Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Information

Palladium-Catalyzed Olefin Epoxidation with Electrophilic Reagents as Oxidizing Agents

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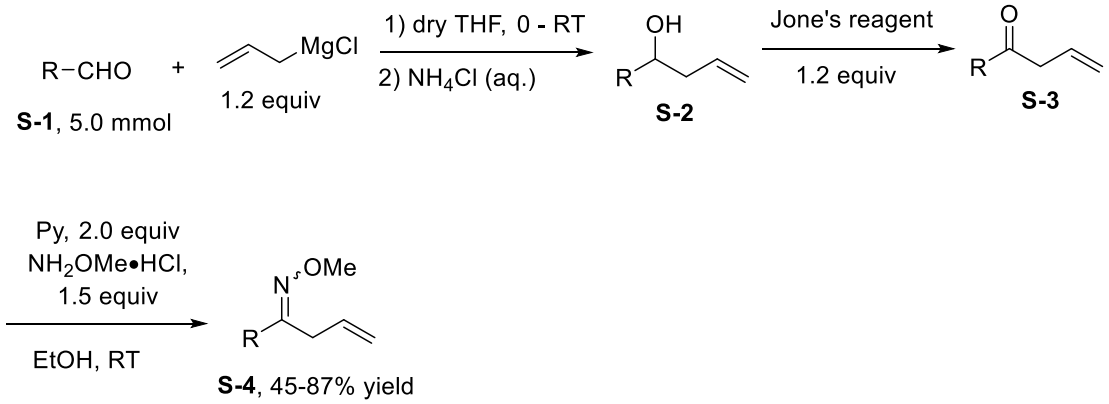
1. General Information

All purchased reagents and solvents were used without further purification unless otherwise noted. Analytical thin layer chromatography was performed by using commercially prepared 100-400 mesh silica gel plates (GF_{254}) and visualization was effected at 254 nm. All the *ortho*-alkynyl phenylacetonitrile were prepared according to known procedures. All commercially available aryl alkynes were purchased from Innochem, Energy Chemical, Bidepharm. All the reaction temperatures reported are oil bath temperature. ^{1}H and ^{13}C NMR spectra were recorded using a Bruker Asend-400 spectrometer using $CDCl_3$. The chemical shifts are referenced to signals at 0.00 and 77.0 ppm, respectively. NMR data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, hept = heptet, qd = quartet of doublet, dd = doublet of doublet, td = triplet of doublet, m = multiplet, *etc.*), coupling constants (Hz) and integration. Coupling constants (*J*) were reported in Hz and referred to apparent peak multiplications. The data of HRMS was carried out on a high-resolution mass spectrometer (LCMS-ESI-TOF). GC-MS analyses were performed on a Thermo Scientific ISQ gas chromatograph-mass spectrometer at an ionization voltage of 70 eV and equipped with a DB-WAX capillary column (internal diameter: 0.25 mm, length: 30 m). IR spectra were obtained as potassium bromide pellets with a Bruker TENSOR 27 spectrometer. Chiral HPLC analyses were performed on an Aglient 1200 system.

2. Experimental Section

2.1 Synthesis of Substrates

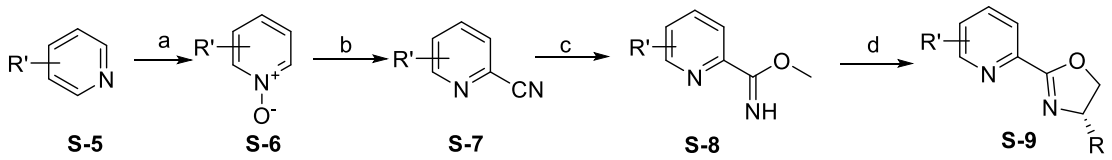


According to the known literature[17,18], aldehyde **S-1** (5 mmol) was dissolved in 10 mL of dried THF in 50 mL Schlenk tube under N2. The mixture was cooled to 0 °C and Grignard reagent (1.2 equiv) was added dropwise with stirring under ice bath. Then it was allowed to warm to room temperature and stirred for 12 h. After completion, the mixture was quenched with NH4Cl (aq.). The aqueous layer was extracted with ethyl acetate (3×25 mL). The combined organic layers weredried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The crudemixture was purified by flash column chromatography on silica gel to give the desired products **S-2.**

Products **S-2** was dissolved in 10 mL DCM in round bottom flask, Jone′s reagent (1.2 equiv) was added into solution in batches with stirring under ice bath. Then it was allowed to warm to room temperature and stirred for 5 h. After completion, the aqueous layer was extracted with DCM (3×25 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The crude mixture was purified by flash column chromatography on silica gel to give the desired products **S-3**.

Products **S-3** was dissolved in 5 mL EtOH in round bottom flask, Py (2.0 equiv) and NH_2OMe•HCl (1.5 equiv) was added into solution with stirring under room temperature. Then it was allowed to warm to room temperature and stirred for 12 h. After completion, the mixture was quenched with NaCl (aq.). the aqueous layer was extracted with EA. The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The crude mixture was purified by flash column chromatography on silica gel to give the desired products **S-4**.

2.2 Synthesis of Ligands



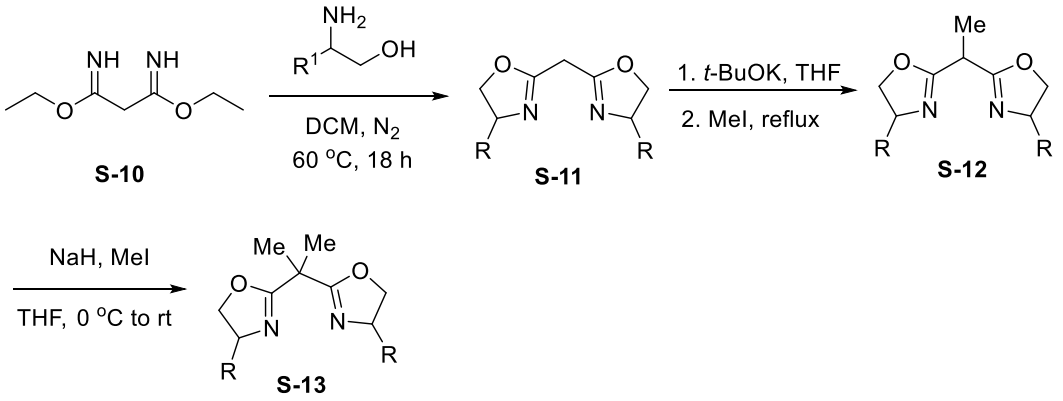
General Procedure for the Synthesis of **S-9**[12]

(a) To a 150 mL round bottom flask with a stir bar was charged with **S-5** (15 mmol) and 30 mL DCM at 0 °C. A solution of *m*-CPBA (1.7 euqiv) in 20 mL of DCM was added to reaction vail. The reaction mixture was stirred for 12 h at room temperature. Then quenched with 4,0 equiv of K_2CO_3, the reaction mixture was stirred for 30 minutes. To the reaction mixture was added aqueous NH_4Cl (10 mL), extracted by DCM for three times, dried over Na_2SO_4, and evaporated in vacuum to afford the crude product, which was purified by flash chromatography on silica gel with PE/EA to give compounds **S-6**.

(b) To a 150 mL round bottom flask with a stir bar was charged with **S-6** (10 mmol), TMSCN (1.2 equiv) and 20 mL DCM at 0 °C. A solution of N, N-Dimethylaminoformyl (1.2 equiv) in 5.0 mL of DCM was added to reaction vail. The reaction mixture was stirred for 24 h at room temperature. Then quenched with aqueous K_2CO_3, extracted by DCM for three times, dried over Na_2SO_4, and evaporated in vacuum to afford the crude product, which was purified by flash chromatography on silica gel with PE/EA to give compound **S-7**.

(c) To a 50 mL round bottom flask with a stir bar was charged with **S-7** (5.0 mmol), MeONa(0.3 equiv) and 10 mL dry MeOH under N_2. The mixture was stirred for 12 h at 40 °C. Then evaporated in vacauum to afford the crude product. To the crude product was added aqueous NH_4Cl, extracted by EtOAc for three times, dired over Na_2SO_4, and ecaprorated in vacuum to affoed the product **S-8**. No further purification is required for the next step.

(d) To a 25 mL round bottom flask with **S-8** (2.0 mmol), amino alcohol (2.0 mmol) and 5.0 mL THF. Concentrated HCl (1 drops) was added to the solution and the mixture was heated to 80 °C under N_2 atmosphere. After the reaction was completed, the organic solvent was removed under vacuum. The residue was purified by flash column chromatography on silica gel to afford **S-9**.



General Procedure for the Synthesis of **S-13**[19]

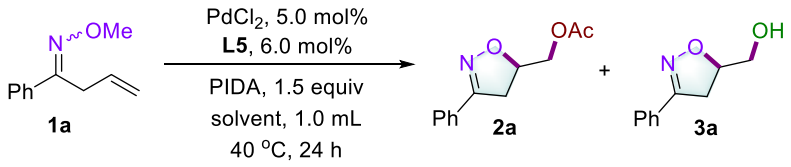
To a 50 mL round bottom flask with **S-10** (10.0 mmol), amino alcohol (11 mmol, 1.1 equiv) and 10.0 mL dry DCM under N_2. The mixture was stirred for 18 h at 60 °C. After the reaction was completed, the organic solvent was removed under vacuum. The residue was purified by flash column chromatography on silica gel to afford **S-11** (31-75% yield).

t-BuOK (5.0 mmol) was added to a solution of **S-11** (5.0 mmol) in 20 mL dry THF at room temperature and the mixture was stirred for 1 h under N_2. Methyl iodide (10 mmol) was added S-11 and the reaction was heated to reflux for 4 h. After evaporating solvent under reduced pressure, brine (35 mL) was added to the crude product and the aqueous phase was extracted with ethyl acetate (3×50 mL). The combined organic phases were dried over Na_2SO_4 and filtered, and evaporated in vacuum to afford the crude product, which was purified by flash chromatography on silica gel with PE/EA to give compound **S-12** (67-83% yield).

To a solution of **S-12** (3.0 mmol) in dry THF (5.0 mL) was added slowly NaH (4.5 mmol) at 0 °C under N_2, then slowly add MeI (20.0 mmol) to the reaction system. After the addition was completed, the reaction mixture was allowed to reach room temperature, and the reaction was completed as monitored by TLC. The reaction was quenched by dropwise addition of water until effervescence ceased and then extracted with ethyl acetate, dried over Na_2SO_4, filtered and the filtrate was concentrated under reduced pressure, purified by flash column chromatography (PE/EA = 10/1) to give **S-13**(53-76% yield).

2.3 Optimization reaction conditions

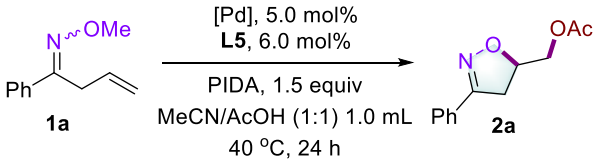
Table S1 The effect of solvent on the reaction



Entry[a]	Solvent	V:V	2a/Yield(%)	3a/Yield[b](/%)
1	DMSO	-	N. D.	N. D.
2	THF	-	N. D.	N. D.
3	1,4-Dioxane	-	N. D.	N. D.
4	DMF	-	N. D.	N. D.
5	MeCN	-	N. D.	N. D.
6	DCE	-	N. D.	N. D.
7	Toluene	-	N. D.	N. D.
8	AcOH	-	43	N. D.
9	DMSO/AcOH	1:1	N.D.	41 (0% ee)
10	THF/AcOH	1:1	5	N. D.
11	1,4-Dioxane /AcOH	1:1	trace	N. D.
12	DMF/AcOH	1:1	trace	N. D.
13	MeCN/AcOH	1:1	41(0% ee)	N. D.
14	DCE/AcOH	1:1	12	N. D.
15	Toluene/AcOH	1:1	7	N. D.

[a] Reaction conditions: **1a** (0.3 mmol), $PdCl_2$ (5 mol%)，**L5** (6.0 mol%), PIDA (1.5 euqiv) in solvent 1.0 mL at 40 °C for 24 h unless otherwise noted. [b] Isolated yield. N. D = Not detected. The ee values were determined by HPLC.

Table S2 The effect of catalysts on the reaction

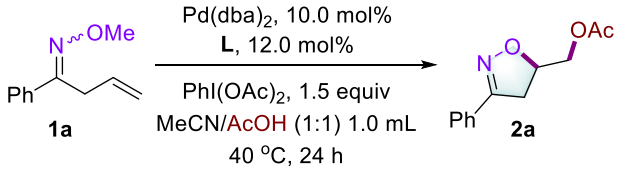


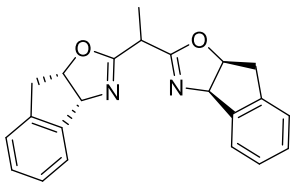
Entry[a]	[Pd]	**2a**/Yield[b](/%)
1	$Pd(OAc)_2$	42
2	$Pd(TFA)_2$	45
3	$Pd(MeCN)_2Cl_2$	43

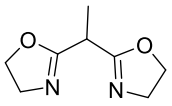
4	$Pd(acac)_2$	29
5	$Pd_2(dba)_3$	62
6	$Pd(dba)_2$	67
7	$Pd(PPh_3)_4$	trace
8[c]	10 mol% $Pd(dba)_2$	75

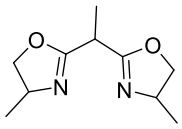
[a] Reaction conditions: **1a** (0.3 mmol), [Pd] (5 mol%), **L5** (6.0 mol%), PIDA (1.5 euqiv) in solvent 1.0 mL at 40 °C for 24 h unless otherwise noted. [b] Isolated yield. [c] 10 mol% $Pd(dab)_2$, 12 mol% **L5**. N. D = Not detected.

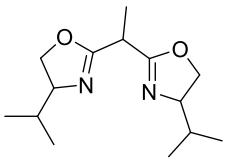
Table S3 The effect of Ligand on the reaction

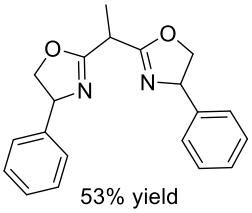


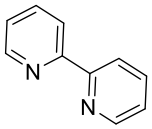

70% yield

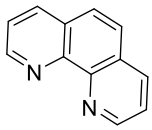

25% yield

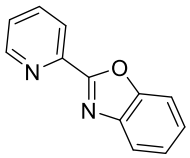

43% yield

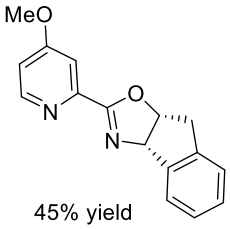

51% yield

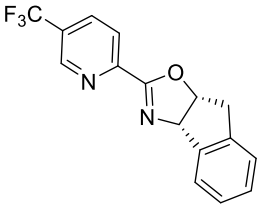

53% yield

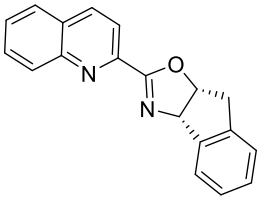

3% yield

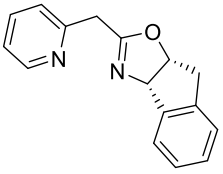

11% yield

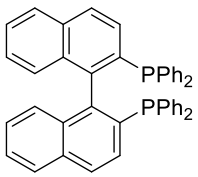

5% yield

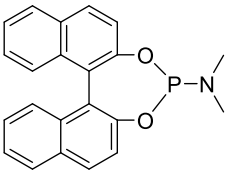

45% yield

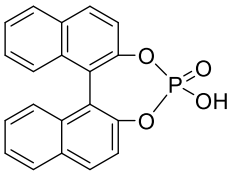

53%% yield

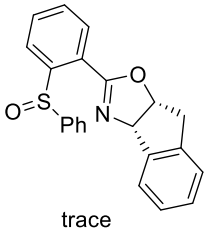

23% yield


32% yield


N.D.

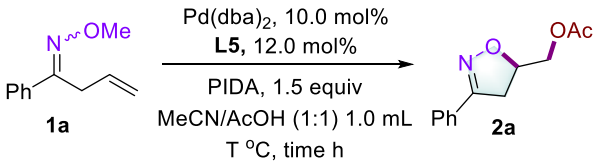

trace


N.D.


trace

[a] Reaction conditions: **1a** (0.3 mmol), $Pd(dba)_2$ (10.0 mol%), **L5** (12.0 mol%), PIDA (1.5 euqiv) in MeCN/AcOH (1:1) 1.0 mL at 40 oC for times h unless otherwise noted. [b] Isolated yield. N. D = Not detected.

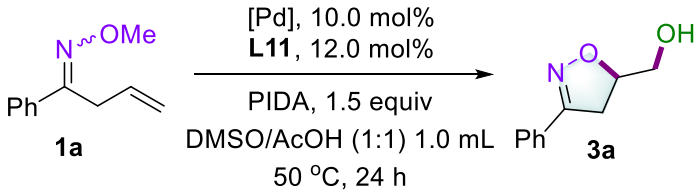
Table S4 Optimization of temperature and time conditions



Entry[a]	T/°C	Time/h	**2a**/Yield[b](/%)
1	R.T	24	33
2	30	24	46
3	50	24	72
4	60	24	69
5	40	12	35
6	40	36	83
7	40	48	81
8	40	72	83

[a] Reaction conditions: **1a** (0.3 mmol), $Pd(dba)_2$ (10.0 mol%), **L5** (12.0 mol%), PIDA (1.5 euqiv) in MeCN/AcOH (1:1) 1.0 mL at T °C for times (h) unless otherwise noted. [b] Isolated yield. N. D = Not detected. R. T = Room Temperature.

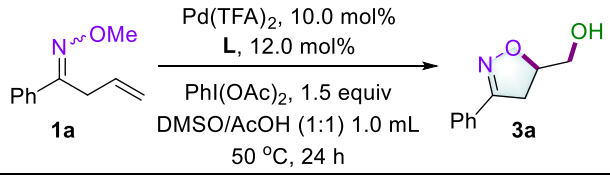
Table S5 The effect of catalysts on the reaction

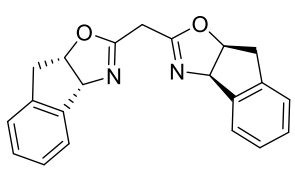


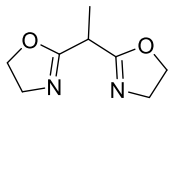
Entry[a]	[Pd]	3a/Yield[b](/%)
1	$Pd(OAc)_2$	71
2	$Pd(TFA)_2$	84
3	$Pd(MeCN)_2Cl_2$	65
4	$Pd(acac)_2$	53
5	$Pd_2(dba)_3$	57
6	$Pd(dba)_2$	55
7	$Pd(PPh_3)_4$	23
8[c]	10 mol% $Pd(TFA)_2$	90

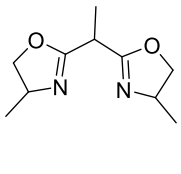
[a] Reaction conditions: **1a** (0.3 mmol), [Pd] (5.0 mol%)**,** **L11** (6.0 mol%), PIDA (1.5 euqiv) in DMSO/AcOH 1.0 mL at 40 °C for 24 h unless otherwise noted. [b] Isolated yield. [c] 10 mol% $Pd(TFA)_2$, 12 mol% **L11**. N. D = Not detected.

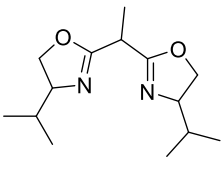
Table S6 The effect of Ligand on the reaction

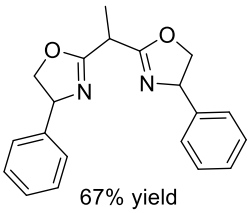


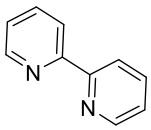

85% yield

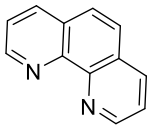

61% yield

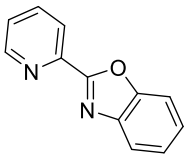

63% yield

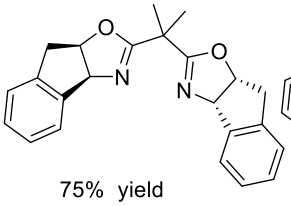

63% yield

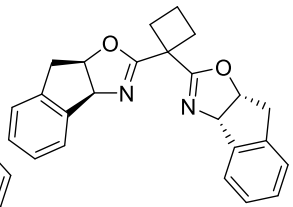

67% yield

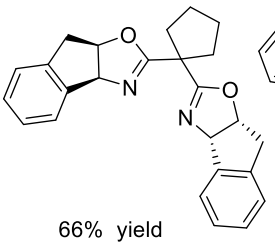

43% yield

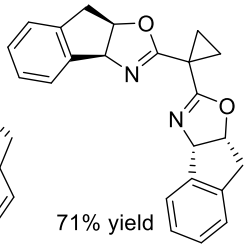

31% yield

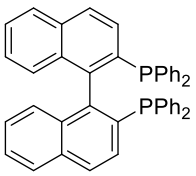

37% yield


75% yield

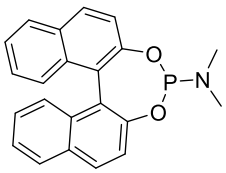

68% yield

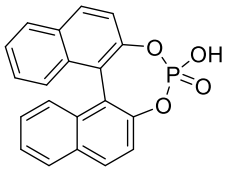

66% yield

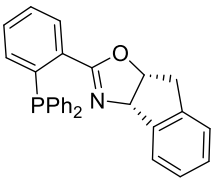

71% yield



N. D.


3% yield

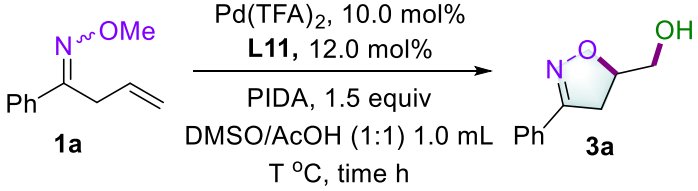

N. D.



13% yield

[a] Reaction conditions: **1a** (0.3 mmol), $Pd(TFA)_2$ (10.0 mol%), **L** (12.0 mol%), PIDA (1.5 euqiv) in DMSO/AcOH (1:1) 1.0 mL at 50 °C for 24 h unless otherwise noted. [b] Isolated yield.

Table S7 Optimization of temperature and time conditions

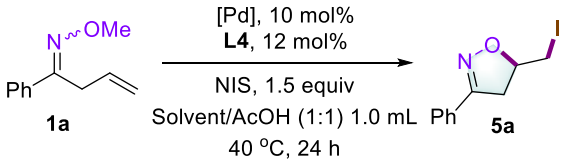


Entry[a]	T/°C	Time/h	3a/Yield[b](/%)
1	30	24	57

2	40	24	78
3	60	24	89
4	70	24	85
5	50	12	52
6	50	36	90
7	50	48	89
8[c]	50	72	88

[a] Reaction conditions: **1a** (0.3 mmol), $Pd(TFA)_2$ (10.0 mol%)，**L11** (12.0 mol%), PIDA (1.5 euqiv) in DMSO/AcOH (1:1) 1.0 mL at T ºC for times (h) unless otherwise noted. [b] Isolated yield.

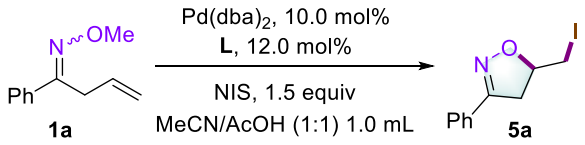
Table S8 The effect of catalysts on the reaction

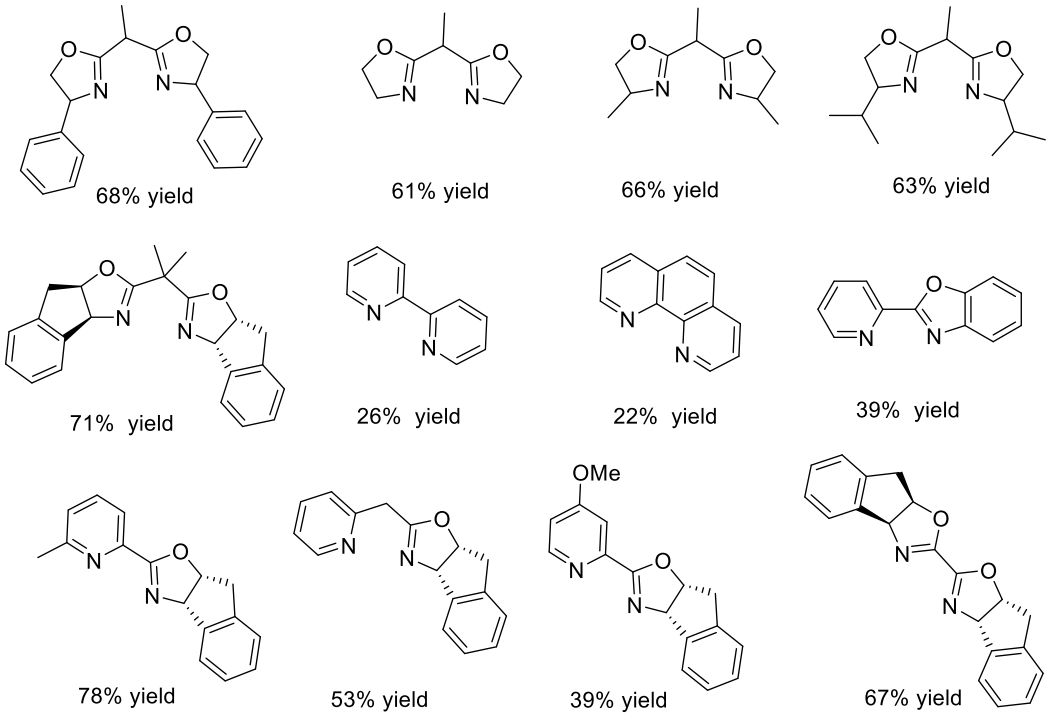


Entry[a]	[Pd]	Solvent/(1;1)	**5a**/Yield[b](/%)
1	$Pd(OAc)_2$	MeCN/AcOH	27
2	$Pd(MeCN)_2Cl_2$	MeCN/AcOH	67
3	$Pd(acac)_2$	MeCN/AcOH	49
4	$Pd_2(dba)_3$	MeCN/AcOH	83
5	$Pd(PPh_3)_4$	MeCN/AcOH	14
6	10 mol% $Pd(dba)_2$	DMSO/AcOH	13

[a] Reaction conditions: **1a** (0.3 mmol), [Pd] (10.0 mol%)，**L4** (12.0 mol%), PIDA (1.5 euqiv) in solvent/AcOH (1:1) 1.0 mL at 40 ºC for 24 h unless otherwise noted. [b] Isolated yield.

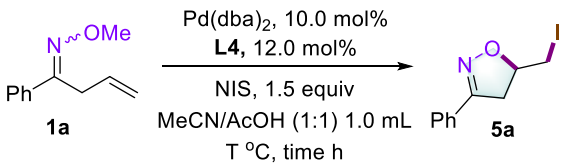
Table S9 The effect of Ligand on the reaction





[a] Reaction conditions: **1a** (0.3 mmol), Pd(dba) $_2$ (10.0 mol%), **L** (12.0 mol%), NIS (1.5 euqiv) in MeCN/ AcOH (1:1) 1.0 mL at 40 °C for 24 h unless otherwise noted. [b] Isolated yield.

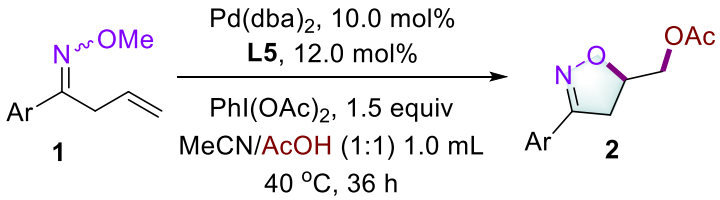
Table S10 Optimization of temperature and time conditions



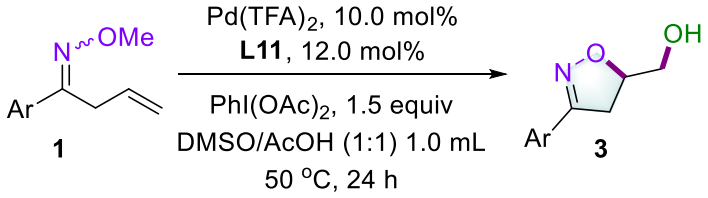
Entry[a]	T/°C	Time/h	3a/Yield[b](/%)
1	R. T	24	79
2	50	24	80
3	60	24	69
4	40	12	71
5	50	36	94
6	50	48	95

[a] Reaction conditions: **1a** (0.3 mmol), Pd(dba) $_2$ (10.0 mol%)，**L4** (12.0 mol%), NIS (1.5 euqiv) in MeCN/AcOH (1:1) 1.0 mL at T °C for times (h) unless otherwise noted. [b] Isolated yield. N. D = Not detected.

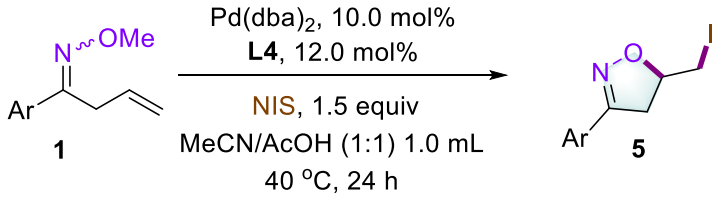
2.4 Synthesis of Products



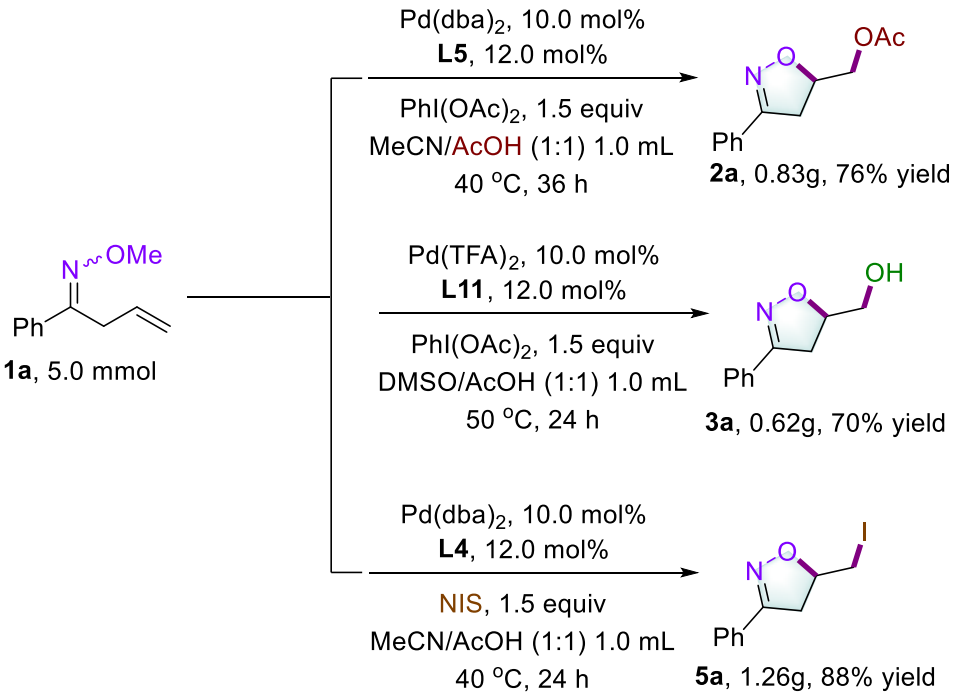
To a 25 ml reaction tube containing a stirring bar was added $Pd(dba)_2$ (10 mol%), **L5** (12 mol%) was added into 0.5 mL MeCN with stirring 10 min under room temperature. **1** (0.3 mmol), PIDA (1.5 equiv) and 0.5 mL AcOH sequentially. The tube was sealed and stirred at 40 °C for 36 h. After completion, the reaction mixture was concentrated and purified by silica gel column chromatography to provide the product **2**.



To a 25 ml reaction tube containing a stirring bar was added $Pd(TFA)_2$ (10 mol%), **L11** (12 mol%) was added into 0.5 mL DMSO with stirring 10 min under room temperature. **1** (0.3 mmol), PIDA (1.5 equiv) and 0.5 mL AcOH sequentially. The tube was sealed and stirred at 50 °C for 24 h. After completion, the reaction mixture was concentrated and purified by silica gel column chromatography to provide the product **3**.



To a 25 ml reaction tube containing a stirring bar was added $Pd(dba)_2$ (10 mol%), **L4** (12 mol%) was added into 0.5 mL MeCN with stirring 10 min under room temperature. **1** (0.3 mmol), NIS (1.5 equiv) and 0.5 mL AcOH sequentially. The tube was sealed and stirred at 40 °C for 24 h. After completion, the reaction mixture was concentrated and purified by silica gel column chromatography to provide the product **5**.

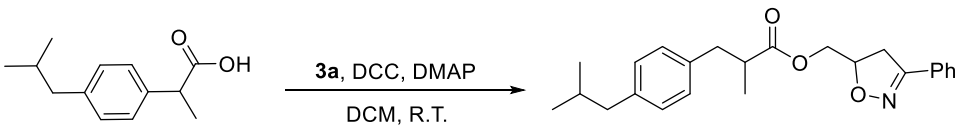


To a 100 ml round bottom flask containing a stirring bar was added $Pd(dba)_2$ (10 mol%), **L5** (12 mol%) was added into 10 mL MeCN with stirring 30 min under room temperature. **1a** (5.0 mmol), PIDA (1.5 equiv) and 10 mL AcOH sequentially. The tube was sealed and stirred at 40 °C for 36 h. After completion, the reaction mixture was concentrated and purified by silica gel column chromatography to provide the product **2a** in 76% yield (0.83g).

To a 100 ml round bottom flask containing a stirring bar was added $Pd(TFA)_2$ (10 mol%), **L11** (12 mol%) was added into 10 mL DMSO with stirring 30 min under room temperature. **1a** (5.0 mmol), PIDA (1.5 equiv) and 10 mL AcOH sequentially. The tube was sealed and stirred at 50 °C for 24 h. After completion, the reaction mixture was concentrated and purified by silica gel column chromatography to provide the product **3a** in 70% yield (0.62g).

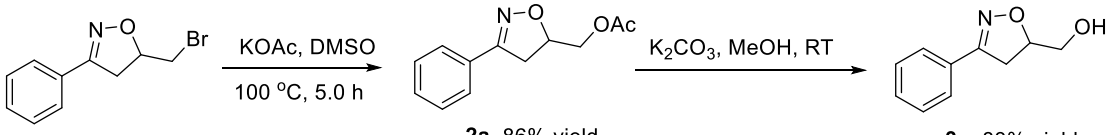
To a 100 ml round bottom flask containing a stirring bar was added $Pd(dba)_2$ (10 mol%), **L4** (12 mol%) was added into 10 mL MeCN with stirring 30 min under room temperature. **1a** (5.0 mmol), NIS (1.5 equiv) and 10 mL AcOH sequentially. The tube was sealed and stirred at 40 °C for 24 h. After completion, the reaction mixture was concentrated and purified by silica gel column chromatography to provide the product **5a** in 88% yield (1.26g).

2.5 Further Synthetic Applications



6a, Ibuprofen (0.2 mmol) **7a,** 89% yield

To a solution of **3a** (0.2 mmol, 1.0 equiv), DMAP (5.0 mol%) and **6a** (0.2 mmol, 1.0 equiv) in DCM (1.0 mL) was slowly added DCC (2.4 mmol, 1.2 equiv; in 1.0 mL DCM). Then, the mixture was stirred overnight at room temperature. The mixture was quenched by aq. NaCl and extracted with DCM. The organic layer was dried over Na_2SO_4. After completion, the reaction mixture was concentrated and purified by silica gel column chromatography to provide the product **7a** in 89% yield.

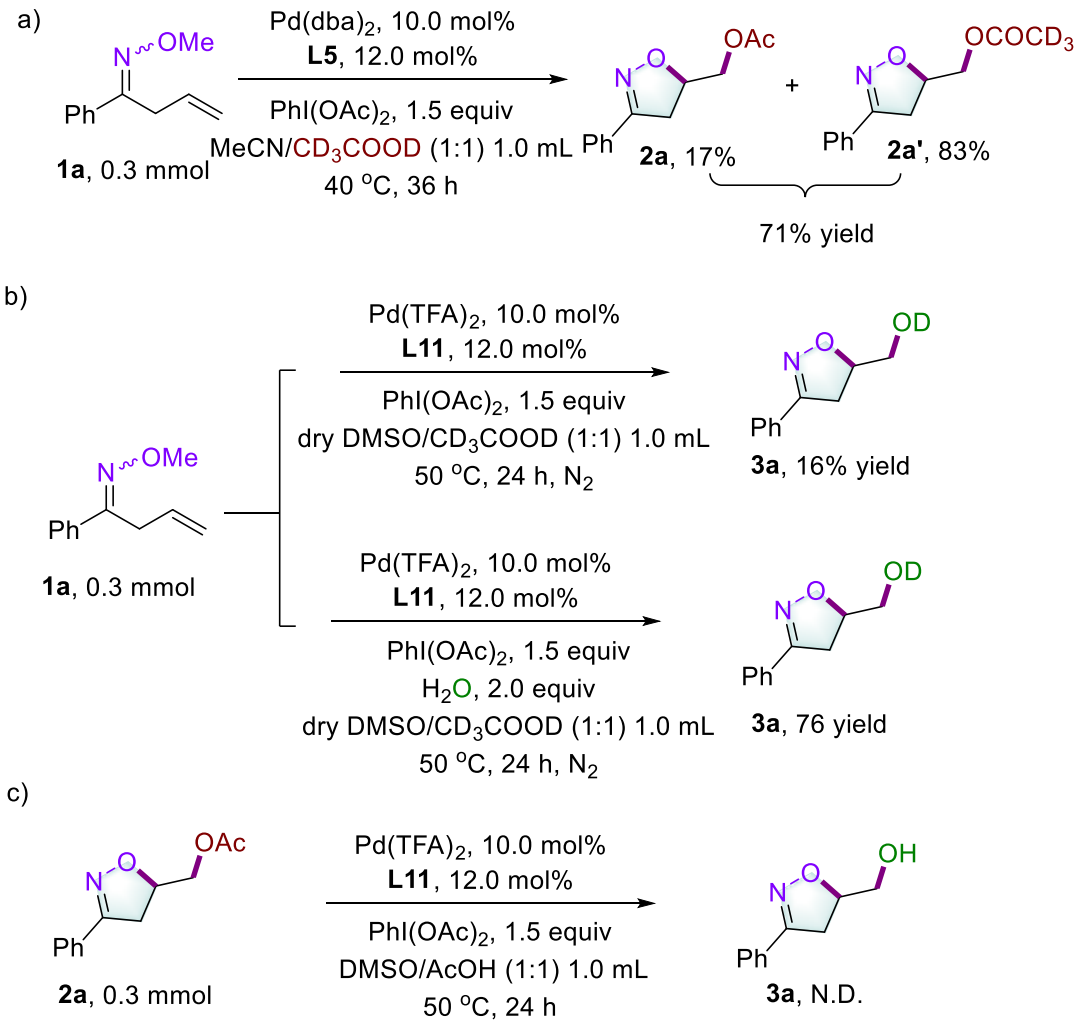


4a, 0.5 mmol **2a**, 86% yield **3a**, 83% yield

To a 25 ml reaction tube containing a stirring bar was added **4a** (0.5 mol) and KOAc (30 equiv) was added into 10 mL DMSO sequentially. The tube was sealed and stirred at 120 °C for 5 h. After completion, the reaction mixture was concentrated and purified by silica gel column chromatography to provide the product **2a** in 86% yield.

