.20 (d, $J = 9.0$ Hz, 1H), 7.74 (d, $J = 8.0$ Hz, 2H), 7.46-7.36 (m, 4H), 6.92 (t, $J = 6.5$ Hz, 1H), 1.46 (s, 9H). ^{13}C NMR (125 MHz, CDCl_3) δ 162.9, 156.7, 142.5, 132.9, 129.9, 128.6, 128.5, 127.6, 126.8, 119.6, 113.5, 102.2, 80.4, 28.3. HRMS calcd for $\text{C}_{18}\text{H}_{18}\text{O}_2\text{N}_2\text{Na}$: 317.1266. Found: 317.1270.

Cyclohexyl-2-phenylpyrazolo[1,5-a]pyridine-3-carboxylate (3e)



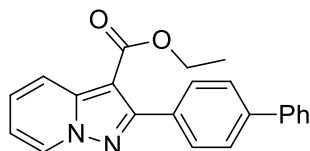
(Eluent: 5% EtOAc/hexane); 60% yield (58 mg); colour less liquid; ^1H NMR (500 MHz, CDCl_3) δ 8.52 (d, $J = 6.5$ Hz, 1H), 8.23 (d, $J = 8.5$ Hz, 1H), 7.78- 7.76 (m, 2H), 7.46-7.38 (m, 4H), 6.94 (t, $J = 7.0$ Hz, 1H), 5.00 (sept, $J = 4.0$ Hz, 1H), 1.93-1.89 (m, 2H), 1.65-1.63 (m, 2H), 1.53-1.23 (m, 6H). ^{13}C NMR (125 MHz, CDCl_3) δ 163.1, 156.9, 142.6, 132.7, 129.7, 128.79, 128.74, 127.7, 127.1, 119.7, 113.7, 101.2, 72.2, 31.7, 25.4, 23.6. HRMS calcd for $\text{C}_{20}\text{H}_{21}\text{O}_2\text{N}_2$: 321.1603. Found: 321.1590.

Ethyl-2-(p-tolyl)pyrazolo[1,5-a]pyridine-3-carboxylate (4a)



(Eluent: 5% EtOAc/hexane); 32% yield (32 mg); White solid; M.p.90-95°C; ^1H NMR (500 MHz, CDCl_3) δ 8.52 (d, $J = 7.0$ Hz, 1H), 8.20 (d, $J = 9.0$ Hz, 1H), 7.70 (d, $J = 8.0$ Hz, 2H), 7.40 (t, $J = 8.0$ Hz, 2H), 7.27-7.25 (m, 2H), 6.94 (t, $J = 7.0$ Hz, 1H), 4.34 (q, $J = 7.0$ Hz, 2H), 2.41 (s, 3H), 1.33 (t, $J = 7.0$ Hz, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 162.4, 155.8, 141.4, 137.5, 128.6, 128.3, 127.5, 127.2, 125.8, 118.4, 112.4, 99.4, 58.6, 20.1, 13.1. HRMS calcd for $\text{C}_{17}\text{H}_{17}\text{O}_2\text{N}_2$: 281.1290. Found: 281.1297.

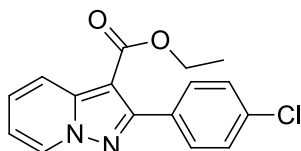
Ethyl-2-([1,1'-biphenyl]-4-yl)pyrazolo[1,5-a]pyridine-3-carboxylate (4b)



Eluent: 5% EtOAc/hexane); 52% yield (53 mg); White solid; M.p.106-111°C; ^1H NMR (500 MHz, CDCl_3) δ 8.55 (d, $J = 7.5$ Hz, 1H), 8.24 (d, $J = 9.0$ Hz, 1H), 7.92 (d, $J = 8.0$ Hz, 2H), 7.71-7.61 (m, 4H), 7.49-7.37 (m, 4H), 6.98-6.96 (m, 1H), 4.36 (q, $J = 7.5$ Hz, 2H), 1.36 (t, $J = 7.5$ Hz, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 163.5, 156.6, 142.6, 141.5, 140.8, 131.4,

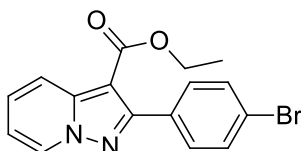
130.3, 128.8, 128.7, 127.3, 127.18, 127.13, 126.4, 119.7, 113.8, 100.7, 59.9, 14.3. HRMS calcd for C₂₂H₁₉O₂N₂: 343.1447. Found: 343.1448.

Ethyl-2-(4-chlorophenyl)pyrazolo[1,5-a]pyridine-3-carboxylate (4c)



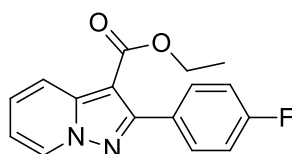
(Eluent: 5% EtOAc/hexane); 63% yield (57 mg); White solid; M.p.124-129°C; ¹H NMR (500 MHz, CDCl₃) δ 8.51 (d, *J* = 6.5 Hz, 1H), 8.20 (d, *J* = 9.0 Hz, 1H), 7.76 (d, *J* = 8.5 Hz, 2H), 7.43-7.35 (m, 3H), 6.95 (t, *J* = 6.5 Hz, 1H), 4.34 (q, *J* = 7.5 Hz, 2H), 1.33 (t, *J* = 7.0 Hz, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 163.6, 155.6, 142.6, 134.9, 131.3, 130.9, 128.7, 127.9, 127.3, 119.7, 113.9, 100.7, 59.9, 14.2. HRMS calcd for C₁₆H₁₄ClN₂O₂: 301.0744. Found: 301.0744.

Ethyl-2-(4-bromophenyl)pyrazolo[1,5-a]pyridine-3-carboxylate (4d)



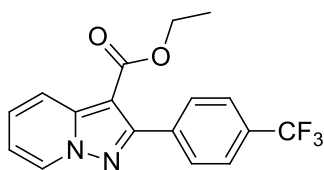
(Eluent: 5% EtOAc/hexane); 63% yield (65 mg); White solid; M.p.119-124°C; ¹H NMR (500 MHz, CDCl₃) δ 8.52 (d, *J* = 6.5 Hz, 1H), 8.20 (d, *J* = 9.0 Hz, 1H), 7.70 (d, *J* = 7.5 Hz, 2H), 7.59 (d, *J* = 7.5 Hz, 2H) 7.43 (t, *J* = 8.0 Hz, 1H), 6.98 (t, *J* = 7.0 Hz, 1H), 4.33 (q, *J* = 7.0 Hz, 2H), 1.33 (t, *J* = 7.0 Hz, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 163.4, 155.8, 142.7, 131.6, 131.5, 130.9, 128.8, 127.4, 123.3, 119.8, 114.0, 100.7, 60.0, 14.3. HRMS calcd for C₁₆H₁₄O₂N₂ Br: 345.0239. Found: 345.0229.

Ethyl-2-(4-fluorophenyl)pyrazolo[1,5-a]pyridine-3-carboxylate (4e)



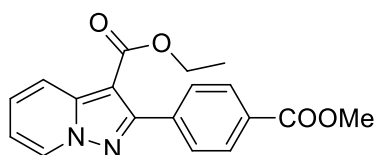
(Eluent: 5% EtOAc/hexane); 62% yield (53 mg); White solid; M.p.90-95°C; ^1H NMR (500 MHz, CDCl_3) δ 8.51 (d, $J = 7.0$ Hz, 1H), 8.20 (d, $J = 9.0$ Hz, 1H), 7.79 (s, 2H), 7.40 (t, $J = 7.5$ Hz, 1H), 7.13 (t, $J = 8.0$ Hz, 2H), 6.96 (d, $J = 6.5$ Hz, 1H), 4.23 (q, $J = 7.0$ Hz, 2H), 1.32 (t, $J = 7.0$ Hz, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 164.2 (d, $J = 246.2$ Hz), 163.4, 155.9, 142.6, 131.8, (d, $J = 8.1$ Hz), 128.7, (d, $J = 28.5$ Hz), 127.2, 119.7, 114.7, (d, $J = 21.3$ Hz), 113.8, 100.6, 59.9, 14.2. HRMS calcd for $\text{C}_{16}\text{H}_{14}\text{O}_2\text{N}_2\text{F}$: 285.1039. Found: 285.1028.

Ethyl-2-(4-(trifluoromethyl)phenyl)pyrazolo[1,5-a]pyridine-3-carboxylate(4f)



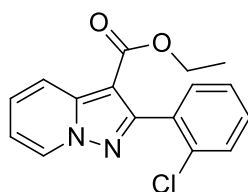
(Eluent: 5% EtOAc/hexane); 70% yield (70.2 mg); White solid; M.p.97-102°C ^1H NMR (500 MHz, CDCl_3) δ 8.53 (d, $J = 7.0$ Hz, 1H), 8.23 (d, $J = 9.0$ Hz, 1H), 7.93 (d, $J = 7.5$ Hz, 2H), 7.71 (d, $J = 7.5$ Hz, 2H), 7.44 (t, $J = 7.5$ Hz, 1H), 6.99 (t, $J = 6.5$ Hz, 1H), 4.34 (q, $J = 7.5$ Hz, 2H), 1.32 (t, $J = 7.5$ Hz, 3H) ^{13}C NMR (125 MHz, CDCl_3) δ 163.2, 155.4, 142.5, 136.2, 130.7 (d $J = 111$ Hz), 128.8, 127.5 (d $J = 51.5$ Hz), 124.8 (d $J = 81$ Hz), 119.8, 114.2, 100.9, 60.0, 14.2. HRMS calcd for $\text{C}_{17}\text{H}_{14}\text{O}_2\text{N}_2\text{F}_3$: 335.1007. Found: 335.1011.

Ethyl-2-(4-(methoxycarbonyl)phenyl)pyrazolo[1,5-a]pyridine-3-carboxylate (4g)



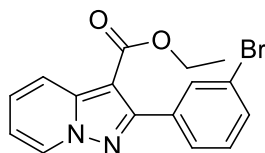
(Eluent: 5% EtOAc/hexane); 62% yield (60.5 mg); White solid; M.p.128-133°C ¹H NMR (500 MHz, CDCl₃) δ 8.54 (d, *J* = 7.5 Hz, 1H), 8.25 (d, *J* = 9.0 Hz, 1H), 8.13 (d, *J* = 9.0 Hz, 2H), 7.88 (d, *J* = 8.5 Hz, 2H), 7.45 (t, *J* = 7.0 Hz, 1H), 7.00 (t, *J* = 6.5 Hz, 1H), 4.34 (q, *J* = 7.0 Hz, 2H), 3.95 (s, 3H), 1.30 (t, *J* = 7.0 Hz, 3H) ¹³C NMR (125 MHz, CDCl₃) δ 167.0, 163.3, 155.8, 142.7, 137.2, 130.2, 130.1, 129.0, 128.9, 127.4, 119.8, 114.1, 101.1, 60.0, 52.1, 14.2. HRMS calcd for C₁₈H₁₇O₄N₂: 325.1188. Found: 325.1191.

Ethyl-2-(2-chlorophenyl)pyrazolo[1,5-a]pyridine-3-carboxylate(4j)



(Eluent: 5% EtOAc/hexane); 61% yield (55 mg); White solid; M.p.102-107°C; ¹H NMR (500 MHz, CDCl₃) δ 8.53 (d, *J* = 7.0 Hz, 1H), 8.23 (d, *J* = 9.0 Hz, 1H), 7.48-7.32 (m, 5H), 6.97 (t, *J* = 7.0 Hz, 1H), 4.22 (q, *J* = 7.0 Hz, 2H), 1.13 (t, *J* = 7.0 Hz, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 163.1, 154.4, 141.8, 134.1, 132.7, 131.2, 129.8, 129.1, 128.9, 127.3, 126.2, 119.4, 113.9, 102.7, 59.8, 13.9 HRMS calcd for C₁₆H₁₄ClN₂O₂: 301.0744. Found: 301.0744.

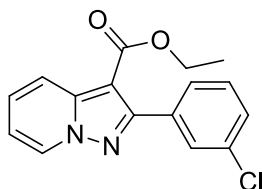
Ethyl-2-(3-bromophenyl)pyrazolo[1,5-a]pyridine-3-carboxylate (4k)



(Eluent: 5% EtOAc/hexane); 51% yield (52.5 mg); White solid; M.p.120-125°C; ¹H NMR (500 MHz, CDCl₃) δ 8.53 (d, *J* = 7.0 Hz, 1H), 8.24 (d, *J* = 9.0 Hz, 1H), 7.96-7.95 (m, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.57-7.56 (m, 1H), 7.45 (d, *J* = 6.5 Hz, 1H), 7.34 (t, *J* = 7.0 Hz, 1H), 7.00-6.95 (m, 1H), 4.34 (q, *J* = 7.0 Hz, 2H), 1.34 (t, *J* = 7.0 Hz, 3H). ¹³C NMR (125 MHz,

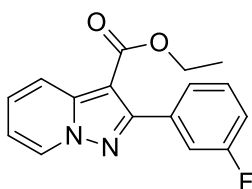
CDCl₃) δ 163.3, 155.2, 142.7, 134.6, 133.0, 131.8, 129.2, 128.8, 128.7, 127.4, 121.7, 119.8, 114.1, 100.9, 60.0, 14.2. HRMS calcd for C₁₆H₁₄O₂N₂Br: 345.0239. Found: 345.0243.

Ethyl-2-(3-chlorophenyl)pyrazolo[1,5-a]pyridine-3-carboxylate (4l)



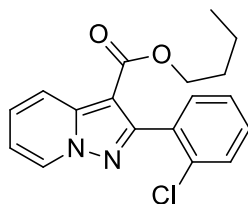
(Eluent: 5% EtOAc/hexane); 58% yield (52.6 mg); White solid; M.p.128-133°C; ¹H NMR (500 MHz, CDCl₃) δ 8.53 (d, *J* = 6.5 Hz, 1H), 8.24 (d, *J* = 9.0 Hz, 1H), 7.806-7.802 (m 1H), 7.70-7.68 (m, 1H), 7.45-7.37 (m, 3), 7.00-6.98 (m, 1H), 4.34 (q, *J* = 7.0 Hz, 2H), 1.32 (t, *J* = 7.0 Hz, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 163.3, 155.3, 142.7, 134.3, 133.5, 130.1, 128.9, 128.88, 128.84, 128.2, 127.4, 119.8, 114.1, 100.9, 60.0, 14.2. HRMS calcd for C₁₆H₁₄ClN₂O₂: 301.0744. Found: 301.0747.

Ethyl-2-(3-fluorophenyl)pyrazolo[1,5-a]pyridine-3-carboxylate (4m)



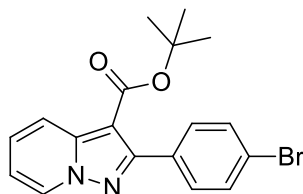
(Eluent: 5% EtOAc/hexane); 61% yield (52 mg); White solid; M.p.116-121°C; ¹H NMR (500 MHz, CDCl₃) δ 8.52 (d, *J* = 7.0 Hz, 1H), 8.23 (d, *J* = 9.0 Hz, 1H), 7.60 (d, *J* = 7.5 Hz, 1H), 7.54 (d, *J* = 10.0 Hz, 1H), 7.44-7.39 (m, 2H), 7.15-7.11 (m, 1H), 6.99 (t, *J* = 6.5 Hz, 1H), 4.35 (q, *J* = 7.0 Hz, 2H), 1.33 (t, *J* = 7.0 Hz, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 163.3, (d, *J* = 20.6 Hz), 161.2, 155.5, 142.7, 134.6, (d, *J* = 8.1 Hz), 129.2, (d, *J* = 8.1 Hz), 128.8, 127.3, 125.7, 119.8, 117.2, (d, *J* = 22.8 Hz), 115.7, (d, *J* = 21.0 Hz), 114.0, 100.8, 59.9, 14.1. HRMS calcd for C₁₆H₁₄O₂N₂F: 285.1039. Found: 285.1032.

Butyl-2-(2-chlorophenyl)pyrazolo[1,5-a]pyridine-3-carboxylate (4n)



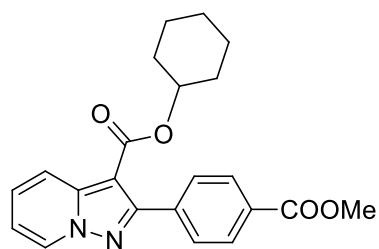
(Eluent: 5% EtOAc/hexane); 60% yield (52.0 mg); White solid; M.p.78-83°C; ¹H NMR (500 MHz, CDCl₃) δ 8.54 (d, *J* = 7.0 Hz, 1H), 8.25 (d, *J* = 9.0 Hz, 1H), 7.49-7.43 (m, 3H), 7.40-7.33 (m, 2H), 6.99 (t, *J* = 7.0 Hz, 1H), 4.15 (t, *J* = 7.5 Hz, 2H), 1.46 (quin, *J* = 6,5 Hz 2H), 1.13 (sextet, *J* = 7.5 Hz, 2H), 0.82 (t, *J* = 7.5 Hz, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 163.3, 154.2, 141.9, 134.1, 132.8, 131.1, 129.8, 129.1, 128.9, 127.3, 126.2, 119.4, 113.9, 102.7, 63.7, 30.5, 19.0, 13.6, HRMS calcd for C₁₈ H₁₈ O₂ N₂ Cl: 329.1057. Found: 329.10565.

Tert-butyl-2-(4-bromophenyl)pyrazolo[1,5-a]pyridine-3-carboxylate (4o)



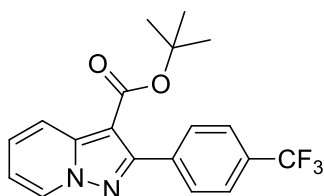
(Eluent: 5% EtOAc/hexane); 60% yield (67.0 mg); White solid; M.p.116-121°C ; ¹H NMR (500 MHz, CDCl₃) δ 8.50 (d, *J* = 7.0 Hz, 1H), 8.19 (d, *J* = 9.0 Hz, 1H), 7.66 (d, *J* = 8.5 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.39 (t, *J* = 8.0 Hz, 1H), 6.95 (t, *J* = 7.0 Hz, 1H), 1.52 (s, 9H). ¹³C NMR (125 MHz, CDCl₃) δ 162.7, 155.6, 142.5, 131.8, 131.6, 130.8, 128.7, 127.0, 123.1, 119.7, 113.8, 80.7, 28.4. HRMS calcd for C₁₈ H₁₈ O₂ N₂ Br: 373.0552. Found: 373.0557.

Cyclohexyl-2-(4-(methoxycarbonyl)phenyl)pyrazolo[1,5-a]pyridine-3-carboxylate (4p)



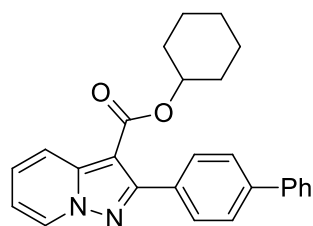
(Eluent: 5% EtOAc/hexane); 72% yield (80.5 mg); White solid; M.p.121-126°C; ¹H NMR (500 MHz, CDCl₃) δ 8.52 (d, *J* = 7.0 Hz, 1H), 8.23 (d, *J* = 9.0 Hz, 1H), 8.12 (d, *J* = 8.5 Hz, 2H), 7.86 (d, *J* = 8.5 Hz, 2H), 7.41 (t, *J* = 7.5 Hz, 1H), 6.96 (t, *J* = 7.0 Hz, 1H), 4.97 (sept, *J* = 5.0 Hz, 1H), 3.90 (s, 3H), 1.91-1.89 (m, 2H), 1.65-1.62 (m, 2H), 1.52-1.21(m, 6H). ¹³C NMR (125 MHz, CDCl₃) δ 165.7, 161.8, 154.4, 141.4, 136.1, 128.9, 128.8, 127.7, 127.5, 126.5, 118.6, 112.8, 100.2, 71.3, 50.9, 30.5, 24.1, 22.5. HRMS calcd for C₂₂H₂₃N₂O₄: 379.1658. Found: 379.1650.

Tert-butyl-2-(4-(trifluoromethyl)phenyl)pyrazolo[1,5-a]pyridine-3-carboxylate (4q)



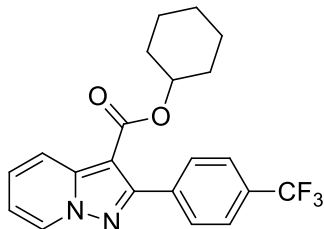
(Eluent: 5% EtOAc/hexane); 79% yield (85.5 mg); White solid; M.p.119-124°C; ¹H NMR (500 MHz, CDCl₃) δ 8.51 (d, *J* = 7.0 Hz, 1H), 8.21 (d, *J* = 9.0 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 2H), 7.72 (d, *J* = 8.0 Hz, 2H), 7.41 (t, *J* = 7.5 Hz, 1H), 6.69 (t, *J* = 6.5 Hz, 1H), 1.51 (s, 9H). ¹³C NMR (125 MHz, CDCl₃) δ 162.6, 155.2, 142.4, 136.9, 130.7(d *J* = 162 Hz), 128.7, 127.7(d *J* = 56.6 Hz), 124.8(d *J* = 86.0 Hz), 119.8, 113.9, 102.5, 80.8, 28.3. HRMS calcd for C₁₉ H₁₈ O₂ N₂ F₃: 363.1320. Found: 363.1326.

Cyclohexyl-2-([1,1'-biphenyl]-4-yl)pyrazolo[1,5-a]pyridine-3-carboxylate (4r)



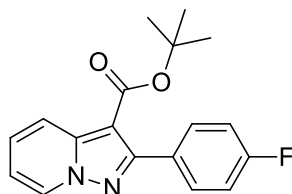
Eluent: 5% EtOAc/hexane); 59% yield (70 mg); White solid; M.p.143-148°C; ¹H NMR (500 MHz, CDCl₃) δ 8.54 (d, *J* = 7.0 Hz, 1H), 8.24 (d, *J* = 9.0 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 2H), 7.69-7.65 (m, 4H), 7.47-7.35 (m, 4H), 6.95 (t, *J* = 6.5 Hz, 1H), 5.03 (sept, *J* = 4.0 Hz, 1H), 1.95-1.92 (m, 2H), 1.68-1.65 (m, 2H), 1.55-1.50 (m, 3H), 1.41-1.35 (m, 2H), 1.28-1.25 (m, 1H). ¹³C NMR (125 MHz, CDCl₃) δ 163.1, 142.7, 141.5, 140.9, 131.7, 130.4, 128.8, 128.7, 127.4, 127.2, 126.5, 119.8, 113.8, 101.2, 72.3, 31.8, 25.4, 23.7, HRMS calcd for C₂₆ H₂₅ O₂ N₂: 397.1916. Found: 397.1922.

Cyclohexyl-2-(4-(trifluoromethyl)phenyl)pyrazolo[1,5-a]pyridine-3-carboxylate (4s)



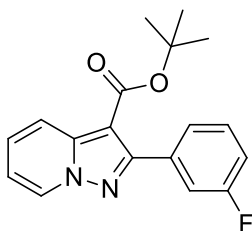
(Eluent: 5% EtOAc/hexane); 68% yield (79.5 mg); White solid; M.p.66-71°C; ¹H NMR (500 MHz, CDCl₃) δ 8.53 (d, *J* = 7.0 Hz, 1H), 8.24 (d, *J* = 8.5 Hz, 1H), 7.92 (d, *J* = 8.0 Hz, 2H), 7.72 (d, *J* = 8.5 Hz, 2H), 7.46 (t, *J* = 7.0 Hz, 1H), 7.01 (t, *J* = 6.5 Hz, 1H), 5.00 (sept, *J* = 5.0 Hz, 1H), 1.94-1.90 (m, 2H), 1.65-1.63 (m, 2H), 1.52-1.26 (m, 6H). ¹³C NMR (125 MHz, CDCl₃) δ 162.8, 155.4, 142.5, 136.4, 130.5, 130.5(d *J* = 72.5 Hz), 128.8, 127.4, 124.8(d *J* = 86.5 Hz), 119.9, 114.1, 101.5, 72.5, 31.7, 25.3, 23.6. HRMS calcd for C₂₁ H₂₀ O₂ N₂ F₃: 389.1477. Found: 389.1489.

Tert-butyl-2-(4-fluorophenyl)pyrazolo[1,5-a]pyridine-3-carboxylate (4t)



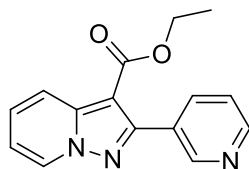
(Eluent: 5% EtOAc/hexane); 79% yield (74 mg); White solid; M.p.132-137°C; ^1H NMR (500 MHz, CDCl_3) δ 8.50 (d, $J = 7.0$ Hz, 1H), 8.20 (d, $J = 9.0$ Hz, 1H), 7.76-7.73 (m, 2H), 7.39 (t, $J = 8.5$ Hz, 1H), 7.14 (t, $J = 8.5$ Hz, 2H), 6.94 (t, $J = 7.0$ Hz, 1H), 1.52 (s, 9H). ^{13}C NMR (125 MHz, CDCl_3) δ 164.1, (d, $J = 246.2$ Hz), 162.9, 155.8, 142.5, 131.9, (d, $J = 8.2$ Hz), 128.9, (d, $J = 28.2$ Hz), 127.0, 119.7, 114.8, (d, $J = 21.3$ Hz), 113.7, 102.1, 80.7, 28.4. HRMS calcd for $\text{C}_{18}\text{H}_{18}\text{O}_2\text{N}_2\text{F}$: 313.1352. Found: 313.1368.

Tert-butyl-2-(3-fluorophenyl)pyrazolo[1,5-a]pyridine-3-carboxylate (4u)



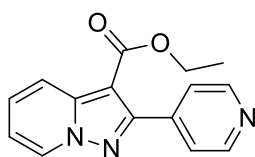
(Eluent: 5% EtOAc/hexane); 82% yield (76.5 mg); White solid; M.p.118-123°C; ^1H NMR (500 MHz, CDCl_3) δ 8.51 (d, $J = 7.0$ Hz, 1H), 8.22 (d, $J = 9.0$ Hz, 1H), 7.55 (d, $J = 7.5$ Hz, 1H), 7.44-7.39 (m, 3H), 7.14-7.11 (m, 1H), 6.96 (t, $J = 6.5$ Hz, 1H), 1.51 (s, 9H). ^{13}C NMR (125 MHz, CDCl_3) δ 163.1 (d, $J = 118.2$ Hz), 162.7, 155.3, 142.6, 135.0 (d, $J = 8.5$ Hz), 129.2 (d, $J = 8.1$ Hz), 128.7, 127.1, 125.7, 119.8, 117.3(d, $J = 22.6$ Hz), 115.6 (d, $J = 21$ Hz), 113.9, 102.3, 80.7, 28.3. HRMS calcd for $\text{C}_{18}\text{H}_{18}\text{O}_2\text{N}_2\text{F}$: 313.1352. Found: 313.1368.

Ethyl-2-(pyridin-3-yl)pyrazolo[1,5-a]pyridine-3-carboxylate (4v)



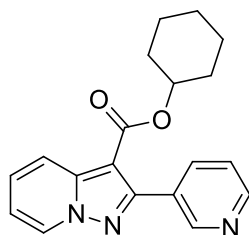
(Eluent: EtOAc); 72% yield (57.5 mg); White solid; M.p.138-143°C; ^1H NMR (500 MHz, CDCl_3) δ 9.01-9.00 (m, 1H), 8.68-8.66 (m, 1H), 8.55 (d, $J = 7.0$ Hz, 1H), 8.25 (d, $J = 7.0$ Hz, 1H), 8.15-8.12 (m, 1H), 7.45 (t, $J = 7.0$ Hz, 1H), 7.40-7.38 (m, 1H), 7.01 (t, $J = 7.0$ Hz, 1H), 4.33 (quar, $J = 7.0$ Hz, 2H), 1.31 (t, $J = 7.0$ Hz, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 163.2, 153.7, 150.5, 149.6, 142.7, 137.4, 128.8, 128.7, 127.5, 122.5, 119.8, 114.2, 101.2, 60.0, 14.2. HRMS calcd for $\text{C}_{15}\text{H}_{14}\text{O}_2\text{N}_3$: 268.1086. Found: 268.1081.

Ethyl-2-(pyridin-4-yl)pyrazolo[1,5-a]pyridine-3-carboxylate (4w)



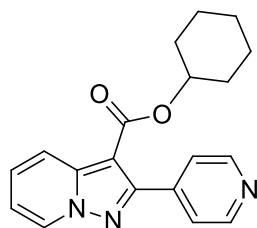
(Eluent: EtOAc); 81% yield (66 mg); White solid; M.p.154-159°C; ^1H NMR (500 MHz, CDCl_3) δ 8.72 (d, $J = 5.5$ Hz, 2H), 8.55 (d, $J = 7.0$ Hz, 1H), 8.25 (d, $J = 9.0$ Hz, 1H), 7.75 (d, $J = 5.5$ Hz, 2H), 7.46 (t, $J = 7.5$ Hz, 1H), 7.02 (t, $J = 6.5$ Hz, 1H), 4.35 (q, $J = 7.0$ Hz, 2H), 1.33 (t, $J = 7.0$ Hz, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 163.1, 154.1, 149.3, 142.6, 140.5, 128.5, 127.6, 124.4, 119.9, 114.2, 101.2, 60.2, 14.2. HRMS calcd for $\text{C}_{15}\text{H}_{14}\text{O}_2\text{N}_3$: 268.1086. Found: 268.1075.

Cyclohexyl-2-(pyridin-3-yl)pyrazolo[1,5-a]pyridine-3-carboxylate (4x)



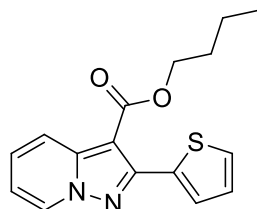
(Eluent: EtOAc); 74% yield (71.5 mg); liquid: ^1H NMR (500 MHz, CDCl_3) δ 8.99 (s, 1H), 8.67 (d, $J = 4.5$ Hz, 1H), 8.55 (d, $J = 6.5$ Hz, 1H), 8.26 (d, $J = 8.5$ Hz, 1H), 8.14 (d, $J = 7.5$ Hz, 1H), 7.46-7.38 (m, 2H), 7.00 (t, $J = 7.0$ Hz, 1H), 4.99 (sept, $J = 5.0$ Hz, 1H), 1.99 (s, 2H), 1.65-1.25 (m, 8H). ^{13}C NMR (125 MHz, CDCl_3) δ 162.7, 153.5, 150.4, 149.4, 142.5, 137.3, 128.8, 128.7, 127.4, 122.4, 119.7, 144.1, 101.5, 72.5, 31.6, 25.2, 23.6. HRMS calcd for $\text{C}_{19}\text{H}_{20}\text{O}_2\text{N}_3$: 322.1556. Found: 322.1566.

Cyclohexyl-2-(pyridin-4-yl)pyrazolo[1,5-a]pyridine-3-carboxylate (4y)



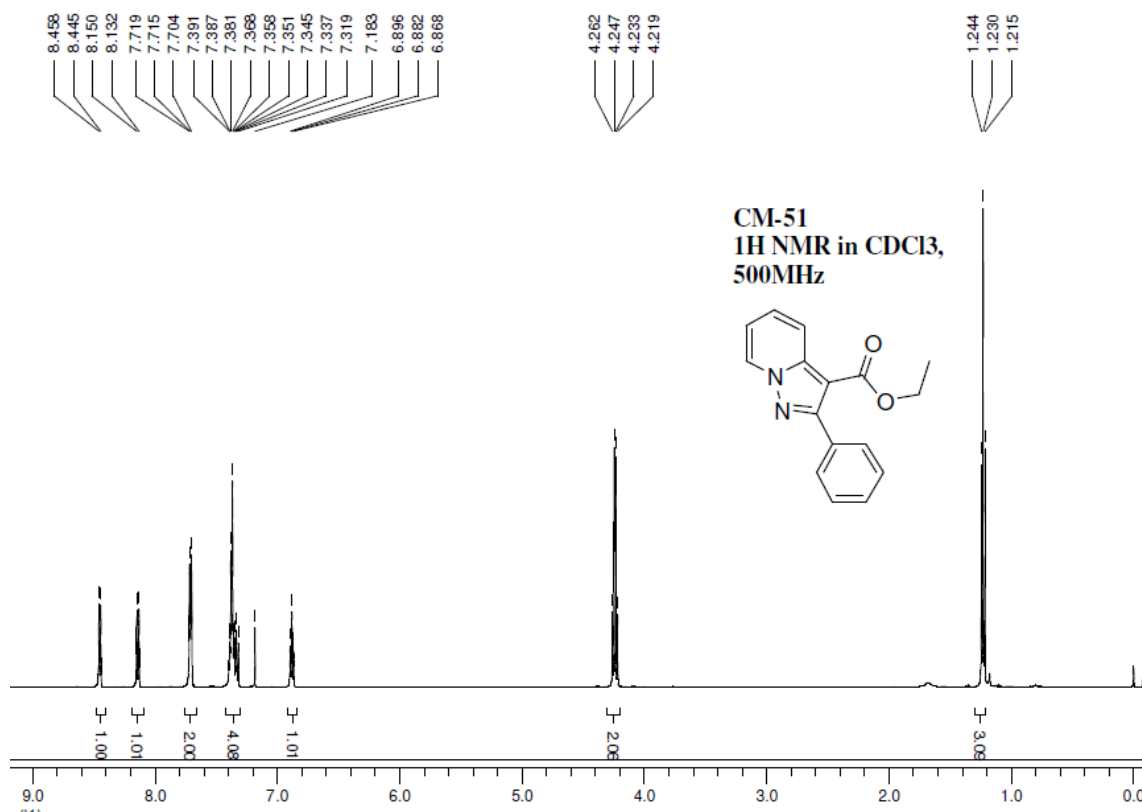
(Eluent: EtOAc); 84% yield (81 mg); White solid; M.p.98-103°C; ^1H NMR (500 MHz, CDCl_3) δ 8.76 (d, $J = 5.0$ Hz, 2H), 8.56 (d, $J = 7.0$ Hz, 1H), 8.28 (d, $J = 9.0$ Hz, 1H), 7.76 (d, $J = 5.5$ Hz, 2H), 7.48 (t, $J = 7.5$ Hz, 1H), 7.03 (t, $J = 7.0$ Hz, 1H), 5.03 (sept, $J = 5.0$ Hz, 1H), 1.97-1.96 (m, 2H), 1.70-1.68 (m, 2H), 1.58-1.27 (m, 6H). ^{13}C NMR (125 MHz, CDCl_3) δ 162.6, 154.0, 149.2, 142.6, 140.6, 128.8, 127.4, 124.4, 119.9, 114.3, 101.6, 72.7, 31.7, 25.2, 23.6. HRMS calcd for $\text{C}_{19}\text{H}_{20}\text{O}_2\text{N}_3$: 322.1556. Found: 322.1555.

