Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.


# Copper Catalysed Aerobic Oxidative Amination of C (sp3)-H bonds: Synthesis of Imidazo[1, 5-*a*]pyridine derivatives

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## Experimental Section

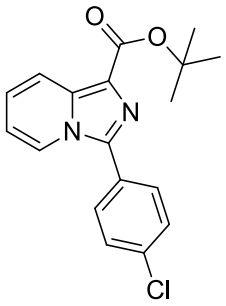
**General:** All commercially available chemicals and reagents were used without any further purification unless otherwise indicated. $^{1}H$ and $^{13}C$ NMR spectra were recorded at 500 and 125 MHz respectively. The spectra were recorded in $CDCl_3$ as solvent. Multiplicity was indicated as follows: s (singlet); d (doublet); t (triplet); m (multiplet); dd (doublet of doublets), etc. and coupling constants (J) were given in Hz. Chemical shifts are reported in ppm relative to TMS as an internal standard. The peaks around delta values of $^{1}H$ 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 using hexane/ethyl acetate as eluent unless otherwise indicated.

## General procedure

Typical general procedure for the synthesis of imidazo[1,5-a]pyridine (**3a**): To a reaction tube without cap equipped with a magnetic stir bar was added tert-butyl 2-(pyridin-2-yl) acetate **1a** (48.2mg, 0.25 mmol), 4-chloro benzyl amine **2a** (70.7mg, 0.5 mmol), PivOH (0.25 mmol) and copper iodide (0.025 mmol) and 1.0 mL of DMSO. The mixture was heated in an oil bath at 65 $^{o}C$ under an open air. Reaction was monitored by TLC, after completion of the reaction, it was allowed to attain room temperature. Then the mixture was poured into 30 mL of sodium chloride solution. The product was extracted with EtOAc (15 mL X 3) and dried with anhydrous $Na_2SO_4$. Removal of the solvent under reduced pressure the left out residue was purified by column chromatography using silica gel (20% EtOAc/hexane) to afford **3a** (74.5 mg; 91% yield).

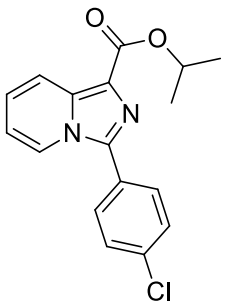
# Characterization data

**Tert-butyl 3-(4-chlorophenyl)imidazo[1,5-a]pyridine-1-carboxylate (3a)**




(Eluent: 20% EtOAc/hexane); 91% yield (74.5 mg); solid; M.p 129-134 $^{o}$C; $^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.25 (d, $J$ = 7.0 Hz, 1H), 8.18 (d, $J$ = 9.0 Hz, 1H), 7.75 (d, $J$ = 8.5 Hz, 2H), 7.50 (d, $J$ = 8.0 Hz, 2H), 7.10 (t, $J$ = 7.0 Hz, 1H), 6.77 (t, $J$ = 7.0 Hz, 1H), 1.65 (s, 9H).$^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 162.7, 137.6, 135.3, 134.7, 129.8, 129.2, 127.7, 123.7, 122.1, 120.3, 144.4, 81.0, 28.4. IR (KBr) 3050, 2976, 2931, 1702, 1700, 1508, 1403, 1364, 1214, 1162, 1125, 1046, 1035, 835, 784, 686. HRMS calcd for $C_{18}$ $H_{17}$ $O_2$ $N_2$ Cl Na: 351.0876. Found: 351.0878.

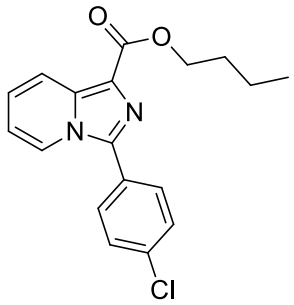
**Isopropyl 3-(4-chlorophenyl)imidazo[1,5-a]pyridine-1-carboxylate (3b)**




(Eluent: 20% EtOAc/hexane); 85% yield (66.7 mg); solid; M.p 68-73$^{o}$C; $^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.15 (t, $J$ = 7.0 Hz, 2H), 7.65 (d, $J$ = 8.5 Hz, 2H), 7.41 (d, $J$ = 8.5 Hz, 2H), 7.06-7.03 (m, 1H), 6.71 (t, $J$ = 7.0 Hz, 1H), 5.29 (qn, $J$ = 6.0 Hz, 1H), 1.37 (d, $J$ = 6.5 Hz, 6H). $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 163.0, 137.9, 135.4, 135.2, 129.9, 129.2, 127.6, 124.1,

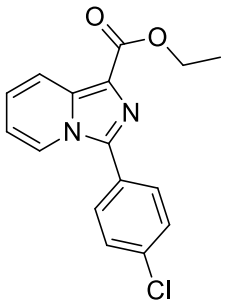
122.3, 122.2, 120.2, 114.6, 67.8, 22.1. IR (KBr) 3067, 2978, 2934, 1706, 1505, 1469, 1405, 1372, 1317, 1224, 1179, 1108, 1039, 1012, 836, 783, 740, 688. HRMS calcd for $C_{17}$ $H_{15}$ $O_2$ $N_2$ Cl Na: 337.0720. Found: 337.0721.

**Butyl 3-(4-chlorophenyl)imidazo[1,5-a]pyridine-1-carboxylate(3c)**



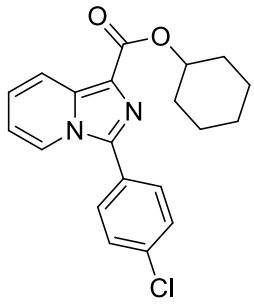

(Eluent: 20% EtOAc/hexane); 73% yield (59.8 mg); solid; M.p 110-115°C; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.26-8.22 (m, 2H), 7.75 (d, $J$ = 9.0 Hz, 2H), 7.51 (d, $J$ = 8.5 Hz, 2H), 7.15-7.12 (m, 1H), 6.80 (t, $J$ = 7.5 Hz, 1H), 4.44 (t, $J$ = 6.5 Hz, 2H), 1.83 (qen, $J$ = 7.0 Hz, 2H), 1.50 (se, $J$ = 7.0 Hz, 2H), 0.99 (t, $J$ = 7.0 Hz, 3H). $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 163.5, 135.5, 135.3, 129.9, 129.2, 127.6, 124.2, 122.2, 120.1, 114.6, 64.3, 31.0, 19.2, 13.8. IR (KBr) 3140, 2959, 2929, 2869, 2362, 1699, 1505, 1468, 1410, 1330, 1314, 1191, 1125, 1045, 1014, 959, 839, 785, 759, 690. HRMS calcd for $C_{18}$ $H_{17}$ $O_2$ $N_2$ Cl Na: 351.0876. Found: 351.08801.

**Ethyl 3-(4-chlorophenyl)imidazo[1,5-a]pyridine-1-carboxylate(3d)**



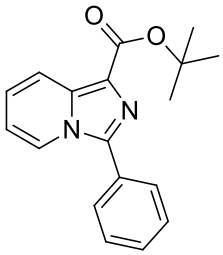
(Eluent: 20% EtOAc/hexane); 70% yield (53 mg); solid; M.p 106-111°C; $^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.17-8.15 (m, 2H), 7.66 (d, $J$ = 8.5 Hz, 2H), 7.42 (d, $J$ = 8.5 Hz, 2H), 7.07-7.04 (m, 1H), 6.72 (t, $J$ = 7.5 Hz, 1H), 4.21 (q, $J$ = 7.0 Hz, 2H), 1.38 (t, $J$ = 7.0 Hz, 3H). $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 163.4, 137.9, 135.5, 129.9, 129.2, 127.5, 124.3, 122.2, 122.0, 120.1, 114.7, 60.4, 14.6. IR (KBr) 3090, 2976, 2927, 2340, 2333, 1708, 1509, 1465, 1412, 1335, 1312, 1199, 1126, 1047, 836, 780, 740, 687. HRMS calcd for $C_{16}$ $H_{13}$ $O_2$ $N_2$ Cl Na: 323.0563. Found: 323.05600.

**Cyclohexyl 3-(4-chlorophenyl)imidazo[1,5-a]pyridine-1-carboxylate (3e)**




(Eluent: 20% EtOAc/hexane); 76% yield(67.6 mg); solid; M.p 144-149°C; $^{1}$H NMR (200 MHz, $CDCl_3$) $\delta$ 8.26-8.20 (m, 2H), 7.77 (d, $J$ = 8.6 Hz, 2H), 7.17-7.09 (m, 2H), 6.79 (t, $J$ = 7.4 Hz, 1H), 5.20-5.07 (m, 1H), 2.11-2.04 (m, 2H), 1.86-1.80 (m, 2H), 1.74-1.23 (m, 6H). $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 162.9, 137.9, 135.4, 135.1, 129.9, 129.2, 127.6, 124.1, 122.5, 122.2, 120.2, 114.5, 72.9, 31.9, 15.4, 24.1. IR (KBr) 3086, 3059, 3032, 2933, 2854, 1635, 1532, 1508, 1406, 1467, 1407, 1351, 1332, 1312, 1190, 1121, 1090, 1041, 1014, 960, 840, 747, 689. HRMS calcd for $C_{20}$ $H_{20}$ $O_2$ $N_2$ Cl: 355.1213. Found: 355.1218

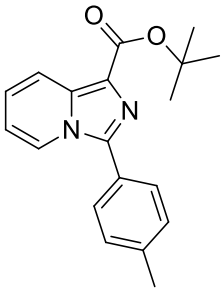
**Tert-butyl 3-phenylimidazo[1,5-a]pyridine-1-carboxylate (4a) [1]**



(Eluent: 20% EtOAc/hexane); 85% yield (63 mg); solid; M.p 108-113°C; $^{1}$H NMR (500 MHz, CDCl3) $\delta$ 8.29 (d, $J$ = 7.5 Hz, 1H), 8.17 (d, $J$ = 9.0 Hz, 1H), 7.80 (d, $J$ =7.0 Hz, 2H), 7.51 (t, $J$ = 7.0 Hz, 2H), 7.46 (t, $J$ = 7.5 Hz, 1H), 7.09-7.06 (m, 1H), 6.73 (t, $J$ = 6.5 Hz, 1H), 1.68 (s, 9H).$^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 162.9, 138.9, 134.7, 129.3, 128.9, 128.6,n 123.6, 122.4, 120.3, 114.1, 80.8, 28.5. IR (KBr) 3143, 3098, 3070, 3034, 2977, 2931, 1697, 1505, 1471, 1404, 1363, 1334, 1212, 1155, 1226, 1044, 772, 760, 690.

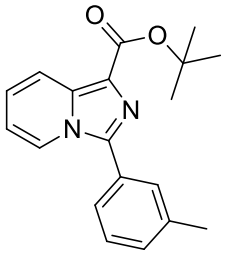
**1.** Yan, Y. Zhang, Z. Zha, Wang, Z. *Org. Lett.* **2013,** *15***,** 2274**.**

**Tert-butyl 3-(p-tolyl)imidazo[1,5-a]pyridine-1-carboxylate (4b)**



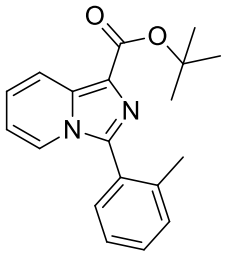
(Eluent: 20% EtOAc/hexane); 84% yield (64.2 mg); liquid; $^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.26 (d, $J$ = 7.0 Hz, 1H), 8.14 (d, $J$ = 7.0 Hz, 1H), 7.67 (d, $J$ = 7.5 Hz, 2H), 7.30 (d, $J$ = 7.5 Hz, 2H), 7.05 (t, $J$ = 7.0 Hz, 1H), 6.71 (t, $J$ = 7.0 Hz, 1H), 2.40 (s, 3H), 1.68 (s, 9H).$^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 161.8, 138.3, 138.0, 133.8, 128.5, 127.4, 125.3, 124.6, 121.8, 121.4, 119.0, 113.0, 79.7, 27.5, 20.3. IR (KBr) 2975, 2929, 1704, 1512, 1477, 1452, 1406, 1364, 1406, 1337, 1240, 1162, 1125, 1041, 833, 785, 741. HRMS calcd for $C_{19}$ $H_{20}$ $O_2$ $N_2$ Na: 331.1422. Found: 331.1420.

**Tert-butyl 3-(m-tolyl)imidazo[1,5-a]pyridine-1-carboxylate (4c)**



(Eluent: 20% EtOAc/hexane); 86% yield (66.5 mg); $^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.29 (d, $J$ = 7.5 Hz, 1H), 8.16 (d, $J$ = 7.0 Hz, 1H), 7.63(s, 1H), 7.56 (d, $J$ = 7.5 Hz, 1H), 7.38 (t, $J$ = 7.0 Hz, 1H), 7.26 (d, $J$ = 7.5 Hz, 1H), 7.08-7.04 (m, 1H), 6.73 (t, $J$ = 7.0 Hz, 1H), 2.41 (s, 3H), 1.68 (s, 9H).$^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 162.7, 138.9, 138.7, 138.4, 130.0, 129.4, 129.0, 128.5, 128.2, 123.5, 122.9, 122.4, 120.0, 113.9, 80.6, 28.4, 21.2. IR (KBr) 3054, 2930, 2978, 1708, 1523, 1467, 1408, 1365, 1339, 1264, 1239, 1162, 1047, 842, 788, 740. HRMS calcd for $C_{19}$ $H_{20}$ $O_2$ $N_2$ Na: 331.1422. Found: 331.1426.

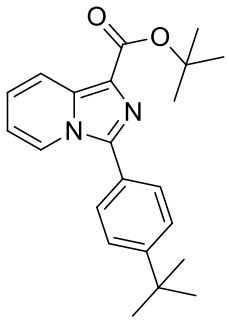
**Tert-butyl 3-(o-tolyl)imidazo[1,5-a]pyridine-1-carboxylate (4d)**



(Eluent: 20% EtOAc/hexane); 83% yield(64 mg); solid; M.p 136-141 $^{o}$C; $^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.18 (d, $J$ = 7.5 Hz, 1H), 7.66 (d, $J$ = 7.0 Hz, 1H), 7.45-7.38 (m, 2H), 7.35-7.28 (m, 2H), 7.10-7.07 (m, 1H), 6.70 (t, $J$ = 7.0 Hz, 1H), 2.16 (s, 3H), 1.68 (s, 9H).$^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 162.2, 133.7, 130.7, 130.5, 129.8, 128.3, 125.9, 123.5, 122.5,

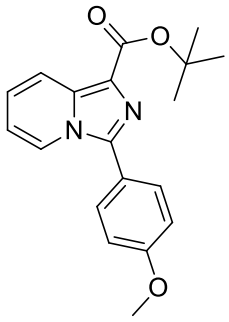
122.3, 119.8, 113.7, 8.06, 28.4, 19.5. IR (KBr) 3099, 3067, 2971, 2930, 2868, 1690, 1532, 1505, 1439, 1402, 1332, 1310, 1234, 1139, 1043, 1023, 771, 759, 726, 694. HRMS calcd for $C_{19}H_{20}O_2N_2Na$: 331.1422. Found: 331.1421.

**Tert-butyl 3-(4-(tert-butyl)phenyl)imidazo[1,5-a]pyridine-1-carboxylate (4e)**



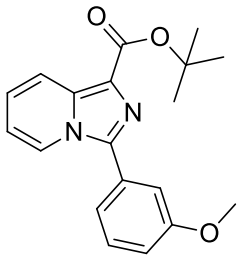
(Eluent: 20% EtOAc/hexane); 82% yield (73.6 mg); solid; M.p 138-143 °C; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.31 (d, $J$ = 7.0 Hz, 1H), 8.17 (d, $J$ = 9.5 Hz, 1H), 7.74 (d, $J$ = 8.5 Hz, 2H), 7.54 (d, $J$ = 8.5 Hz, 2H), 7.07-7.04 (m, 1H), 6.72 (t, $J$ = 6.5 Hz, 1H), 1.68 (s, 9H), 1.36 (s, 9H). $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 162.9, 152.6, 139.1, 134.6, 128.3, 126.4, 125.8, 123.5, 123.10, 122.5, 120.2, 113.9, 8.7, 34.8, 31.2, 28.5. IR (KBr) 3096, 3055, 2962, 2926, 2364, 1679, 1536, 1511, 1406, 1334, 1237, 1164, 1128, 1041, 130, 962, 840, 787, 755, 693. HRMS calcd for $C_{22}H_{27}N_2O_2$: 351.2073. Found: 351.2074.

**Tert-butyl 3-(4-methoxyphenyl)imidazo[1,5-a]pyridine-1-carboxylate (4f)**



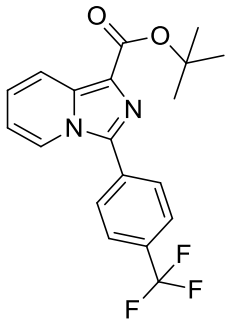
(Eluent: 20% EtOAc/hexane); 83% yield (67 mg); $^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.25 (d, $J$ = 7.0 Hz, 1H), 8.18 (d, $J$ = 9.0 Hz, 1H), 7.75 (d, $J$ = 8.5 Hz, 2H), 7.50 (d, $J$ = 8.0 Hz, 2H), 7.10 (t, $J$ = 7.0 Hz, 1H), 6.77 (t, $J$ = 7.0 Hz, 1H), 3.85 (s, 3H), 1.65 (s, 9H).$^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 162.7, 160.0, 137.6, 135.3, 134.7, 129.8, 129.2, 127.7, 123.7, 122.1, 120.3, 144.4, 81.0, 28.4. IR (KBr) 3054, 2978, 2930, 1708, 1523, 1408, 1339, 1264, 1239, 1162, 1047, 788, 708, 703. HRMS calcd for $C_{19}H_{21}O_3N_2$: 325.1552. Found: 325.1548.

**Tert-butyl 3-(3-methoxyphenyl)imidazo[1,5-a]pyridine-1-carboxylate (4g)**



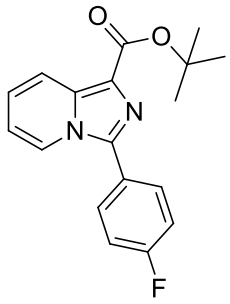
(Eluent: 20% EtOAc/hexane); 79% yield(65.5 mg); $^{1}$H NMR (200 MHz, $CDCl_3$) $\delta$ 8.34 (d, $J$ = 7.2 Hz, 1H), 8.18 (d, $J$ = 9.2 Hz, 1H), 7.44-7.31 (m, 3H), 7.19-6.98 (m, 2H), 6.74 (t, $J$ = 6.8 Hz, 1H), 3.86 (s, 3H), 1.60 (s, 9H). $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 162.9, 160.0, 138.8, 134.7, 130.5, 129.8, 123.7, 123.1, 120.5, 120.7, 115.6, 144.1, 80.9, 55.3, 28.5. IR (KBr) 3011, 2977, 2931, 2825, 1707, 1529, 1502, 1452, 1410, 1366, 1339, 1242, 1163, 1094, 1019, 839, 786, 748. HRMS calcd for $C_{19}H_{21}O_3N_2$: 325.1552. Found: 325.1555.

**Tert-butyl 3-(4-(trifluoromethyl)phenyl)imidazo[1,5-a]pyridine-1-carboxylate (4h)**



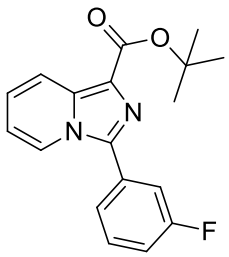
(Eluent: 20% EtOAc/hexane); 74% yield (67.0 mg); solid; M. p. 94-99 $^{o}$C; $^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.33 (d, $J$ = 7.5 Hz, 1H), 8.19 (d, $J$ = 9.5 Hz, 1H), 7.96 (d, $J$ = 8.0 Hz, 2H), 7.77 (d, $J$ = 8.0 Hz, 2H), 7.14-7.11 (m, 1H), 6.82 (t, $J$ = 7.0 Hz, 1H), 1.69 (s, 9H). $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 162.6, 137.2, 134.9, 132.8, 131.0, 130.8, 128.7, 125.8, 124.0, 123.8, 122.1, 120.3, 114.7, 81.1, 28.4. IR (KBr) 3153, 3095, 3068, 3011, 2936, 2979, 1691, 1621, 1511, 1408, 1351, 1368, 1320, 1217, 1165, 1124, 1064, 1034, 1013, 850, 783, 738, 687. HRMS calcd for $C_{19}$ $H_{17}$ $O_2$ $N_2$ $F_3$ Na: 385.1140. Found: 385.1143.

**Tert-butyl 3-(4-fluorophenyl)imidazo[1,5-a]pyridine-1-carboxylate (4i)**



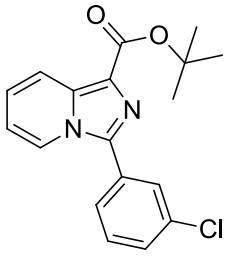

(Eluent: 20% EtOAc/hexane); 87% yield (68 mg); $^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.23 (d, $J$ = 7.5 Hz, 1H), 8.18 (d, $J$ = 9.5 Hz, 1H), 7.79-7.18 (m, 2H), 7.21 (t, $J$ = 8.5 Hz, 2H), 7.11-7.08 (m, 1H), 6.78 (t, $J$ = 7.0 Hz, 1H), 1.60 (s, 9H).$^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 164.1 (d, $J$ = 247.5 Hz), 162.7, 137.8, 134.5, 130.6, (d, $J$ = 7.5 Hz), 123.6, (d, $J$ = 73.5 Hz), 122.0, 120.2, , 116.1, 115.9, 114.2, 80.9, 28.4. IR (KBr) 308, 2933, 2977, 1703, 1519, 1462, 1406, 1366, 1338, 1264, 1161, 1046, 892, 839,740, 594. HRMS calcd for $C_{18}$ $H_{17}$ $O_2$ $N_2$ F Na: 335.1172. Found: 335.1170.

**Ttert-butyl 3-(3-fluorophenyl)imidazo[1,5-a]pyridine-1-carboxylate (4j)**



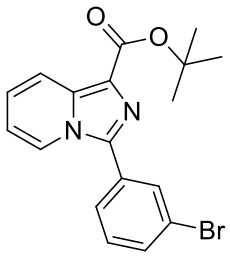

(Eluent: 20% EtOAc/hexane); 88% yield (69.0 mg); $^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.31 (d, $J$ = 7.0 Hz, 1H), 8.18 (d, $J$ = 9.20 Hz, 1H), 7.59-7.46 (m, 3H), 7.17-7.09 (m, 2H), 6.79 (t, $J$ = 6.5 Hz, 1H), 1.608 (s, 9H). $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 163.8, (d, $J$ = 245.8 Hz), 162.6, 137.4, 134.8, 131.3, (d, $J$ = 7.5 Hz), 130.6, (d, $J$ = 8.1 Hz), 124.0, 123.8, 123.4, 122.2, 120.2, 116.3, (d, $J$ = 21 Hz), 115.7, 115.5, 114.5, 80.9, 28.4. IR (KBr) 3055, 2925, 2858, 1706, 1517, 1460, 1402, 1368, 1340, 1311, 1241, 1163, 1044, 784, 741, 698. HRMS calcd for $C_{18}$ $H_{17}$ $O_2$ $N_2$ F N: 313.1352. Found: 313.1327.

**Tert-butyl 3-(3-chlorophenyl)imidazo[1,5-a]pyridine-1-carboxylate (4k)**



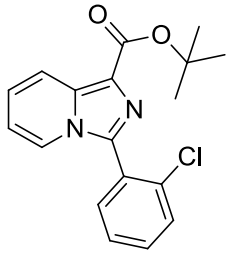

(Eluent: 20% EtOAc/hexane); 89% yield (72.7 mg); $^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.19 (d, $J$ = 7.0 Hz, 1H), 8.08 (d, $J$ = 9.0 Hz, 1H), 7.72 (s, 1H), 7.59 (d, $J$ = 6.5 Hz, 1H), 7.36-7.31 (m, 2H), 7.01 (t, $J$ = 8.0 Hz, 1H), 6.70 (t, $J$ = 7.0 Hz, 1H), 1.60 (s, 9H).$^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 161.5, 136.2, 133.9, 133.7, 129.9, 129.1, 128.3, 127.6, 125.4, 122.9, 122.4, 121.1, 119.2, 113.6, 80.0, 27.4. IR (KBr) 3055, 2925, 2858, 1706, 1571, 1517, 1460, 1409, 1368, 1241, 1163, 1044, 784, 741, 698. HRMS calcd for $C_{18}$ $H_{17}$ $O_2$ $N_2$ Cl Na: 351.0876. Found: 351.0875.

**Tert-butyl 3-(3-bromophenyl)imidazo[1,5-a]pyridine-1-carboxylate (4l)**




(Eluent: 20% EtOAc/hexane); 95% yield (89.2 mg); $^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.29 (d, $J$ = 7.0 Hz, 1H), 8.18 (d, $J$ = 9.0 Hz, 1H), 7.98 (s, 1H), 7.73 (d, $J$ = 8.0 Hz, 1H), 7.58 (d, $J$ = 8.0 Hz, 1H), 7.37 (t, $J$ = 8.0 Hz, 1H), 7.12-7.09 (m, 1H), 6.80 (t, $J$ = 7.5 Hz, 1H), 1.65 (s, 9H).$^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 162.5, 132.1, 131.4, 130.2, 126.7, 123.8, 122.0, 120.1, 114.5, 80.9, 20.3. IR (KBr) 3055, 2979, 2932, 1704, 1596, 1566, 1517, 1457, 1409, 1366, 1338, 1264, 1162, 1045, 893, 840, 789, 701. HRMS calcd for $C_{18}$ $H_{17}$ $O_2$ $N_2$ Br Na: 395.0371. Found: 395.0362.

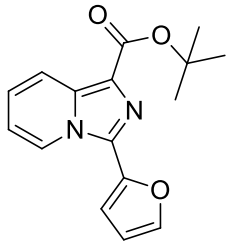
**Tert-butyl 3-(2-chlorophenyl)imidazo[1,5-a]pyridine-1-carboxylate (4m)**




(Eluent: 20% EtOAc/hexane); 82% yield(367.7 mg); solid; M. p 194-199$^{o}$C; $^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.12 (d, $J$ = 9.0 Hz, 1H), 7.59 (d, $J$ = 7.0 Hz, 1H), 7.45 (d, $J$ = 8.0 Hz, 2H), 7.40-7.33 (m, 2H), 7.06-7.03 (m, 1H), 6.68 (d, $J$ = 6.5 Hz, 1H), 1.68 (s, 9H).$^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 161.8, 135.9 133.3, 133.2, 132.6, 130.3, 128.7, 127.5, 126.2, 122.9, 122.1, 188.9, 112.8, 79.8, 27.5. IR (KBr) 3138, 3104, 3052, 2973, 2930, 1689, 1531, 1505, 1441,

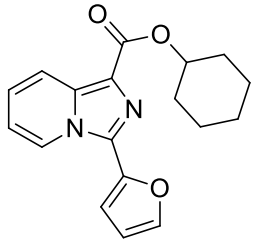
1405, 1366, 1317, 1236, 1160, 1125, 1059, 1028, 775, 755, 689, 679. HRMS calcd for $C_{18}$ $H_{17}$ $O_2$ $N_2$ Cl Na: 351.0876. Found: 351.0881.

**Tert-butyl 3-(furan-2-yl)imidazo[1,5-a]pyridine-1-carboxylate (4o)**



(Eluent: 20% EtOAc/hexane); 84% yield (59.7 mg); $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.81 (d, $J$ = 8.0 Hz, 1H), 8.16(d, $J$ = 9.0 Hz, 1H), 7.58 (s, 1H), 7.20 (d, $J$ = 3.5 Hz, 1H), 7.12-7.09 (m, 1H), 6.83 (t, $J$ = 7.5 Hz, 1H), 6.66-6.59 (m, 1H), 1.68 (s, 9H).$^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 161.5, 144.4, 141.4, 133.6, 129.9, 122.9, 122.2, 188.9, 133.6, 110,8, 109.3, 80.0, 27.4. IR (KBr) 3128, 3955, 2931, 2979, 1706, 1519, 1462, 1406, 1366, 1338, 1264, 1161, 1046, 740. HRMS calcd for $C_{16}$ $H_{16}$ $O_3$ $N_2$ Na: 307.1059. Found: 307.10602.

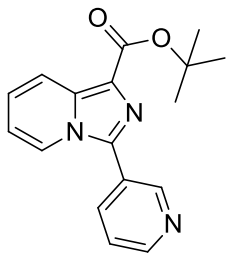
**Cyclohexyl 3-(furan-2-yl)imidazo[1,5-a]pyridine-1-carboxylate (4p)**



(Eluent: 20% EtOAc/hexane); 76% yield (54.2 mg); $^1$H NMR (200 MHz, $CDCl_3$) $\delta$ 8.82 (d, $J$ = 7.2 Hz, 1H), 8.21 (d, $J$ = 9.2 Hz, 1H), 7.59 (s, 1H), 7.7.20-7.09 (m, 2H), 6.85 (t, $J$ = 6.6 Hz, 1H), 6.61-6.58 (m, 1H), 5.18-5.08 (m, 1H), 2.11-1.20 (m, 10H). $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 184.0, 162.2, 158.9, 148.8, 144.6, 135.9, 123.7, 133.5, 130.5, 124.0, 120.5, 188.8,

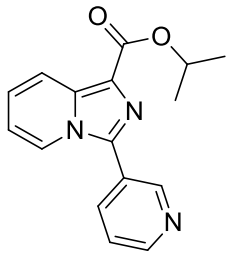
71.9, 20.6, 12.5, 10.8. IR (KBr) 3055, 2932, 2860, 1708, 1511, 1416, 1338, 1265, 1164, 1121, 1044, 896, 742. HRMS calcd for $C_{18}$ $H_{18}$ $O_3$ $N_2$ Na: 333.1215. Found: 333.1213

**Tert-butyl 3-(pyridin-3-yl)imidazo[1,5-a]pyridine-1-carboxylate (4q)**



(Eluent: EtOAc); 93% yield (68.4 mg); M.p 104-109°C; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.98 (s, 1H), 8.62 (s, 1H), 8.21-8.08 (m,1H), 8.10 (t, $J$ = 8.5 Hz, 2H), 7.41-7.39 (m, H), 7.07-7.04 (m, 1H), 6.74 (d, $J$ = 7.0 Hz, 1H), 1.60 (s, 9H).$^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 162.4, 149.9, 148.7, 136.2, 134.8, 124.0, 123.7, 121.8, 120.3, 114.7, 81.0, 20.3. IR (KBr) 3134, 3038, 3089, 3003, 2967, 2928, 2647, 1709, 1502, 1404, 1356, 1343, 1309, 1248, 1211, 1157, 1130, 1050, 1028, 957, 835, 785, 551, 708, 690. HRMS calcd for $C_{17}$ $H_{17}$ $O_2$ $N_3$ Na: 318.1218. Found: 318.1218.

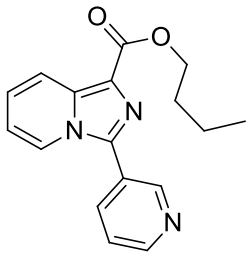
**Isopropyl 3-(pyridin-3-yl)imidazo[1,5-a]pyridine-1-carboxylate (4r)**



(Eluent: EtOAc); 65% yield (54.9 mg); M.p 68-73 °C; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.96 (d, $J$ = 2.5 Hz, 1H), 8.62-8.61 (m, 1H), 8.20-8.06 (m, 3H), 7.41-7.38 (m,1H),7.10-7.07 (m, 1H), 6.76 (t, $J$ = 7.0 Hz, 1H), 5.30 (qen, $J$ = 6.0 Hz, 1H), 1.37 (d, $J$ = 7.0 Hz, 6H).$^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 162.7, 150.1, 148.9, 136.2, 135.8, 135.2, 125.5, 124.3, 123.6, 122.7, 121.8,

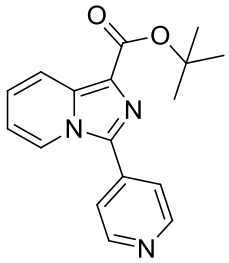
120.1, 114.8, 67.8, 22.0. IR (KBr) 308, 3040, 2982, 2934, 2878, 1702, 1641, 1520, 1411, 1341, 1314, 1227, 1197, 1111, 1052, 1032, 815, 789, 744, 692. HRMS calcd for $C_{16}$ $H_{15}$ $O_2$ $N_3$ Na: 304.1062. Found: 304.1064.

**Butyl 3-(pyridin-3-yl)imidazo[1,5-a]pyridine-1-carboxylate (4s)**



(Eluent: EtOAc); 54% yield (40 mg); M.p 60-65 °C; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.98 (s, 1H),8.64 (d, *J* = 5.0 Hz, 1H), 8.22-8.08 (m, 3H), 7.42-7.42 (m,1H), 7.12(m, 1H), 6.78 (t, *J* = 7.0 Hz, 1H), 4.37 (t, *J* = 7.0Hz, 2H), 1.76 (pen, *J* = 7.0 Hz, 2H), 1.44-1.33 (m,2H), 0.91 (t, *J* = 7.0 Hz, 3H). $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 163.4, 150.3, 149.0, 136.4, 136.0, 135.5, 125.6, 124.5, 123.8, 122.6, 12.0, 120.2, 155.0, 64.4, 30.9, 192, 13.8. IR (KBr) 3090, 2959, 2934, 2873,1707, 1693, 1523, 1417, 1340, 1312, 1219, 1197, 1133, 1058, 1031, 14, 781, 744, 701, 698. HRMS calcd for $C_{17}$ $H_{17}$ $O_2$ $N_3$ Na: 318.1218. Found: 318.1211.

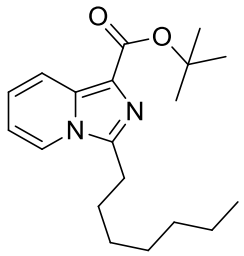
**Tert-butyl 3-(pyridin-4-yl)imidazo[1,5-a]pyridine-1-carboxylate (4u)**



(Eluent: EtOAc); 68% yield (49 mg); M.p 124-129 °C; $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.68(s, 1H), 8.34 (d, *J* = 6.5 Hz, 2H), 8.14 (d, *J* = 9.0 Hz, 1H), 7.70 (d, *J* = 2.5 Hz, 2H), 7.07 (d, *J* = 7.5 Hz, 1H), 6.80 (s, 1H), 1.61 (s, 9H). $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 162.3, 150.4, 136.7,

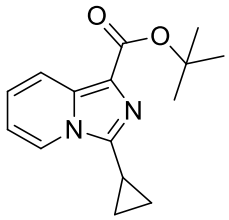
135.8, 135.2, 124.3, 122.1, 122.0, 120.4, 115.0, 81.2, 28.4. IR (KBr) 3091, 3002, 2967, 2929, 2365, 1707, 1597, 1507, 1411, 1365, 1347, 1244, 1261, 1168, 1129, 1097, 1031, 800, 754, 684. HRMS calcd for $C_{17}$ $H_{17}$ $O_2$ $N_3$ Na: 318.1218. Found: 318.1220.

**Tert-butyl 3-heptylimidazo[1,5-a]pyridine-1-carboxylate (4v)**



(Eluent: 20% EtOAc/hexane); 59% yield (47 mg); $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.09 (d, $J$ = 9.2 Hz, 1H), 7.88 (d, $J$ = 7.2 Hz, 1H), 7.06-6.98 (m, 1H), 6.79 (t, $J$ = 6.7 Hz, 1H), 3.03 (t, $J$ = 7.8 Hz, 2H), 1.88-1.77 (m, 2H), 1.66 (s, 9H), 1,43-1.29 (m, 6H), 0.94-0.88 (m, 5H), $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 162.8, 140.0, 133.8, 122.8, 121.5, 121.4, 120.1, 113.4, 80.5, 31.6, 28.5, 26.6, 26.5, 26.1, 22.4, 22.3, 13.9. IR (KBr) 3327, 3095, 3045, 2928, 2857, 1708, 1531, 1457, 1409, 1367, 1330, 1245, 1211, 1161, 1110, 1073, 1012, 839, 784, 746. HRMS calcd for $C_{19}H_{29}N_2O_2$: 317.2229. Found: 317.2222.

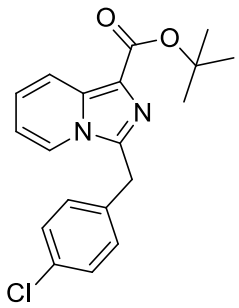
**Tert-butyl 3-cyclopropylimidazo[1,5-a]pyridine-1-carboxylate (4w)**



(Eluent: 20% EtOAc/hexane); 68% yield(44 mg); $^1$H NMR (200 MHz, $CDCl_3$) $\delta$ 8.14 (d, $J$ = 7.2 Hz, 1H), 8.05 (d, $J$ = 9.2 Hz, 1H), 7.05 (t, $J$ = 6.6 Hz, 1H), 6.77 (d, $J$ = 6.6 Hz, 1H), 2.06-1.95 (m, 1H), 1.66 (s, 9H), 1.18-1.05 (m, 4H). $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 162.7, 140.6, 133.9, 123.2, 121.6, 120.8, 119.8, 133.3, 80.4, 28.4, 6.58, 6.08. . IR (KBr) 2978, 2823, 1768,

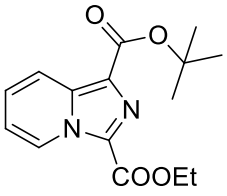
1531, 1486, 1425, 1398, 1348, 1278, 1231, 1189, 1115, 1098, 1029, 889, 756, 731. HRMS calcd for $C_{15}$ $H_{18}$ $O_2$ $N_2$ Na: 281.1266. Found: 281.1268.

**Tert-butyl 3-(4-chlorobenzyl)imidazo[1,5-a]pyridine-1-carboxylate (4x) new compound**




(Eluent: 20% EtOAc/hexane); 39% yield (34 mg); M.p 130-134 $^{o}$C; $^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.12 (d, $J$ = 9.2 Hz, 1H), 7.63 (t, $J$ = 7.0 Hz, 1H), 7.28-6.99 (m, 5H). 6.64 (t, $J$ = 6.8 Hz, 1H), 4.45 (s, 2H), 1.60 (s, 9H). $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 1 84.1, 152.1, 148.1, 148.0, 146.7, 143.4, 142.6, 141.9, 141.7, 134.8, 132.7, 130.8, 122.9, 81.7, 21.8, 16.4. IR (KBr) 3390, 3276, 3086, 2977, 2931, 2859, 1705, 1702, 1526, 1493, 1410, 1410, 1366, 1333, 1248, 1207, 1160, 1138, 1022, 989, 856, 836, 789, 746, 689. HRMS calcd for C19 H20 O2 N2 Cl: 343.1213. Found: 343.1219.

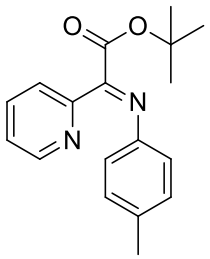
**1-Tert-butyl 3-ethyl imidazo[1,5-a]pyridine-1,3-dicarboxylate (6a)**




(Eluent: 20% EtOAc/hexane); 47% yield(33.8 mg); M.p 143-148 $^{o}$C; $^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.25 (d, $J$ = 7.0 Hz, 1H), 8.26 (d, $J$ = 7.0 Hz, 1H), 7.28-7.21 (m, 1H), 6.93 (t, $J$ = 7.0 Hz, 1H), 4.43 (q, $J$ = 7.0 Hz, 2H), 1.66 (s, 9H), 1.40 (t, $J$ = 7.0 Hz, 3H). $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 161.9, 159.5, 136.1, 127.1, 126.2, 126.1, 124.4, 119.8, 116.2, 81.6, 61.7,

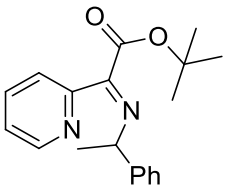
28.3, 14.2. IR (KBr) 3125, 3098, 3048, 2980, 2932, 1714, 1632, 1502, 1472, 1401, 1361, 1337, 1219, 1171, 1134, 1064, 1036, 1002, 873, 842, 836, 770, 651. HRMS calcd for $C_{15}$ $H_{18}$ $O_4$ $N_2$ Na: 226.12313.1164. Found: 313.1165.

