Synthesis of Poly-functionalized Imidazoles *via* Vinyl Azides Participated Annulation

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Supporting Information

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General Information

All solvents were purified according to standard methods prior to use. Purifications of products were carried out by chromatography using silica gel (200-300 mesh). Melting points were recorded on a BÜCHI B-540 melting point apparatus. NMR spectra were recorded on a Bruker DRX-500 [Bruker Biospin, Germany] and Mercury plus Varian 300MHz. NMR spectra were recorded for ^{1}H NMR at 500 MHz and for ^{13}C NMR at 125 MHz. For ^{1}H NMR, tetramethylsilane (TMS) served as internal standard (δ=0) and data are reported as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), and coupling constant(s) in Hz. For ^{13}C NMR, TMS (δ=0) or CDCl3 (δ=77.26) was used as internal standard and spectra were obtained with complete proton decoupling. HPLC analysis and the HRMS of all biologically evaluated compounds was confirmed on a Agilent 1290 HPLC-6224 Time of Fight Mass Spectrometer using PhenomenexLuna 5μ C18, 100 Å, 150 × 4.60 mm 5 micron column at a flow rate of 0.5 mL/min using liner gradients buffer B in A (B: CH3OH containing 0.1 % formic acid, A: H_2O containing 0.1% formic acid). Mobile phase B was increased linearly from 5% to 95% over 7 min and 95% over the next 2 min, after which the column was equilibrated to 5% for 1 min.

The starting material **1** and **2** were prepared according to literature methods.[1, 2]

References:

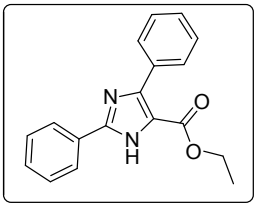
1. Chiba, S.; Wang, Y.-F.; Lapointe, G.; Narasaka, K. *Org. Lett.* **2008**, 10, 313.
2. Caron, S.; Wei, L.; Douville, J.; Ghosh, A. *J. Org. Chem.* **2010**, 75, 945.

General Procedure for the Synthesis of 3

A mixture of vinyl azide **1** (0.1 mmol), imidate or thioamidium **2** (0.11 mmol, 1.1 equiv) was stirred in *t*-BuOH (1.0 mL) in a sealed tube at 110 °C for 8 h. After the completeness of the reaction, the mixture was cooled down to room temperature and diluted with water, extracted three times with EtOAc (3 × 10 mL). The combined organic extracts were washed with brine, dried over Na_2SO_4, concentrated and purified by flash chromatography (DCM/MeOH) on silica gel to afford **3**.

Characterization Data

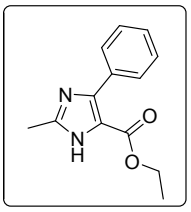
Ethyl 2, 4-diphenyl-*1H*-imidazole-5-carboxylate (3a)



Yellow solid, m.p. 158.9-159.1 °C; Yield: 269 mg (92%); ^{1}H NMR (500 MHz, $CDCl_3$) δ10.43 (s, 1H), 7.97 (m, 4H), 7.48-7.36 (m, 6H), 4.33 (q, *J* = 6.4 Hz, 2H), 1.30 (t, *J* = 6.4 Hz, 3H); ^{13}C NMR

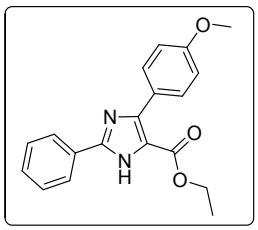
(125 MHz, $CDCl_3$) δ 160.8, 148.1, 133.6, 130.0, 129.6, 129.2, 129.0, 128.7, 128.0, 126.3, 119.0, 61.2, 14.3. HRMS (ESI) calcd. for $C_{18}H_{17}N_2O_2$ [M+H]+ = 293.1285, found 293.1285.

Ethyl 2-methyl-4-phenyl-*1H*-imidazole-5-carboxylate (3b)



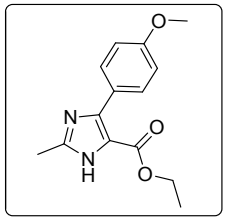
Yellow oil; Yield: 159 mg (69%); ^1H NMR (500 MHz, $CDCl_3$) δ 7.59 (dd, *J* = 7.7, 1.7 Hz, 2H), 7.22-7.16 (m, 3H), 4.10 (q, *J* = 7.1 Hz, 2H), 2.09 (s, 3H), 1.07 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.1, 146.4, 142.5, 131.5, 129.2, 128.3, 127.8, 122.0, 60.4, 14.0, 13.3. HRMS (ESI) calcd. for $C_{13}H_{15}N_2O_2$[M+H]+ = 231.1128, found 231.1128.

Ethyl 4-(4-methoxyphenyl)-2-phenyl-*1H*-imidazole-5-carboxylate (3c):



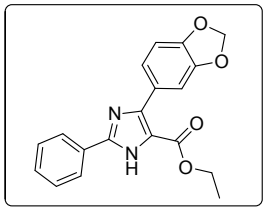
Yellow solid, m.p. 122.9-123.3 ℃; Yield: 258 mg (80%);^1H NMR (500 MHz, $CDCl_3$) δ 10.18 (s, 1H), 7.97 (m, 3H), 7.48-7.36 (m, 6H), 4.35 (q, *J* = 7.1 Hz, 2H), 1.69 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.2, 162.1, 158.8, 138.0, 131.2, 126.4, 123.3, 121.8, 114.1, 112.2, 109.0, 93.7, 60.8, 55.4, 14.4. HRMS (ESI) calcd for $C_{19}H_{19}N_2O_3$ [M+H]+ = 323.1390, found 323.1391.

Ethyl 4-(4-methoxyphenyl)-2-methyl-*1H*-imidazole-5-carboxylate (3d):



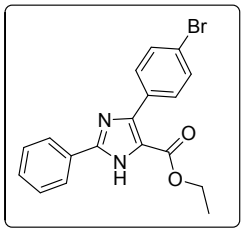
Yellow oil; Yield: 177 mg (68%); ^1H NMR (500 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.7 Hz, 2H), 6.88-6.83 (m, 2H), 4.24 (q, *J* = 7.1 Hz, 2H), 3.78 (s, 3H), 2.28 (s, 3H), 1.23 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.9, 159.9, 146.2, 130.6, 124.5, 113.4, 60.6, 55.4, 14.3, 13.9. HRMS (ESI) calcd. for $C_{14}H_{17}N_2O_3$[M+H]$^+$ = 261.1234, found 261.1234;

Ethyl 4-(benzo[*d*][1,3]dioxol-5-yl)-2-phenyl-*1H*-imidazole-5-carboxylate (3e):



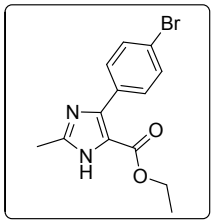
Yellow solid, m.p. 202.5-202.8 °C; Yield: 221 mg (66%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.01 (s, 1H), 7.95 (d, *J* = 6.8 Hz, 2H), 7.49-7.43 (m, 5H), 6.87 (d, *J* = 8.1 Hz, 1H), 6.00 (s, 2H), 4.37 (q, *J* = 7.1 Hz, 2H), 1.36 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.1, 147.5, 1230.1, 129.2, 129.1, 126.1, 123.8, 122.3, 118.3, 110.2, 108.1, 101.3, 61.2, 14.5. HRMS (ESI) calcd. for $C_{19}H_{17}N_2O_4$ $[M+H]^+$ = 337.1183, found 337.1184.

Ethyl 4-(4-bromophenyl)-2-phenyl-1H-imidazole-5-carboxylate (3f):



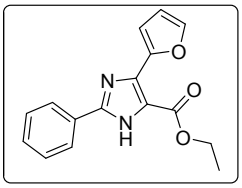
Yellow solid, m.p. 159.0-159.3 °C; Yield: 344 mg (93%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.23 (s, 1H), 7.96 (d, *J* = 6.7 Hz, 2H), 7.88 (m, 2H), 7.55 (d, *J* = 8.4 Hz, 2H), 7.47 (d, *J* = 7.3 Hz, 3H), 4.36 (q, *J* = 7.1 Hz, 2H), 1.34 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.0, 148.1, 132.0, 130.3, 130.1, 129.7, 129.1, 128.4, 126.0, 124.2, 123.5, 123.1, 61.5, 14.3. HRMS (ESI) calcd for$C_{18}H_{16}BrN_2O_2$ $[M+H]^+$ = 371.0390, found 371.0392.

Ethyl 4-(4-bromophenyl)-2-methyl-*1H*-imidazole-5-carboxylate (3g):



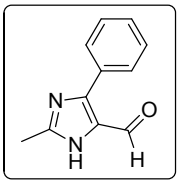
Yellow solid, m.p.137.3-137.5 °C. Yield: 271 mg (88%);^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.3 Hz, 2H), 7.69 (d, *J* = 8.3 Hz, 2H), 7.47-7.45(m, 2H), 7.41-7.38 (m, 2H), 7.35-7.33(m, 1H), 7.31 (d, *J* = 7.8 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.15-7.13 (m, 1H), 7.08 (d, *J* = 8.0 Hz, 2H), 5.11 (s, 2H), 3.73 (s, 2H), 3.59 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.4, 158.3, 147.2, 146.0, 142.1, 136.8, 130.4, 130.0, 129.3, 128.9, 128.6, 128.0, 127.8, 127.7, 127.6, 127.4, 124.2, 119.1, 115.3, 70.0, 51.9. HRMS (ESI) calcd. for$C_{27}H_{23}N_2O_5$ [M+H]+= 455.1601, found 455.1601.

Ethyl 4-(furan-2-yl)-2-phenyl-*1H*-imidazole-5-carboxylate (3i):



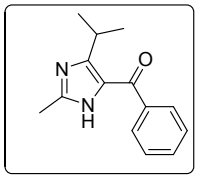
Yellow solid, m.p. 117.7-118.0 ^{o}C; Yield: 155 mg (55%); ^{1}H NMR (500 MHz, $CDCl_3$) δ10.19 (s, 1H), 7.98 (m, 3H), 7.44 (m, 5H), 4.35 (q, J = 7.1 Hz, 2H), 1.33 (t, J = 7.1 Hz, 3H).; ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.4, 148.3, 147.7, 133.3, 129.9, 129.4,129.0, 128.9, 128.5, 127.8, 126.0, 118.5, 61.1, 14.2. HRMS (ESI) calcd. for $C_{16}H_{15}N_2O_3$ $[M+H]^+$ = 283.1077, found 283.1077.

2-Methyl-4-phenyl-*1H*-imidazole-5-carbaldehyde (3k):



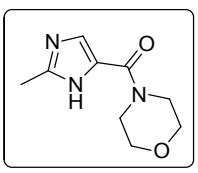
Yellow solid, m.p. 164.9-165.2 ^{o}C; Yield: 52 mg (28%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.04 (s, 1H), 8.19-8.09 (m, 2H), 7.46-7.37 (m, 3H), 7.09 (s, 1H), 2.40 (s, 3H).; ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.6, 161.2, 139.7, 134.1, 132.4, 130.6, 129.0, 128.0, 16.8. HRMS (ESI) calcd. for $C_{11}H_{11}N_2O$ $[M+H]^+$= 187.0866, found 187.0866.

(4-Isopropyl-2-methyl-*1H*-imidazol-5-yl)(phenyl)methanone (3l):



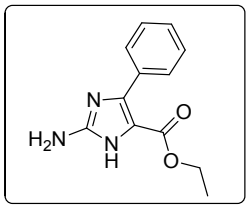
Yellow solid, m.p.95.8-96.2 ^{o}C; Yield: 217 mg (95%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (s, 2H), 7.53 (t, J = 7.3 Hz, 1H), 7.45 (t, J = 7.4 Hz, 2H), 3.71 (d, J = 7.0 Hz, 1H), 2.42 (s, 3H), 1.21 (d, J = 6.8 Hz, 6H). ^{13}C NMR (125MHz, $CDCl_3$) δ 188.7, 145.8, 139.4, 132.0, 129.3, 128.2, 26.2, 22.3, 14.2. HRMS (ESI) calcd. for $C_{14}H_{17}N_2O$ $[M+H]^+$=229.1335, found 229.1337.

(2-Methyl-*1H*-imidazol-5-yl)(morpholino)methanone (3m):



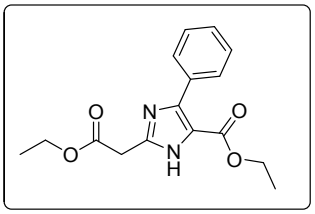
Yellow solid, m.p.174.1-174.3 ^{o}C; Yield: 176 mg (90%); ^{1}H NMR (500 MHz, DMSO-d6) δ 12.21 (s, 1H), 7.46 (s, 1H), 4.11 -4.51 (m, 8H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d6) δ 171.9, 162.3, 162.2, 144.3, 66.9, 22.9, 14.20. HRMS (ESI) calcd. for $C_9H_{14}N_3O_2$ [M+H]+ = 196.1081, found 196.1083.

Ethyl 2-amino-4-phenyl-*1H*-imidazole-5-carboxylate (3n):



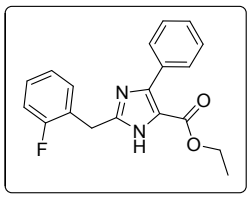
Yellow oil. Yield: 169 mg (73%); ^{1}H NMR (500 MHz, DMSO-d6) δ 10.86(s, 1H), 7.86 (d, *J* = 7.4 Hz, 2H), 7.32-7.24 (m, 3H), 5.73 (s, 2H), 4.13 (q, *J* = 7.1 Hz, 2H), 1.19 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, DMSO-d6) δ 164.8, 156.6, 139.0, 137.0, 133.9, 132.8, 132.6, 64.5, 19.5. HRMS (ESI) calcd. for $C_{12}H_{14}N_3O_2$[M+H]+ = 232.1081, found 232.1082.

Ethyl 2-(2-ethoxy-2-oxoethyl)-4-phenyl-*1H*-imidazole-5-carboxylate (3o):



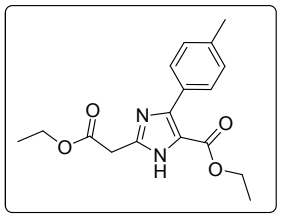
Yellow solid, m.p.116.3-116.7 ^{o}C. Yield: 193 mg (64%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.22 (s, 1H), 7.24-7.16 (m, 5H), 5.14 (s, 2H), 4.26 (q, *J* = 7.1 Hz, 2H), 4.16 (t, *J* = 7.1 Hz, 2H), 1.26 (t, *J* = 7.1 Hz , 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.5, 165.6, 147.1, 131.2, 128.8, 127.3, 126.3, 125.1, 111.6, 93.3, 61.6, 59.7, 14.6, 14.2. HRMS (ESI) calcd. for $C_{16}H_{19}N_2O_4$ $[M+H]^+$ =303.1339, found 303.1339.

Ethyl 2-(2-fluorobenzyl)-4-phenyl-*1H*-imidazole-5-carboxylate (3p):



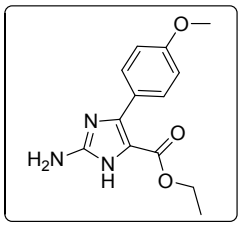
Yellow oil; Yield: 185 mg (57%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (s, 2H), 7.40-7.33 (m, 3H), 7.26 (s, 2H), 7.12-7.04 (m, 2H), 4.27 (q, *J* = 7.1 Hz, 2H), 4.15 (s, 2H), 1.27 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.6(d, *J* = 245.1 Hz), 159.4, 146.8, 131.1, 130.2, 130.0 (d, *J* = 3.8 Hz), 128.3,128.2, 126.8, 123.7,123.6, 122.1 (d, *J* = 15.6 Hz), 120.7, 114.5 (d, *J* = 21.6 Hz), 60.1, 27.2 (d, *J* = 3.3 Hz), 13.1. HRMS (ESI) calcd. for $C_{19}H_{18}FN_2O_2$ $[M+H]^+$=325.1347, found 325.1348.

Ethyl 2-(2-ethoxy-2-oxoethyl)-4-(p-tolyl)-*1H*-imidazole-5-carboxylate (3q):



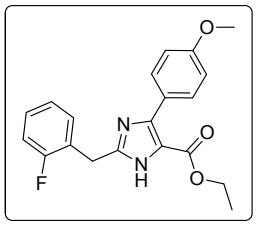
Yellow oil. Yield: 250 mg (79%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.07 (s, 1H), 7.16 (d, *J* = 8.1 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 2H), 5.15 (s, 2H), 4.28 (d, *J* = 7.2 Hz, 2H), 4.19 (d, *J* = 7.1 Hz, 2H), 2.31 (s, 3H), 1.32-1.26 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.4, 165.6, 146.8, 137.3, 129.5, 128.4, 126.3, 125.3, 111.2, 93.1, 61.5, 59.6, 21.3, 14.6, 14.2. HRMS (ESI) calcd. for $C_{17}H_{21}N_2O_4$ $[M+H]^+$ =317.1496, found 317.1498.

Ethyl 2-amino-4-(4-methoxyphenyl)-*1H*-imidazole-5-carboxylate (3r):



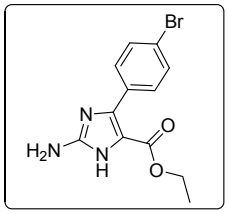
Yellow oil. Yield: 178 mg (68%); ^{1}H NMR (500 MHz, DMSO-d6) δ 10.68 (s, 1H), 7.86 (d, *J* = 8.6 Hz, 2H), 6.86 (d, *J* = 9.0 Hz, 2H), 5.68 (s, 2H), 4.12 (q, *J* = 7.1 Hz, 2H), 3.73 (s, 3H), 1.20 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, DMSO-d6) δ 160.2, 159.3, 151.8, 130.4, 113.3, 59.6, 55.5, 14.8. HRMS (ESI) calcd. for $C_{13}H_{16}N_3O_3[M+H]^+$ = 262.1186, found 262.1188.