Butyl-2-(thiophen-2-yl)pyrazolo[1,5-a]pyridine-3-carboxylate (4z)

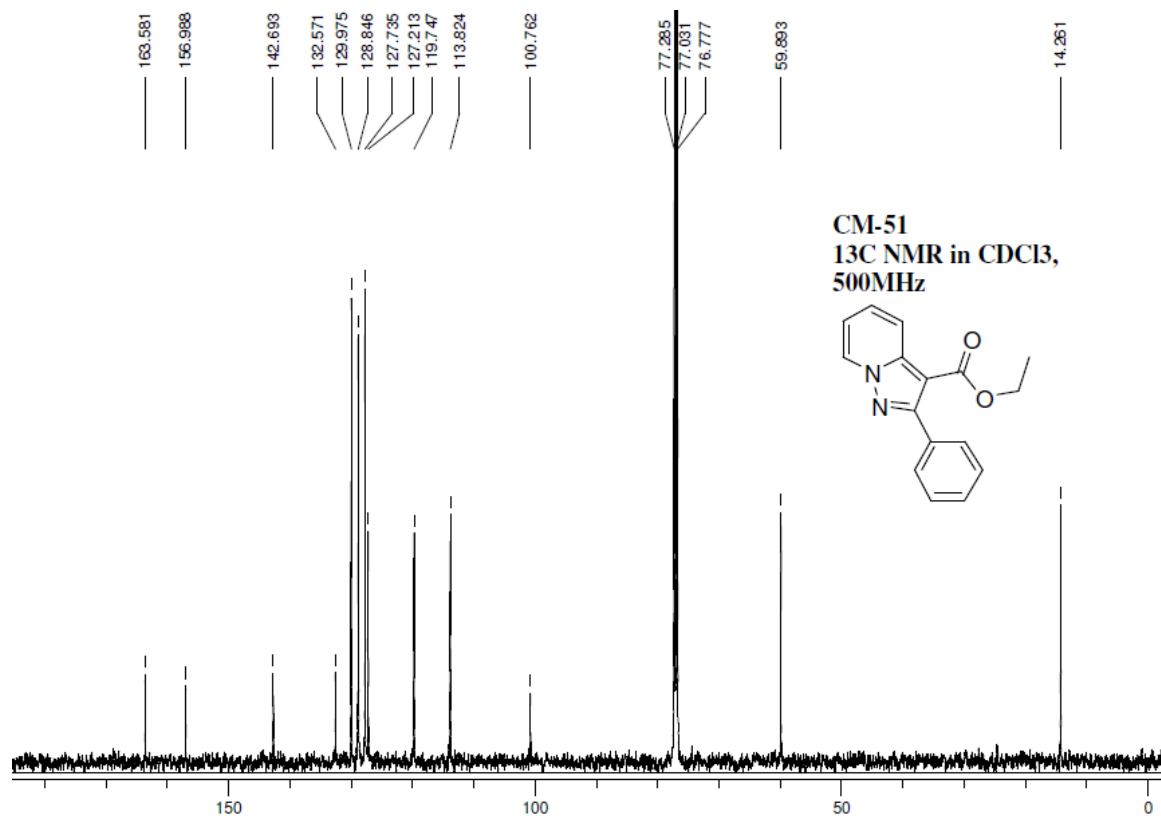


(Eluent: 5% EtOAc/hexane); 37% yield (32 mg); White solid; M.p.68-73°C; ^1H NMR (500 MHz, CDCl_3) δ 8.50 (d, $J = 7.0$ Hz, 1H), 8.18-8.15 (m, 2H), 7.43-7.37 (m, 2H), 7.15 (t, $J =$

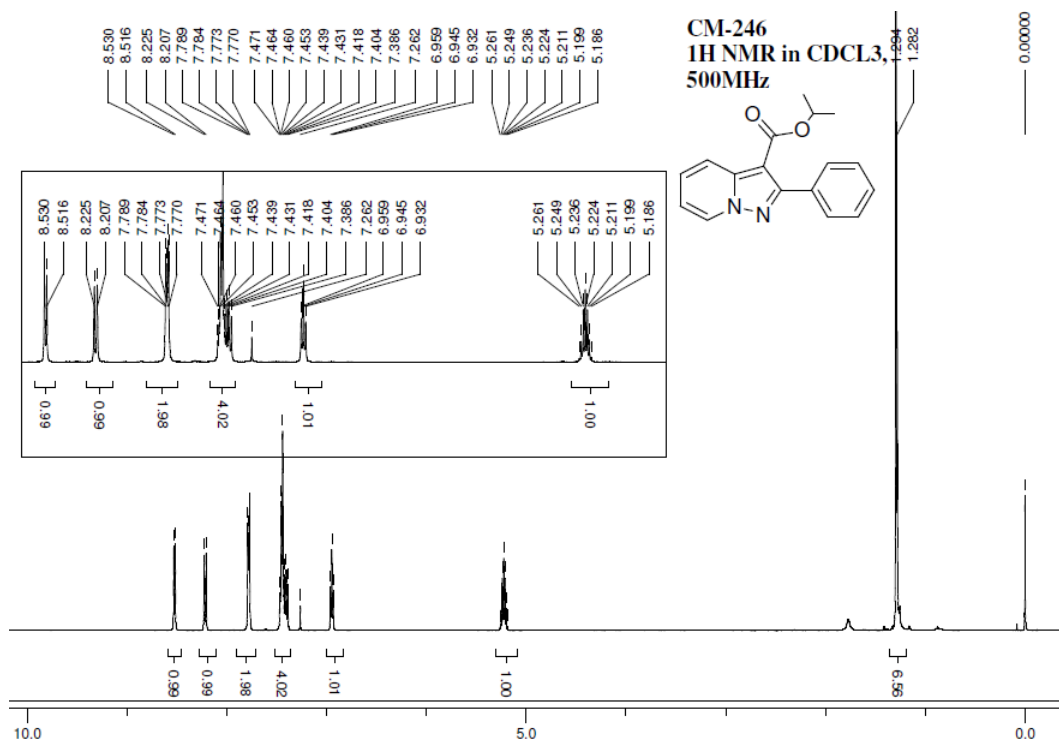
5.5 Hz, 1H), 6.94 (t, $J = 7.0$ Hz, 1H), 4.37 (t, $J = 7.0$ Hz, 2H), 1.79 (quin, $J = 7.0$ Hz 2H), 1.51-1.41 (m, 2H), 0.98 (t, $J = 7.0$ Hz, 3H).. ^{13}C NMR (125 MHz, CDCl_3) δ 163.5, 150.4, 142.8, 133.8, 130.4, 128.6, 127.47, 127.42, 119.7, 113.9, 100.0, 64.0, 30.8, 19.3, 13.7. HRMS calcd for $\text{C}_{16}\text{H}_{17}\text{O}_2\text{N}_2\text{S}$: 301.1011. Found: 301.1001.