**(E)-tert-butyl 2-(pyridin-2-yl)-2-(p-tolylimino)acetate (9a)**



Eluent: 10% EtOAc/hexane); 89% yield; M.p 111-116 $^{o}$C; $^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.68 (d, $J$ = 5.0 Hz, 1H), 8.18 (d, $J$ = 6.5 Hz, 1H), 7.79 (d, $J$ = 7.5 Hz, 1H), 7.37-7.35 (m, 1H), 7.15 (d, $J$ = 8.0 Hz, 2H), 6.96 (d, $J$ = 8.0 Hz, 2H), 2.34 (s, 3H), 1.34 (s, 9H), $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 164.2, 160.8, 153.5, 149.2, 146.9, 136.5, 134.7, 129.2, 1251, 119.9, 83.5, 27.9, 20.9. IR (KBr) 3390, 3276, 3086, 2977, 2931, 2859, 1705, 1702, 1526, 1493, 1410, 1410, 1366, 1333, 1248, 1207, 1160, 1138, 1022, 989, 856, 836, 789, 746, 689. HRMS calcd for $C_{18}$ $H_{21}$ $O_2$ $N_2$: 297.1603. Found: 297.1598.

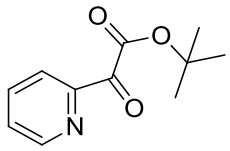
**(*E*)-Tert-butyl 2-((1-phenylethyl)imino)-2-(pyridin-2-yl)acetate (10a)**



(Eluent: 10% EtOAc/hexane); 85% yield (64.8 mg); $^{1}$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.50 (d, $J$ = 4.5 Hz, 1H), 8.05 (d, $J$ = 8.0 Hz, 1H), 7.62-7.59 (m, 1H), 7.38 (d, $J$ = 7.5 Hz, 2H), 7.25 (t, $J$ = 7.5 Hz, 2H), 7.17-7.14 (m, 2H), 4.74 (q, $J$ = 6.5 Hz, 1H), 1.54-1.51 (m, 12H). $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 164.9, 159.3, 153.8, 148.8, 144.1, 136.2, 128.3, 126.9, 126.6, 121.3,

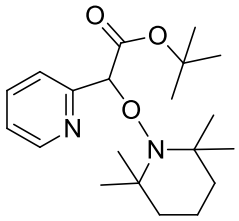
83.5, 63.0, 28.2, 23.9. IR (KBr) 3060, 3029, 2978, 2931, 1730, 1642, 1583, 1456, 1392, 1369, 1320, 1251, 1232, 1159, 1081, 1071, 847, 803, 75, 69, 618, 532. HRMS calcd for $C_{19}$ $H_{22}$ $O_2$ $N_2$ Na: 333.1579. Found: 333.1575.

**Tert-butyl 2-oxo-2-(pyridin-2-yl)acetate (11a)**



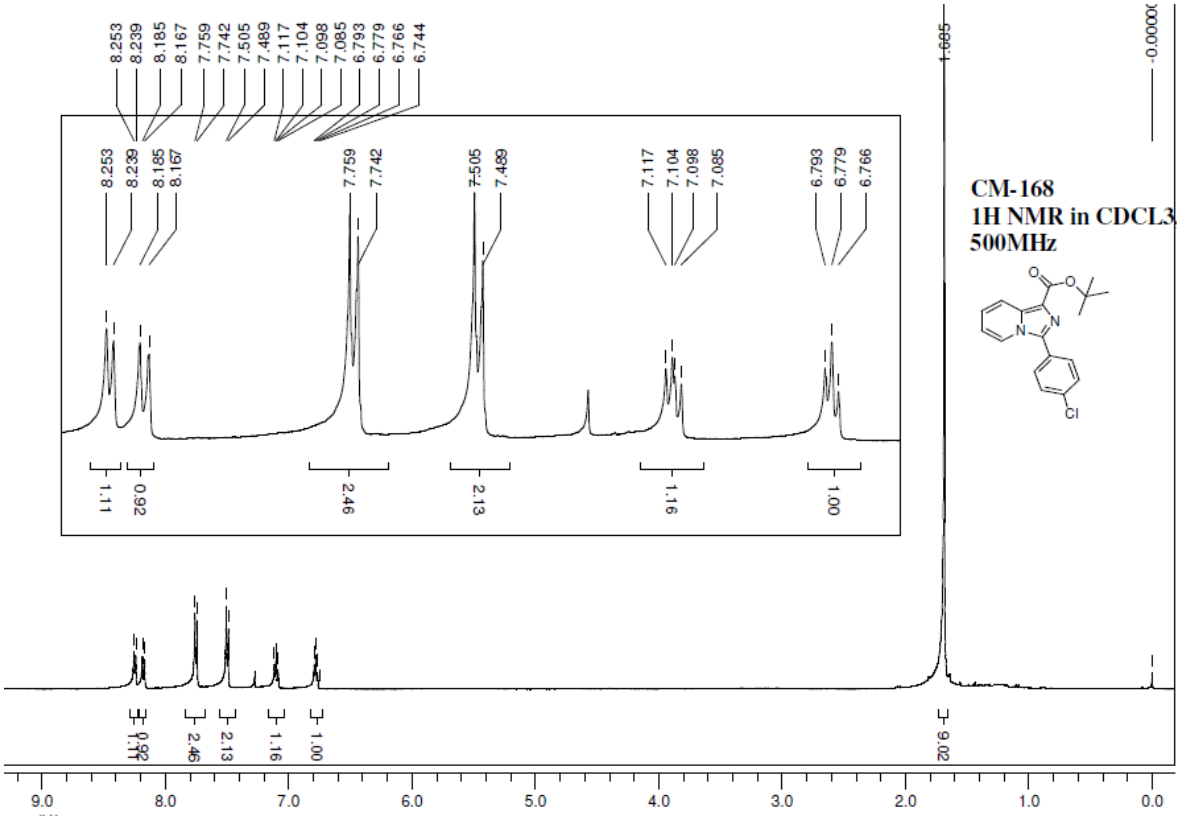
(Eluent: 15% EtOAc/hexane); 65% yield (33.3 mg); 1H NMR (500 MHz, $CDCl_3$) δ 8.75 (d, *J* = 5.0 Hz, 1H), 8.09 (d, *J* = 8.0 Hz, 1H), 7.90-7.87 (m, 1H), 7.53-7.51 (m, 1H), 1.63 (s, 9H). 13C NMR (125 MHz, $CDCl_3$) δ 187.4, 164.7, 150.5, 149.7, 137.0, 127.9, 123.3, 84.7, 28.1. IR (KBr) 2987, 2924, 1789, 1708, 1532, 1501, 1478, 1432, 1255, 1209, 1143, 1042, 992, 904, 867, 803, 746. HRMS calcd for $C_{11}$ $H_{13}$ $O_3$ N Na: 230.0793. Found: 230.0789.

**Tert-butyl 2-(pyridin-2-yl)-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)acetate (12a)**

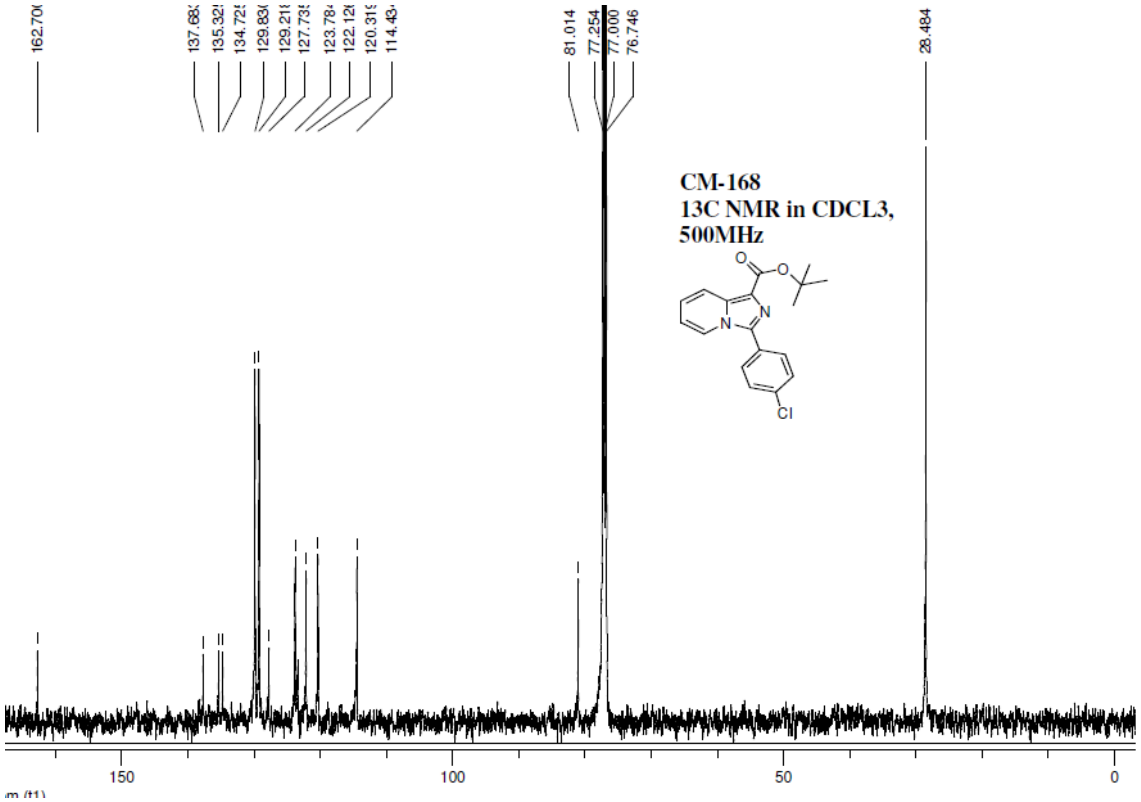


(Eluent: 15% EtOAc/hexane); 92% yield(80 mg); $^1$H NMR (500 MHz, $CDCl_3$) *δ* 8.49 (d, *J* = 4.5 Hz, 1H), 7.62(d, *J* = 7.5 Hz, 1H), 7.46(d, *J* = 7.5 Hz, 1H), 7.12 (t, *J* = 7.0 Hz, 1H), 5.20 (s, 1H), 1.41-1.30 (m, 14H), 1.17 (d, *J* = 7.0 Hz, 7H), 1.0 (s, 3H), 0.55 (s, 3H). $^{13}$C NMR (125 MHz, $CDCl_3$) *δ* 169.7, 158.1, 148.3, 136.1, 122.2, 121.3, 89.7, 81.0, 59.6, 59.3, 396, 32.9, 32.5, 27.4, 19.7, 16.6. IR (KBr) 2976, 2934, 1739, 1589, 1469, 1368, 1255, 1218, 1153, 1058, 994, 958, 924, 845, 801, 756. HRMS calcd for $C_{20}$ $H_{32}$ $O_3$ $N_2$ Na: 371.2311. Found: 371.2316.