Ethyl 2-(2-fluorobenzyl)-4-(4-methoxyphenyl)-*1H*-imidazole-5-carboxylate (3s):



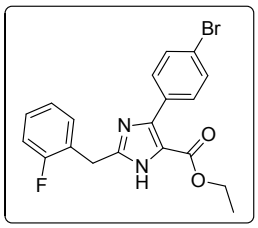
Yellow oil; Yield: 163 mg (46%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.58 (s, 1H), 7.87 (s, 1H), 7.31-7.25 (m, 2H), 7.09 (d, *J* = 6.8 Hz, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 4.34-4.24 (m, 2H), 4.15 (s, 2H), 3.83 (s, 3H), 1.30 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.7, 159.8, 159.8, 131.2, 131.2, 130.5, 129.3, 129.2, 124.7, 124.7, 115.7, 115.5, 113.3, 60.7, 55.2, 28.5, 14.2. HRMS (ESI) calcd. for $C_{20}H_{20}FN_2O_3$ $[M+H]^+$=355.1452, found 355.1452.

Ethyl 2-amino-4-(3-bromophenyl)-*1H*-imidazole-5-carboxylate (3t):



Yellow solid, m.p. 182.6-182.9 ^{o}C; Yield: 273 mg (88%); ^{1}H NMR (500 MHz, DMSO-d6) δ 10.86 (s,1H),7.86 (d, *J* = 7.4 Hz, 2H), 7.32-7.24 (m, 3H), 5.73 (s, 2H), 4.13 (q, *J* = 7.1 Hz, 2H), 1.19 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, DMSO-d6) δ 164.8, 156.6, 139.0, 137.0, 133.9, 132.8, 132.6, 64.5, 19.5; HRMS (ESI) calcd. for $C_{12}H_{13}BrN_3O_2[M+H]^+$ = 310.0186, found 310.0186.

Ethyl 4-(3-bromophenyl)-2-(2-fluorobenzyl)-*1H*-imidazole-5-carboxylate (3u):



Yellow oil; Yield: 330 mg (88%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.89 (s, 1H), 7.93 (s,1H), 7.93 (s,1H),7.40 (m, , 1H), 7.39 (m, 1H), 7.20-7.16 (m, 2H), 7.06-6.99 (m, 2H), 4.22 (q, *J* = 7.1 Hz, 2H), 4.10 (s, 2H), 1.23 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.6(d *J* = 245.1 Hz), 159.4, 146.8, 131.1, 130.2, 130.0 (d, *J* = 3.8 Hz), 128.3, 128.2, 126.8, 123.7, 123.6, 122.1 (d, *J* = 15.6 Hz), 120.7, 114.5 (d, *J* = 21.6 Hz), 60.1, 27.2 (d, *J* = 3.3 Hz), 13.1. HRMS (ESI) calcd. for $C_{19}H_{17}BrFN_2O_2$ [M+H]+= 403.0452, found 403.0452.

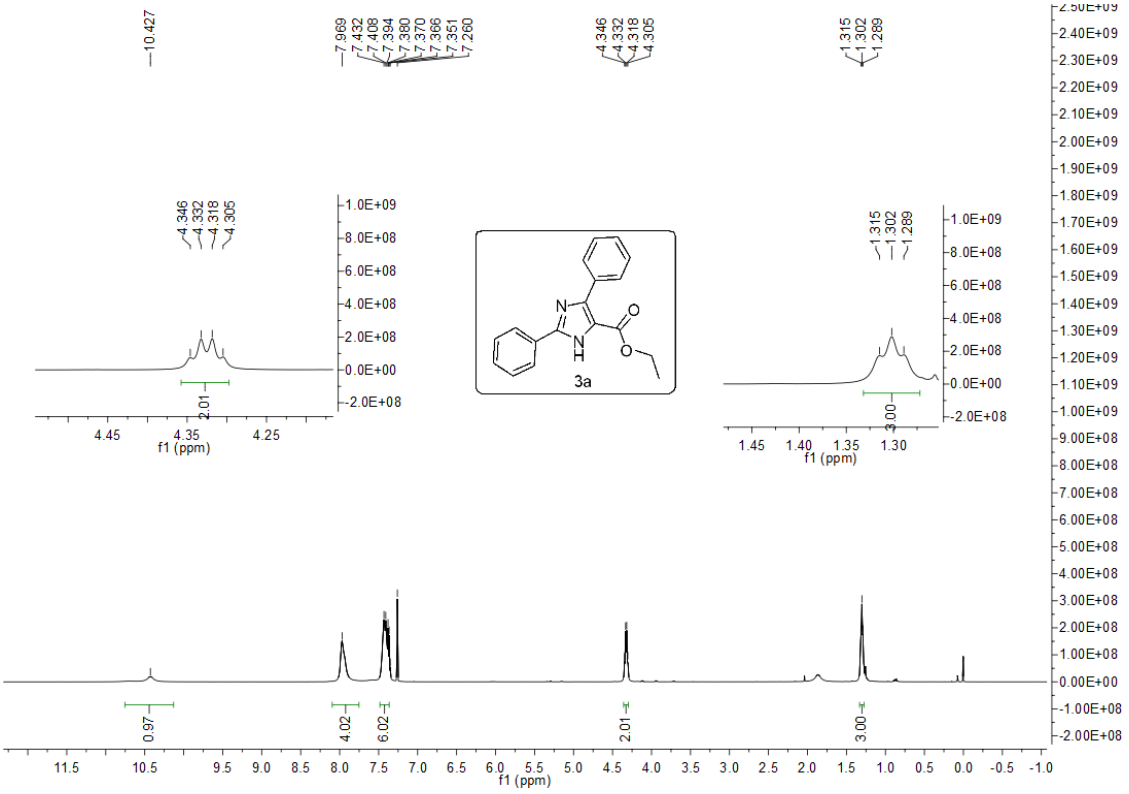
X-ray crystallography Data of 3g (CCDC No: 1045551):

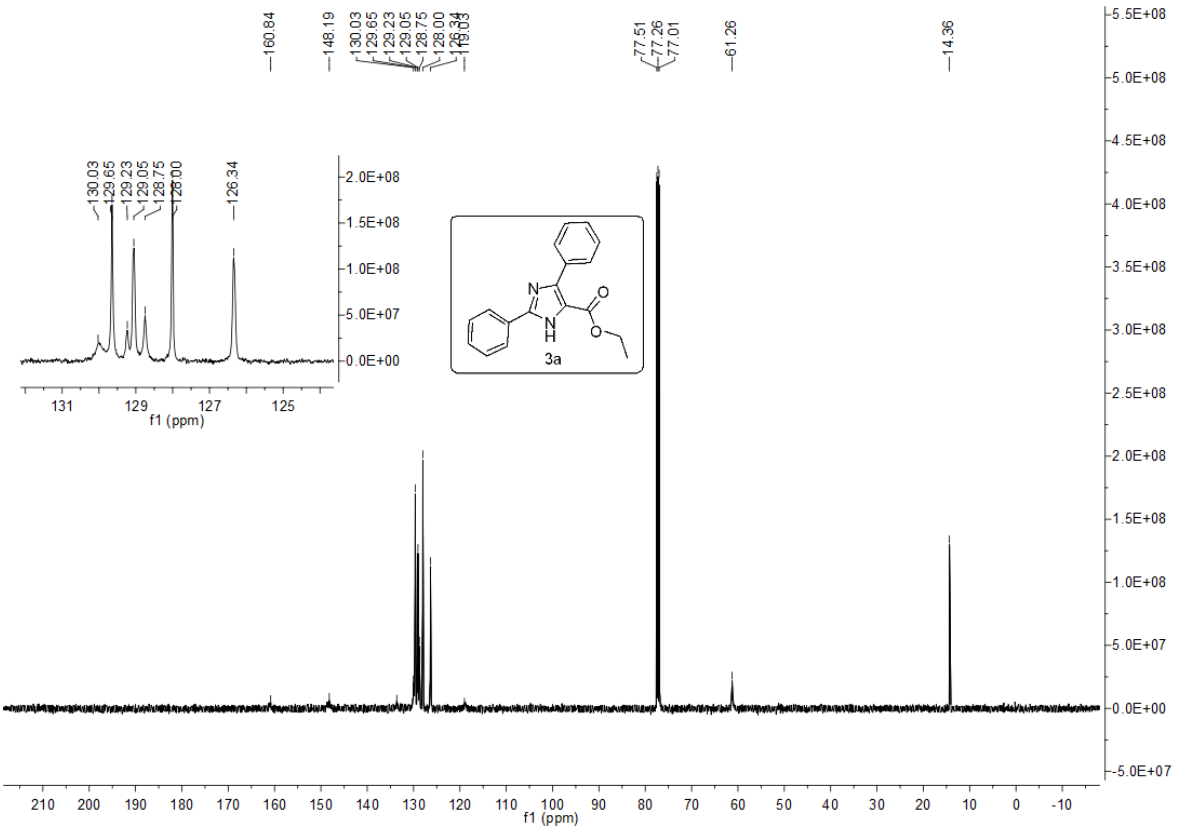
Single crystals of compound **3g** were measured on a Rigaku RAXIS-RAPID single-crystal diffractometer. The recrystallization solvent of **3g** was EtOH.

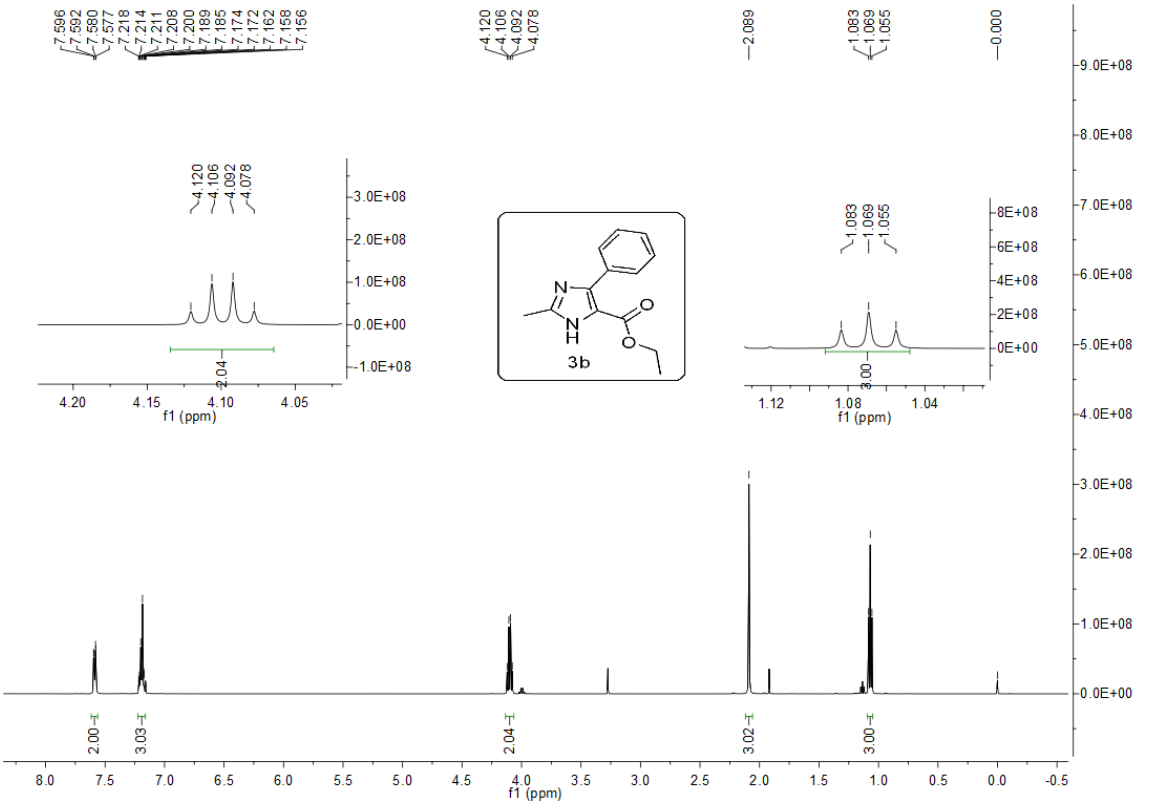
Table S1 X-ray crystallography data of **3g**

Formula moiety	$C_{13}H_{13}BrN_2O_2$
Formula sum	$C_{13}H_{13}BrN_2O_2$
Formula weight	309.16
Temperature	293 K
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	a= 9.0885(9) Å b= 10.1681(9) Å c= 15.4664(10) Å alpha= 88.451(6) deg. beta = 87.493(7) deg. gamma = 66 deg.
Volume	1307.0(2) $Å^3$
Z	4
Calculated density	1.571 g/cm^3
Absorption coefficient	3.141mm^{-1}
F(000)	624
Crystal size	0.18 x 0.16 x 0.13 mm
Theta range for data collection	3.4 to 25.3 deg
Reflections collected / unique	8223 / 4768 [R(int) = 0.0385]
Data / restraints / parameters	4768 / 0 / 329
Goodness-of-fit on F2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0461, wR2 = 0.0883
R indices (all data)	R1 = 0.0889, wR2 = 0.1089

^{1}H NMR (500 MHz) and^{13}C NMR (125 MHz) Spectra of 3:



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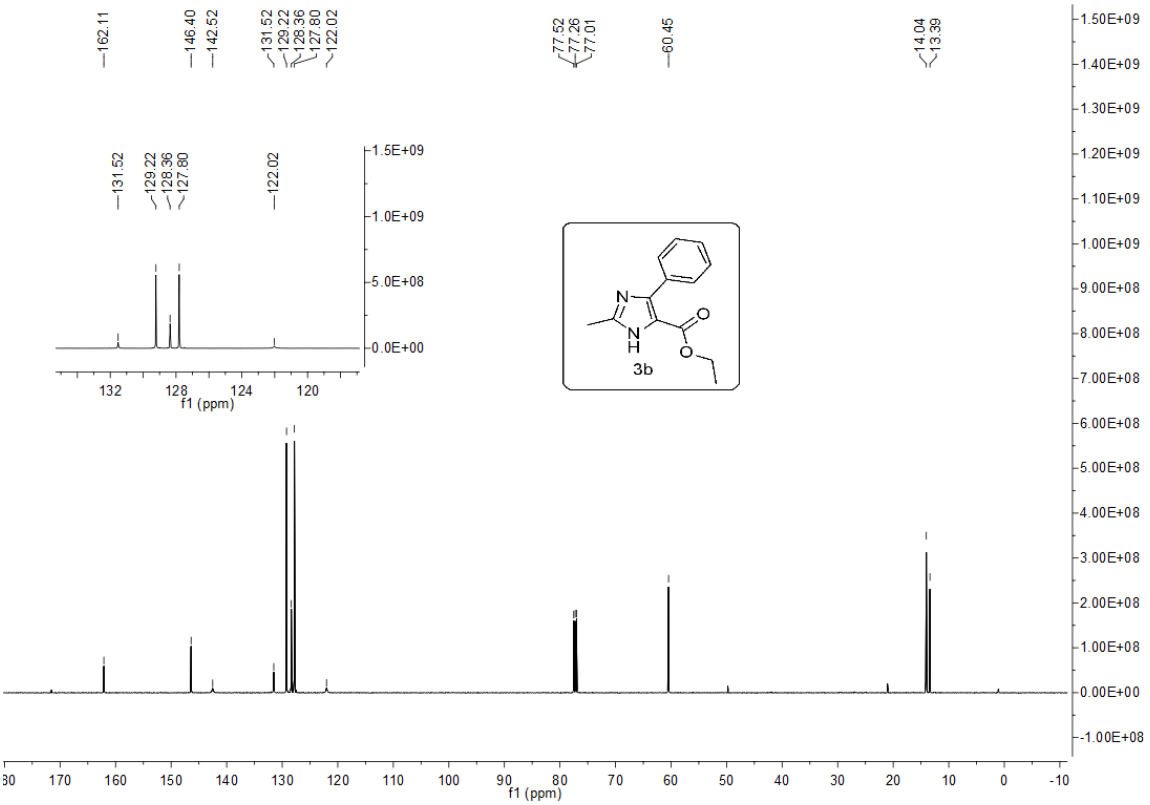
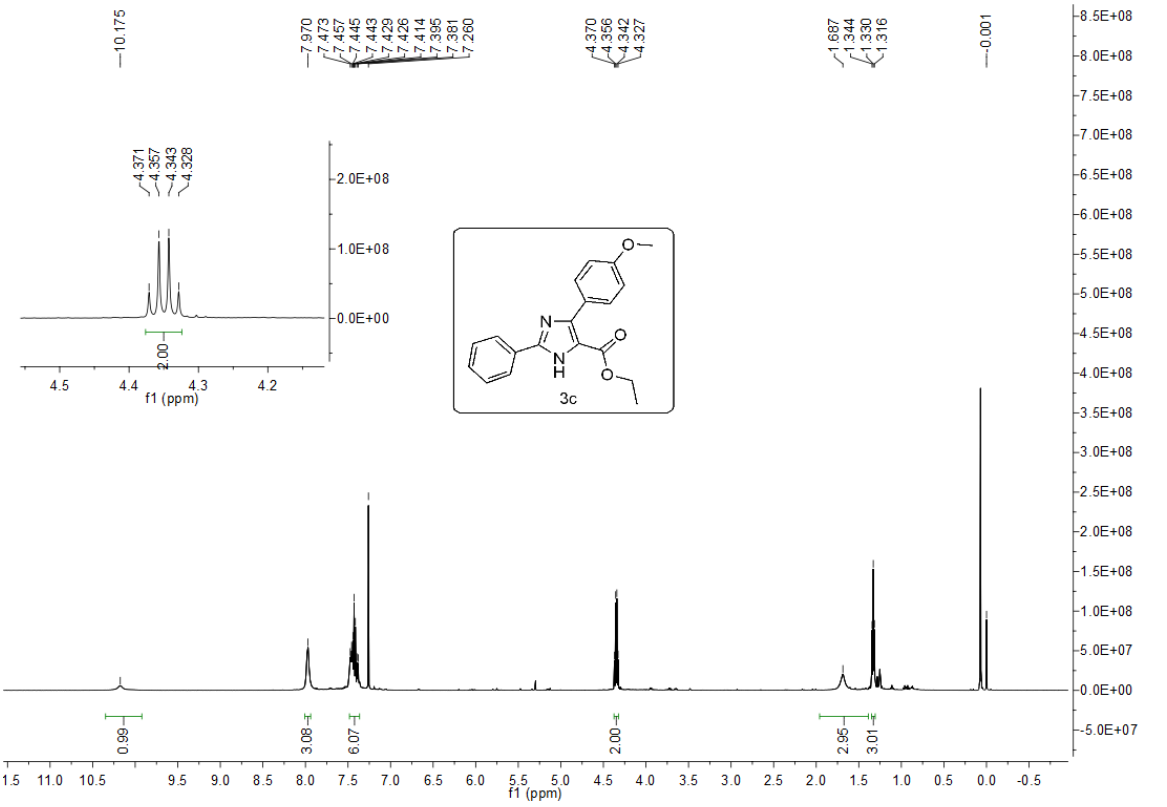
7.592
7.580
7.577
7.218
7.214
7.211
7.208
7.200
7.189
7.185
7.174
7.172
7.162
7.158
7.156
4.120
4.106
4.092
4.078
2.089
1.083
1.069
1.055
0.000
3b
f1 (ppm)