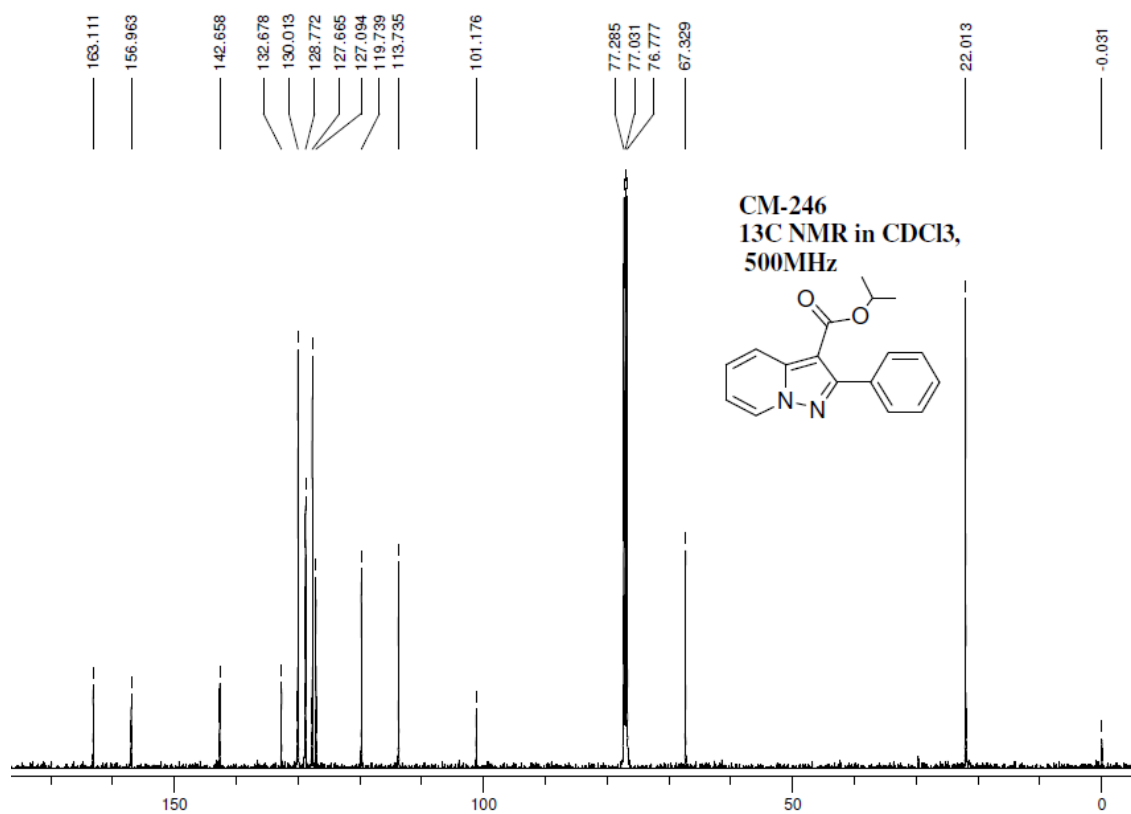
¹H NMR of **3a**



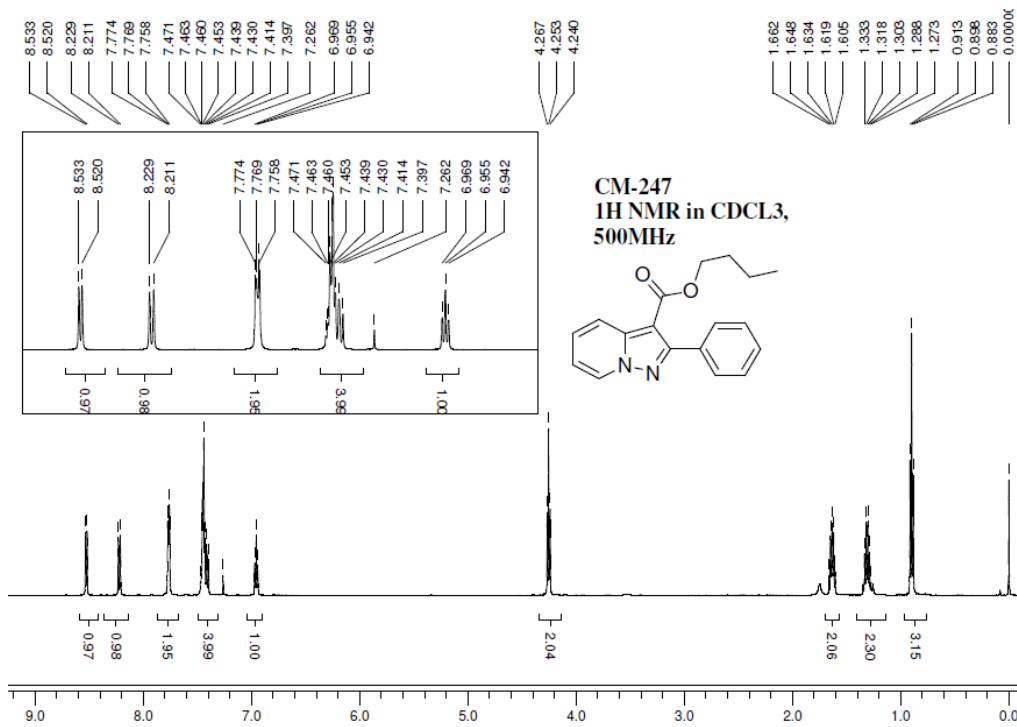
¹³C NMR of **3a**



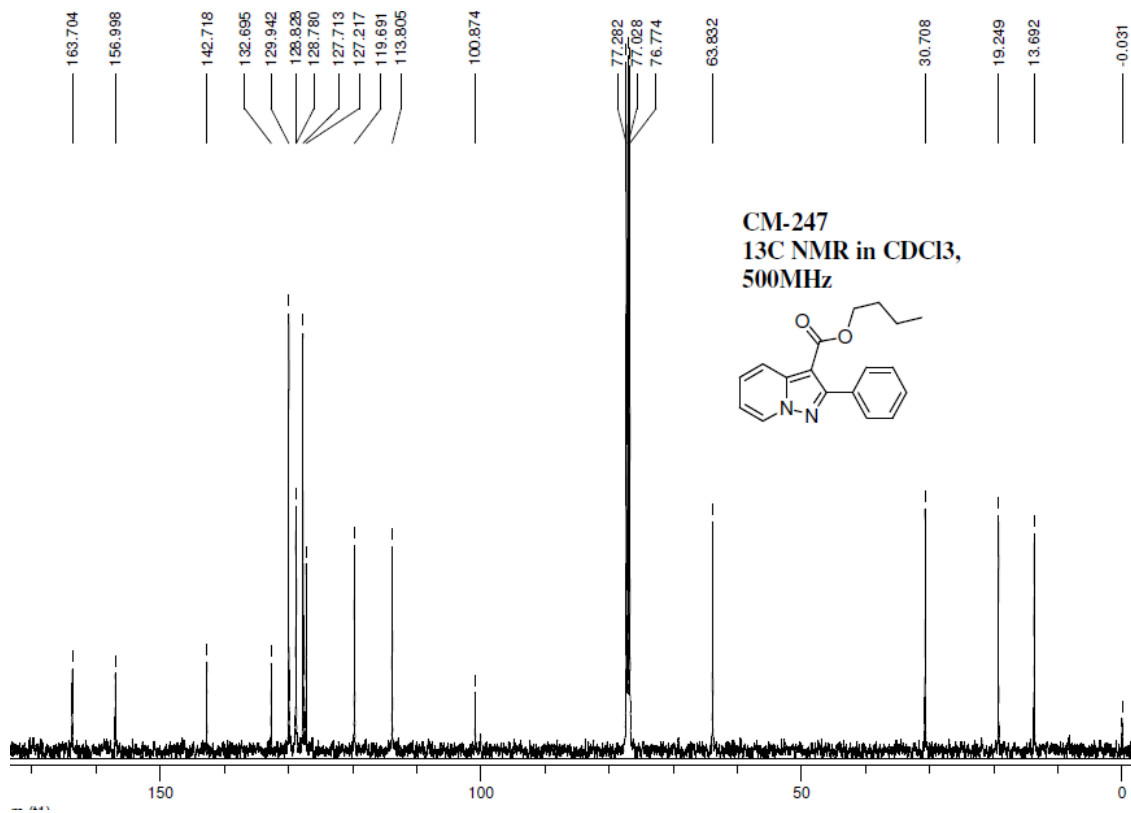
¹H NMR of **3b**



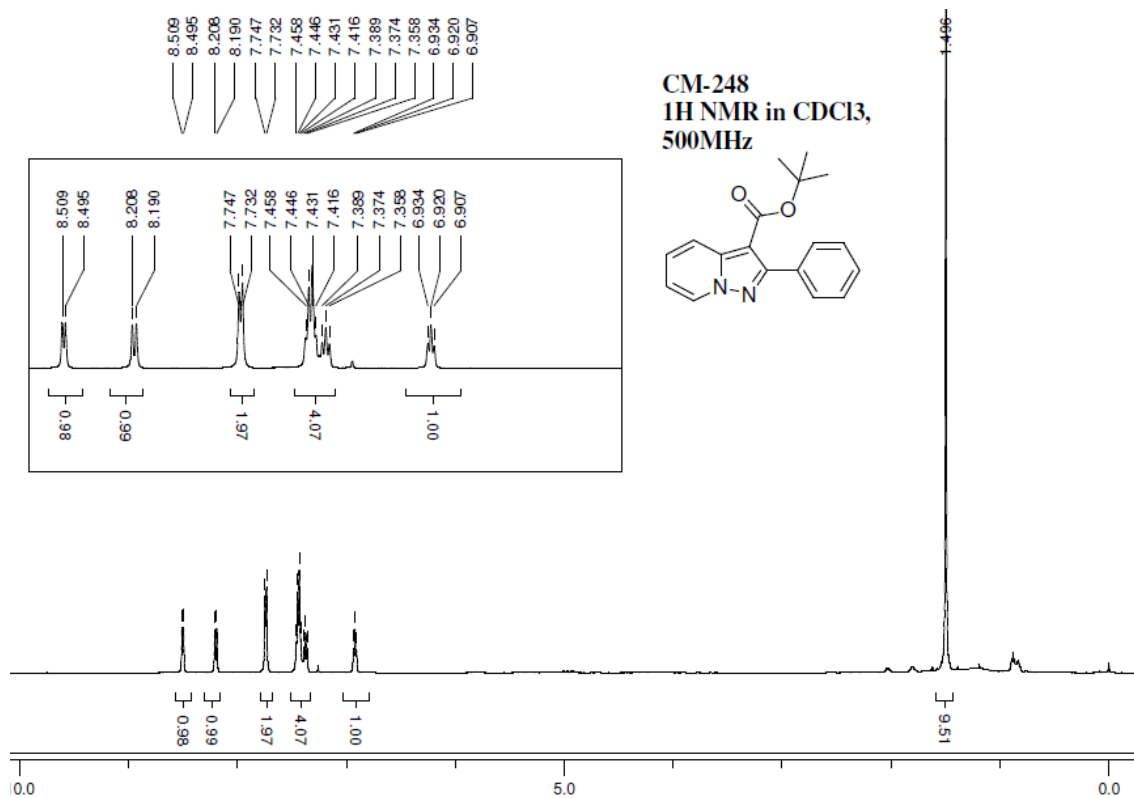
¹³C NMR of **3b**



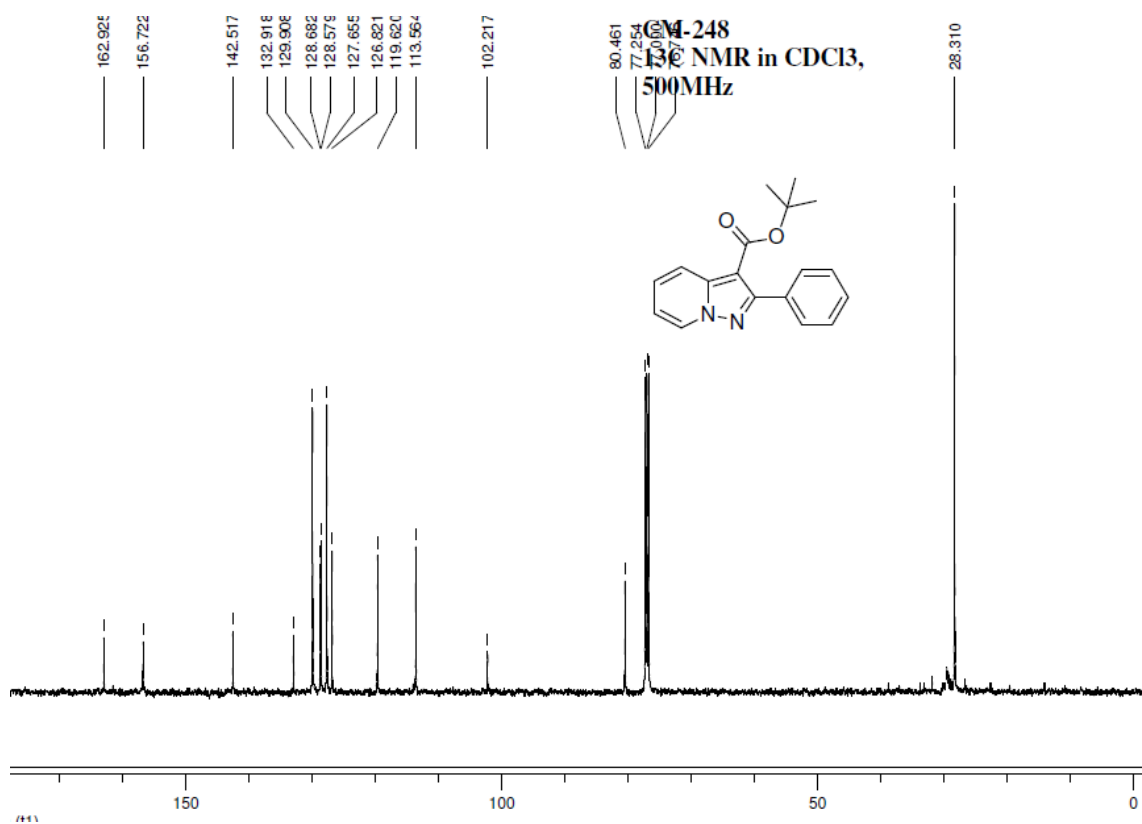
¹H NMR of **3c**



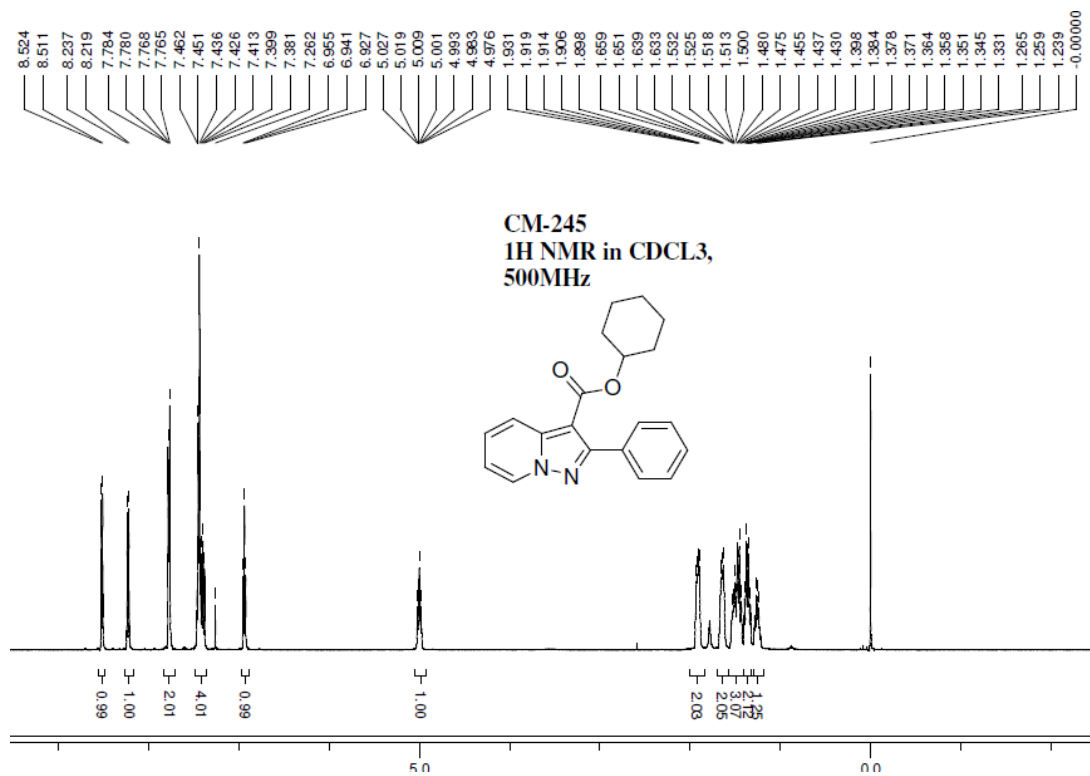
¹³C NMR of **3c**



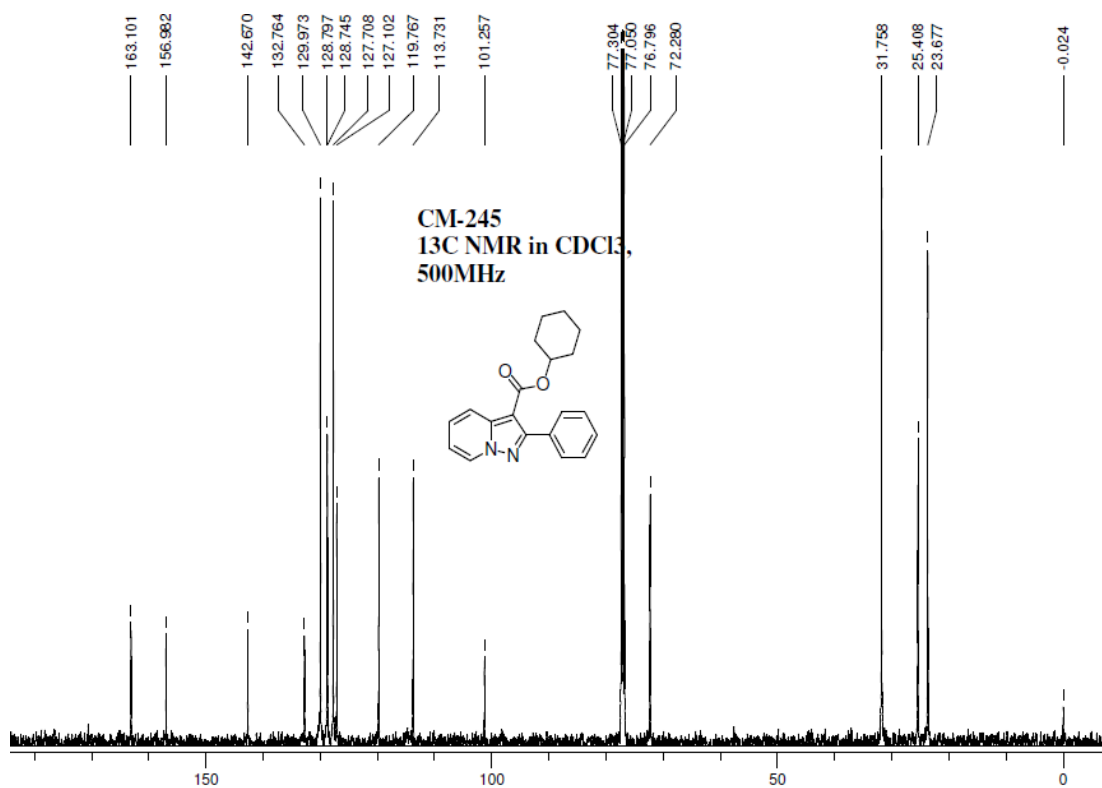
¹H NMR of 3d



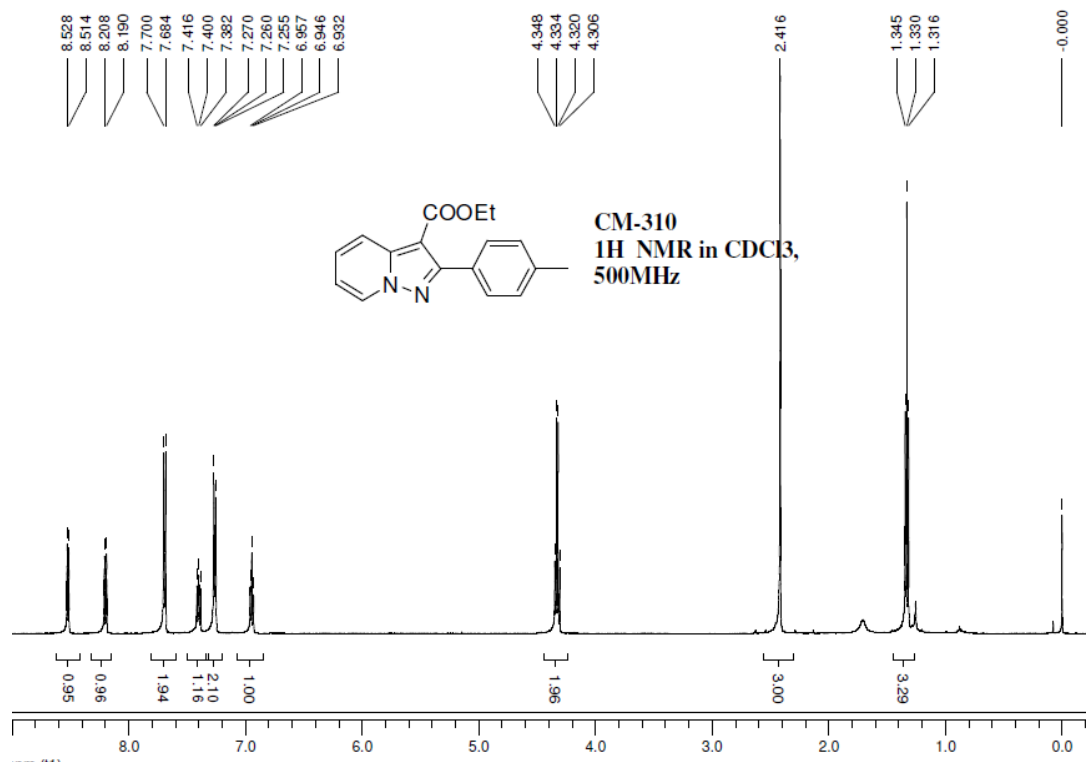
¹³C NMR of 3d



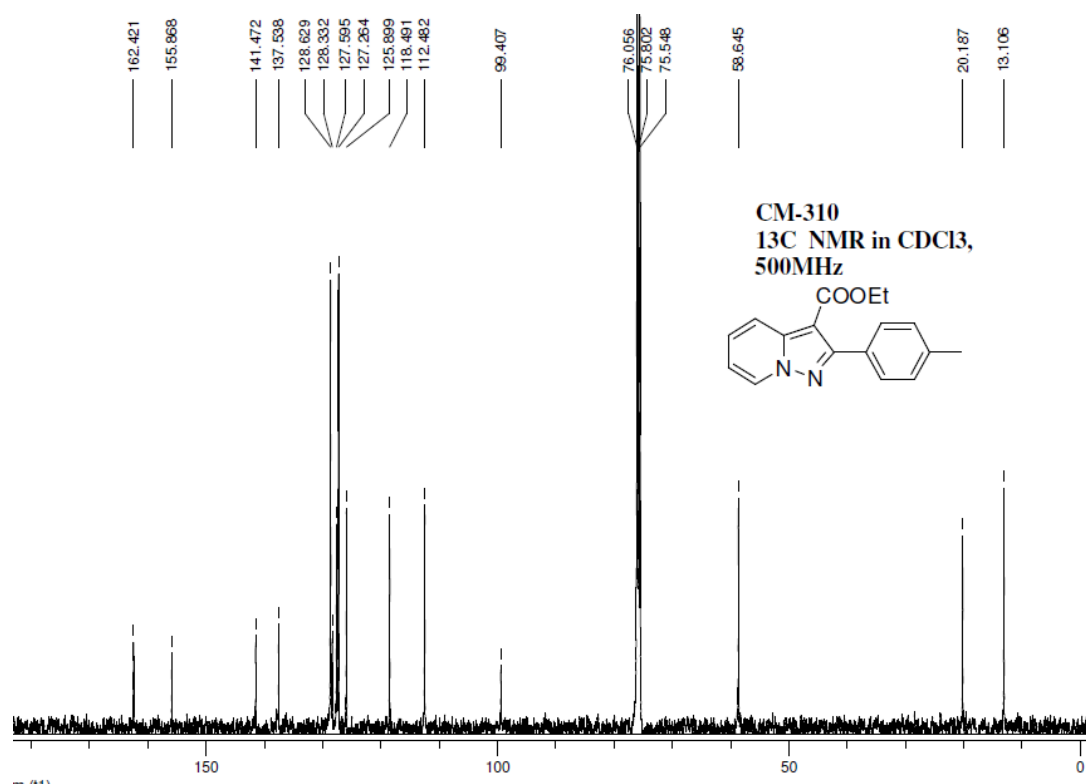
¹H NMR of 3e



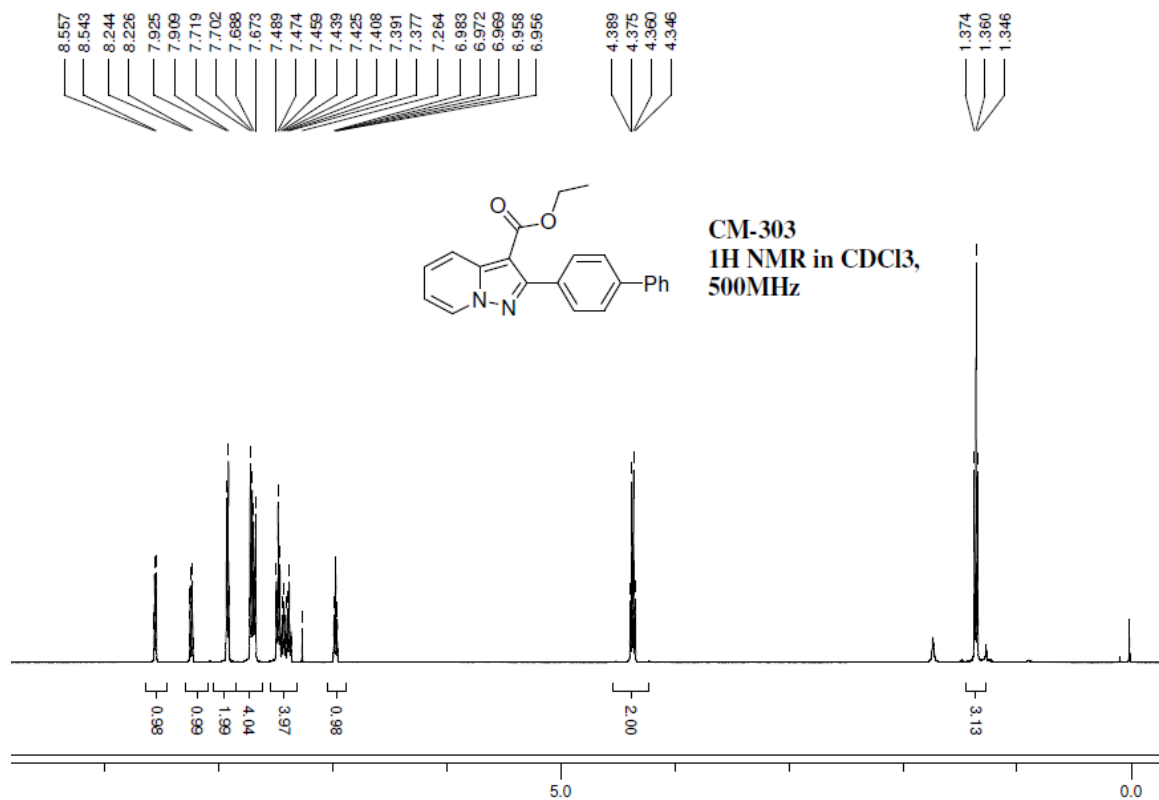
¹³C NMR of 3e



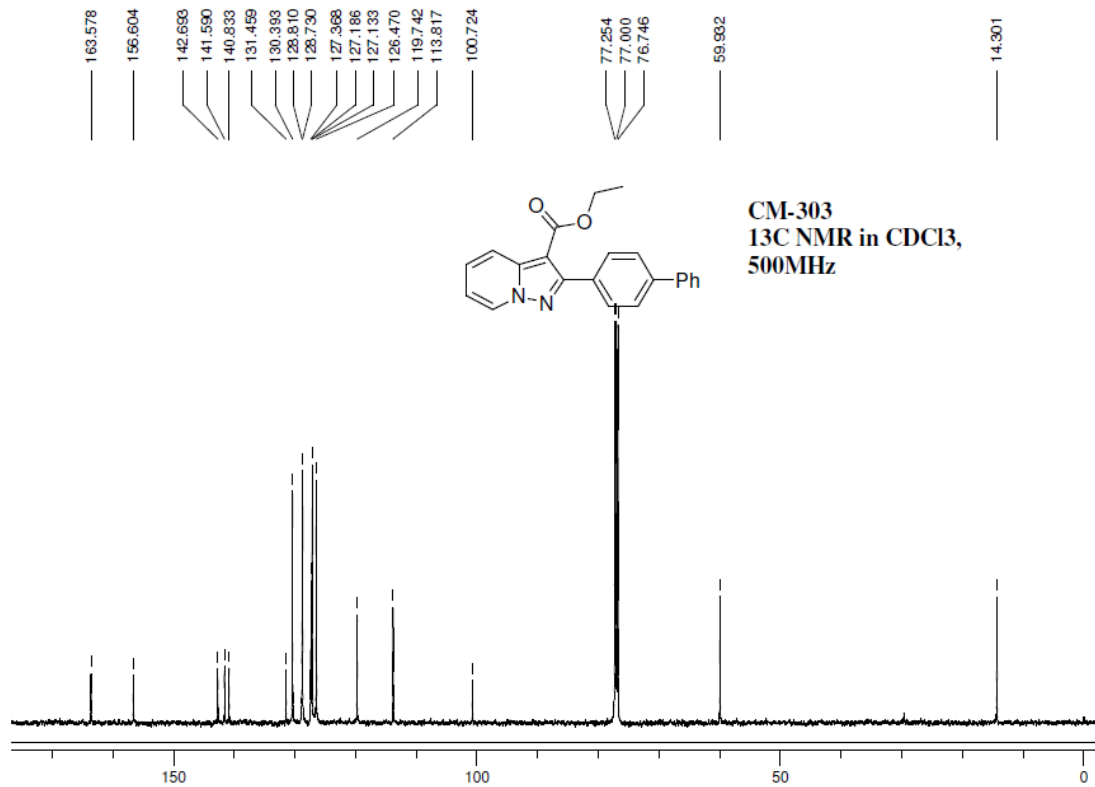
¹H NMR of **4a**



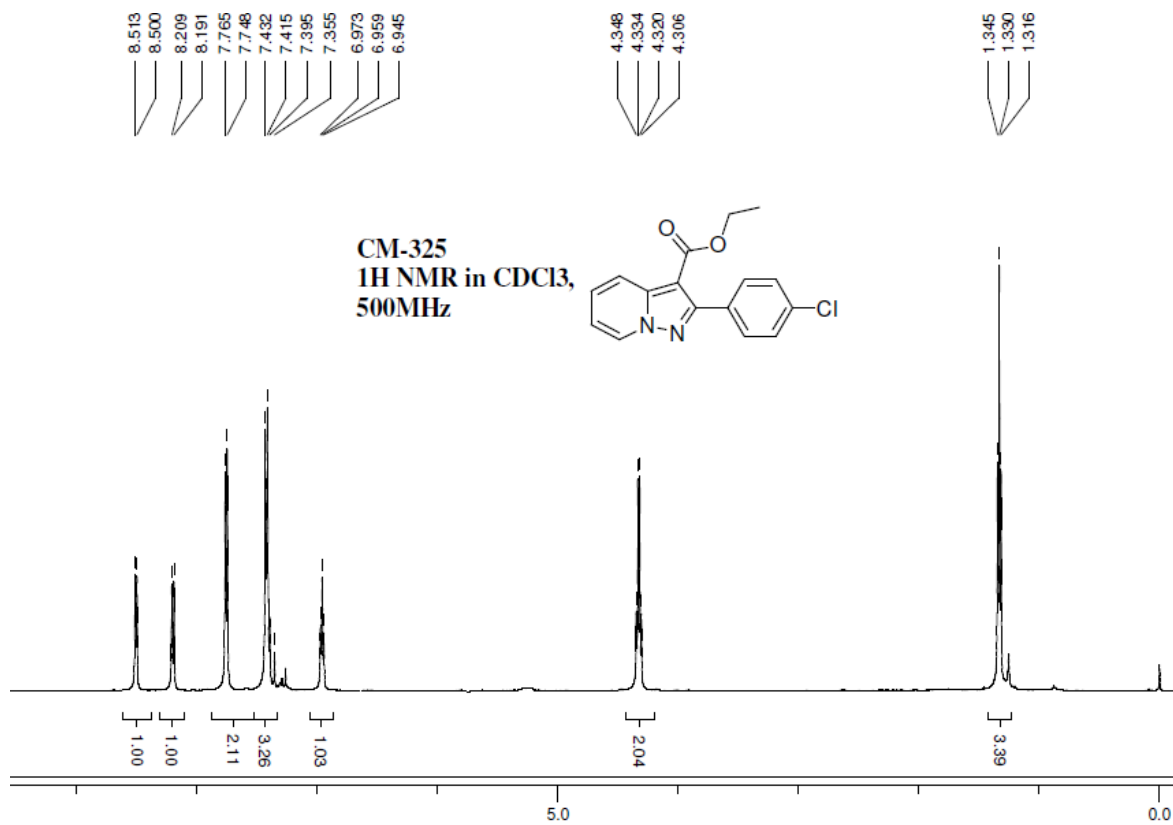
¹³C NMR of **4a**



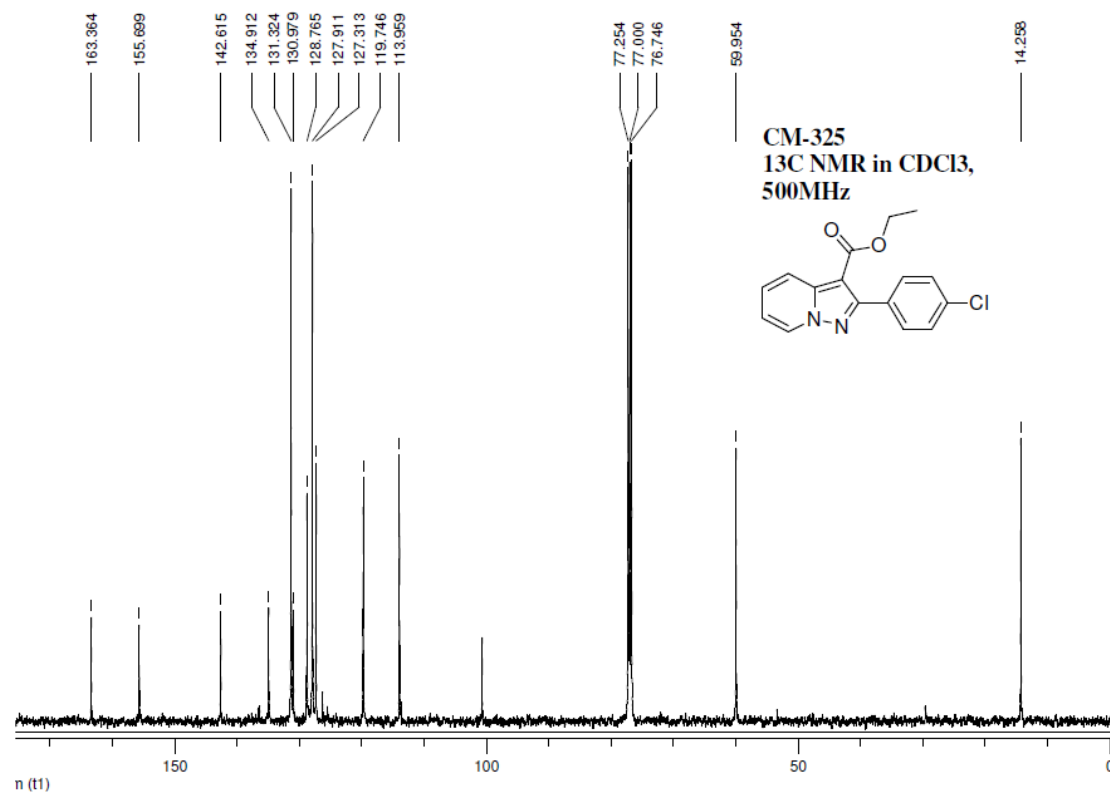
¹H NMR of **4b**



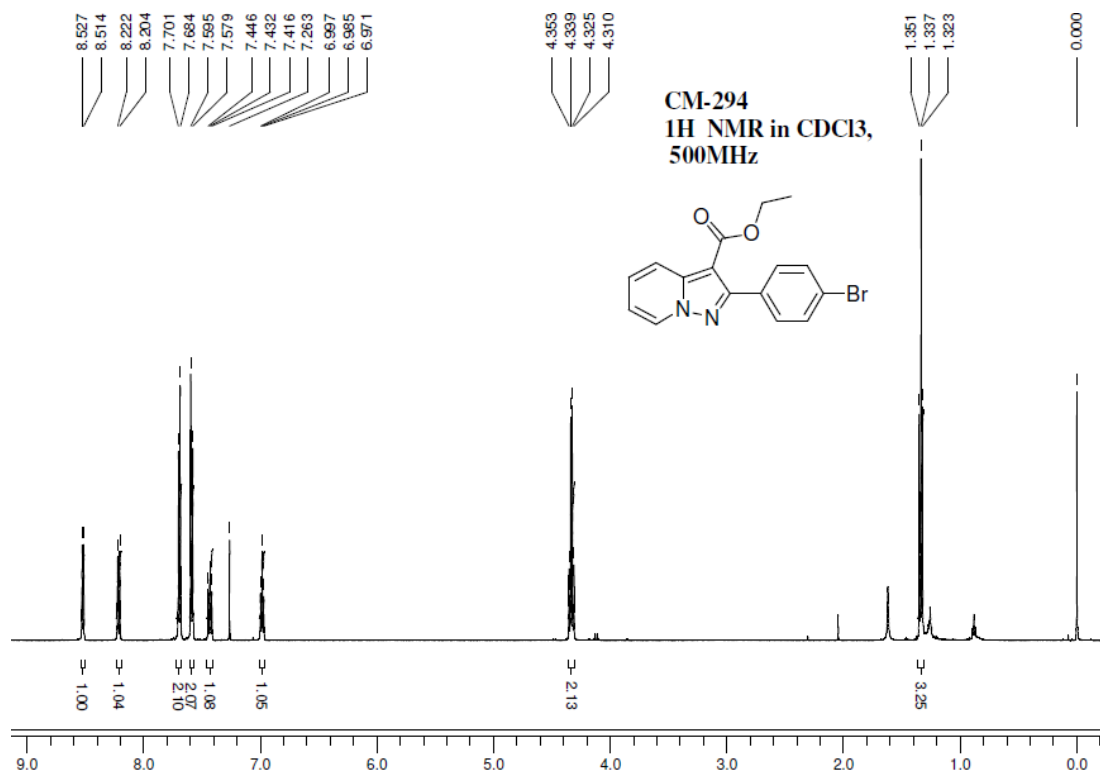
¹³C NMR of **4b**



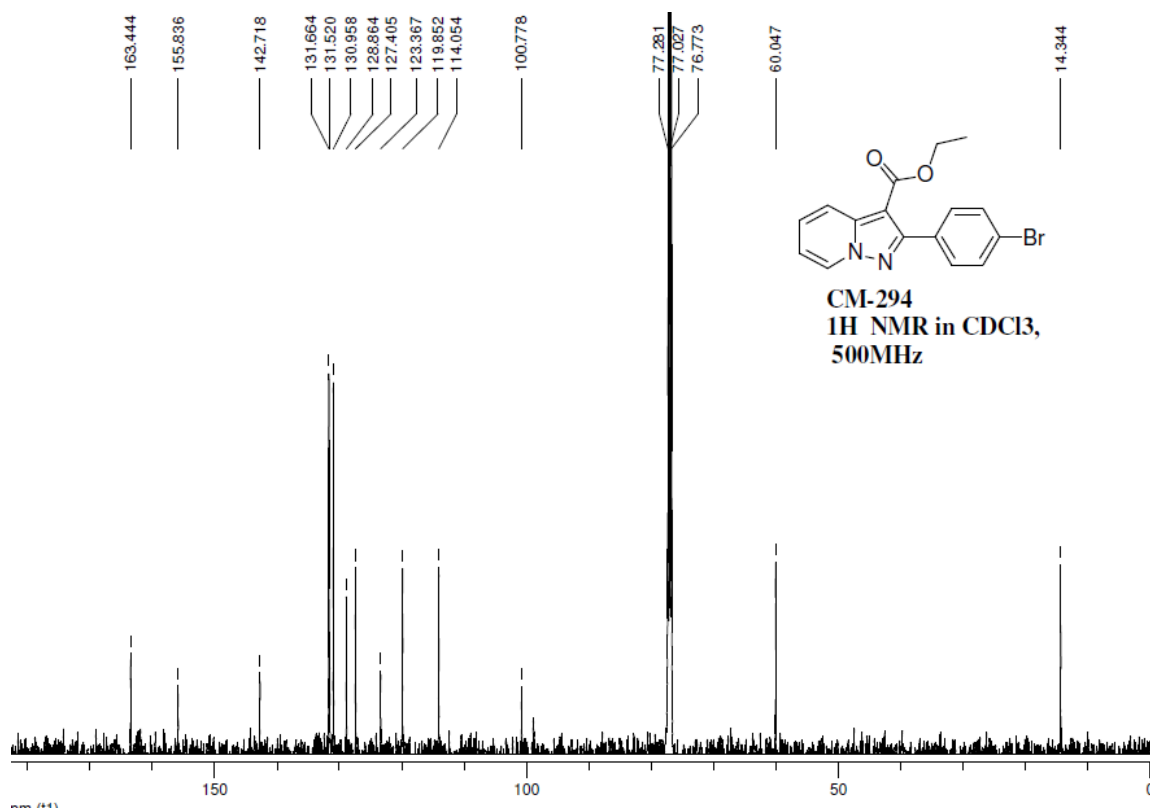
¹H NMR of **4c**



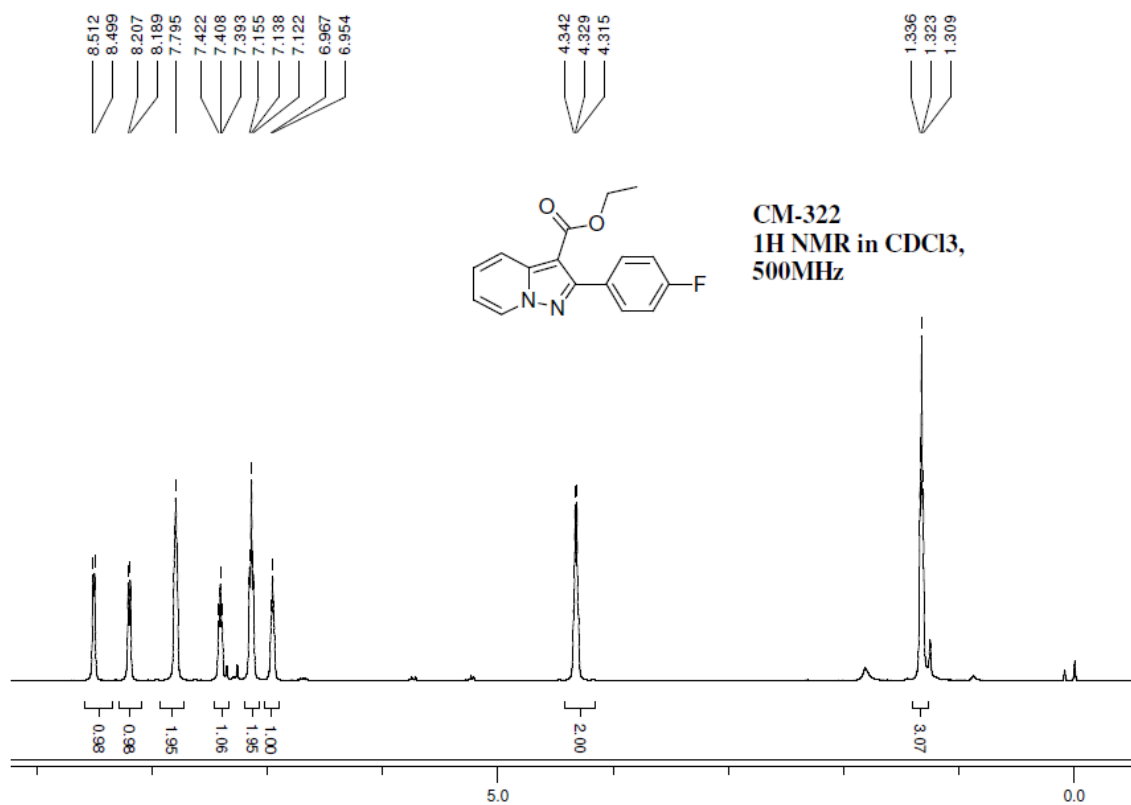
¹³C NMR of **4c**



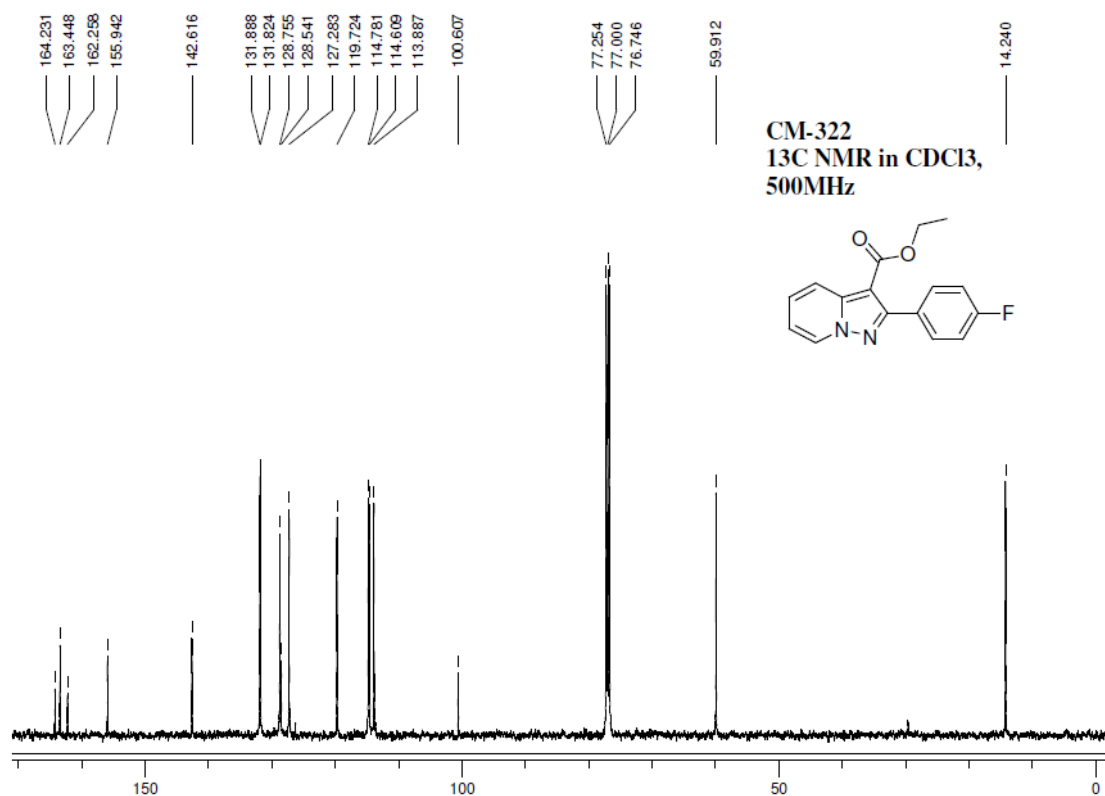
¹H NMR of **4d**



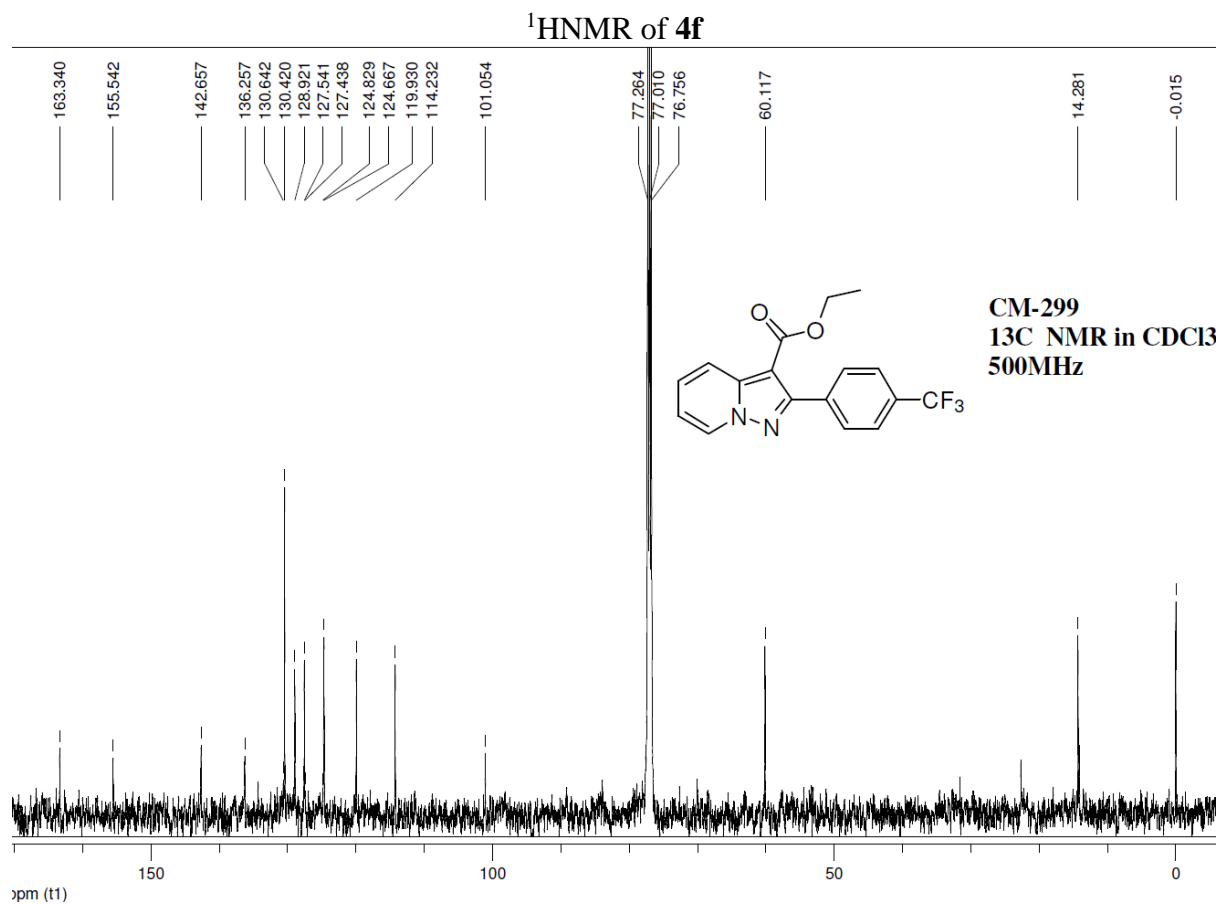
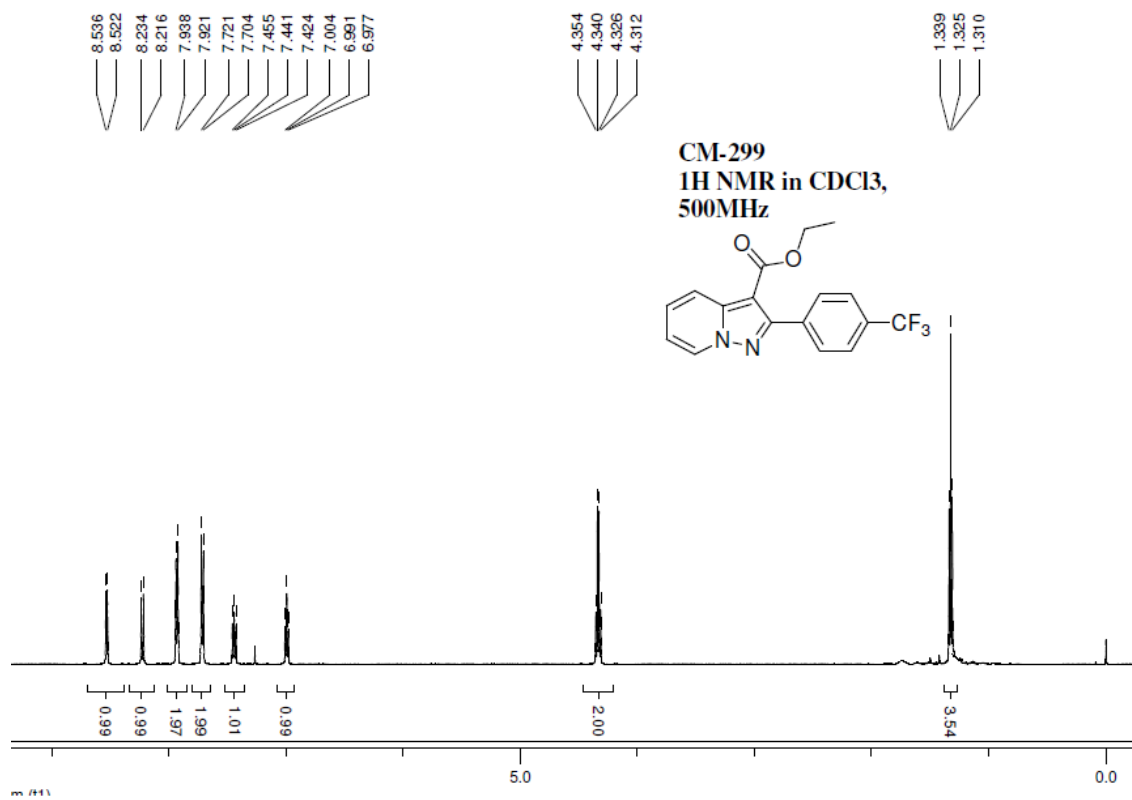
¹³C NMR of **4d**