To a 25 ml reaction tube containing a stirring bar was added K_2CO_3 (2.0 equiv), **2a** (0.3 mmol) and 5mL MeOH sequentially. The tube was sealed and stirred at room temperature for 2 h. After completion, the reaction mixture was concentrated and purified by silica gel column chromatography to provide the product **3a** in 83% yield.

2.6 Mechanism verification experiments



a) To a 25 ml flame-dried Schlenk tube containing a stirring bar was added $Pd(dba)_2$ (10 mol%), **L5** (12 mol%) was added into 0.5 mL MeCN with stirring 10 min under room temperature. **1a** (0.3 mmol), PIDA (1.5 equiv) and 0.5 mL CD_3COOD sequentially under N_2. The tube was sealed and stirred at 40 °C for 36 h. After completion, the reaction mixture was concentrated and purified by silica gel column chromatography to provide the product **2a**/**2a'** (17:83) in 71% yield.

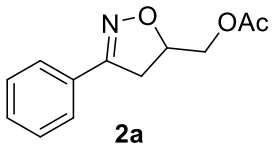
b) To a 25 ml flame-dried Schlenk tube containing a stirring bar was added $Pd(TFA)_2$ (10 mol%), **L11** (12 mol%) was added into 0.5 mL anhydrous DMSO with stirring 10 min at room temperature under N_2. **1a** (0.3 mmol), PIDA (1.5 equiv) and 0.5 mL CD_3COOD sequentially under N_2. The tube was sealed and stirred at 50 °C for 24 h. After completion, the reaction mixture was concentrated and purified by silica gel column chromatography to provide the product **3a** in 16% yield.

To a 25 ml flame-dried Schlenk tube containing a stirring bar was added $Pd(TFA)_2$ (10 mol%), **L11** (12 mol%) was added into 0.5 mL anhydrous DMSO with stirring 10 min at room temperature under N_2. **1a** (0.3 mmol), PIDA (1.5 equiv), H_2O (2.0 equiv) and 0.5 mL CD_3COOD sequentially under

N_2. The tube was sealed and stirred at 50 °C for 24 h. After completion, the reaction mixture was concentrated and purified by silica gel column chromatography to provide the product **3a** in 76% yield.

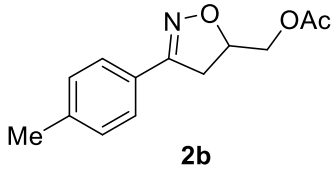
c) To a 25 ml reaction tube containing a stirring bar was added $Pd(TFA)_2$ (10 mol%), **L11** (12 mol%) was added into 0.5 mL DMSO with stirring 10 min under room temperature. **2a** (0.3 mmol), PIDA (1.5 equiv) and 0.5 mL AcOH sequentially. The tube was sealed and stirred at 40 °C for 24 h. After completion, The reaction did not detect the formation of products **3a**.

3. NMR Spectroscopic Data



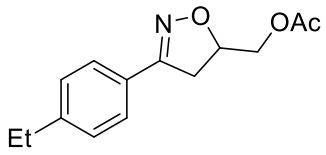
2a

(3-phenyl-4,5-dihydroisoxazol-5-yl)methyl acetate (2a). 54.6 mg, 83% yield, yellow solid, **M. P.** 79.3-82.1 °C. **^{1}H NMR (400 MHz, $CDCl_3$) δ** 7.69-7.65 (m, 2H), 7.42-7.38 (m, 3H), 5.01-4.93 (m, 1H), 4.24 (qd, *J* = 11.9, 5.0 Hz, 2H), 3.46 (dd, *J* = 16.7, 10.8 Hz, 1H), 3.16 (dd, *J* = 16.7, 7.3 Hz, 1H), 2.08 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ** 170.8, 156.2, 130.2, 129.1, 128.7, 126.6, 78.1, 64.8, 37.2, 20.7; **ν (KBr)/cm^{-1}:** 3731.3, 2928.3, 2361.4, 1744.0, 1363.0, 1235.0, 900.5, 763.9, 691.5; **HRMS** (ESI) m/z: **calcd for** $C_{12}H_{14}NO_3^+$, **[M+H]$^+$**: 220.0968, **found**: 220.0965.



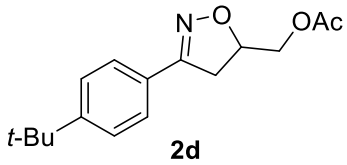
2b

(3-(p-tolyl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2b). 56.7 mg, 81% yield, yellow solid, **M. P.** 89.8-91.8 °C. **^{1}H NMR (400 MHz, $CDCl_3$) δ** 7.56 (d, *J* = 8.3 Hz, 2H), 7.21 (d, *J* = 7.7 Hz, 2H), 4.98-4.91 (m, 1H), 4.23 (qd, *J* = 11.8, 5.1 Hz, 2H), 3.44 (dd, *J* = 16.7, 10.8 Hz, 1H), 3.14 (dd, *J* = 16.7, 7.2 Hz, 1H), 2.38 (s, 3H), 2.08 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ** 170.8, 156.1, 140.5, 129.4, 126.6, 126.3, 77.9, 64.9, 37.3, 21.4, 20.7; **ν (KBr)/cm^{-1}:** 2921.9, 1739.7, 1513.4, 1446.7, 1239.9, 1045.8, 894.5, 817.1, 749.3; **HRMS** (ESI) m/z: **calcd for** $C_{13}H_{16}NO_3^+$, **[M+H]$^+$**: 234.1125, **found**: 234.1122.



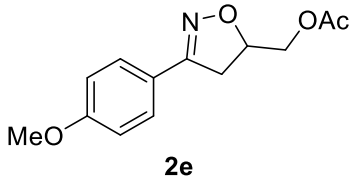
2c

(3-(4-ethylphenyl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2c). 57.9 mg, 78% yield, yellow solid, **M. P.** 81.2-83.8 °C. **^{1}H NMR (400 MHz, $CDCl_3$) δ** 7.59 (d, *J* = 8.3 Hz, 2H), 7.24 (d, *J* = 8.2 Hz, 2H), 4.99-4.92 (m, 1H), 4.23 (qd, *J* = 11.8, 5.1 Hz, 2H), 3.44 (dd, *J* = 16.7, 10.8 Hz, 1H), 3.14 (dd, *J* = 16.7, 7.2 Hz, 1H), 2.68 (q, *J* = 7.6 Hz, 2H), 2.08 (s, 3H), 1.25 (t, *J* = 7.6 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ** 170.7, 156.1, 146.7, 128.2, 126.7, 126.5, 77.9, 64.8, 37.3, 28.7, 20.7, 15.3; **ν (KBr)/cm^{-1}:** 3446.9, 2964.9, 2361.0, 1736.9, 1443.8, 1241.1, 1046.5, 898.2, 838.0, 553.7; **HRMS** (ESI) m/z: **calcd for** $C_{14}H_{18}NO_3^+$, **[M+H]$^+$**: 248.1281, **found**: 248.1276.



2d

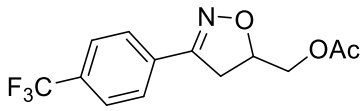
(3-(4-(tert-butyl)phenyl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2d). 70.2 mg, 85% yield, white solid, **M. P.** 89.3-92.1 °C. **^{1}H NMR (400 MHz, $CDCl_3$) δ** 7.62-7.59 (m, 2H), 7.45-7.41 (m, 2H), 4.99-4.92 (m, 1H), 4.23 (qd, *J* = 11.8, 5.0 Hz, 2H), 3.45 (dd, *J* = 16.7, 10.8 Hz, 1H), 3.15 (dd, *J* = 16.7, 7.2 Hz, 1H), 2.08 (s, 3H), 1.33 (s, 9H); **^{13}C NMR (100 MHz, $CDCl_3$) δ** 170.7, 156.0, 153.6, 126.5, 126.2, 125.6, 77.9, 64.8, 37.3, 34.8, 31.1, 20.7; **ν (KBr)/cm^{-1}:** 3460.7, 2960.6, 2361.5, 1743.5, 1363.1, 1236.1, 1046.3, 899.5, 832.5, 568.1; **HRMS** (ESI) m/z: **calcd for** $C_{16}H_{22}NO_3^+$, **[M+H]$^+$**: 276.1594, **found**: 276.1589.



2e

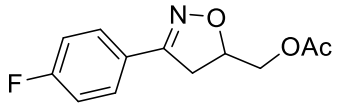
(3-(4-methoxyphenyl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2e). 33.7 mg, 45% yield, white solid, **M. P.** 125.3-127.6 °C. **^{1}H NMR (400 MHz, $CDCl_3$) δ** 7.63-7.59 (m, 2H), 6.94-6.90 (m, 2H), 4.97-4.90 (m, 1H), 4.27-4.18 (m, 2H), 3.84 (s, 3H), 3.43 (dd, *J* = 16.6, 10.8 Hz, 1H), 3.13 (dd, *J* = 16.6, 7.2 Hz, 1H), 2.09 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ** 170.8, 161.1, 155.8, 128.2,

121.7, 114.1, 77.9, 64.9, 55.3, 37.5, 20.7; **ν (KBr)/cm^{-1}:** 3434.8, 2988.8, 2362.1, 1744.5, 1603.9, 1367.3, 1243.4, 1048.6, 828.3; **HRMS** (ESI) m/z: **calcd for** $C_{13}H_{16}NO_4^+$, **[M+H]$^+$**: 250.1074, **found**: 250.1069.



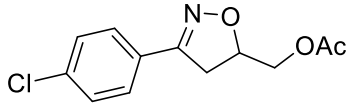
2f

(3-(4-(trifluoromethyl)phenyl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2f). 31.9 mg, 31% yield, white solid, **M. P.** 88.2-90.3 °C. **^{1}H NMR (400 MHz, CDCl$_3$) δ** 7.71 (d, *J* = 8.2 Hz, 2H), 7.59 (d, *J* = 8.1 Hz, 2H), 4.99-4.92 (m, 1H), 4.24-4.13 (m, 2H), 3.40 (dd, *J* = 16.8, 11.0 Hz, 1H), 3.11 (dd, *J* = 16.8, 7.5 Hz, 1H), 2.01 (s, 3H); **^{13}C NMR (100 MHz, CDCl$_3$) δ** 170.7, 155.2, 132.6, 131.8 (q, *J* = 32.6 Hz), 126.9, 125.7 (q, *J* = 3.7 Hz), 123.7 (q, *J* = 270.6 Hz), 78.8, 64.7, 36.8, 20.7; **ν (KBr)/cm^{-1}:** 2947.7, 2394.9, 1745.3, 1407.5, 1240.1, 1165.7, 905.6, 838.9, 599.8; **HRMS** (ESI) m/z: **calcd for** $C_{13}H_{13}F_3NO_3^+$, **[M+H]$^+$**: 288.0842, **found**: 288.0837.



2g

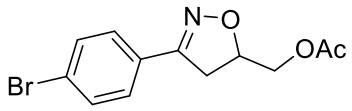
(3-(4-fluorophenyl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2g). 34.9 mg, 49% yield, yellow oil. **^{1}H NMR (400 MHz, CDCl$_3$) δ** 7.68-7.64 (m, 2H), 7.13-7.08 (m, 2H), 5.01-4.94 (m, 1H), 4.24 (qd, *J* = 11.8, 4.2 Hz 2H), 3.44 (dd, *J* = 16.6, 10.8 Hz, 1H), 3.14 (dd, *J* = 16.6, 7.3 Hz, 1H), 2.09 (s, 3H); **^{13}C NMR (100 MHz, CDCl$_3$) δ** 170.8, 163.8 (d, *J* = 249.6 Hz), 155.2, 128.6 (d, *J* = 8.3 Hz), 125.4 (d, *J* = 3.4 Hz), 115.9 (d, *J* = 22 Hz), 78.3, 64.8, 37.3, 20.7; **ν (KBr)/cm^{-1}:** 2921.5, 2359.8, 1742.4, 1508.6, 1237.8, 1047.1, 898.5, 832.1, 597.6; **HRMS** (ESI) m/z: **calcd for** $C_{12}H_{13}FNO_3^+$, **[M+H]$^+$**: 238.0874, **found**: 238.0869.



2h

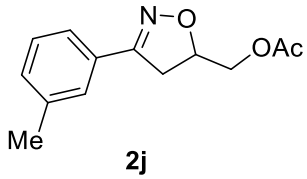
(3-(4-chlorophenyl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2h). 43.4 mg, 57% yield, yellow oil. **^{1}H NMR (400 MHz, CDCl$_3$) δ** 7.62-7.59 (m, 2H), 7.40-7.37 (m, 2H), 5.02-4.95 (m, 1H), 4.24

(qd, J = 11.8, 4.3 Hz 2H), 3.43 (dd, J = 16.6, 10.8 Hz, 1H), 3.13 (dd, J = 16.6, 7.3 Hz, 1H), 2.09 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ** 170.7, 155.3, 136.2, 129.0, 127.9, 127.6, 78.4, 64.7, 37.0, 20.7; **ν (KBr)/cm^{-1}:** 3445.3, 2988.9, 2361.8, 1761.0, 1601.6, 1369.2, 1241.9, 1052.6, 907.4, 825.5; **HRMS** (ESI) m/z: **calcd for** $C_{12}H_{13}ClNO_3^+$, **[M+H]$^+$**: 254.0578, **found**: 254.0573.



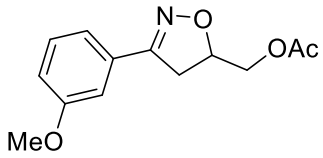
2i

(3-(4-bromophenyl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2i). 60.8 mg, 68% yield, white solid, **M. P.** 103.2-105.4 °C. **^{1}H NMR (400 MHz, $CDCl_3$) δ** 7.56-7.28 (m, 4H), 5.02-4.95 (m, 1H), 4.24 (qd, J = 11.8, 4.3 Hz, 2H), 3.43 (dd, J = 16.7, 10.9 Hz, 1H), 3.13 (dd, J = 16.7, 7.3 Hz, 1H), 2.08 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ** 170.7, 155.4, 131.9, 128.1, 128.0, 124.5, 78.4, 64.7, 36.9, 20.7; **ν (KBr)/cm^{-1}:** 3448.4, 2923.3, 2361.1, 1742.1, 1386.7, 1241.9, 1049.6, 892.9, 819.3, 538.8; **HRMS** (ESI) m/z: **calcd for** $C_{12}H_{13}BrNO_3^+$, **[M+H]$^+$**: 298.0073, **found**: 298.0068.



2j

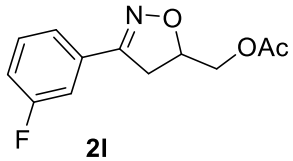
(3-(m-tolyl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2j). 49.7 mg, 71% yield, yellow oil. **^{1}H NMR (400 MHz, $CDCl_3$) δ** 7.50 (s, 1H), 7.45 (d, J = 7.6 Hz, 1H), 7.29 (t, J = 7.6 Hz, 1H), 7.23 (d, J = 7.7 Hz, 1H), 4.99-4.92 (m, 1H), 4.23 (qd, J = 11.8, 4.3 Hz, 2H), 3.44 (dd, J = 16.7, 10.8 Hz, 1H), 3.15 (dd, J = 16.7, 7.2 Hz, 1H), 2.38 (s, 3H), 2.08 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ** 170.7, 156.3, 138.4, 131.0, 128.9, 128.5, 127.2, 123.8, 78.0, 64.8, 37.2, 21.2, 20.7; **ν (KBr)/cm^{-1}:** 3734.5, 2926.8, 2361.6, 1743.2, 1608.2, 1368.5, 1240.1, 1047.8, 910.6, 778.7, 690.0; **HRMS** (ESI) m/z: **calcd for** $C_{13}H_{16}NO_3^+$, **[M+H]$^+$**: 234.1125, **found**: 234.1120.



2k

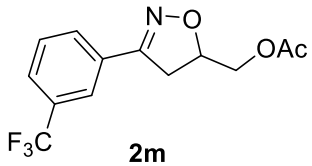
(3-(3-methoxyphenyl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2k). 49.4 mg, 66% yield, yellow oil. **^{1}H NMR (400 MHz, $CDCl_3$) δ** 7.32 (t, J = 7.8 Hz, 1H), 7.28-7.27 (m, 1H), 7.18 (d, J = 7.6 Hz,

1H), 6.97 (dd, *J* = 8.3, 2.2 Hz, 1H), 5.00-4.93 (m, 1H), 4.23 (qd, J = 11.7, 4.2 Hz, 2H), 3.83 (s, 3H), 3.45 (dd, *J* = 16.8, 10.8 Hz, 1H), 3.14 (dd, *J* = 16.8, 7.2 Hz, 1H), 2.08 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ** 170.7, 159.6, 156.2, 130.3, 129.7, 119.3, 116.5, 111.3, 78.2, 64.8, 55.3, 37.2, 20.7; **ν (KBr)/cm^{-1}:** 3733.6, 2928.4, 2361.0, 1741.8, 1565.2, 1431.9, 1369.2, 1237.8, 1042.2, 910.9, 777.0, 684.0; **HRMS** (ESI) m/z: **calcd for** $C_{13}H_{16}NO_4^+$, **[M+H]$^+$**: 250.1074, **found**: 250.1069.



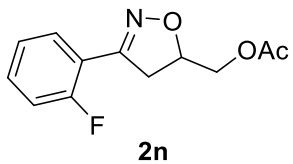
2l

(3-(3-fluorophenyl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2l). 46.3 mg, 65% yield, yellow oil. **^{1}H NMR (400 MHz, $CDCl_3$) δ** 7.43-7.36 (m, 3H), 7.15-7.10 (m, 1H), 5.04-4.97 (m, 1H), 4.25 (qd, J = 11.8, 4.1 Hz, 2H), 3.44 (dd, *J* = 16.7, 10.9 Hz, 1H), 3.15 (dd, *J* = 16.9, 7.5 Hz, 1H), 2.09 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$) δ** 170.7, 162.7 (d, *J* = 244.8 Hz), 155.4 (d, *J* = 2.9 Hz), 131.2 (d, *J* = 8.0 Hz), 130.3 (d, *J* = 8.1 Hz), 122.4 (d, *J* = 3.0 Hz), 117.2 (d, *J* = 21.3 Hz), 113.5 (d, *J* = 23.0 Hz), 78.5, 64.7, 37.0, 20.7; **ν (KBr)/cm^{-1}:** 3458.2, 2988.8, 2361.7, 1745.7, 1377.4, 1241.3, 1049.0, 917.4, 792.7; **HRMS** (ESI) m/z: **calcd for** $C_{12}H_{13}FNO_3^+$, **[M+H]$^+$**: 238.0874, **found**: 238.0869.



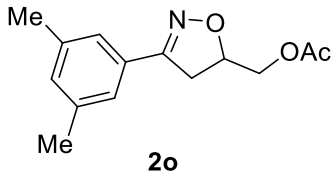
2m

(3-(3-(trifluoromethyl)phenyl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2m). 31.9 mg, 37% yield, yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.89 (d, *J* = 7.2 Hz, 2H), 7.68 (d, *J* = 7.9 Hz, 1H), 7.55 (d, *J* = 7.9 Hz, 1H), 5.07-5.00 (m, 1H), 4.26 (qd, J = 11.8, 4.3 Hz, 2H), 3.49 (dd, *J* = 16.7, 10.9 Hz, 1H), 3.20 (dd, *J* = 16.7, 7.4 Hz, 1H), 2.10 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 170.7, 155.2, 131.3 (q, *J* = 32.5 Hz), 130.1, 129.7, 129.3, 126.7 (q, *J* = 3.6 Hz), 123.7 (q, *J* = 270.6 Hz), 123.4 (q, *J* = 3.7 Hz), 78.7, 64.6, 36.9, 20.7; **ν (KBr)/cm^{-1}:** 29227, 2359.8, 1744.0, 1239.3, 1167.0, 1047.4, 690.1; **HRMS** (ESI) m/z: **calcd for** $C_{13}H_{13}F_3NO_3^+$, **[M+H]$^+$**: 288.0842, **found**: 288.0837.



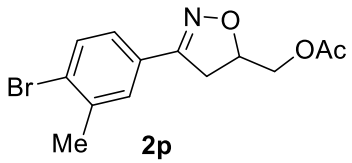
2n

(3-(2-fluorophenyl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2n). 33.4 mg, 47% yield, yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.85 (td, *J* = 7.6, 1.5 Hz, 1H), 7.44-7.38 (m, 1H), 7.21-7.10 (m, 1H), 5.02-4.95 (m, 1H), 4.24 (qd, *J* = 11.9, 4.2 Hz, 2H), 3.55 (dd, *J* = 10.4, 2.8 Hz, 1H), 3.25 (dd, *J* = 7.2, 2.3 Hz, 1H), 2.10 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 170.8, 160.3 (d, *J* = 250.7), 153.1 (d, *J* = 2.8 Hz), 131.9 (d, *J* = 8.6 Hz), 129.0 (d, *J* = 3.1 Hz), 124.5 (d, *J* = 3.4 Hz), 117.2 (d, J = 11.5 Hz), 116.4 (d, *J* = 21.8 Hz), 78.4 (d, *J* = 2.1 Hz), 64.6, 38.9 (d, *J* = 7.2 Hz), 20.7; **ν (KBr)/cm^{-1}:** 3446.2, 2926.5, 2361.7, 1743.5, 1603.2, 1366.8, 1047.0, 911.3, 761.4, 551.9; **HRMS** (ESI) m/z: **calcd for** $C_{12}H_{13}FNO_3^+$, **[M+H]$^+$**: 238.0874, **found**: 238.0870.



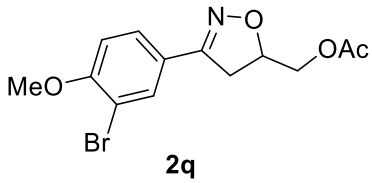
2o

(3-(3,5-dimethylphenyl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2o). 50.4 mg, 68% yield, white solid, **M. P.** 91.3.3-93.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.29 (s, 2H), 7.05 (s, 1H), 4.98-4.91 (m, 1H), 4.22 (qd, *J* = 11.7, 4.3 Hz, 2H), 3.43 (dd, *J* = 16.7, 10.8 Hz, 1H), 3.25 (dd, *J* = 16.7, 7.2 Hz, 1H), 2.33 (s, 6H), 2.08 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 170.7, 156.4, 138.2, 131.9, 128.8, 124.4, 77.9, 64.8, 37.3, 21.1, 20.7; **ν (KBr)/cm^{-1}:** 3460.9, 2922.0, 1743.1, 1606.9, 1367.9, 1238.8, 1046.5, 910.0, 847.1, 792.0, 533.7; **HRMS** (ESI) m/z: **calcd for** $C_{14}H_{18}NO_3^+$, **[M+H]$^+$**: 248.1281, **found**: 248.1277.



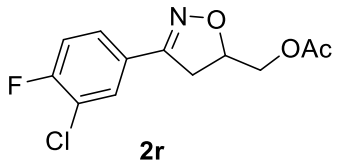
2p

(3-(4-bromo-3-methylphenyl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2p). 51.5 mg, 55% yield, white solid, **M. P.** 113.3-115.7 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.49-7.46 (m, 2H), 7.24 (dd, *J* = 8.3, 1.9 Hz, 1H), 4.93-4.86 (m, 1H), 4.16 (qd, *J* = 11.9, 4.3 Hz, 2H), 3.35 (dd, *J* = 16.8, 10.9 Hz, 1H), 3.05 (dd, *J* = 16.8, 7.3 Hz, 1H), 2.34 (s, 3H), 2.01 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 170.7, 155.5, 138.5, 132.7, 128.7, 128.2, 127.0, 125.4, 78.3, 64.7, 37.0, 22.8, 20.7; **ν (KBr)/cm^{-1}:** 3734.1, 3448.7, 2921.7, 2361.4, 1744.7, 1605.9, 1370.2, 1240.7, 1050.2, 913.3, 773.3, 681.2; **HRMS** (ESI) m/z: **calcd for** $C_{13}H_{15}BrNO_3^+$, **[M+H]$^+$**: 312.0230, **found**: 312.0224.



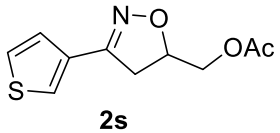
2q

(3-(3-bromo-4-methoxyphenyl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2q). 62.0 mg, 63% yield, white solid, **M. P.** 110.3-113.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.76 (d, *J* = 2.1 Hz, 1H), 7.52 (dd, *J* = 8.6, 2.0 Hz, 1H), 6.84 (d, *J* = 8.6 Hz, 1H), 4.92-4.85 (m, 1H), 4.15 (qd, *J* = 11.8, 4.4 Hz, 2H), 3.86 (s, 3H), 3.34 (dd, *J* = 16.7, 10.8 Hz, 1H), 3.04 (dd, *J* = 16.6, 7.2 Hz, 1H), 2.01 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 170.7, 157.2, 154.7, 131.6, 127.1, 122.9, 111.9, 111.7, 78.2, 64.7, 56.3, 37.2, 20.7; **ν (KBr)/cm^{-1}:** 2921.5, 2359.8, 1742.4, 1508.6, 1385.9, 1345.0, 1237.8, 1047.1, 898.5, 832.1, 537.7; **HRMS** (ESI) m/z: **calcd for** $C_{13}H_{15}BrNO_4^+$, **[M+H]$^+$**: 328.0179, **found**: 328.0173.



2r

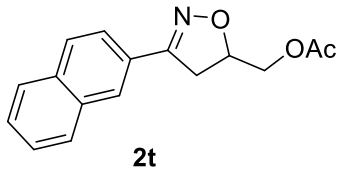
(3-(3-chloro-4-fluorophenyl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2r). 52.4 mg, 52% yield, yellow solid, **M. P.** 90.8-93.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49-7.36 (m, 3H), 5.05-4.98 (m, 1H), 4.25 (qd, *J* = 12.3, 4.3 Hz, 2H), 3.42 (dd, *J* = 16.8, 11.0 Hz, 1H), 3.12 (dd, *J* = 16.6, 7.3 Hz, 1H), 2.09 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.7, 158.1 (d, *J* = 248.3 Hz), 154.7 (d, *J* = 2.8 Hz), 131.0, 129.6 (d, *J* = 7.2 Hz), 123.0 (d, *J* = 17.8 Hz), 123.0 (d, *J* = 3.6 Hz), 114.6 (d, *J* = 22.6 Hz), 78.8, 64.6, 36.8, 20.7; **ν (KBr)/cm^{-1}:** 3447.5, 2924.2, 2363.7, 1745.2, 1557.2, 1370.7, 1241.6, 1049.4, 922.3, 810.7, 609.6; **HRMS** (ESI) m/z: **calcd for** $C_{12}H_{12}ClFNO_3^+$, **[M+H]$^+$**: 272.0484, **found**: 272.0478.



2s

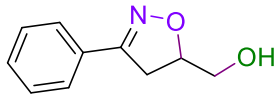
(3-(thiophen-3-yl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2s). 27.7 mg, 41% yield, yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.50 (dd, *J* = 5.0, 1.0 Hz, 1H), 7.46 (dd, *J* = 2.9, 1.1 Hz, 1H), 7.37 (q, *J* = 2.7 Hz, 1H), 4.97-4.90 (m, 1H), 4.23 (qd, *J* = 10.9, 4.3 Hz, 2H), 3.44 (dd, *J* = 16.6, 10.7 Hz, 1H), 3.14 (dd, *J* = 16.8, 7.5 Hz, 1H), 2.09 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 170.8, 152.4,

131. 126.9, 125.6, 125.6, 77.9, 64.8, 37.9, 20.8; **ν (KBr)/cm^{-1}:** 3729.3, 2919.9, 2361.8, 1744.7, 1518.1, 1240.1, 1048.8, 915.2, 778.4, 681.9; **HRMS** (ESI) m/z: **calcd for** $C_{10}H_{12}NO_3S$, **[M+H]$^+$**: 226.0532, **found**: 226.0527.



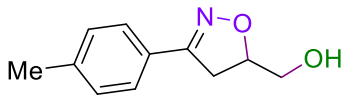
2t

(3-(naphthalen-2-yl)-4,5-dihydroisoxazol-5-yl)methyl acetate (2t). 61.4 mg, 76% yield, white solid, **M. P.** 98.8-100.3 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.95 (dd, J = 8.7, 1.6 Hz, 1H), 7.87-7.81 (m, 4H), 7.54-7.48 (m, 2H), 5.04-4.97 (m, 1H), 4.26 (qd, J = 11.9, 4.3 Hz, 2H), 3.53 (dd, *J* = 16.6, 10.8 Hz, 1H), 3.26 (dd, *J* = 16.6, 7.3 Hz, 1H), 2.08 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 170.7, 156.3, 134.0, 132.8, 128.5, 128.3, 127.8, 127.1, 126.9, 126.6, 123.4, 78.3, 64.8, 37.1, 20.7; **ν (KBr)/cm^{-1}:** 3735.0, 2927.2, 2361.1, 1741.2, 1381.8, 1236.9, 1044.9, 907.8, 907.8, 812.7, 755.4, 683.2; **HRMS** (ESI) m/z: **calcd for** $C_{16}H_{16}NO_3^+$, **[M+H]$^+$**: 270.1125, **found**: 270.1120.



3a

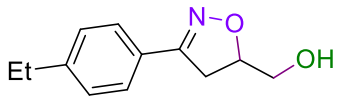
(3-phenyl-4,5-dihydroisoxazol-5-yl)methanol (3a). 47.9 mg, 90% yield, white solid, **M. P.** 69.3-72.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.68-7.63 (m, 2H), 7.43-7.36 (m, 3H), 4.90-4.83 (m, 1H), 3.87 (dd, *J* = 12.2, 3.1 Hz, 1H), 3.68 (dd, *J* = 12.2, 4.6 Hz, 1H), 3.38 (dd, *J* = 16.7, 10.8 Hz, 1H), 3.27 (dd, *J* = 16.6, 7.9 Hz, 1H), 2.39 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 170.7, 156.3, 134.0, 132.8, 128.5, 128.3, 127.8, 127.1, 126.9, 126.6, 123.4, 78.3, 64.8, 37.1; **ν (KBr)/cm^{-1}:** 3445.0, 2922.0, 1763.5, 1385.0, 1243.0, 1053.5, 904.5, 753.0, 691.9; **HRMS** (ESI) m/z: **calcd for** $C_{10}H_{12}NO_2^+$, **[M+H]$^+$**: 178.0863, **found**: 178.0859.



3b

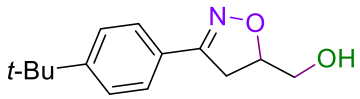
(3-(p-tolyl)-4,5-dihydroisoxazol-5-yl)methanol (3b). 49.9 mg, 87% yield, white solid, **M. P.** 107.3-109.6 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.54 (d, *J* = 8.1 Hz, 2H), 7.19 (d, *J* = 7.9 Hz, 2H), 4.87-4.80 (m, 1H), 3.84 (dd, *J* = 12.1, 3.2 Hz, 1H), 3.67 (dd, *J* = 12.1, 4.6 Hz, 1H), 3.31 (qd, *J* = 19.4, 10.7 Hz, 2H), 2.37 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 157.0, 140.4, 129.3, 126.6, 126.4,

81.0, 63.6, 36.4, 21.4; **ν (KBr)/cm^{-1}:** 3445.8, 2926.1, 1747.3, 1603.3, 1464.2, 1242.4, 1168.1, 1047.5, 819.1, 542.5; **HRMS** (ESI) m/z: **calcd for** $C_{11}H_{14}NO_2^+$, **[M+H]$^+$**: 192.1019, **found**: 192.1016.



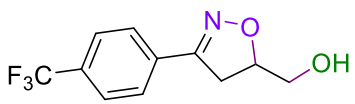
3c

(3-(4-ethylphenyl)-4,5-dihydroisoxazol-5-yl)methanol (3c). 52.4 mg, 85% yield, white solid, **M. P.** 81.3-83.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.57 (d, *J* = 8.2 Hz, 2H), 7.22 (d, *J* = 8.4 Hz, 2H), 4.87-4.81 (m, 1H), 3.84 (dd, *J* = 12.3, 3.2 Hz, 1H), 3.67 (dd, *J* = 12.3, 4.7 Hz, 1H), 3.36 (qd, *J* = 19.2, 10.7 Hz, 2H), 2.66 (q, *J* = 7.6 Hz, 2H), 2.46 (s, 1H), 1.24 (t, J = 7.6 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 157.0, 146.7, 128.2, 126.7, 126.6, 81.0, 63.6, 36.4, 28.7, 15.3; **ν (KBr)/cm^{-1}:** 3780.5, 3398.1, 2959.2, 1746.5, 1602.7, 1464.0, 1404.0, 1359.0, 1102.4, 1047.1, 902.1, 833.6, 567.7; **HRMS** (ESI) m/z: **calcd for** $C_{12}H_{16}NO_2^+$, **[M+H]$^+$**: 206.1176, **found**: 206.1173.



3d

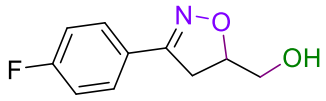
(3-(4-(tert-butyl)phenyl)-4,5-dihydroisoxazol-5-yl)methanol (3d). 60.2 mg, 86% yield, white solid, **M. P.** 79.3-82.5 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.61-7.59 (m, 2H), 7.43-7.40 (m, 2H), 4.87-4.81 (m, 1H), 3.84 (dd, *J* = 12.2, 3.4 Hz, 1H), 3.67 (dd, *J* = 12.2, 4.8 Hz, 1H), 3.32 (qd, *J* = 19.2, 10.5 Hz, 2H), 2.49 (s, 1H), 1.32 (s, 9H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 156.9, 153.5, 126.5, 126.4, 125.6, 81.0, 63.6, 36.4, 34.8, 31.1; **ν (KBr)/cm^{-1}:** 3347.4, 2963.0, 2924.1, 1739.2, 1598.1, 1364.3, 1243.1, 1048.7, 828.4, 778.5, 551.1; **HRMS** (ESI) m/z: **calcd for** $C_{14}H_{20}NO_2^+$, **[M+H]$^+$**: 234.1489, **found**: 234.1484.



3e

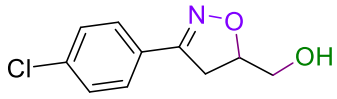
(3-(4-(trifluoromethyl)phenyl)-4,5-dihydroisoxazol-5-yl)methanol (3e). 41.9 mg, 57% yield, white solid, **M. P.** 72.6-75.3 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.70 (d, *J* = 8.1 Hz, 2H), 7.58 (d, *J* = 8.2 Hz, 2H), 4.89 -4.80 (m, 1H), 3.84 (dd, *J* = 12.3, 3.1 Hz, 1H), 3.63 (dd, *J* = 12.4, 4.4 Hz, 1H),

3.28 (qd, *J* = 16.6, 9.4 Hz, 2H), 1.91 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 156.0, 132.7, 131.8 (q, *J* = 32.7 Hz), 126.9, 125.7 (q, *J* = 3.8 Hz), 123.8 (q, *J* = 270.5 Hz), 81.9, 64.1, 34.2; **ν (KBr)/cm^{-1}:** 3436.1, 2926.4, 1762.7, 1604.7, 1324.2, 1243.7, 1061.1, 908.9, 839.8, 599.3; **HRMS** (ESI) m/z: **calcd for** $C_{11}H_{11}F_3NO_2^+$, **[M+H]$^+$**: 246.0736, **found**: 246.0732.



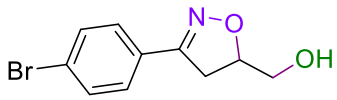
3f

(3-(4-fluorophenyl)-4,5-dihydroisoxazol-5-yl)methanol (3f). 39.2 mg, 67% yield, yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.67-7.64 (m, 2H), 7.11-7.07 (m, 2H), 4.91-4.84 (m, 1H), 3.88 (dd, *J* = 12.2, 3.1 Hz, 1H), 3.53 (dd, *J* = 12.2, 4.4 Hz, 1H), 3.40-3.24 (m, 2H), 2.09 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 163.8 (d, *J* = 246.5 Hz), 156.1, 128.6 (d, *J* = 8.4 Hz), 125.5, 115.8 (d, *J* = 21.8 Hz), 81.3, 63.6, 36.3; **ν (KBr)/cm^{-1}:** 3771.0, 3348.6, 2922.6, 1756.4, 1598.5, 1436.9, 1242.8, 1049.9, 825.3, 540.9; **HRMS** (ESI) m/z: **calcd for** $C_{10}H_{11}NO_2F$, **[M+H]$^+$**: 196.0768, **found**: 196.0767.