162.11
146.40
142.52
131.52
129.22
128.36
127.80
122.02
77.52
77.26
77.01
60.45
14.04
13.39
3b
f1 (ppm)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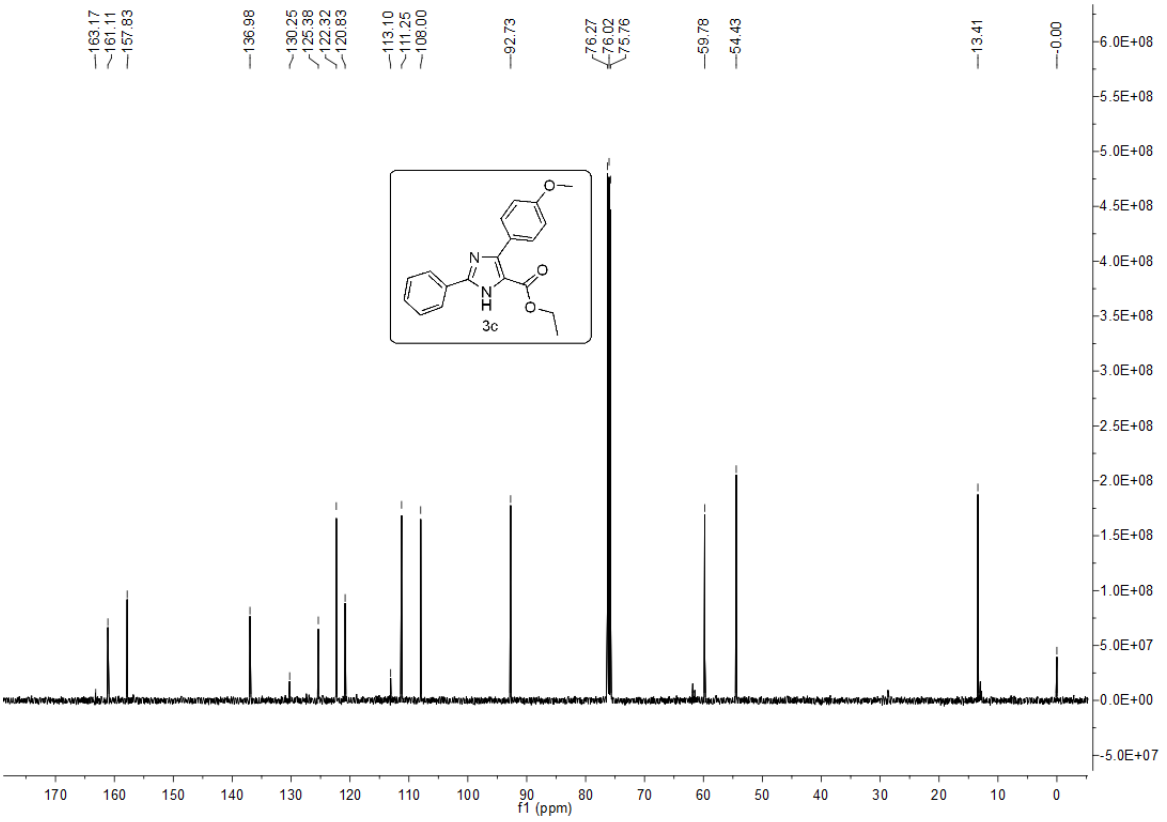
7.473
7.457
7.445
7.443
7.429
7.426
7.414
7.395
7.381
7.260
4.370
4.356
4.342
4.327
1.687
1.344
1.330
1.316
0.001
4.371
4.357
4.343
4.328
2.00
f1 (ppm)
3c
0.99
3.08
6.07
2.00
2.95
3.01
f1 (ppm)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157.83
136.98
130.25
125.38
122.32
120.83
113.10
111.25
108.00
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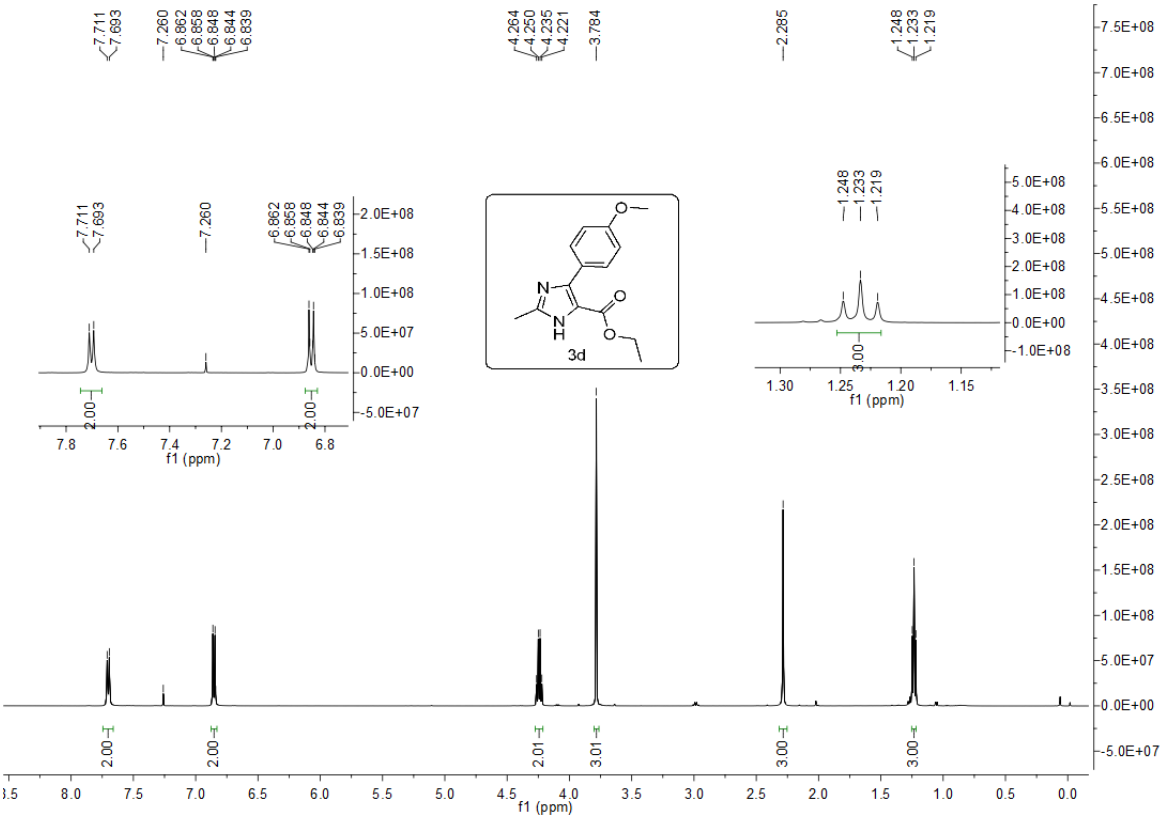
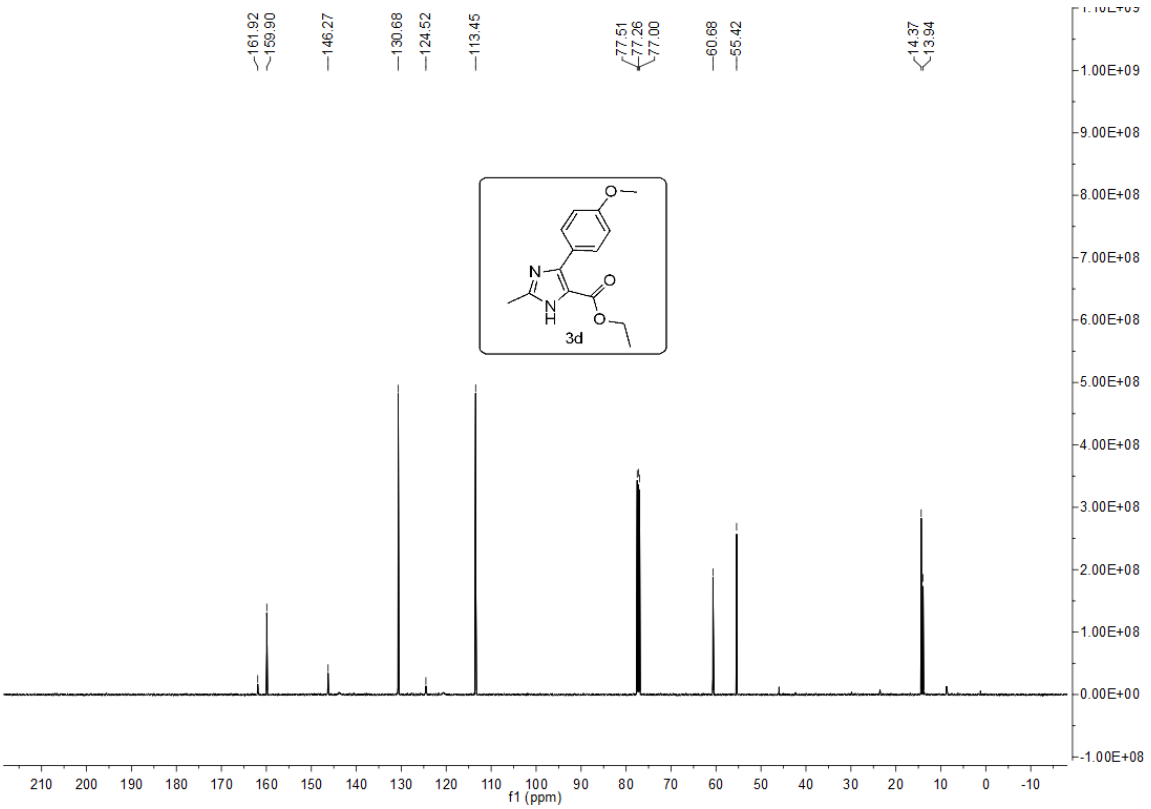
76.27
76.02
75.76
59.78
54.43
13.41
0.00
3c
f1 (ppm)


7.711
7.693
7.260
6.862
6.858
6.848
6.844
6.839
4.264
4.250
4.235
4.221
3.784
2.285
1.248
1.233
1.219
3d
f1 (ppm)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159.90
146.27
130.68
124.52
113.45
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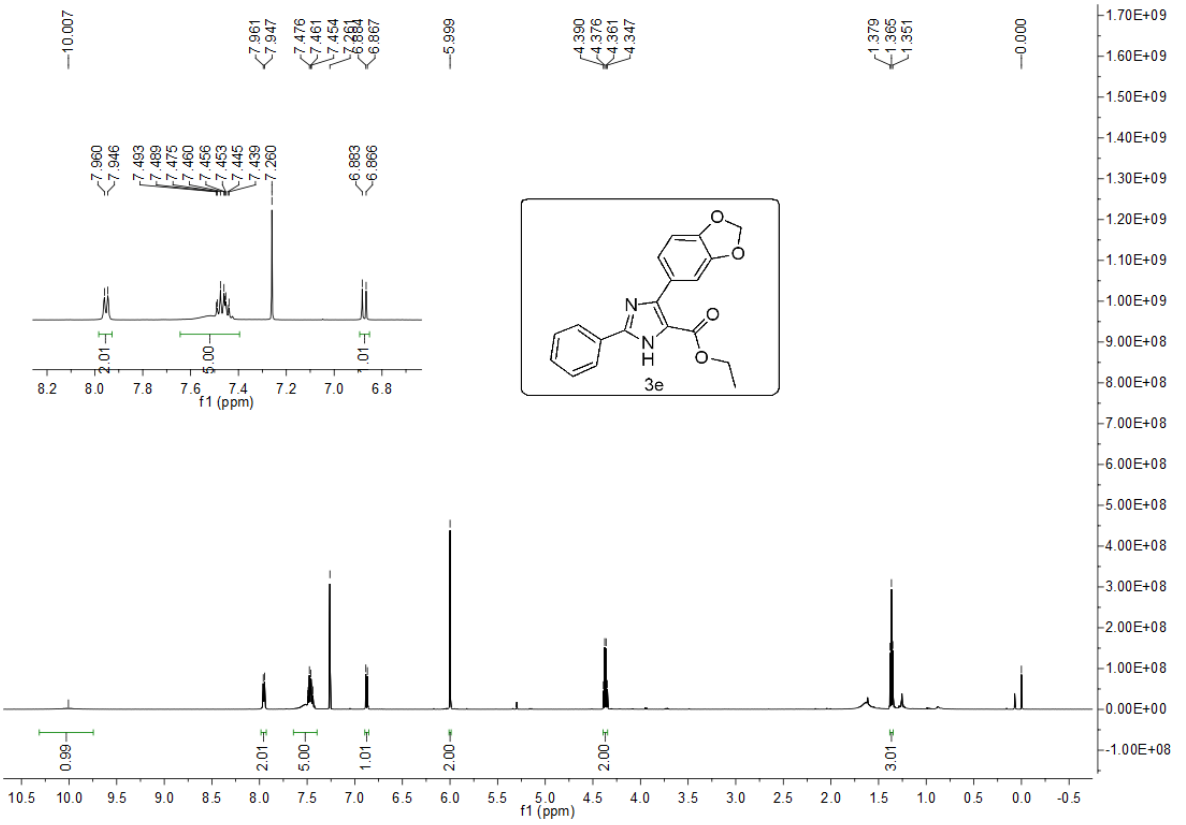
77.26
77.00
60.68
55.42
14.37
13.94
3d
f1 (ppm)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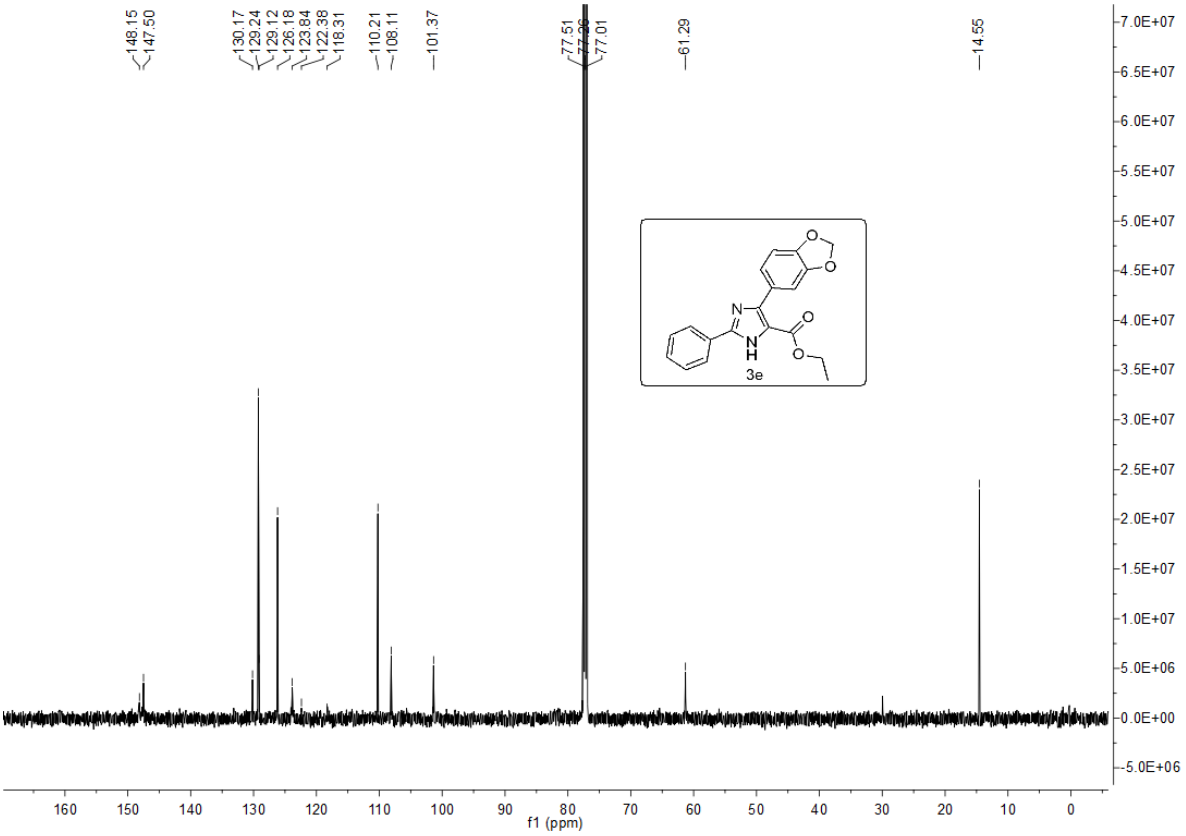
7.947
7.476
7.461
7.454
7.261
6.884
6.867
5.999
4.390
4.376
4.361
4.347
1.379
1.365
1.351
0.000
7.960
7.946
7.493
7.489
7.475
7.460
7.456
7.453
7.445
7.439
7.260
6.883
6.866
2.01
5.00
1.01
f1 (ppm)
3e
0.99
2.01
5.00
1.01
2.00
2.00
3.01
f1 (ppm)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147.50
130.17
129.24
129.12
126.18
123.84
122.38
118.31
110.21
108.11
101.37
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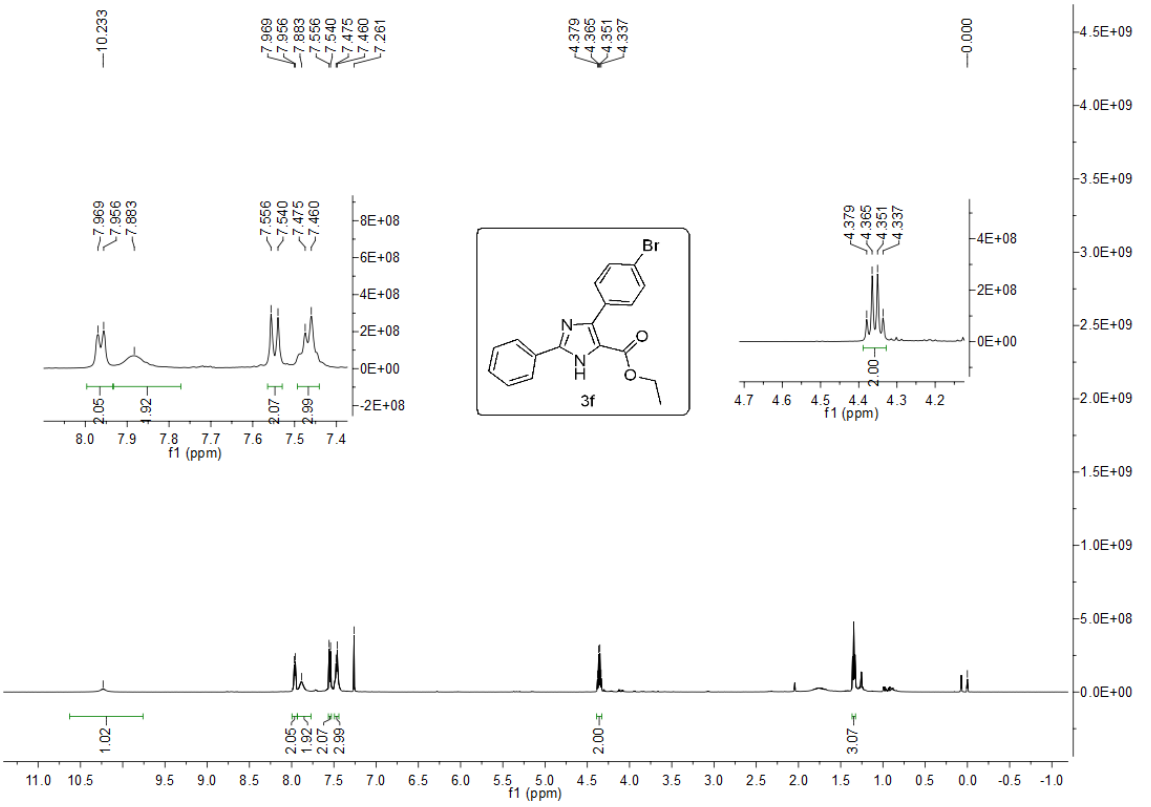
77.26
77.01
61.29
14.55
3e
f1 (ppm)