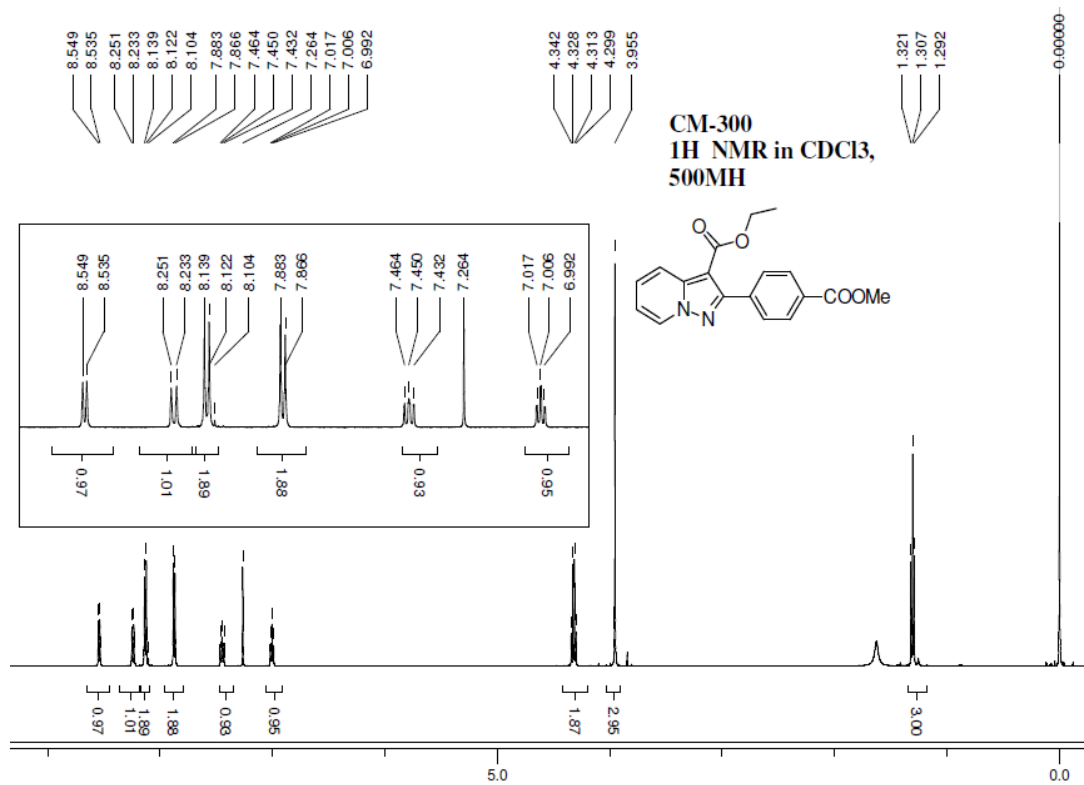
¹H NMR of 4e



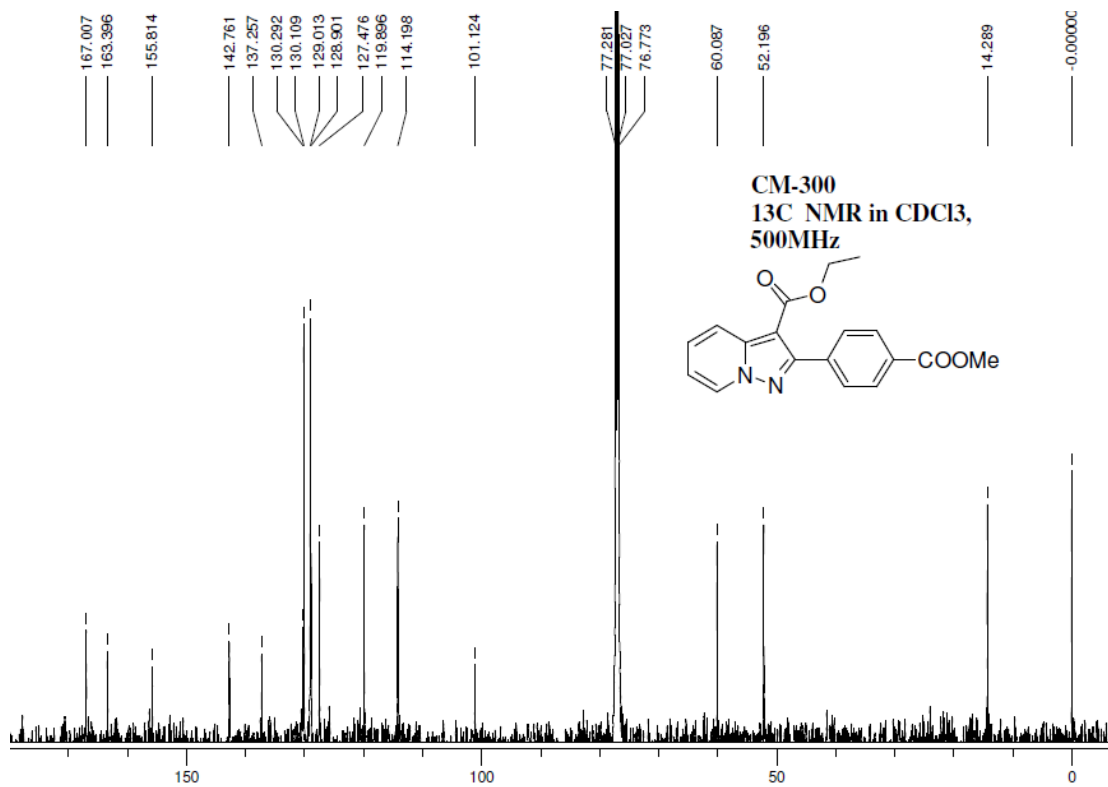
¹³C NMR of 4e



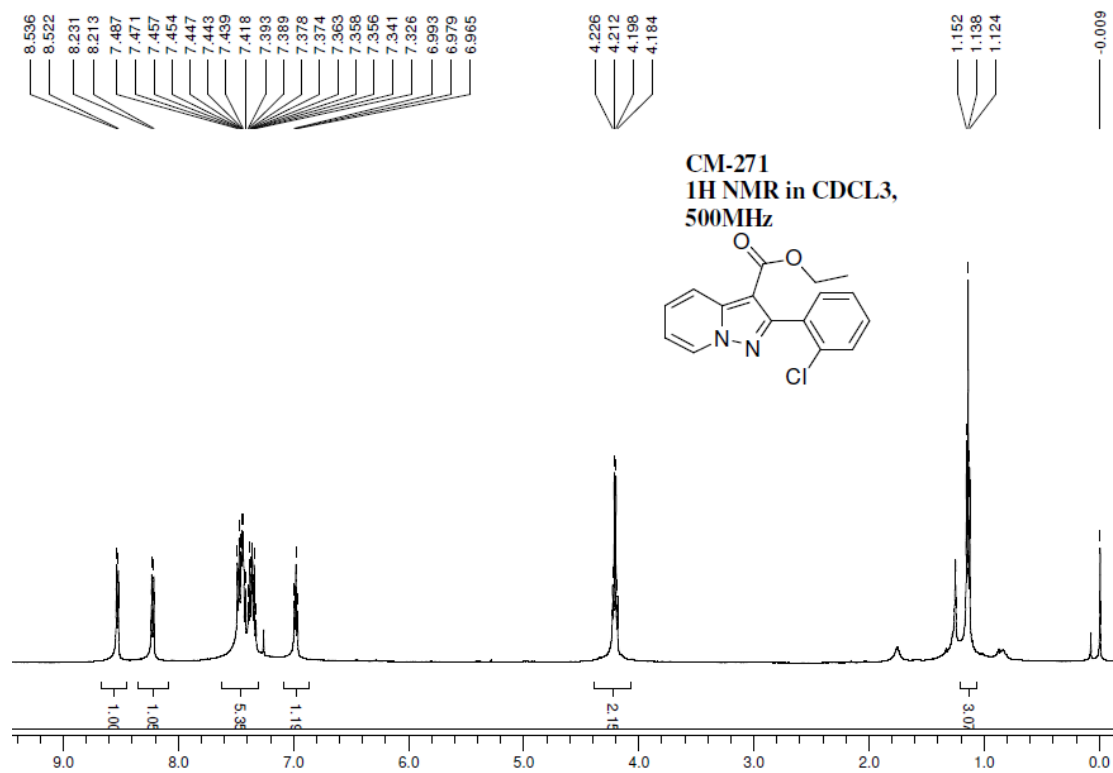
¹³C NMR of **4f**



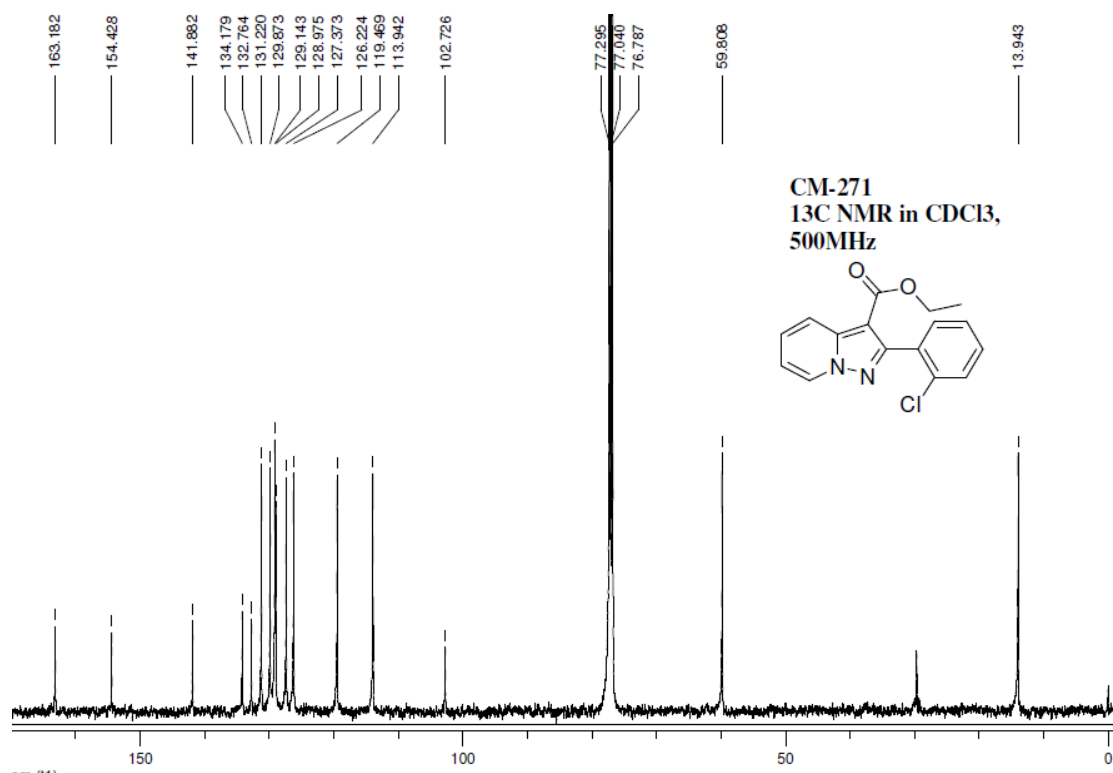
¹H NMR of 4g



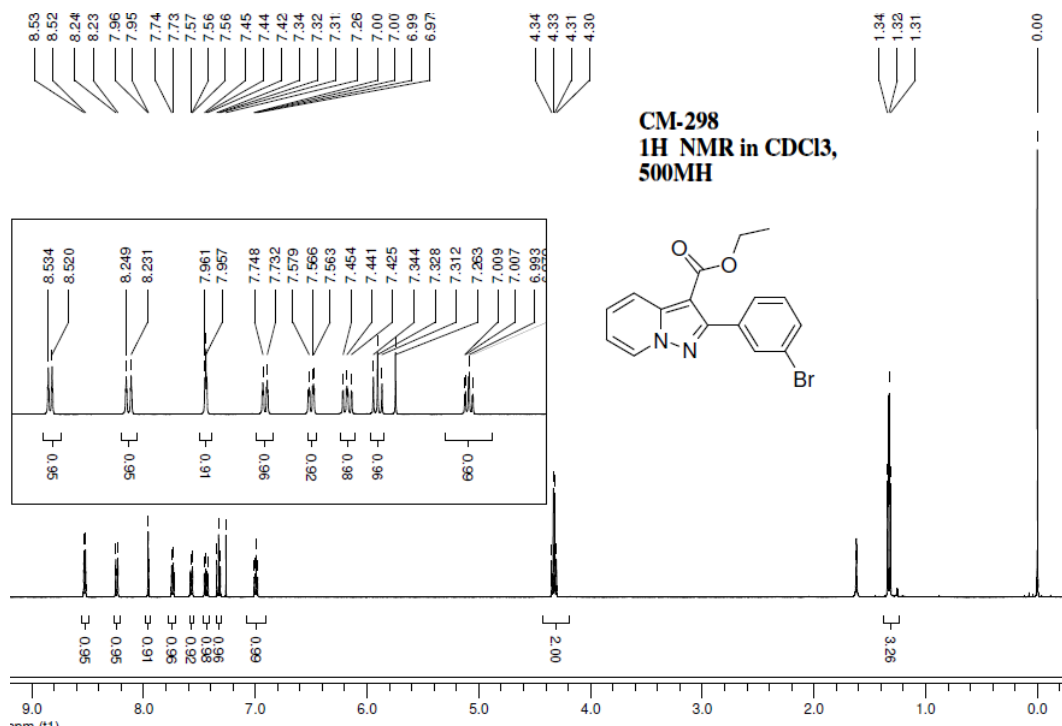
¹³C NMR of 4g



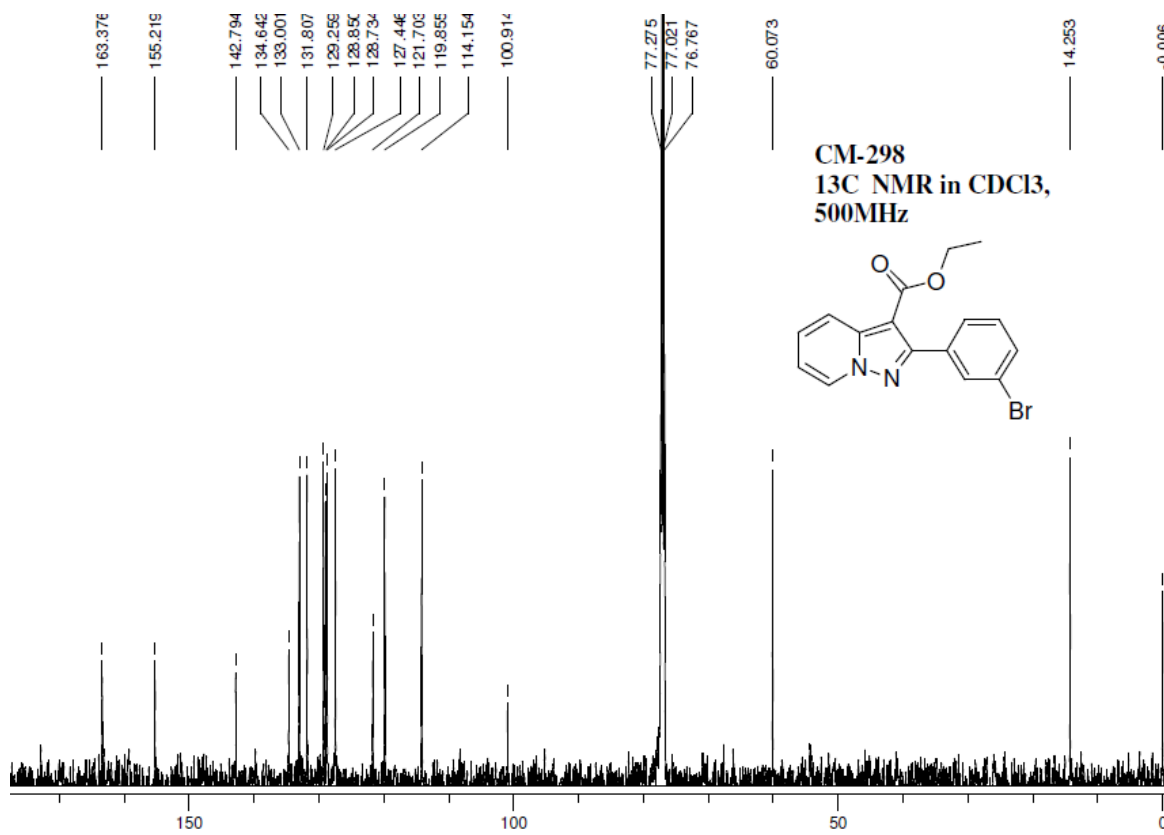
¹H NMR of **4j**



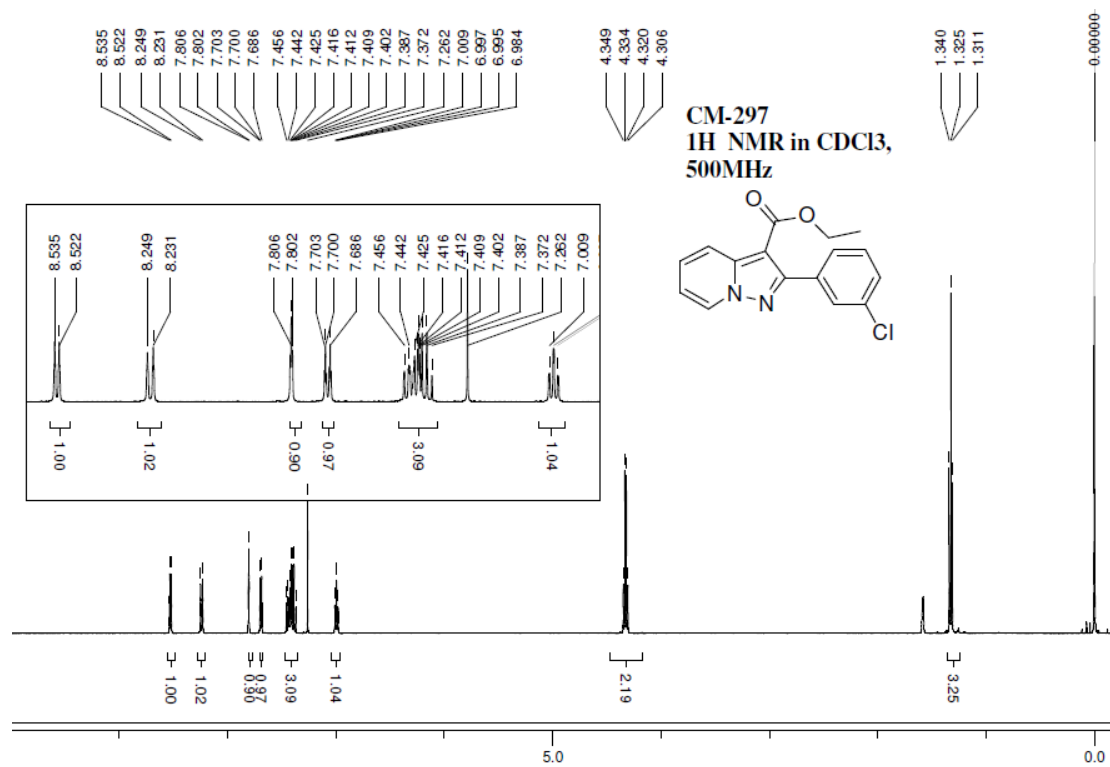
¹³C NMR of **4j**



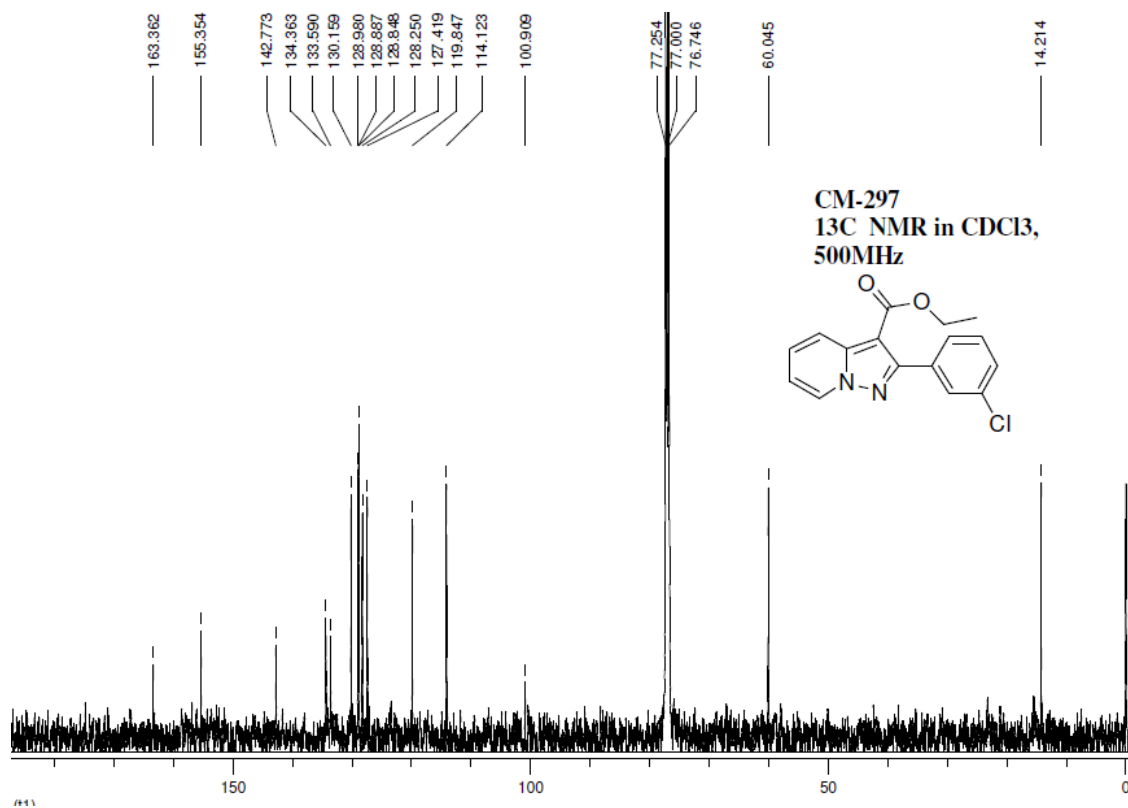
¹H NMR of **4k**



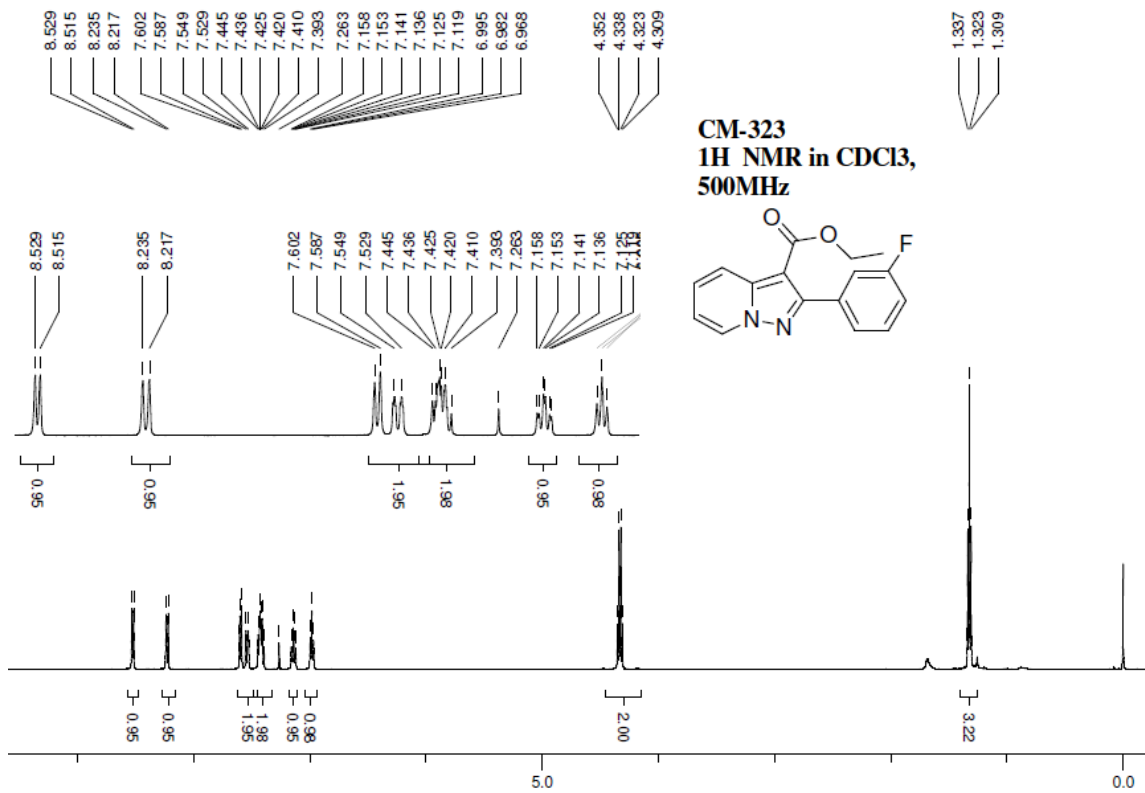
¹³C NMR of **4k**



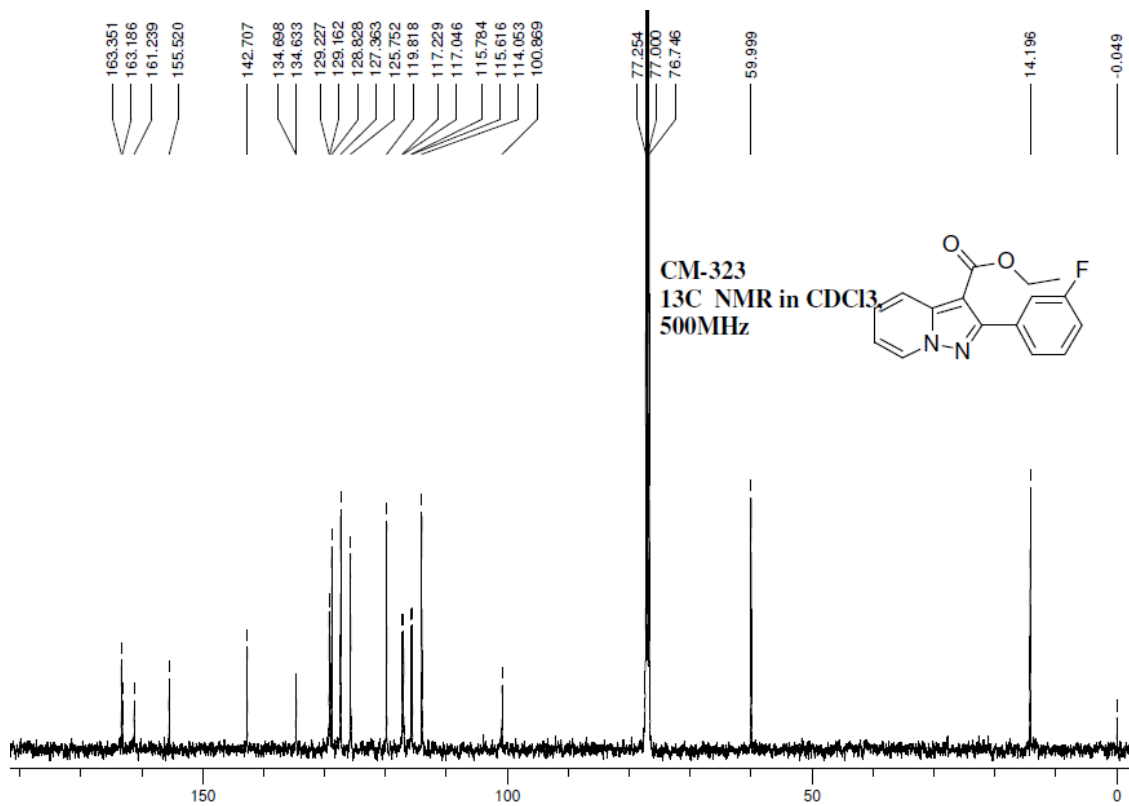
¹H NMR of 41



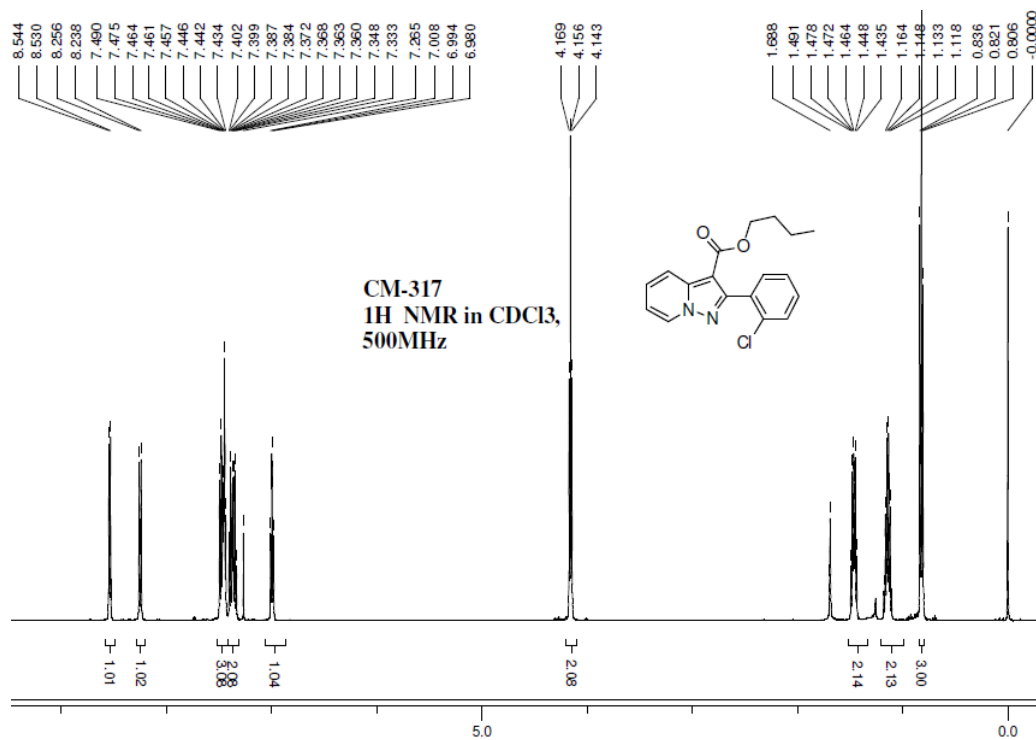
¹³C NMR of 41



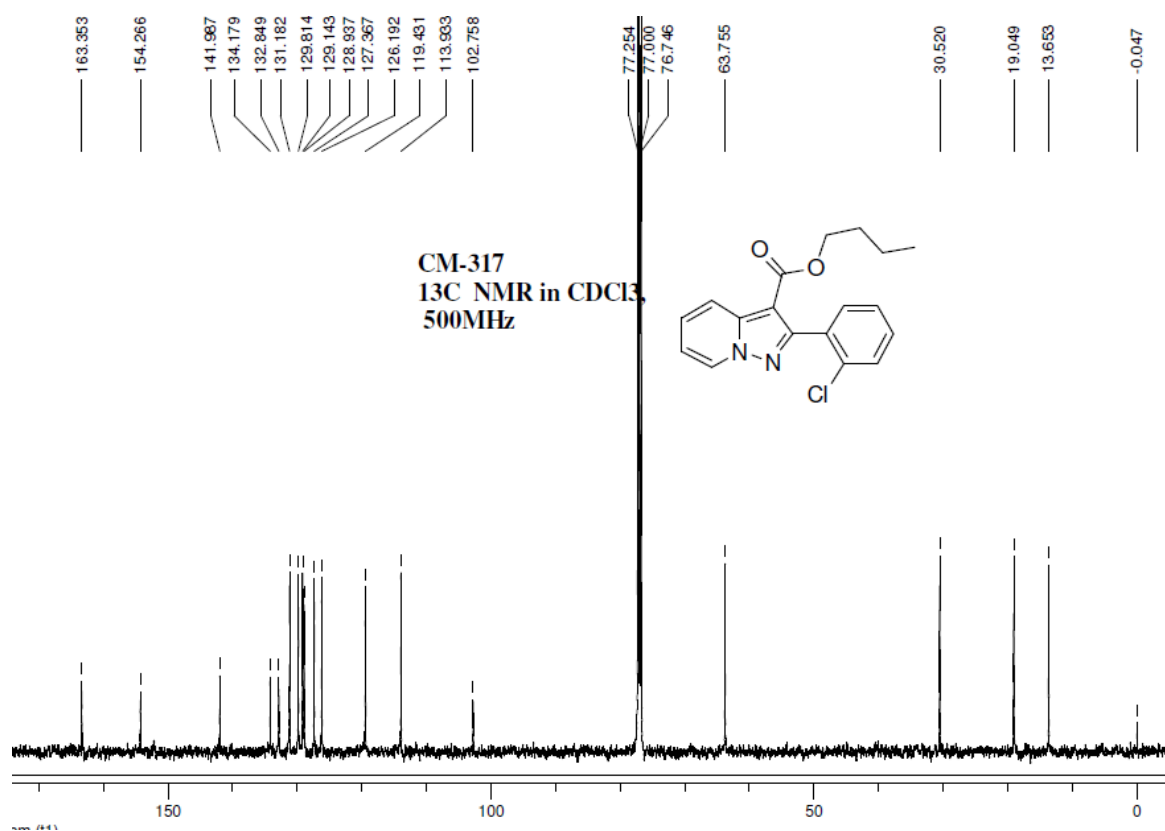
¹H NMR of **4m**



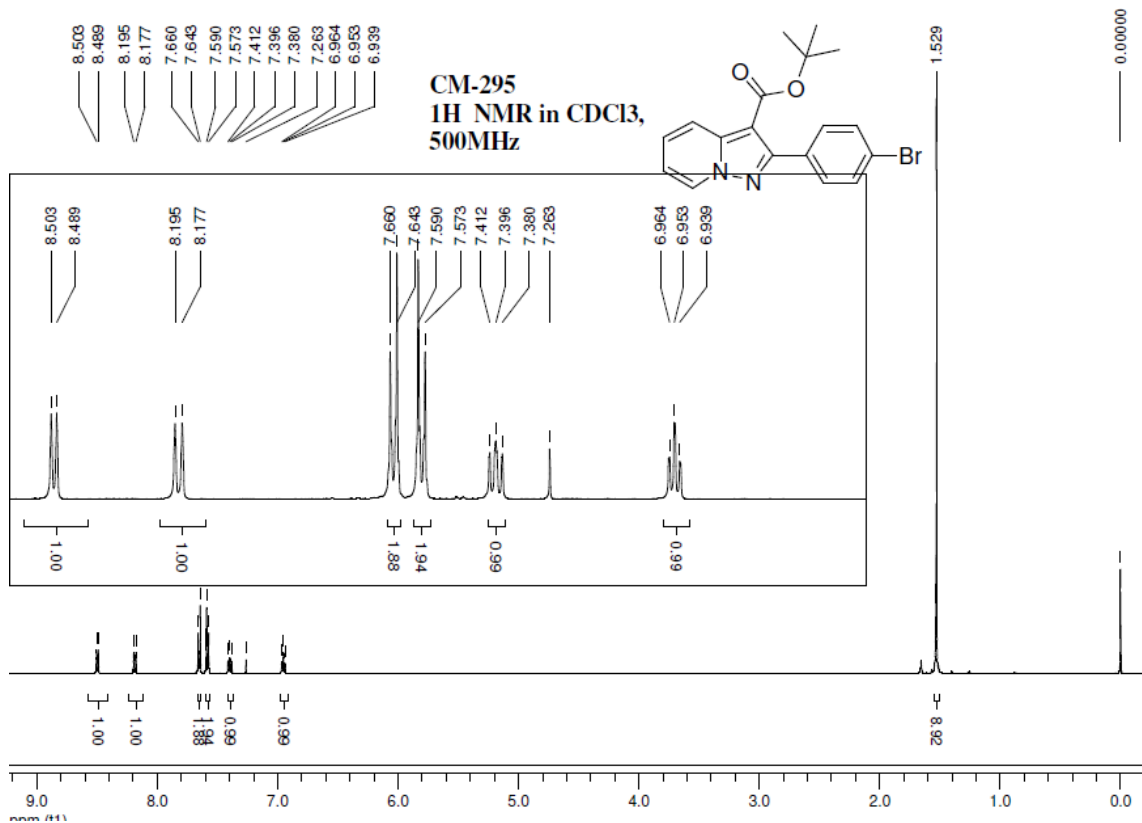
¹³C NMR of **4m**



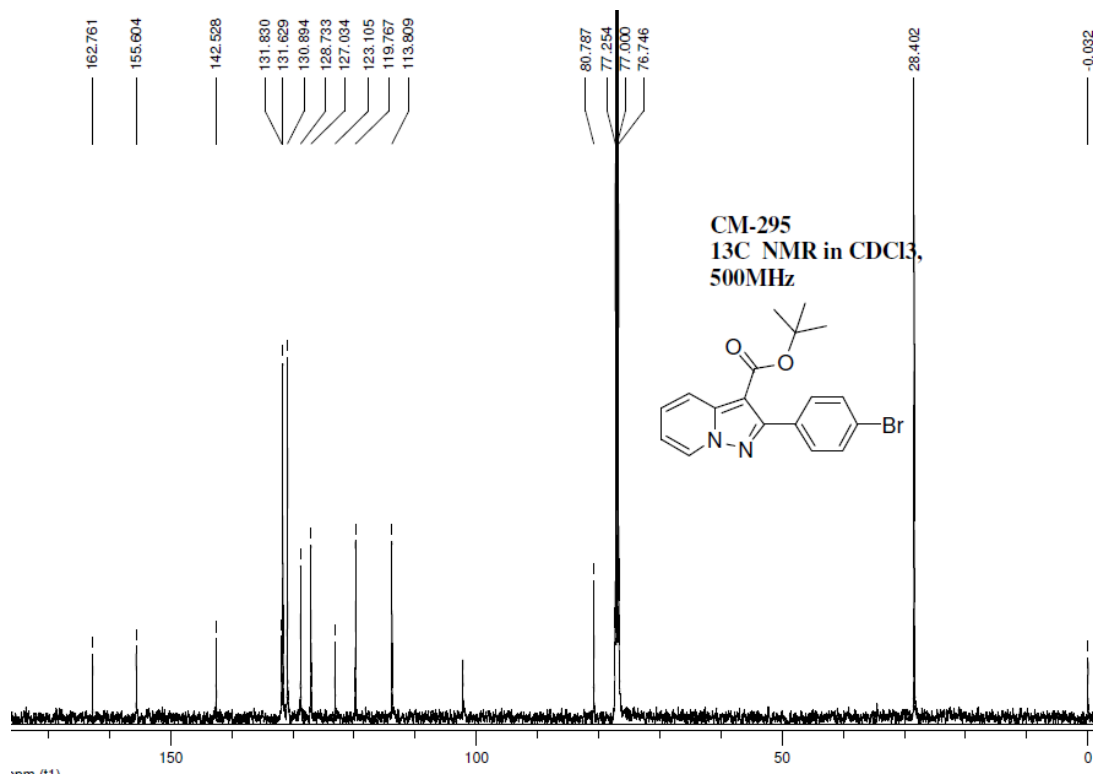
¹H NMR of 4n



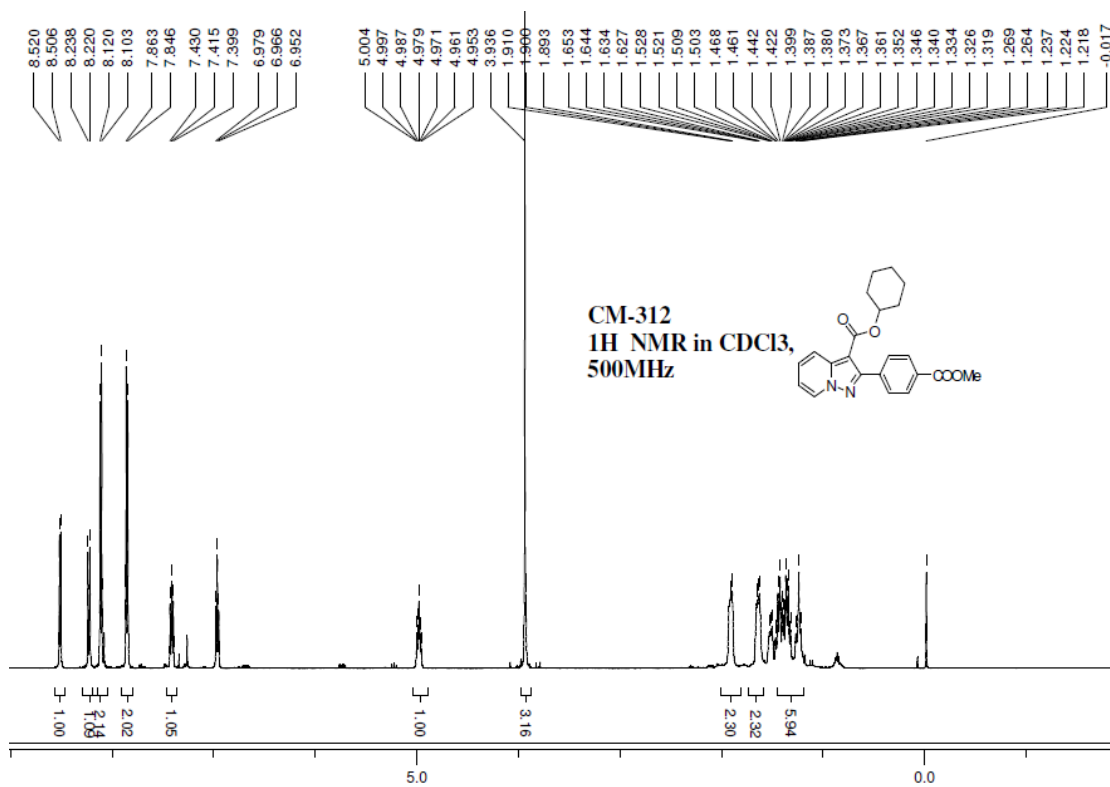
¹³C NMR of 4n



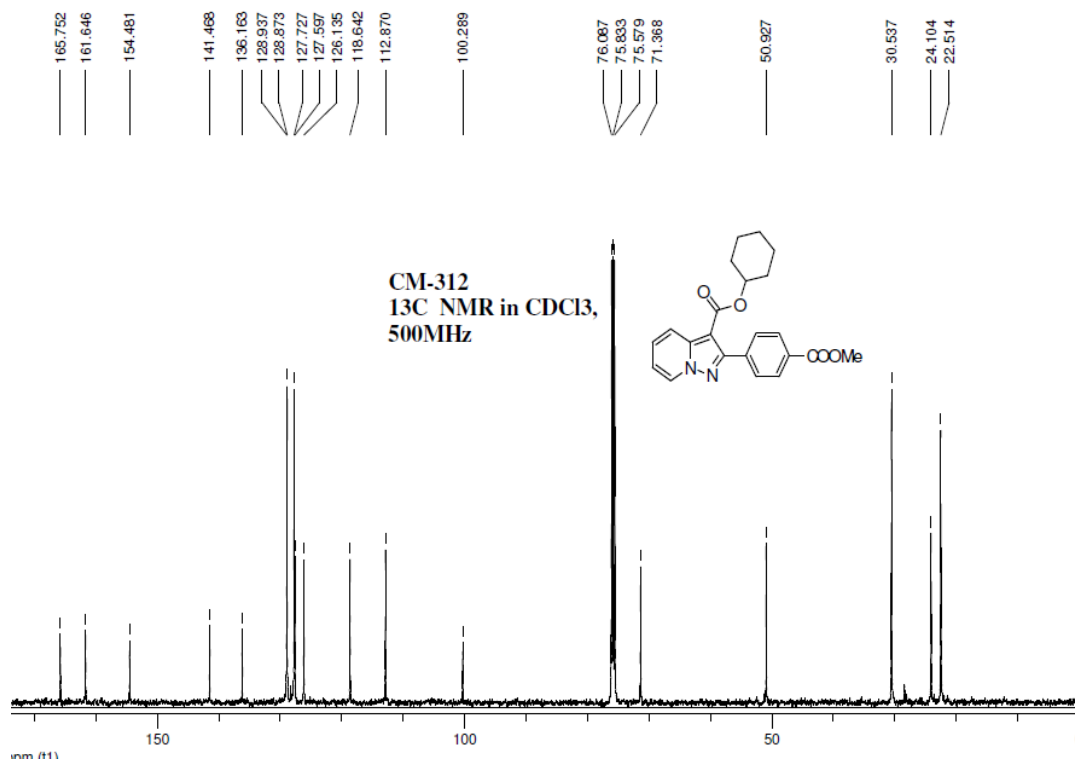
¹H NMR of **4o**



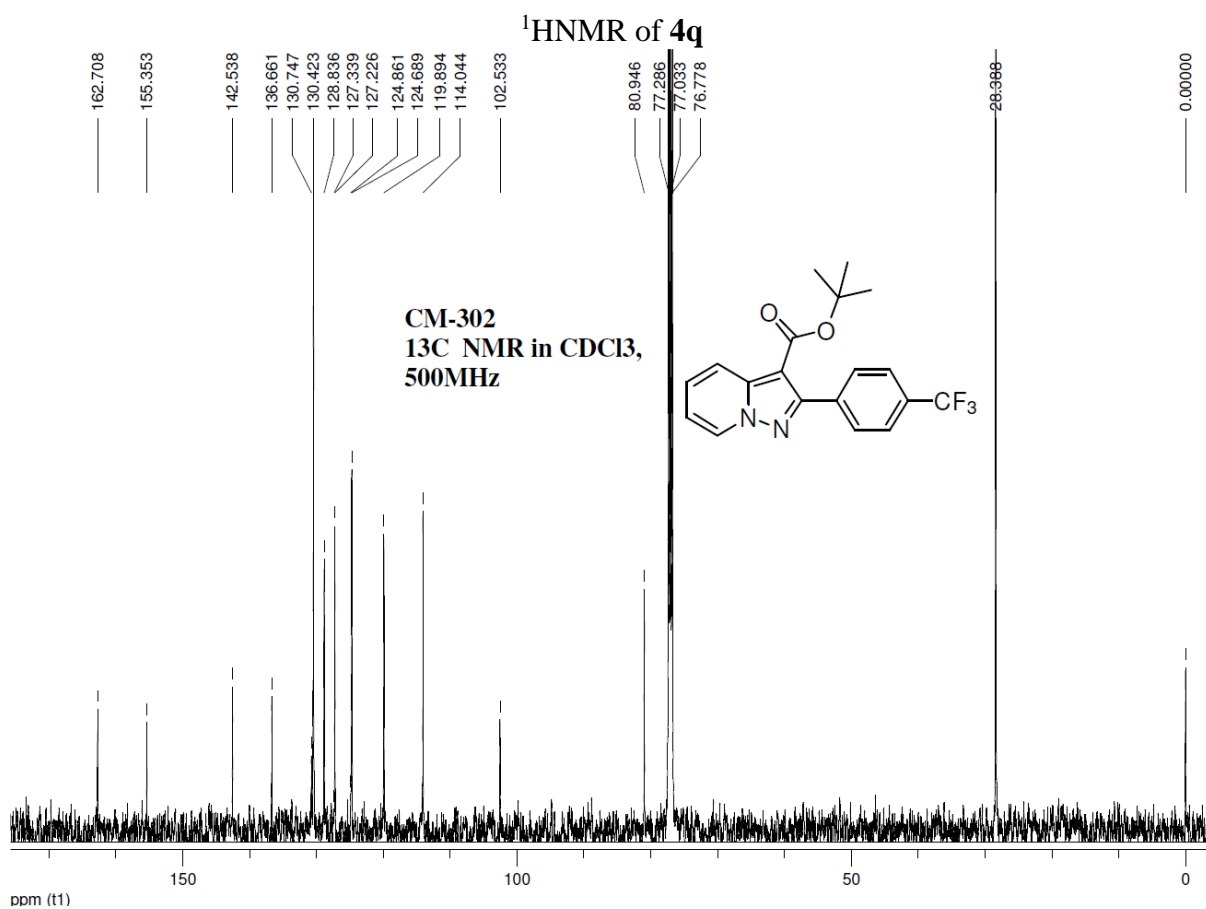
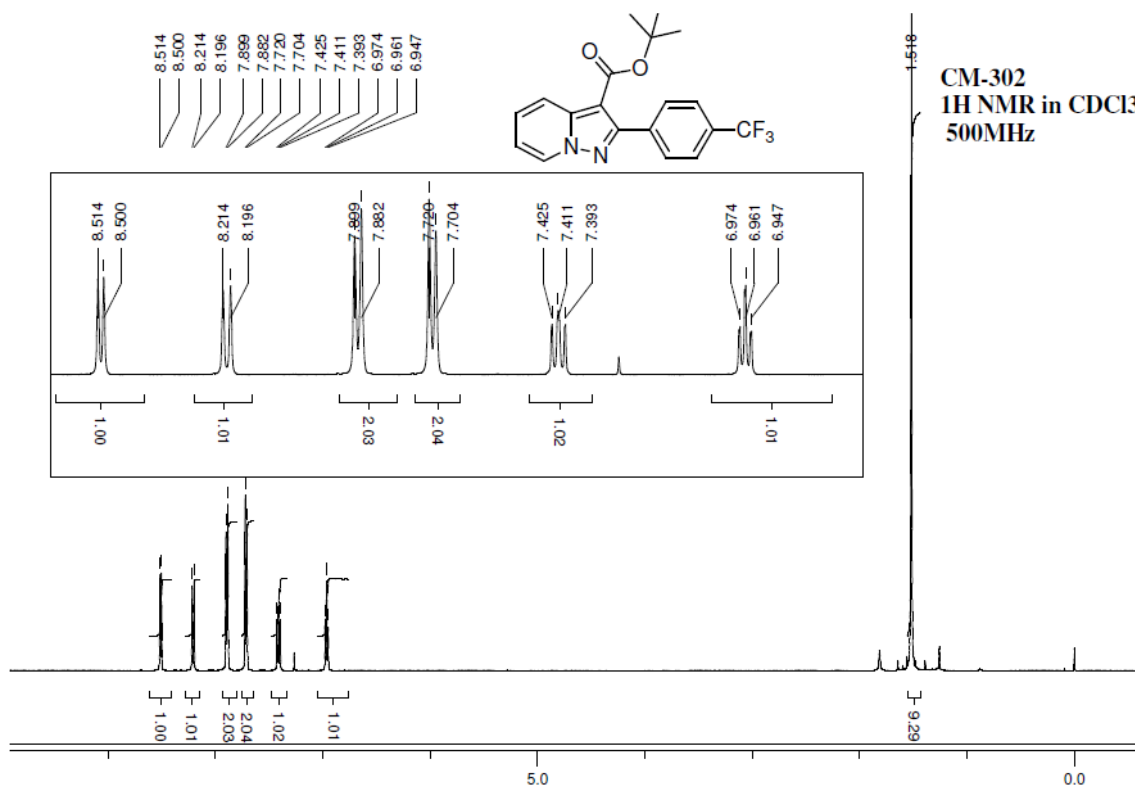
¹³C NMR of **4o**