3g

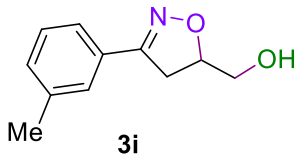
(3-(4-chlorophenyl)-4,5-dihydroisoxazol-5-yl)methanol (3g). 45.0 mg, 71% yield, yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.57 (d, J = 8.4 Hz, 2H), 7.36 (d, J = 8.4 Hz, 2H), 4.91-4.84 (m, 1H), 3.88 (dd, *J* = 12.3, 3.2 Hz, 1H), 3.68 (dd, *J* = 12.3, 4.4 Hz, 1H), 3.31 (qd, J = 17.1, 10.7 Hz, 2H), 2.27 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 156.1, 136.1, 128.9, 127.9, 127.8, 81.5, 63.5, 36.1; **ν (KBr)/cm^{-1}:** 3351.1, 2923.7, 1745.9, 1597.6, 1400.5, 1361.7, 1097.4, 1049.9, 899.1, 826.3, 543.0; **HRMS** (ESI) m/z: **calcd for** $C_{10}H_{11}ClNO_2^+$, **[M+H]$^+$**: 212.0473, **found**: 212.0469.



3h

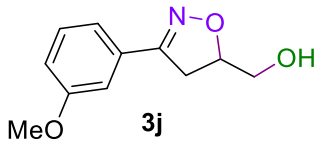
(3-(4-chlorophenyl)-4,5-dihydroisoxazol-5-yl)methanol (3h). 61.5 mg, 80% yield, white solid, **M. P.** 103.9-105.7 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.54-7.49 (m, 4H), 4.91-4.84 (m, 1H), 3.88 (dd, *J* = 12. 4, 3.2 Hz, 1H), 3.68 (dd, *J* = 12.4, 4.4 Hz, 1H), 3.31 (qd, J = 17.1, 10.7 Hz, 2H), 2.34 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 156.2, 131.9, 128.2, 128.1, 124.4, 81.5, 63.5, 36.0; **ν**

(KBr)/cm^{-1}: 3338.0, 2923.5, 1912.6, 1736.2, 1595.6, 1362.7, 1049.8, 898.9, 541.8; **HRMS** (ESI) m/z: **calcd for** $C_{10}H_{11}BrNO_2^+$, **[M+H]$^+$**: 255.9968, **found**: 255.9965.



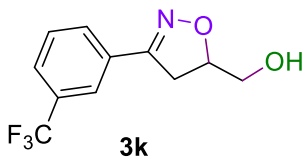
3i

(3-(m-tolyl)-4,5-dihydroisoxazol-5-yl)methanol (3i). 52.8 mg, 92% yield, yellow solid, **M. P.** 73.9-76.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.49 (s, 1H), 7.43 (d, *J* = 7.8 Hz, 1H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.21 (d, *J* = 7.5 Hz, 1H), 4.88-4.82 (m, 1H), 3.85 (dd, *J* = 12.3, 3.2 Hz, 1H), 3.68 (dd, *J* = 12.3, 4.7 Hz, 1H), 3.32 (qd, *J* = 18.9, 10.8 Hz, 2H), 2.37 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 157.1, 138.4, 130.9, 129.1, 128.5, 127.2, 123.8, 81.1, 63.6, 36.3, 21.3; **ν (KBr)/cm^{-1}:** 3770.8, 3395.36, 2922.7, 1733.5, 1575.8, 1439.0, 1092.0, 1045.5, 913.2, 791.9, 692.2, 525.3; **HRMS** (ESI) m/z: **calcd for** $C_{11}H_{14}NO_2^+$, **[M+H]$^+$**: 192.1019, **found**: 192.1016.



3j

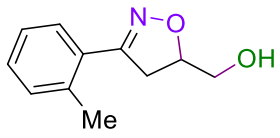
(3-(3-methoxyphenyl)-4,5-dihydroisoxazol-5-yl)methanol (3j). 41.0 mg, 66% yield, yellow solid, **M. P.** 99.3-102.7 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.32-7.25 (m, 2H), 7.19-7.17 (m, 1H), 6.97-6.94 (m, 1H), 4.90-4.83 (m, 1H), 3.86 (dd, *J* = 12.3, 3.2 Hz, 1H), 3.83 (s, 3H), 3.68 (dd, *J* = 12.2, 4.7 Hz, 1H), 3.32 (qd, J = 19.4, 10.7 Hz, 2H), 2.26 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 159.6, 157.0, 130.5, 129.7, 119.3, 116.4, 111.3, 81.3, 63.6, 55.3, 36.3; **ν (KBr)/cm^{-1}:** 3399.6, 2926.2, 1760.4, 1602.9, 1574.7, 1356.4, 1219.3, 1040.4, 790.9, 688.0, 564.9; **HRMS** (ESI) m/z: **calcd for** $C_{11}H_{14}NO_3^+$, **[M+H]$^+$**: 208.0968, **found**: 208.0967.



3k

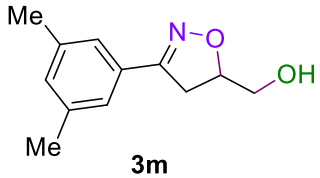
(3-(3-(trifluoromethyl)phenyl)-4,5-dihydroisoxazol-5-yl)methanol (3k). 53.0 mg, 72% yield, yellow solid, **M. P.** 75.8-79.0 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.89 (s, 1H), 7.86 (d, J = 7.9 Hz, 1H), 7.66 (d, J = 7.9 Hz, 1H), 7.53 (t, *J* = 7.8 Hz, 1H), 4.96-4.89 (m, 1H), 3.92 (dd, *J* = 12.3, 3.1 Hz, 1H), 3.70 (dd, *J* = 12.4, 4.3 Hz, 1H), 3.37 (qd, *J* = 16.6, 10.7 Hz, 2H), 2.27 (s, 1H); **^{13}C**

NMR (100 MHz, $CDCl_3$) **δ** 156.0, 131.2 (q, *J* = 32.6 Hz), 130.2, 129.7, 129.3, 126.6 (q, *J* = 3.6 Hz), 123.5 (q, *J* = 270.8 Hz), 123.4 (q, *J* = 3.8 Hz), 81.8, 63.5, 35.9; **ν (KBr)/cm^{-1}:** 3428.6, 2928.2, 1763.8, 1603.3, 1367.8, 1313.8, 1243.2, 1051.9, 915.3, 693.0; **HRMS** (ESI) m/z: **calcd for** $C_{11}H_{11}F_3NO_2^+$, **[M+H]$^+$**: 246.0736, **found**: 246.0732.



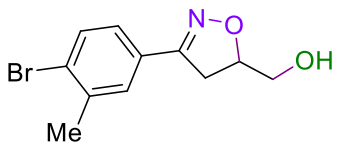
3l

(3-(o-tolyl)-4,5-dihydroisoxazol-5-yl)methanol (3l). 36.1 mg, 63% yield, yellow solid, **M. P.** 78.3-81.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.35-7.22 (m, 4H), 4.85-4.78 (m, 1H), 3.87 (dd, *J* = 12.3, 3.2 Hz, 1H), 3.69 (dd, *J* = 12.2, 4.7 Hz, 1H), 3.38 (qd, J = 21.3, 10.6 Hz, 2H), 2.55 (s, 3H), 2.09 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 158.0, 137.9, 131.5, 129.4, 128.8, 128.4, 125.8, 80.1, 63.7, 39.0, 22.8; **ν (KBr)/cm^{-1}:** 2991.2, 2389.8, 1763.9, 1531.1, 1399.2, 1243.0, 1053.3, 909.2, 751.5; **HRMS** (ESI) m/z: **calcd for** $C_{11}H_{14}NO_2^+$, **[M+H]$^+$**: 192.1019, **found**: 192.1015.



3m

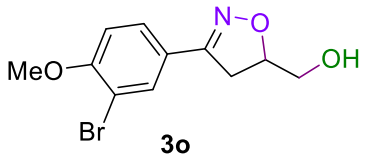
(3-(3,5-dimethylphenyl)-4,5-dihydroisoxazol-5-yl)methanol (3m). 51.1 mg, 83% yield, yellow solid, **M. P.** 132.1-135.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.28 (s, 2H), 7.05 (s, 1H), 4.86-4.81 (m, 1H), 3.84 (dd, *J* = 12.1, 2.9 Hz, 1H), 3.67 (dd, *J* = 12.2, 4.7 Hz, 1H), 3.30 (qd, *J* = 19.7, 10.7 Hz, 2H), 2.32 (s, 7H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 157.2, 138.2, 131.8, 129.0, 124.5, 81.0, 63.7, 36.5, 21.1; **ν (KBr)/cm^{-1}:** 3359.3, 2919.2, 1733.6, 1436.9, 1097.0, 1047.2, 943.1, 626.4; **HRMS** (ESI) m/z: **calcd for** $C_{12}H_{16}NO_2^+$, **[M+H]$^+$**: 206.1176, **found**: 206.1175.



3n

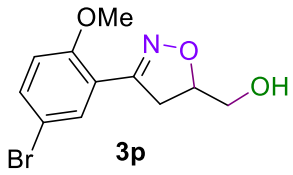
(3-(4-bromo-3-methylphenyl)-4,5-dihydroisoxazol-5-yl)methanol (3n). 56.7 mg, 70% yield, yellow solid, **M. P.** 109.3-112.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.54-7.52 (m, 2H), 7.14 (dd, *J* = 10.2, 2.0 Hz, 1H), 4.90-4.83 (m, 1H), 3.87(dd, *J* = 12.3, 3.1 Hz, 1H), 3.68 (dd, *J* = 12.3, 4.5 Hz,

1H), 3.30 (qd, *J* = 17.1, 9.8 Hz, 2H), 2.40 (s, 4H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 156.4, 138.4, 132.6, 128.7, 128.4, 126.9, 125.4, 81.4, 63.5, 36.1, 22.8; **ν (KBr)/cm^{-1}:** 3391.6, 2923.1, 2390.7, 1745.8, 1243.6, 1029.4, 915.9, 810.2, 539.4; **HRMS** (ESI) m/z: **calcd for** $C_{11}H_{13}BrNO_2^+$, **[M+H]$^+$**: 270.0124, **found**: 270.0119.



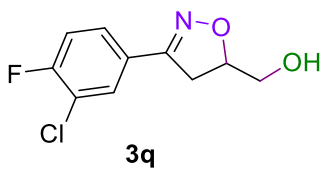
3o

(3-(3-bromo-4-methoxyphenyl)-4,5-dihydroisoxazol-5-yl)methanol (3o). 30.9 mg, 36% yield, yellow solid, **M. P.** 119.2-121.5 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.83 (d, *J* = 2.1 Hz, 1H), 7.56 (dd, *J* = 8.6, 2.1 Hz, 1H), 6.89 (d, *J* = 8.6 Hz, 1H), 4.88-4.81 (m, 1H), 3.92 (s, 3H), 3.86 (dd, *J* = 12.3, 3.2 Hz, 1H), 3.67 (dd, *J* = 12.3, 4.6 Hz, 1H), 3.28 (qd, *J* = 17.8, 10.6 Hz, 2H), 2.34 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 157.2, 155.5, 131.6, 127.1, 123.2, 111.9, 111.6, 81.3, 63.5, 56.3, 36.2; **ν (KBr)/cm^{-1}:** 3391.4, 2927.8, 1734.9, 1598.9, 1553.4, 1348.9, 1049.7, 905.6, 682.5, 591.6; **HRMS** (ESI) m/z: **calcd for** $C_{11}H_{13}BrNO_3^+$, **[M+H]$^+$**: 286.0073, **found**: 286.0072.



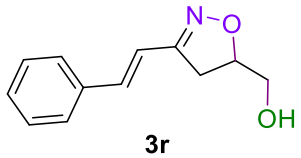
3p

(3-(5-bromo-2-methoxyphenyl)-4,5-dihydroisoxazol-5-yl)methanol (3p). 45.0 mg, 52% yield, yellow solid, **M. P.** 110.3-112.5 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.76 (d, *J* = 2.5 Hz, 1H), 7.38 (dd, *J* = 8.9, 2.6 Hz, 1H), 6.74 (d, *J* = 8.9 Hz, 1H), 4.78-4.71 (m, 1H), 3.78-3.74 (m, 4H), 3.60 (dd, *J* = 12.2, 4.9 Hz, 1H), 3.39 (dd, *J* = 17.4, 10.7 Hz, 1H), 3.30 (dd, *J* = 17.4, 7.9 Hz, 1H), 2.03 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 156.6, 155.6, 133.8, 131.8, 120.3, 113.1, 113.0, 81.4, 63.7, 55.8, 38.7; **ν (KBr)/cm^{-1}:** 3477.6, 2972.8, 1831.9, 1601.9, 1599.4, 1356.9, 1051.7, 935.6, 703.5, 603.6; **HRMS** (ESI) m/z: **calcd for** $C_{11}H_{13}BrNO+3$, **[M+H]$^+$**: 286.0073, **found**: 286.0072.



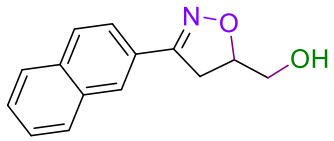
3q

(3-(3-chloro-4-fluorophenyl)-4,5-dihydroisoxazol-5-yl)methanol (3q). 61.3 mg, 89% yield, yellow solid, **M. P.** 112.0-115.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.45-7.40 (m, 2H), 7.34 (dd, *J* = 8.4, 1.5 Hz, 1H), 4.94-4.87 (m, 1H), 3.90 (dd, *J* = 12.0, 3.0 Hz, 1H), 3.69 (dd, *J* = 12.4, 4.2 Hz, 1H), 3.30 (qd, *J* = 16.3, 10.8 Hz, 2H), 2.25 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 168.0 (d, *J* = 248.2 Hz), 155.5 (d, *J* = 2.7 Hz), 130.9, 129.8 (d, *J* = 7.2 Hz), 123.0 (d, *J* = 3.8 Hz), 122.9 (d, *J* = 17.9 Hz), 114.6 (d, *J* = 22.8 Hz), 81.9, 63.4, 35.8; **ν (KBr)/cm^{-1}:** 3409.2, 2923.8, 2390.7, 1763.4, 1243.2, 1052.8, 922.6, 809.9, 749.2; **HRMS** (ESI) m/z: **calcd for** $C_{10}H_{10}ClFNO_2^+$, **[M+H]$^+$**: 230.0379, **found**: 230.0374.



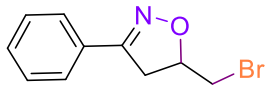
3r

(*E*)-(3-styryl-4,5-dihydroisoxazol-5-yl)methanol (3r). 47.5 mg, 78% yield, white solid, **M. P.** 96.7-99.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.47-7.45 (m, 2H), 7.38-7.30 (m, 3H), 7.05 (d, *J* = 16.3 Hz, 1H), 6.76 (d, *J* = 16.3 Hz, 1H), 4.85-4.79 m, 1H), 3.86 (dd, *J* = 12.1, 3.1 Hz, 1H), 3.66 (dd, *J* = 12.4, 4.6 Hz, 1H), 3.25 (dd, *J* = 16.3, 10.8 Hz, 1H), 3.13 (dd, *J* = 16.3, 7.7 Hz, 1H), 2.10 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 158.2, 136.9, 135.6, 129.0, 128.8, 127.0, 117.6, 81.3, 63.7, 34.9; **ν (KBr)/cm^{-1}:** 3346.9, 2921.9, 2397.2, 1761.7, 1457.2, 1242.9, 1051.5, 958.2, 913.5, 692.9; **HRMS** (ESI) m/z: **calcd for** $C_{12}H_{14}NO_2^+$, **[M+H]$^+$**: 204.1019, **found**: 204.1016.



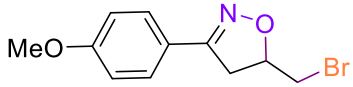
3s

(3-(naphthalen-2-yl)-4,5-dihydroisoxazol-5-yl)methanol (3s). 45.0 mg, 66% yield, white solid, **M. P.** 154.3-156.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.95-7.83 (m, 5H), 7.52-7.50 (m, 2H), 4.92 (d, *J* = 2.5 Hz, 1H), 3.91 (d, *J* = 10.5 Hz, 1H), 3.73 (dd, *J* = 12.0, 4.1 Hz, 1H), 3.45 (qd, *J* = 18.3, 10.7 Hz, 2H), 2.13 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 157.2, 134.0, 132.9, 128.5, 128.4, 127.8, 127.1, 127.0, 126.9, 126.7, 123.5, 81.4, 63.7, 36.3; **ν (KBr)/cm^{-1}:** 3467.3, 2926.1, 1736.4, 1242.6, 1052.9, 918.9, 799.7, 647.3; **HRMS** (ESI) m/z: **calcd for** $C_{14}H_{14}NO_2^+$, **[M+H]$^+$**: 228.1019, **found**: 228.1015.



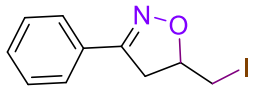
4a

5-(bromomethyl)-3-phenyl-4,5-dihydroisoxazole (4a). 54.7 mg, 74% yield, white solid, **M. P.** 69.8-73.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.69-7.64 (m, 2H), 7.43-7.38 (m, 3H), 5.03-4.96 (m, 1H), 3.91 (d, *J* = 10.5 Hz, 1H), 3.57 (dd, *J* = 10.3, 4.3 Hz, 1H), 3.50 (dd, *J* = 17.0, 10.4 Hz, 1H), 3.41 (dd, *J* = 10.2, 8.1 Hz, 1H), 3.32 (dd, *J* = 17.1, 6.5 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 156.0, 130.3, 128.9, 128.7, 1, 79.6, 39.5, 33.2; **ν (KBr)/cm^{-1}:** 3447.6, 2923.7, 1747.7, 1603.5, 1362.5, 1243.1, 1050.9, 896.9, 752.9, 540.7; **HRMS** (ESI) m/z: **calcd for** $C_{10}H_{11}BrNO^+$, **[M+H]$^+$**: 240.0019, **found**: 240.0014.



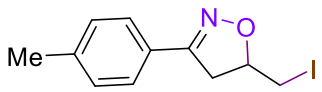
4b

5-(bromomethyl)-3-(4-methoxyphenyl)-4,5-dihydroisoxazole (4b). 29.2 mg, 36% yield, yellow solid, **M.P.** 59.3-62.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.55-7.52 (m, 2H), 5.87-6.83 (m, 2H), 4.93-4.86 (m, 1H), 3.77 (s, 3H), 3.50 (dd, *J* = 10.3, 4.2 Hz, 1H), 3.41 (dd, *J* = 17.0, 10.4 Hz, 1H), 3.32 (dd, *J* = 10.2, 8.4 Hz, 1H), 3.22 (dd, *J* = 17.0, 6.4 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 161.2, 155.6, 128.3, 121.5, 114.1, 79.4, 55.3, 39.8, 33.2; **ν (KBr)/cm^{-1}:** 2990.8, 1761.3, 1513.0, 1244.6, 1050.1, 831.8, 749.3; **HRMS** (ESI) m/z: **calcd for** $C_{11}H_{13}BrNO_2^+$, **[M+H]$^+$**: 270.0124, **found**: 270.0118.



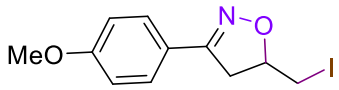
5a

5-(iodomethyl)-3-phenyl-4,5-dihydroisoxazole (5a). 81.8 mg, 95% yield, yellow solid, **M. P.** 69.3.-73.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.62-7.57 (m, 2H), 7.37-7.30 (m, 3H), 4.89-4.81 (m, 1H), 3.44 (dd, *J* = 16.9, 10.3 Hz, 1H), 3.34 (dd, *J* = 10.0, 4.0 Hz, 1H), 3.18-3.13 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 155.8, 130.3, 129.0, 128.7, 126.7, 80.3, 41.0, 7.6; **ν (KBr)/cm^{-1}:** 3449.6, 2991.2, 1763.4, 1362.9, 1243.3, 1054.3, 898.1, 753.6, 689.5; **HRMS** (ESI) m/z: **calcd for** $C_{10}H_{11}INO^+$, **[M+H]$^+$**: 287.9880, **found**: 287.9874.



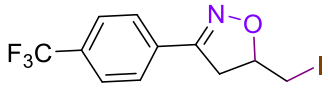
5b

5-(iodomethyl)-3-(p-tolyl)-4,5-dihydroisoxazole (5b). 63.2 mg, 70% yield, yellow solid, **M. P.** 108.3-112.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.96 (d, *J* = 8.1 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 4.86-4.78 (m, 1H), 3.42 (dd, *J* = 17.0, 10.3 Hz, 1H), 3.33 (dd, *J* = 10.3, 4.1 Hz, 1H), 3.17-3.10 (m, 2H), 2.30 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 155.8, 130.3, 129.0, 128.7, 126.7, 80.3, 41.0, 7.6; **ν (KBr)/cm^{-1}:** 3445.8, 2926.1, 1747.3, 1603.3, 1364.2, 1324.4, 1242.4, 1047.5, 898.9, 542.5; **HRMS** (ESI) m/z: **calcd for** $C_{11}H_{13}INO^+$, **[M+H]$^+$**: 302.0036, **found**: 302.0031.



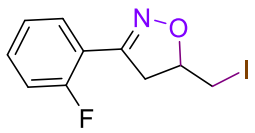
5c

5-(iodomethyl)-3-(4-methoxyphenyl)-4,5-dihydroisoxazole (5c). 47.6 mg, 50% yield, yellow solid, **M. P.** 86.8-90.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.55-7.51 (m, 2H), 6.87-6.83 (m, 2H), 4.85-4.76 (m, 1H), 3.77 (s, 3H), 3.42 (dd, *J* = 17.0, 10.3 Hz, 1H), 3.33 (dd, *J* = 10.0, 4.1 Hz, 1H), 317-3.10 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 161.2, 155.3, 128.3, 121.6, 114.1, 80.1, 55.3, 41.2, 7.7; **ν (KBr)/cm^{-1}:** 2925.6, 2392.4, 1746.3, 1513.6, 1248.0, 1044.2, 896.5, 754.4, 610.3; **HRMS** (ESI) m/z: **calcd for** $C_{11}H_{13}INO_2^+$, **[M+H]$^+$**: 317.9985, **found**: 317.9980.



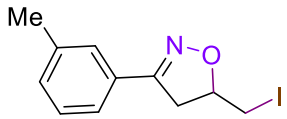
5d

5-(iodomethyl)-3-(4-(trifluoromethyl)phenyl)-4,5-dihydroisoxazole (5d). 75.6 mg, 71% yield, yellow solid, **M. P.** 76.5-79.3 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.70 (d, *J* = 8.3 Hz, 2H), 7.58 (d, *J* = 8.4 Hz, 2H), 4.92-4.85 (m, 1H), 3.45 (dd, *J* = 17.0, 10.5 Hz, 1H), 3.37 (dd, *J* = 10.1, 4.0 Hz, 1H), 3.21-3.12 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 154.7, 132.5, 131.7 (q, *J* = 32.5 Hz), 126.9, 125.7 (q, *J* = 3.7 Hz), 123.7 (q, *J* = 270.6 Hz), 80.8, 40.7, 7.2; **ν (KBr)/cm^{-1}:** 3447.1, 2926.5, 1758.2, 1605.3, 1325.4, 1243.5, 1125.1, 1067.8 840.1, 694.0; **HRMS** (ESI) m/z: **calcd for** $C_{11}H_{10}F_3INO^+$, **[M+H]$^+$**: 355.9754, **found**: 355.9748.



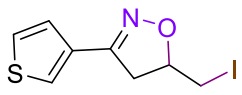
5e

3-(2-fluorophenyl)-5-(iodomethyl)-4,5-dihydroisoxazole (5e). 89.7 mg, 98% yield, yellow solid, **M. P.** 79.3-82.5 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.76 (td, *J* = 7.6, 1.7 Hz, 1H), 7.35-7.29 (m, 1H), 7.12-7.01 (m, 2H), 4.87-4.79 (m, 1H), 3.52 (ddd, *J* = 17.6, 10.3, 2.4 Hz, 1H), 3.32 (dd, *J* = 10.2, 4.2 Hz, 1H), 3.25-3.15 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 161.3 (d, *J* = 251.0 Hz), 152.6 (d, *J* = 3.0 Hz), 131.9 (d, *J* = 8.6 Hz), 129.0 (d, *J* = 2.9 Hz), 124.4 (d, *J* = 3.4 Hz), 117.2 (d, *J* = 11.6 Hz), 116.4 (d, *J* = 21.8 Hz), 80.4 (d, *J* = 2.1 Hz), 42.6 (d, *J* = 6.9 Hz) 7.3; **ν (KBr)/cm^{-1}:** 2927.4, 2360.6, 1756.4, 1599.3, 1449.7, 1239.0, 908.9, 757.8, 507.4; **HRMS** (ESI) m/z: **calcd for** $C_{10}H_{10}FINO^+$, **[M+H]$^+$**: 305.9786, **found**: 305.9780.



5f

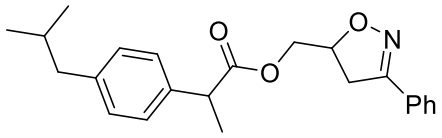
5-(iodomethyl)-3-(m-tolyl)-4,5-dihydroisoxazole (5f). 86.7 mg, 96% yield, yellow solid, **M. P.** 92.3-95.4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.4 (s, 1H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.20 (t, *J* = 7.6 Hz, 1H), 7.14 (d, *J* = 7.6 Hz, 1H), 4.84-4.77 (m, 1H), 3.40 (dd, *J* = 17.7, 10.5 Hz, 1H), 3.31 (dd, *J* = 10.0, 4.0 Hz, 1H), 3.16-3.09 (m, 2H), 2.29 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 155.8, 138.4, 131.0, 128.8, 128.5, 127.2, 123.8, 80.2, 40.9, 21.3, 7.6; **ν (KBr)/cm^{-1}:** 2990.3, 2392.7, 1762.9, 1545.7, 1242.8, 1053.2, 902.6, 692.0; **HRMS** (ESI) m/z: **calcd for** $C_{11}H_{13}INO^+$, **[M+H]$^+$**: 302.0036, **found**: 302.0030.



5g

5-(iodomethyl)-3-(thiophen-3-yl)-4,5-dihydroisoxazole (5g). 84.4 mg, 96% yield, yellow solid, **M. P.** 86.3-89.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.41-7.9 (m, 2H), 7.29 (d, *J* = 5.0, 3.1 Hz, 1H), 4.85-4.77 (m, 1H), 3.42 (dd, *J* = 16.9, 10.3 Hz, 1H), 3.33 (dd, *J* = 10.1, 4.1 Hz, 1H), 3.16-3.10 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 151.9, 130.8, 126.9, 125.8, 125.5, 80.0, 41.6, 7.5; **ν**

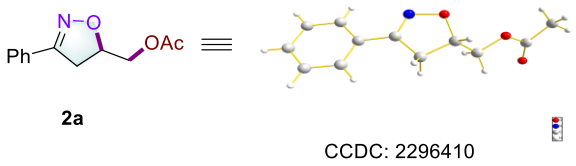
(KBr)/cm^{-1}: 3447.5, 2921.0, 1763.7, 1605.1, 1243.2, 1055.1, 786.9, 623.9; **HRMS** (ESI) m/z: **calcd for** $C_8H_9INOS^+$, **[M+H]$^+$**: 293.9444, **found**: 293.9438.



7a

(3-phenyl-4,5-dihydroisoxazol-5-yl)methyl 3-(4-isobutylphenyl)-2-methylpropanoate (7a). 67.6 mg, 89% yield, yellow solid, **M. P.** 102.1-105.2 ^oC. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 7.66-7.61 (m, 2H), 7.47-7.40 (m, 3H), 7.17 (dd, J = 17.4, 7.9 Hz, 1H), 7.20 (dd, J = 19.1, 7.9 Hz, 1H), 4.97-4.90 (m, 1H), 4.30-4.22 (m, 2H), 3.78-3.72 (m, 1H), 3.33 (td, J = 16.6, 11.0 Hz, 1H), 3.05-2.94 (m, 1H), 2.42 (t, J = 6.8 Hz, 2H), 1.89-1.78 (m, 1H), 1.50 (dd, J = 7.2, 2.4 Hz, 3H), 0.91 (d, J = 6.6 Hz, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) **δ** 174.4(174.4), 156.1(156.1), 140.6(140.5), 137.3(137.2), 130.2(130.1), 129.3 (129.2), 128.7(128.6), 127.1(127.1), 126.6, 78.1(78.1), 64.8, 45.0, 44.9(44.8), 37.0(36.8), 30.1, 22.3, 18.2(17.9); **ν (KBr)/cm^{-1}:** 2927.1, 2358.8, 1744.8, 1602.7, 1365.4, 1237.0, 1048.5, 758.1, 545.9; **HRMS** (ESI) m/z: **calcd for** $C_{24}H_{30}NO_3^+$, **[M+H]$^+$**: 380.2220, **found**: 380.2217.

4. X-ray Crystallographic Analysis



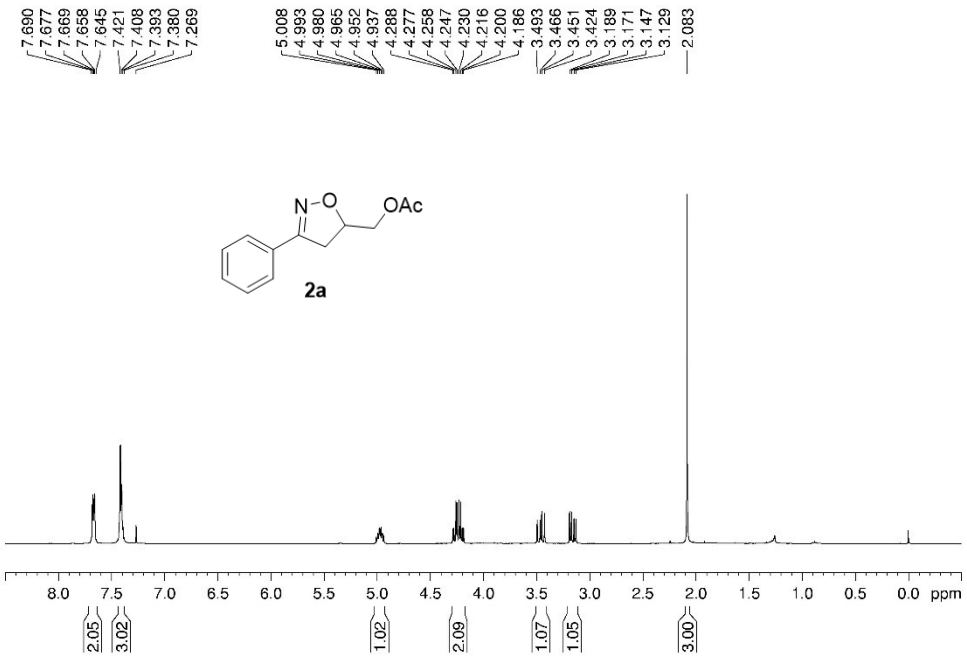
2a

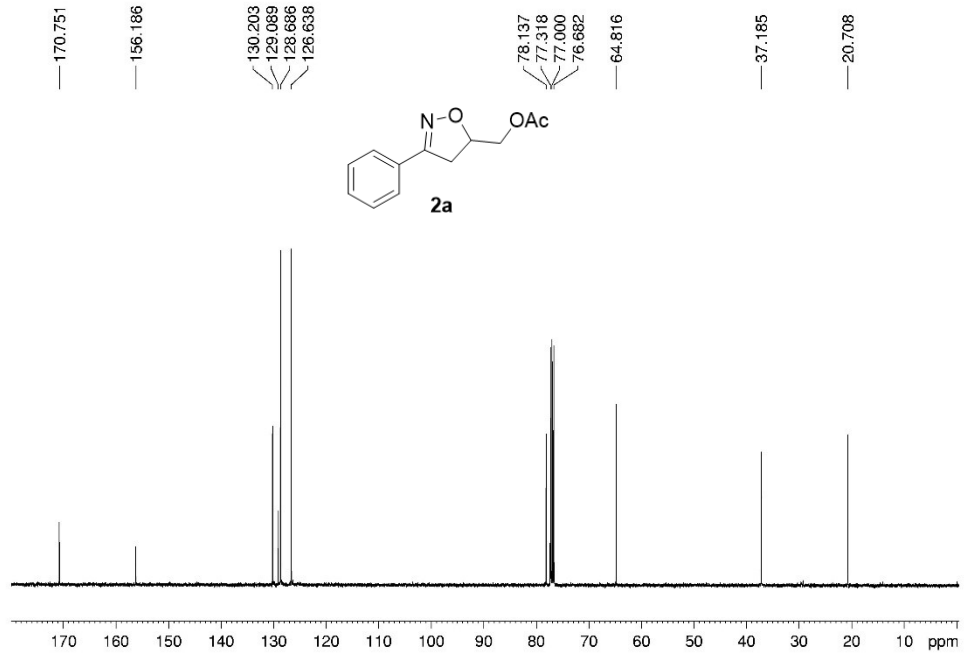
CCDC: 2296410

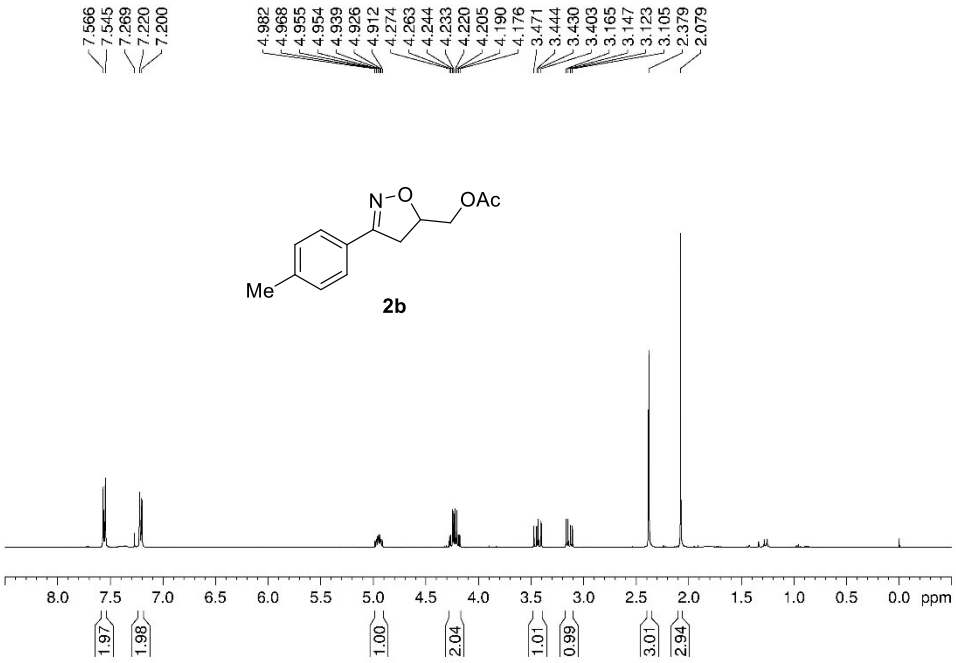
Table 1 Crystal data and structure refinement for 2a.