10.233
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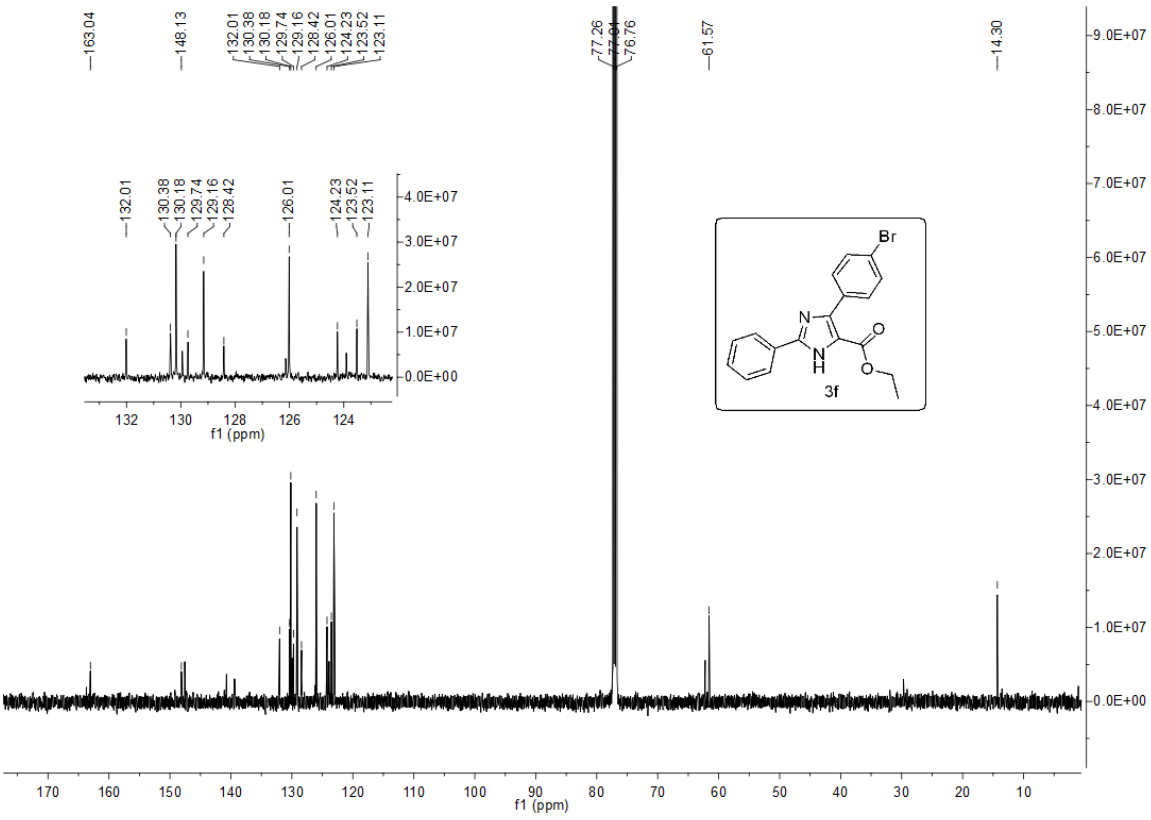
7.956
7.883
7.556
7.540
7.475
7.460
7.261
4.379
4.365
4.351
4.337
0.000
Br
N
H
O
O
3f
f1 (ppm)
1.02
2.05
1.92
2.07
2.99
2.00
3.07