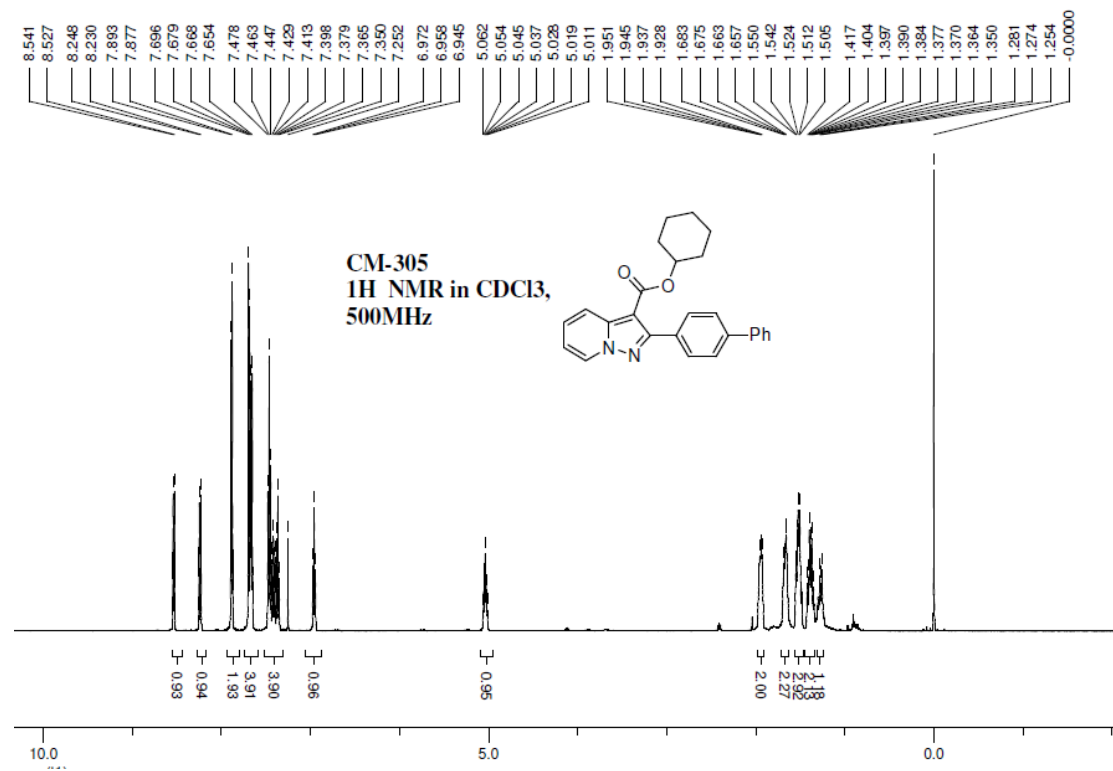
¹H NMR of **4p**



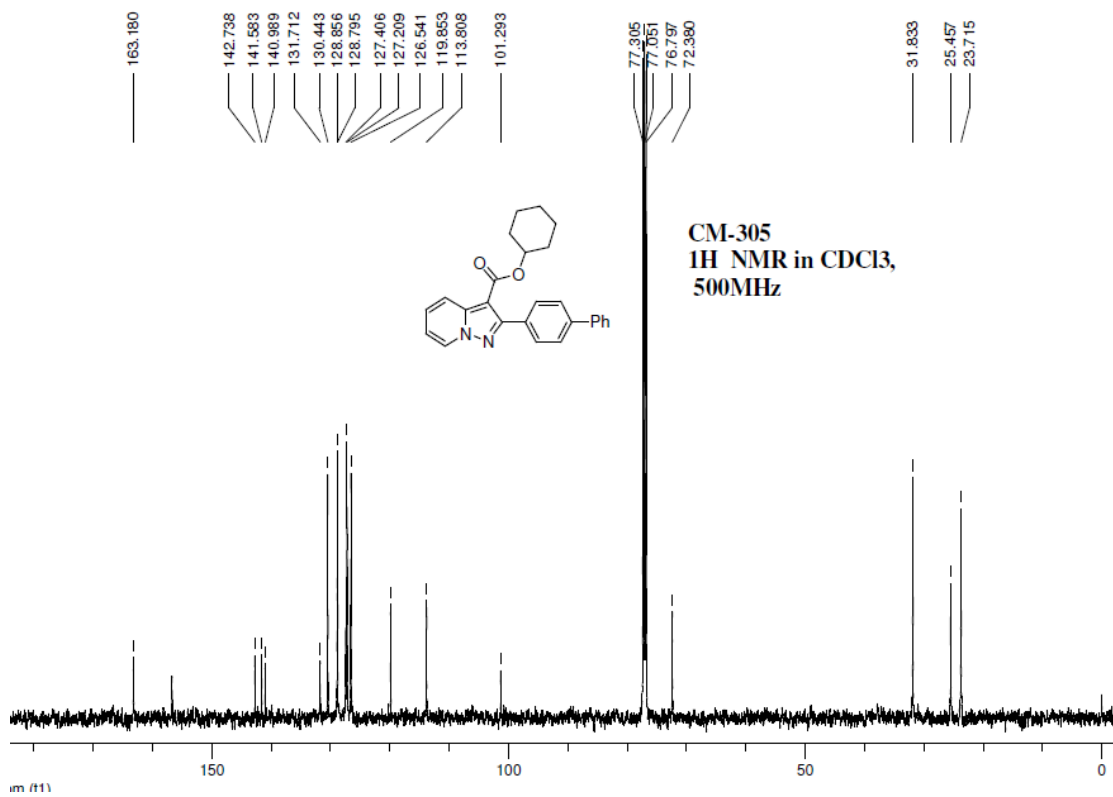
¹³C NMR of **4p**



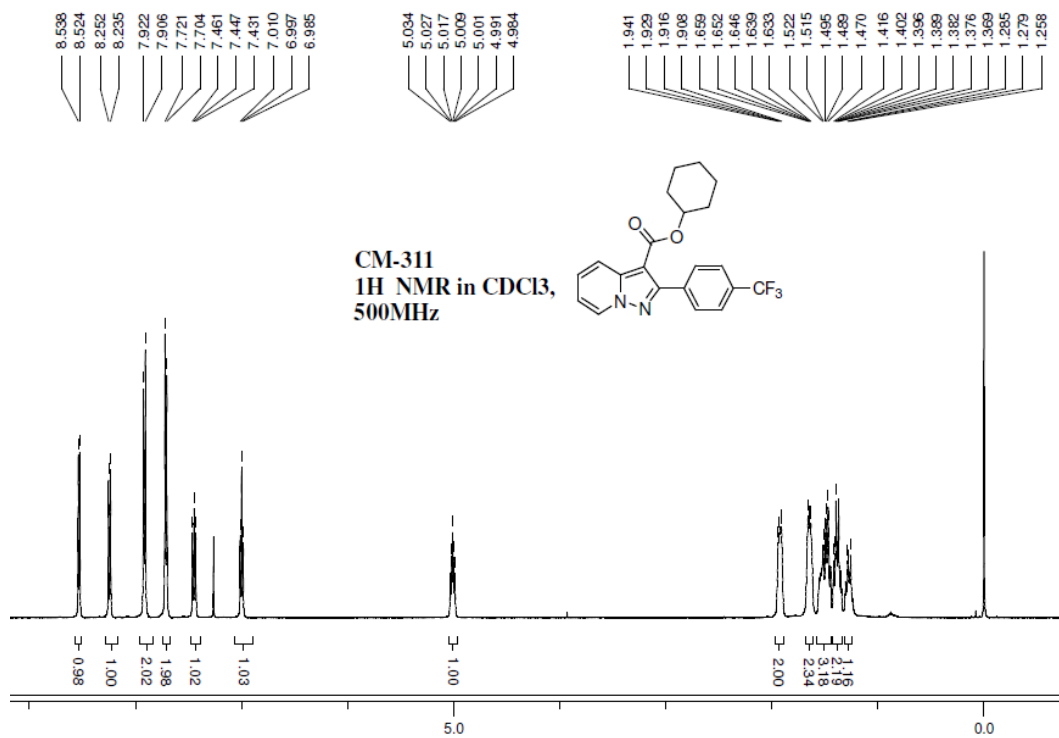
¹³C NMR of **4q**



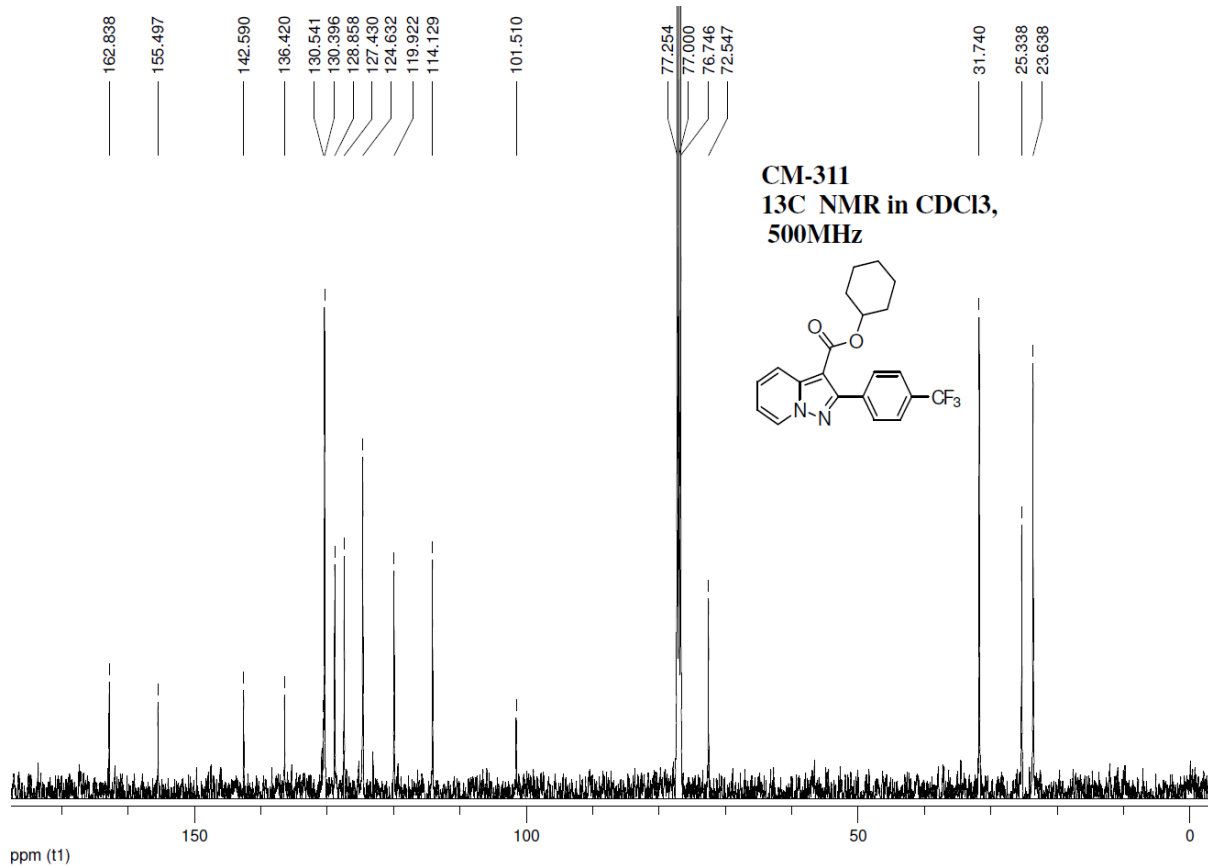
¹H NMR of **4r**



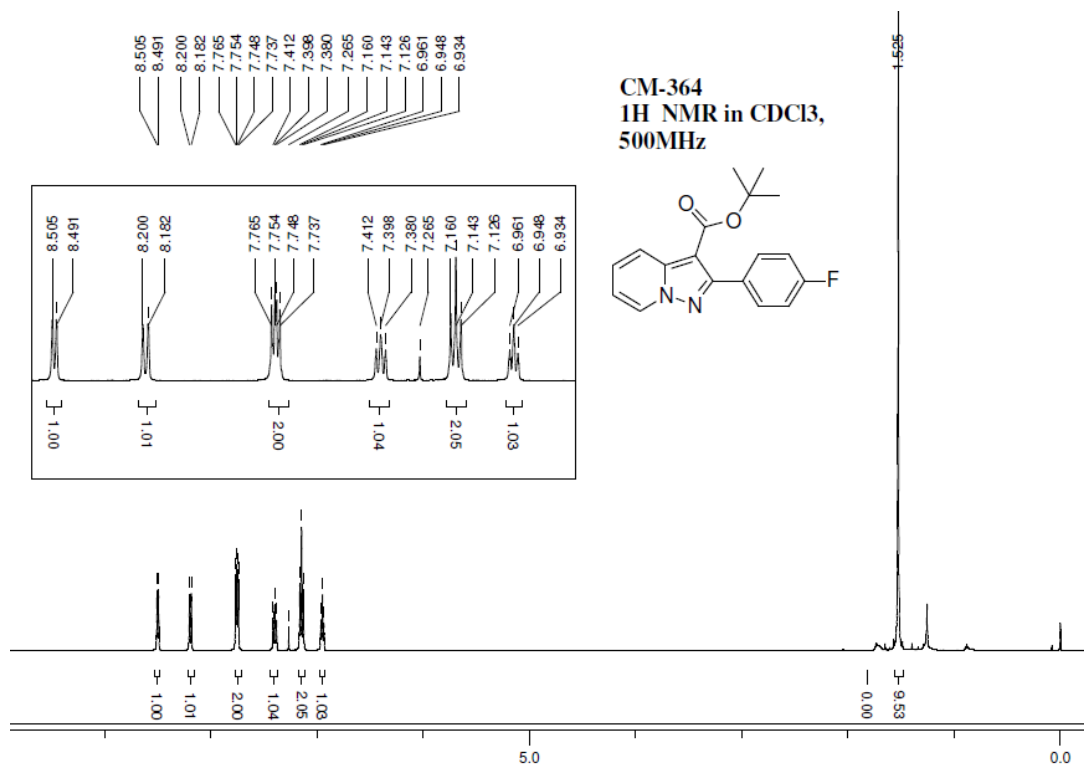
¹³C NMR of **4r**



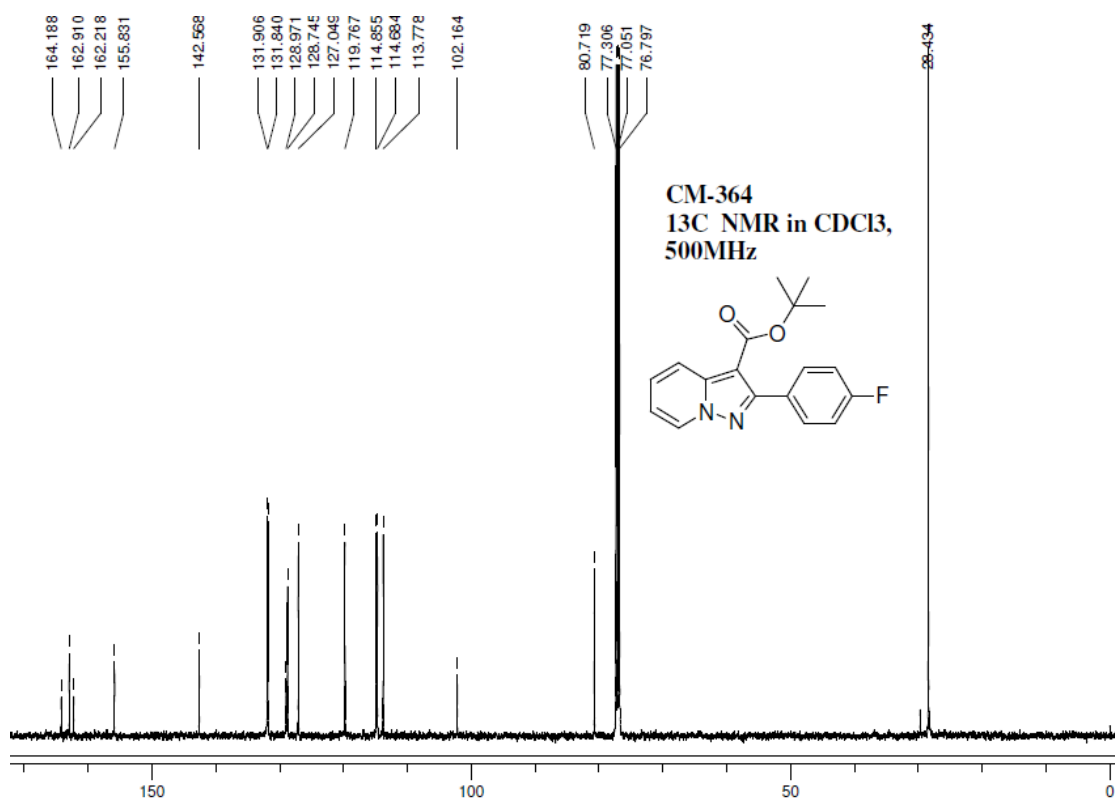
¹H NMR of **4s**



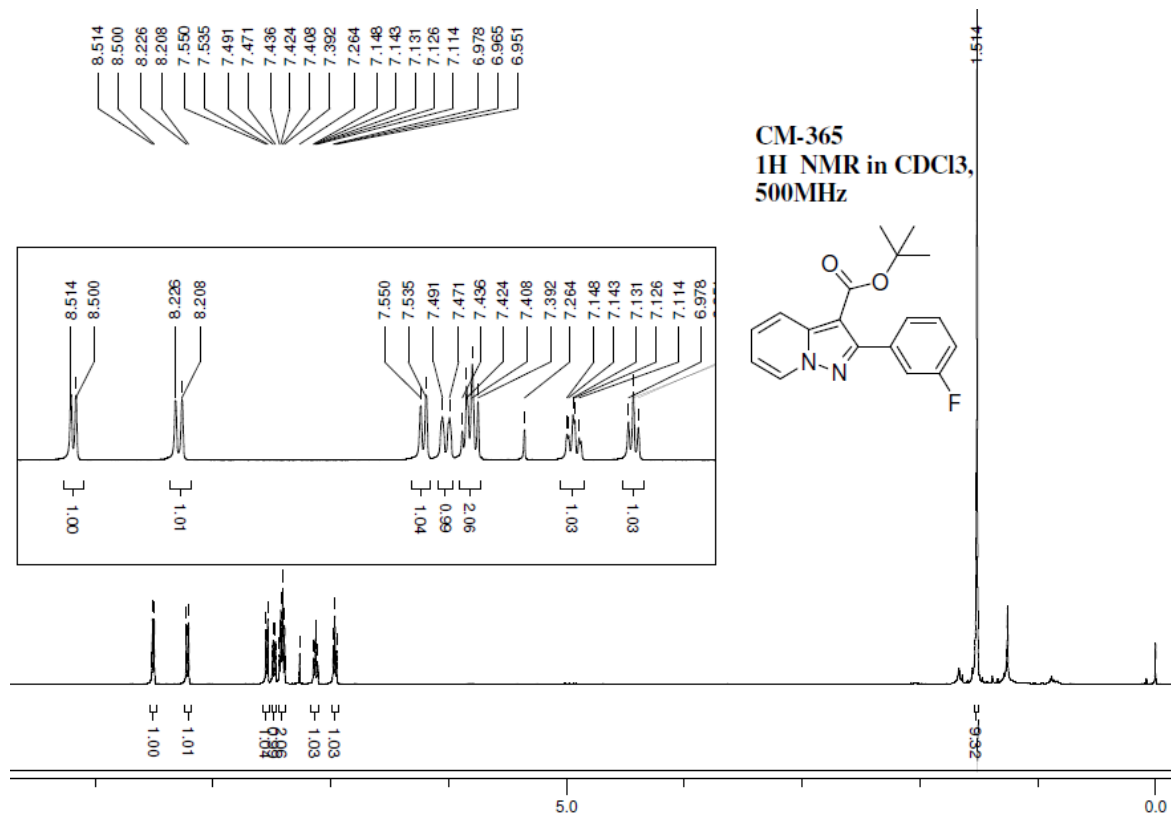
¹³C NMR of **4s**



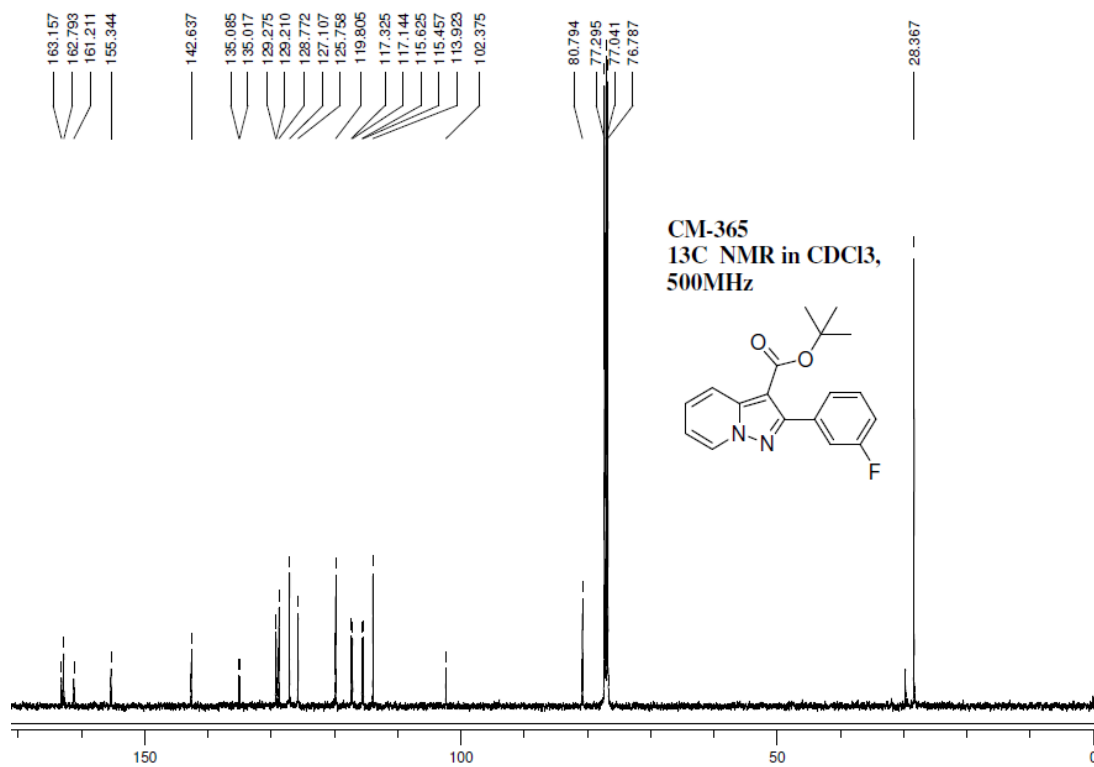
¹H NMR of 4t



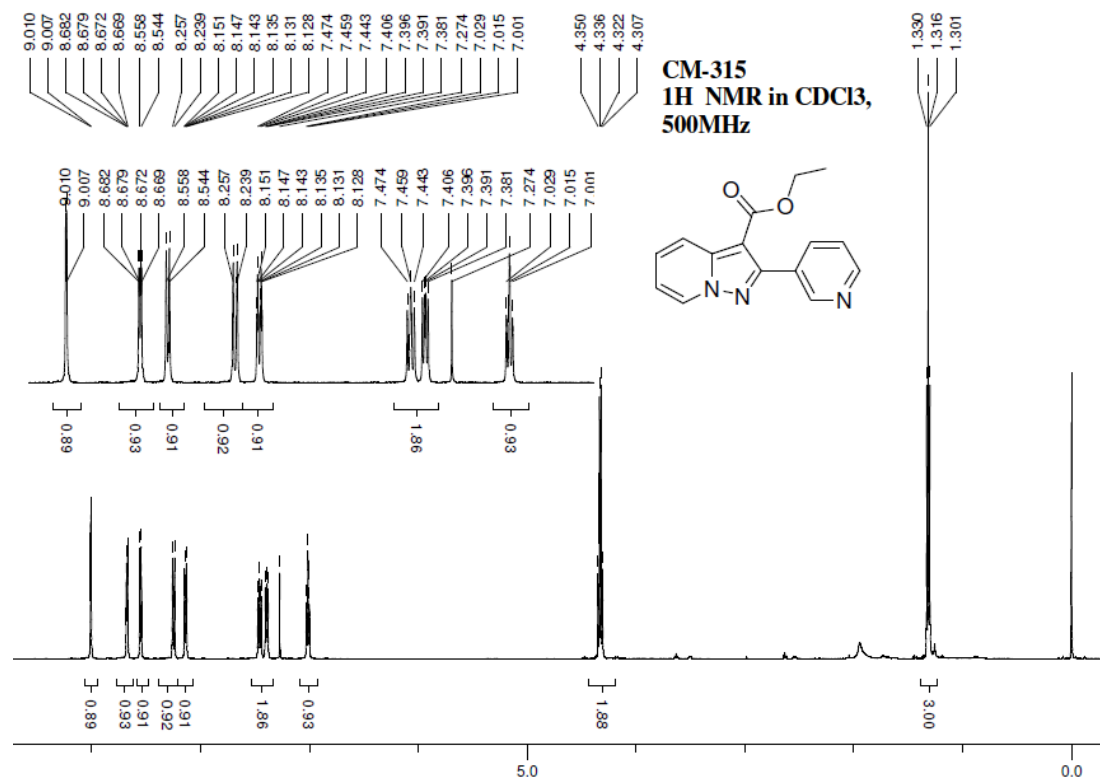
¹³C NMR of 4t



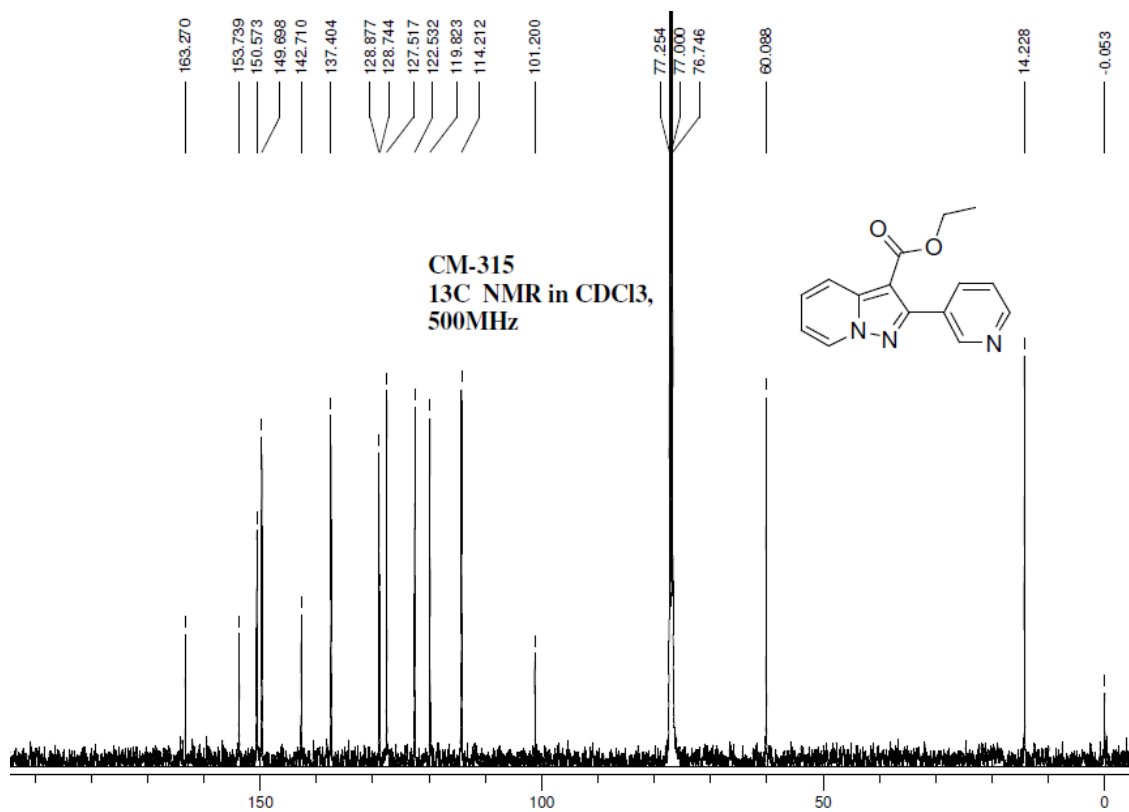
¹H NMR of **4u**



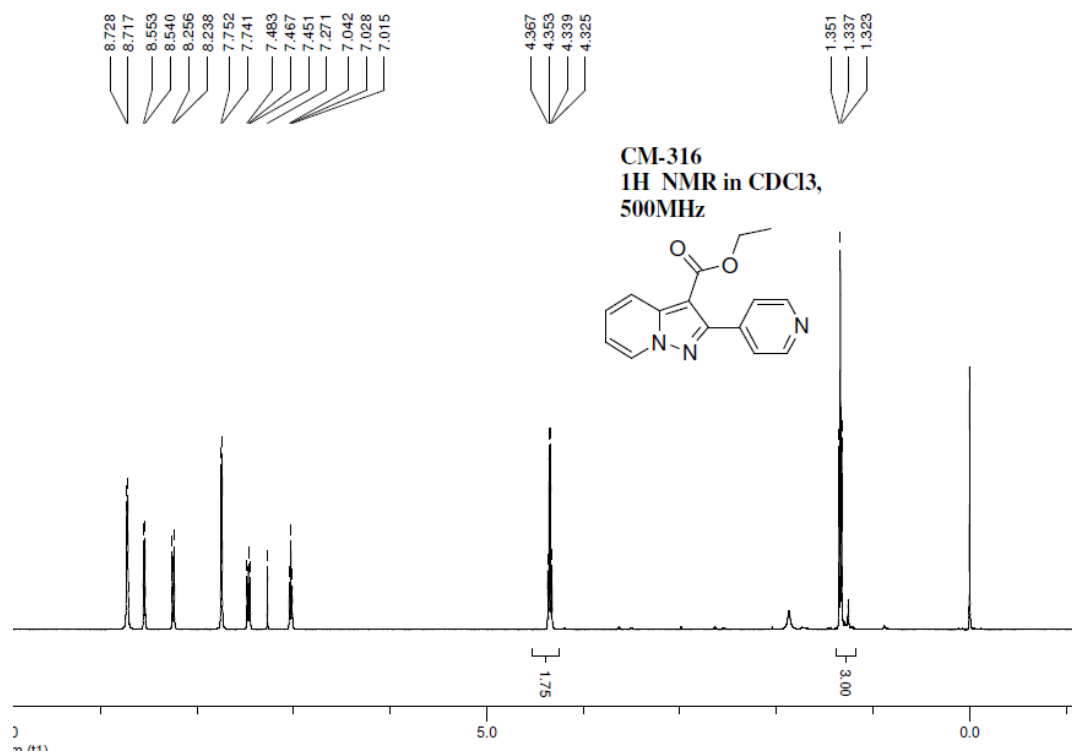
¹³C NMR of **4u**



