Supporting Information

For

Visible-light-induced photocatalytic oxytrifluoromethylation of *N*-allylamides for the synthesis of CF_3-containing oxazolines and benzoxazines

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1. General Information

^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on 400/600 MHz spectrophotometers. Chemical shifts (δ) are reported in parts per million (ppm) relative to residual solvent signals ($CDCl_3$, 7.26 ppm for ^{1}H NMR, $CDCl_3$, 77.0 ppm for ^{13}C NMR). Data are reported as follows: chemical shift (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, dt = doublet of triplets, m = multiplet, br = broad signal), coupling constants (Hz). Mass spectra were measured on MS spectrometer (EI) or LC/MS/MS (ESI-MS). HRMS was recorded on Bruker ultrafleXtreme MALDI-TOF/TOF mass spectrometer.

2. Materials

Unless otherwise noted, materials were purchased from commercial suppliers and used without further purification. All the solvents were treated according to general methods.[1] Flash column chromatography was performed using 200-300 mesh silica gel. The *N*-allylamides were prepared according to literature procedures from commercially available substrates.[2,3]

References

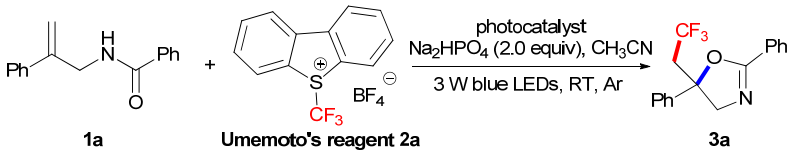
1 D. D. Perrin, W. L. F.Armarego, Purification of Laboratory Chemicals, 4th ed.; Pergamon Press, Oxford, 1997.

2 A. Jaganathan, A. Garzan, D. C. Whitehead, R. J. Staples and B. Borhan, *Angew. Chem. Int. Ed.*, 2011, **50**, 2593.

3 Y.-M. Wang, J. Wu, C. Hoong, V. Rauniyar and F. D. Toste, *J. Am. Chem. Soc.*, 2012, **134**, 12928.

3. Detailed Optimization of Reaction Conditions

Table S1. Studies of the effect of photocatalysts[a]

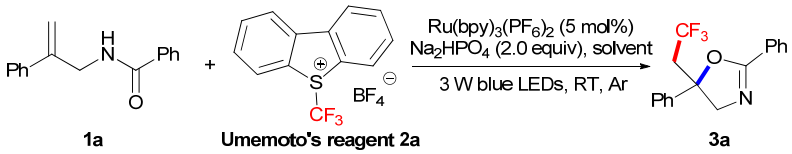


1a Umemoto's reagent 2a 3a

entry	Catalyst	*t* (h)	yield (%)[b]
1	$Ru(bpy)_3Cl_2 \cdot 6H_2O$	5	86
2	$Ir(ppy)_2(dtbbpy)PF_6$	5	88
3	$Ir(dF(CF_3)ppy)_2(dtbbpy)PF_6$	5	60
4	*fac*-$Ir(ppy)_3$	5	85
5	EosinY	5	0
6	$Ir(ppy)_2(bpy)PF_6$	5	91
7	$Ru(bpm)_3(BArF)_2$	5	0
8	2,4,6-triphenylpyrylium tetrafluoroborate	5	0
9	$Ru(bpy)_3(PF_6)_2$	5	93

[a] Reaction conditions: **1a** (0.1 mmol), **2a** (0.11 mmol), catalyst (5 mol%), Na_2HPO_4 (0.2 mmol) in CH_3CN (1.0 mL) under Ar with 3 W blue LEDs irradiation at room temperature. [b] GC yield using biphenyl as an internal standard.

Table S2. Studies of the effect of solvents[a]

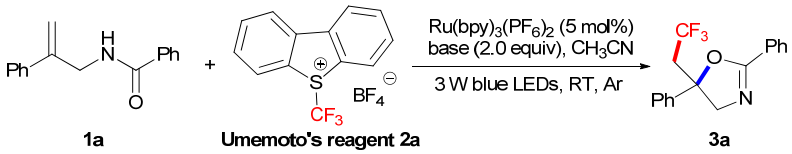


1a **Umemoto's reagent 2a** **3a**

entry	solvent	*t* (h)	yield (%)[b]
1	CH_3CN	5	93
2	DMF	5	59
3	DMSO	5	33
4	CH_2Cl_2	5	85
5	$CHCl_3$	5	66
6	DCE	5	90
7	EtOH	5	20
8	Toluene	5	0
9	THF	5	9
10	Et_2O	24	0

[a] Reaction conditions: **1a** (0.1 mmol), **2a** (0.11 mmol), $Ru(bpy)_3(PF_6)_2$ (5 mol%), Na_2HPO_4 (0.2 mmol) in the solvent (1.0 mL) under Ar with 3 W blue LEDs irradiation at room temperature. [b] GC yield using biphenyl as an internal standard.

Table S3. Studies of the effect of bases[a]



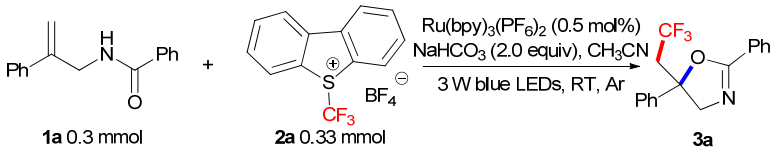
1a Umemoto's reagent 2a 3a

entry	base	*t* (h)	yield (%)[b]
1	Na_2HPO_4	5	93
2	$NaHCO_3$	5	95
3	K_2CO_3	5	73
4	Cs_2CO_3	5	26
5	NaOH	5	29
6	^tBuOK	5	0
7	K_2HPO_4	5	91

[a] Reaction conditions: **1a** (0.1 mmol), **2a** (0.11 mmol), $Ru(bpy)_3(PF_6)_2$ (5 mol%), Base (0.2 mmol) in the CH_3CN (1.0 mL) under Ar with 3 W blue LEDs irradiation at room temperature. [b] GC yield using biphenyl as an internal standard.

4. Time profile of photocatalytic oxytrifluoromethylation of 1a with 2a

The oxytrifluoromethylation of **1a** was performed with/without visible light irradiation. The time profile is shown in Figure S1. As a result, continuous irradiation of visible light is essential for efficient reaction. Furthermore, the result of this experiment suggests that radical chain propagation mechanism isn't main component in this reaction.



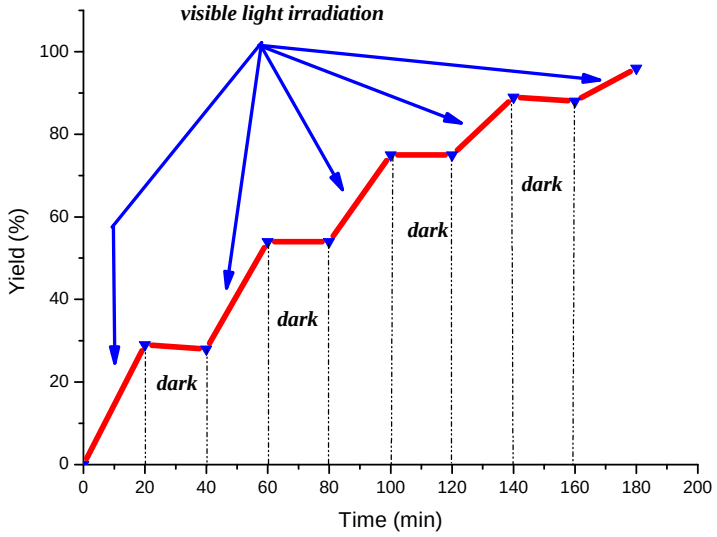


Figure S1.

5. Crystal Structure of 5f

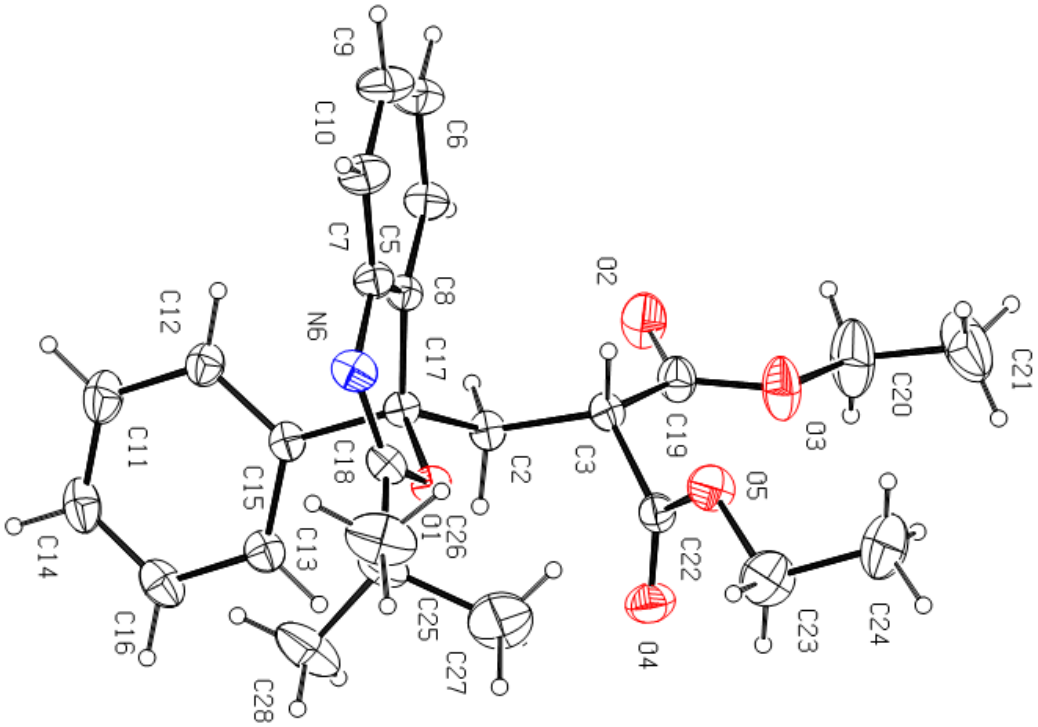
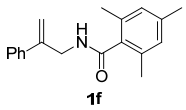
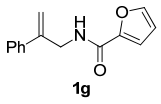


Figure S2.

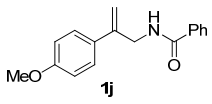
6. Spectral Data of Substrates



2,4,6-Trimethyl-*N*-(2-phenylallyl)benzamide (1f)[2] : ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.48 (d, *J* = 7.2 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 2H), 7.30 (s, 1H), 6.77 (s, 2H), 5.63 (br s, 1H), 5.48 (s, 1H), 5.34 (s, 1H), 4.56 (d, *J* = 5.6 Hz, 2H), 2.23 (s, 3H), 2.13 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 170.2, 144.4, 138.2, 138.2, 134.6, 134.1, 128.4, 128.0, 128.0, 126.2, 114.6, 43.3, 20.9, 18.9; HRMS (ESI): calculated for $[C_{19}H_{21}NO+Na]^+$ requires 302.1515, found 302.1518.

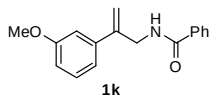


***N*-(2-phenylallyl)furan-2-carboxamide (1g)**[2]: ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.48 (d, *J* = 7.5 Hz, 2H), 7.39 (s, 1H), 7.36 (t, *J* = 7.4 Hz, 2H), 7.30 (t, *J* = 7.3 Hz, 1H), 7.12 (d, *J* = 3.0 Hz, 1H), 6.48 (s, 1H), 6.45 (br s, 1H), 5.52 (s, 1H), 5.31 (s, 1H), 4.50 (d, *J* = 5.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 158.1, 147.6, 143.9, 143.8, 138.2, 128.4, 128.0, 125.9, 114.2, 113.8, 112.0, 42.6; HRMS (ESI): calculated for $[C_{14}H_{13}NO_2+Na]^+$ requires 250.0838, found 250.0837.



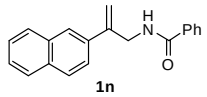
***N*-(2-(4-methoxyphenyl)allyl)benzamide (1j)**[2]: ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.71 (d, *J* = 7.6 Hz, 2H), 7.48 (t, *J* = 7.3 Hz, 1H), 7.45 – 7.37 (m, 4H), 6.89 (d, *J* = 8.5 Hz, 2H), 6.17 (br s, 1H), 5.45 (s, 1H), 5.23 (s, 1H), 4.52 (d, *J* = 5.5 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 167.3, 159.4, 143.4, 134.3, 131.3, 130.6, 128.4, 127.1, 126.8, 113.8, 112.2, 55.1,

43.7; HRMS (ESI): calculated for $[C_{17}H_{17}NO_2+Na]^+$ requires 290.1151, found 290.1143.



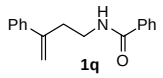
1k

***N*-(2-(3-methoxyphenyl)allyl)benzamide (1k)**[2]: ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.74 – 7.68 (m, 2H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.30 – 7.26 (m, 1H), 7.07 (d, *J* = 7.7 Hz, 1H), 7.02 (s, 1H), 6.87 – 6.83 (m, 1H), 6.23 (br s, 1H), 5.52 (s, 1H), 5.32 (s, 1H), 4.53 (d, *J* = 5.5 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 167.3, 159.6, 144.0, 139.8, 134.3, 131.4, 129.4, 128.4, 126.8, 118.4, 113.8, 113.5, 111.7, 55.1, 43.5; HRMS (ESI): calculated for $[C_{17}H_{17}NO_2+Na]^+$ requires 290.1151, found 290.1157.



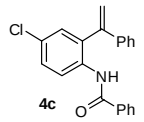
1n

***N*-(2-(naphthalen-2-yl)allyl)benzamide (1n)**[2]: ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.92 (s, 1H), 7.86 – 7.80 (m, 3H), 7.71 (d, *J* = 8.2 Hz, 2H), 7.64 (d, *J* = 8.5 Hz, 1H), 7.49 – 7.43 (m, 3H), 7.38 (t, *J* = 7.5 Hz, 2H), 6.26 (br s, 1H), 5.67 (s, 1H), 5.43 (s, 1H), 4.66 (d, *J* = 5.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 167.4, 143.8, 135.5, 134.2, 133.2, 132.9, 131.3, 128.4, 128.2, 128.0, 127.4, 126.9, 126.2, 126.1, 124.8, 124.1, 114.2, 43.6; HRMS (ESI): calculated for $[C_{20}H_{17}NO+Na]^+$ requires 310.1202, found 310.1203.



1q

***N*-(3-phenylbut-3-en-1-yl)benzamide (1q)**[2]: ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.65 (d, *J* = 8.0 Hz, 2H), 7.49 – 7.44 (m, 3H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.31 (d, *J* = 7.2 Hz, 1H), 6.16 (br s, 1H), 5.43 (s, 1H), 5.19 (s, 1H), 3.59 (q, *J* = 6.3 Hz, 2H), 2.86 (t, *J* = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 167.5, 145.4, 140.0, 134.4, 131.3, 128.5, 128.4, 127.7, 126.7, 126.0, 114.3, 38.7, 34.8; HRMS (ESI): calculated for $[C_{17}H_{17}NO+Na]^+$ requires 274.1202, found 274.1220.



4c

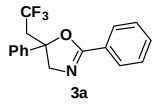
***N*-(4-chloro-2-(1-phenylvinyl)phenyl)benzamide (4c)**[3]: ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.47 (d, *J* = 8.8 Hz, 1H), 7.73 (br s, 1H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.42 – 7.37 (m, 6H), 7.34 (d, *J* = 2.4 Hz, 1H), 7.30 (t, *J* = 7.8 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 5.93 (s, 1H), 5.45 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 164.9, 145.2, 138.2, 134.4, 134.1, 133.1, 131.7, 130.2, 129.2, 129.0, 128.8, 128.5, 126.7, 126.6, 122.2, 118.5, 109.7; HRMS (ESI): calculated for $[C_{21}H_{16}ClNO+Na]^+$ requires 356.0813, found 356.0805.

7. General Procedures and Data of Products

Conditions A: To a 10 mL schlenk tube equipped with a magnetic stir bar were added substrate **1** or **4** (0.30 mmol, 1.0 equiv), Umemoto's reagent **2** (0.33 mmol, 1.1 equiv), $Ru(bpy)_3(PF_6)_2$ (0.0015 mmol, 0.005 equiv), $NaHCO_3$ (0.60 mmol, 2.0 equiv) and dry CH_3CN (3.0 mL) under Ar. The resulting mixture was degassed via 'freeze-pump-thaw' procedure (3 times). Then the reaction mixture was stirred under irradiation with the 3 W blue LEDs. The reaction was monitored via TLC (petroleum ether : ethyl acetate). Upon consumption of the starting materials, the solvent was evaporated under reduced pressure, the residue was purified by flash chromatography on silica gel (petroleum ether : ethyl acetate = 4:1) to give the desired product **3**

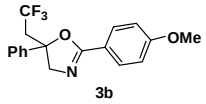
or **5**.

Conditions B: To a 10 mL schlenk tube equipped with a magnetic stir bar were added substrate **1** or **4** (0.30 mmol, 1.0 equiv), $BrCH(CO_2Et)_2$ **2b** (0.6 mmol 2.0 equiv), $Ru(bpy)_3Cl_2{\cdot}6H_2O$ (0.003 mmol, 0.01 equiv), 4-methoxy-*N*,*N*-diphenylaniline (0.60 mmol, 2.0 equiv), 4 Å MS (100 mg), Na_2HPO_4 (0.60 mmol, 2.0 equiv) and dry CH_3CN (3.0 mL) under Ar. The resulting mixture was degassed via 'freeze-pump-thaw' procedure (3 times). Then the reaction mixture was stirred under irradiation with the 3 W blue LEDs. The reaction was monitored via TLC (petroleum ether : ethyl acetate). Upon consumption of the starting materials, the solvent was evaporated under reduced pressure, the residue was purified by flash chromatography on silica gel (petroleum ether : ethyl acetate = 5:1) to give the desired product **3** or **5**.



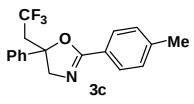
3a

2,5-Diphenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrooxazole (3a): Colorless oil, 88% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.05 (d, *J* = 7.3 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.42 – 7.37 (m, 4H), 7.34 – 7.29 (m, 1H), 4.39 (d, *J* = 14.8 Hz, 1H), 4.23 (d, *J* = 14.9 Hz, 1H), 2.95 – 2.85 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 162.9, 142.5, 131.7, 128.7, 128.5, 128.2, 127.9, 127.3, 124.8 (q, *J* = 277.2 Hz) 124.3, 84.6, 68.2, 44.2 (q, *J* = 26.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -61.61 (s, 3F); IR (in KBr): 3438, 3065, 2938, 1655, 1450, 1377, 1349, 1262, 1133, 1084, 696 cm^{-1}; HRMS (ESI): calculated for $[C_{17}H_{14}F_3NO+Na]^+$ requires 328.0920, found 328.0923.



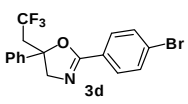
3b

2-(4-Methoxyphenyl)-5-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrooxazole (3b): Colorless oil, 91% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.99 (d, *J* = 8.6 Hz, 2H), 7.38 (m, 4H), 7.31 (m, 1H), 6.96 (d, *J* = 8.6 Hz, 2H), 4.35 (d, *J* = 14.7 Hz, 1H), 4.18 (d, *J* = 14.7 Hz, 1H), 3.85 (s, 3H), 2.92 – 2.85 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 162.7, 162.3, 142.6, 130.0, 128.6, 127.8, 124.8 (q, *J* = 276.9 Hz), 124.3, 119.7, 113.8, 84.4, 68.2, 55.3, 44.1 (q, *J* = 27.3 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -61.59 (s, 3F); IR (in KBr): 3441, 2936, 1654, 1609, 1514, 1350, 1259, 1169, 1133, 1078, 1030, 913, 841, 744, 702 cm^{-1}; HRMS (ESI): calculated for $[C_{18}H_{16}F_3NO_2+Na]^+$ requires 358.1025, found 358.1042.



3c

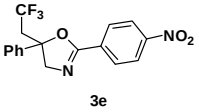
5-Phenyl-2-(*p*-tolyl)-5-(2,2,2-trifluoroethyl)-4,5-dihydrooxazole (3c): White solid, 89% yield. M.P.: 39 - 41 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.94 (d, *J* = 8.1 Hz, 2H), 7.41 – 7.36 (m, 4H), 7.32 – 7.29 (m, 1H), 7.28 – 7.24 (m, 2H), 4.36 (d, *J* = 14.7 Hz, 1H), 4.20 (d, *J* = 14.7 Hz, 1H), 2.89 – 2.86 (m, 2H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 163.0, 142.6, 142.1, 129.2, 128.6, 128.2, 127.9, 124.8 (q, *J* = 277.4 Hz) 124.5, 124.3, 84.5, 68.1, 44.1 (q, *J* = 27.1 Hz), 21.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -61.60 (s, 3F); IR (in KBr): 3425, 2927, 1654, 1377, 1349, 1262, 1133, 1079, 913, 745, 676 cm^{-1}; HRMS (ESI): calculated for $[C_{18}H_{16}F_3NO+Na]^+$ requires 342.1076, found 342.1092.



3d

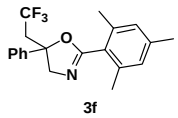
2-(4-Bromophenyl)-5-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrooxazole(3d): Colorless

oil, 95% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.91 (d, *J* =8.5 Hz, 2H), 7.60 (d, *J* = 8.5 Hz, 2H), 7.40 – 7.38 (m, 4H), 7.34 – 7.32 (m, 1H), 4.38 (d, *J* = 14.9, 1H), 4.21 (d, *J* = 14.9 Hz, 1H), 2.95 – 2.84 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 162.0, 142.3, 131.7, 129.7, 128.7, 128.0, 126.4, 126.2, 124.8 (q, *J* = 276.9 Hz), 124.2, 84.9, 68.1,44.1 (q, *J* = 27.5 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -61.67 (s, 3F); IR (in KBr): 3424, 2928, 1656, 1593, 1488, 1398, 1377, 1348, 1262, 1134, 1079, 1011, 837, 727, 703 cm^{-1}; HRMS (ESI): calculated for $[C_{17}H_{13}BrF_3NO+H]^+$ requires 384.0205, found 384.0204.



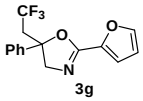
3e

2-(4-Nitrophenyl)-5-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrooxazole (3e): White Solid**,** 69% yield. M.P.: 93 - 95 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.32 (d, *J* = 8.4 Hz, 2H), 8.22 (d, *J* = 8.5 Hz, 2H), 7.44 – 7.38 (m, 4H), 7.35 (t, *J* = 6.8 Hz, 1H), 4.47 (d, *J* = 15.5 Hz, 1H), 4.30 (d, *J* = 15.4 Hz, 1H), 3.00 – 2.84 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 161.0, 149.6, 142.1, 133.0, 129.2, 128.9, 128.2, 124.7 (q, *J* = 276.7 Hz), 124.1, 123.7, 85.5, 68.1, 44.2 (q, *J* = 27.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -61.72 (s, 3F); IR (in KBr): 3438, 2973, 1655, 1630, 1601, 1526, 1378, 1343, 1261, 1133, 1081, 1043, 911, 867, 742, 703 cm^{-1}; HRMS (ESI): calculated for $[C_{17}H_{13}F_3N_2O_3+H]^+$ requires 351.0951, found 351.0963.



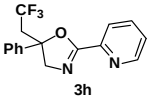
3f

2-Mesityl-5-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrooxazole (3f): Colorless oil, 75% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.46 – 7.36 (m, 4H), 7.33 (s, 1H), 6.90 (s, 2H), 4.42 (d, *J* = 14.6 Hz, 1H), 4.35 (d, *J* = 14.7 Hz, 1H), 2.93 – 2.88 (m, 2H), 2.30 (s, 3H), 2.29 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 163.3, 142.5, 139.5, 137.0, 128.6, 128.3, 127.9, 125.5, 124.7 (q, *J* = 276.7 Hz) 124.6, 84.2, 68.1, 45.0 (q, *J* = 27.1 Hz), 21.1, 19.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -61.37 (s, 3F); IR (in KBr): 3425, 2925, 1670, 1376, 1260, 1131, 1062, 1036, 744, 703 cm^{-1}, HRMS (ESI): calculated for $[C_{20}H_{20}F_3NO+Na]^+$ requires 370.1389, found 370.1371.



3g

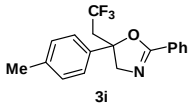
2-(Furan-2-yl)-5-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrooxazole (3g): Colorless oil, 45% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.60 (d, *J* = 0.9 Hz, 1H), 7.41 – 7.37 (m, 4H), 7.35 – 7.31 (m, 1H), 7.10 (d, *J* = 3.4 Hz, 1H), 6.54 (dd, *J* = 3.4 Hz, *J* = 1.8 Hz, 1H), 4.39 (d, *J* = 14.9 Hz, 1H), 4.23 (d, *J* = 14.9 Hz, 1H), 2.91 – 2.88 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.2, 145.6, 142.5, 142.0, 128.7, 128.1, 124.7 (q, *J* = 276.8 Hz), 124.3, 114.9, 111.6, 85.0, 67.7, 44.0 (q, *J* = 27.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -61.73 (s, 3F); IR (in KBr): 3435, 2930, 1678, 1483, 1378, 1261, 1140, 1093, 750, 701 cm^{-1}; HRMS (ESI): calculated for $[C_{15}H_{12}F_3NO_2+Na]^+$ requires 318.0712, found 318.0699.



3h

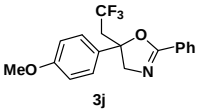
5-Phenyl-2-(pyridin-2-yl)-5-(2,2,2-trifluoroethyl)-4,5-dihydrooxazole (3h): Colorless oil, 94% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.26 (s, 1H), 8.82 – 8.72 (m, 1H), 8.31 (d, *J* = 7.9 Hz, 1H), 7.44 – 7.39 (m, 5H), 7.36 – 7.33 (m, 1H), 4.44 (d, *J* = 15.0 Hz, 1H), 4.26 (d, *J* = 15.1 Hz, 1H), 2.96 – 2.86 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 160.8, 152.2, 149.3, 142.2, 135.5, 128.7, 128.1, 124.8 (q, *J* = 280.4 Hz), 124.1, 123.4, 123.3, 85.0, 67.8, 44.1 (q, *J* = 27.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -61.70 (s, 3F); IR (in KBr): 3441, 2925, 1659, 1592, 1379, 1352, 1261, 1129, 1083, 1021, 705 cm^{-1}; HRMS

(ESI): calculated for $[C_{16}H_{13}F_3N_2O+H]^+$ requires 307.1047, found 307.1033.



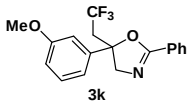
3i

2-Phenyl-5-(*p*-tolyl)-5-(2,2,2-trifluoroethyl)-4,5-dihydrooxazole (3i): Colorless oil, 94% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.08 (d, *J* = 7.3 Hz, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.7 Hz, 2H), 7.31 (d, *J* = 7.9 Hz, 2H), 7.20 (d, *J* = 7.9 Hz, 2H), 4.38 (d, *J* = 14.8 Hz, 1H), 4.22 (d, *J* = 14.8 Hz, 1H), 2.95 – 2.83 (m, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 162.8, 139.6, 137.6, 131.6, 129.3, 128.4, 128.2, 127.4, 124.9 (q, *J* = 276.8 Hz), 124.2, 84.6, 68.1,44.1 (q, *J* = 27.2 Hz), 20.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -61.57 (s, 3F); IR (in KBr): 3402, 2975, 2928, 1655, 1451, 1377, 1350, 1263, 1134, 1086, 1027, 911, 741, 696 cm^{-1}; HRMS (ESI): calculated for $[C_{18}H_{16}F_3NO+Na]^+$ requires 342.1076, found 342.1087.



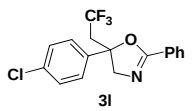
3j

5-(4-Methoxyphenyl)-2-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrooxazole (3j): Colorless oil, 81% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.04 (d, *J* = 7.4 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.33 (d, *J* = 8.7 Hz, 2H), 6.91 (d, *J* =8.8 Hz, 2H), 4.36 (d, *J* = 14.7 Hz, 1H), 4.21 (d, *J* = 14.8 Hz, 1H), 3.81 (s, 3H), 2.91 – 2.85 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 162.8, 159.2, 134.5, 131.6, 128.4, 128.2, 127.4, 125.6, 124.9 (q, *J* = 276.9 Hz), 114.0, 84.5, 68.0, 55.2, 44.2 (q, *J* = 27.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -61.79 (s, 3F); IR (in KBr): 3431, 2968, 1655, 1614, 1515, 1377, 1349, 1259, 1179, 1134, 1084, 1030, 912, 744, 696 cm^{-1}; HRMS (ESI): calculated for $[C_{18}H_{16}F_3NO_2+Na]^+$ requires 358.1025, found 358.0969.



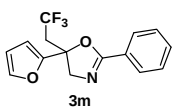
3k

5-(3-Methoxyphenyl)-2-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrooxazole (3k): Colorless oil, 92% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.04 (d, *J* = 7.8 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.9 Hz, 1H), 7.06 – 6.90 (m, 2H), 6.85 (d, *J* = 8.3 Hz, 1H), 4.37 (d, *J* = 14.9 Hz, 1H), 4.21 (d, *J* = 14.9 Hz, 1H), 3.82 (s, 3H), 2.94 – 2.83 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 162.8, 159.8, 144.2, 131.6, 129.8, 128.4, 128.2, 127.3, 124.8 (q, *J* = 276.9 Hz), 116.6, 112.6, 110.8, 84.5, 68.2, 55.2, 44.1 (q, *J* = 27.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -61.65 (s, 3F); IR (in KBr): 3440, 2942, 1656, 1607, 1585, 1491, 1377, 1349, 1264, 1231, 1129, 1085, 1058, 1026, 911, 745, 695 cm^{-1}; HRMS (ESI): calculated for $[C_{18}H_{16}F_3NO_2+Na]^+$ requires 358.1025, found 358.1052.



3l

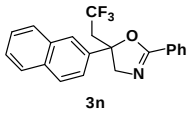
5-(4-Chlorophenyl)-2-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrooxazole (3l): Colorless oil, 94% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.03 (d, *J* = 7.9 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.7 Hz, 2H), 7.38 – 7.34 (m, 4H), 4.37 (d, *J* = 14.8 Hz, 1H), 4.18 (d, *J* = 14.8 Hz, 1H), 2.91 – 2.86 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 162.7, 140.9, 133.8, 131.8, 128.9, 128.5, 128.2, 127.0, 125.8, 124.7 (q, *J* = 275.1 Hz), 84.2, 68.3, 44.1 (q, *J* = 27.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -61.55 (s, 3F); IR (in KBr): 3446, 2937, 1656, 1494, 1377, 1349, 1261, 1133, 1086, 1065, 1022, 909, 744, 695 cm^{-1}; HRMS (ESI): calculated for $[C_{17}H_{13}ClF_3NO+H]^+$ requires 340.0705, found 340.0708.



3m

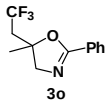
5-(Furan-2-yl)-2-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrooxazole (3m): Colorless oil,

48% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.96 (d, *J* = 7.2 Hz, 2H), 7.56 – 7.35 (m, 4H), 6.43 (d, *J* = 3.3 Hz, 1H), 6.37 (m, 1H), 4.43 (d, *J* = 15.3 Hz, 1H), 4.28 (d, *J* = 15.3 Hz, 1H), 3.11 – 2.99 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 162.6, 152.2, 143.4, 131.7, 128.4, 128.2, 127.0, 124.7 (q, *J* = 276.0 Hz), 110.5, 107.4, 80.3, 64.0, 41.0 (q, *J* = 27.8 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -62.48 (s, 3F); IR (in KBr): 3434, 2948, 1655, 1408, 1371, 1348, 1260, 1132, 1092, 1026, 913, 743, 696 cm^{-1}; HRMS (ESI): calculated for $[C_{15}H_{12}F_3NO_2+H]^+$ requires 296.0893, found 296.0899.



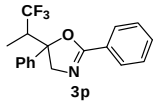
3n

5-(Naphthalen-2-yl)-2-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrooxazole (3n): Colorless oil, 71% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.11 (d, *J* = 7.1 Hz, 2H), 7.92 – 7.84 (m, 2H), 7.84 – 7.79 (m, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.50 – 7.44 (m, 4H), 7.42 (d, *J* = 8.6 Hz, 1H), 4.43 (d, *J* = 14.9 Hz, 1H), 4.29 (d, *J* = 14.8 Hz, 1H), 3.02 – 2.90 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 162.9, 139.6, 133.0, 132.70, 131.70, 128.8, 128.50, 128.3, 128.2, 127.6, 127.3, 126.6, 126.4, 124.9 (q, *J* = 276.8 Hz), 123.1, 122.3, 84.8, 68.2, 44.1 (q, *J* = 27.4 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -61.55 (s, 3F); IR (in KBr): 3444, 3061, 2932, 1655, 1377, 1264, 1138, 1084, 910, 747, 695, 477 cm^{-1}; HRMS (ESI): calculated for $[C_{21}H_{16}F_3NO+Na]^+$ requires 378.1076, found 378.1116.



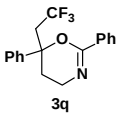
3o

5-Methyl-2-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrooxazole (3o): Colorless oil, 35% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.93 (d, *J* = 7.2 Hz, 2H), 7.49 (t, *J* = 7.2 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 2H), 4.01 (d, *J* = 14.8 Hz, 1H), 3.85 (d, *J* = 14.9 Hz, 1H), 2.69 – 2.53 (m, 2H), 1.60 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 162.8, 131.5, 128.3, 128.1, 127.5, 125.2 (q, *J* = 276.0 Hz) 81.8, 66.3, 43.1 (q, *J* = 27.4 Hz), 25.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -62.20 (s, 3F); IR (in KBr): 3430, 2976, 2877, 1651, 1452, 1378, 1350, 1270, 1220, 1167, 1108, 1085, 1062, 1026, 911, 779, 741, 695 cm^{-1}; HRMS (ESI): calculated for $[C_{12}H_{12}F_3NO+Na]^+$ requires 266.0763, found 266.0784.



3p

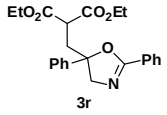
2,5-Diphenyl-5-(1,1,1-trifluoropropan-2-yl)-4,5-dihydrooxazole (3p): Colorless oil, 70% yield, dr = 1.1:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) major + minor: ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.03 (m, 4H), 7.50 (m, 2H), 7.47 – 7.41 (m, 6H), 7.40 – 7.34 (m, 6H), 7.31 – 7.29 (m, 2H), 4.60 (d, *J* = 15.2 Hz, 1H), 4.49 (d, *J* = 15.2 Hz, 1H), 4.35 (d, *J* = 15.1 Hz, 1H), 4.28 (d, *J* = 15.1 Hz, 1H), 3.00 – 2.80 (m, 2H), 1.28 (d, *J* = 7.0 Hz, 3H), 1.20 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 162.9, 162.6, 142.5, 141.9, 131.6, 131.5, 128.6, 128.5, 128.4, 128.2, 128.1, 127.9, 127.8, 127.4, 127.2, 127.0 (q, *J* = 267.0 Hz), 126.8 (q, *J* = 264.0 Hz), 125.2, 125.0, 87.8, 87.5, 67.1, 65.7, 47.5 (q, *J* = 24.0 Hz), 46.7 (q, *J* = 24.5 Hz), 10.4, 9.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -66.82 (s, 3F), -66.98 (s, 3F); IR (in KBr): 3424, 2973, 1658, 1451, 1348, 1267, 1175, 1120, 1084, 1047, 913, 745, 696 cm^{-1}; calculated for $[C_{18}H_{16}F_3NO+H]^+$ requires 320.1257, found 320.1259.



3q

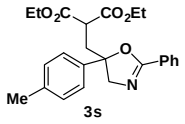
2,6-Diphenyl-6-(2,2,2-trifluoroethyl)-5,6-dihydro-4*H*-1,3-oxazine (3q): Colorless oil, 78% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.11 – 8.05 (m, 2H), 7.51 – 7.42 (m, 3H), 7.38 – 7.34 (m, 2H), 7.34 – 7.29 (m, 3H), 3.64 – 3.54 (m, 1H), 3.17 – 2.98 (m, 1H), 2.89 – 2.77 (m, 2H), 2.39 –

2.35 (m, 1H), 2.27 – 2.22 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 154.3, 141.1, 133.1, 130.8, 128.8, 128.2, 128.0, 127.0, 125.0 (q, *J* = 276.9 Hz), 124.4, 77.4, 45.8 (q, *J* = 26.3 Hz), 40.0, 31.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -60.70 (s, 3F); IR (in KBr): 3432, 3064, 2931, 1659, 1448, 1379, 1262, 1126, 1069, 911, 699 cm^{-1}; HRMS (ESI): calculated for $[C_{18}H_{16}F_3NO+Na]^+$ requires 342.1076, found 342.1068.



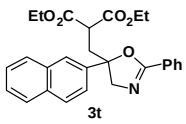
3r

Diethyl 2-((2,5-diphenyl-4,5-dihydrooxazol-5-yl)methyl)malonate (3r): Brown oil, 82% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.99 (d, *J* = 7.7 Hz, 2H), 7.51 (d, *J* = 7.1 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.39 – 7.35 (m, 4H), 7.30 (d, *J* = 5.9 Hz, 1H), 4.27 (d, *J* = 14.8 Hz, 1H), 4.17 (d, *J* = 15.0 Hz, 1H), 4.15 – 3.93 (m, 3H), 3.87 – 3.82 (m, 1H), 3.43 (t, *J* = 6.3 Hz, 1H), 2.78 (d, *J* = 6.4 Hz, 2H), 1.16 (t, *J* = 7.1 Hz, 3H), 1.08 (t, *J* = 7.1 Hz, 3H), ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 169.0, 168.9, 162.6, 142.9, 131.4, 128.6, 128.3, 128.1, 127.6, 127.5, 124.7, 87.8, 68.5, 61.5 (overlap), 48.2, 39.8, 13.8, 13.7; IR (in KBr): 3429, 2977, 2932, 1733, 1653, 1633, 1448, 1370, 1268, 1151, 1050, 1026, 778, 697 cm^{-1}; HRMS (ESI): calculated for $[C_{23}H_{25}NO_5+Na]^+$ requires 418.1625, found 418.1612.



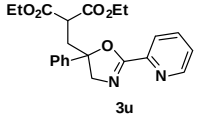
3s

Diethyl 2-((2-phenyl-5-(*p*-tolyl)-4,5-dihydrooxazol-5-yl)methyl)malonate (3s): Brown oil, 85% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.98 (d, *J* = 7.6 Hz, 2H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.27 (d, *J* = 5.5 Hz, 2H), 7.18 (d, *J* = 7.9 Hz, 2H), 4.23 (d, *J* = 14.6 Hz, 1H), 4.17 – 4.10 (m, 2H), 4.09 – 3.98 (m, 2H), 3.89 – 3.82 (m, 1H), 3.41 (t, *J* = 6.4 Hz, 1H), 2.75 (d, *J* = 6.4 Hz, 2H), 2.34 (s, 3H), 1.16 (t, *J* = 7.1 Hz, 3H), 1.09 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 169.0, 168.8, 162.6, 139.8, 137.2, 131.3, 129.2, 128.2, 128.0, 127.5, 124.5, 87.8, 68.4, 61.4 (overlap), 48.1, 39.7, 20.8, 13.7, 13.6; IR (in KBr): 2982, 2933, 2871, 1733, 1653, 1580, 1514, 1449, 1347, 1269, 1236, 1152, 1099, 1053, 1025, 818, 696 cm^{-1}; HRMS (ESI): calculated for $[C_{24}H_{27}NO_5+Na]^+$ requires 432.1781, found 432.1771.