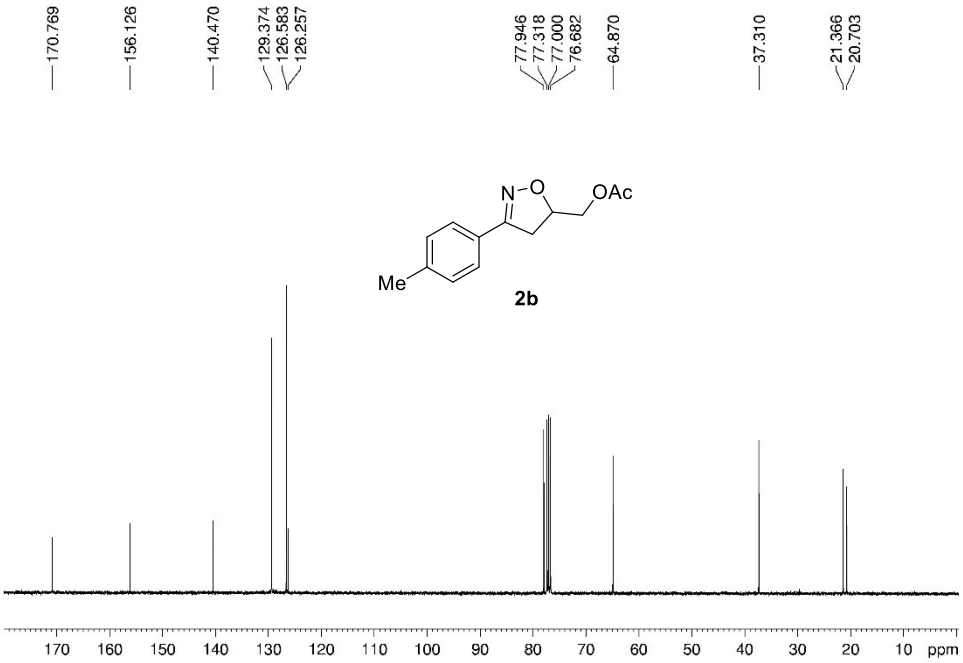
Identification code	2a
Empirical formula	$C_{12}H_{13}NO_3$
Formula weight	219.23
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	25.4531(15)
b/Å	5.4653(3)
c/Å	7.6438(4)
α/°	90
β/°	95.309(2)
γ/°	90
Volume/Å^3	1058.76(10)
Z	4
ρ_{calc}g/cm^3	1.375
μ/mm^{-1}	0.099
F(000)	464.0
Crystal size/mm^3	0.11 × 0.04 × 0.02
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.822 to 52.752
Index ranges	-31 ≤ h ≤ 31, -6 ≤ k ≤ 6, -9 ≤ l ≤ 9
Reflections collected	9339
Independent reflections	2123 [R_{int}= 0.0791, R_{sigma}= 0.0673]
Data/restraints/parameters	2123/0/146
Goodness-of-fit on F^2	1.088
Final R indexes [I>=2σ (I)]	R_1= 0.0522, wR_2= 0.1065
Final R indexes [all data]	R_1= 0.0867, wR_2= 0.1236
Largest diff. peak/hole / e Å^{-3}	0.20/-0.26

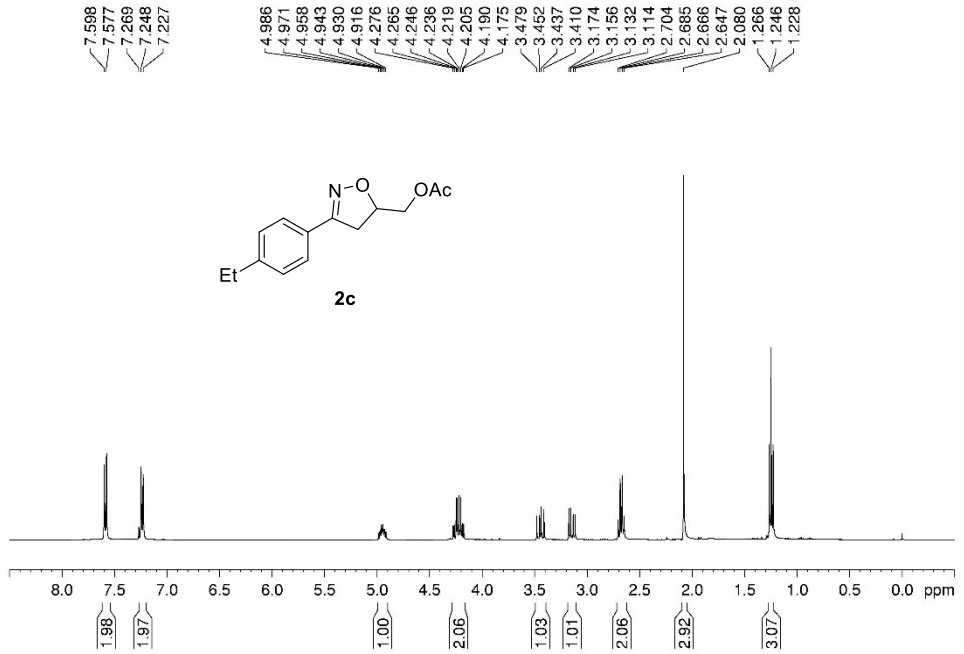
5. ^{1}H NMR and ^{13}C NMR Spectra of Compounds

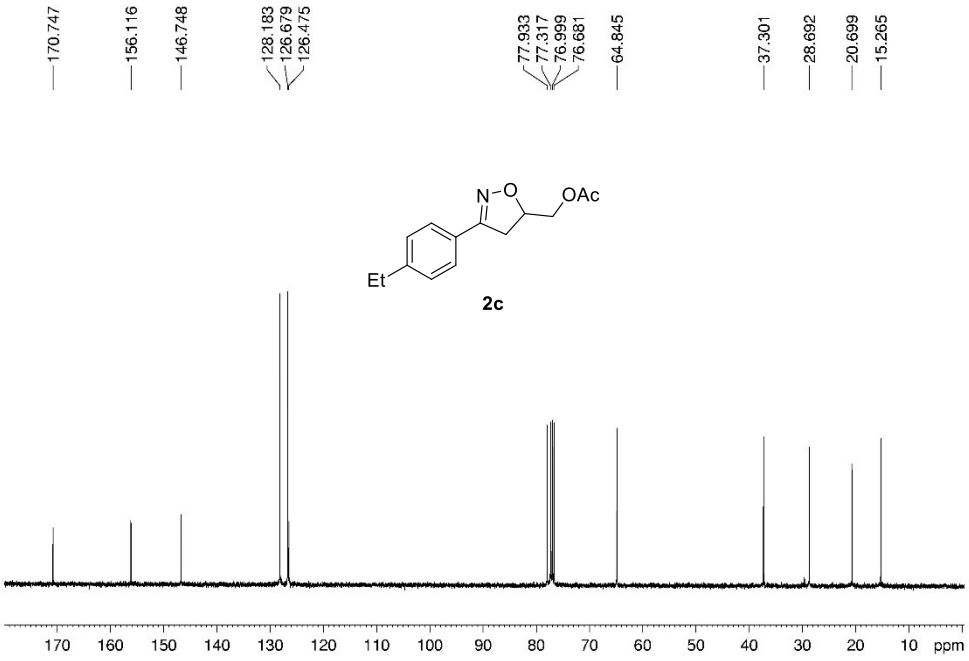


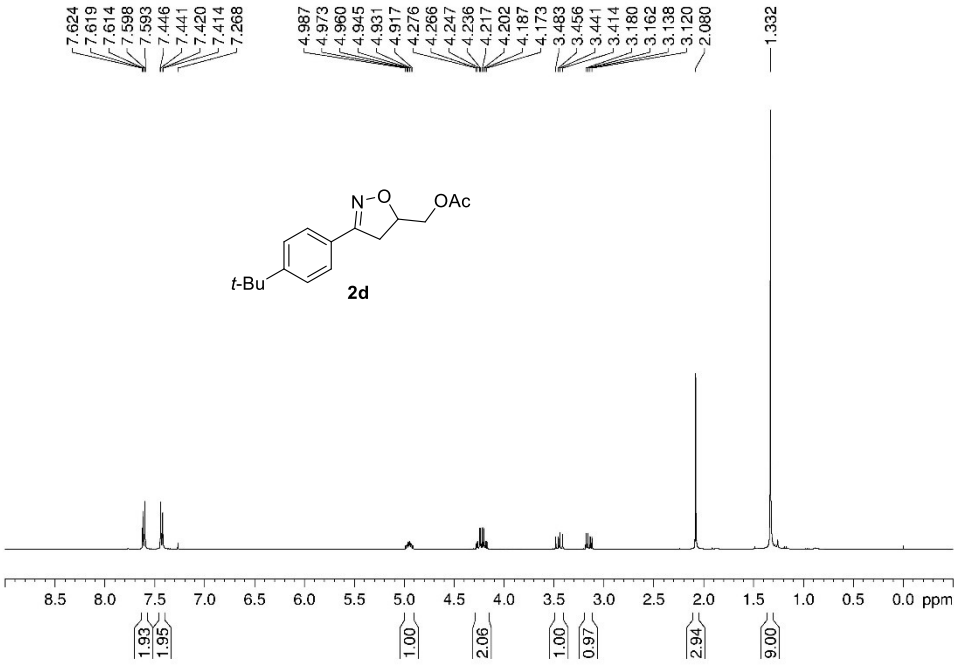


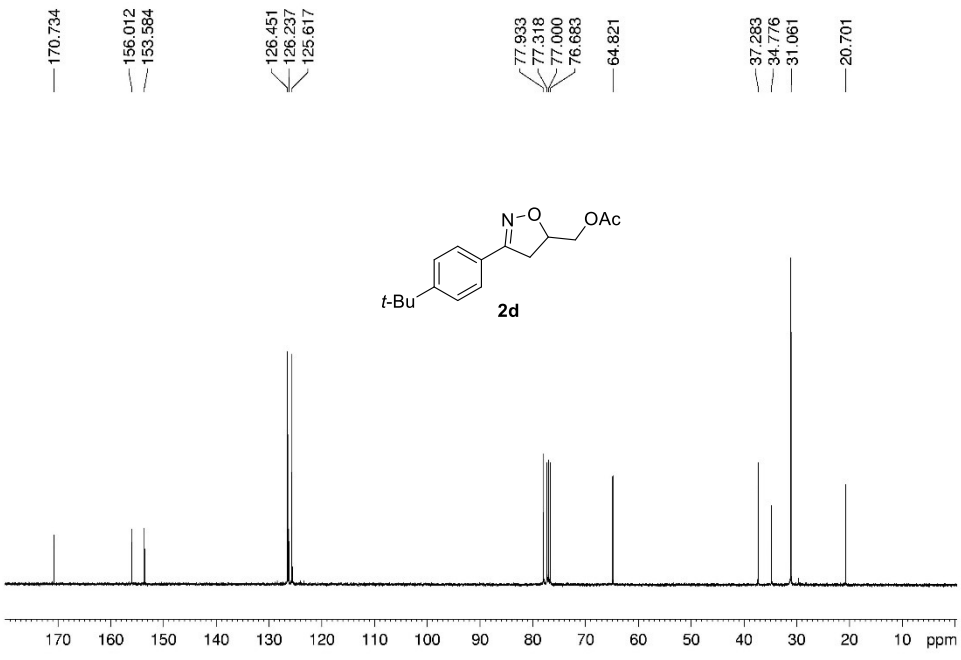

7.566
7.545
7.269
7.220
7.200
4.982
4.968
4.955
4.954
4.939
4.926
4.912
4.274
4.263
4.244
4.233
4.220
4.205
4.190
4.176
3.471
3.444
3.430
3.403
3.165
3.147
3.123
3.105
2.379
2.079
N
O
OAc
Me
2b
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.97
1.98
1.00
2.04
1.01
0.99
3.01
2.94

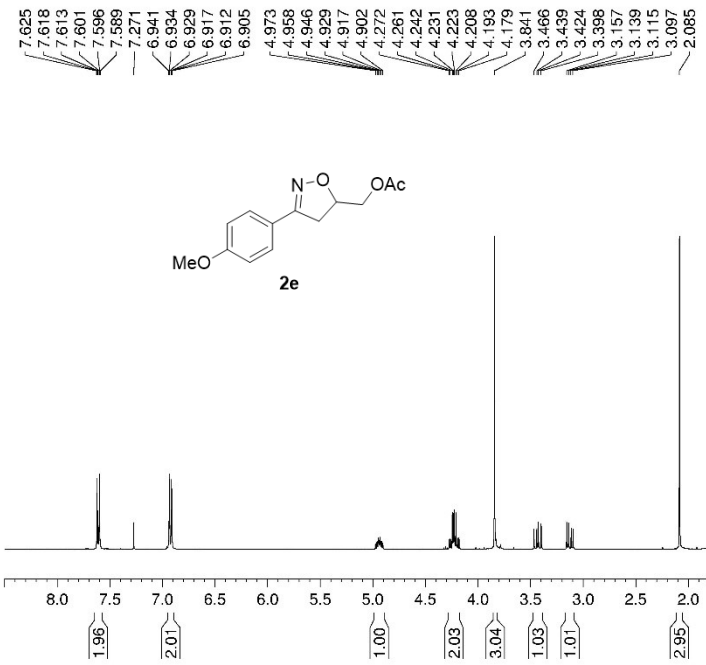

170.769
156.126
140.470
129.374
126.583
126.257
77.946
77.318
77.000
76.682
64.870
37.310
21.366
20.703
N
O
OAc
Me
2b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

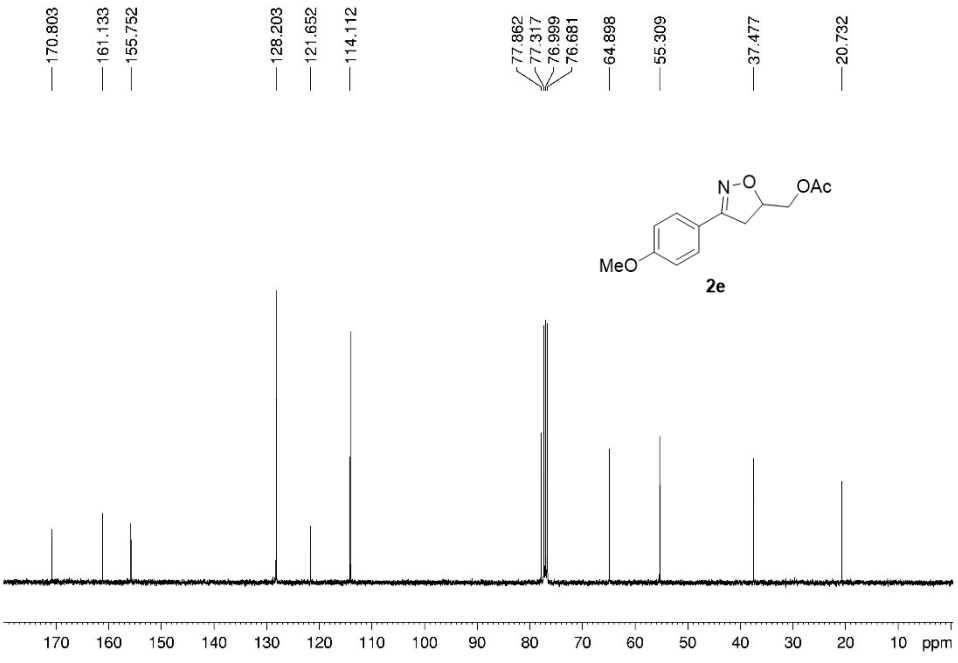

7.598
7.577
7.269
7.248
7.227
4.986
4.971
4.958
4.943
4.930
4.916
4.276
4.265
4.246
4.236
4.219
4.205
4.190
4.175
3.479
3.452
3.437
3.410
3.174
3.156
3.132
3.114
2.704
2.685
2.666
2.647
2.080
1.266
1.246
1.228
N
O
OAc
Et
2c
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
1.98
1.97
1.00
2.06
1.03
1.01
2.06
2.92
3.07

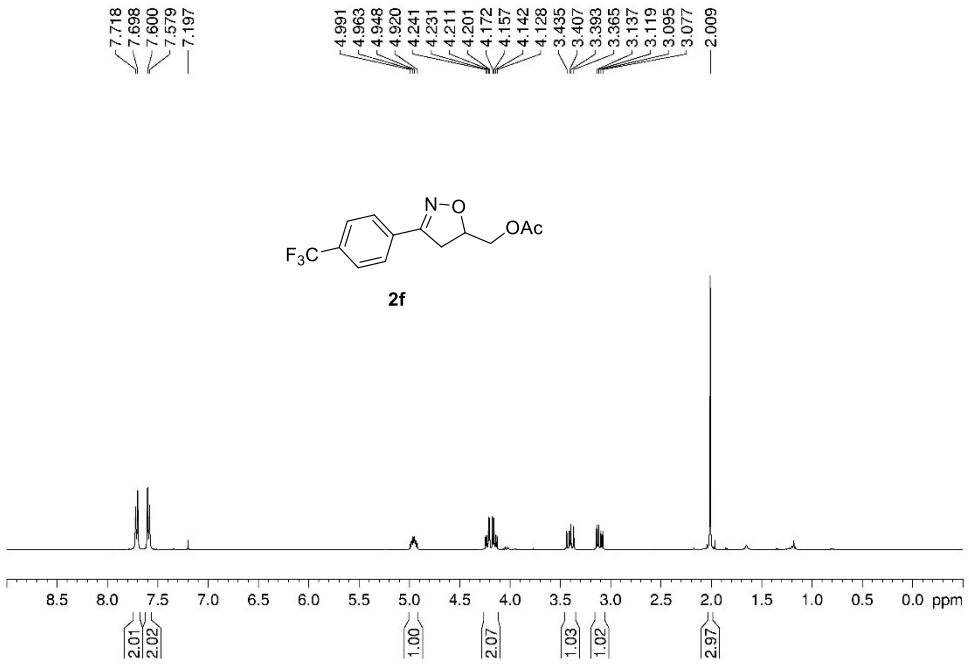

170.747
156.116
146.748
128.183
126.679
126.475
77.933
77.317
76.999
76.681
64.845
37.301
28.692
20.699
15.265
N
O
OAc
Et
2c
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

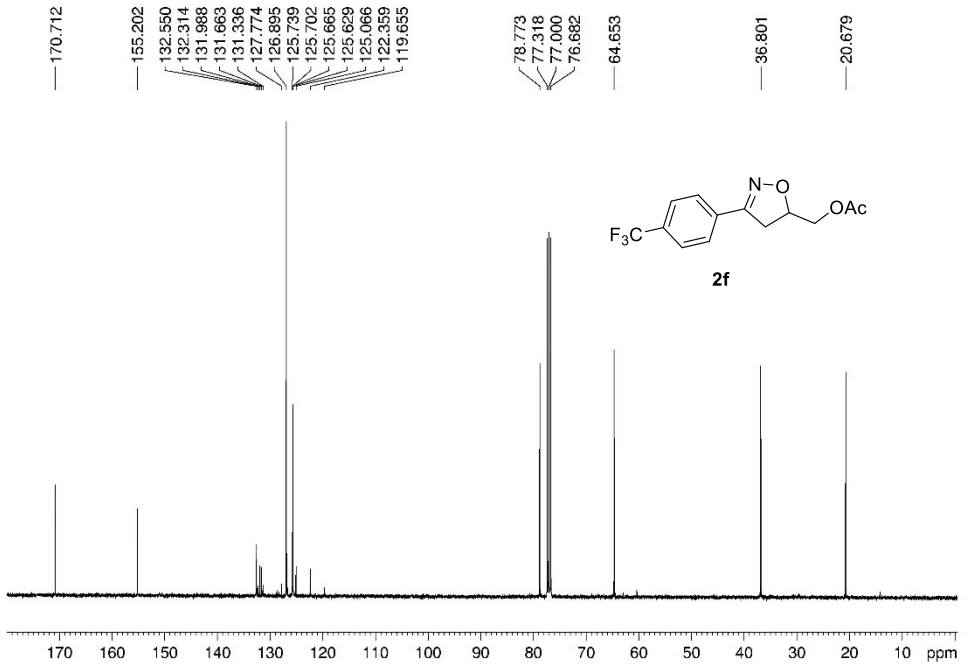

7.624
7.619
7.614
7.598
7.593
7.446
7.441
7.420
7.414
7.268
4.987
4.973
4.960
4.945
4.931
4.917
4.276
4.266
4.247
4.236
4.217
4.202
4.187
4.173
3.483
3.456
3.441
3.414
3.180
3.162
3.138
3.120
2.080
1.332
N
O
OAc
t-Bu
2d
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.93
1.95
1.00
2.06
1.00
0.97
2.94
9.00

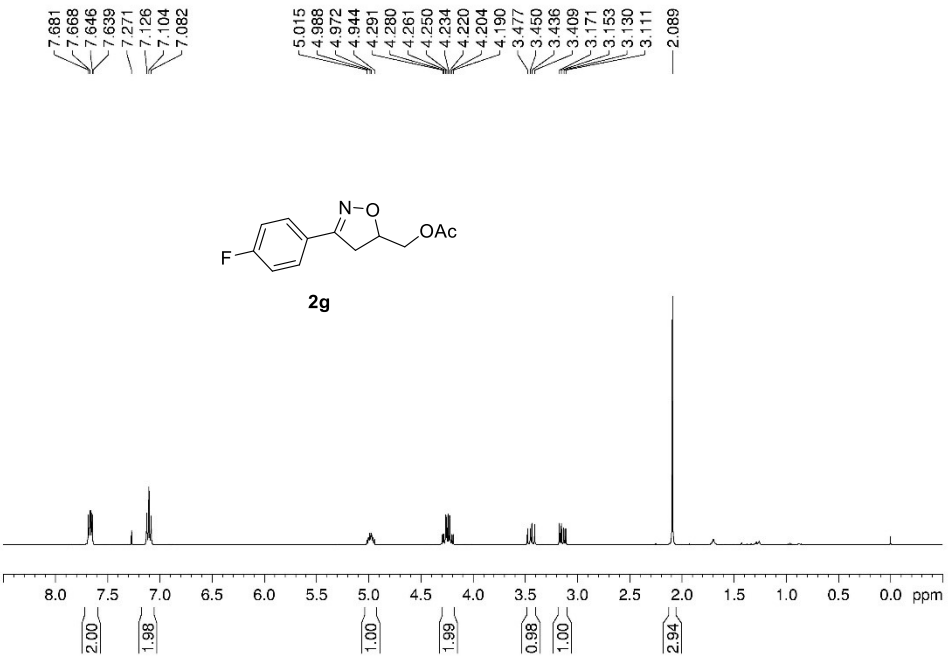

170.734
156.012
153.584
126.451
126.237
125.617
77.933
77.318
77.000
76.683
64.821
37.283
34.776
31.061
20.701
N
O
OAc
t-Bu
2d
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

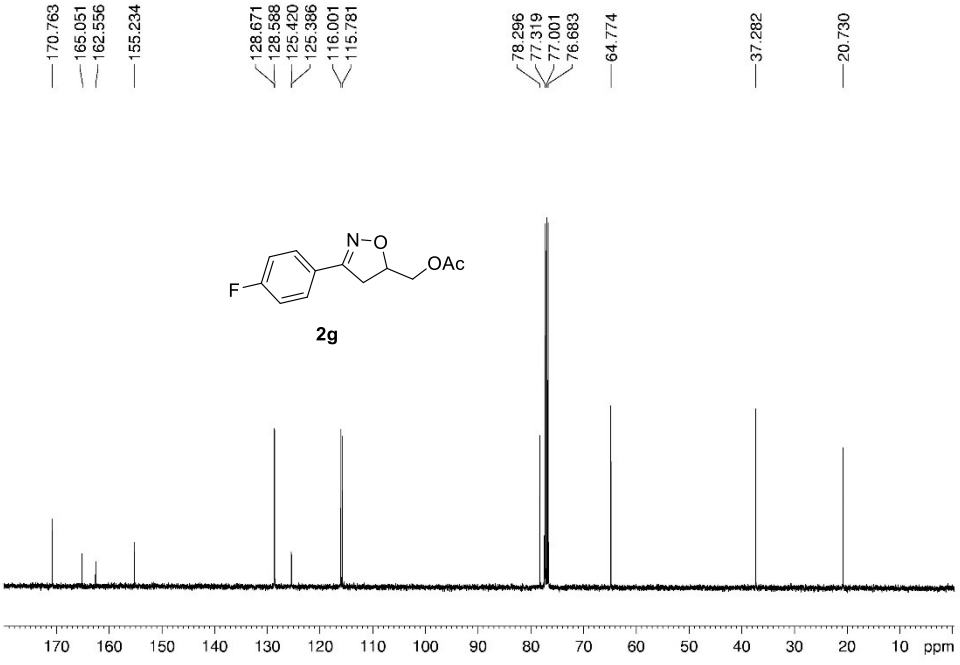

7.625
7.618
7.613
7.601
7.596
7.589
7.271
6.941
6.934
6.929
6.917
6.912
6.905
4.973
4.958
4.946
4.929
4.917
4.902
4.272
4.261
4.242
4.231
4.223
4.208
4.193
4.179
3.841
3.466
3.439
3.424
3.398
3.157
3.139
3.115
3.097
2.085
N
O
OAc
MeO
2e
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.96
2.01
1.00
2.03
3.04
1.03
1.01
2.95

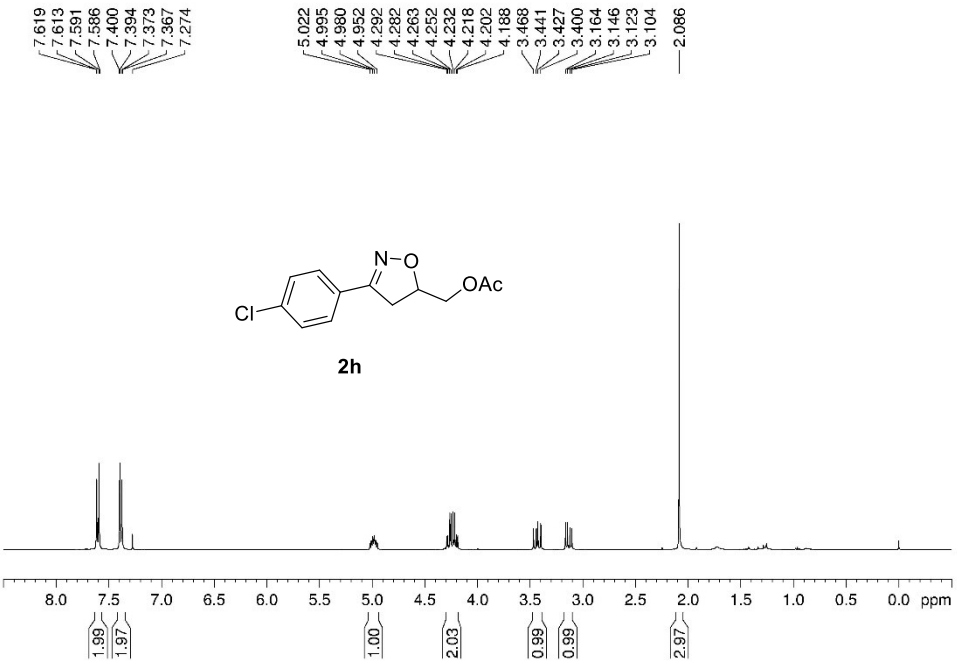

170.803
161.133
155.752
128.203
121.652
114.112
77.862
77.317
76.999
76.681
64.898
55.309
37.477
20.732
N
O
OAc
MeO
2e
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

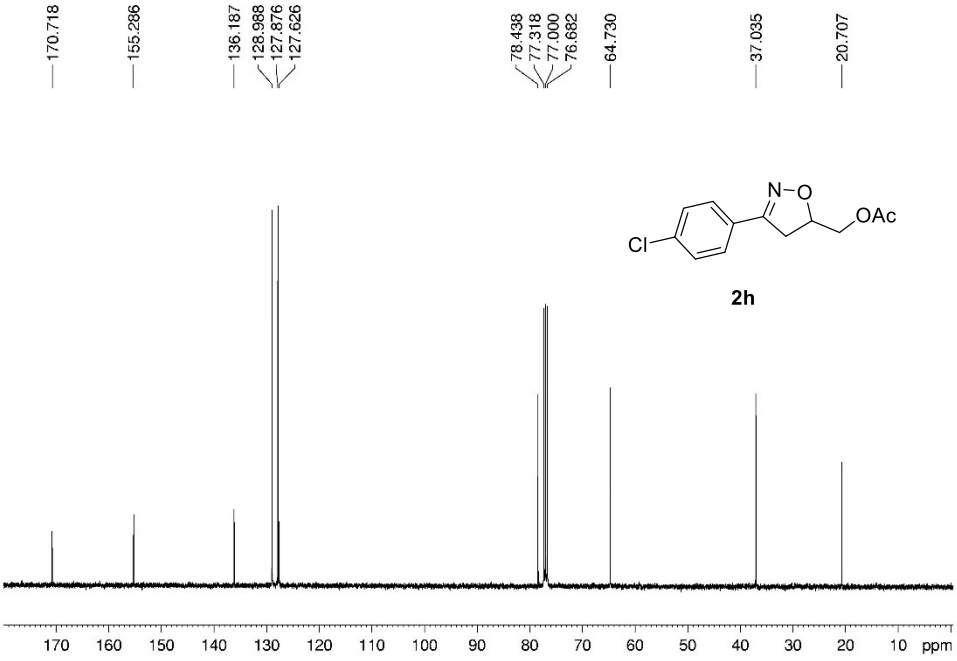

7.718
7.698
7.600
7.579
7.197
4.991
4.963
4.948
4.920
4.241
4.231
4.211
4.201
4.172
4.157
4.142
4.128
3.435
3.407
3.393
3.365
3.137
3.119
3.095
3.077
2.009
N–O
OAc
F3C
2f
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.01
2.02
1.00
2.07
1.03
1.02
2.97

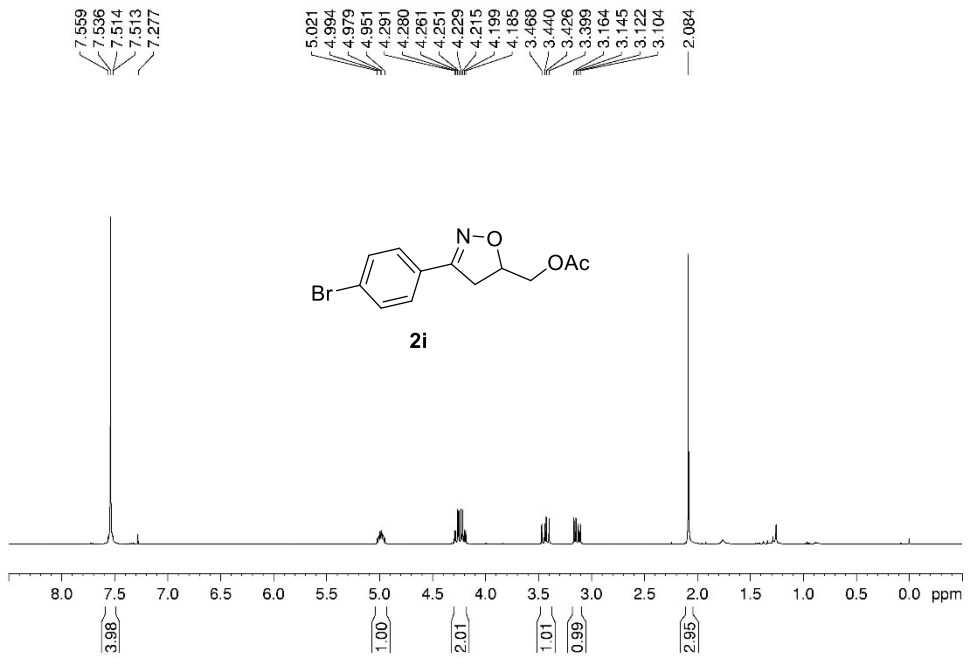

170.712
155.202
132.550
132.314
131.988
131.663
131.336
127.774
126.895
125.739
125.702
125.665
125.629
125.066
122.359
119.655
78.773
77.318
77.000
76.682
64.653
36.801
20.679
N–O
OAc
F3C
2f
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

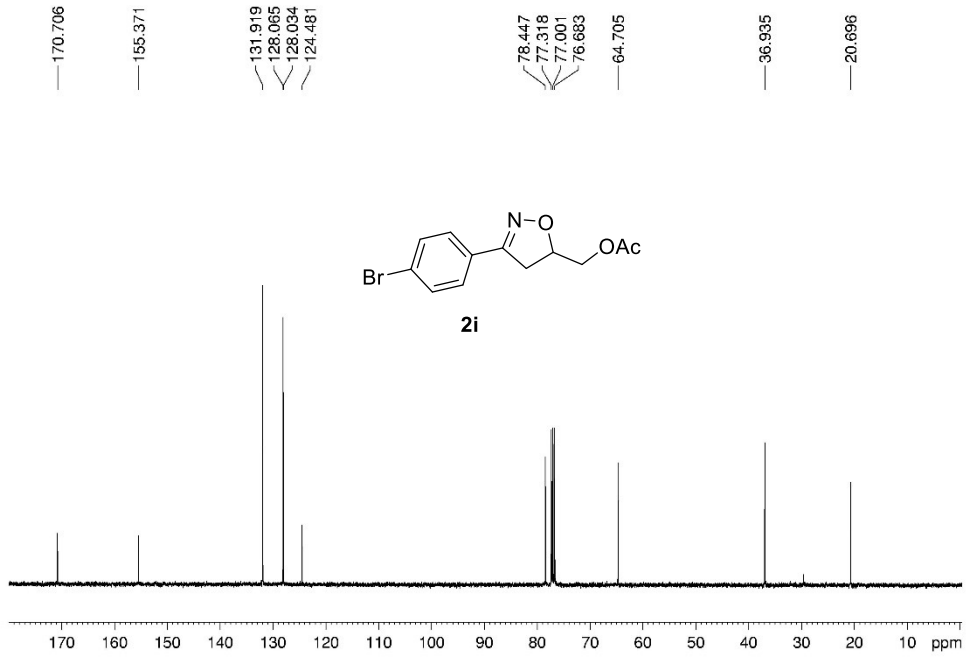

7.681
7.668
7.646
7.639
7.271
7.126
7.104
7.082
5.015
4.988
4.972
4.944
4.291
4.280
4.261
4.250
4.234
4.220
4.204
4.190
3.477
3.450
3.436
3.409
3.171
3.153
3.130
3.111
2.089
N
O
OAc
F
2g
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.00
1.98
1.00
1.99
0.98
1.00
2.94

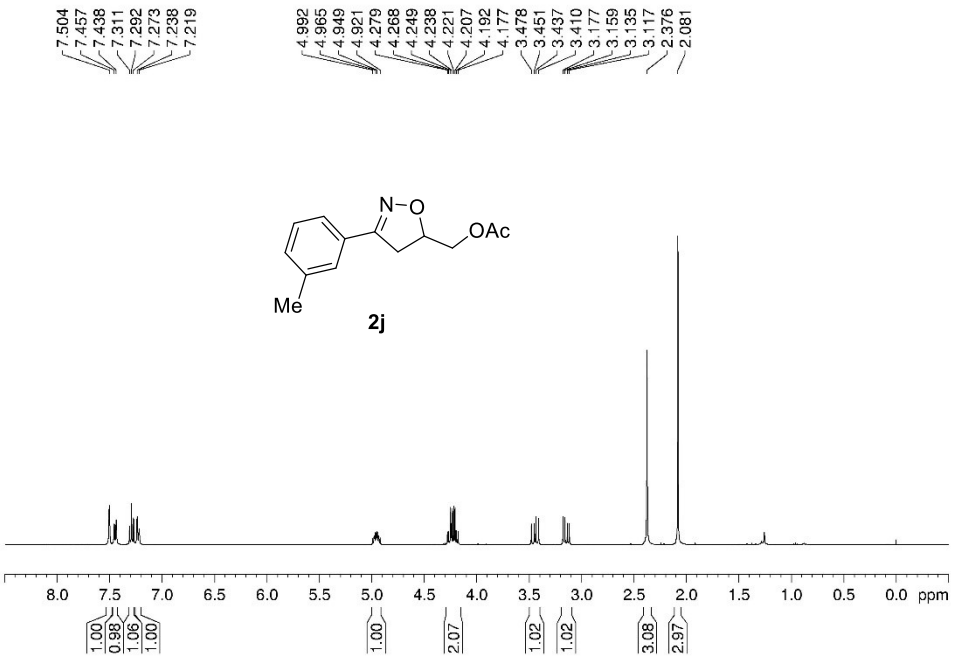

170.763
165.051
162.556
155.234
128.671
128.588
125.420
125.386
116.001
115.781
78.296
77.319
77.001
76.683
64.774
37.282
20.730
N
O
OAc
F
2g
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

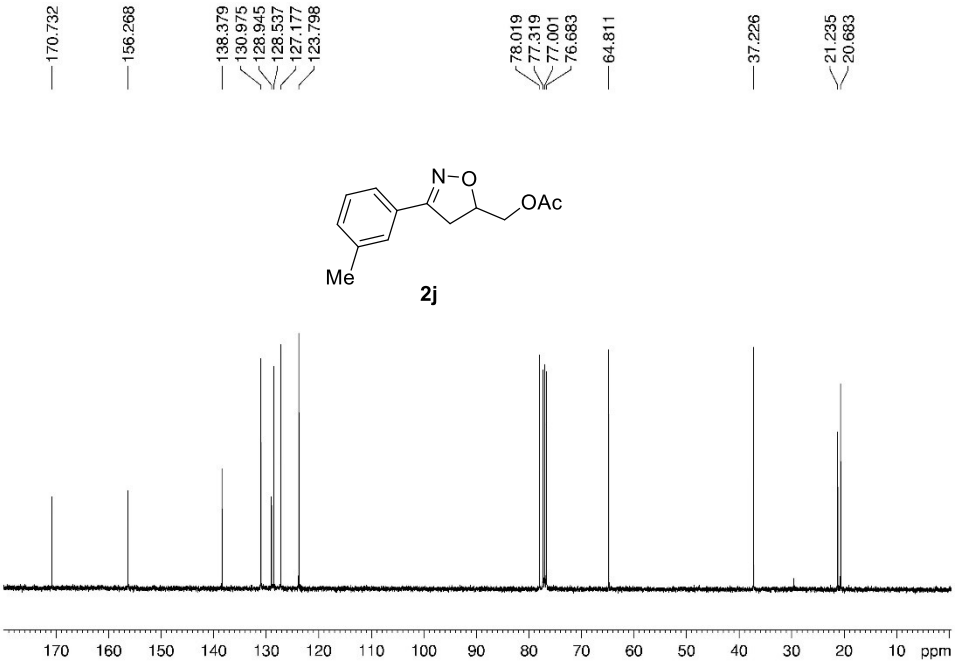

7.619
7.613
7.591
7.586
7.400
7.394
7.373
7.367
7.274
5.022
4.995
4.980
4.952
4.292
4.282
4.263
4.252
4.232
4.218
4.202
4.188
3.468
3.441
3.427
3.400
3.164
3.146
3.123
3.104
2.086
N–O
OAc
Cl
2h
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.99
1.97
1.00
2.03
0.99
0.99
2.97

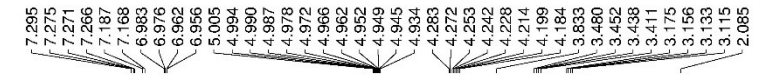

170.718
155.286
136.187
128.988
127.876
127.626
78.438
77.318
77.000
76.682
64.730
37.035
20.707
N–O
OAc
Cl
2h
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

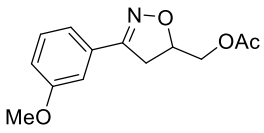

7.559
7.536
7.514
7.513
7.277
5.021
4.994
4.979
4.951
4.291
4.280
4.261
4.251
4.229
4.215
4.199
4.185
3.468
3.440
3.426
3.399
3.164
3.145
3.122
3.104
2.084
N
O
OAc
Br
2i
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
3.98
1.00
2.01
1.01
0.99
2.95


170.706
155.371
131.919
128.065
128.034
124.481
78.447
77.318
77.001
76.683
64.705
36.935
20.696
N
O
OAc
Br
2i
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