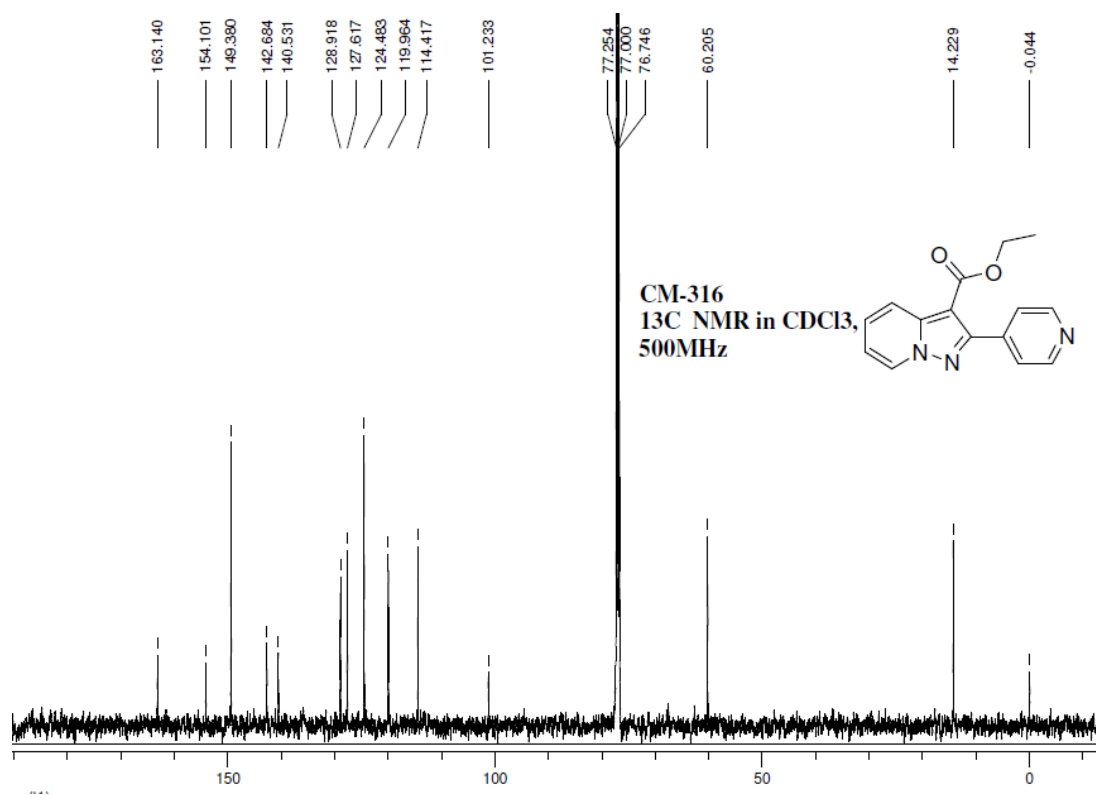
¹H NMR of **4v**



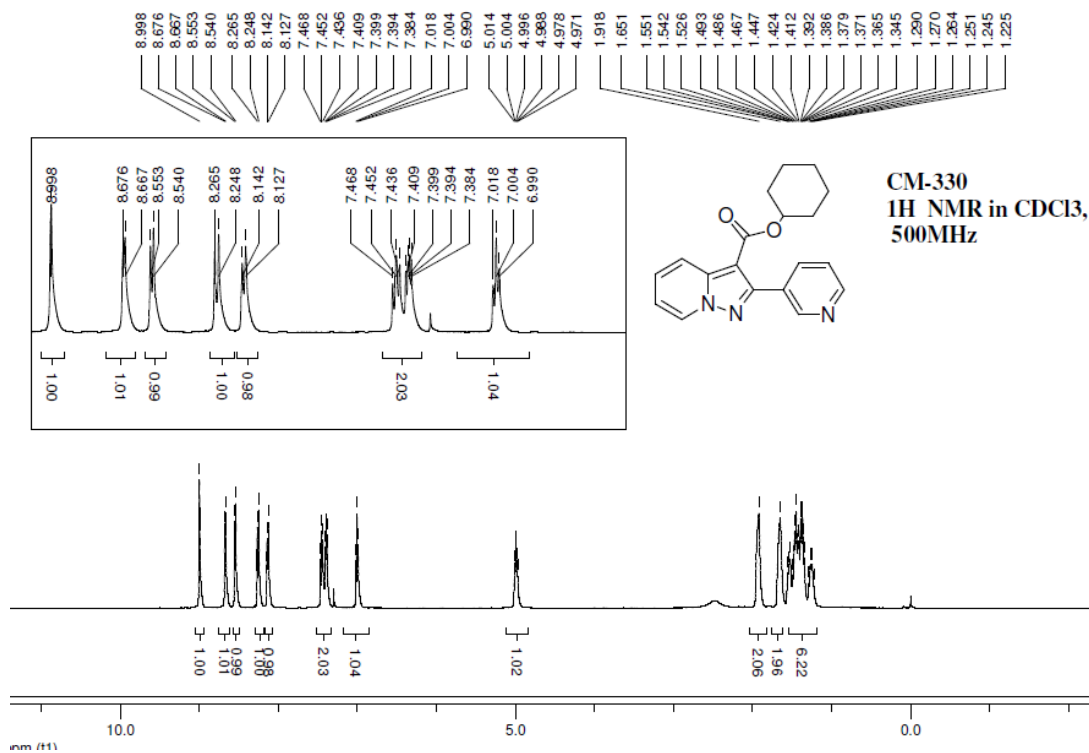
¹³C NMR of **4v**



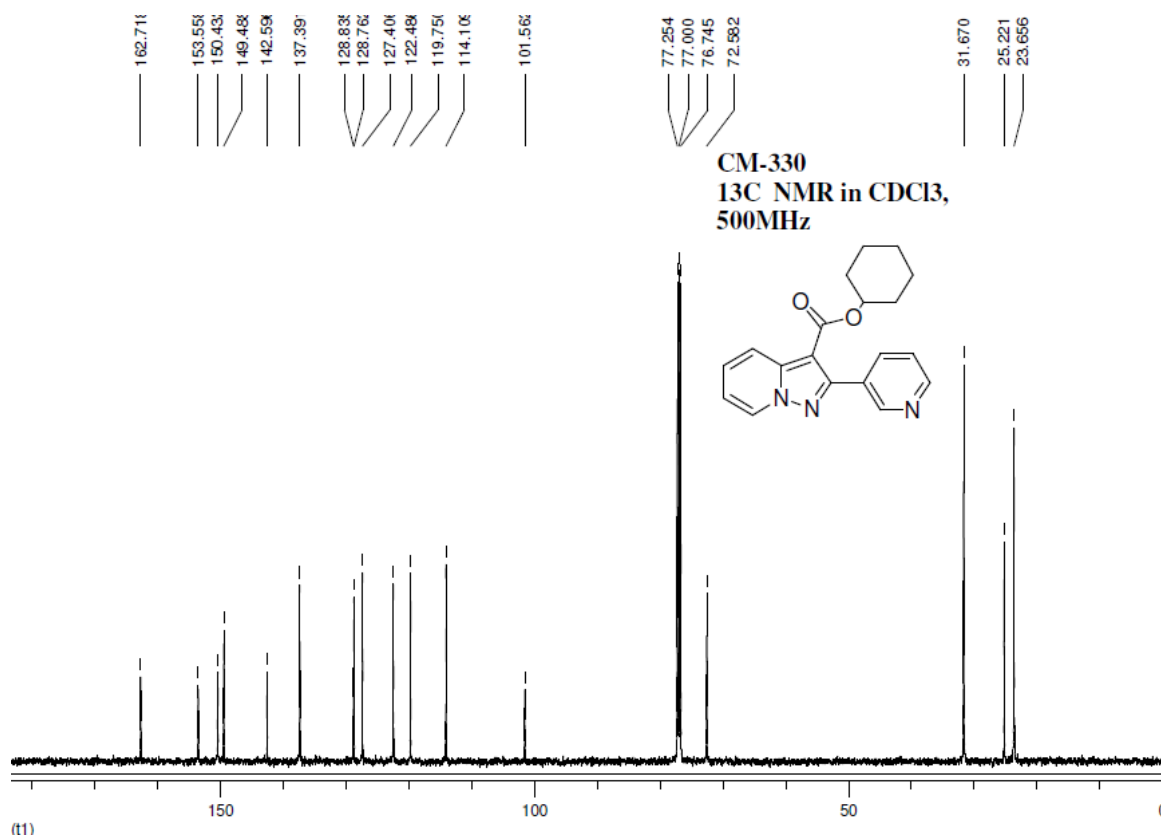
¹H NMR of **4w**



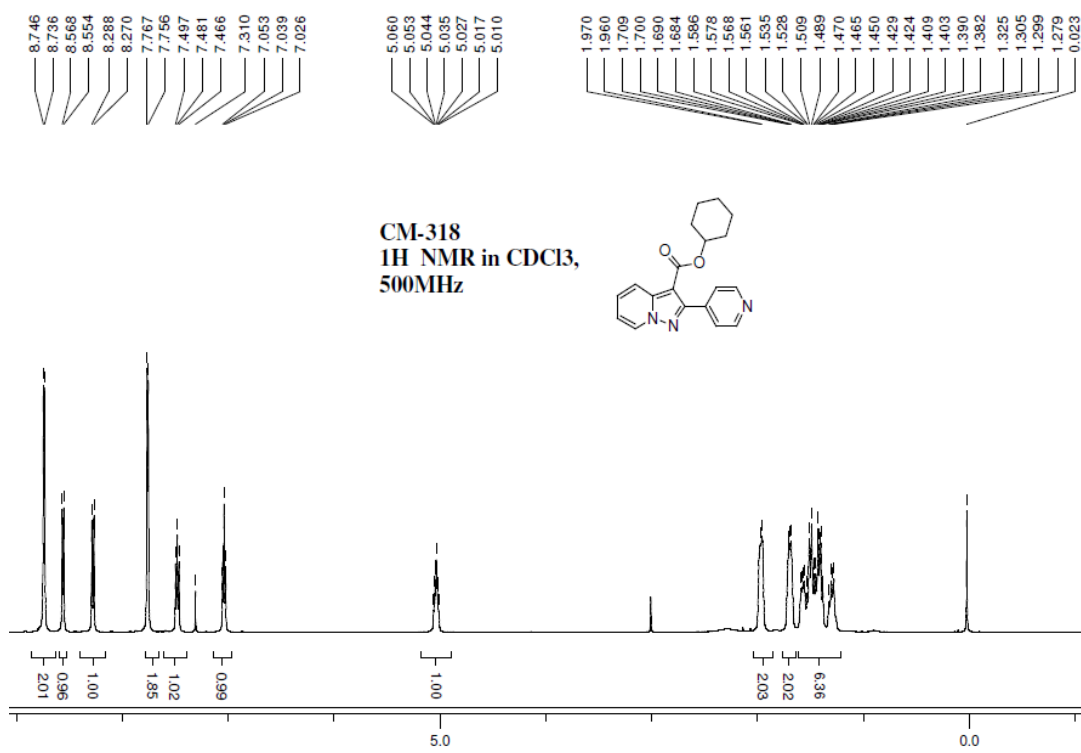
¹³C NMR of **4w**



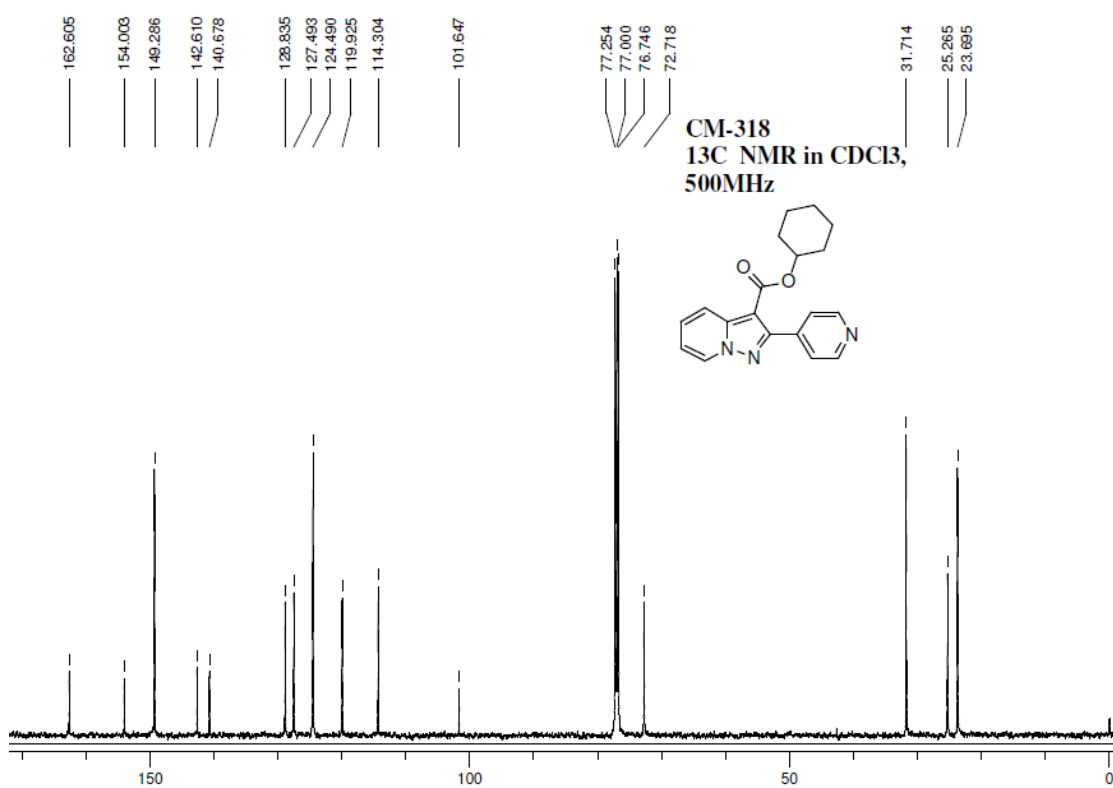
¹H NMR of **4x**



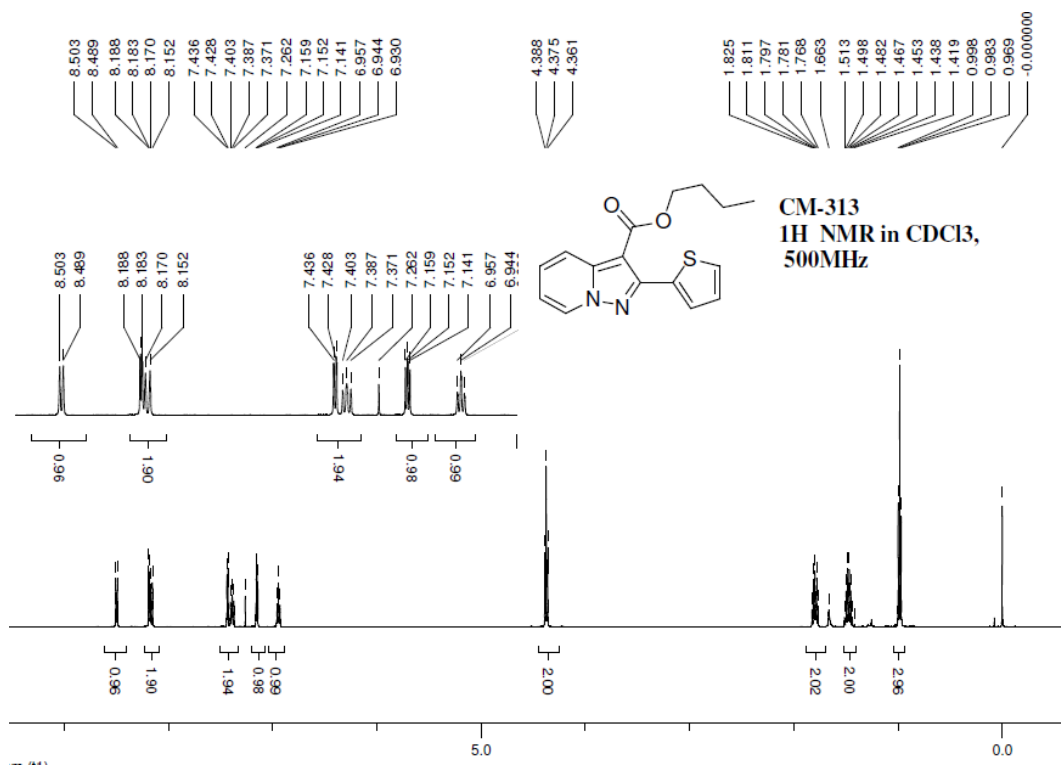
¹³C NMR of **4x**



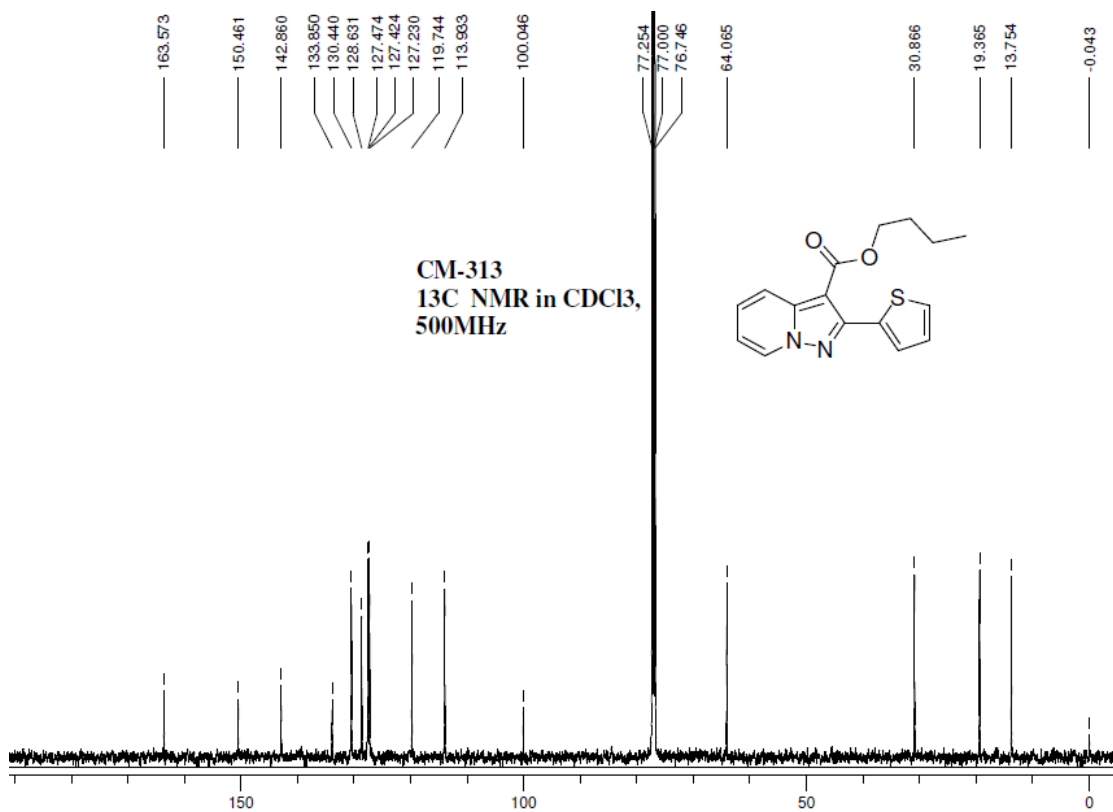
¹H NMR of **4y**



¹³C NMR of **4y**



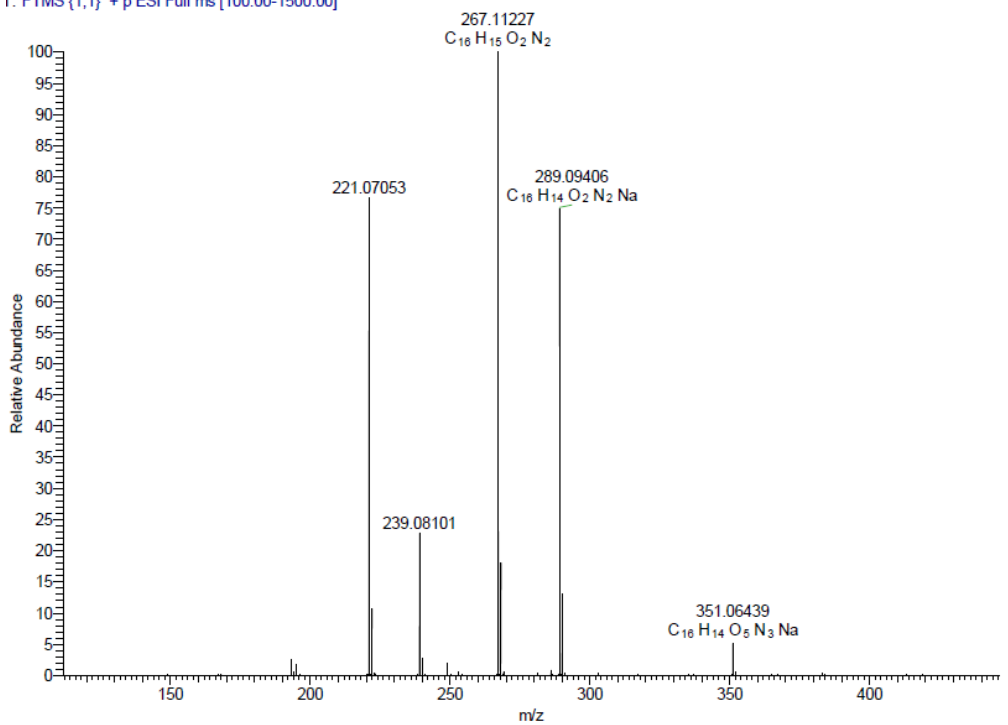
¹H NMR of **4z**



¹³C NMR of **4z**

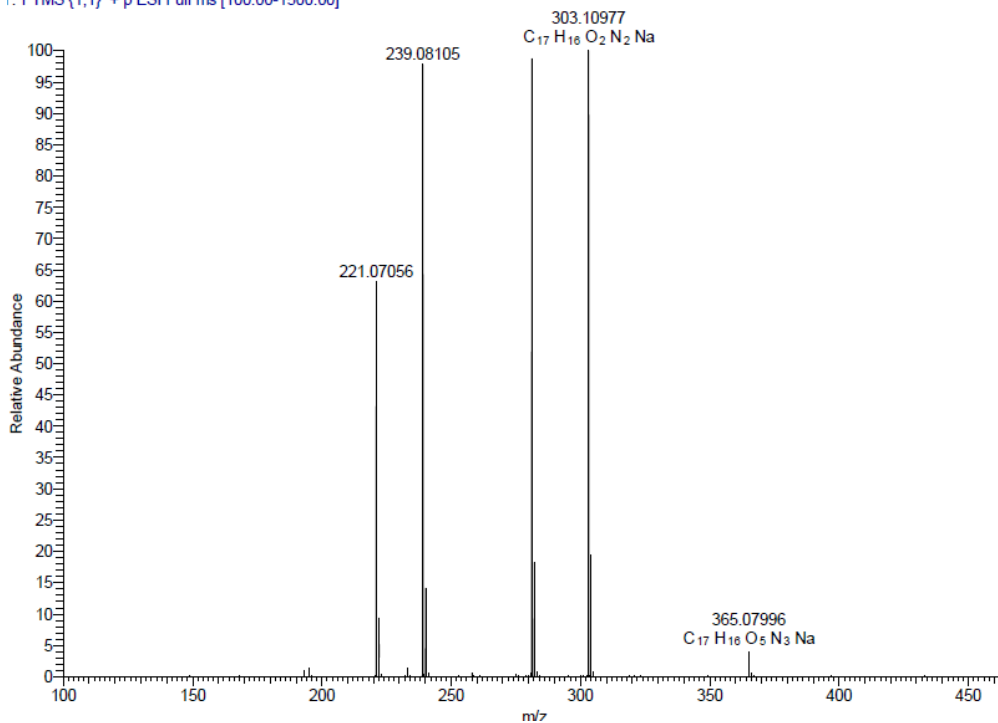
HRMS SPECTRA

2C-51-A #77 RT: 1.14 AV: 1 NL: 9.79E7
F: FTMS (1,1) + p ESI Full ms [100.00-1500.00]