3t

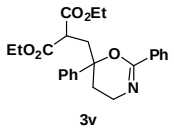
Diethyl 2-((5-(naphthalen-2-yl)-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)malonate (3t): Brown oil, 77% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.04 (d, *J* = 7.5 Hz, 2H), 7.91 – 7.86 (m, 2H), 7.84 (t, *J* = 8.1 Hz, 2H), 7.54 (t, *J* = 7.3 Hz, 1H), 7.51 – 7.45 (m, 4H), 7.42 (d, *J* = 8.6 Hz, 1H), 4.34 (d, *J* = 14.7 Hz, 1H), 4.26 (d, *J* = 14.7 Hz, 1H), 4.18 – 4.12 (m, 1H), 4.11 – 4.04 (m, 1H), 3.94 – 3.89 (m, 1H), 3.74 – 3.69 (m, 1H), 3.47 (t, *J* = 6.3 Hz, 1H), 2.92 – 2.83 (m, 2H), 1.17 (t, *J* = 7.1 Hz, 3H), 0.98 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 169.0, 168.8, 162.7, 139.8, 132.8, 132.5, 131.5, 128.7, 128.3, 128.1, 128.1, 127.5, 126.4, 126.2, 123.5, 122.7, 88.0, 68.3, 61.5, 61.4, 48.2, 39.6, 13.8, 13.5; IR (in KBr): 3441, 2981, 2852, 1732, 1653, 1448, 1334, 1269, 1151, 1053, 1025, 859, 778, 696 cm^{-1}; HRMS (ESI): calculated for $[C_{27}H_{27}NO_5+Na]^+$ requires 468.1781, found 468.1773.



3u

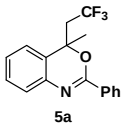
Diethyl 2-((5-phenyl-2-(pyridin-2-yl)-4,5-dihydrooxazol-5-yl)methyl)malonate (3u): Brown oil, 42% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.17 (s, 1H), 8.74 (d, *J* = 4.8 Hz, 1H), 8.26 (d, *J* = 8.0 Hz, 1H), 7.42 – 7.36 (m, 5H), 7.31 (t, *J* = 6.7 Hz, 1H), 4.28 (d, *J* = 15.0 Hz, 1H), 4.20 – 4.09 (m, 3H), 4.05 – 4.00 (m, 1H), 3.92 – 3.85 (m, 1H), 3.41 (t, *J* = 6.4 Hz, 1H), 2.79 (d, *J* = 6.4

Hz, 2H), 1.20 (t, *J* = 7.1 Hz, 3H), 1.11 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 169.0, 168.7, 160.6, 152.1, 149.2, 142.3, 135.5, 128.7, 127.8, 124.6, 123.6, 123.2, 88.4, 68.4, 61.6, 61.6, 48.0, 39.7, 13.8, 13.7; IR (in KBr): 3450, 2982, 2934, 1732, 1657, 1592, 1447, 1332, 1272, 1236, 1153, 1081, 1023, 745, 706 cm^{-1}; HRMS (ESI): calculated for $[C_{22}H_{24}N_2O_5+Na]^+$ requires 419.1577, found 419.1562.



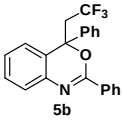
3v

Diethyl 2-(2,6-diphenyl-5,6-dihydro-4*H*-1,3-oxazin-6-yl)malonate (3v): Brown oil, 55% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.01 (d, *J* = 7.3 Hz, 2H), 7.47 (t, *J* = 7.3 Hz, 1H), 7.42 (t, *J* = 7.4 Hz, 2H), 7.36 – 7.32 (m, 2H), 7.28 (d, *J* = 8.0 Hz, 3H), 4.15 – 4.08 (m, 2H), 4.01 – 3.95 (m, 1H), 3.91 – 3.84 (m, 1H), 3.61 – 3.54 (m, 1H), 3.47 (t, *J* = 6.2 Hz, 1H), 3.16 – 3.03 (m, 1H), 2.72 (d, *J* = 6.2 Hz, 2H), 2.32 – 2.20 (m, 1H), 2.15 – 2.05 (m, 1H), 1.20 (t, *J* = 7.1 Hz, 3H), 1.12 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 169.3, 169.0, 154.3, 141.6, 133.6, 130.5, 128.7, 128.0, 127.6, 127.0, 124.8, 80.0, 61.5 (overlap), 47.3, 40.7, 40.5, 32.4, 13.9, 13.8; IR (in KBr): 3435, 2981, 2935, 1732, 1658, 1493, 1447, 1370, 1349, 1279, 1140, 1099, 1067, 1029, 765, 699 cm^{-1}; HRMS (ESI): calculated for $[C_{24}H_{27}NO_5+Na]^+$ requires 432.1781, found 432.1768.



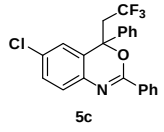
5a

4-Methyl-2-phenyl-4-(2,2,2-trifluoroethyl)-4*H*-benzo[*d*][1,3]oxazine (5a): White Solid**,** 74% yield. M.P.: 66 - 68 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.17 (d, *J* = 7.3 Hz, 2H), 7.49 (t, *J* = 7.3 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.36 – 7.30 (m, 2H), 7.23 – 7.21 (m, 1H), 7.11 (d, *J* = 7.6 Hz, 1H), 2.89 – 2.81 (m, 1H), 2.64 – 2.55 (m, 1H), 1.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.6, 138.3, 132.2, 131.5, 129.3, 128.2, 128.0, 126.9, 125.6, 125.9, 125.1 (q, *J* = 275.7 Hz), 122.5, 76.6, 43.6 (q, *J* = 27.1 Hz), 26.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -60.99 (s, 3F); IR (in KBr): 3443, 1628, 1600, 1574, 1485, 1452, 1370, 1323, 1258, 1154, 1133, 1066, 1089, 913, 764, 747, 696 cm^{-1}; HRMS (ESI): calculated for $[C_{17}H_{14}F_3NO+Na]^+$ requires 328.0920, found 328.0887.



5b

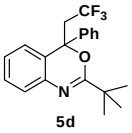
2,4-Diphenyl-4-(2,2,2-trifluoroethyl)-4*H*-benzo[*d*][1,3]oxazine (5b): White Solid**,** 94% yield. M.P.: 97 - 99 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.35 (d, *J* = 8.0 Hz, 2H), 7.59 – 7.55 (m, 1H), 7.53 (t, *J* = 7.2 Hz, 2H), 7.45 – 7.40 (m, 4H), 7.33 (t, *J* = 7.4 Hz, 2H), 7.32 – 7.26 (m, 3H), 3.37 – 3.29 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 155.4, 141.5, 138.6, 131.9, 131.6, 129.4, 128.5, 128.4, 128.3, 127.9, 126.5, 126.2, 125.8, 125.4, 124.8 (q, *J* = 277.7 Hz), 124.2, 80.0, 43.3 (q, *J* = 27.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -59.65 (s, 3F); IR (in KBr): 3442, 1628, 1598, 1574, 1485, 1453, 1375, 1321, 1264, 1129, 1082, 912, 764, 745, 697 cm^{-1}; HRMS (ESI): calculated for $[C_{22}H_{16}F_3NO+H]^+$ requires 368.1251, found 368.1270.



5c

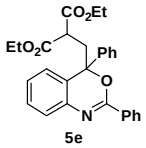
6-Chloro-2,4-diphenyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (5c): White Solid**,** 98% yield. M.P.: 118 - 120 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.23 (d, *J* = 7.4 Hz, 2H), 7.56 – 7.50 (m, 1H), 7.50 – 7.42 (m, 2H), 7.38 – 7.25 (m, 7H), 7.17 (d, *J* = 6.2 Hz, 1H), 3.33 – 3.15 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.6, 140.9, 137.3, 131.8, 131.6, 129.6, 128.7, 128.6, 128.4, 128.0, 127.7, 127.2, 125.3, 124.6 (q, *J* = 277.5 Hz), 124.3, 79.8, 43.3 (q, *J* = 27.6 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -59.74 (s, 3F); IR (in KBr): 3446, 3065, 1626, 1576, 1474, 1374, 1315, 1260, 1133, 1082, 911, 833, 743,

695 cm^{-1}; HRMS (ESI): calculated for $[C_{22}H_{15}ClF_3NO+H]^+$ requires 402.0867, found 402.0908.



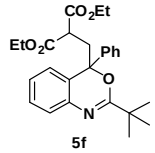
5d

2-(Tert-butyl)-4-phenyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (5d): Colorless oil, 88% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.34 – 7.29 (m, 4H), 7.28 – 7.25 (m, 2H), 7.24 (d, *J* = 7.8 Hz, 1H), 7.20 (t, *J* = 7.5 Hz, 1H), 7.08 (d, *J* = 7.6 Hz, 1H), 3.25 – 3.16 (m, 2H), 1.24 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 166.1, 142.9, 138.6, 129.2, 128.5, 128.3, 125.9, 125.8, 125.6, 124.9, 124.8 (q, *J* = 277.7 Hz), 124.0, 79.3, 43.5 (q, *J* = 27.0 Hz), 37.2, 27.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -59.67 (s, 3F); IR (in KBr): 3423, 2975, 1638, 1601, 1485, 1456, 1372, 1306, 1261, 1129, 914, 768, 746, 698 cm^{-1}; HRMS (ESI): calculated for $[C_{20}H_{20}F_3NO+Na]^+$ requires 370.1389, found 370.1386.



5e

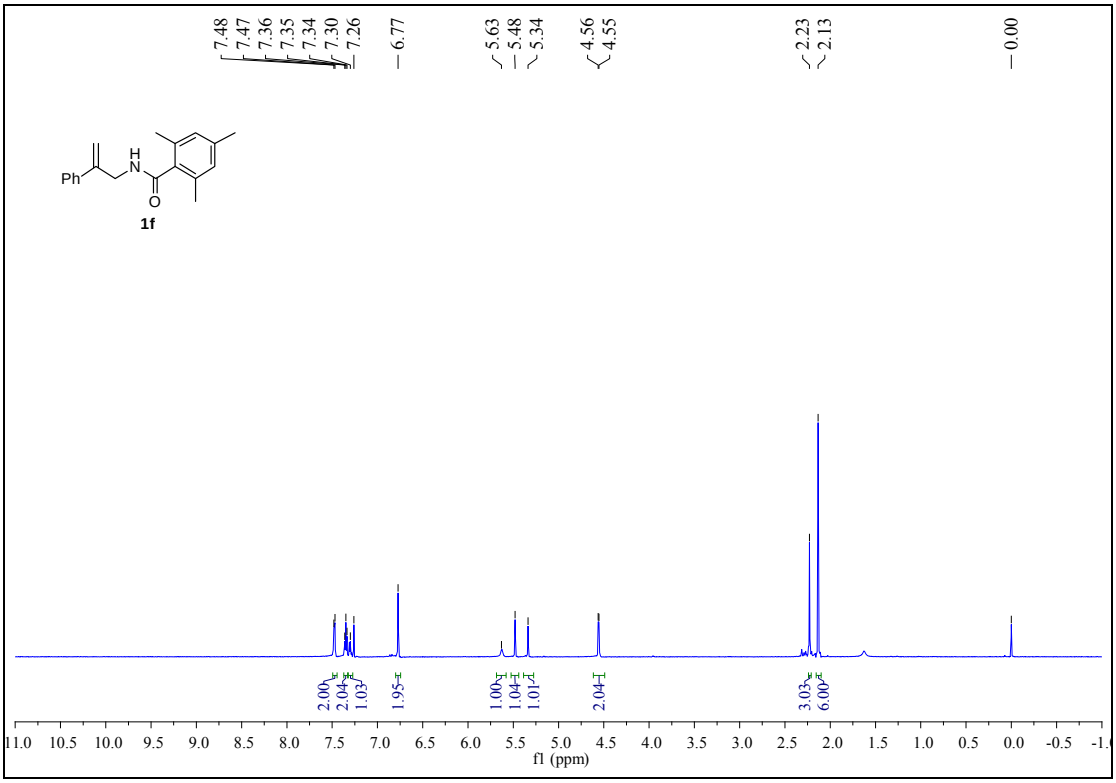
Diethyl 2-((2,4-diphenyl-4H-benzo[*d*][1,3]oxazin-4-yl)methyl)malonate (5e):White solid, 56% yield. M.P.: 107 - 109 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.18 (d, *J* = 7.7 Hz, 2H), 7.50 (t, *J* = 7.1 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.40 – 7.37 (m, 1H), 7.35 (d, *J* = 4.6 Hz, 2H), 7.33 – 7.28 (m, 3H), 7.25 – 7.18 (m, 3H), 4.15 – 4.03 (m, 3H), 3.90 – 3.83 (m, 1H), 3.68 – 3.64 (m, 1H), 3.29 – 3.22 (m, 1H), 3.18 – 3.11 (m, 1H), 1.20 (t, *J* = 7.1 Hz, 3H), 1.05 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 169.5, 169.1, 155.8, 142.8, 139.8, 132.1, 131.5, 129.3, 128.3, 128.2, 127.8, 126.6, 126.2, 125.9, 125.8, 125.4, 124.2, 83.4, 61.7, 61.4, 48.8, 39.1, 13.8, 13.7; IR (in KBr): 3450, 3063, 2982, 1732, 1626, 1598, 1573, 1480, 1451, 1370, 1319, 1262, 1181, 1152, 1089, 1048, 913, 767, 745, 697 cm^{-1}; HRMS (ESI): calculated for $[C_{28}H_{27}NO_5+Na]^+$ requires 480.1781, found 480.1766.

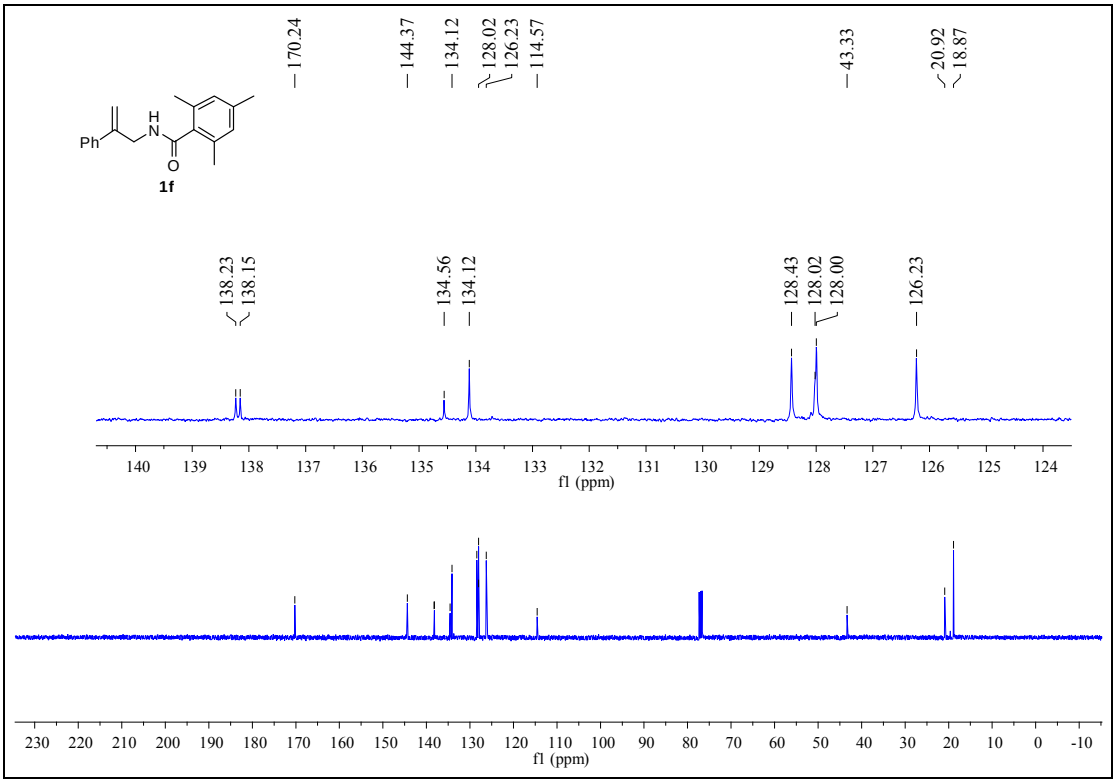


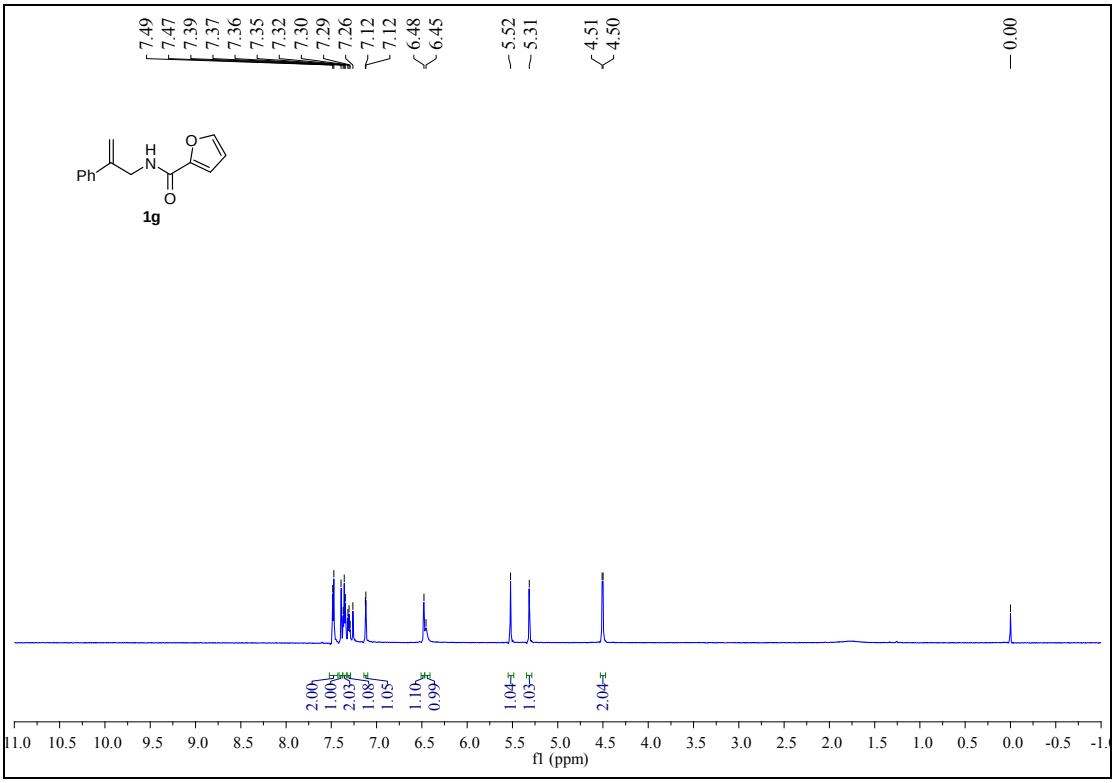
5f

Diethyl 2-((2-(tert-butyl)-4-phenyl-4*H*-benzo[*d*][1,3]oxazin-4-yl)methyl)malonate (5f): White solid, 55% yield. M.P.: 105 - 107 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.34 (t, *J* = 7.3 Hz, 1H), 7.26 – 7.23 (m, 4H), 7.23 – 7.18 (m, 4H), 4.29 – 4.24 (m, 1H), 4.14 – 4.01 (m, 3H), 3.64 – 3.60 (m, 1H), 3.29 – 3.22 (m, 1H), 3.05 – 3.01 (m, 1H), 1.24 (t, *J* = 7.1 Hz, 3H), 1.20 (t, *J* = 7.1 Hz, 3H), 1.14 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 169.2, 167.2, 143.0, 140.2, 129.2, 128.2, 128.0, 126.3, 126.2, 126.1, 125.4, 124.7, 124.7, 82.8, 61.7, 61.4, 48.8, 38.4, 37.2, 27.4, 13.9, 13.8; IR (in KBr): 3452, 2979, 2933, 1734, 1633, 1600,1580, 1484, 1454, 1369, 1265, 1185, 1148, 1030, 804, 770, 700, 588 cm^{-1}; HRMS (ESI): calculated for $[C_{26}H_{31}NO_5+Na]^+$ requires 460.2054, found 460.2058.

8. Copies of ^{1}H NMR, ^{13}C NMR and ^{19}F NMR Spectra



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5.52
5.31
4.51
4.50
0.00
Ph
H
N
O
O
1g
2.00
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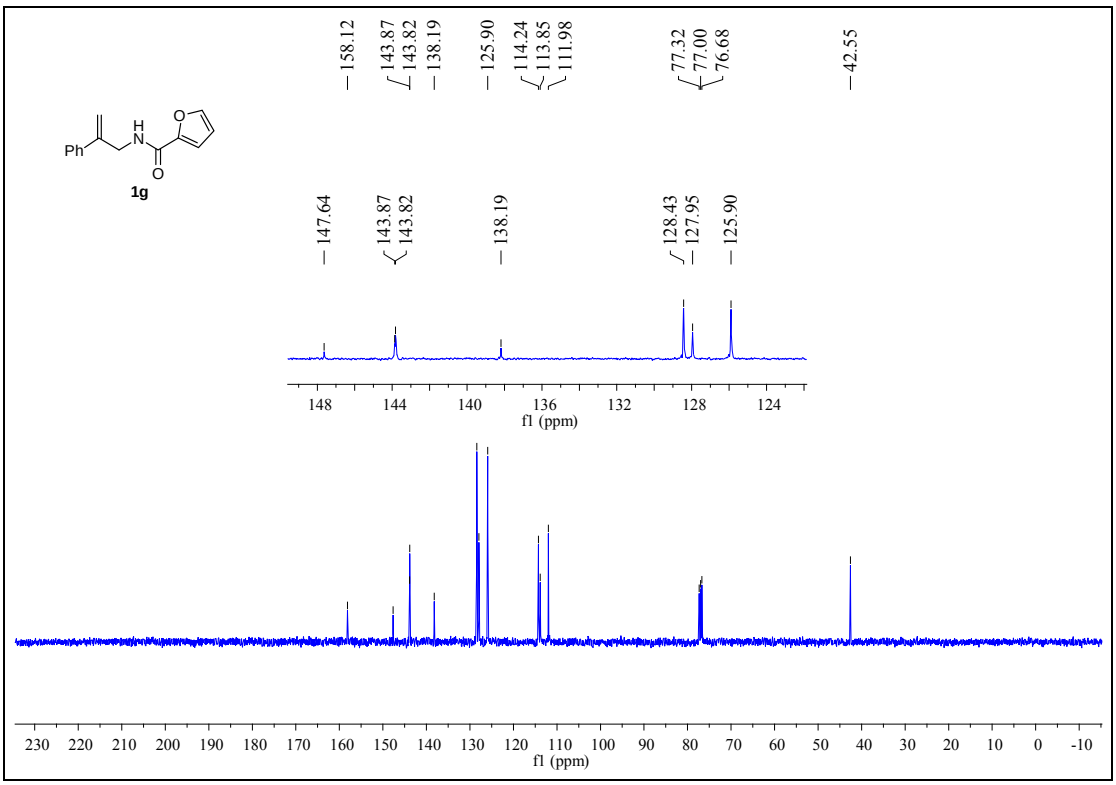
2.03
1.08
1.05
1.10
0.99
1.04
1.03
2.04
fl (ppm)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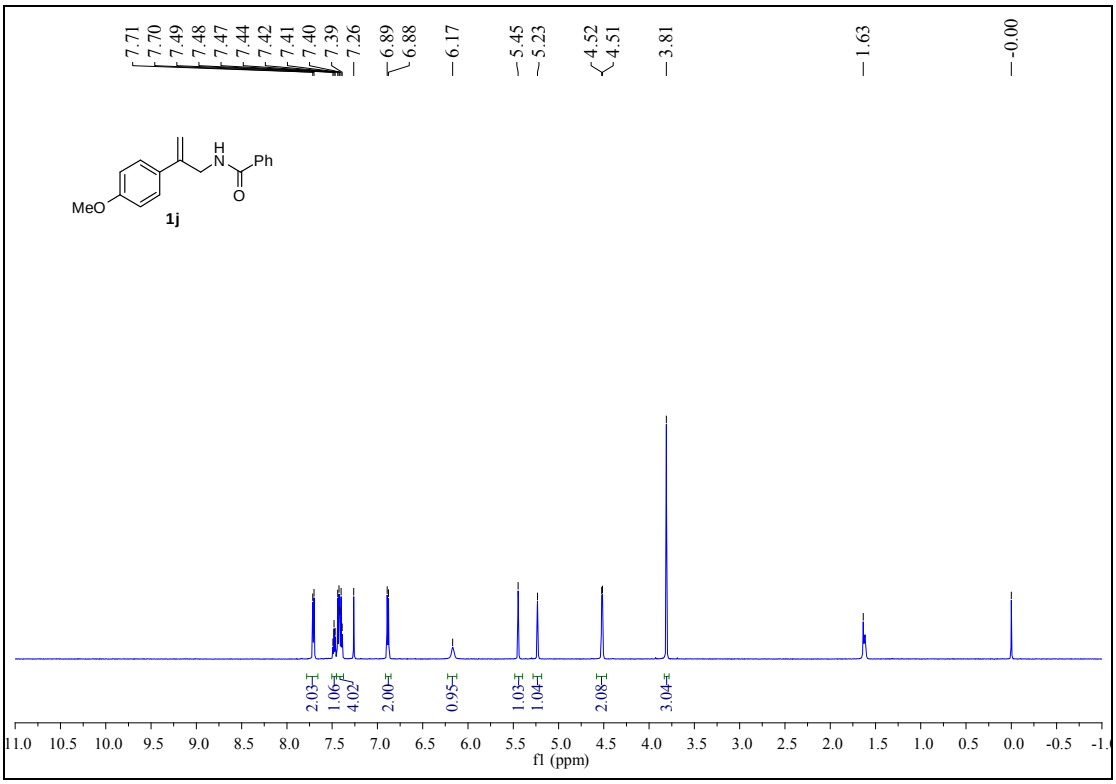
fl (ppm)
fl (ppm)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4.51
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1.63
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H
N
Ph
O
1j
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1.06
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2.00
0.95
1.03
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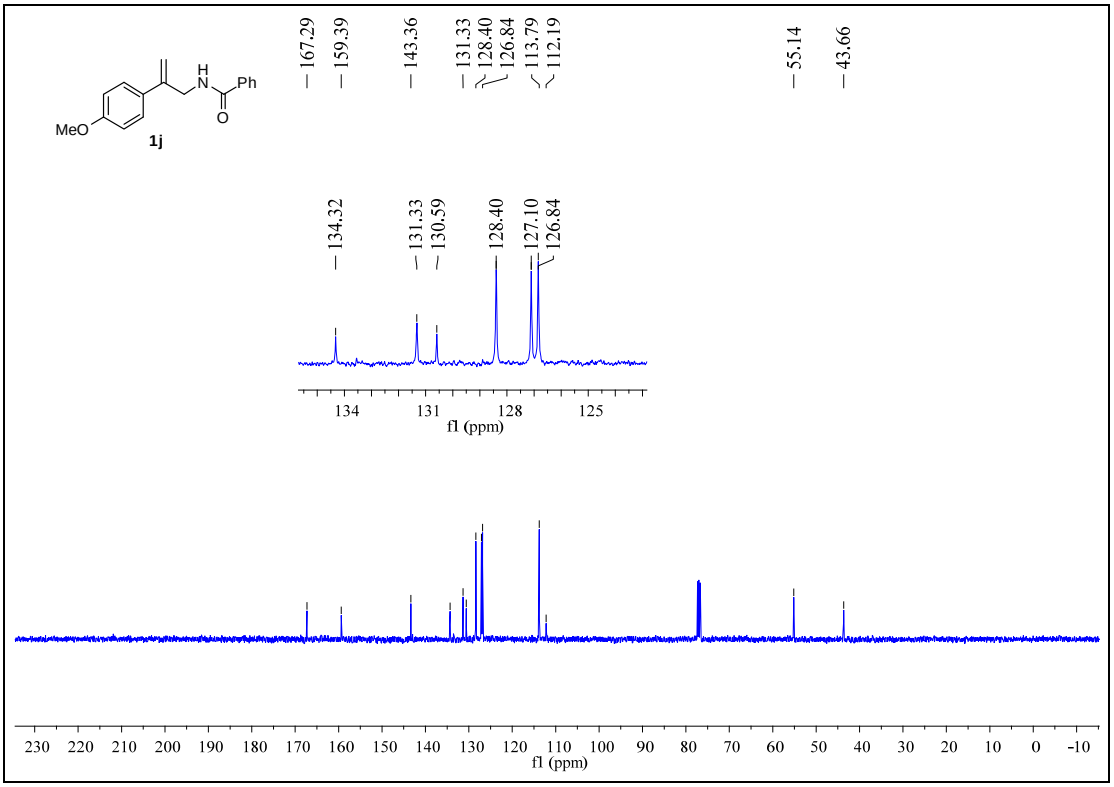
3.04
fl (ppm)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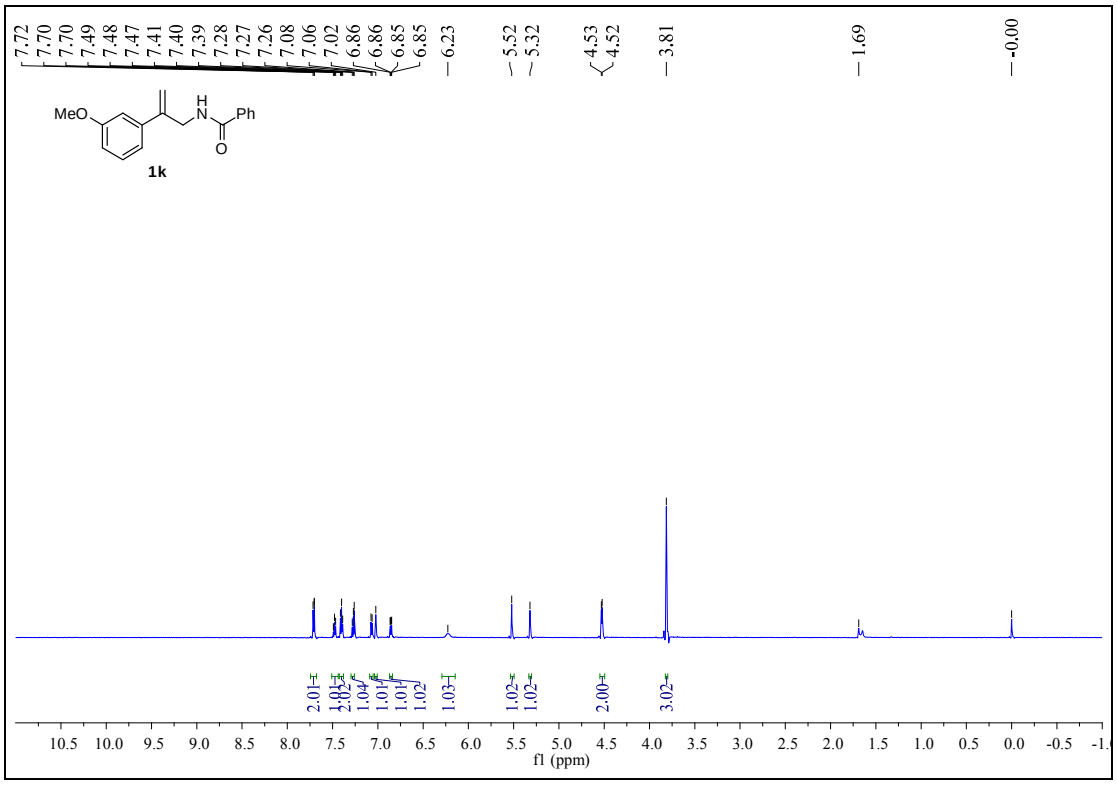
127.10
126.84
fl (ppm)
fl (ppm)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N
Ph
O
1k
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2.01
2.02
1.04
1.01
1.01
1.02
1.03
1.02
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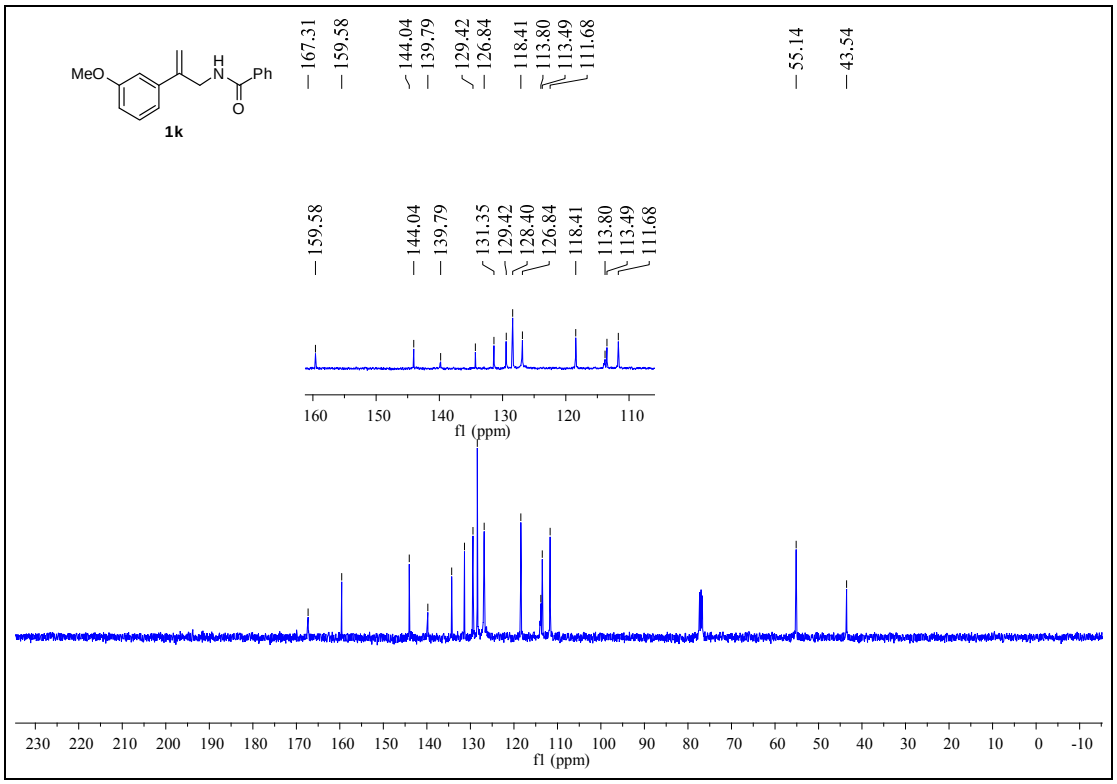
3.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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N
Ph
O
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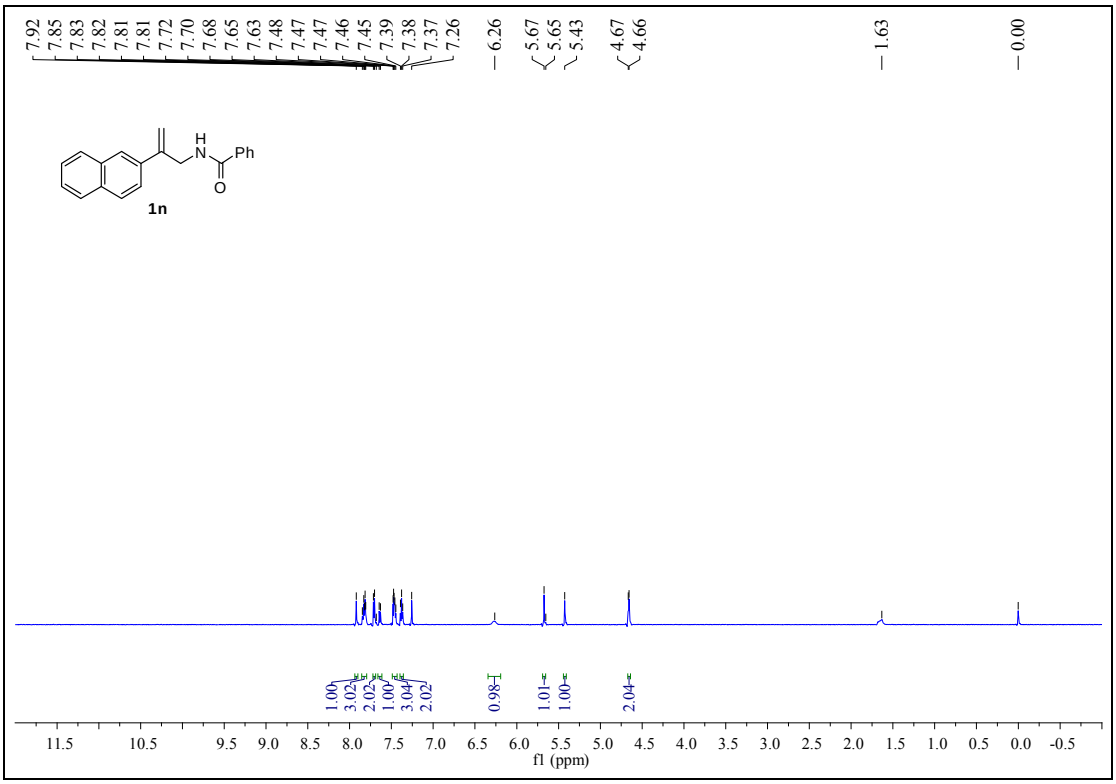
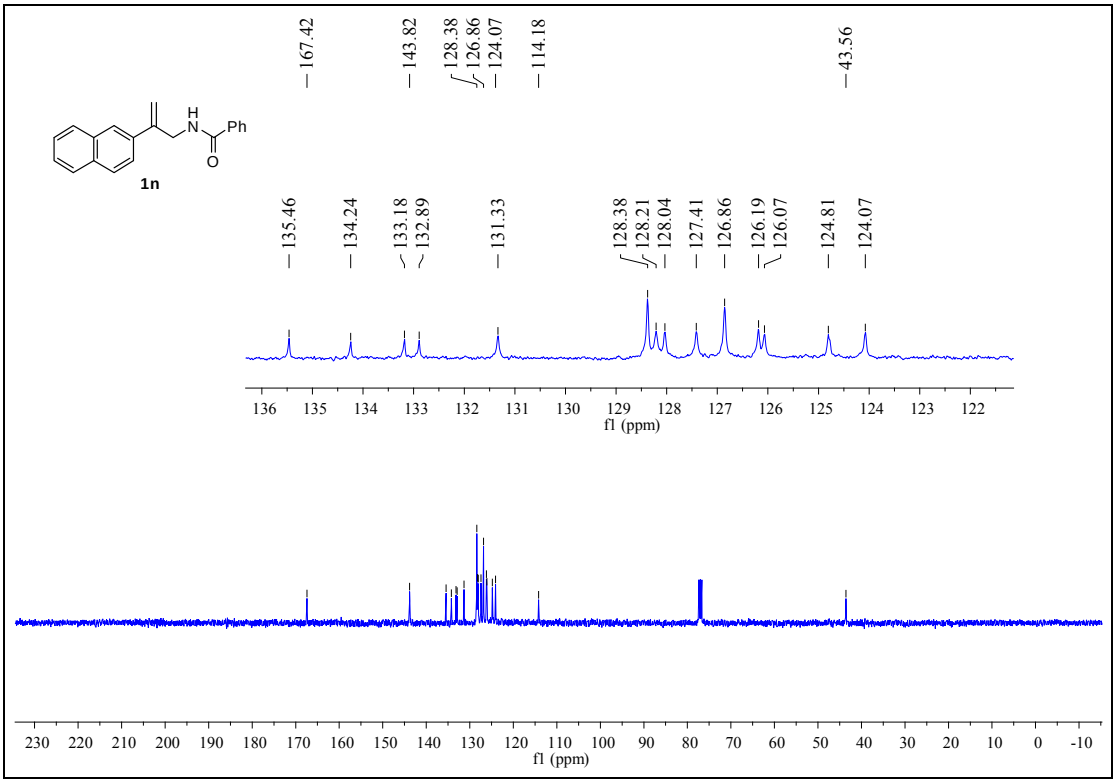
128.40
126.84
118.41
113.80
113.49
111.68
160 150 140 130 120 110
f1 (ppm)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.92
7.85
7.83
7.82
7.81
7.81
7.72
7.70
7.68
7.65
7.63
7.48
7.47
7.47
7.46
7.45
7.39
7.38
7.37
7.26
6.26
5.67
5.65
5.43
4.67
4.66
1.63
0.00
H
N
Ph
O
1n
1.00
3.02
2.02
1.00
3.04
2.02
0.98
1.01
1.00
2.04
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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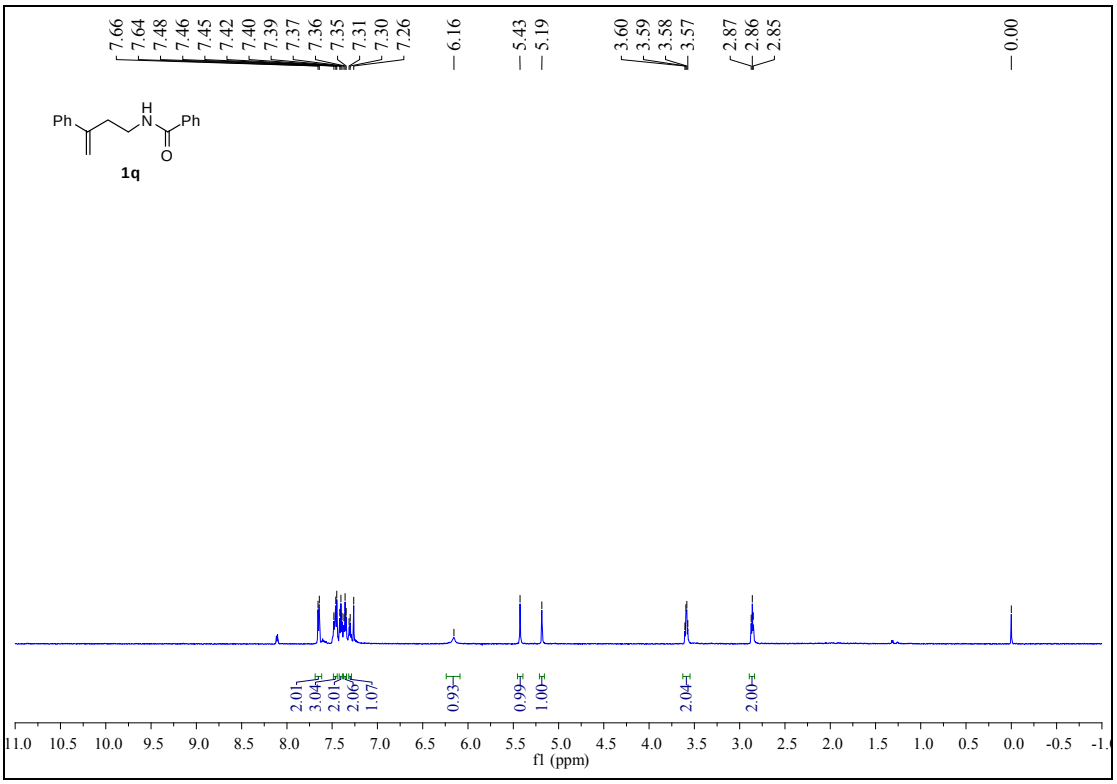
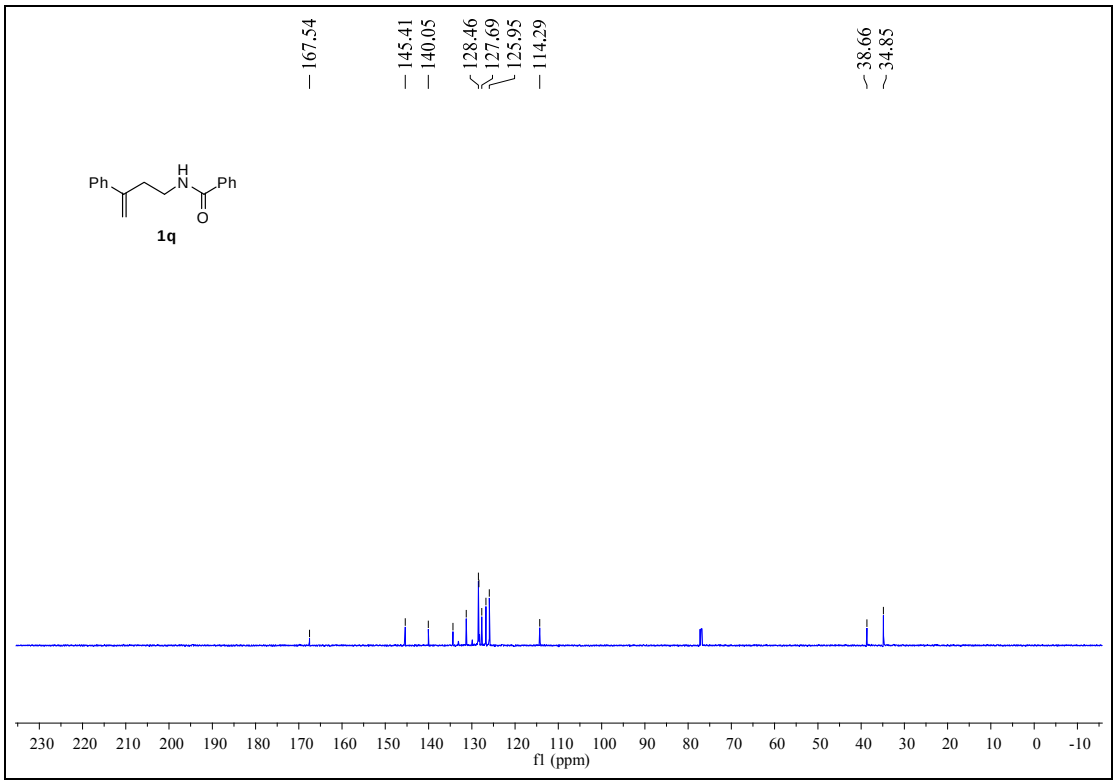
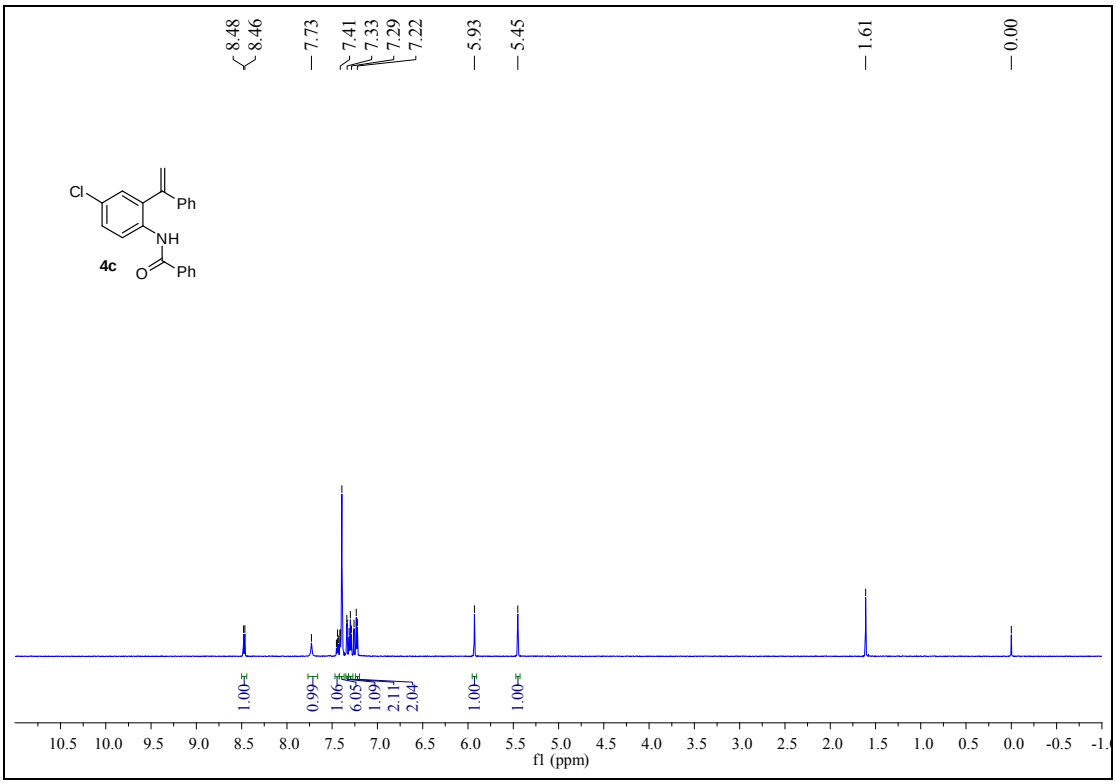
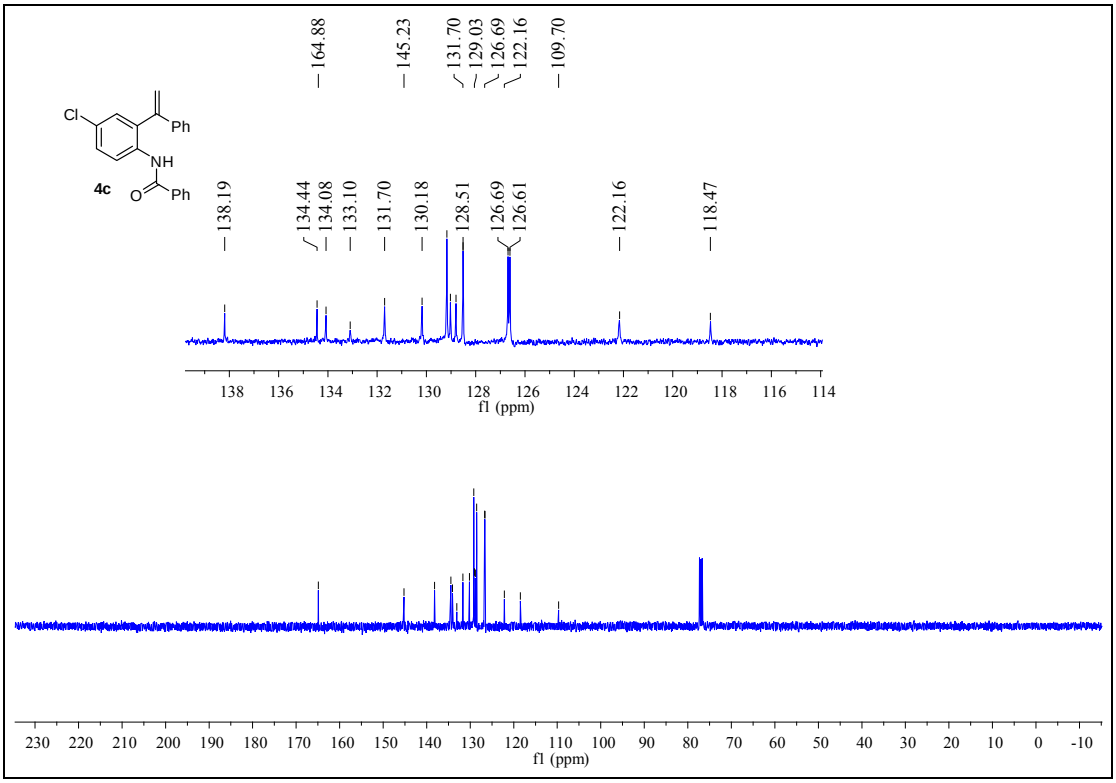
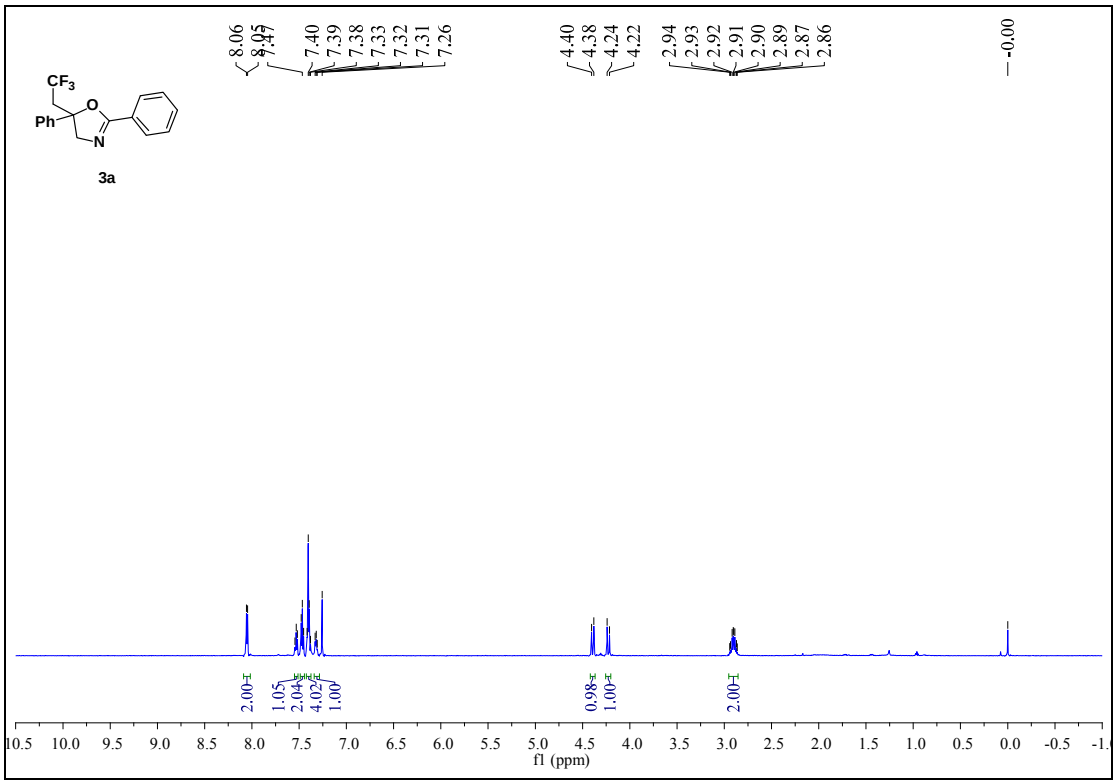
143.82
128.38
126.86
124.07
114.18
43.56
H
N
Ph
O
1n
135.46
134.24
133.18
132.89
131.33
128.38
128.21
128.04
127.41
126.86
126.19
126.07
124.81
124.07
136
135
134
133
132
131
130
129
128
127
126
125
124
123
122
f1 (ppm)
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.66
7.64
7.48
7.46
7.45
7.42
7.40
7.39
7.37
7.36
7.35
7.31
7.30
7.26
6.16
5.43
5.19
3.60
3.59
3.58
3.57
2.87
2.86
2.85
0.00
Ph
H
N
Ph
O
1q
2.01
3.04
2.01
2.06
1.07
0.93
0.99
1.00
2.04
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