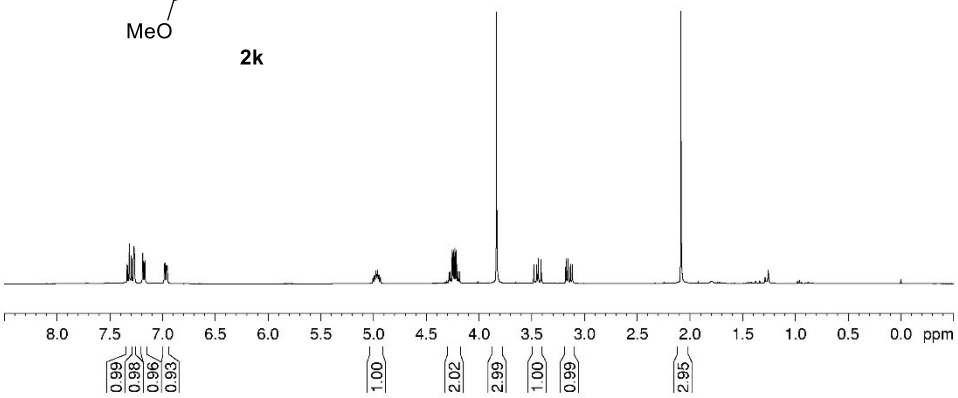

7.504
7.457
7.438
7.311
7.292
7.273
7.238
7.219
4.992
4.965
4.949
4.921
4.279
4.268
4.249
4.238
4.221
4.207
4.192
4.177
3.478
3.451
3.437
3.410
3.177
3.159
3.135
3.117
2.376
2.081
N–O
OAc
Me
2j
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
1.00
0.98
1.06
1.00
1.00
2.07
1.02
1.02
3.08
2.97


170.732
156.268
138.379
130.975
128.945
128.537
127.177
123.798
78.019
77.319
77.001
76.683
64.811
37.226
21.235
20.683
N–O
OAc
Me
2j
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

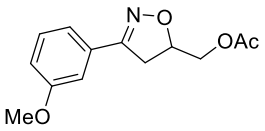

7.295
7.275
7.271
7.266
7.187
7.168
6.983
6.976
6.962
6.956
5.005
4.994
4.990
4.987
4.978
4.972
4.966
4.962
4.952
4.949
4.945
4.934
4.283
4.272
4.253
4.242
4.228
4.214
4.199
4.184
3.833
3.480
3.452
3.438
3.411
3.175
3.156
3.133
3.115
2.085


N
O
OAc
MeO

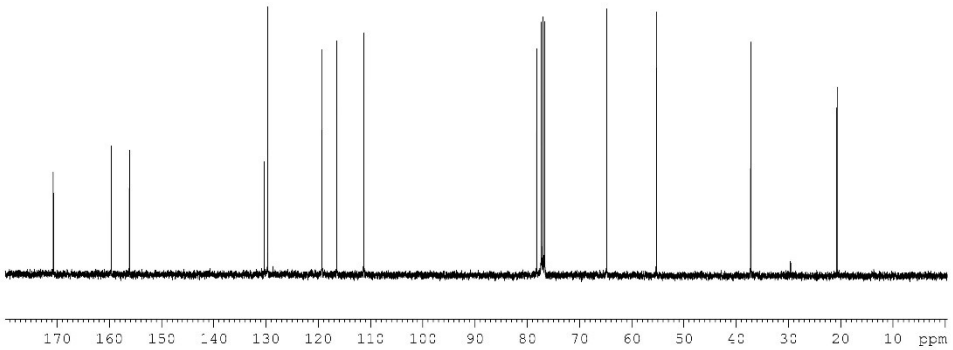
2k

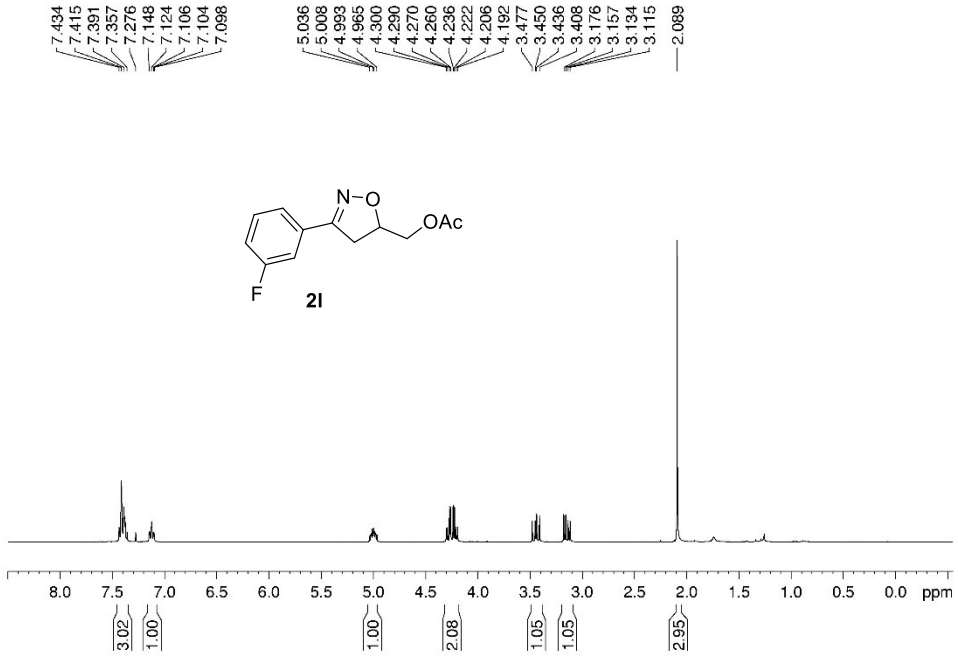

8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.99
0.98
0.96
0.93
1.00
2.02
2.99
1.00
0.99
2.95

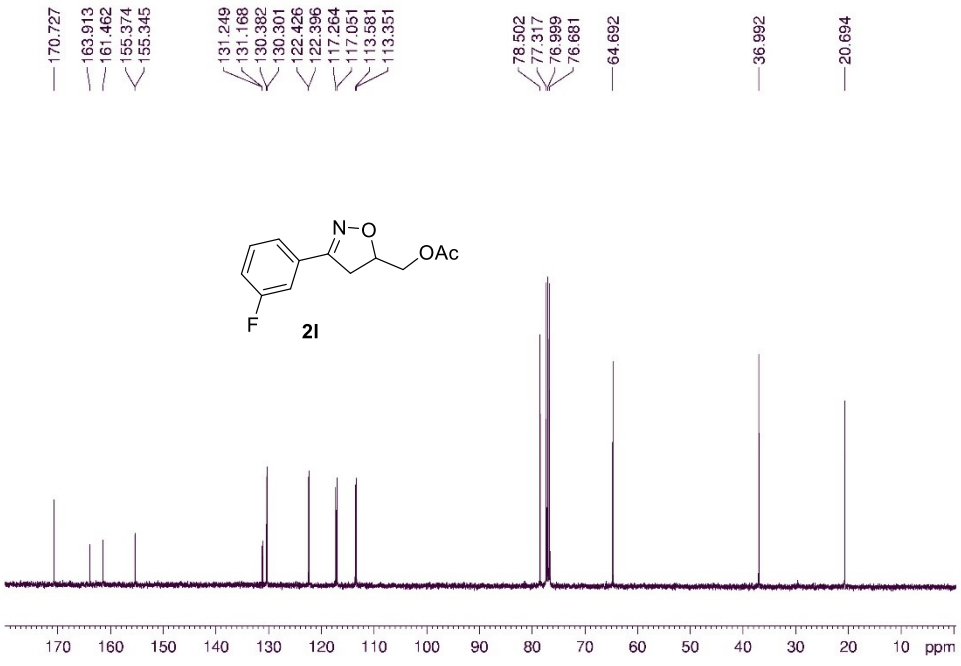

170.732
159.625
156.159
130.327
129.678
119.269
116.463
111.256
78.192
77.317
76.999
76.681
64.777
55.275
37.201
20.693


N
O
OAc
MeO

2k


170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.434
7.415
7.391
7.357
7.276
7.148
7.124
7.106
7.104
7.098
5.036
5.008
4.993
4.965
4.300
4.290
4.270
4.260
4.236
4.222
4.206
4.192
3.477
3.450
3.436
3.408
3.176
3.157
3.134
3.115
2.089
N–O
OAc
F
2l
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
ppm
3.02
1.00
1.00
2.08
1.05
1.05
2.95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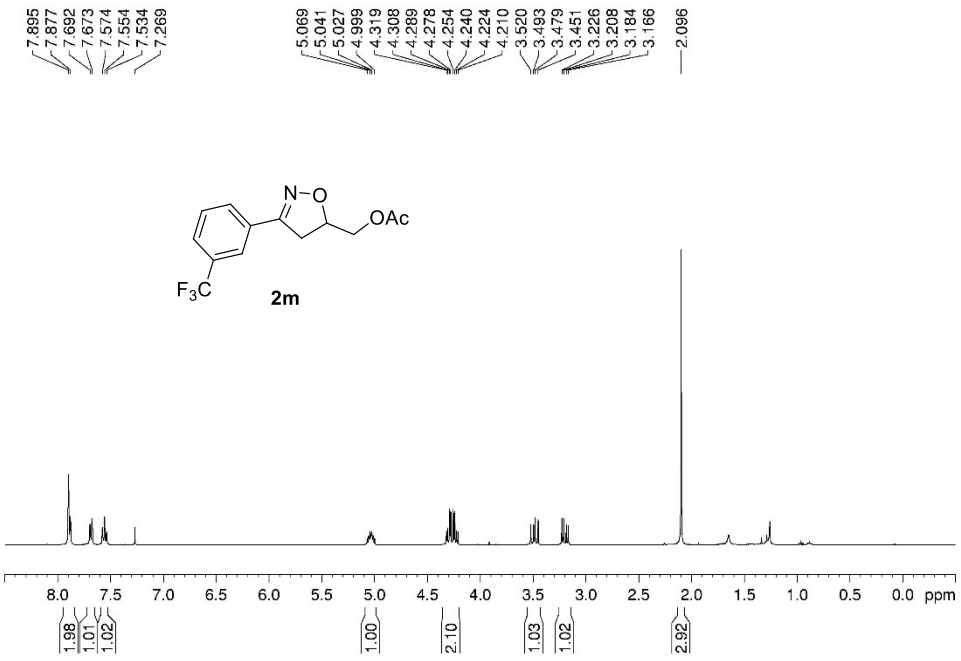
155.374
155.345
131.249
131.168
130.382
130.301
122.426
122.396
117.264
117.051
113.581
113.351
78.502
77.317
76.999
76.681
64.692
36.992
20.694
N–O
OAc
F
2l
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.692
7.673
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7.269
5.069
5.041
5.027
4.999
4.319
4.308
4.289
4.278
4.254
4.240
4.224
4.210
3.520
3.493
3.479
3.451
3.226
3.208
3.184
3.166
2.096
N
O
OAc
F3C
2m
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 ppm
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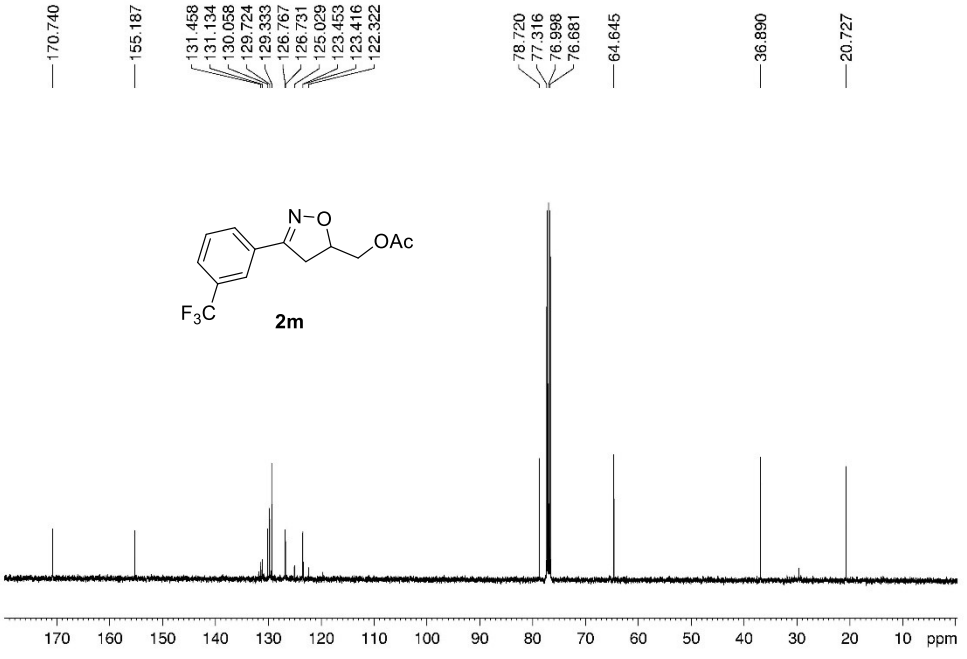
1.01
1.02
1.00
2.10
1.03
1.02
2.92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131.458
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129.724
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126.767
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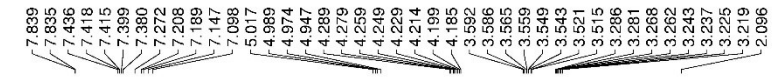
125.029
123.453
123.416
122.322
78.720
77.316
76.998
76.681
64.645
36.890
20.727
N
O
OAc
F3C
2m
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm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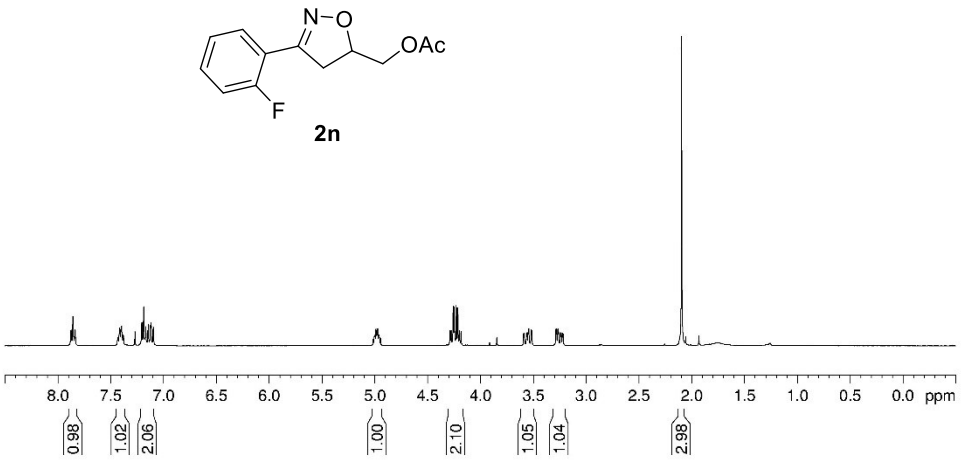
7.835
7.436
7.418
7.415
7.399
7.380
7.272
7.208
7.189
7.147
7.098
5.017
4.989
4.974
4.947
4.289
4.279
4.259
4.249
4.229
4.214
4.199
4.185
3.592
3.586
3.565
3.559
3.549
3.543
3.521
3.515
3.286
3.281
3.268
3.262
3.243
3.237
3.225
3.219
2.096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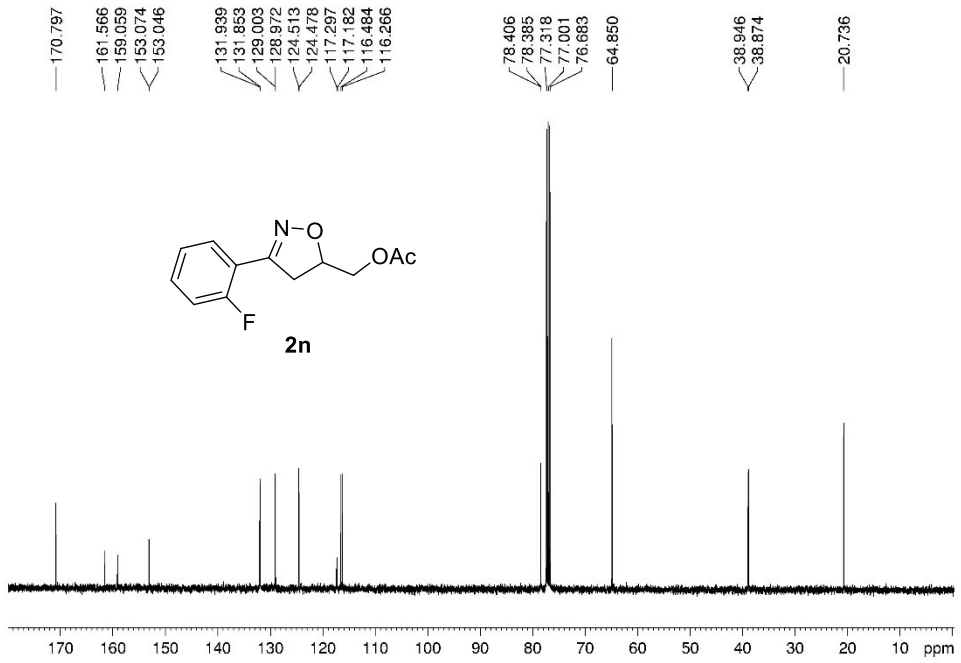
O
OAc
F
2n
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
0.98
1.02
2.06
1.00
2.10
1.05
1.04
2.98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159.059
153.074
153.046
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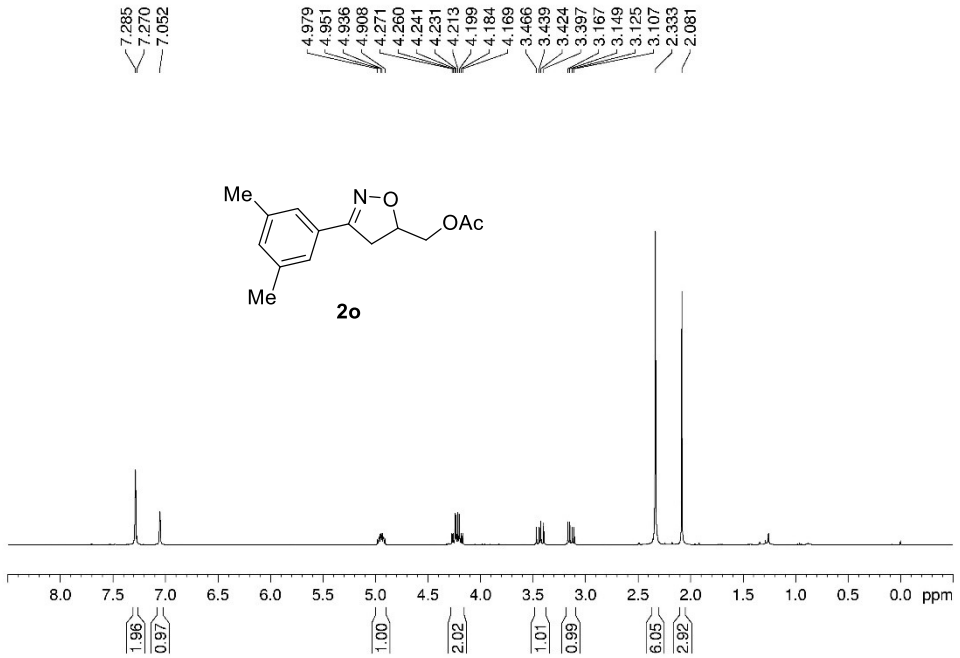
131.853
129.003
128.972
124.513
124.478
117.297
117.182
116.484
116.266
78.406
78.385
77.318
77.001
76.683
64.850
38.946
38.874
20.736
N
O
OAc
F
2n
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm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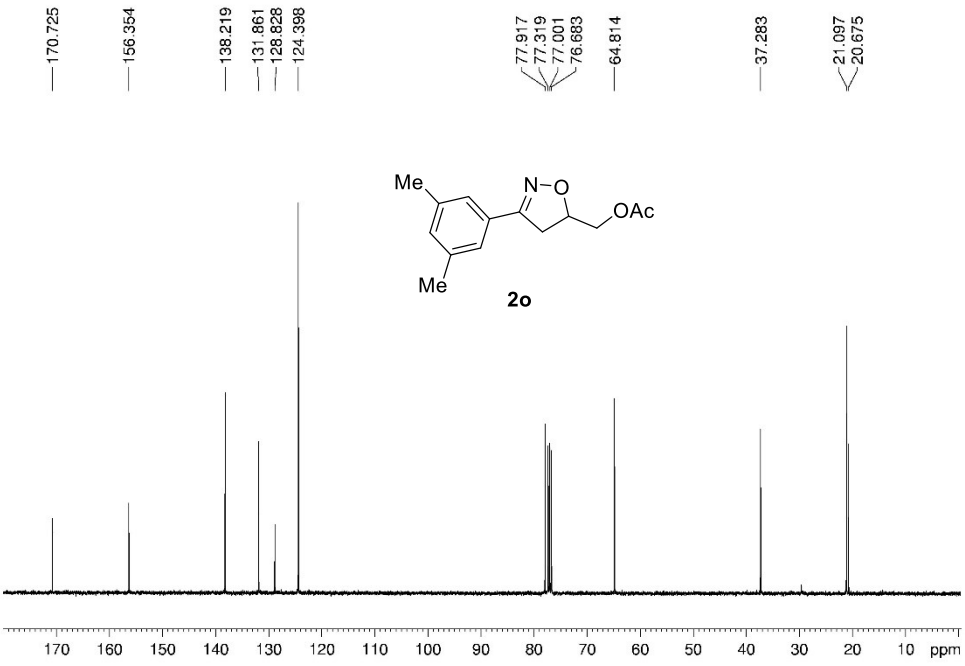
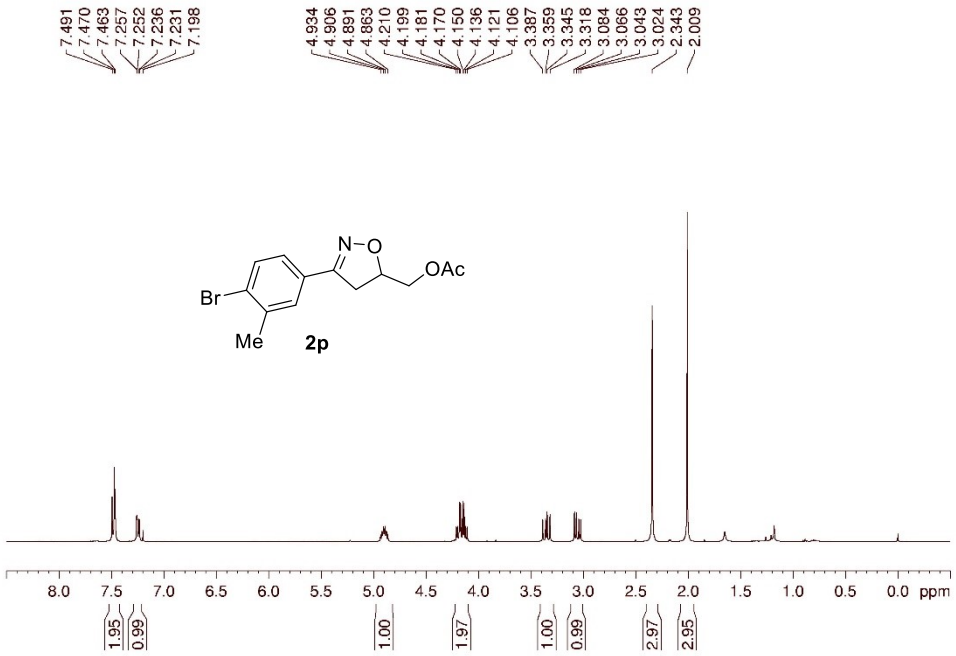
7.270
7.052
4.979
4.951
4.936
4.908
4.271
4.260
4.241
4.231
4.213
4.199
4.184
4.169
3.466
3.439
3.424
3.397
3.167
3.149
3.125
3.107
2.333
2.081
Me
N–O
OAc
Me
2o
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.96
0.97
1.00
2.02
1.01
0.99
6.05
2.92


170.725
156.354
138.219
131.861
128.828
124.398
77.917
77.319
77.001
76.683
64.814
37.283
21.097
20.675
Me
N–O
OAc
Me
2o
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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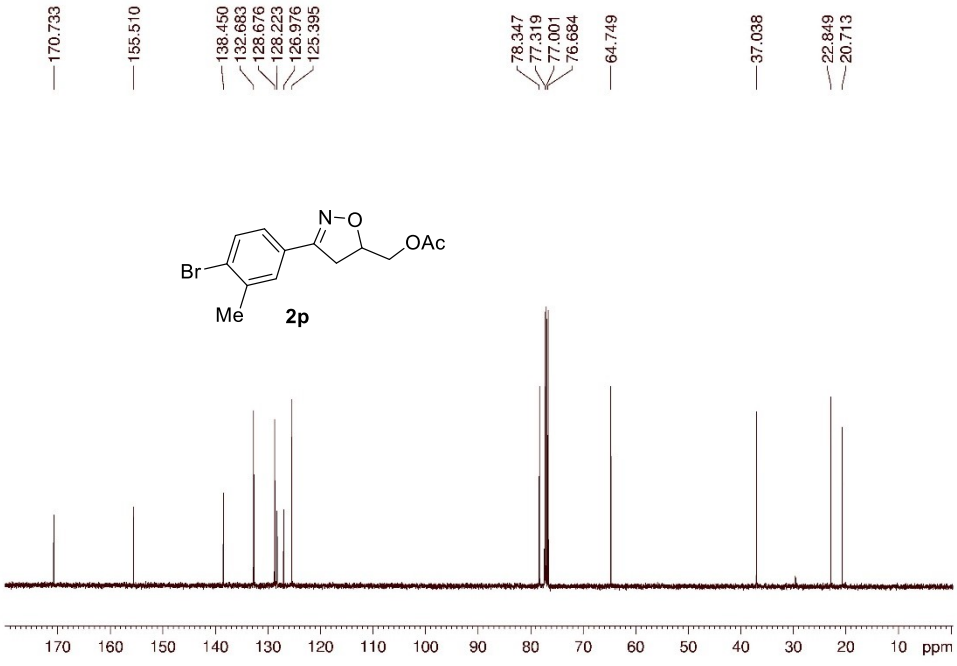
7.470
7.463
7.257
7.252
7.236
7.231
7.198
4.934
4.906
4.891
4.863
4.210
4.199
4.181
4.170
4.150
4.136
4.121
4.106
3.387
3.359
3.345
3.318
3.084
3.066
3.043
3.024
2.343
2.009
N–O
OAc
Br
Me
2p
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
1.95
0.99
1.00
1.97
1.00
0.99
2.97
2.95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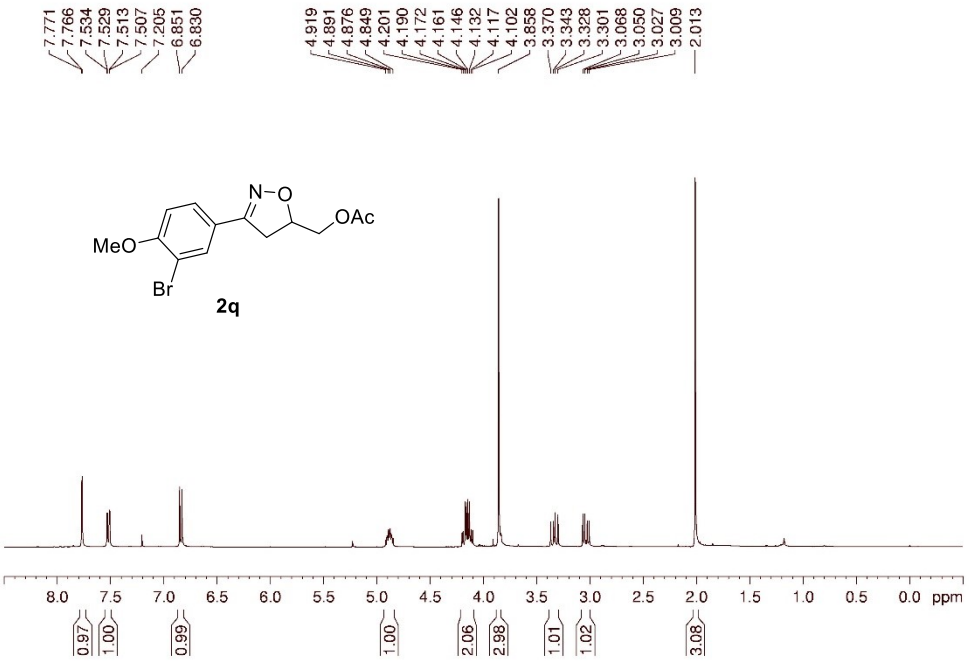
155.510
138.450
132.683
128.676
128.223
126.976
125.395
78.347
77.319
77.001
76.684
64.749
37.038
22.849
20.713
N–O
OAc
Br
Me
2p
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm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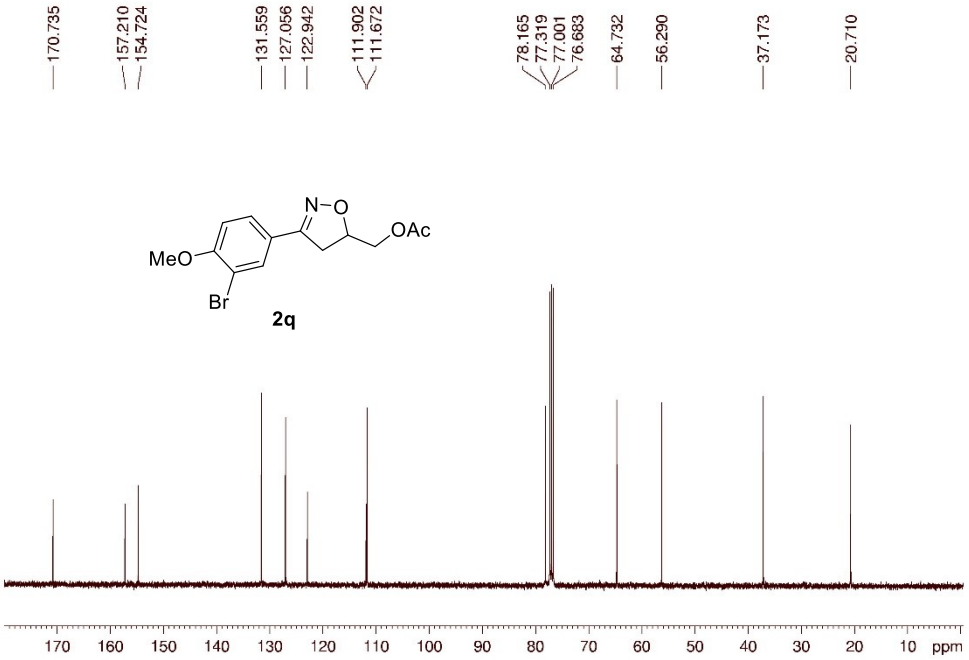
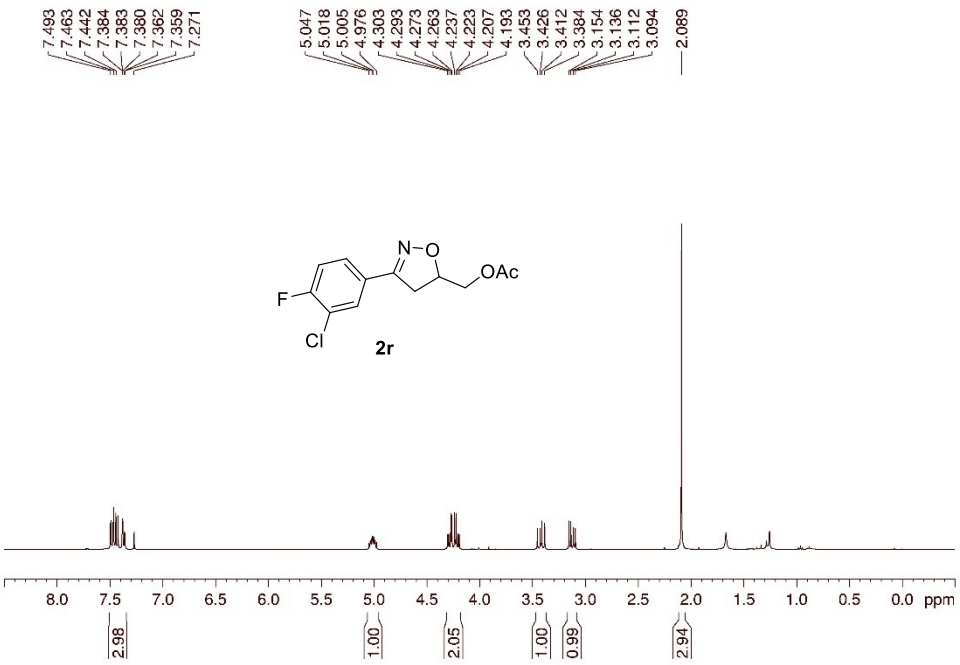
7.766
7.534
7.529
7.513
7.507
7.205
6.851
6.830
4.919
4.891
4.876
4.849
4.201
4.190
4.172
4.161
4.146
4.132
4.117
4.102
3.858
3.370
3.343
3.328
3.301
3.068
3.050
3.027
3.009
2.013
N
O
OAc
MeO
Br
2q
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
0.97
1.00
0.99
1.00
2.06
2.98
1.01
1.02
3.08


170.735
157.210
154.724
131.559
127.056
122.942
111.902
111.672
78.165
77.319
77.001
76.683
64.732
56.290
37.173
20.710
N
O
OAc
MeO
Br
2q
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm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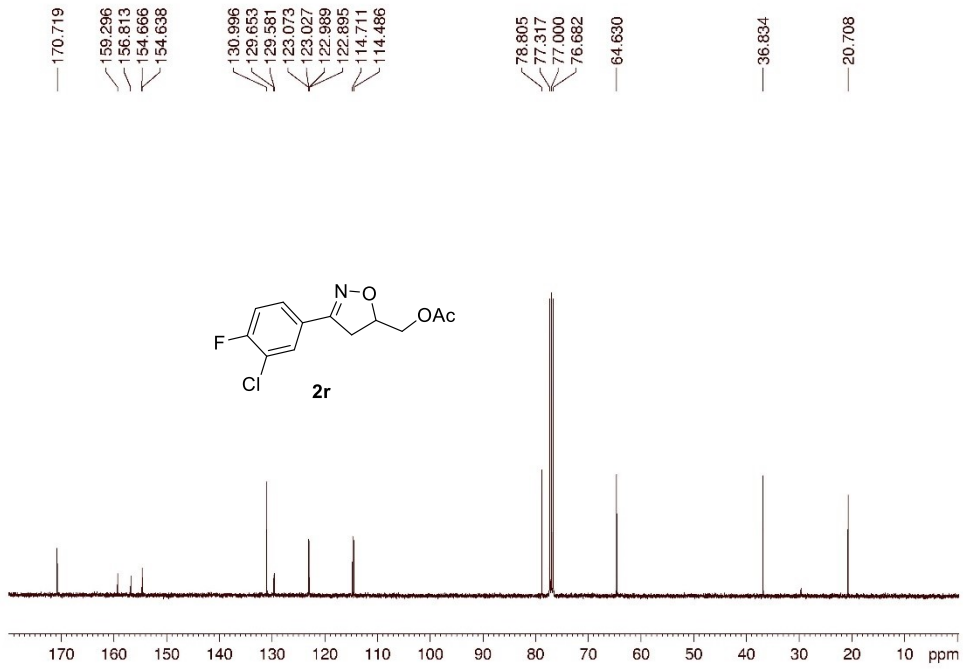
7.463
7.442
7.384
7.383
7.380
7.362
7.359
7.271
5.047
5.018
5.005
4.976
4.303
4.293
4.273
4.263
4.237
4.223
4.207
4.193
3.453
3.426
3.412
3.384
3.154
3.136
3.112
3.094
2.089
N
O
OAc
F
Cl
2r
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
2.98
1.00
2.05
1.00
0.99
2.94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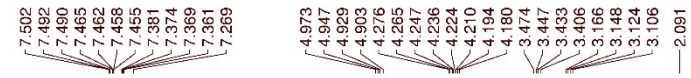
159.296
156.813
154.666
154.638
130.996
129.653
129.581
123.073
123.027
122.989
122.895
114.711
114.486
78.805
77.317
77.000
76.682
64.630
36.834
20.708
N
O
OAc
F
Cl
2r
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm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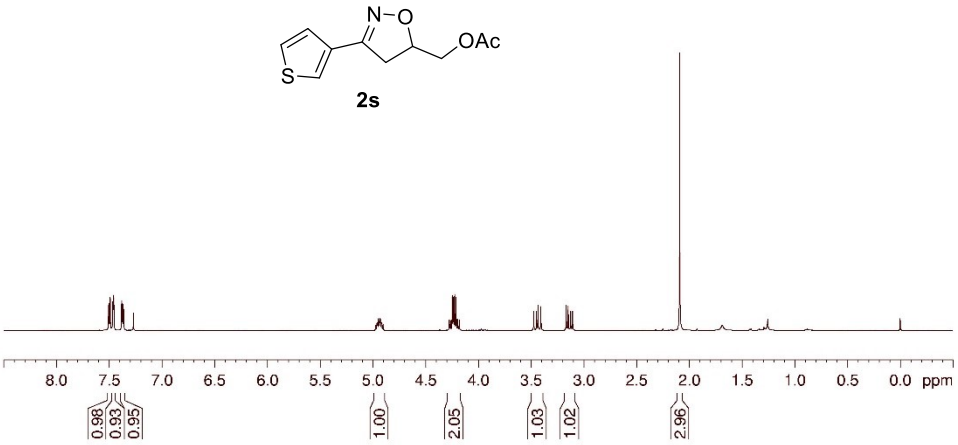
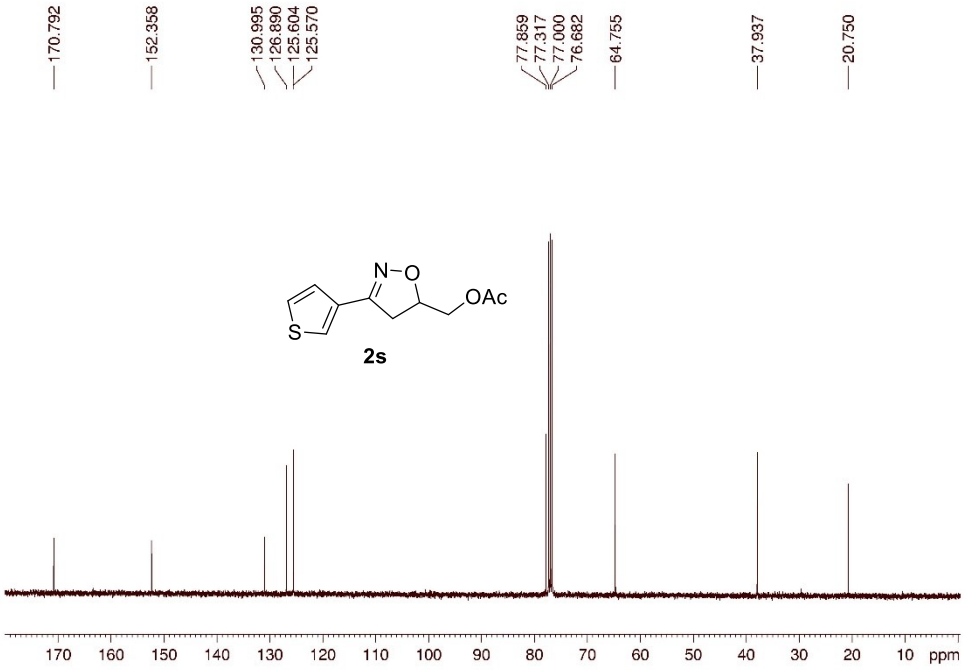
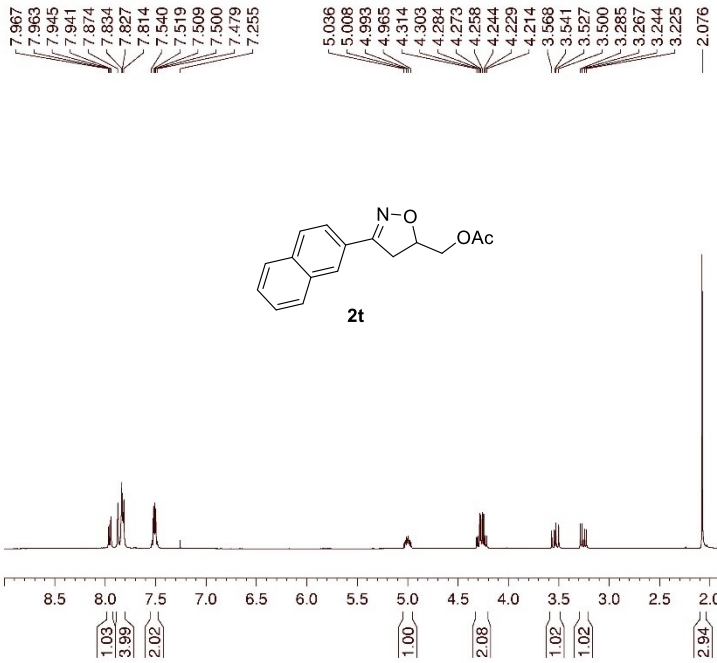
7.492
7.490
7.465
7.462
7.458
7.455
7.381
7.374
7.369
7.361
7.269
4.973
4.947
4.929
4.903
4.276
4.265
4.247
4.236
4.224
4.210
4.194
4.180
3.474
3.447
3.433
3.406
3.166
3.148
3.124
3.106
2.091