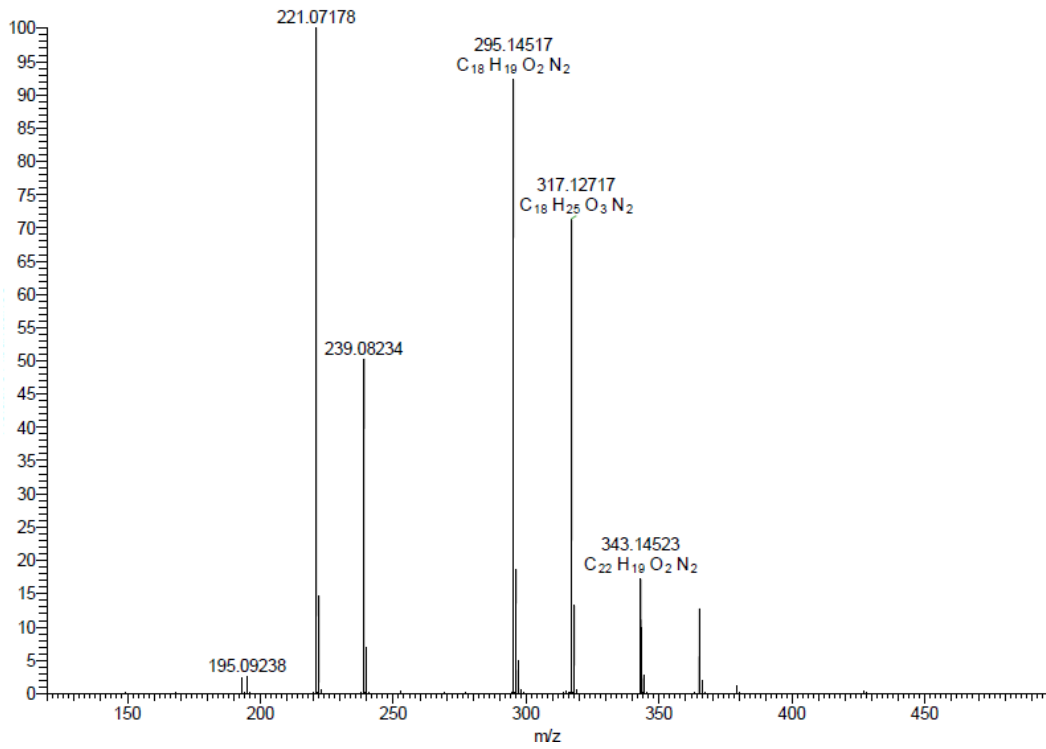
HRMS of 3a

2C-246 #77 RT: 1.14 AV: 1 NL: 1.60E8
F: FTMS (1,1) + p ESI Full ms [100.00-1500.00]

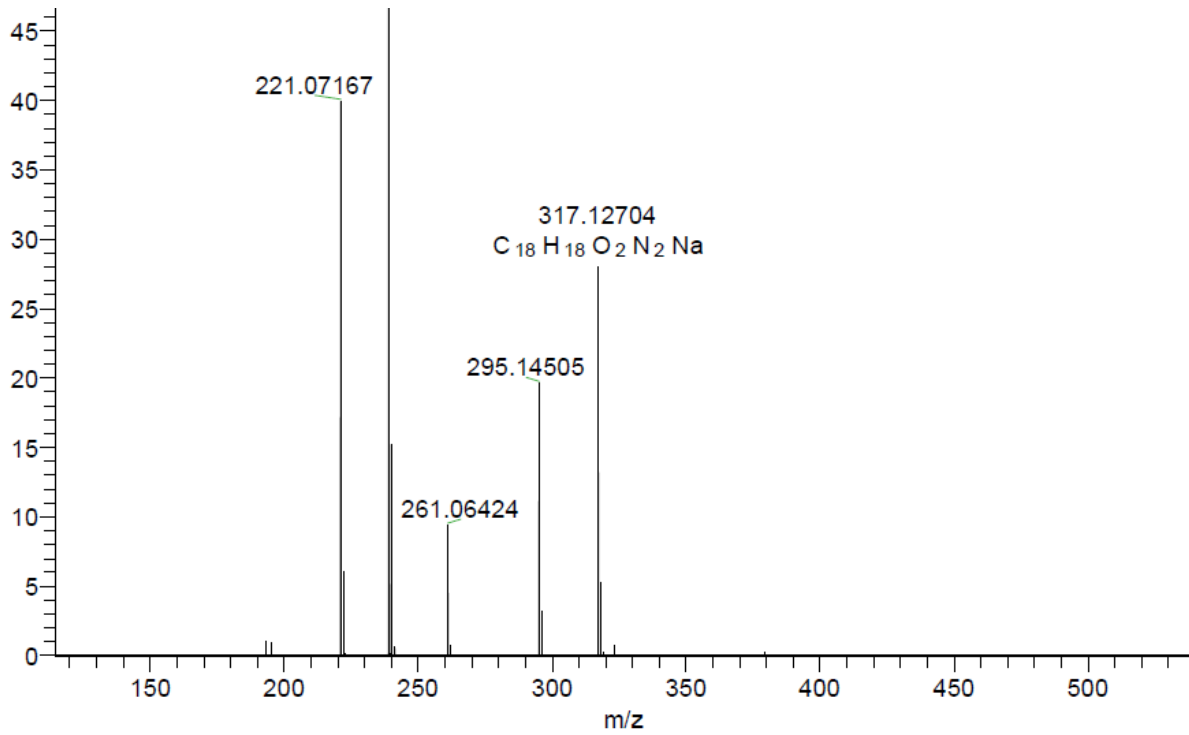


HRMS of 3b

247 #85 RT: 1.20 AV: 1 NL: 9.24E7
FTMS (1,1) + p ESI Full ms [100.00-1500.00]

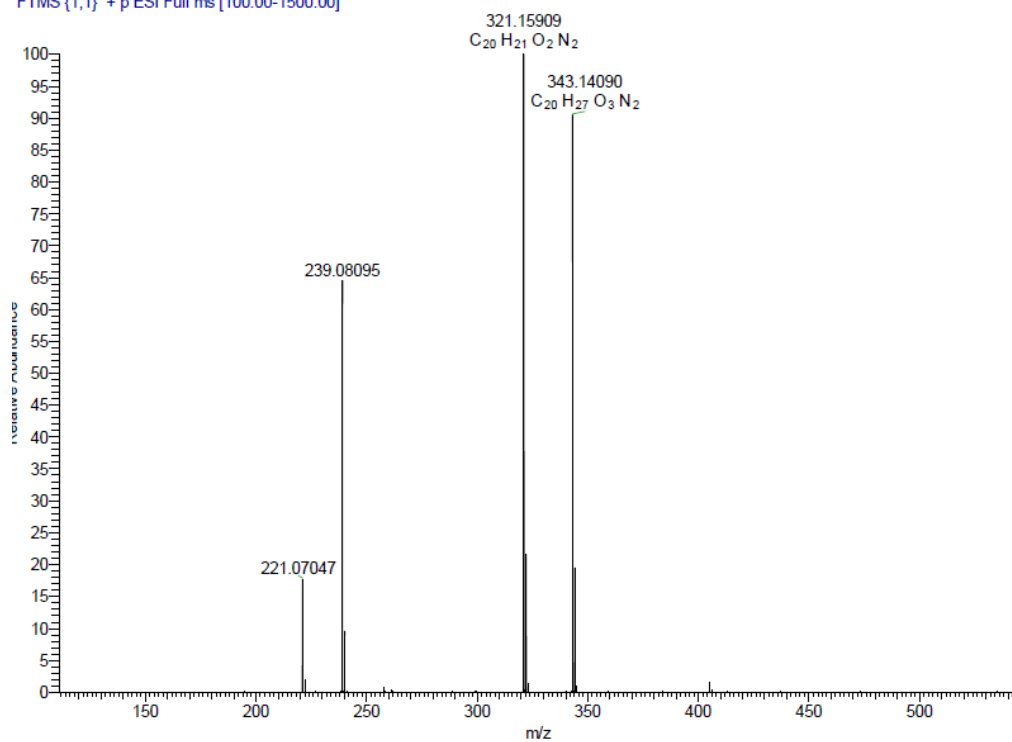


HRMS of 3c



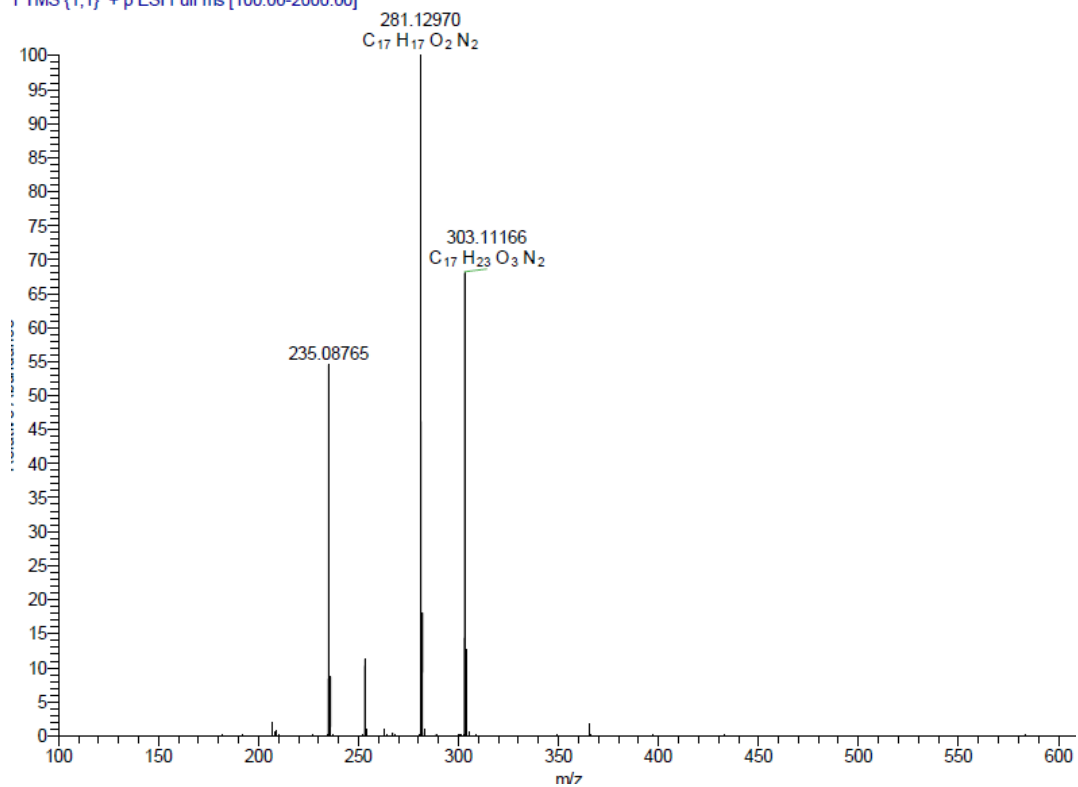
HRMS of 3d

2-245 #87 RT: 1.28 AV: 1 NL: 1.06E8
FTMS (1,1) + p ESI Full ms [100.00-1500.00]



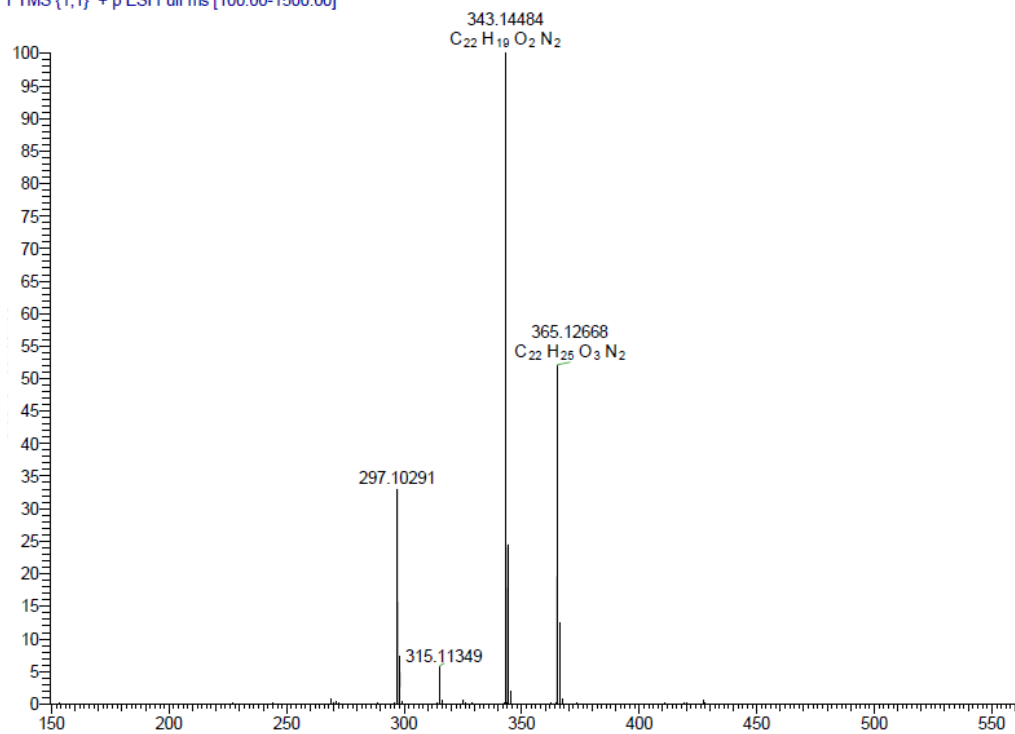
HRMS of 3e

1-1-310 #77 RT: 1.14 AV: 1 NL: 1.21E8
FTMS (1,1) + p ESI Full ms [100.00-2000.00]



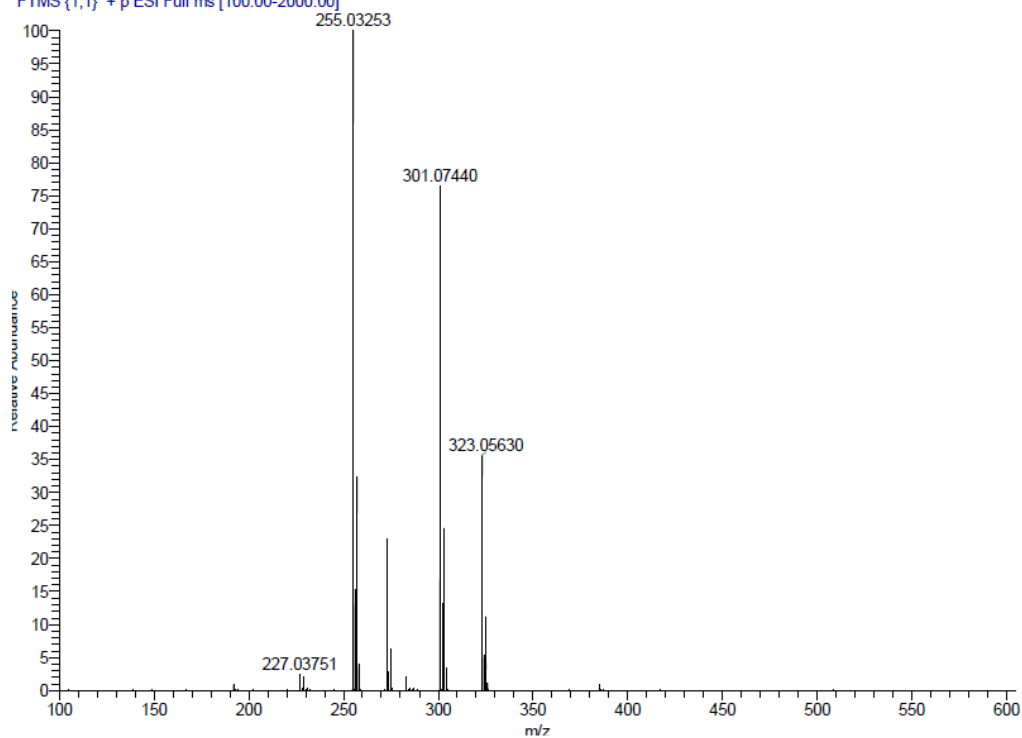
HRMS of 4a

303 #89 RT: 1.25 AV: 1 NL: 9.87E7
FTMS (1,1) + p ESI Full ms [100.00-1500.00]



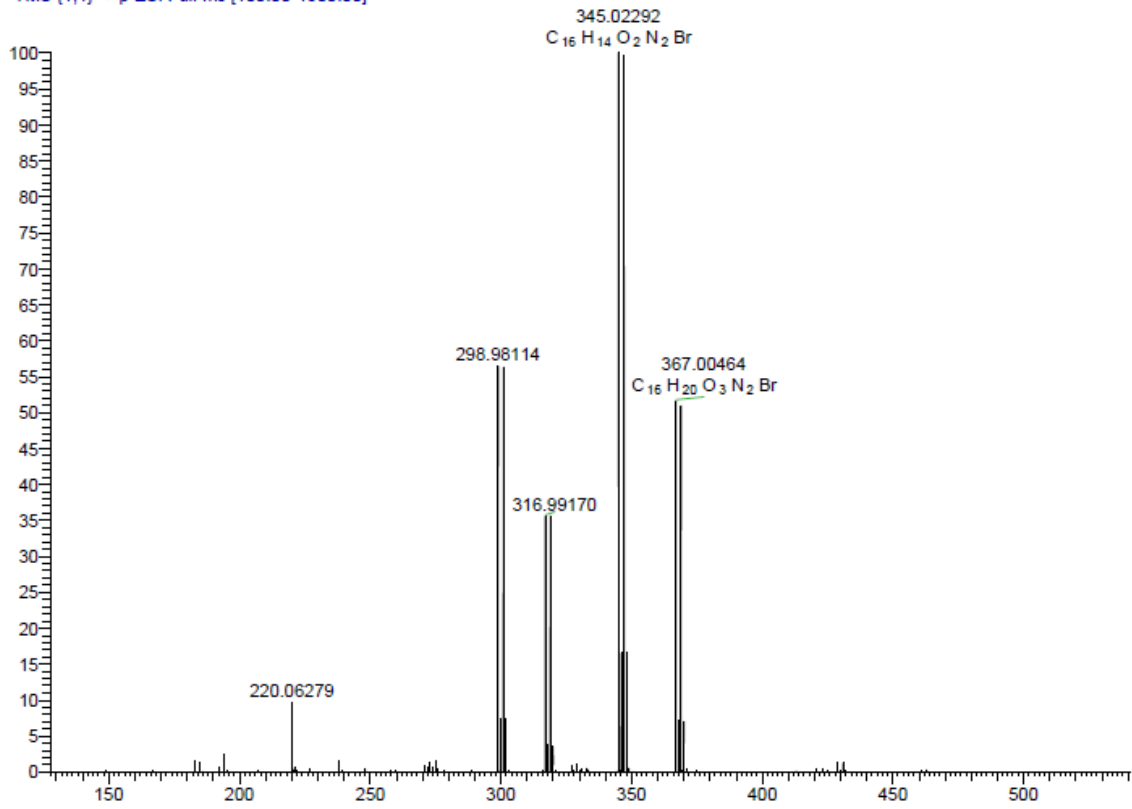
HRMS of 4b

296-A #83 RT: 1.17 AV: 1 NL: 4.68E7
FTMS (1,1) + p ESI Full ms [100.00-2000.00]



HRMS of 4c

-294 #87 RT: 1.23 AV: 1 NL: 2.62E7
 TMS (1,1) + p ESI Full ms [100.00-1500.00]



HRMS of 4d

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

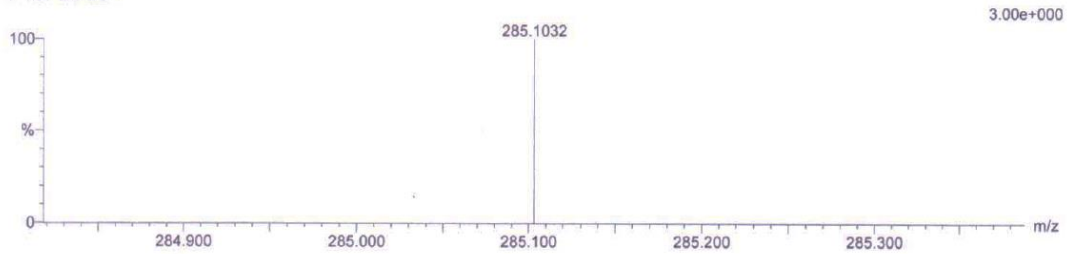
11 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-17 H: 0-14 N: 0-2 O: 0-2 F: 0-1

CM323 9 (0.125)

1: TOF MS ES+

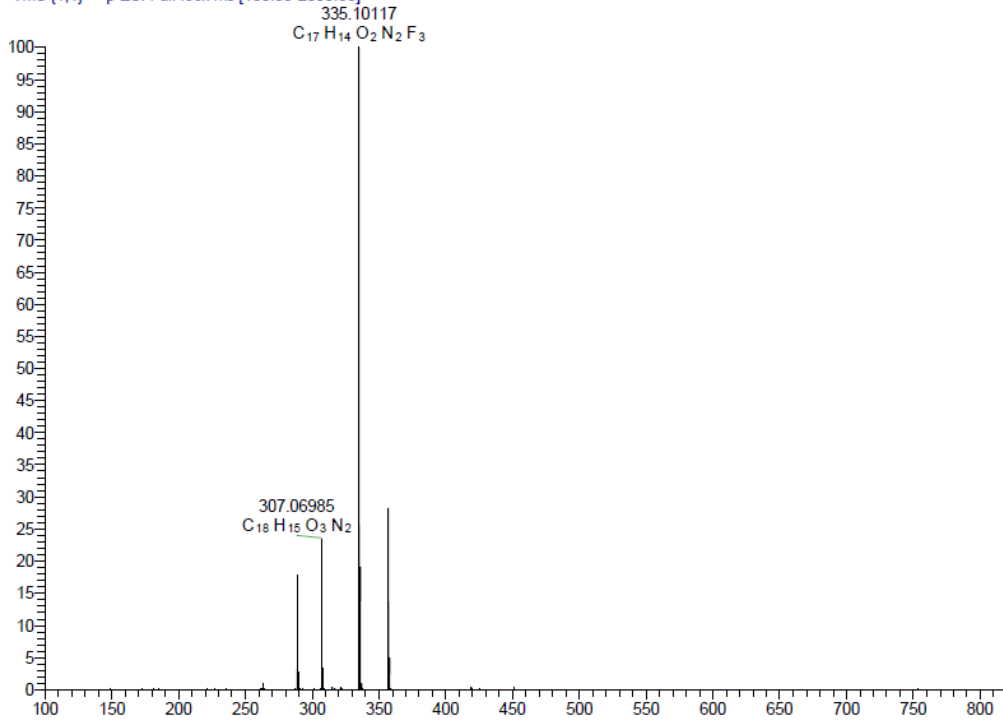


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
285.1032	285.1039	-0.7	-2.5	10.5	n/a	C ₁₆ H ₁₄ N ₂ O ₂ F

HRMS of 4e

1-299 #78 RT: 1.16 AV: 1 NL: 1.01E8

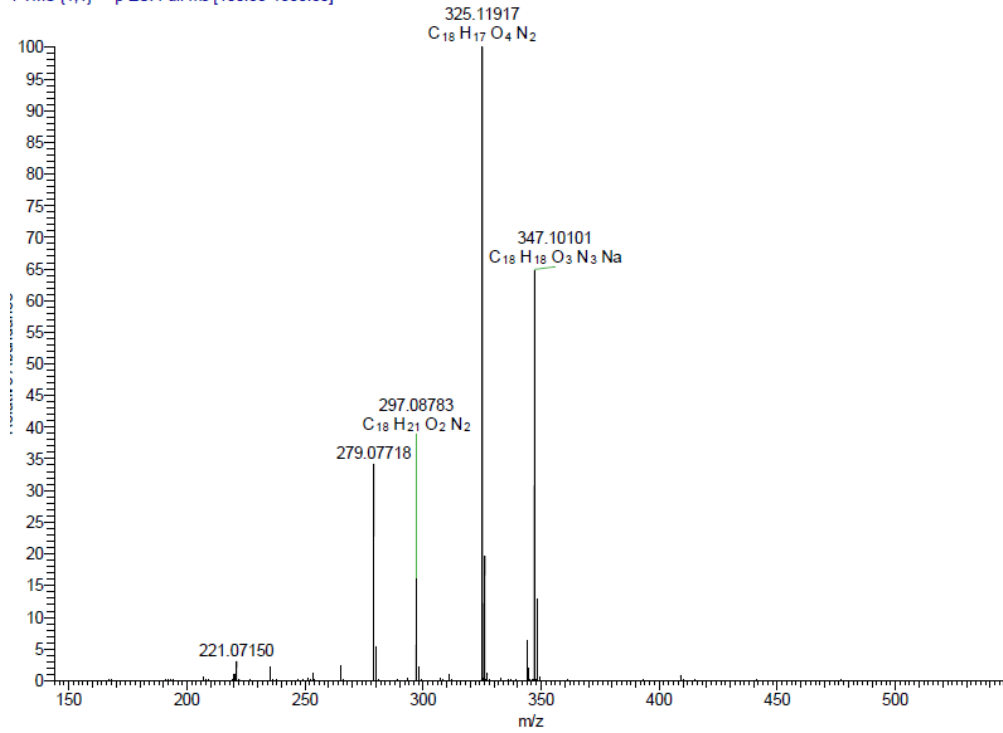
FTMS (1,1) + p ESI Full lock ms [100.00-2000.00]



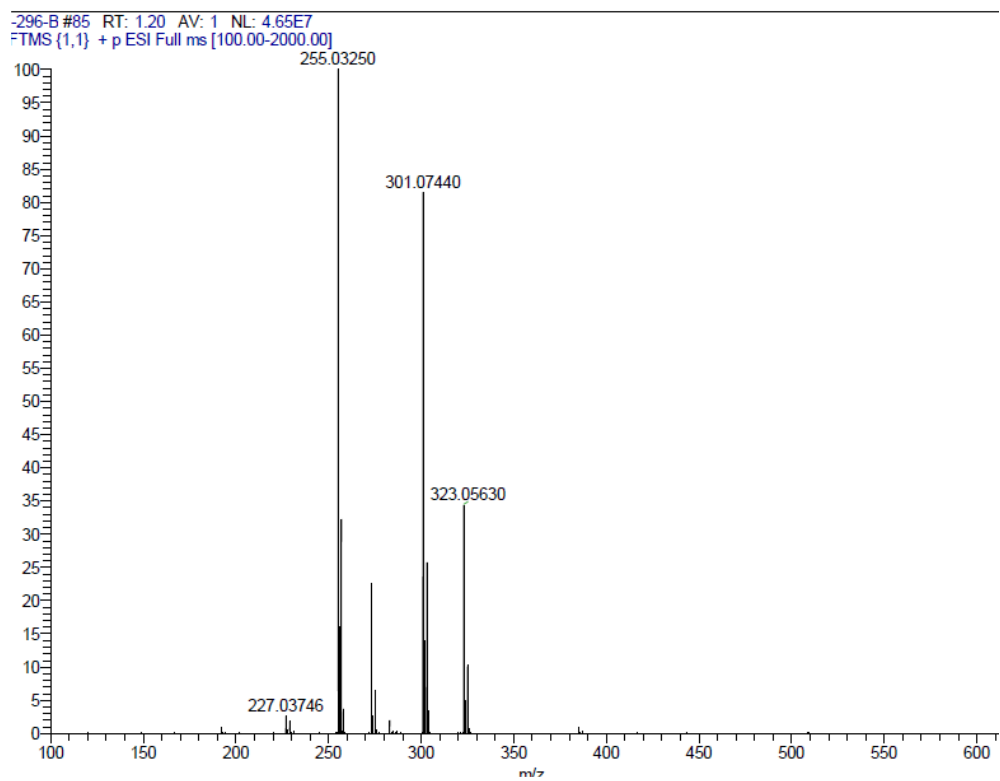
HRMS of 4f

>300 #81 RT: 1.14 AV: 1 NL: 1.05E8

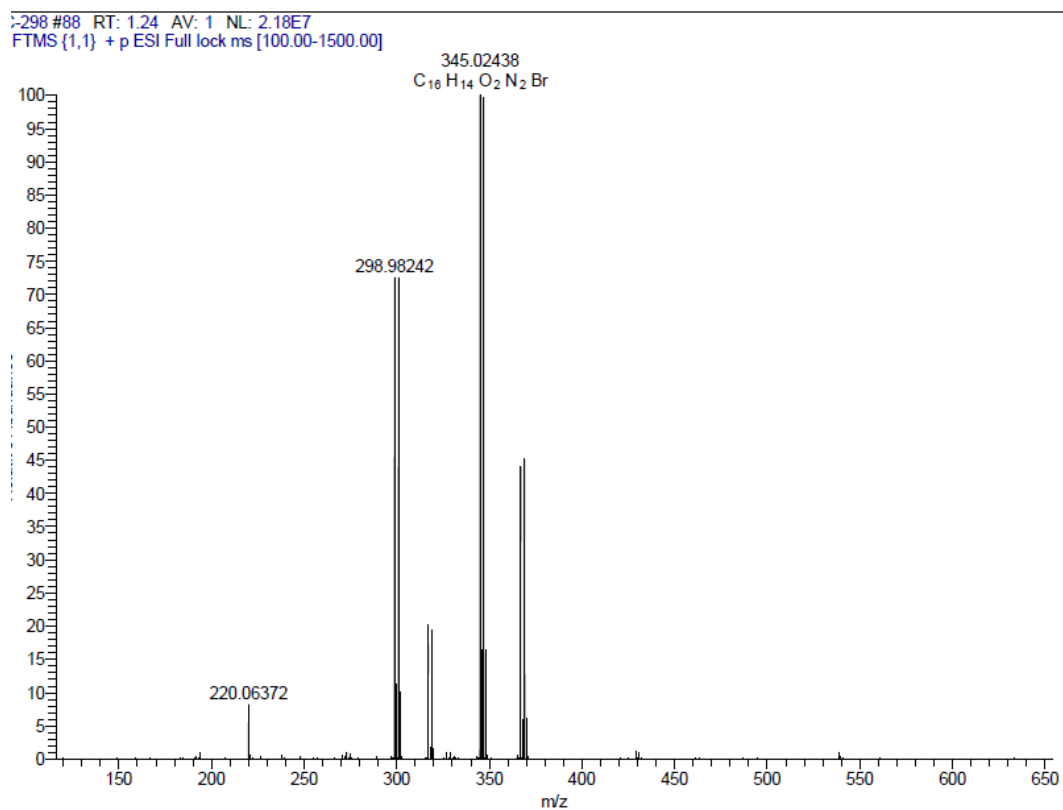
FTMS (1,1) + p ESI Full ms [100.00-1500.00]



HRMS of 4g

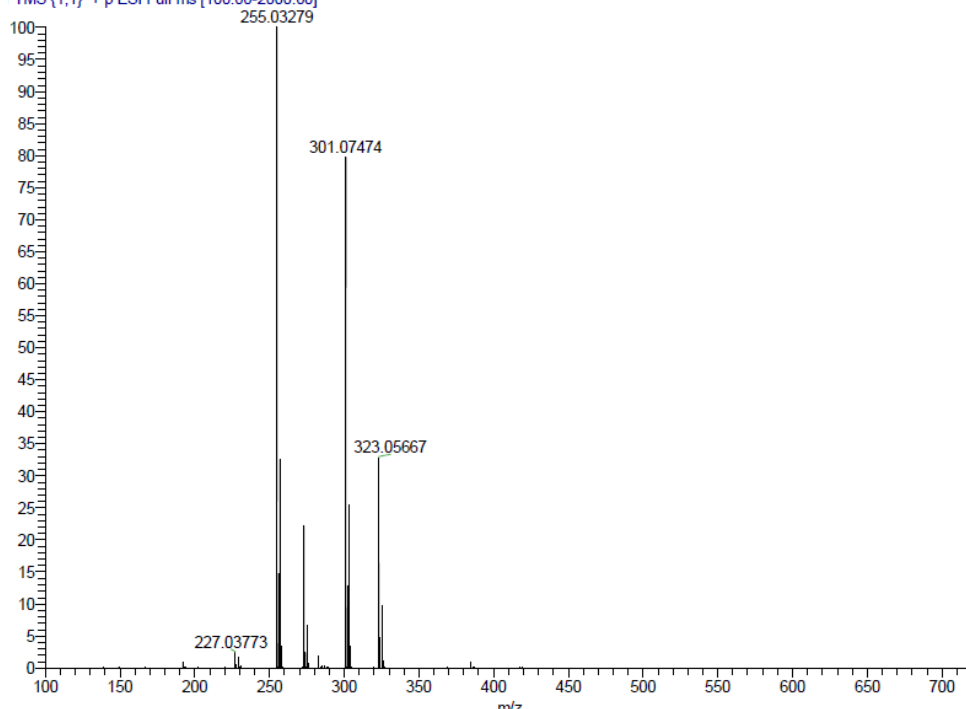


HRMS of 4j



HRMS of 4k

-296-C #85 RT: 1.20 AV: 1 NL: 5.31E7
 TMS (1,1) + p ESI Full ms [100.00-2000.00]