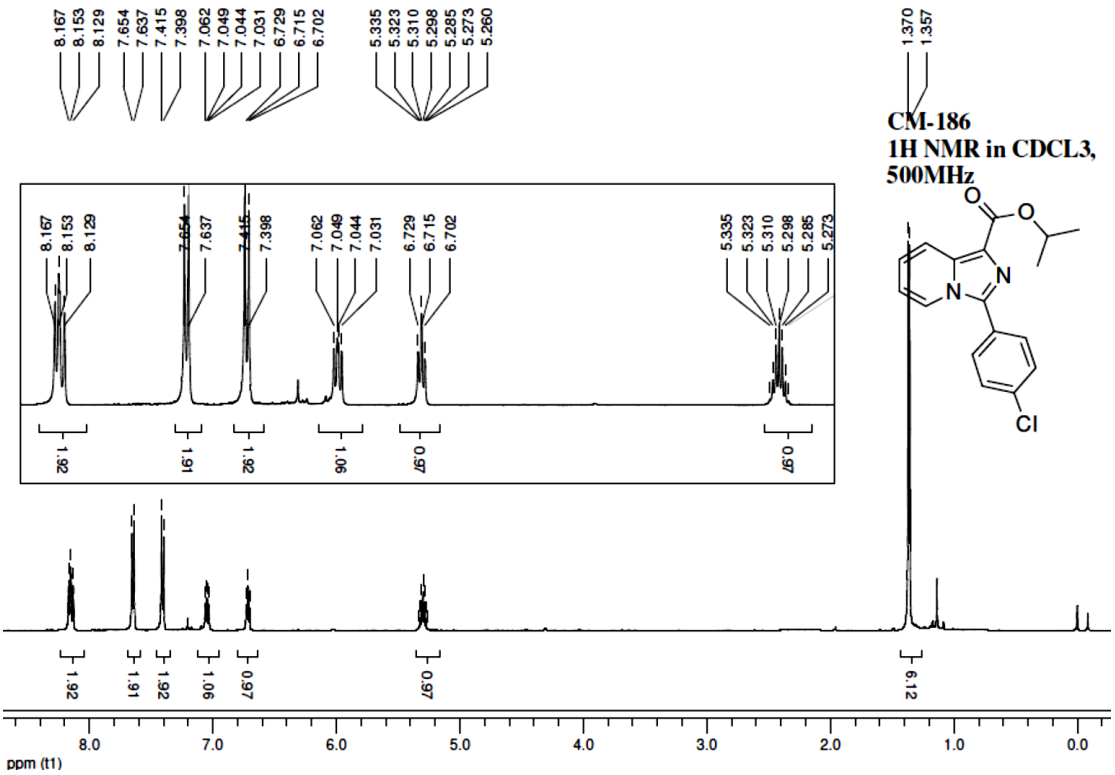
# $^{1}H$ &$^{13}$ C NMR spectral data



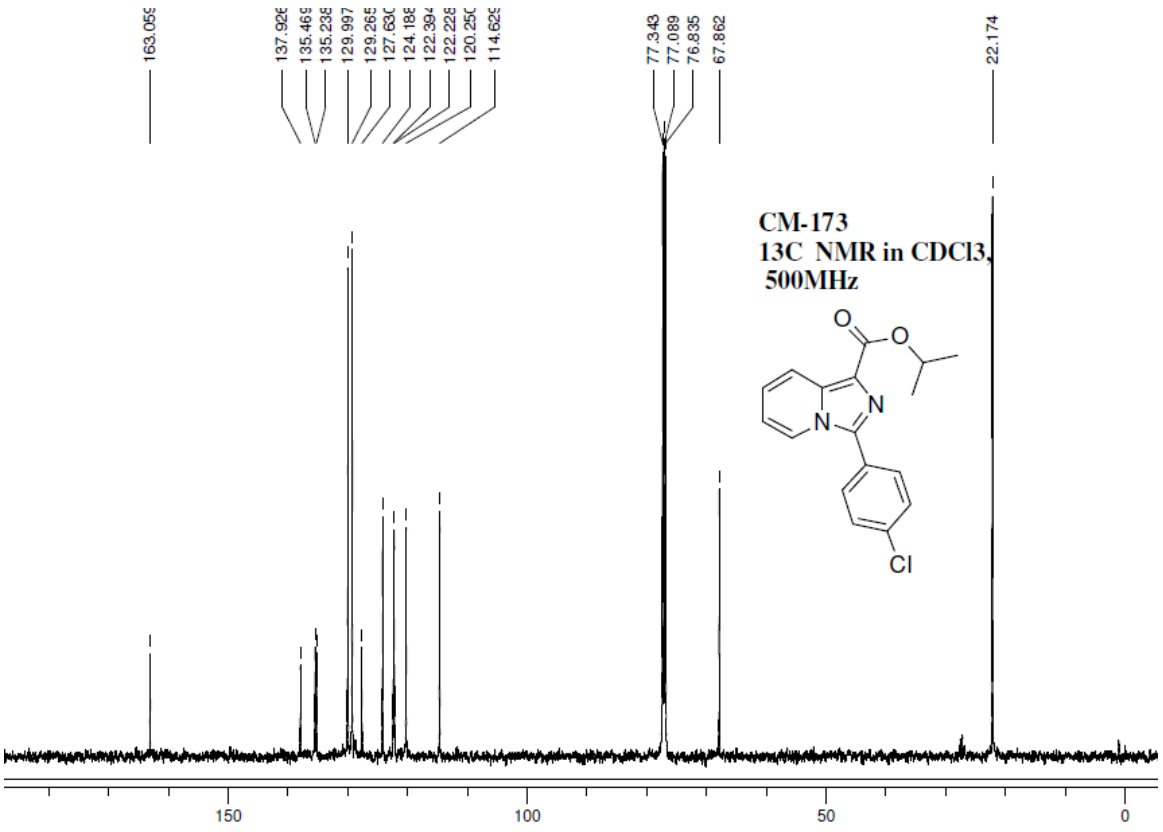

1H NMR of **3a**



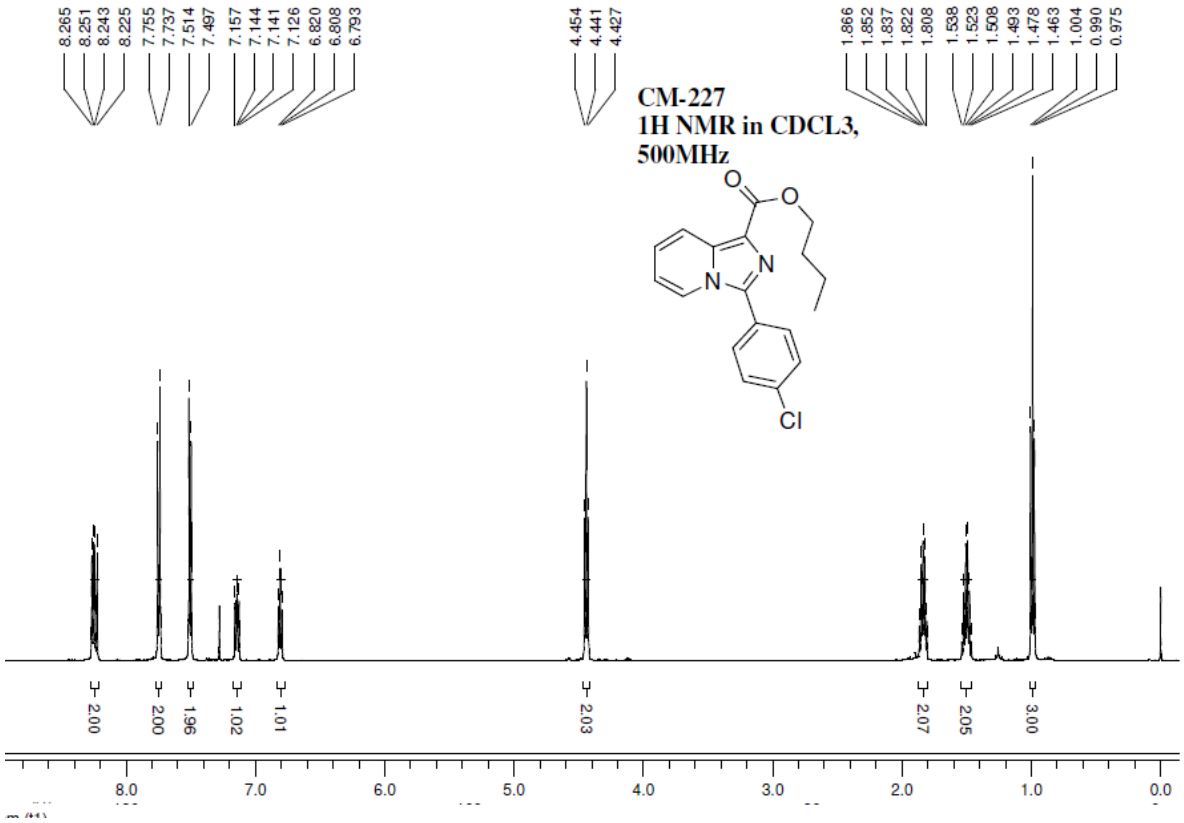

$^{13}$C NMR of **3a**



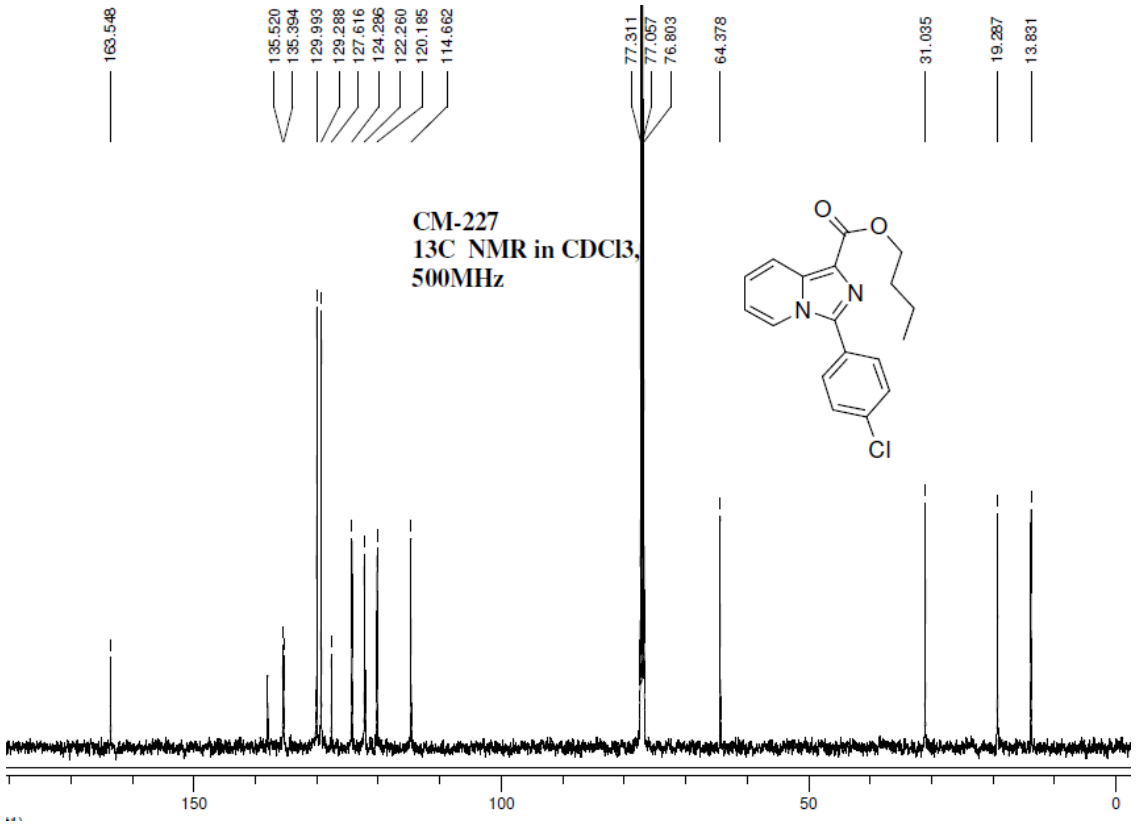

1H NMR of **3b**



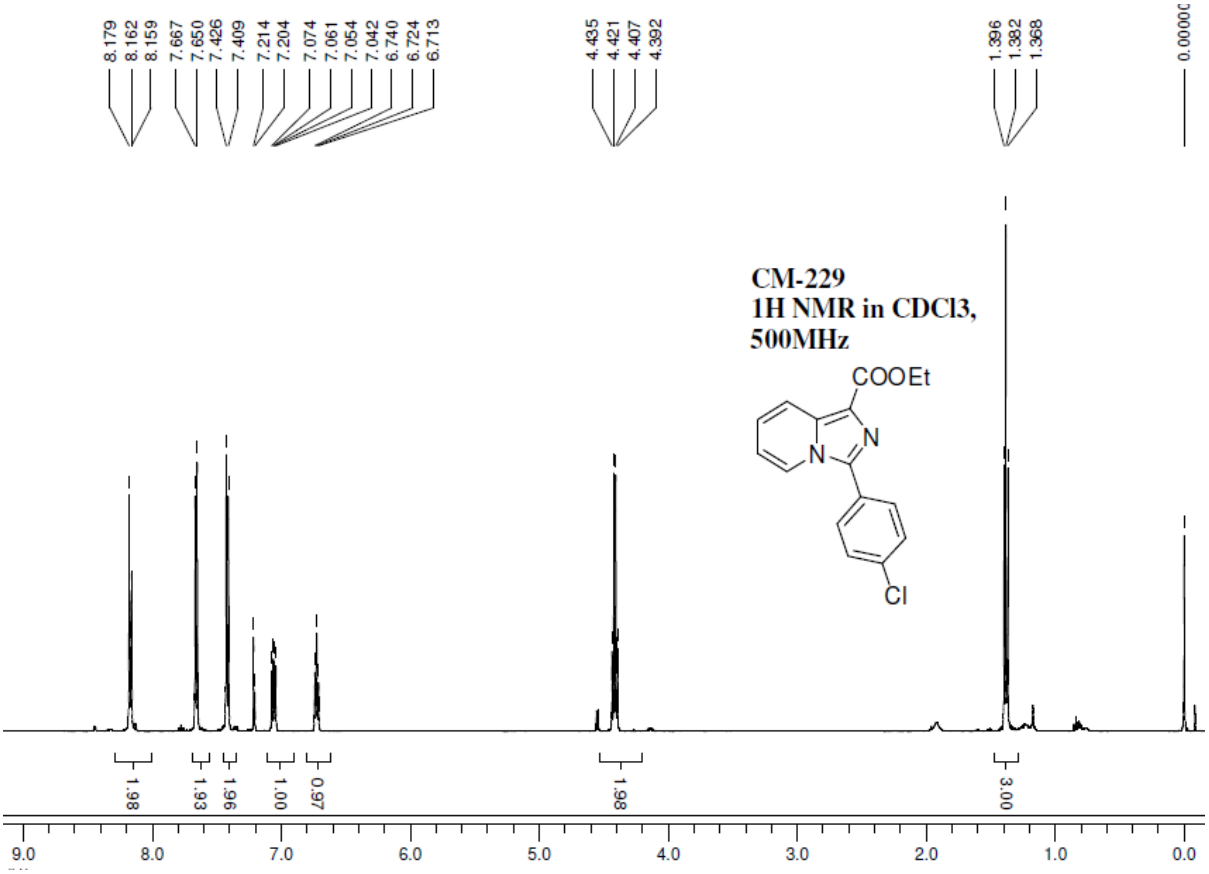

$^{13}$C NMR of **3b**



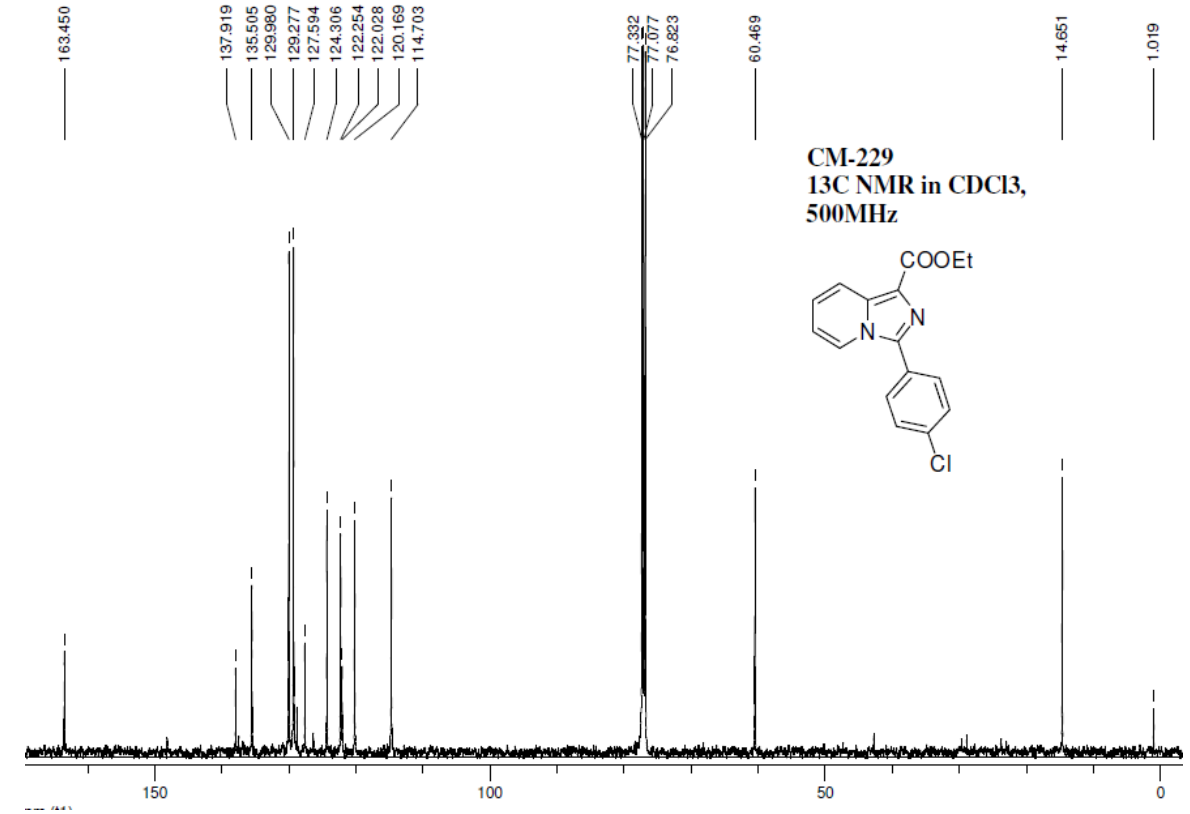

1H NMR of **3c**



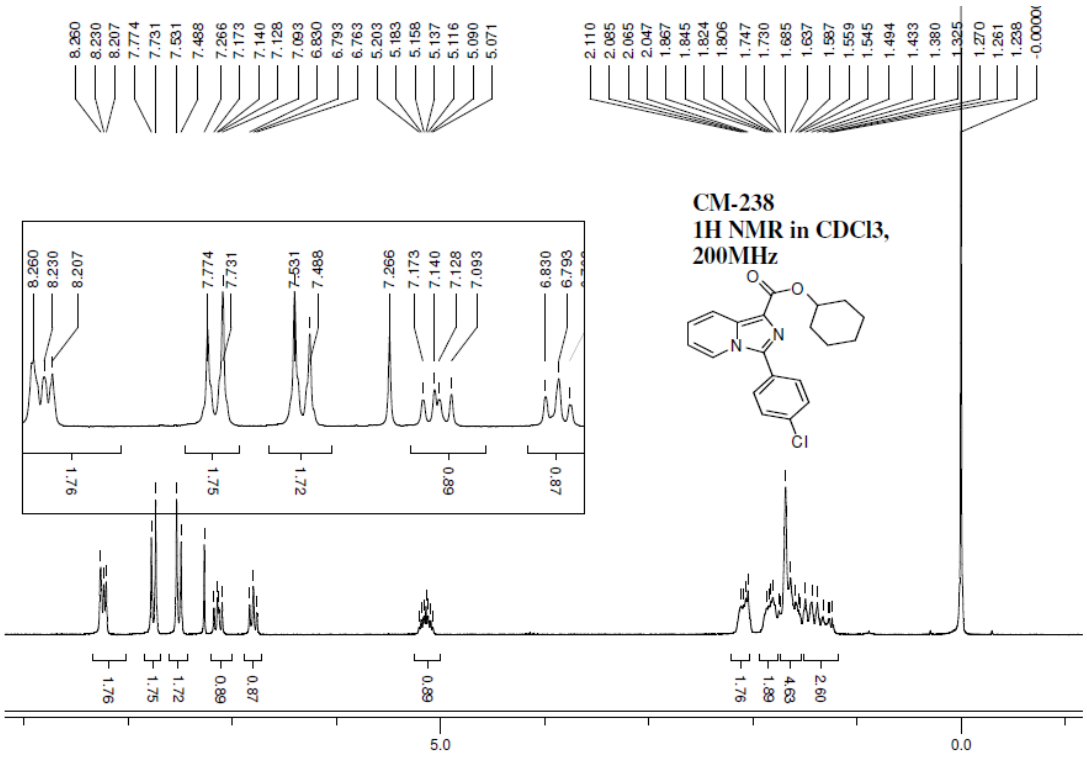

**$^{13}$C** NMR of **3c**



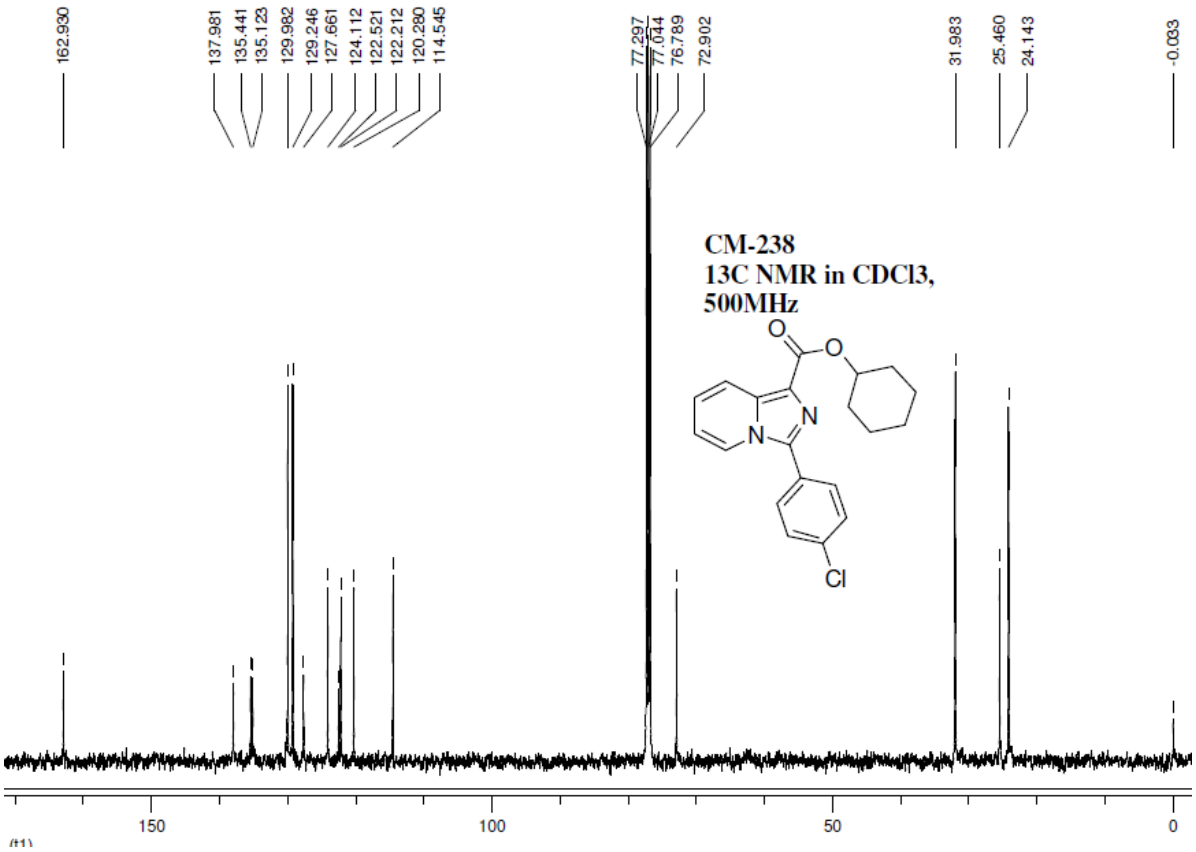

**1H NMR of 3d**



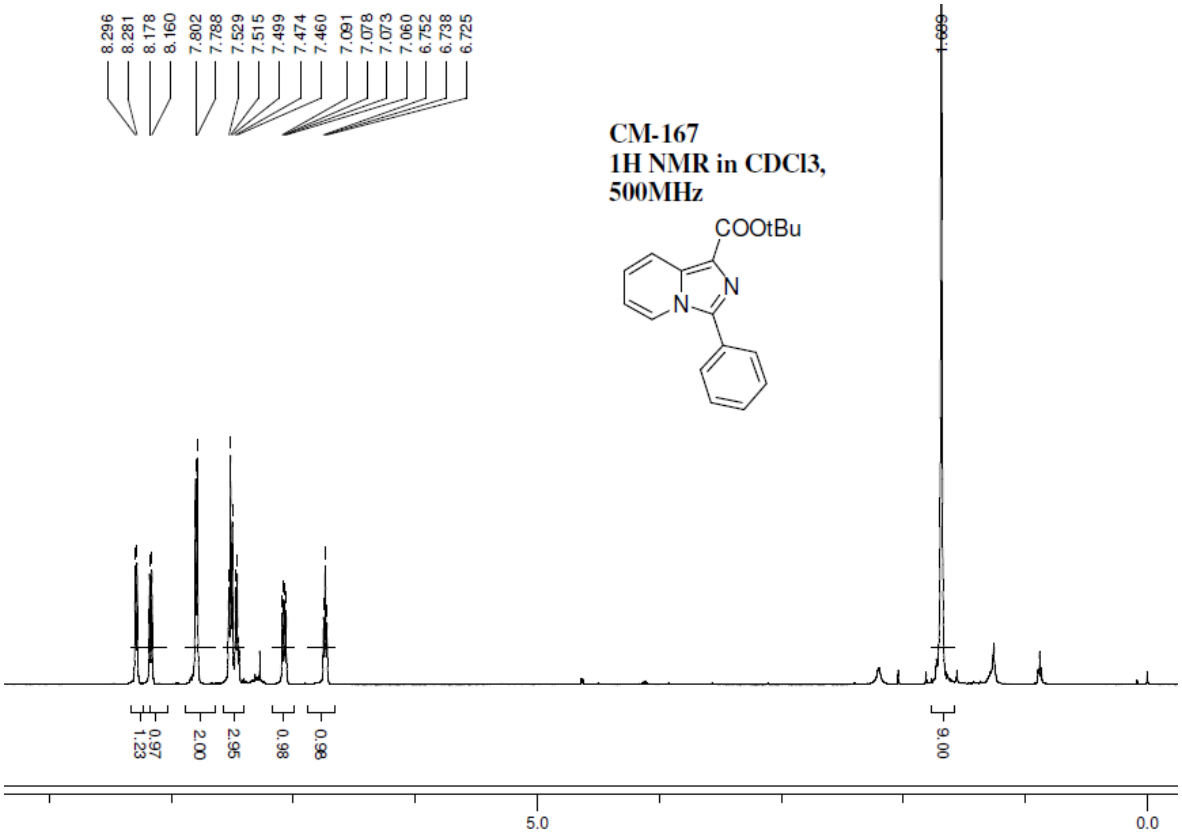

$^{13}$C NMR of **3d**



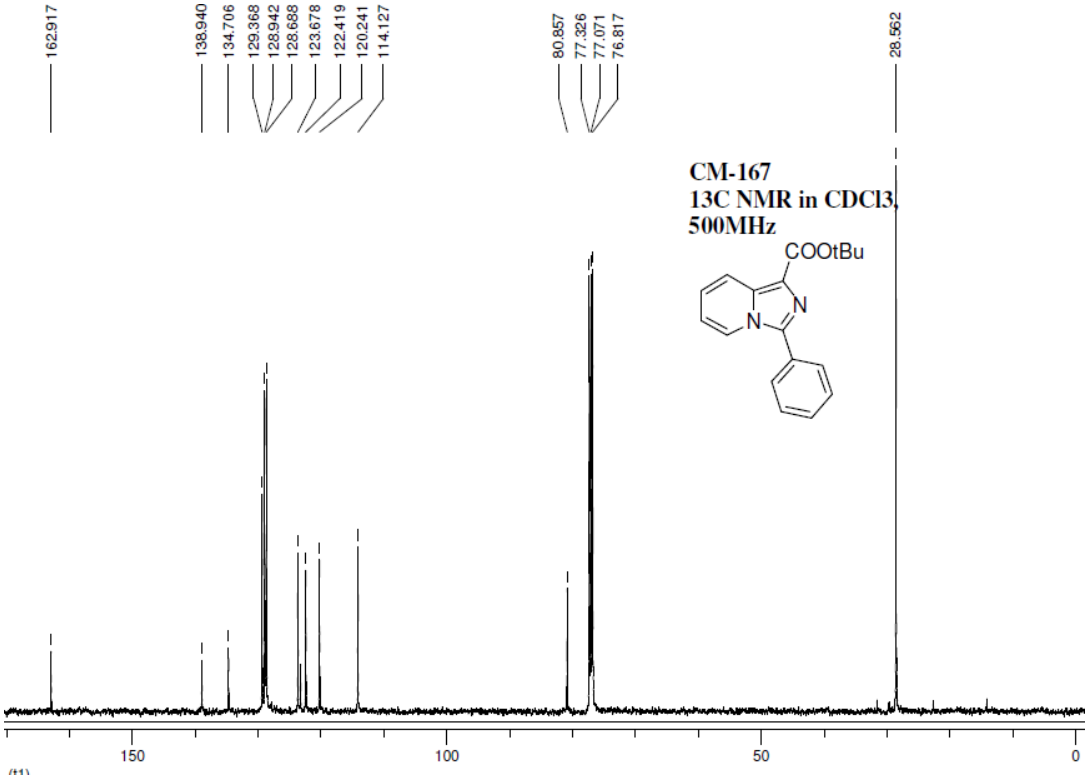

1H NMR of **3e**



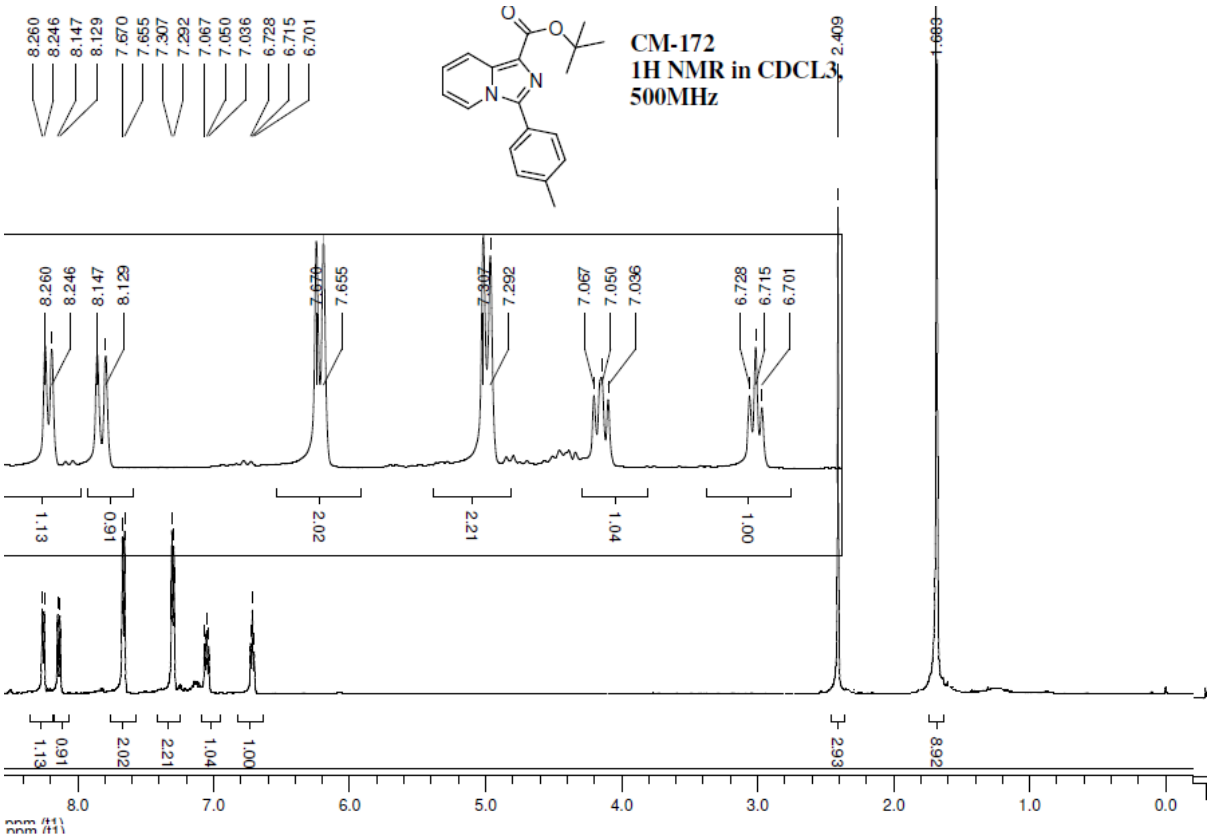

$^{13}$C NMR of **3e**



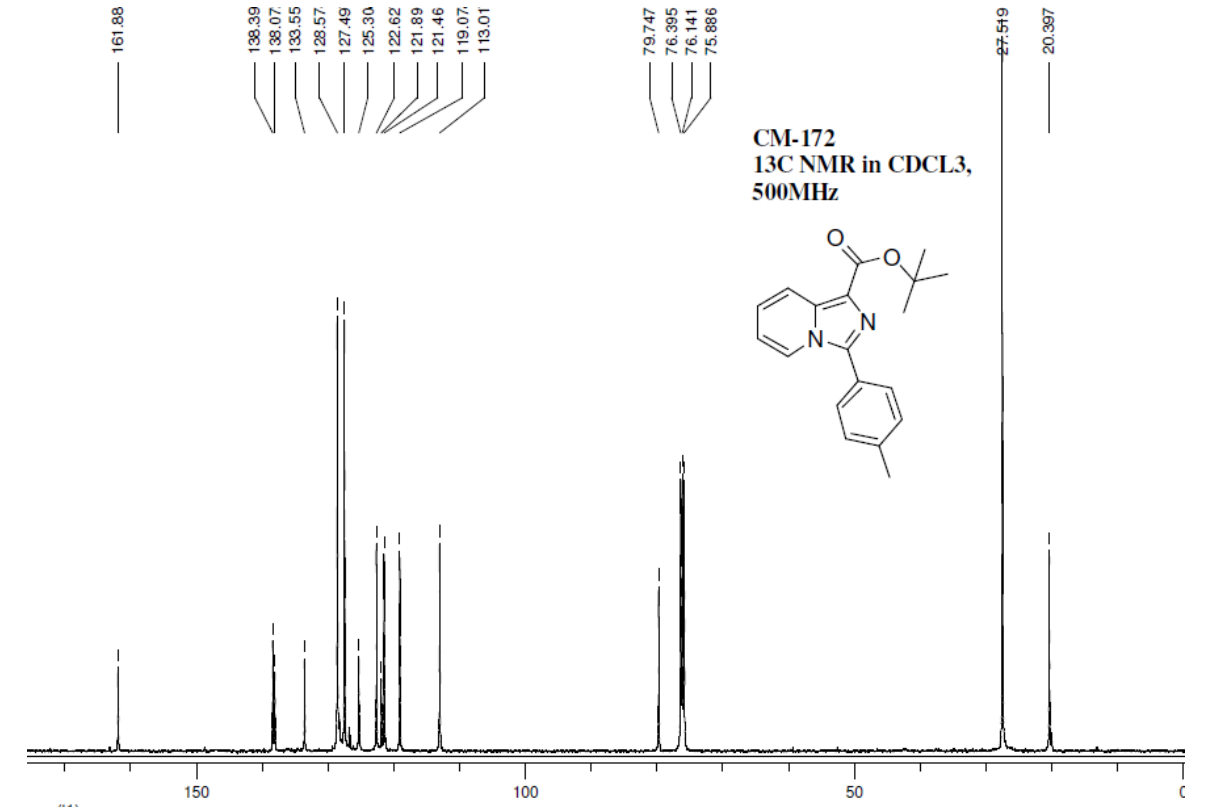

1H NMR of **4a**



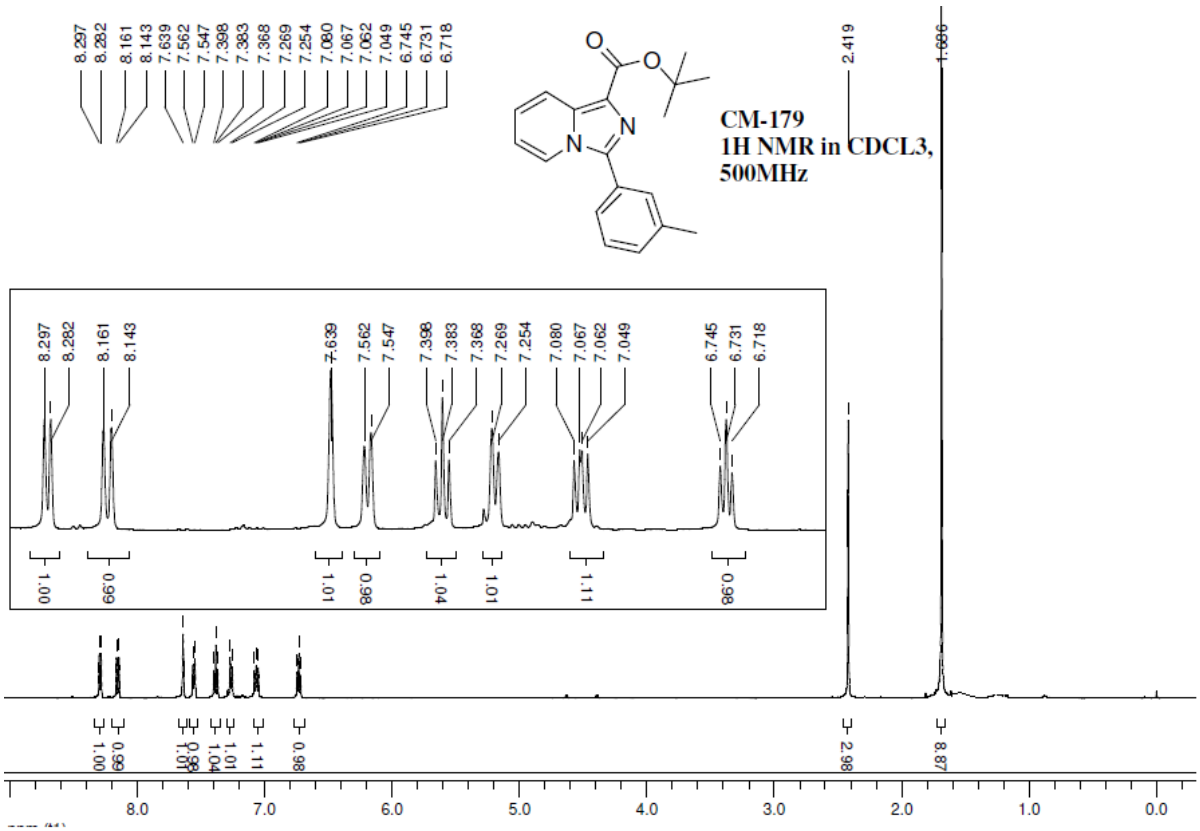

$^{13}$C NMR of **4a**



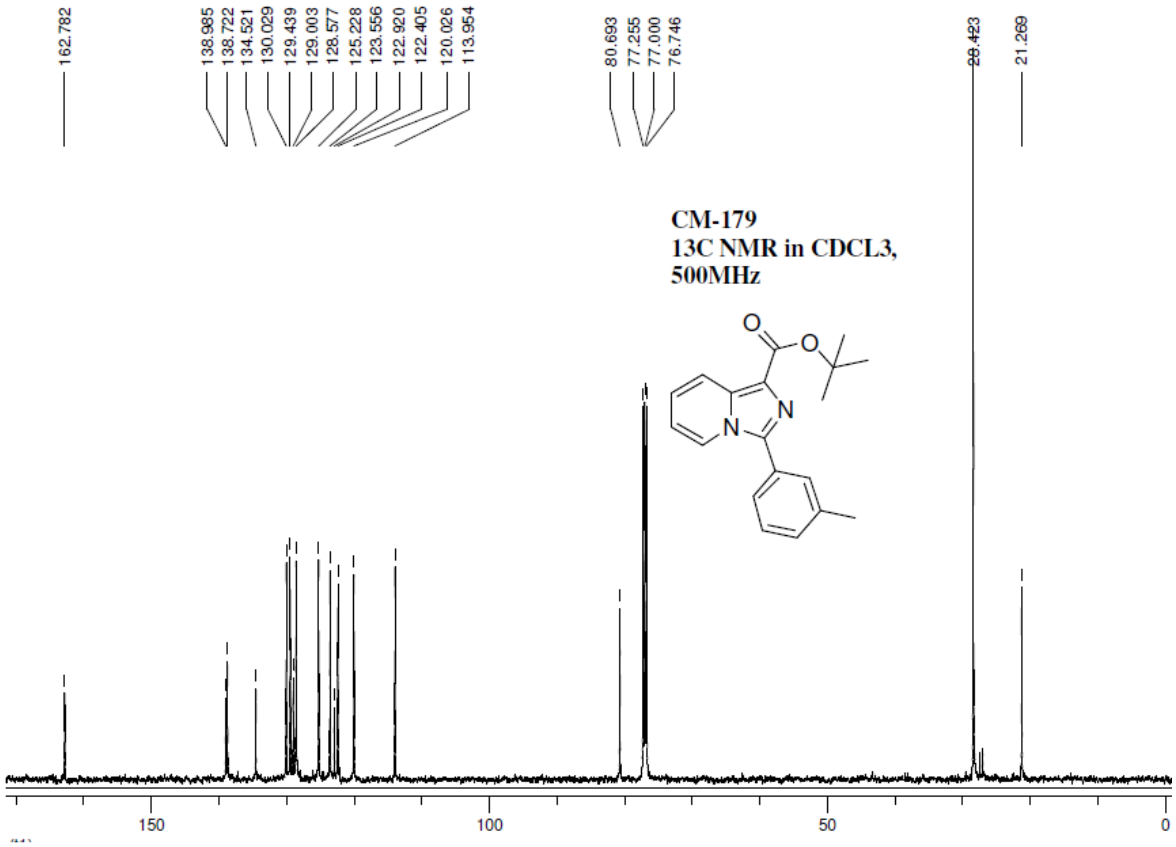

1H NMR of **4b**



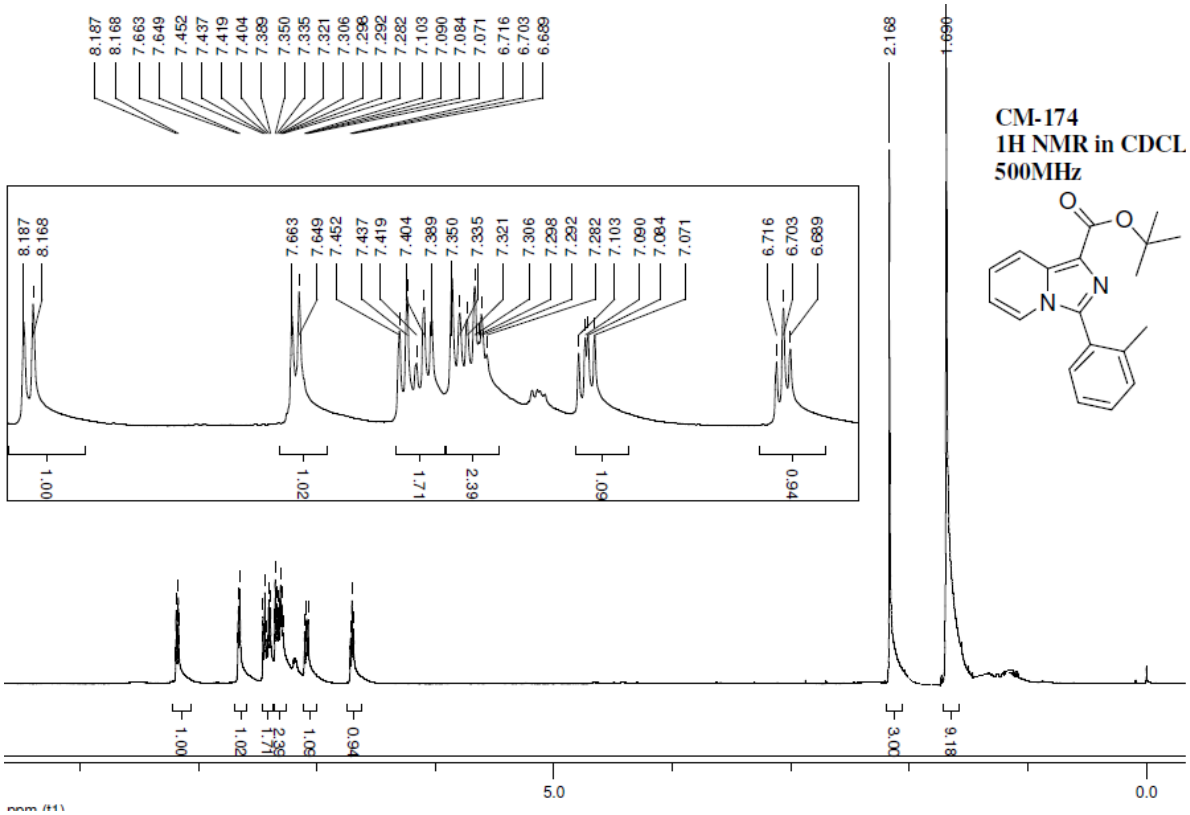

$^{13}$C NMR of **4b**



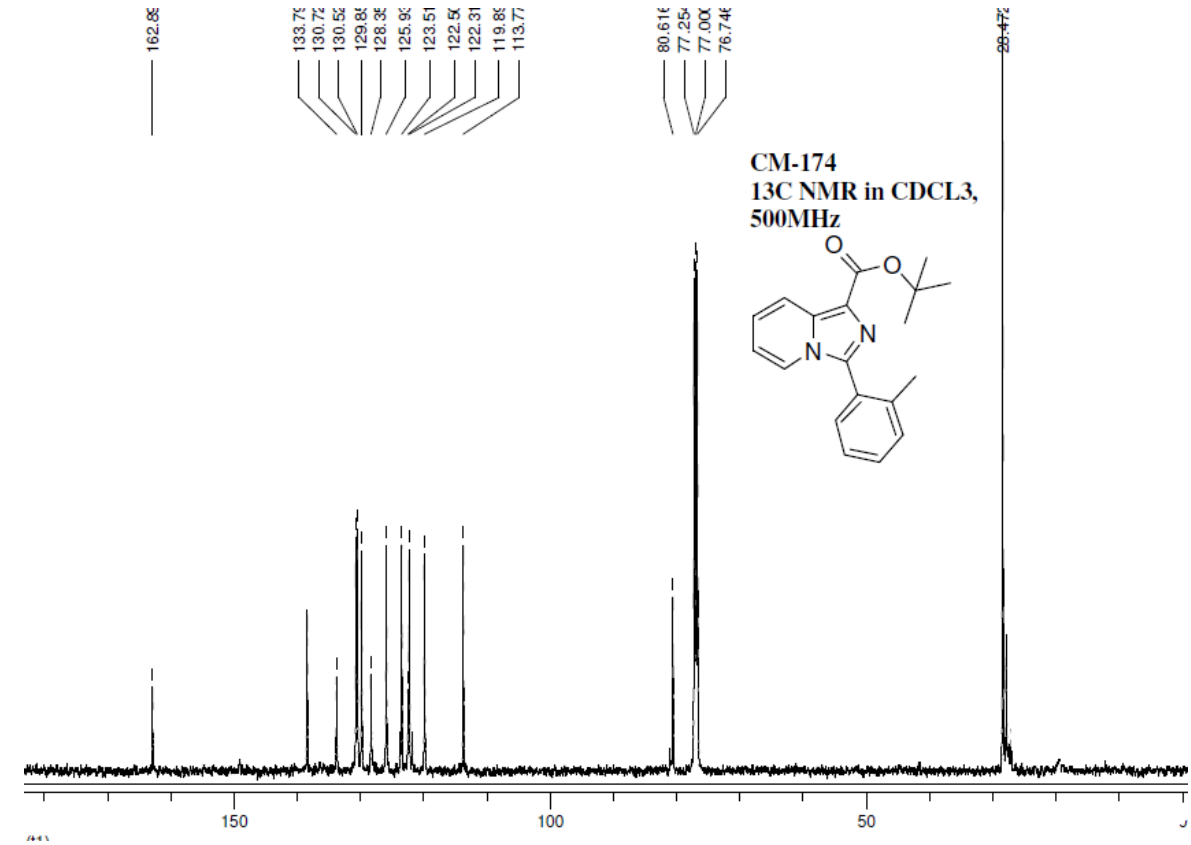

1H NMR of **4c**



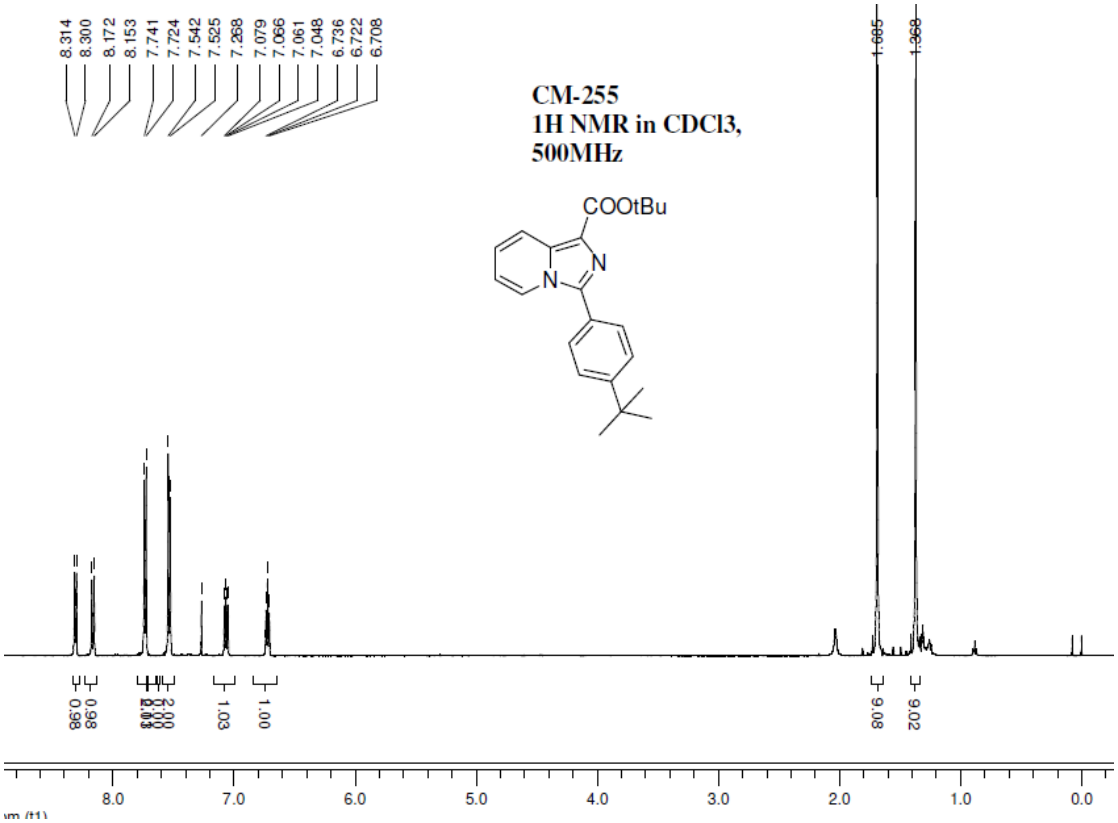

$^{13}$C NMR of **4c**



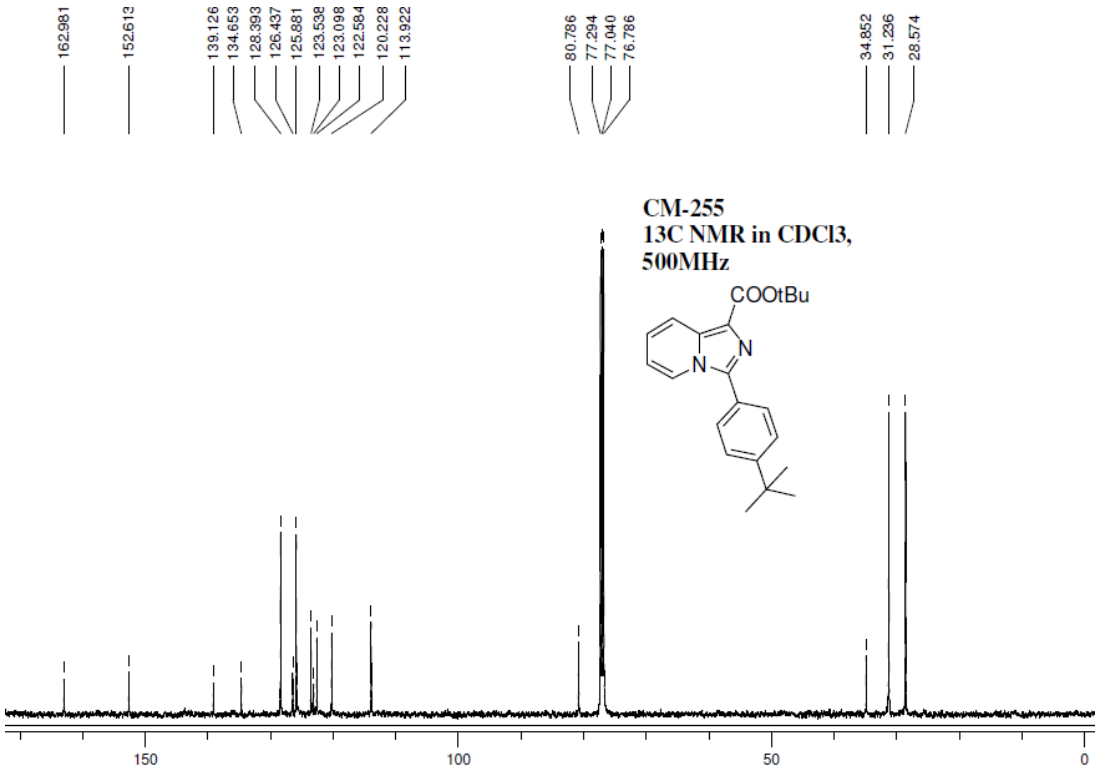

$^{1}$H NMR of **4d**



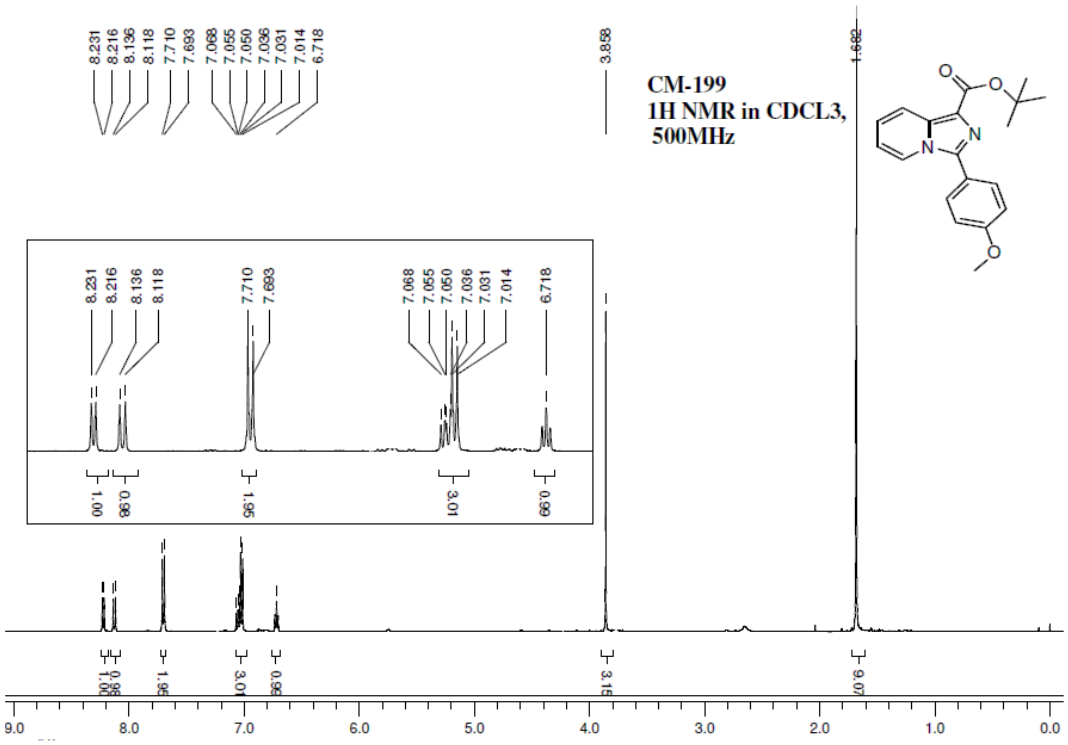

13C NMR of **4d**



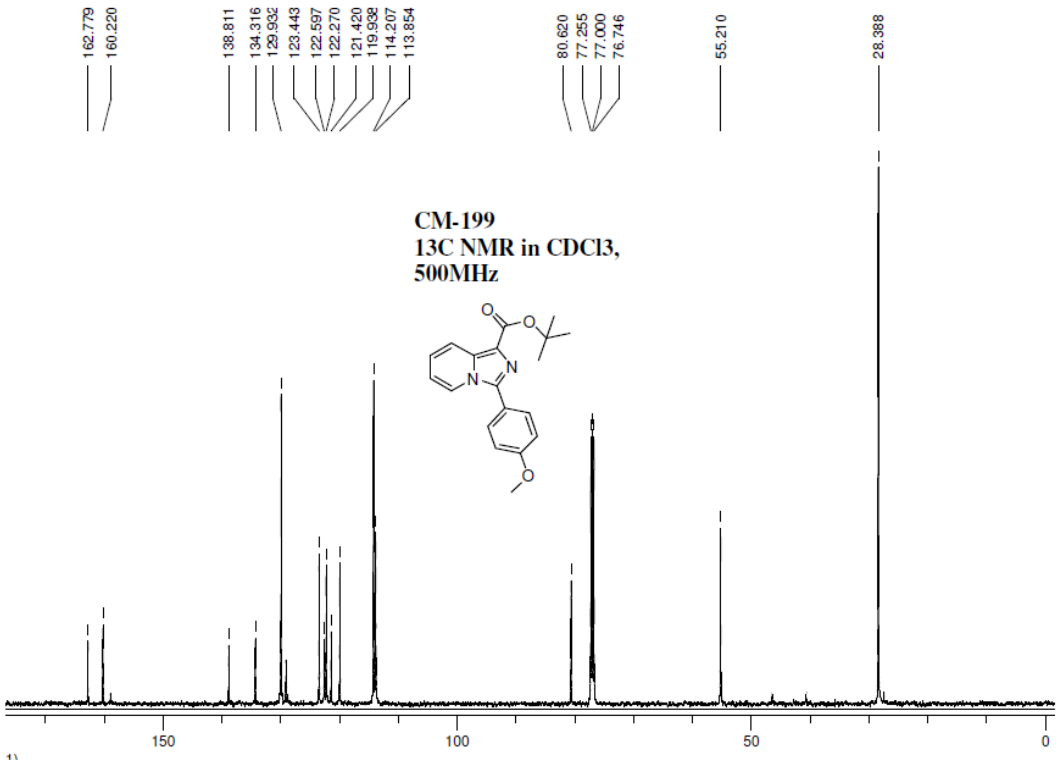

1H NMR of **4e**



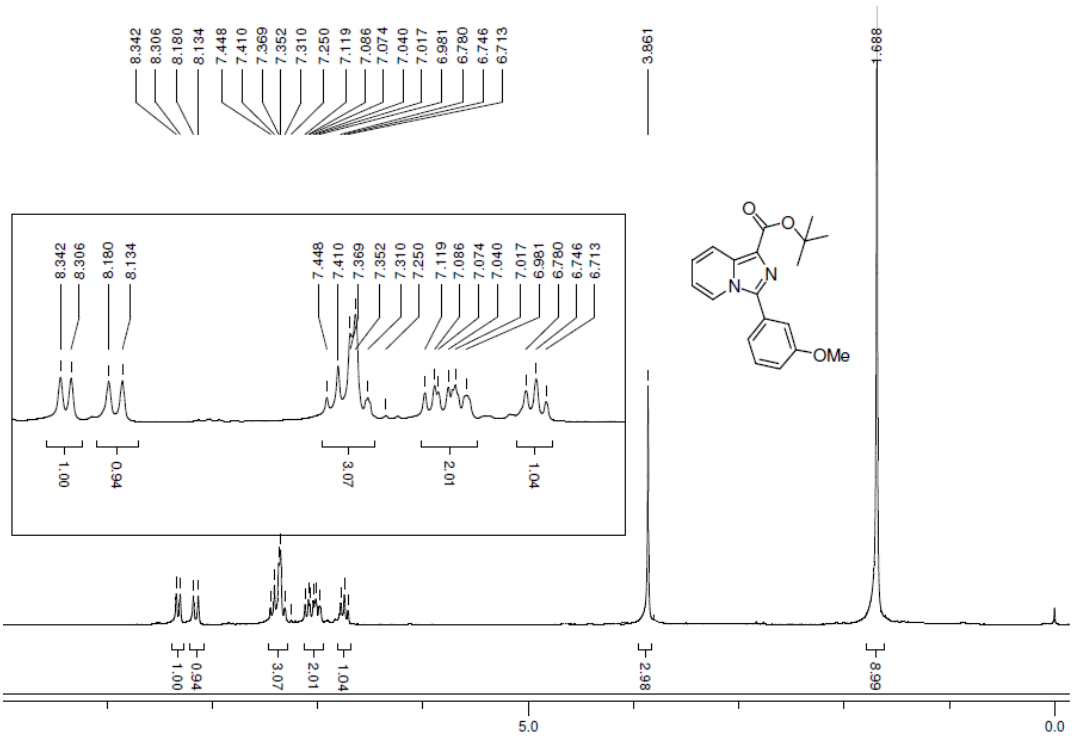

**13C NMR of 4e**



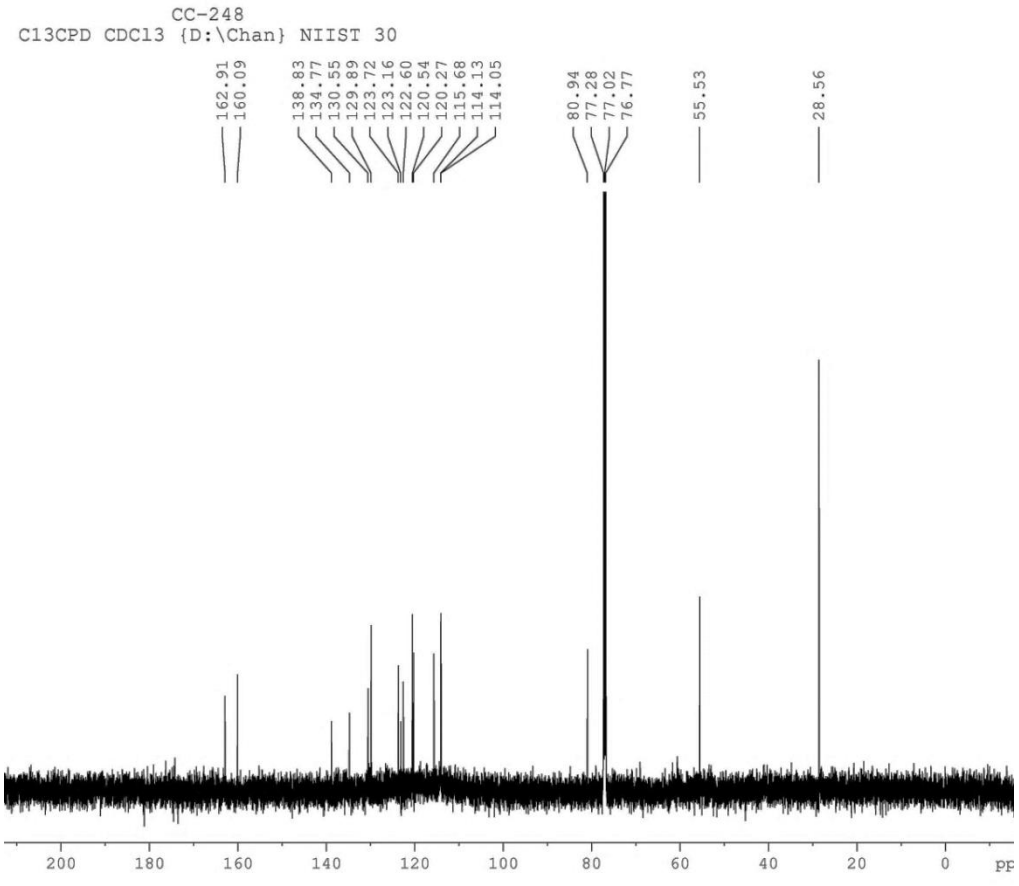

1H NMR of **4f**



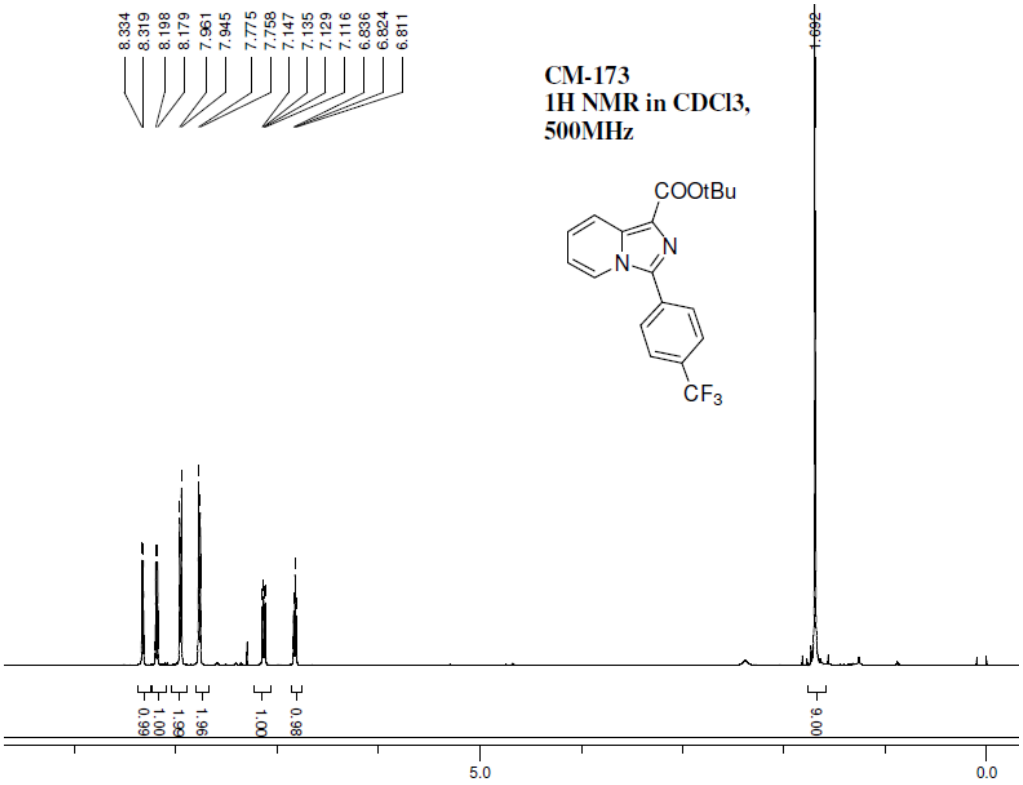

13C NMR of **4f**



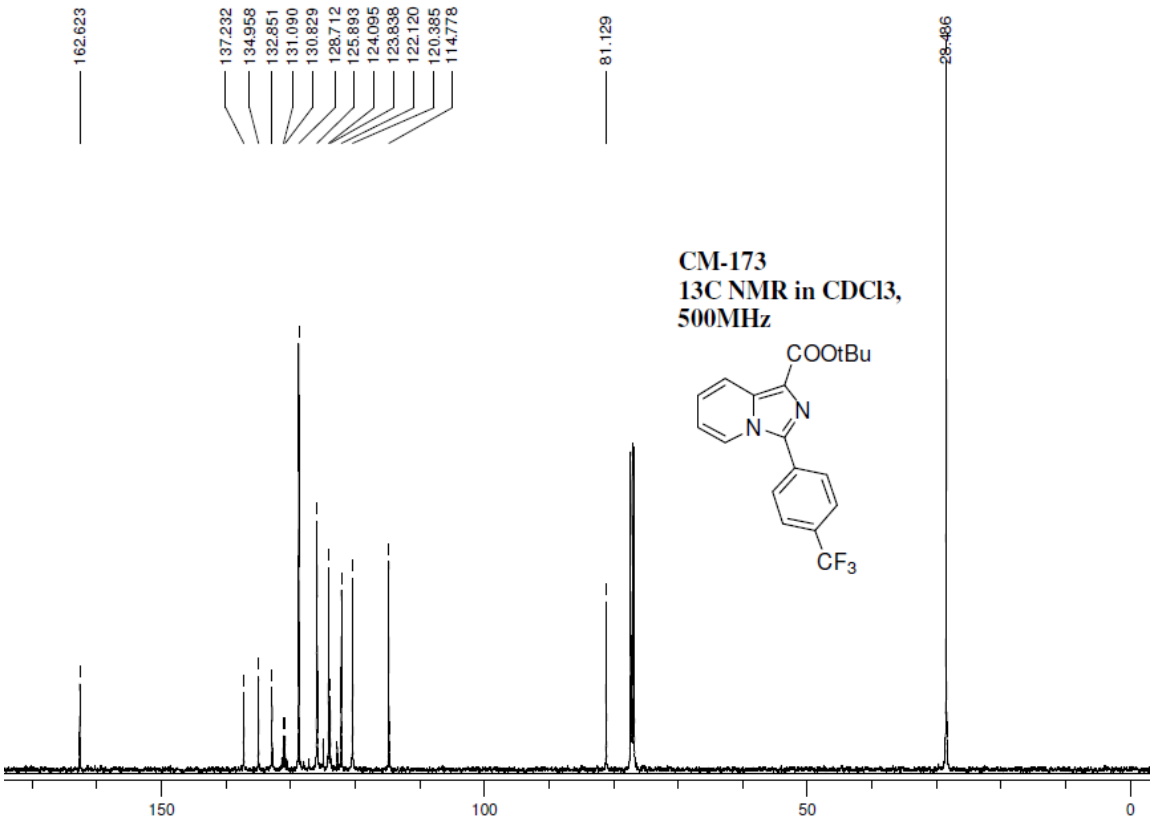

1H NMR of **4g**



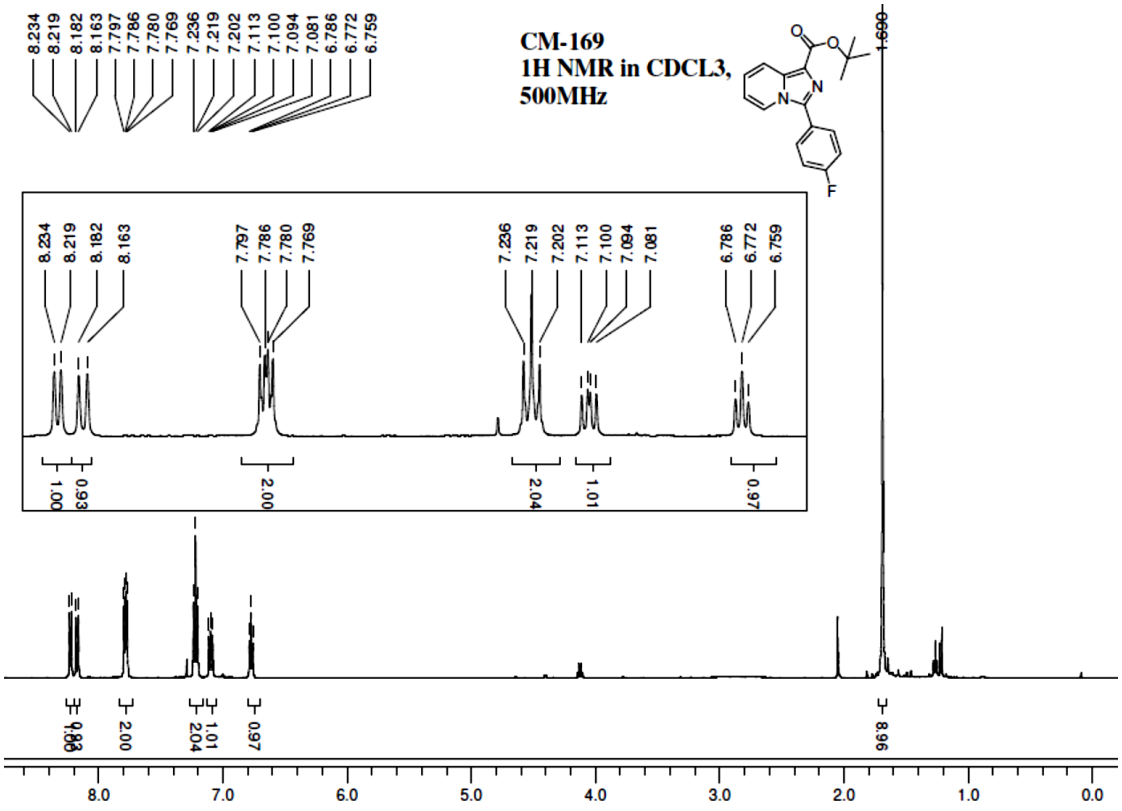

13C NMR of **4g**



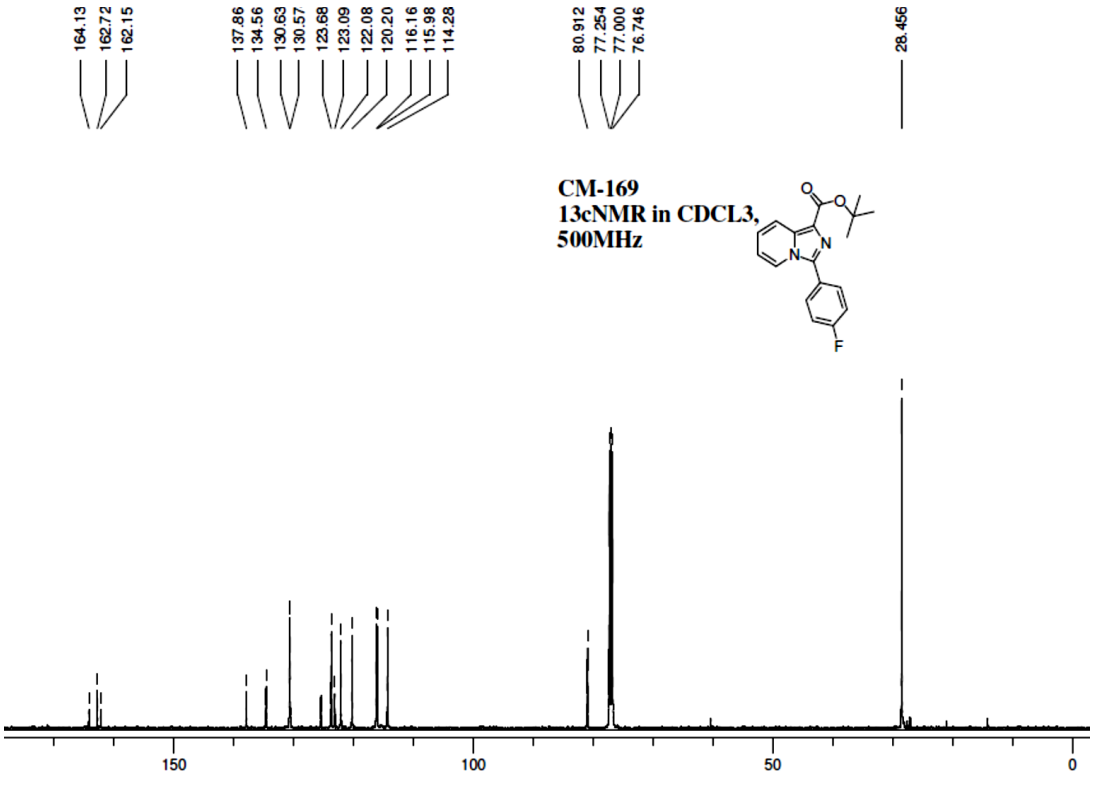

**1H NMR of 4h**



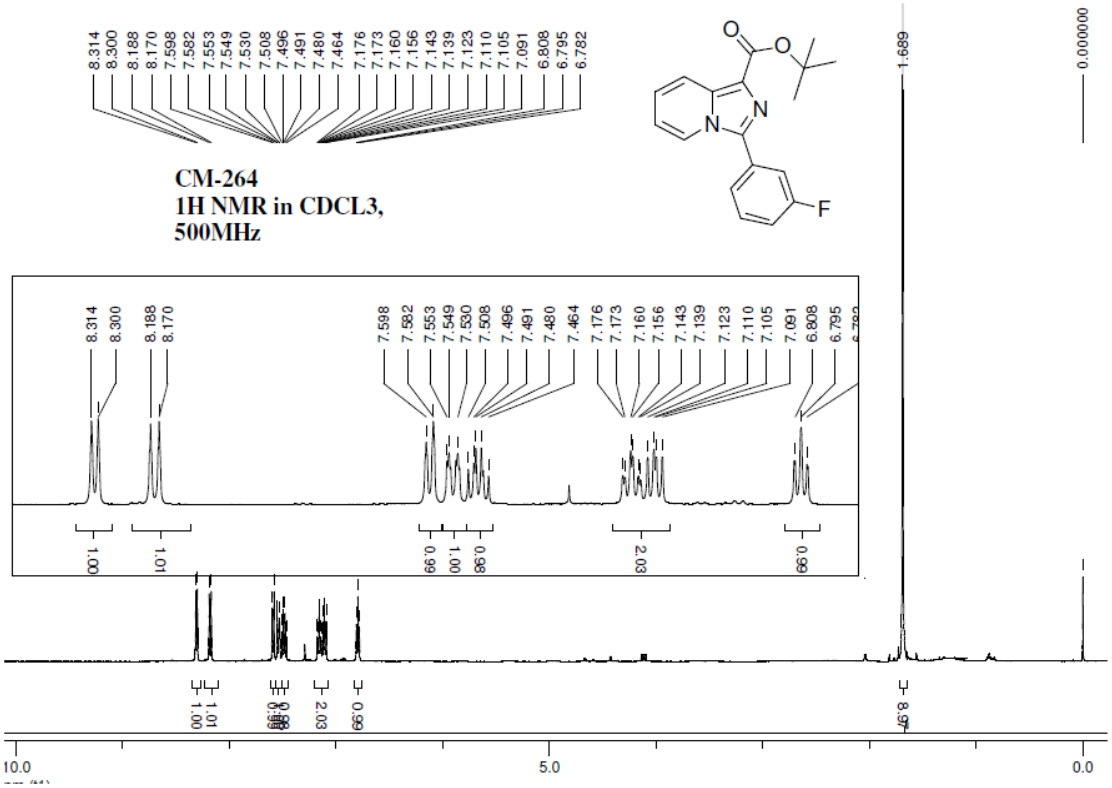

13C NMR of **4h**



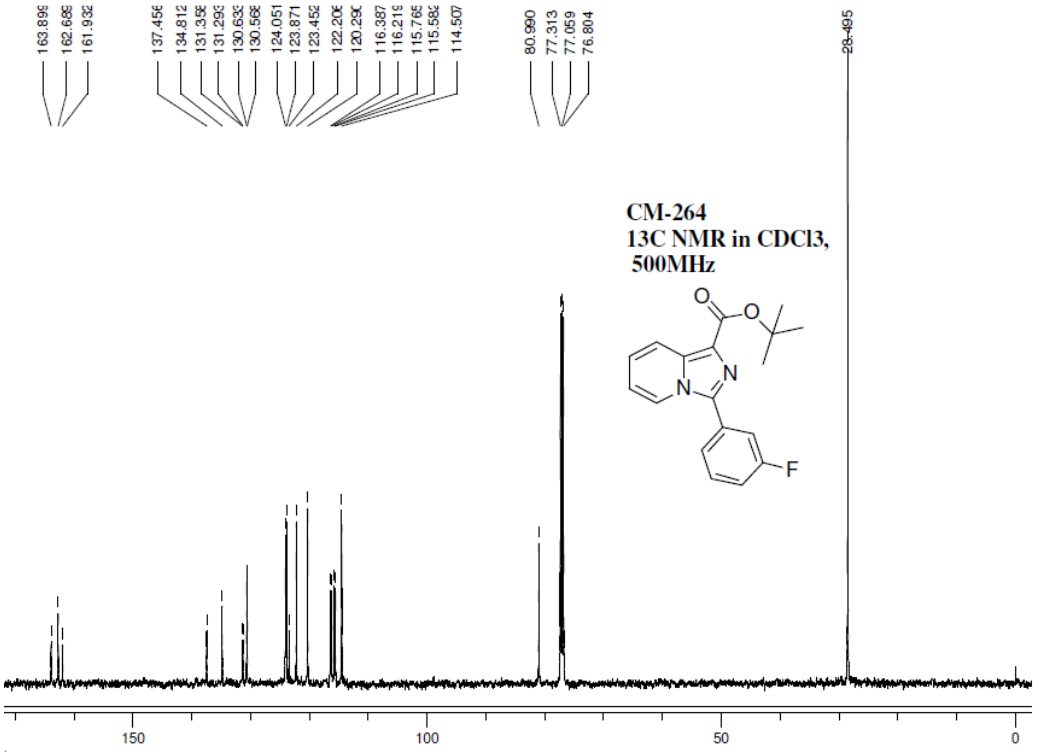

**1H NMR of 4i**



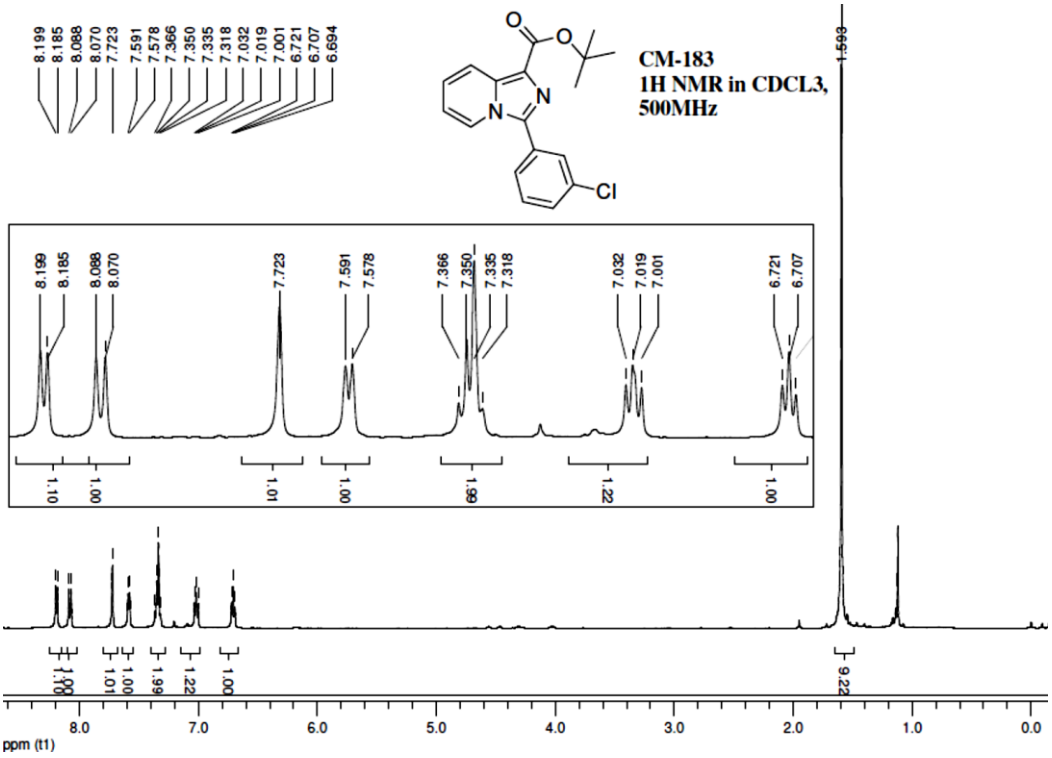

**13C NMR of 4i**



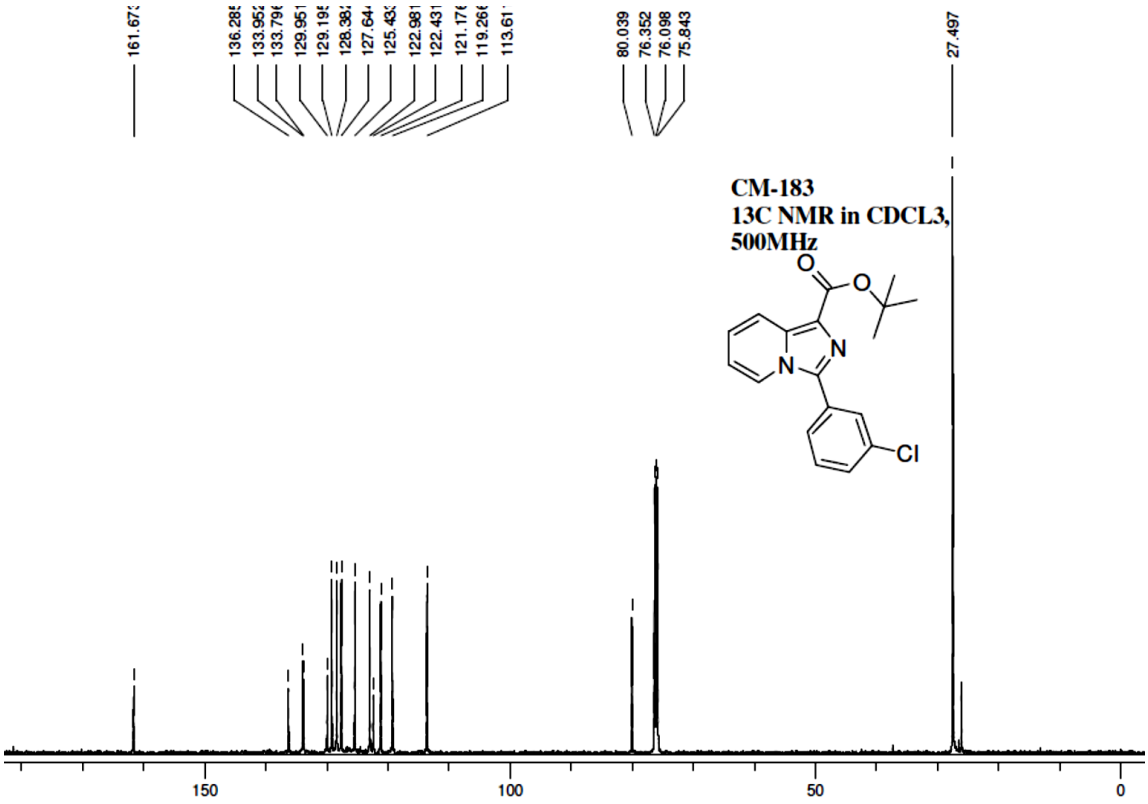

**1H NMR of 4j**



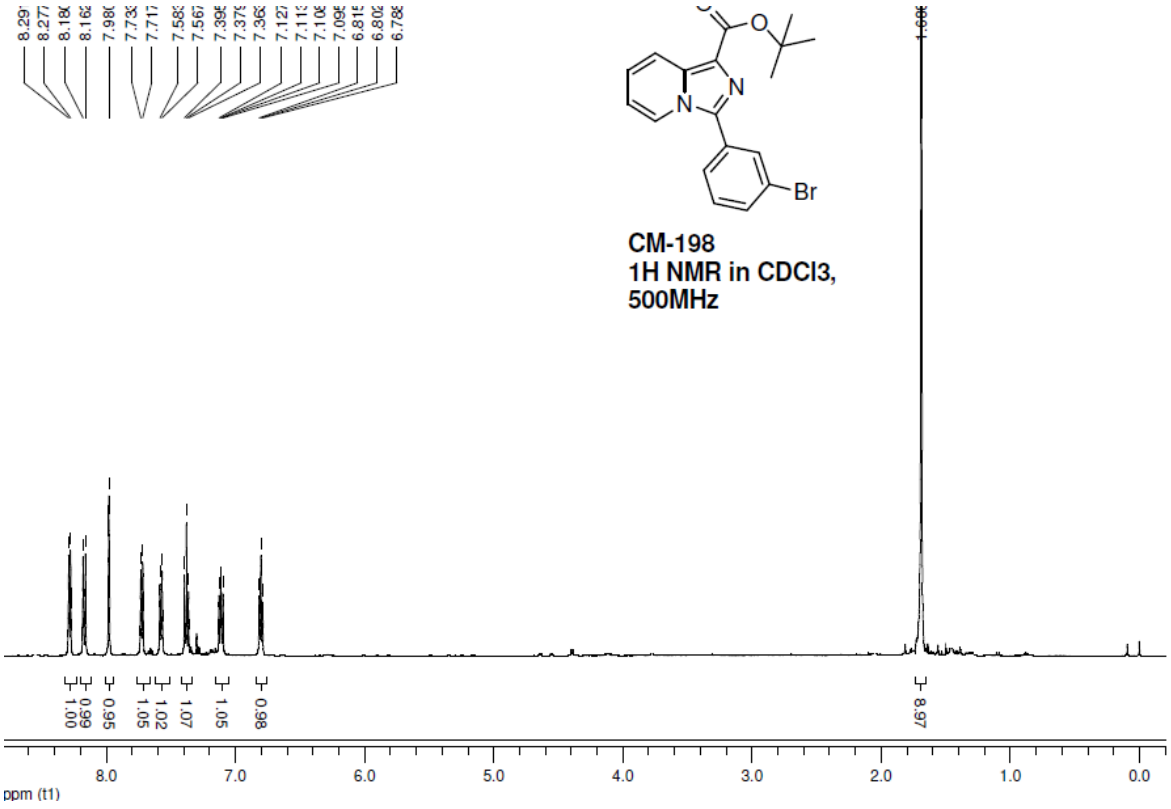

**13C NMR of 4j**



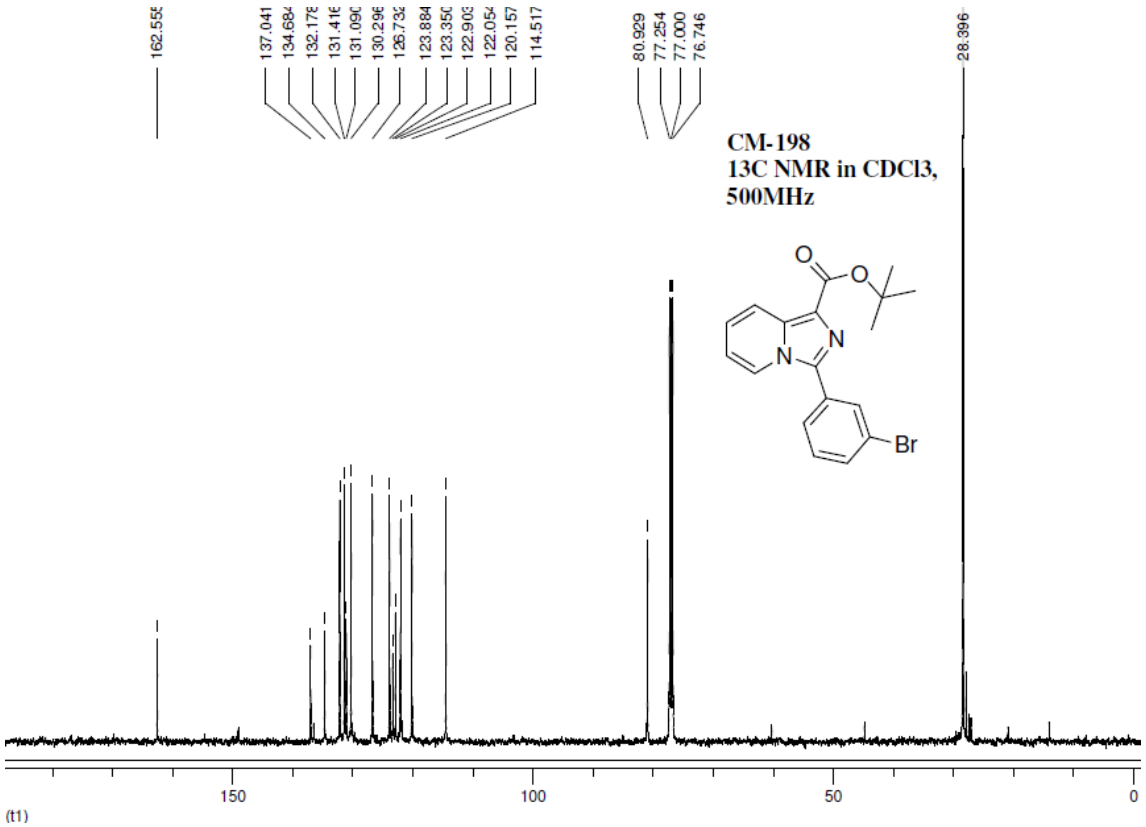

**1H NMR of 4k**



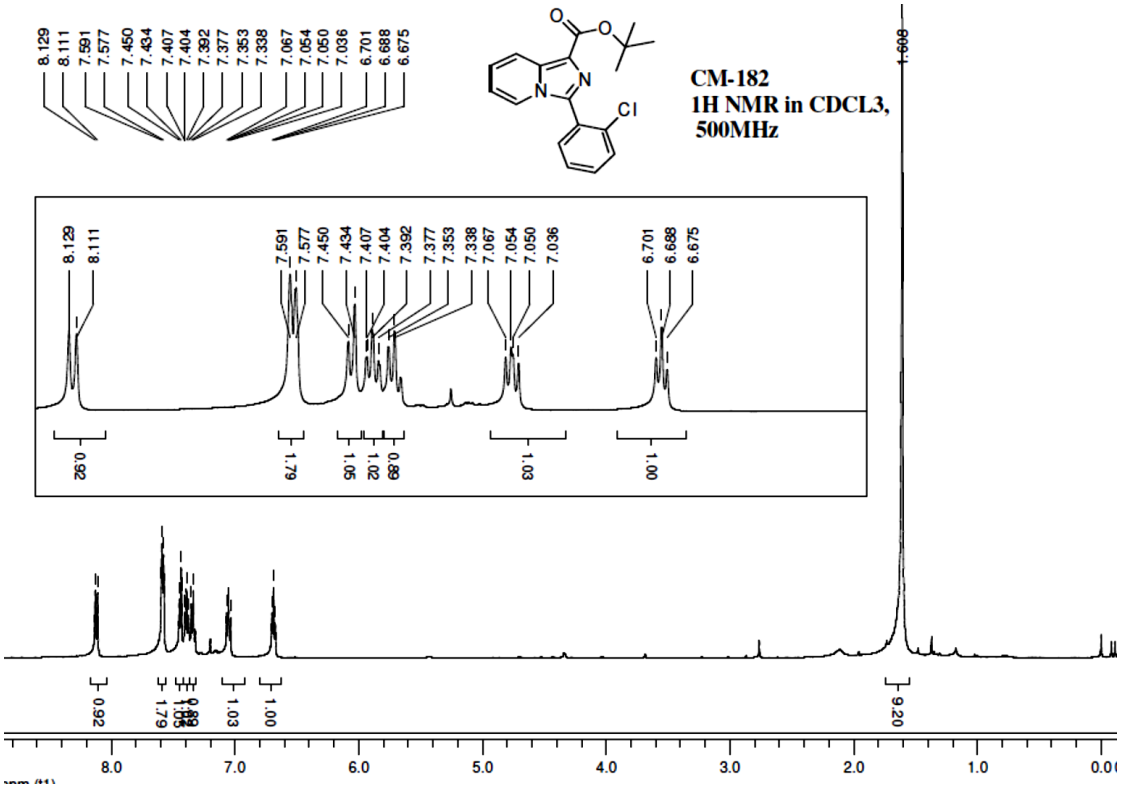

**13C NMR of 4k**



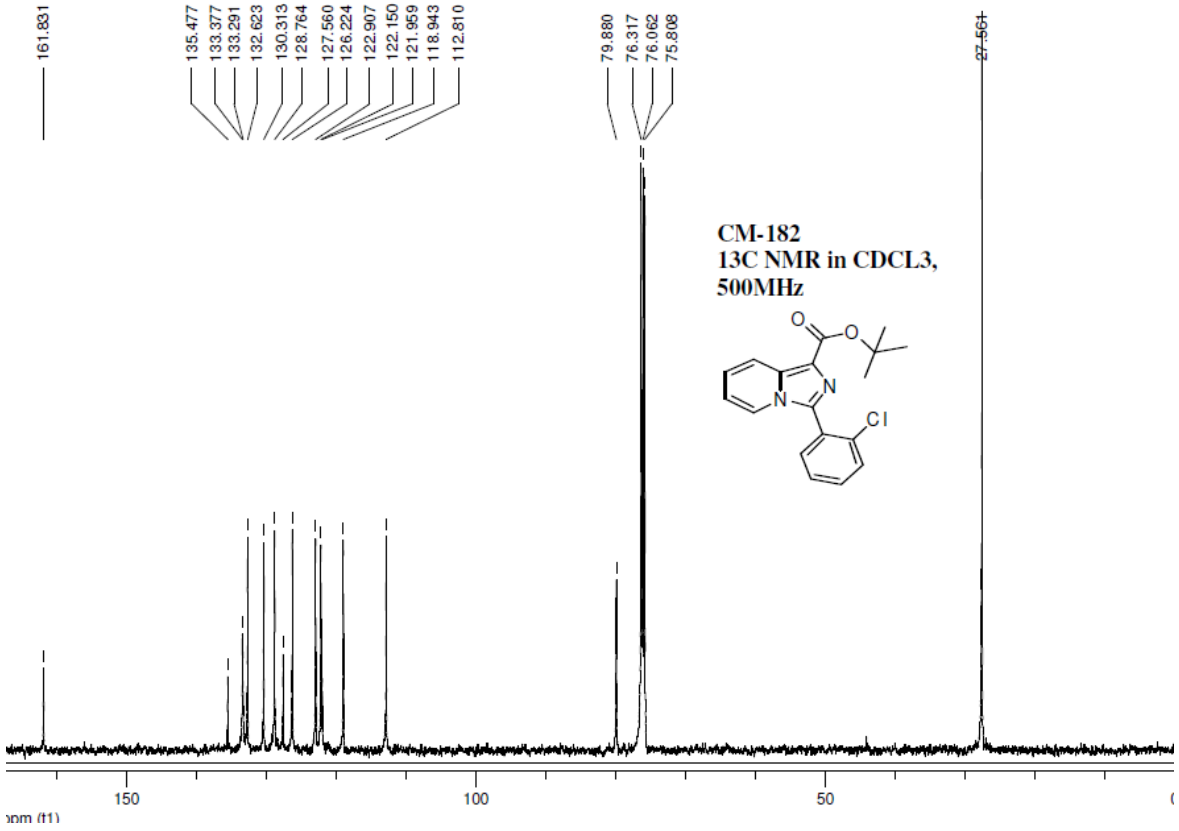

**1H NMR of 4l**



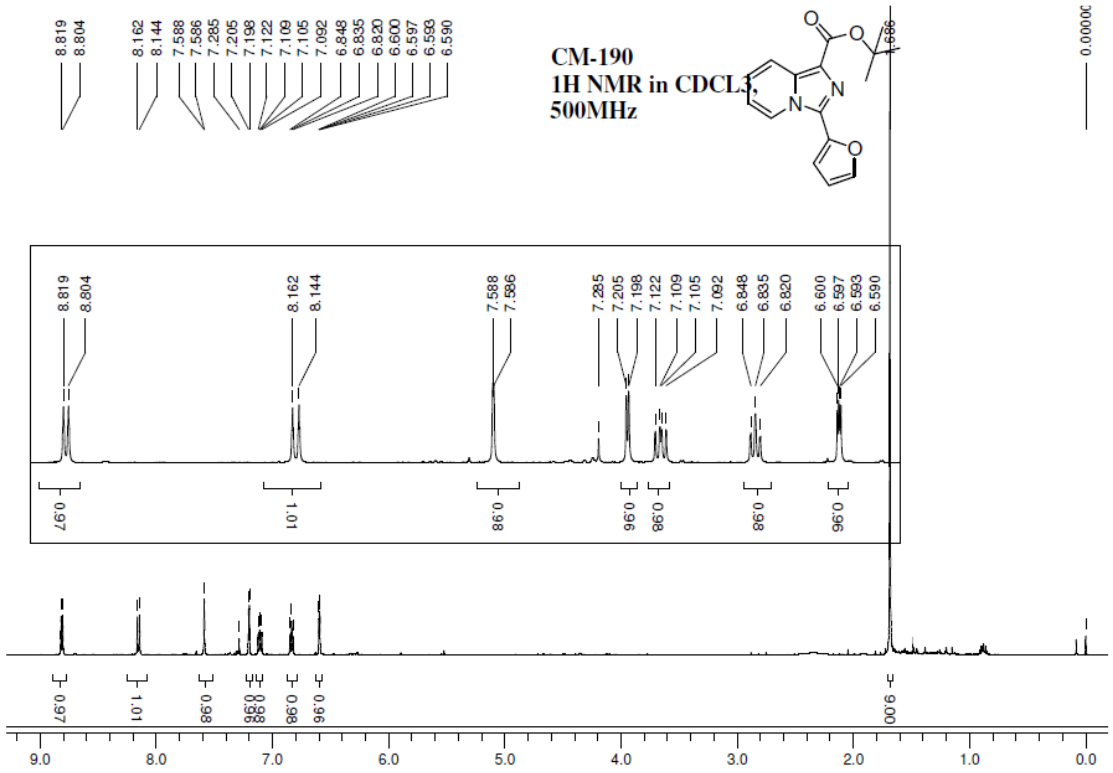

**13C NMR of 4l**



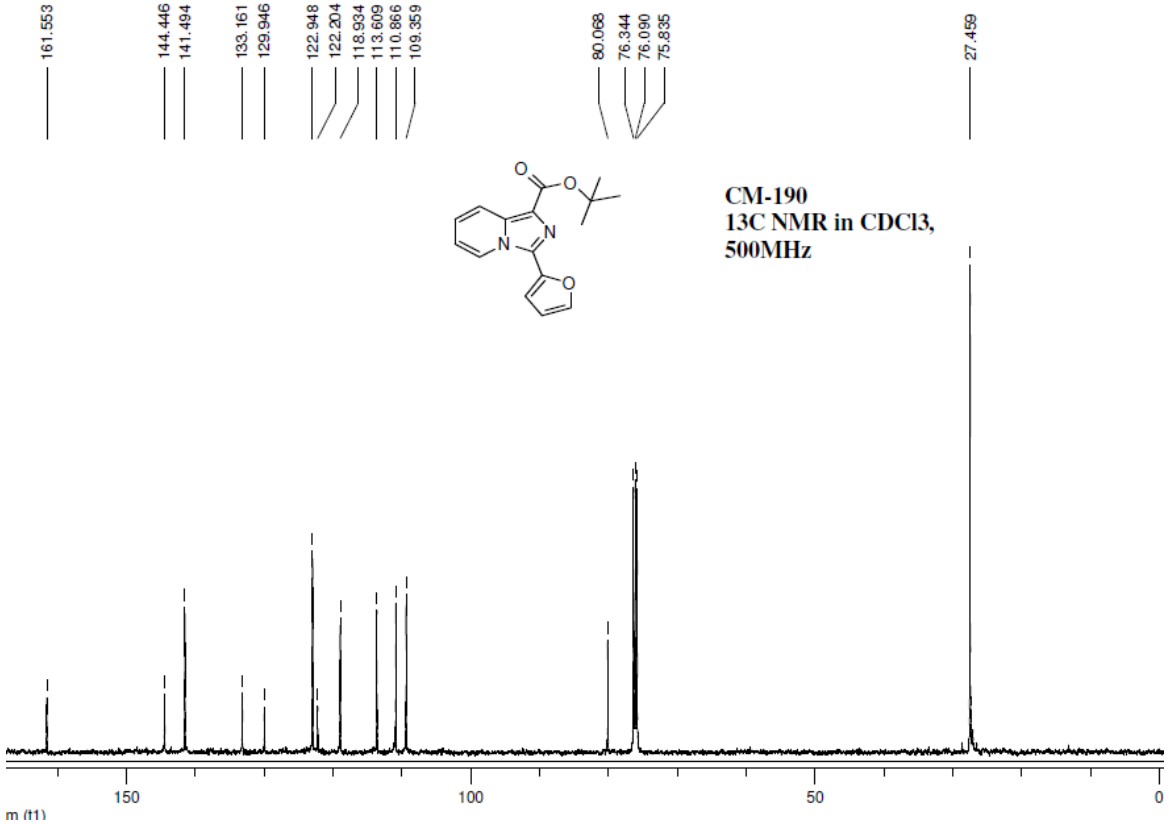

**1H NMR of 4m**



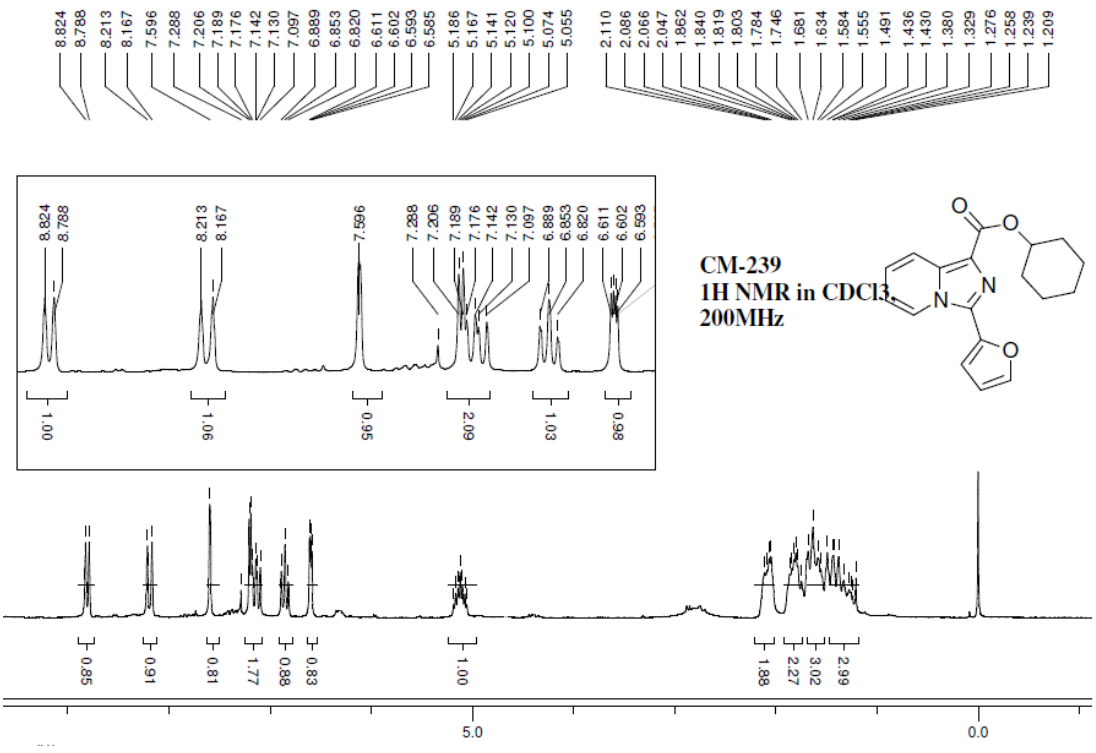