167.54
145.41
140.05
128.46
127.69
125.95
114.29
38.66
34.85
Ph
H
N
Ph
O
1q
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.48
8.46
7.73
7.41
7.33
7.29
7.22
5.93
5.45
1.61
0.00
Cl
Ph
NH
O
Ph
4c
1.00
0.99
1.06
6.05
1.09
2.11
2.04
1.00
1.00
fl (ppm)


164.88
145.23
131.70
129.03
126.69
122.16
109.70
Cl
Ph
NH
O
Ph
4c
138.19
134.44
134.08
133.10
131.70
130.18
128.51
126.69
126.61
122.16
118.47
fl (ppm)
fl (ppm)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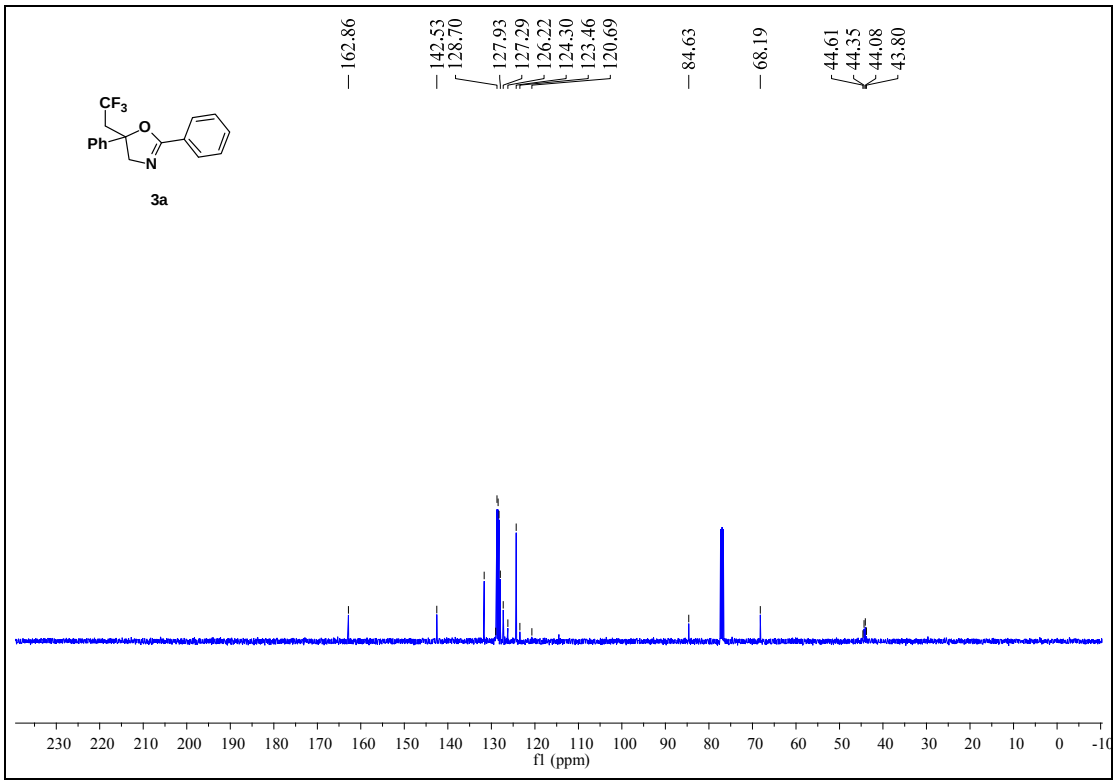
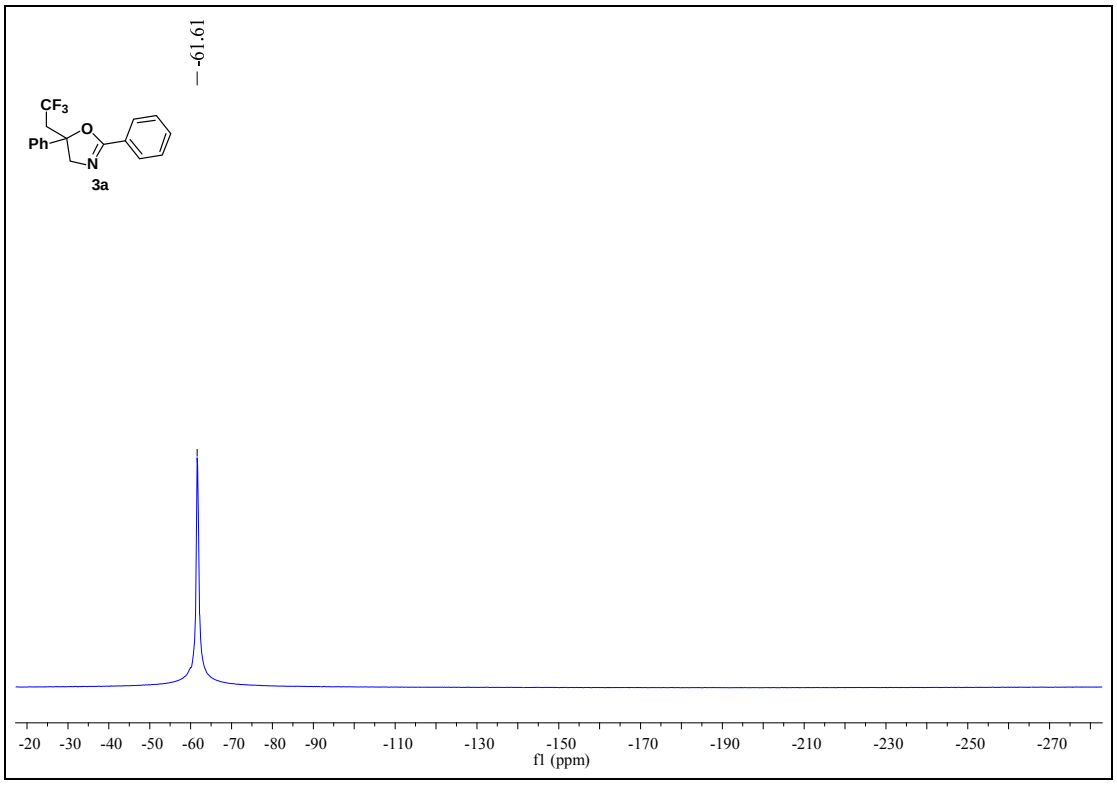
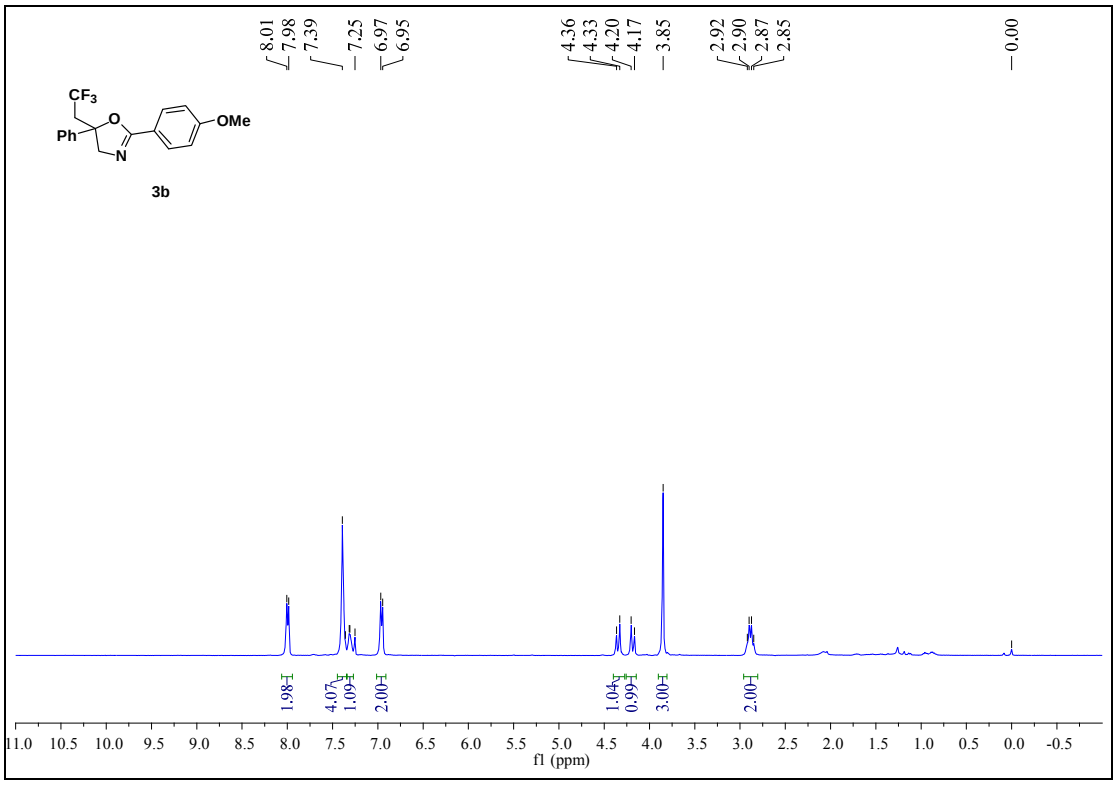
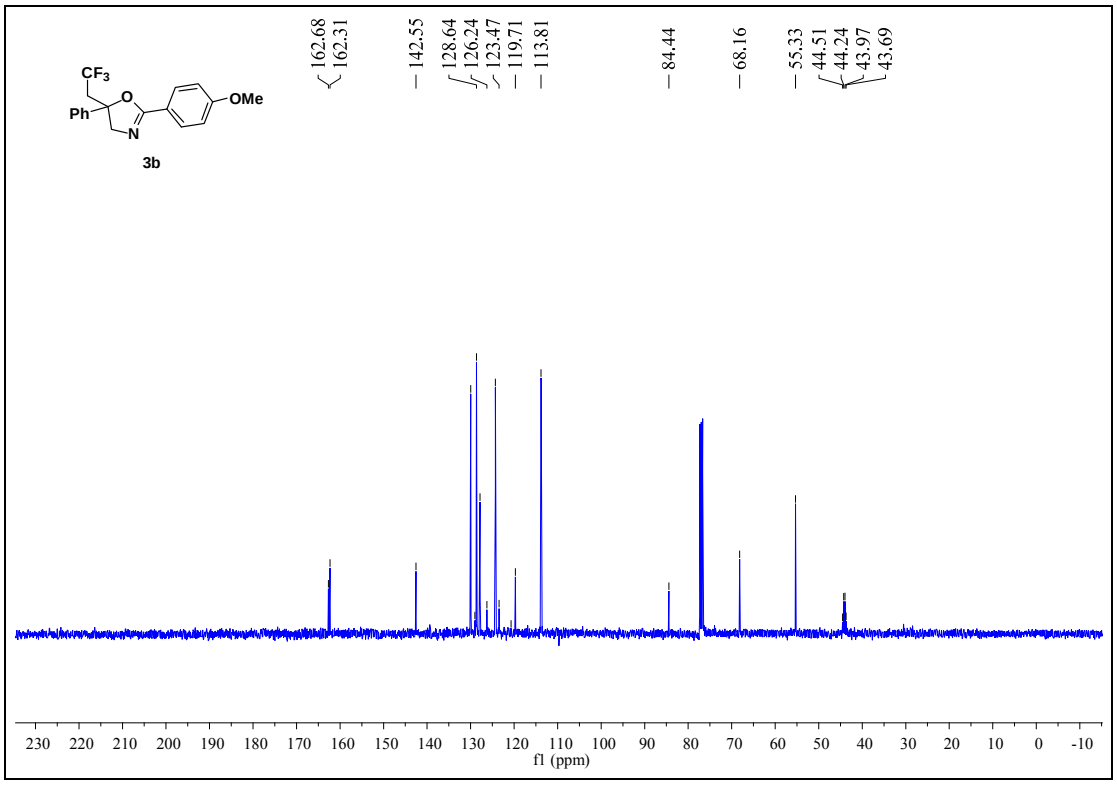
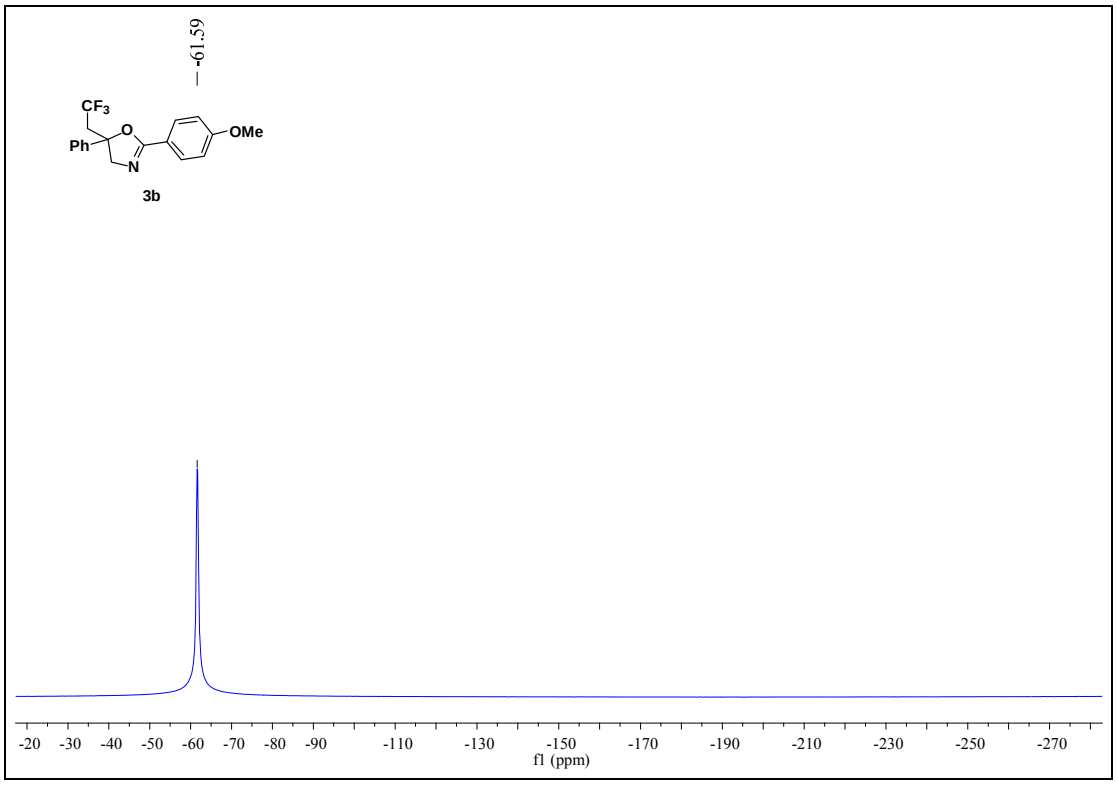
8.05
7.47
7.40
7.39
7.38
7.33
7.32
7.31
7.26
4.40
4.38
4.24
4.22
2.94
2.93
2.92
2.91
2.90
2.89
2.87
2.86
-0.00
CF3
Ph
O
N
3a
2.00
1.05
2.04
4.02
1.00
0.98
1.00
2.00
fl (ppm)

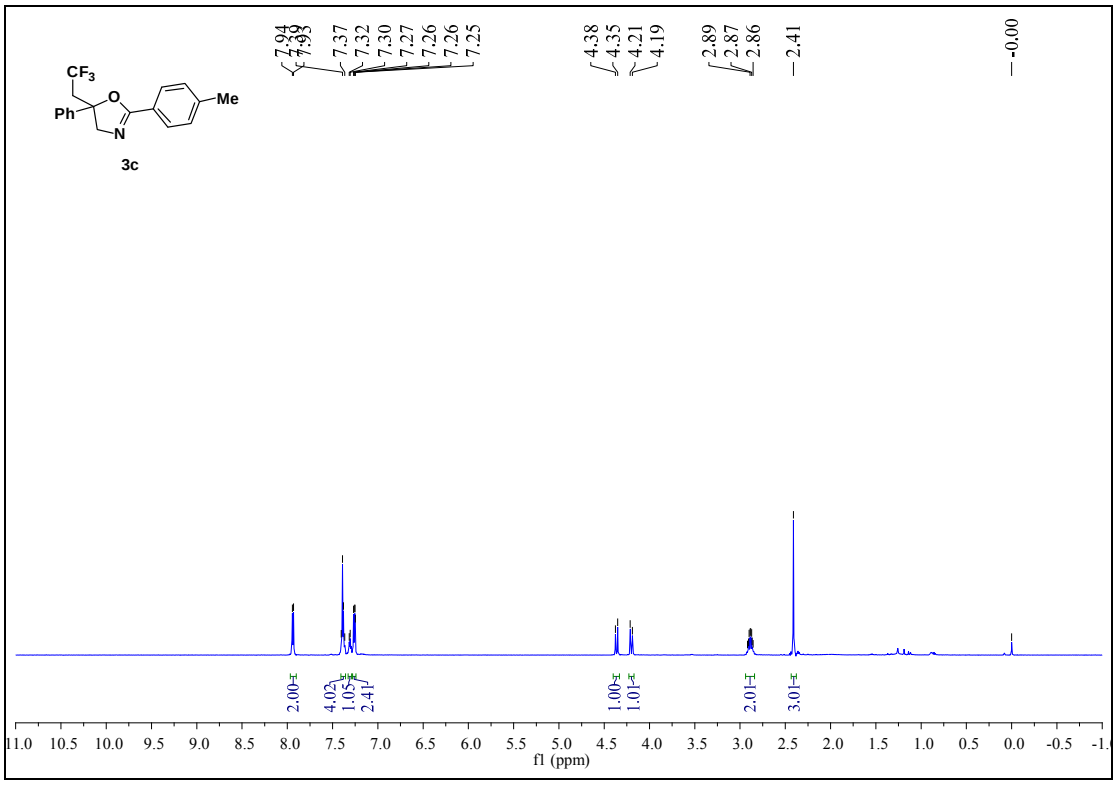

162.86
142.53
128.70
127.93
127.29
126.22
124.30
123.46
120.69
84.63
68.19
44.61
44.35
44.08
43.80
CF3
Ph
O
N
3a
fl (ppm)

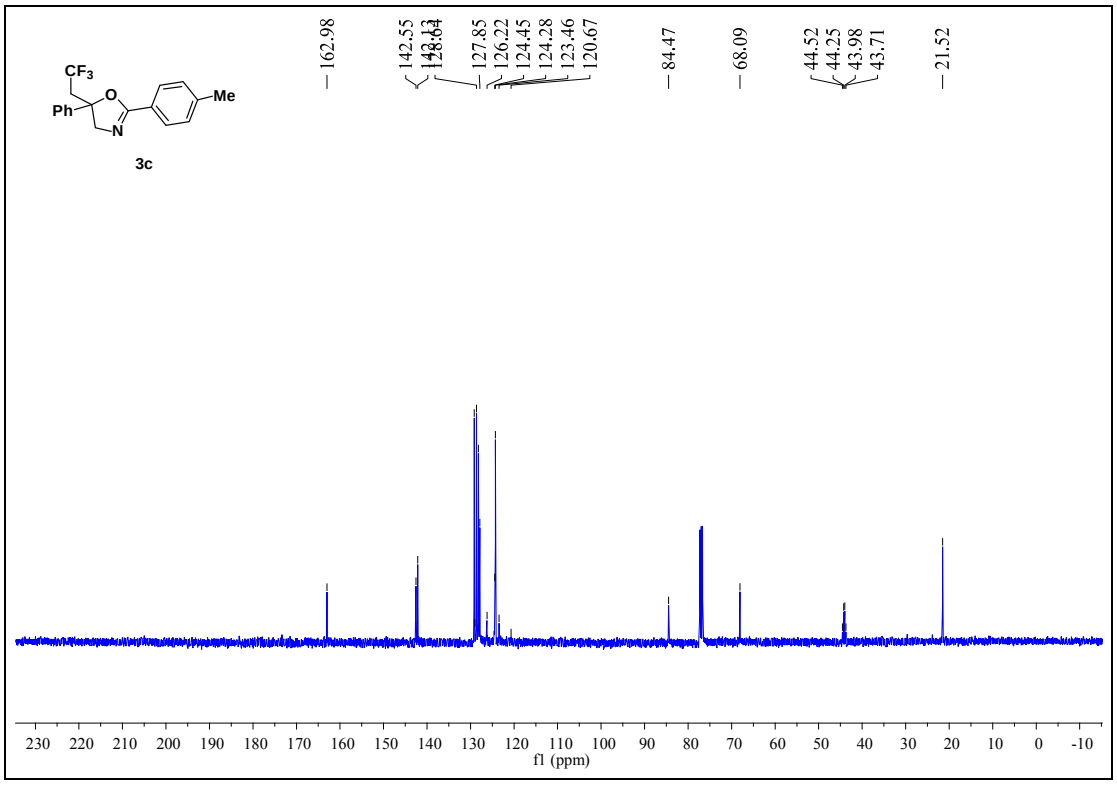

-61.61
CF3
Ph
O
N
3a
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)

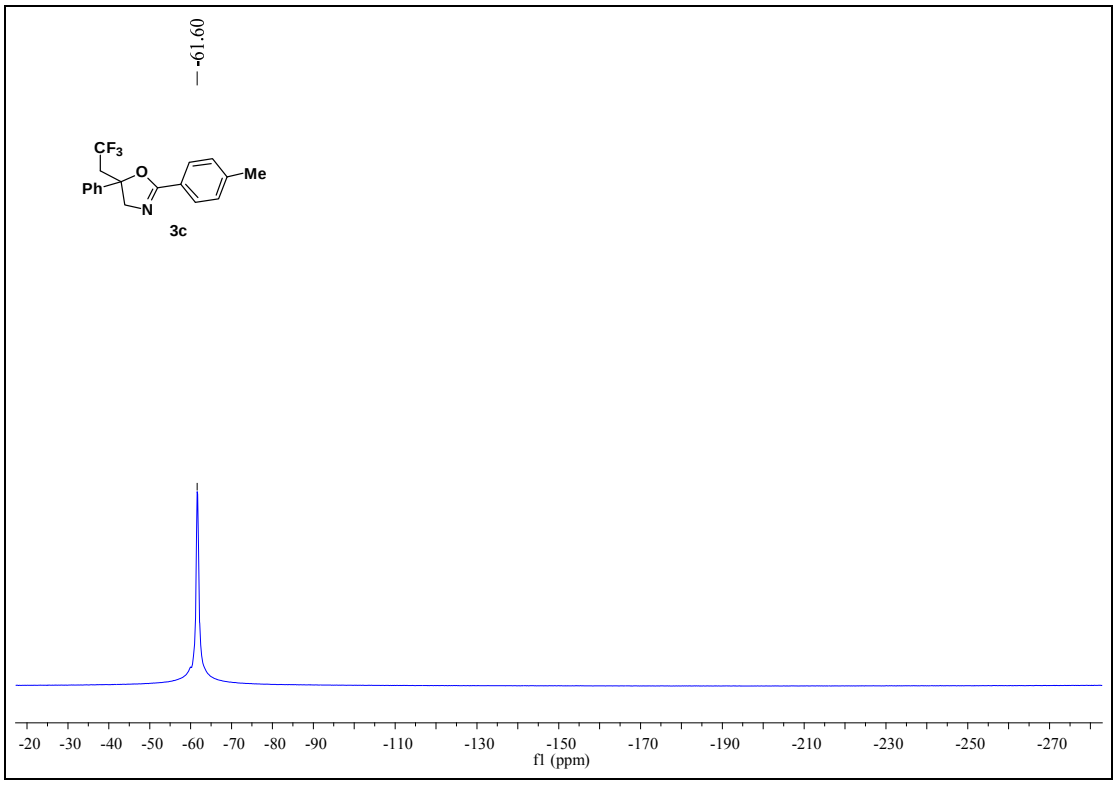

8.01
7.98
7.39
7.25
6.97
6.95
4.36
4.33
4.20
4.17
3.85
2.92
2.90
2.87
2.85
0.00
CF3
Ph
O
N
OMe
3b
1.98
4.07
1.09
2.00
1.04
0.99
3.00
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

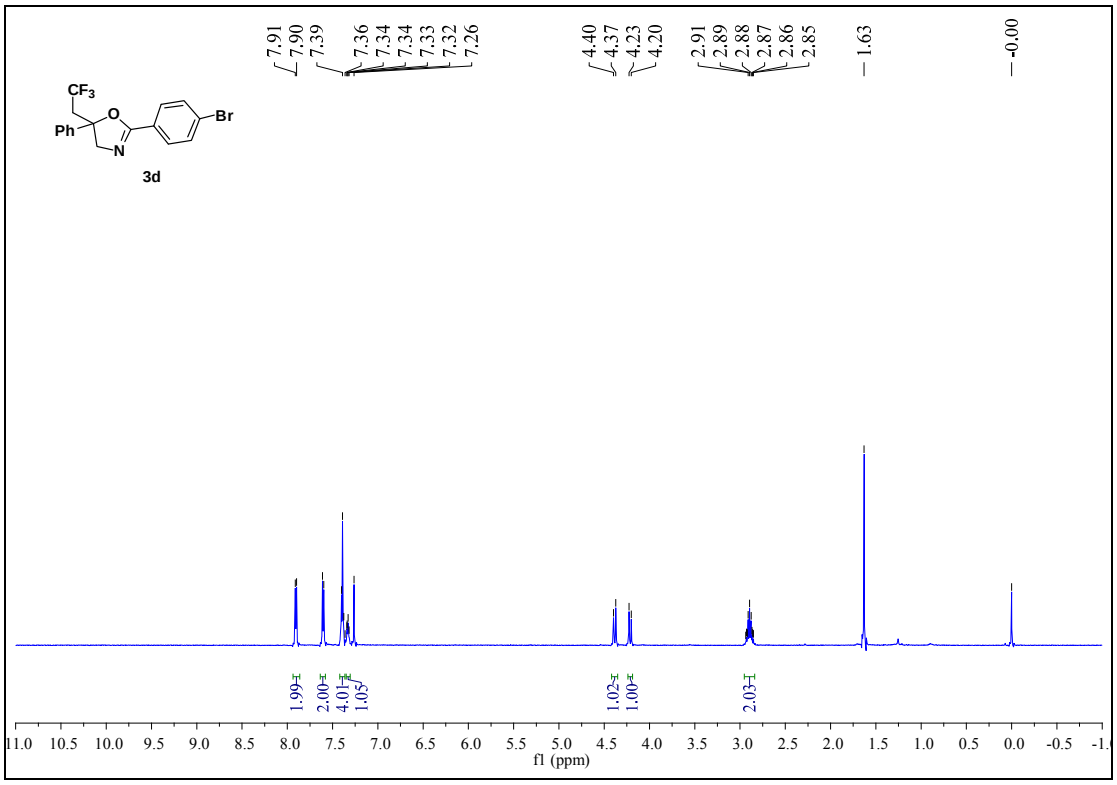

CF3
Ph
O
N
OMe
3b
162.68
162.31
142.55
128.64
126.24
123.47
119.71
113.81
84.44
68.16
55.33
44.51
44.24
43.97
43.69
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

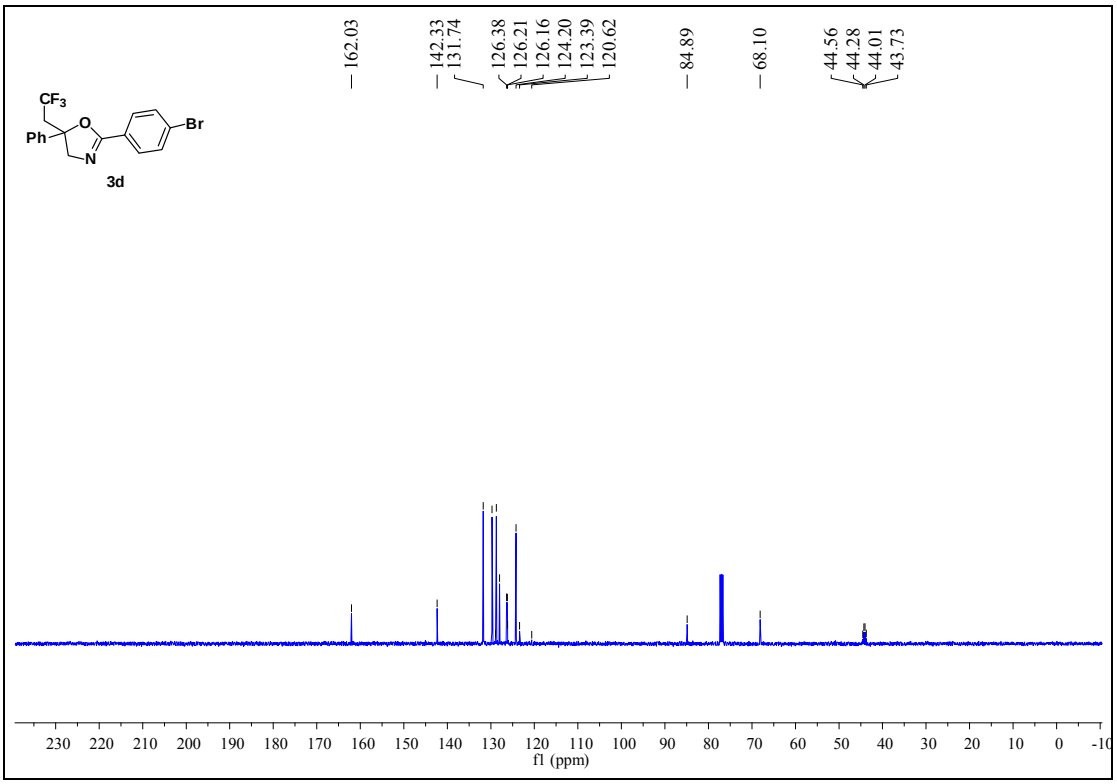

-61.59
CF3
Ph
O
N
OMe
3b
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)

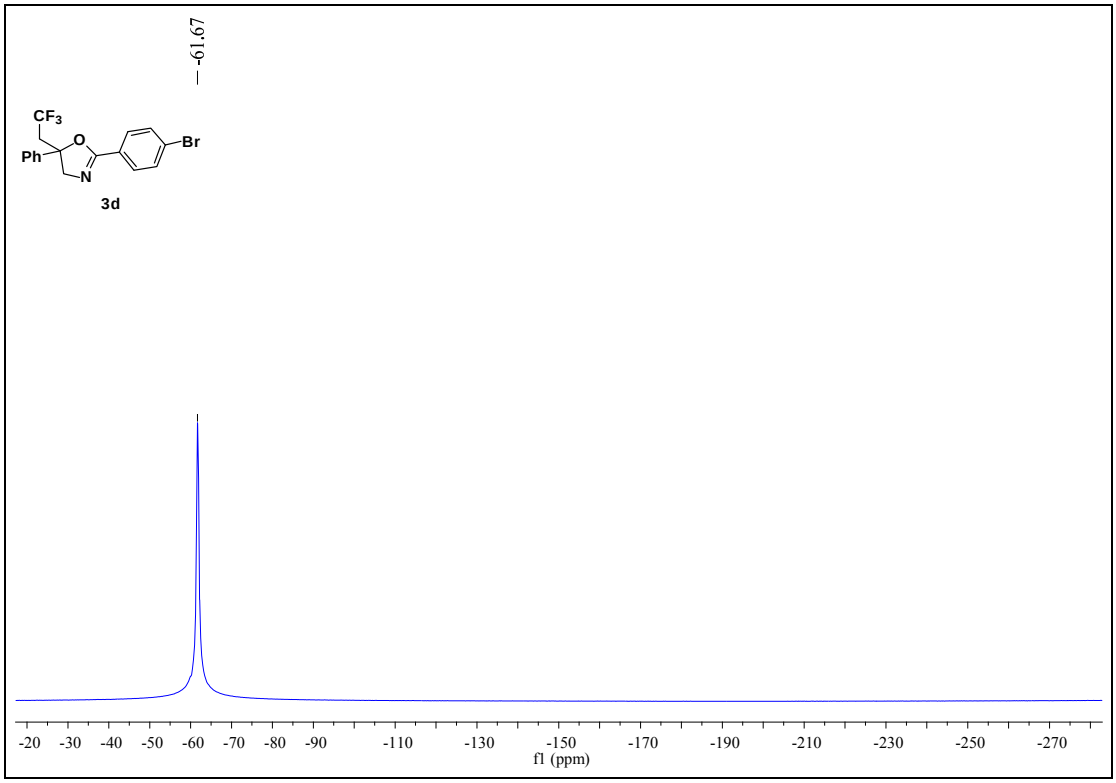

CF3
Ph
O
N
Me
3c
7.94
7.93
7.37
7.32
7.30
7.27
7.26
7.26
7.25
4.38
4.35
4.21
4.19
2.89
2.87
2.86
2.41
0.00
2.00
4.02
1.05
2.41
1.00
1.01
2.01
3.01
fl (ppm)

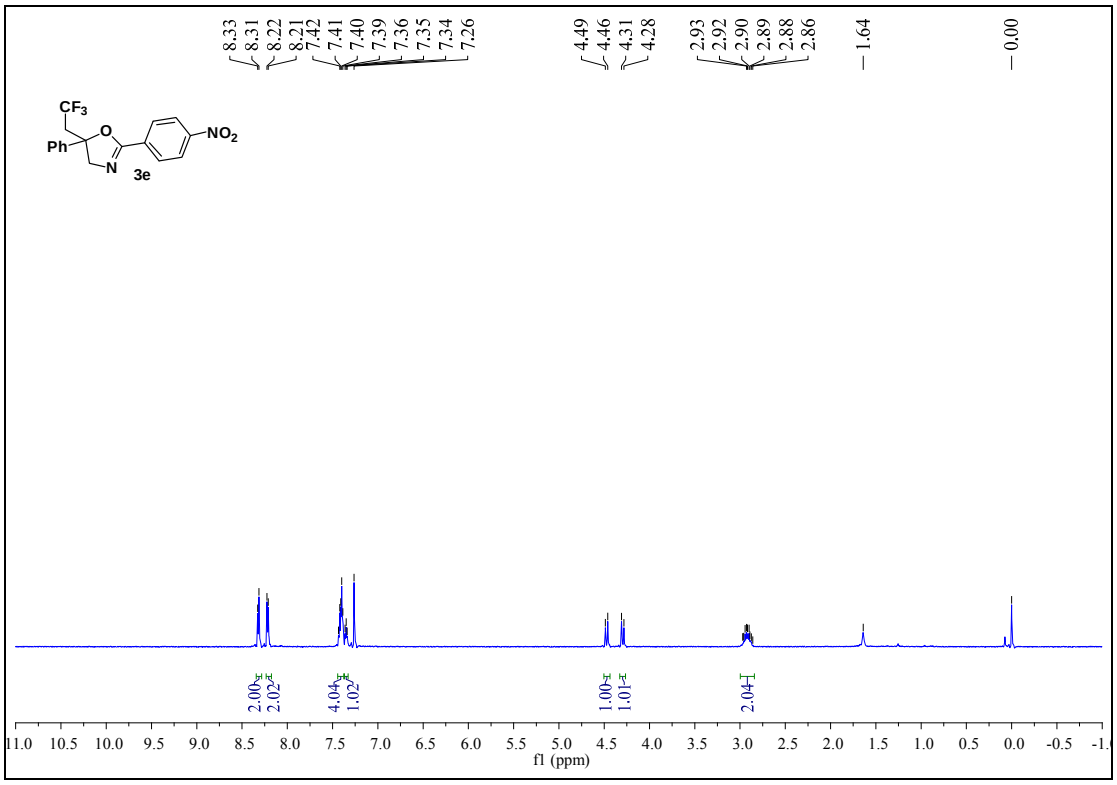

CF3
Ph
O
N
Me
3c
162.98
142.55
128.64
127.85
126.22
124.45
124.28
123.46
120.67
84.47
68.09
44.52
44.25
43.98
43.71
21.52
fl (ppm)

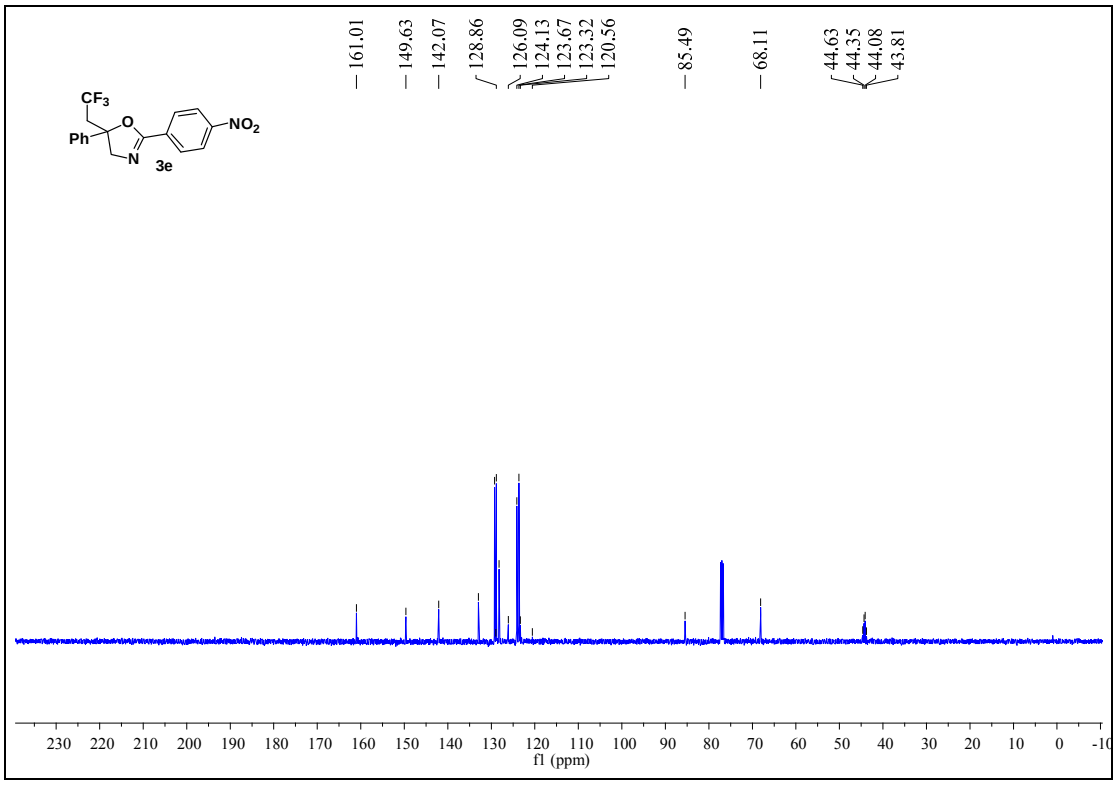

-61.60
CF3
Ph
O
N
Me
3c
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)

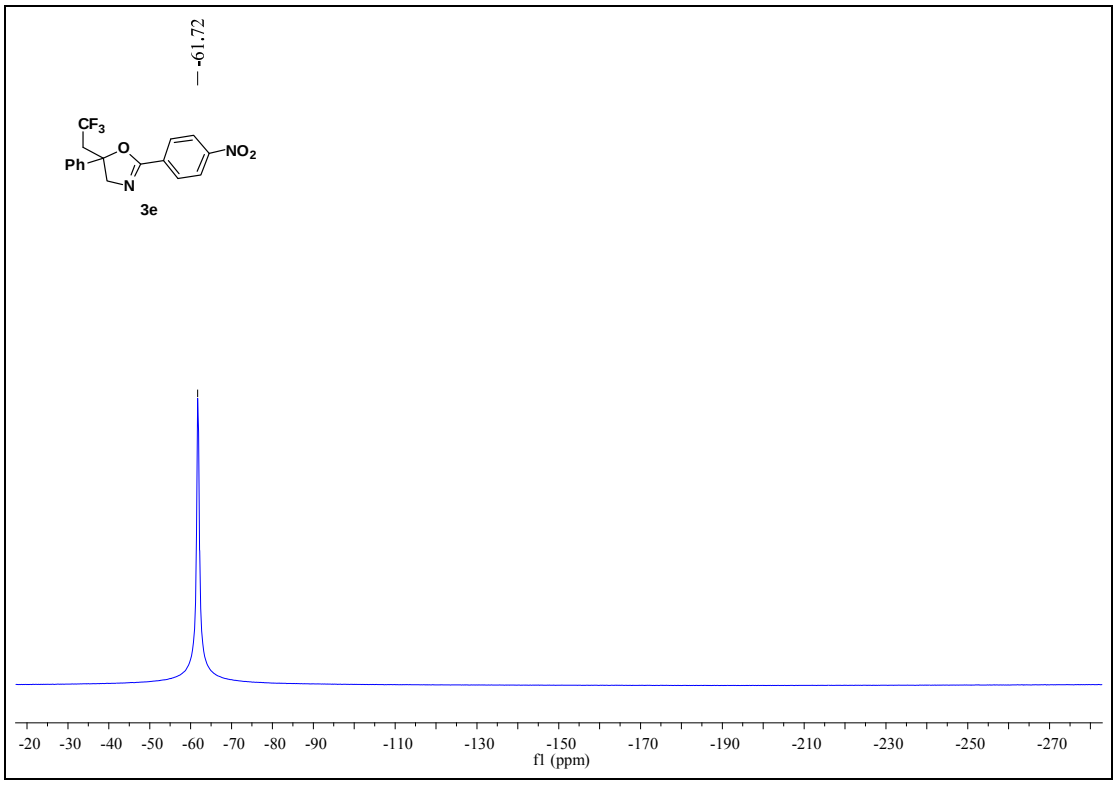

7.91
7.90
7.39
7.36
7.34
7.34
7.33
7.32
7.26
4.40
4.37
4.23
4.20
2.91
2.89
2.88
2.87
2.86
2.85
1.63
0.00
CF3
Ph
O
N
Br
3d
1.99
2.00
4.01
1.05
1.02
1.00
2.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

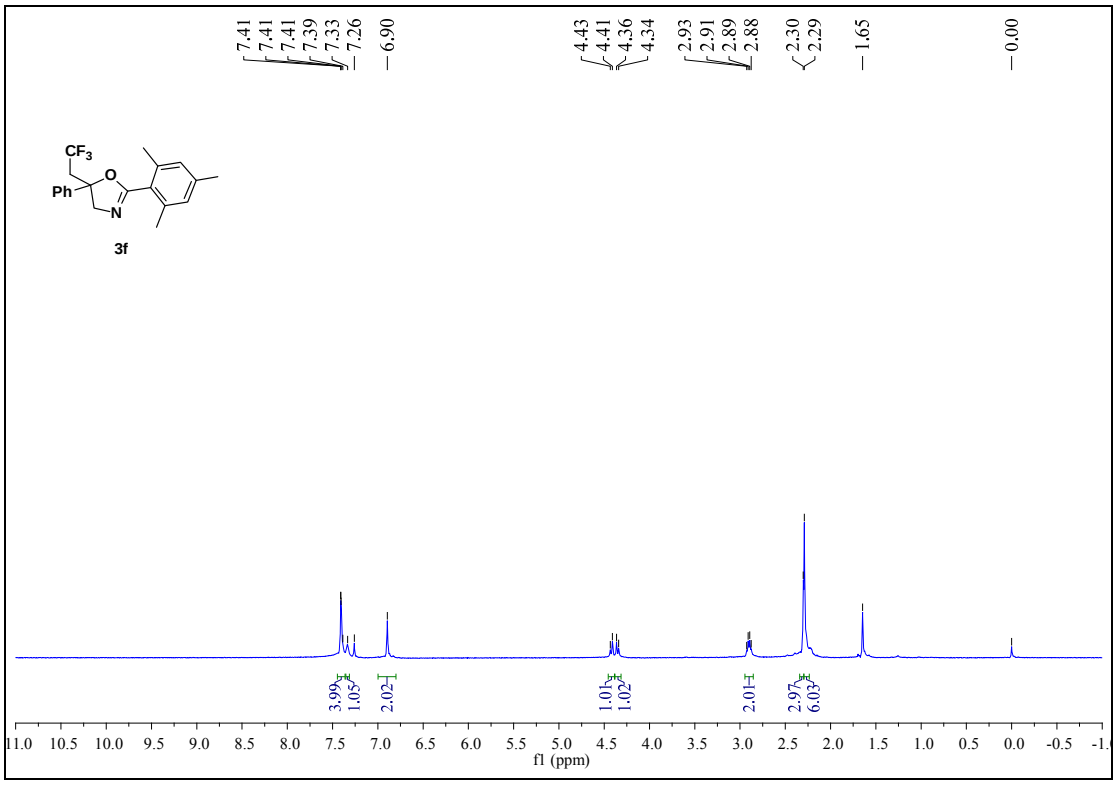

162.03
142.33
131.74
126.38
126.21
126.16
124.20
123.39
120.62
84.89
68.10
44.56
44.28
44.01
43.73
CF3
Ph
O
N
Br
3d
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-61.67
CF3
Ph
O
N
Br
3d
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)


8.33
8.31
8.22
8.21
7.42
7.41
7.40
7.39
7.36
7.35
7.34
7.26
4.49
4.46
4.31
4.28
2.93
2.92
2.90
2.89
2.88
2.86
1.64
0.00
CF3
Ph
O
N
NO2
3e
2.00
2.02
4.04
1.02
1.00
1.01
2.04
f1 (ppm)


161.01
149.63
142.07
128.86
126.09
124.13
123.67
123.32
120.56
85.49
68.11
44.63
44.35
44.08
43.81
CF3
Ph
O
N
NO2
3e
f1 (ppm)


-61.72
CF3
Ph
O
N
NO2
3e
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)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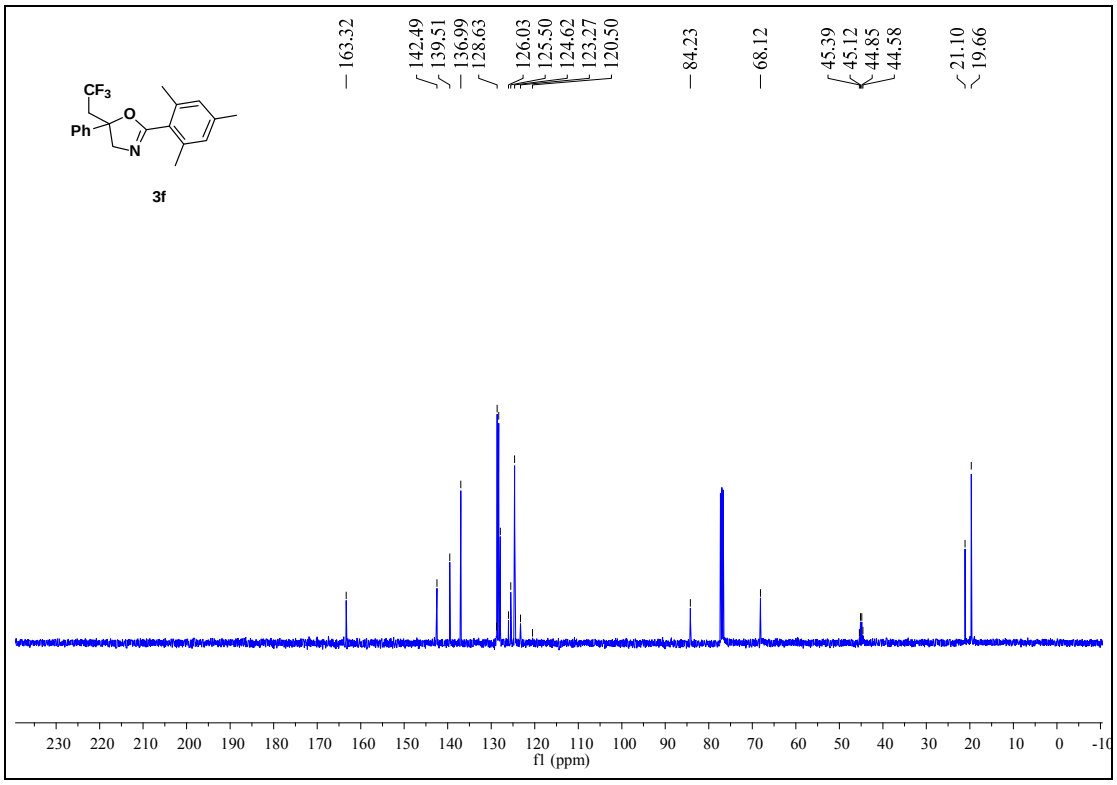
7.41
7.41
7.39
7.33
7.26
6.90
4.43
4.41
4.36
4.34
2.93
2.91
2.89
2.88
2.30
2.29
1.65
0.00
CF3
Ph
O
N
3f
3.99
1.05
2.02
1.01
1.02
2.01
2.97
6.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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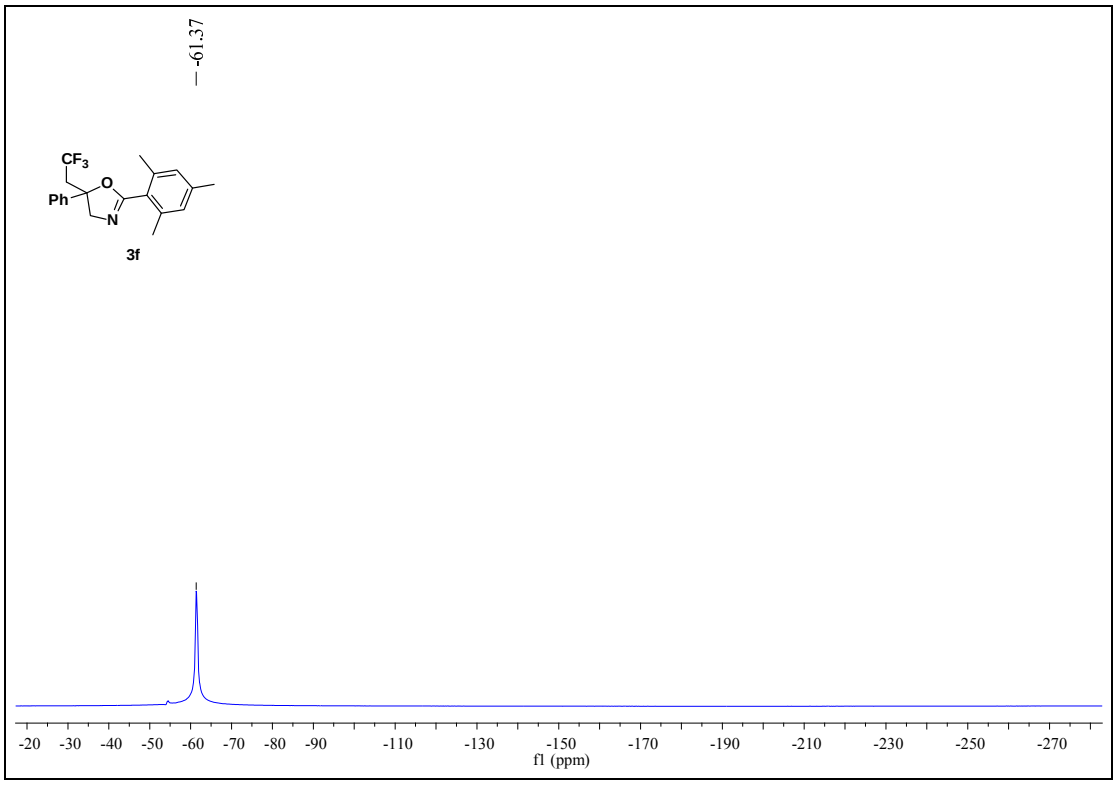
136.99
128.63
126.03
125.50
124.62
123.27
120.50
84.23
68.12
45.39
45.12
44.85
44.58
21.10
19.66
CF3
Ph
O
N
3f
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-61.37
CF3
Ph
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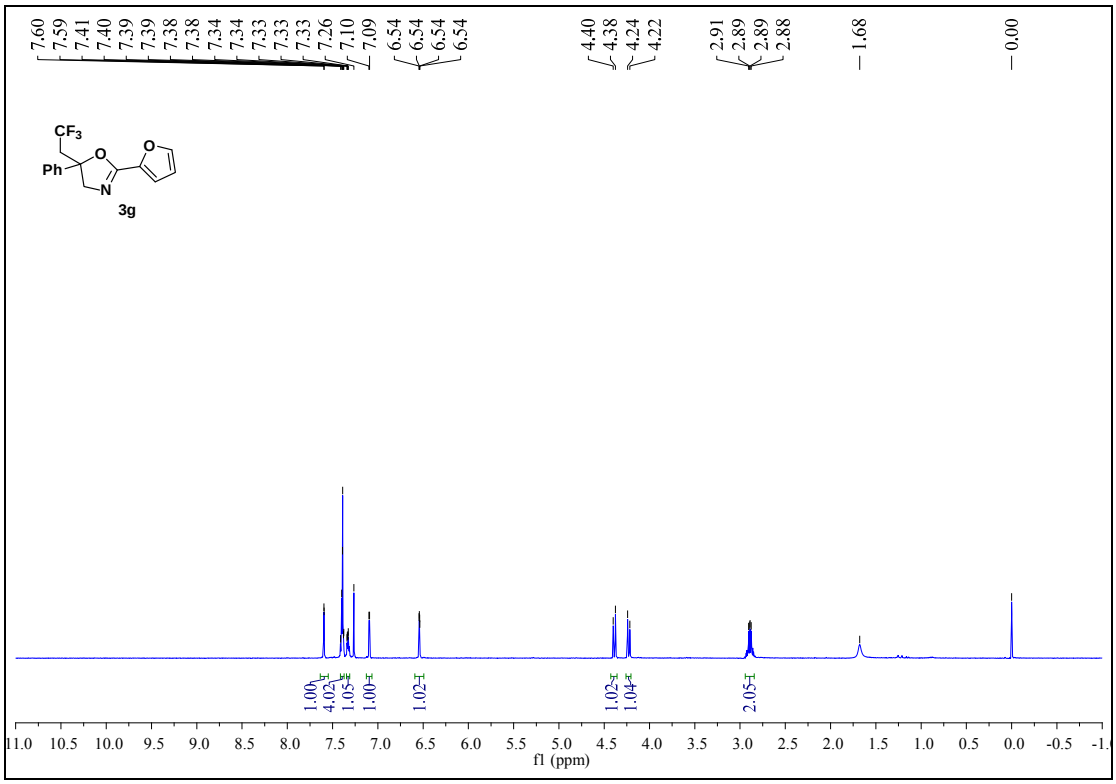
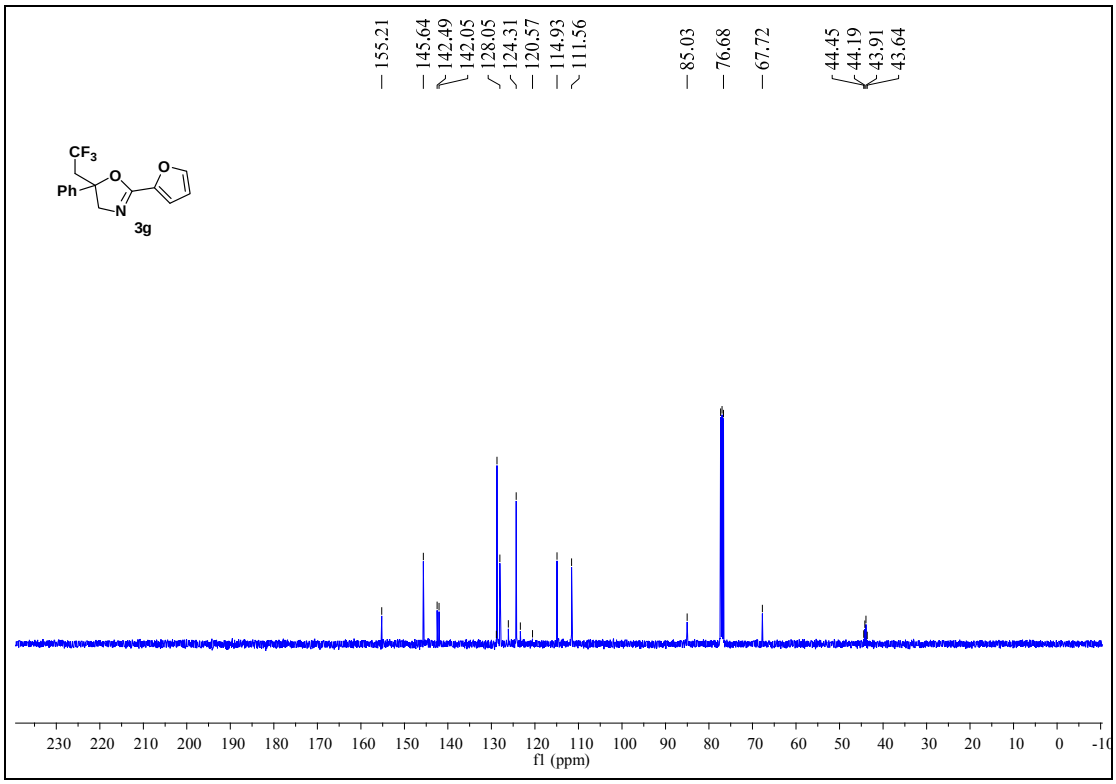
N
3f
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)


7.60
7.59
7.41
7.40
7.39
7.39
7.38
7.38
7.34
7.34
7.33
7.33
7.33
7.26
7.10
7.09
6.54
6.54
6.54
6.54
4.40
4.38
4.24
4.22
2.91
2.89
2.89
2.88
1.68
0.00
CF3
Ph
O
O
N
3g
1.00
4.02
1.05
1.00
1.02
1.02
1.04
2.05
f1 (ppm)


155.21
145.64
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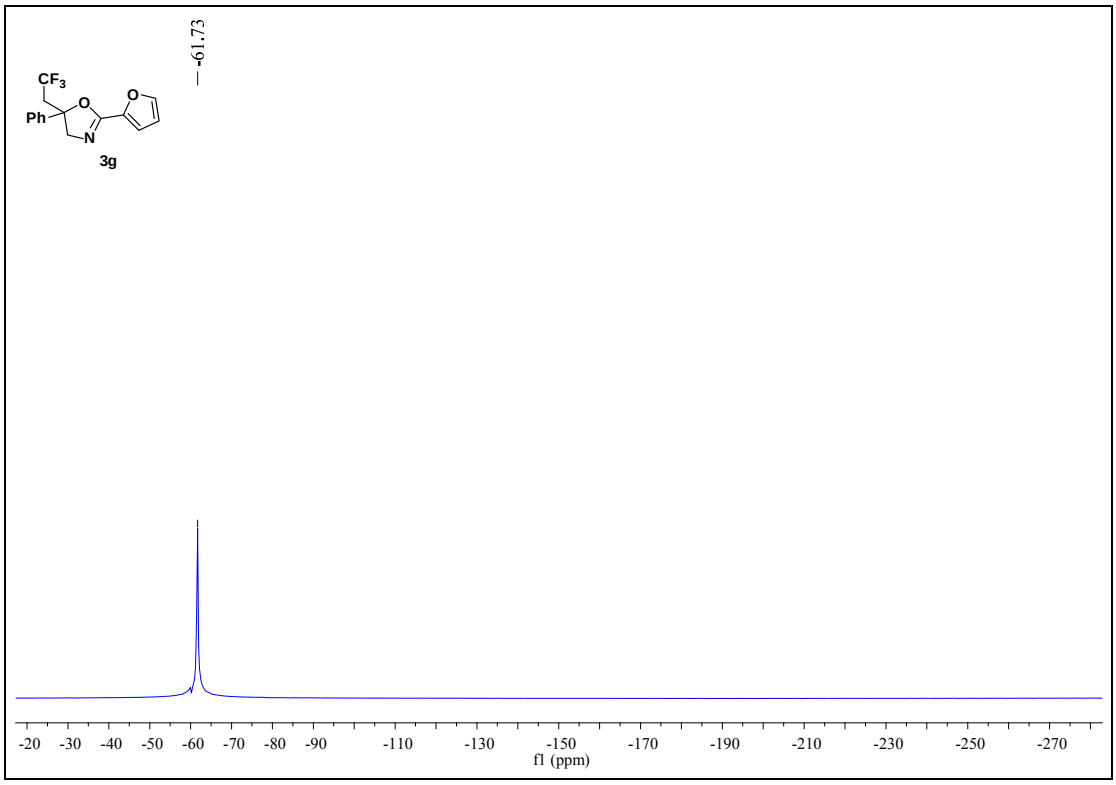
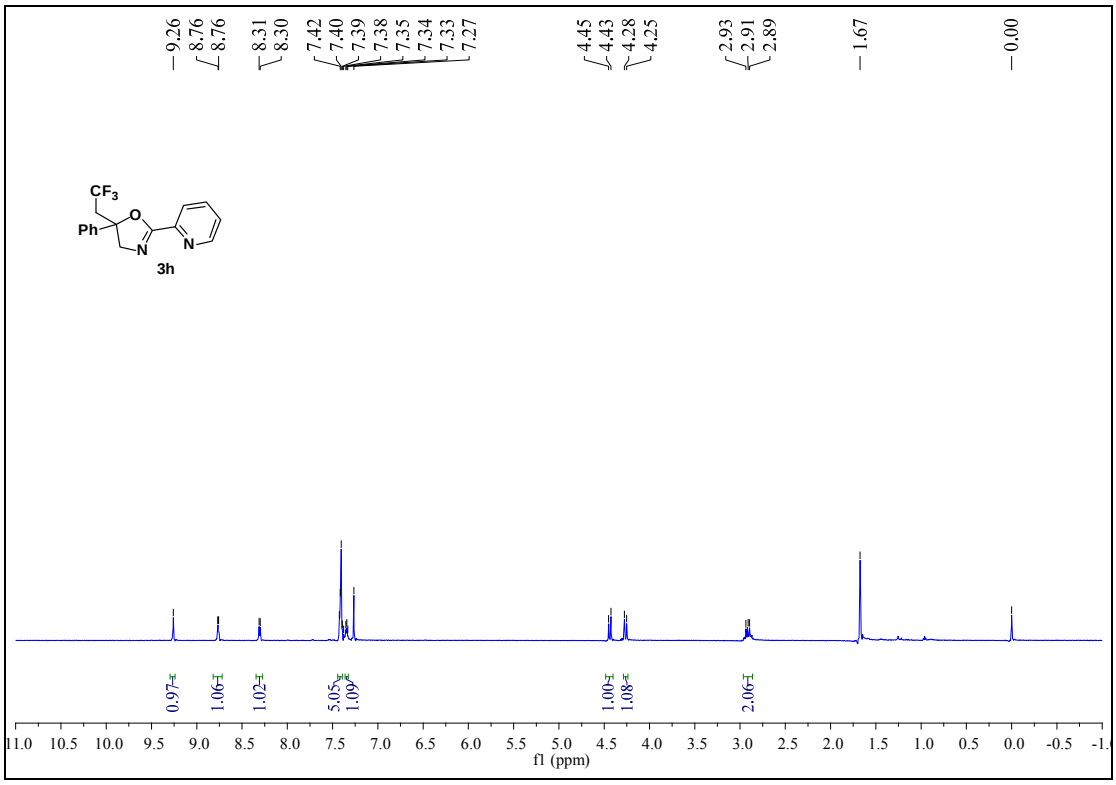
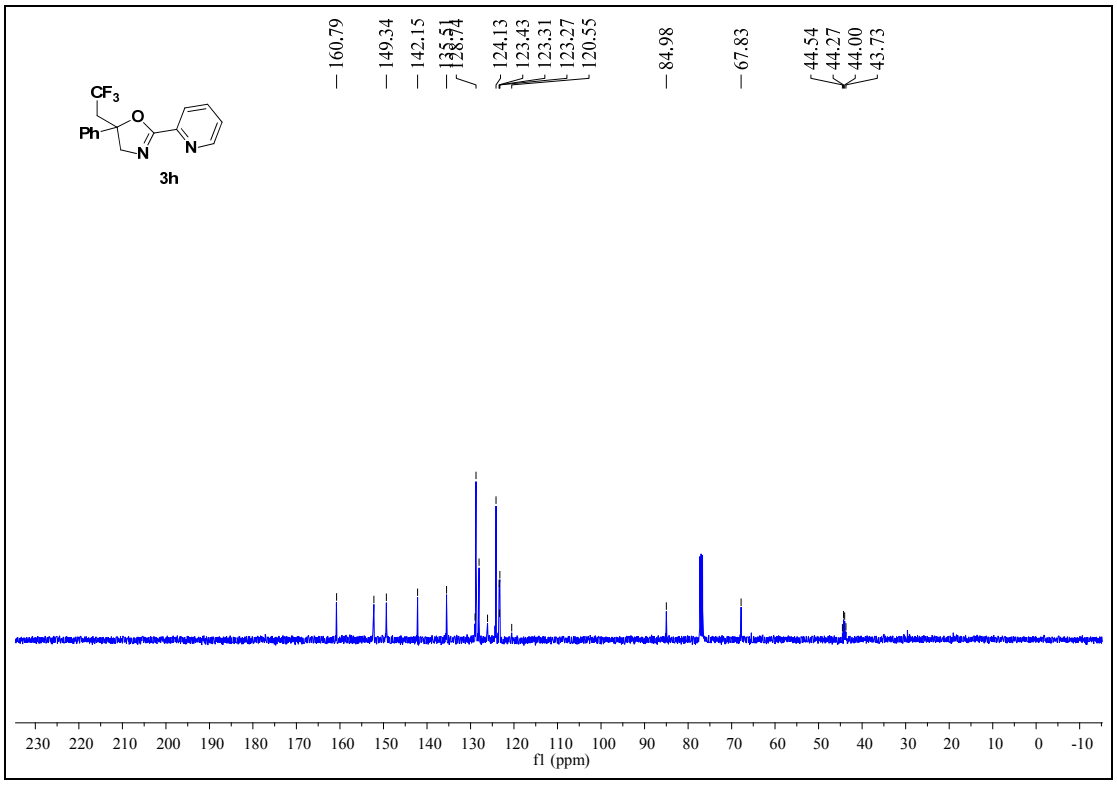
128.05
124.31
120.57
114.93
111.56
85.03
76.68
67.72
44.45
44.19
43.91
43.64
CF3
Ph
O
O
N
3g
f1 (ppm)


-61.73
CF3
Ph
O
O
N
3g
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)


9.26
8.76
8.76
8.31
8.30
7.42
7.40
7.39
7.38
7.35
7.34
7.33
7.27
4.45
4.43
4.28
4.25
2.93
2.91
2.89
1.67
0.00
CF3
Ph
O
N
N
3h
0.97
1.06
1.02
5.05
1.09
1.00
1.08
2.06
f1 (ppm)


160.79
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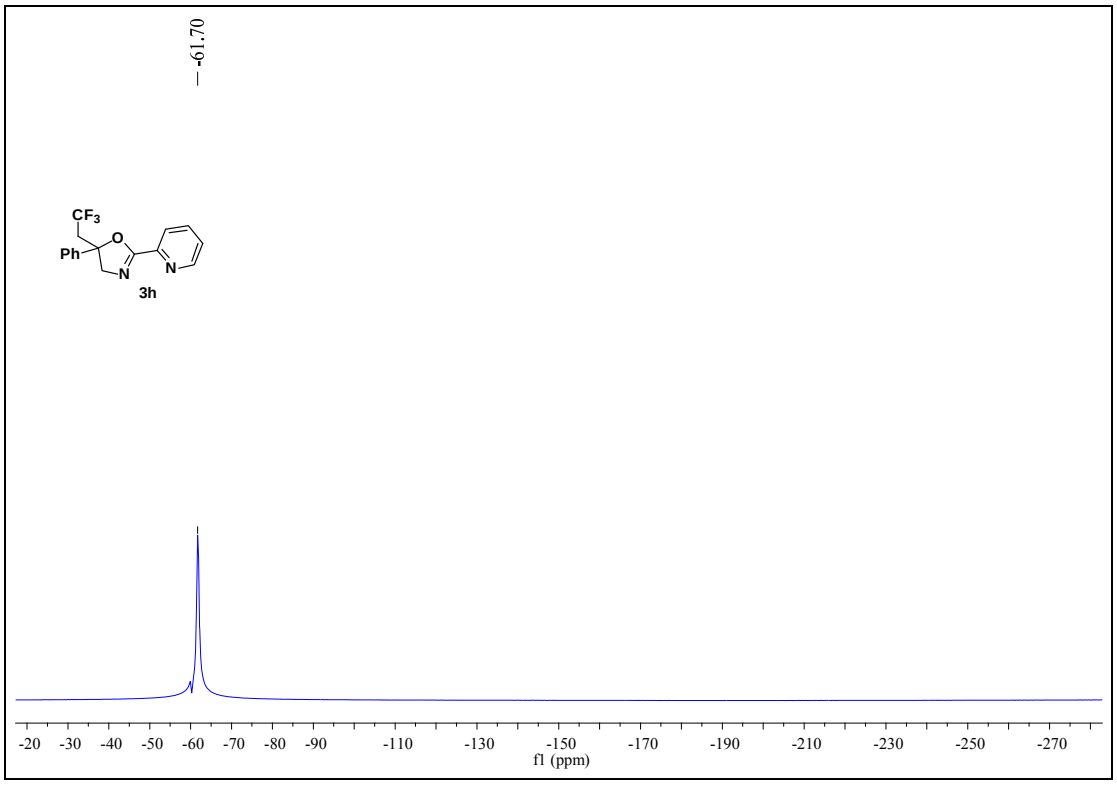
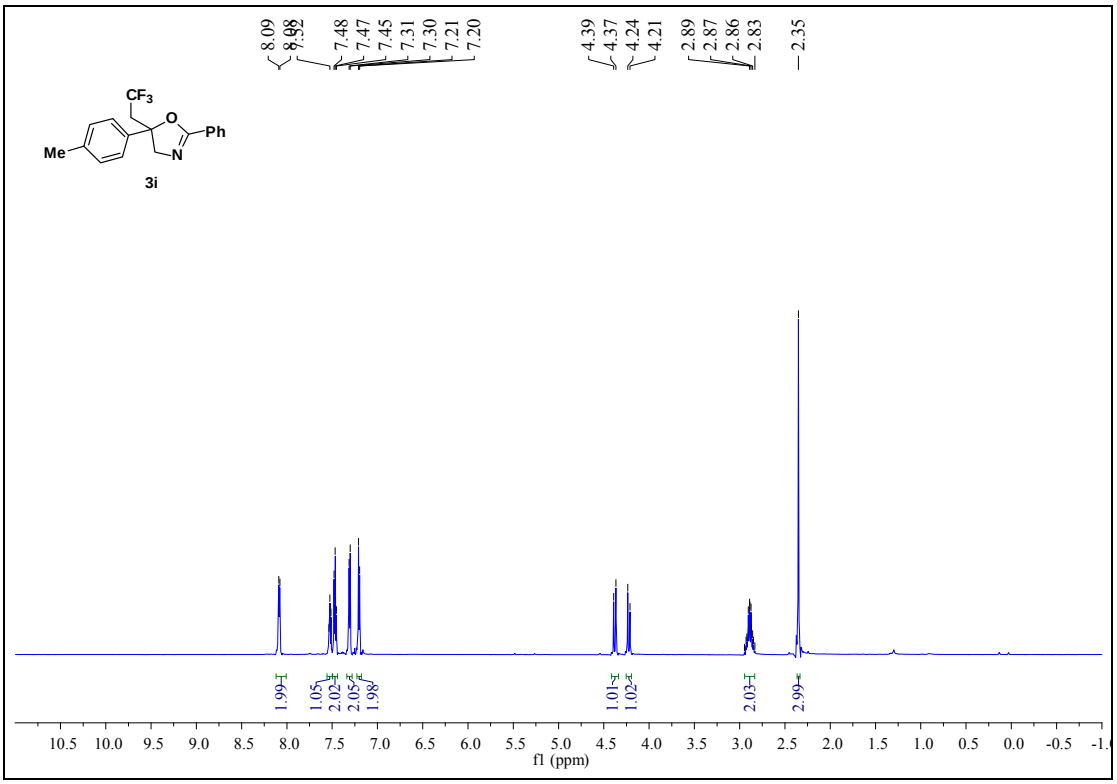
142.15
135.51
128.74
124.13
123.43
123.31
123.27
120.55
84.98
67.83
44.54
44.27
44.00
43.73
CF3
Ph
O
N
N
3h
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-61.70
CF3
Ph
O
N
N
3h
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)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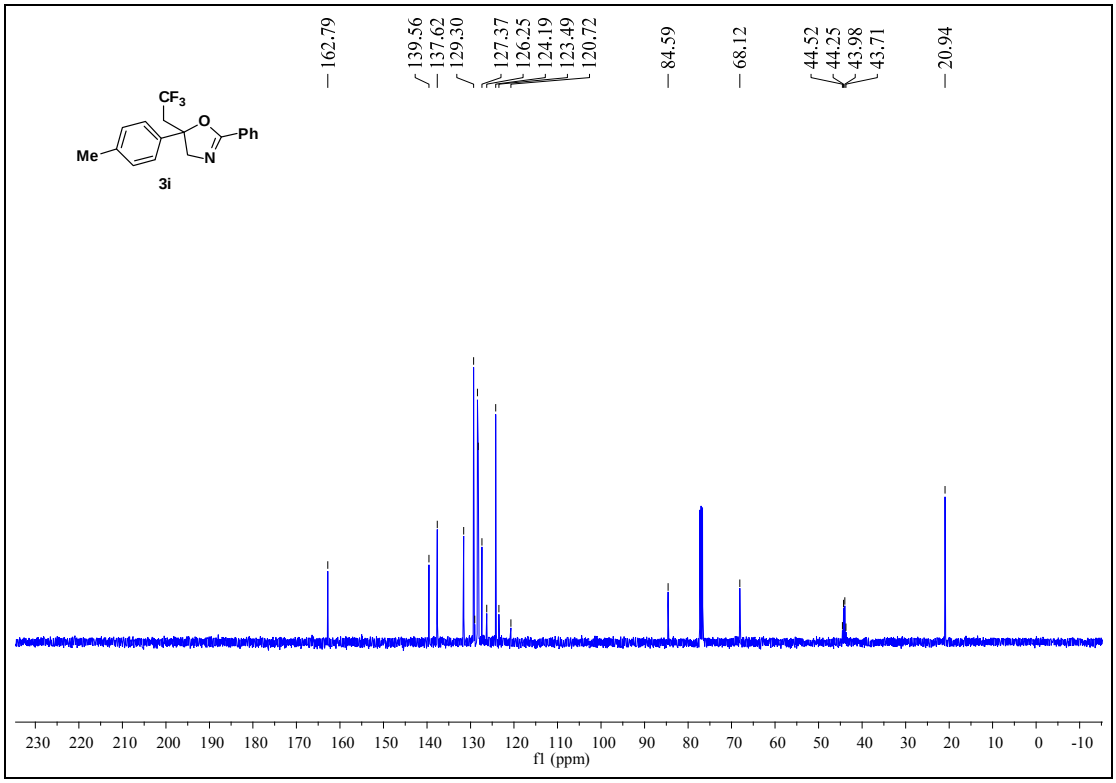
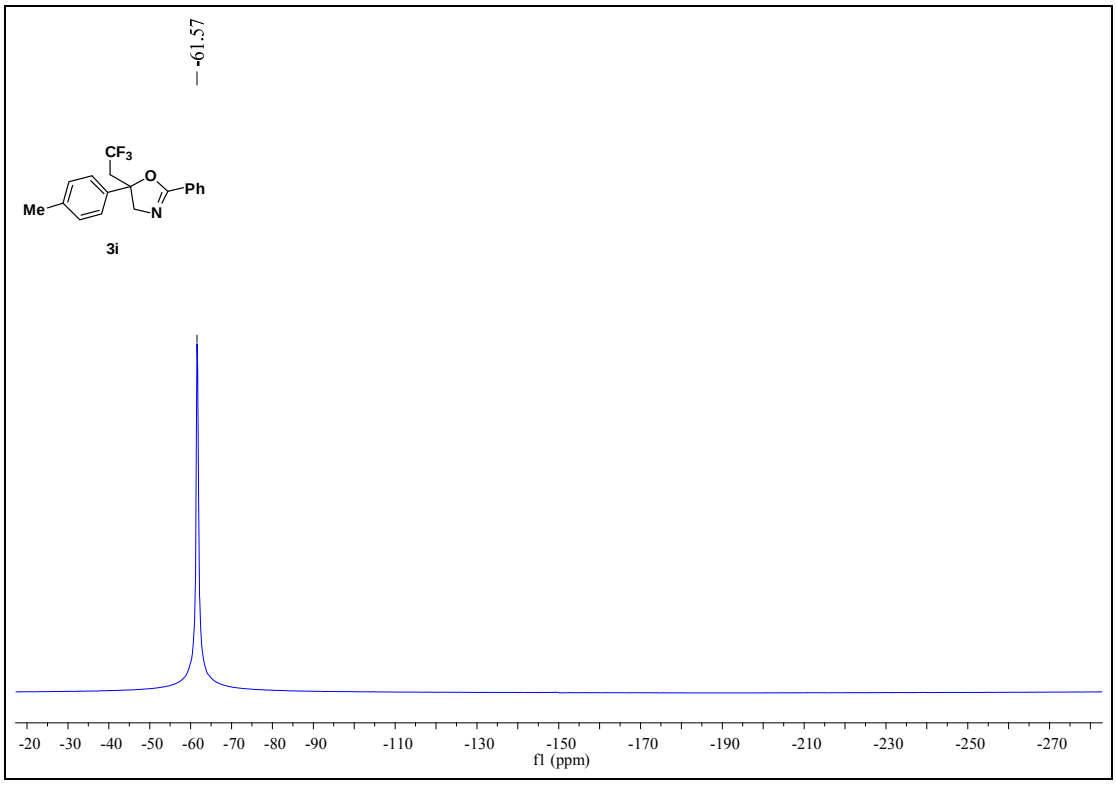
8.08
8.07
7.48
7.47
7.45
7.31
7.30
7.21
7.20
4.39
4.37
4.24
4.21
2.89
2.87
2.86
2.83
2.35
CF3
O
Ph
Me
N
3i
1.99
1.05
2.02
2.05
1.98
1.01
1.02
2.03
2.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


162.79
139.56
137.62
129.30
127.37
126.25
124.19
123.49
120.72
84.59
68.12
44.52
44.25
43.98
43.71
20.94
CF3
O
Ph
Me
N
3i
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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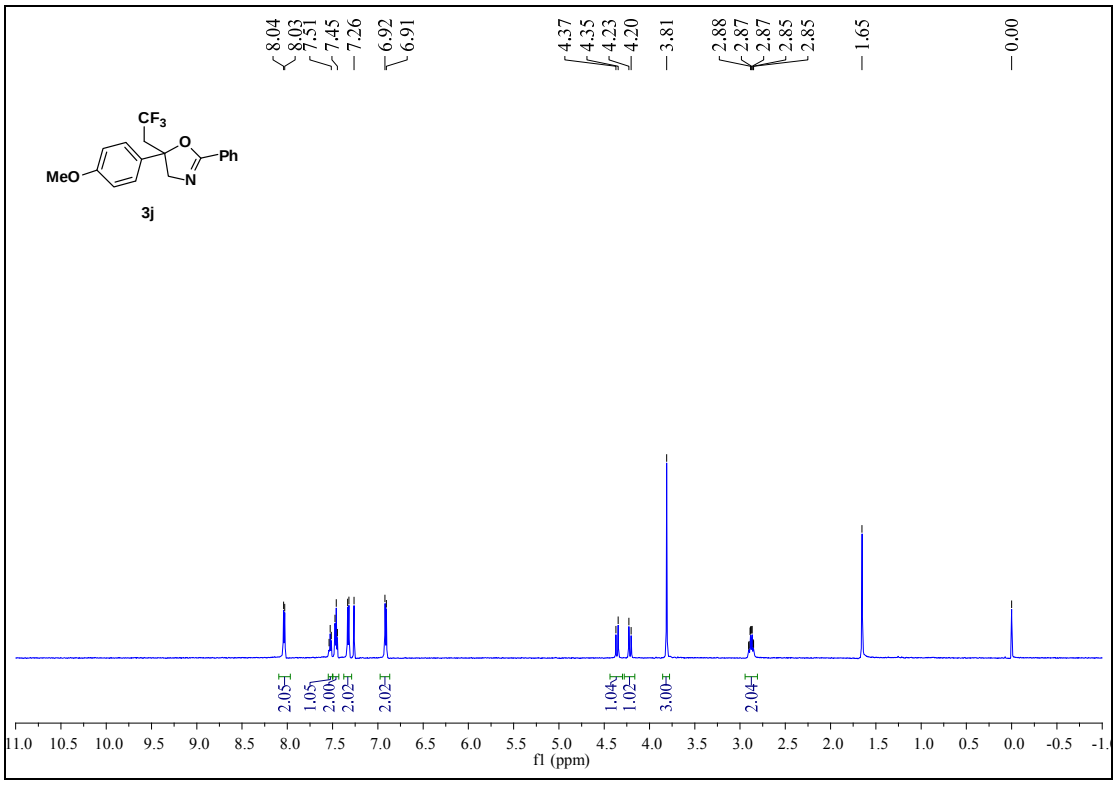
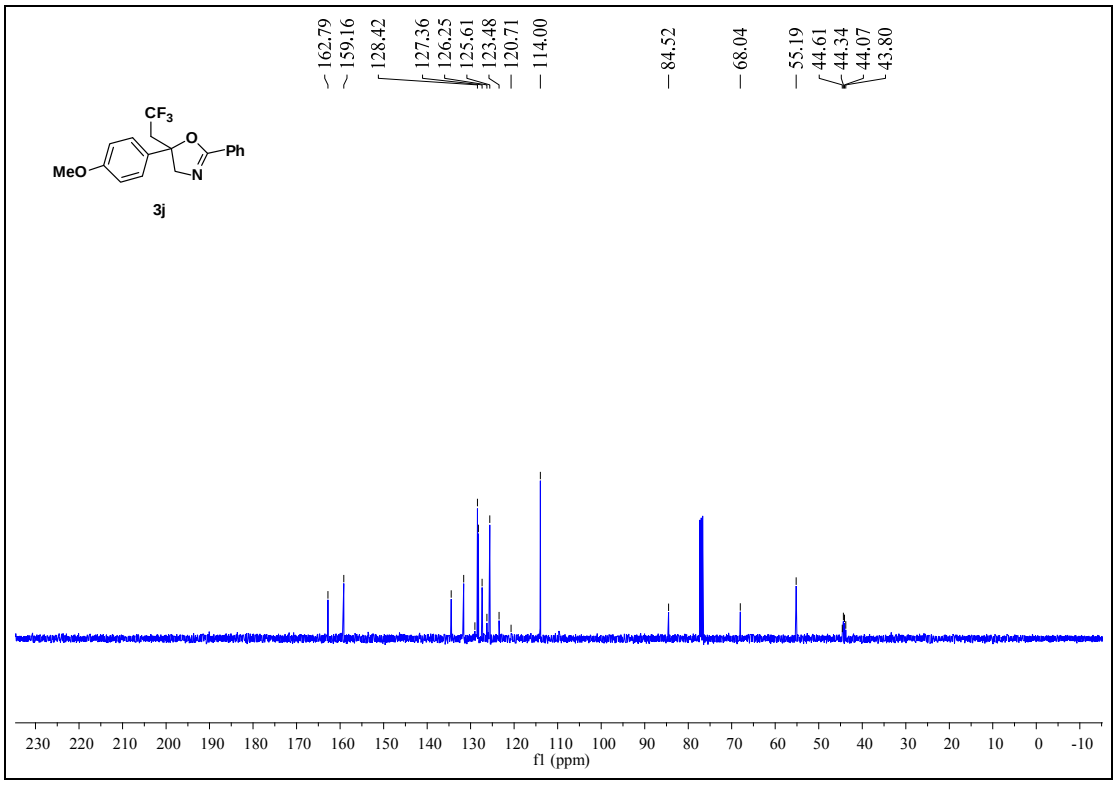
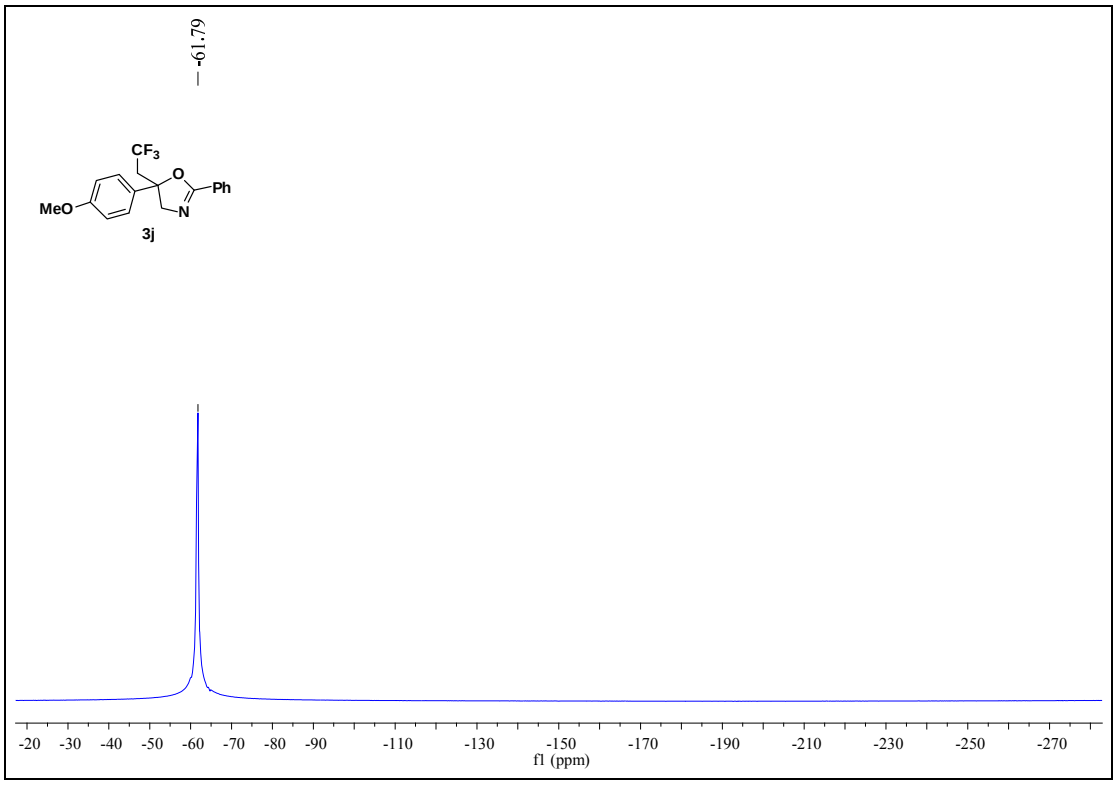
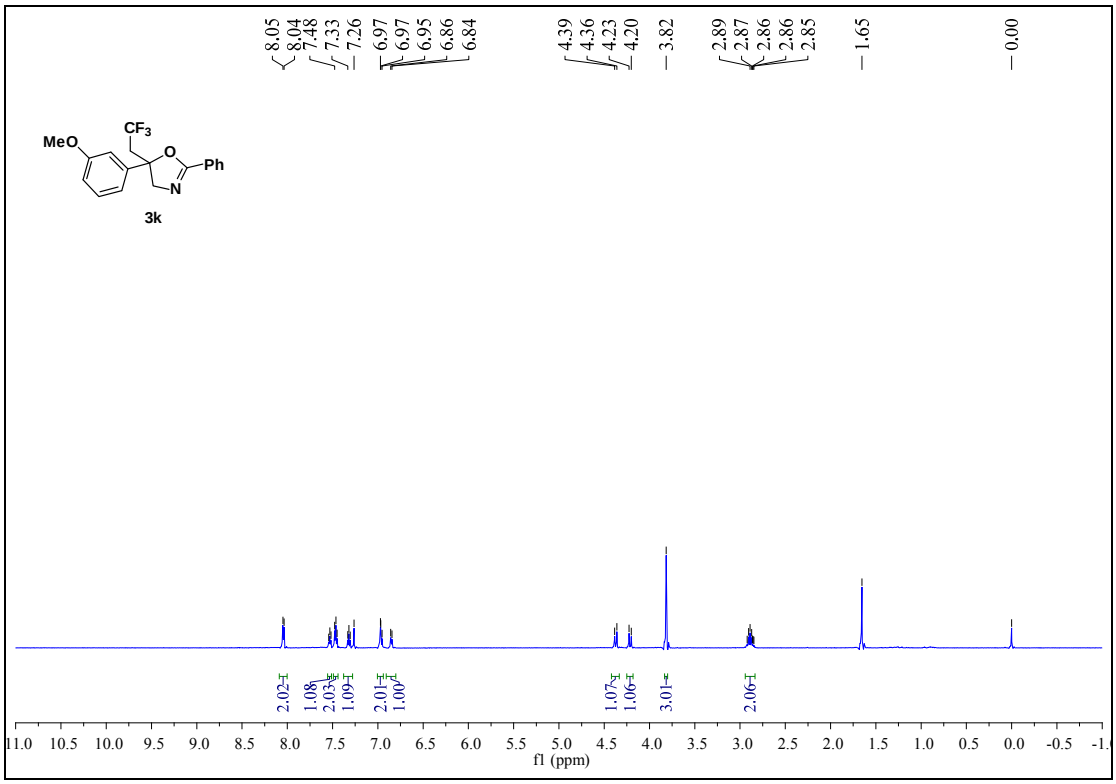
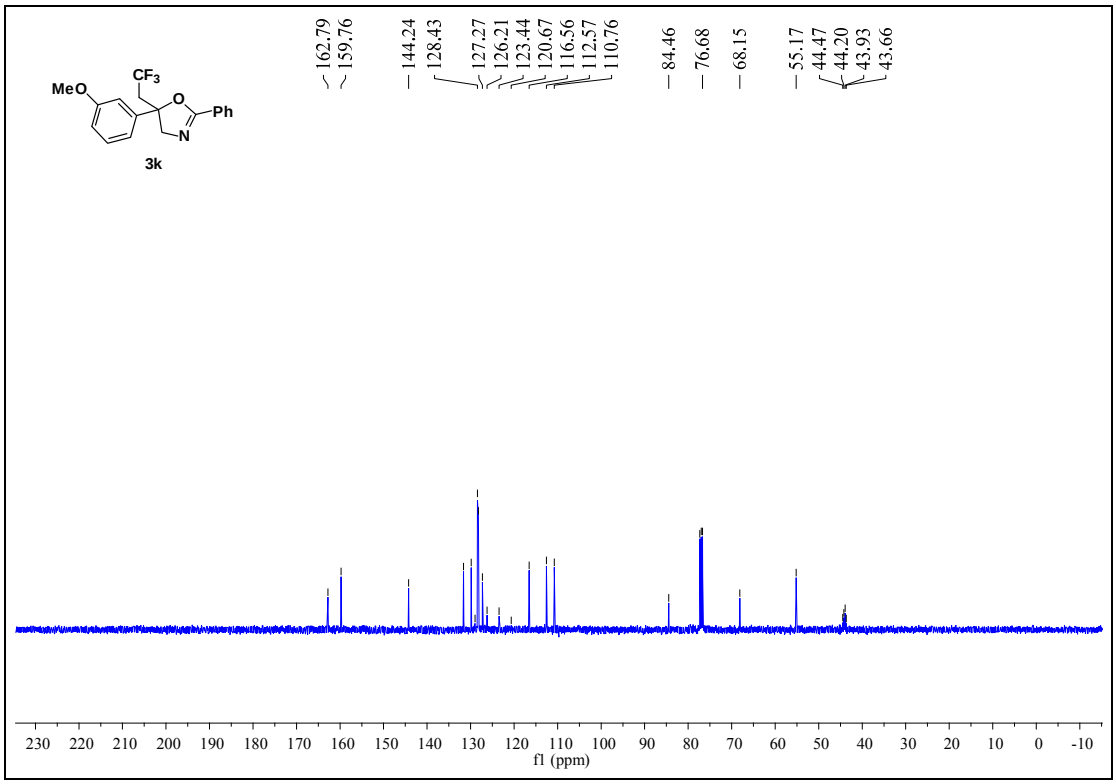
CF3
O
Ph
Me
N
3i
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)

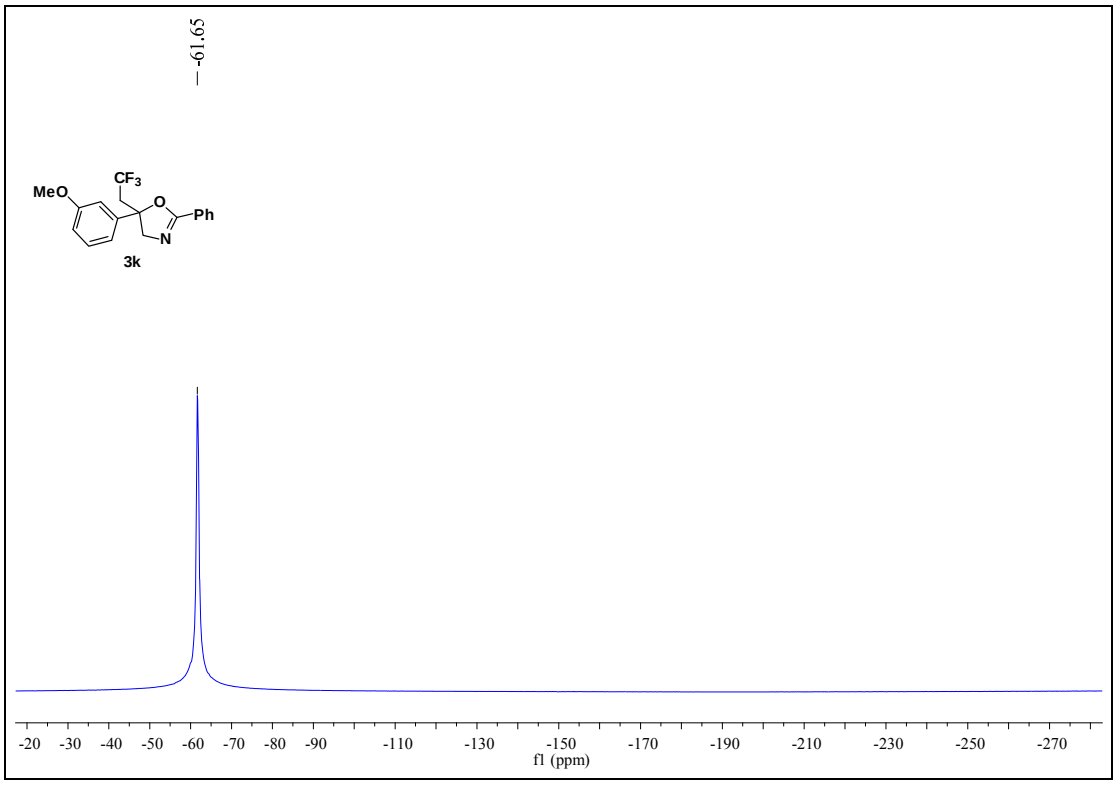

8.04
8.03
7.51
7.45
7.26
6.92
6.91
4.37
4.35
4.23
4.20
3.81
2.88
2.87
2.87
2.85
2.85
1.65
0.00
CF3
O
Ph
MeO
N
3j
2.05
1.05
2.00
2.02
2.02
1.04
1.02
3.00
2.04
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

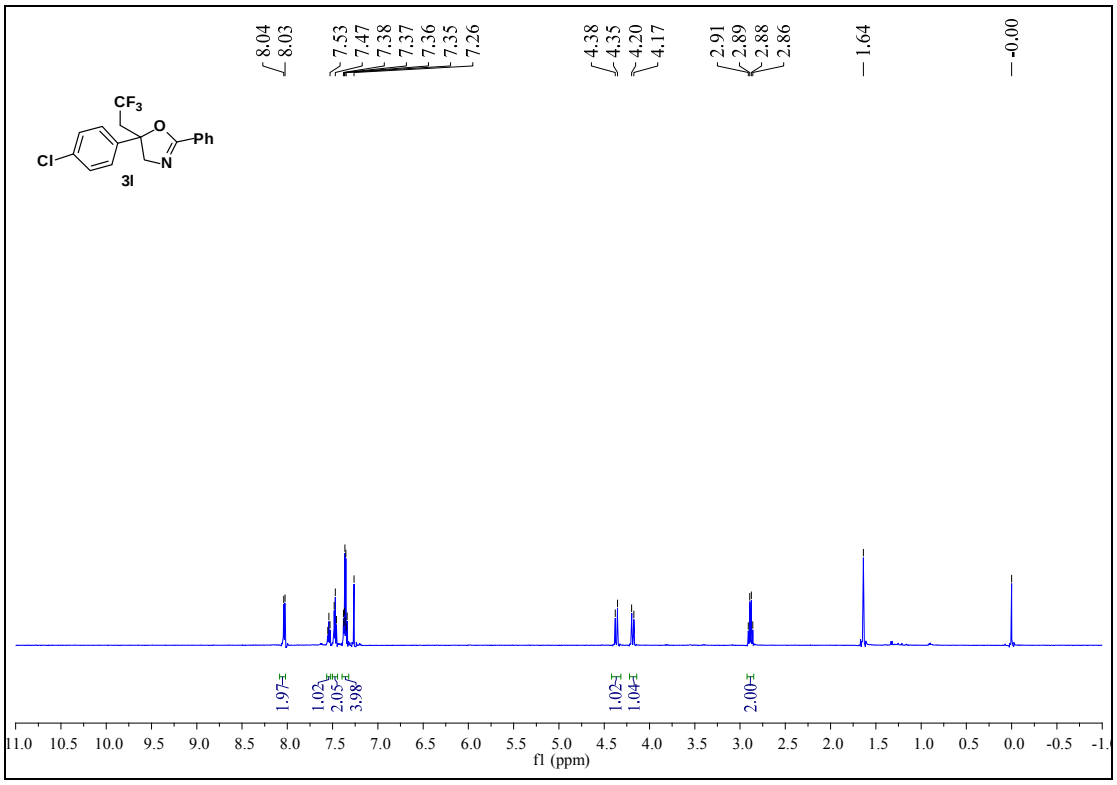

162.79
159.16
128.42
127.36
126.25
125.61
123.48
120.71
114.00
84.52
68.04
55.19
44.61
44.34
44.07
43.80
CF3
O
Ph
MeO
N
3j
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

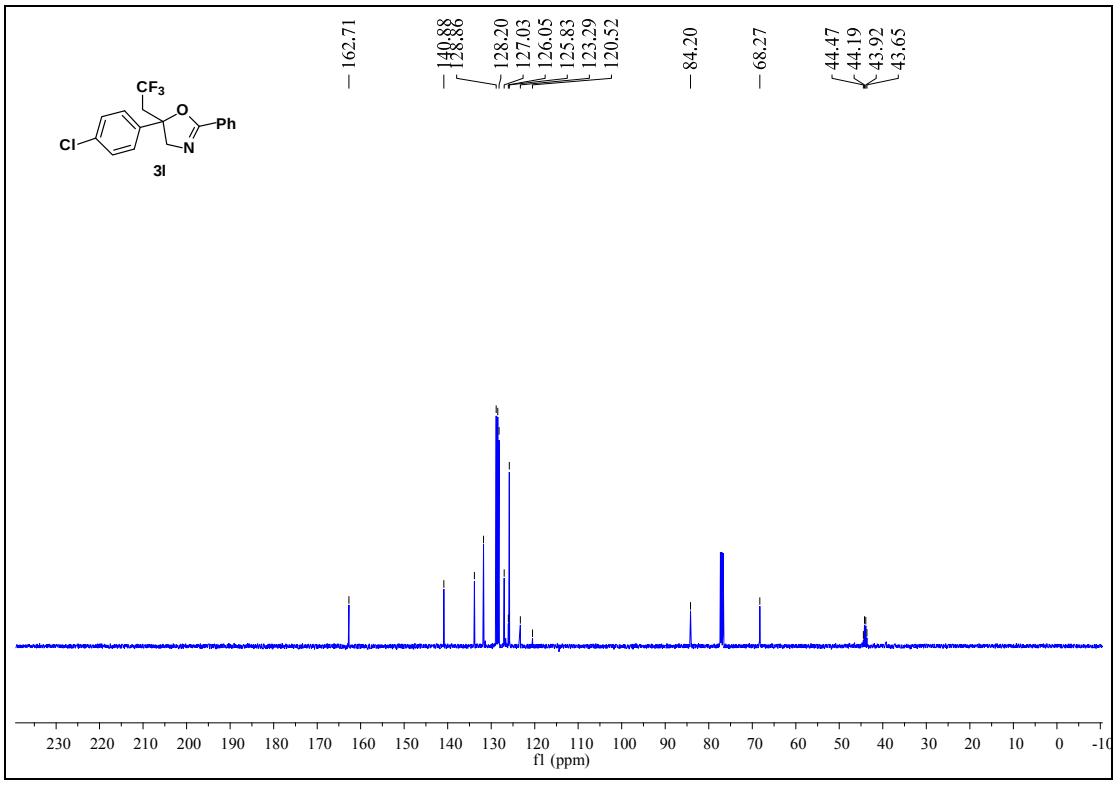

-61.79
CF3
O
Ph
MeO
N
3j
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)

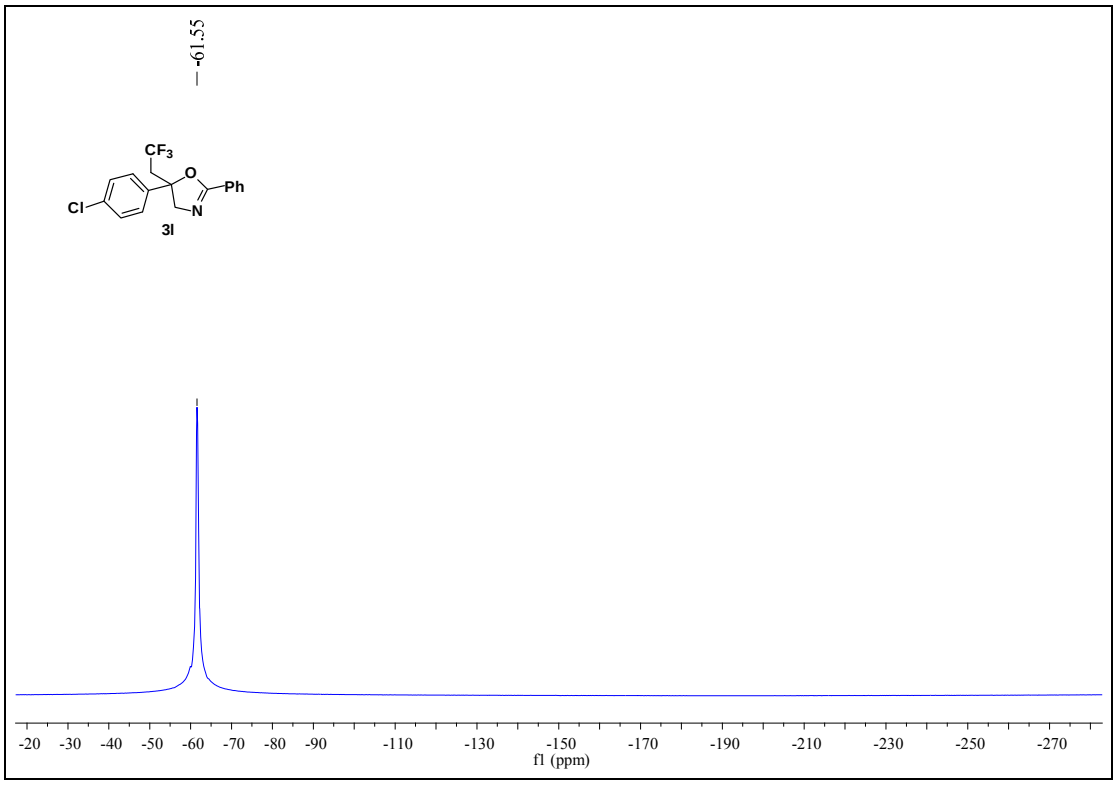

8.05
8.04
7.48
7.33
7.26
6.97
6.97
6.95
6.86
6.84
4.39
4.36
4.23
4.20
3.82
2.89
2.87
2.86
2.86
2.85
1.65
0.00
MeO
CF3
O
Ph
N
3k
2.02
1.08
2.03
1.09
2.01
1.00
1.07
1.06
3.01
2.06
fl (ppm)

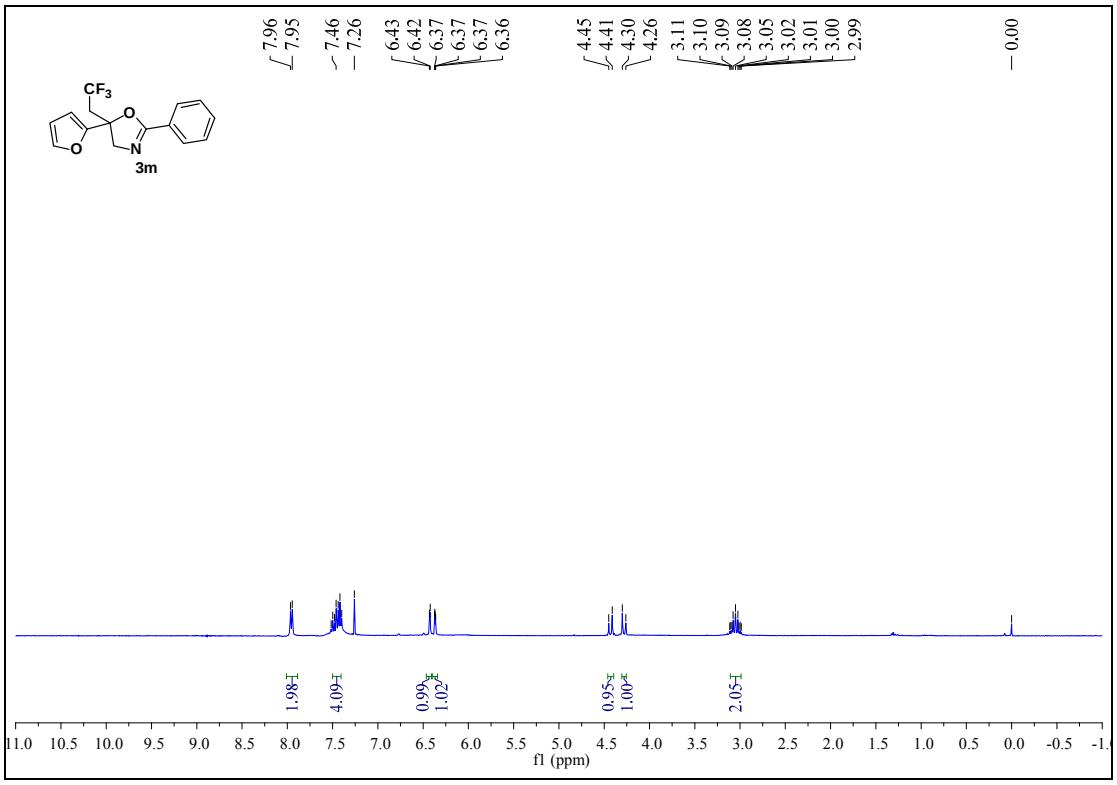

162.79
159.76
144.24
128.43
127.27
126.21
123.44
120.67
116.56
112.57
110.76
84.46
76.68
68.15
55.17
44.47
44.20
43.93
43.66
MeO
CF3
O
Ph
N
3k
fl (ppm)

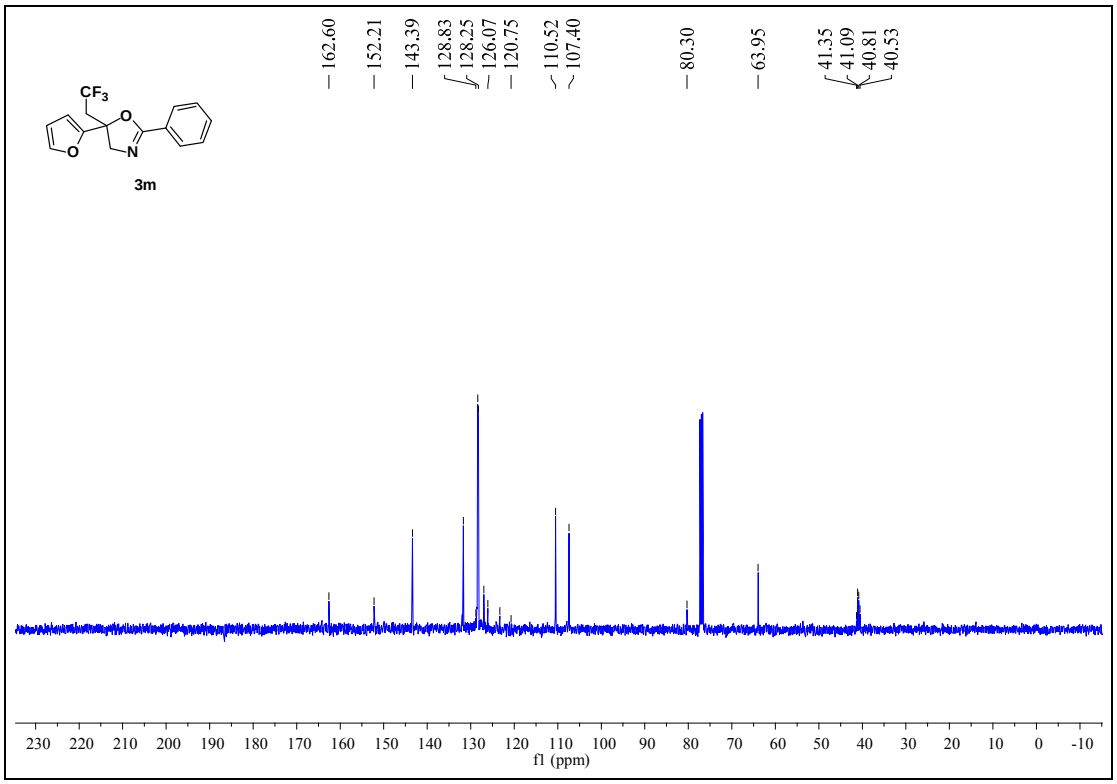

-61.65
MeO
CF3
O
Ph
N
3k
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)

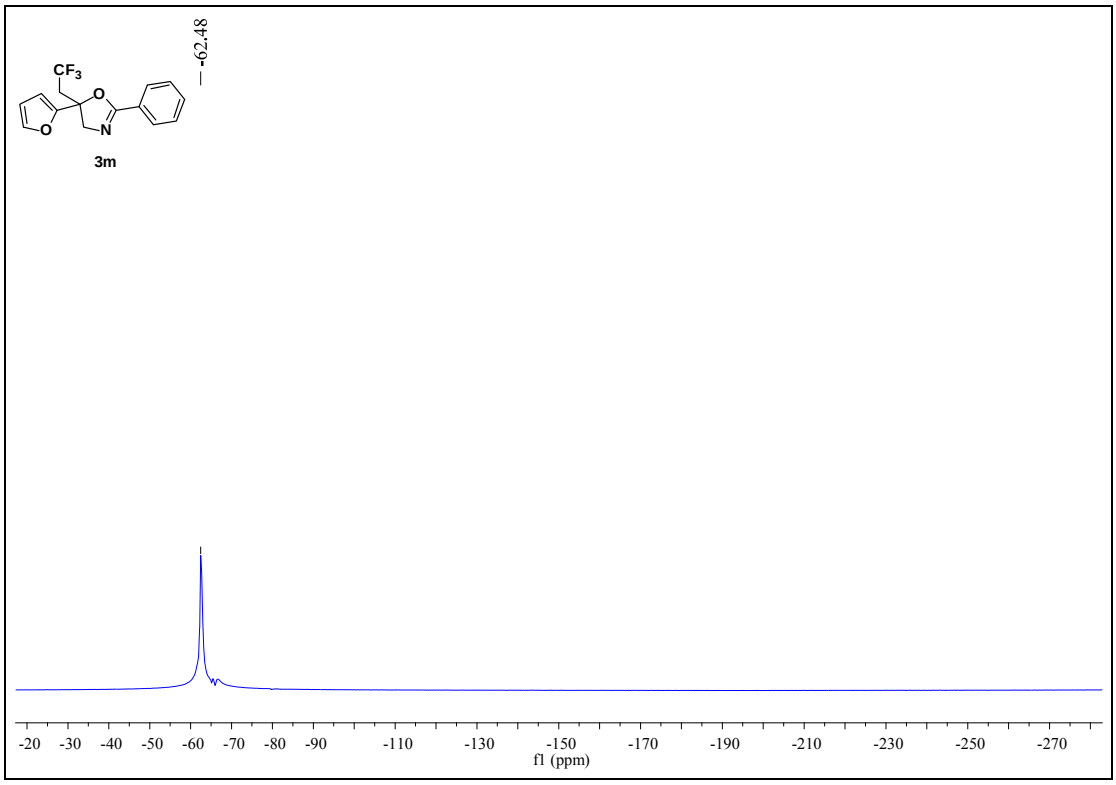

8.04
8.03
7.53
7.47
7.38
7.37
7.36
7.35
7.26
4.38
4.35
4.20
4.17
2.91
2.89
2.88
2.86
1.64
0.00
CF3
O
Ph
Cl
N
3l
1.97
1.02
2.05
3.98
1.02
1.04
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

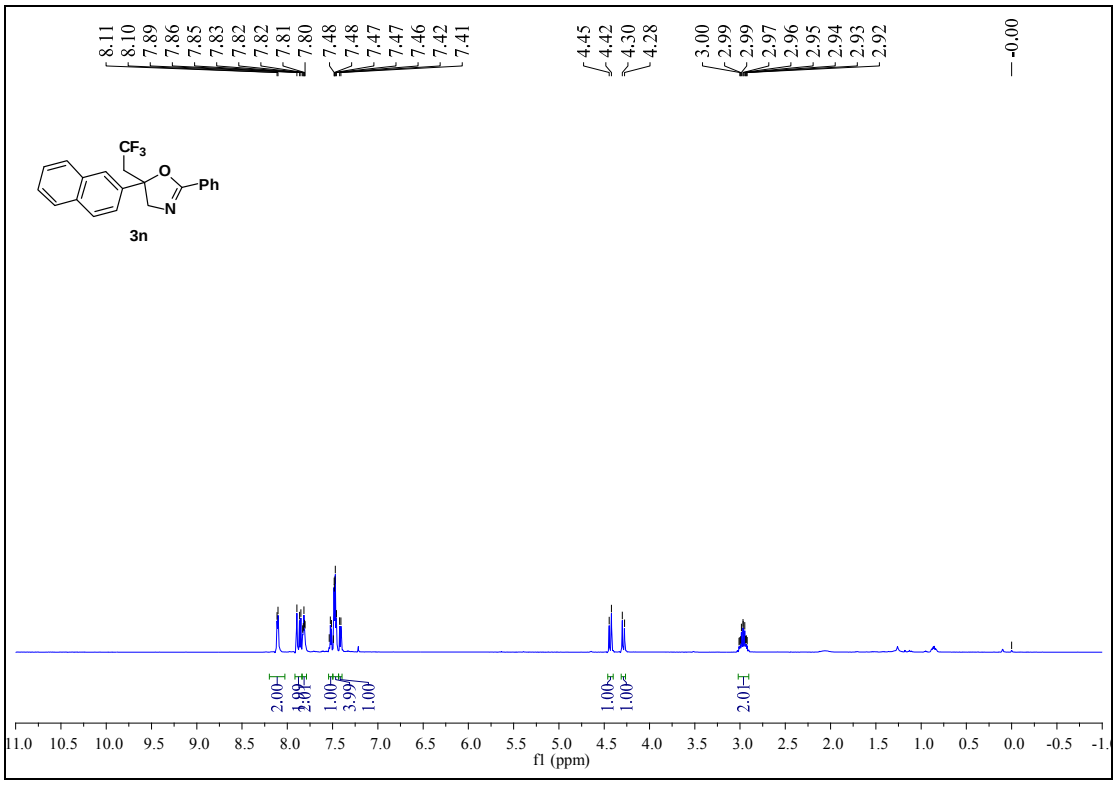

162.71
140.88
128.86
128.20
127.03
126.05
125.83
123.29
120.52
84.20
68.27
44.47
44.19
43.92
43.65
CF3
O
Ph
Cl
N
3l
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

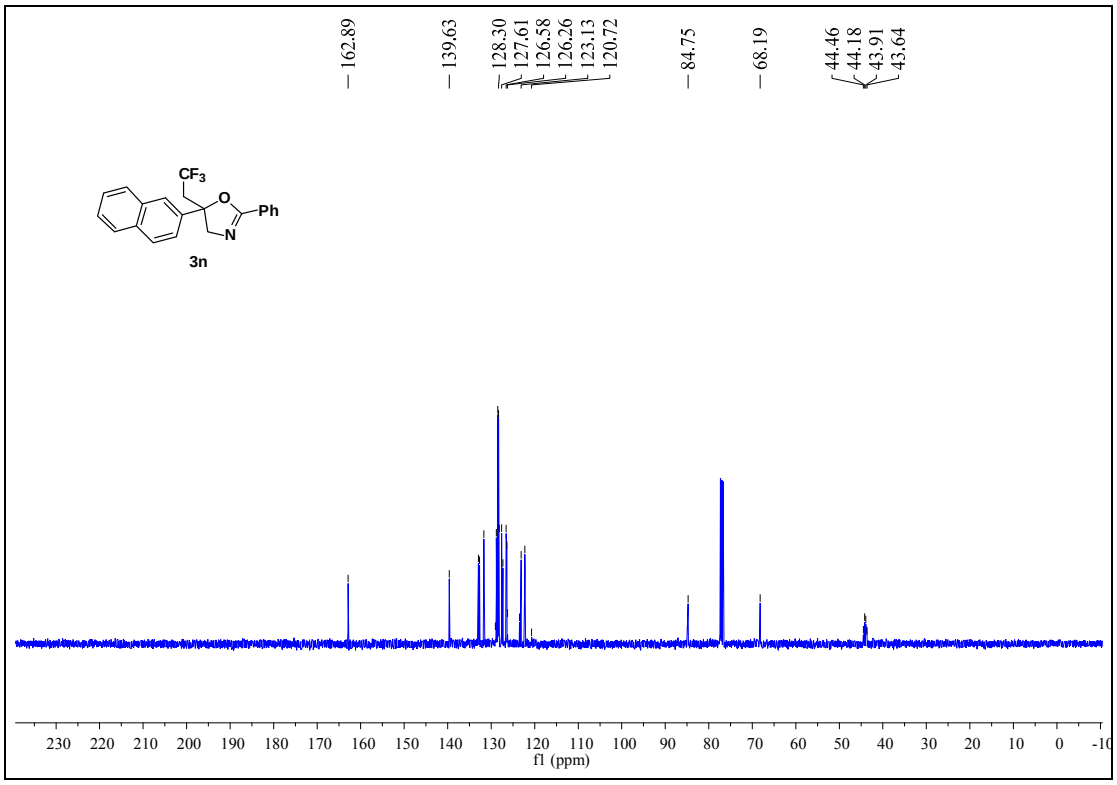

-61.55
CF3
O
Ph
Cl
N
3l
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)

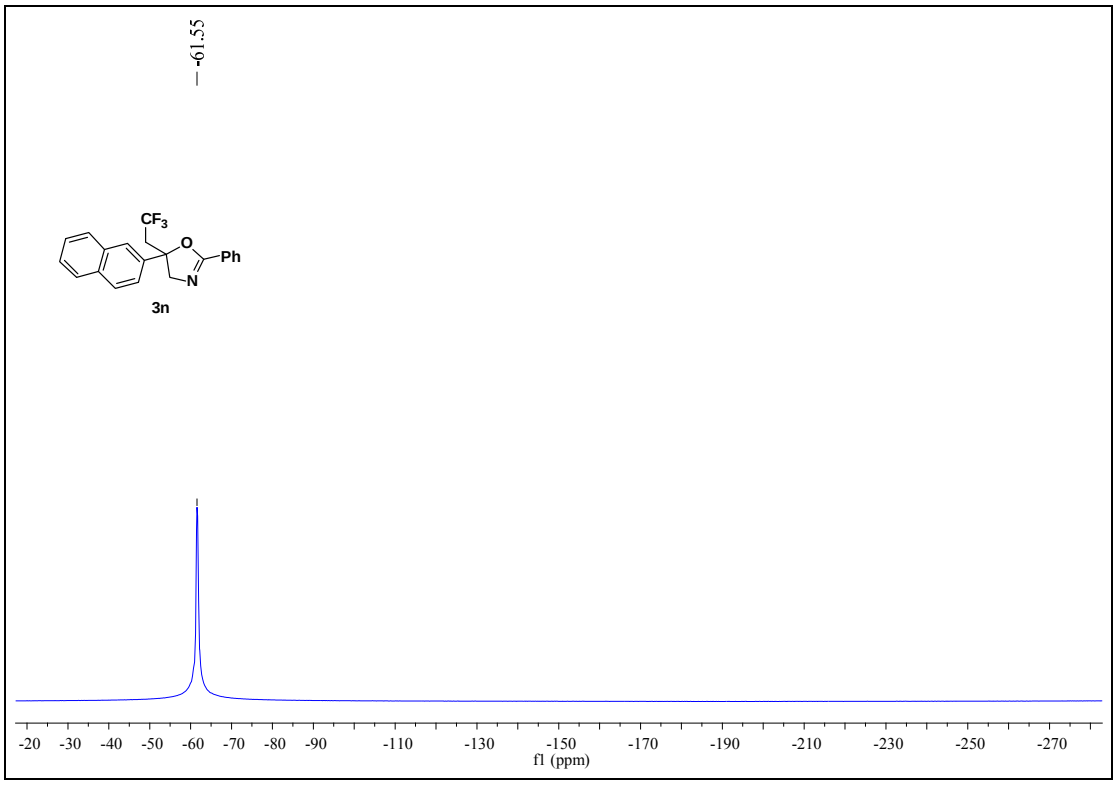

7.96
7.95
7.46
7.26
6.43
6.42
6.37
6.37
6.37
6.36
4.45
4.41
4.30
4.26
3.11
3.10
3.09
3.08
3.05
3.02
3.01
3.00
2.99
0.00
CF3
O
O
N
3m
1.98
4.09
0.99
1.02
0.95
1.00
2.05
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

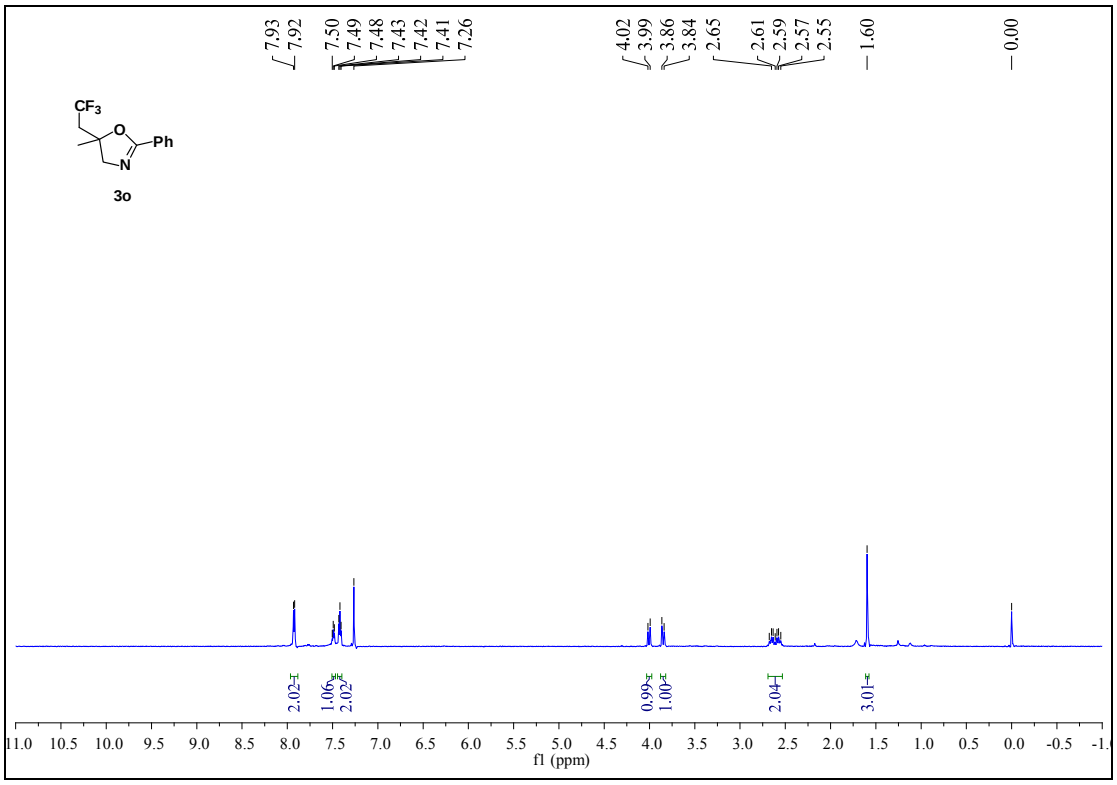

162.60
152.21
143.39
128.83
128.25
126.07
120.75
110.52
107.40
80.30
63.95
41.35
41.09
40.81
40.53
CF3
O
O
N
3m
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

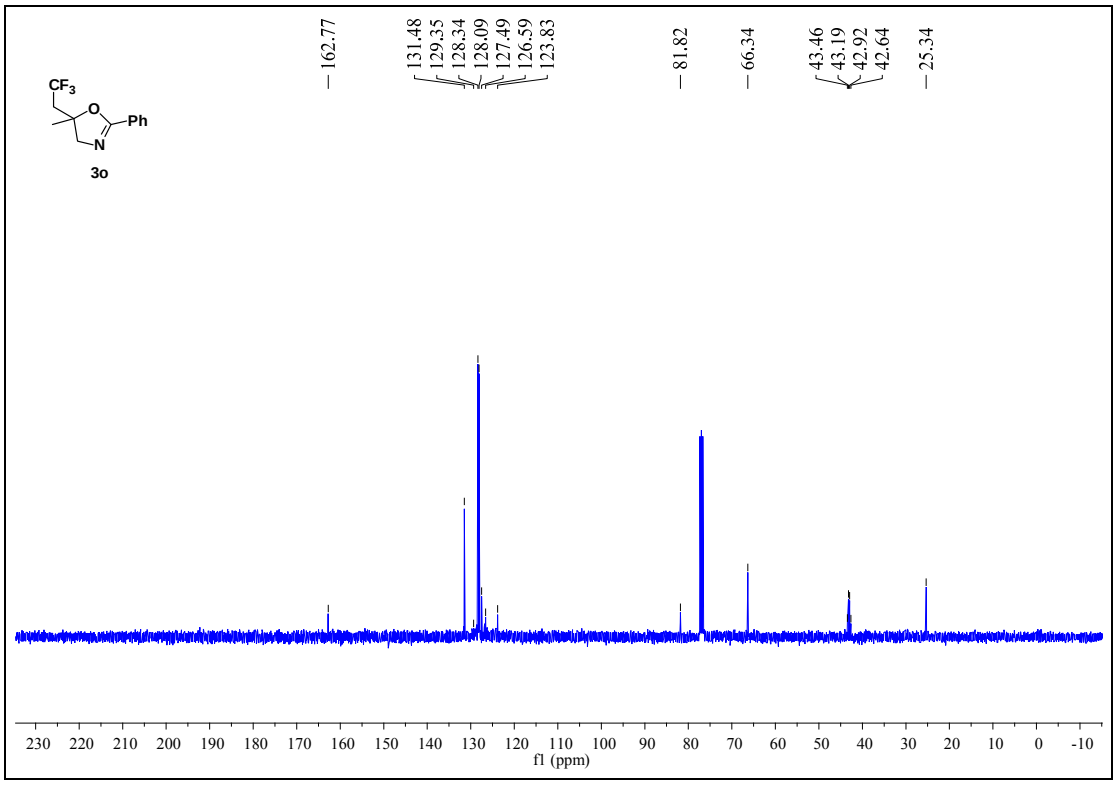

-62.48
CF3
O
N
O
3m
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)


8.11
8.10
7.89
7.86
7.85
7.83
7.82
7.82
7.81
7.80
7.48
7.48
7.47
7.47
7.46
7.42
7.41
4.45
4.42
4.30
4.28
3.00
2.99
2.99
2.97
2.96
2.95
2.94
2.93
2.92
-0.00
CF3
O
Ph
N
3n
2.00
1.00
3.99
1.00
1.00
1.00
2.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


162.89
139.63
128.30
127.61
126.58
126.26
123.13
120.72
84.75
68.19
44.46
44.18
43.91
43.64
CF3
O
Ph
N
3n
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-61.55
CF3
O
Ph
N
3n
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)


7.93
7.92
7.50
7.49
7.48
7.43
7.42
7.41
7.26
4.02
3.99
3.86
3.84
2.65
2.61
2.59
2.57
2.55
1.60
0.00
CF3
O
Ph
N
3o
2.02
1.06
2.02
0.99
1.00
2.04
3.01
f1 (ppm)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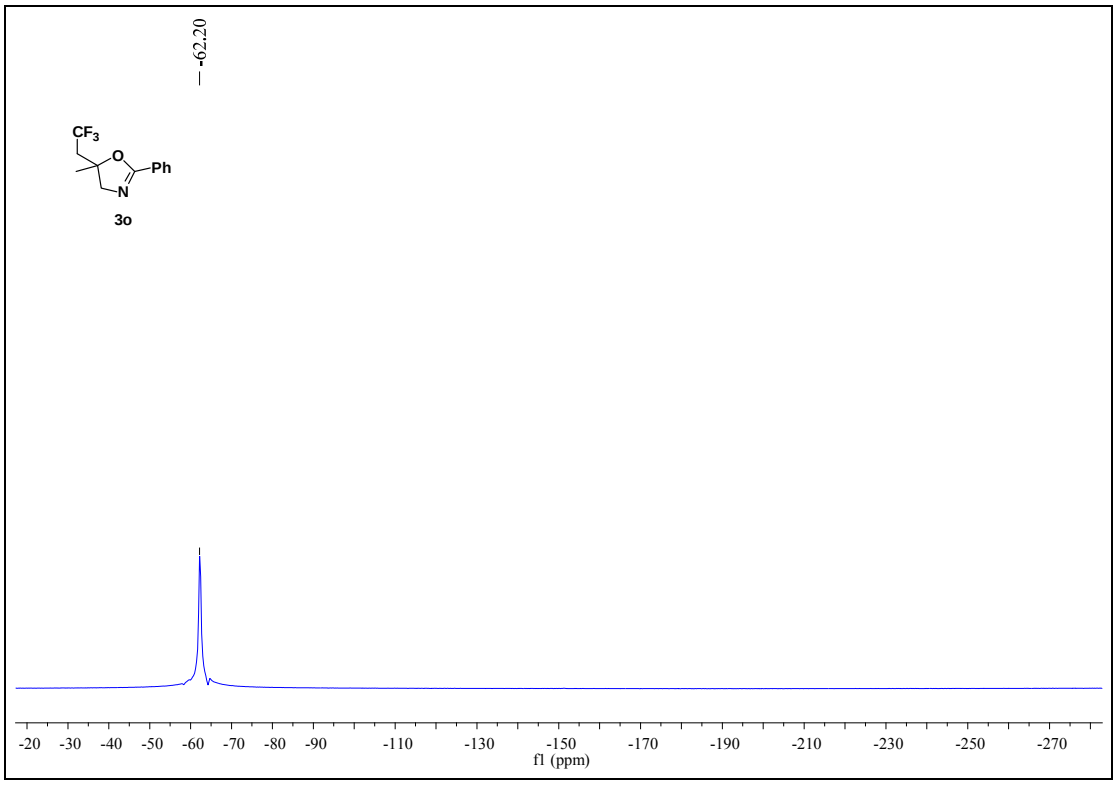
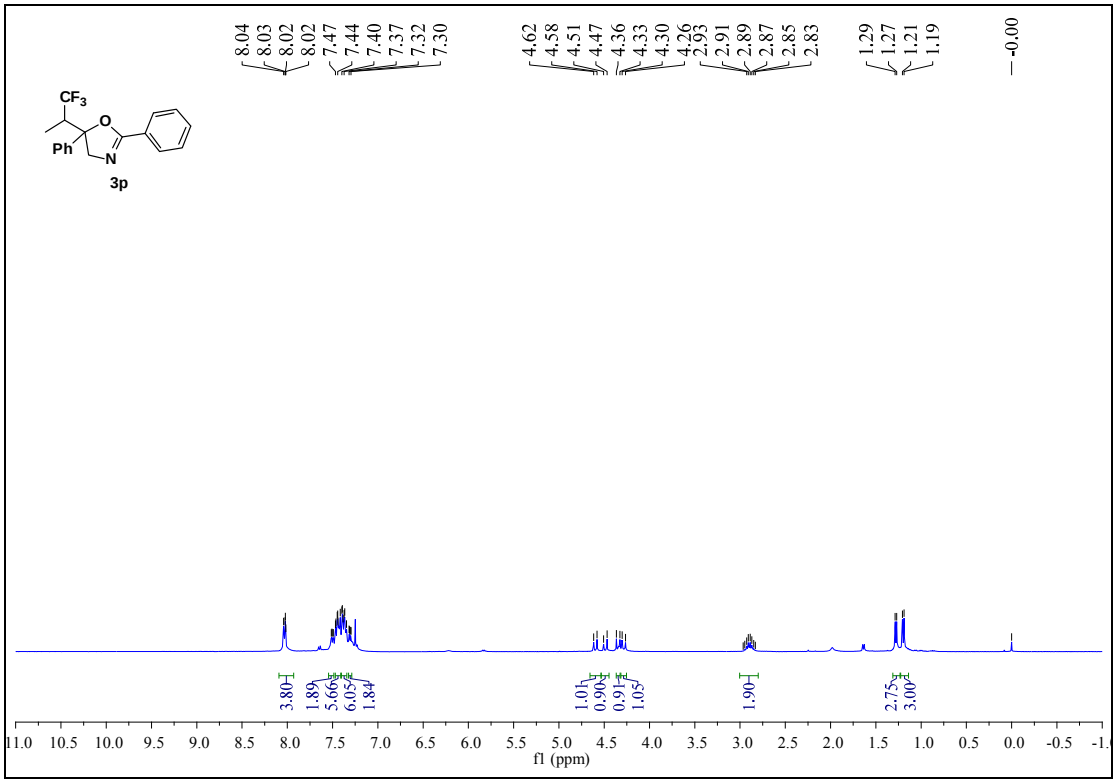
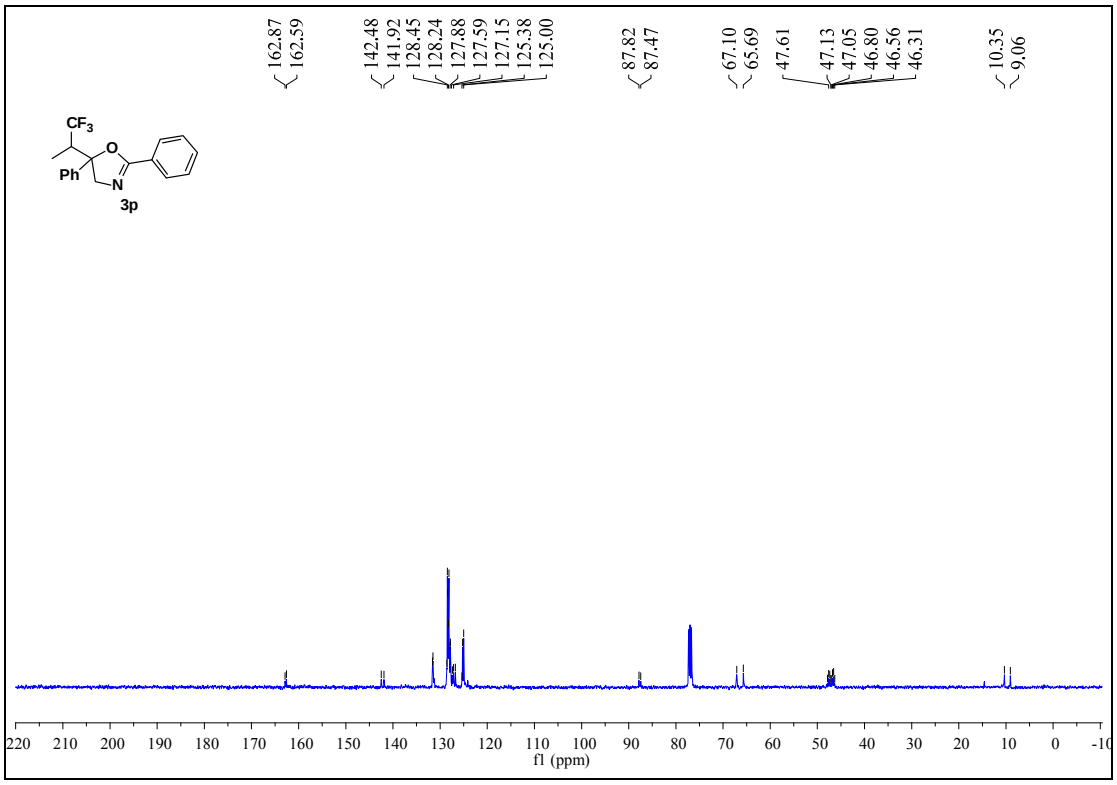
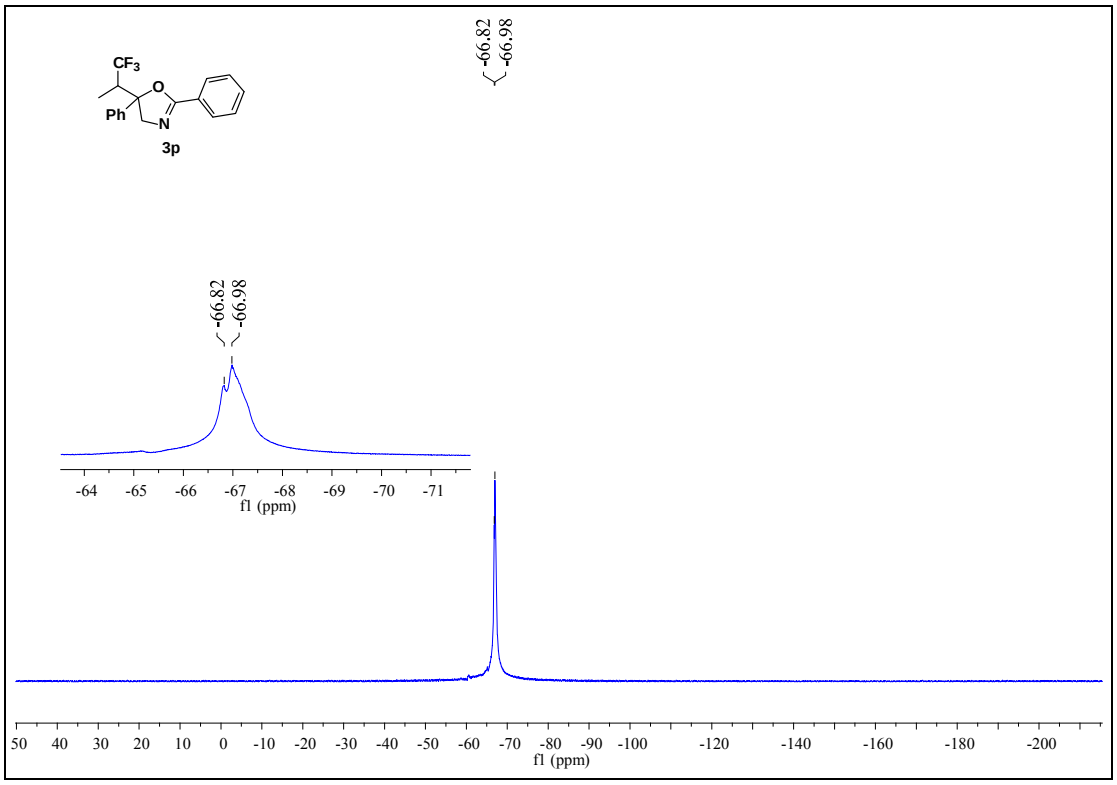
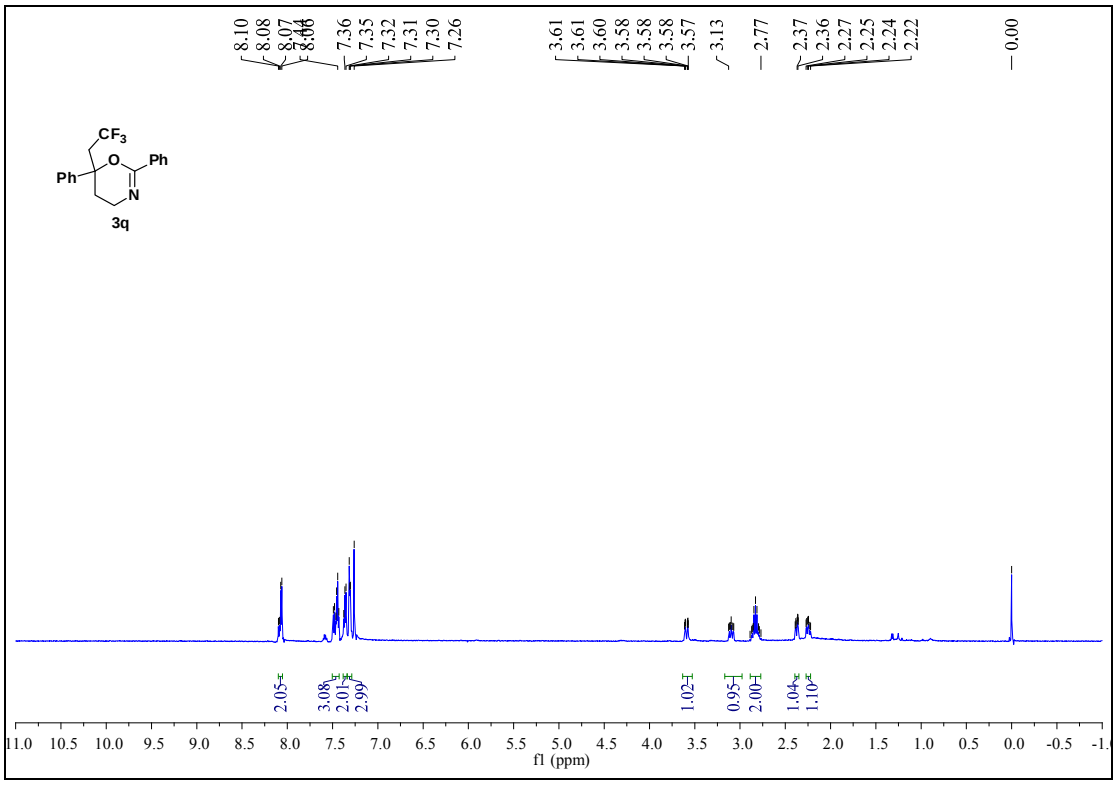
131.48
129.35
128.34
128.09
127.49
126.59
123.83
81.82
66.34
43.46
43.19
42.92
42.64
25.34
CF3
O
Ph
N
3o
f1 (ppm)

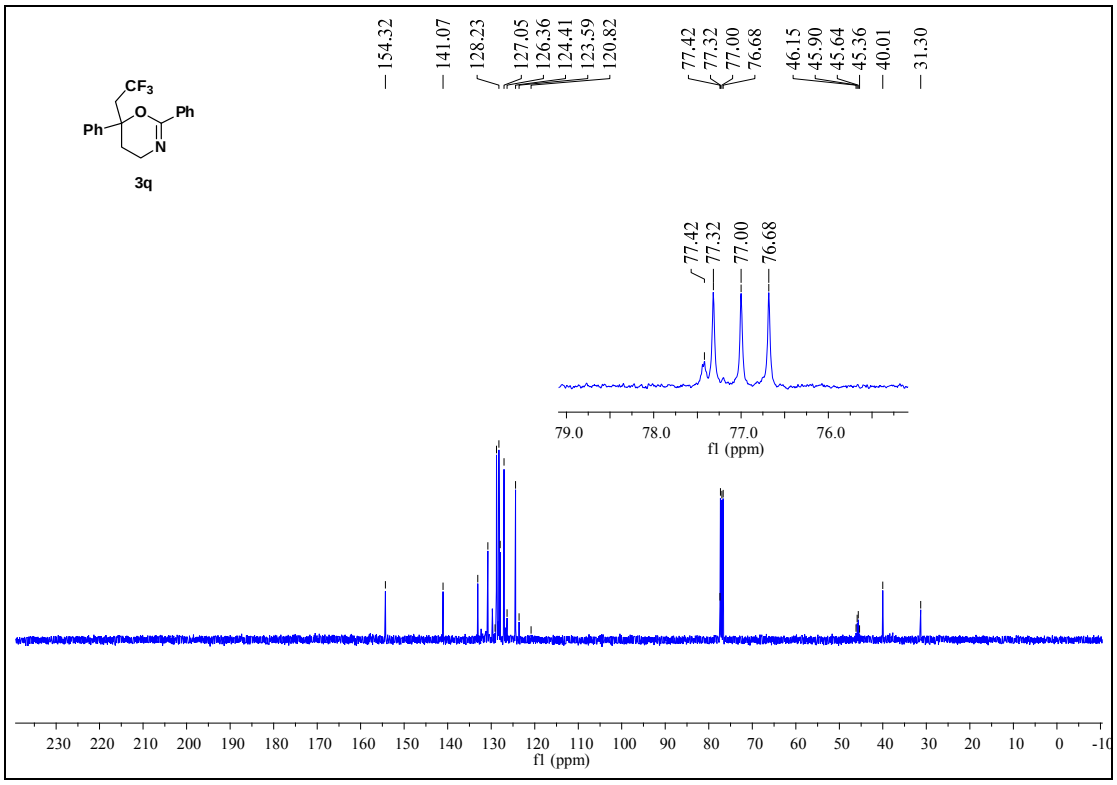

-62.20
CF3
O
Ph
N
3o
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)

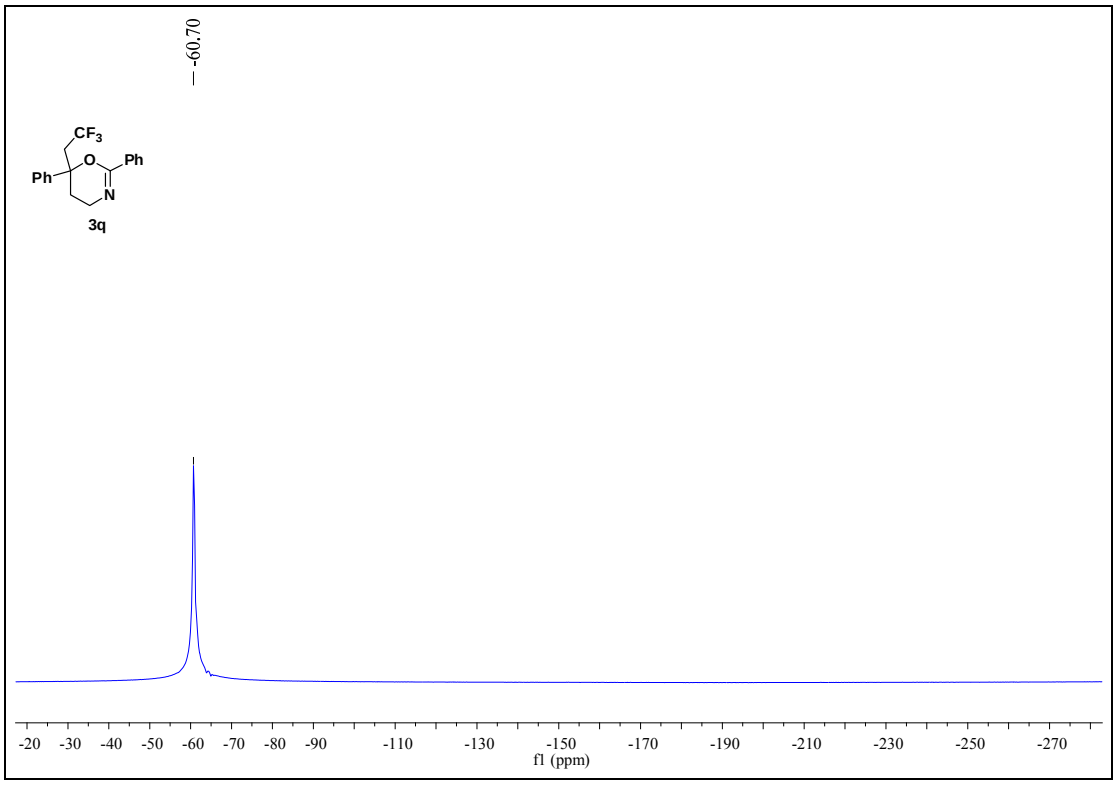

8.04
8.03
8.02
8.02
7.47
7.44
7.40
7.37
7.32
7.30
4.62
4.58
4.51
4.47
4.36
4.33
4.30
4.26
2.93
2.91
2.89
2.87
2.85
2.83
1.29
1.27
1.21
1.19
-0.00
CF3
Ph
O
N
3p
3.80
1.89
5.66
6.05
1.84
1.01
0.90
0.91
1.05
1.90
2.75
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

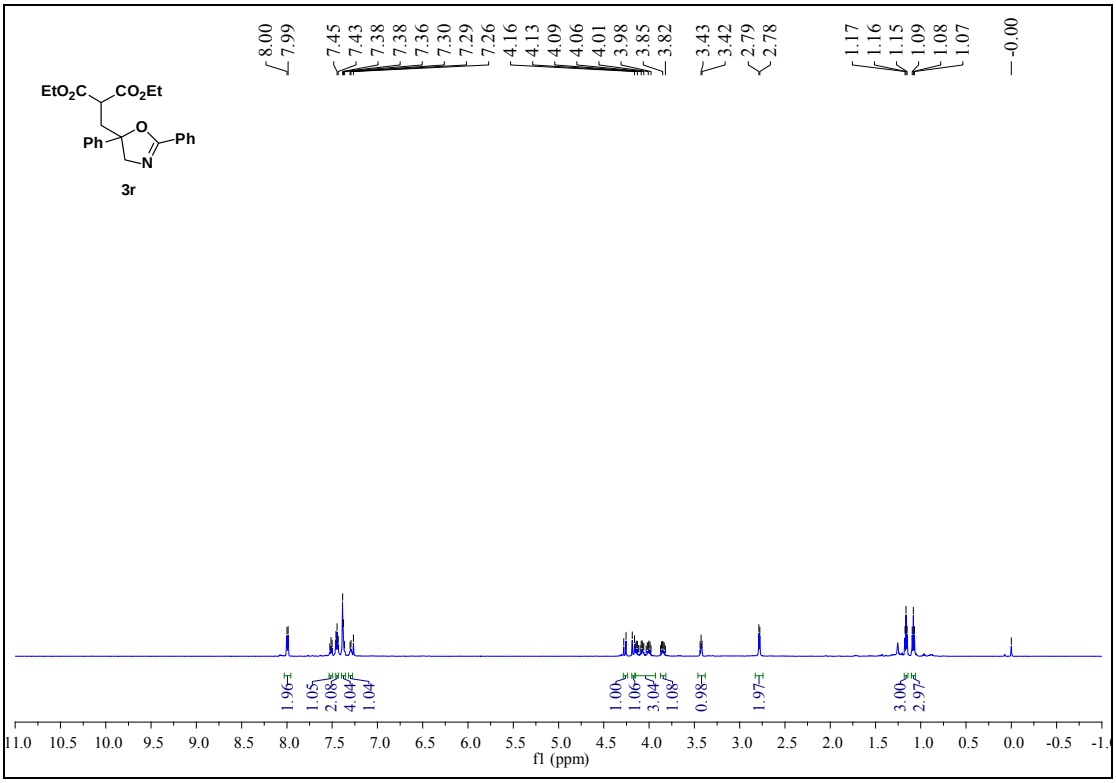

162.87
162.59
142.48
141.92
128.45
128.24
127.88
127.59
127.15
125.38
125.00
87.82
87.47
67.10
65.69
47.61
47.13
47.05
46.80
46.56
46.31
10.35
9.06
CF3
O
Ph
N
3p
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

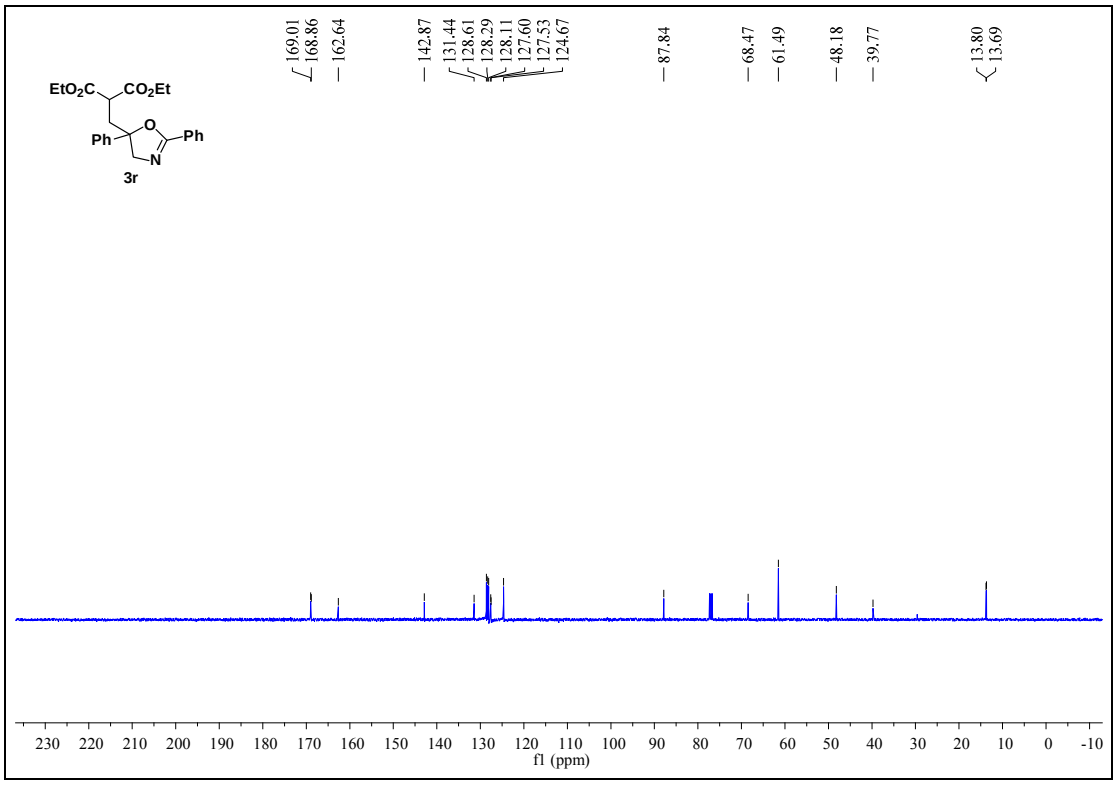

-66.82
-66.98
CF3
O
Ph
N
3p
-66.82
-66.98
-64 -65 -66 -67 -68 -69 -70 -71
f1 (ppm)
50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)


8.10
8.08
8.07
8.04
8.03
7.36
7.35
7.32
7.31
7.30
7.26
3.61
3.61
3.60
3.58
3.58
3.58
3.57
3.13
2.77
2.37
2.36
2.27
2.25
2.24
2.22
0.00
CF3
Ph
O
Ph
N
3q
2.05
3.08
2.01
2.99
1.02
0.95
2.00
1.04
1.10
fl (ppm)


154.32
141.07
128.23
127.05
126.36
124.41
123.59
120.82
77.42
77.32
77.00
76.68
46.15
45.90
45.64
45.36
40.01
31.30
CF3
Ph
O
Ph
N
3q
fl (ppm)


-60.70
CF3
Ph
O
Ph
N
3q
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)


8.00
7.99
7.45
7.43
7.38
7.38
7.36
7.30
7.29
7.26
4.16
4.13
4.09
4.06
4.01
3.98
3.85
3.82
3.43
3.42
2.79
2.78
1.17
1.16
1.15
1.09
1.08
1.07
-0.00
EtO2C
CO2Et
Ph
O
Ph
N
3r
1.96
1.05
2.08
4.04
1.04
1.00
1.06
3.04
1.08
0.98
1.97
3.00
2.97
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.29
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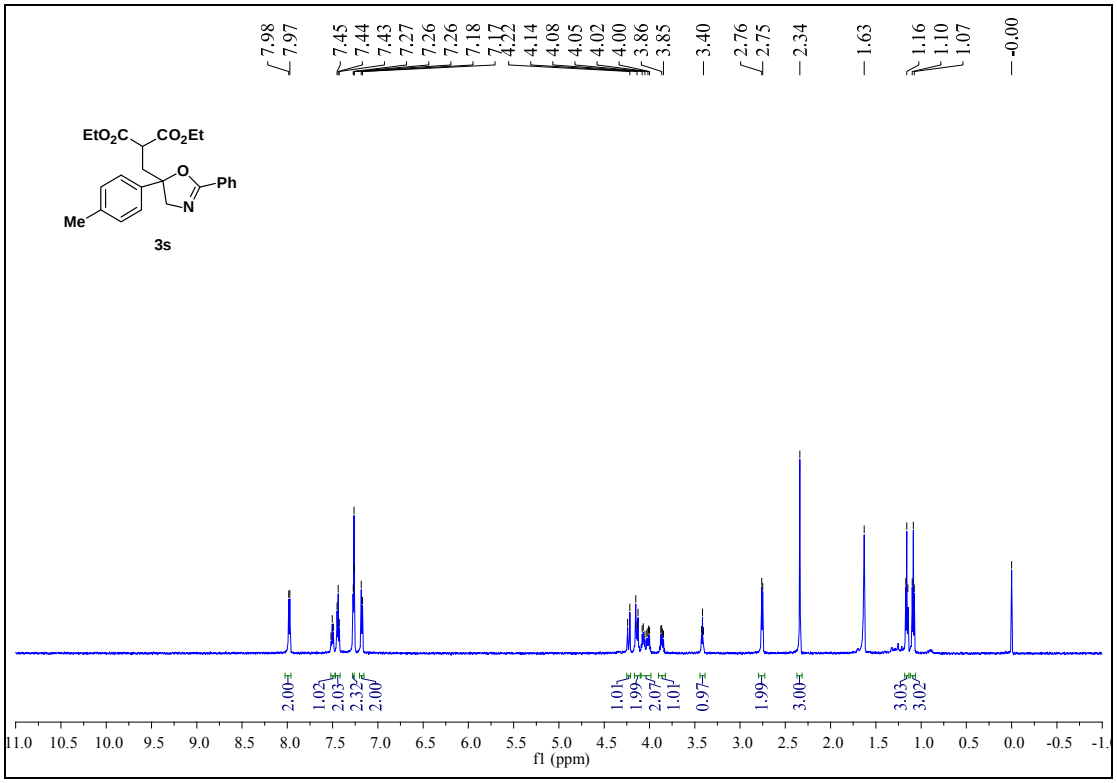
127.53
124.67
87.84
68.47
61.49
48.18
39.77
13.80
13.69
EtO2C
CO2Ph
Ph
O
Ph
N
3r
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.97
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7.43
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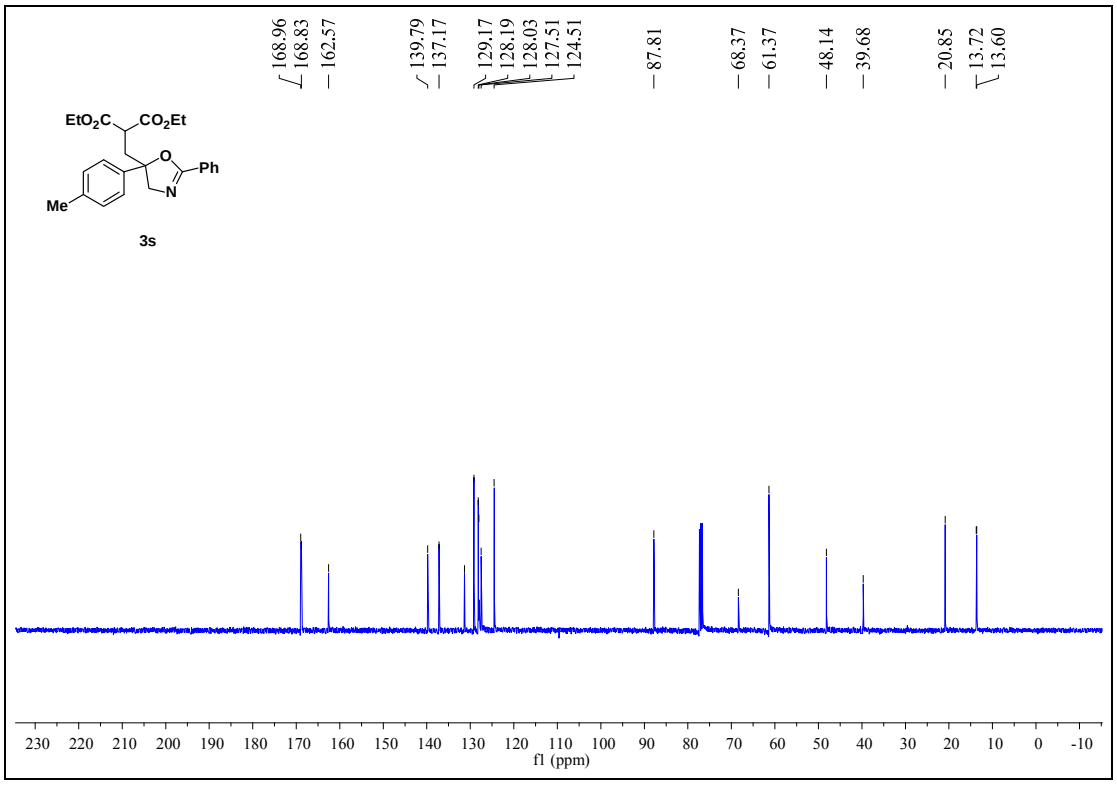
7.26
7.26
7.18
7.17
4.22
4.14
4.08
4.05
4.02
4.00
3.86
3.85
3.40
2.76
2.75
2.34
1.63
1.16
1.10
1.07
0.00
EtO2C
CO2Et
O
Ph
N
Me
3s
2.00
1.02
2.03
2.32
2.00
1.01
1.99
2.07
1.01
0.97
1.99
3.00
3.03
3.02
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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129.17
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128.03
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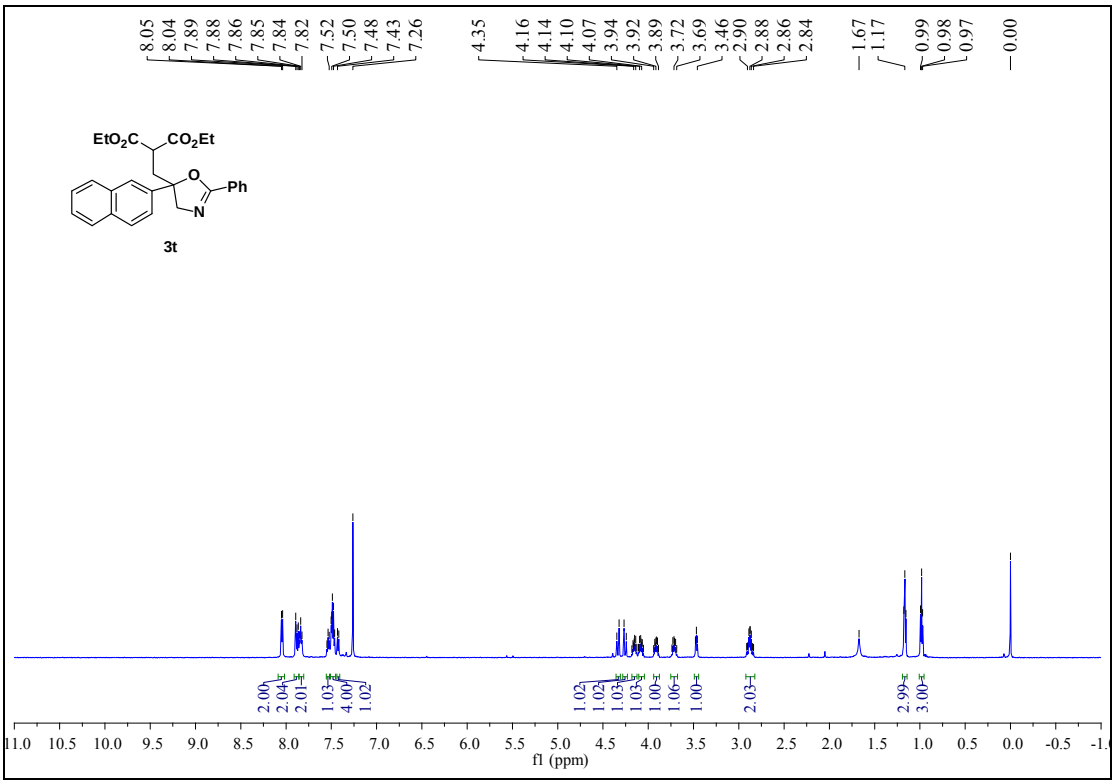
124.51
87.81
68.37
61.37
48.14
39.68
20.85
13.72
13.60
EtO2C
CO2Ph
O
Ph
N
Me
3s
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.04
7.89
7.88
7.86
7.85
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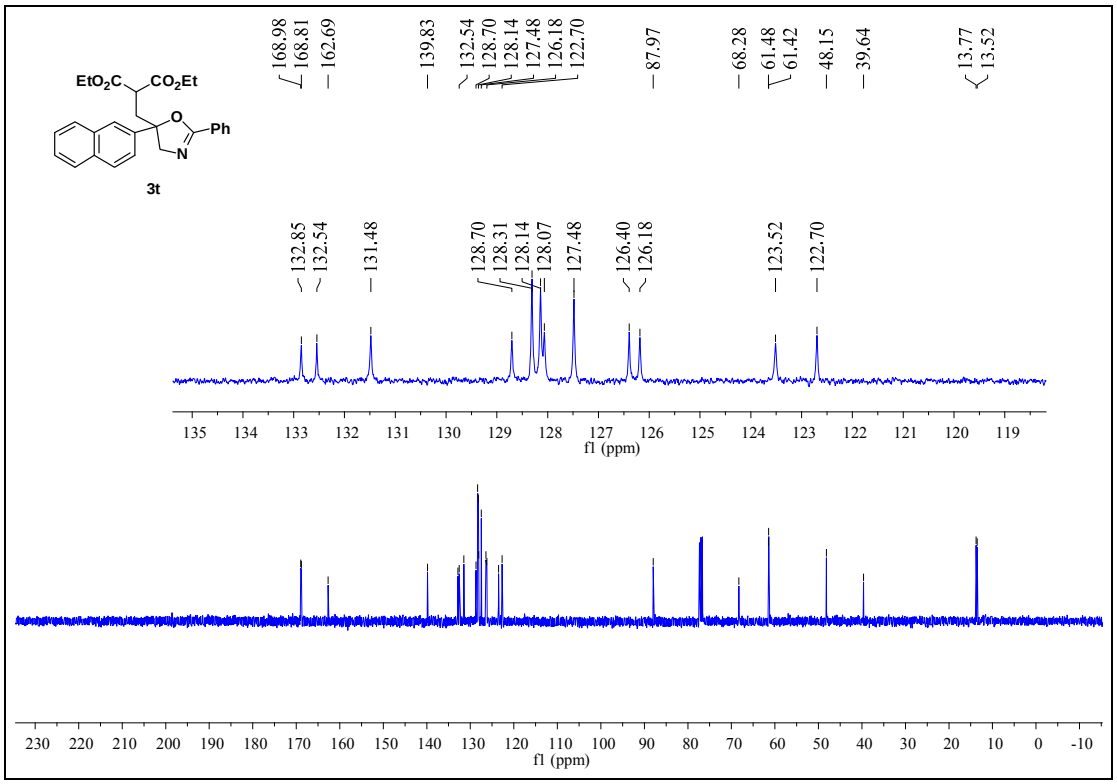
7.82
7.52
7.50
7.48
7.43
7.26
4.35
4.16
4.14
4.10
4.07
3.94
3.92
3.89
3.72
3.69
3.46
2.90
2.88
2.86
2.84
1.67
1.17
0.99
0.98
0.97
0.00
EtO2C
CO2Ph
O
Ph
N
3t
2.00
2.04
2.01
1.03
4.00
1.02
1.02
1.02
1.03
1.03
1.00
1.06
1.00
2.03
2.99
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


EtO2C
CO2Ph
O
N
Ph
3t
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168.81
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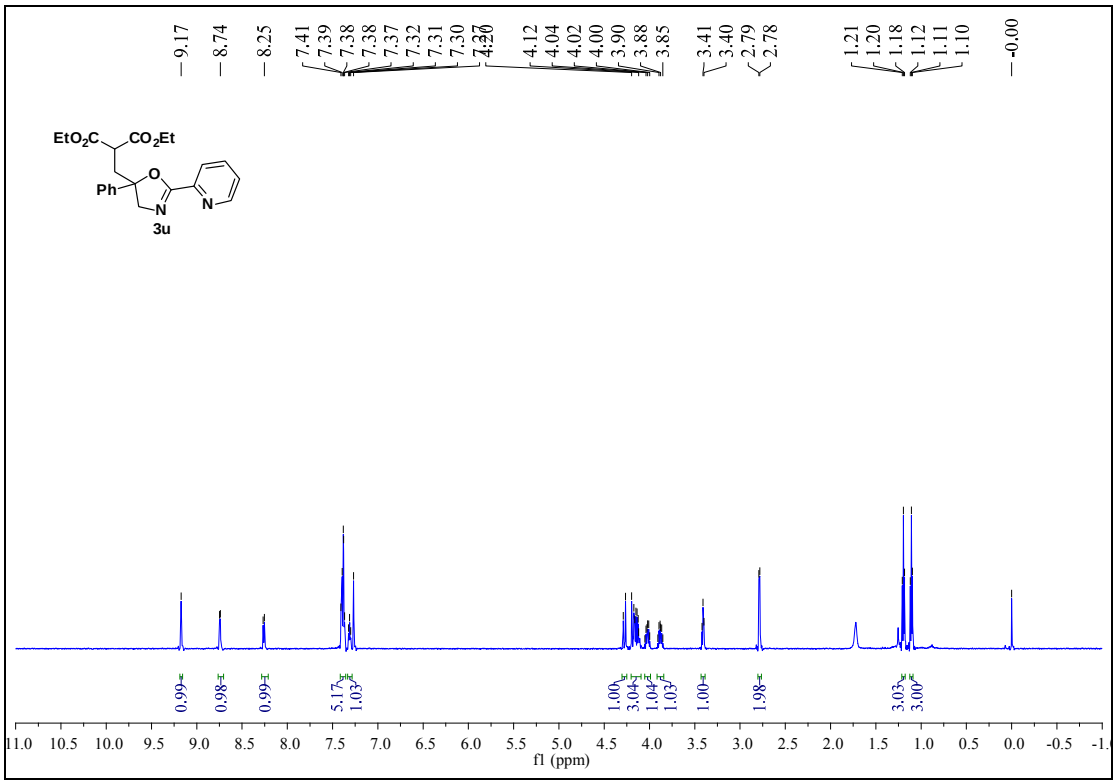
139.83
132.54
128.70
128.14
127.48
126.18
122.70
87.97
68.28
61.48
61.42
48.15
39.64
13.77
13.52
132.85
132.54
131.48
128.70
128.31
128.14
128.07
127.48
126.40
126.18
123.52
122.70
f1 (ppm)
f1 (ppm)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8.74
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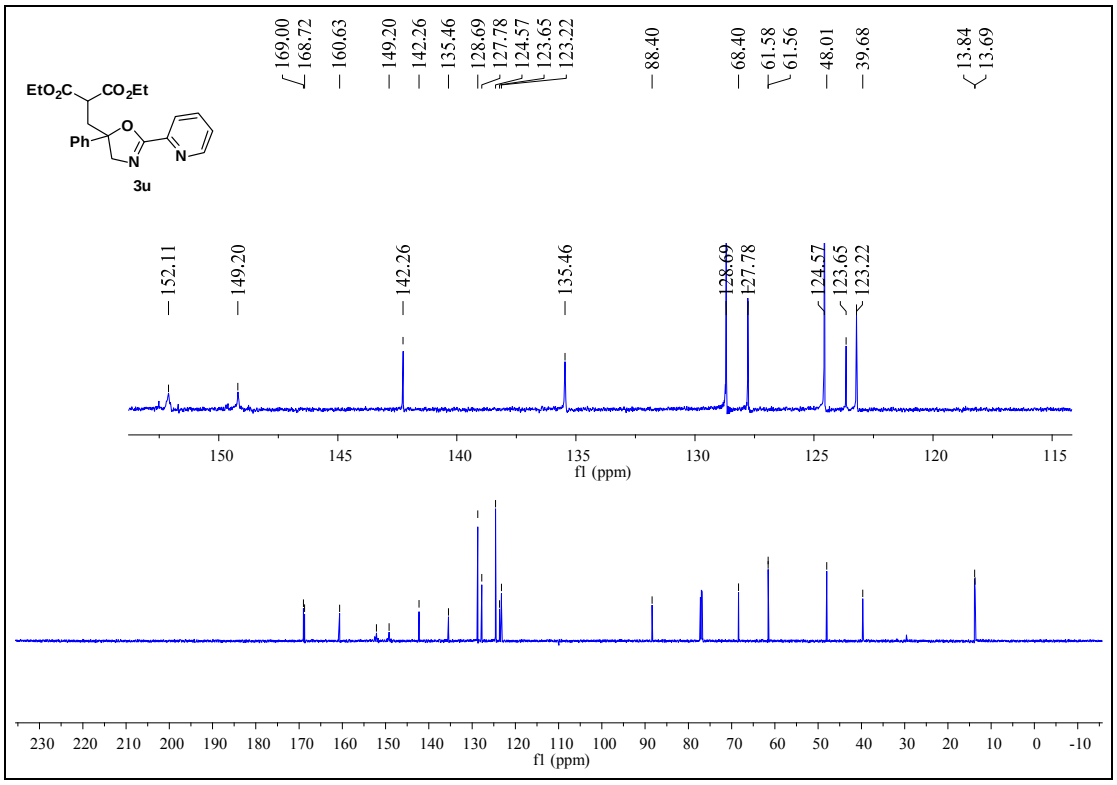
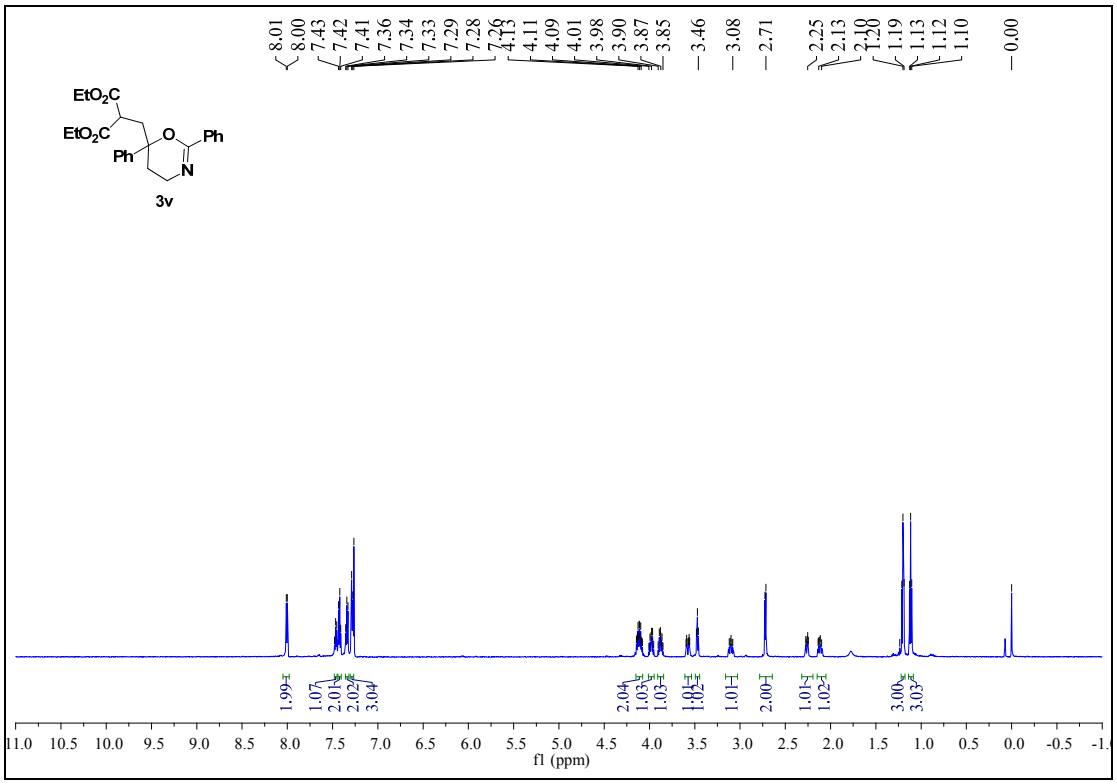
7.38
7.38
7.37
7.32
7.31
7.30
4.12
4.04
4.02
4.00
3.90
3.88
3.85
3.41
3.40
2.79
2.78
1.21
1.20
1.18
1.12
1.11
1.10
-0.00
EtO2C
CO2Et
Ph
O
N
N
3u
0.99
0.98
0.99
5.17
1.03
1.00
3.04
1.04
1.03
1.00
1.98
3.03
3.00
f1 (ppm)


169.00
168.72
160.63
149.20
142.26
135.46
128.69
127.78
124.57
123.65
123.22
88.40
68.40
61.58
61.56
48.01
39.68
13.84
13.69
EtO2C
CO2Et
Ph
O
N
N
3u
152.11
149.20
142.26
135.46
128.69
127.78
124.57
123.65
123.22
150
145
140
135
130
125
120
115
f1 (ppm)
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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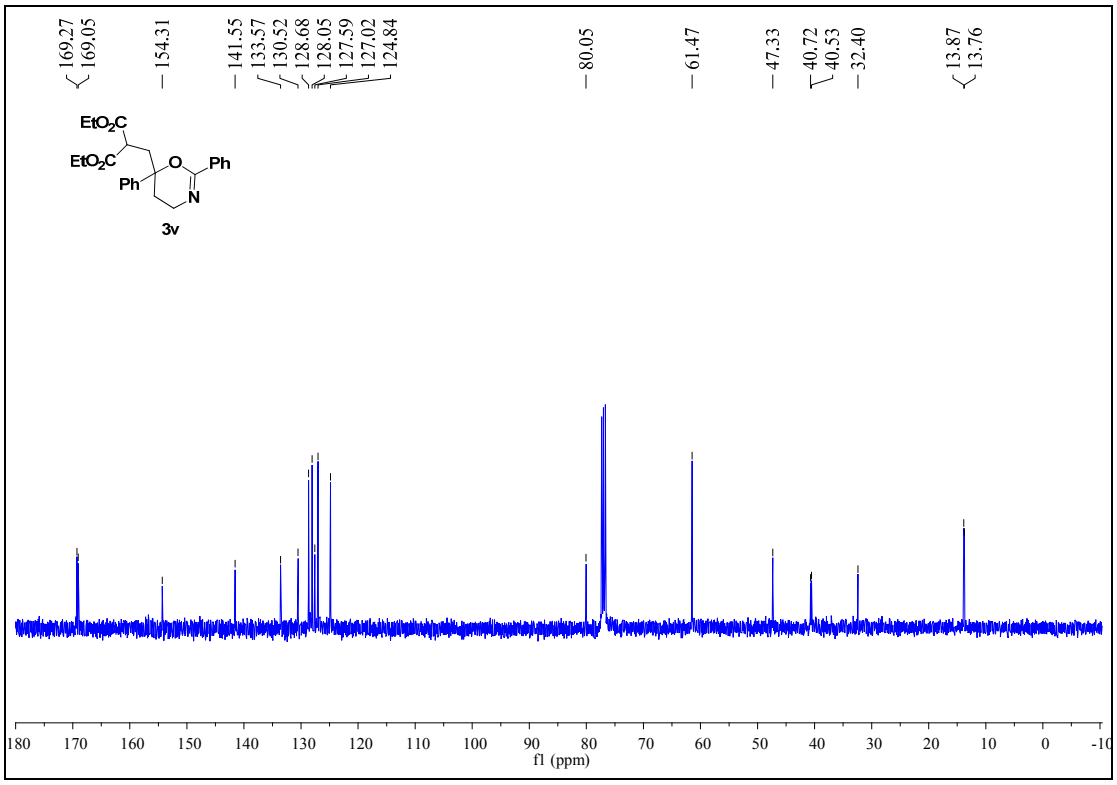
8.00
7.43
7.42
7.41
7.36
7.34
7.33
7.29
7.28
7.26
4.13
4.11
4.09
4.01
3.98
3.90
3.87
3.85
3.46
3.08
2.71
2.25
2.13
2.10
2.00
1.19
1.13
1.12
1.10
0.00
EtO2C
EtO2C
Ph
O
Ph
N
3v
1.99
1.07
2.01
2.02
3.04
2.04
1.03
1.03
1.02
1.02
1.01
2.00
1.01
1.02
3.00
3.03
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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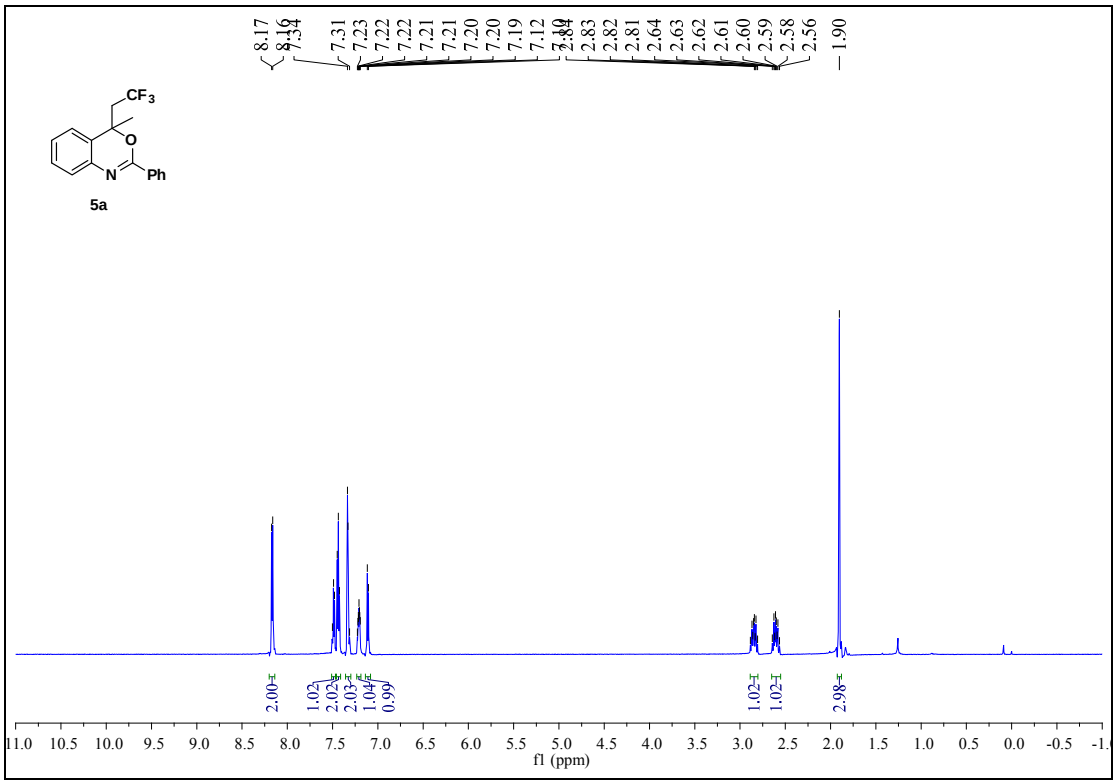
169.05
154.31
141.55
133.57
130.52
128.68
128.05
127.59
127.02
124.84
80.05
61.47
47.33
40.72
40.53
32.40
13.87
13.76
EtO2C
EtO2C
Ph
O
Ph
N
3v
f1 (ppm)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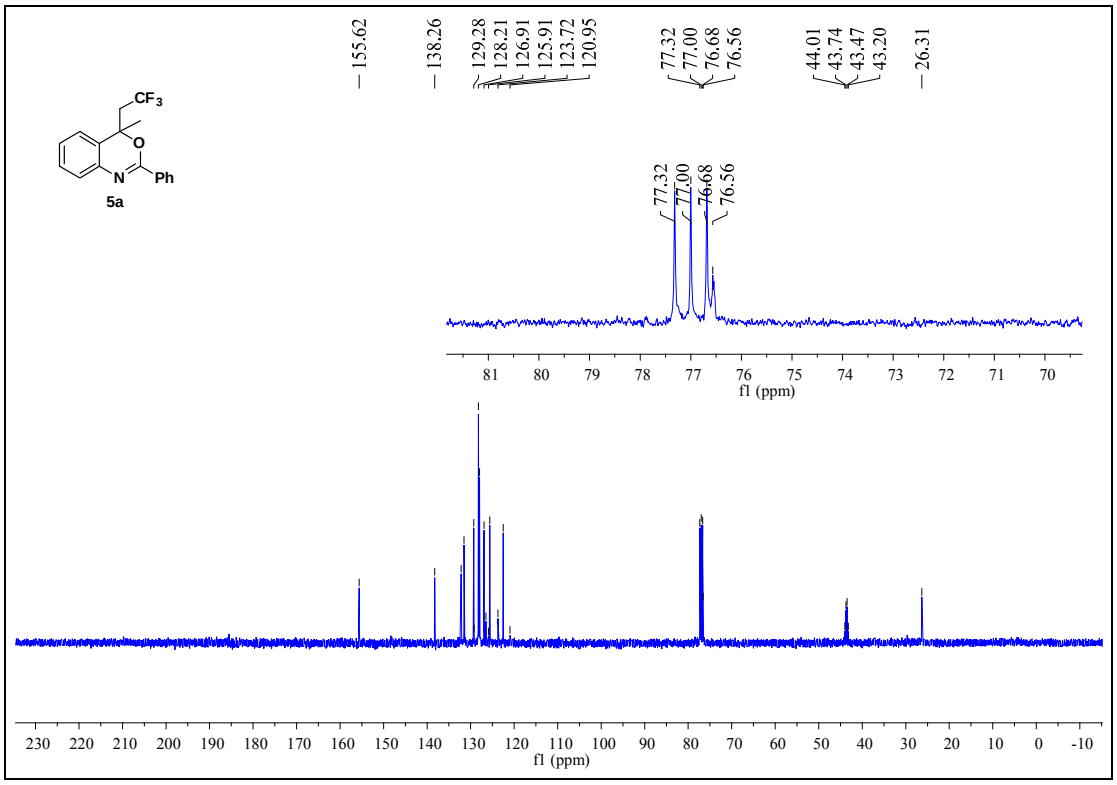
8.16
7.34
7.31
7.23
7.22
7.22
7.21
7.21
7.20
7.20
7.19
7.12
2.83
2.82
2.81
2.64
2.63
2.62
2.61
2.60
2.59
2.58
2.56
1.90
CF3
O
N
Ph
5a
2.00
1.02
2.02
2.03
1.04
0.99
1.02
1.02
2.98
f1 (ppm)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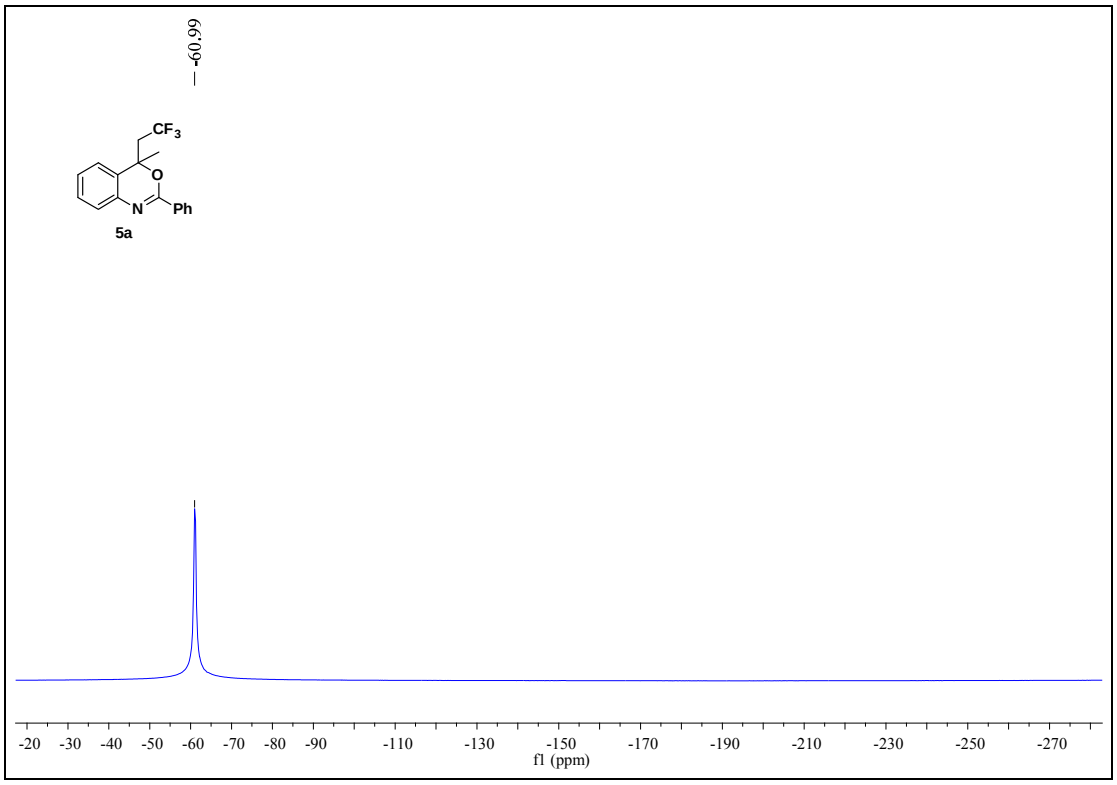
138.26
129.28
128.21
126.91
125.91
123.72
120.95
77.32
77.00
76.68
76.56
44.01
43.74
43.47
43.20
26.31
CF3
O
N
Ph
5a
fl (ppm)
fl (ppm)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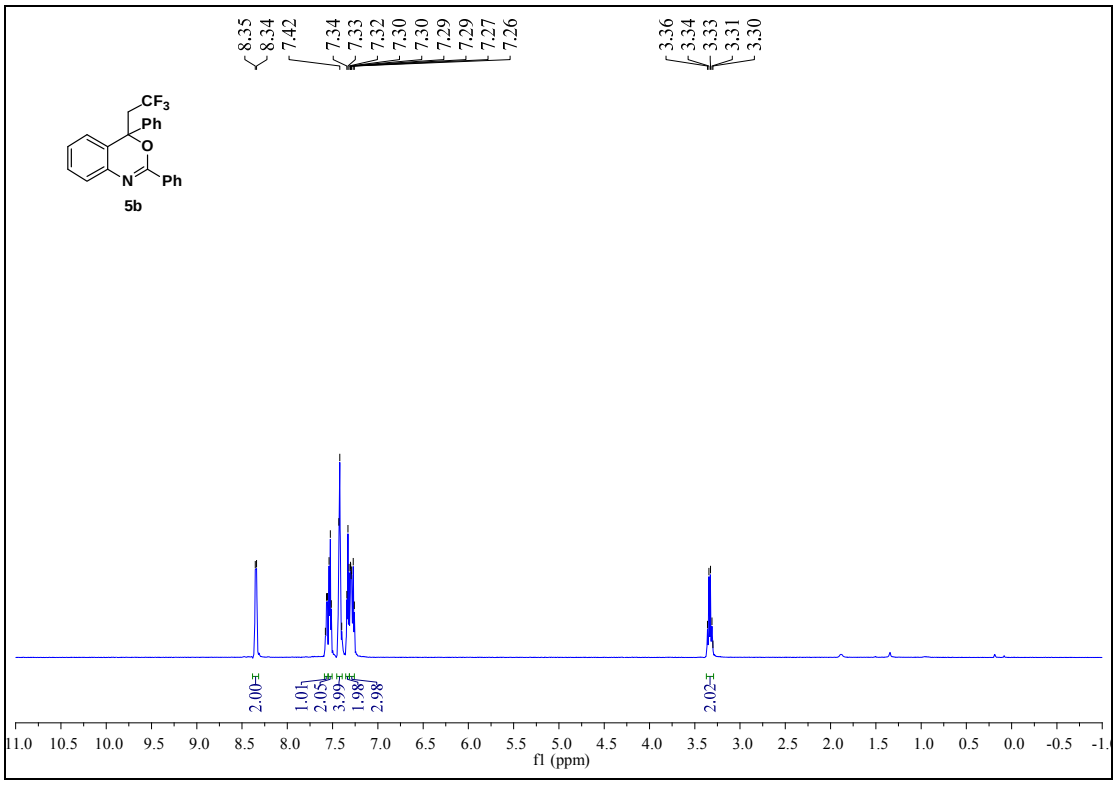
CF3
O
N
Ph
5a
fl (ppm)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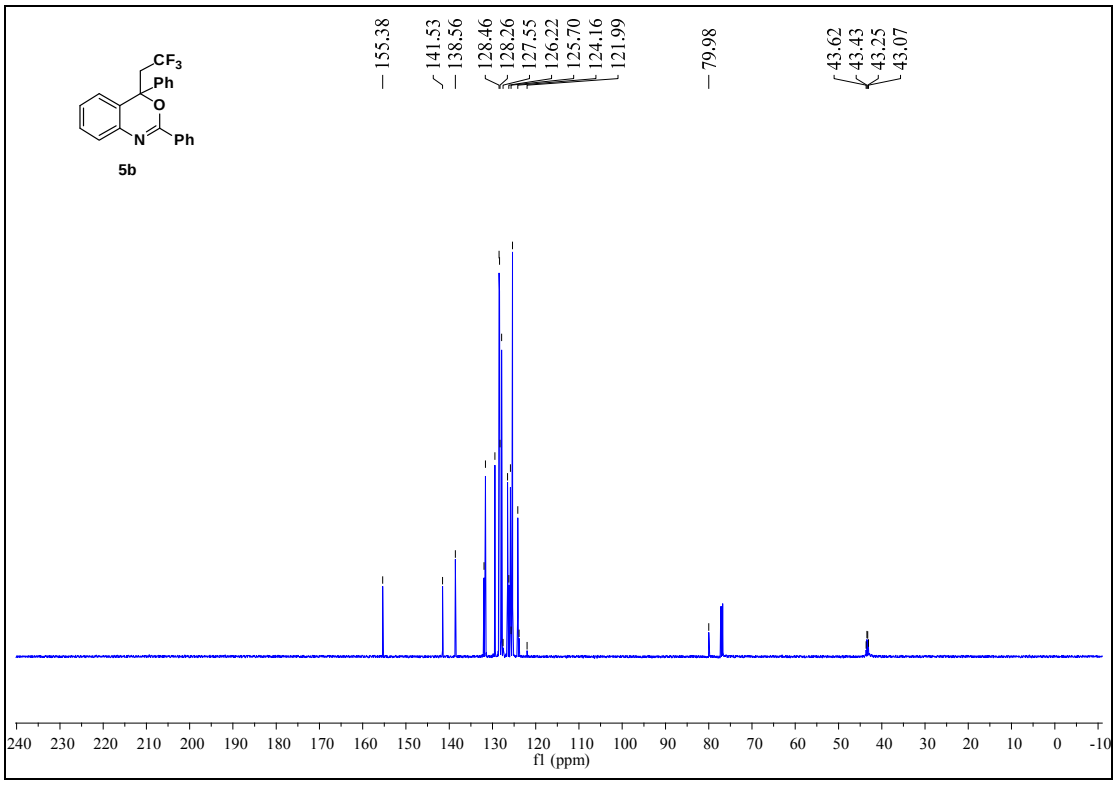
8.34
7.42
7.34
7.33
7.32
7.30
7.30
7.29
7.29
7.27
7.26
3.36
3.34
3.33
3.31
3.30
CF3
Ph
O
N
Ph
5b
2.00
1.01
2.05
3.99
1.98
2.98
2.02
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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141.53
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128.46
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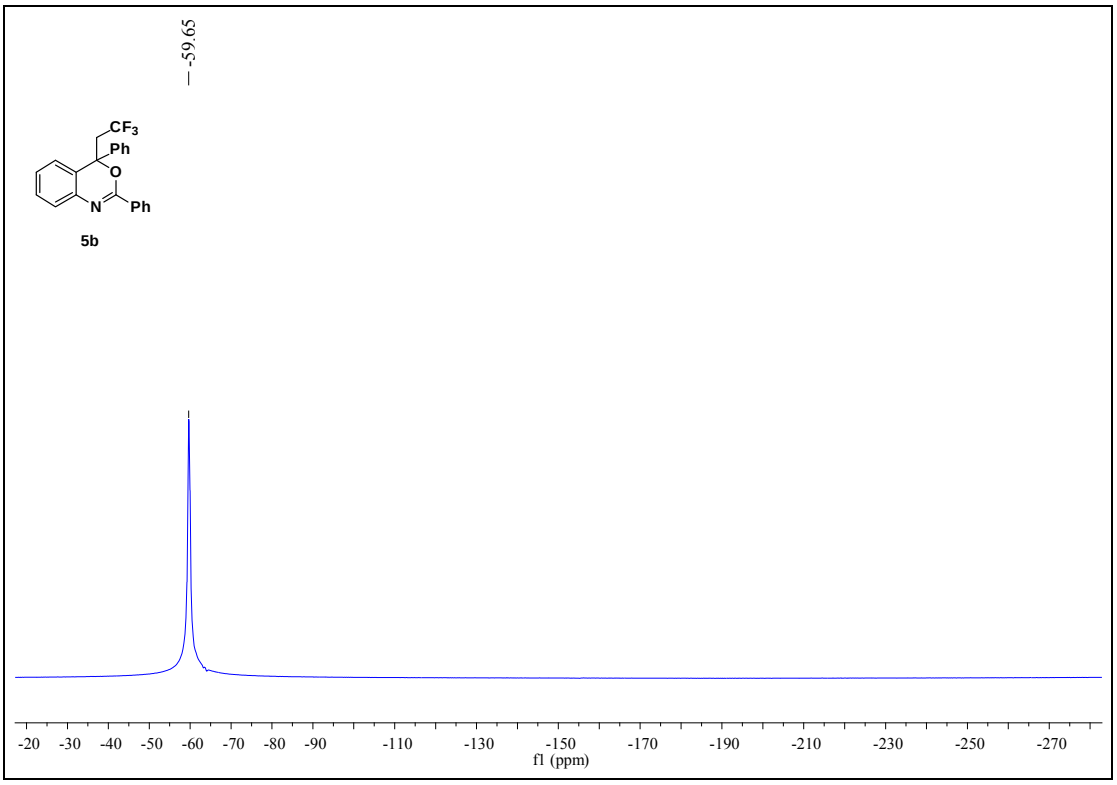
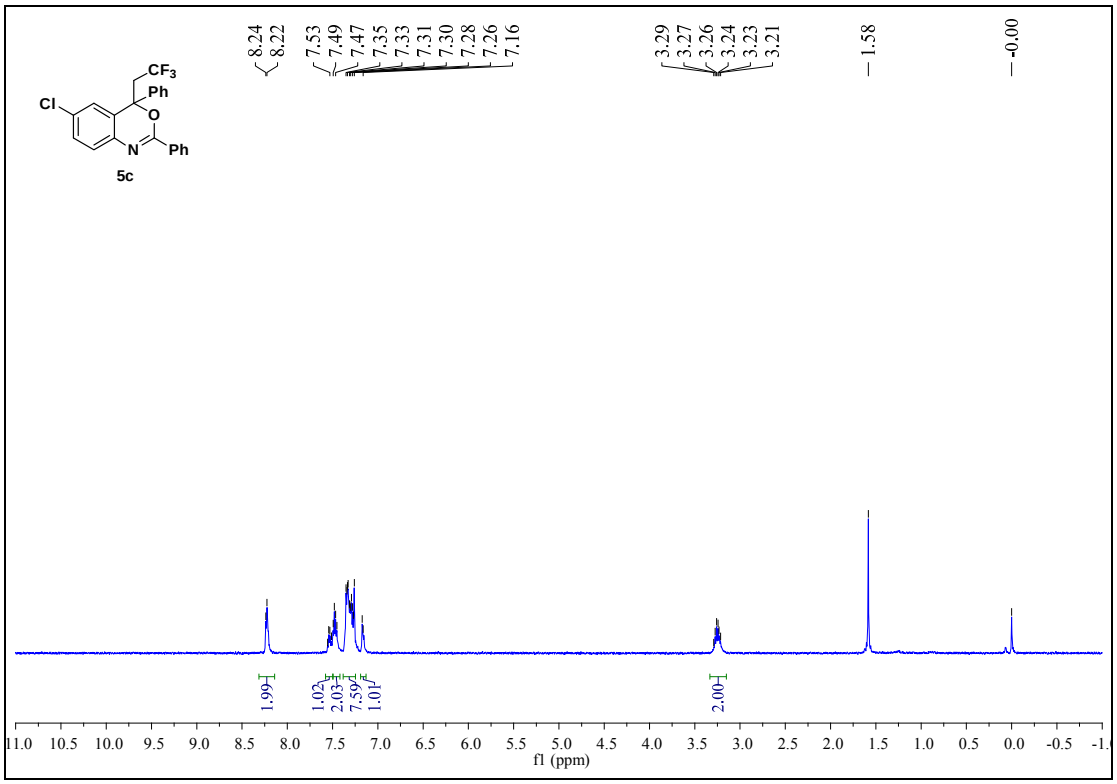
127.55
126.22
125.70
124.16
121.99
79.98
43.62
43.43
43.25
43.07
CF3
Ph
O
N
Ph
5b
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-59.65
CF3
Ph
O
N
Ph
5b
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)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8.22
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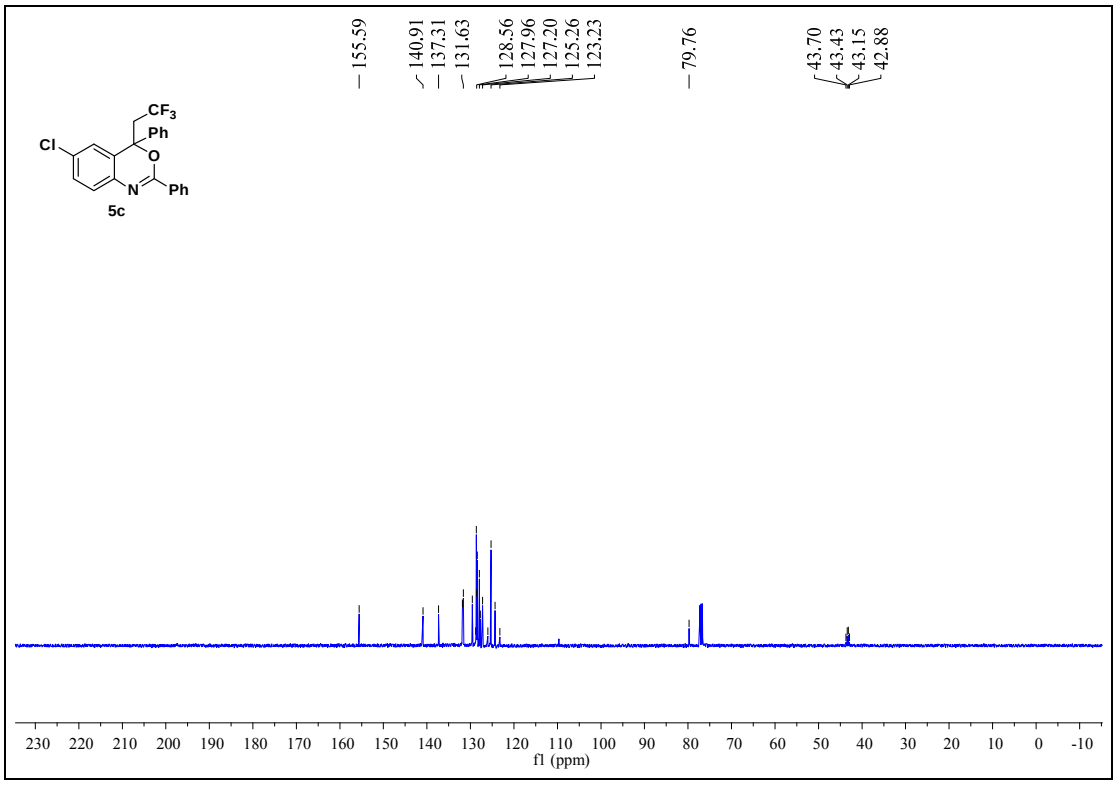
7.35
7.33
7.31
7.30
7.28
7.26
7.16
3.29
3.27
3.26
3.24
3.23
3.21
1.58
0.00
CF3
Ph
Cl
O
N
Ph
5c
1.99
1.02
2.03
7.59
1.01
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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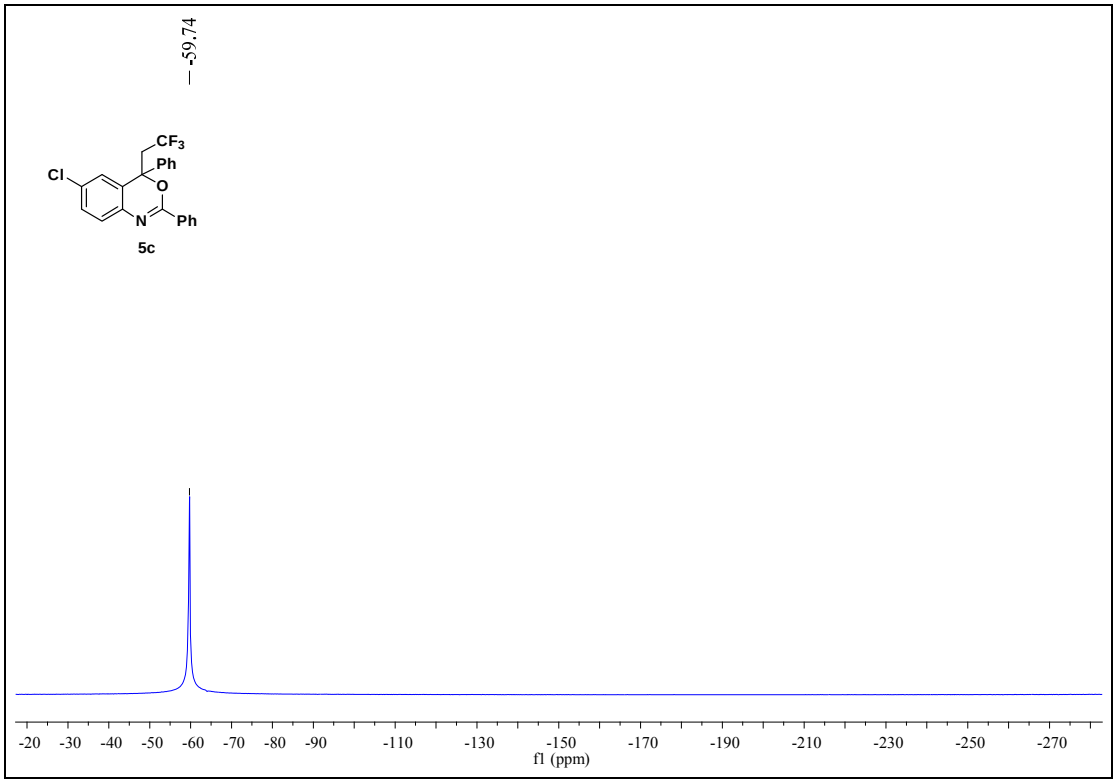
128.56
127.96
127.20
125.26
123.23
79.76
43.70
43.43
43.15
42.88
CF3
Ph
Cl
O
N
Ph
5c
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-59.74
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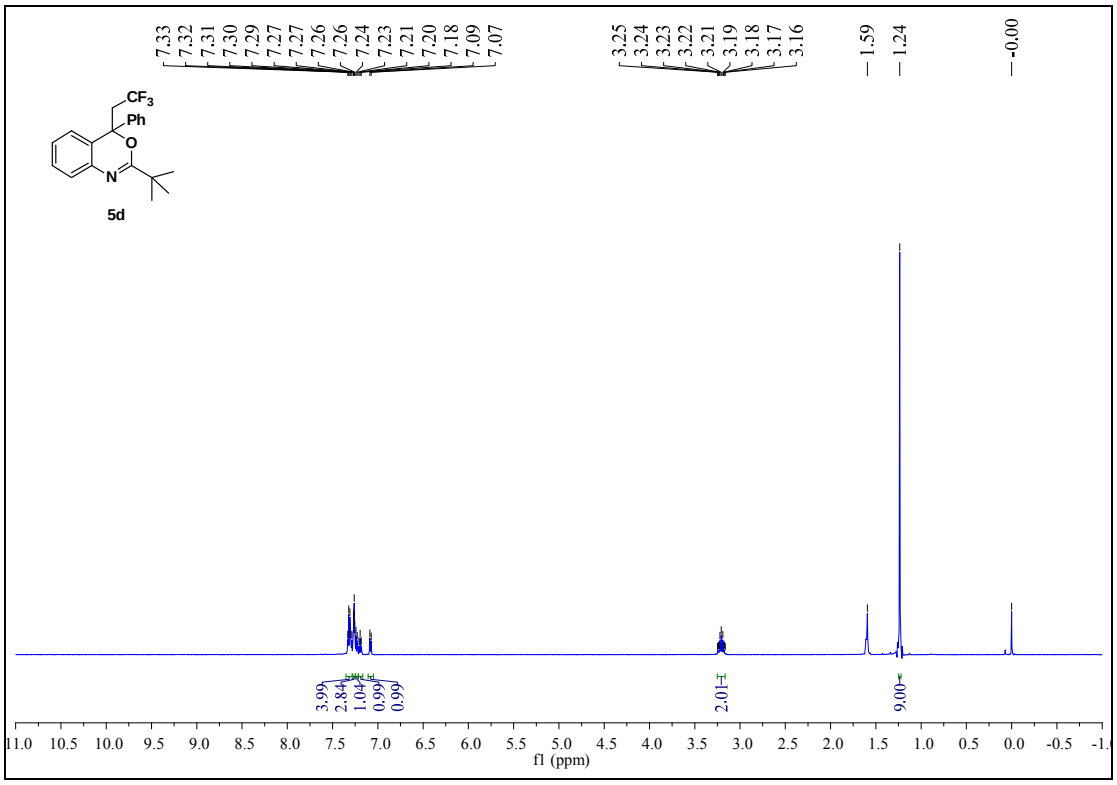
Ph
Cl
O
N
Ph
5c
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)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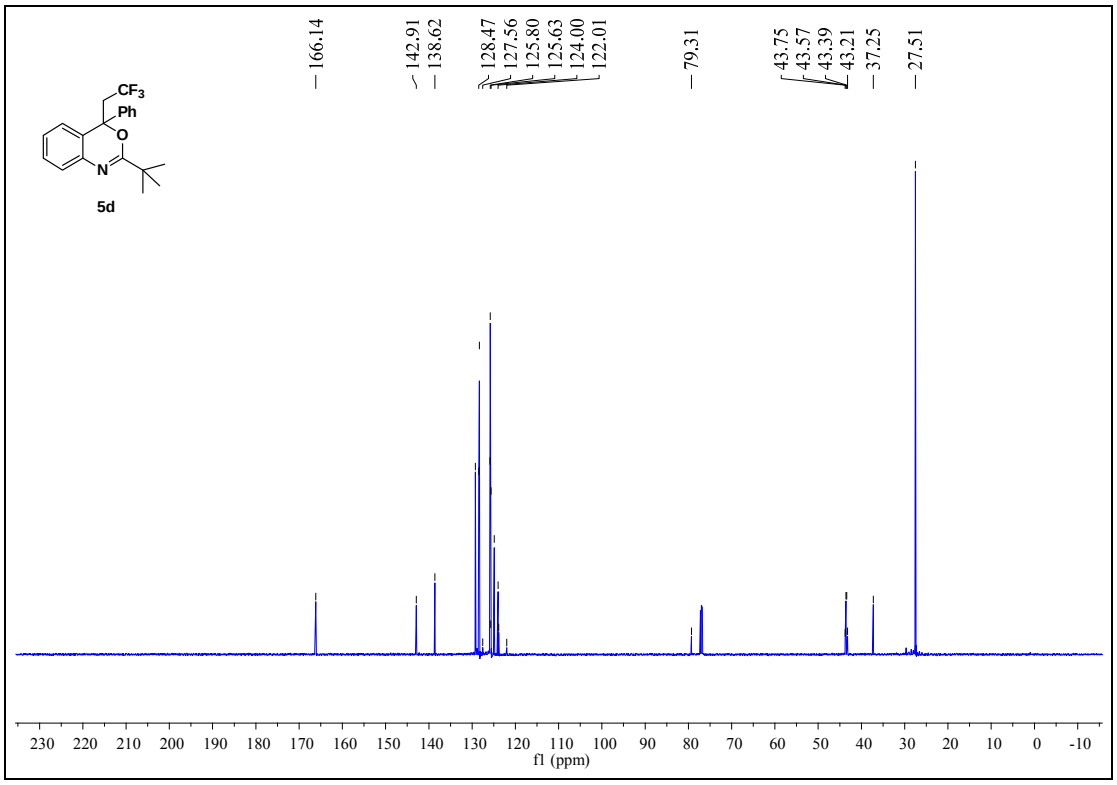
7.27
7.27
7.26
7.26
7.24
7.23
7.21
7.20
7.18
7.09
7.07
3.25
3.24
3.23
3.22
3.21
3.19
3.18
3.17
3.16
1.59
1.24
0.00
CF3
Ph
O
N
5d
3.99
2.84
1.04
0.99
0.99
2.01
9.00
f1 (ppm)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124.00
122.01
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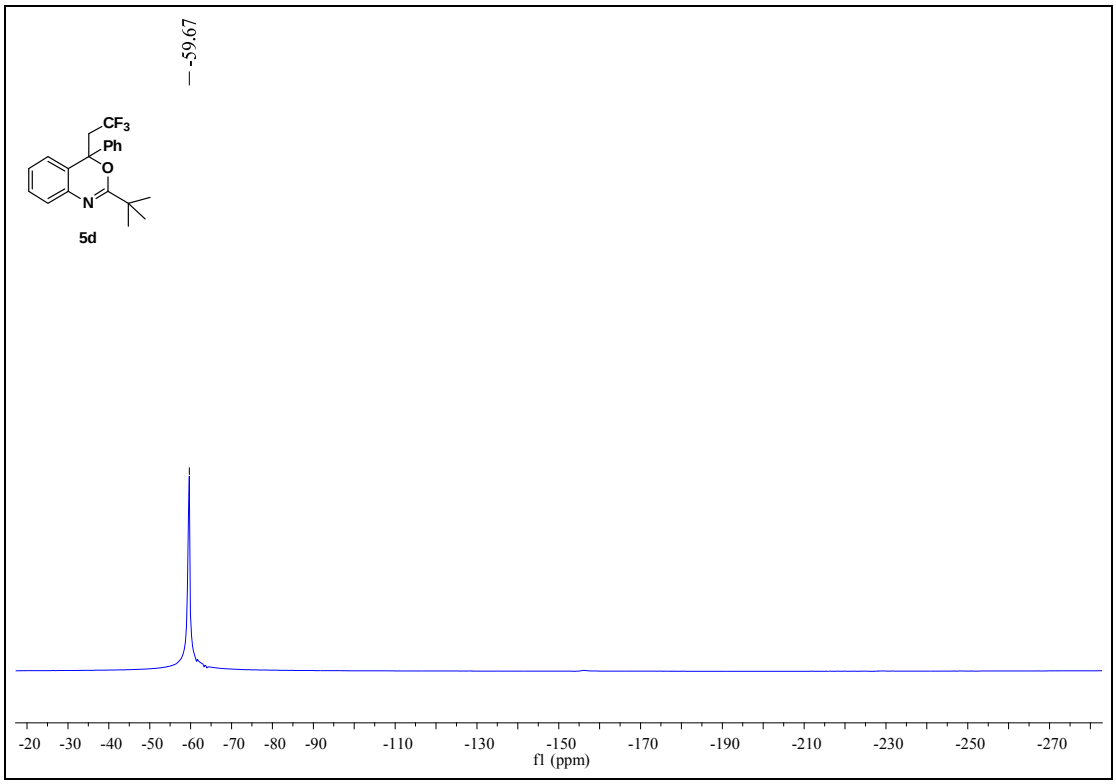
43.57
43.39
43.21
37.25
27.51
CF3
Ph
O
N
5d
f1 (ppm)


-59.67
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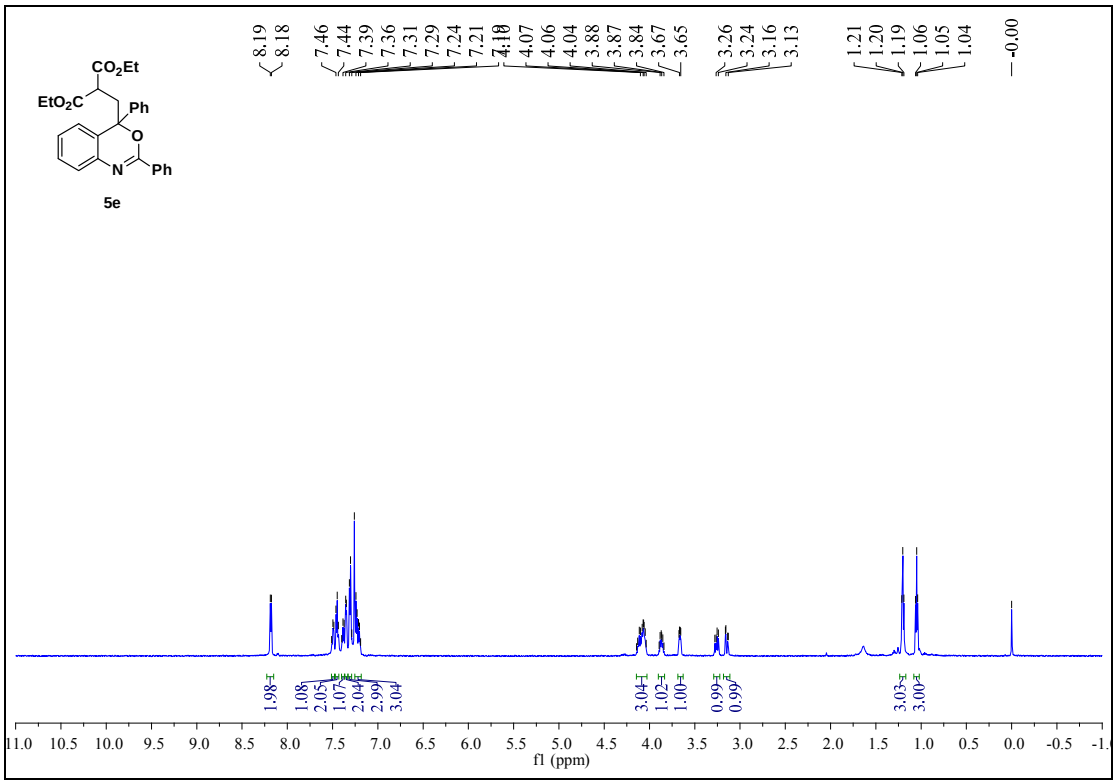
Ph
O
N
5d
-20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)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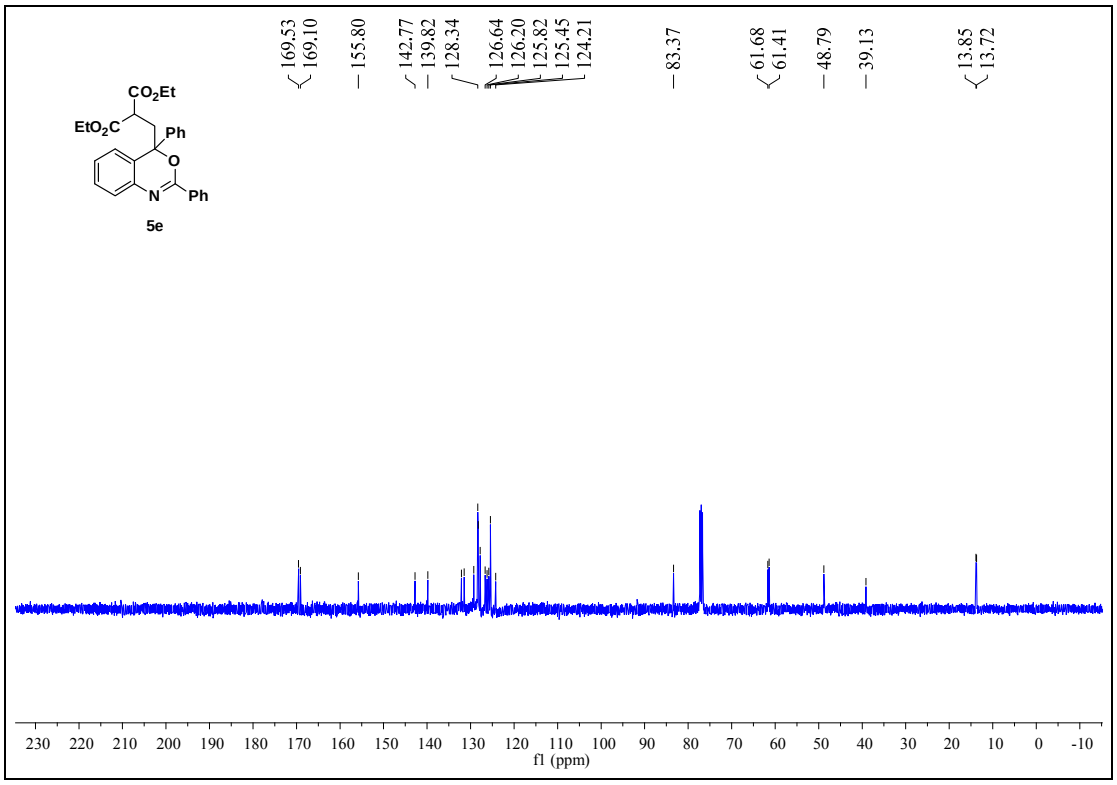
7.31
7.29
7.24
7.21
4.10
4.07
4.06
4.04
3.88
3.87
3.84
3.67
3.65
3.26
3.24
3.16
3.13
1.21
1.20
1.19
1.06
1.05
1.04
-0.00
CO2Et
EtO2C
Ph
O
N
Ph
5e
1.98
1.08
2.05
1.07
2.04
2.99
3.04
3.04
1.02
1.00
0.99
0.99
3.03
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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169.10
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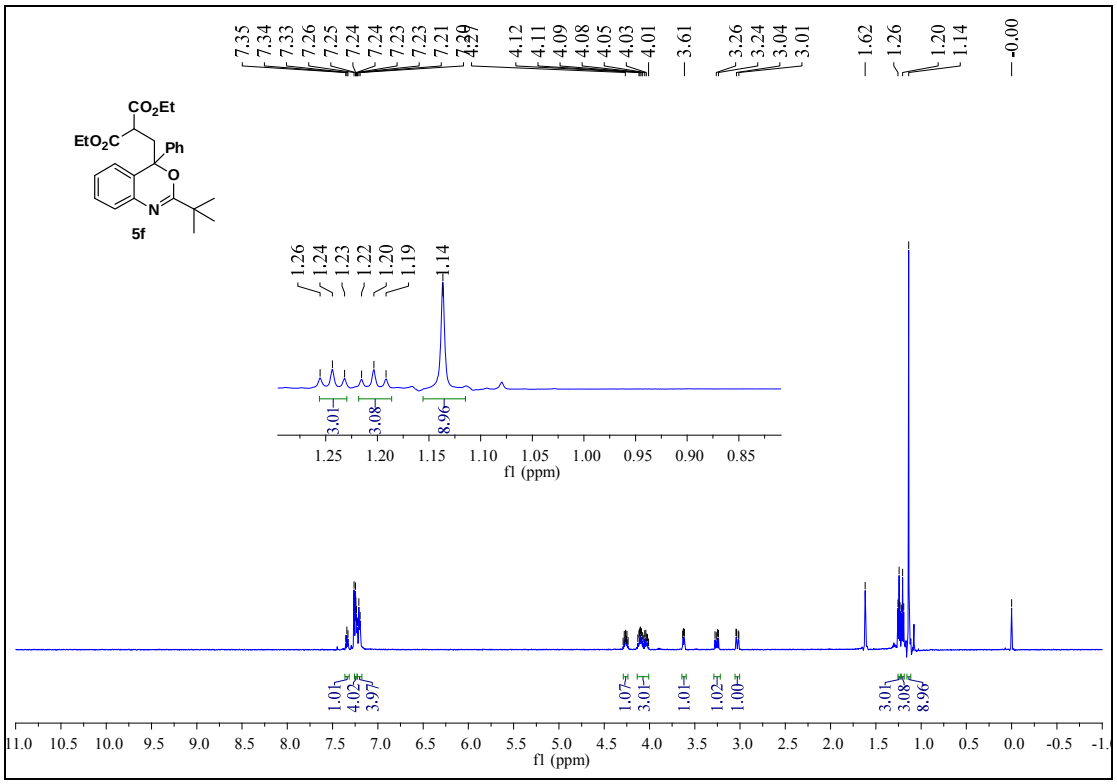
126.64
126.20
125.82
125.45
124.21
83.37
61.68
61.41
48.79
39.13
13.85
13.72
CO2Et
EtO2C
Ph
O
N
Ph
5e
fl (ppm)


7.35
7.34
7.33
7.26
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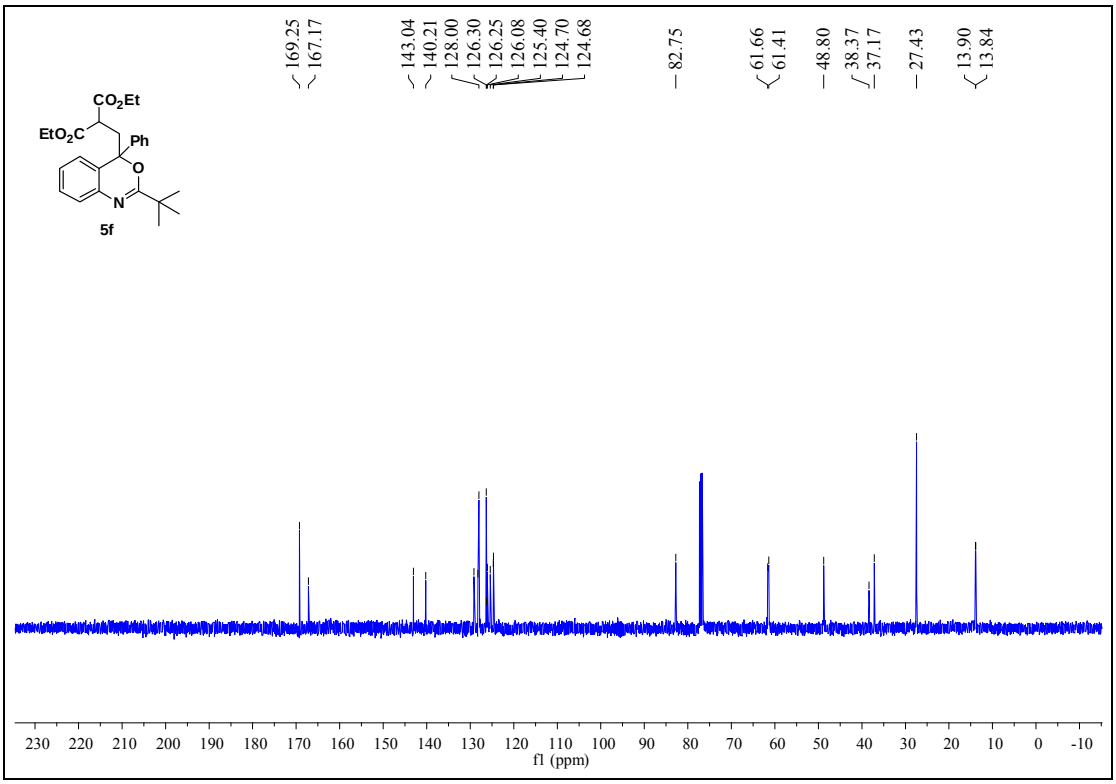
7.24
7.24
7.23
7.23
7.21
4.12
4.11
4.09
4.08
4.05
4.03
4.01
3.61
3.26
3.24
3.04
3.01
1.62
1.26
1.20
1.14
0.00
CO2Et
EtO2C
Ph
O
N
5f
1.26
1.24
1.23
1.22
1.20
1.19
1.14
3.01
3.08
8.96
fl (ppm)
1.01
4.02
3.97
1.07
3.01
1.01
1.02
1.00
3.01
3.08
8.96
fl (ppm)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126.25
126.08
125.40
124.70
124.68
82.75
61.66
61.41
48.80
38.37
37.17
27.43
13.90
13.84
CO2Et
EtO2C
Ph
O
N
5f
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)