HRMS of 4l

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

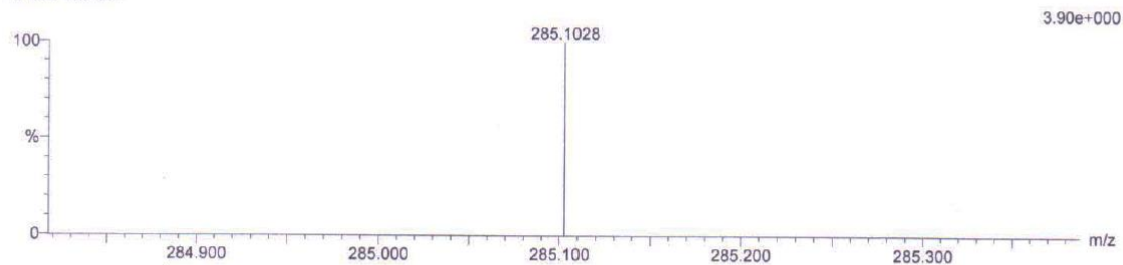
11 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-17 H: 0-14 N: 0-2 O: 0-2 F: 0-1

CM322 10 (0.139)

1: TOF MS ES+



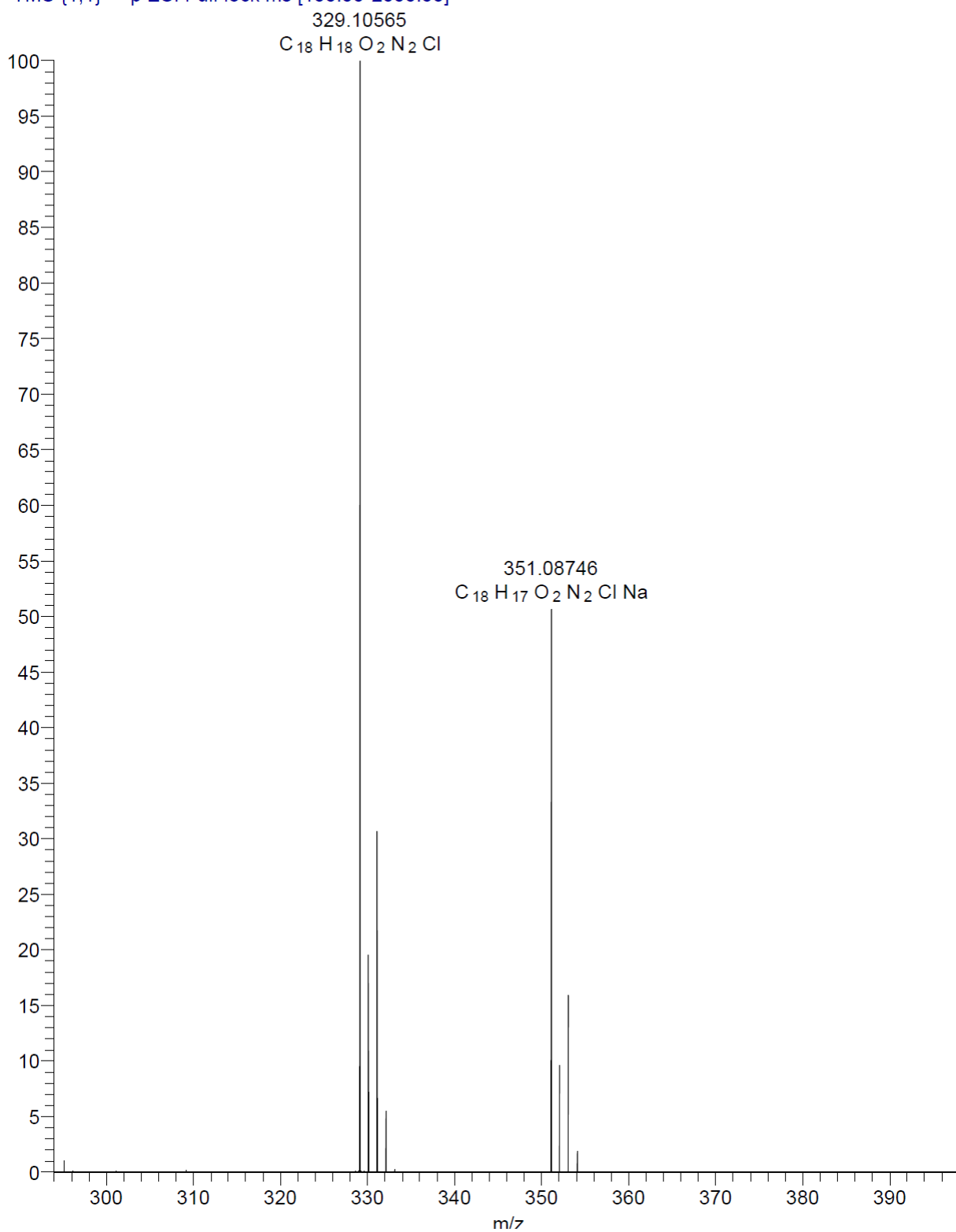
Minimum:
 Maximum:

5.0 50.0 -1.5
 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
285.1028	285.1039	-1.1	-3.9	10.5	n/a	C16 H14 N2 O2 F

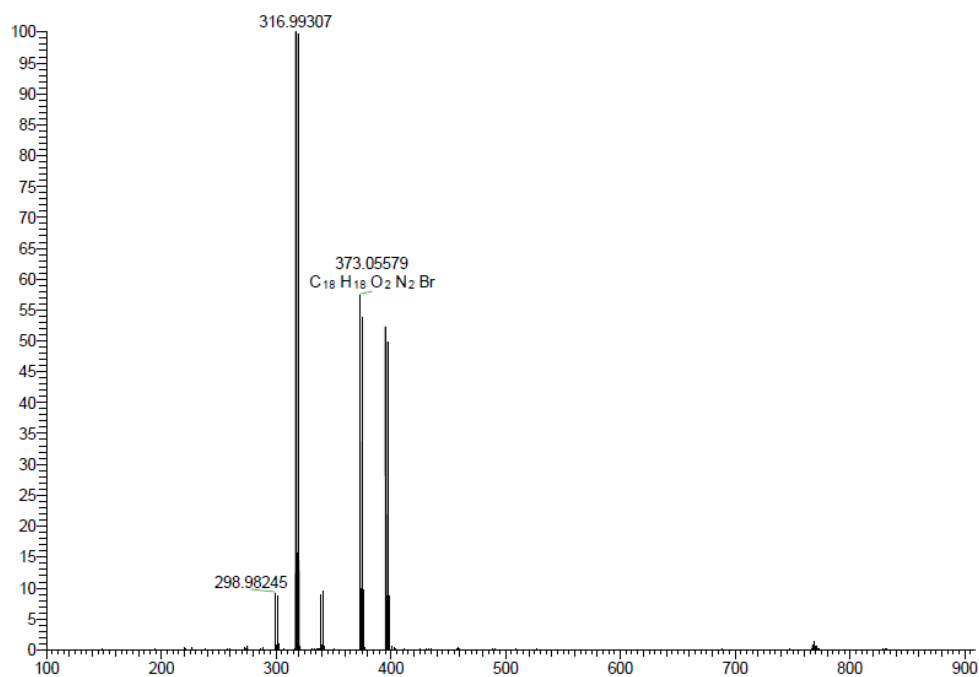
HRMS of 4m

317 #84 RT: 1.24 AV: 1 NL: 2.14E7
TMS {1,1} + p ESI Full lock ms [100.00-2000.00]



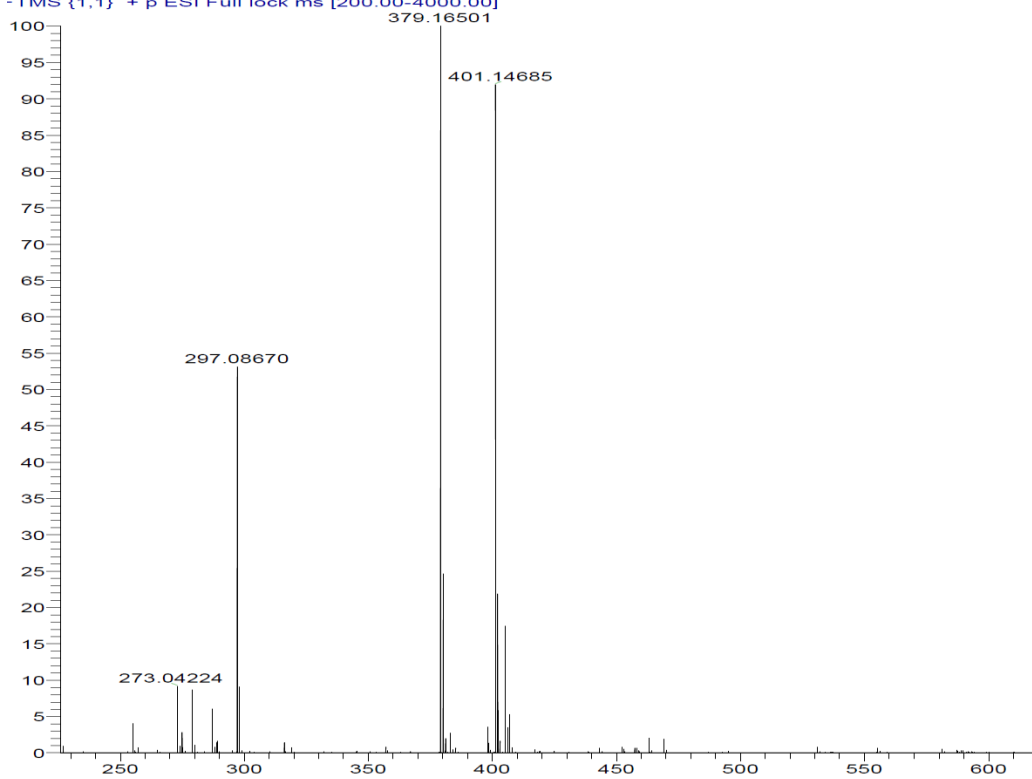
HRMS of 4n

-1-295 #86 RT: 1.27 AV: 1 NL: 5.19E7
FTMS (1,1) + p ESI Full lock ms [100.00-2000.00]



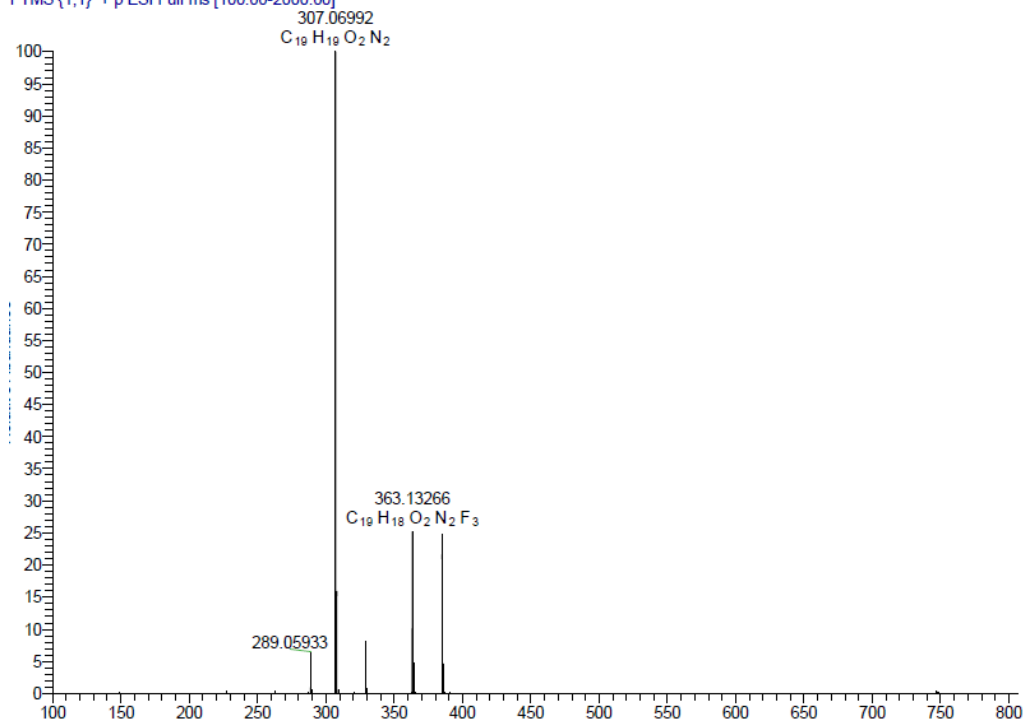
HRMS of 4o

✓VK-122 #86 RT: 1.28 AV: 1 NL: 3.30E7
FTMS (1,1) + p ESI Full lock ms [200.00-4000.00]



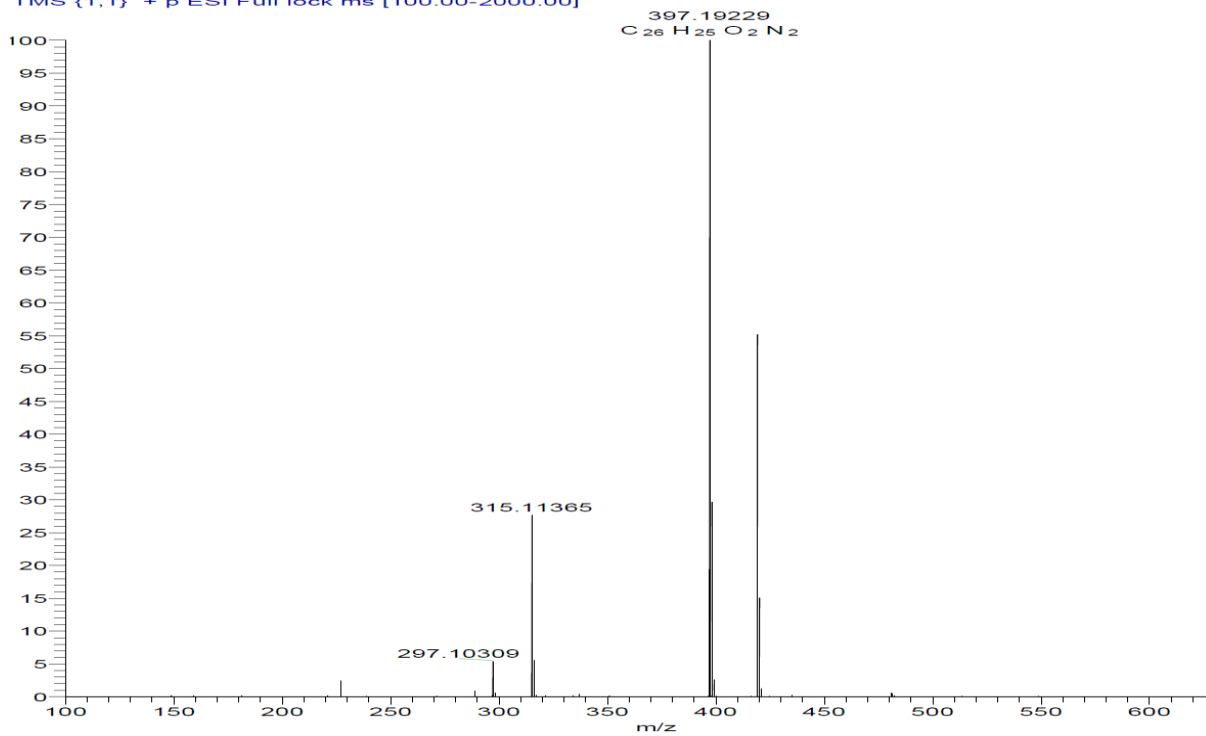
HRMS of 4p

1-302 #80 RT: 1.19 AV: 1 NL: 1.16E8
FTMS (1,1) + p ESI Full ms [100.00-2000.00]



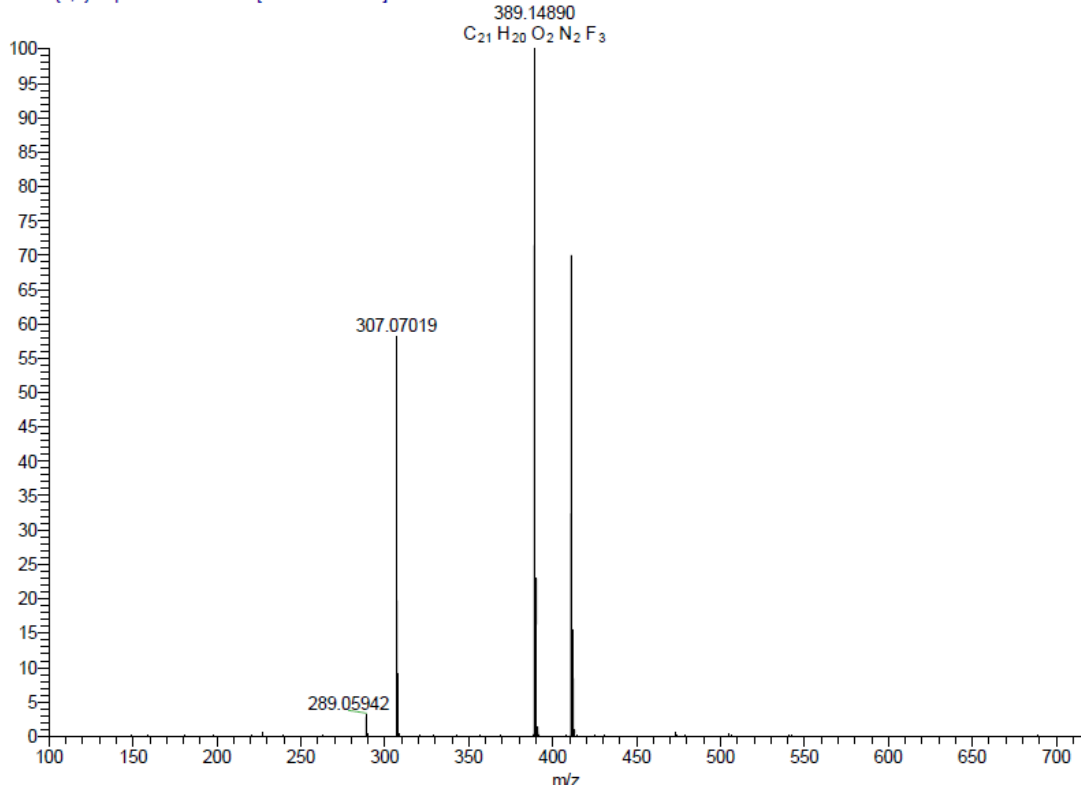
HRMS of 4q

305 #99 RT: 1.47 AV: 1 NL: 2.14E7
TMS (1,1) + p ESI Full lock ms [100.00-2000.00]



HRMS of 4r

1-311 #86 RT: 1.28 AV: 1 NL: 5.87E7
 TMS (1,1) + p ESI Full lock ms [100.00-2000.00]



HRMS of 4s

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

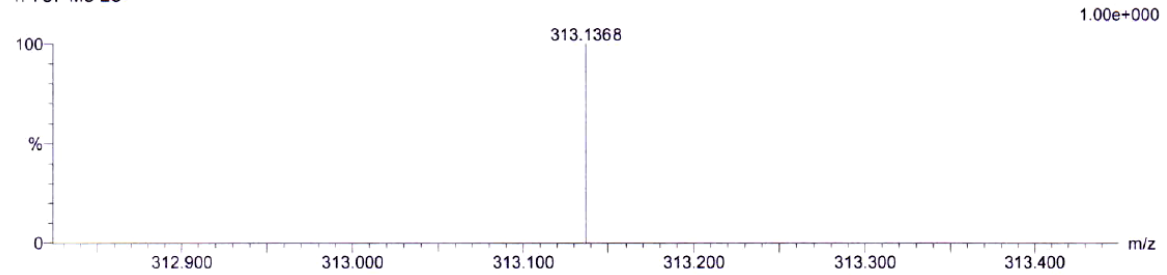
11 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-19 H: 0-18 N: 0-2 O: 0-2 F: 0-1

CM364 9 (0.125)

1: TOF MS ES+



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
313.1368	313.1352	1.6	5.1	10.5	n/a	C18 H18 N2 O2 F

HRMS of 4t

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

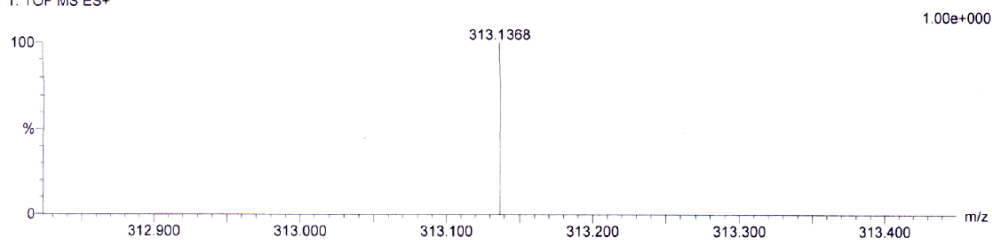
11 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-19 H: 0-18 N: 0-2 O: 0-2 F: 0-1

CM365 7 (0.097)

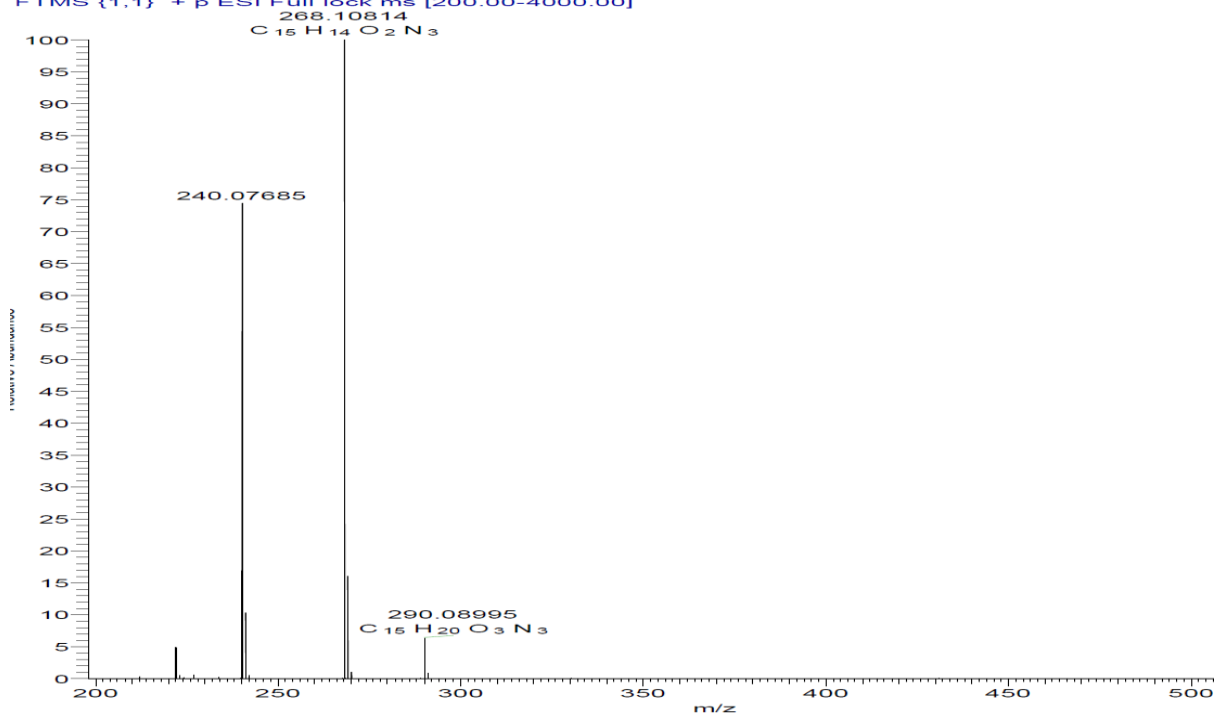
1: TOF MS ES+



Minimum:				-1.5			
Maximum:	5.0	50.0		50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula	
313.1368	313.1352	1.6	5.1	10.5	n/a	C18 H18 N2 O2 F	

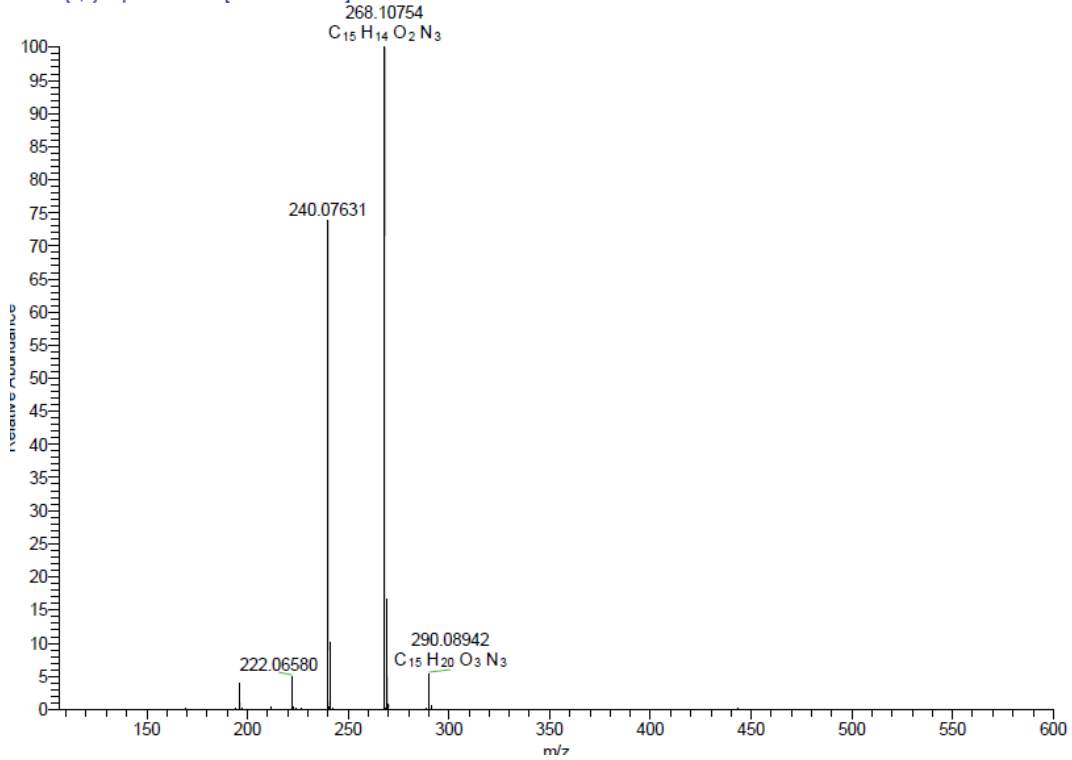
HRMS of 4u

IV-VK-127 #68-76 RT: 1.01-1.12 AV: 9 NL: 1.41E8
FTMS (1,1) + p ESI Full lock MS [200.00-4000.00]



HRMS of 4v

D-316 #72 RT: 1.07 AV: 1 NL: 1.90E8
 FTMS (1,1) + p ESI Full ms [100.00-1500.00]



HRMS of 4w

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

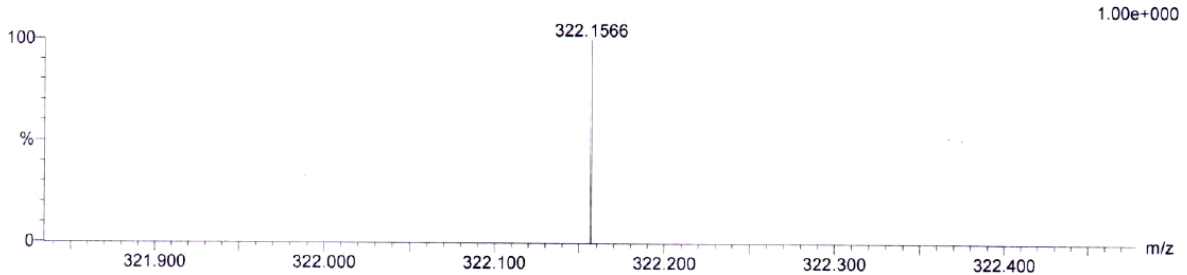
5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-20 H: 0-20 N: 0-3 O: 0-2

CM330 6 (0.083)

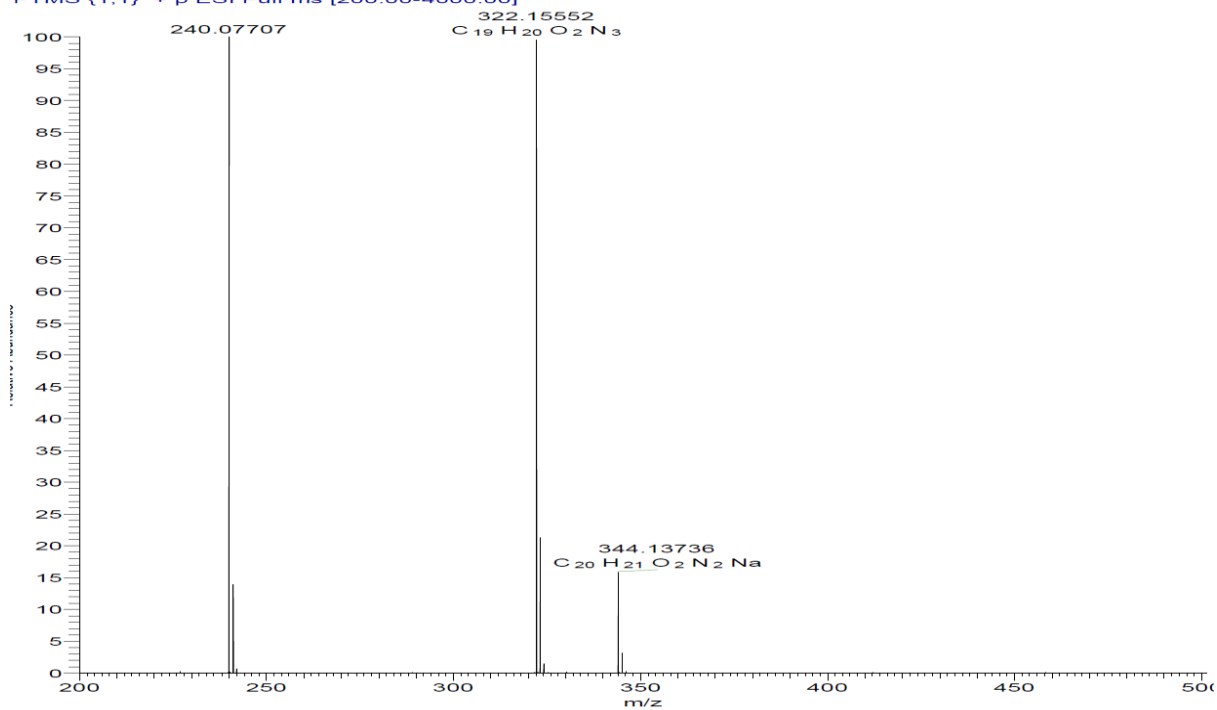
1: TOF MS ES+



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
322.1566	322.1556	1.0	3.1	11.5	n/a	C ₁₉ H ₂₀ N ₃ O ₂

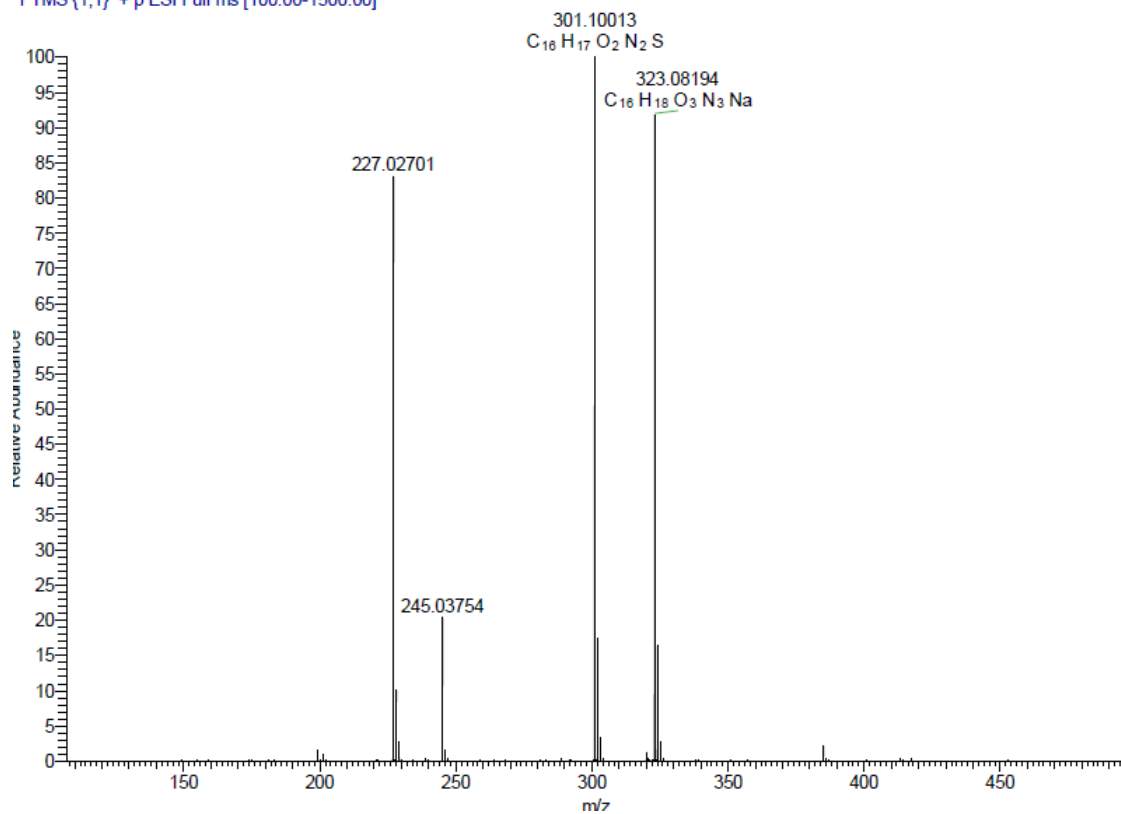
HRMS of 4x

IV-VK-108 #80 RT: 1.19 AV: 1 NL: 2.05E8
FTMS (1,1) + p ESI Full ms [200.00-4000.00]



HRMS of 4y

C-313 #83 RT: 1.24 AV: 1 NL: 3.11E7
FTMS (1,1) + p ESI Full ms [100.00-1500.00]



HRMS of 4z