163.04
148.13
132.01
130.38
130.18
129.74
129.16
128.42
126.01
124.23
123.52
123.11
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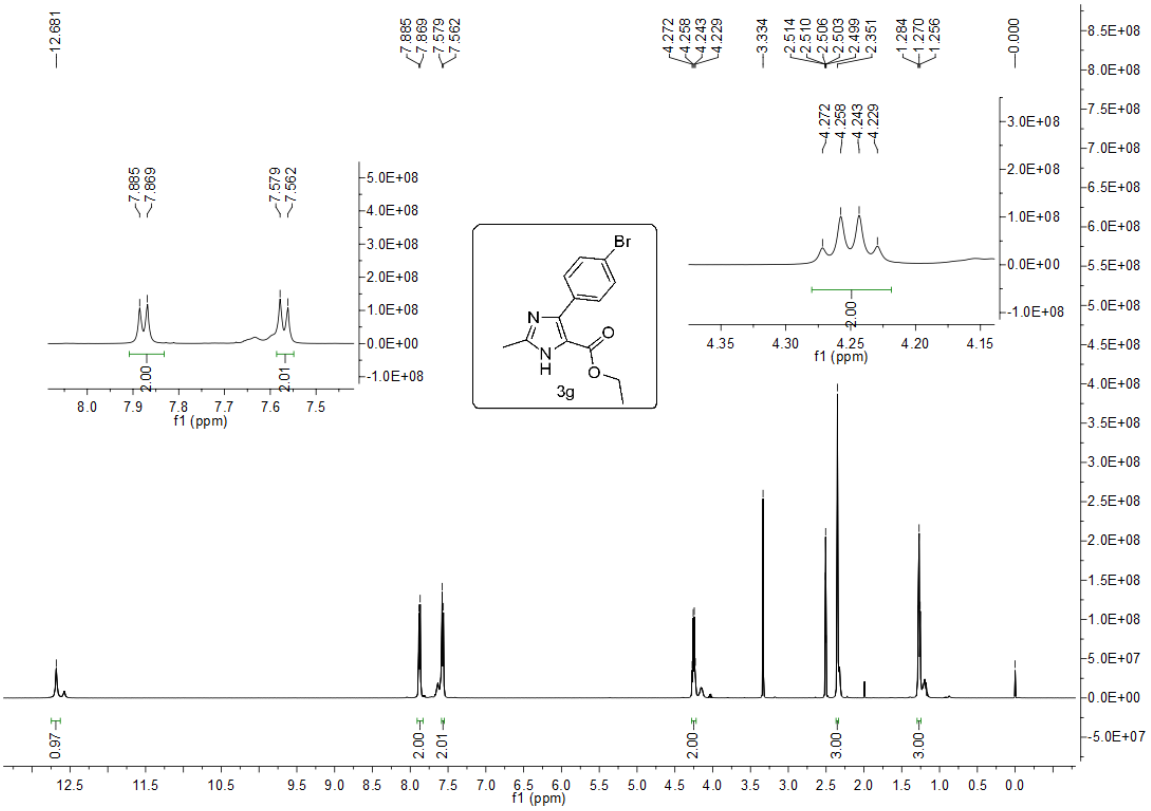
77.04
76.76
61.57
14.30
Br
N
H
O
O
3f
f1 (ppm)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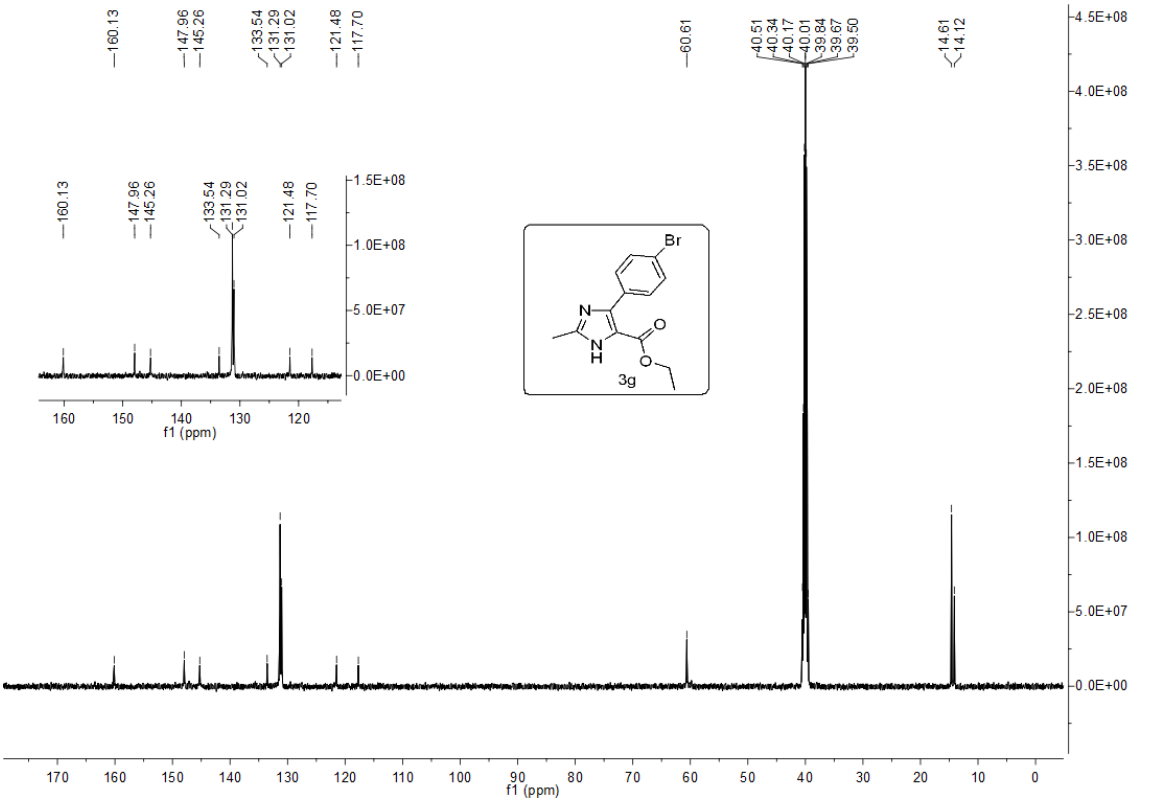
7.869
7.579
7.562
4.272
4.258
4.243
4.229
3.334
2.514
2.510
2.506
2.503
2.499
2.351
1.284
1.270
1.256
0.000
Br
N
H
O
O
3g
f1 (ppm)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145.26
133.54
131.29
131.02
121.48
117.70
60.61
40.51
40.34
40.17
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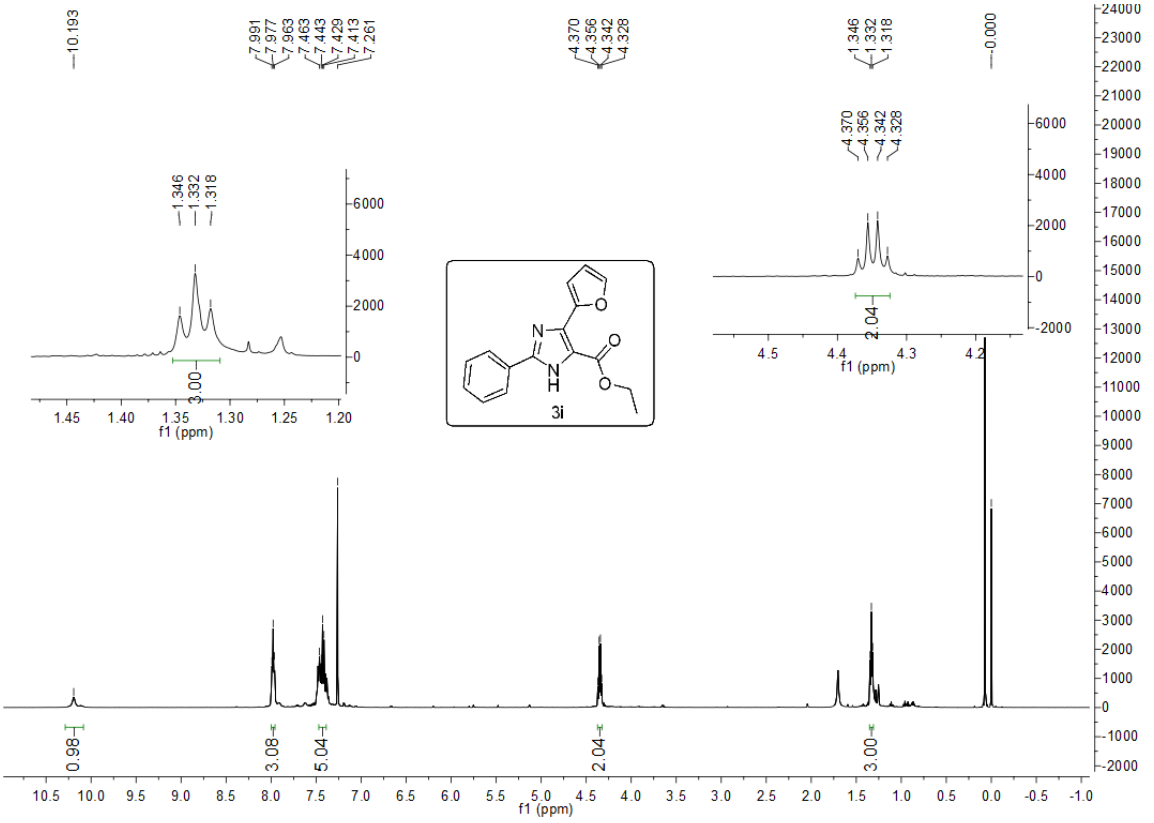
Br
N
H
O
O
3g
f1 (ppm)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7.977
7.963
7.463
7.443
7.429
7.413
7.261
4.370
4.356
4.342
4.328
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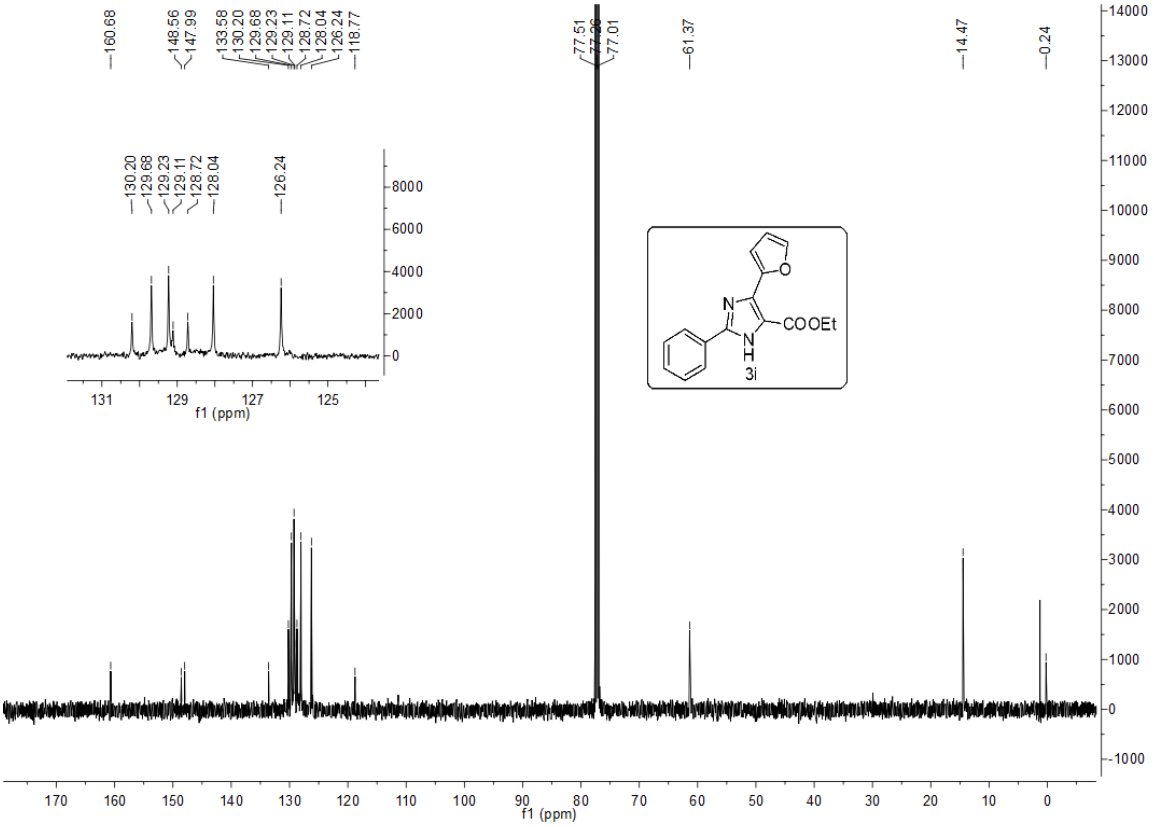
1.332
1.318
0.000
3i
0.98
3.08
5.04
2.04
3.00
f1 (ppm)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133.58
130.20
129.68
129.23
129.11
128.72
128.04
126.24
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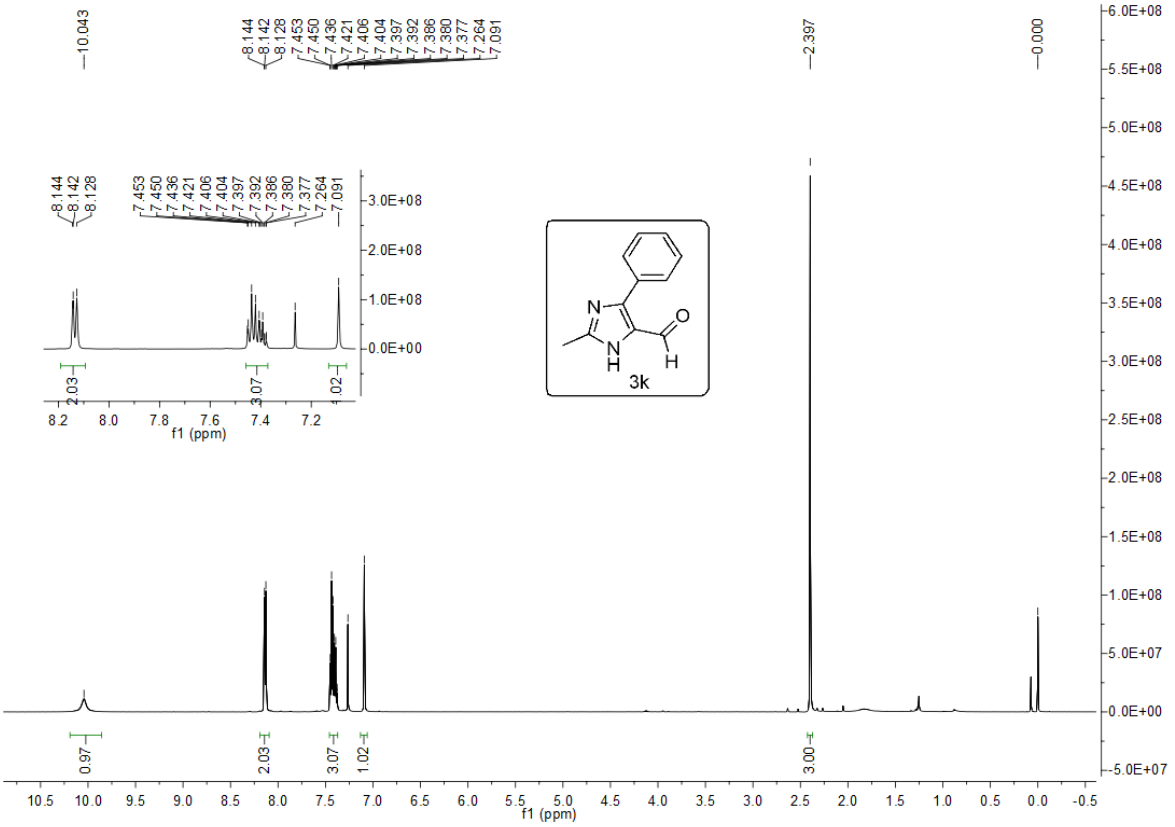
77.00
61.37
14.47
0.24
COOEt
3i
f1 (ppm)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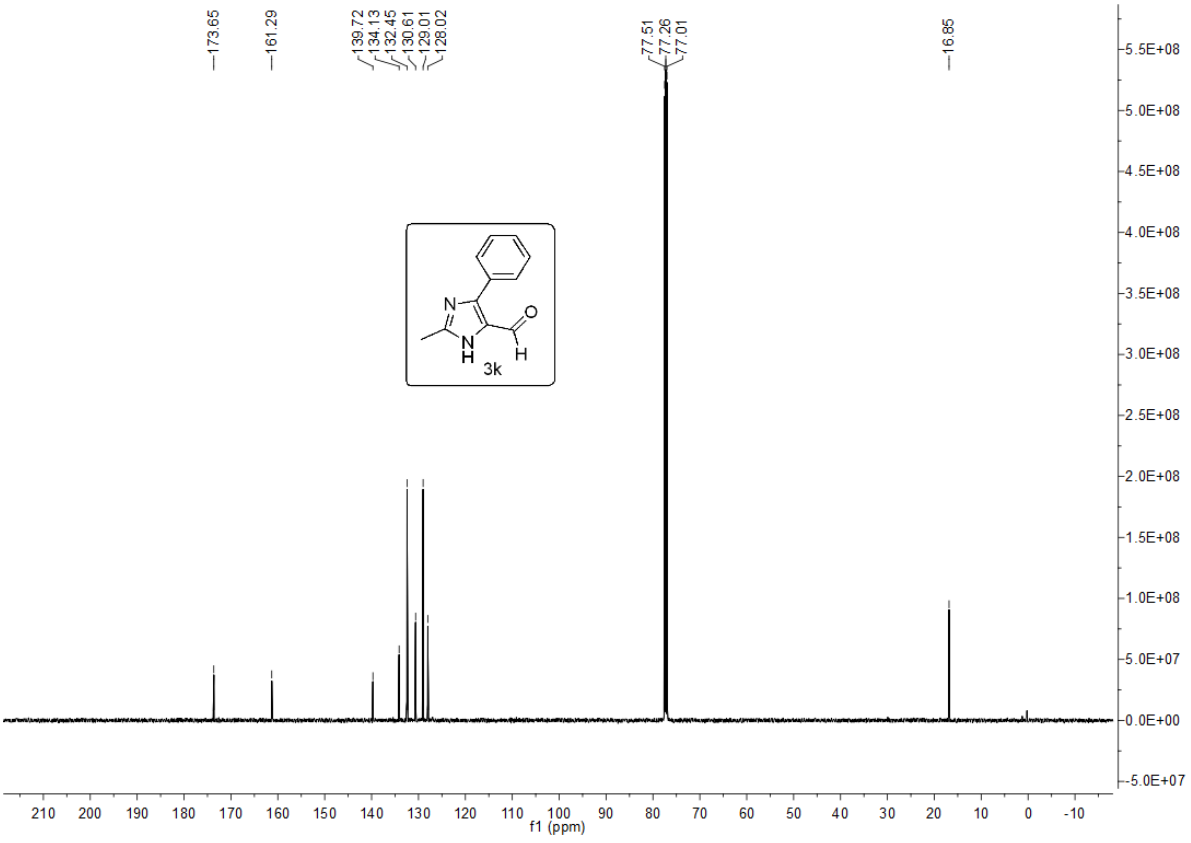
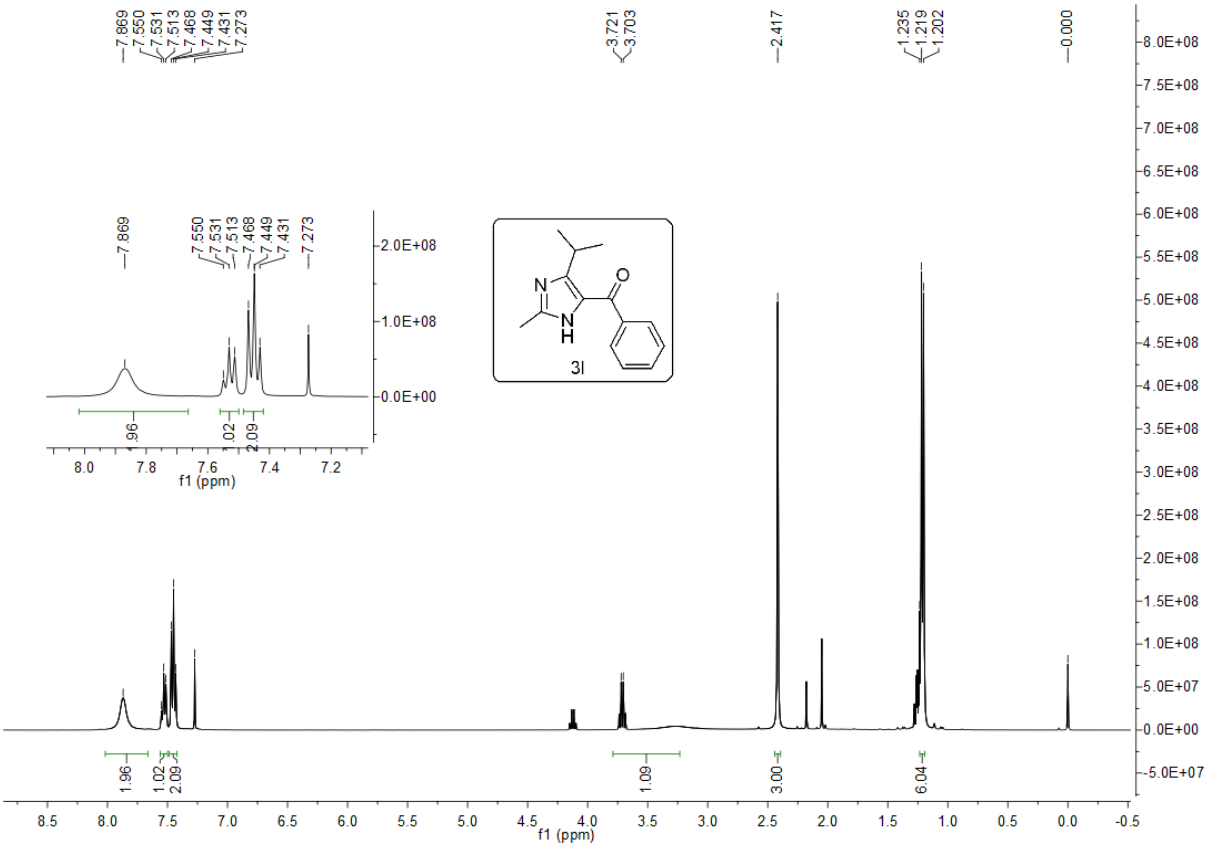
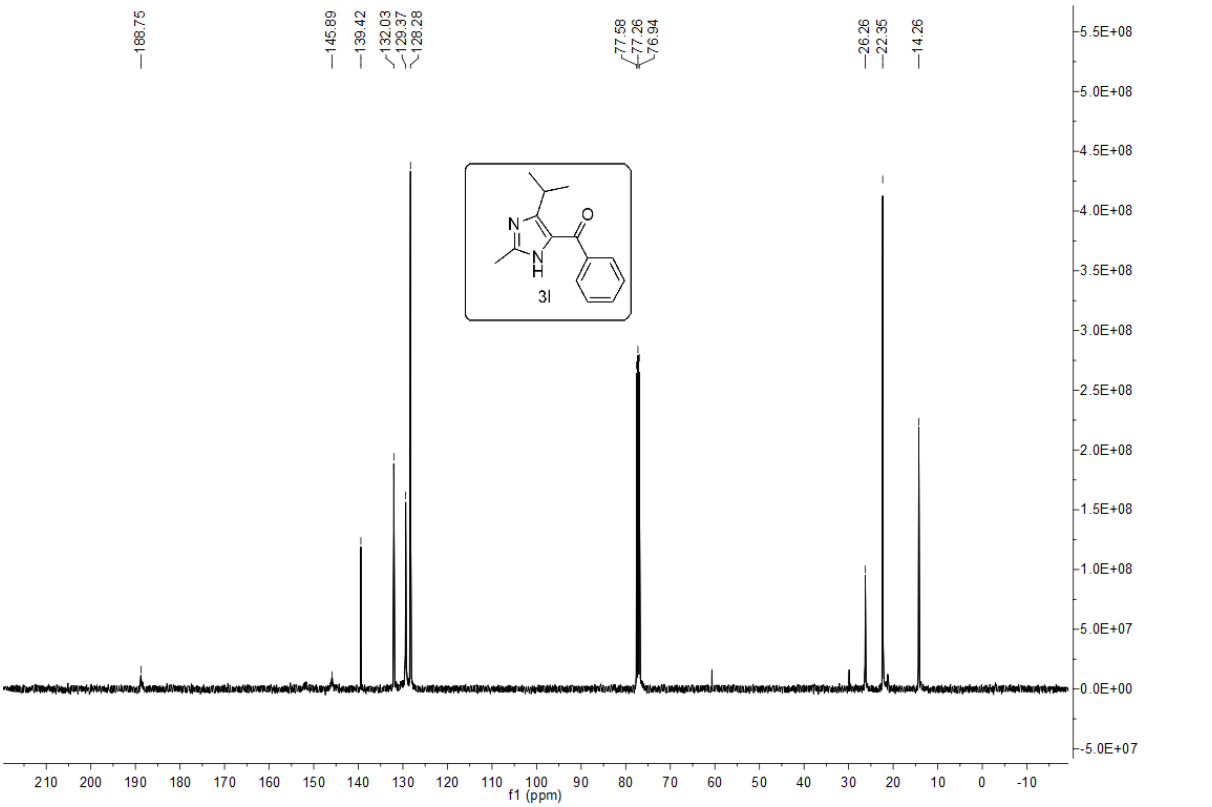
8.142
8.128
7.453
7.450
7.436
7.421
7.406
7.404
7.397
7.392
7.386
7.380
7.377
7.264
7.091
2.397
0.000
3k
0.97
2.03
3.07
1.02
3.00
f1 (ppm)


173.65
161.29
139.72
134.13
132.45
130.61
129.01
128.02
77.51
77.26
77.01
16.85
3k
f1 (ppm)


7.869
7.550
7.531
7.513
7.468
7.449
7.431
7.273
3.721
3.703
2.417
1.235
1.219
1.202
0.000
3l
f1 (ppm)


188.75
145.89
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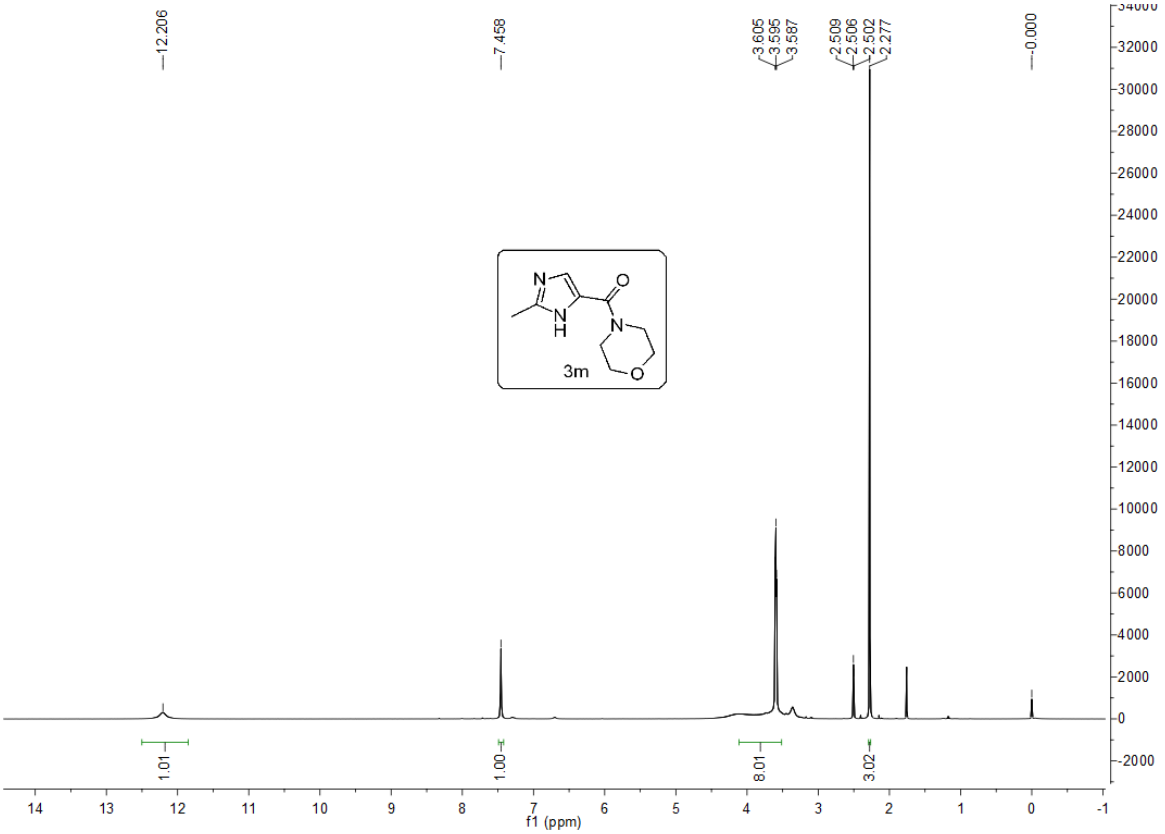
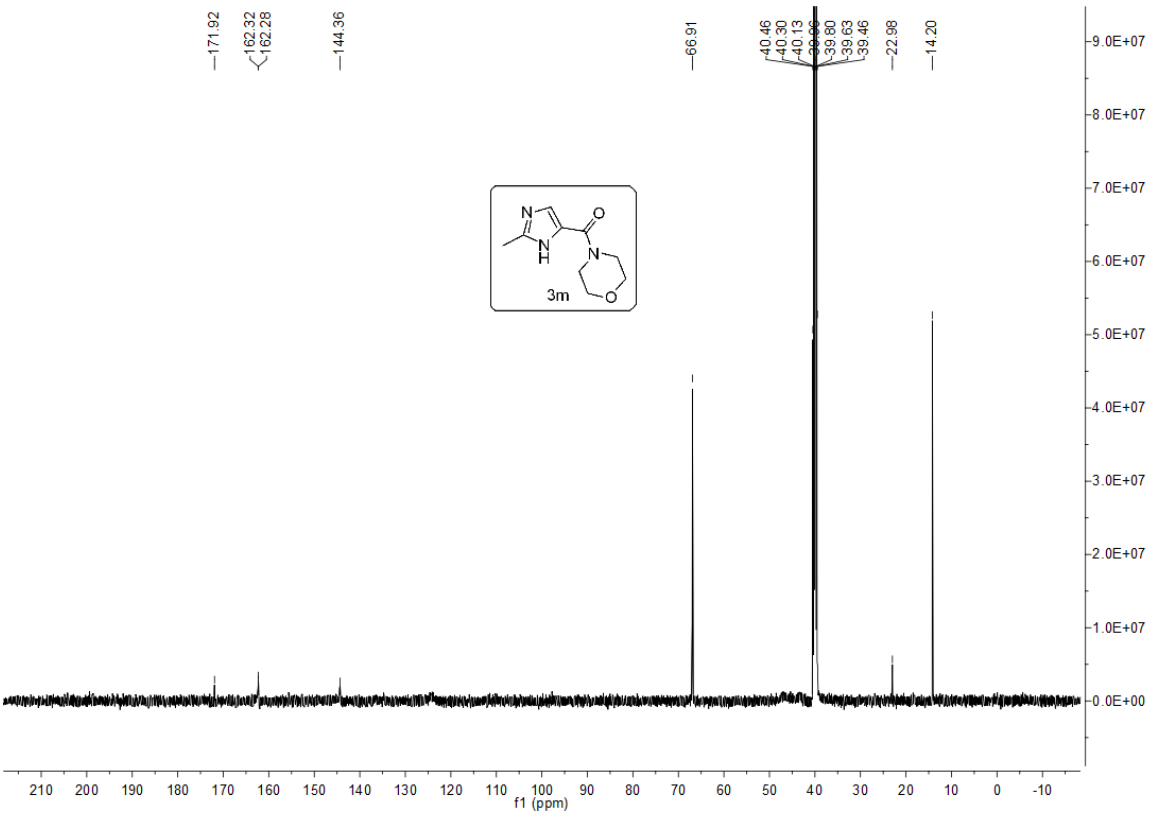
132.03
129.37
128.28
77.58
77.26
76.94
26.26
22.35
14.26
3l
f1 (ppm)


12.206
7.458
3.605
3.595
3.587
2.509
2.506
2.502
2.277
0.000
3m
1.01
1.00
8.01
3.02
f1 (ppm)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162.32
162.28
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40.13
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39.46
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14.20
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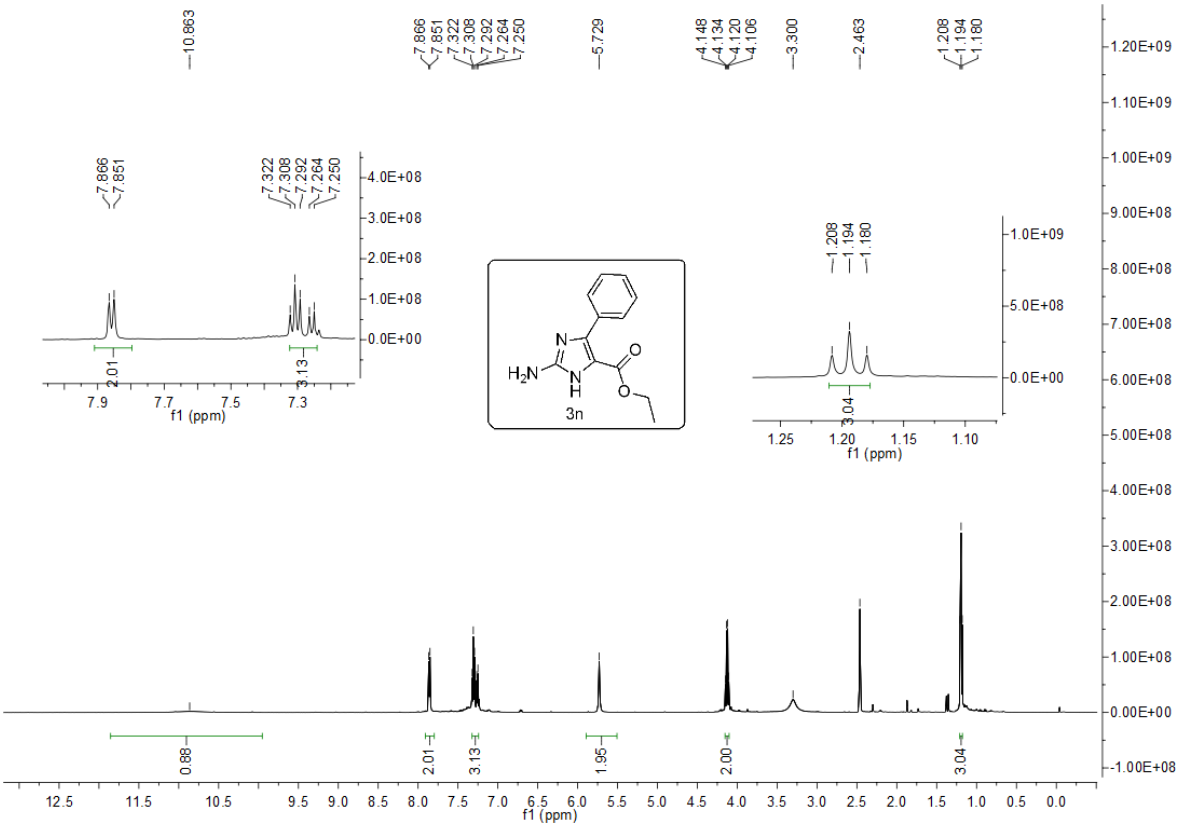
f1 (ppm)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7.292
7.264
7.250
5.729
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4.120
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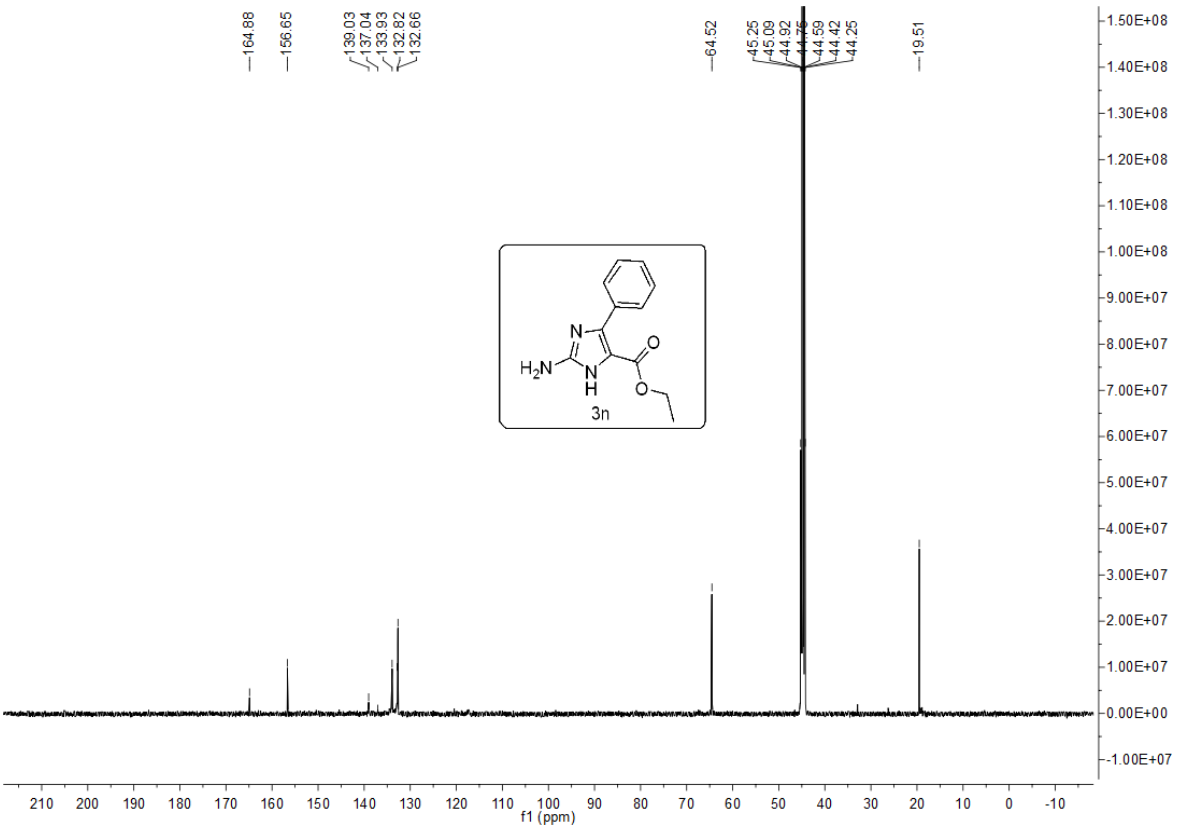
3.300
2.463
1.208
1.194
1.180
3n
f1 (ppm)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137.04
133.93
132.82
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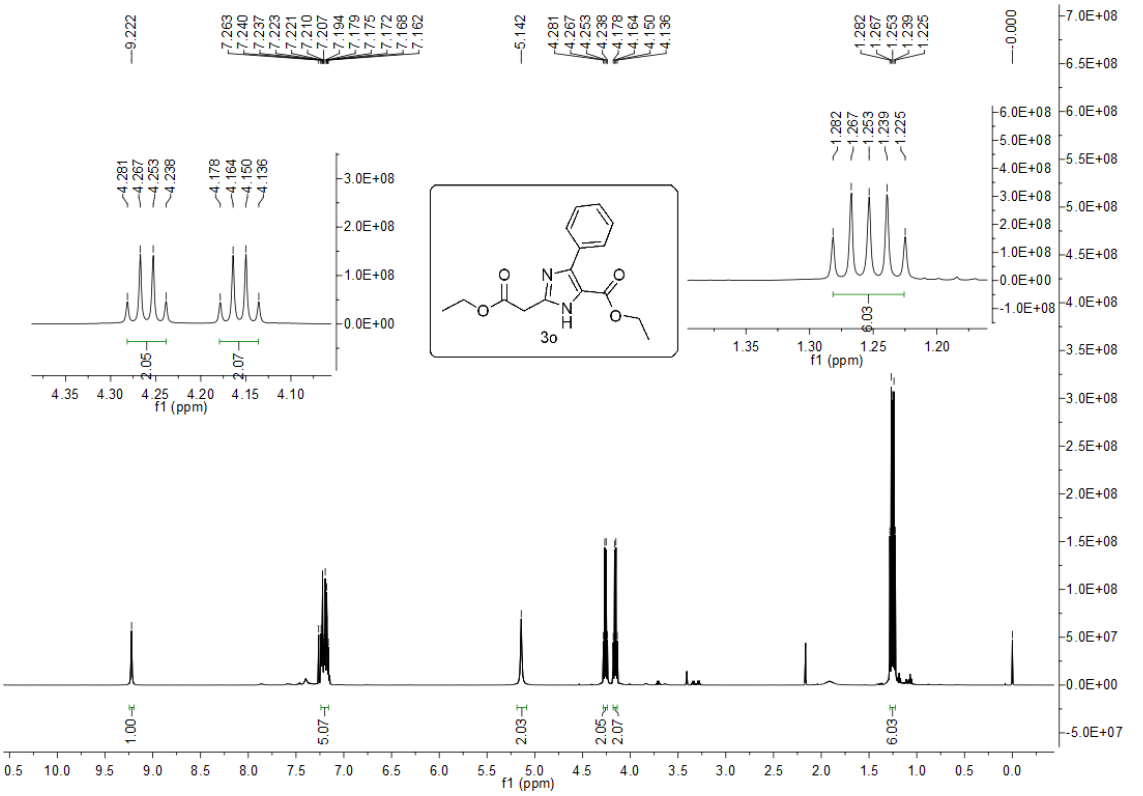
45.09
44.92
44.59
44.42
44.25
19.51
3n
f1 (ppm)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7.221
7.210
7.207
7.194
7.179
7.175
7.172
7.168
7.162
5.142
4.281
4.267
4.253
4.238
4.178
4.164
4.150
4.136
1.282
1.267
1.253
1.239
1.225
0.000
3o
f1 (ppm)
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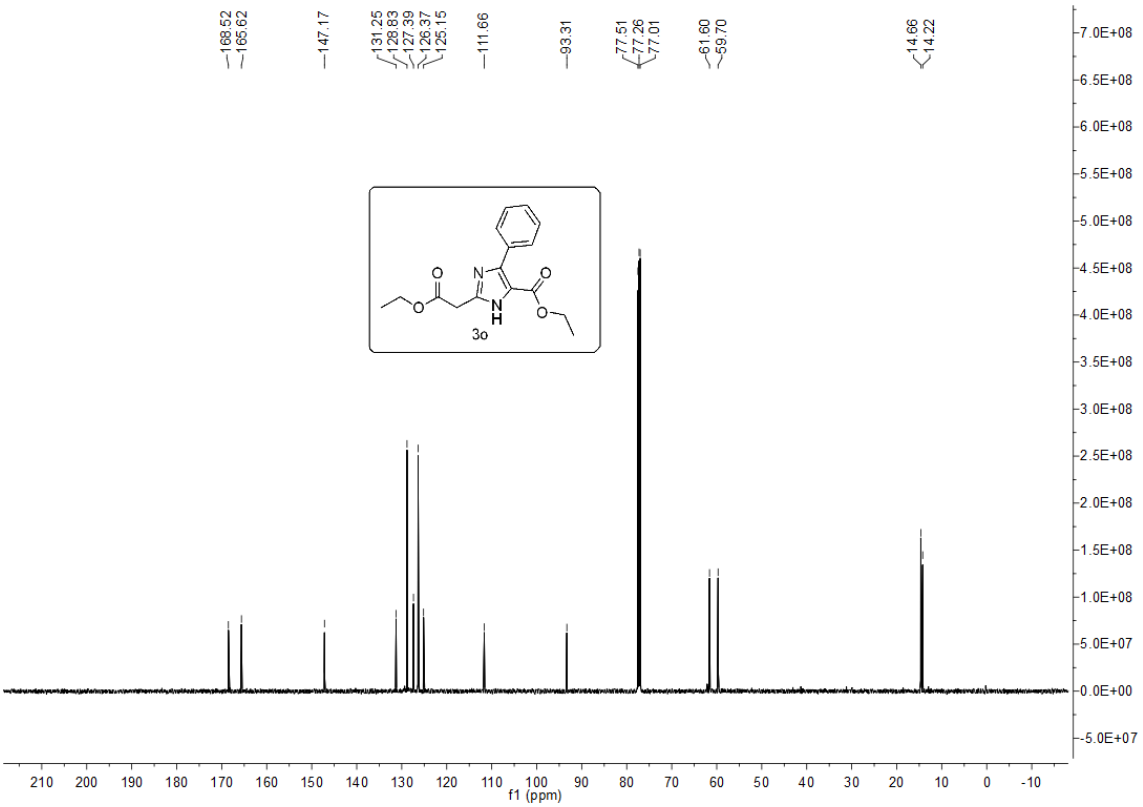
5.07
2.03
2.05
2.07
6.03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131.25
128.83
127.39
126.37
125.15
111.66
93.31
77.51
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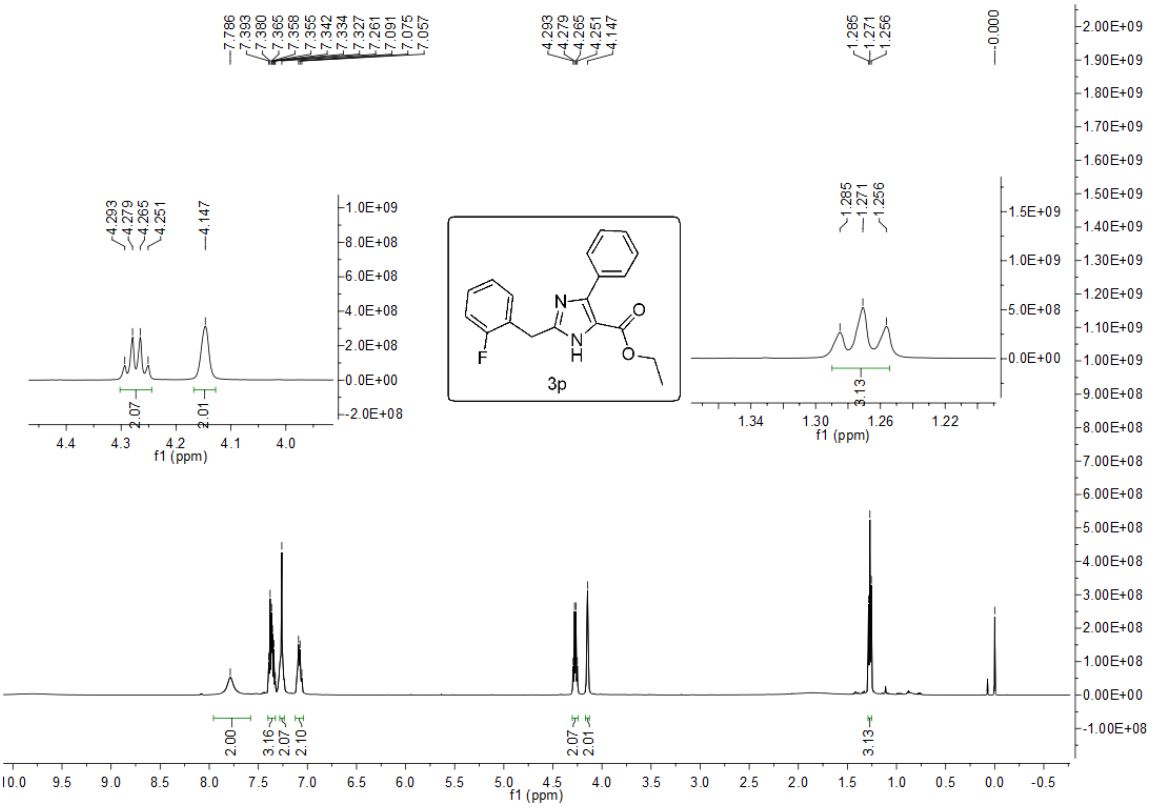
59.70
14.66
14.22
3o
f1 (ppm)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7.355
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7.334
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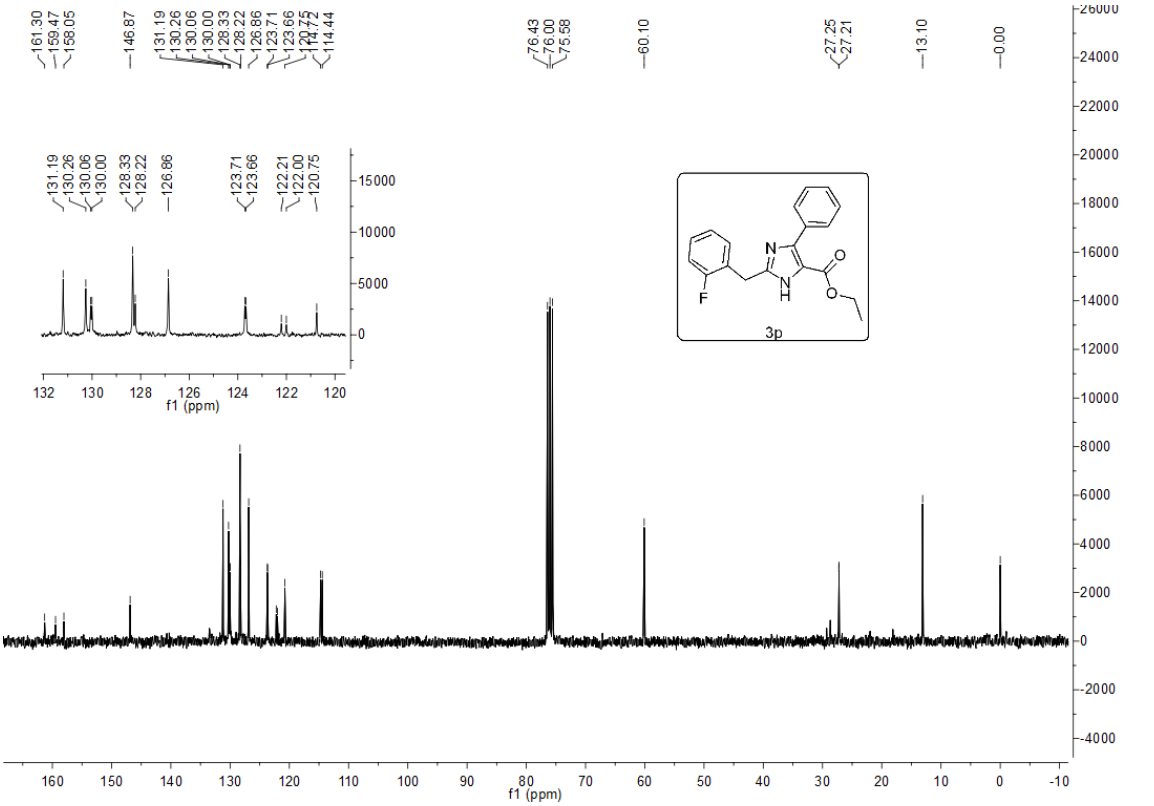
7.261
7.091
7.075
7.057
4.293
4.279
4.265
4.251
4.147
1.285
1.271
1.256
0.000
3p
2.00
3.16
2.07
2.10
2.07
2.01
3.13
f1 (ppm)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131.19
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130.06
130.00
128.33
128.22
126.86
123.71
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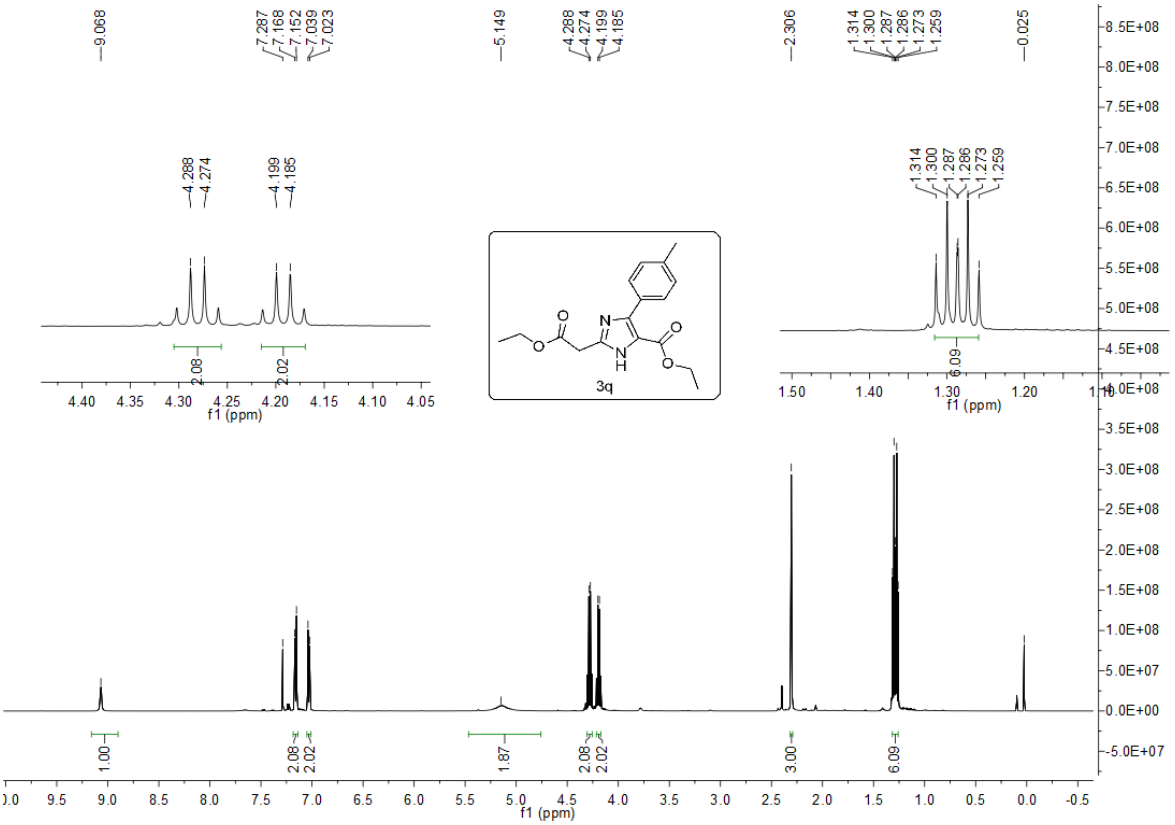
122.21
122.00
120.75
114.72
114.44
76.43
76.00
75.58
60.10
27.25
27.21
13.10
0.00
3p
f1 (ppm)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7.023
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4.288
4.274
4.199
4.185
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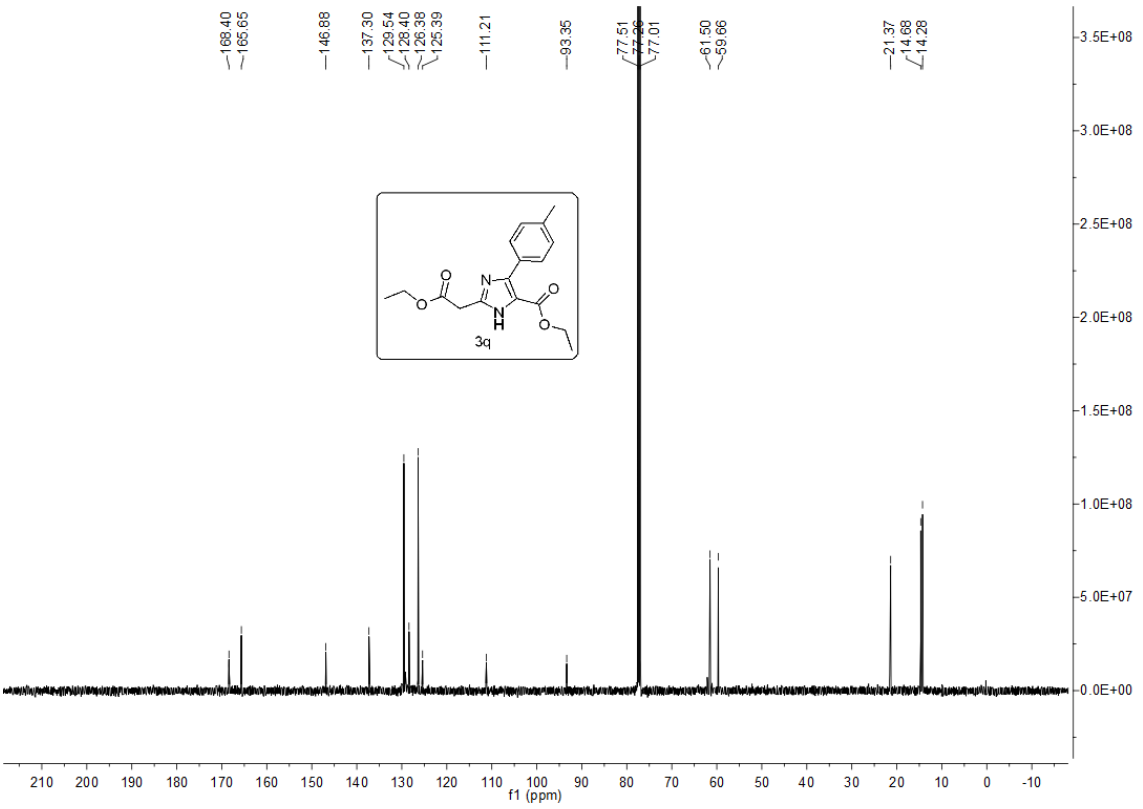
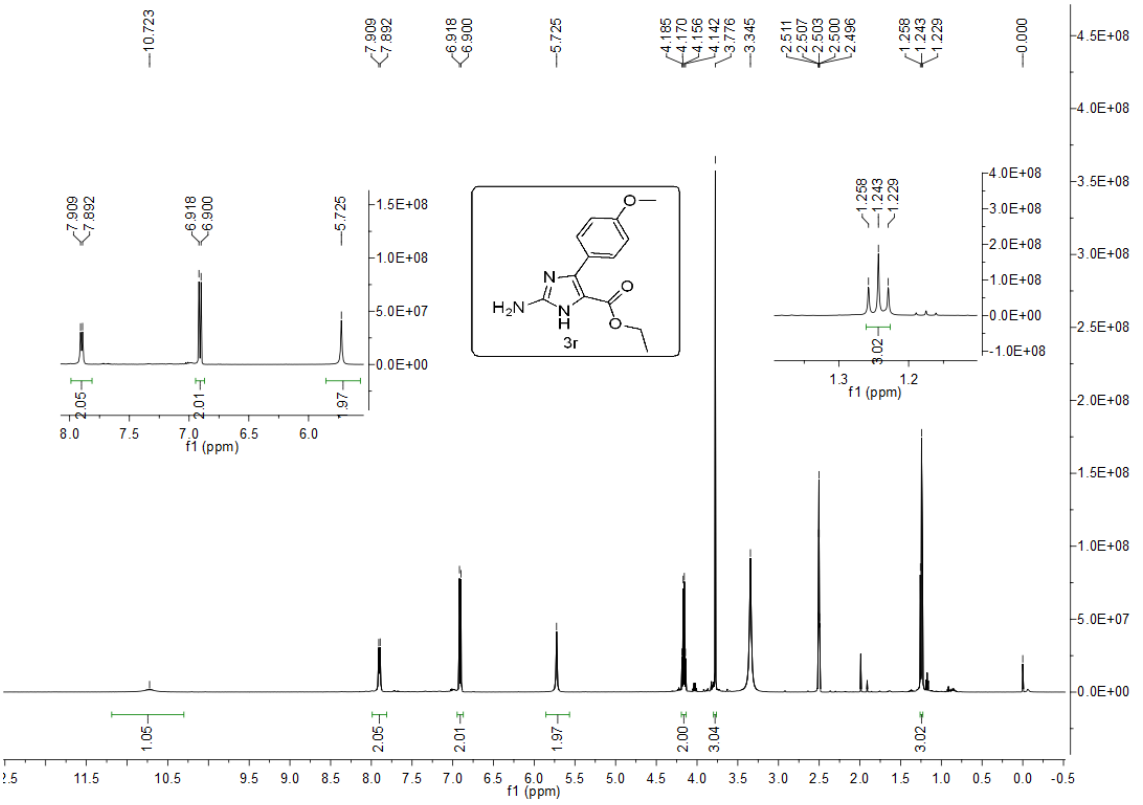
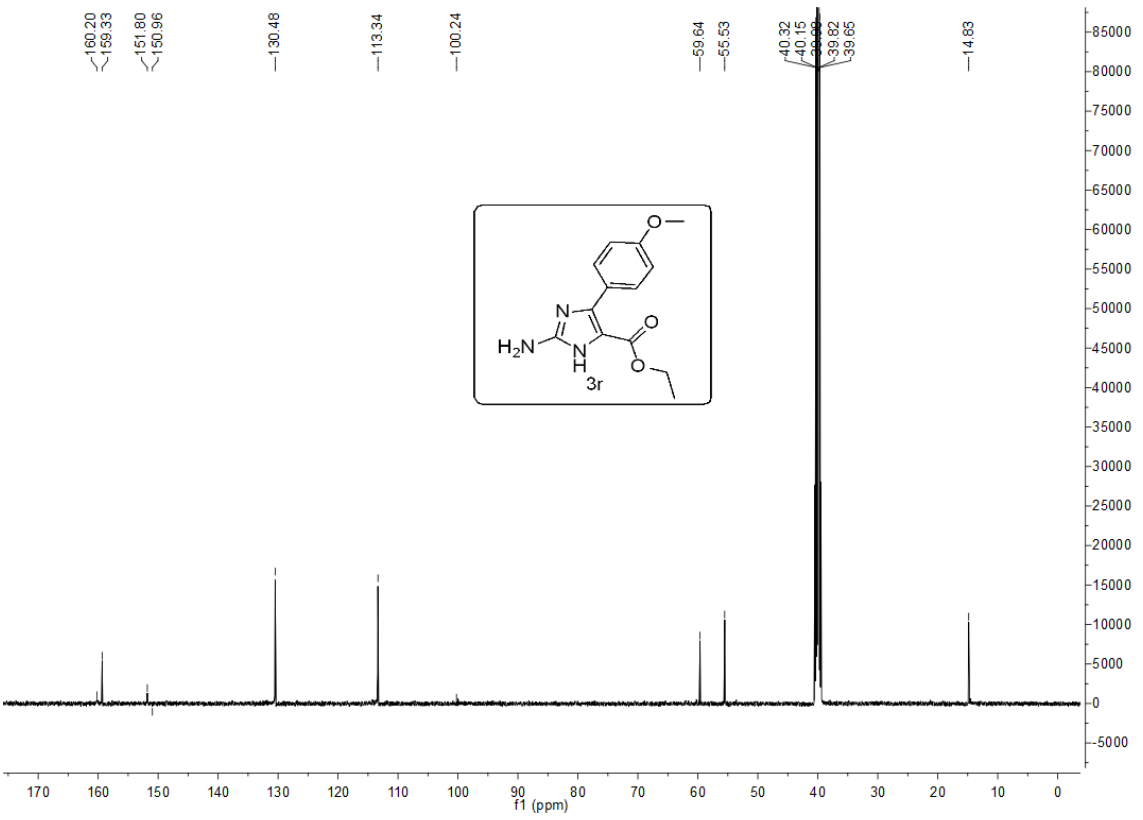
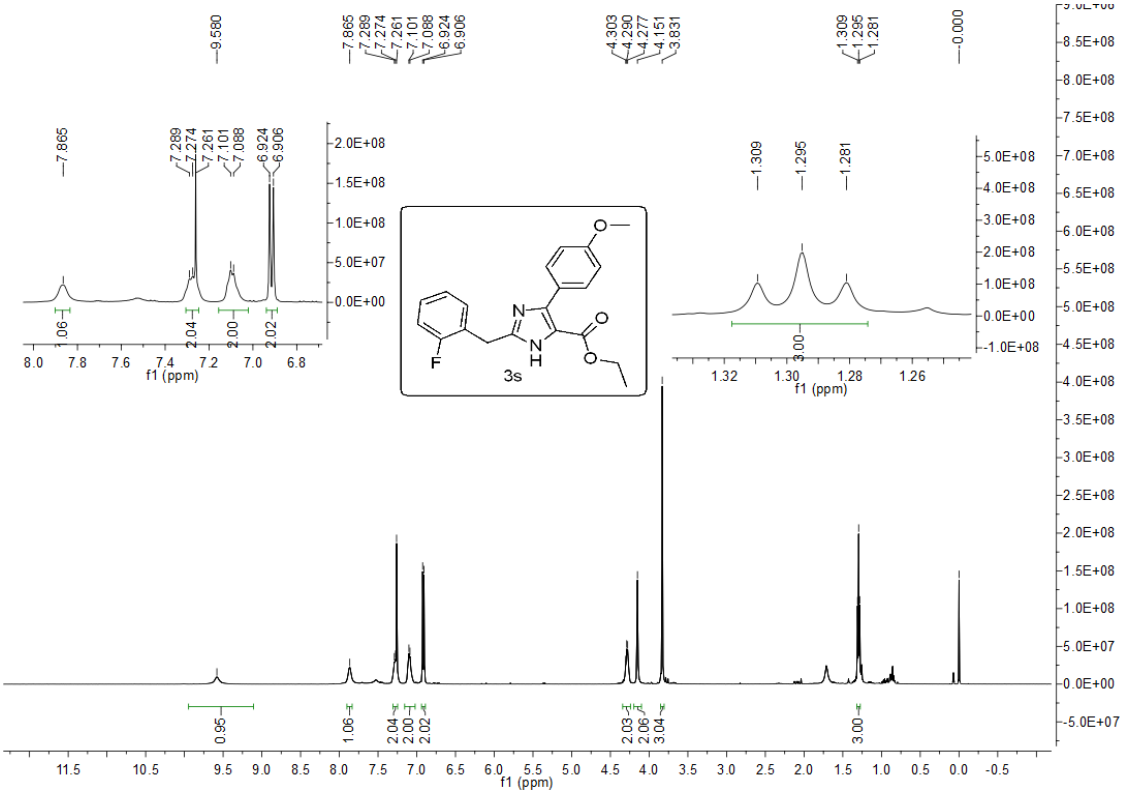
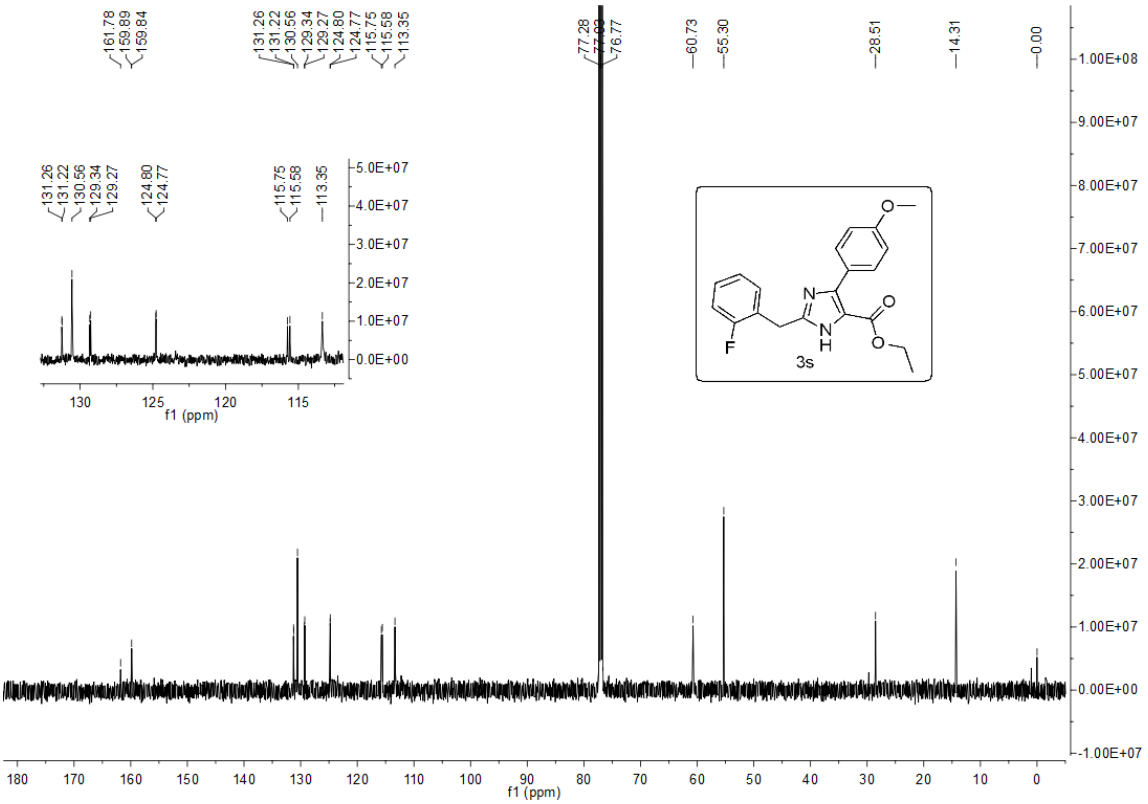
1.300
1.287
1.286
1.273
1.259
0.025
3q
f1 (ppm)

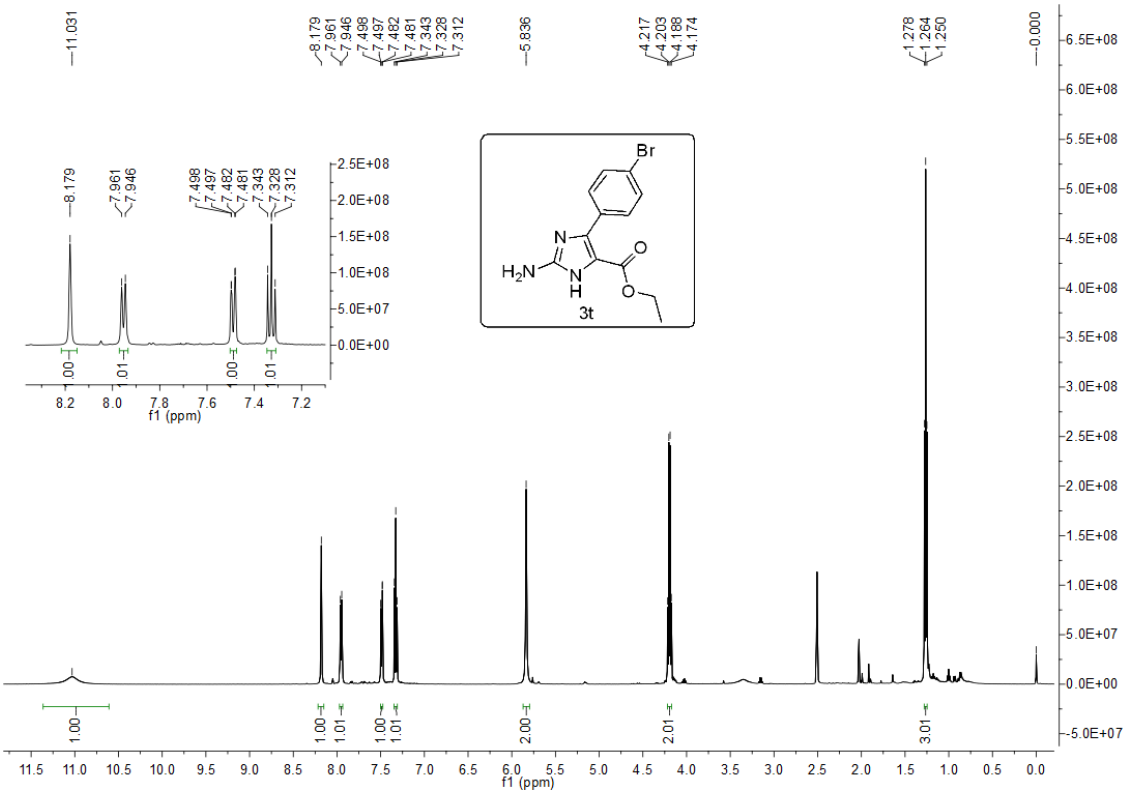

168.40
165.65
146.88
137.30
129.54
128.40
126.38
125.39
111.21
93.35
77.51
77.26
77.01
61.50
59.66
21.37
14.68
14.28
3q
f1 (ppm)

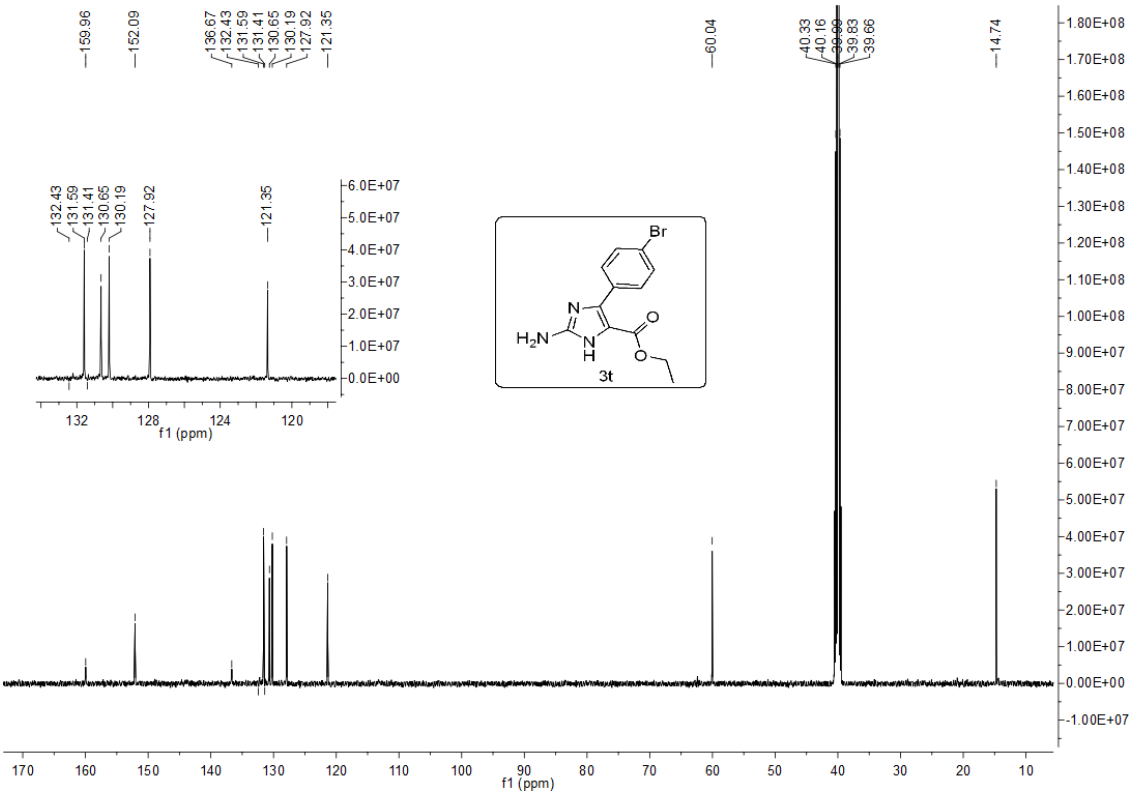

10.723
7.909
7.892
6.918
6.900
5.725
4.185
4.170
4.156
4.142
3.776
3.345
2.511
2.507
2.503
2.500
2.496
1.258
1.243
1.229
0.000
3r
f1 (ppm)

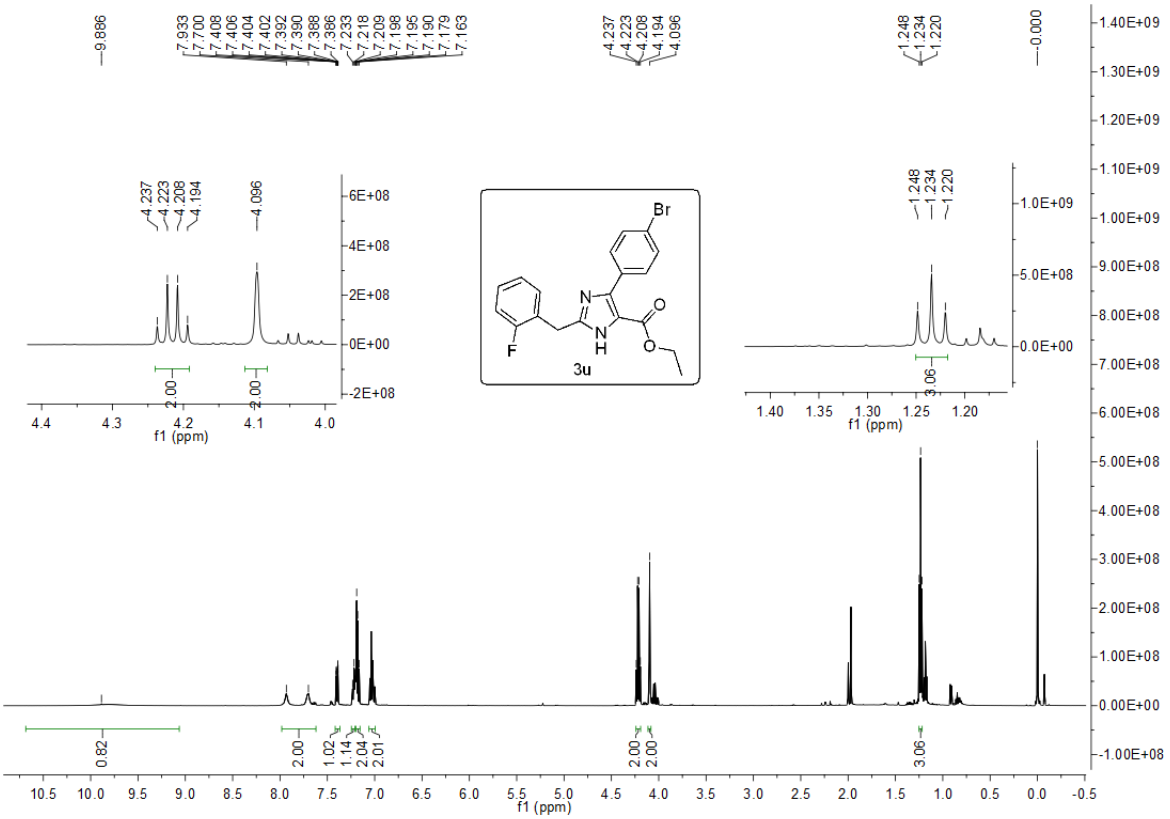

160.20
159.33
151.80
150.96
130.48
113.34
100.24
59.64
55.53
40.32
40.15
39.82
39.65
14.83
3r
f1 (ppm)

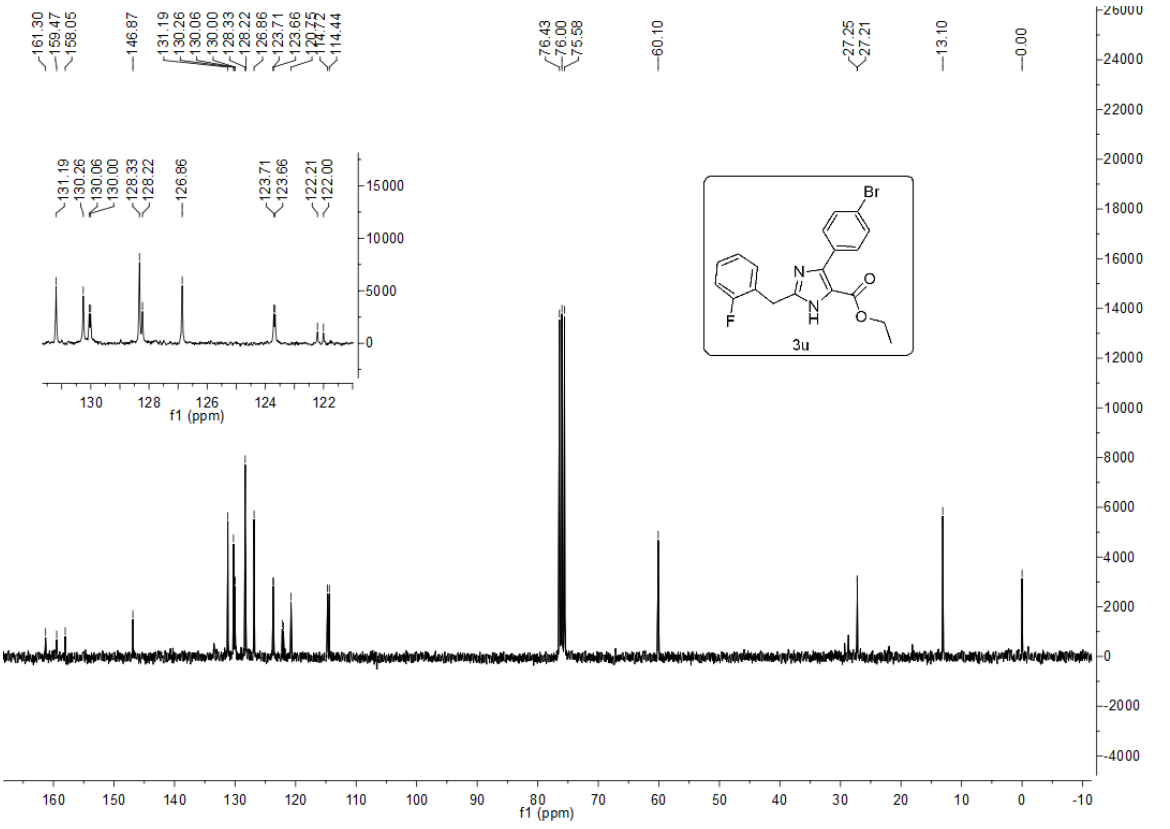

9.580
7.865
7.289
7.274
7.261
7.101
7.088
6.924
6.906
4.303
4.290
4.277
4.151
3.931
1.309
1.295
1.281
0.000
3s
f1 (ppm)


161.78
159.89
159.84
131.26
131.22
130.56
129.34
129.27
124.80
124.77
115.75
115.58
113.35
77.28
77.00
76.77
60.73
55.30
28.51
14.31
0.00
3s
f1 (ppm)


11.031
8.179
7.961
7.946
7.498
7.497
7.482
7.481
7.343
7.328
7.312
5.836
4.217
4.203
4.188
4.174
1.278
1.264
1.250
0.000
Br
N
H2N
N
H
O
O
3t
f1 (ppm)


159.96
152.09
136.67
132.43
131.59
131.41
130.65
130.19
127.92
121.35
60.04
40.33
40.16
39.99
39.83
39.66
14.74
Br
N
H2N
N
H
O
O
3t
f1 (ppm)


9.886
7.933
7.700
7.408
7.406
7.404
7.402
7.392
7.390
7.388
7.386
7.233
7.218
7.209
7.198
7.195
7.190
7.179
7.163
4.237
4.223
4.208
4.194
4.096
1.248
1.234
1.220
0.000
Br
N
H
O
O
F
3u
f1 (ppm)


161.30
159.47
158.05
146.87
131.19
130.26
130.06
130.00
128.33
128.22
126.86
123.71
123.66
122.21
122.00
114.72
114.44
76.43
76.00
75.58
60.10
27.25
27.21
13.10
0.00
Br
N
H
O
O
F
3u
f1 (ppm)