N
O
OAc
S
2s
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 ppm
0.98
0.93
0.95
1.00
2.05
1.03
1.02
2.96


170.792
152.358
130.995
126.890
125.604
125.570
77.859
77.317
77.000
76.682
64.755
37.937
20.750
N
O
OAc
S
2s
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm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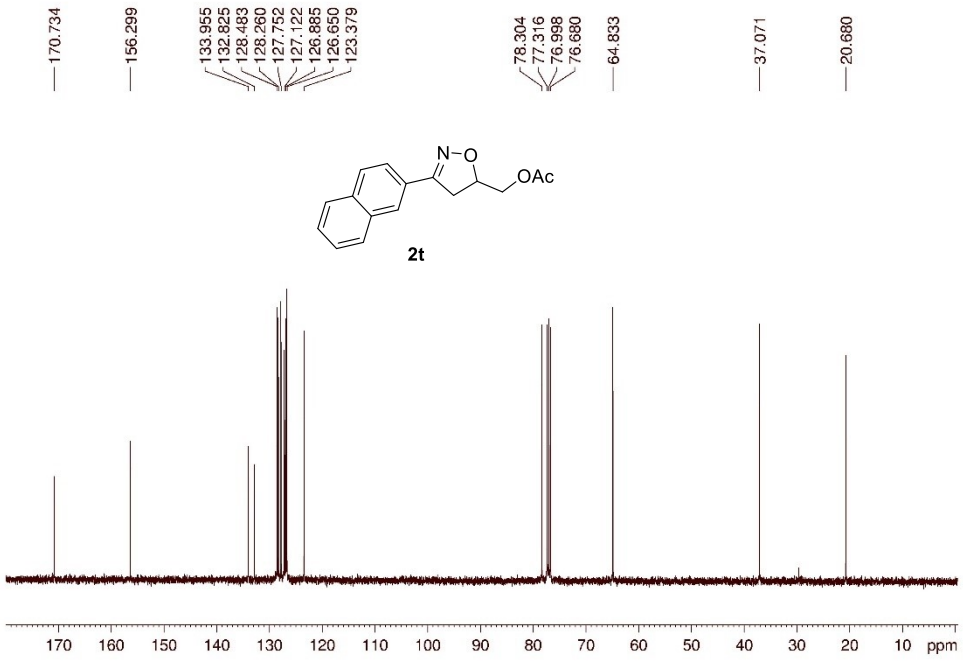
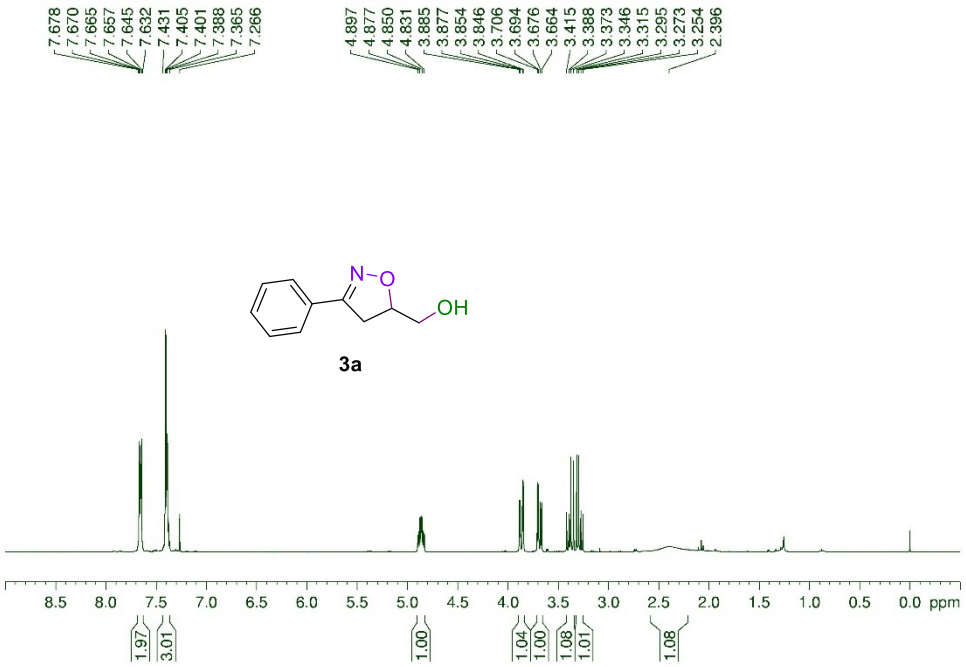
7.963
7.945
7.941
7.874
7.834
7.827
7.814
7.540
7.519
7.509
7.500
7.479
7.255
5.036
5.008
4.993
4.965
4.314
4.303
4.284
4.273
4.258
4.244
4.229
4.214
3.568
3.541
3.527
3.500
3.285
3.267
3.244
3.225
2.076
N
O
OAc
2t
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
1.03
3.99
2.02
1.00
2.08
1.02
1.02
2.94


170.734
156.299
133.955
132.825
128.483
128.260
127.752
127.122
126.885
126.650
123.379
78.304
77.316
76.998
76.680
64.833
37.071
20.680
N
O
OAc
2t
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm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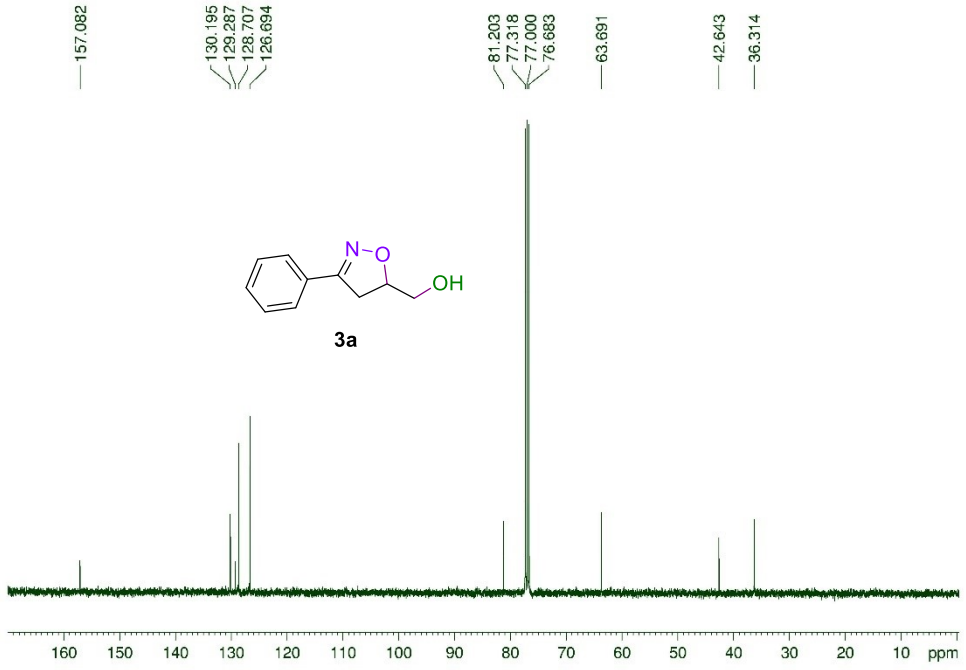
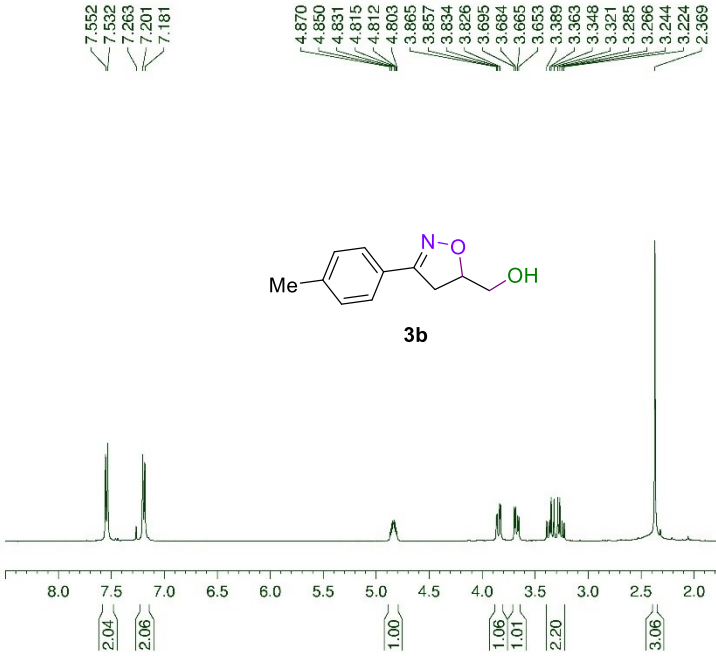
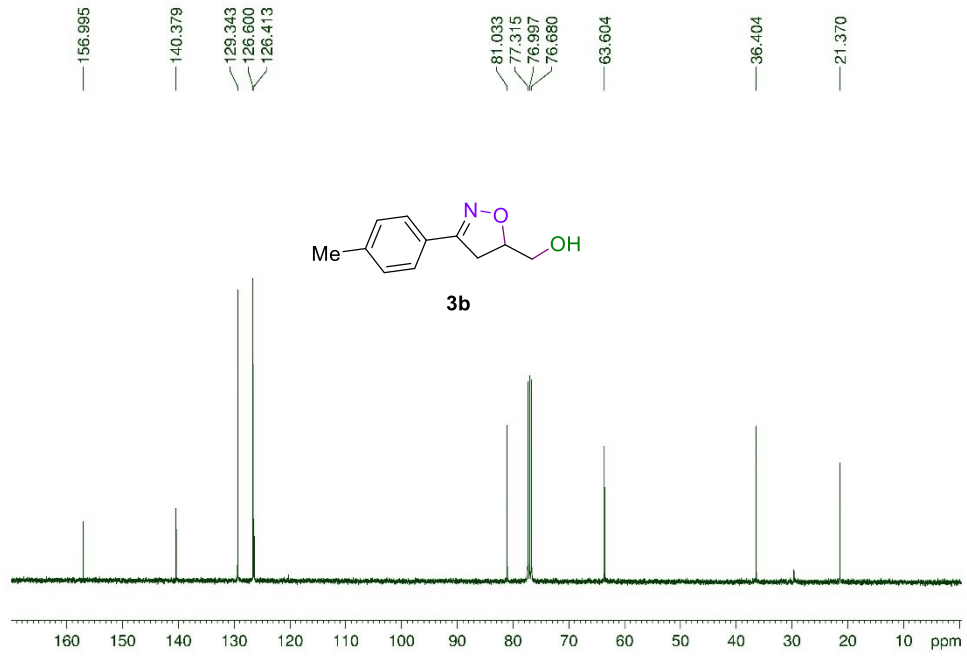
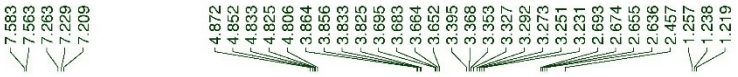
7.670
7.665
7.657
7.645
7.632
7.431
7.405
7.401
7.388
7.365
7.266
4.897
4.877
4.850
4.831
3.885
3.877
3.854
3.846
3.706
3.694
3.676
3.664
3.415
3.388
3.373
3.346
3.315
3.295
3.273
3.254
2.396
N
O
OH
3a
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
1.97
3.01
1.00
1.04
1.00
1.08
1.01
1.08


157.082
130.195
129.287
128.707
126.694
81.203
77.318
77.000
76.683
63.691
42.643
36.314
N
O
OH
3a
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm


7.552
7.532
7.263
7.201
7.181
4.870
4.850
4.831
4.815
4.812
4.803
3.865
3.857
3.834
3.826
3.695
3.684
3.665
3.653
3.389
3.363
3.348
3.321
3.285
3.266
3.244
3.224
2.369
N
O
Me
OH
3b
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
ppm
2.04
2.06
1.00
1.06
1.01
2.20
3.06


156.995
140.379
129.343
126.600
126.413
81.033
77.315
76.997
76.680
63.604
36.404
21.370
N
O
Me
OH
3b
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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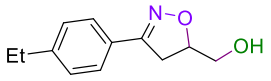
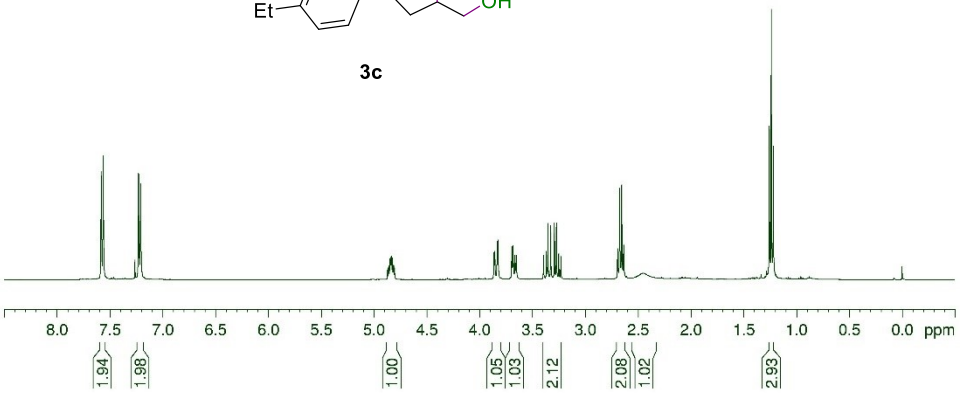
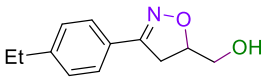
7.563
7.263
7.229
7.209
4.872
4.852
4.833
4.825
4.806
3.864
3.856
3.833
3.825
3.695
3.683
3.664
3.652
3.395
3.368
3.353
3.327
3.292
3.273
3.251
3.231
2.693
2.674
2.655
2.636
2.457
1.257
1.238
1.219


N
O
Et
OH

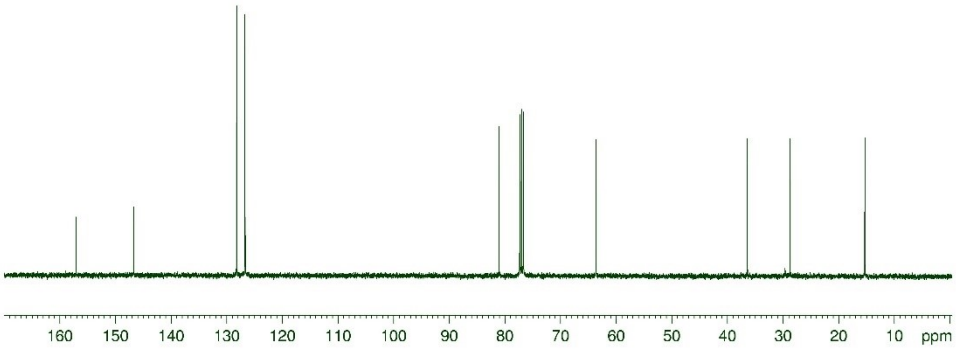
3c

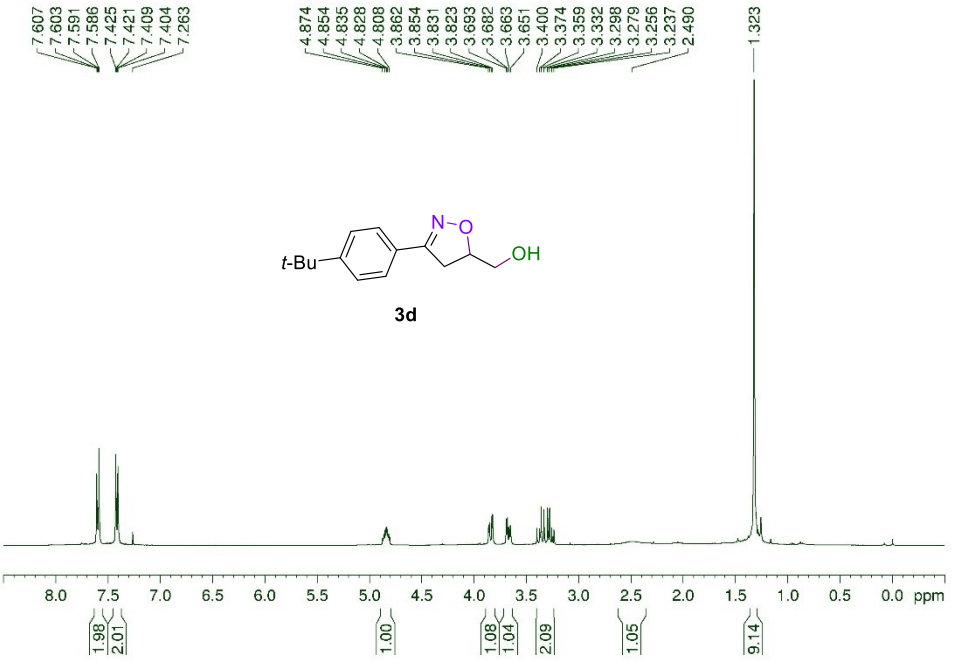

8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
1.94
1.98
1.00
1.05
1.03
2.12
2.08
1.02
2.93

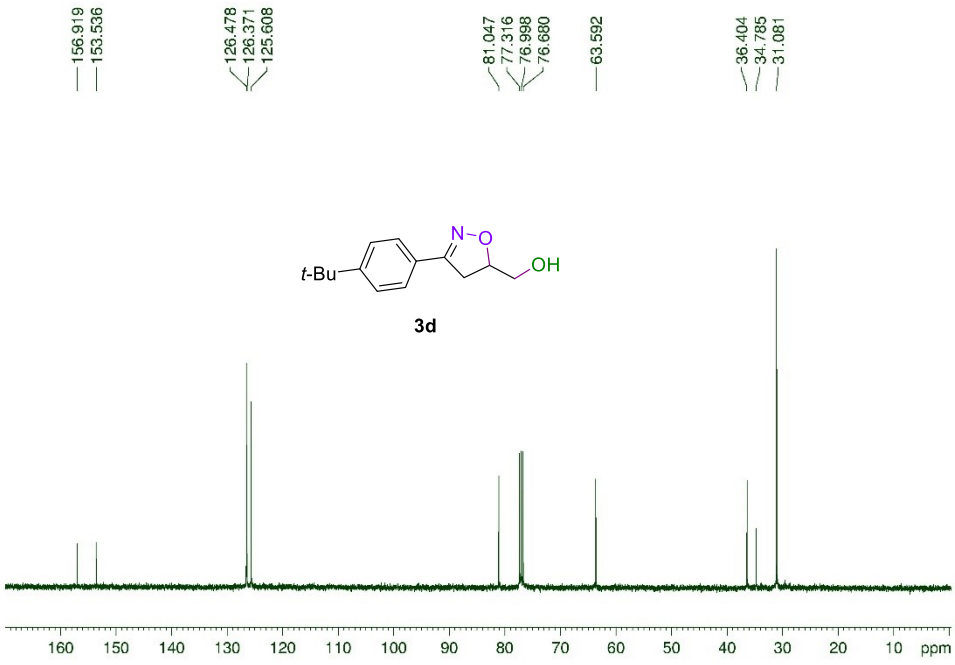

156.997
146.677
128.162
126.704
126.628
81.033
77.316
76.998
76.680
63.595
36.405
28.707
15.289


N
O
Et
OH

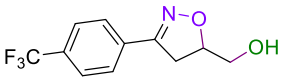
3c


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

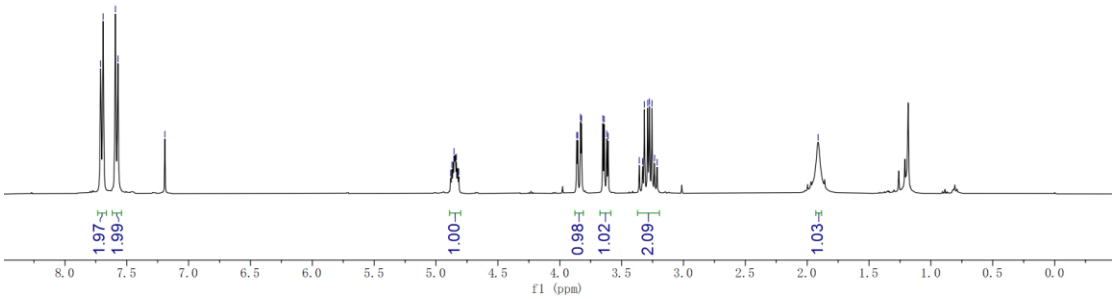

7.607
7.603
7.591
7.586
7.425
7.421
7.409
7.404
7.263
4.874
4.854
4.835
4.828
4.808
3.862
3.854
3.831
3.823
3.693
3.682
3.663
3.651
3.400
3.374
3.359
3.332
3.298
3.279
3.256
3.237
2.490
1.323
N
O
t-Bu
OH
3d
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.98
2.01
1.00
1.08
1.04
2.09
1.05
9.14


156.919
153.536
126.478
126.371
125.608
81.047
77.316
76.998
76.680
63.592
36.404
34.785
31.081
N
O
t-Bu
OH
3d
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

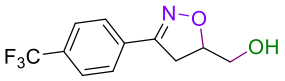

7.711
7.691
7.592
7.571
7.191
4.882
4.871
4.854
4.835
4.816
3.863
3.855
3.832
3.824
3.651
3.641
3.620
3.610
3.357
3.330
3.316
3.289
3.275
3.255
3.234
3.213
1.912


N
O
F3C
OH

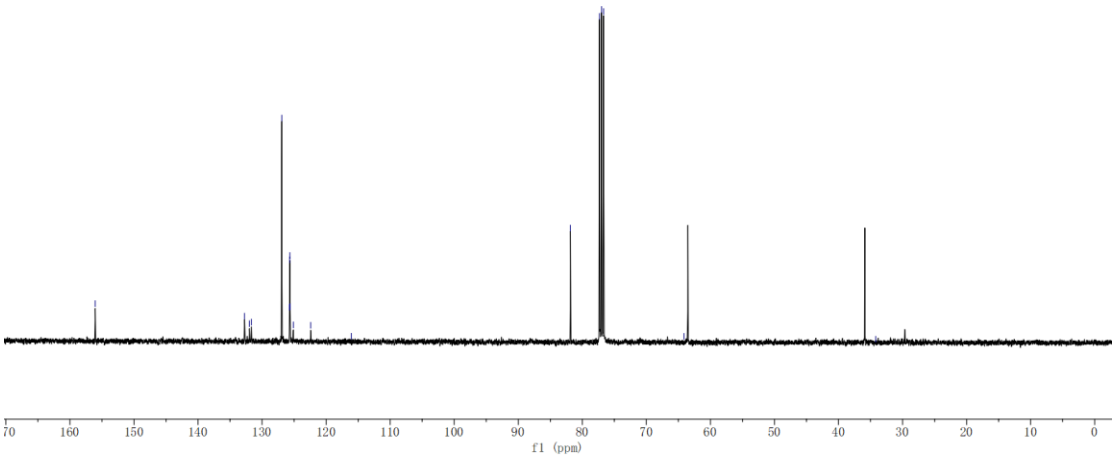
3e

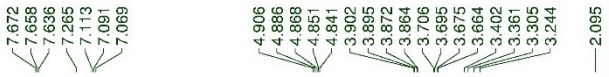

1.97
1.99
1.00
0.98
1.02
2.09
1.03
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

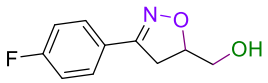

156.055
132.743
131.988
131.661
126.923
125.731
125.695
125.655
125.617
125.114
122.409
116.077
81.850
77.317
76.999
76.682
64.125
34.185


N
O
F3C
OH

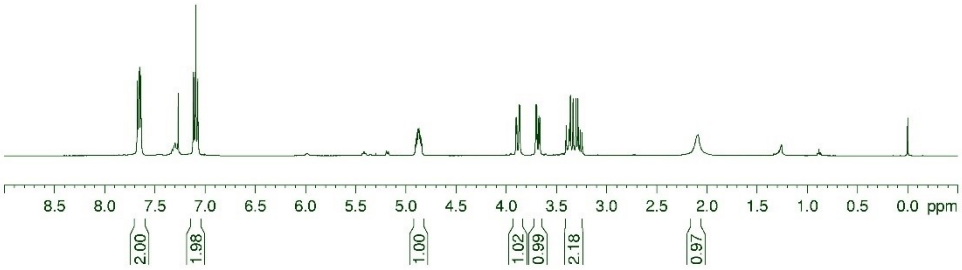
3e


70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

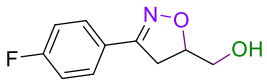

7.672
7.658
7.636
7.265
7.113
7.091
7.069
4.906
4.886
4.868
4.851
4.841
3.902
3.895
3.872
3.864
3.706
3.695
3.675
3.664
3.402
3.361
3.305
3.244
2.095


N
O
F
OH

3f

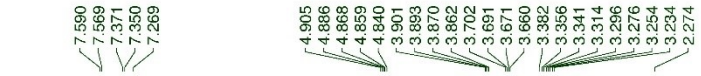

8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.00
1.98
1.00
1.02
0.99
2.18
0.97

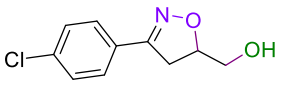

165.025
162.533
156.097
128.678
128.594
125.548
115.958
115.740
81.335
77.319
77.001
76.683
63.590
36.347


N
O
F
OH

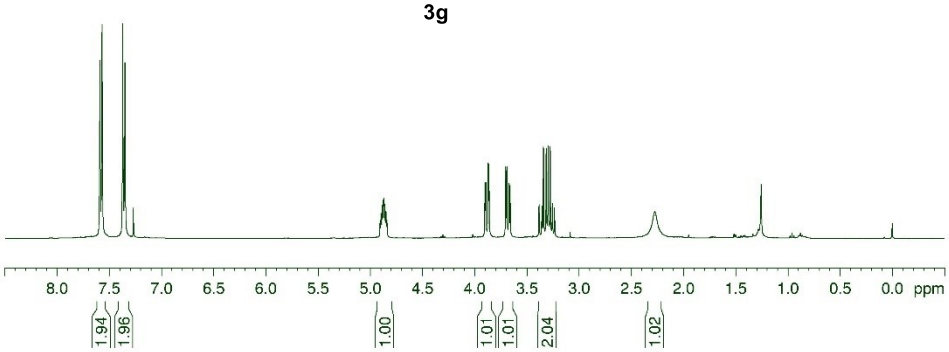
3f

160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

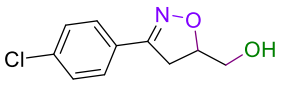

7.590
7.569
7.371
7.350
7.269
4.905
4.886
4.868
4.859
4.840
3.901
3.893
3.870
3.862
3.702
3.691
3.671
3.660
3.382
3.356
3.341
3.314
3.296
3.276
3.254
3.234
2.274


N
O
Cl
OH

3g

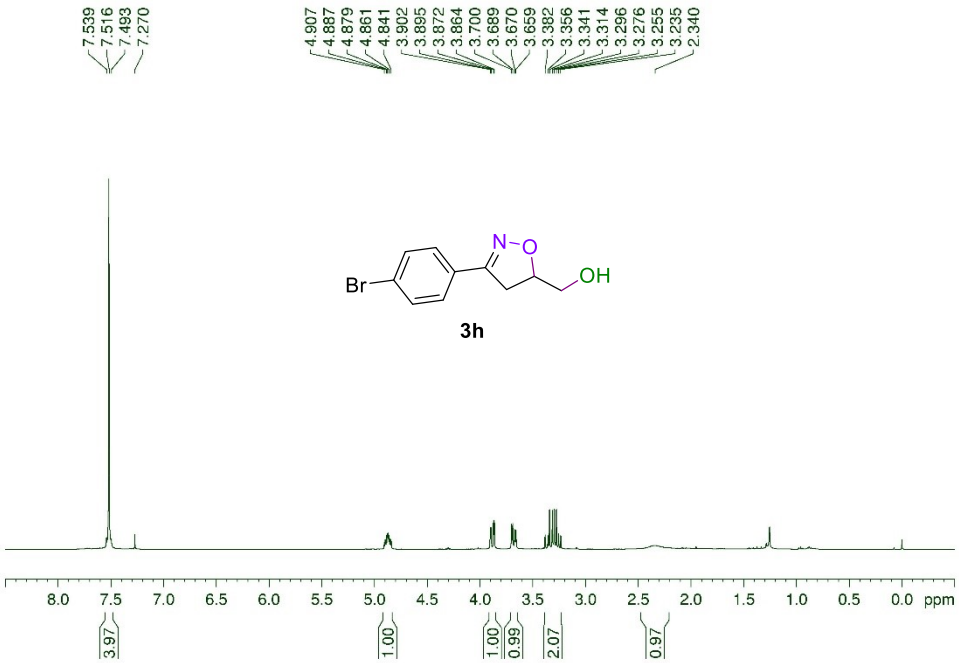

8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.94
1.96
1.00
1.01
1.01
2.04
1.02

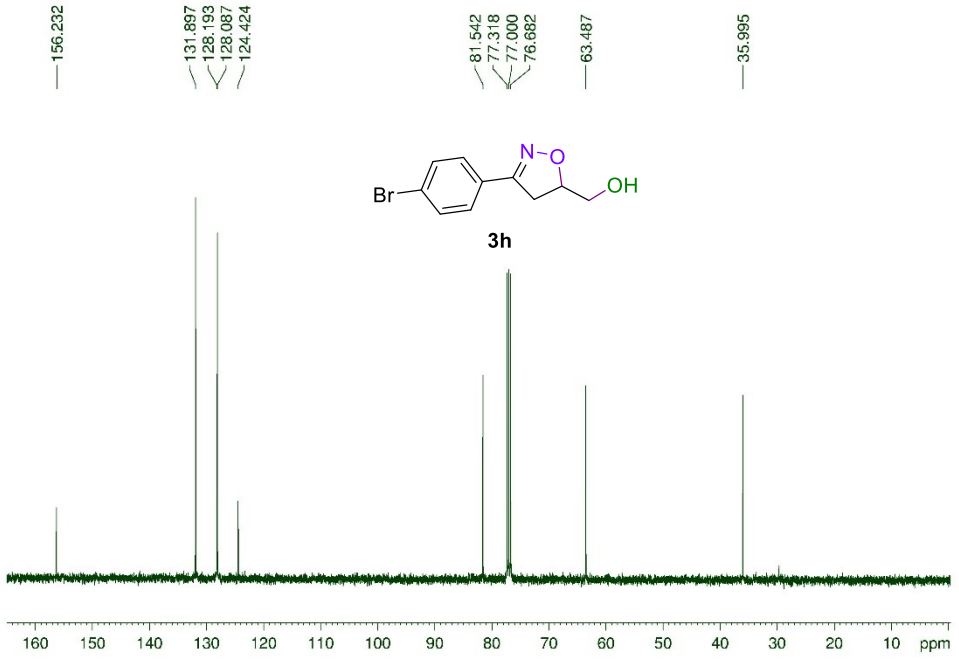

156.137
136.096
128.939
127.878
127.763
81.516
77.319
77.001
76.683
63.493
36.071

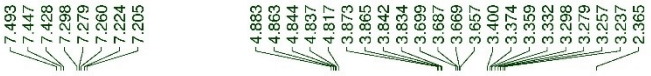

N
O
Cl
OH

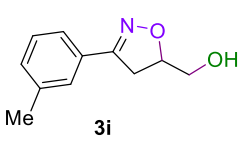
3g

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.539
7.516
7.493
7.270
4.907
4.887
4.879
4.861
4.841
3.902
3.895
3.872
3.864
3.700
3.689
3.670
3.659
3.382
3.356
3.341
3.314
3.296
3.276
3.255
3.235
2.340
N
O
Br
OH
3h
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
ppm
3.97
1.00
1.00
0.99
2.07
0.97


156.232
131.897
128.193
128.087
124.424
81.542
77.318
77.000
76.682
63.487
35.995
N
O
Br
OH
3h
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

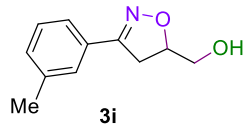

7.493
7.447
7.428
7.298
7.279
7.260
7.224
7.205
4.883
4.863
4.844
4.837
4.817
3.873
3.865
3.842
3.834
3.699
3.687
3.669
3.657
3.400
3.374
3.359
3.332
3.298
3.279
3.257
3.237
2.365


N
O
OH
Me

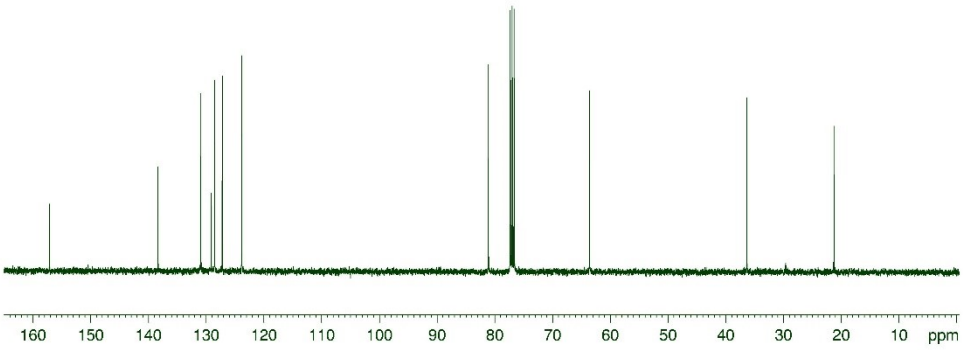
3i

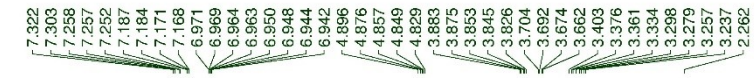
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.97
0.96
1.09
0.99
1.00
1.02
1.03
2.10
3.13

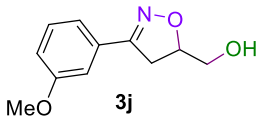

157.150
138.357
130.931
129.113
128.534
127.220
123.842
81.121
77.319
77.001
76.683
63.610
36.350
21.274


N
O
OH
Me

3i


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

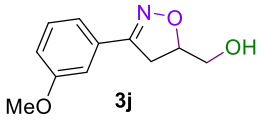

7.322
7.303
7.258
7.257
7.252
7.187
7.184
7.171
7.168
6.971
6.969
6.964
6.963
6.950
6.948
6.944
6.942
4.896
4.876
4.857
4.849
4.829
3.883
3.875
3.853
3.845
3.826
3.704
3.692
3.674
3.662
3.403
3.376
3.361
3.334
3.298
3.279
3.257
3.237
2.262