**13C NMR of 4m**



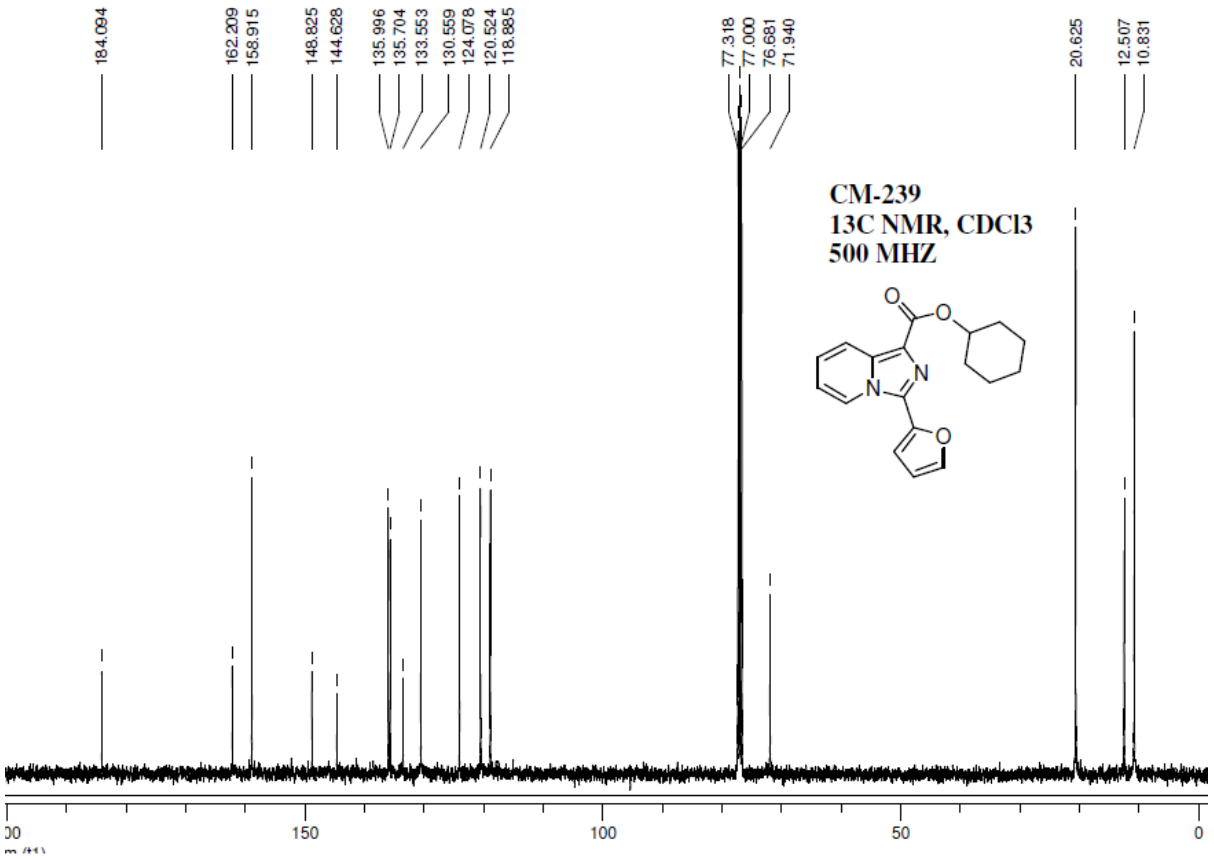

**1H NMR of 4o**



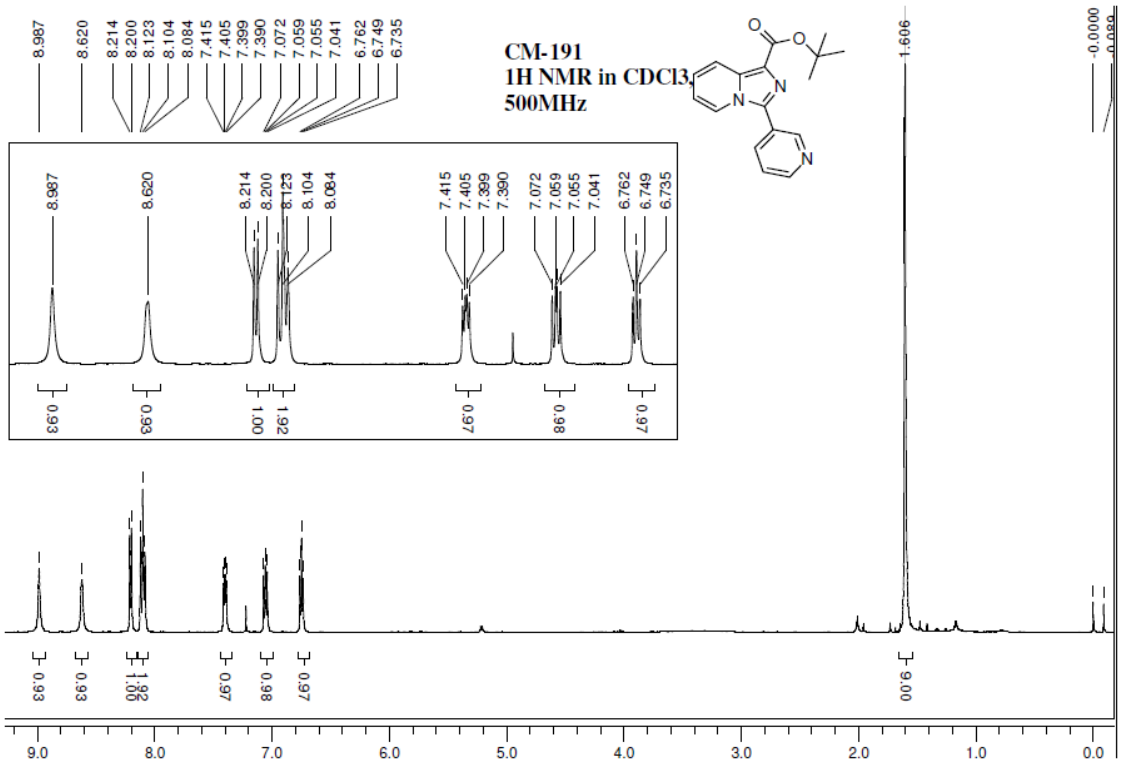

**13C NMR of 4o**



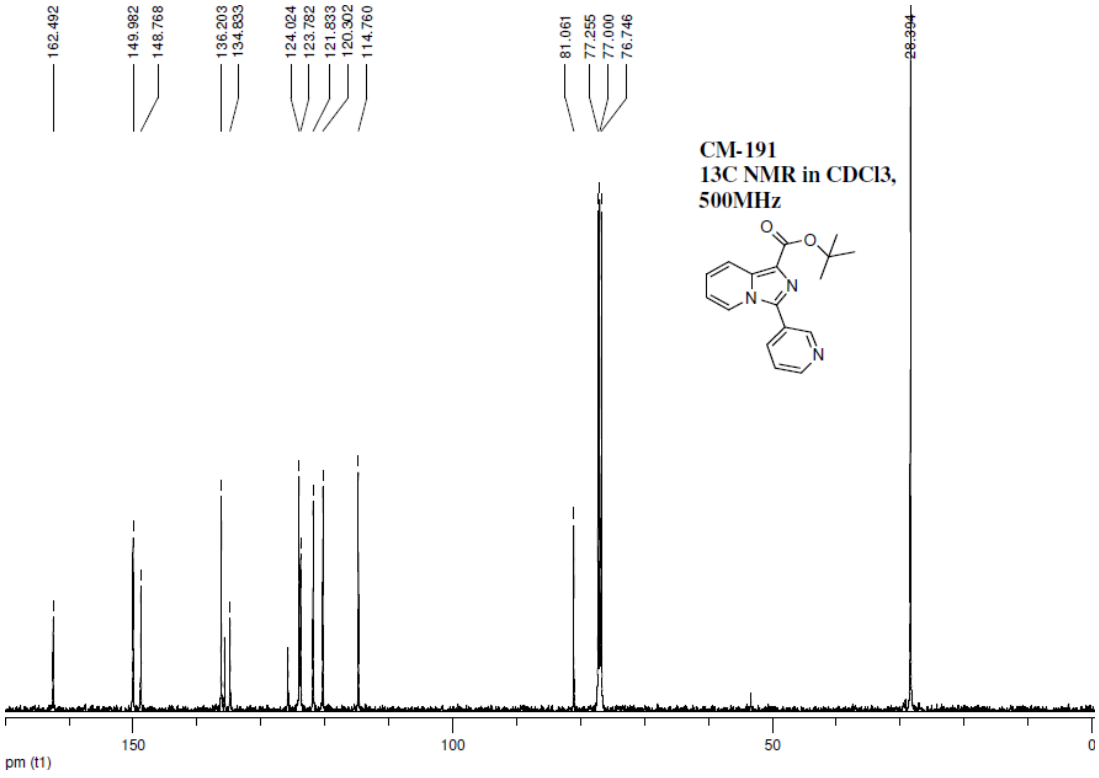

**1H NMR of 4p**



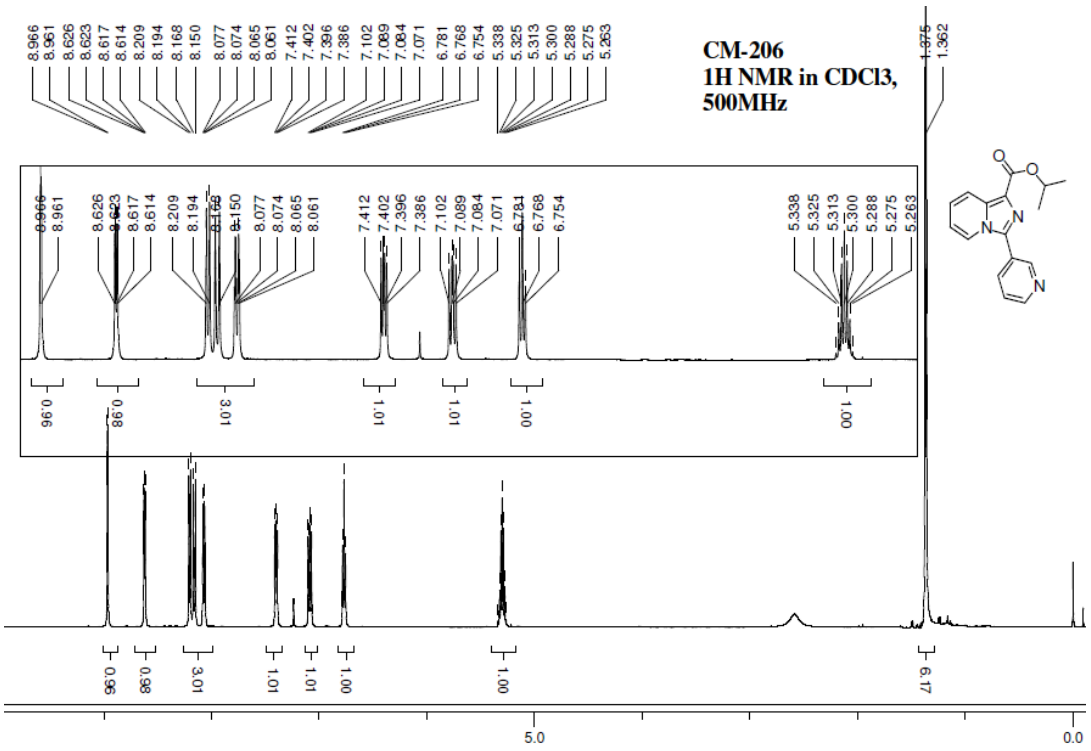

**13C NMR of 4p**



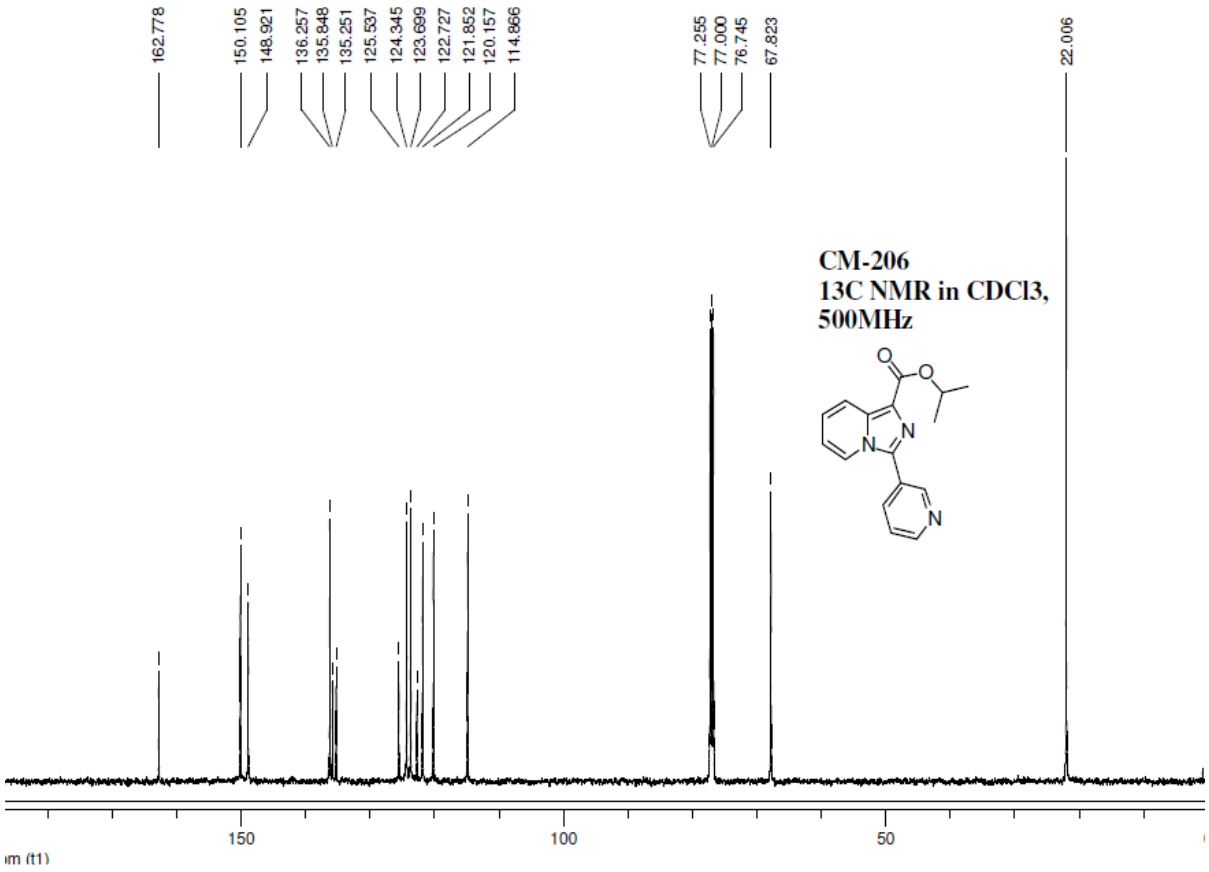

**1H NMR of 4q**



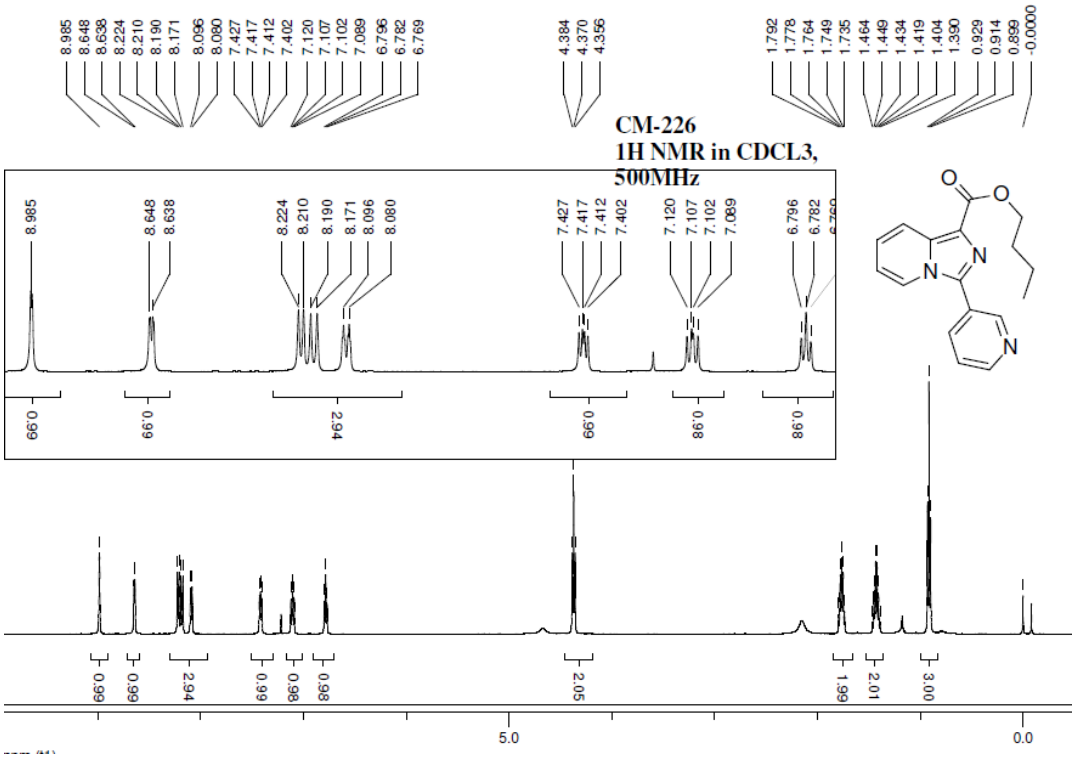

**13C NMR of 4q**



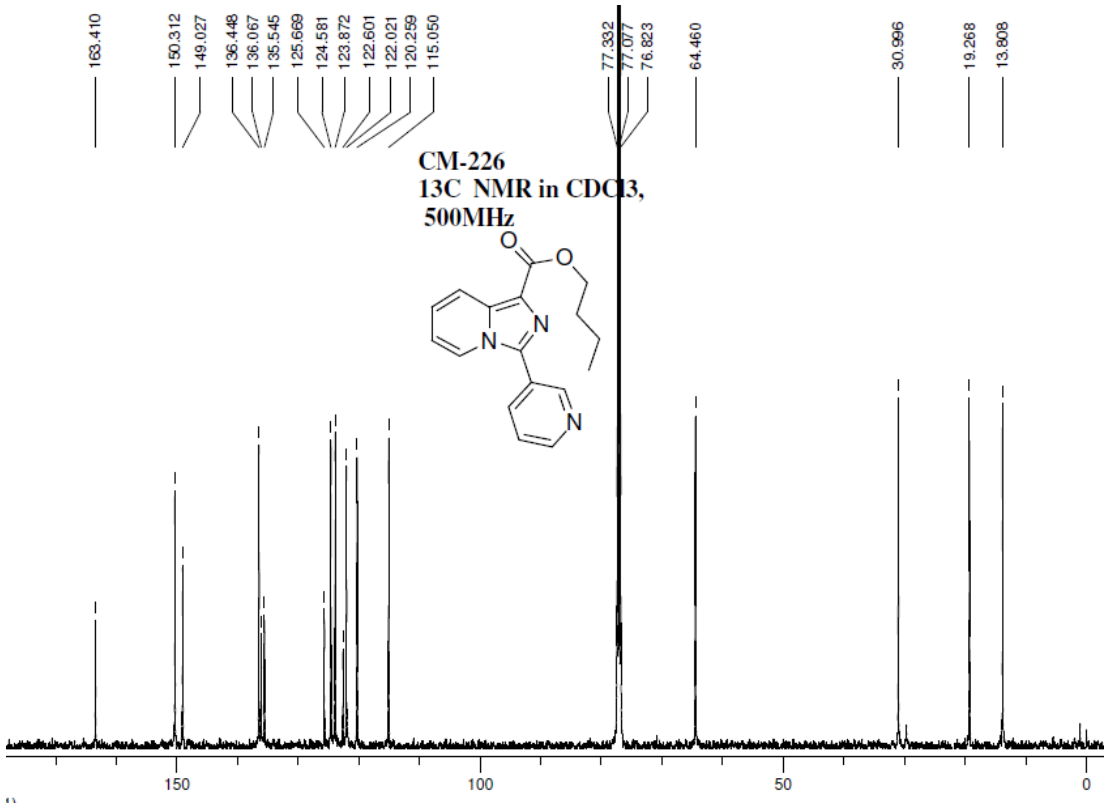

**1H NMR of 4r**



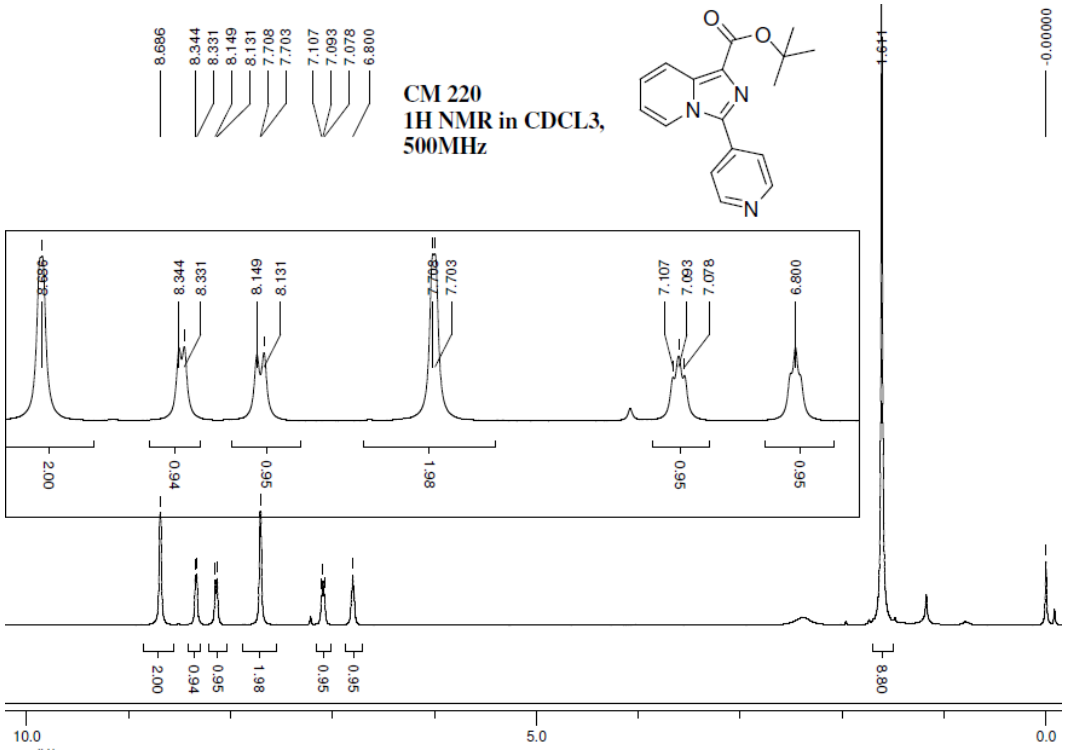

**13C NMR of 4r**



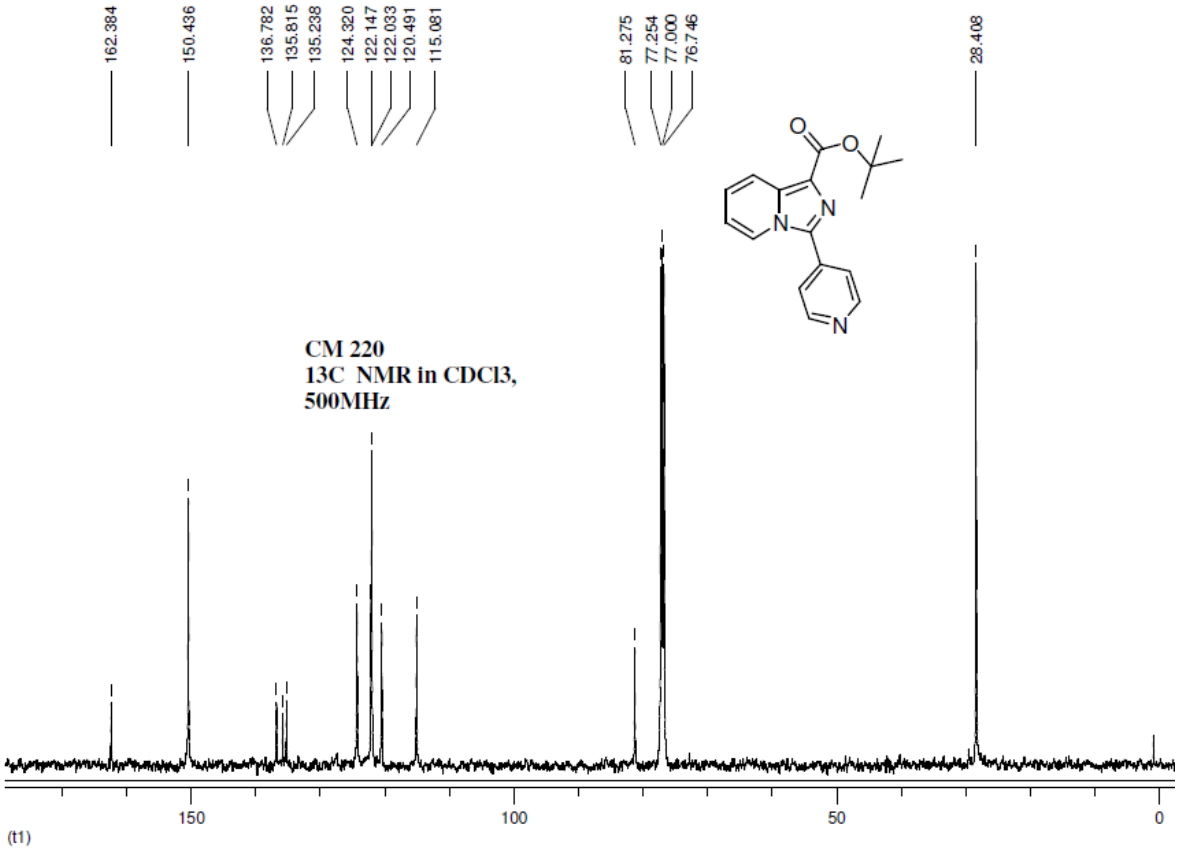

**1H NMR of 4s**



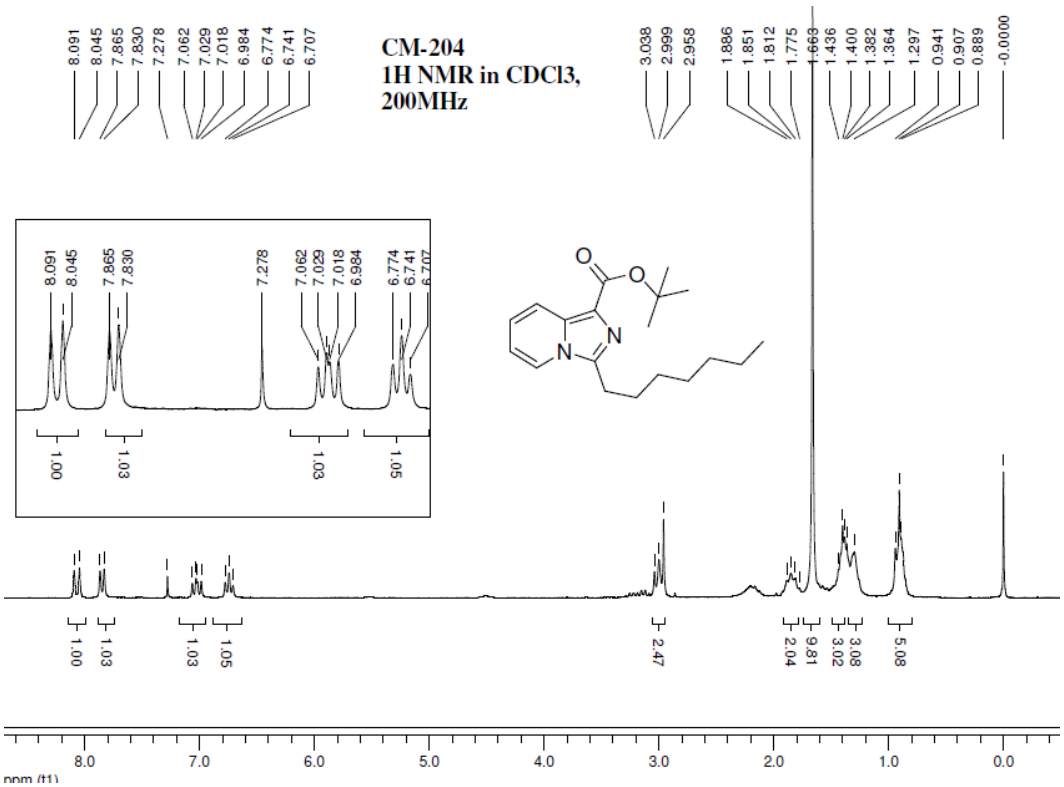

**13C NMR of 4s**



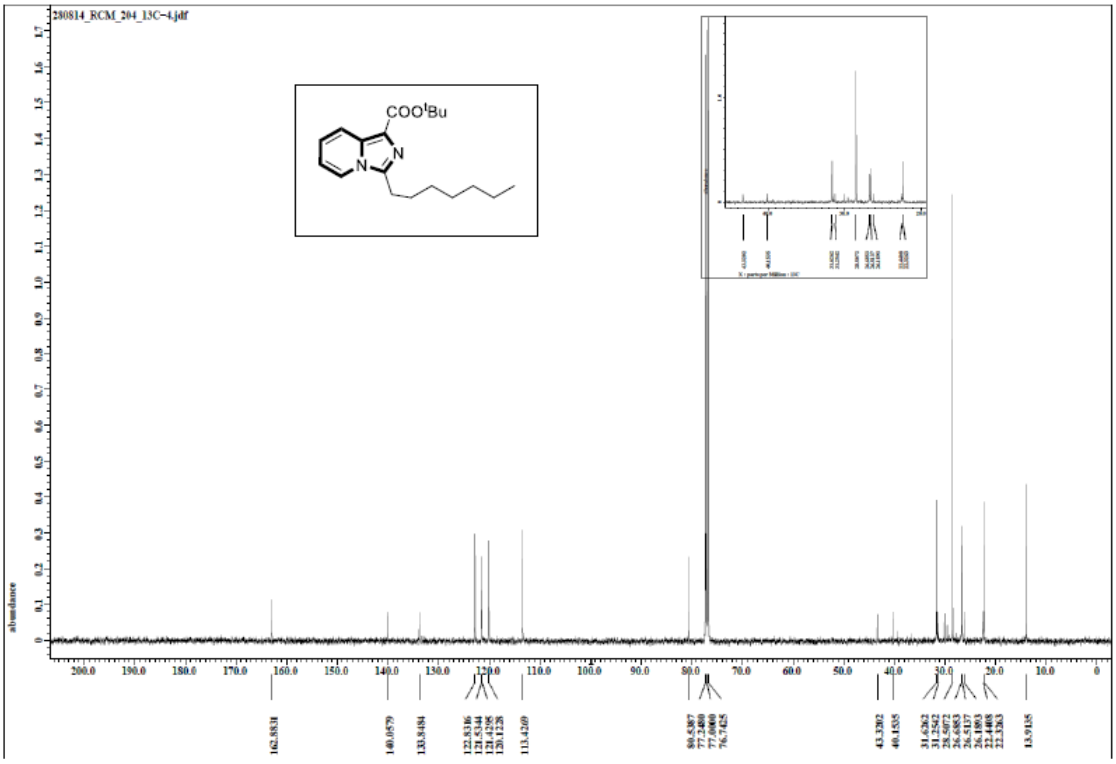

**1H NMR of 4u**



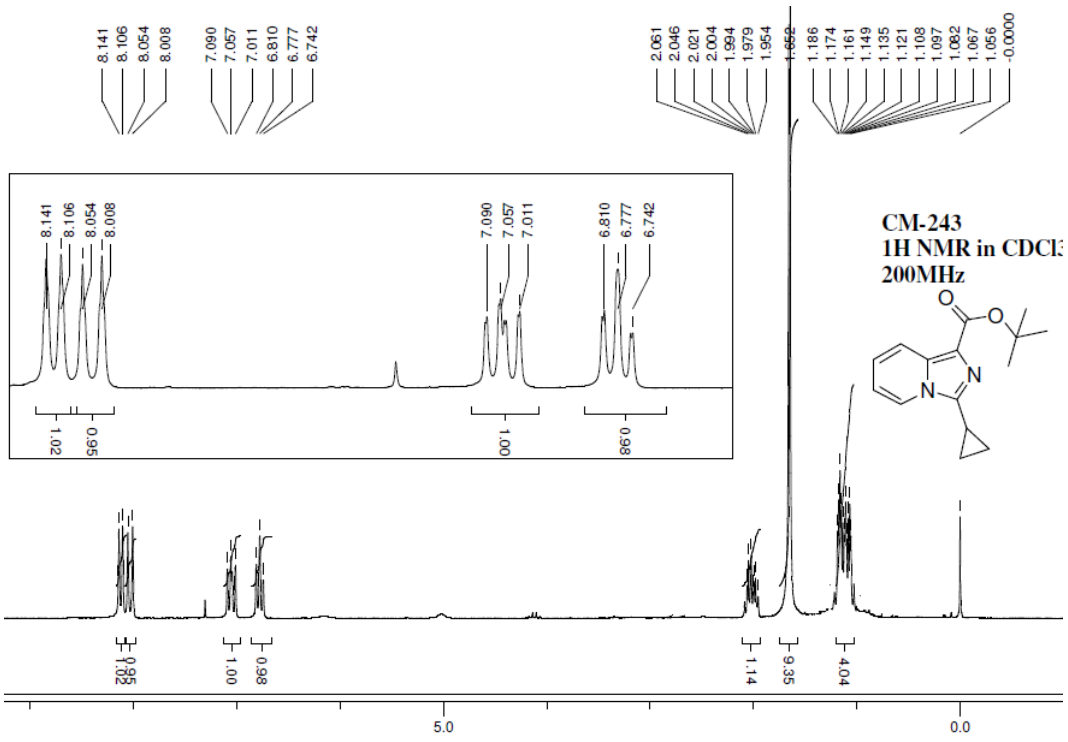

**13C NMR of 4u**



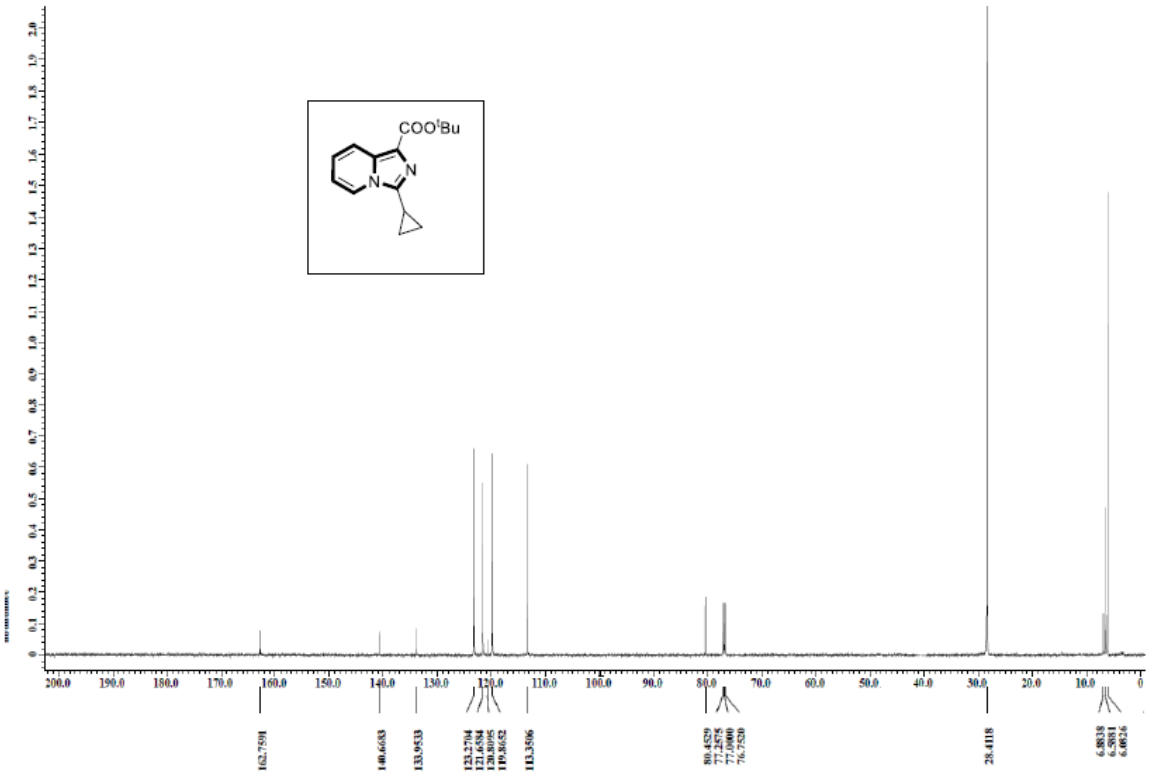

**1H NMR of 4v**



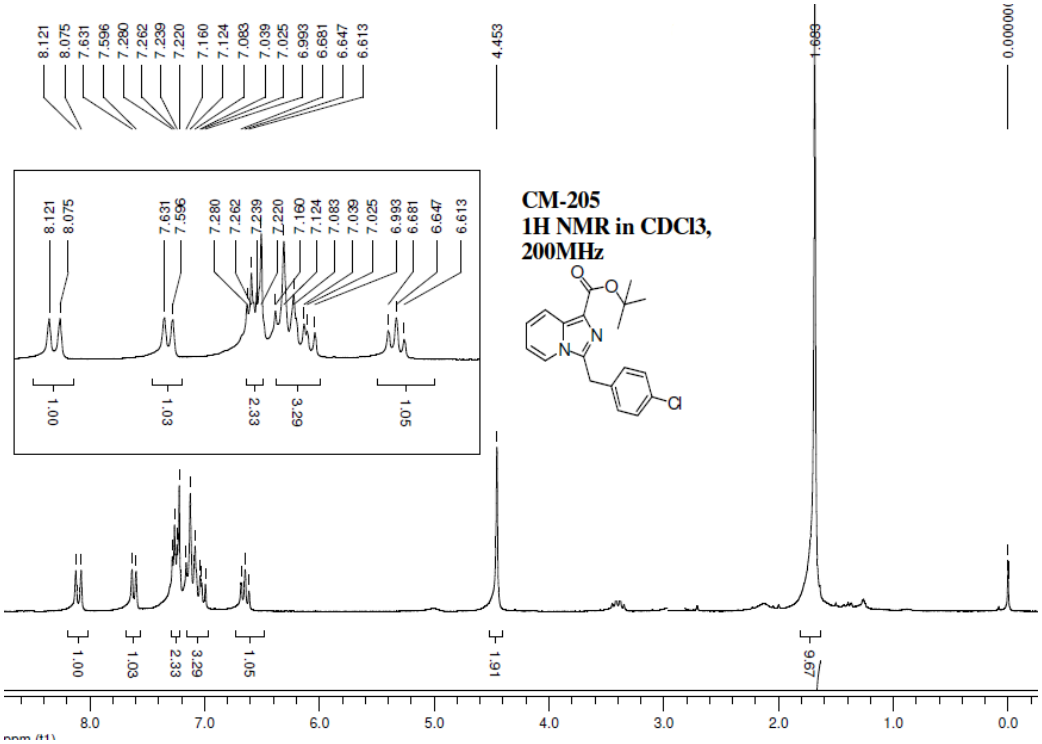

**13C NMR of 4v**



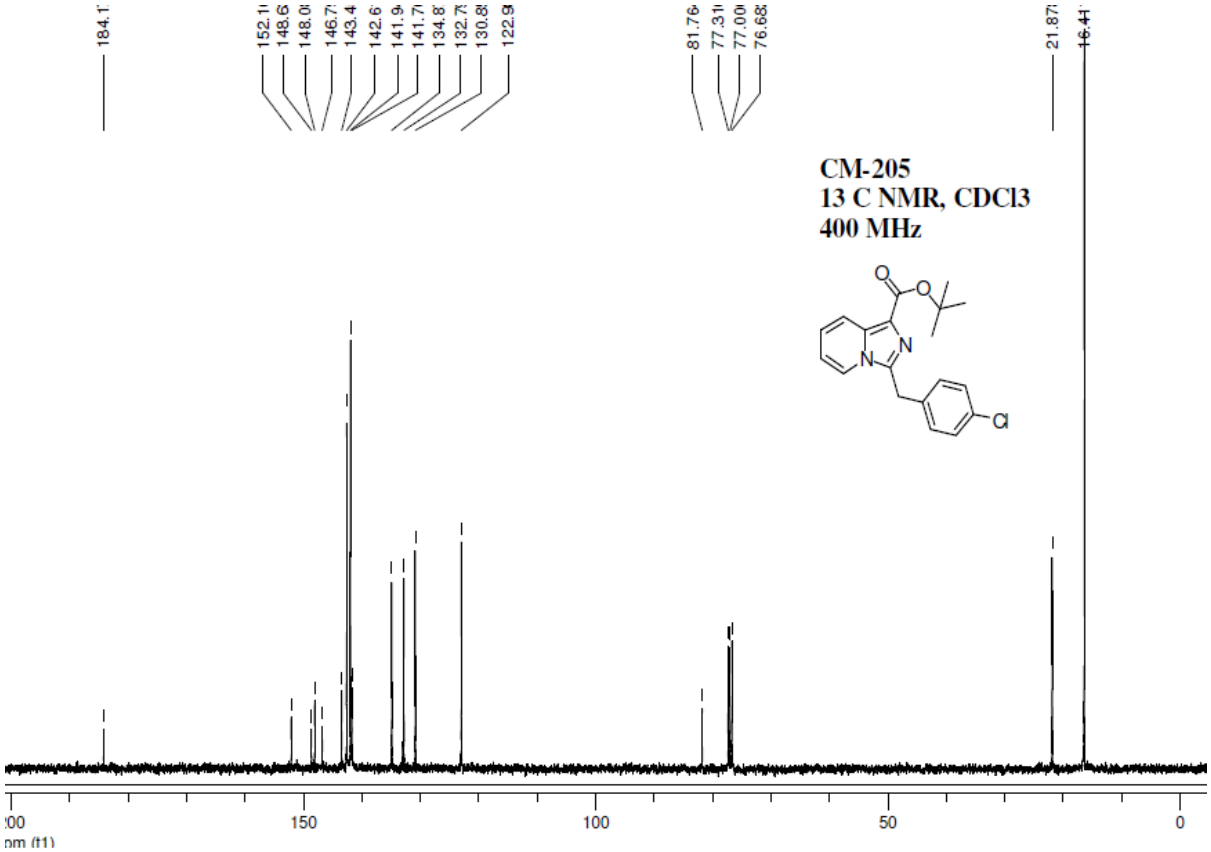

**1H NMR of 4w**



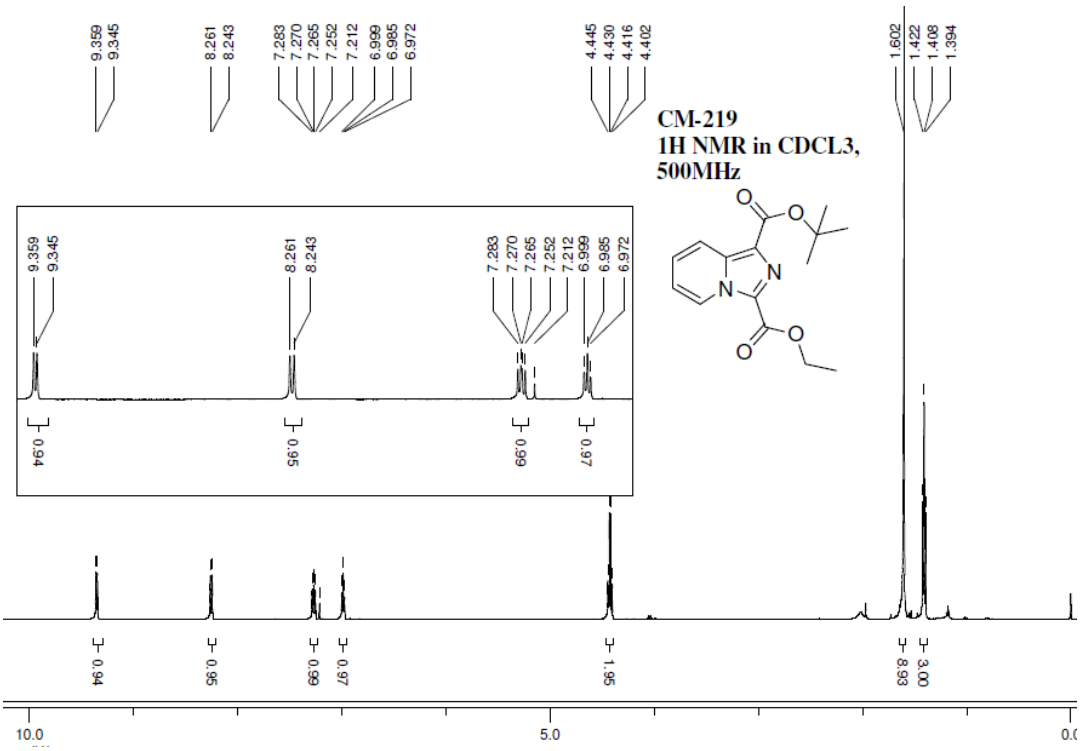
**13C NMR of 4w**



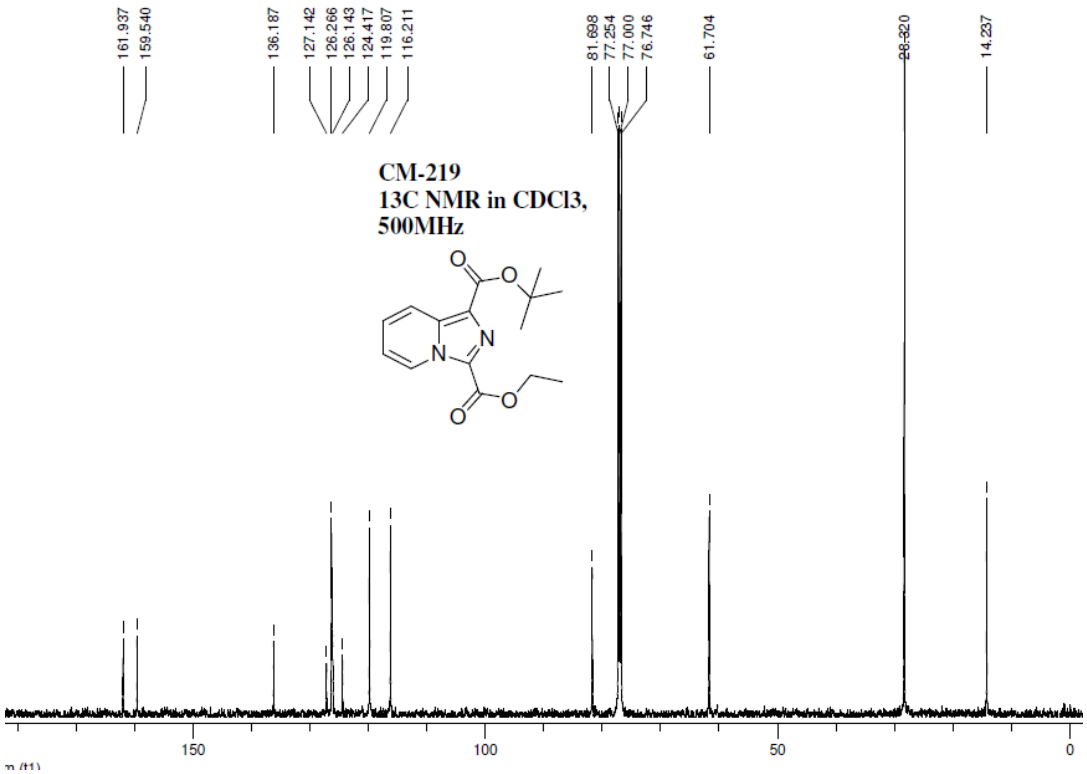

**1H NMR of 4x**



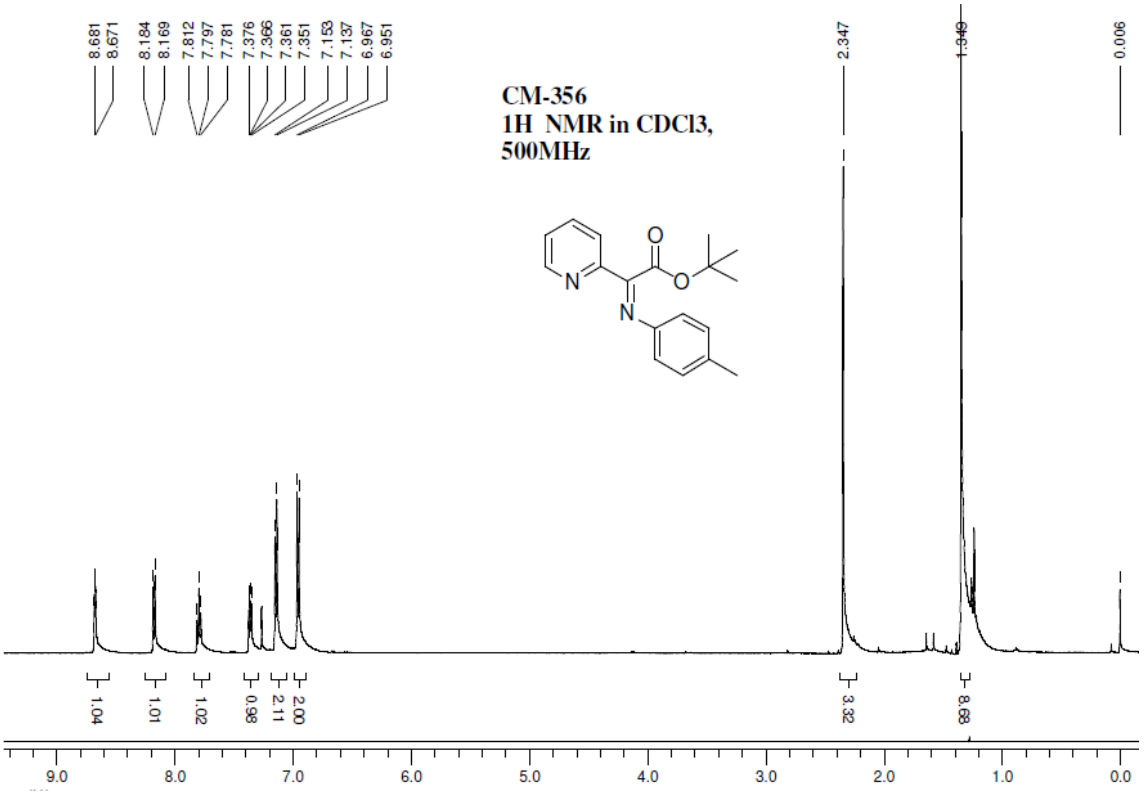

**13C NMR of 4x**



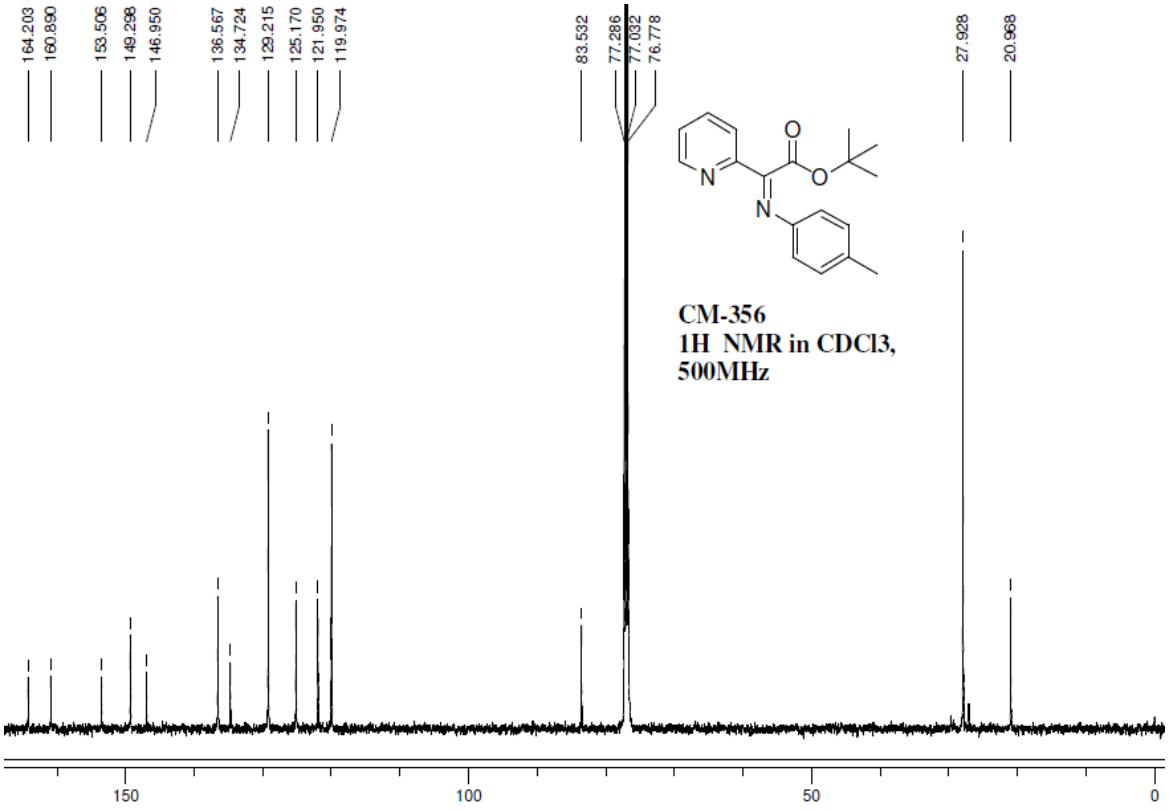

**1H NMR of 6a**



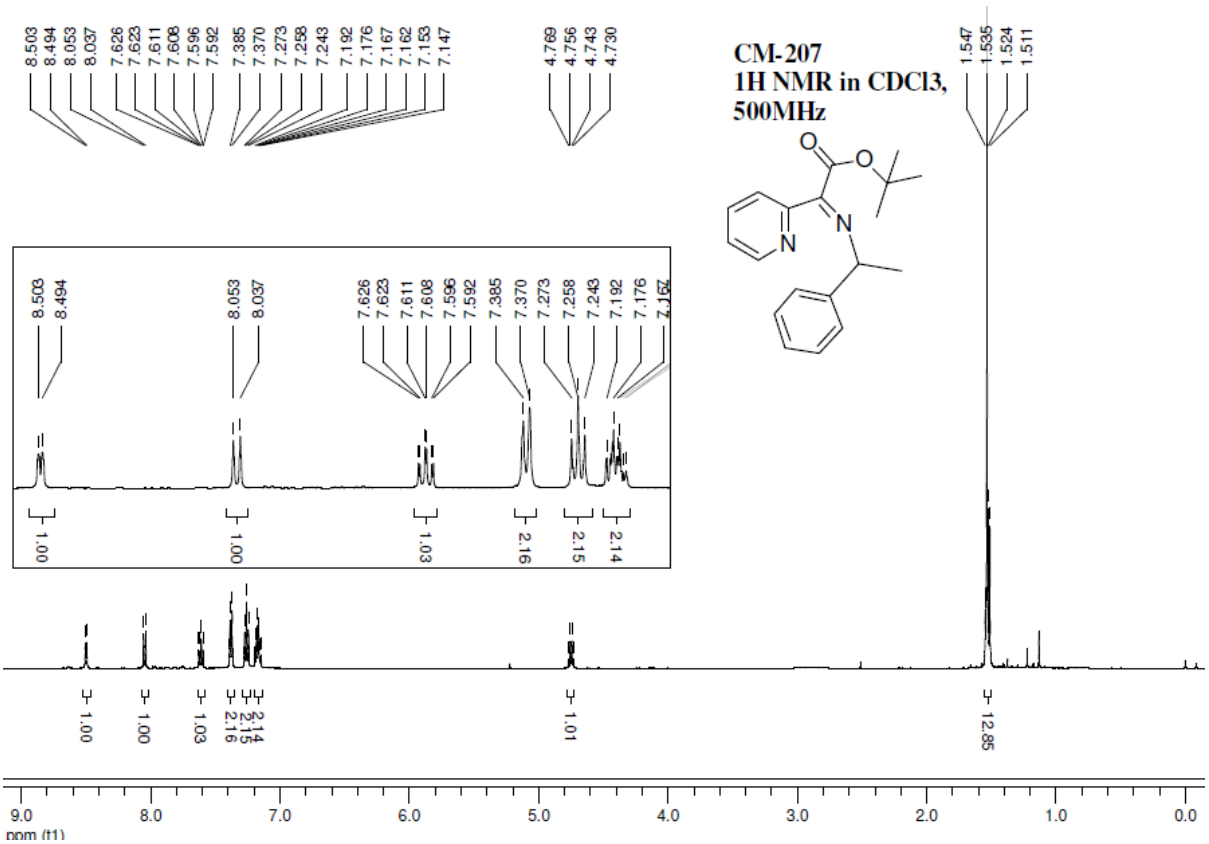

**13C NMR of 6a**



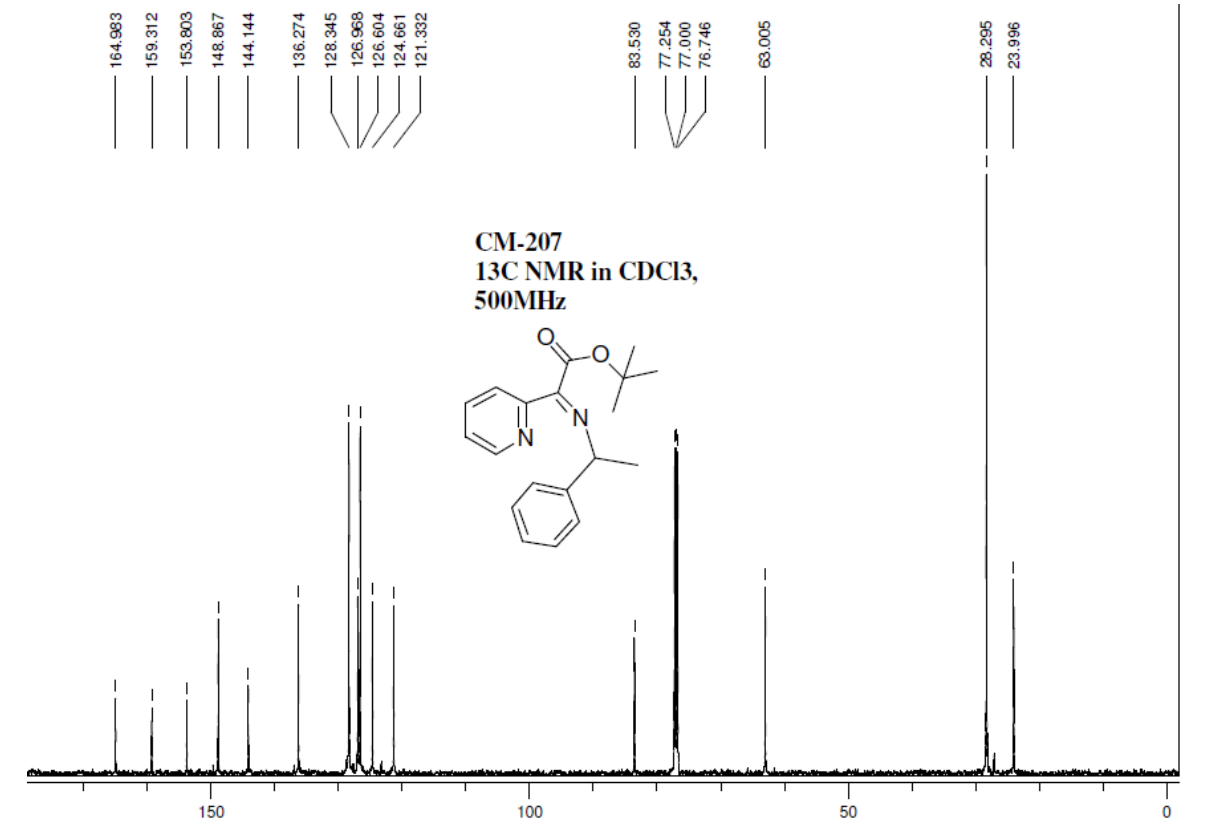

**1H NMR of 9a**



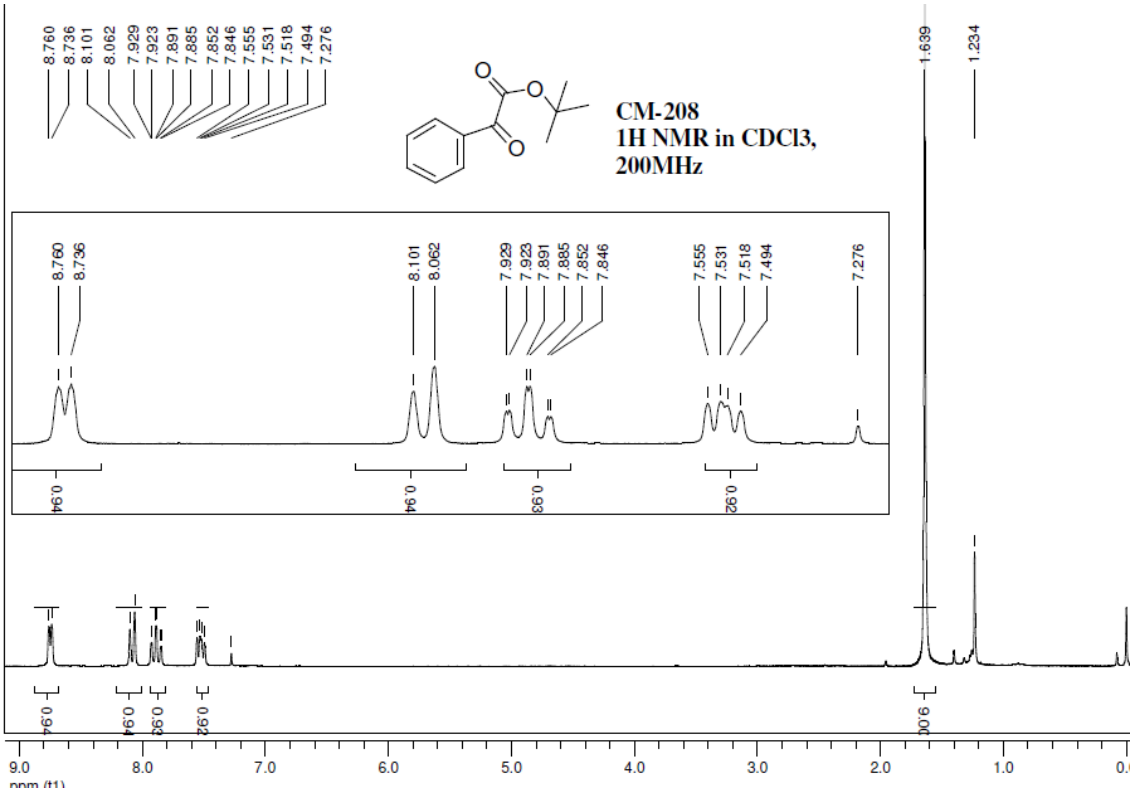

**13C NMR of 9a**



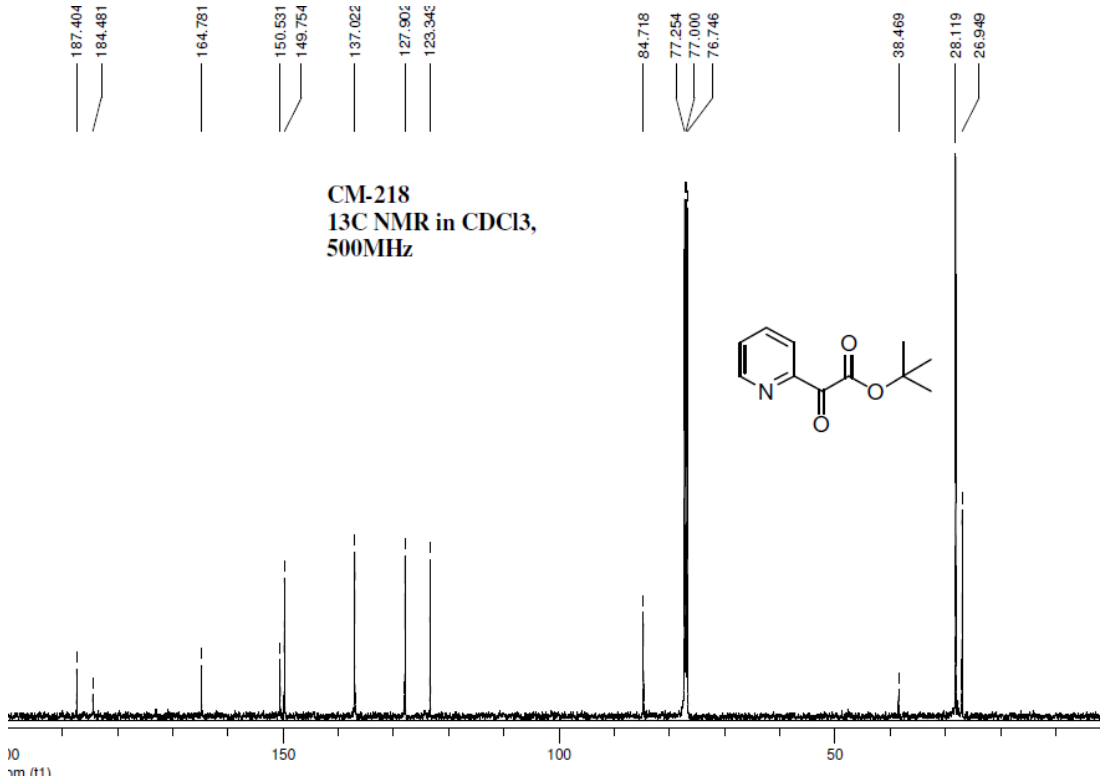

**1H NMR of 10a**



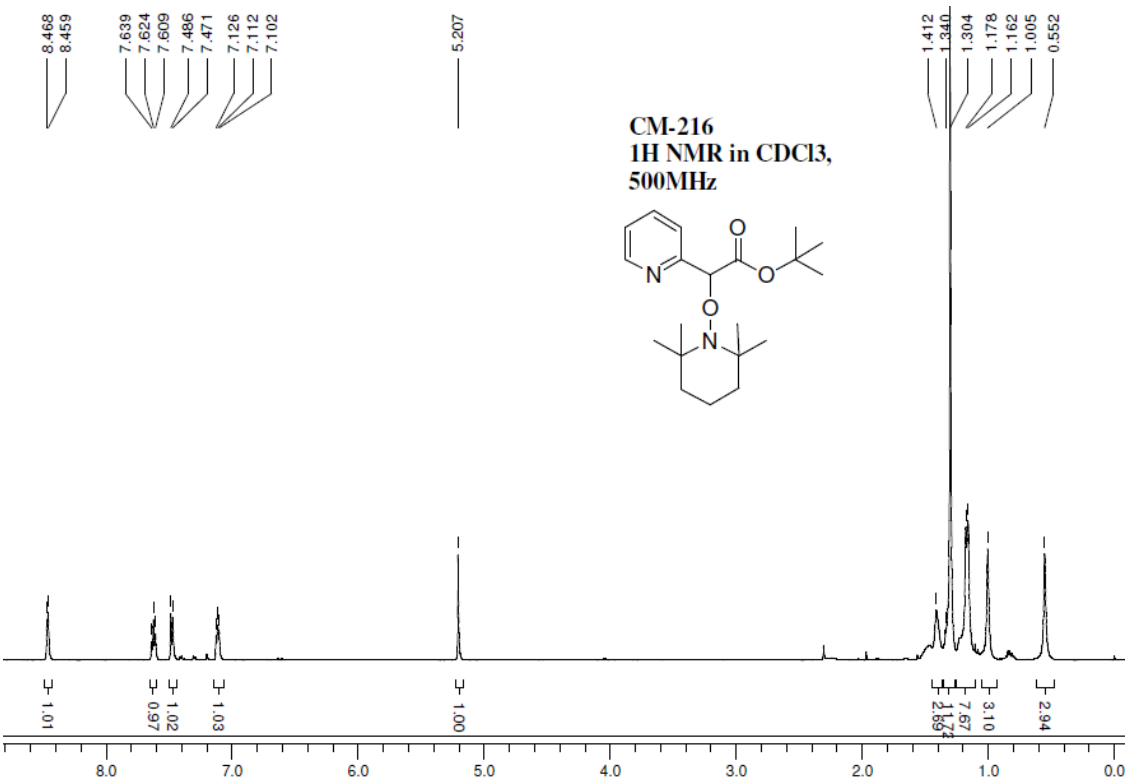

**13C NMR of 10a**



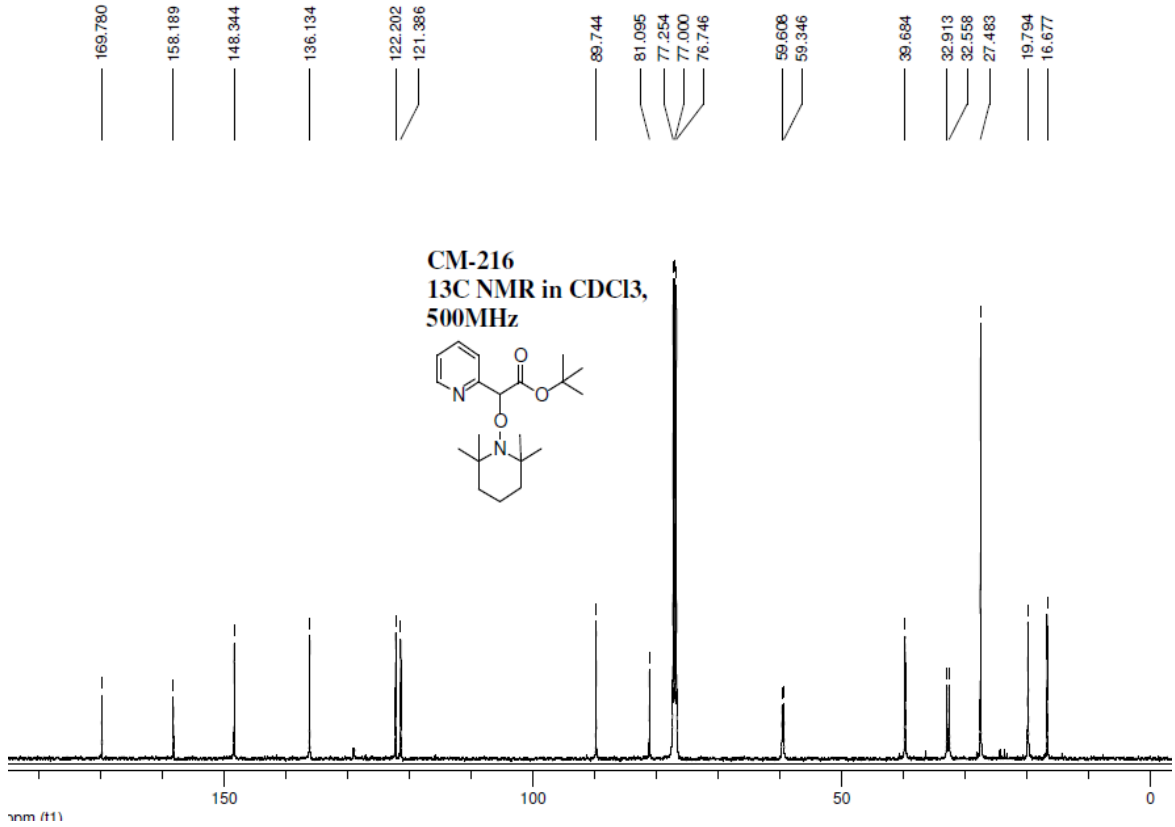

**1H NMR of 11a**




**13C NMR of 11a**

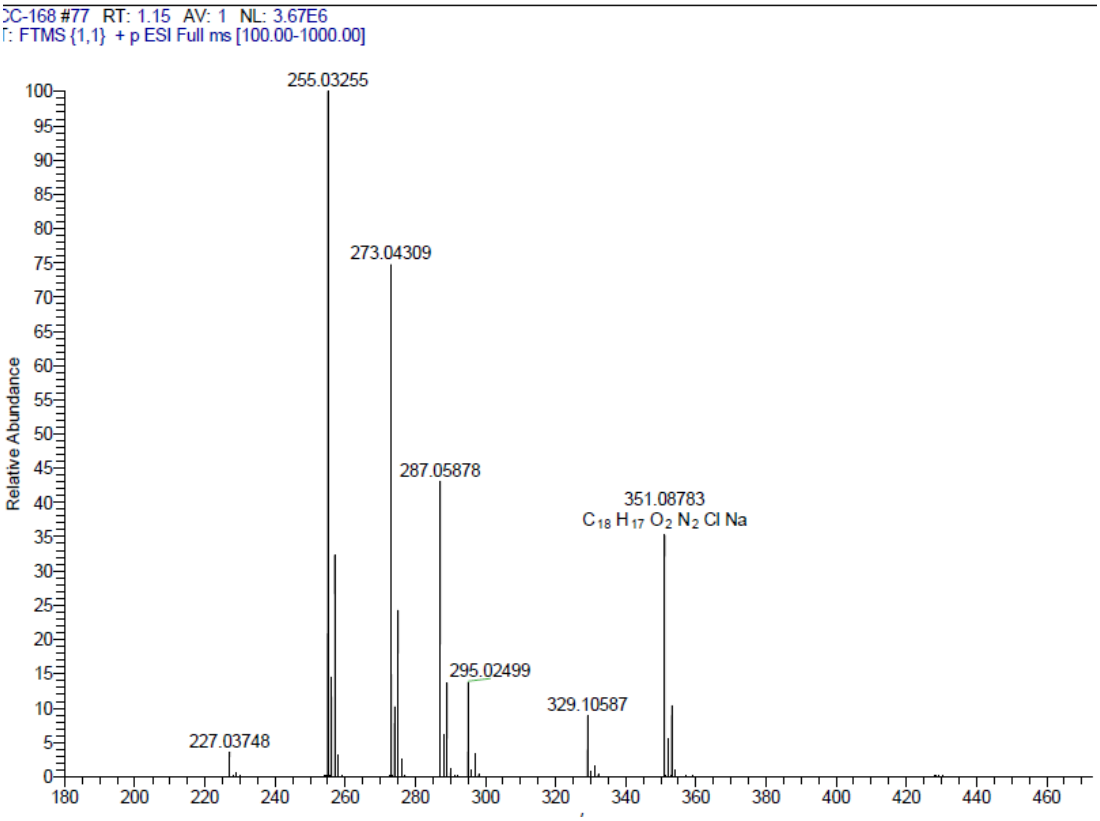



**1H NMR of 12a**

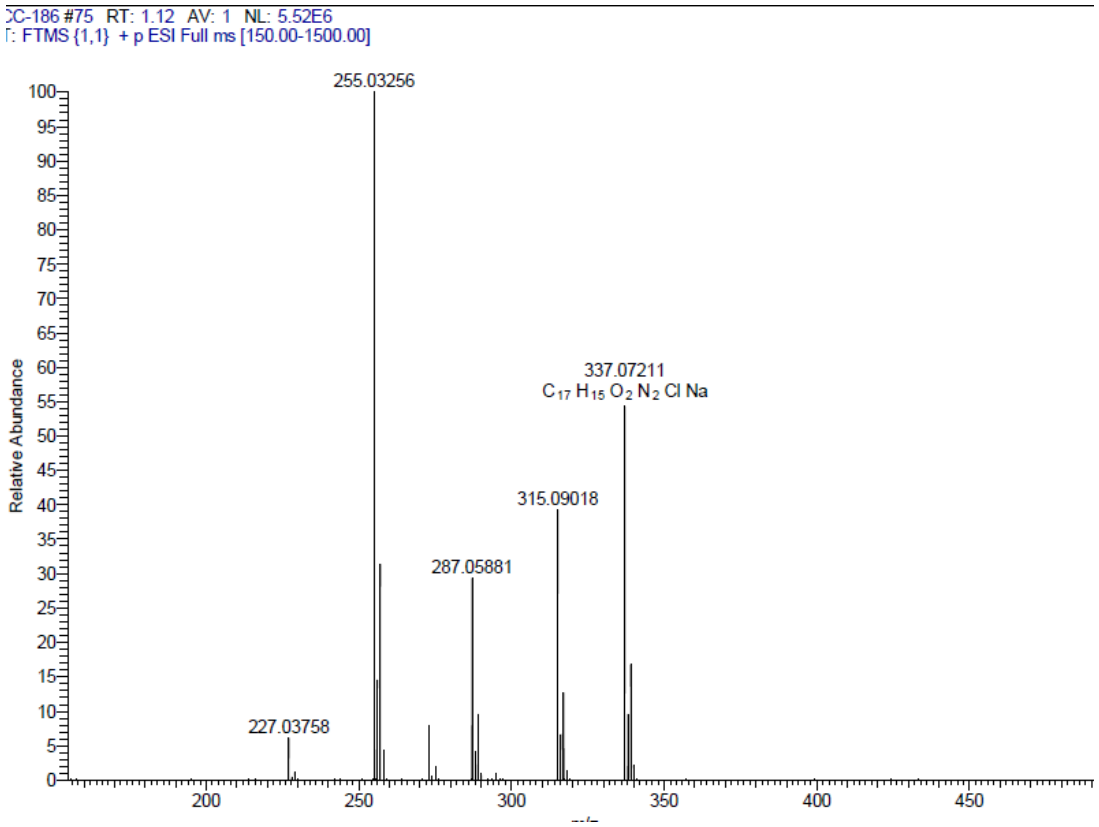



**13C NMR of 12a**

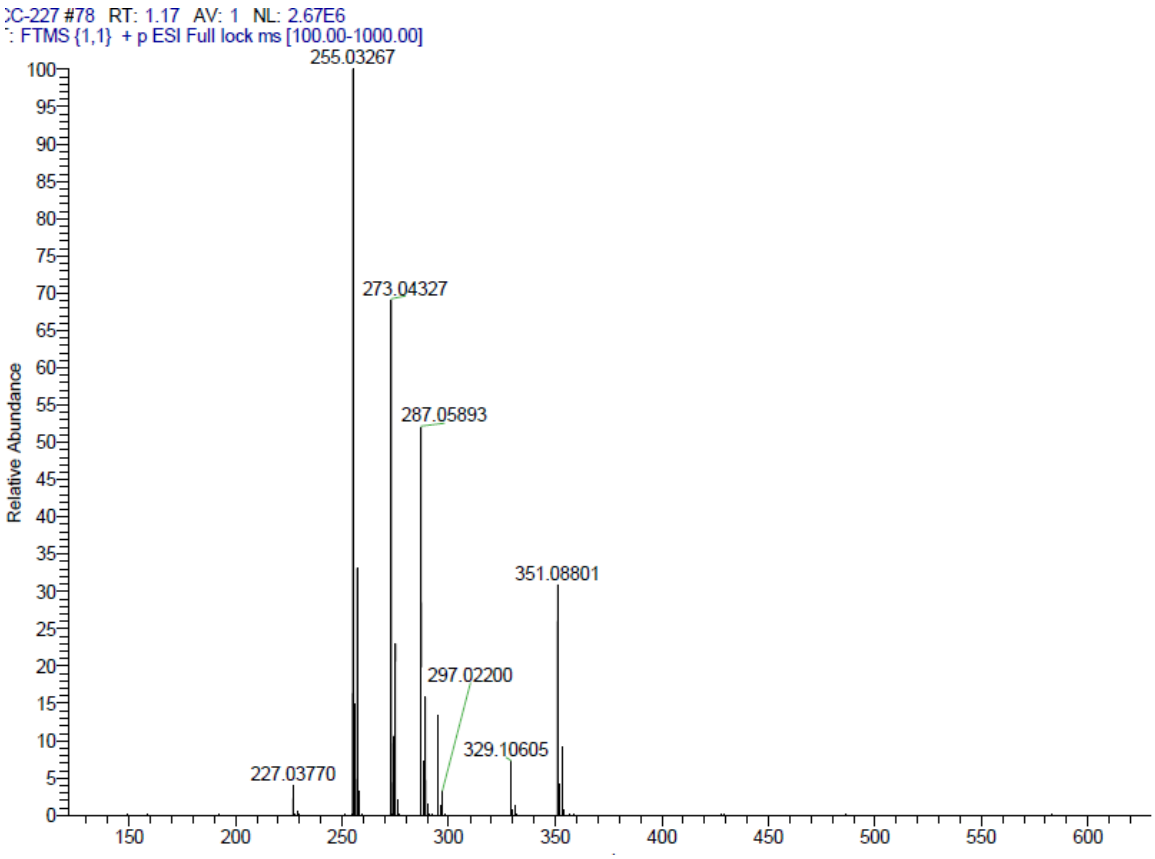
# HRMS spectral data



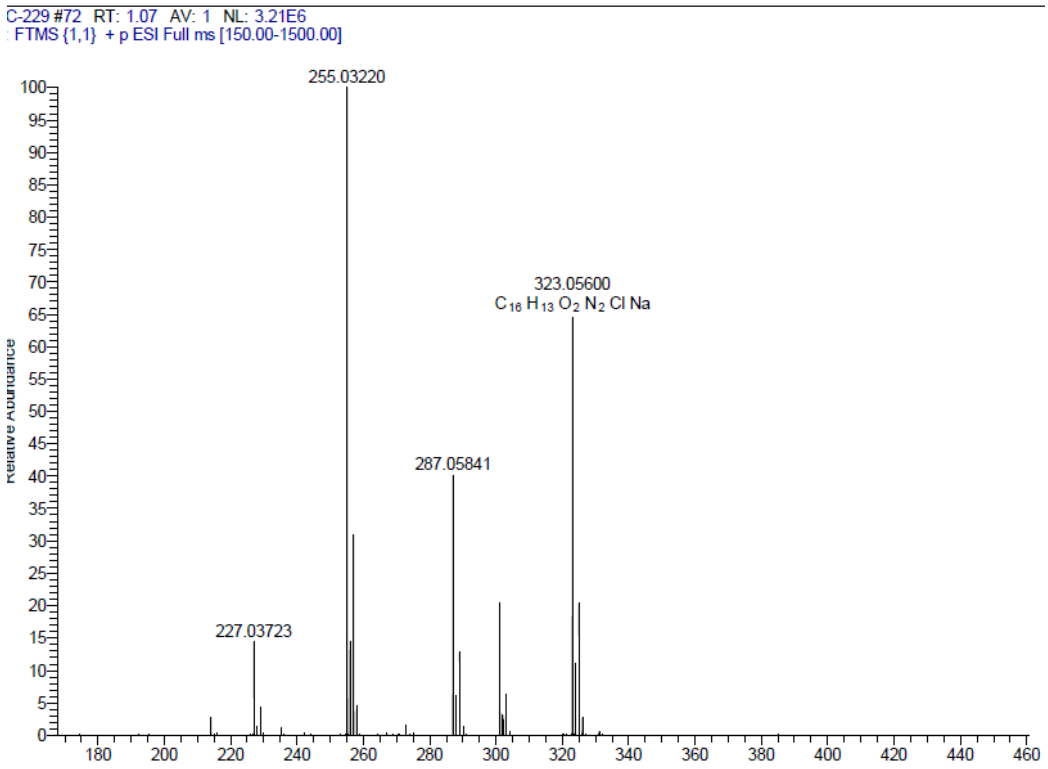

**HRMS of 3a**



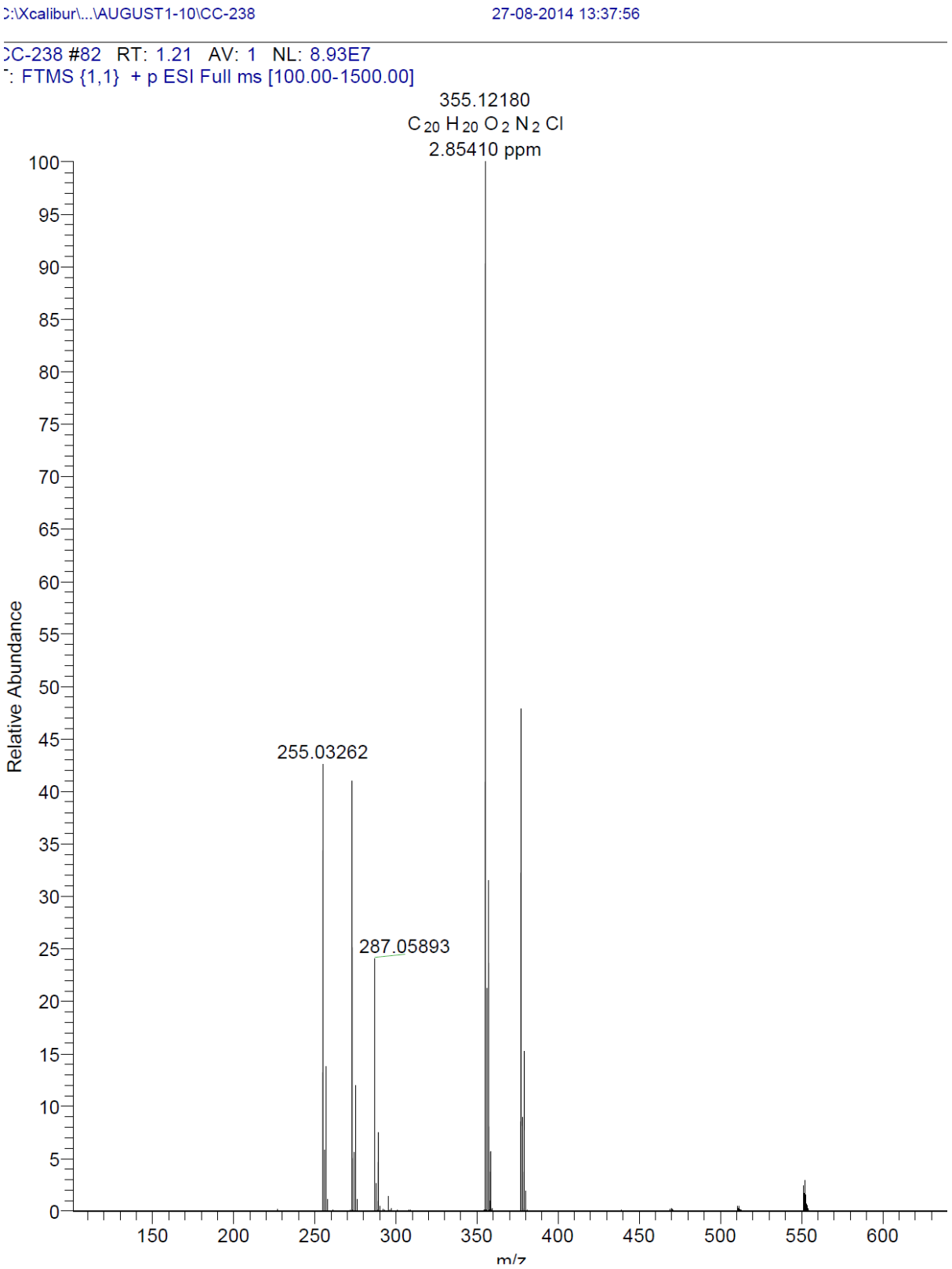

**HRMS of 3b**



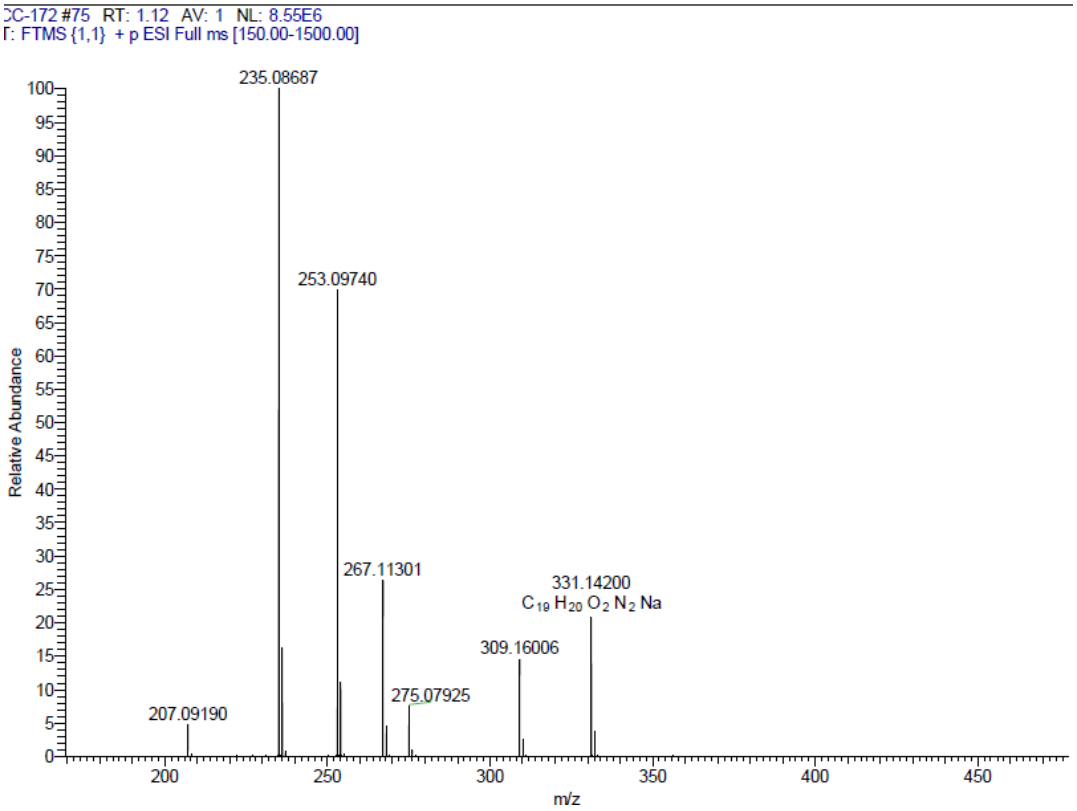

**HRMS of 3c**



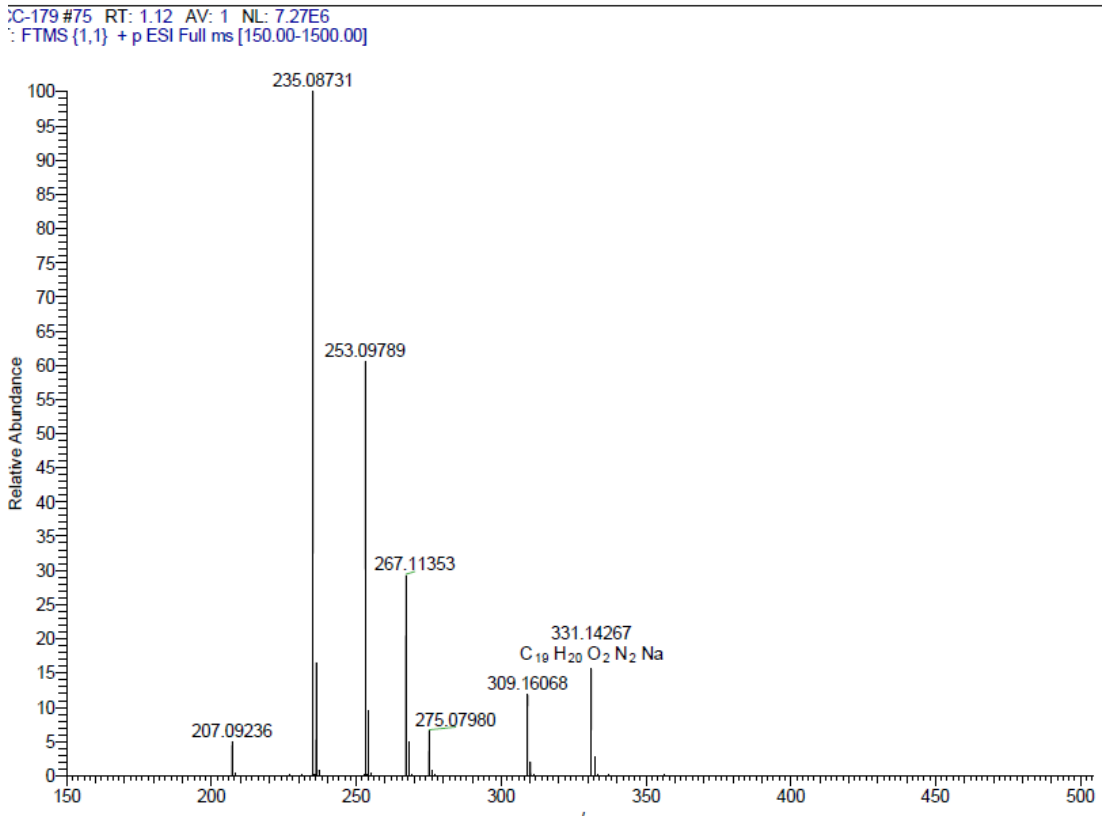

**HRMS of 3d**


C:\Xcalibur\...\AUGUST1-10\CC-238
27-08-2014 13:37:56
CC-238 #82 RT: 1.21 AV: 1 NL: 8.93E7
T: FTMS {1,1} + p ESI Full ms [100.00-1500.00]
355.12180
C20 H20 O2 N2 Cl
2.85410 ppm
255.03262
287.05893
Relative Abundance
m/z

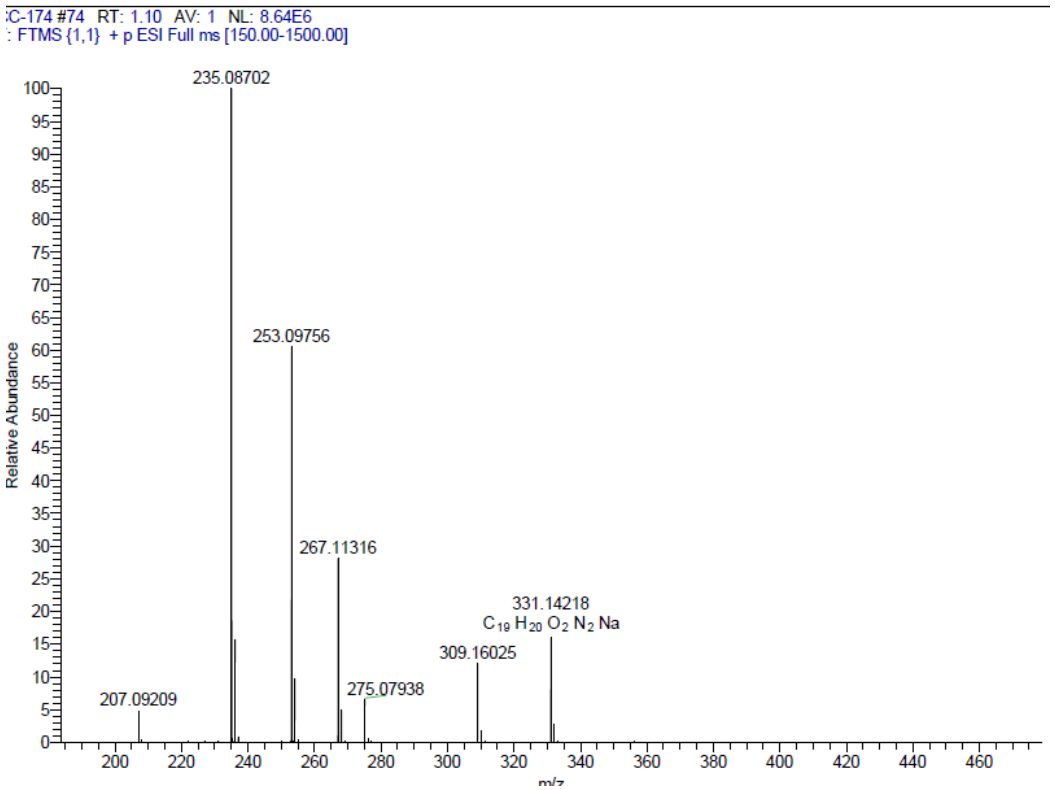
**HRMS of 3e**



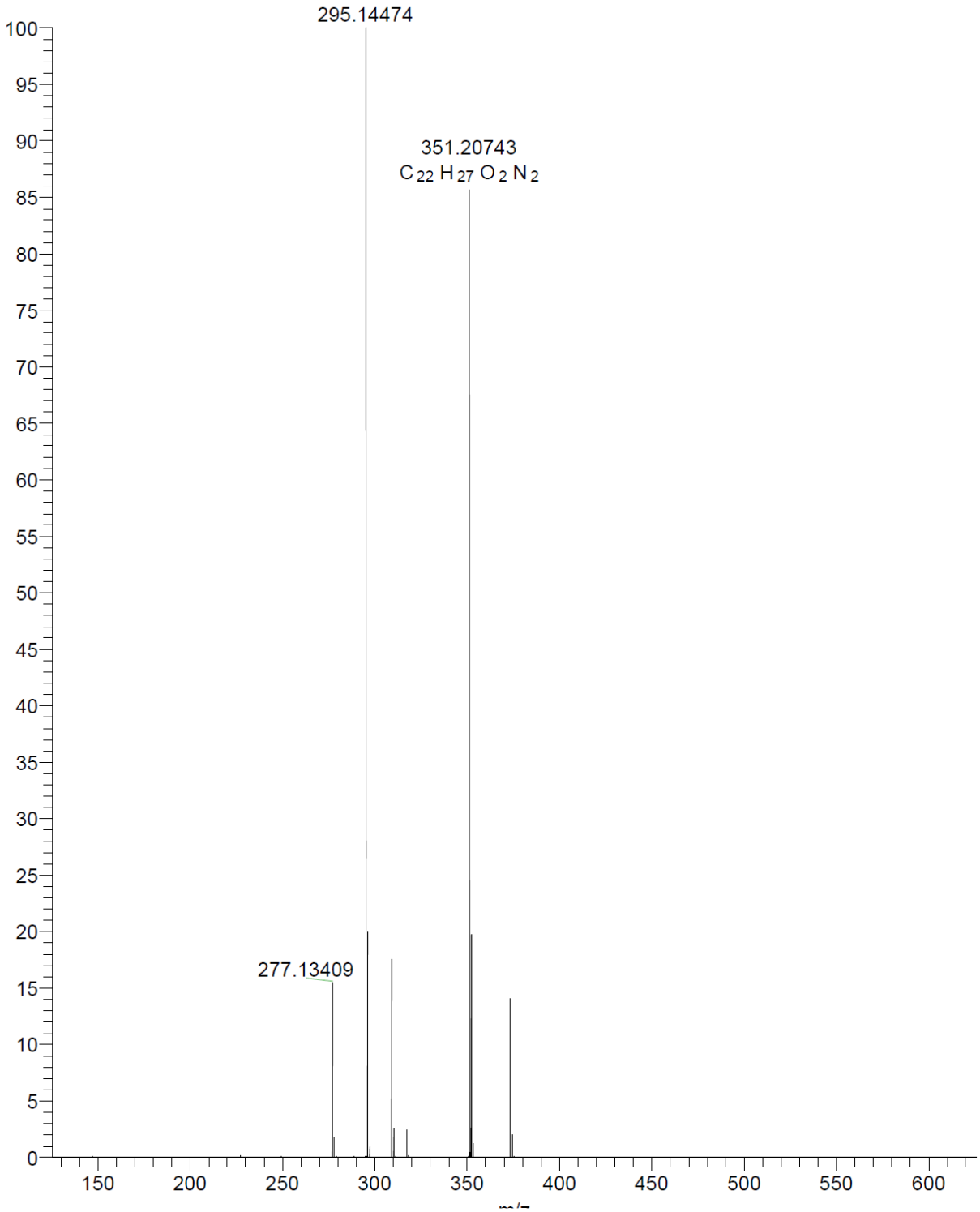

**HRMS of 4b**



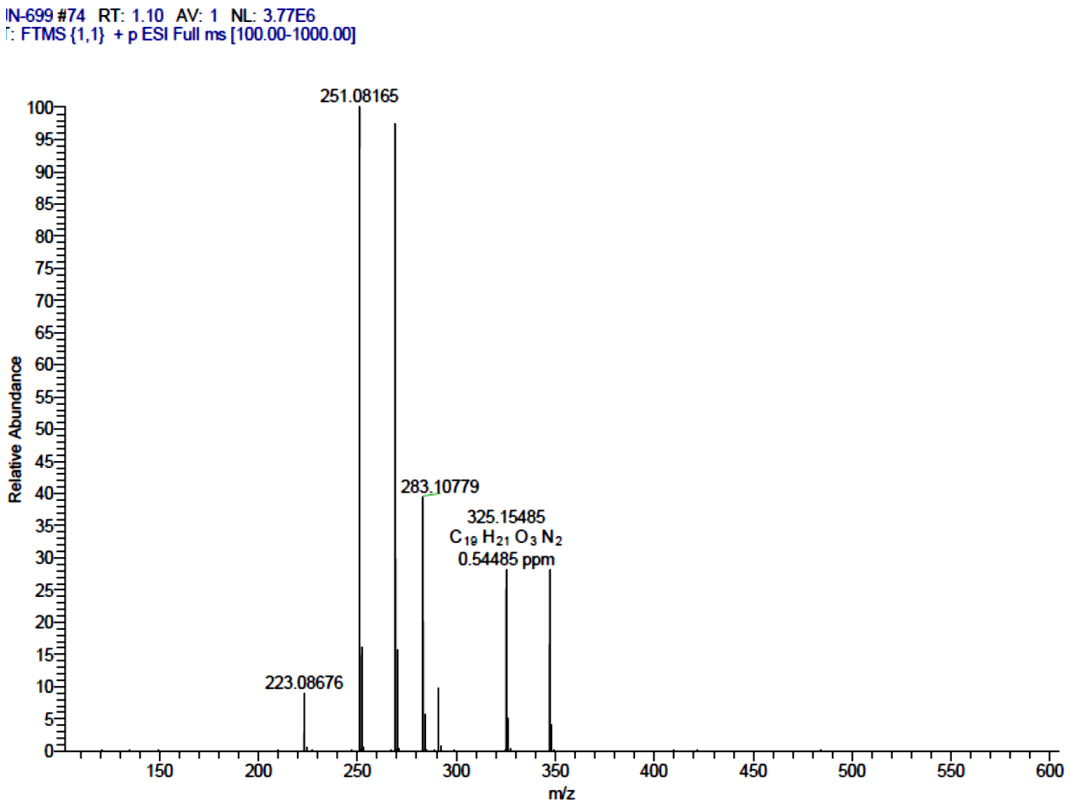

**HRMS of 4c**


C-174 #74 RT: 1.10 AV: 1 NL: 8.64E6
FTMS {1,1} + p ESI Full ms [150.00-1500.00]
235.08702
253.09756
267.11316
331.14218
C19 H20 O2 N2 Na
309.16025
275.07938
207.09209
Relative Abundance
m/z

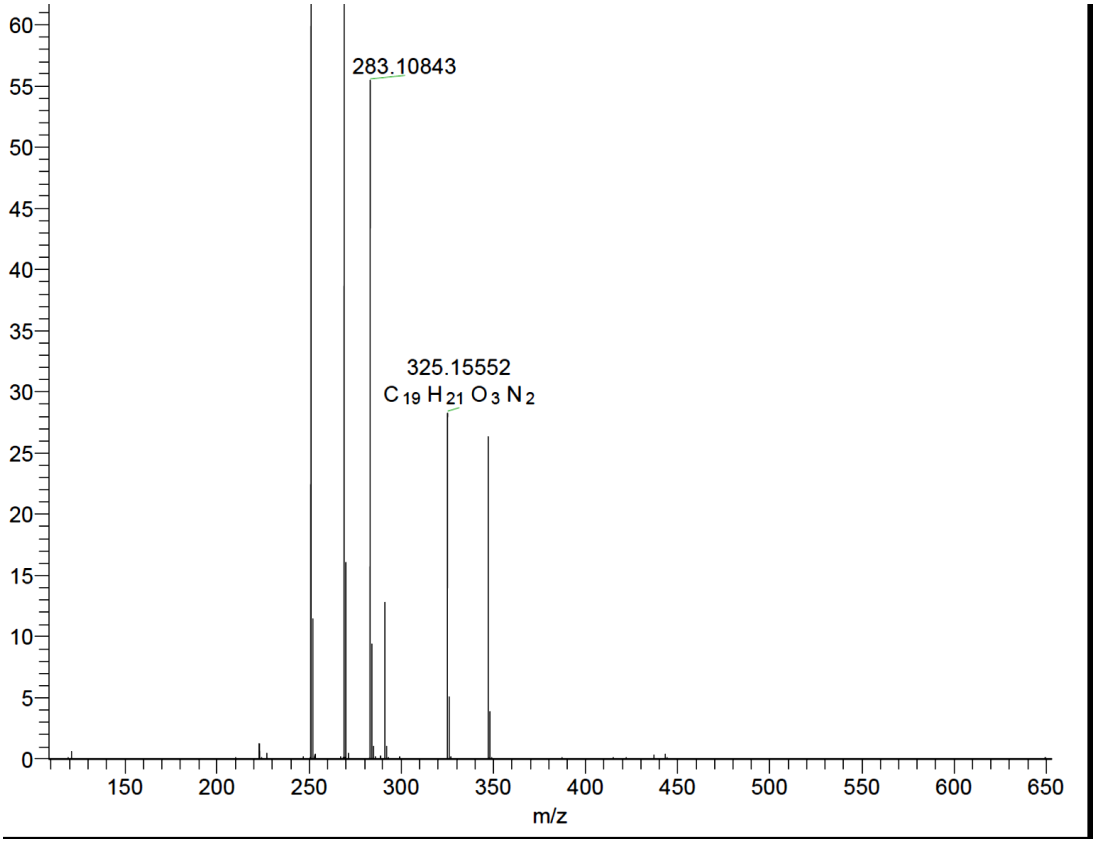
**HRMS of 4d**


295.14474
351.20743
C 22 H 27 O 2 N 2
277.13409
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
150
200
250
300
350
400
450
500
550
600

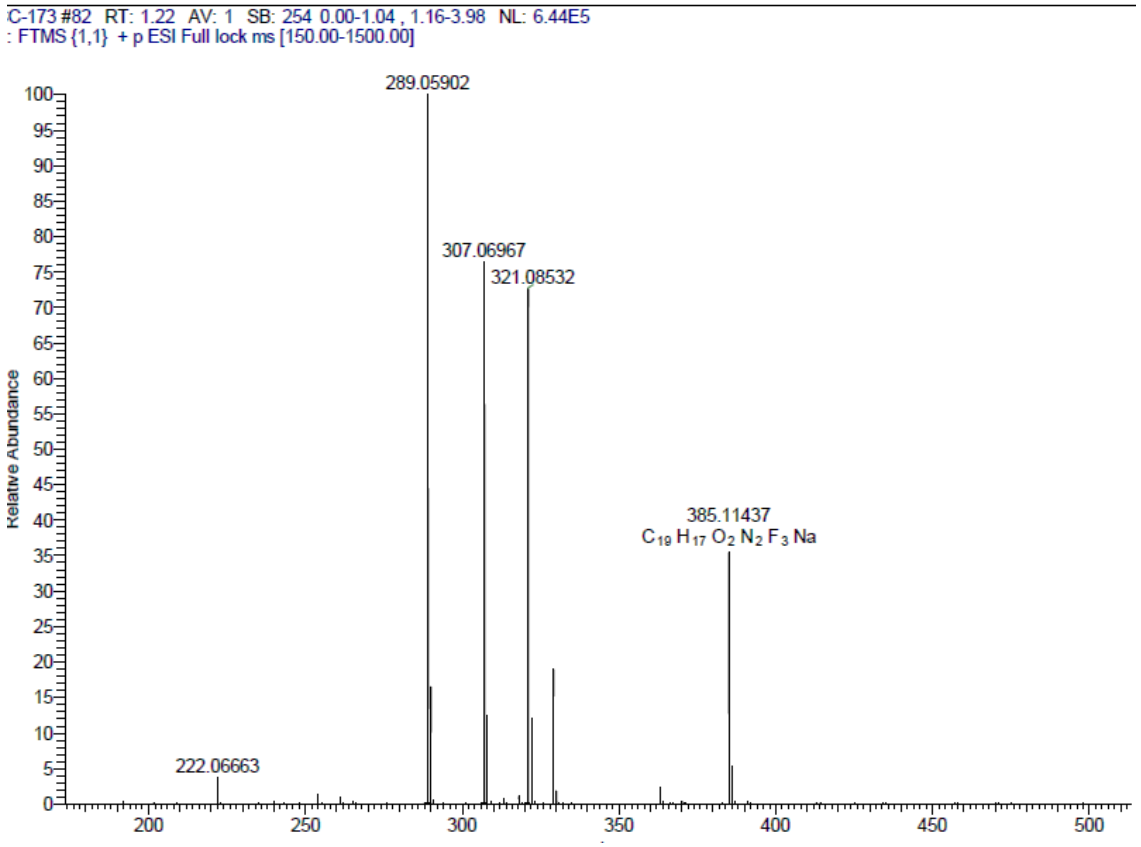
**HRMS of 4e**



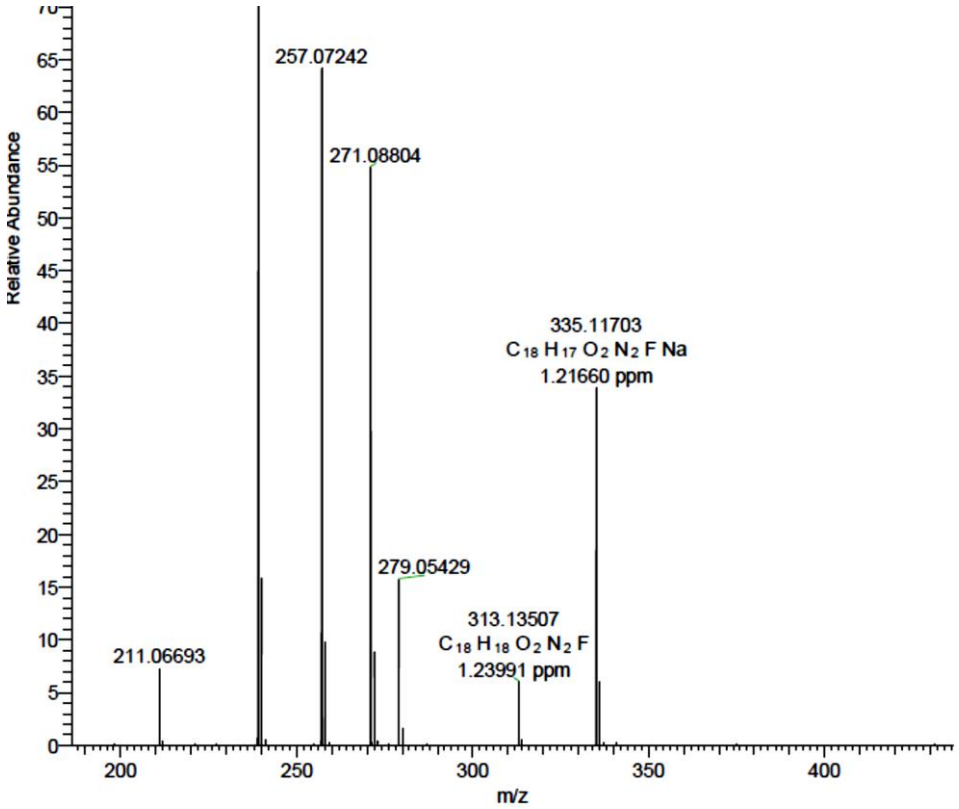

**HRMS of 4f**




**HRMS of 4g**




**HRMS of 4h**




**HRMS of 4i**

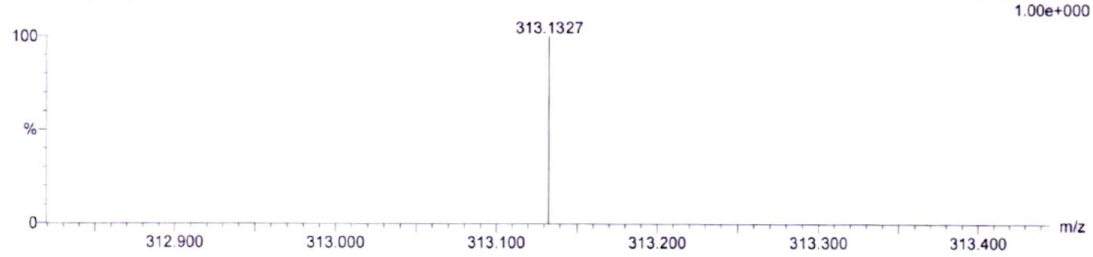
**Elemental Composition Report** **Page 1**

**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
83 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 Al: 0-1 I: 0-1 F: 0-1

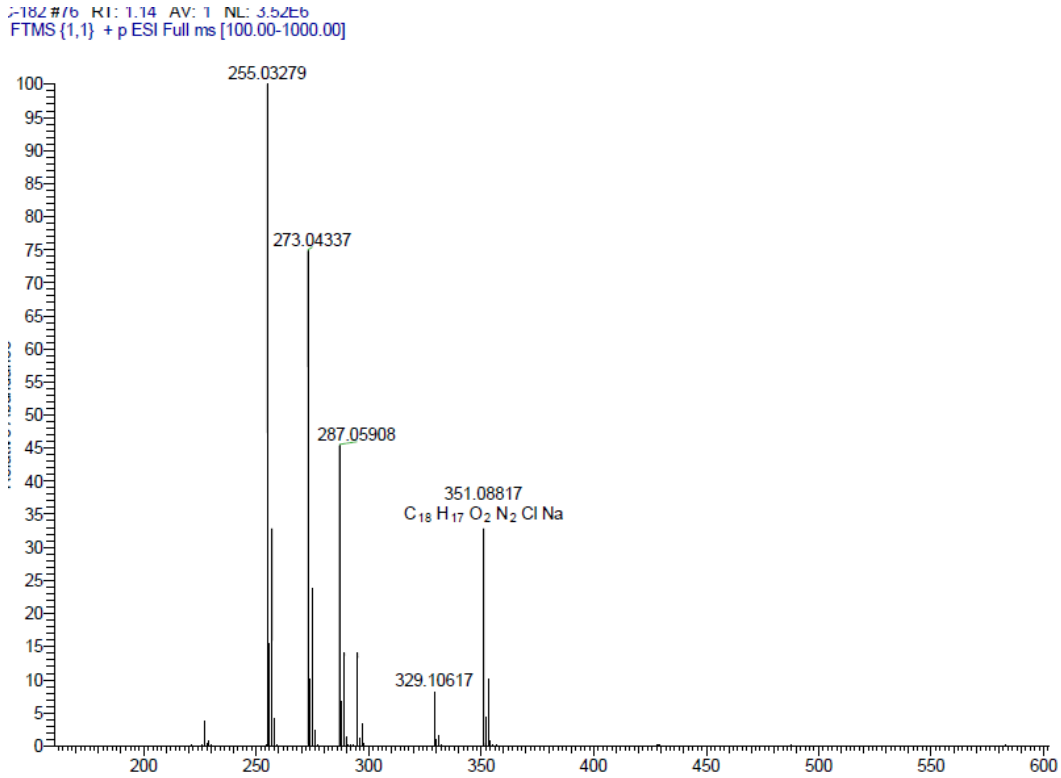
CM264
CM264 70 (2.285)

1: TOF MS ES+
1.00e+000

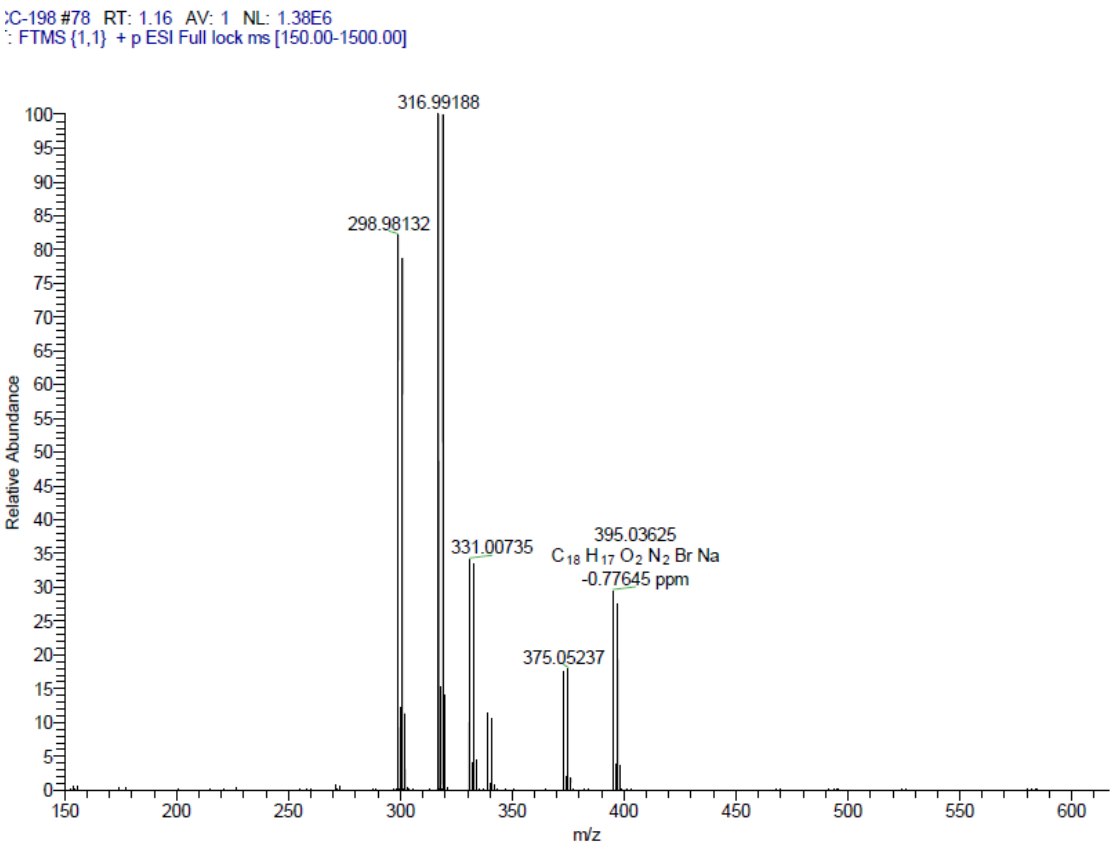



| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 5.0 | 50.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 313.1327 | 313.1352 | -2.5 | -8.0 | 10.5 | n/a | C18 H18 N2 O2 F |

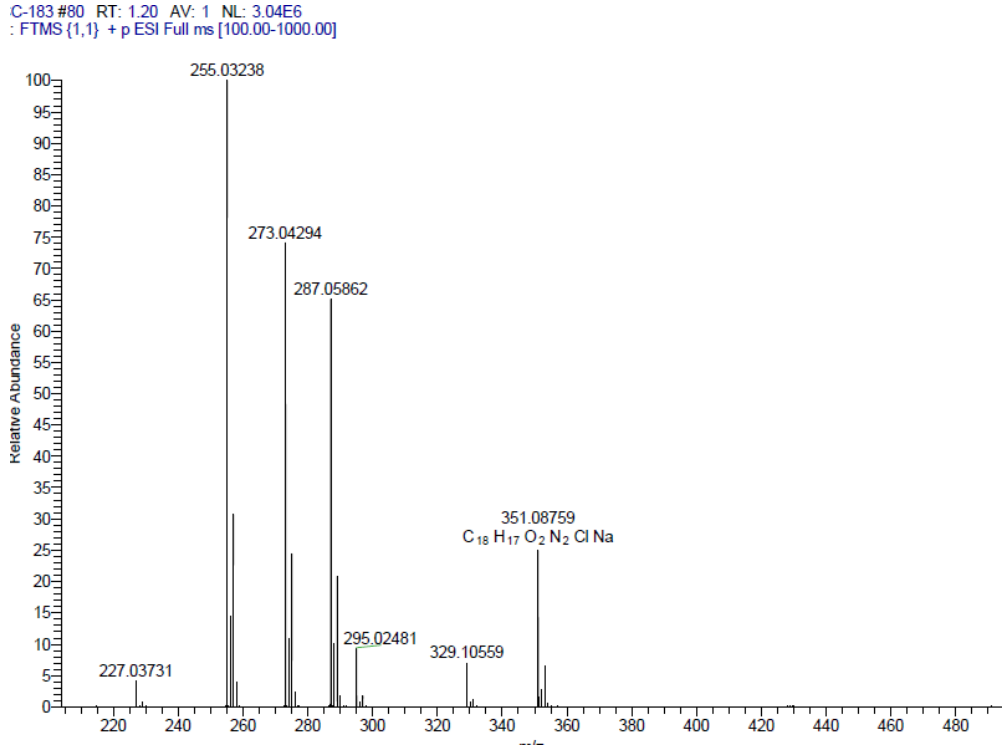
**HRMS of 4j**



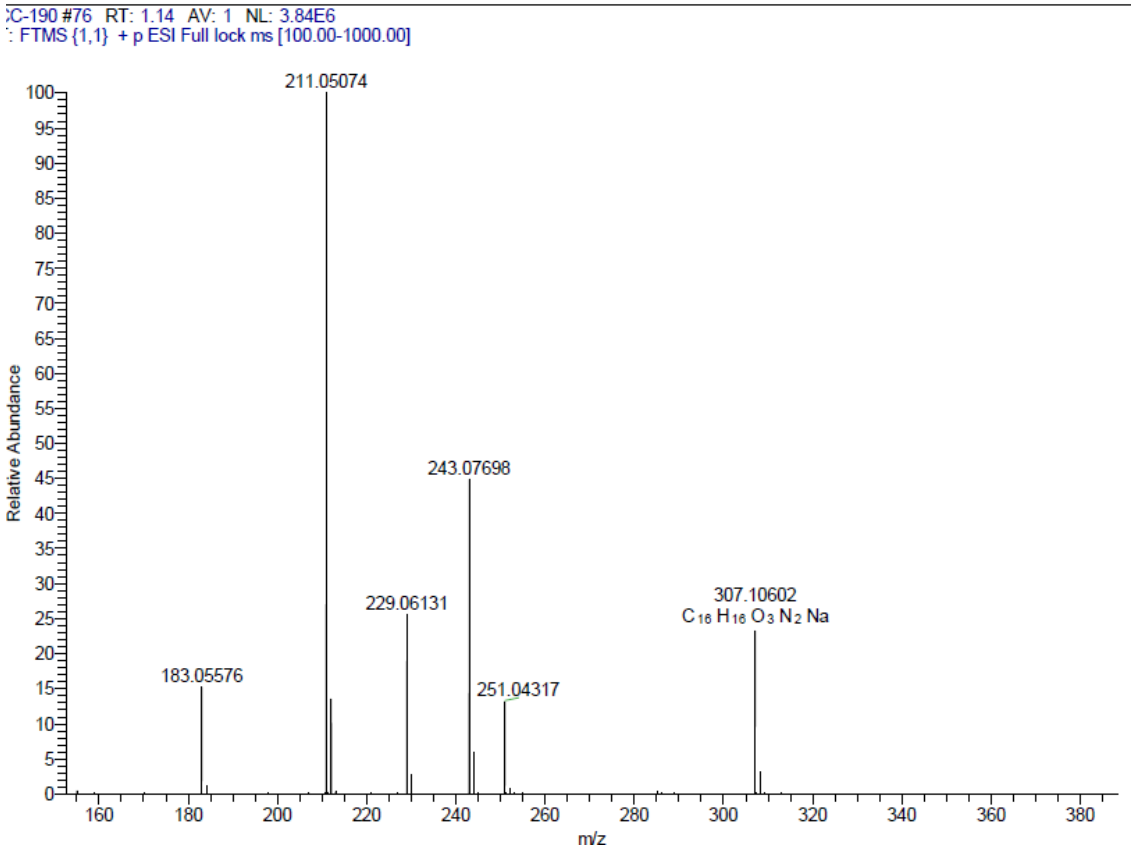

**HRMS of 4k**



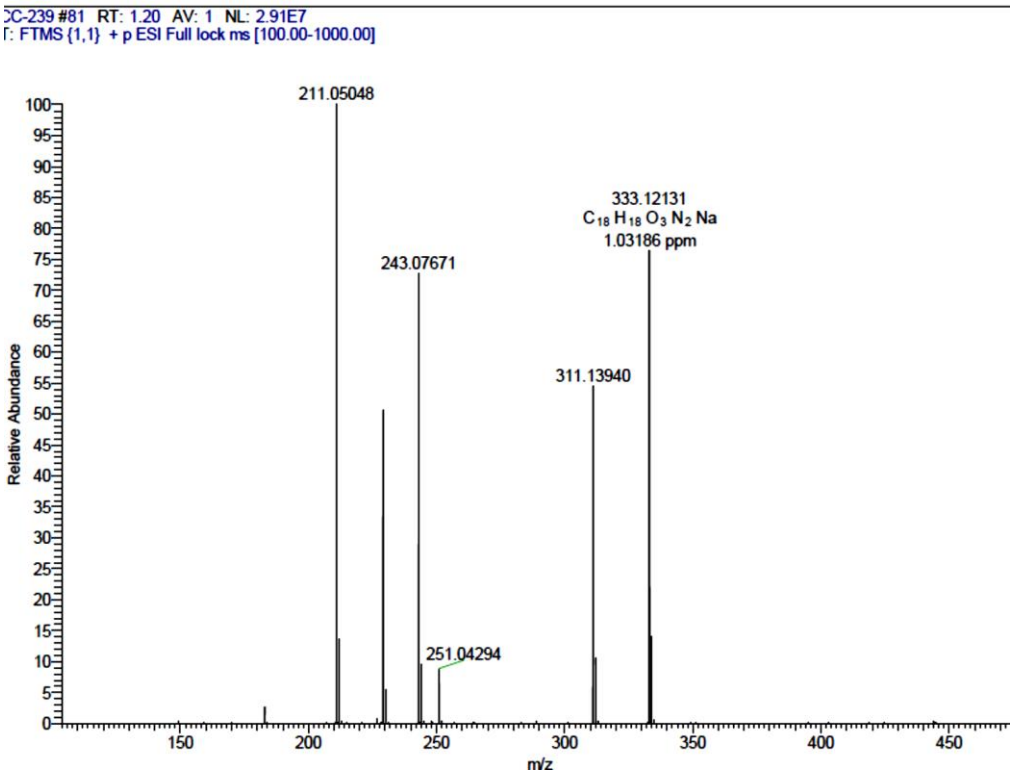

**HRMS of 4l**



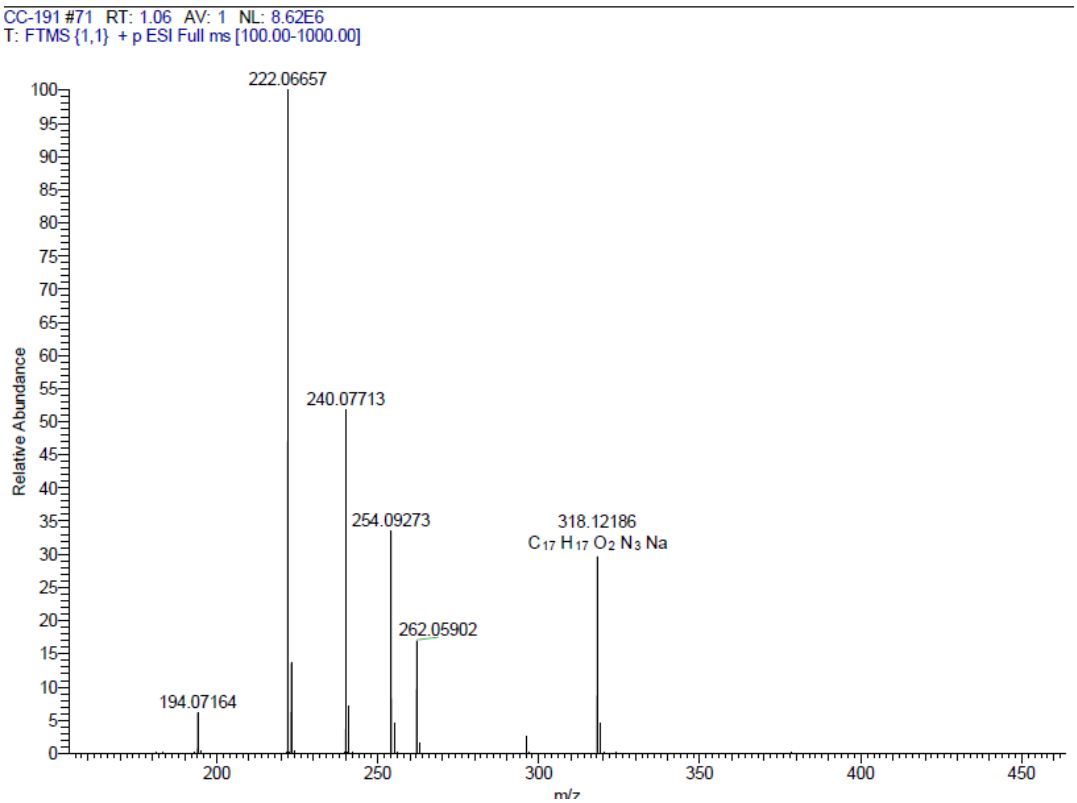

**HRMS of 4m**



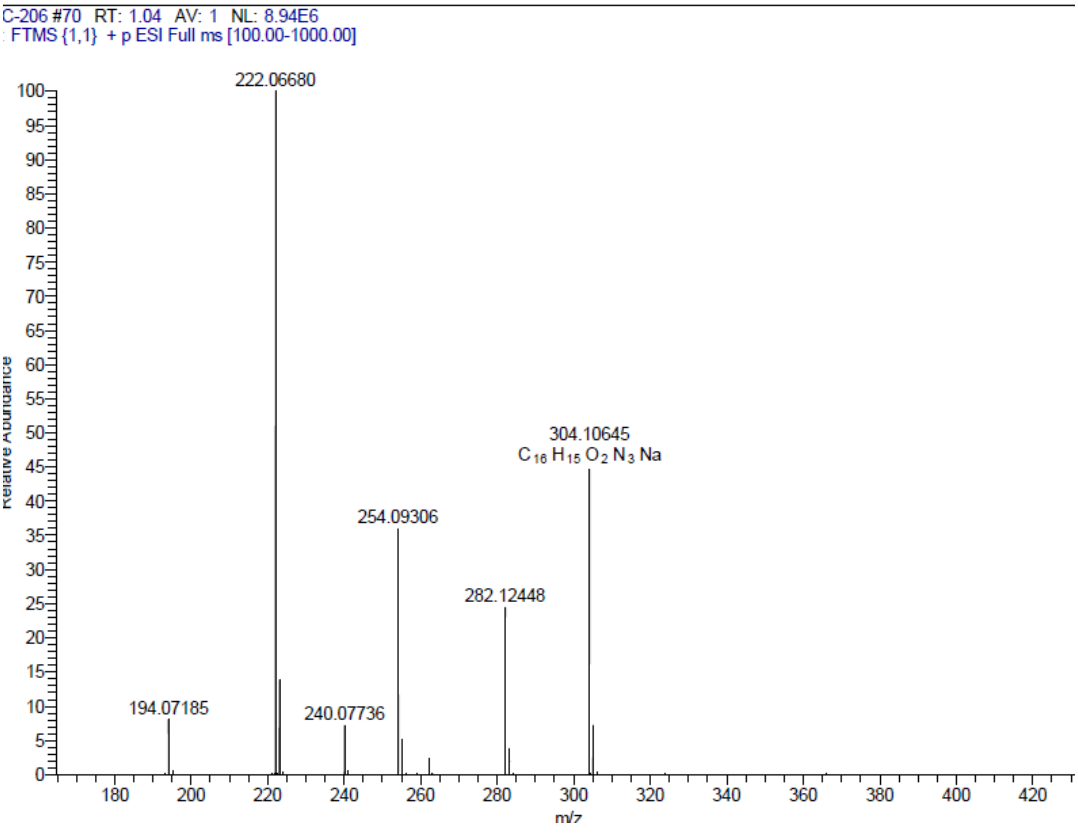

**HRMS of 4o**



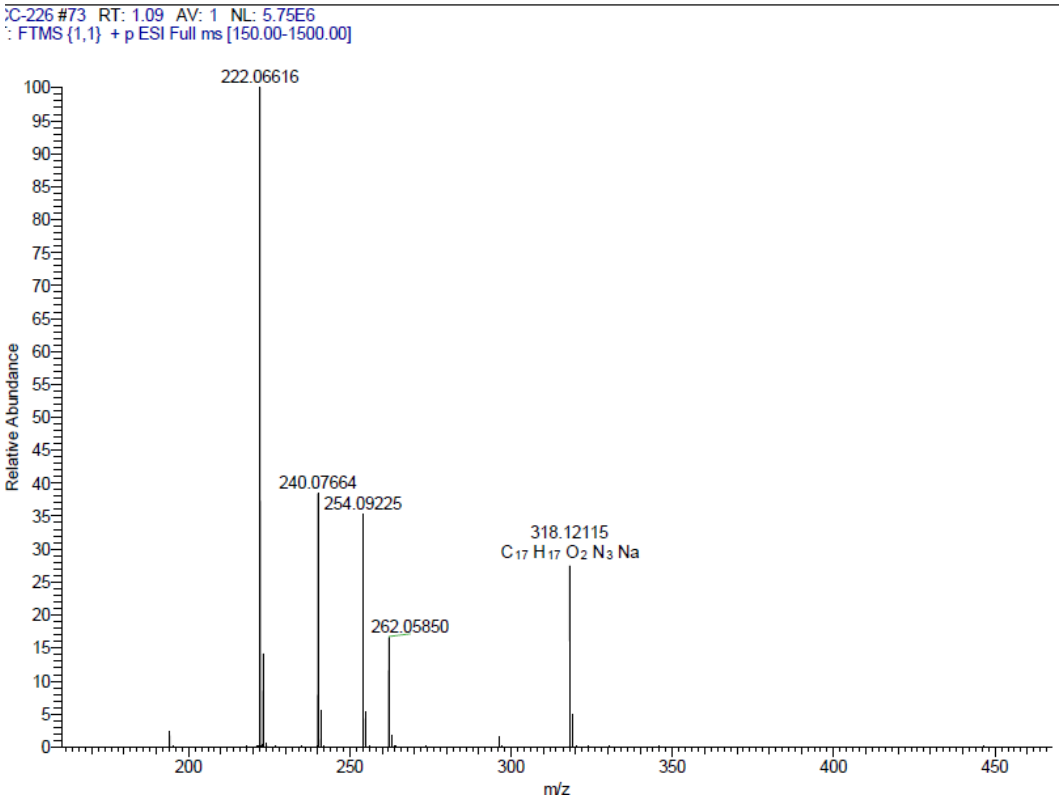

**HRMS of 4p**



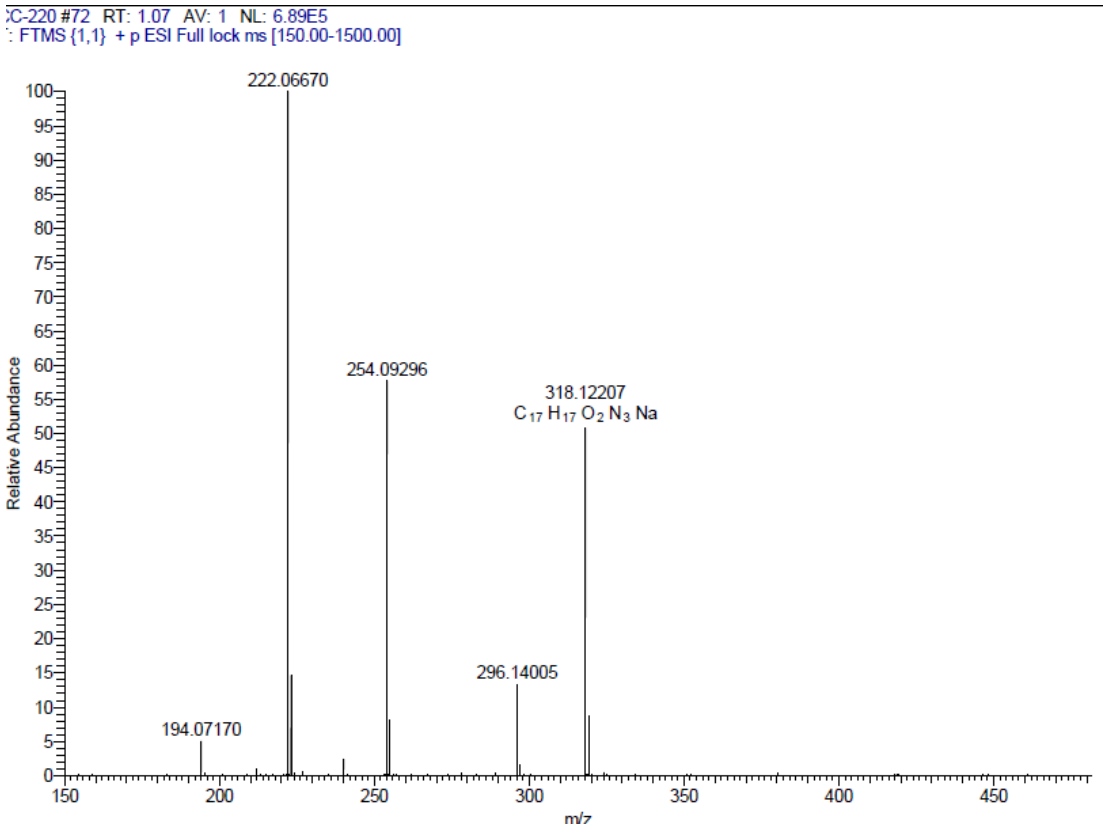

**HRMS of 4q**



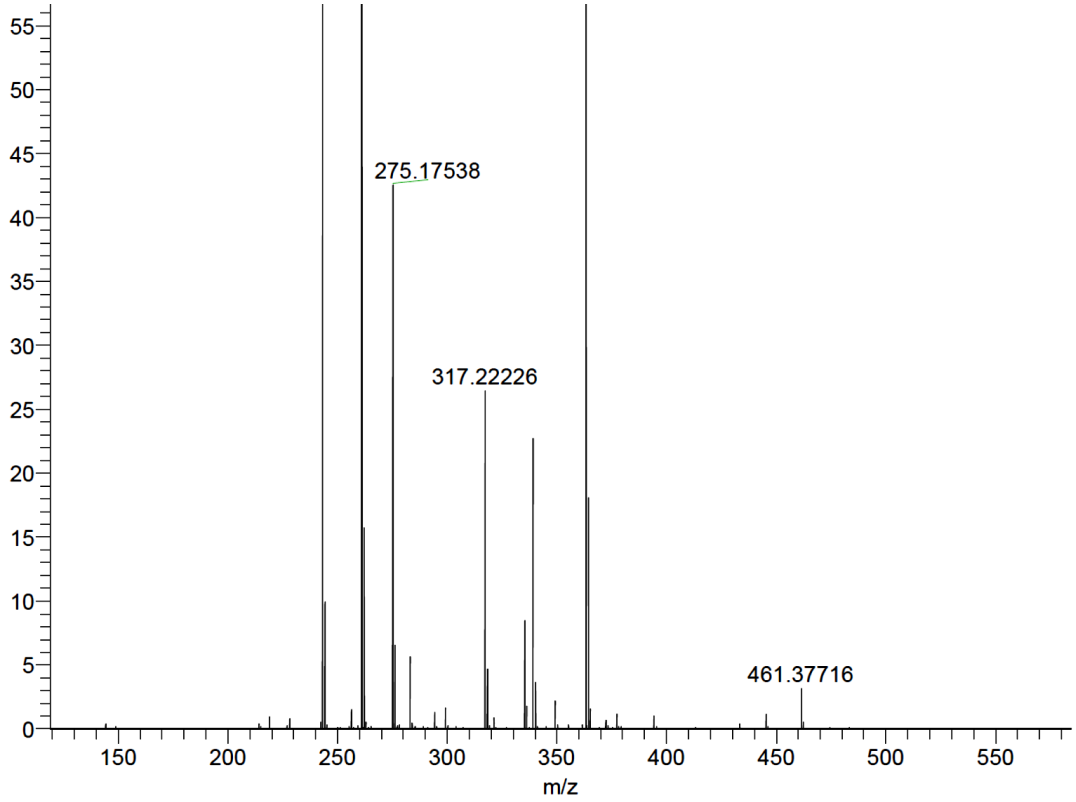

**HRMS of 4r**



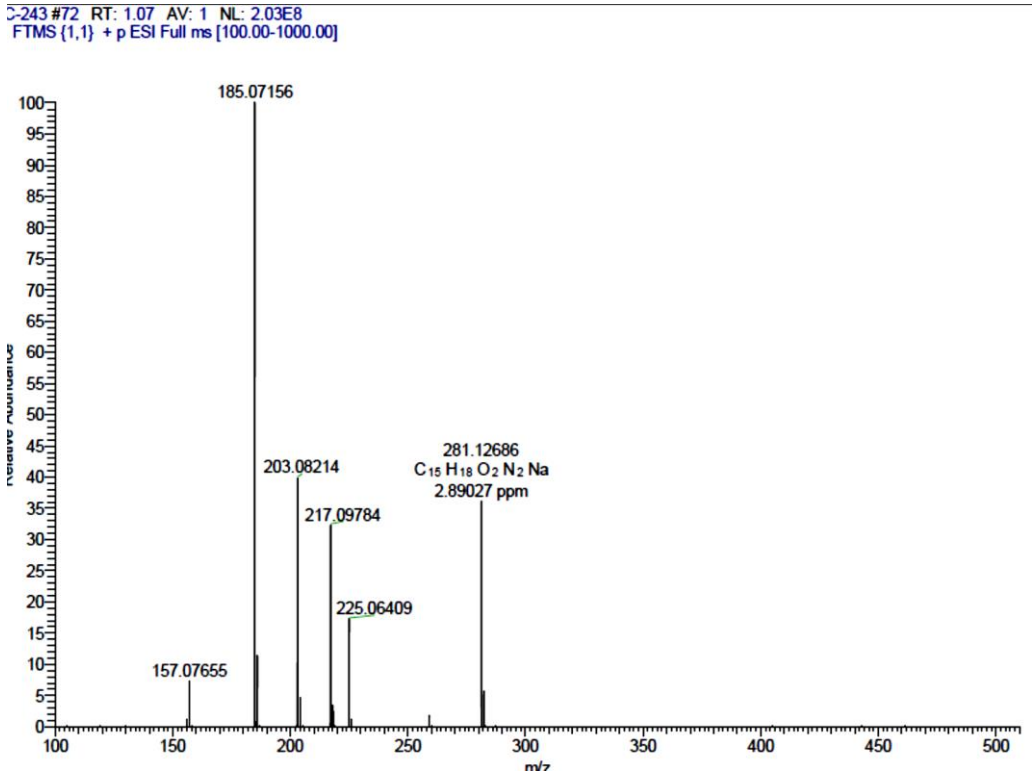

**HRMS of 4s**



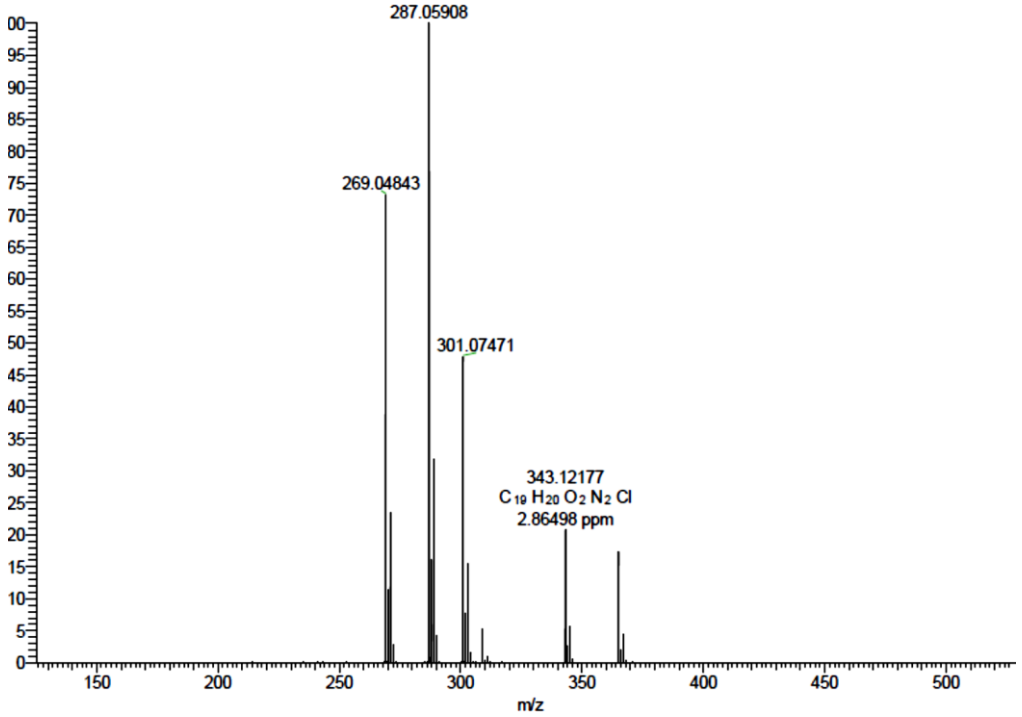

**HRMS of 4u**



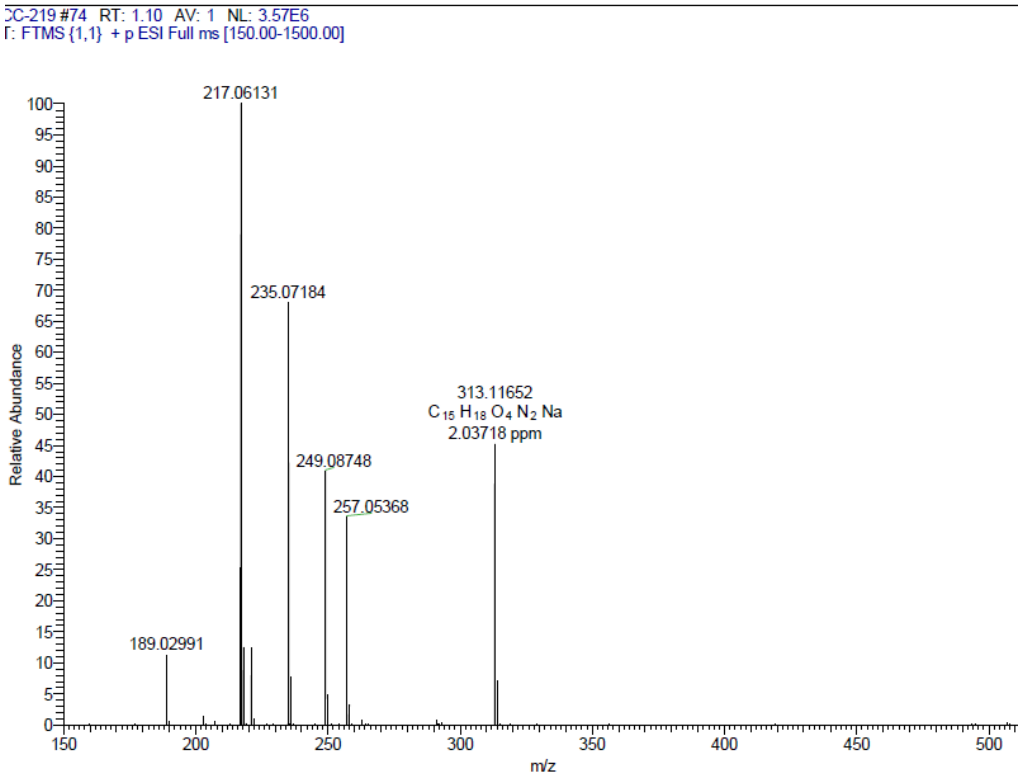

**HRMS of 4v**




**HRMS of 4w**




**HRMS of 4x**

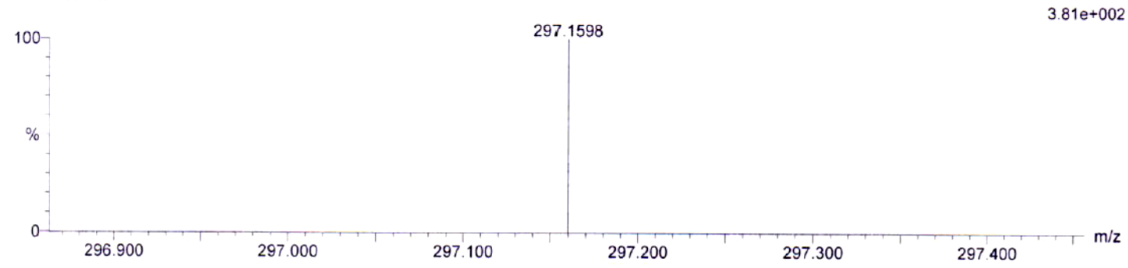



**HRMS of 6a**

**Elemental Composition Report** **Page 1**

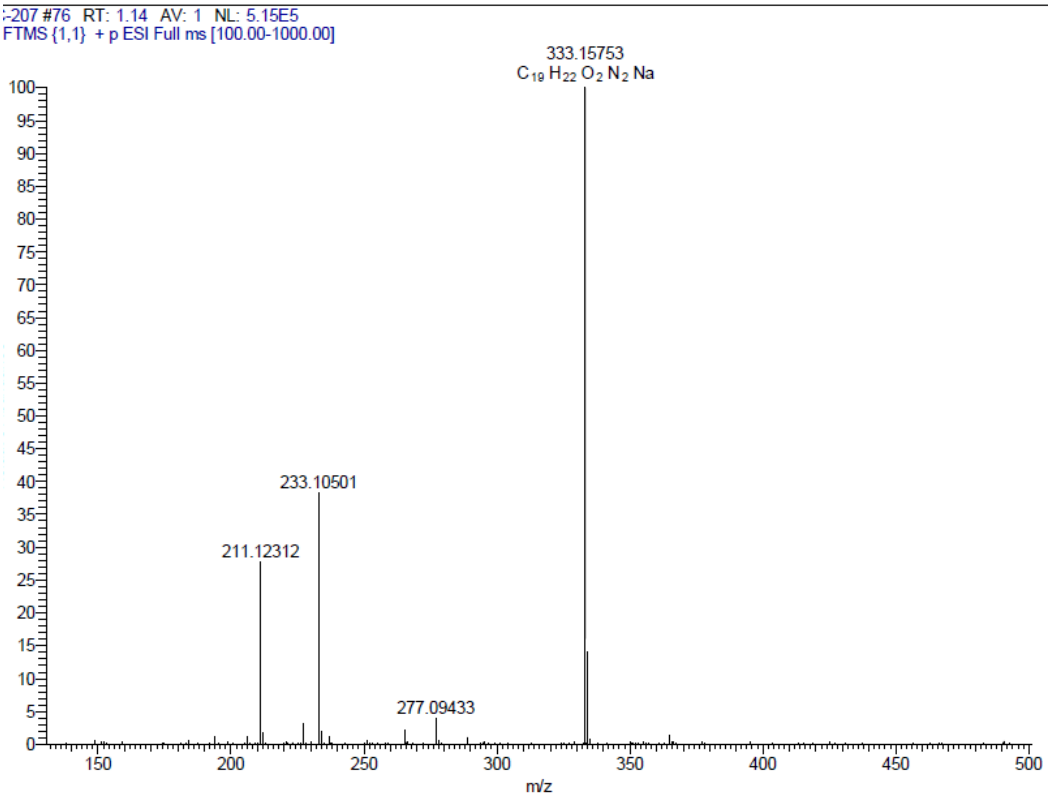
**Single Mass Analysis**
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
15 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-19 H: 0-21 N: 0-2 O: 0-2 Si: 0-1
CM 356 HR 30 (0.356)
1: TOF MS ES+

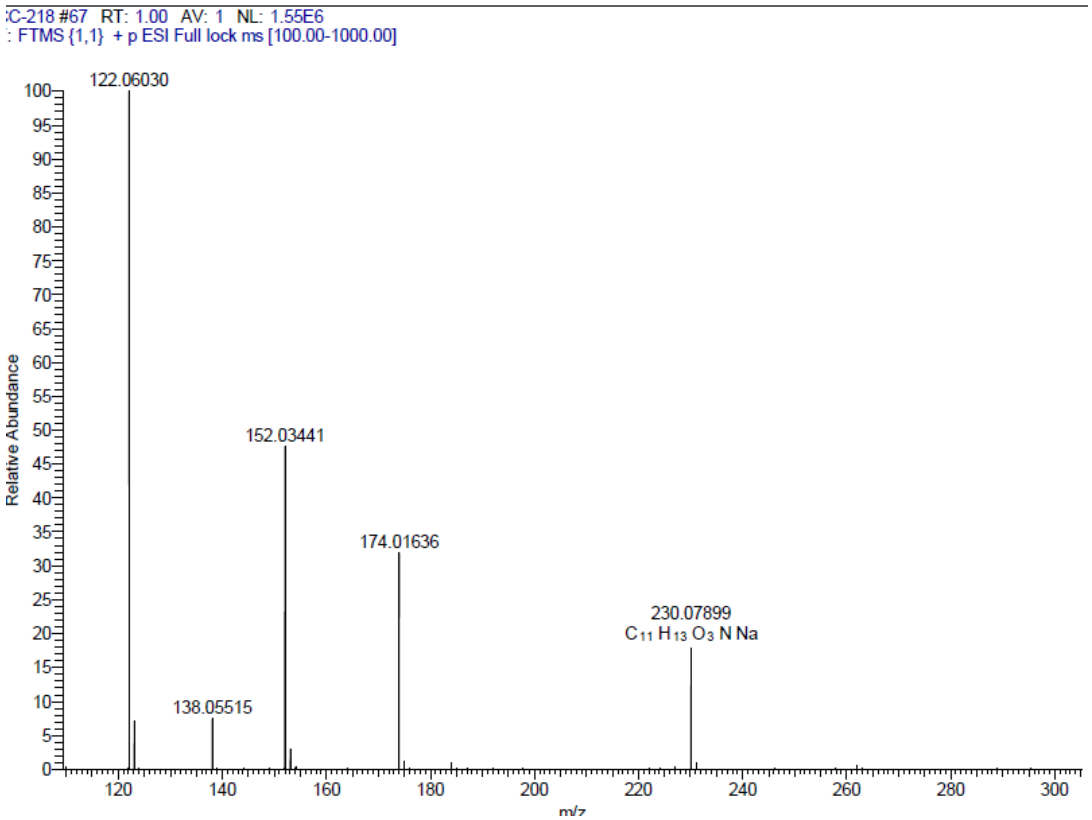



| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 5.0 | 50.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 297.1598 | 297.1603 | -0.5 | -1.7 | 9.5 | n/a | C18 H21 N2 O2 |

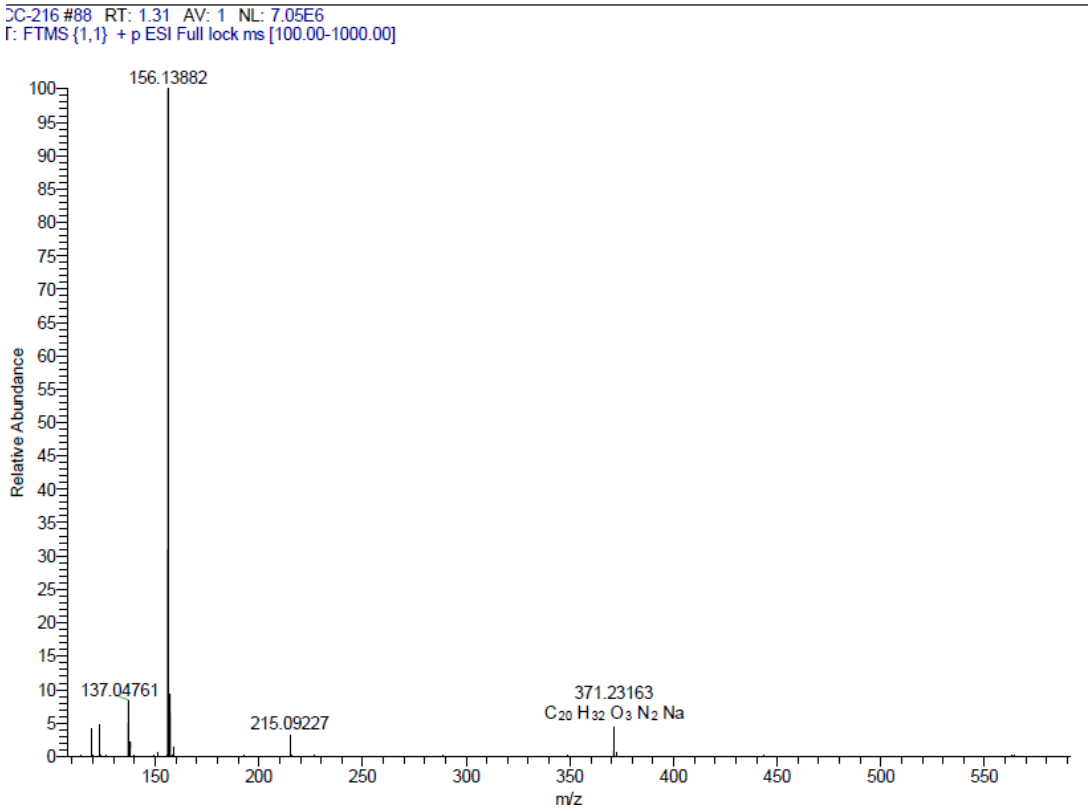
**HRMS of 9a**




**HRMS of 10a**




**HRMS of 11a**




**HRMS of 12a**