N
O
OH
MeO

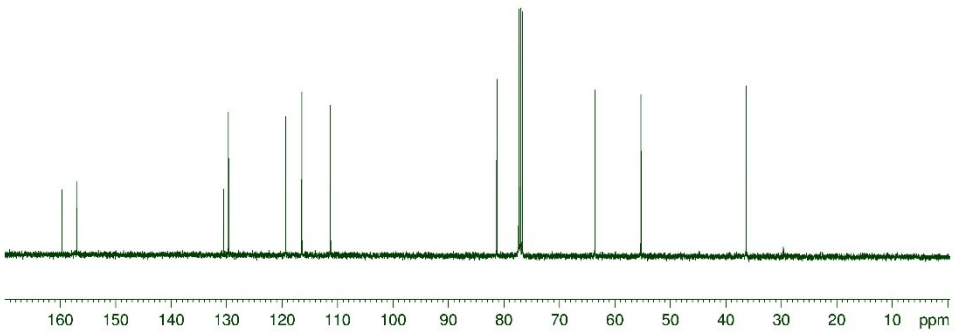
3j

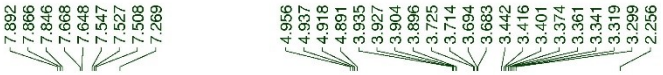
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.14
1.02
1.03
1.00
1.01
2.93
1.01
2.13
1.04

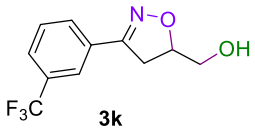

159.619
157.025
130.501
129.672
119.339
116.447
111.275
81.287
77.318
77.000
76.683
63.594
55.302
36.325


N
O
OH
MeO

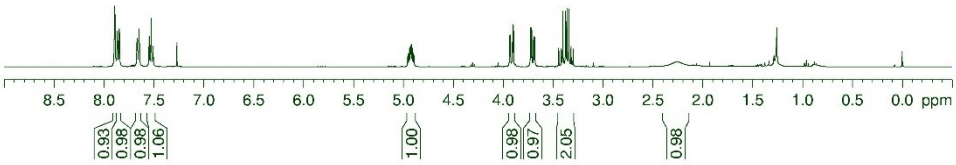
3j


160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

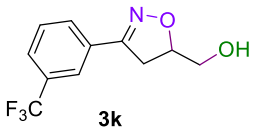

7.892
7.866
7.846
7.668
7.648
7.547
7.527
7.508
7.269
4.956
4.937
4.918
4.891
3.935
3.927
3.904
3.896
3.725
3.714
3.694
3.683
3.442
3.416
3.401
3.374
3.361
3.341
3.319
3.299
2.256


N
O
OH
F3C

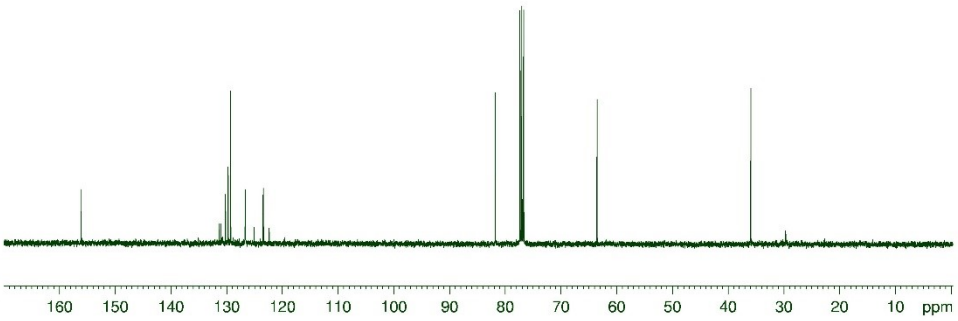
3k

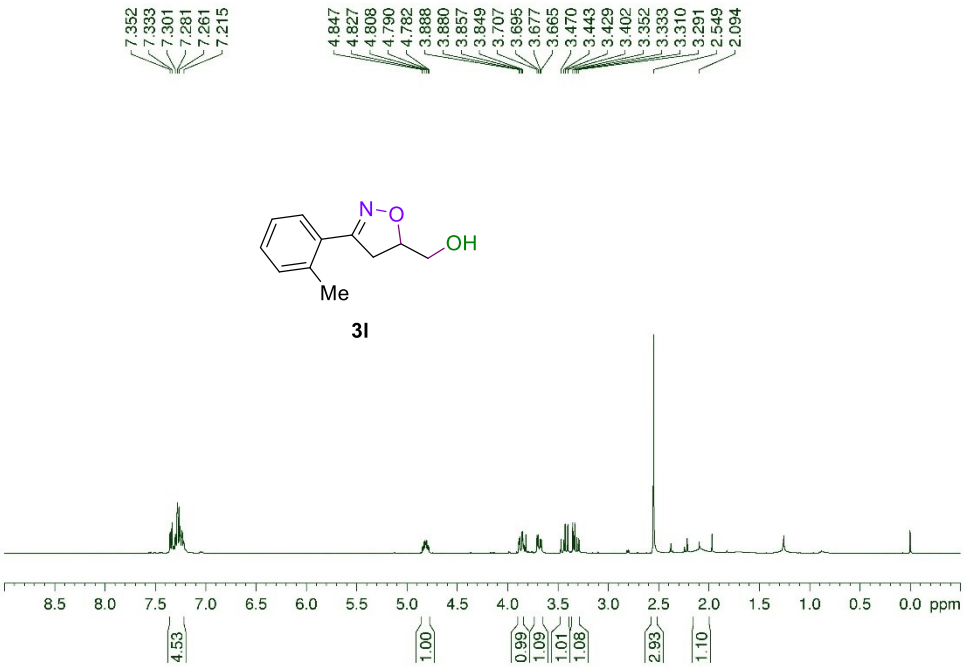

8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
0.93
0.98
0.98
1.06
1.00
0.98
0.97
2.05
0.98


156.008
131.369
131.043
130.187
129.709
129.259
126.646
126.609
126.573
125.041
123.487
123.447
123.409
123.372
122.334
81.776
77.319
77.001
76.683
63.502
35.906

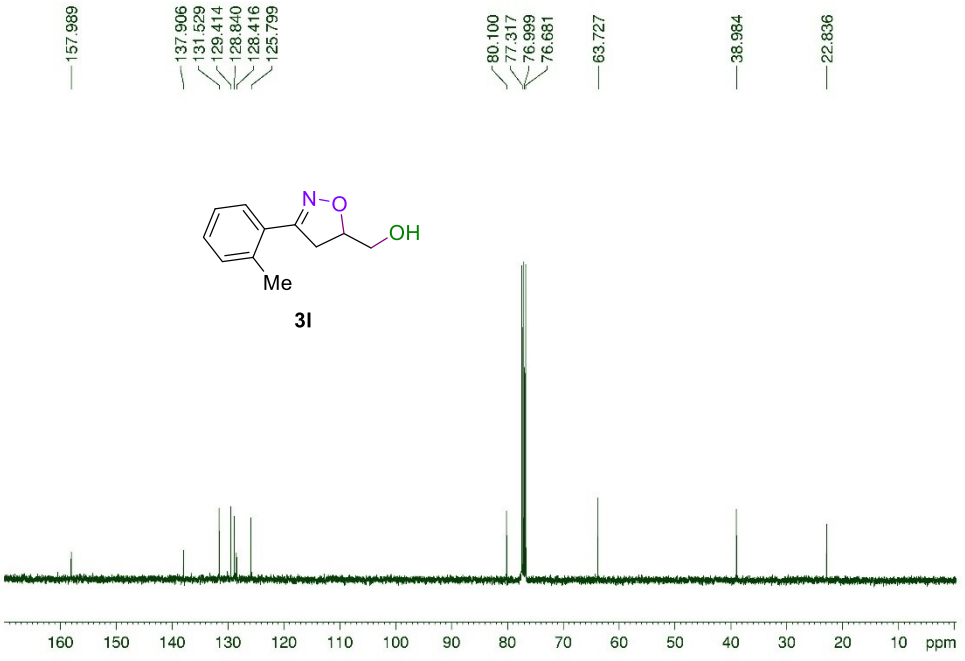

N
O
OH
F3C

3k


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm


7.352
7.333
7.301
7.281
7.261
7.215
4.847
4.827
4.808
4.790
4.782
3.888
3.880
3.857
3.849
3.707
3.695
3.677
3.665
3.470
3.443
3.429
3.402
3.352
3.333
3.310
3.291
2.549
2.094
N
O
OH
Me
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 ppm
4.53
1.00
0.99
1.09
1.01
1.08
2.93
1.10

3l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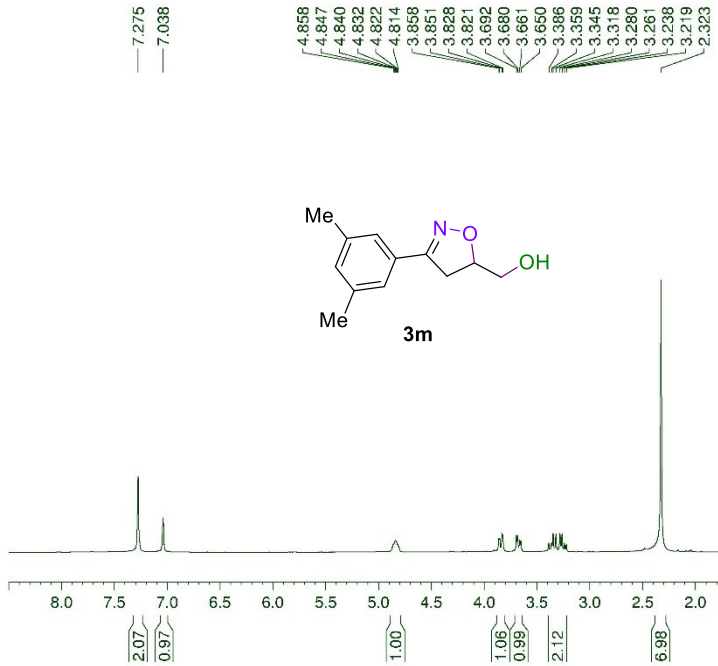
137.906
131.529
129.414
128.840
128.416
125.799
80.100
77.317
76.999
76.681
63.727
38.984
22.836
N
O
OH
Me
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

3l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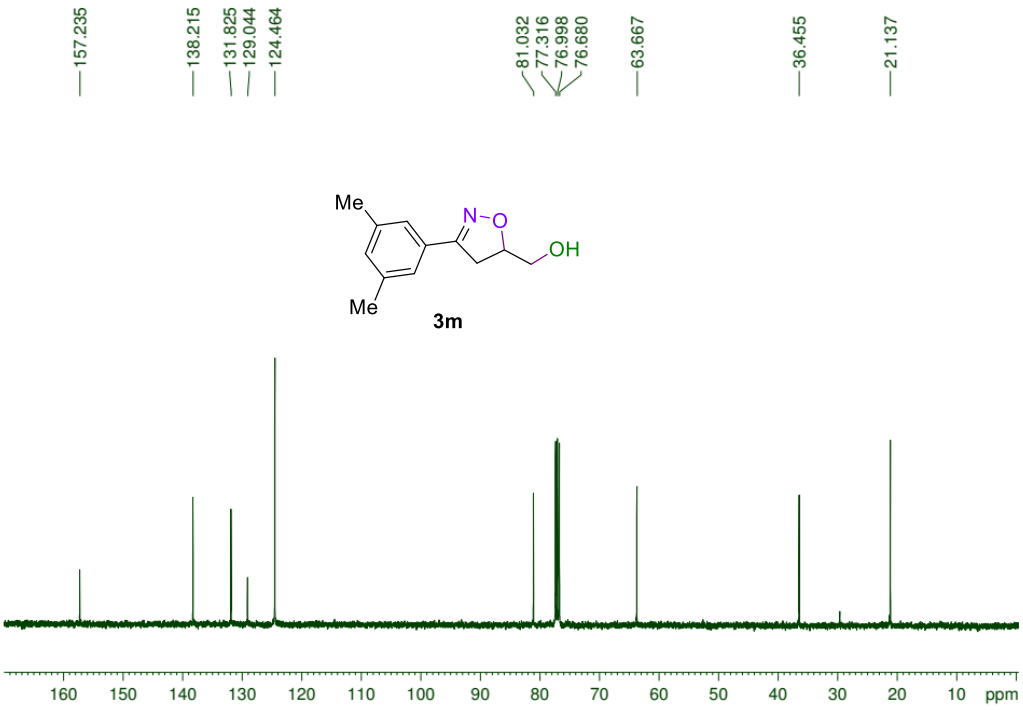
7.038
4.858
4.847
4.840
4.832
4.822
4.814
3.858
3.851
3.828
3.821
3.692
3.680
3.661
3.650
3.386
3.359
3.345
3.318
3.280
3.261
3.238
3.219
2.323
Me
N
O
OH
Me
3m
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.07
0.97
1.00
1.06
0.99
2.12
6.98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138.215
131.825
129.044
124.464
81.032
77.316
76.998
76.680
63.667
36.455
21.137
Me
N
O
OH
Me
3m
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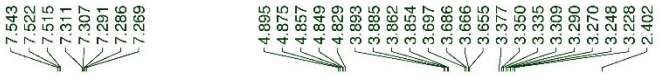
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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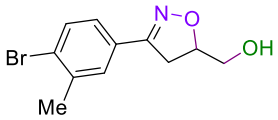
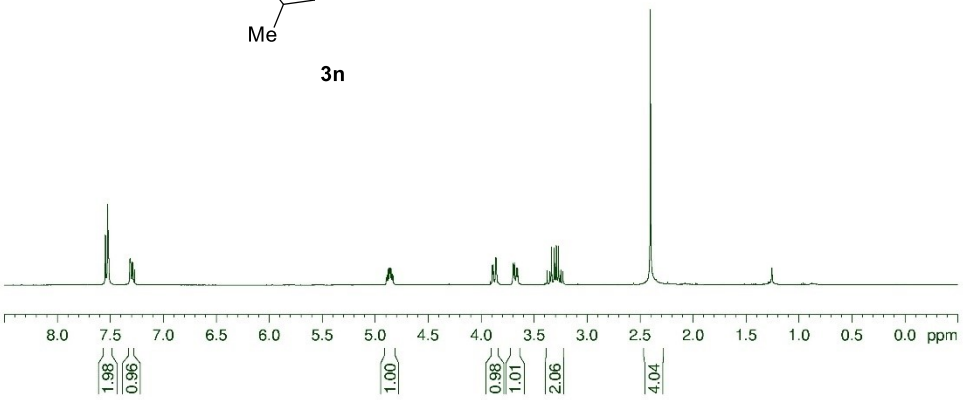
7.522
7.515
7.311
7.307
7.291
7.286
7.269
4.895
4.875
4.857
4.849
4.829
3.893
3.885
3.862
3.854
3.697
3.686
3.666
3.655
3.377
3.350
3.335
3.309
3.290
3.270
3.248
3.228
2.402


N
O
Br
OH
Me

3n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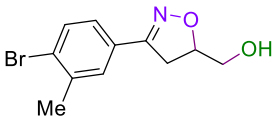
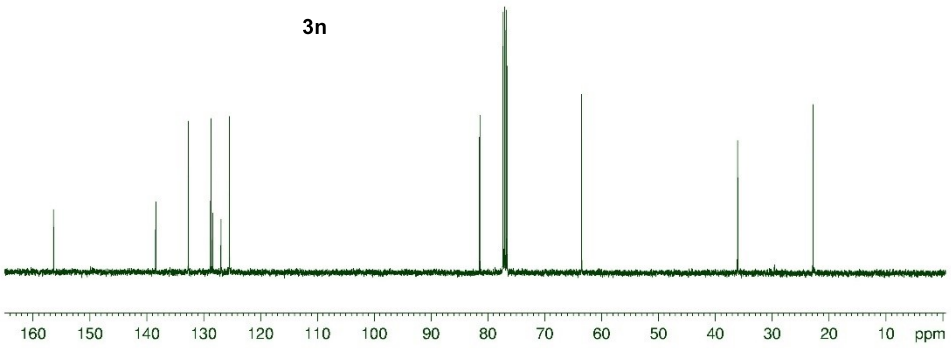
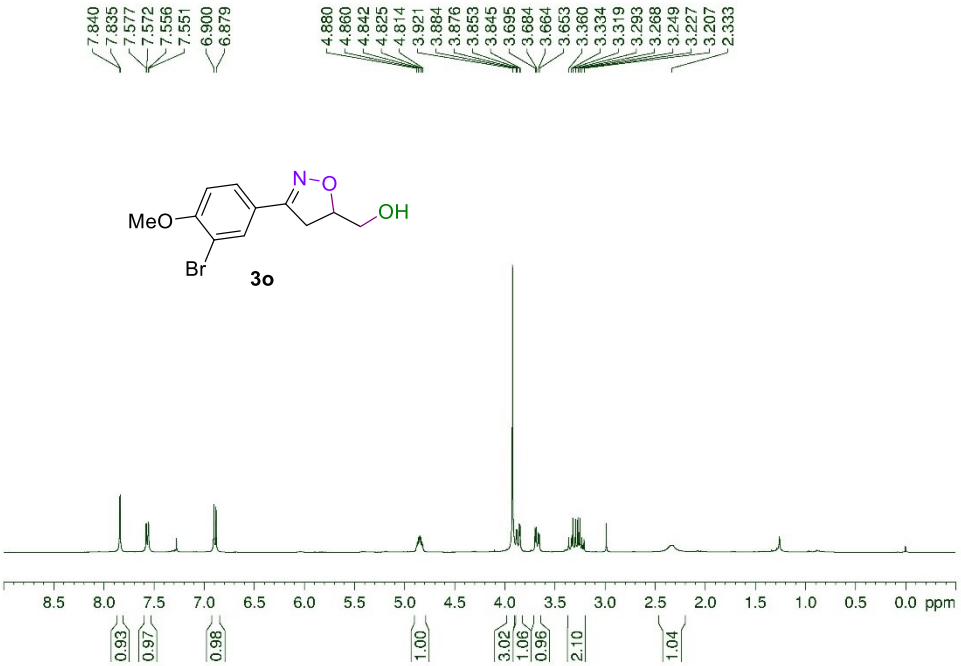
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.98
0.96
1.00
0.98
1.01
2.06
4.04

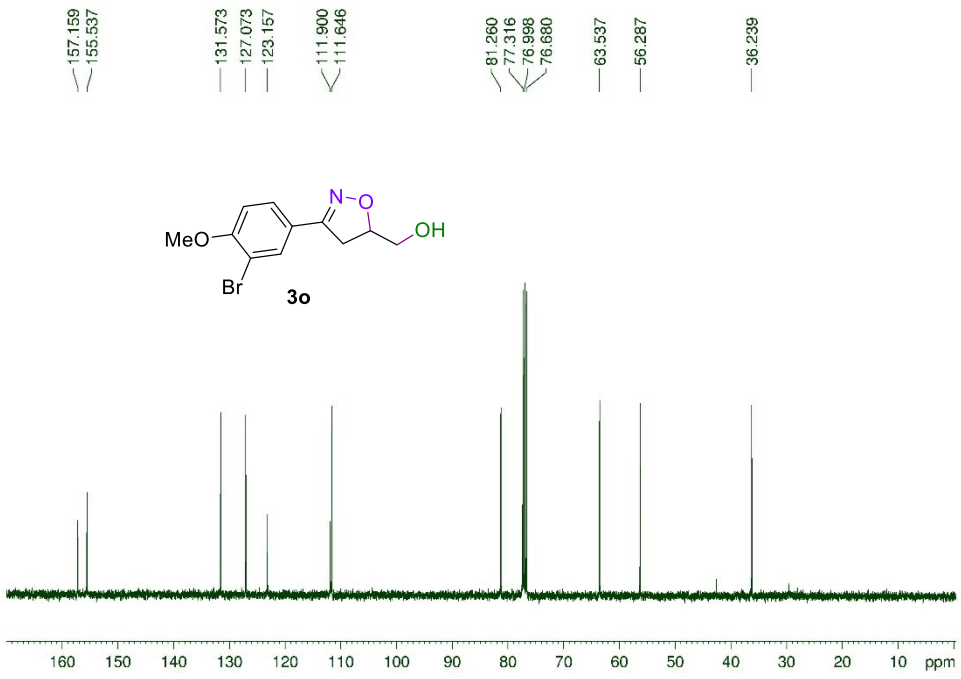

156.356
138.378
132.637
128.685
128.372
126.887
125.405
81.435
77.318
77.000
76.682
63.517
36.087
22.846

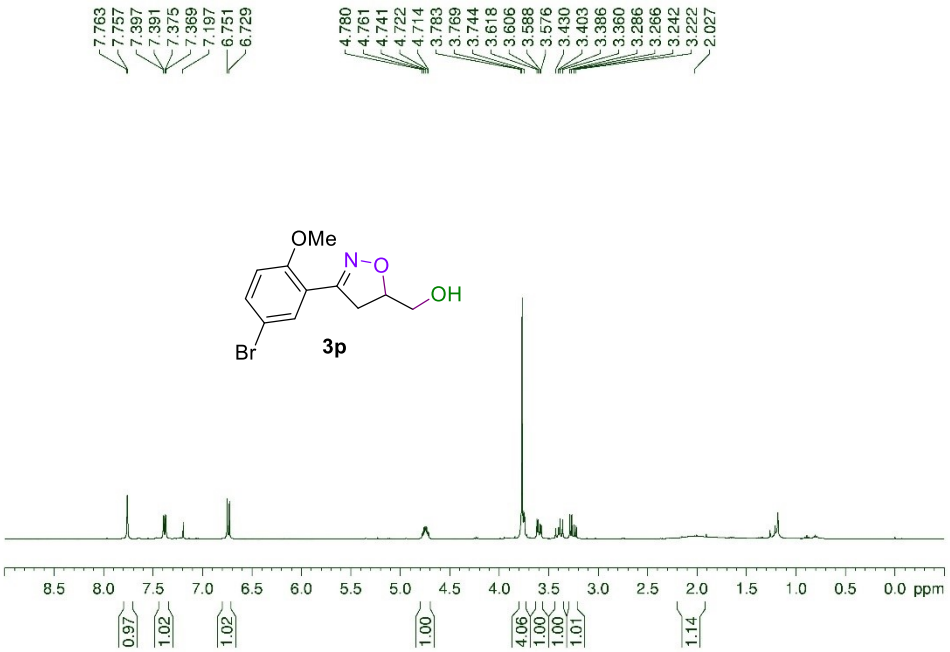

N
O
Br
OH
Me

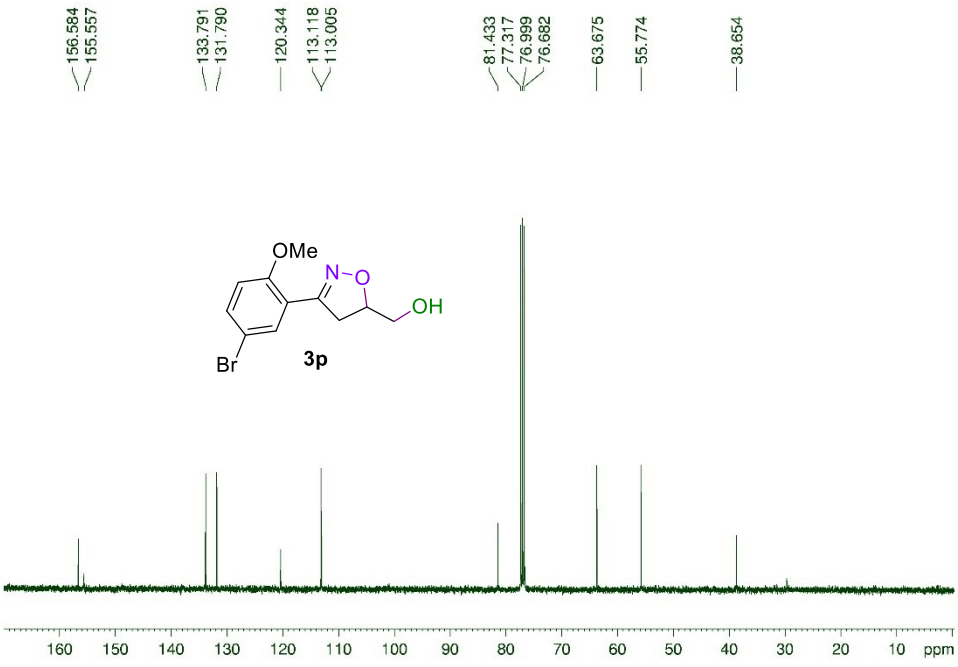
3n

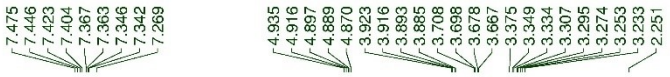

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

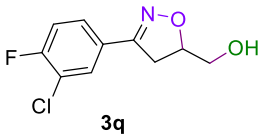

7.840
7.835
7.577
7.572
7.556
7.551
6.900
6.879
4.880
4.860
4.842
4.825
4.814
3.921
3.884
3.876
3.853
3.845
3.695
3.684
3.664
3.653
3.360
3.334
3.319
3.293
3.268
3.249
3.227
3.207
2.333
MeO
Br
N
O
OH
3o
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
0.93
0.97
0.98
1.00
3.02
1.06
0.96
2.10
1.04


157.159
155.537
131.573
127.073
123.157
111.900
111.646
81.260
77.316
76.998
76.680
63.537
56.287
36.239
MeO
Br
N
O
OH
3o
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

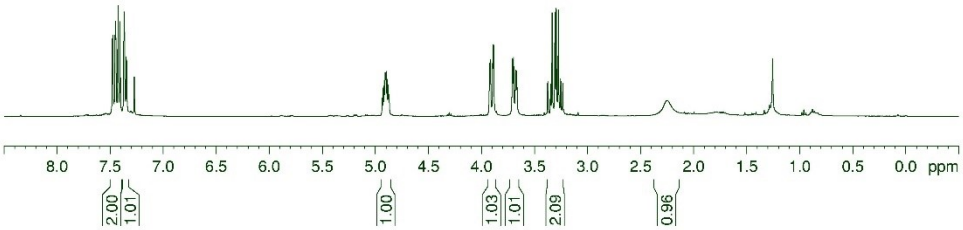

7.763
7.757
7.397
7.391
7.375
7.369
7.197
6.751
6.729
4.780
4.761
4.741
4.722
4.714
3.783
3.769
3.744
3.618
3.606
3.588
3.576
3.430
3.403
3.386
3.360
3.286
3.266
3.242
3.222
2.027
OMe
N
O
OH
Br
3p
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.97
1.02
1.02
1.00
4.06
1.00
1.00
1.01
1.14


156.584
155.557
133.791
131.790
120.344
113.118
113.005
81.433
77.317
76.999
76.682
63.675
55.774
38.654
OMe
N
O
OH
Br
3p
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

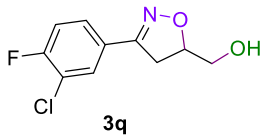

7.475
7.446
7.423
7.404
7.367
7.363
7.346
7.342
7.269
4.935
4.916
4.897
4.889
4.870
3.923
3.916
3.893
3.885
3.708
3.698
3.678
3.667
3.375
3.349
3.334
3.307
3.295
3.274
3.253
3.233
2.251


N
O
F
Cl
OH

3q

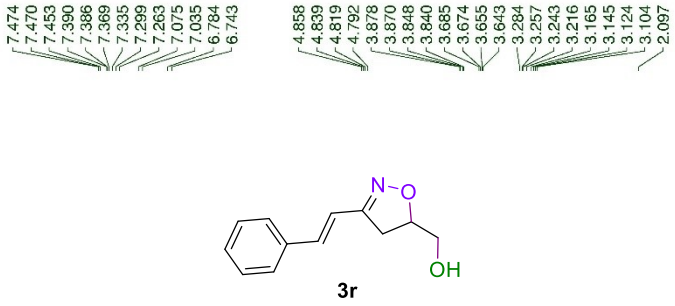

8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.00
1.01
1.00
1.03
1.01
2.09
0.96


159.251
156.769
155.496
155.469
130.925
129.810
129.739
123.034
122.997
122.950
122.771
114.679
114.451
81.867
77.317
76.999
76.681
63.438
35.846


N
O
F
Cl
OH

3q

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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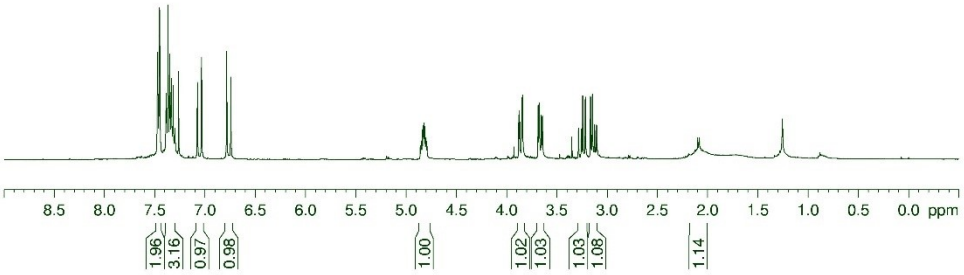
7.453
7.390
7.386
7.369
7.335
7.299
7.263
7.075
7.035
6.784
6.743
4.858
4.839
4.819
4.792
3.878
3.870
3.848
3.840
3.685
3.674
3.655
3.643
3.284
3.257
3.243
3.216
3.165
3.145
3.124
3.104
2.097
N
O
OH
3r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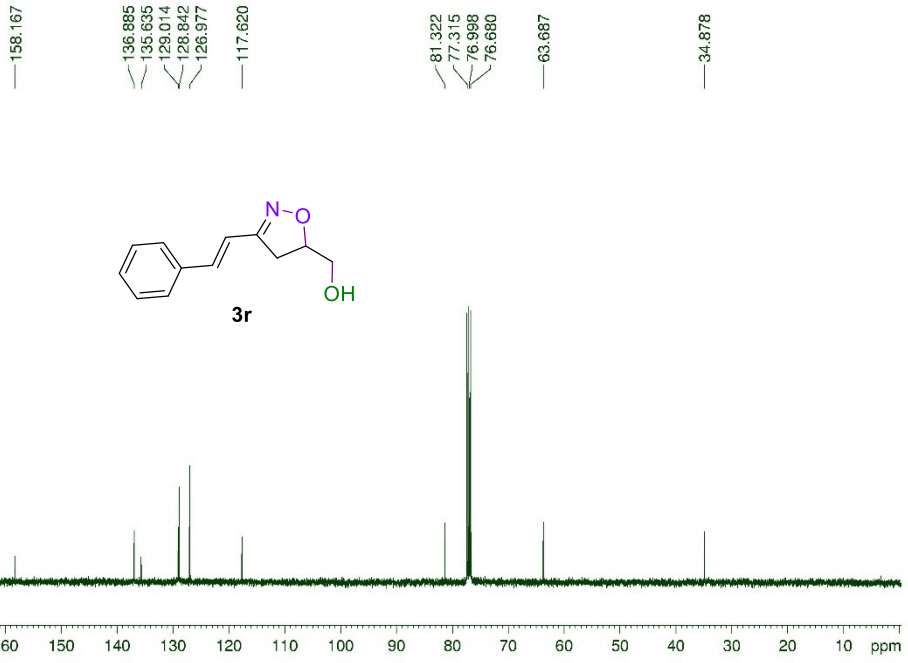
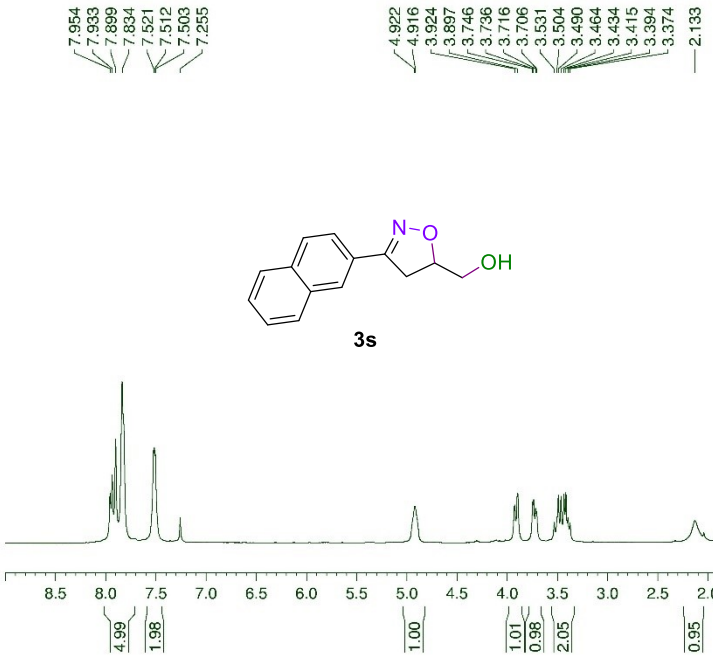
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
1.96
3.16
0.97
0.98
1.00
1.02
1.03
1.03
1.08
1.14


158.167
136.885
135.635
129.014
128.842
126.977
117.620
81.322
77.315
76.998
76.680
63.687
34.878
N
O
OH
3r
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.899
7.834
7.521
7.512
7.503
7.255
4.922
4.916
3.924
3.897
3.746
3.736
3.716
3.706
3.531
3.504
3.490
3.464
3.434
3.415
3.394
3.374
2.133
N
O
OH
3s
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 ppm
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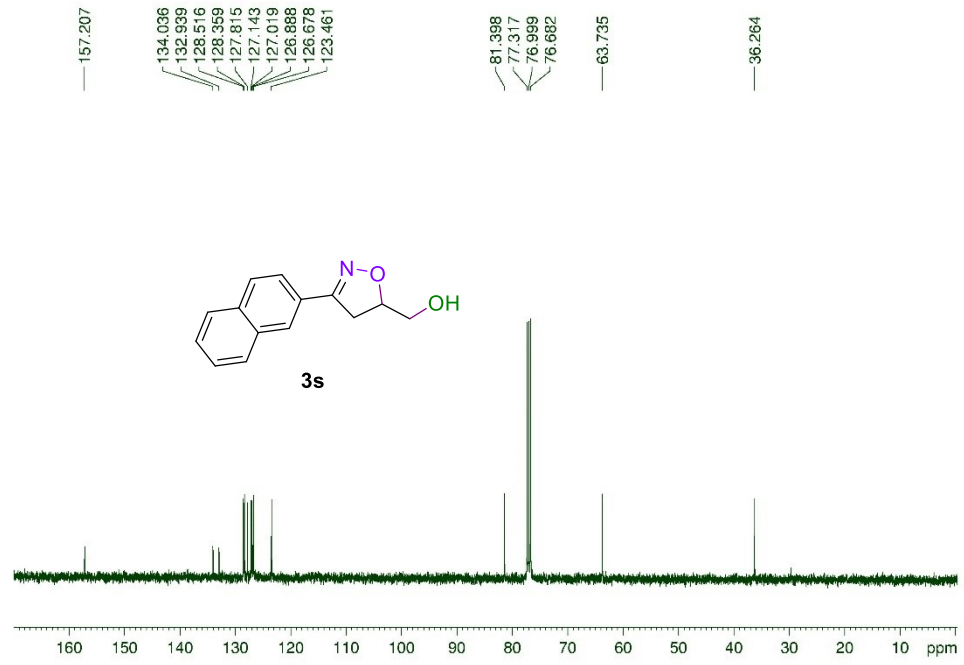
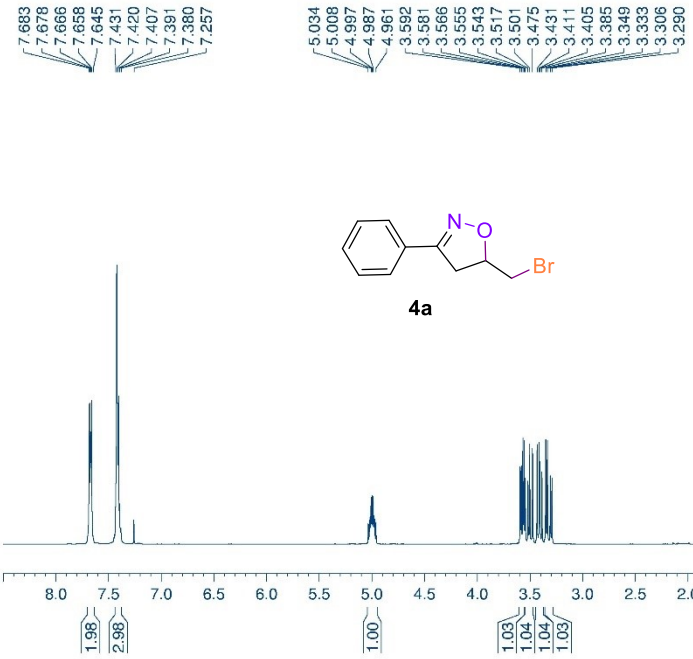
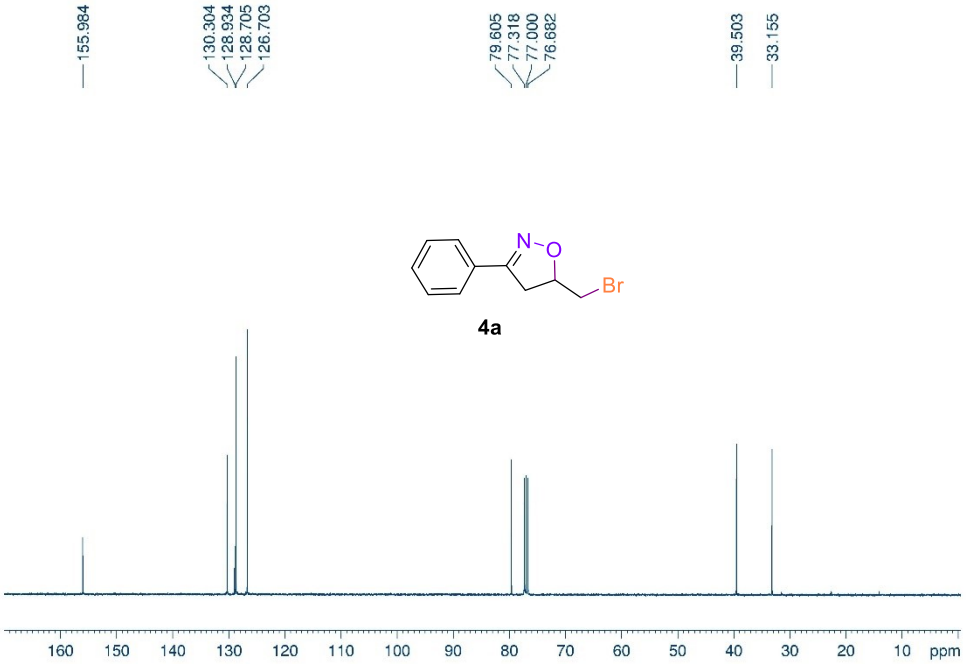
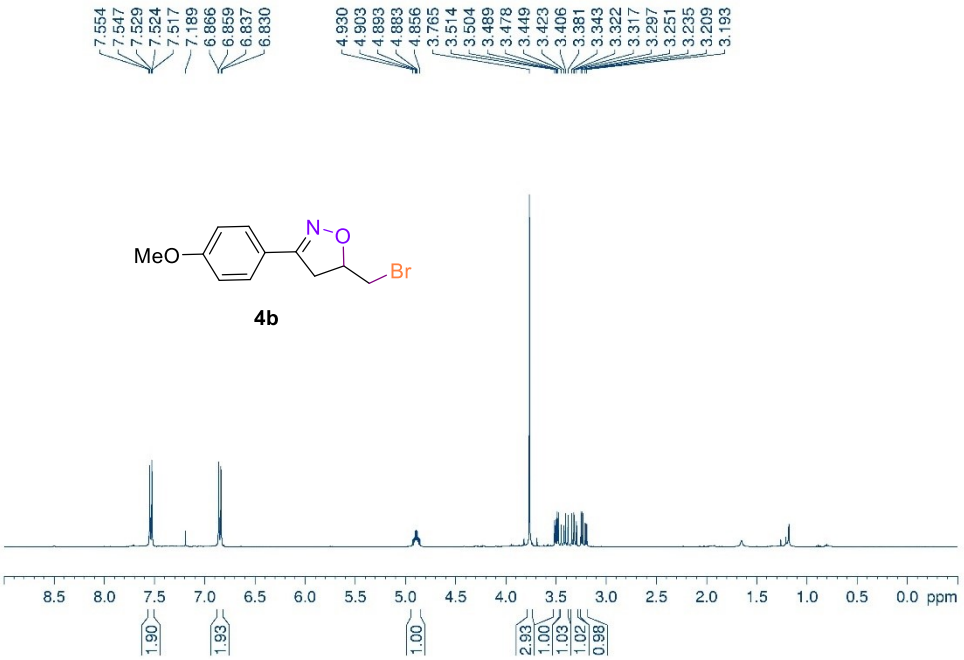
1.98
1.00
1.01
0.98
2.05
0.95


157.207
134.036
132.939
128.516
128.359
127.815
127.143
127.019
126.888
126.678
123.461
81.398
77.317
76.999
76.682
63.735
36.264
N
O
OH
3s
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm


7.683
7.678
7.666
7.658
7.645
7.431
7.420
7.407
7.391
7.380
7.257
5.034
5.008
4.997
4.987
4.961
3.592
3.581
3.566
3.555
3.543
3.517
3.501
3.475
3.431
3.411
3.405
3.385
3.349
3.333
3.306
3.290
N
O
Br
4a
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 ppm
1.98
2.98
1.00
1.03
1.04
1.04
1.03


155.984
130.304
128.934
128.705
126.703
79.605
77.318
77.000
76.682
39.503
33.155
N
O
Br
4a
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm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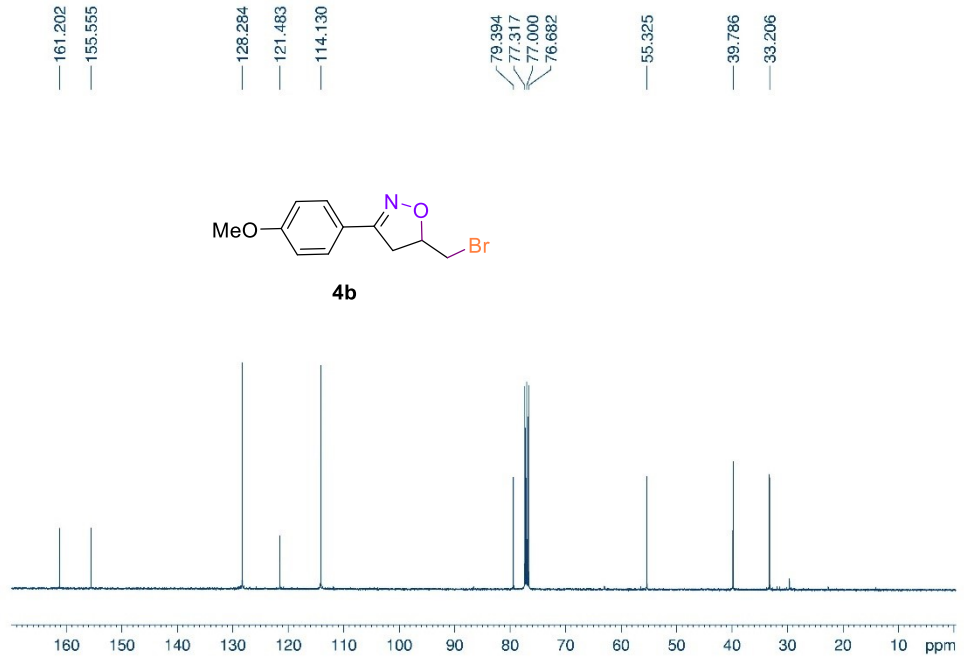
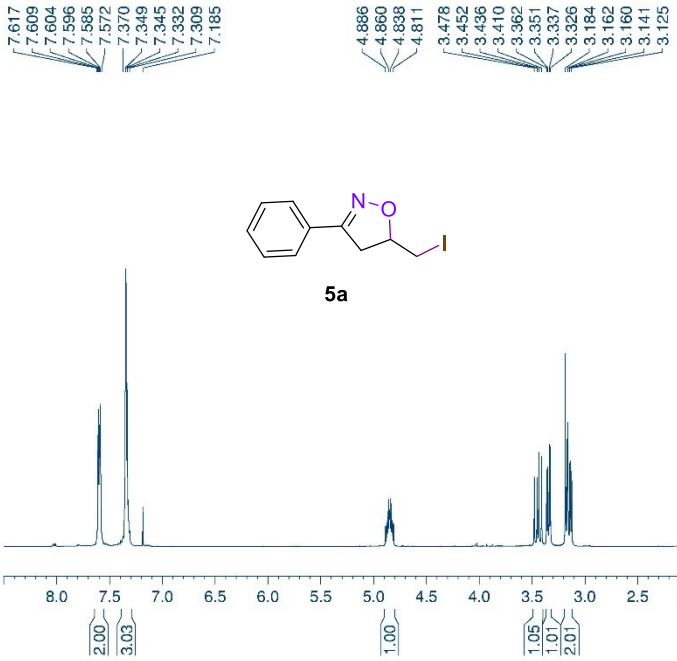
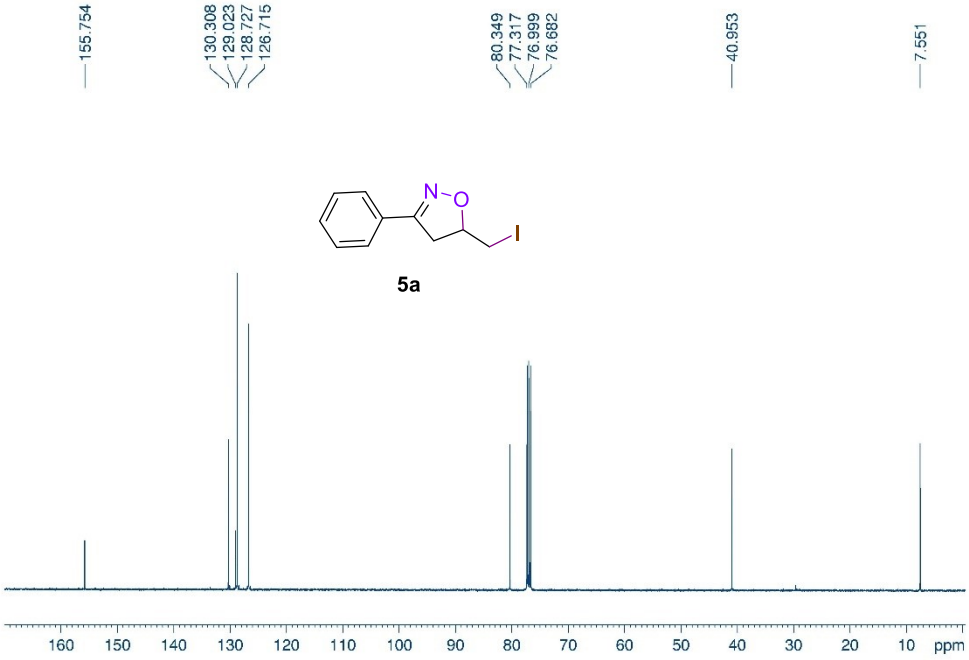
7.547
7.529
7.524
7.517
7.189
6.866
6.859
6.837
6.830
4.930
4.903
4.893
4.883
4.856
3.765
3.514
3.504
3.489
3.478
3.449
3.423
3.406
3.381
3.343
3.322
3.317
3.297
3.251
3.235
3.209
3.193
MeO
N
O
Br
4b
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.90
1.93
1.00
2.93
1.00
1.03
1.02
0.98

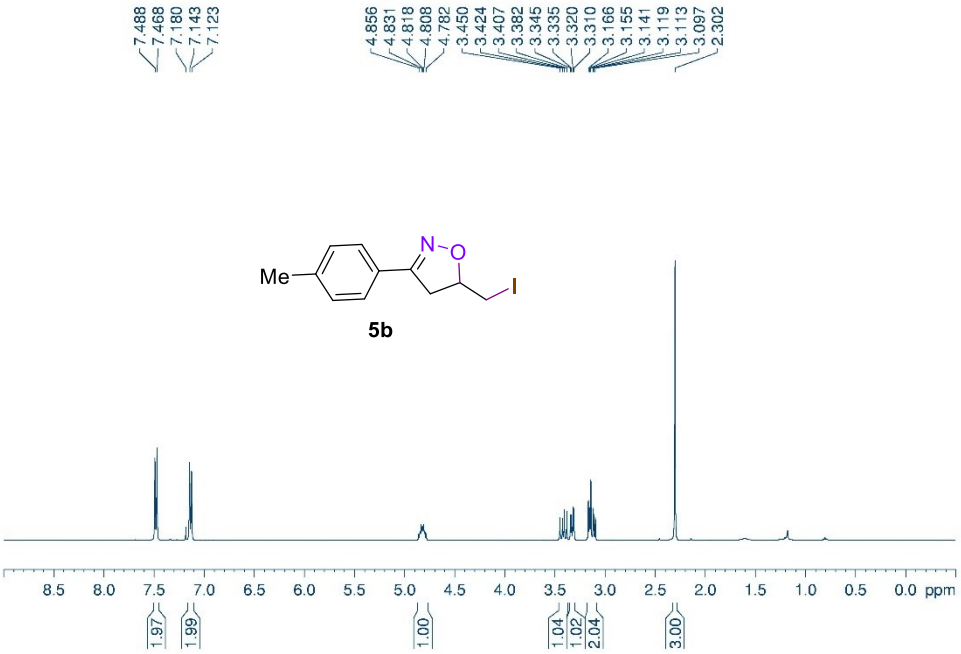

161.202
155.555
128.284
121.483
114.130
79.394
77.317
77.000
76.682
55.325
39.786
33.206
MeO
N
O
Br
4b
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

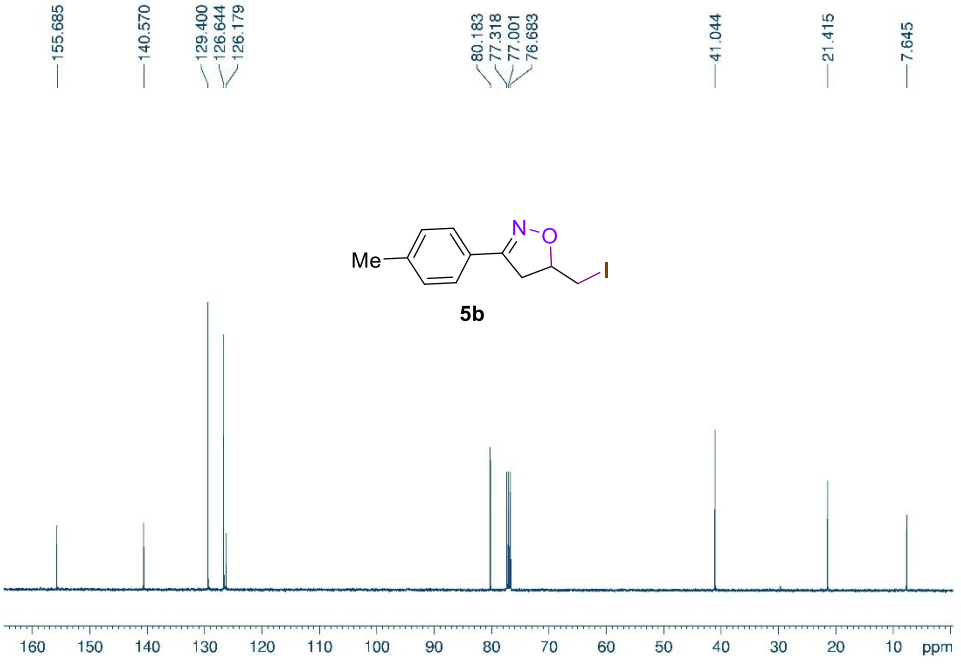

7.617
7.609
7.604
7.596
7.585
7.572
7.370
7.349
7.345
7.332
7.309
7.185
4.886
4.860
4.838
4.811
3.478
3.452
3.436
3.410
3.362
3.351
3.337
3.326
3.184
3.162
3.160
3.141
3.125
N
O
I
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.00
3.03
1.00
1.05
1.01
2.01

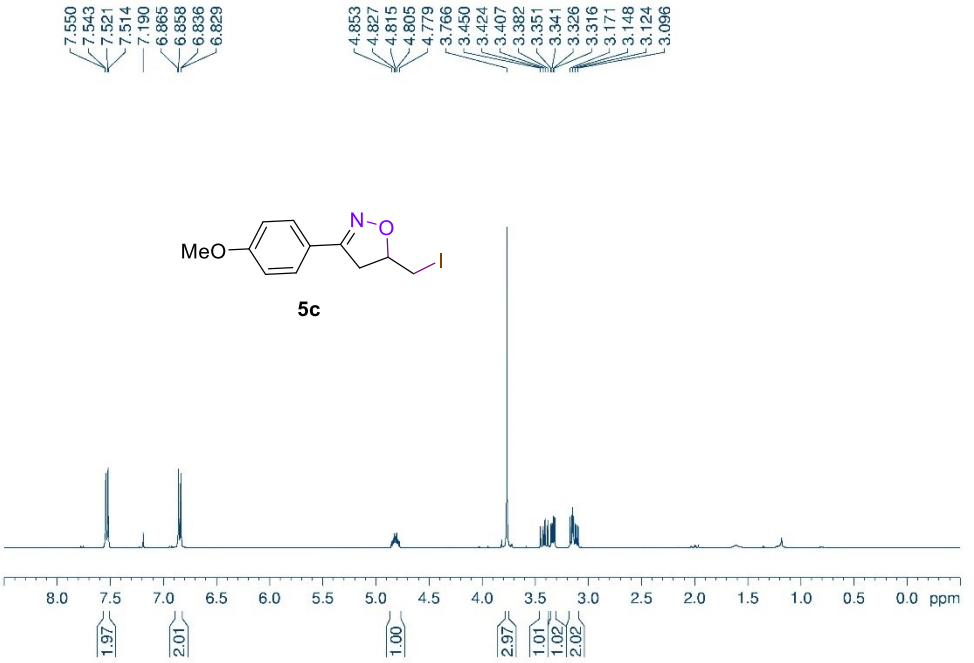
5a

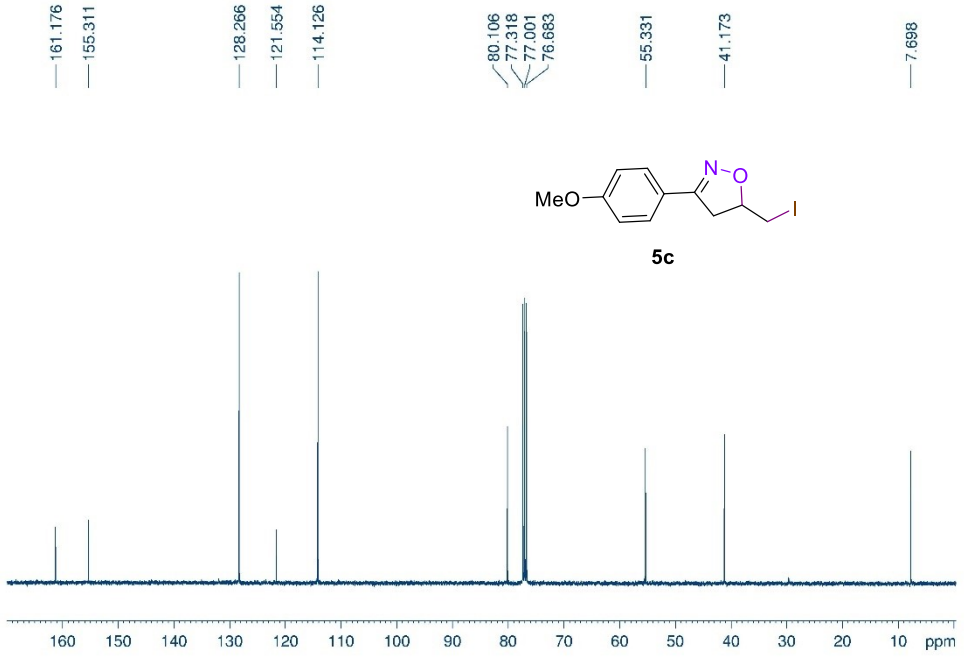

155.754
130.308
129.023
128.727
126.715
80.349
77.317
76.999
76.682
40.953
7.551
N
O
I
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

5a

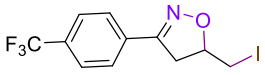

7.488
7.468
7.180
7.143
7.123
4.856
4.831
4.818
4.808
4.782
3.450
3.424
3.407
3.382
3.345
3.335
3.320
3.310
3.166
3.155
3.141
3.119
3.113
3.097
2.302
Me
N
O
I
5b
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.97
1.99
1.00
1.04
1.02
2.04
3.00


155.685
140.570
129.400
126.644
126.179
80.183
77.318
77.001
76.683
41.044
21.415
7.645
Me
N
O
I
5b
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

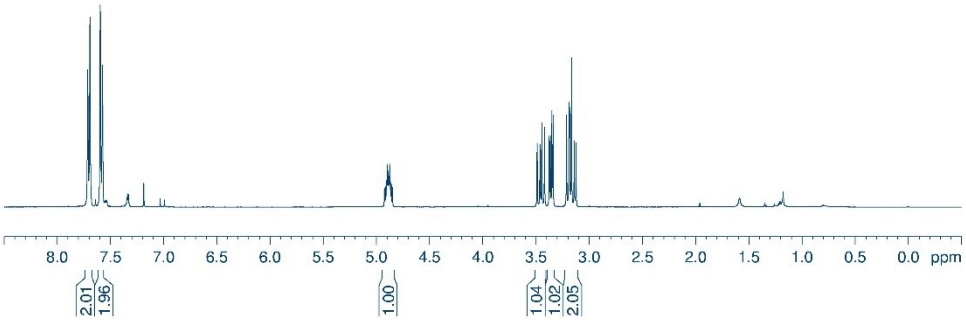

7.550
7.543
7.521
7.514
7.190
6.865
6.858
6.836
6.829
4.853
4.827
4.815
4.805
4.779
3.766
3.450
3.424
3.407
3.382
3.351
3.341
3.326
3.316
3.171
3.148
3.124
3.096
MeO
N
O
I
5c
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
1.97
2.01
1.00
2.97
1.01
1.02
2.02


161.176
155.311
128.266
121.554
114.126
80.106
77.318
77.001
76.683
55.331
41.173
7.698
MeO
N
O
I
5c
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

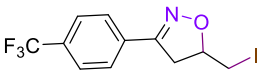

7.713
7.692
7.595
7.574
7.186
4.924
4.897
4.875
4.849
3.488
3.462
3.445
3.419
3.375
3.365
3.349
3.339
3.212
3.191
3.166
3.140
3.123


N
O
F3C
I

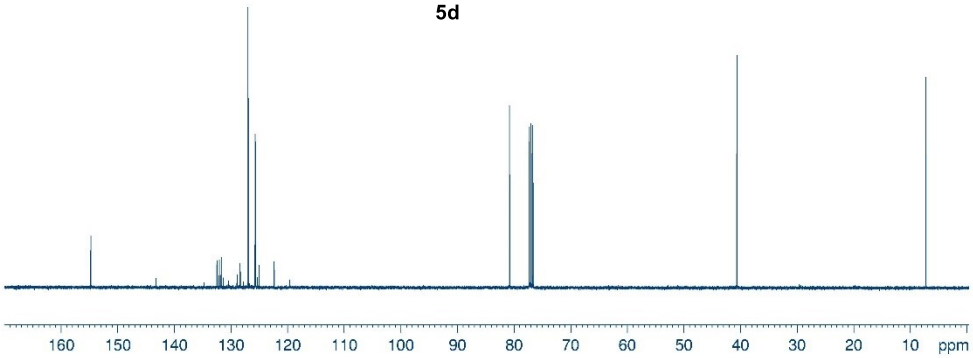
5d

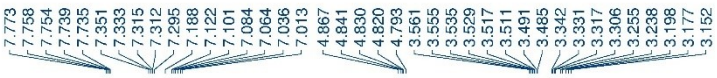

8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.01
1.96
1.00
1.04
1.02
2.05

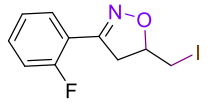

154.748
132.469
132.356
132.032
131.707
131.381
127.751
126.943
125.741
125.705
125.668
125.629
125.047
122.340
119.633
80.818
77.316
76.998
76.680
40.666
7.237


N
O
F3C
I

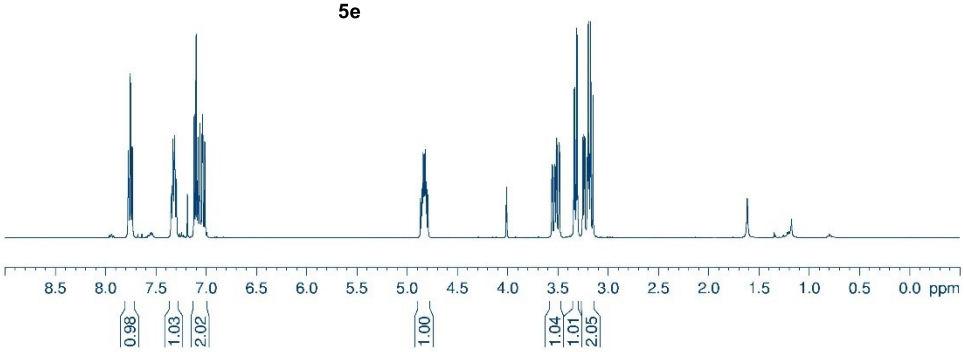
5d


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

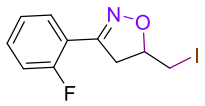

7.773
7.758
7.754
7.739
7.735
7.351
7.333
7.315
7.312
7.295
7.188
7.122
7.101
7.084
7.064
7.036
7.013
4.867
4.841
4.830
4.820
4.793
3.561
3.555
3.535
3.529
3.517
3.511
3.491
3.485
3.342
3.331
3.317
3.306
3.255
3.238
3.198
3.177
3.152


N
O
I
F

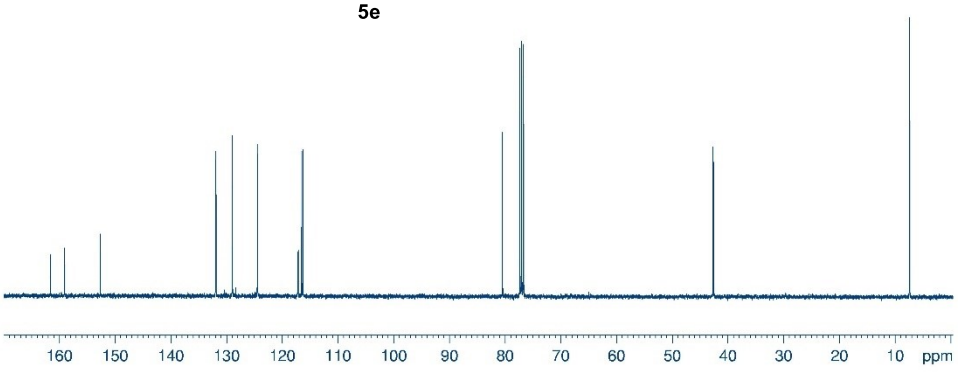
5e

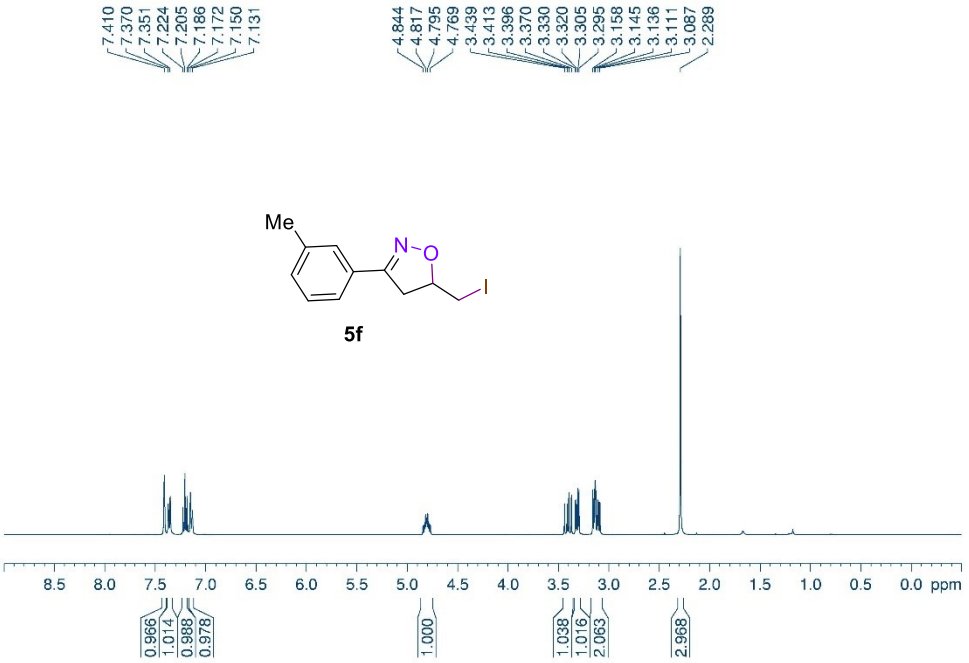

8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.98
1.03
2.02
1.00
1.04
1.01
2.05

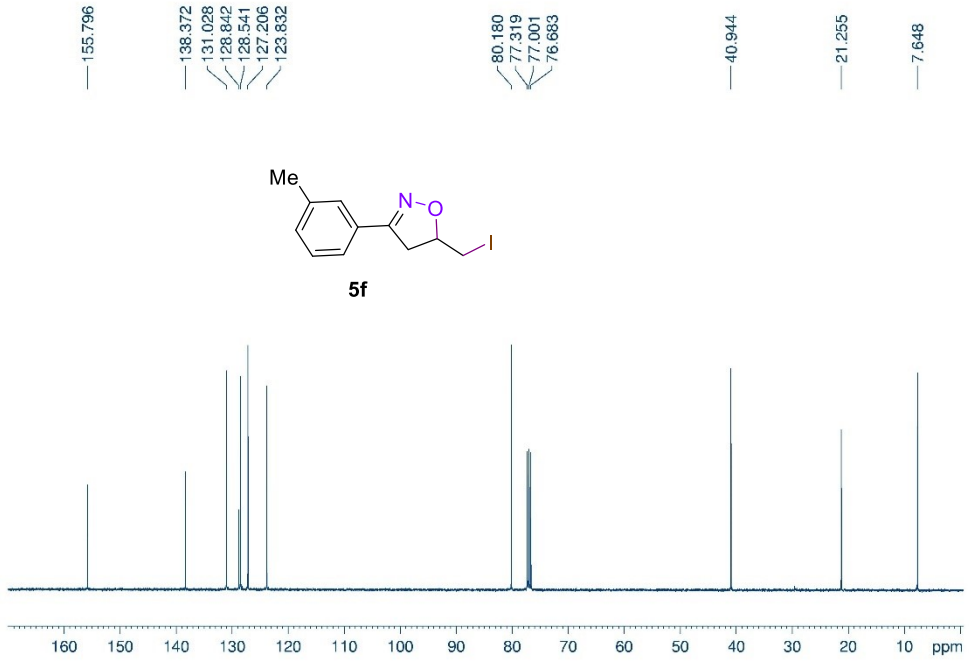

161.527
159.017
152.606
152.577
131.957
131.871
128.976
128.947
124.463
124.430
117.227
117.112
116.484
116.266
80.455
80.433
77.317
76.999
76.681
42.638
42.569
7.346

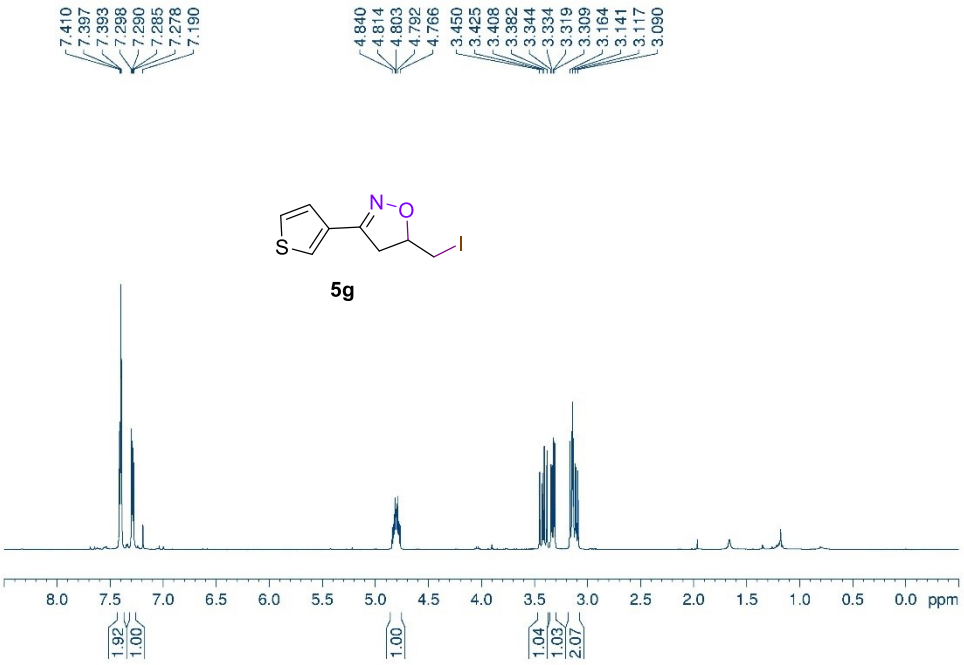

N
O
I
F

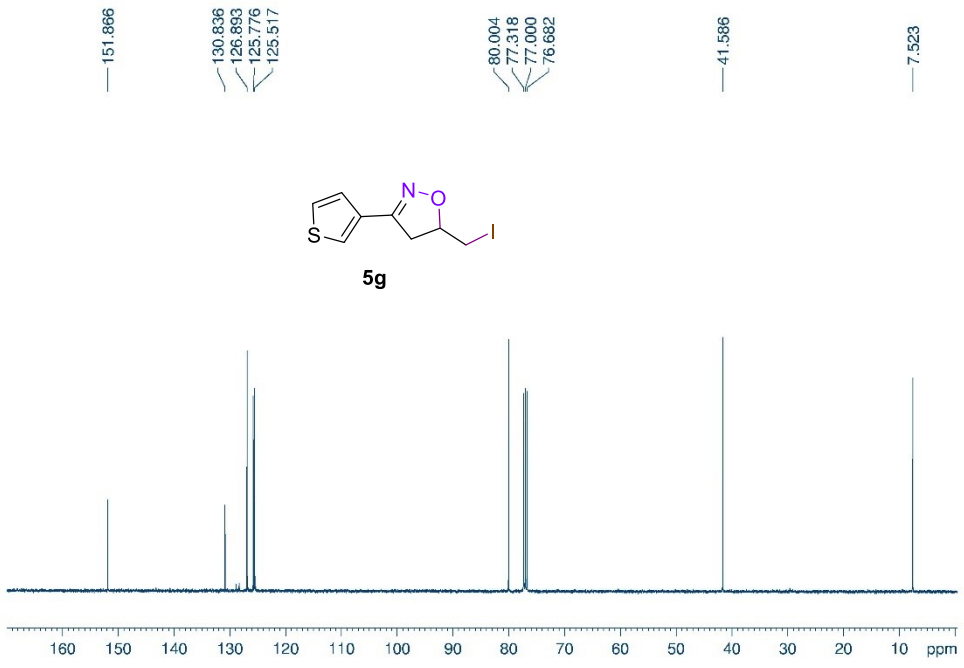
5e

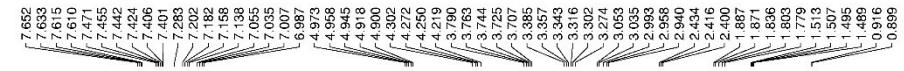

160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

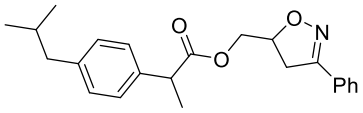

7.410
7.370
7.351
7.224
7.205
7.186
7.172
7.150
7.131
4.844
4.817
4.795
4.769
3.439
3.413
3.396
3.370
3.330
3.320
3.305
3.295
3.158
3.145
3.136
3.111
3.087
2.289
Me
N
O
I
5f
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.966
1.014
0.988
0.978
1.000
1.038
1.016
2.063
2.968


155.796
138.372
131.028
128.842
128.541
127.206
123.832
80.180
77.319
77.001
76.683
40.944
21.255
7.648
Me
N
O
I
5f
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

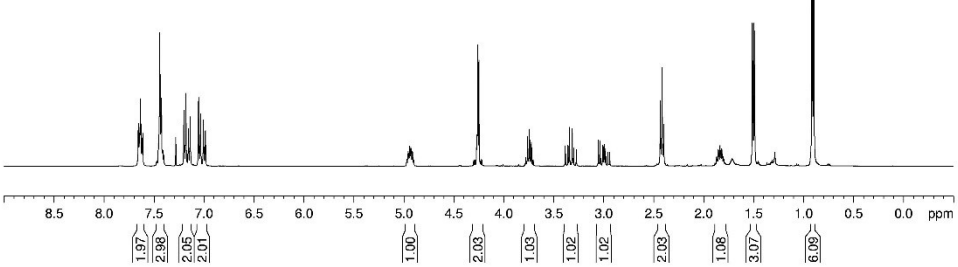

7.410
7.397
7.393
7.298
7.290
7.285
7.278
7.190
4.840
4.814
4.803
4.792
4.766
3.450
3.425
3.408
3.382
3.344
3.334
3.319
3.309
3.164
3.141
3.117
3.090
N
O
S
I
5g
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.92
1.00
1.00
1.04
1.03
2.07

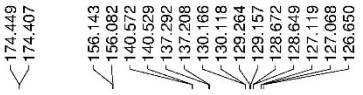

151.866
130.836
126.893
125.776
125.517
80.004
77.318
77.000
76.682
41.586
7.523
N
O
S
I
5g
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

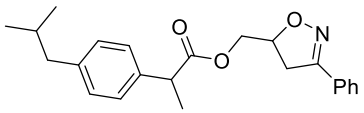

7.652
7.633
7.615
7.610
7.471
7.455
7.442
7.424
7.406
7.401
7.283
7.202
7.182
7.158
7.138
7.055
7.035
7.007
6.987
4.973
4.958
4.945
4.918
4.900
4.302
4.272
4.250
4.219
3.790
3.763
3.744
3.725
3.707
3.385
3.357
3.343
3.316
3.302
3.274
3.053
3.035
2.993
2.958
2.940
2.434
2.416
2.400
1.887
1.871
1.836
1.803
1.779
1.513
1.507
1.495
1.489
0.916
0.899


O
O
O
N
Ph

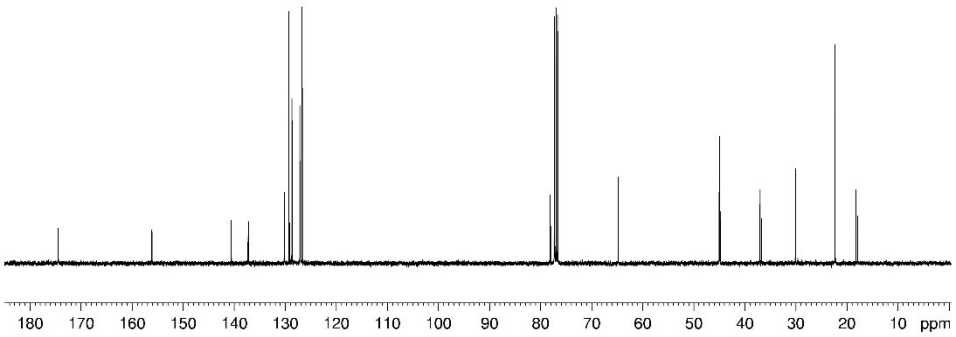
7a


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
ppm
1.97
2.98
2.05
2.01
1.00
2.03
1.03
1.02
1.02
2.03
1.08
3.07
6.09


174.449
174.407
156.143
156.082
140.572
140.529
137.292
137.208
130.166
130.118
129.264
129.157
128.672
128.649
127.119
127.068
126.650
78.139
78.086
77.319
77.001
76.684
64.798
45.038
44.932
44.824
37.032
36.769
30.077
22.330
18.219
17.925


O
O
O
N
Ph

7a


180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm