Supporting Information

Transition-metal-free C-C, C-O and C-N cross-couplings enabled by light

Wenbo Liu, Jianbin Li, Pierre Querard and Chao-Jun Li*

Department of Chemistry and FRQNT Centre for Green Chemistry and Catalysis, McGill University, 801 Sherbrooke St. W., Montreal, Quebec H3A 0B8, Canada.

E-mail: cj.li@mcgill.ca

Table of Contents

1. General information

All the reactions were carried out under argon atmosphere using standard Schlenk technique. ^{1}H NMR (500 MHz), ^{19}F NMR (471 MHz), ^{13}C NMR (126 MHz) and ^{11}B NMR (161 MHz) were recorded on an NMR spectrometer with $CDCl_3$ or DMSO-d_6 as the solvent. Chemical shifts of ^{1}H, ^{19}F, and ^{13}C spectra are reported in parts per million (ppm). The residual solvent signals were used as references and the chemical shifts were converted to the TMS scale ($CDCl_3$: δ H = 7.26 ppm, δ C = 77.16 ppm). All coupling constants (*J* values) were reported in Hertz (Hz). High-resolution mass spectrometry was conducted through using atmospheric pressure chemical ionization (APCI) or electro-spraying ionization (ESI), and was performed at McGill University on a Thermo-Scientific Exactive Orbitrap. Protonated molecular ions $[M+H]^+$ or sodium adducts $[M+Na]^+$, or $[M-K]^-$ (for organotrifluoroborate) were used for empirical formula confirmation. Column chromatography was performed on silica gel 200−300 mesh.

2. General procedure for the synthesis of aryl triflate and organotrifluoroborate

2.1. Synthesis of aryl triflate

The phenol (2 mmol) was dissolved in DCM (20 mL) and cooled to 0 °C. NEt_3 (330 μL, 2.4 mmol, 1.2 equiv) was added dropwise to the solution, which was followed by the addition of triflic anhydride (400 μL, 2.4 mmol, 1.2 equiv). After 5 mins, the ice bath was removed, and the reaction was monitored by TLC. Once the phenol was completely consumed, the reaction was stopped. The solvent was evaporated under vacuum and the residue was purified by flash column chromatography to get the desired aryl triflate.

2.2. Synthesis of organotrifluoroborate

The boronic acid was dissolved in MeOH (5 mL) and cooled to 0 °C. Saturated KHF_2 (4 equiv, 4.5 M) was added dropwise to the reaction, and the resulting mixture was allowed to warm to rt. After 30 min, the solid was filtered and washed with H_2O and Et_2O to result in the aromatic potassium trifluoroborates.

3. General procedures for the coupling of aryl triflate with potassium aryl trifluoroborate, alcohol and nitrile

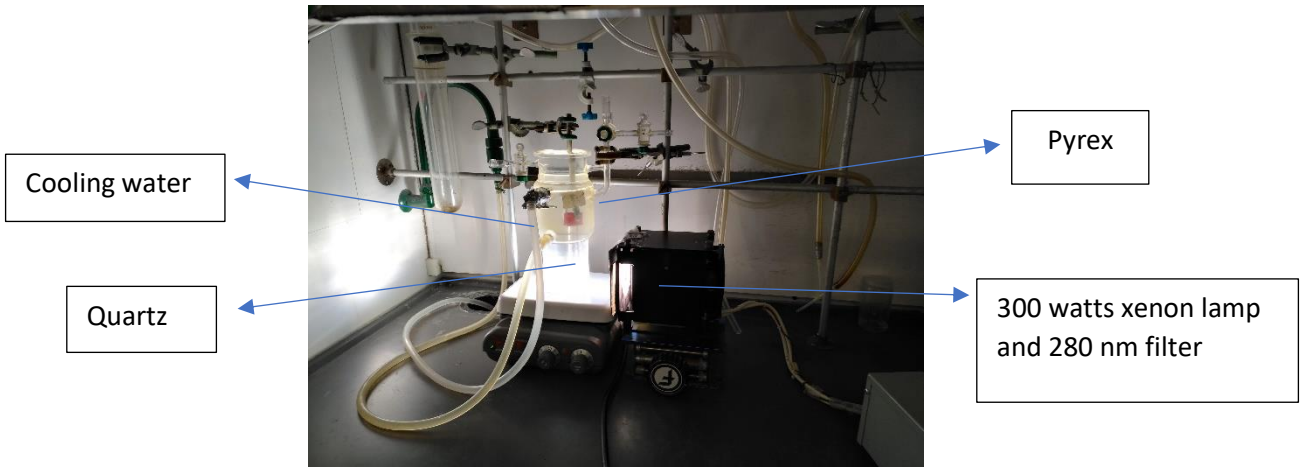


Figure S1. Reaction setup.

The reaction vessel we used in the study is the quartz tube, which has a cut-off wavelength of 175 nm. That is to say, the UV light (including UVA, UVB and UVC) can penetrate this quartz tube. For the cooling reactor, we designed this reactor together with the glass blower in the department. Although the top part of this cooling chamber is made from the regular pyrex (cut-off wavelength of 300 nm), the bottom part, which is on the pathway of the light beam, is made from quartz. This combination of pyrex and quartz will lower the price of the whole chamber but will also allow the light to penetrate the chamber to fully take use of the light.

The light source we used is a 300 watts xenon lamp. Although only the UV light (280 nm – 400 nm) is able to promote the reactions, this lamp also emits visible light. Please see below for the emission spectrum of the UV lamp we used in the study. Since our naked eye can not see the UV light, we can only see the white light from the picture. Because this lamp emits a large amount of visible light, which will generate heat, the cooling chamber to stabilize the temperature is very crucial for this reaction.

Figure S2. UV xenon lamp used in this study.

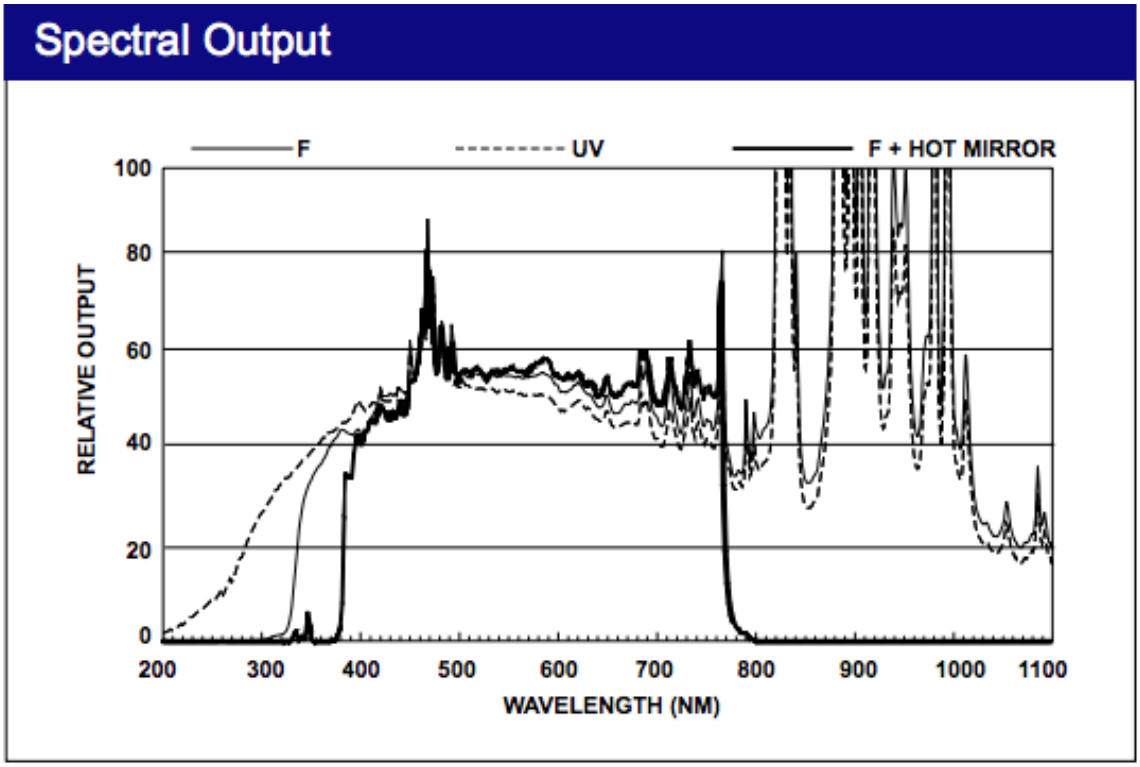


Figure S3. Emission spectrum of the lamp used in this study.

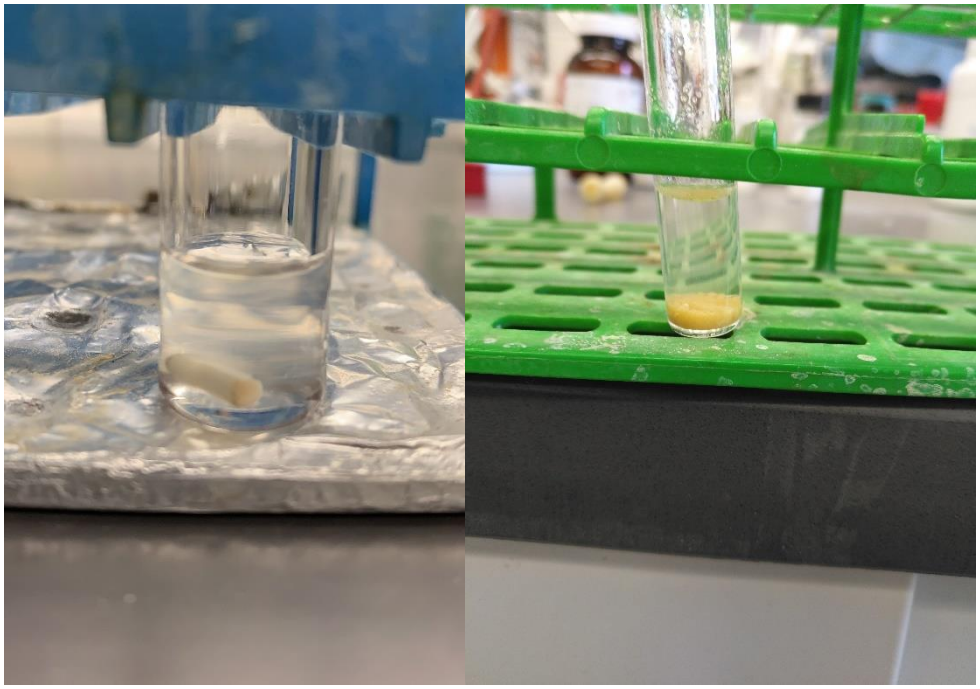


Figure S4. Reaction mixture before and after the reaction.

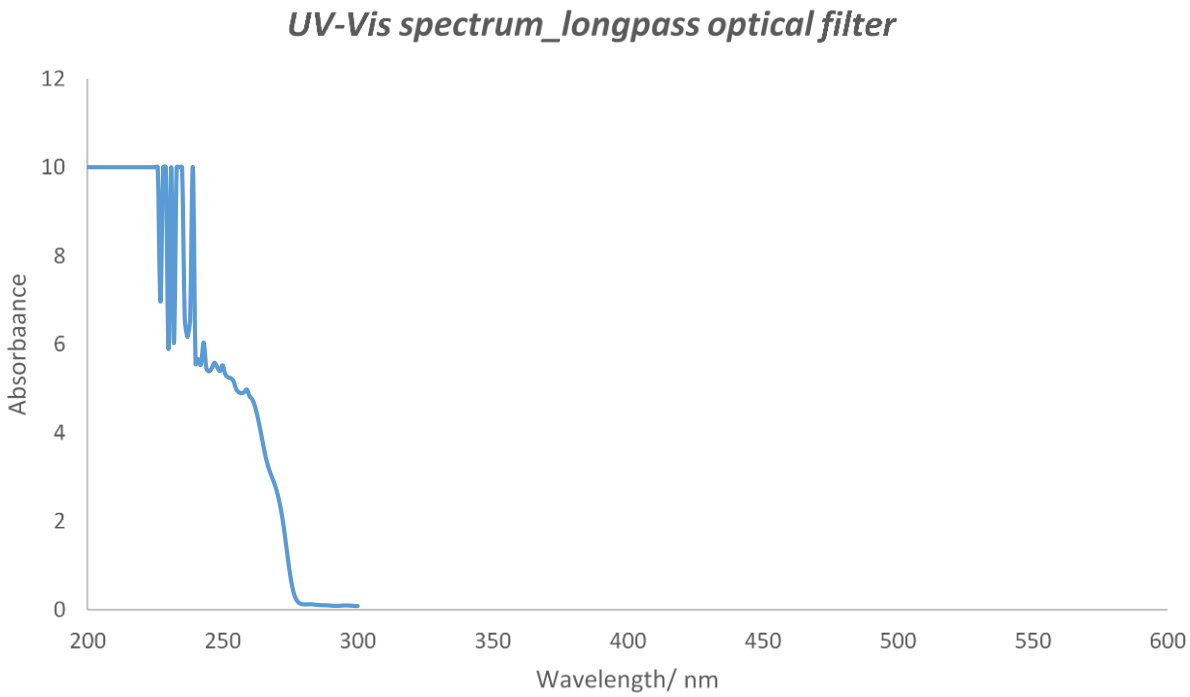


Figure S5. UV_Vis spectrum of the 280 nm optical filter.

The effective optical filtration range of the longpass optical filter employed in our reaction was measure by attaching it to inner wall of chamber (the side close to the light source) and blocking the light emission from 300 nm to 200 nm. The detailed experimental setup could be seen in the picture as below.

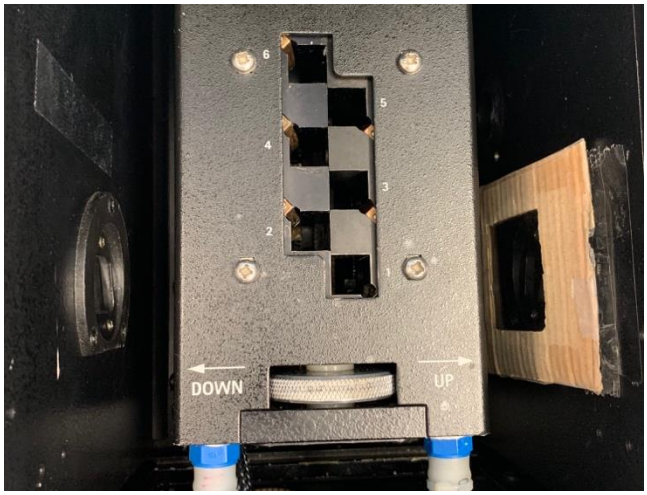


Figure S6. Set-up to collect the UV_Vis spectrum of the 280 nm optical filter.

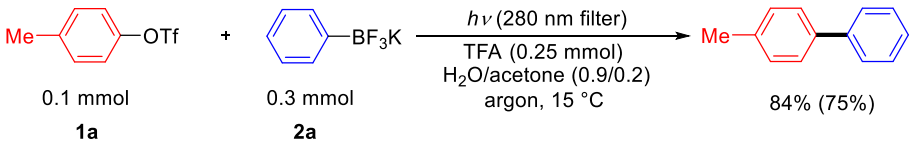
As shown in the UV-Vis spectra, irradiation below 275 nm was partially blocked by the longpass filter and 275 nm was in the absorption band of both acetone and Ar-OTf. Therefore, 275 nm was chosen as the excitation wavelength for fluorescence quenching experiments.

The fluctuation from 250 nm to 200 nm in the spectra of longpass optical filter was caused by saturation of signals during the measurement.

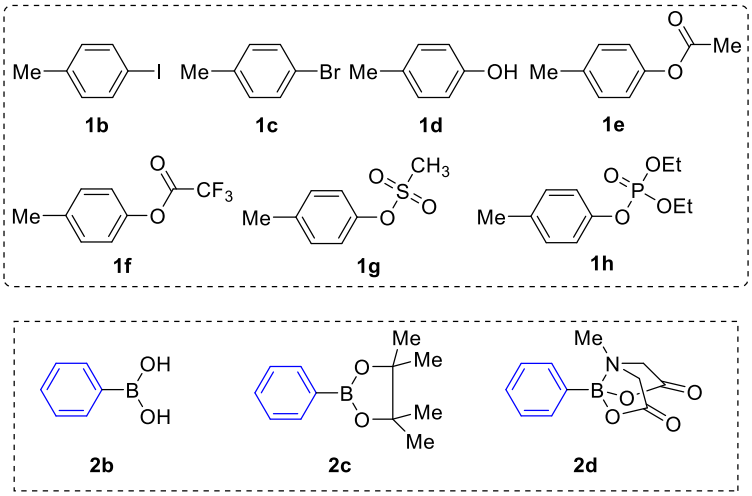
3.1. Procedure of coupling between aryl triflate and potassium aryl trifluoroborates

Potassium aryl trifluoroborates (0.3 mmol, 3 equiv), aryl triflate (0.1 mmol, 1 equiv) and trifluoroacetic acid (20 μL, 0.25 mmol, 2.5 equiv) were added into 0.9 mL water and 0.2 mL acetone. The air-tight quartz tube (10 mL, 1 cm diameter) containing these reactants and solvents with a teflon-coated stir bar was evacuated by three frozen-pump-thaw cycles and back-filled with argon prior to use. The reaction was stirred at 15 ºC (cooled by flowing water) under photo irradiation by using a 300 watts xenon lamp with a 280 nm long pass optical filter. The reaction was monitored by GC/MS. When aryl triflate was gone, the resulting crude mixture was extracted with EtOAc and purified by flash column chromatography on silica gel to provide the desired product.

Table S1. Impact of various factors on the metal-free Suzuki coupling [a]



entry	Variation from standard conditions	yield
1	no change	84% (75%)
2	no light	0%
3	no 280 nm filter	46%
4	400 nm filter	0%
5	no acetone (pure water)	0%
6	no water (pure acetone)	21%
7	no TFA	25%
8	air instead of argon	57%
9	CH_3CN instead of water	28%
10	DMSO instead of water	0%
11	CH_2Cl_2 instead of water	trace
12	THF instead of water	12%
13	^{t}BuOH instead of water	8%
14	0.12 mmol **2a** instead of 0.3 mmol	60%
15	0.12 mmol TFA instead of 0.25 mmol	64%
16	**1b** instead of **1a**	0%
17	**1c** instead of **1a**	0%
18	**1d** instead of **1a**	0%
19	**1e** instead of **1a**	0%
20	**1f** instead of **1a**	0%
21	**1g** instead of **1a**	36%
22	**1h** instead of **1a**	17%
23	**2b** instead of **2a**	26%
24	**2c** instead of **2a**	23%
25	**2d** instead of **2a**	7%



***a*:** The standard conditions are **1a** (0.1 mmol), **2a** (0.3 mmol), with the addition of TFA (0.25 mmol) in the acetone/water mixture (0.2 mL/0.9 mL) under argon at 15 °C. The light is a 300 watts xenon lamp with a 280 nm optical filter. The yields were calculated with GC/MS based on the calibrated curve and the isolated yield was given in the parenthesis.

During the screening, we have also evaluated other common photosensitizers including benzophenone, diacetyl, Eosine, Xanthanone, $Ru(bpy)_3(PF_6)_2$, Fukuzumi's photocatalyst (9-Mesityl-10-phenylacridinium tetrafluoroborate), none of which gave the desired coupling product. Moreover, we have attempted to measure the quantum yield of this reaction at 300 nm. However, aryl triflate, potassium phenyl trifluoroborate and acetone all have absorption in this area. Therefore, we did not get the accurate quantum yield.

3.2. Procedure of coupling between aryl triflate and alcohol

Aryl triflate (0.1 mmol, 1 equiv), alcohol (0.3 mL, primary and secondary alcohols), trifluoroacetic acid (0.25 mmol, 20 μL, 2.5 equiv) and $B(OMe)_3$ (0.2 mmol, 22 μL, 2 equiv) were added into 0.1 mL acetone. The air-tight quartz tube (5 mL, 0.5 cm diameter) containing these reactants and solvents with a teflon-coated stir bar was evacuated by three frozen-pump-thaw cycles and back-filled with argon prior to use. The reaction was stirred at 15 ºC (cooled by flowing water) under photo irradiation by using a 300 watts xenon lamp with a 280 nm long pass optical filter. The reaction was monitored by GC/MS. When aryl triflate was completely consumed, the resulting crude mixture was purified by flash column chromatography on silica gel to provide the desired product.

3.3. Procedure of coupling between aryl triflate and nitrile

Aryl triflate (0.1 mmol, 1 equiv), nitrile (0.3 mL), H_2O (3.6 μL, 0.2 mmol, 2 equiv), trifluoroacetic acid (0.25 mmol, 20 μL, 2.5 equiv) and $B(OMe)_3$ (0.2 mmol, 22 μL, 2 equiv) were added into 0.1 mL acetone.

The air-tight quartz tube (5 mL, 0.5 cm diameter) containing these reactants and solvents with a teflon-coated stir bar was evacuated by three frozen-pump-thaw cycles and back-filled with argon prior to use. The reaction was stirred at 15 ºC (cooled by flowing water) under photo irradiation by using a 300 watts xenon lamp (*Attention: No 280 nm long-pass cutoff optical filter*). The reaction was monitored by GC/MS. When aryl triflate was completely consumed, the resulting crude mixture was purified by flash column chromatography on silica gel to provide the desired product.

3.4. Some mechanistic concerns regarding reductive nucleophiles and non-reductive nucleophiles

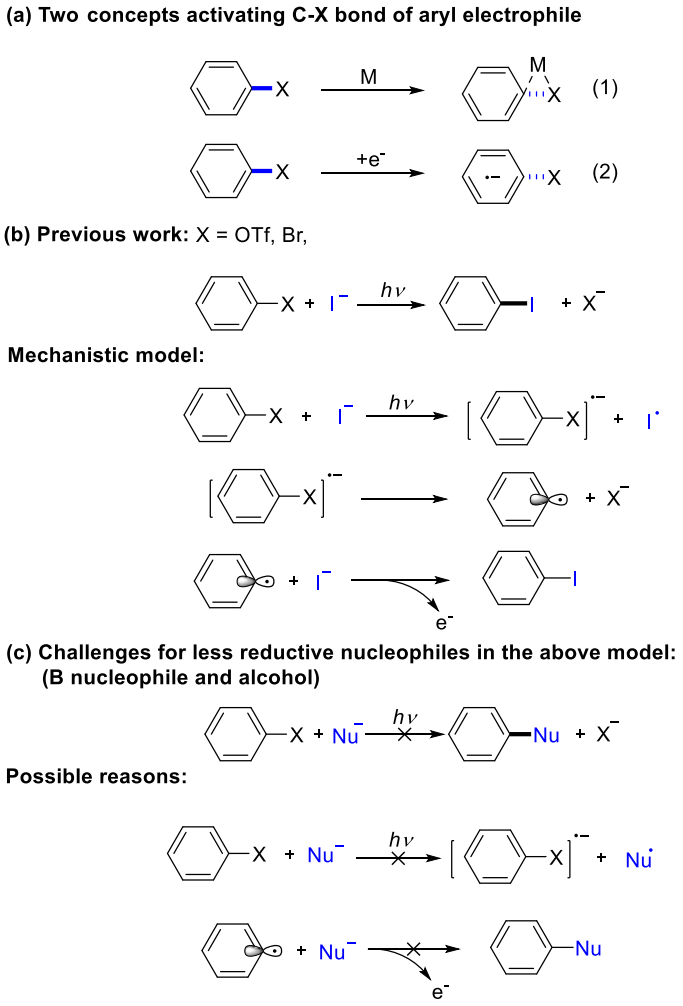
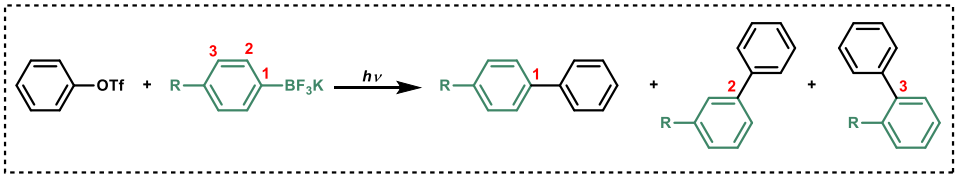
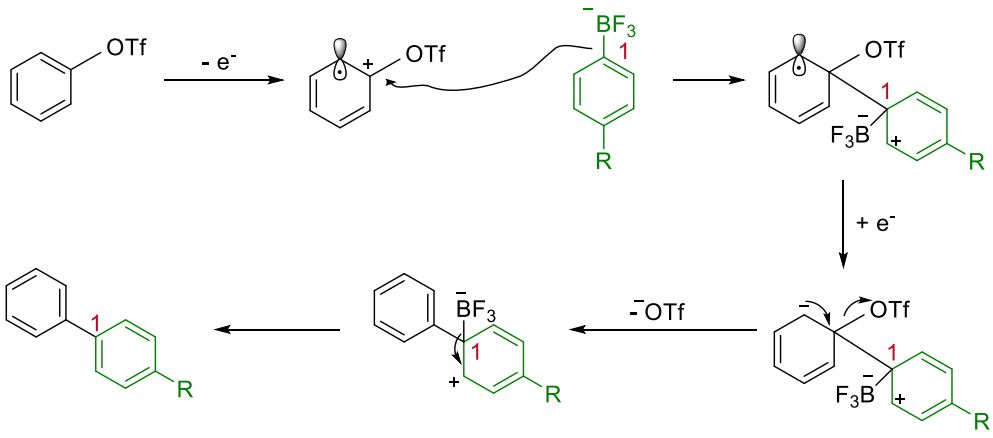


Figure S7. Discussion on the reductive nucleophile and non-reductive nucleophile in the context of electron catalysis

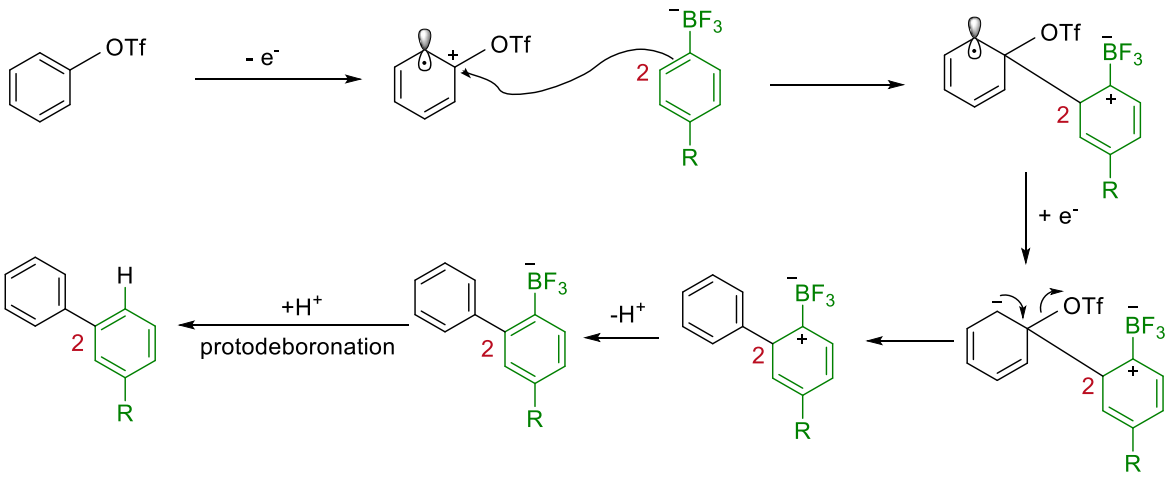
3.5. Mechanism to generate regioisomers for the metal-free Suzuki coupling



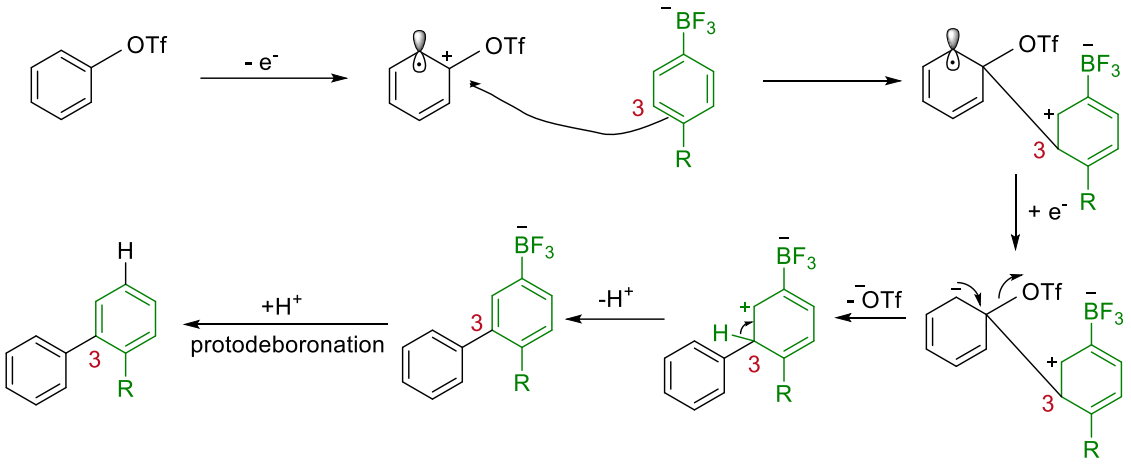
1): The generation of 1-substitution isomer.



2): The generation of 2-substitution isomer.

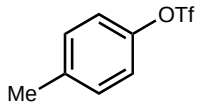
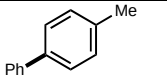
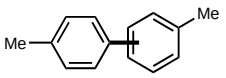
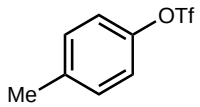
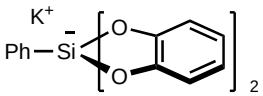
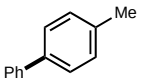
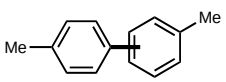
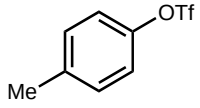
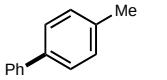
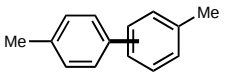


3): The generation of 3-substitution isomer.

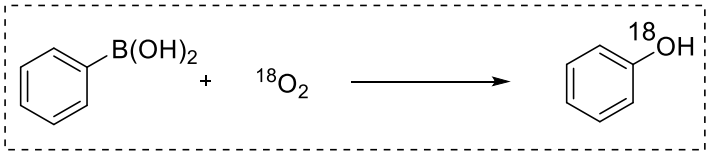


3.6. Procedure of cross coupling of aryl triflates (Ar-OTf) and aryl silanes (Ar-[Si])

The general operation of cross coupling described as below unless otherwise specified. To an air-tight quartz tube (10 mL, 1 cm diameter) were added toly triflate (0.10 mmol, 1.0 equiv) and a specific type of phenyl silane reagent (Ar-[Si], 0.30 mmol, 3.0 equiv) (Table 2) with additive (indicated in the table below, 0.25 mmol, 2.5 equiv) in 0.9 mL water and 0.2 mL acetone. The tube containing these reactants and solvents with a teflon-coated stir bar was evacuated by three frozen-pump-thaw cycles and back-filled with argon prior to use. The reaction was stirred at 15 °C (cooled by flowing water) under photo irradiation by using a 300 watts xenon lamp with a 275 nm long pass optical filter. After 10 hours, internal standard (1, 3, 5-trimethoxybenzene, 0.10 mmol) was added into the reaction crude and the resulted mixture was extracted with EtOAc for three times. Then, the combined organic layers were dried over Na_2SO_4, concentrated in vacuo and subjected to GC-MS analysis. The results of examination were summarized in the following table.

aryl triflate	***aryl silane***	***additive***	***product observed***	
	Ph-Si(OMe)$_3$	TBAF·3H$_2$O	 ***Cross coupling product*** ~5%	 ***Homo coupling product*** ~5%
		TFA	 ***Cross coupling product*** trace	 ***Homo coupling product*** trace
	Ph-SiH$_3$	-	 ***Cross coupling product*** ~5%	 ***Homo coupling product*** ~5%

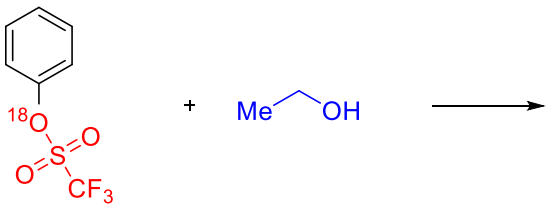
4. Isotopic labelling studies between aryl triflate and alcohol



Phenyl boronic acid (61 mg, 0.5 mmol), $Ru(bpy)_3Cl_2 \cdot 6H_2O$ (7.5 mg, 0.01 mmol), DIPEA (174 μL, 1 mmol) were added into 5 mL DMF. The 10 mL pyrex tube containing all these chemicals and solvent with an injectable septum and teflon stir bar was evacuated by three frozen-pump-thaw cycles and back-filled with argon prior to use. Then a low pressure cylinder containing $^{18}O_2$ with a long needed was connected with the pyrex tube. A 34 watts CFL was turned on, which was used to irradiate the reaction. After 48 hours, the reaction was stopped and the product was purified (40.3 mg, 0.42 mmol, 84%). The product was confirmed by ^{1}H NMR and GC/MS.

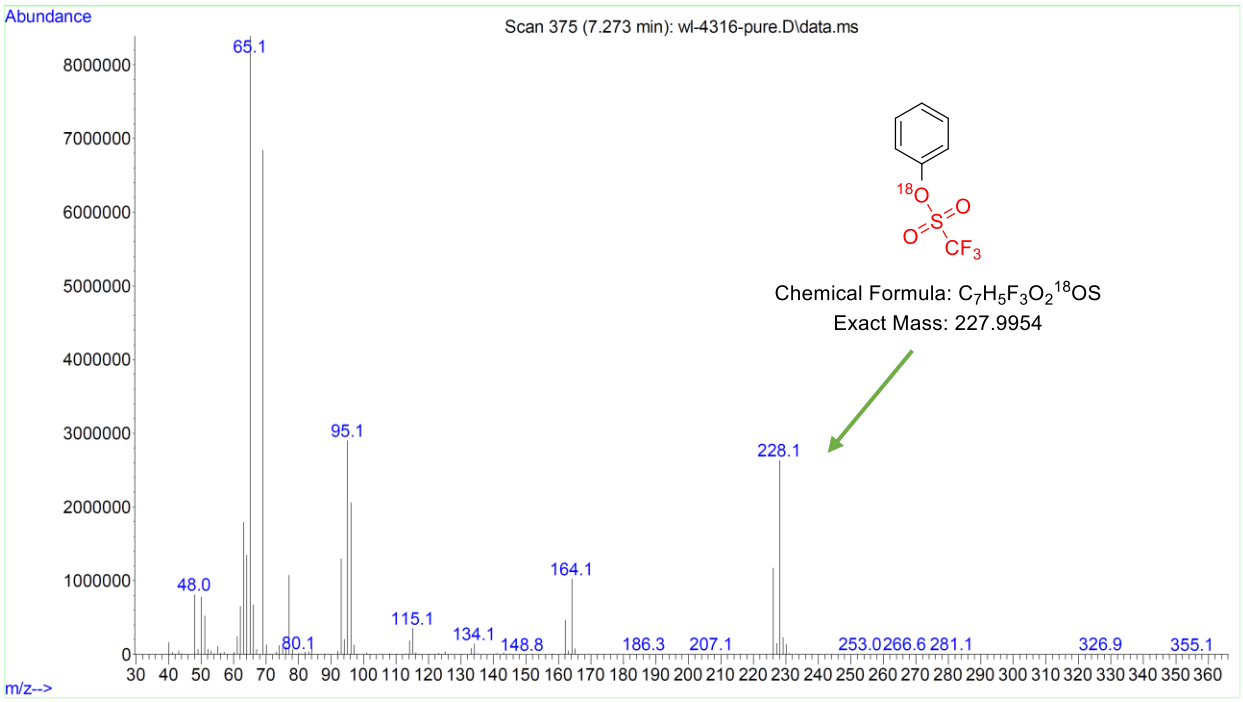
Following the general procedures to prepare aryl triflate, the ^{18}O labelled phenyl triflate can be prepared with 93% yield.

The ^{18}O labelled phenyl triflate (23 mg, 0.1 mmol) was subjected to the standard conditions between aryl triflate with ethanol. The aryl ethyl ether was purified in 52% yield (6.1 mg), whose GC/MS was shown below. The GC/MS result clearly suggests that the O atom in the product comes from the alcohol instead of the aryl triflate.



Chemical Formula: $C_7H_5F_3O_2{}^{18}OS$
Exact Mass: 227.9954

Chemical Formula: $C_8H_{10}O$
Exact Mass: 122.0732



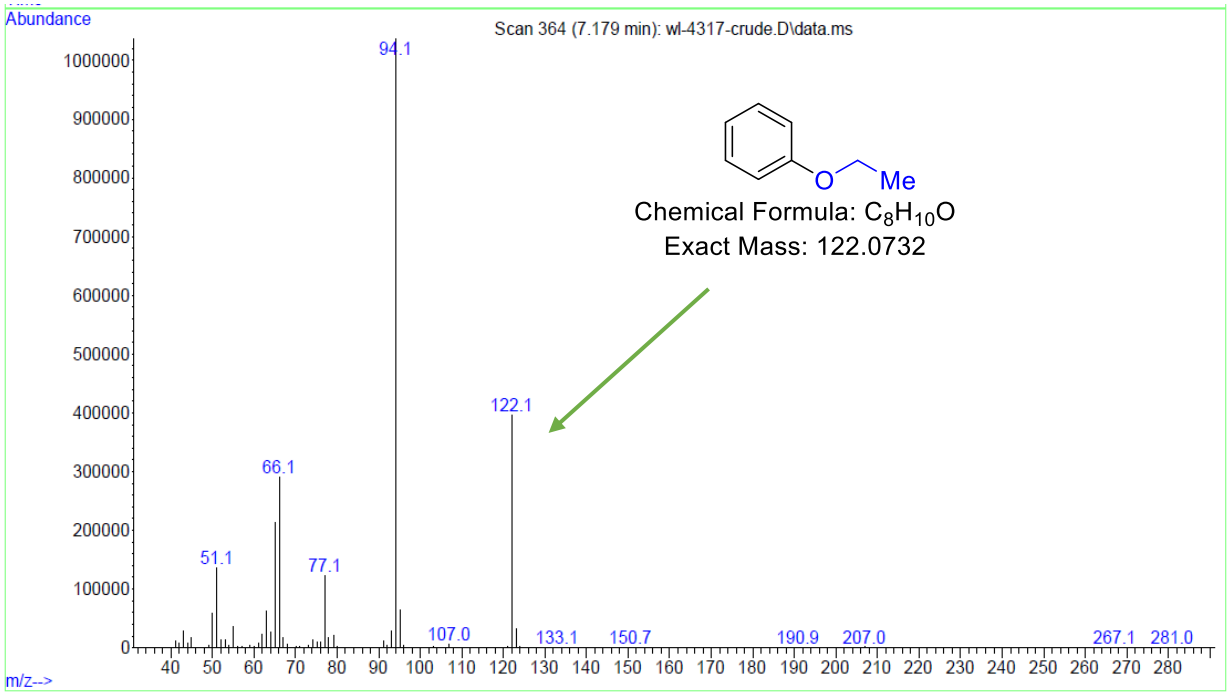


Figure S8: Isotopic labelling study for the C-O coupling.

5. Fluorescence quenching studies between acetone and aryl triflate

The UV-Vis spectrometric experiments of acetone, p-tolyl trifluoromethanesulfonate (Ar-OTf) and the long pass optical filter was performed on Agilent Cary 5000 series UV-Vis-NIR spectrometer under the conditions as below.

A Stock solution of acetone (0.10 M, in HPLC grade CH_3CN) was prepared in a volumetric flask and diluted by HPLC grade CH_3CN to 0.10 mM for the UV-Vis experiment. A quartz cuvette (1 cm x 1 cm x 3 cm) was filled with the above-mentioned 0.10 mM acetone solution and its spectrum was recorded from 800 nm to 200 nm in the spectrometer.

The same procedure is applicable to the spectroscopic experiment of Ar-OTf solution.

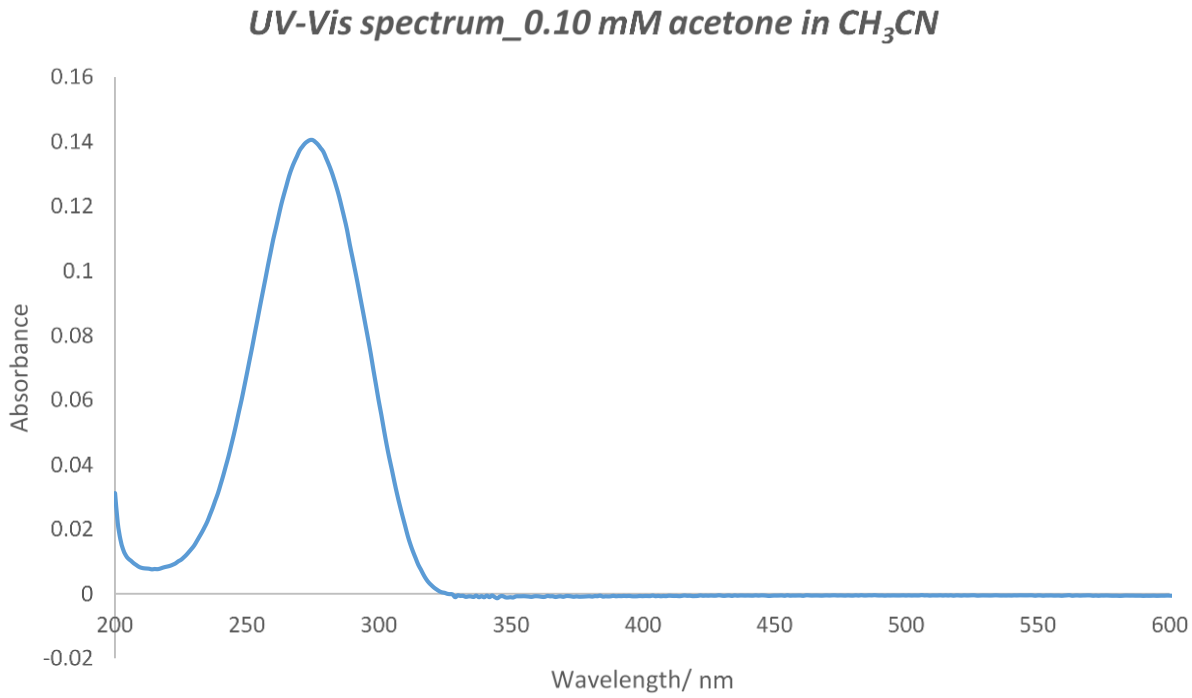


Figure S9. UV-Vis spectrum of acetone.

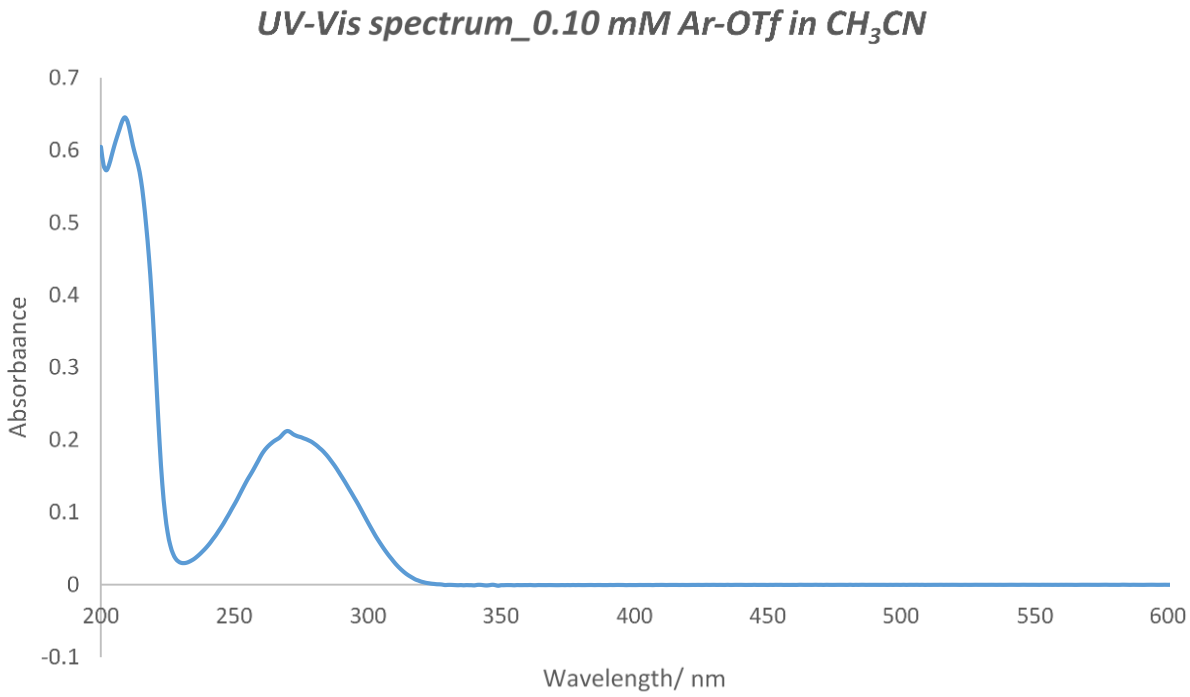
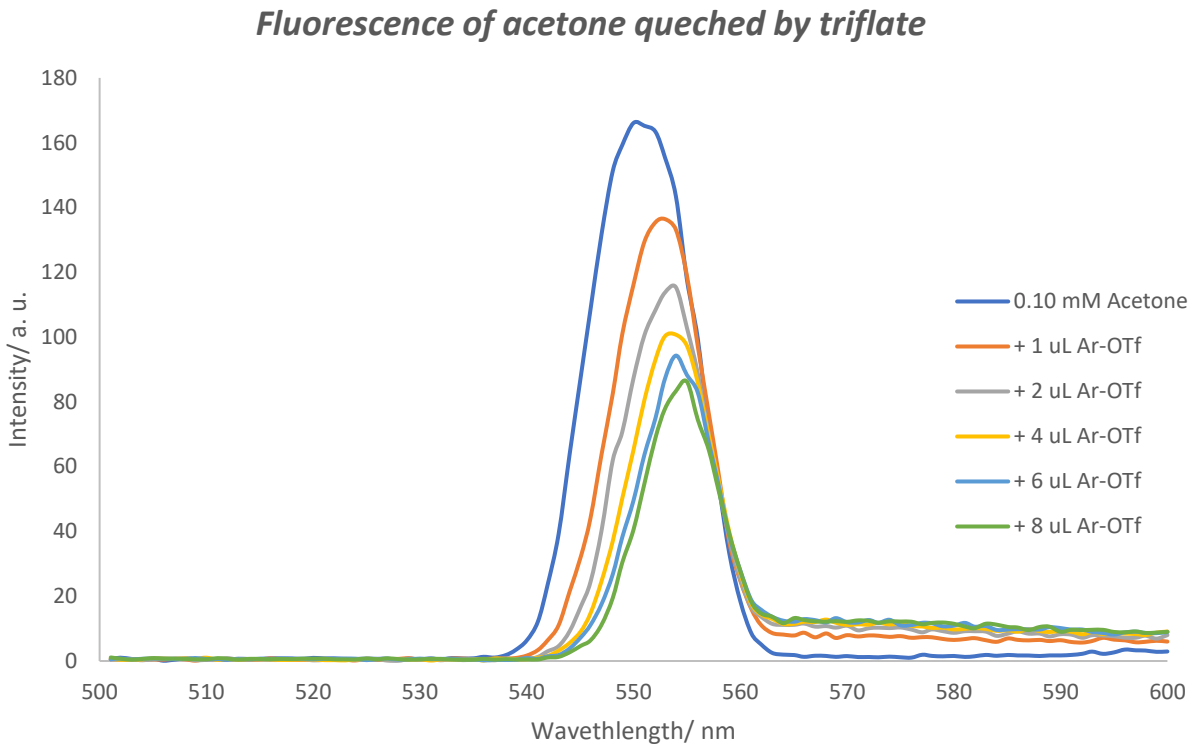
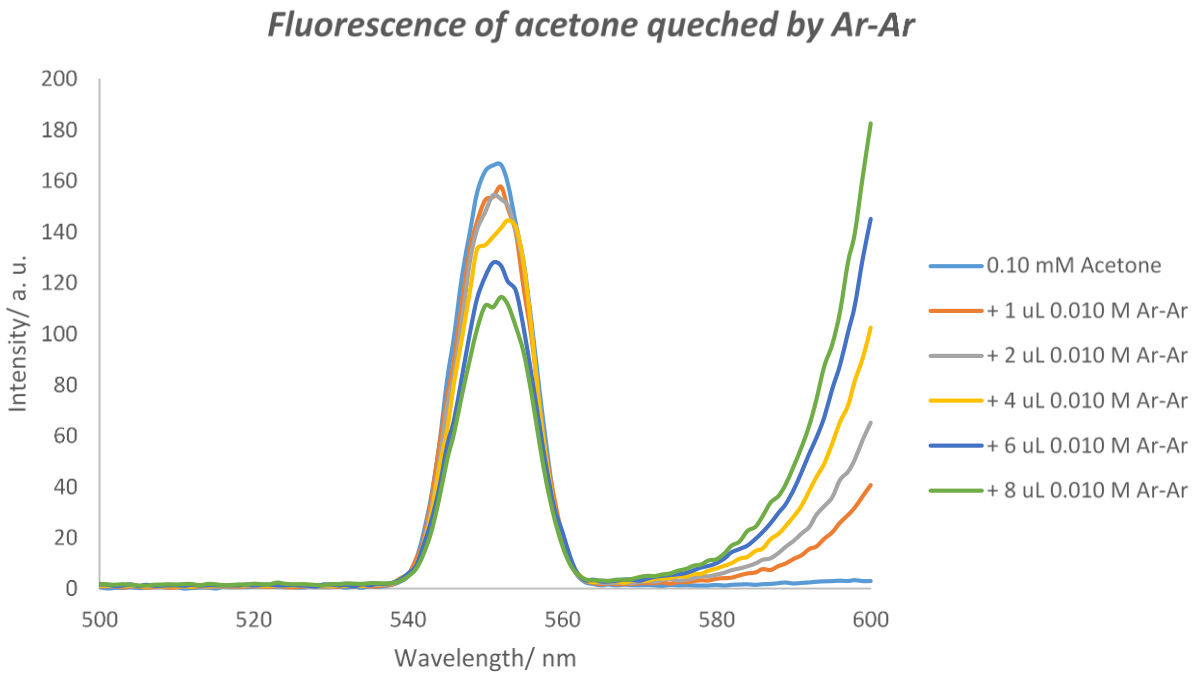


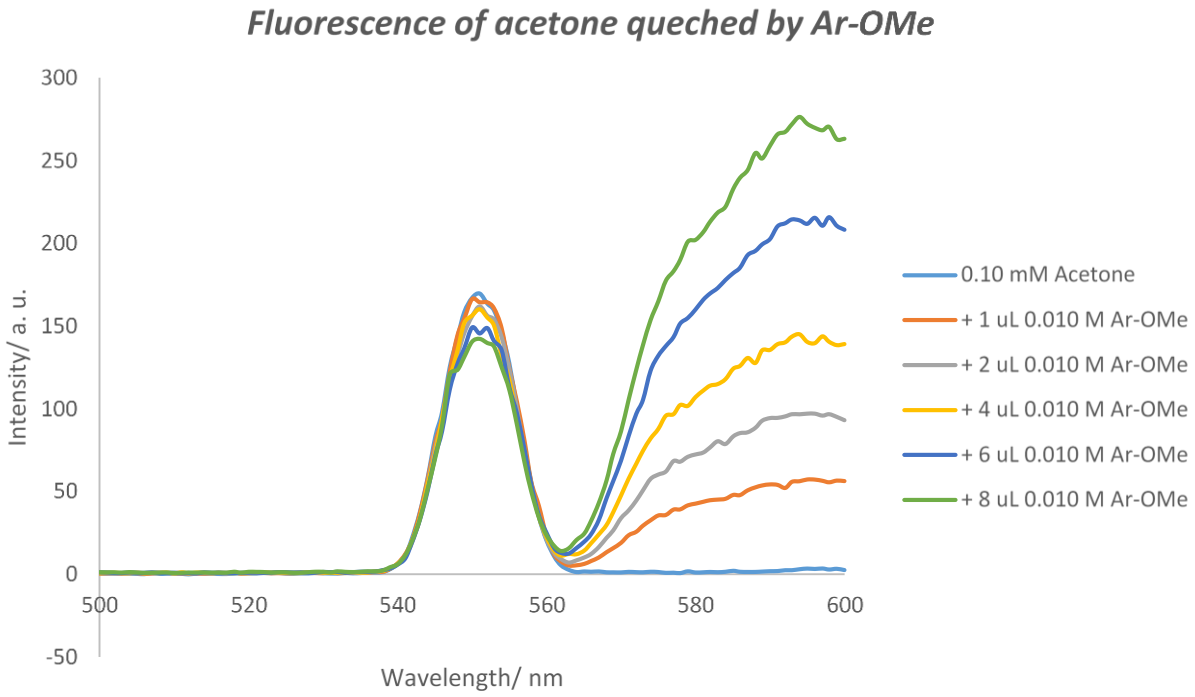
Figure S10. UV-Vis spectrum of phenyl triflate.

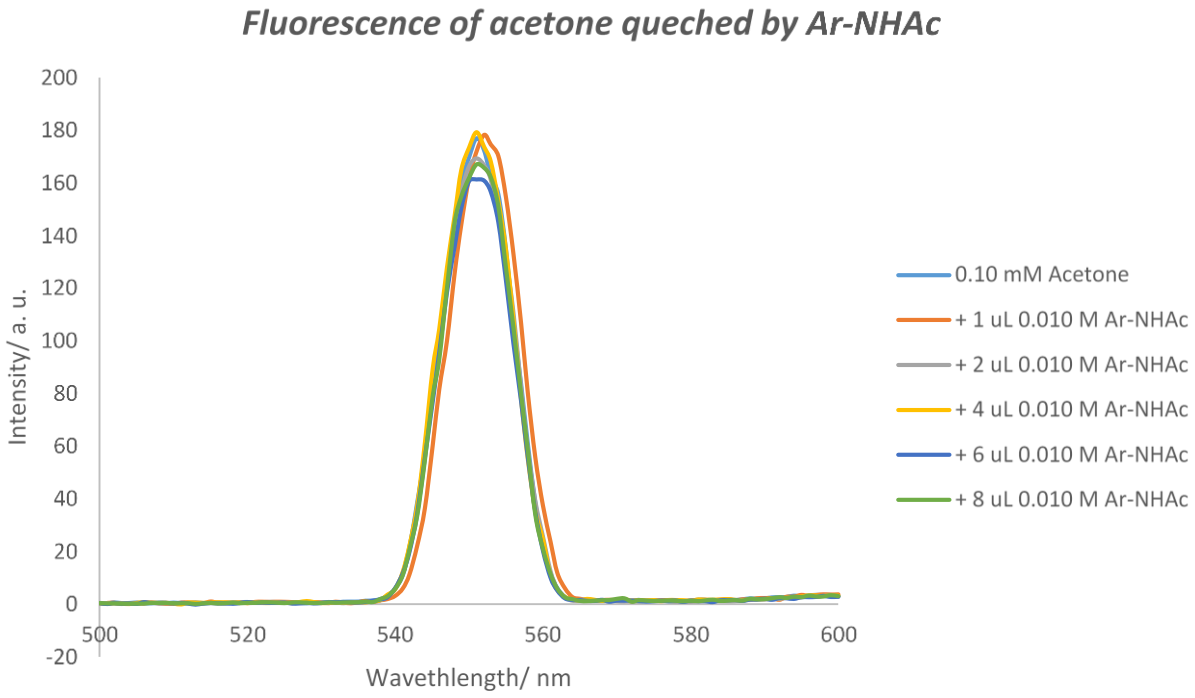
The quenching experiment for the fluorescence of acetone by *p*-tolyl trifluoromethanesulfonate (Ar-OTf was performed on VARIAN CARY Eclipse fluorescence spectrophotometer.

A stock solution of acetone (0.10 M, in HPLC grade CH_3CN) was prepared in a volumetric flask and diluted by HPLC grade CH_3CN to 0.10 mM for the quenching experiment. A quartz cuvette (1 cm × 1 cm × 3 cm) was filled with the abovementioned 0.10 mM acetone solution and its fluorescence was recorded with excitation at 275 nm in the spectrometer. Quenching experiments were performed under duplicate conditions with the injection of 2 μL, 4 μL, 6 μL, 8 μL and 10 μL Ar-OTf respectively by auto-pipette.


Fluorescence of acetone queched by triflate
Intensity/ a. u.
Wavethlength/ nm
0.10 mM Acetone
+ 1 uL Ar-OTf
+ 2 uL Ar-OTf
+ 4 uL Ar-OTf
+ 6 uL Ar-OTf
+ 8 uL Ar-OTf


Fluorescence of acetone queched by Ar-Ar
Intensity/ a. u.
Wavelength/ nm
0.10 mM Acetone
+ 1 uL 0.010 M Ar-Ar
+ 2 uL 0.010 M Ar-Ar
+ 4 uL 0.010 M Ar-Ar
+ 6 uL 0.010 M Ar-Ar
+ 8 uL 0.010 M Ar-Ar


Fluorescence of acetone queched by Ar-OMe
Intensity/ a. u.
Wavelength/ nm
0.10 mM Acetone
+ 1 uL 0.010 M Ar-OMe
+ 2 uL 0.010 M Ar-OMe
+ 4 uL 0.010 M Ar-OMe
+ 6 uL 0.010 M Ar-OMe
+ 8 uL 0.010 M Ar-OMe


Fluorescence of acetone queched by Ar-NHAc
Intensity/ a. u.
Wavethlength/ nm
0.10 mM Acetone
+ 1 uL 0.010 M Ar-NHAc
+ 2 uL 0.010 M Ar-NHAc
+ 4 uL 0.010 M Ar-NHAc
+ 6 uL 0.010 M Ar-NHAc
+ 8 uL 0.010 M Ar-NHAc

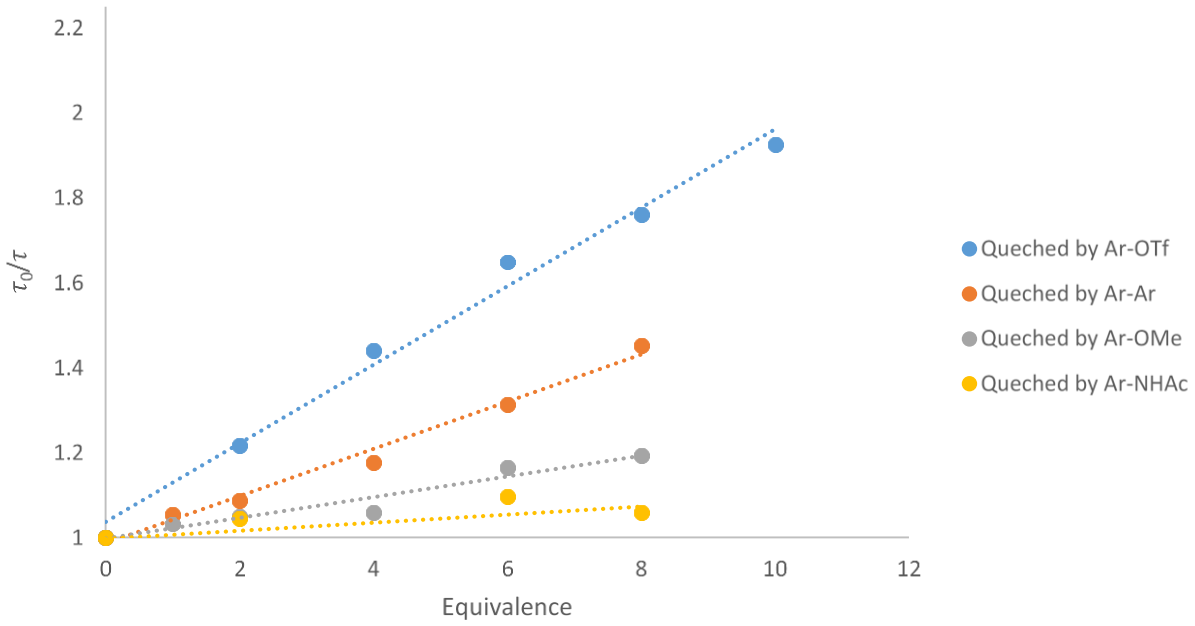


Figure S11. Fluorescence quenching effect of acetone by different aryl compounds.

The quenching experiment for the fluorescence of Ar-OTf by acetone was performed on VARIAN CARY Eclipse fluorescence spectrophotometer and the general procedure is described as below.

A Stock solution of Ar-OTf (0.10 M, in HPLC grade CH_3CN) was prepared in a volumetric flask and diluted by HPLC grade CH_3CN to 0.10 mM for the quenching experiment. A quartz cuvette (1 cm x 1 cm x 3 cm) was filled with the abovementioned 0.10 mM Ar-OTf solution and its fluorescence was recorded with excitation at 260 nm in the spectrometer. Quenching experiments were performed under duplicate conditions with the injection of 1 μL, 2 μL, 4 μL, 6 μL, 8 μL, 10 μL and 12 μL HPLC grade acetone respectively by auto-pippette. The results were stacked in the following figure and the Stern-Volmer relationship was plotted as below.

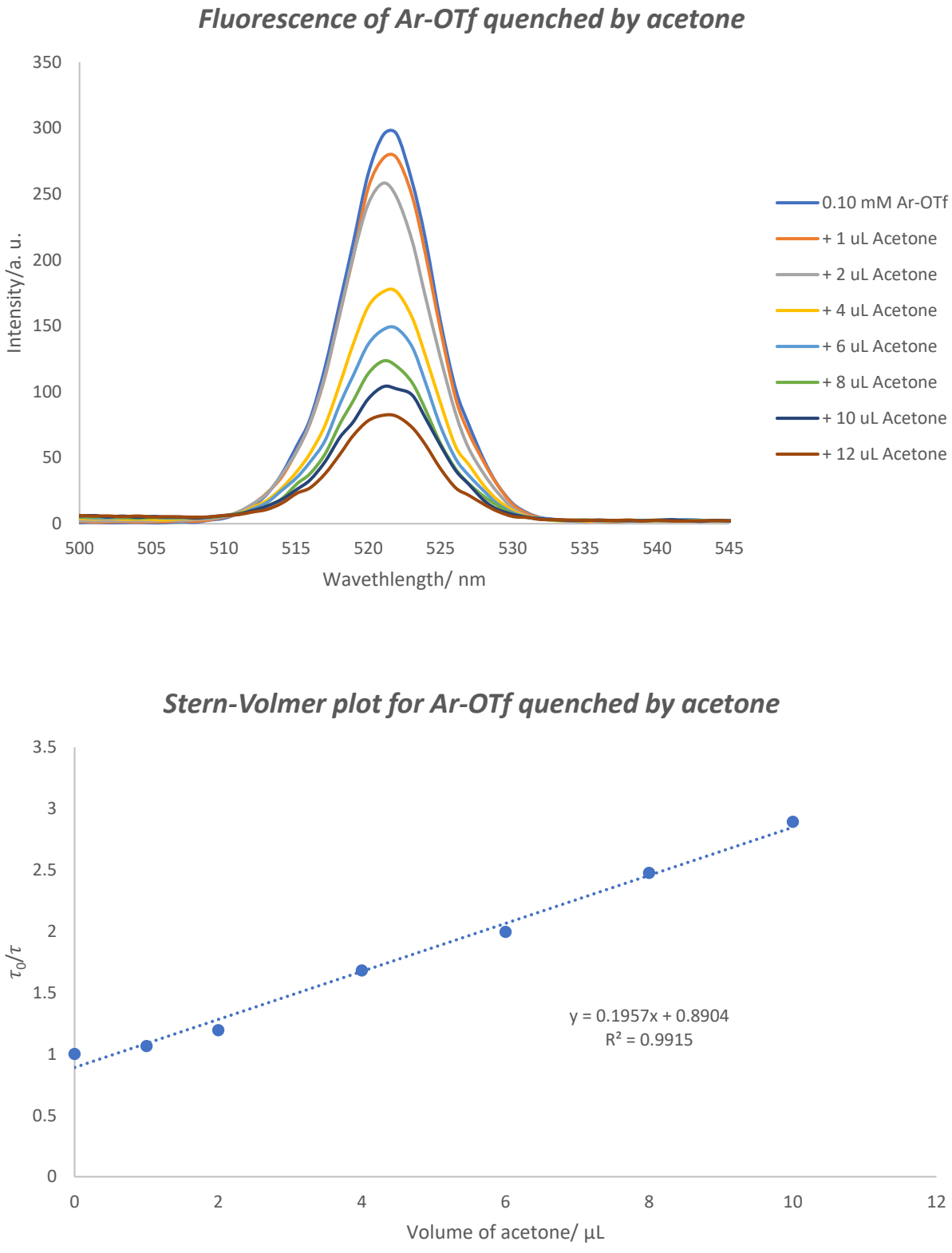
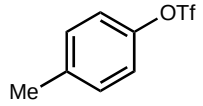
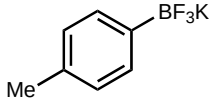
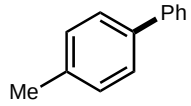
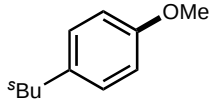
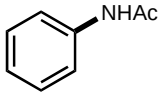
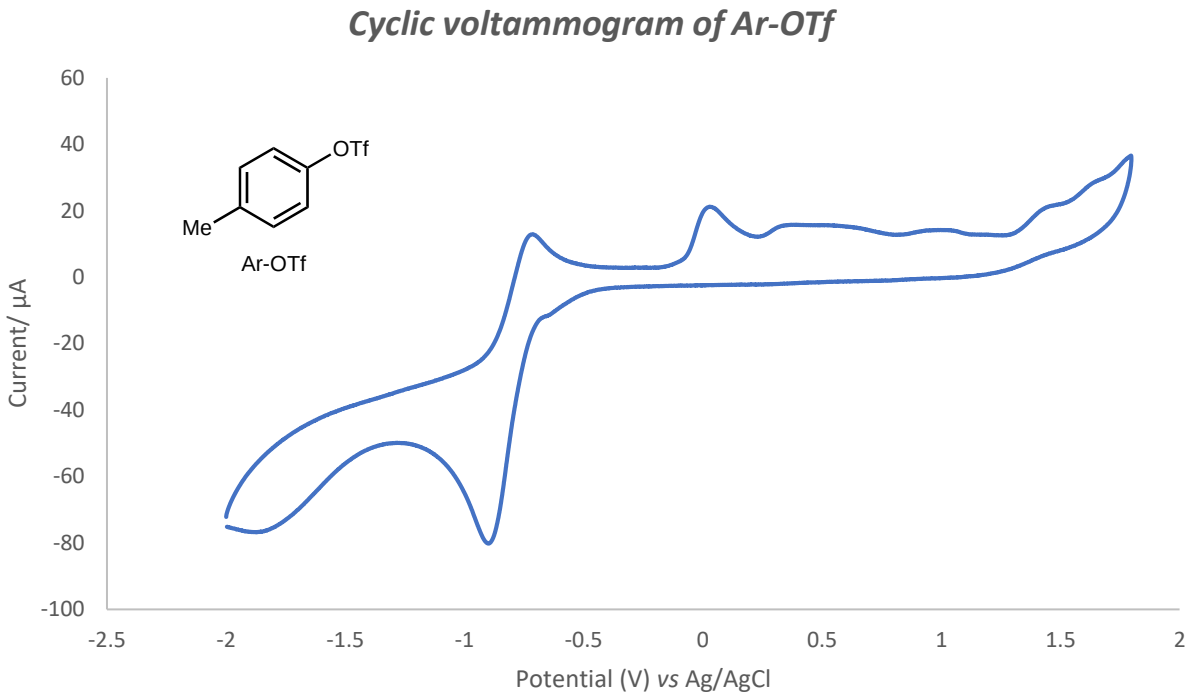


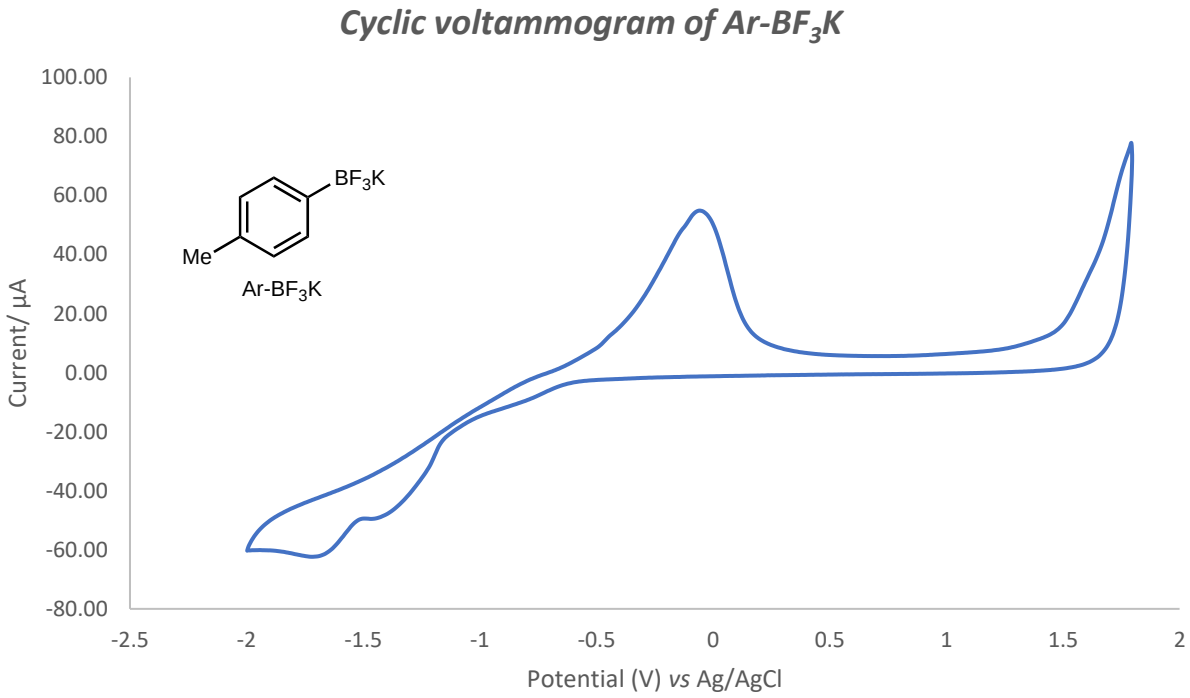
Figure S12. Fluorescence quenching effect of triflate by acetone.

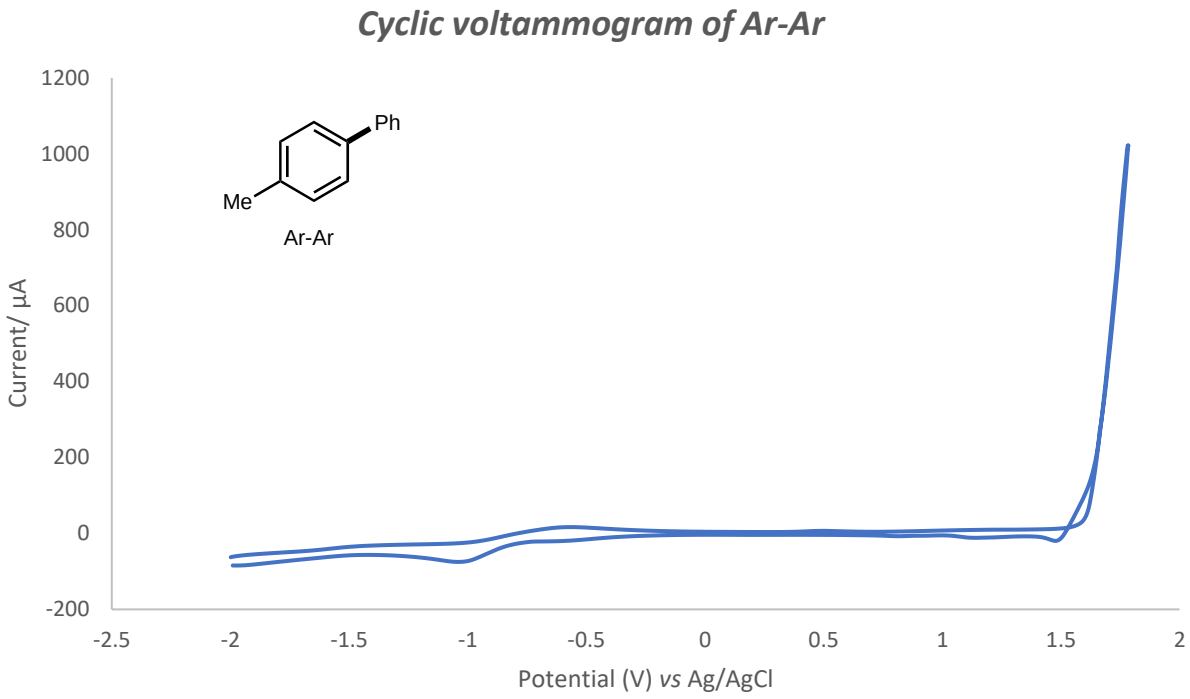
6. Measurement of cyclic voltammetry of some representative reactants

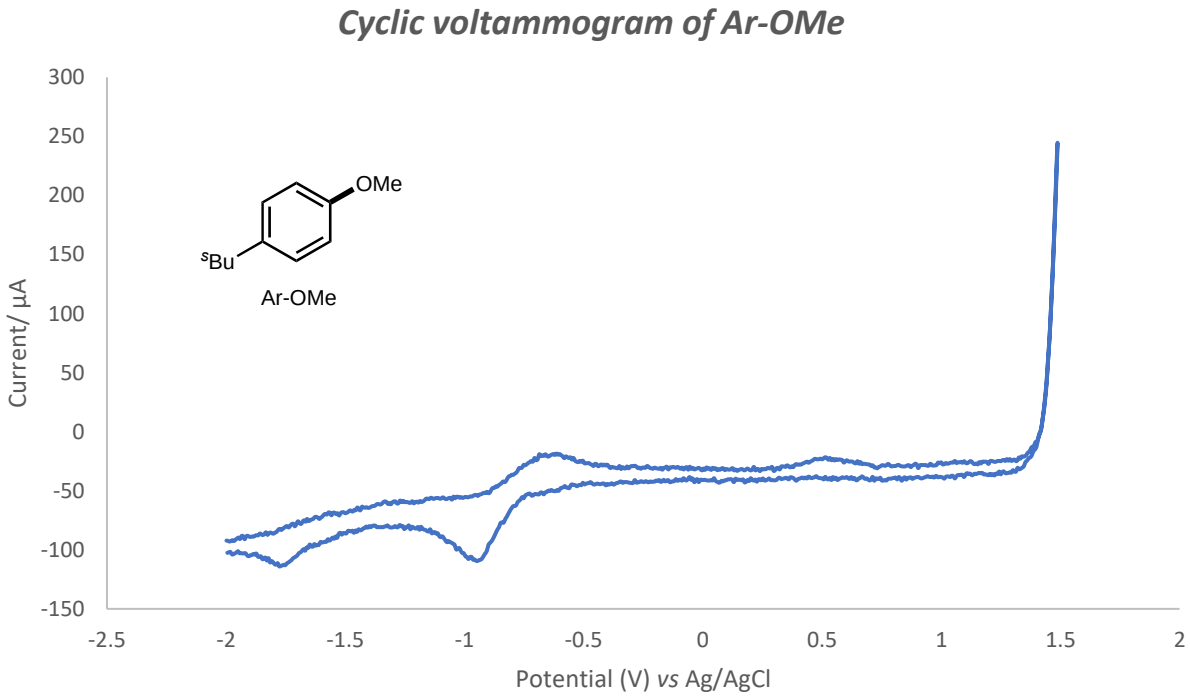
Procedure of cyclic voltammetry experiment for substrates and products in C-C/C-O/C-N cross coupling reactions are described below. The cyclic voltammetry experiments of *p*-tolyl trifluoromethanesulfonate (Ar-OTf), potassium p-tolyltrifluoroborate (PhBF3K), 4-methyl-1,1'-biphenyl (Ar-Ar), 1-(sec-butyl)-4-methoxybenzene (Ar-OMe) N-phenylacetamide (Ar-NHAc) were performed under the conditions in the following table.

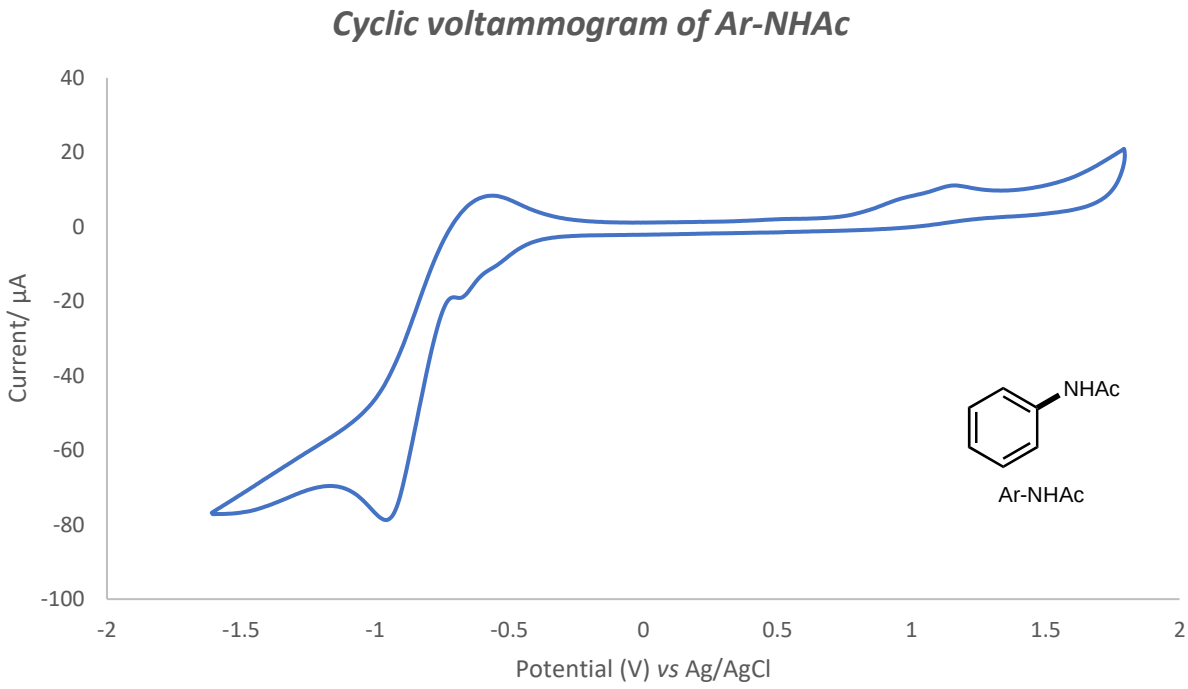
compound	***concentration***	***experimental parameters***
 Ar-OTf	0.10 M	Electrolyte: 0.10 M $^{n}Bu_4NBF_4$ Solvent: HPLC grade CH_3CN Reference electrode: Ag/AgCl Scanning rate: 100 mV/s
 Ar-BF_3K	0.050 M	Electrolyte: 0.050 M $^{n}Bu_4NBF_4$ Solvent: HPLC grade CH_3CN Reference electrode: Ag/AgCl Scanning rate: 100 mV/s
 Ar-Ar	0.10 M	Electrolyte: 0.10 M $^{n}Bu_4NBF_4$ Solvent: HPLC grade CH_3CN Reference electrode: Ag/AgCl Scanning rate: 100 mV/s
 Ar-OMe	0.10 M	Electrolyte: 0.10 M $^{n}Bu_4NBF_4$ Solvent: HPLC grade CH_3CN Reference electrode: Ag/AgCl Scanning rate: 100 mV/s
 Ar-NHAc	0.10 M	Electrolyte: 0.10 M $^{n}Bu_4NBF_4$ Solvent: HPLC grade CH_3CN Reference electrode: Ag/AgCl Scanning rate: 100 mV/s

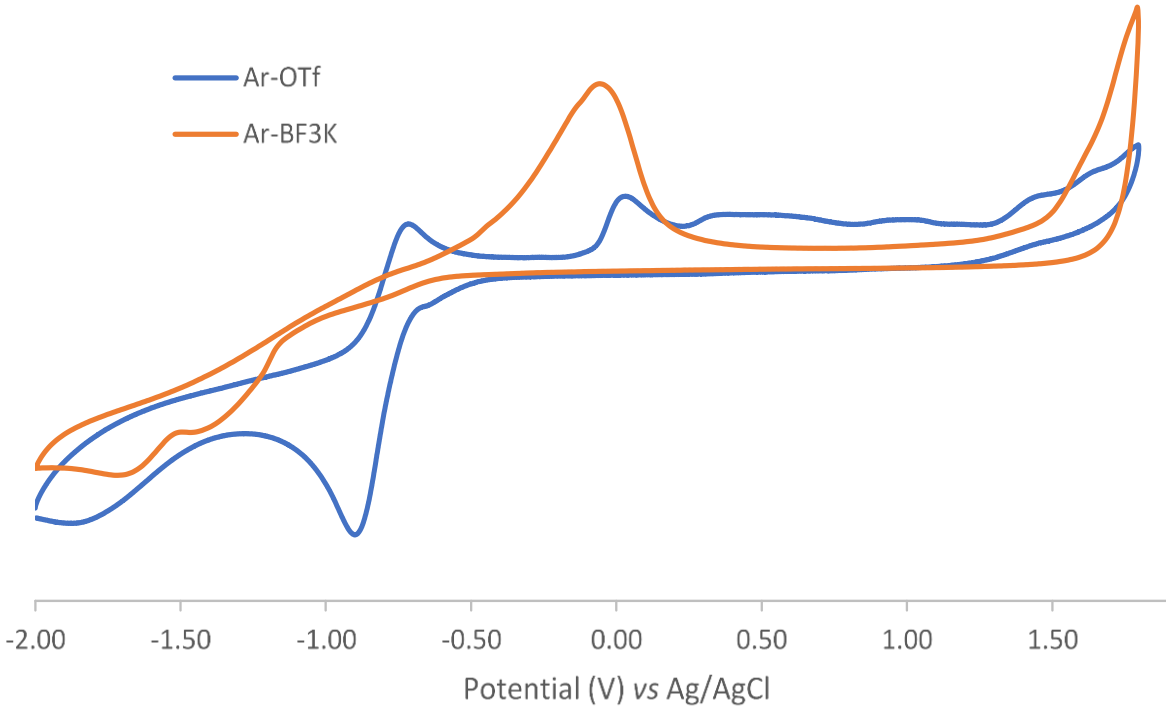

Cyclic voltammogram of Ar-OTf
60
40
20
0
-20
-40
-60
-80
-100
Current/ µA
OTf
Me
Ar-OTf
-2.5
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2
Potential (V) vs Ag/AgCl


Cyclic voltammogram of Ar-BF3K
100.00
80.00
60.00
40.00
20.00
0.00
-20.00
-40.00
-60.00
-80.00
Current/ µA
BF3K
Me
Ar-BF3K
-2.5
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2
Potential (V) vs Ag/AgCl


Cyclic voltammogram of Ar-Ar
1200
1000
800
600
400
200
0
-200
Current/ µA
-2.5
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2
Potential (V) vs Ag/AgCl
Ph
Me
Ar-Ar


Cyclic voltammogram of Ar-OMe
300
250
200
150
100
50
0
-50
-100
-150
Current/ µA
-2.5
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2
Potential (V) vs Ag/AgCl
OMe
sBu
Ar-OMe


Cyclic voltammogram of Ar-NHAc
Current/ µA
40
20
0
-20
-40
-60
-80
-100
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2
Potential (V) vs Ag/AgCl
NHAc
Ar-NHAc


Ar-OTf
Ar-BF3K
-2.00
-1.50
-1.00
-0.50
0.00
0.50
1.00
1.50
Potential (V) vs Ag/AgCl

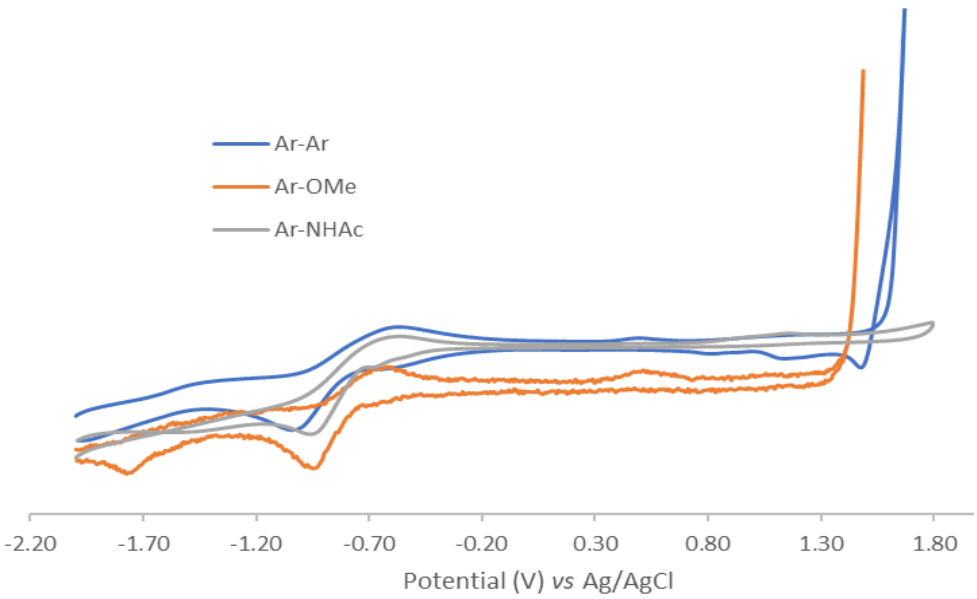
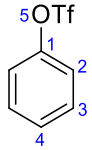


Figure S13: CV of different compounds in this study.

7. Computational studies

The theoretical natural population analysis (NPA) calculationsi were carried out by using Gaussian 09 program.[1] Geometry optimizations were performed using the B3LYP functional with a standard 6-31G(d) basis set.

Summary of NPA analysis of phenyl triflate at ground and radical cation state.

	Atom	Neutral	Cation	Δ
	**C1**	0.261	**0.456**	**0.195**
	C2	-0.236	-0.242	-0.006
	C3	-0.238	-0.197	**0.041**
	C4	-0.212	-0.044	**0.168**
	O5	-0.600	-0.594	**0.006**

Various energy values for all the relevant intermediates and transition states

Neutral form

Zero-point correction= 0.115273 (Hartree/Particle)

Thermal correction to Energy= 0.128000

Thermal correction to Enthalpy= 0.128944

Thermal correction to Gibbs Free Energy= 0.074048

Sum of electronic and zero-point Energies= -1192.554419

Sum of electronic and thermal Energies= -1192.541693

Sum of electronic and thermal Enthalpies= -1192.540749

[1] Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

Sum of electronic and thermal Free Energies= -1192.595645

Cationic form

Zero-point correction= 0.117358 (Hartree/Particle)

Thermal correction to Energy= 0.130480

Thermal correction to Enthalpy= 0.131424

Thermal correction to Gibbs Free Energy= 0.073970

Sum of electronic and zero-point Energies= -1192.651261

Sum of electronic and thermal Energies= -1192.638138

Sum of electronic and thermal Enthalpies= -1192.637194

Sum of electronic and thermal Free Energies= -1192.694648

Cartesian coordinates for all the relevant intermediates and transition states

Neutral form

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-3.65467	0.9387	0.15538
C	-2.88024	-0.21294	-0.03932
C	-1.50382	-0.18429	0.22254
C	-0.90183	0.996	0.67909
C	-1.67626	2.14764	0.87379
C	-3.05268	2.11899	0.61193
H	-4.7056	0.91682	-0.04455
H	-3.33988	-1.11412	-0.38791
H	0.1491	1.01787	0.87902
H	-1.21662	3.04881	1.22238
H	-3.64397	2.99829	0.76059
O	-0.71359	-1.35944	0.02386
S	-0.13197	-1.38108	-1.54144
O	0.69591	-0.18912	-1.77294

O	-1.26013	-1.38439	-2.48322
C	0.85168	-2.84384	-1.78874
F	1.32185	-2.86134	-3.0541
F	1.88803	-2.8408	-0.9236
F	0.09118	-3.93879	-1.57608

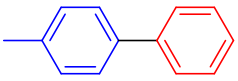
Cationic form

Symbolic Z-matrix:

Charge = 1 Multiplicity = 2

C	-3.65467	0.9387	0.15538
C	-2.88024	-0.21294	-0.03932
C	-1.50382	-0.18429	0.22254
C	-0.90183	0.996	0.67909
C	-1.67626	2.14764	0.87379
C	-3.05268	2.11899	0.61193
H	-4.7056	0.91682	-0.04455
H	-3.33988	-1.11412	-0.38791
H	0.1491	1.01787	0.87902
H	-1.21662	3.04881	1.22238
H	-3.64397	2.99829	0.76059
O	-0.71359	-1.35944	0.02386
S	-0.13197	-1.38108	-1.54144
O	0.69591	-0.18912	-1.77294
O	-1.26013	-1.38439	-2.48322
C	0.85168	-2.84384	-1.78874
F	1.32185	-2.86134	-3.0541
F	1.88803	-2.8408	-0.9236
F	0.09118	-3.93879	-1.57608

8. Characterization data



3a

4-Methylbiphenyl (3a) (CAS: 644-08-6)[1]

White solid (12.5 mg, 75%)

^{1}H-NMR ($CDCl_3$, 500 MHz): 7.63-7.61 (m, 2H), 7.55-7.53 (m, 2H), 7.49-7.45 (m, 2H), 7.37 (tt, J_1 = 1.25 Hz, J_2 = 7.5 Hz, 1H), 7.29 (d, J = 7.5 Hz, 2H), 2.44 (s, 3H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 141.2, 138.4, 137.1, 129.5, 128.7, 127.1, 127.0, 126.9, 21.1.

GCMS: $C_{13}H_{12}$ calculated: 168.1, found: 168.1.

3b

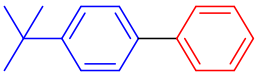
Biphenyl (3b) (CAS: 92-52-4)[2]

White solid (12.6 mg, 82%)

^{1}H-NMR ($CDCl_3$, 500 MHz): 7.67-7.65 (m, 4H), 7.52-7.49 (m, 4H), 7.41 (tt, J_1 = 1.25 Hz, J_2 = 7.40 Hz, 2H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 141.3, 128.8, 127.3, 127.2.

GCMS: $C_{12}H_{10}$ calculated: 154.1, found: 154.1.



3c

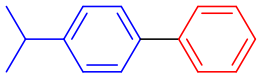
4-(tert-Butyl)-1,1'-biphenyl (3c)[3]

White solid (14.9 mg, 71%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.74-7.71 (m, 2H), 7.69-7.66 (m, 2H), 7.61-7.58 (m, 2H), 7.57-7.53 (m, 2H), 7.46-7.42 (m, 1H), 1.50 (s, 9H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 150.3, 141.2, 138.5, 128.8, 127.2, 127.1, 126.9, 125.8, 34.7, 31.5.

GCMS: $C_{16}H_{18}$ calculated: 210.1, found: 210.1.



3d

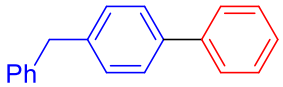
4-Isopropyl-1,1'-biphenyl (3d)[4]

White solid (15.4 mg, 79%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.79-7.76 (m, 2H), 7.74-7.71 (m, 2H), 7.62-7.58 (m, 2H), 7.52-7.48 (m, 3H), 3.14 (septet, *J* = 8.0 Hz, 1H) 1.49 (d, *J* = 8.0 Hz, 6H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 148.1, 141.4, 138.9, 128.9, 127.3, 127.2, 127.1, 127.0, 34.0, 24.2.

GCMS: $C_{15}H_{16}$ calculated: 196.1, found: 196.1.



3e

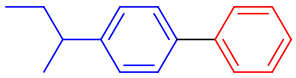
4-Benzyl-1,1'-biphenyl (3e)[5]

White solid (12.3 mg, 51%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.63-7.61 (m, 2H), 7.59-7.54 (m, 2H), 7.46 (t, *J* = 8.0 Hz, 2H), 7.39-7.33 (m, 8H), 4.07 (s, 2H);

^{13}C-NMR ($CDCl_3$, 125 MHz): 141.0, 140.3, 139.1, 129.3, 129.0, 128.7, 128.5, 127.2, 127.1, 127.0, 126.1, 41.6.

GCMS: $C_{19}H_{16}$ calculated: 244.1, found: 244.1.



3f

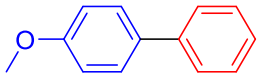
4-(Sec-butyl)-1,1'-biphenyl (3f)[6]

White solid (15.1 mg, 72%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.65-7.61 (m, 2H), 7.59-7.54 (m, 2H), 7.50-7.42 (m, 2H), 7.38-7.32 (m, 1H), 7.29 (d, *J* = 8.0 Hz, 2H), 2.68 (sextet, *J* = 8.0 Hz, 1H), 1.71-1.62 (m, 2H), 1.31 (d, *J* = 8.0 Hz, 3H), 0.90 (t, *J* = 8.0 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 146.9, 141.2, 138.7, 128.8, 128.7, 127.5, 127.2, 127.1, 127.0, 126.9, 41.4, 31.2, 21.8, 12.3.

GCMS: $C_{16}H_{18}$ calculated: 210.1, found: 210.1.



3g

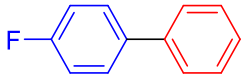
4-Methoxy-1,1'-biphenyl (3g)[7]

White solid (12.3 mg, 70%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.57-7.52 (m, 4H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 1H), 6.99 (d, *J* = 8.7 Hz, 2H), 3.86 (s, 2H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 159.2, 140.8, 133.8, 128.7, 128.2, 126.8, 126.7, 114.2, 55.4.

GCMS: $C_{13}H_{12}O$ calculated: 184.1, found: 184.1.



3h

4-Fluoro-1,1'-biphenyl (3h)[8]

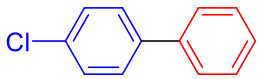
White solid (8.1 mg, 47%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.60-7.54 (m, 4H), 7.46 (t, *J* = 8.0 Hz, 2H), 7.37 (t, *J* = 8.0 Hz, 1H), 7.15 (t, *J* = 8.0 Hz, 2H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 162.4 (d, $J_{C\text{-}F}$ = 244.1 Hz), 140.3, 137.3 (d, $J_{C\text{-}F}$ = 3.0 Hz), 128.8, 128.7 (d, $J_{C\text{-}F}$ = 8.0 Hz), 127.3, 127.0, 115.6 (d, $J_{C\text{-}F}$ = 21.0 Hz).

^{19}F-NMR ($CDCl_3$, 376 MHz): -115.9

GCMS: $C_{12}H_{19}F$ calculated: 172.1, found: 172.1.



3i

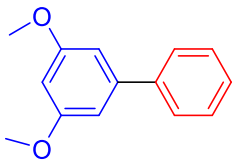
4-Chloro-1,1'-biphenyl (3i)[9]

White solid (9.4 mg, 50%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.60-7.53 (m, 4H), 7.50-7.37 (m, 5H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 140.0, 139.7, 133.4, 128.9, 128.8, 128.4, 127.6, 127.0.

GCMS: $C_{12}H_{19}Cl$ calculated: 188.0, 190.0, found: 188.0, 190.0.



3j

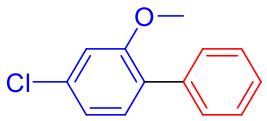
3,5-Dimethoxy-1,1'-biphenyl (3j)[10]

White solid (14.5 mg, 68%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.58 (d, *J* = 7.0 Hz, 2H), 7.44 (t, *J* = 7.0 Hz, 2H), 7.36 (t, *J* = 7.0 Hz, 1H), 6.74 (d, *J* = 2.0 Hz, 2H), 6.48 (t, *J* = 2.0 Hz, 1H), 3.86 (s, 6H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 161.0, 143.5, 141.2, 128.7, 127.8, 127.2, 105.5, 99.3, 55.4.

GCMS: $C_{14}H_{14}O_2$ calculated: 214.1, found: 214.1.



3k

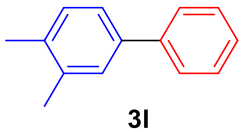
4-Chloro-2-methoxy-1,1'-biphenyl (3k)

White solid (7.3 mg, 34%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.50-7.47 (m, 2H), 7.43-7.38 (m, 2H), 7.36-7.31 (m, 1H), 7.25 (d, *J* = 8.0 Hz, 1H), 7.01 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 6.96 (d, *J* = 4.0 Hz, 1H), 3.81 (s, 3H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 157.0, 137.5, 133.9, 131.5, 129.4, 129.3, 128.1, 127.2, 120.8, 111.9, 55.8.

HRMS (APCI): $C_{13}H_{12}ClO$ $[M+H]^+$ calculated: 219.0577, found: 219.0585.



3l

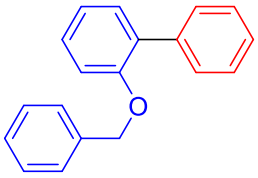
3,4-Dimethylbiphenyl (3l)[11]

White solid (14.0 mg, 77%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.59-7.56 (m, 2H), 7.43-7.29 (m, 5H), 7.20 (d, *J* = 8.0 Hz, 1H), 2.33 (s, 3H), 2.30 (s, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 141.3, 138.9, 136.9, 135.7, 130.1, 128.7, 128.4, 127.0, 126.9, 124.5, 19.9, 19.4.

GCMS: $C_{14}H_{14}$ calculated: 182.1, found: 182.1.



3m

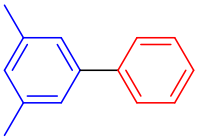
2-(Benzyloxy)-1,1'-biphenyl (3m)[12]

White solid (10.4 mg, 40%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.62 (d, *J* = 8.0 Hz, 2H), 7.46-7.29 (m, 10H), 7.11-7.05 (m, 2H), 5.12 (s, 2H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 155.6, 138.5, 137.3, 131.4, 131.0, 129.7, 128.6, 128.4, 127.9, 127.6, 126.9, 126.8, 121.4, 113.4, 70.5.

GCMS: $C_{19}H_{16}O$ calculated: 260.1, found: 260.1.



3n

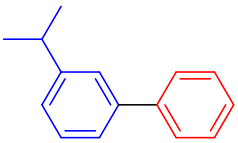
3,5-dimethylbiphenyl (3n)[13]

White solid (14.6 mg, 81%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.68 (d, *J* = 8.0 Hz, 2H), 7.51 (t, *J* = 8.0 Hz, 2H), 7.42 (t, *J* = 8.0 Hz, 1H), 7.32 (s, 2H), 7.10 (s, 1H), 2.48 (s, 6H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 141.6, 141.4, 138.3, 129.0, 128.7, 127.3, 127.2, 125.2, 21.5.

GCMS: $C_{14}H_{14}$ calculated: 182.1, found: 182.1.



3o

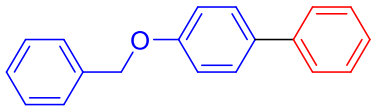
3-Isopropyl-biphenyl (3o)[14]

White solid (9.8 mg, 50%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.61 (d, *J* = 8.0 Hz, 2H), 7.48-7.32 (m, 6H), 7.23 (d, *J* = 8.0 Hz, 1H), 2.99 (septet, *J* = 8.0 Hz, 1H), 1.31 (d, *J* = 8.0 Hz, 6H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 149.4, 141.6, 141.3, 128.7, 128.6, 127.3, 127.1, 125.5, 125.4, 124.7, 34.3, 24.1.

GCMS: $C_{15}H_{16}$ calculated: 196.1, found: 196.1.



3p

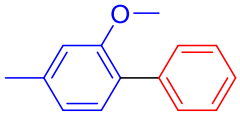
4-(benzyloxy)-1,1'-biphenyl (3p)[15]

White solid (10.9 mg, 42%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.60-7.55 (m, 4H), 7.52-7.40 (m, 6H), 7.38-7.30 (m, 2H), 7.08 (dt, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 2H), 5.15 (s, 2H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 158.4, 140.8, 137.0, 134.0, 128.7, 128.6, 128.2, 128.0, 127.5, 126.7, 126.6, 115.2, 70.1.

GCMS: $C_{19}H_{16}O$ calculated: 260.1, found: 260.1.



3q

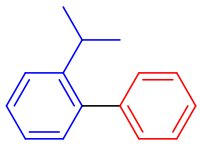
2-methoxy-4-methyl-1,1'-biphenyl (3q) [16]

Colorless oil (9.9 mg, 50%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.52 (d, *J* = 8.0 Hz, 2H), 7.40 (t, *J* = 8.0 Hz, 2H), 7.30 (t, *J* = 8.0 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 1H), 6.86 (d, *J* = 8.0 Hz, 1H), 6.81 (s, 1H), 3.80 (s, 3H), 2.41 (s, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 156.3, 138.7, 138.6, 130.7, 129.5, 127.9, 127.8, 126.7, 121.5, 112.2, 55.5, 21.6.

GCMS: $C_{14}H_{14}O$ calculated: 198.1, found: 198.1.



3r

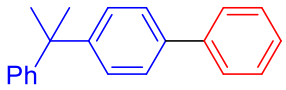
2-Isopropyl-biphenyl (3r)[17]

Colorless oil (8.8 mg, 45%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.43-7.28 (m, 7H), 7.24-7.17 (m, 2H), 3.06 (sept, *J* = 7.0 Hz, 1H), 1.16 (d, *J* = 7.0 Hz, 6H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 146.4, 142.1, 141.1, 129.9, 129.3, 128.0, 127.7, 126.7, 125.5, 125.3, 29.4, 24.3.

GCMS: $C_{15}H_{16}$ calculated: 196.1, found: 196.1.



3s

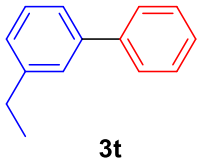
4-(2-phenylpropan-2-yl)-1,1'-biphenyl (3s)

Colorless oil (15.0 mg, 55%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.58 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 2H), 7.42 (t, *J* = 8.0 Hz, 2H), 7.34-7.26 (m, 7H), 7.22-7.18 (m, 1H), 1.73 (s, 6H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 150.5, 149.8, 140.9, 138.4, 128.7, 128.1, 127.2, 127.1, 127.0, 126.8, 126.7, 125.7, 42.8, 30.8.

GCMS (EI): $C_{21}H_{20}$ calculated: 272.1565, found: 272.1560.



3t

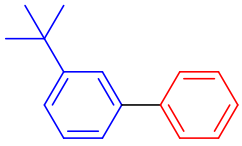
3-ethyl-biphenyl (3t) [18]

White solid (11.6 mg, 64%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.61 (d, *J* = 8.0 Hz, 2H), 7.48-7.42 (m, 4H), 7.39-7.33 (m, 2H), 7.21 (d, *J* = 8.0 Hz, 1H), 2.74 (q, *J* = 8.0 Hz, 2H), 1.31 (t, *J* = 8.0 Hz, 2H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 144.7, 141.5, 141.3, 128.8, 128.74, 128.70, 127.2, 127.1, 126.8, 124.6, 29.0, 15.7.

GCMS: $C_{14}H_{14}$ calculated: 182.1, found: 182.1.



3u

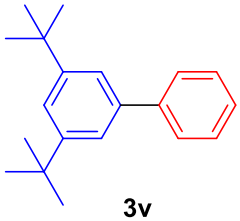
3-*t*-Butyl-biphenyl (3u) [19]

White solid (6.7 mg, 32%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.65 (d, *J* = 8.0 Hz, 3H), 7.51-7.37 (m, 6H), 1.43 (s, 9H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 151.6, 141.9, 141.1, 128.7, 128.5, 127.4, 127.2, 124.5, 124.4, 124.3, 34.9, 31.5.

GCMS: $C_{16}H_{18}$ calculated: 210.1, found: 210.1.



3v

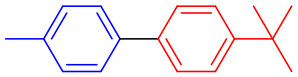
3,5-Di-tert-butyl-1,1'-biphenyl (3v)[20]

White solid (9.0 mg, 34%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.66 (d, *J* = 8.0 Hz, 2H), 7.52-7.47 (m, 5H), 7.40 (t, *J* = 8.0 Hz, 1H), 1.45 (s, 18H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 151.1, 142.6, 140.7, 128.7, 127.5, 127.0, 121.8, 121.4, 35.0, 31.6.

GCMS: $C_{20}H_{26}$ calculated: 266.2, found: 266.2.

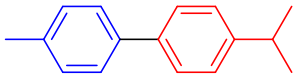


3w

4-(tert-butyl)-4'-methyl-1,1'-biphenyl (3w)[21]

White solid (19.1 mg, 85%) From GCMS, the mixture comprises three isomers.

GCMS: $C_{17}H_{20}$ calculated: 224.2, found: 224.2.

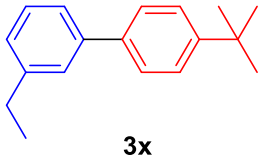


3ab

4-isopropyl-4'-methyl-1,1'-biphenyl (3ab) [22]

White solid (16.8 mg, 80%) From GCMS, the mixture comprises three isomers.

GCMS: $C_{16}H_{18}$ calculated: 210.1, found: 210.1.

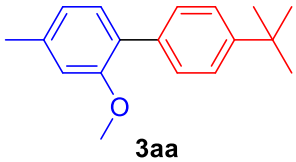


3x

4'-(tert-butyl)-3-ethyl-1,1'-biphenyl (3x)

Colorless oil (14.2 mg, 60%) From GCMS, the mixture comprises three isomers.

GCMS (EI): $C_{18}H_{22}$ calculated: 238.1722, found: 238.1730.

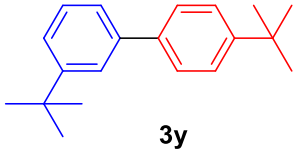


3aa

4'-(tert-butyl)-2-methoxy-4-methyl-1,1'-biphenyl (3aa)

White solid (13.2 mg, 52%) From GCMS, the mixture comprises three isomers.

GCMS (EI): $C_{18}H_{22}O$ calculated: 254.1671, found: 254.1670.

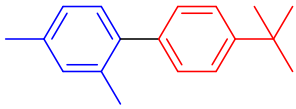


3y

3,4'-di-tert-butyl-1,1'-biphenyl (3y)

Colorless oil (13.0 mg, 50%) From GCMS, the mixture comprises three isomers.

GCMS (EI): $C_{20}H_{26}$ calculated: 266.2035, found: 266.2041.

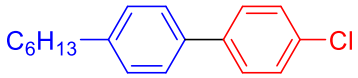


3z

4'-(tert-butyl)-2,4-dimethyl-1,1'-biphenyl (3z)

White solid (10.4 mg, 44%) From GCMS, the mixture comprises three isomers.

GCMS: $C_{18}H_{22}$ calculated: 238.1722, found: 238.1710.

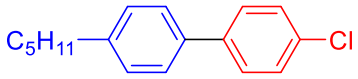


3ac

4-chloro-4'-hexyl-1,1'-biphenyl (3ac)

White solid (10.4 mg, 40%) From GCMS, the mixture comprises three isomers.

GCMS (EI): $C_{18}H_{21}Cl$ calculated: 272.1332, found 272.1340.

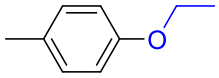


3ad

4-chloro-4'-pentyl-1,1'-biphenyl (3ad)

White solid (13.7 mg, 53%) From GCMS, the mixture comprises three isomers.

GCMS (EI): $C_{17}H_{19}Cl$ calculated: 258.1175, found: 258.1173.



5a

1-ethoxy-4-methylbenzene (5a)[23]

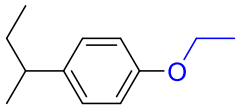
Colorless oil (6.8 mg, 50%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.15 (d, *J* = 8.0 Hz, 2H), 6.87 (d, *J* = 8.0 Hz, 2H), 4.07 (q, *J* = 7.2 Hz, 2H), 2.36 (s, 3H), 1.47 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 156.8, 129.9, 129.7, 114.4, 63.5, 20.5, 14.9.

GCMS: $C_9H_{12}O$ calculated: 136.1, found: 136.1.

Gram scale procedure: *para*-Methyl phenyl triflate (10 mmol, 1 equiv), ethanol (50 mL), trifluoroacetic acid (25 mmol, 2.0 mL, 2.5 equiv) and $B(OMe)_3$ (20 mmol, 2.2 mL, 2 equiv) were added into 10 mL acetone. The quartz round-bottom flask (100 mL) containing these reactants and solvents with a teflon-coated stir bar was evacuated by three frozen-pump-thaw cycles and back-filled with argon prior to use. The reaction was stirred at 15 ºC (cooled by flowing water) under photo irradiation by using a 300 watts xenon lamp with a 280 nm long pass optical filter. After 72 hours, the resulting crude mixture was purified by flash column chromatography on silica gel to provide the desired product as a colorless oil (1.0 g, 5.5 mmol, 55%).



5b

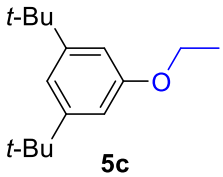
1-(sec-butyl)-4-ethoxybenzene (5b)

Colorless oil (12.5 mg, 70%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.12 (d, *J* = 8.0 Hz, 2H), 6.86 (d, *J* = 8.0 Hz, 2H), 4.04 (q, *J* = 7.2 Hz, 2H), 2.57 (sextet, *J* = 7.2 Hz, 1H), 1.60 (quintet, *J* = 7.2 Hz, 2H), 1.43 (t, *J* = 7.2 Hz, 3H), 1.25 (d, *J* = 7.2 Hz, 3H), 0.85 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 157.1, 139.7, 127.9, 114.2, 63.4, 40.8, 31.4, 22.1, 14.9, 12.3.

GCMS (EI): $C_{12}H_{18}O$ calculated: 178.1358, found: 178.1357.



5c

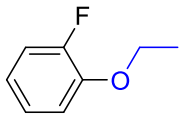
1,3-di-tert-butyl-5-ethoxybenzene (5c)

Colorless oil (19.2 mg, 82%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.08 (t, *J* = 1.6 Hz, 1H), 6.83 (d, *J* = 1.6 Hz, 2H), 4.11 (q, *J* = 7.2 Hz, 2H), 1.49 (t, *J* = 7.2 Hz, 3H), 1.38 (s, 18H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 158.5, 152.1, 114.9, 108.9, 63.2, 35.0, 31.5, 15.0.

GCMS (EI): $C_{16}H_{26}O$ calculated: 234.1984, found: 234.1981.



5d

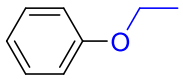
1-ethoxy-2-fluorobenzene (5d)[24]

Colorless oil (5.9 mg, 42%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.09-7.02 (m, 2H), 6.98-6.94 (m, 1H), 6.90-6.85 (m, 1H), 4.11 (q, *J* = 7.2 Hz, 2H), 1.45 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 152.8 (d, *J* = 244.0 Hz), 146.9 (d, *J* = 10.0 Hz), 124.2 (d, *J* = 3.0 Hz), 120.9 (d, *J* = 21.0 Hz), 116.1 (d, *J* = 18.0 Hz), 114.8 (d, *J* = 2.0 Hz), 64.9, 14.8.

GCMS: C_8H_9OF calculated: 140.0, found: 140.0.



5e

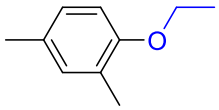
Ethoxybenzene (5e) [25]

Colorless oil (6.5 mg, 54%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.30 (t, *J* = 8.0 Hz, 2H), 6.96 (d, *J* = 8.0 Hz, 1H), 6.92 (d, *J* = 8.0 Hz, 2H), 4.05 (q, *J* = 7.2 Hz, 2H), 1.43 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 158.9, 129.4, 120.5, 114.5, 63.3, 14.9.

GCMS: $C_8H_{10}O$ calculated: 122.1, found: 122.1.



5f

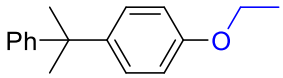
1-ethoxy-2,4-dimethylbenzene (5f)[26]

Colorless oil (6.0 mg, 40%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 6.99 (s, 1H), 6.97 (d, *J* = 8.0 Hz, 1H), 6.75 (d, *J* = 8.0 Hz, 1H), 4.04 (q, *J* = 7.2 Hz, 2H), 2.30 (s, 3H), 2.25 (s, 3H), 1.45 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 155.1, 131.5, 129.3, 126.9, 126.7, 111.3, 63.7, 20.5, 16.2, 15.1.

GCMS: $C_{10}H_{14}O$ calculated: 150.1, found: 150.1.



5g

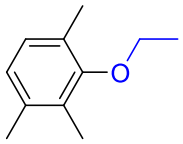
1-ethoxy-4-(2-phenylpropan-2-yl)benzene (5g)[27]

Colorless oil (14.5 mg, 60%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.33-7.29 (m, 4H), 7.23-7.18 (m, 3H), 6.85 (d, *J* = 8.0 Hz, 2H), 4.05 (q, *J* = 7.2 Hz, 2H), 1.71 (s, 6H), 1.45 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 156.8, 151.0, 142.8, 128.0, 127.8, 126.8, 125.6, 113.9, 63.4, 42.4, 31.0, 15.0.

GCMS: $C_{17}H_{20}O$ calculated: 240.1, found: 240.1.



5h

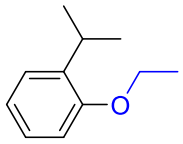
2-ethoxy-1,3,4-trimethylbenzene (5h)

Colorless oil (4.2 mg, 25%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 6.96 (d, *J* = 7.6 Hz, 1H), 6.87 (d, *J* = 7.6 Hz, 1H), 3.85 (q, *J* = 7.2 Hz, 2H), 2.31 (s, 3H), 2.28 (s, 3H), 2.24 (s, 3H), 1.45 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 155.9, 135.7, 129.6, 128.2, 127.8, 125.1, 68.0, 19.9, 16.3, 15.8, 12.5.

GCMS (EI): $C_{11}H_{16}O$ calculated: 164.1201, found: 164.1211.



5i

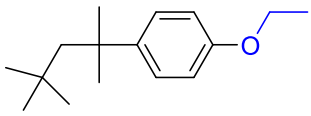
1-ethoxy-2-isopropylbenzene (5i)

Colorless oil (8.2 mg, 50%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.25 (d, *J* = 7.6 Hz, 1H), 7.18 (t, *J* = 7.6 Hz, 1H), 6.95 (t, *J* = 7.6 Hz, 1H), 6.87 (d, *J* = 7.6 Hz, 1H), 4.07 (q, *J* = 7.2 Hz, 2H), 3.39 (heptet, *J* = 7.2 Hz, 1H), 1.46 (t, *J* = 7.2 Hz, 3H), 1.27 (d, *J* = 7.2 Hz, 6H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 156.2, 137.2, 126.5, 126.1, 120.5, 111.4, 63.6, 26.9, 22.7, 15.0.

GCMS (EI): $C_{11}H_{16}O$ calculated: 164.1201, found: 164.1203.



5j

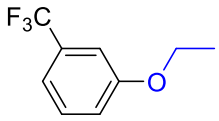
1-ethoxy-4-(2,4,4-trimethylpentan-2-yl)benzene (5j)

Colorless oil (17.1 mg, 73%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.28 (d, *J* = 7.6 Hz, 2H), 6.83 (d, *J* = 7.6 Hz, 2H), 4.02 (q, *J* = 7.2 Hz, 2H), 1.72 (s, 2H), 1.42 (t, *J* = 7.2 Hz, 3H), 1.36 (s, 6H), 0.73 (s, 9H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 156.6, 142.0, 127.0, 113.6, 63.3, 57.1, 37.9, 32.3, 31.8, 31.7, 14.9.

GCMS (EI): $C_{16}H_{26}O$ calculated: 234.1984, found: 234.1990.



5k

1-ethoxy-3-(trifluoromethyl)benzene (5k)

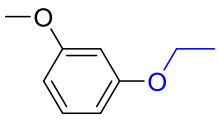
Colorless oil (6.6 mg, 35%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.37 (t, *J* = 7.6 Hz, 1H), 7.19 (d, *J* = 7.6 Hz, 1H), 7.12 (s, 1H), 7.06 (d, *J* = 8.0 Hz, 1H), 4.06 (q, *J* = 7.2 Hz, 2H), 1.42 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 159.1, 131.8 (q, *J* = 32 Hz), 129.9, 124.0 (q, *J* = 271 Hz), 117.9, 117.1 (q, *J* = 4 Hz), 111.2 (q, *J* = 4 Hz), 63.8, 14.7.

^{19}F-NMR ($CDCl_3$, 376 MHz): -62.8.

GCMS (EI): $C_9H_9F_3O$ calculated: 190.0605, found: 190.0609.



5l

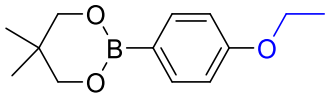
1-ethoxy-3-methoxybenzene (5l)[28]

Colorless oil (4.6 mg, 30%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.18 (t, *J* = 7.6 Hz, 1H), 6.52-6.47 (m, 3H), 4.02 (q, *J* = 7.2 Hz, 2H), 3.79 (s, 3H), 1.42 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 160.9, 160.2, 129.8, 106.7, 106.2, 100.9, 63.4, 55.2, 14.8.

GCMS: $C_9H_{12}O_2$ calculated: 152.1, found: 152.1.



5m

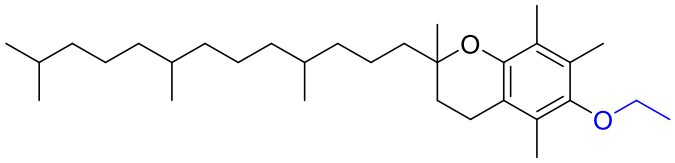
2-(4-Ethoxyphenyl)-5,5-dimethyl-1,3,2-dioxaborinane (5m)

White solid (12.6 mg, 54%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.75 (d, *J* = 7.6 Hz, 2H), 6.89 (d, *J* = 7.6 Hz, 2H), 4.06 (q, *J* = 7.2 Hz, 2H), 3.76 (s, 4H), 1.42 (t, *J* = 7.2 Hz, 3H), 1.02 (s, 6H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 161.2, 135.5, 113.7, 72.3, 63.2, 31.9, 21.9, 14.8.

HRMS (APCI): $C_{13}H_{20}BO_3$ $[M+H]^+$, calculated: 235.1506, found: 235.1510.



5o

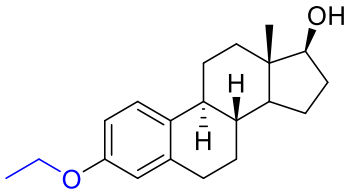
6-Ethoxy-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)chromane (5o)

Colorless oil (16.5 mg, 36%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 3.76 (q, *J* = 7.2 Hz, 2H), 2.62 (t, *J* = 7.2 Hz, 2H), 2.22 (s, 3H), 2.17 (s, 3H), 2.13 (s, 3H), 1.89-1.76 (m, 2H), 1.65-1.55 (m, 3H), 1.44 (t, *J* = 7.2 Hz, 6H), 1.38-1.25 (m, 11H), 1.24-1.05 (m, 7H), 0.95-0.85 (m, 13H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 148.5, 147.6, 127.9, 125.8, 122.7, 117.4, 74.7, 68.5, 40.1, 39.4, 37.6, 37.5, 37.3, 32.8, 32.7, 31.3, 28.0, 24.8, 24.5, 23.9, 22.7, 22.6, 21.0, 20.7, 19.8, 19.7, 19.6, 15.7, 12.8, 11.9, 11.8.

HRMS (APCI): $C_{31}H_{55}O_2$ $[M+H]^+$, calculated: 459.4202, found: 459.4210.



5n

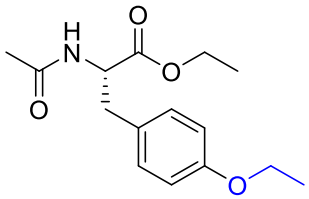
(8R,9S,13S,17S)-3-ethoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-ol (5n)

White solid (15.3 mg, 51%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.22 (d, *J* = 7.6 Hz, 1H), 6.73 (dd, J_1 = 7.6 Hz, J_2 = 2.8 Hz, 1H), 6.65 (d, *J* = 2.8 Hz, 1H), 4.03 (q, *J* = 7.2 Hz, 2H), 3.76 (t, *J* = 7.2 Hz, 2H), 2.90-2.85 (m, 2H), 2.38-2.30 (m, 1H), 2.25-2.10 (m, 2H), 2.01-1.94 (m, 1H), 1.93-1.86 (m, 1H), 1.77-1.68 (m, 1H), 1.58-1.17 (m, 11H), 0.81 (s, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 156.8, 137.9, 132.5, 126.3, 114.5, 112.1, 81.9, 63.3, 50.1, 43.9, 43.3, 38.9, 36.7, 30.6, 29.8, 27.3, 26.3, 23.2, 14.9, 11.1

HRMS (ESI): $C_{20}H_{29}O_2$ $[M+H]^+$, calculated: 301.2160, found: 301.2162.



5p

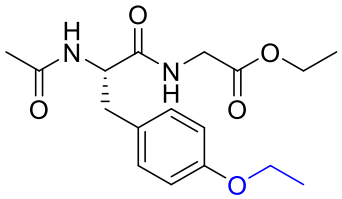
Ethyl (S)-2-acetamido-3-(4-ethoxyphenyl)propanoate (5p)

White solid (16.1 mg, 58%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.00 (d, *J* = 7.6 Hz, 2H), 6.80 (d, *J* = 7.6 Hz, 2H), 6.14 (d, *J* = 7.6 Hz, 1H), 4.80 (d, *J* = 7.2 Hz, 1H), 4.15 (q, *J* = 7.2 Hz, 2H), 3.98 (q, *J* = 7.2 Hz, 2H), 3.03 (t, *J* = 7.2 Hz, 2H), 1.97 (s, 3H), 1.38 (t, *J* = 7.2 Hz, 3H), 1.24 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 171.8, 169.6, 158.0, 130.2, 127.7, 114.5, 63.3, 61.4, 53.3, 37.0, 23.1, 14.8, 14.1.

HRMS (ESI): $C_{15}H_{22}NO_4$ $[M+H]^+$, calculated: 280.1549, found: 280.1553.



5q

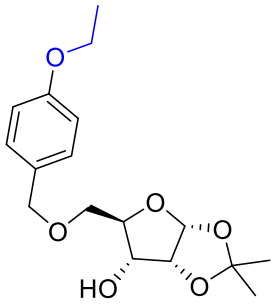
Ethyl (S)-(2-acetamido-3-(4-ethoxyphenyl)propanoyl)glycinate (5q)

White solid (15.1 mg, 45%)

^{1}H-NMR (*d_4*-MeOH, 400 MHz): 7.16 (d, *J* = 7.6 Hz, 2H), 6.83 (d, *J* = 7.6 Hz, 2H), 4.62 (dd, J_1 = 7.2 Hz, J_2 = 10.0 Hz, 1H), 4.19 (q, *J* = 7.2 Hz, 2H), 4.01 (q, *J* = 7.2 Hz, 2H), 3.92 (s, 2H), 3.12 (dd, J_1 = 7.2 Hz, J_2 = 10.0 Hz, 1H), 2.81 (dd, J_1 = 10.0 Hz, J_2 = 14.0 Hz, 1H) 1.92 (s, 3H), 1.38 (t, *J* = 7.2 Hz, 3H), 1.28 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR (*d_4*-MeOH, 100 MHz): 172.9, 171.7, 169.6, 157.9, 129.8, 128.9, 114.0, 63.0, 60.9, 54.7, 40.7, 36.7, 21.0, 13.8, 13.1.

HRMS (ESI): $C_{17}H_{24}N_2O_5Na$ $[M+Na]^+$, calculated: 359.1583, found: 359.1580.



5r

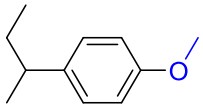
(3aR,5R,6R,6aR)-5-(((4-ethoxybenzyl)oxy)methyl)-2,2-dimethyltetrahydrofuro[2,3-d][1,3]dioxol-6-ol (5r)

White solid (17.8 mg, 55%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.24 (d, *J* = 7.6 Hz, 2H), 6.89 (d, *J* = 7.6 Hz, 2H), 5.99 (d, *J* = 3.5 Hz, 1H), 4.67-4.63 (m, 2H), 4.41 (d, *J* = 15.0 Hz, 1H), 4.27 (q, *J* = 7.2 Hz, 1H), 4.04 (q, *J* = 7.2 Hz, 2H), 4.01 (d, *J* = 3.5 Hz, 1H), 3.92 (dd, J_1 = 5.0 Hz, J_2 = 12.0 Hz, 1H), 3.86-3.83 (m, 1H), 2.18 (br, 1H), 1.49 (s, 3H), 1.42 (t, *J* = 7.2 Hz, 3H), 1.34 (s, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 159.0, 129.4, 128.9, 114.7, 111.8, 105.1, 82.6, 82.4, 79.9, 71.7, 63.5, 61.0, 26.8, 26.3, 14.8.

HRMS (ESI): $C_{17}H_{24}O_6Na$ $[M+Na]^+$, calculated: 347.1465, found: 347.1470.



5s

1-(Sec-butyl)-4-methoxybenzene (5s) [29]

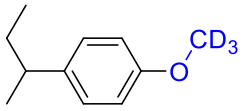
Colorless oil (10.5 mg, 64%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.14 (d, *J* = 7.6 Hz, 2H), 6.88 (d, *J* = 7.6 Hz, 2H), 3.82 (s, 3H), 2.59 (sextet, *J* = 7.2 Hz, 1H), 1.61 (quintet, *J* = 7.2 Hz, 2H), 1.26 (d, *J* = 7.2 Hz, 3H), 0.86 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 157.2, 139.8, 127.9, 113.6, 55.2, 40.9, 31.4, 22.1, 12.3.

GCMS: $C_{11}H_{16}O$, calculated: 164.1, found: 164.1.

Gram scale procedure: *para*-sec-butyl phenyl triflate (10 mmol, 1 equiv), methanol (50 mL), trifluoroacetic acid (25 mmol, 2.0 mL, 2.5 equiv) and $B(OMe)_3$ (20 mmol, 2.2 mL, 2 equiv) were added into 10 mL acetone. The quartz round-bottom flask (100 mL) containing these reactants and solvents with a teflon-coated stir bar was evacuated by three frozen-pump-thaw cycles and back-filled with argon prior to use. The reaction was stirred at 15 ºC (cooled by flowing water) under photo irradiation by using a 300 watts xenon lamp with a 280 nm long pass optical filter. After 72 hours, the resulting crude mixture was purified by flash column chromatography on silica gel to provide the desired product as a colorless oil (0.98 g, 6.0 mmol, 60%).



5t

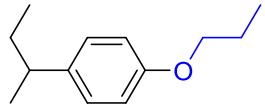
1-(Sec-butyl)-4-(methoxy-d3)benzene (5t)

Colorless oil (10.0 mg, 60%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.11 (d, *J* = 7.6 Hz, 2H), 6.84 (d, *J* = 7.6 Hz, 2H), 2.55 (sextet, *J* = 7.2 Hz, 1H), 1.57 (quintet, *J* = 7.2 Hz, 2H), 1.22 (d, *J* = 7.2 Hz, 3H), 0.82 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 157.7, 139.8, 127.9, 113.6, 40.8, 31.4, 22.1, 12.3.

GCMS (EI): $C_{11}H_{13}D_3O$, calculated: 167.1389, found: 167.1385.



5u

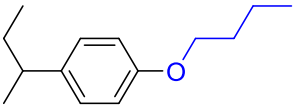
1-(Sec-butyl)-4-propoxybenzene (5u)

Colorless oil (13.6 mg, 71%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.13 (d, *J* = 7.6 Hz, 2H), 6.88 (d, *J* = 7.6 Hz, 2H), 3.94 (t, *J* = 7.2 Hz, 2H), 2.59 (sextet, *J* = 7.2 Hz, 1H), 1.84 (sextet, *J* = 7.2 Hz, 2H), 1.61 (quintet, *J* = 7.2 Hz, 2H), 1.26 (d, *J* = 7.2 Hz, 3H), 1.08 (t, *J* = 7.2 Hz, 3H), 0.86 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 157.3, 139.6, 127.8, 114.3, 69.5, 40.9, 31.4, 22.7, 22.1, 12.3, 10.6.

GCMS (EI): $C_{13}H_{20}O$, calculated: 192.1514, found: 192.1510.



5v

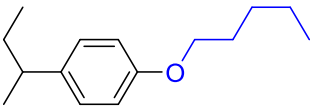
1-Butoxy-4-(sec-butyl)benzene (5v)[30]

Colorless oil (15.4 mg, 75%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.12 (d, *J* = 7.6 Hz, 2H), 6.87 (d, *J* = 7.6 Hz, 2H), 3.98 (t, *J* = 7.2 Hz, 2H), 2.58 (sextet, *J* = 7.2 Hz, 1H), 1.80 (quintet, *J* = 7.2 Hz, 2H), 1.64-1.48 (m, 4H), 1.25 (d, *J* = 7.2 Hz, 3H), 1.01 (t, *J* = 7.2 Hz, 3H), 0.85 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 157.3, 139.6, 127.8, 114.2, 67.6, 40.9, 31.5, 31.4, 22.1, 19.3, 13.9, 12.3.

GCMS: $C_{14}H_{22}O$, calculated: 206.1, found: 206.1.



5w

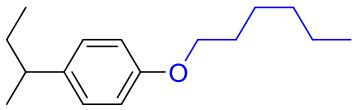
1-(Sec-butyl)-4-(pentyloxy)benzene (5w)

Colorless oil (17.6 mg, 80%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.12 (d, *J* = 7.6 Hz, 2H), 6.87 (d, *J* = 7.6 Hz, 2H), 3.97 (t, *J* = 7.2 Hz, 2H), 2.58 (sextet, *J* = 7.2 Hz, 1H), 1.82 (quintet, *J* = 7.2 Hz, 2H), 1.60 (quintet, *J* = 7.2 Hz, 2H), 1.53-1.37 (m, 4H), 1.25 (d, *J* = 7.2 Hz, 3H), 0.97 (t, *J* = 7.2 Hz, 3H), 0.86 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 157.3, 139.6, 127.8, 114.2, 67.9, 40.8, 31.4, 29.1, 28.3, 22.5, 22.1, 14.1, 12.3.

GCMS (EI): $C_{15}H_{24}O$, calculated: 220.1827, found: 220.1824.



5x

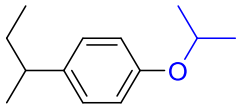
1-(Sec-butyl)-4-(hexyloxy)benzene (5x)

Colorless oil (17.5 mg, 75%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.11 (d, *J* = 7.6 Hz, 2H), 6.86 (d, *J* = 7.6 Hz, 2H), 3.96 (t, *J* = 7.2 Hz, 2H), 2.57 (sextet, *J* = 7.2 Hz, 1H), 1.80 (quintet, *J* = 7.2 Hz, 2H), 1.59 (quintet, *J* = 7.2 Hz, 2H), 1.55-1.45 (m, 2H), 1.45-1.33 (m, 4H), 1.24 (d, *J* = 7.2 Hz, 3H), 0.94 (t, *J* = 7.2 Hz, 3H), 0.85 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 157.3, 139.6, 127.8, 114.2, 67.9, 40.8, 31.6, 31.4, 29.4, 25.8, 22.7, 22.1, 14.1, 12.3.

GCMS (EI): $C_{16}H_{26}O$, calculated: 234.1984, found: 234.1989.



5z

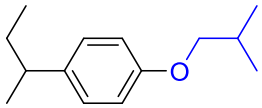
1-(Sec-butyl)-4-isopropoxybenzene (5z)

Colorless oil (9.2 mg, 48%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.08 (d, *J* = 7.6 Hz, 2H), 6.83 (d, *J* = 7.6 Hz, 2H), 4.52 (heptet, *J* = 7.2 Hz, 1H), 2.55 (sextet, *J* = 7.2 Hz, 1H), 1.57 (quintet, *J* = 7.2 Hz, 2H), 1.34 (d, *J* = 7.2 Hz, 6H), 1.22 (d, *J* = 7.2 Hz, 3H), 0.83 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 155.9, 139.7, 127.8, 115.6, 69.8, 40.8, 31.4, 22.2, 22.0, 12.3.

GCMS (EI): $C_{13}H_{20}O$, calculated: 192.1514, found: 192.1520.



5y

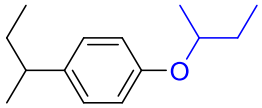
1-(Sec-butyl)-4-isobutoxybenzene (5y)

Colorless oil (16.5 mg, 80%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.12 (d, *J* = 7.6 Hz, 2H), 6.87 (d, *J* = 7.6 Hz, 2H), 3.73 (d, *J* = 7.2 Hz, 2H), 2.57 (sextet, *J* = 7.2 Hz, 1H), 2.11 (heptet, *J* = 7.2 Hz, 1H), 1.59 (quintet, *J* = 7.2 Hz, 2H), 1.25 (d, *J* = 7.2 Hz, 3H), 1.05 (d, *J* = 7.2 Hz, 6H), 0.85 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 157.4, 139.6, 127.8, 114.3, 74.5, 40.9, 31.4, 28.4, 22.1, 19.3, 12.3.

GCMS (EI): $C_{14}H_{22}O$, calculated: 206.1671, found: 206.1670.



5aa

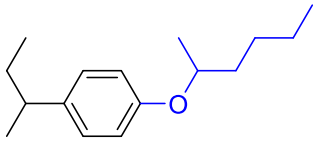
1-(Sec-butoxy)-4-(sec-butyl)benzene (5aa)

Colorless oil (14.4 mg, 70%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.10 (d, *J* = 7.6 Hz, 2H), 6.85 (d, *J* = 7.6 Hz, 2H), 4.28 (sextet, *J* = 7.2 Hz, 1H), 2.56 (sextet, *J* = 7.2 Hz, 1H), 1.77 (heptet, *J* = 7.2 Hz, 1H), 1.68-1.55 (m, 3H), 1.31 (d, *J* = 7.2 Hz, 3H), 1.24 (d, *J* = 7.2 Hz, 3H), 1.00 (d, *J* = 7.2 Hz, 3H), 0.85 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 156.3, 139.6, 127.8, 115.7, 75.1, 40.8, 31.4, 29.3, 22.0, 19.4, 12.3, 9.89.

GCMS (EI): $C_{14}H_{22}O$, calculated: 206.1671, found: 206.1674.



5ab

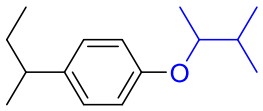
1-(Sec-butyl)-4-(hexan-2-yloxy)benzene (5ab)

Colorless oil (18.7 mg, 80%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.09 (d, *J* = 7.6 Hz, 2H), 6.84 (d, *J* = 7.6 Hz, 2H), 4.33 (sextet, *J* = 7.2 Hz, 1H), 2.56 (sextet, *J* = 7.2 Hz, 1H), 1.81-1.74 (m, 1H), 1.62-1.52 (m, 3H), 1.51-1.32 (m, 4H), 1.31 (d, *J* = 7.2 Hz, 3H), 1.23 (d, *J* = 7.2 Hz, 3H), 0.93 (t, *J* = 7.2 Hz, 3H), 0.85 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 156.3, 139.6, 127.8, 115.6, 73.9, 40.8, 36.4, 31.4, 27.9, 22.8, 22.0, 19.9, 14.1, 12.3.

GCMS (EI): $C_{16}H_{26}O$, calculated: 234.1984, found: 234.1980.



5ac

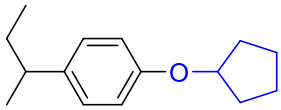
1-(Sec-butyl)-4-((3-methylbutan-2-yl)oxy)benzene (5ac)

Colorless oil (18.5 mg, 84%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.12 (d, *J* = 7.6 Hz, 2H), 6.87 (d, *J* = 7.6 Hz, 2H), 4.15 (quintet, *J* = 7.2 Hz, 1H), 2.59 (sextet, *J* = 7.2 Hz, 1H), 2.03-1.92 (m, 1H), 1.61 (quintet, *J* = 7.2 Hz, 2H), 1.27 (t, *J* = 7.2 Hz, 6H), 1.05 (d, *J* = 7.2 Hz, 3H), 1.02 (d, *J* = 7.2 Hz, 3H), 0.88 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 156.5, 139.5, 127.8, 115.8, 78.5, 40.8, 33.1, 31.4, 22.0, 18.6, 17.8, 16.1, 12.3.

GCMS (EI): $C_{15}H_{24}O$, calculated: 220.1827, found: 220.1824.



5ad

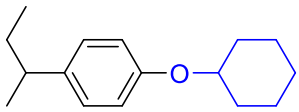
1-(Sec-butyl)-4-(cyclopentyloxy)benzene (5ad)

Colorless oil (18.5 mg, 85%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.07 (d, *J* = 7.6 Hz, 2H), 6.80 (d, *J* = 7.6 Hz, 2H), 4.76-4.70 (m, 1H), 2.53 (sextet, *J* = 7.2 Hz, 1H), 1.93-1.75 (m, 6H), 1.68-1.50 (m, 4H), 1.21 (d, *J* = 7.2 Hz, 3H), 0.82 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 156.2, 139.3, 127.7, 115.2, 79.1, 40.8, 32.9, 31.4, 24.0, 22.0, 12.3.

GCMS (EI): $C_{15}H_{22}O$, calculated: 218.1671, found: 218.1670.



5ae

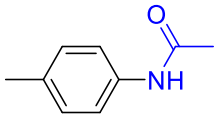
1-(Sec-butyl)-4-(cyclohexyloxy)benzene (5ae)

Colorless oil (17.2 mg, 74%)

^{1}H-NMR ($CDCl_3$, 500 MHz): 7.09 (d, *J* = 7.6 Hz, 2H), 6.85 (d, *J* = 7.6 Hz, 2H), 4.24-4.19 (m, 1H), 2.55 (sextet, *J* = 7.2 Hz, 1H), 2.04-1.99 (m, 2H), 1.84-1.81 (m, 2H), 1.62-1.49 (m, 5H), 1.42-1.22 (m, 3H), 1.23 (d, *J* = 7.2 Hz, 3H), 0.83 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 155.8, 139.7, 127.8, 115.8, 75.5, 40.8, 32.0, 31.4, 25.7, 23.9, 21.9, 12.3.

GCMS (EI): $C_{16}H_{24}O$, calculated: 232.1827, found: 232.1828.



7a

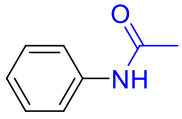
N-(p-tolyl) acetamide (7a)[31]

White solid (10.4 mg, 70%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 9.88 (s, 1H), 7.46 (d, *J* = 7.6 Hz, 2H), 7.05 (d, *J* = 7.6 Hz, 2H), 2.19 (s, 3H), 2.02 (s, 3H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 168.8, 137.1, 132.5, 129.5, 119.6, 24.2, 20.8.

GCMS: $C_9H_{11}NO$, calculated: 149.1, found: 149.1.



7b

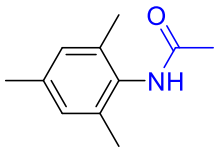
N-phenylacetamide (7b)[32]

White solid (5.4 mg, 40%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.79 (br, 1H), 7.52 (d, *J* = 7.6 Hz, 2H), 7.31 (t, *J* = 7.6 Hz, 2H), 7.11 (t, *J* = 7.6 Hz, 1H), 2.17 (s, 3H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 168.7, 138.0, 128.9, 124.3, 120.0, 24.5.

GCMS: C_8H_9NO, calculated: 135.1, found: 135.1.



7c

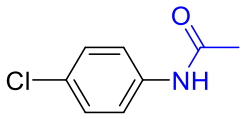
N-mesitylacetamide (7c)[33]

White solid (10.6 mg, 60%)

^{1}H-NMR (*d*$_6$-DMSO, 400 MHz): 9.12 (s, 1H), 6.86 (s, 2H), 2.22 (s, 3H), 2.09 (s, 6H), 2.02 (s, 3H).

^{13}C-NMR (*d*$_6$-DMSO, 100 MHz): 168.3, 135.6, 135.2, 133.2, 128.6, 22.9, 20.9, 18.5.

GCMS: $C_{11}H_{15}NO$, calculated: 177.1, found: 177.1.



7e

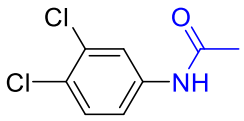
N-(4-chlorophenyl)acetamide (7e)[34]

White solid (6.7 mg, 40%)

^{1}H-NMR (*d*$_4$-MeOH, 400 MHz): 7.55 (d, *J* = 7.6 Hz, 2H), 7.29 (d, *J* = 7.6 Hz, 2H), 4.88 (s, 1H), 2.13 (s, 3H).

^{13}C-NMR (*d*$_4$-MeOH, 125 MHz): 170.2, 137.4, 128.5, 128.3, 121.0, 22.4.

GCMS: C_8H_8ClNO, calculated: 169.1, found: 169.1.



7d

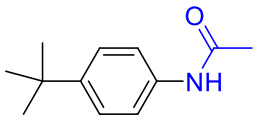
N-(3,4-dichlorophenyl)acetamide (7d)[35]

White solid (7.1 mg, 35%)

^{1}H-NMR (*d*$_6$-DMSO, 400 MHz): 10.2 (s, 1H), 7.98 (d, *J* = 2.4 Hz, 1H), 7.51 (d, *J* = 7.6 Hz, 2H), 7.45 (dd, J_1 = 7.6 Hz, J_2 = 2.4 Hz, 1H), 2.06 (s, 3H).

^{13}C-NMR (*d*$_6$-DMSO, 100 MHz): 169.2, 139.8, 131.4, 130.9, 124.8, 120.5, 119.4, 24.5.

GCMS: $C_8H_7Cl_2NO$, calculated: 203.0, found: 203.0.



7f

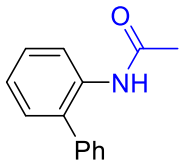
N-(4-(tert-butyl)phenyl)acetamide (7f)[36]

White solid (13.0 mg, 68%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.72 (br, 1H), 7.44 (d, *J* = 7.6 Hz, 2H), 7.34 (d, *J* = 7.6 Hz, 2H), 2.16 (s, 3H), 1.32 (s, 3H).

^{13}C-NMR ($CDCl_3$, 125 MHz): 168.6, 147.2, 135.3, 125.7, 119.9, 34.4, 31.4, 24.4.

GCMS: $C_{12}H_{17}NO$, calculated: 191.1, found: 191.1.



7g

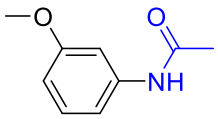
N-([1,1'-biphenyl]-2-yl)acetamide (7g)[37]

White solid (11.4 mg, 54%)

^{1}H-NMR (*d_6*-DMSO, 400 MHz): 9.25 (s, 1H), 7.49-7.29 (m, 9H), 1.90 (s, 3H).

^{13}C-NMR (*d_6*-DMSO, 100 MHz): 169.2, 139.5, 137.1, 135.4, 130.7, 129.1, 128.8, 128.1, 127.8, 127.6, 126.4, 23.5.

GCMS: $C_{14}H_{13}NO$, calculated: 211.1, found: 211.1.



7h

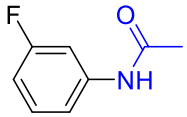
N-(3-methoxyphenyl)acetamide (7h)[38]

White solid (9.2 mg, 56%)

^{1}H-NMR (*d_6*-DMSO, 400 MHz): 9.93 (s, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.21-7.12 (m, 2H), 6.60 (d, *J* = 7.6 Hz, 1H), 3.71 (s, 3H), 2.05 (s, 3H).

^{13}C-NMR (*d_6*-DMSO, 100 MHz): 168.9, 159.9, 140.9, 129.8, 111.8, 108.7, 105.4, 55.3, 24.5.

GCMS: $C_9H_{11}NO_2$, calculated: 165.1, found: 165.1.



7i

N-(3-fluorophenyl)acetamide (7i)[39]

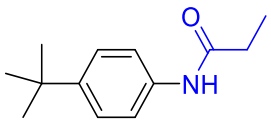
White solid (7.7 mg, 50%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 8.22 (br, 1H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.28-7.16 (m, 2H), 6.81 (t, *J* = 7.6 Hz, 2H), 2.18 (s, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 169.1, 162.9 (d, *J* = 243.1 Hz), 139.5 (d, *J* = 11.0 Hz), 130.0 (d, *J* = 9.0 Hz), 115.2 (d, *J* = 3.1 Hz), 110.9 (d, *J* = 21.0 Hz), 107.5 (d, *J* = 26.0 Hz), 24.5.

^{19}F-NMR ($CDCl_3$, 376 MHz): -111.6.

GCMS: C_8H_8FNO, calculated: 153.1, found: 153.1.



7j

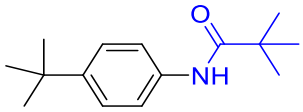
N-(4-(tert-butyl)phenyl)propionamide (7j)[40]

White solid (9.8 mg, 48%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.46 (d, *J* = 7.6 Hz, 2H), 7.35 (d, *J* = 7.6 Hz, 2H), 2.40 (q, *J* = 7.2 Hz, 2H), 1.32 (s, 9H), 1.26 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 173.3, 147.2, 135.5, 125.7, 120.4, 34.4, 31.4, 30.7, 10.2.

GCMS: $C_{13}H_{19}NO$, calculated: 205.1, found: 205.1.



7k

N-(4-(tert-butyl)phenyl)pivalamide (7k)

White solid (14.7 mg, 63%)

^{1}H-NMR ($CDCl_3$, 400 MHz): 7.47 (d, *J* = 7.6 Hz, 2H), 7.35 (d, *J* = 7.6 Hz, 2H), 1.334 (s, 9H), 1.333 (s, 9H).

^{13}C-NMR ($CDCl_3$, 100 MHz): 176.4, 147.2, 135.4, 125.7, 119.7, 39.5, 34.3, 31.4, 27.7.

HRMS (ESI): $C_{15}H_{24}NO$ $[M+H]^+$, calculated: 234.1858, found: 234.1860.

9: Reference

1 Karimi, B.; Akhavan, P. F. *Chem. Commun.* **2009**, 3750-3752.

2 Cheng, Y.; Gu, X.; Li, P. *Org. Lett.* **2013,** *15*, 2664-2667.

3 Paul, S.; Pradhan, K.; Ghosh, S.; De, S. K.; Das, A. R. *Adv. Synth. Catal.* **2014,** *356*, 1301-1316.

4 Mahajani, N. S.; Chisholm, J. D. *J. Org. Chem.* **2018,** *83*, 4131-4139.

5 Sun, Y.-Y.; Yi, J.; Lu, X.; Zhang, Z.-Q.; Xiao, B.; Fu, Y. *Chem. Commun.* **2014,** *50*, 11060-11062.

6 Hansen, A. L.; Ebran, J.-P.; Gøgsig, T. M.; Skrydstrup, T. *J. Org. Chem.* **2007,** *72*, 6464-6472.

7 Xi, Z.; Zhou, Y.; Chen, W. *J. Org. Chem.* **2008,** *73*, 8497-8501.

8 Dewanji, A.; Murarka, S.; Curran, D. P.; Studer, A. *Org. Lett.* **2013,** *15*, 6102-6105.

9 Kumar, A.; Shah, B. A. *Org. Lett.* **2015,** *17*, 5232-5235.

10 El-Deeb, I. Y.; Funakoshi, T.; Shimomoto, Y.; Matsubara, R.; Hayashi, M. *J. Org. Chem.* **2017,** *82*, 2630-2640.

11 Yasukawa, N.; Yokoyama, H.; Masuda, M.; Monguchi, Y.; Sajiki, H.; Sawama, Y. *Green Chem.* **2018,** *20*, 1213-1217.

12 Dey, A.; Sasmal, S.; Seth, K.; Lahiri, G. K.; Maiti, D. *ACS Cat.* **2017,** *7*, 433-437.

13 Tanimoro, K.; Ueno, M.; Takeda, K.; Kirihata, M.; Tanimori, S. *J. Org. Chem.* **2012,** *77*, 7844-7849.

14 Rieke, R. D.; Schulte, L. D.; Dawson, B. T.; Yang, S. S. *J. Am. Chem. Soc.* **1990,** *112*, 8388-8398.

15 Chen, X.; Ke, H.; Chen, Y.; Guan, C.; Zou, G. *J. Org. Chem.* **2012,** *77*, 7572-7578.

16 Bradshaw, J. S.; Loveridge, E. L.; White, L. *J. Org. Chem.* **1968,** *33*, 4127-4132.

17 Liu, Q.; Lan, Y.; Liu, J.; Li, G.; Wu, Y.-D.; Lei, A. *J. Am. Chem. Soc.* **2009,** *131*, 10201-10210.

18 Guan, B.-T.; Xiang, S.-K.; Wang, B.-Q.; Sun, Z.-P.; Wang, Y.; Zhao, K.-Q.; Shi, Z.-J. *J. Am. Chem. Soc.* **2008,** *130*, 3268-3269.

19 Kinoshita, H.; Tohjima, T.; Miura, K. *Org. Lett.* **2014,** *16*, 4762-4765.

20 Li, W.; Lv, G.; Cheng, X.; Sang, R.; Ma, X.; Zhang, Y.; Nie, R.; Li, J.; Guan, M.; Wu, Y. *Tetrahedron* **2016,** *72*, 8557-8564.

21 Luan, Y.-X.; Zhang, T.; Yao, W.-W.; Lu, K.; Kong, L.-Y.; Lin, Y.-T.; Ye, M. *J. Am. Chem. Soc.* **2017,** *139*, 1786-1789.

22 Wang, Z.-Y.; Chen, G.-Q.; Shao, L.-X. *J. Org. Chem.* **2012,** *77*, 6608-6614.

23 Guo, Y.; Fan, X.-M.; Nie, M.; Liu, H.-W.; Liao, D.-H.; Pan, X.-D.; Ji, Y.-F. *Eur. J. Org. Chem.* **2015,** *2015*, 4744-4755.

24 Brenner, E.; Baldwin, R. M.; Tamagnan, G. *Org. Lett.* **2005,** *7*, 937-939.

25 Song, L. X.; Wang, H. M.; Guo, X. Q.; Bai, L. *J. Org. Chem.* **2008,** *73*, 8305-8316.

26 Bates, R. B.; Siahaan, T. J.; Suvannachut, K. *J. Org. Chem.* **1990,** *55*, 1328-1334.

27 Sun, H.-B.; Li, B.; Hua, R.; Yin, Y. *Eur. J. Org. Chem.* **2006,** *2006*, 4231-4236.

28 Yoshioka, E.; Miyabe, H. *Tetrahedron* **2012,** *68*, 179-189.

29 Zhang, K.-F.; Christoffel, F.; Baudoin, O. *Angew. Chem. Int. Ed.* **2018,** *57*, 1982-1986.

30 Spanninger, P. A.; Von Rosenberg, J. L. *J. Am. Chem. Soc.* **1972,** *94*, 1973-1978.

31 Rao, S. N.; Mohan, D. C.; Adimurthy, S. *Org. Lett.* **2013,** *15*, 1496-1499.

32 Escobar, L.; Díaz-Moscoso, A.; Ballester, P. *Chem. Sci.* **2018,** *9*, 7186-7192.

33 Simkó, D. C.; Elekes, P.; Pázmándi, V.; Novák, Z. *Org. Lett.* **2018,** *20*, 676-679.

34 Gao, Y.; Liu, J.; Li, Z.; Guo, T.; Xu, S.; Zhu, H.; Wei, F.; Chen, S.; Gebru, H.; Guo, K. *J. Org. Chem.* **2018,** *83*, 2040-2049.

35 Xiong, B.; Wang, G.; Xiong, T.; Wan, L.; Zhou, C.; Liu, Y.; Zhang, P.; Yang, C.; Tang, K. *Tetrahedron Lett.* **2018,** *59*, 3139-3142.

36 Zhang, X.; Liu, Z.; Gao, Y.; Li, F.; Tian, Y.; Li, C.; Jia, X.; Li, J. *Adv. Synth. Catal.* **2017,** *360*, 272-277.

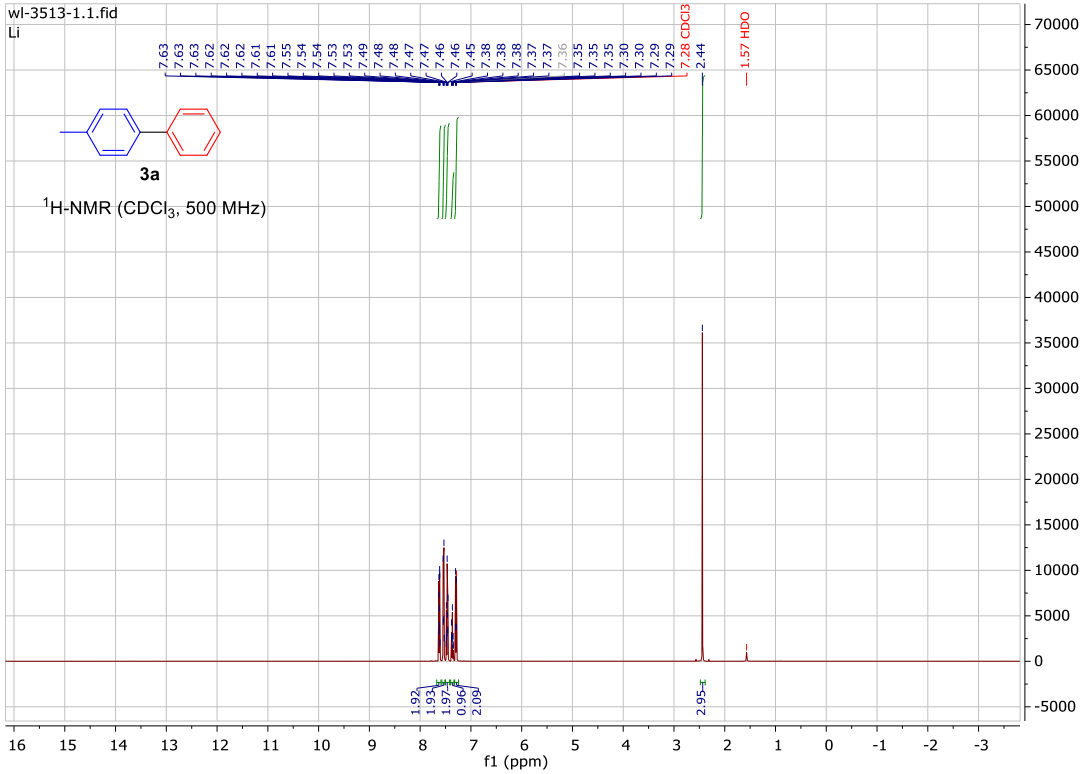
37 Bjørsvik, H.-R.; Elumalai, V. *Eur. J. Org. Chem.* **2016,** *2016*, 5474-5479.

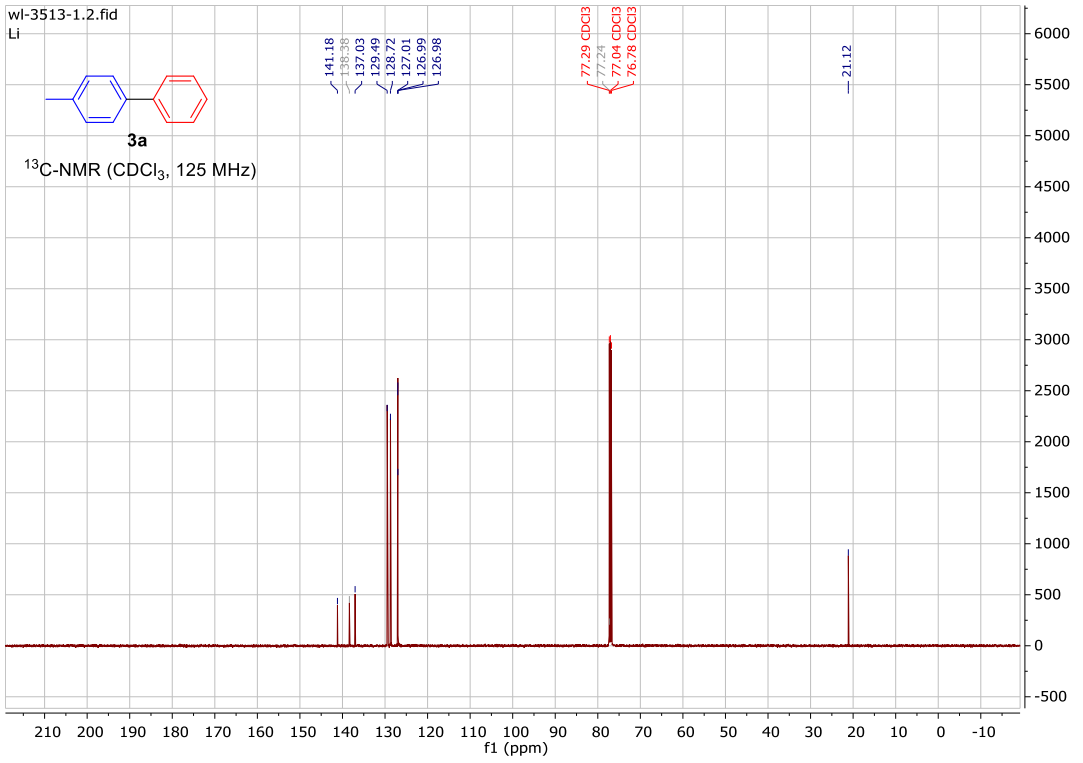
38 Niu, G.; Liu, W.; Wu, J.; Zhou, B.; Chen, J.; Zhang, H.; Ge, J.; Wang, Y.; Xu, H.; Wang, P. *J. Org. Chem.* **2015,** *80*, 3170-3175.

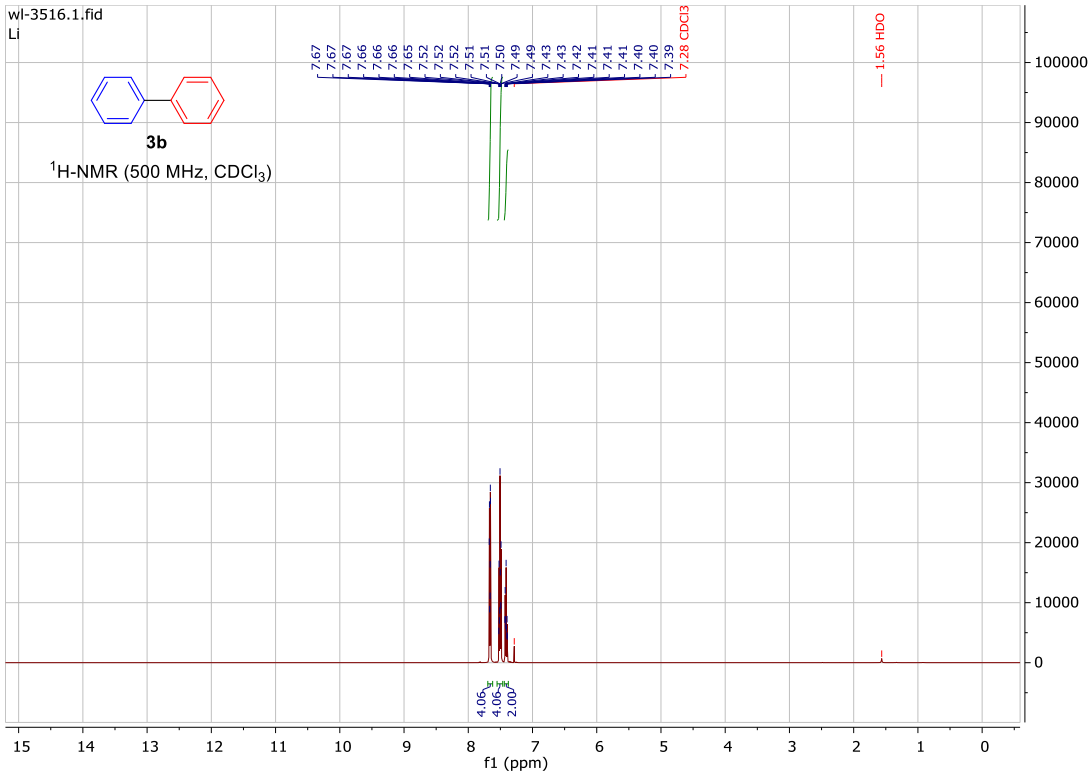
39 Mondal, A.; Subaramanian, M.; Nandakumar, A.; Balaraman, E. *Org. Lett.* **2018,** *20*, 3381-3384.

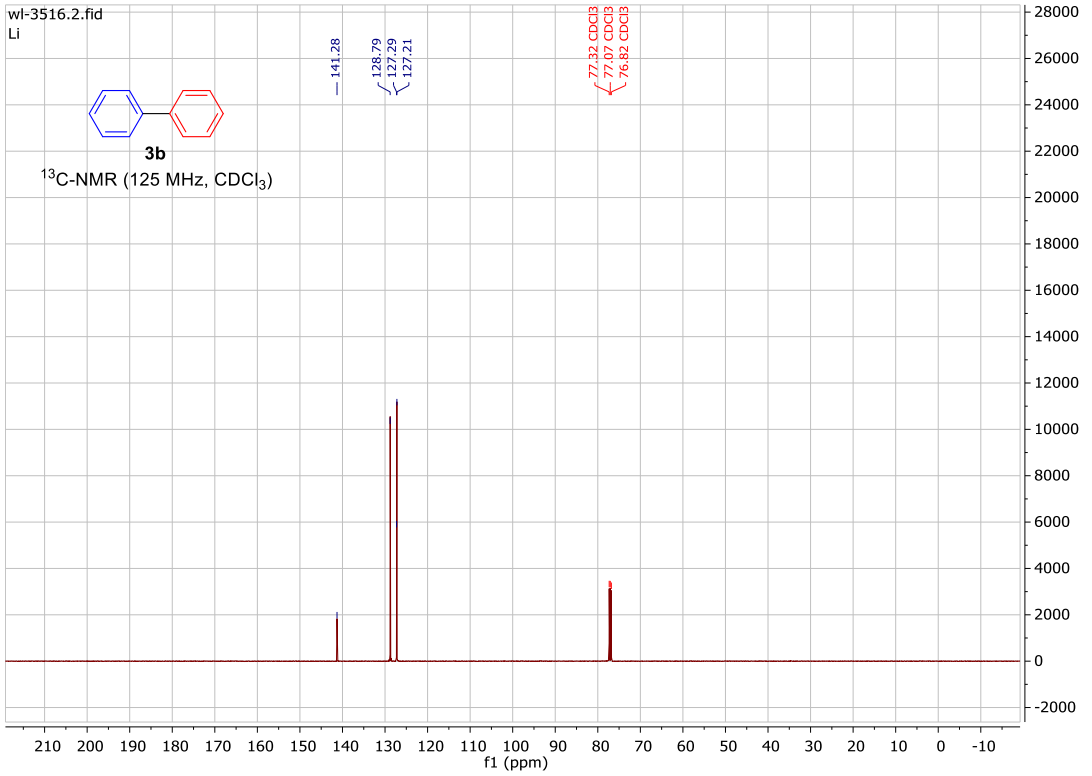
40 Deng, Y.; Gong, W.; He, J.; Yu, J.-Q. *Angew. Chem. Int. Ed.* 2014, 53, 6692-6695.

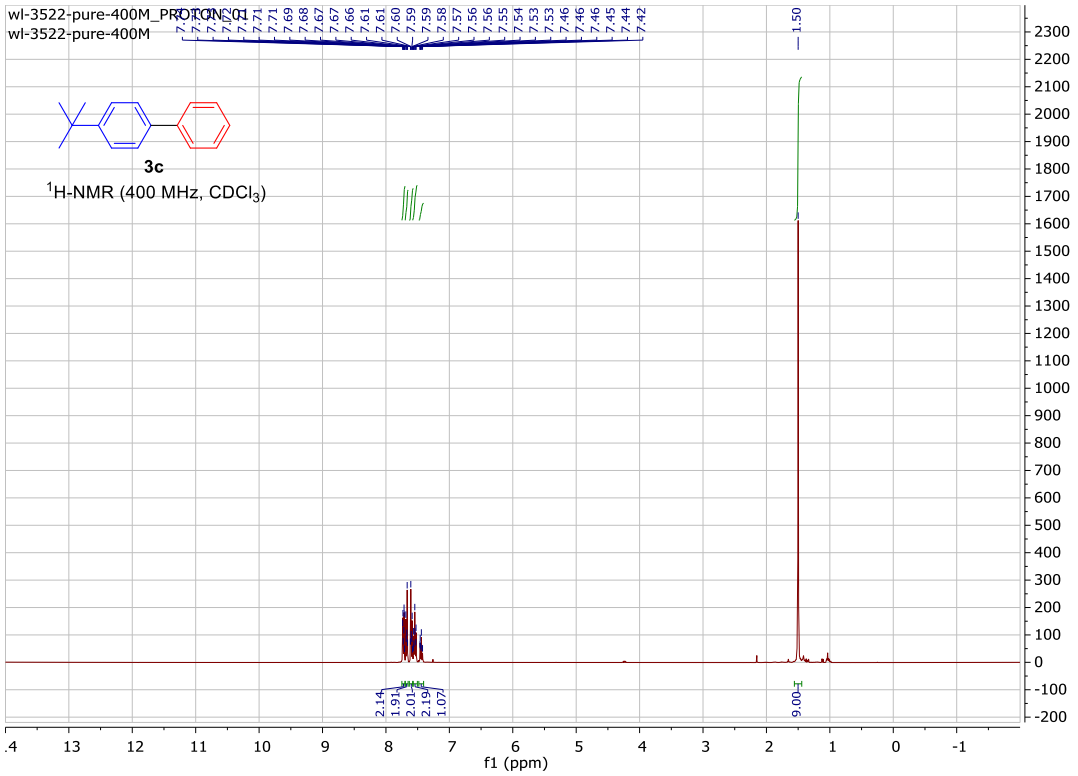
10. Copies of spectra

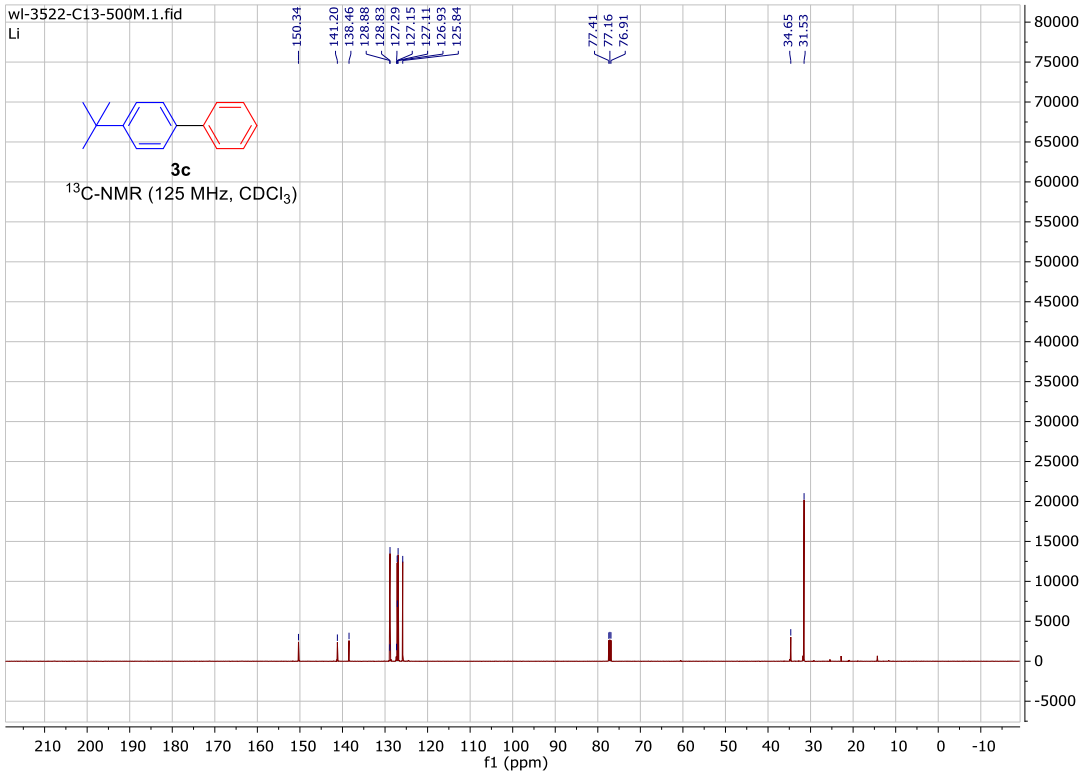


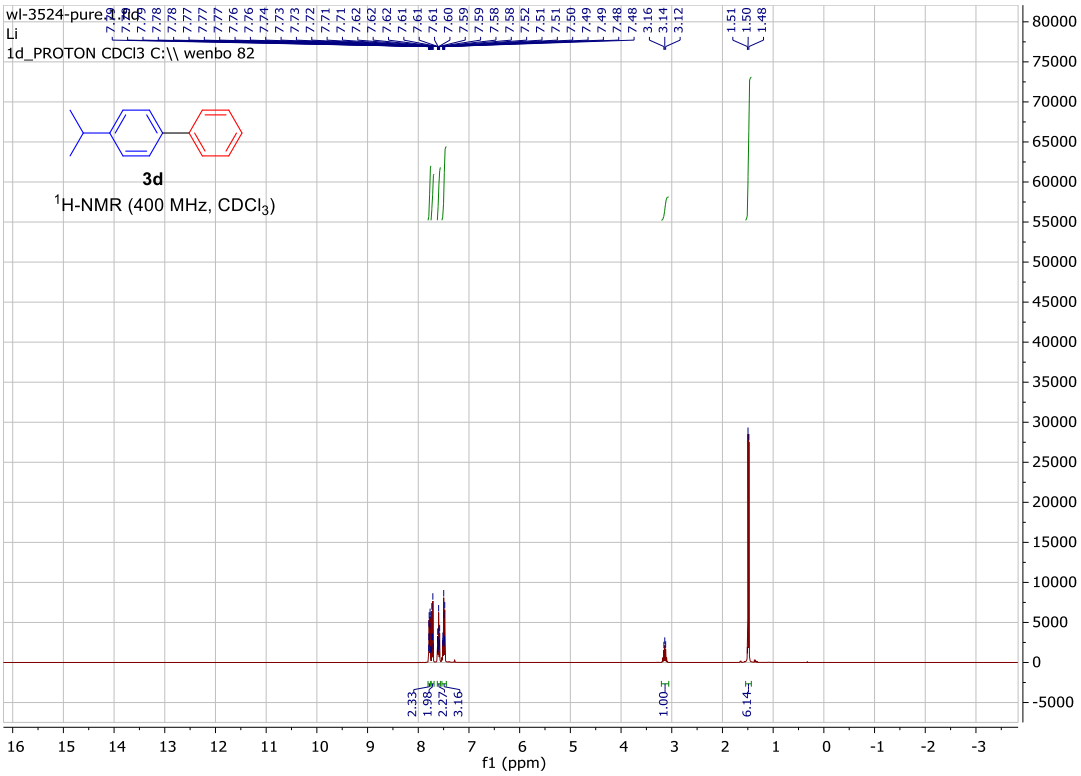


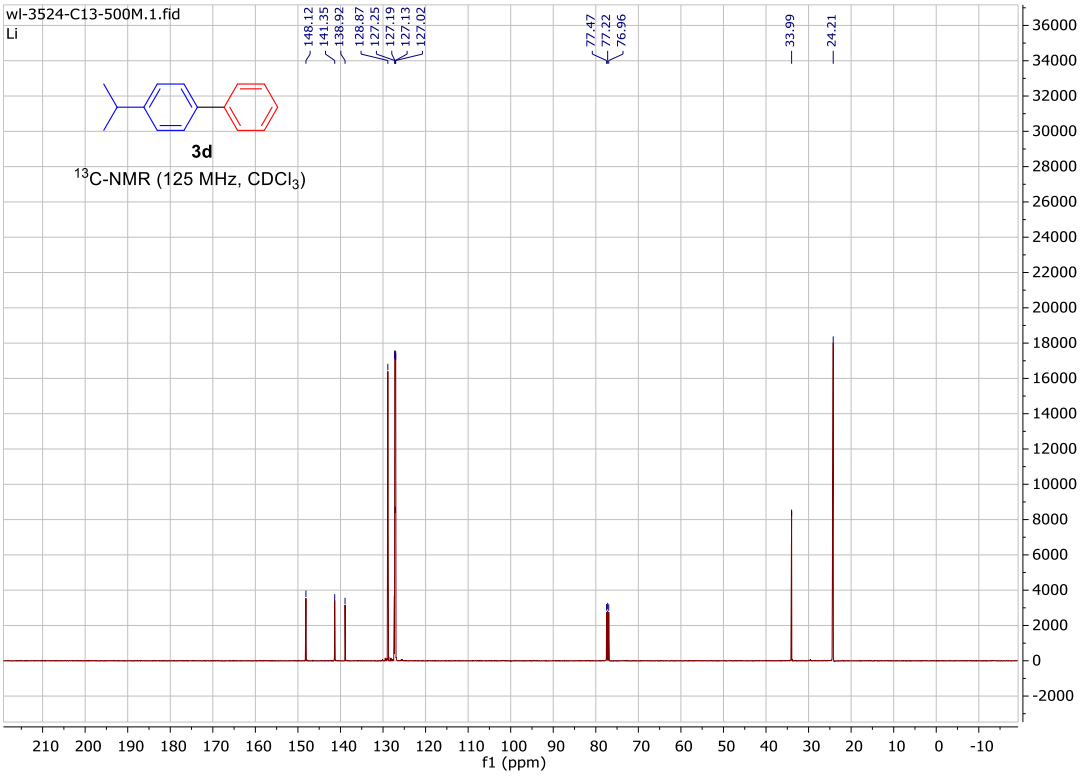

wl-3516.1.fid
Li
3b
^{1}H-NMR (500 MHz, $CDCl_3$)
7.67
7.67
7.67
7.66
7.66
7.66
7.65
7.52
7.52
7.52
7.51
7.51
7.50
7.49
7.49
7.43
7.43
7.42
7.41
7.41
7.41
7.40
7.40
7.39
7.28 CDCl3
1.56 HDO
4.06
4.06
2.00
f1 (ppm)

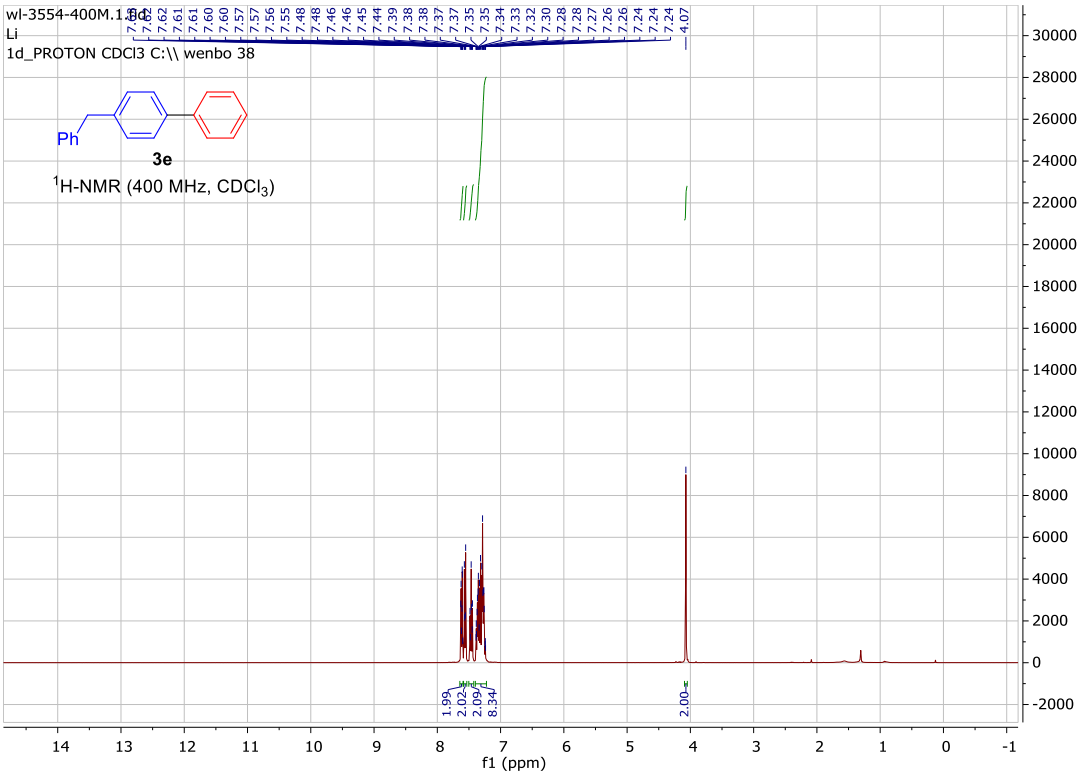

wl-3516.2.fid
Li
3b
^{13}C-NMR (125 MHz, $CDCl_3$)
141.28
128.79
127.29
127.21
77.32 CDCl3
77.07 CDCl3
76.82 CDCl3
f1 (ppm)

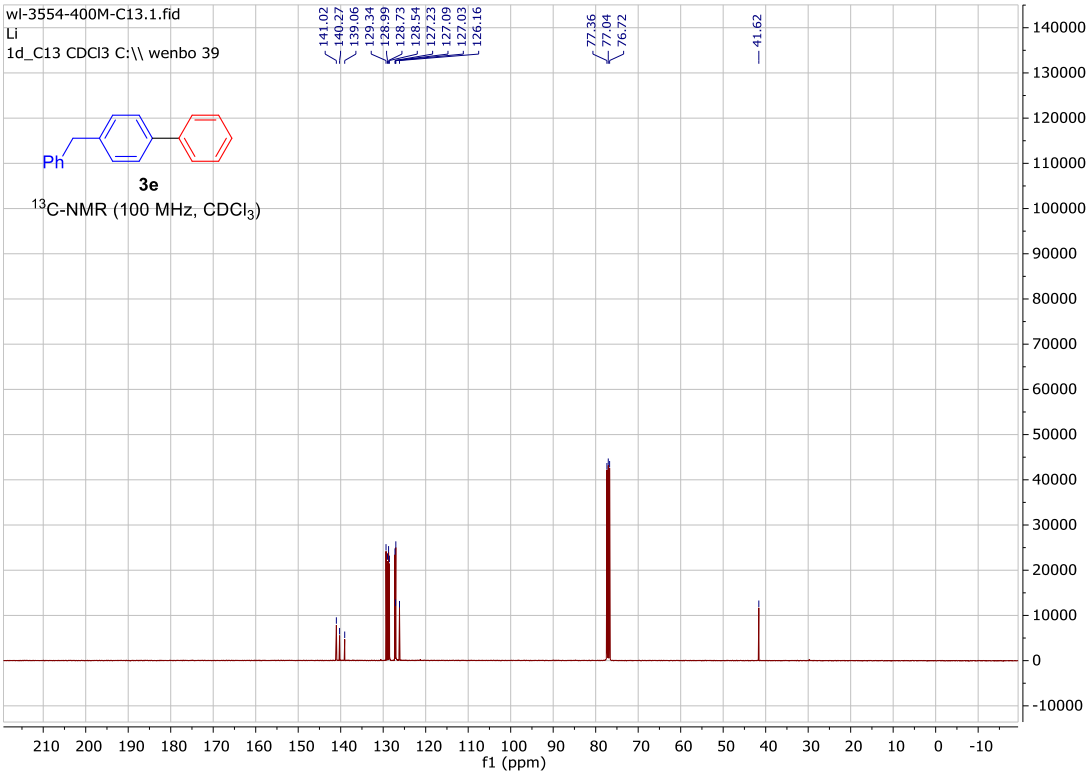

wl-3522-pure-400M_PROTON_01
wl-3522-pure-400M
3c
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

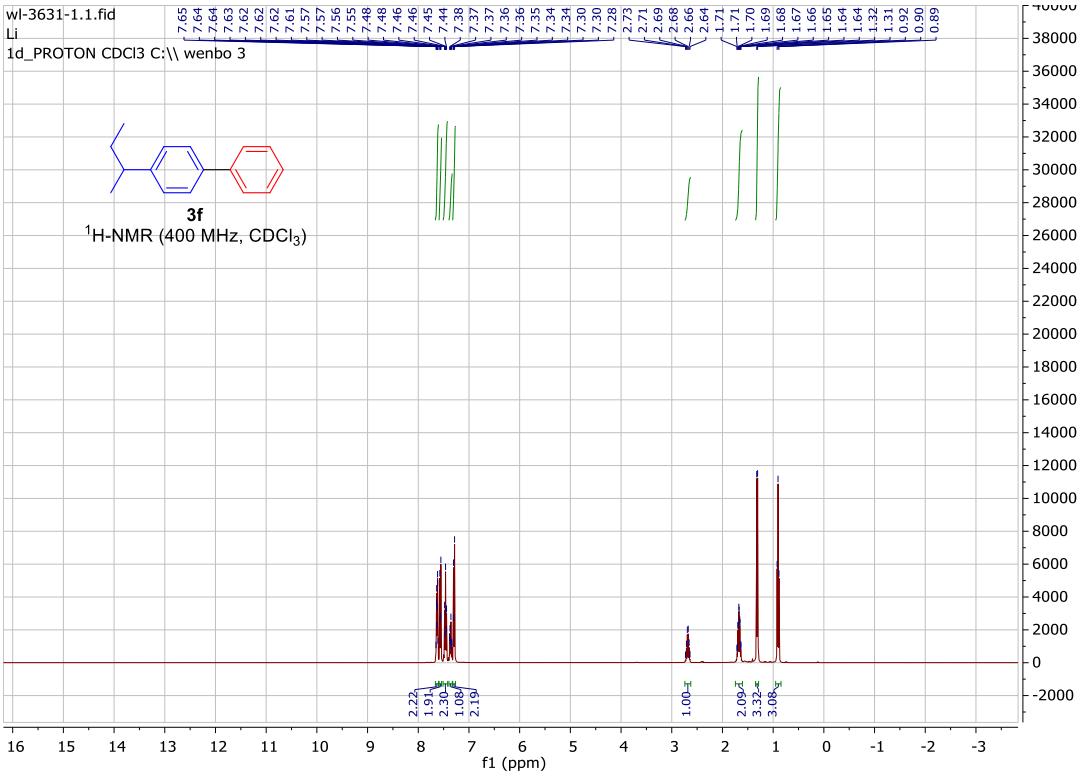

wl-3522-C13-500M.1.fid
Li
3c
13C-NMR (125 MHz, CDCl3)
f1 (ppm)

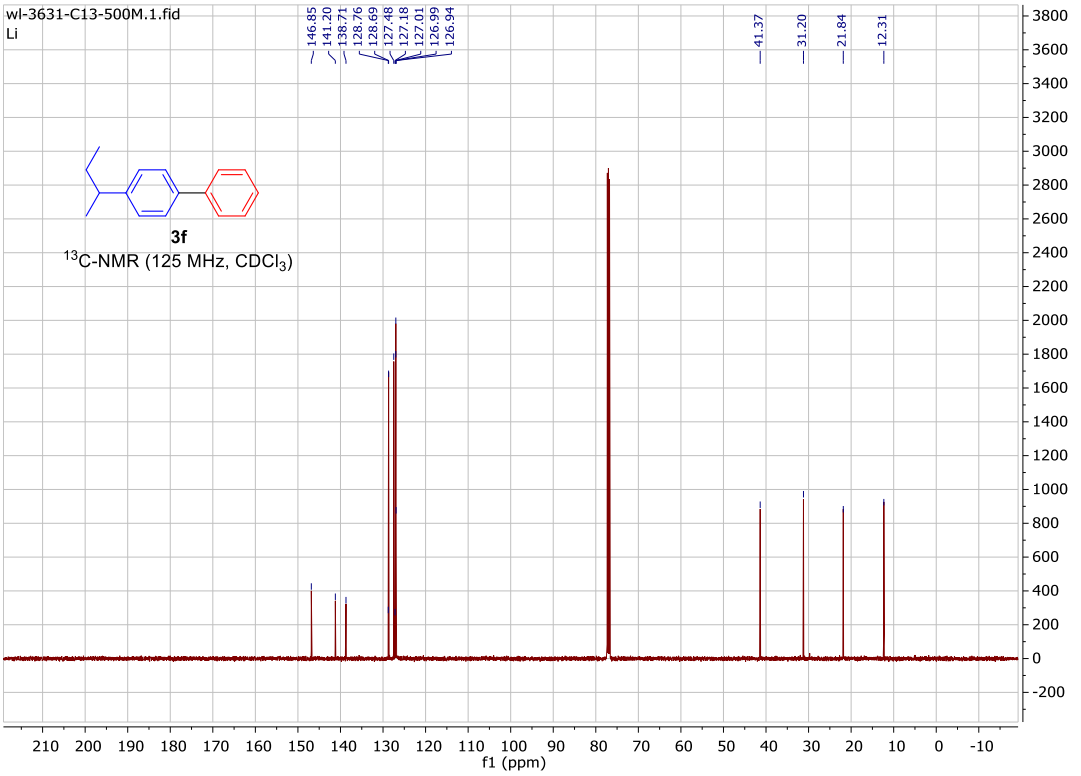

wl-3524-pure1.1.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 82
3d
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

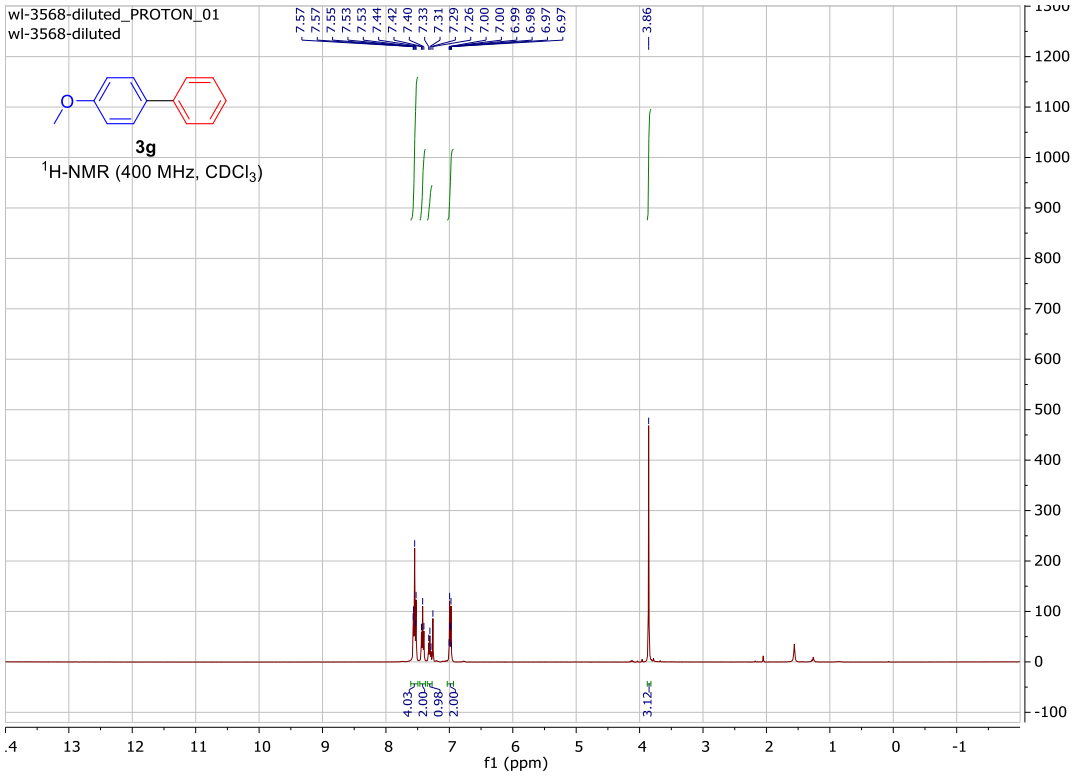

wl-3524-C13-500M.1.fid
Li
3d
13C-NMR (125 MHz, CDCl3)
f1 (ppm)

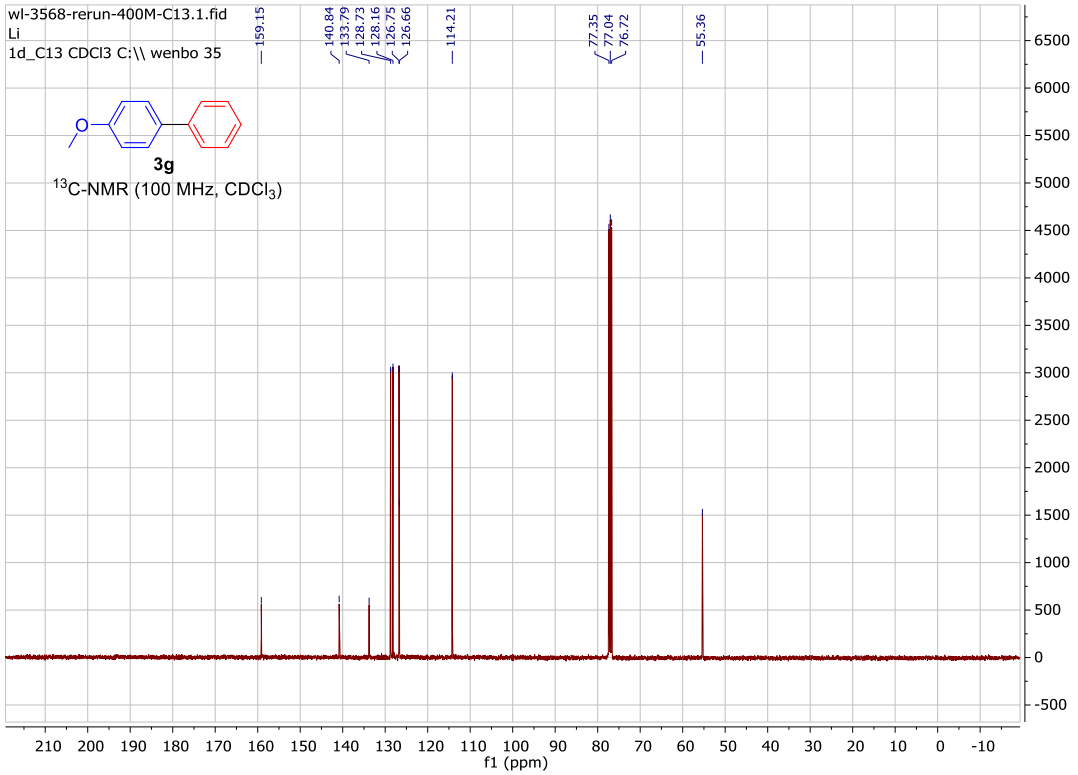

wl-3554-400M.1.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 38
Ph
3e
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

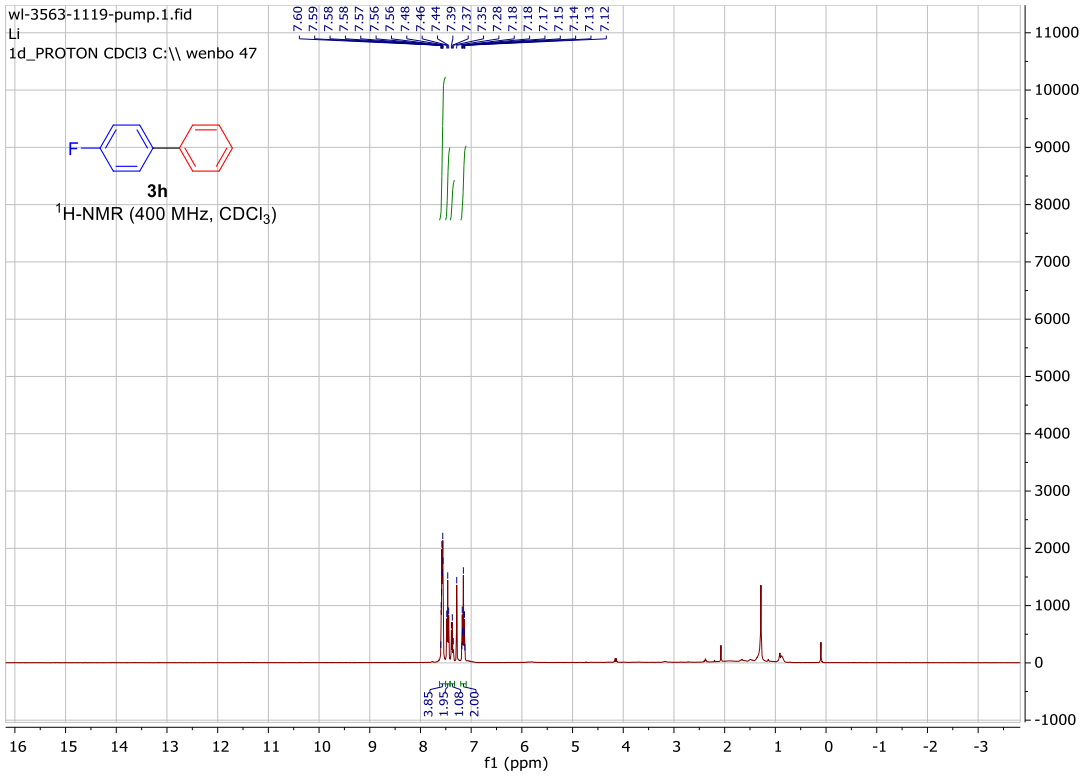

wl-3554-400M-C13.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 39
Ph
3e
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

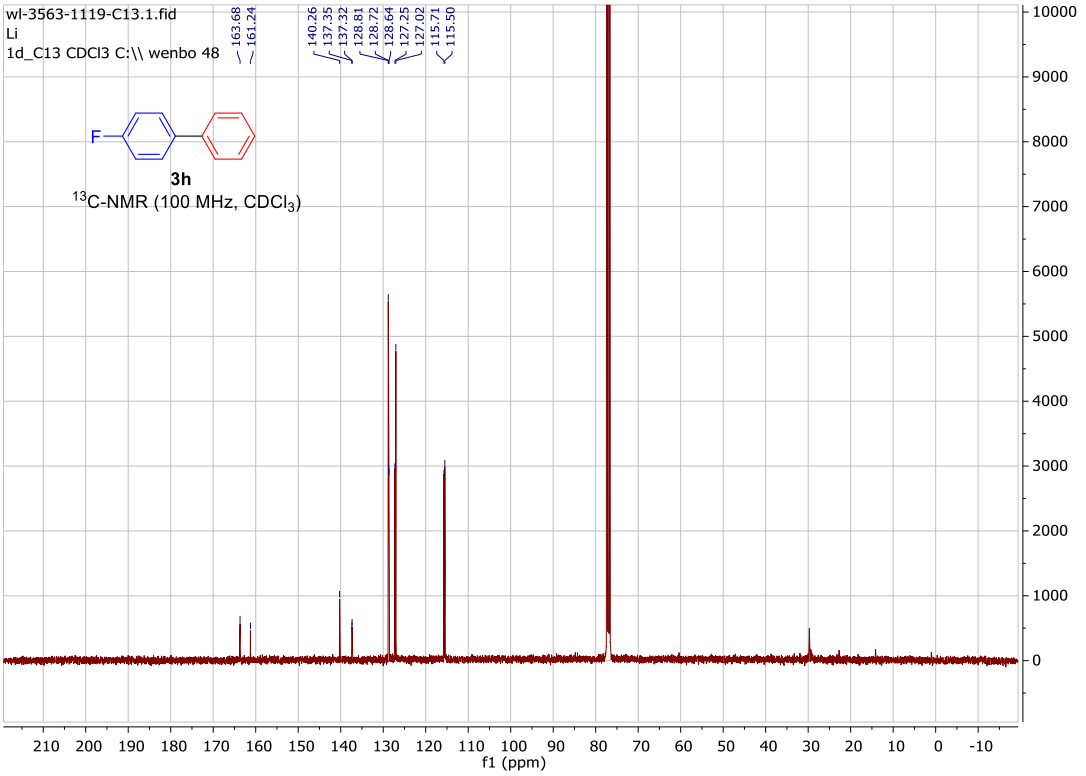

wl-3631-1.1.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 3
3f
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

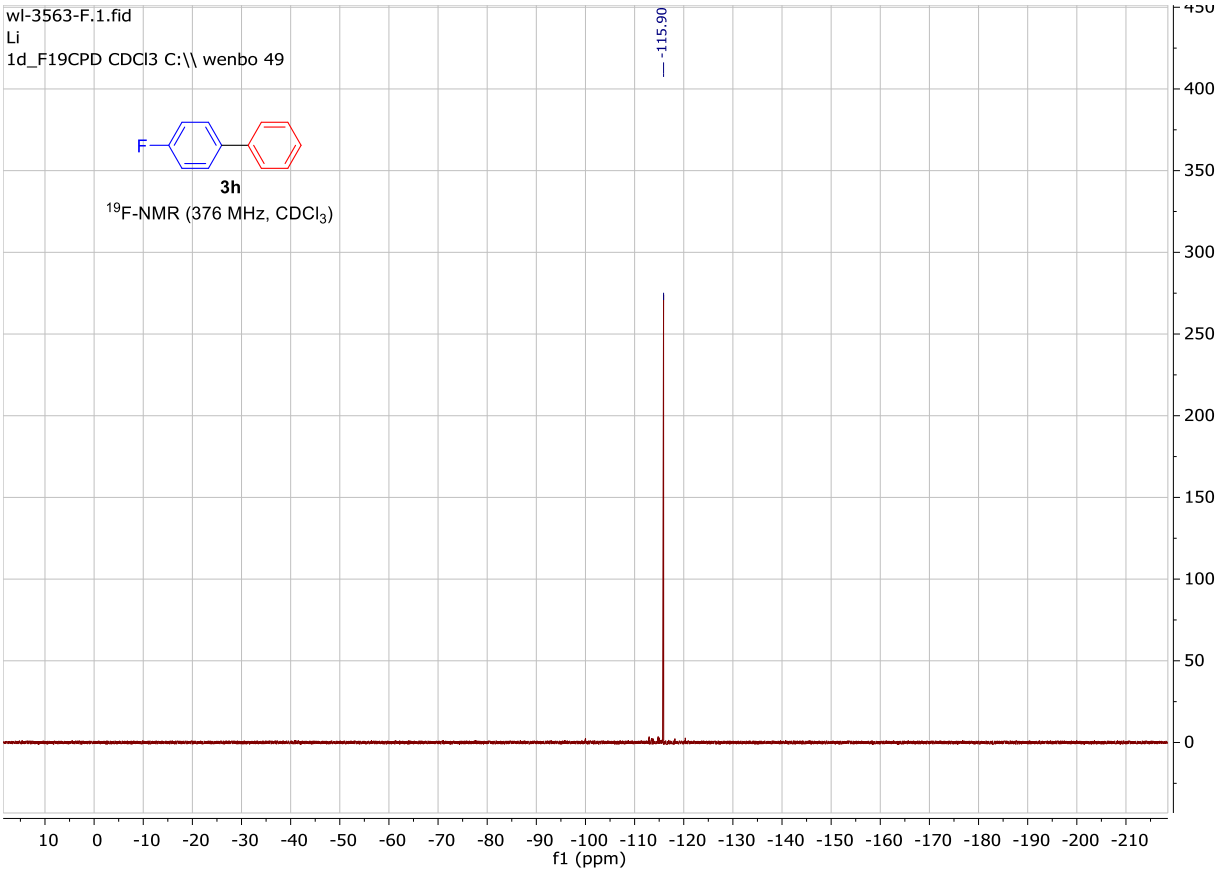

wl-3631-C13-500M.1.fid
Li
3f
13C-NMR (125 MHz, CDCl3)
f1 (ppm)

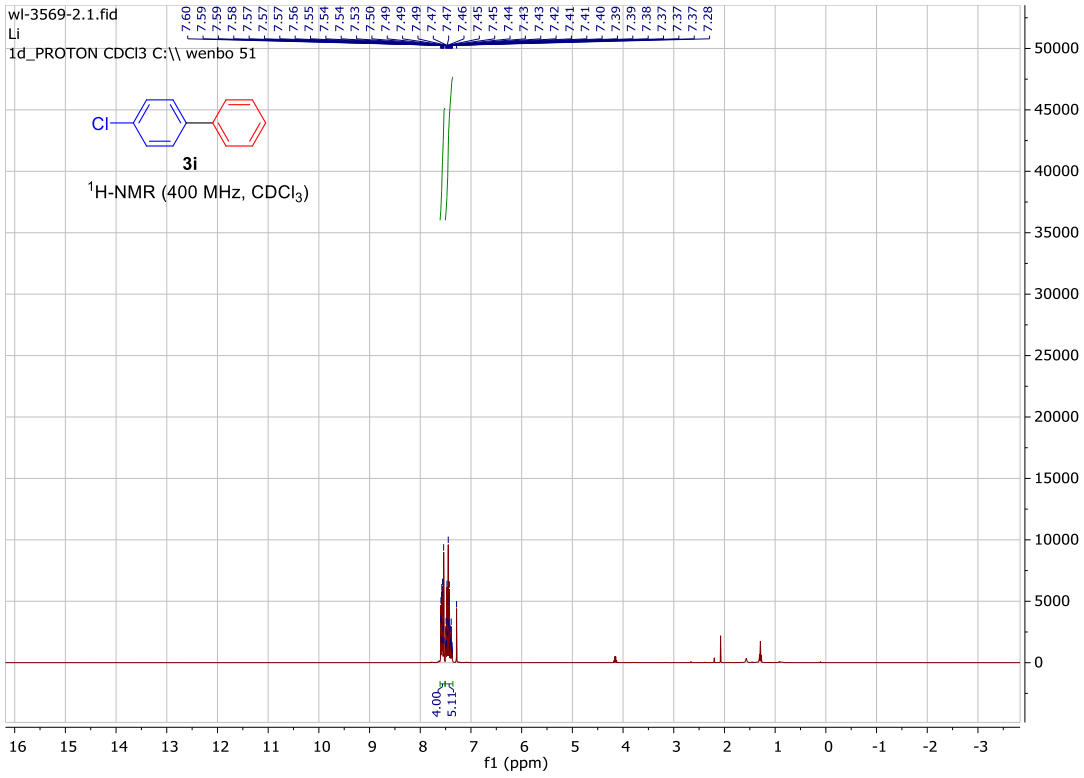

wl-3568-diluted_PROTON_01
wl-3568-diluted
3g
^{1}H-NMR (400 MHz, $CDCl_3$)
7.57
7.57
7.55
7.53
7.53
7.44
7.42
7.40
7.33
7.31
7.29
7.26
7.00
7.00
6.99
6.98
6.97
6.97
3.86
4.03
2.00
0.98
2.00
3.12
f1 (ppm)

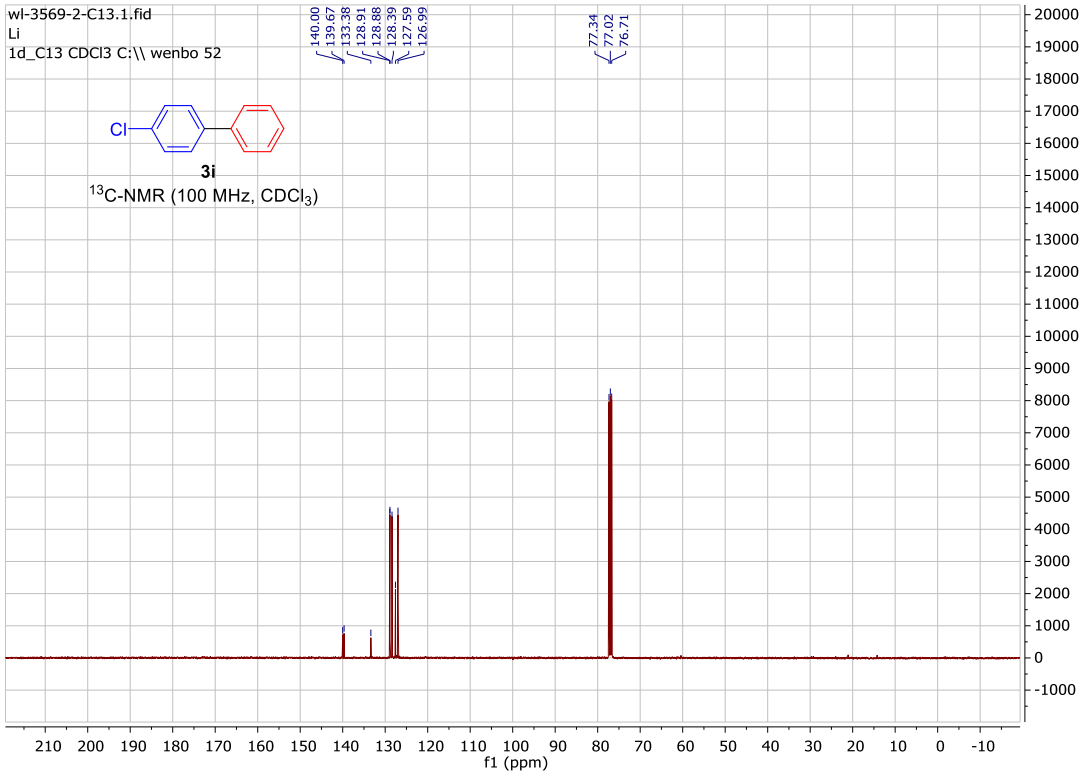

wl-3568-rerun-400M-C13.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 35
3g
^{13}C-NMR (100 MHz, $CDCl_3$)
159.15
140.84
133.79
128.73
128.16
126.75
126.66
114.21
77.35
77.04
76.72
55.36
f1 (ppm)

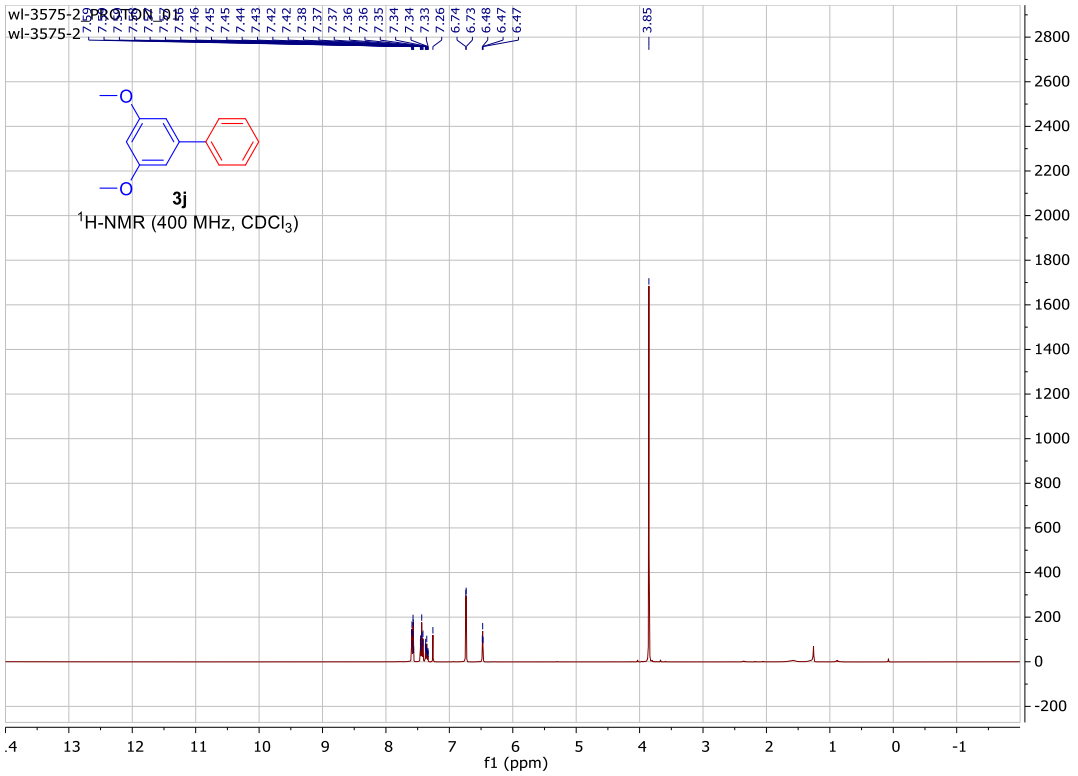

wl-3563-1119-pump.1.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 47
F
3h
1H-NMR (400 MHz, CDCl3)
7.60
7.59
7.58
7.58
7.57
7.56
7.56
7.48
7.46
7.44
7.39
7.37
7.35
7.28
7.18
7.18
7.17
7.15
7.14
7.13
7.12
3.85
1.95
1.08
2.00
f1 (ppm)

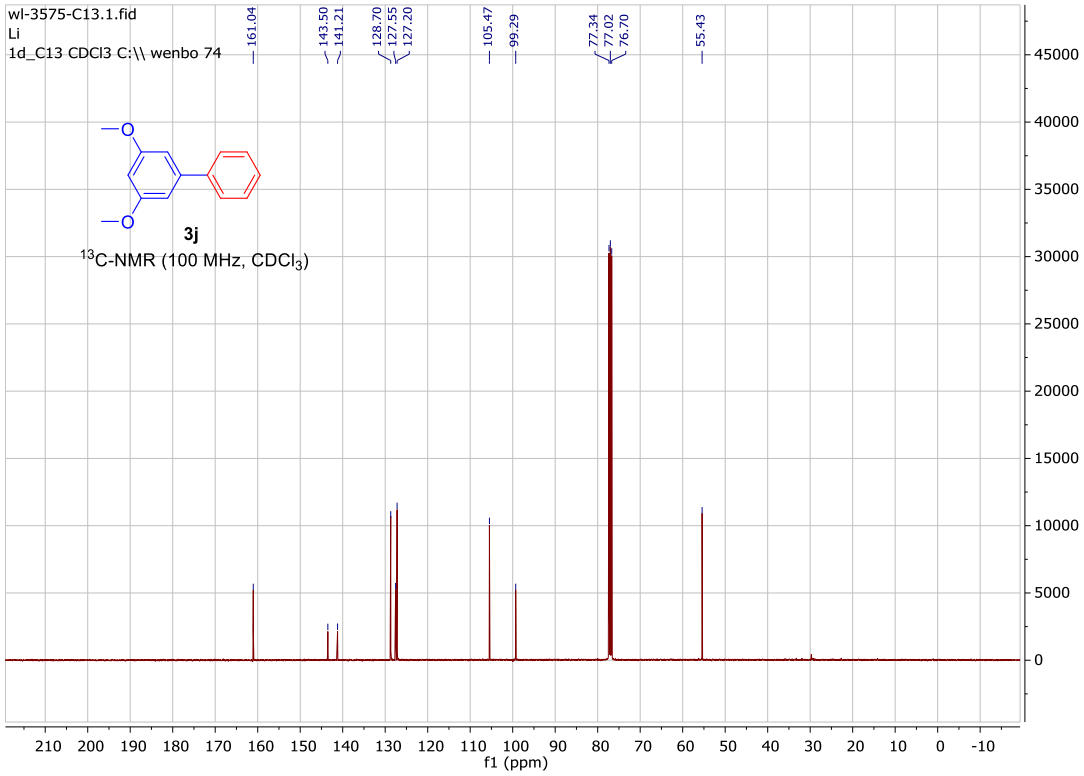

wl-3563-1119-C13.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 48
F
3h
13C-NMR (100 MHz, CDCl3)
163.68
161.24
140.26
137.35
137.32
128.81
128.72
128.64
127.25
127.02
115.71
115.50
f1 (ppm)

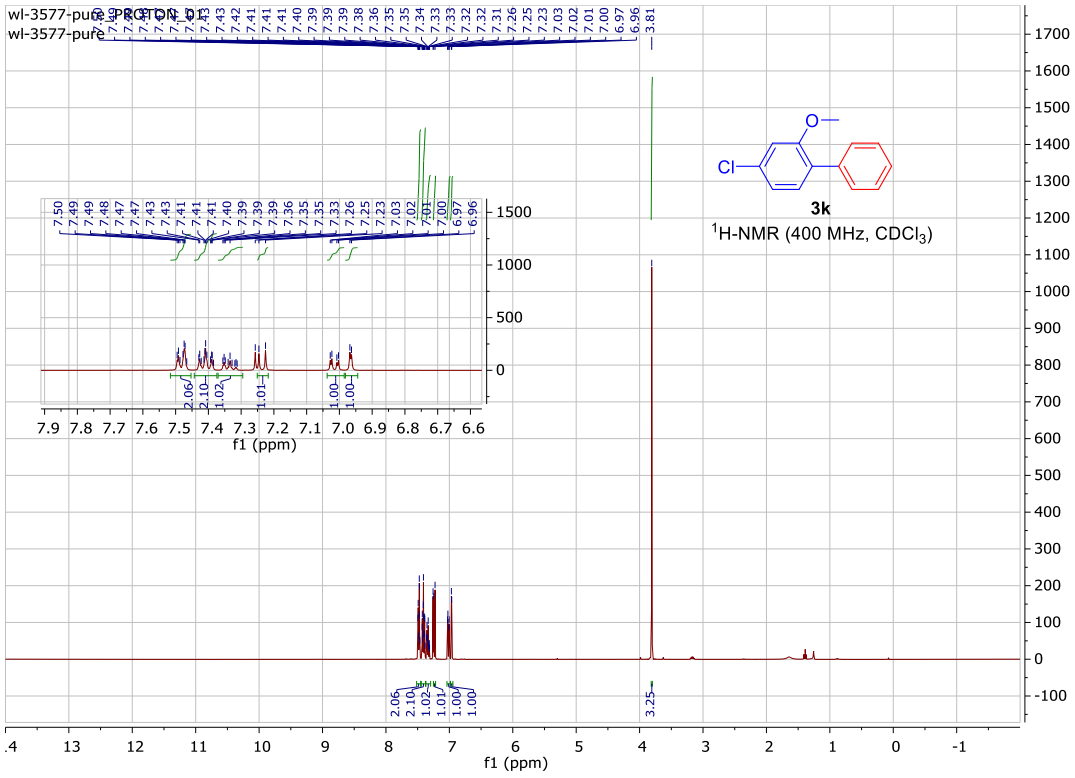

wl-3563-F.1.fid
Li
1d_F19CPD CDCl3 C:\\ wenbo 49
F
3h
19F-NMR (376 MHz, CDCl3)
-115.90
450
400
350
300
250
200
150
100
50
0
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

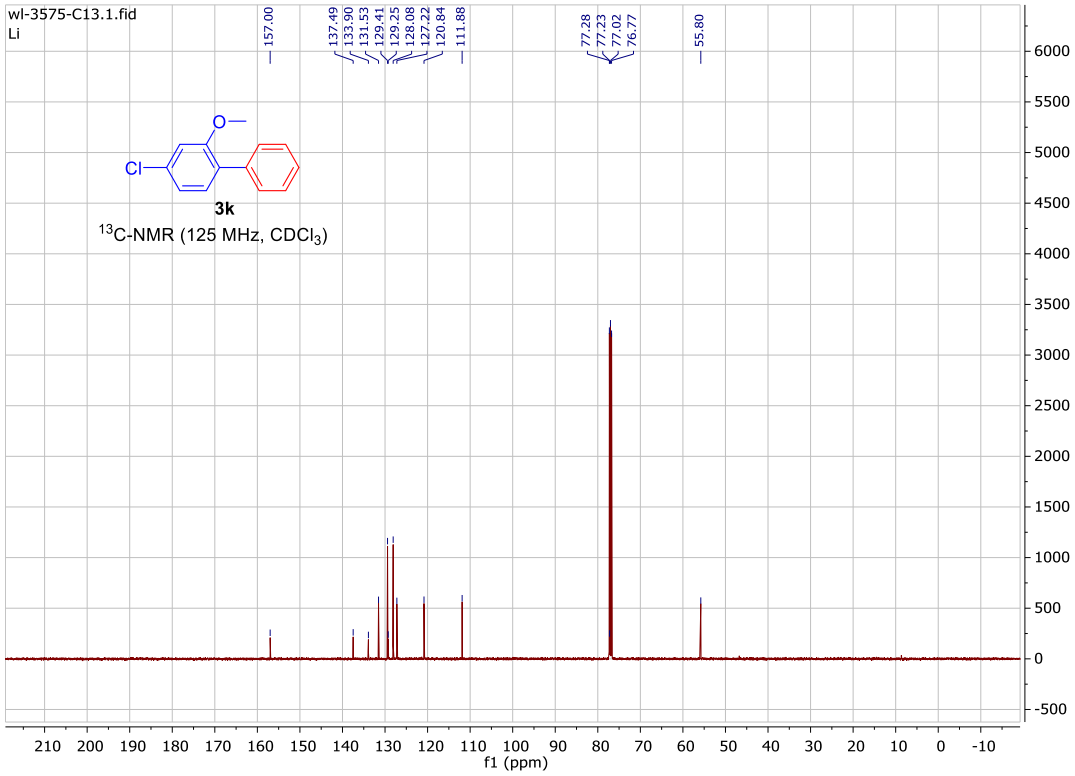

wl-3569-2.1.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 51
7.60 7.59 7.59 7.58 7.57 7.57 7.57 7.56 7.55 7.54 7.54 7.53 7.50 7.49 7.49 7.49 7.47 7.47 7.46 7.45 7.45 7.44 7.43 7.43 7.42 7.41 7.41 7.40 7.39 7.39 7.38 7.37 7.37 7.37 7.28
Cl
3i
1H-NMR (400 MHz, CDCl3)
4.00
5.11
f1 (ppm)

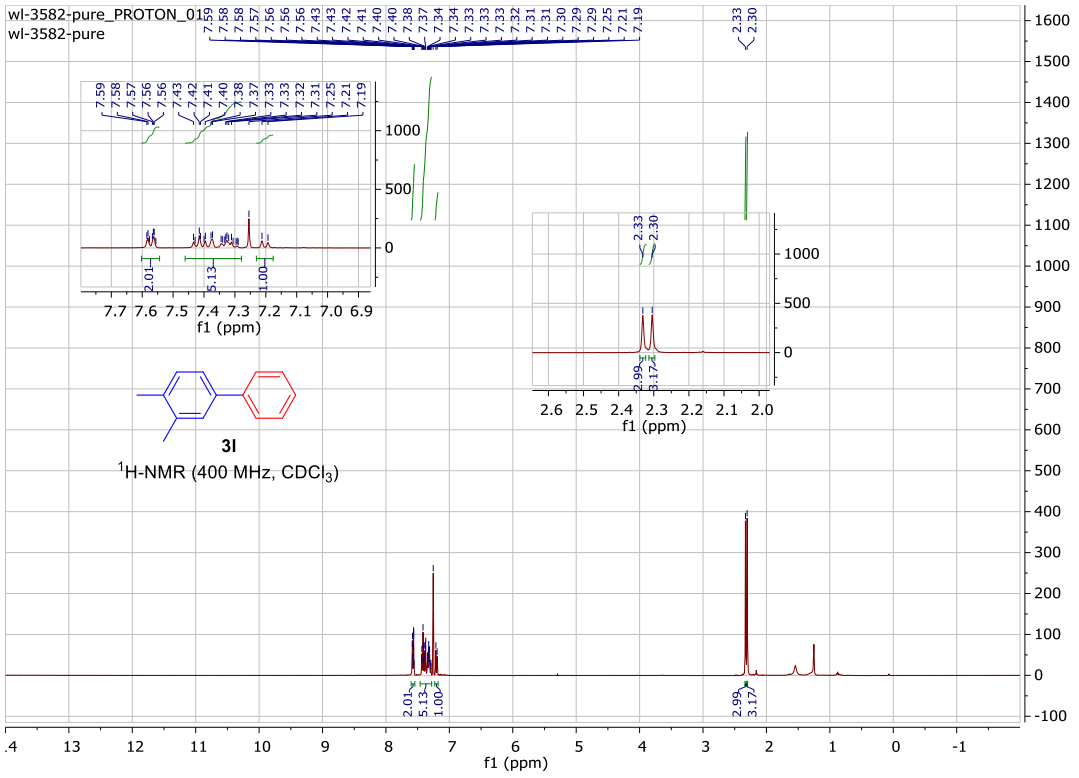

wl-3569-2-C13.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 52
140.00 139.67 133.38 128.91 128.88 128.39 127.59 126.99
77.34 77.02 76.71
Cl
3i
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

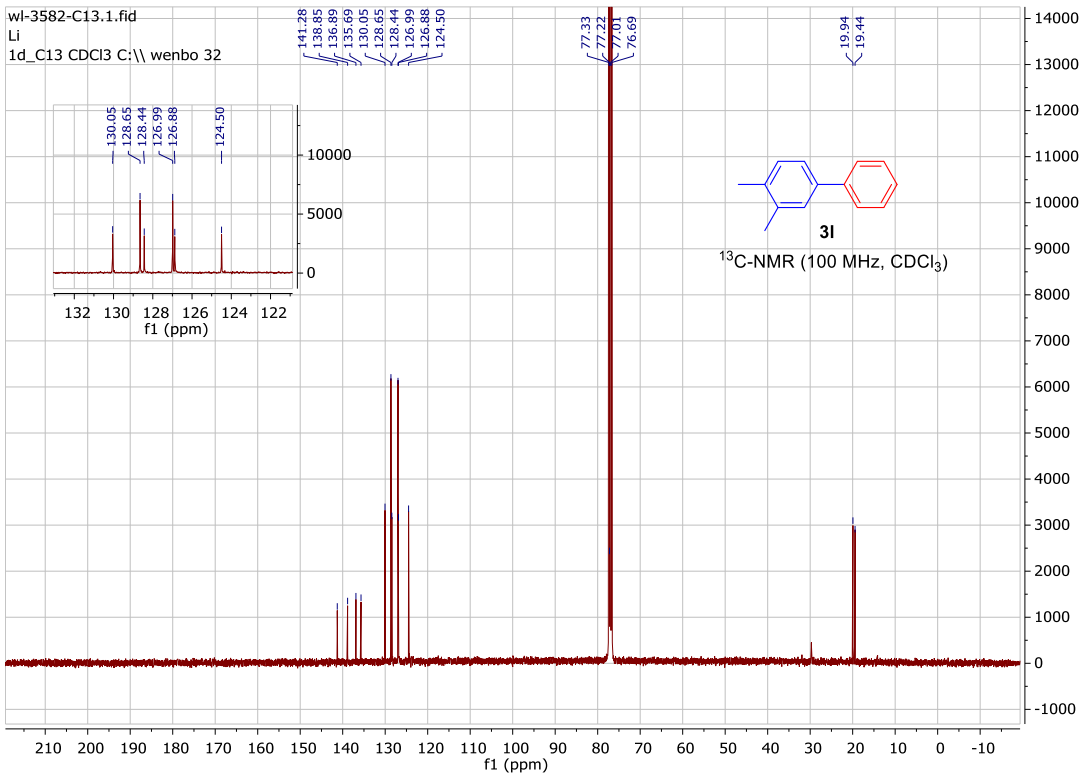

wl-3575-2 PROTON_01
3j
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

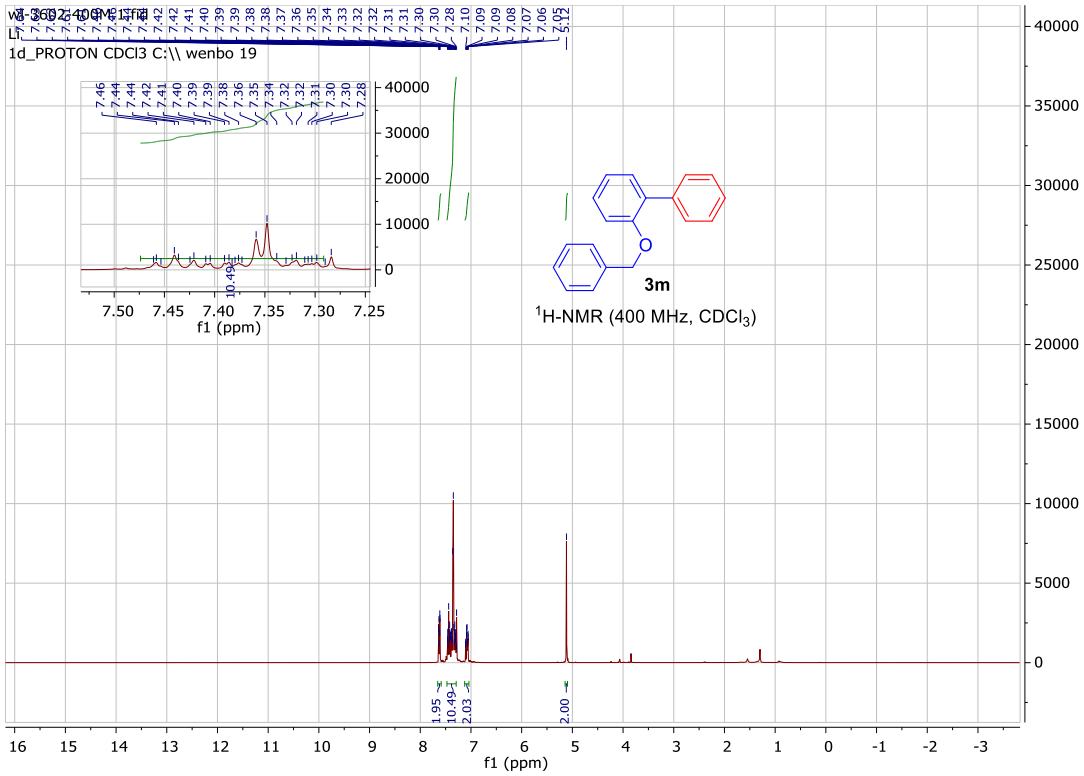

wl-3575-C13.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 74
3j
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

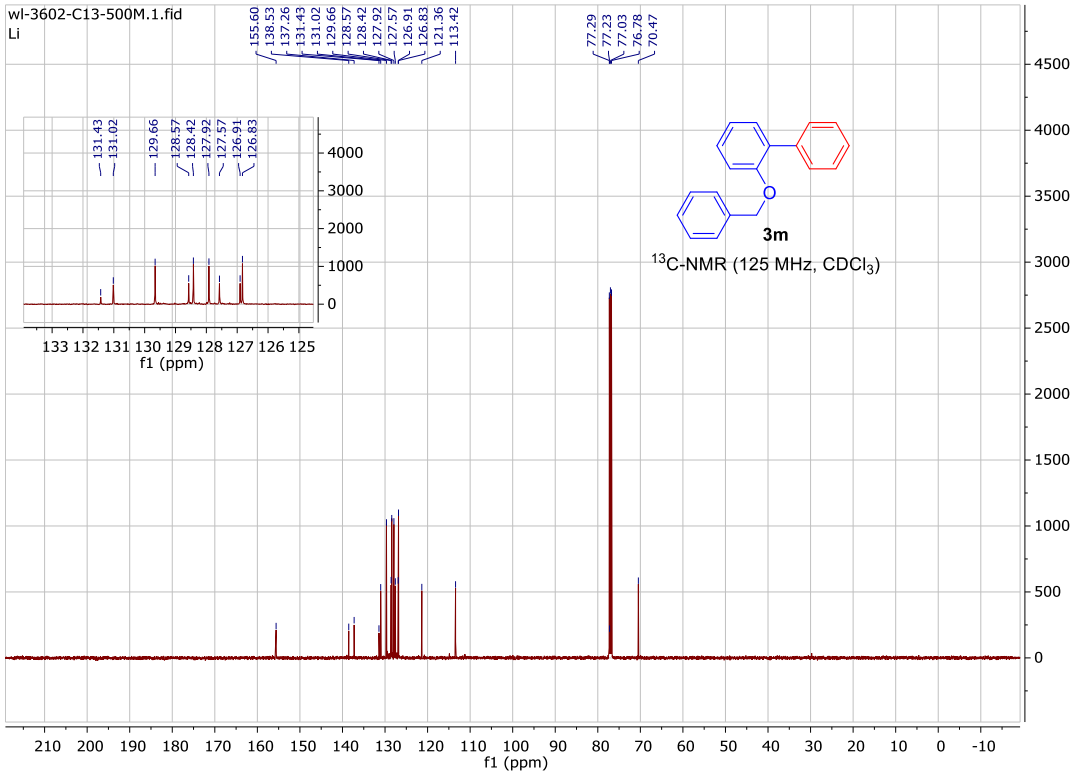

wl-3577-pure 1 PROTON 01
wl-3577-pure
3k
^{1}H-NMR (400 MHz, $CDCl_3$)
f1 (ppm)

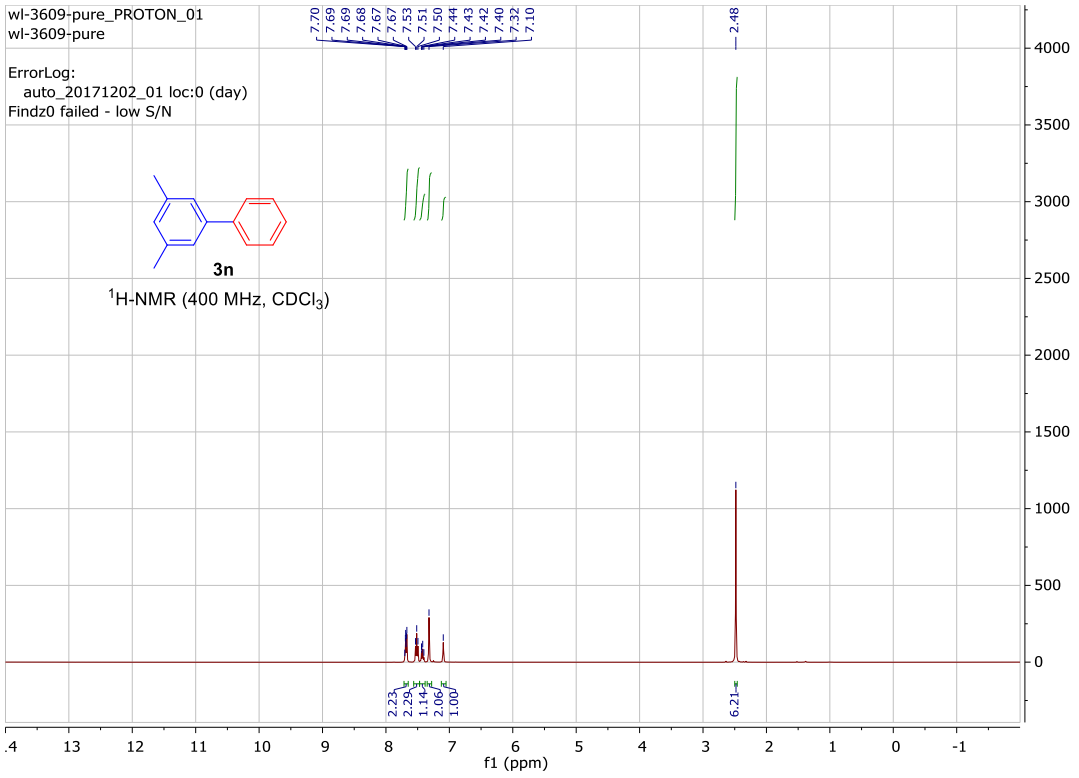

wl-3575-C13.1.fid
Li
3k
^{13}C-NMR (125 MHz, $CDCl_3$)
f1 (ppm)

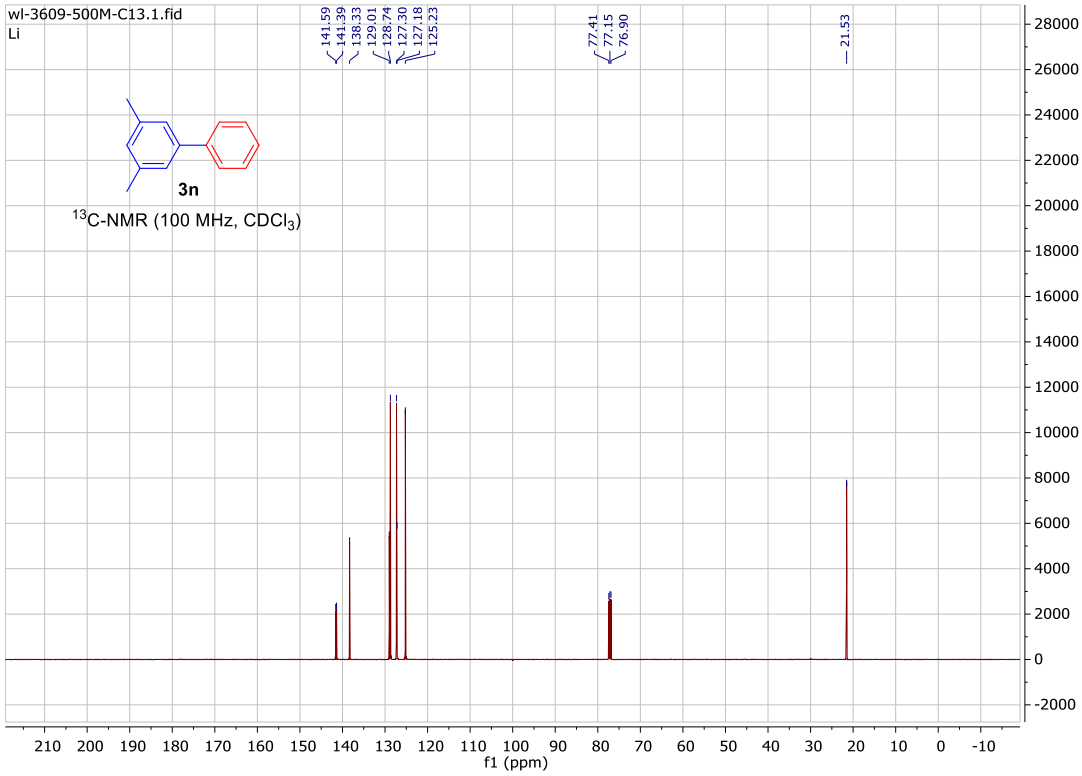

wl-3582-pure_PROTON_01
wl-3582-pure
3l
^{1}H-NMR (400 MHz, $CDCl_3$)
f1 (ppm)

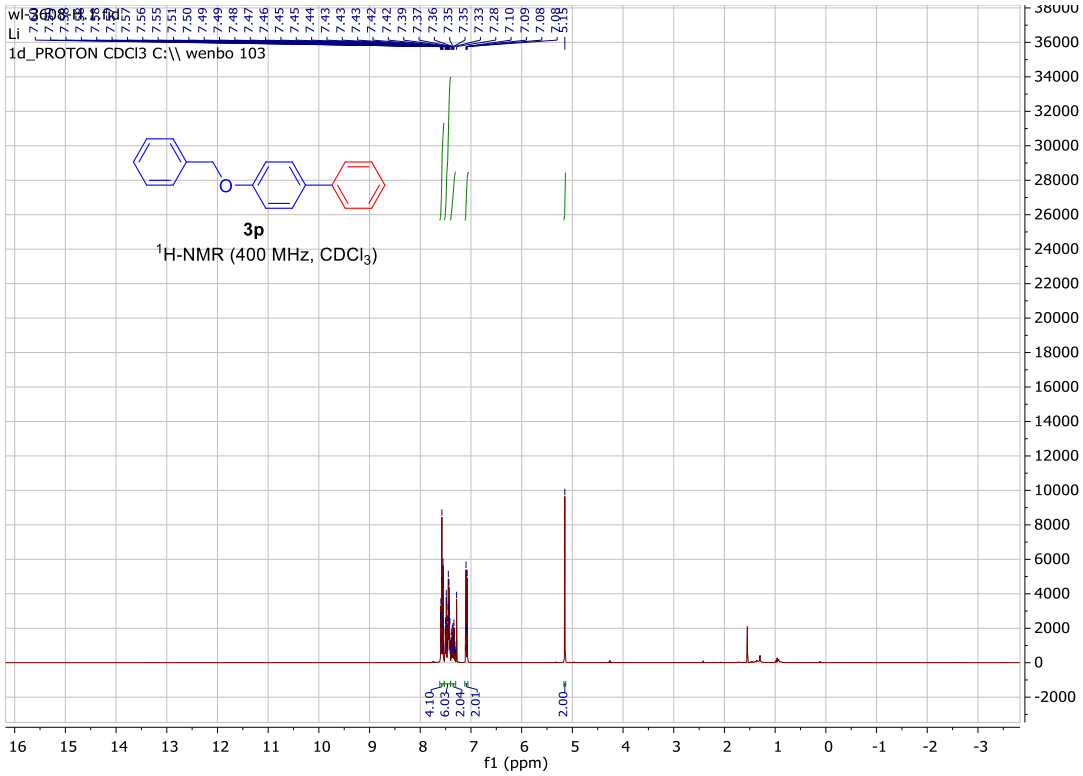

wl-3582-C13.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 32
3l
^{13}C-NMR (100 MHz, $CDCl_3$)
f1 (ppm)

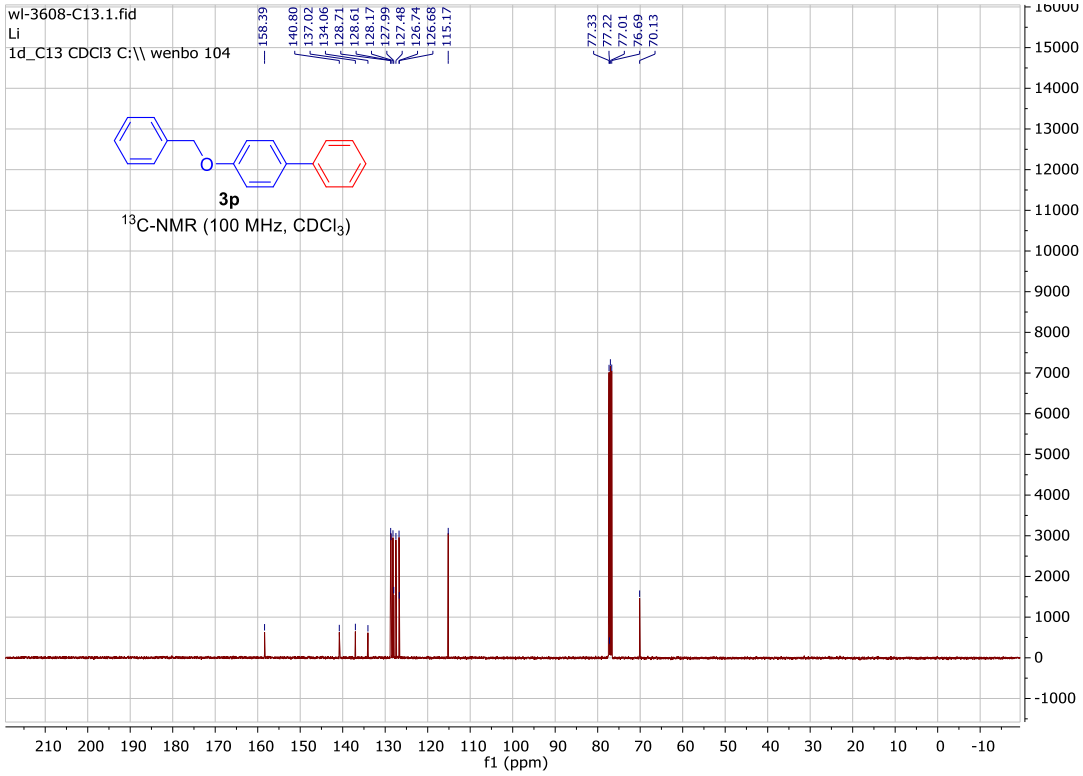

wl-3602-403M.1.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 19
3m
^{1}H-NMR (400 MHz, $CDCl_3$)
f1 (ppm)

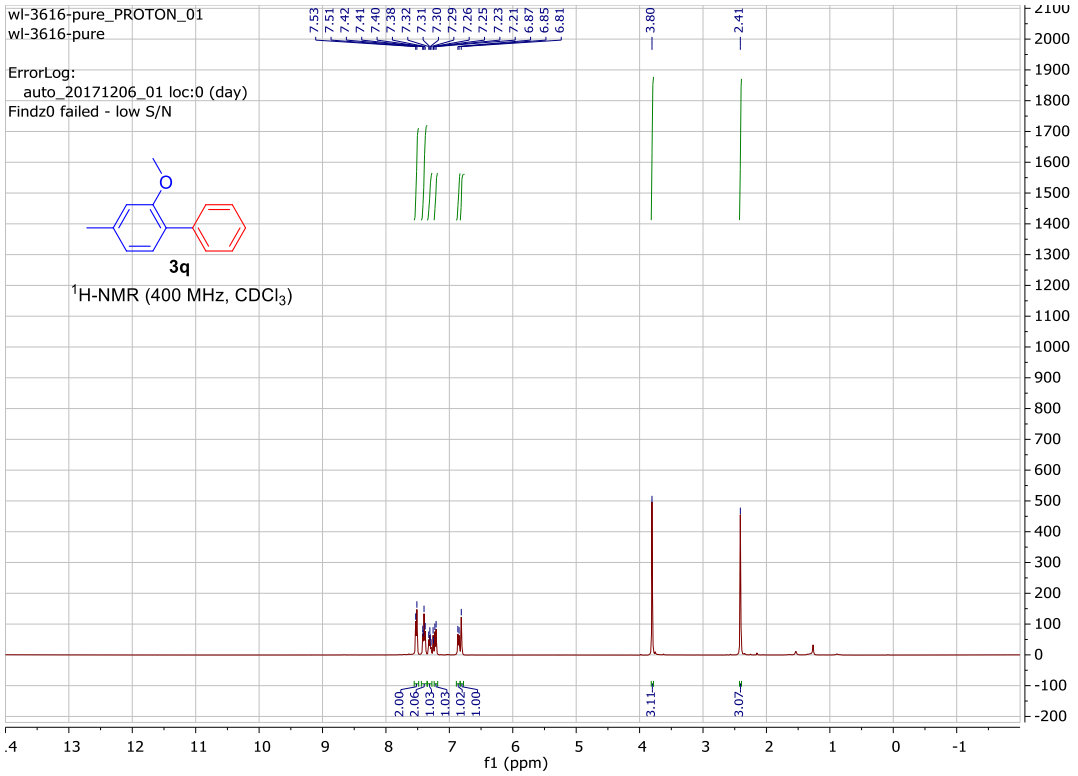

wl-3602-C13-500M.1.fid
Li
3m
^{13}C-NMR (125 MHz, $CDCl_3$)
f1 (ppm)

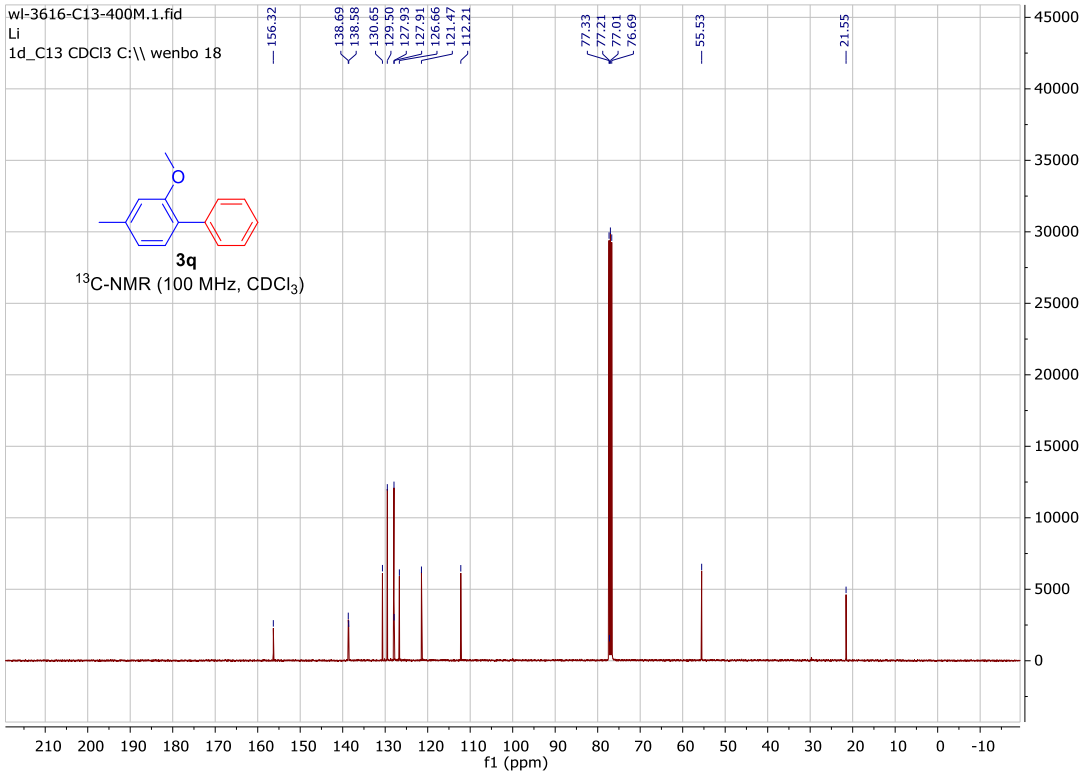

wl-3609-pure_PROTON_01
wl-3609-pure
ErrorLog:
auto_20171202_01 loc:0 (day)
Findz0 failed - low S/N
7.70
7.69
7.69
7.68
7.67
7.67
7.53
7.51
7.50
7.44
7.43
7.42
7.40
7.32
7.10
2.48
3n
1H-NMR (400 MHz, CDCl3)
2.23
2.29
1.14
2.06
1.00
6.21
f1 (ppm)

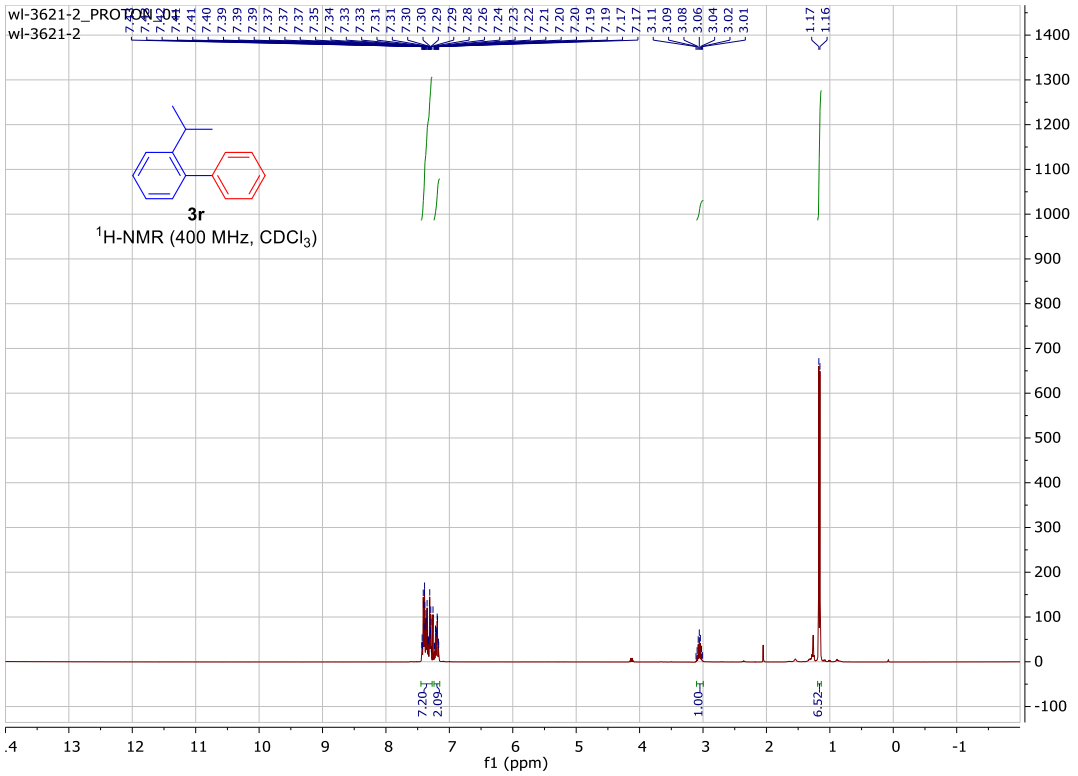

wl-3609-500M-C13.1.fid
Li
141.59
141.39
138.33
129.01
128.74
127.30
127.18
125.23
77.41
77.15
76.90
21.53
3n
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

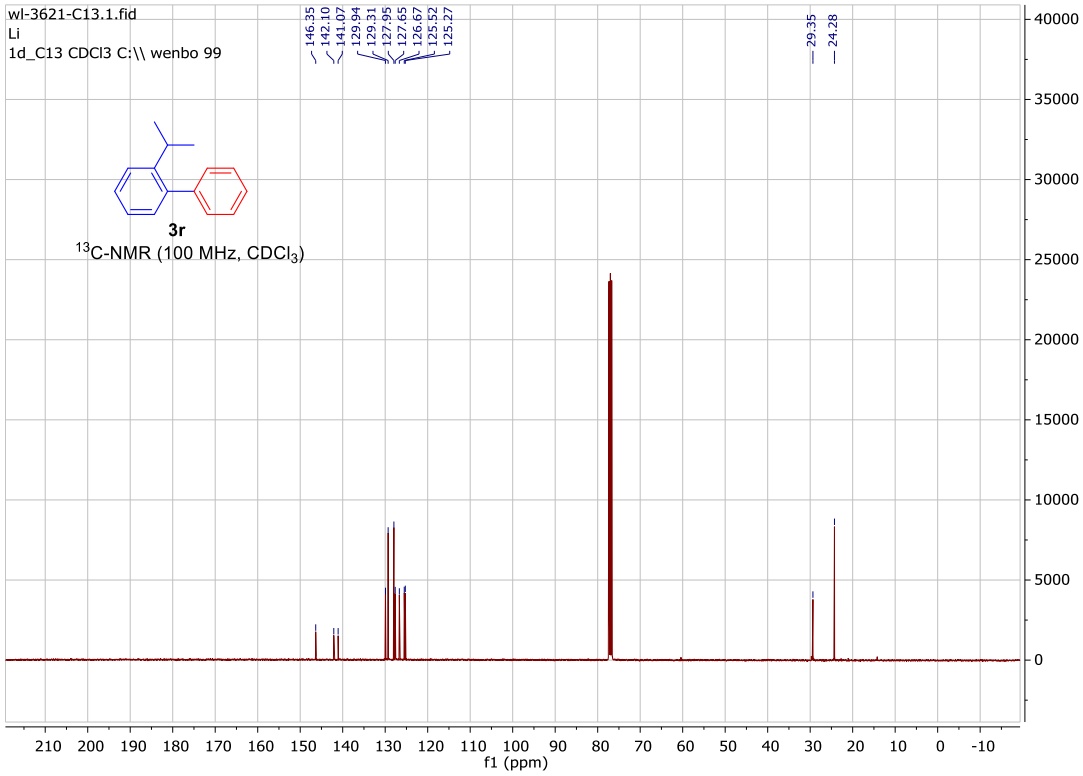

Li
1d_PROTON CDCl3 C:\\ wenbo 103
3p
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

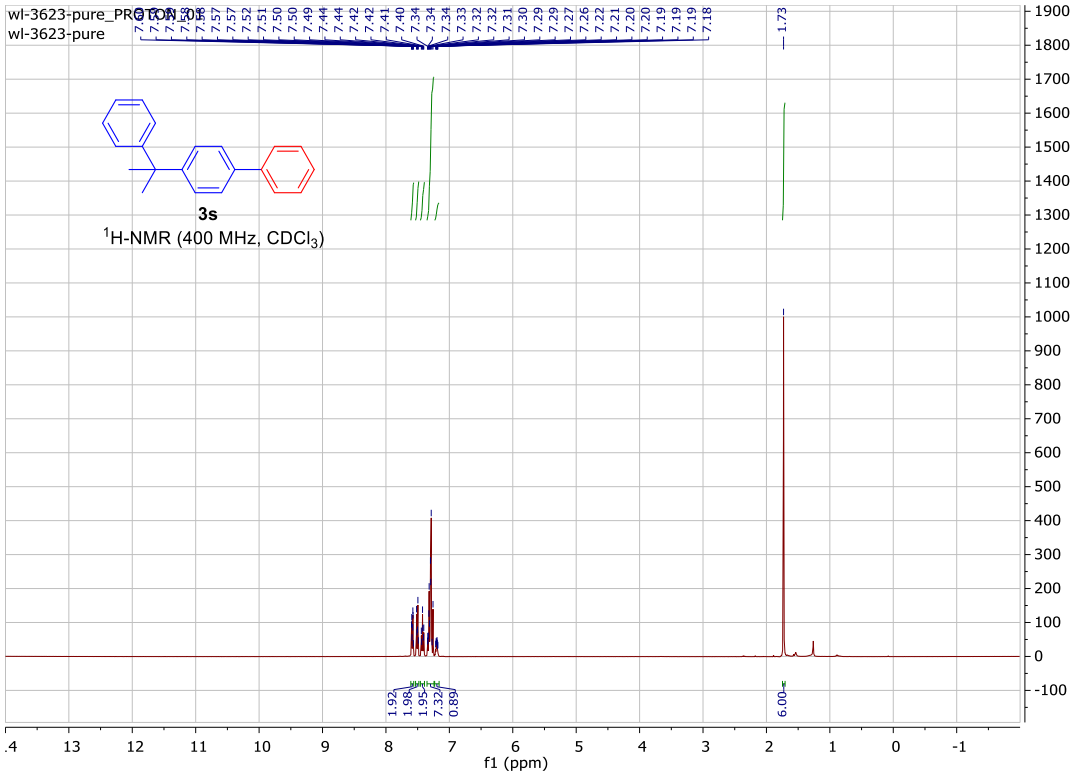

wl-3608-C13.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 104
3p
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

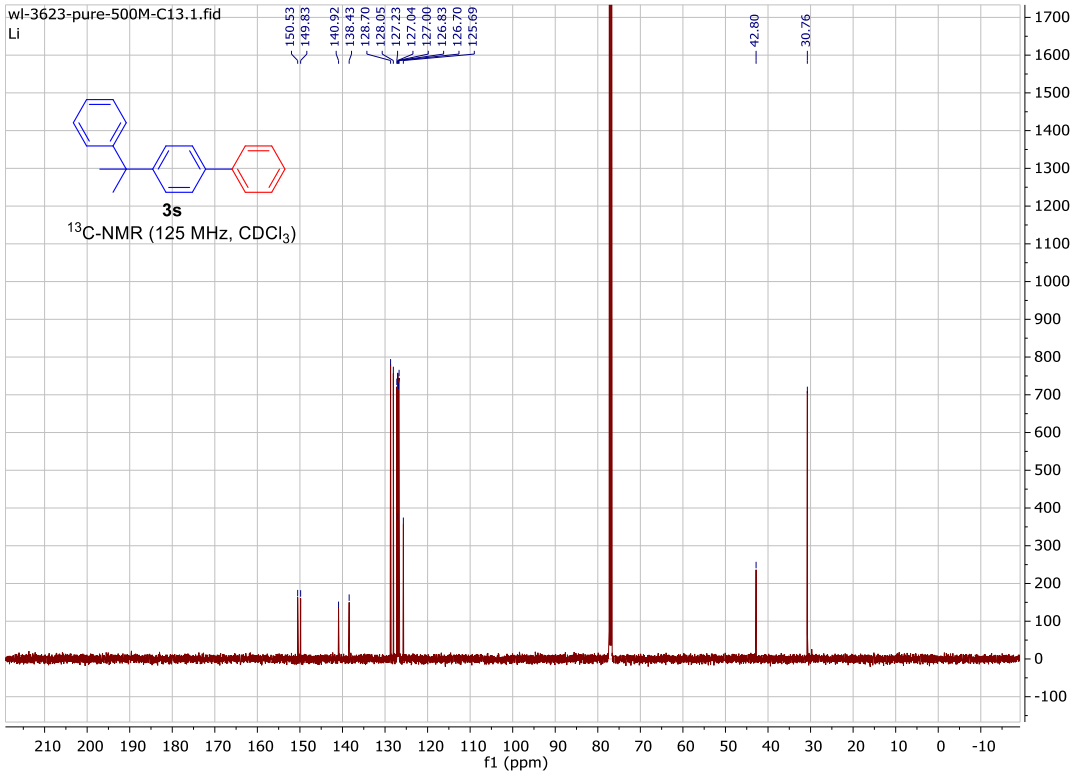

wl-3616-pure_PROTON_01
wl-3616-pure
ErrorLog:
auto_20171206_01 loc:0 (day)
Findz0 failed - low S/N
7.53
7.51
7.42
7.41
7.40
7.38
7.32
7.31
7.30
7.29
7.26
7.25
7.23
7.21
6.87
6.85
6.81
3.80
2.41
2.00
2.06
1.03
1.03
1.02
1.00
3.11
3.07
3q
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

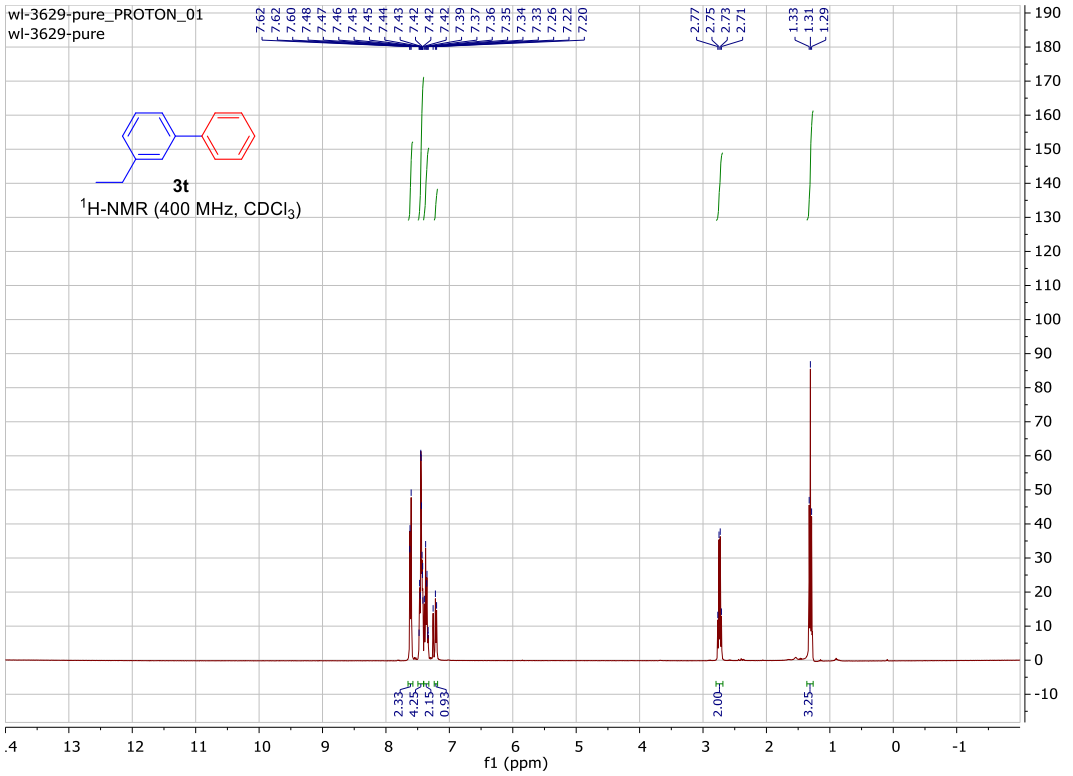

wl-3616-C13-400M.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 18
156.32
138.69
138.58
130.65
129.50
127.93
127.91
126.66
121.47
112.21
77.33
77.21
77.01
76.69
55.53
21.55
3q
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

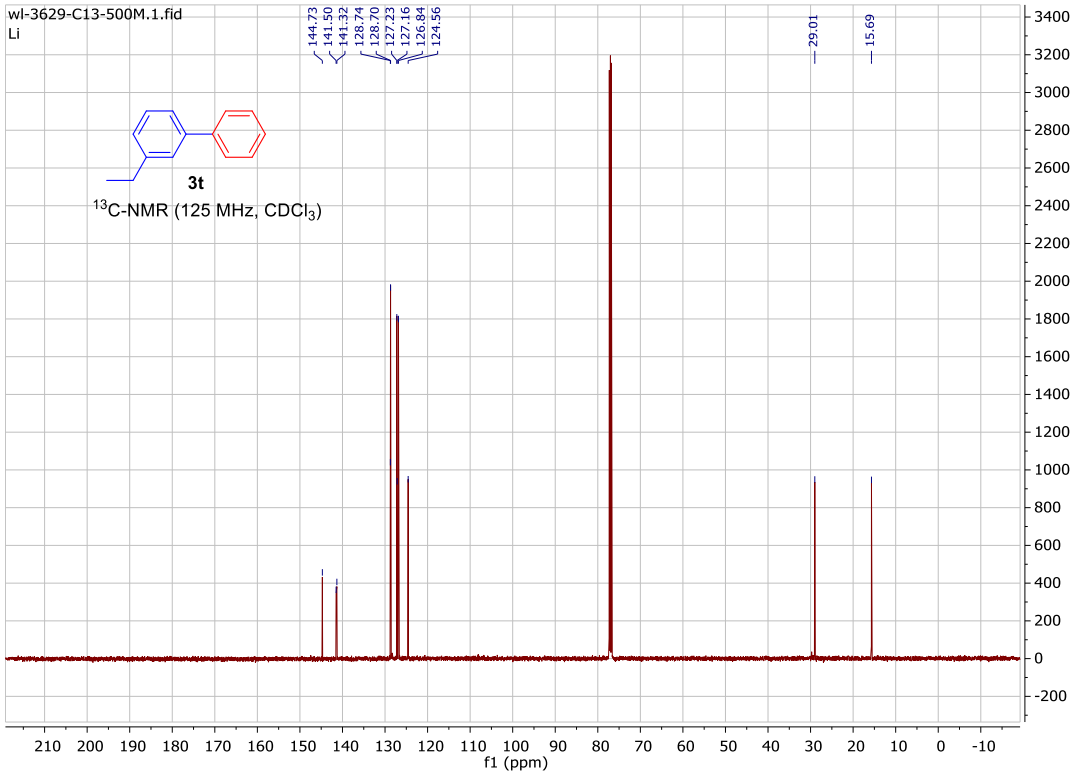

wl-3621-2_PROTON_01
wl-3621-2
3r
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

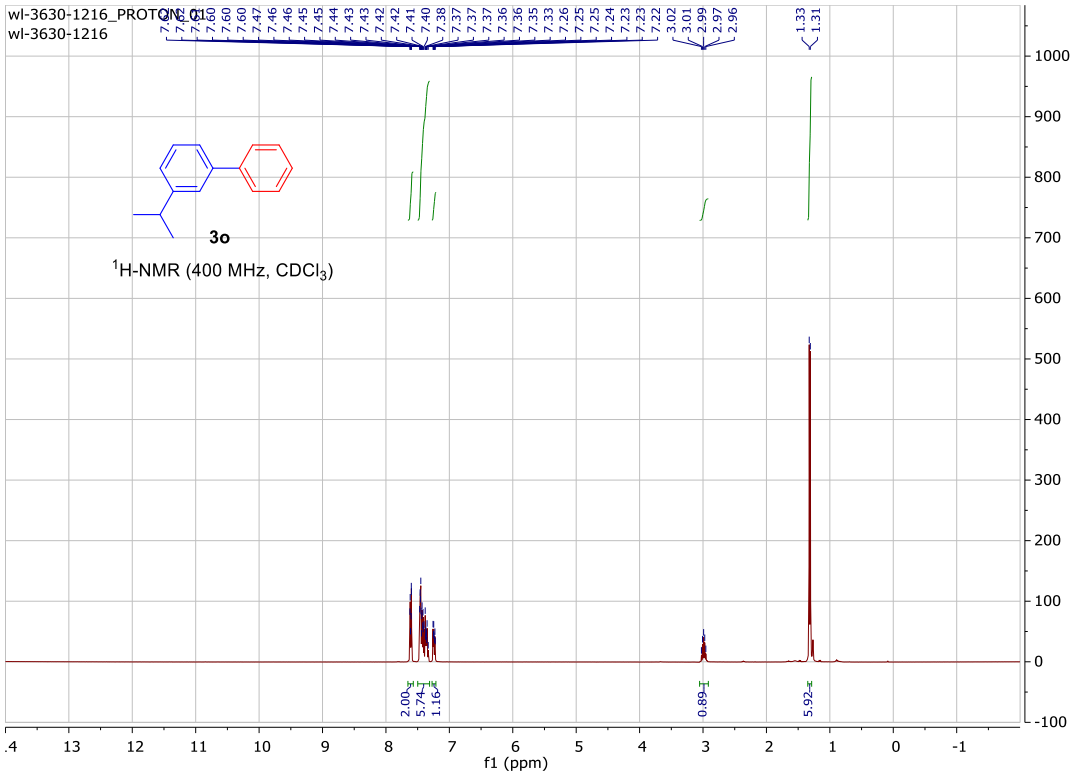

wl-3621-C13.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 99
3r
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

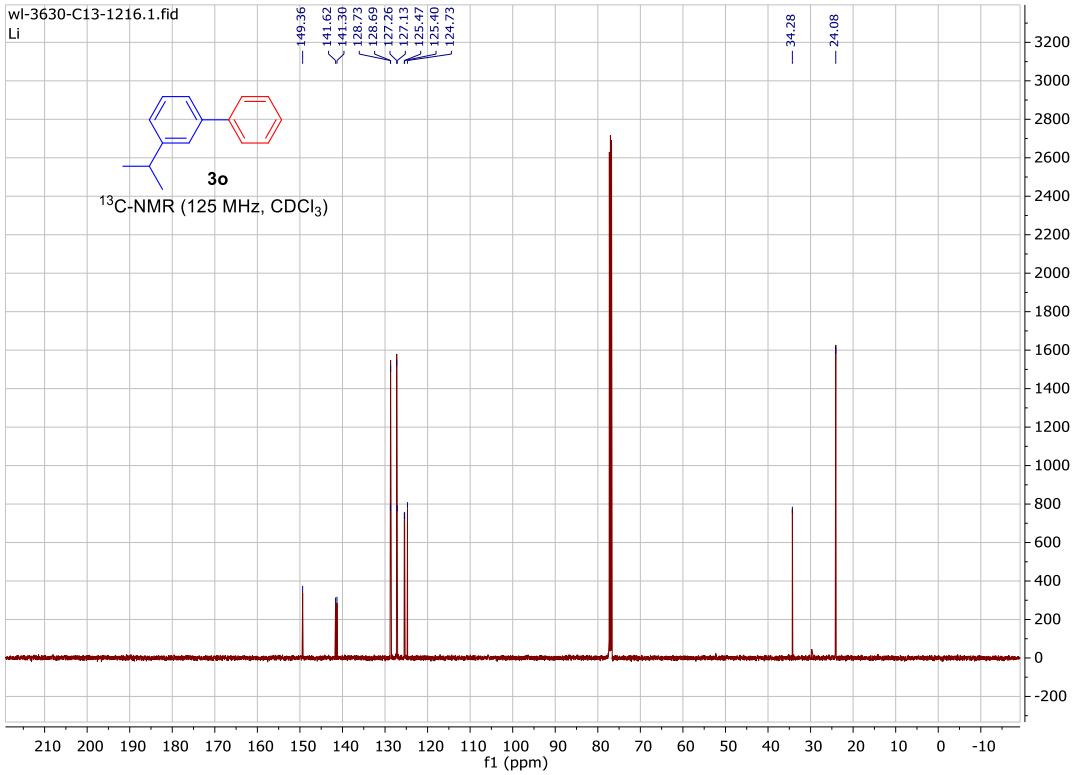

wl-3623-pure_PROTON_01
wl-3623-pure
3s
1H-NMR (400 MHz, CDCl3)
1.92
1.96
1.95
7.32
0.89
1.73
6.00
f1 (ppm)

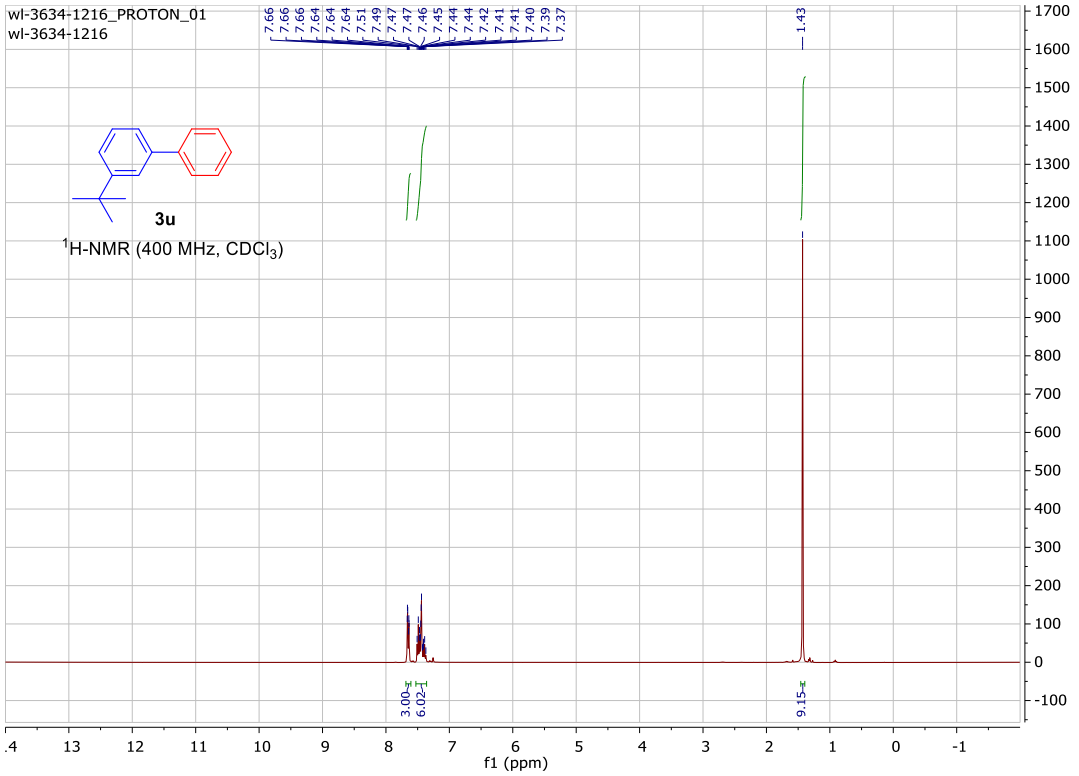

wl-3623-pure-500M-C13.1.fid
Li
150.53
149.83
140.92
138.43
128.70
128.05
127.23
127.04
127.00
126.83
126.70
125.69
42.80
30.76
3s
13C-NMR (125 MHz, CDCl3)
f1 (ppm)

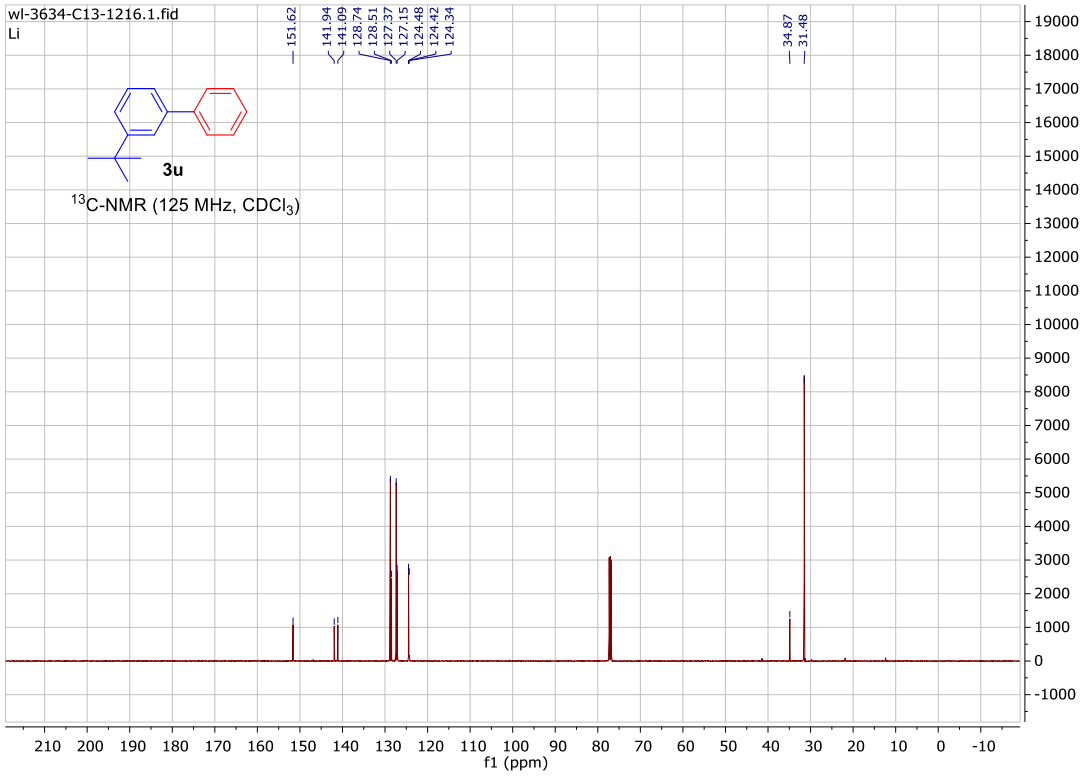

wl-3629-pure_PROTON_01
wl-3629-pure
3t
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

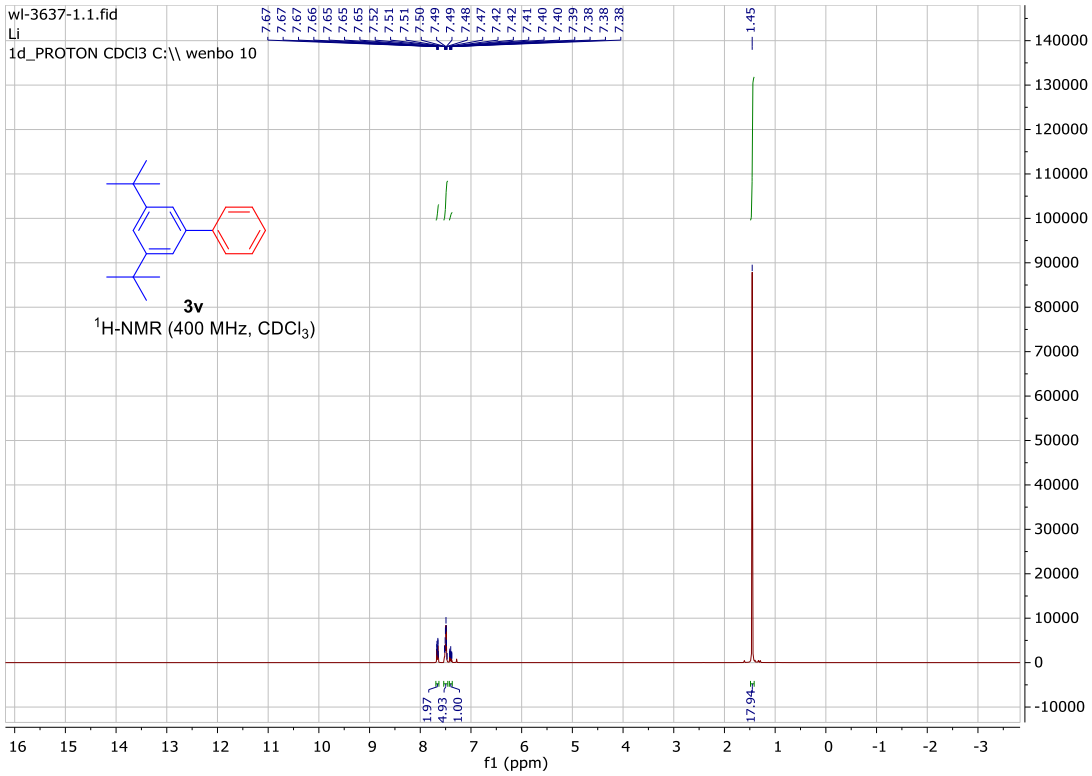

wl-3629-C13-500M.1.fid
Li
3t
13C-NMR (125 MHz, CDCl3)
f1 (ppm)

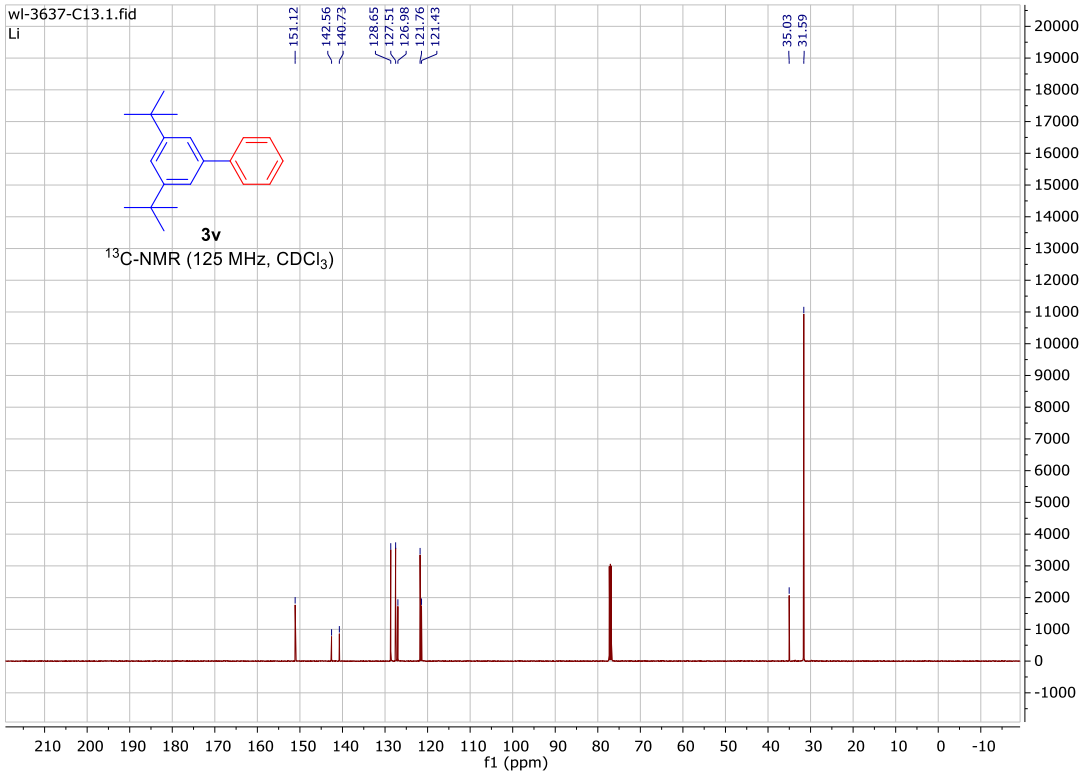

wl-3630-1216_PROTON_01
wl-3630-1216
3o
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

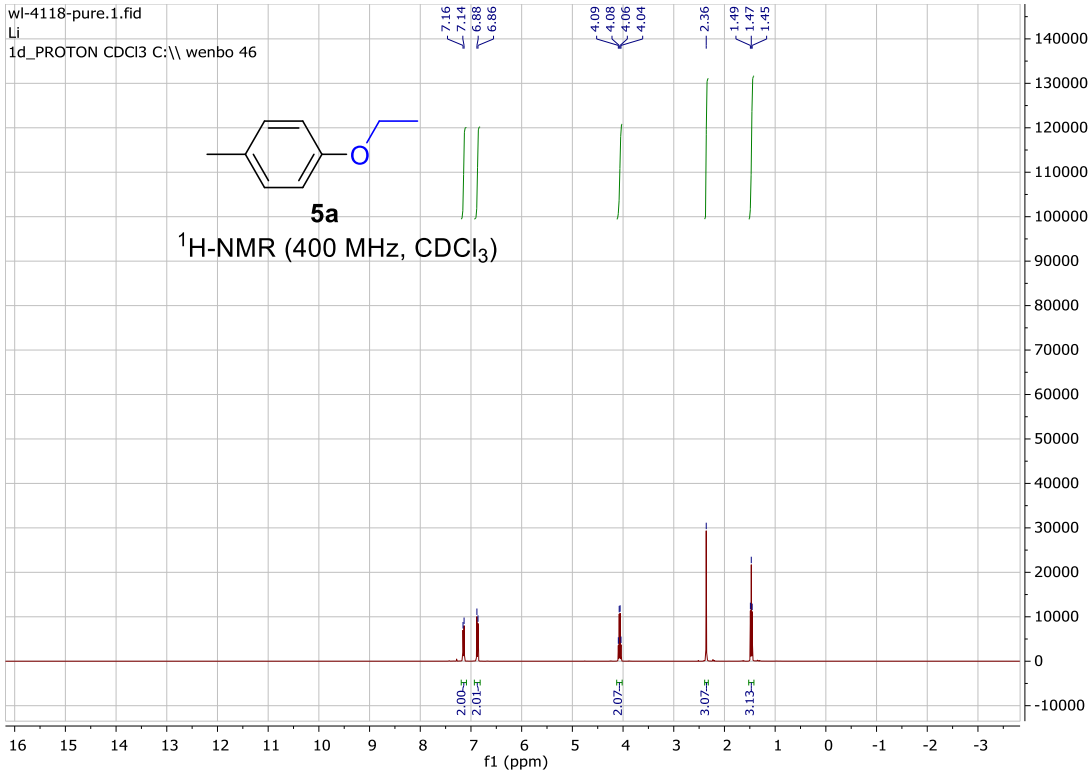

wl-3630-C13-1216.1.fid
Li
3o
13C-NMR (125 MHz, CDCl3)
f1 (ppm)

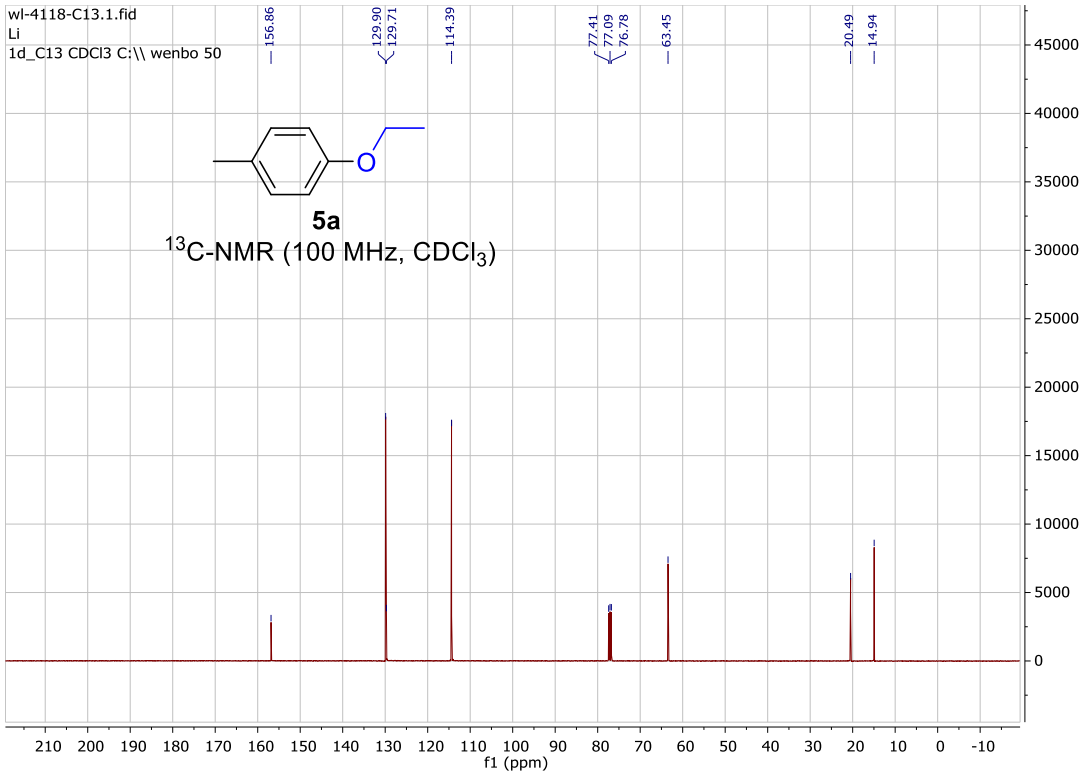

wl-3634-1216_PROTON_01
wl-3634-1216
7.66
7.66
7.66
7.64
7.64
7.64
7.51
7.49
7.47
7.47
7.46
7.45
7.44
7.44
7.42
7.41
7.41
7.40
7.39
7.37
1.43
3u
1H-NMR (400 MHz, CDCl3)
3.00
6.02
9.15
f1 (ppm)

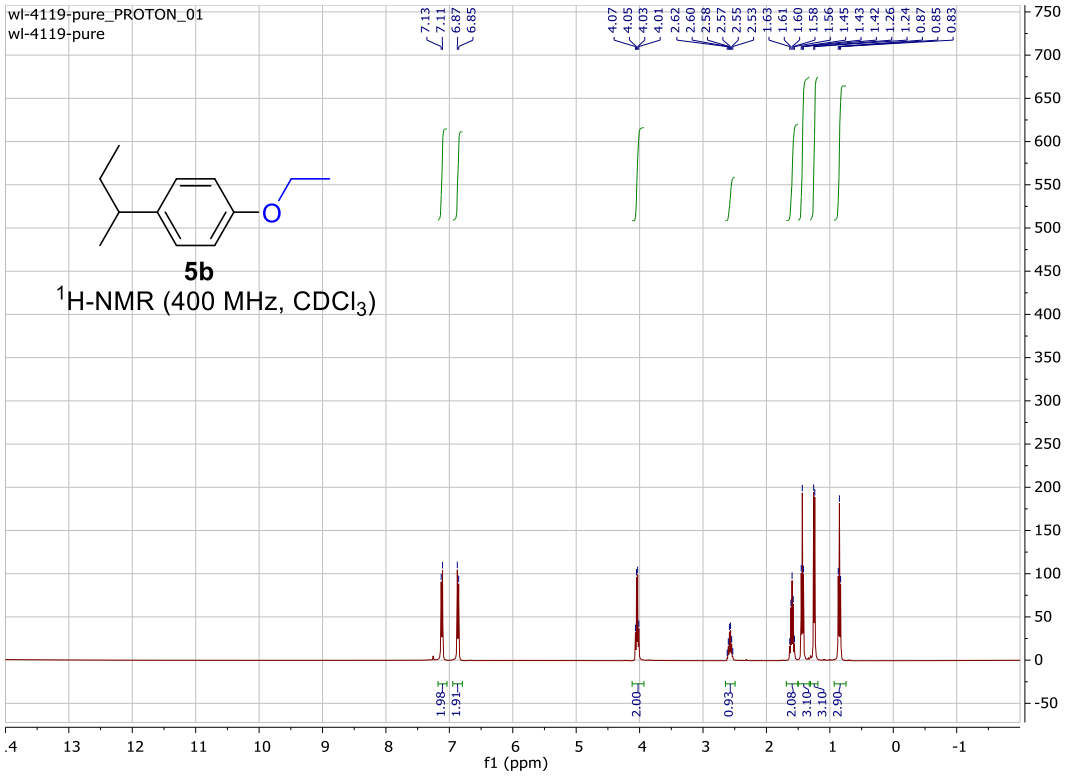

wl-3634-C13-1216.1.fid
Li
151.62
141.94
141.09
128.74
128.51
127.37
127.15
124.48
124.42
124.34
34.87
31.48
3u
13C-NMR (125 MHz, CDCl3)
f1 (ppm)

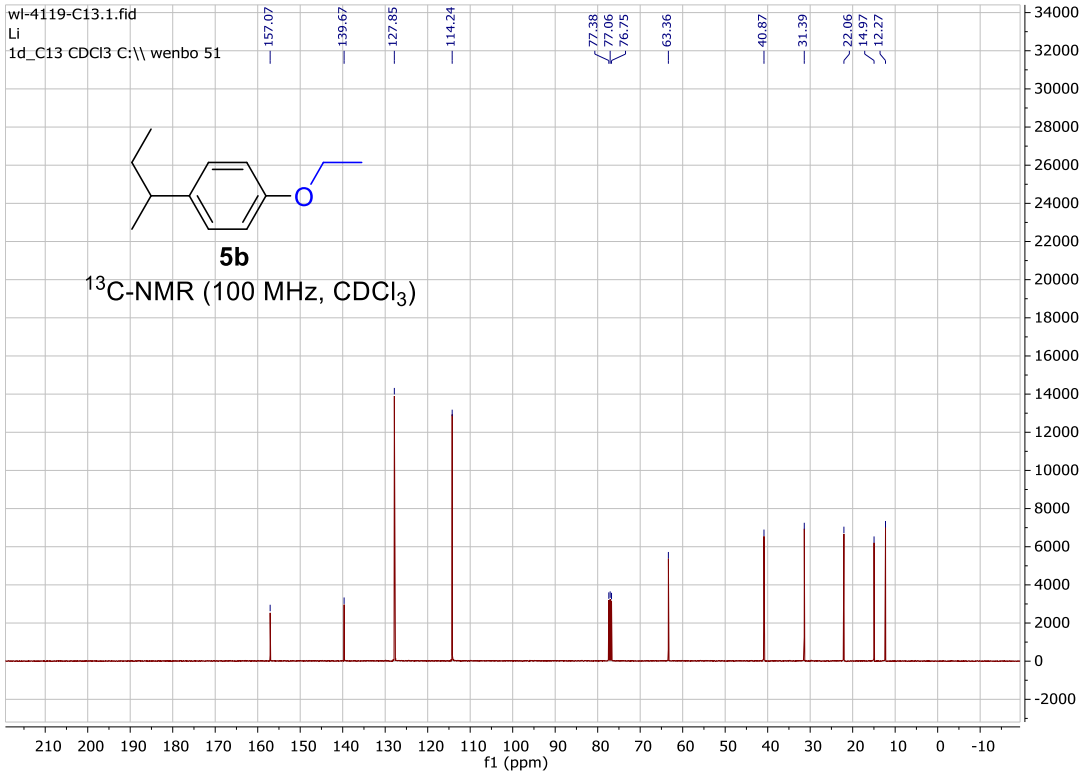

wl-3637-1.1.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 10
7.67
7.67
7.67
7.66
7.65
7.65
7.65
7.52
7.51
7.51
7.50
7.49
7.49
7.48
7.47
7.42
7.42
7.41
7.40
7.40
7.39
7.38
7.38
7.38
1.45
3v
1H-NMR (400 MHz, CDCl3)
1.97
4.93
1.00
17.94
f1 (ppm)

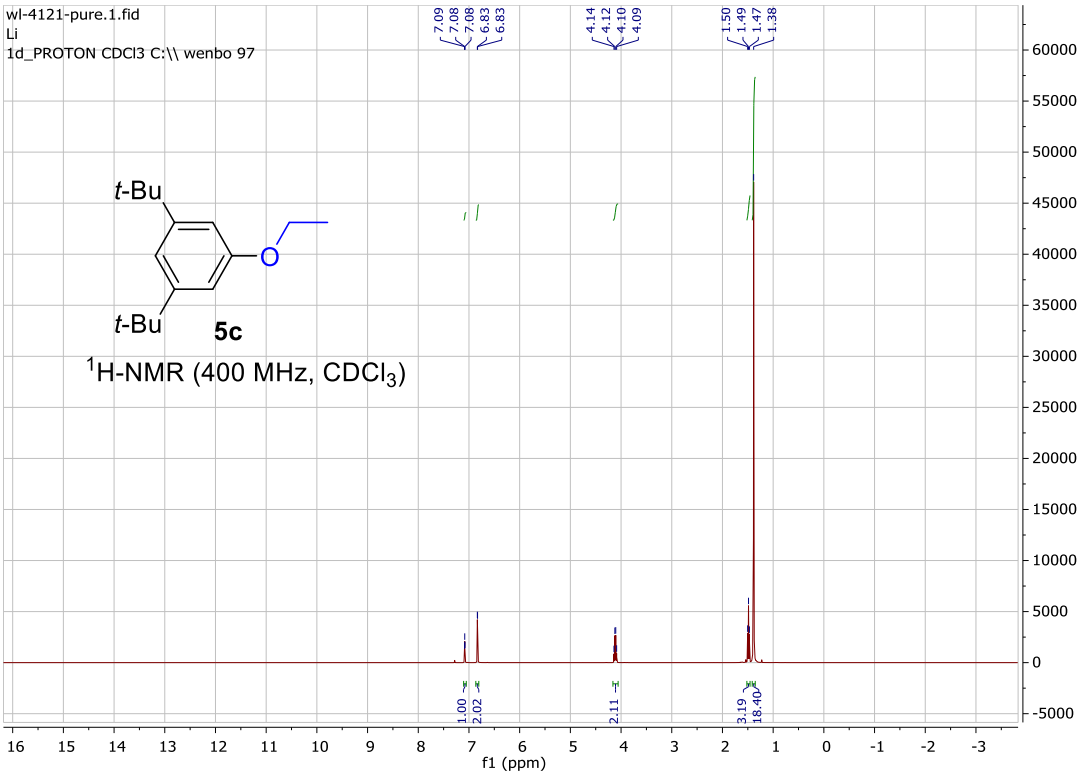

wl-3637-C13.1.fid
Li
151.12
142.56
140.73
128.65
127.51
126.98
121.76
121.43
35.03
31.59
3v
13C-NMR (125 MHz, CDCl3)
f1 (ppm)

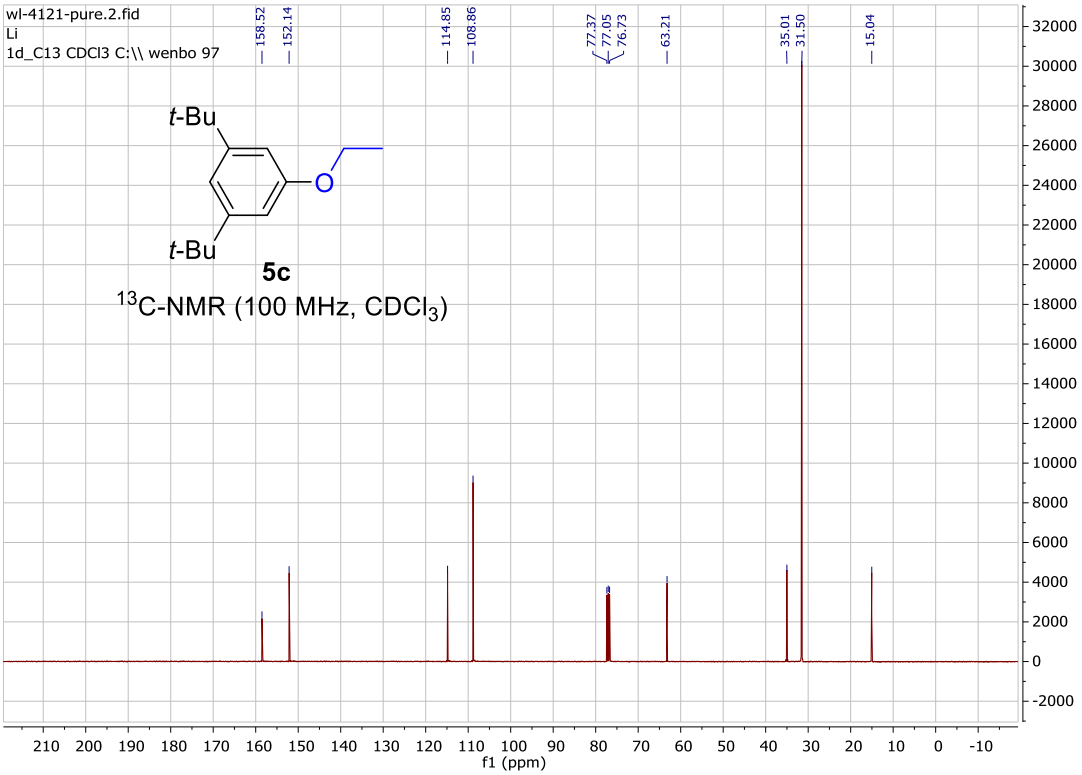

wl-4118-pure.1.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 46
7.16
7.14
6.88
6.86
4.09
4.08
4.06
4.04
2.36
1.49
1.47
1.45
5a
1H-NMR (400 MHz, CDCl3)
2.00
2.01
2.07
3.07
3.13
f1 (ppm)

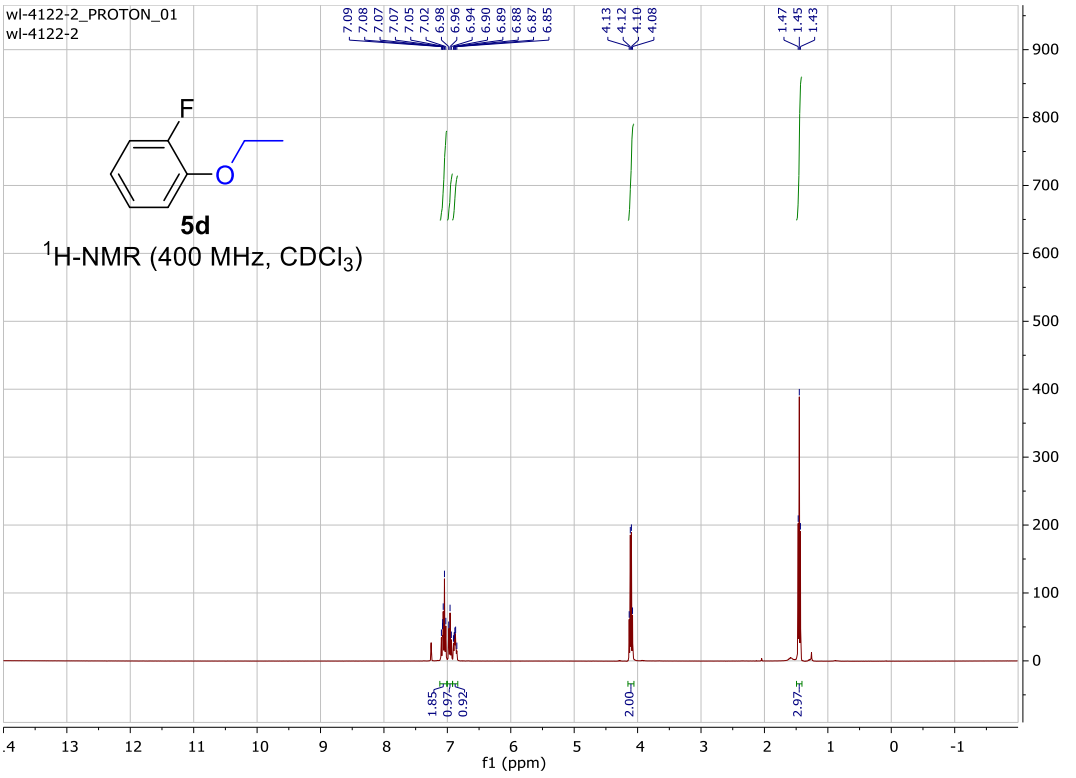

wl-4118-C13.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 50
156.86
129.90
129.71
114.39
77.41
77.09
76.78
63.45
20.49
14.94
5a
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

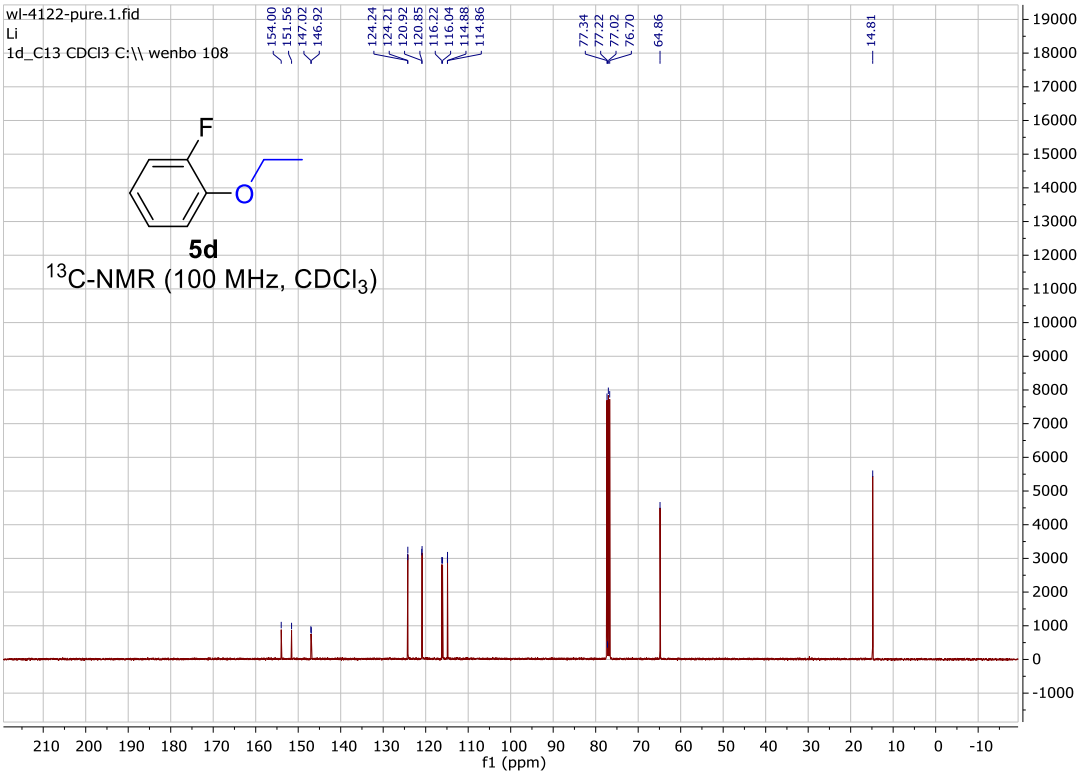

wl-4119-pure_PROTON_01
wl-4119-pure
5b
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

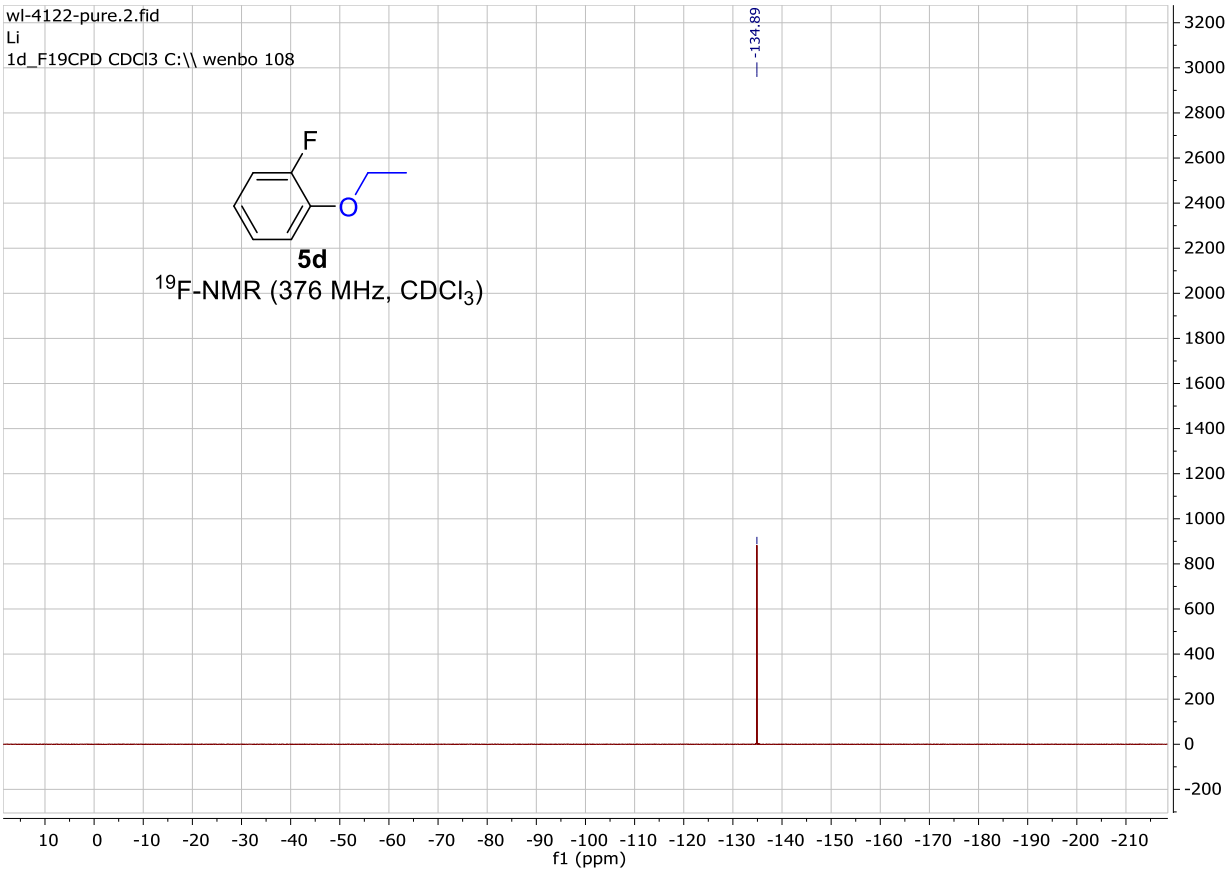

wl-4119-C13.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 51
5b
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

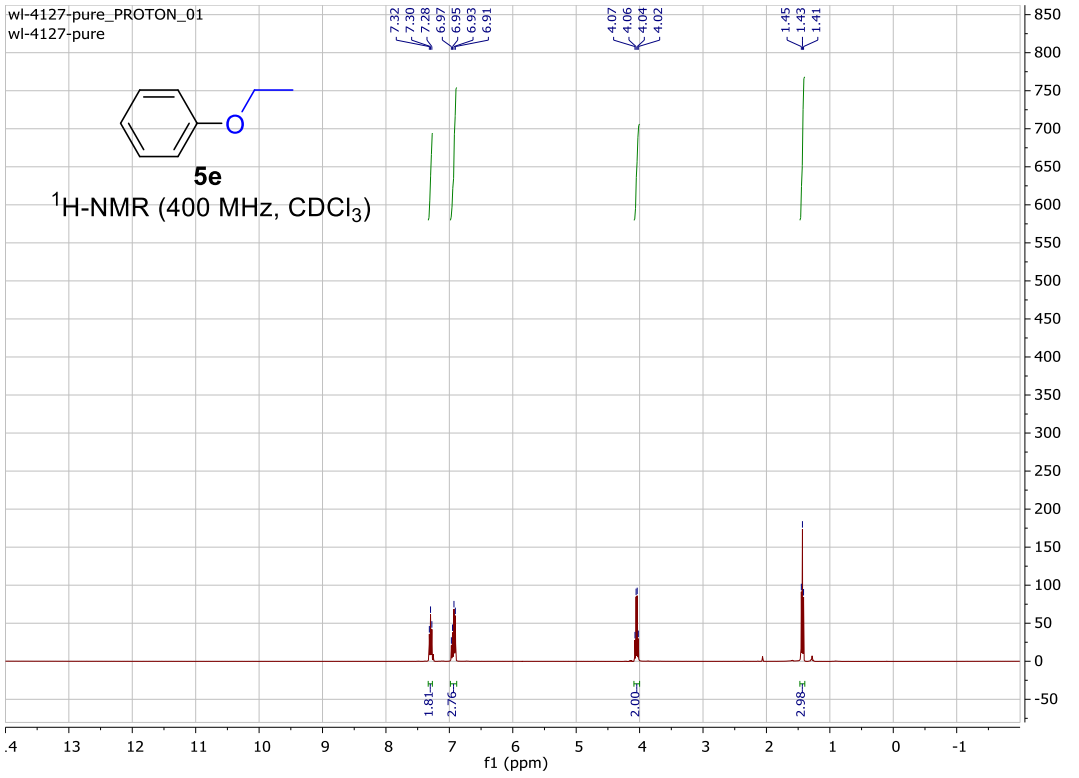

wl-4121-pure.1.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 97
7.09
7.08
7.08
6.83
6.83
4.14
4.12
4.10
4.09
1.50
1.49
1.47
1.38
t-Bu
t-Bu
5c
1H-NMR (400 MHz, CDCl3)
1.00
2.02
2.11
3.19
18.40
f1 (ppm)

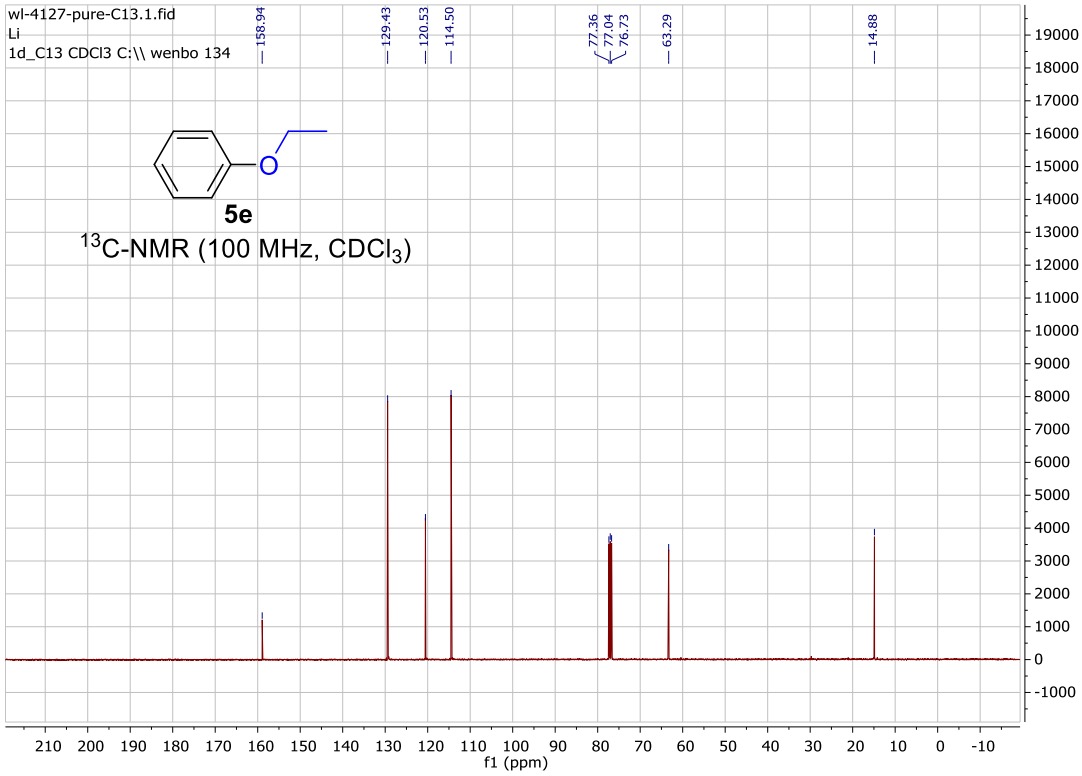

wl-4121-pure.2.fid
Li
1d_C13 CDCl3 C:\\ wenbo 97
158.52
152.14
114.85
108.86
77.37
77.05
76.73
63.21
35.01
31.50
15.04
t-Bu
t-Bu
5c
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

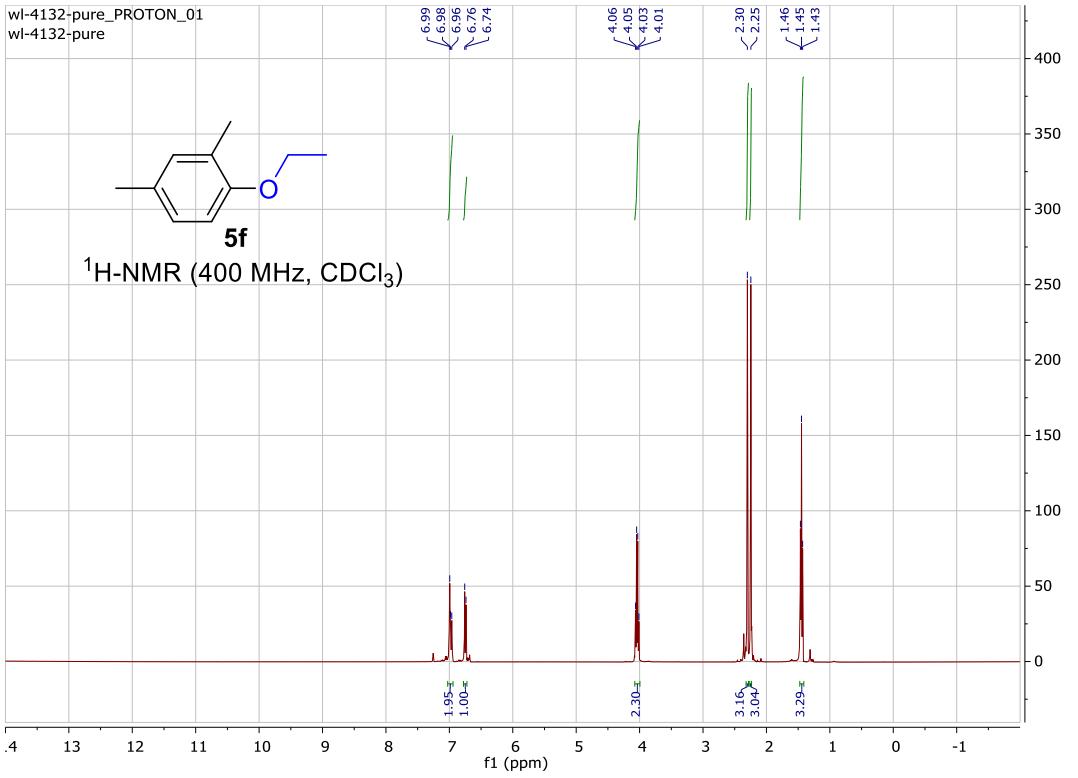

wl-4122-2_PROTON_01
wl-4122-2
7.09
7.08
7.07
7.07
7.05
7.02
6.98
6.96
6.94
6.90
6.89
6.88
6.87
6.85
4.13
4.12
4.10
4.08
1.47
1.45
1.43
F
O
5d
1H-NMR (400 MHz, CDCl3)
1.85
0.97
0.92
2.00
2.97
f1 (ppm)

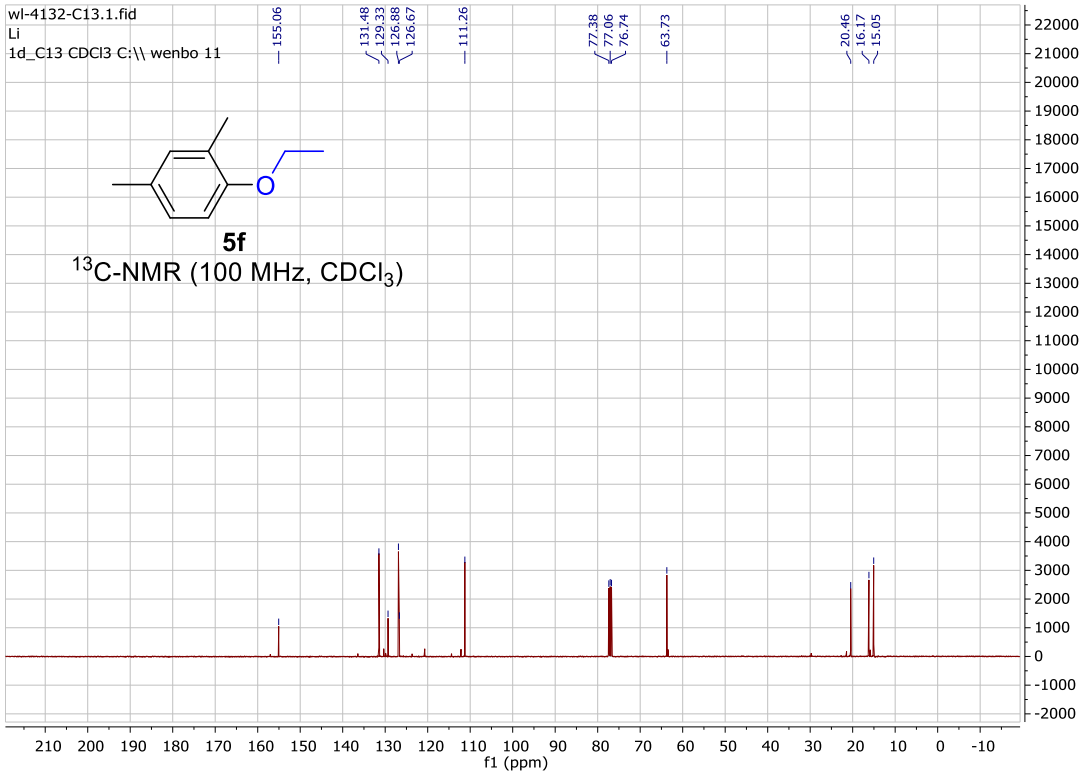

wl-4122-pure.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 108
154.00
151.56
147.02
146.92
124.24
124.21
120.92
120.85
116.22
116.04
114.88
114.86
77.34
77.22
77.02
76.70
64.86
14.81
F
O
5d
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

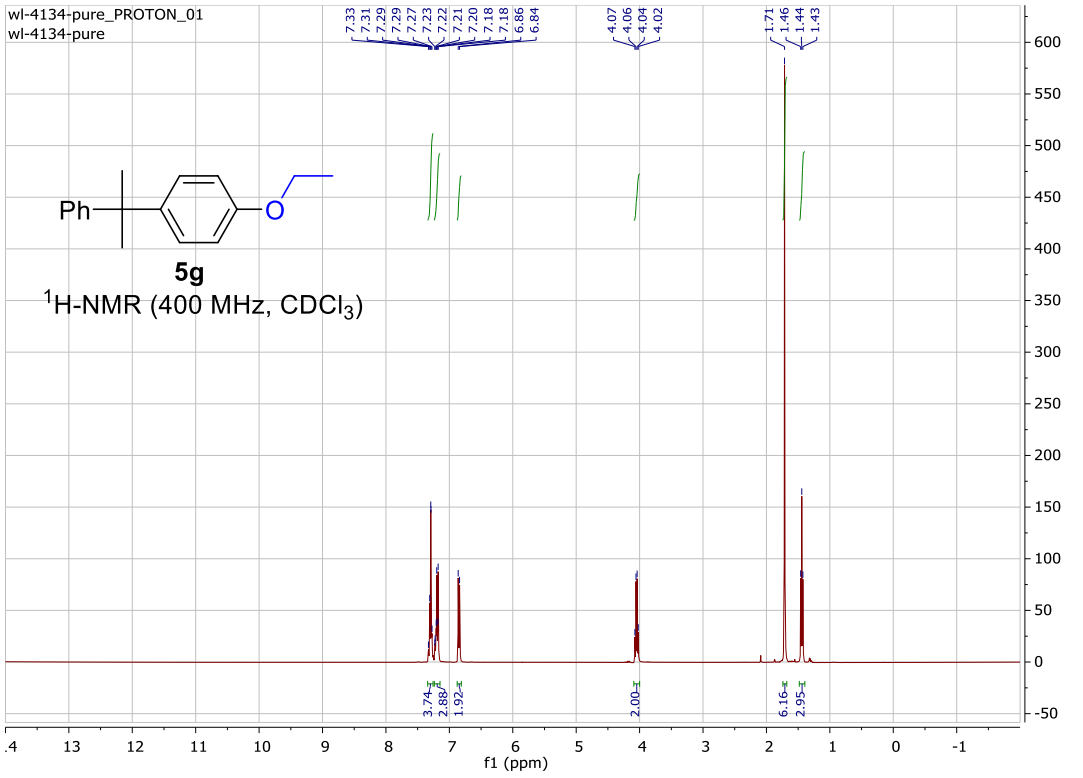

wl-4122-pure.2.fid
Li
1d_F19CPD CDCl3 C:\\ wenbo 108
-134.89
F
O
5d
19F-NMR (376 MHz, CDCl3)
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

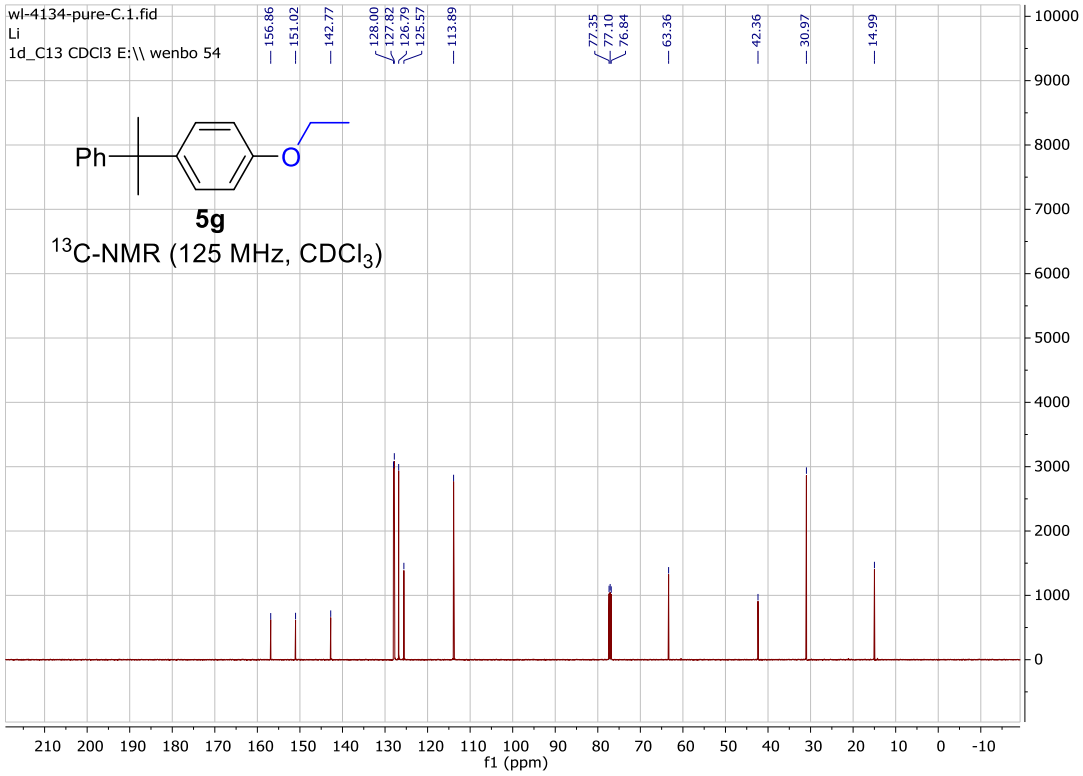

wl-4127-pure_PROTON_01
wl-4127-pure
7.32
7.30
7.28
6.97
6.95
6.93
6.91
4.07
4.06
4.04
4.02
1.45
1.43
1.41
5e
1H-NMR (400 MHz, CDCl3)
1.81
2.76
2.00
2.98
f1 (ppm)

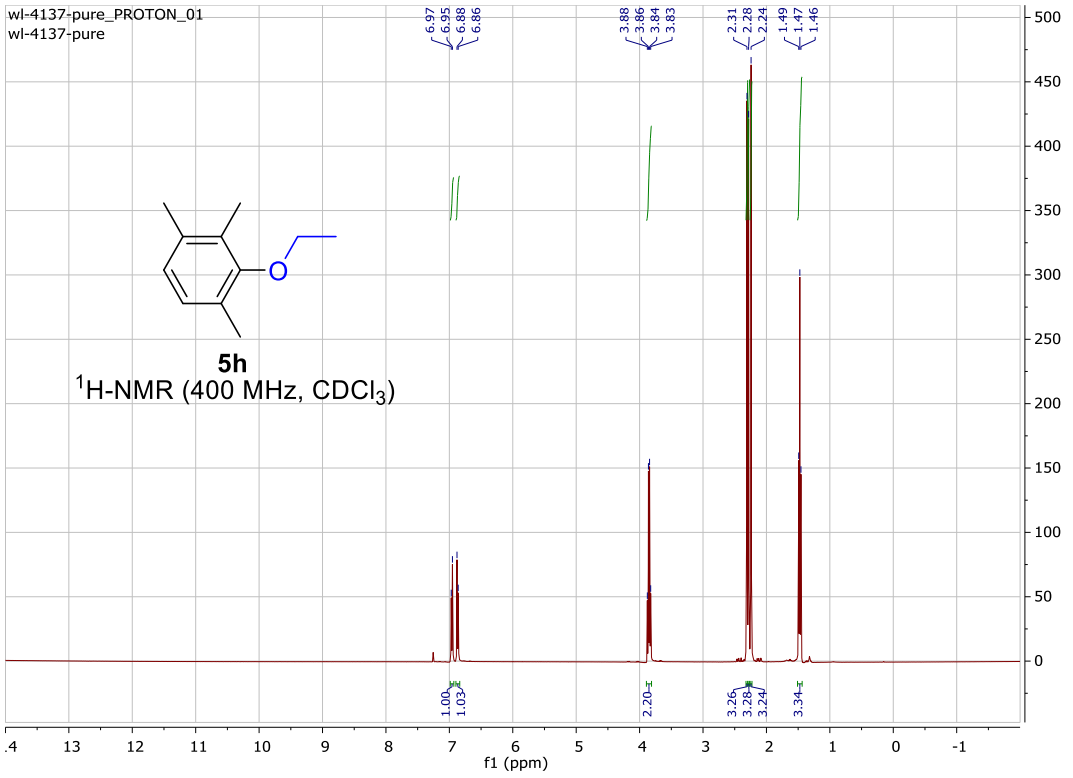

wl-4127-pure-C13.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 134
158.94
129.43
120.53
114.50
77.36
77.04
76.73
63.29
14.88
5e
13C-NMR (100 MHz, CDCl3)
f1 (ppm)


wl-4132-pure_PROTON_01
wl-4132-pure
6.99
6.98
6.96
6.76
6.74
4.06
4.05
4.03
4.01
2.30
2.25
1.46
1.45
1.43
5f
1H-NMR (400 MHz, CDCl3)
1.95
1.00
2.30
3.16
3.04
3.29
f1 (ppm)


wl-4132-C13.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 11
155.06
131.48
129.33
126.88
126.67
111.26
77.38
77.06
76.74
63.73
20.46
16.17
15.05
5f
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

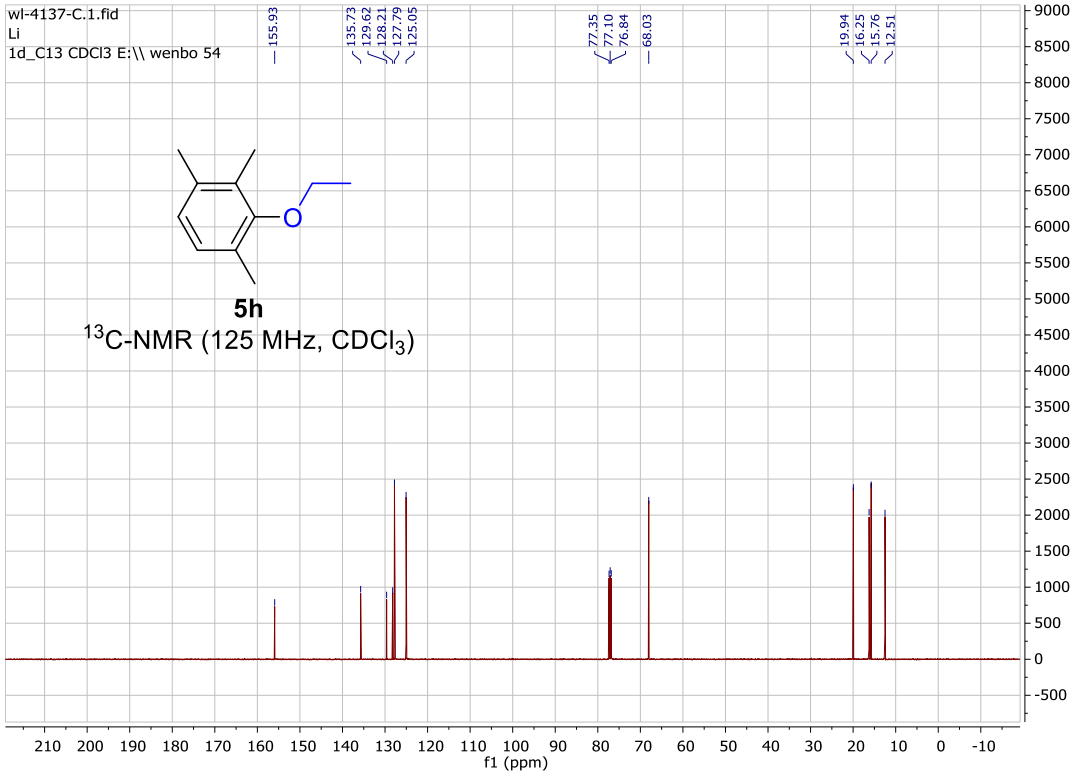

wl-4134-pure_PROTON_01
wl-4134-pure
7.33
7.31
7.29
7.29
7.27
7.23
7.22
7.21
7.20
7.18
7.18
6.86
6.84
4.07
4.06
4.04
4.02
1.71
1.46
1.44
1.43
Ph
O
5g
1H-NMR (400 MHz, CDCl3)
3.74
2.88
1.92
2.00
6.16
2.95
f1 (ppm)


wl-4134-pure-C.1.fid
Li
1d_C13 CDCl3 E:\\ wenbo 54
156.86
151.02
142.77
128.00
127.82
126.79
125.57
113.89
77.35
77.10
76.84
63.36
42.36
30.97
14.99
Ph
O
5g
13C-NMR (125 MHz, CDCl3)
f1 (ppm)



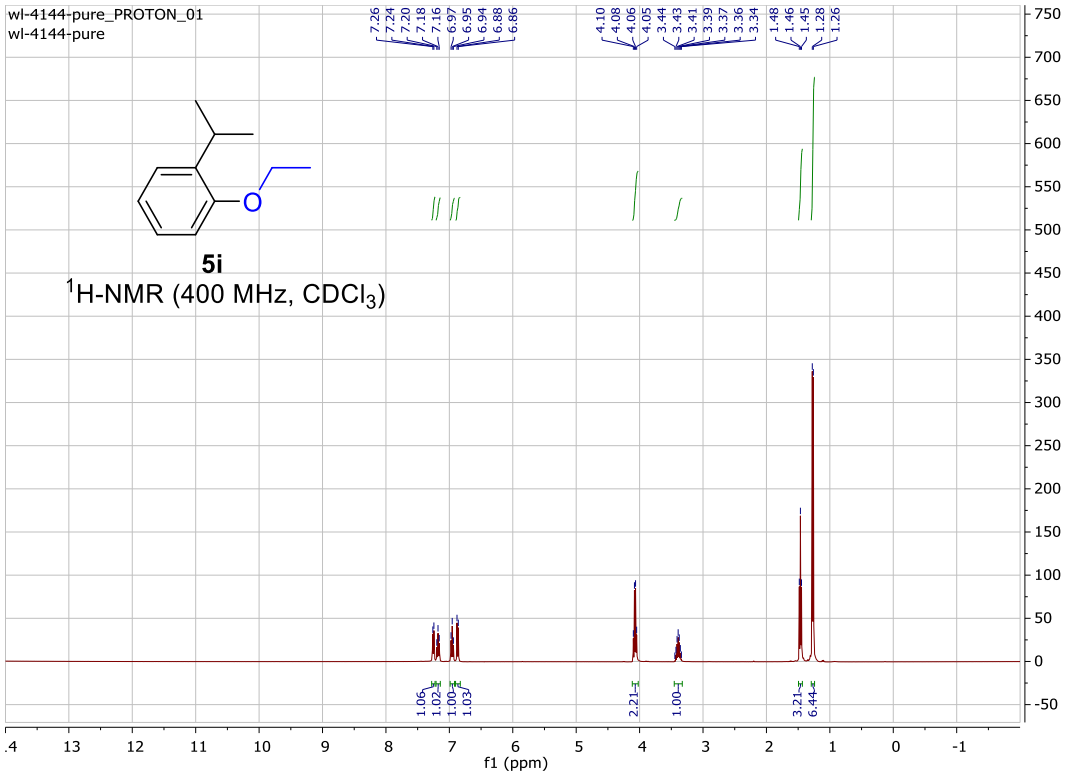
5h

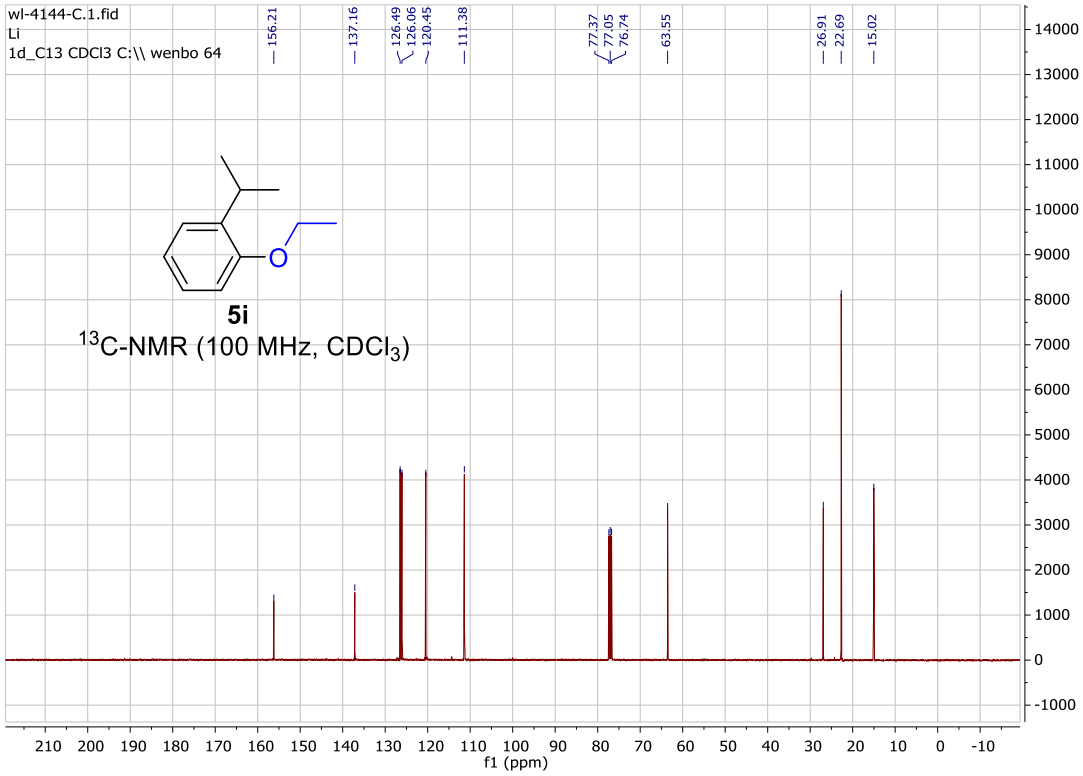
^{1}H-NMR (400 MHz, $CDCl_3$)

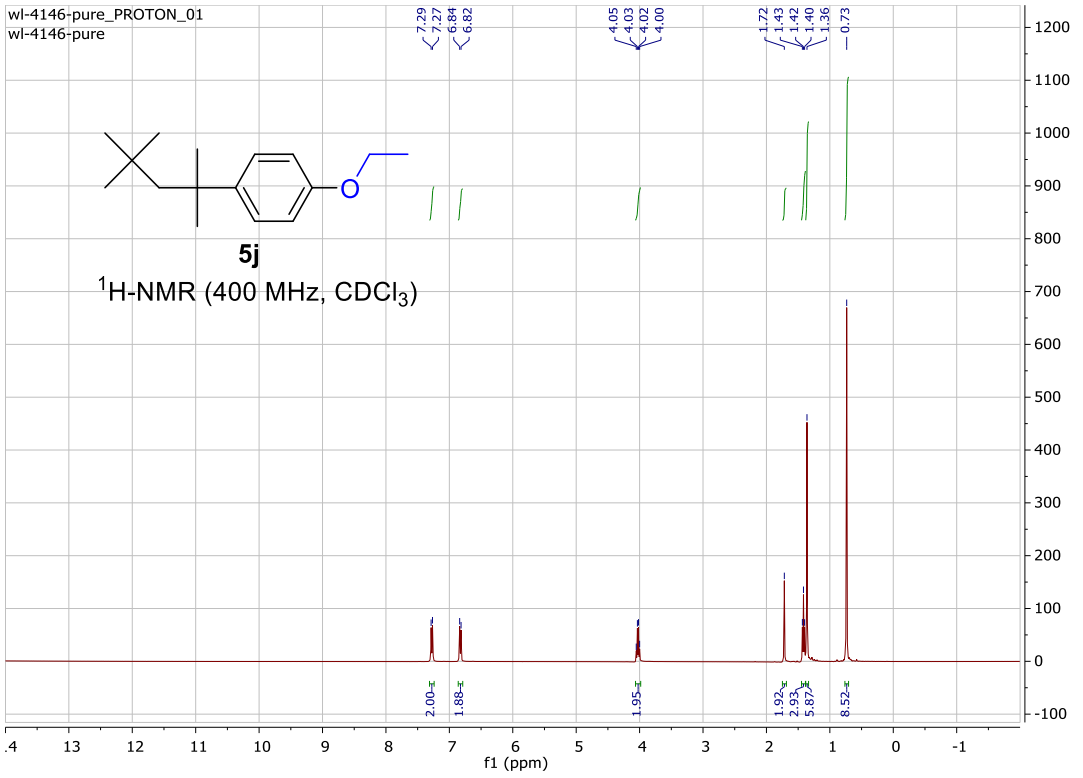


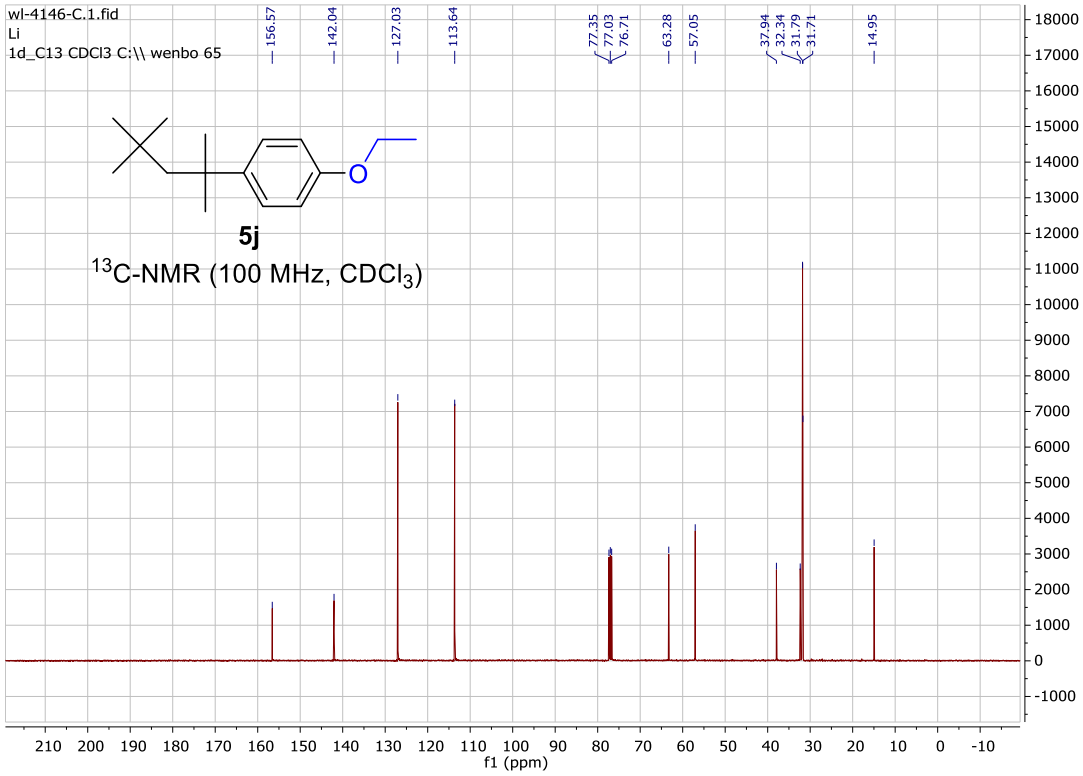
5h

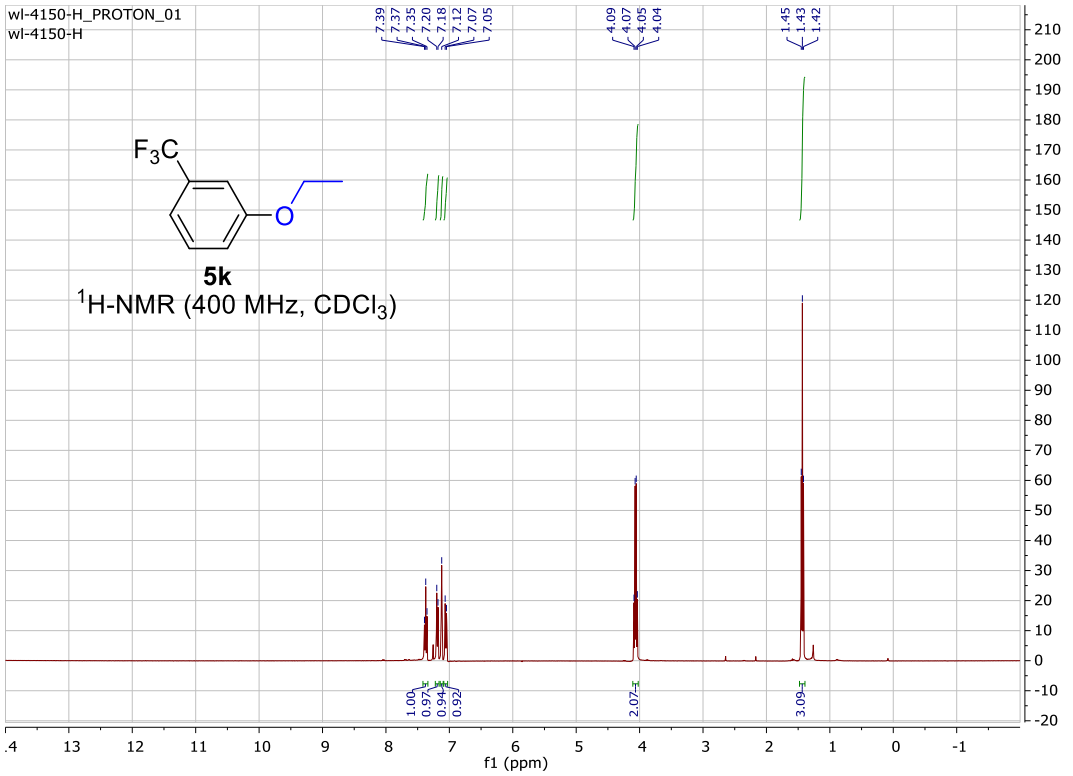
^{13}C-NMR (125 MHz, $CDCl_3$)

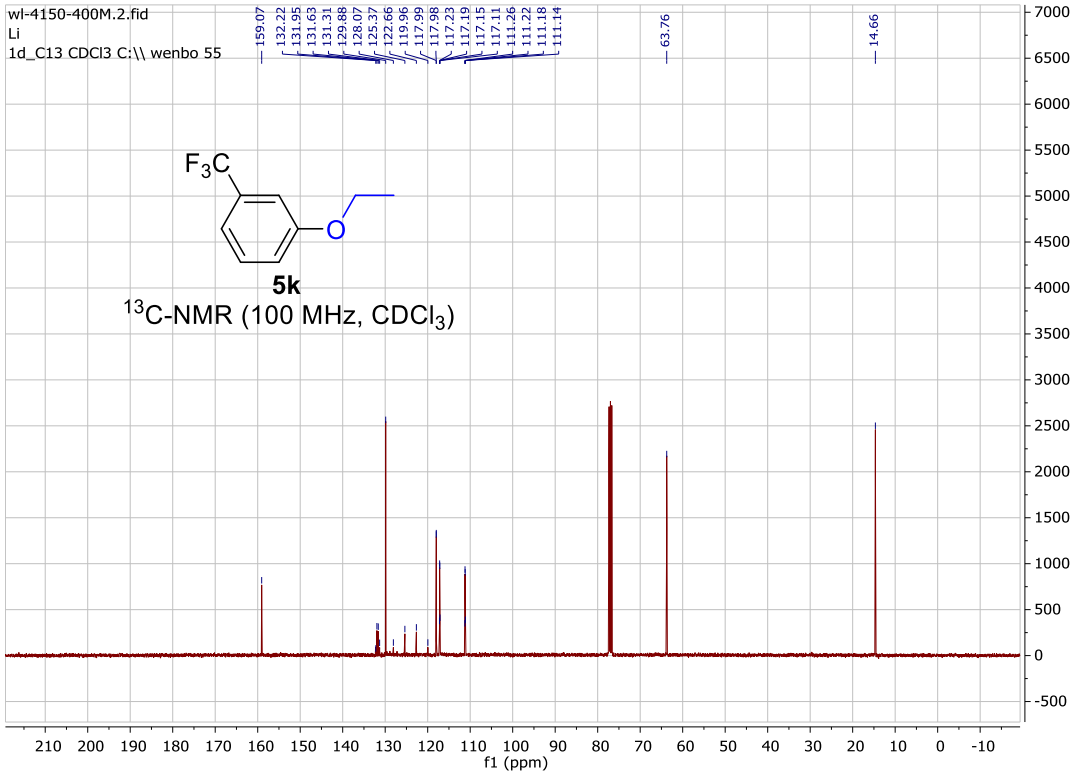

wl-4144-pure_PROTON_01
wl-4144-pure
7.26
7.24
7.20
7.18
7.16
6.97
6.95
6.94
6.88
6.86
4.10
4.08
4.06
4.05
3.44
3.43
3.41
3.39
3.37
3.36
3.34
1.48
1.46
1.45
1.28
1.26
O
5i
1H-NMR (400 MHz, CDCl3)
1.06
1.02
1.00
1.03
2.21
1.00
3.21
6.44
f1 (ppm)

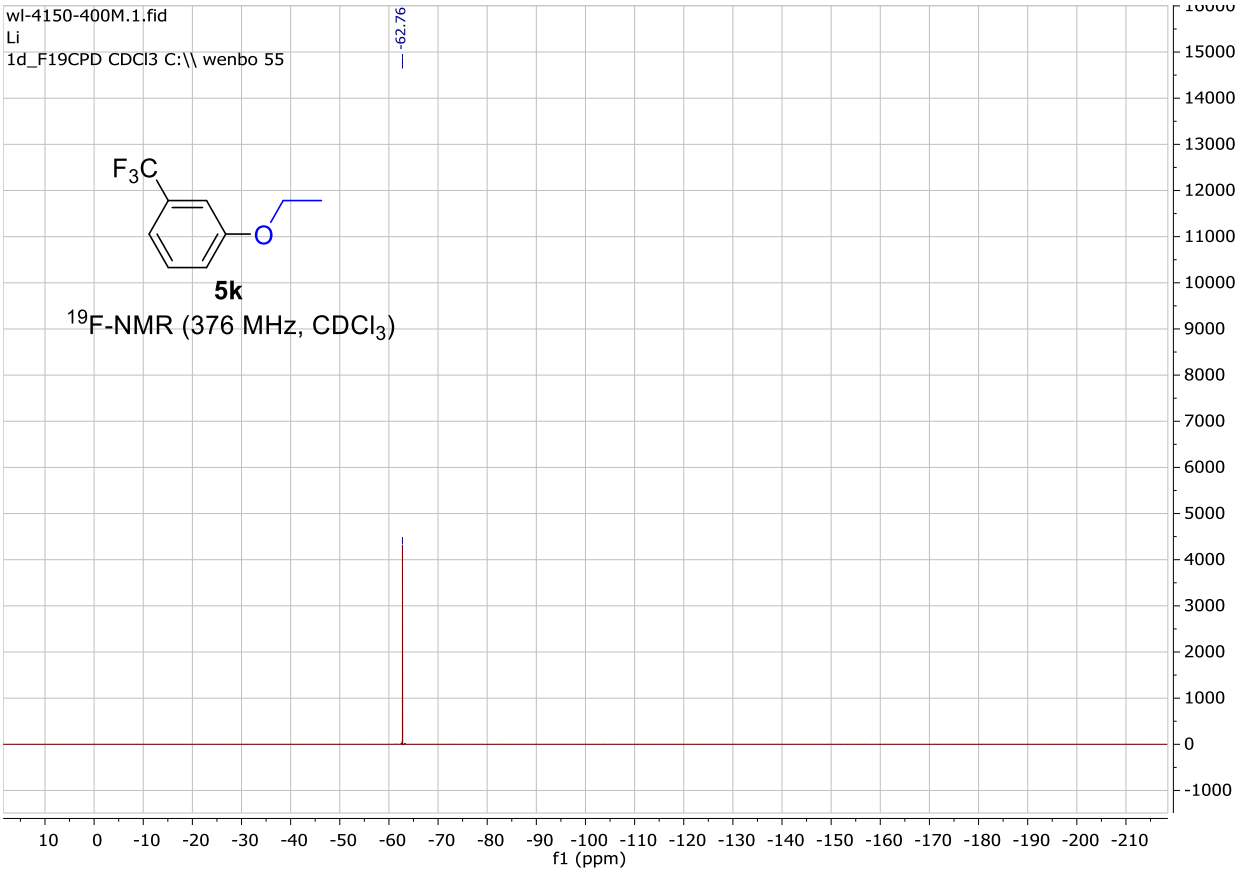

wl-4144-C.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 64
156.21
137.16
126.49
126.06
120.45
111.38
77.37
77.05
76.74
63.55
26.91
22.69
15.02
O
5i
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

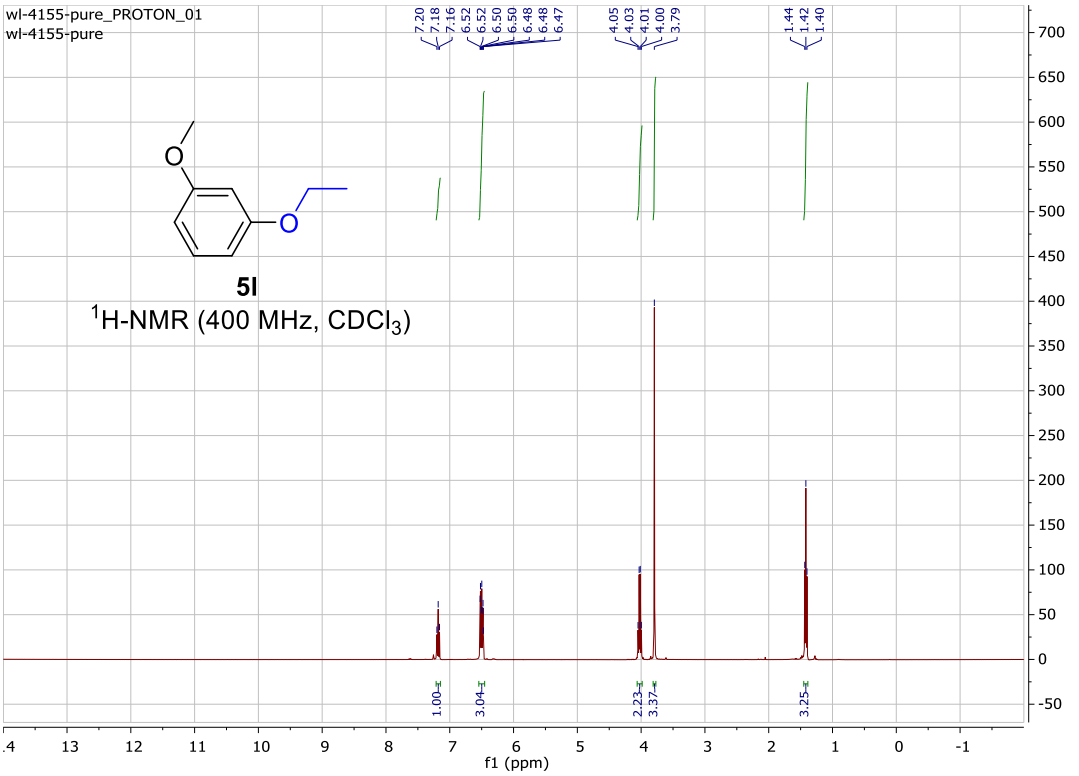

wl-4146-pure_PROTON_01
wl-4146-pure
7.29
7.27
6.84
6.82
4.05
4.03
4.02
4.00
1.72
1.43
1.42
1.40
1.36
0.73
5j
1H-NMR (400 MHz, CDCl3)
2.00
1.88
1.95
1.92
2.93
5.87
8.52
f1 (ppm)

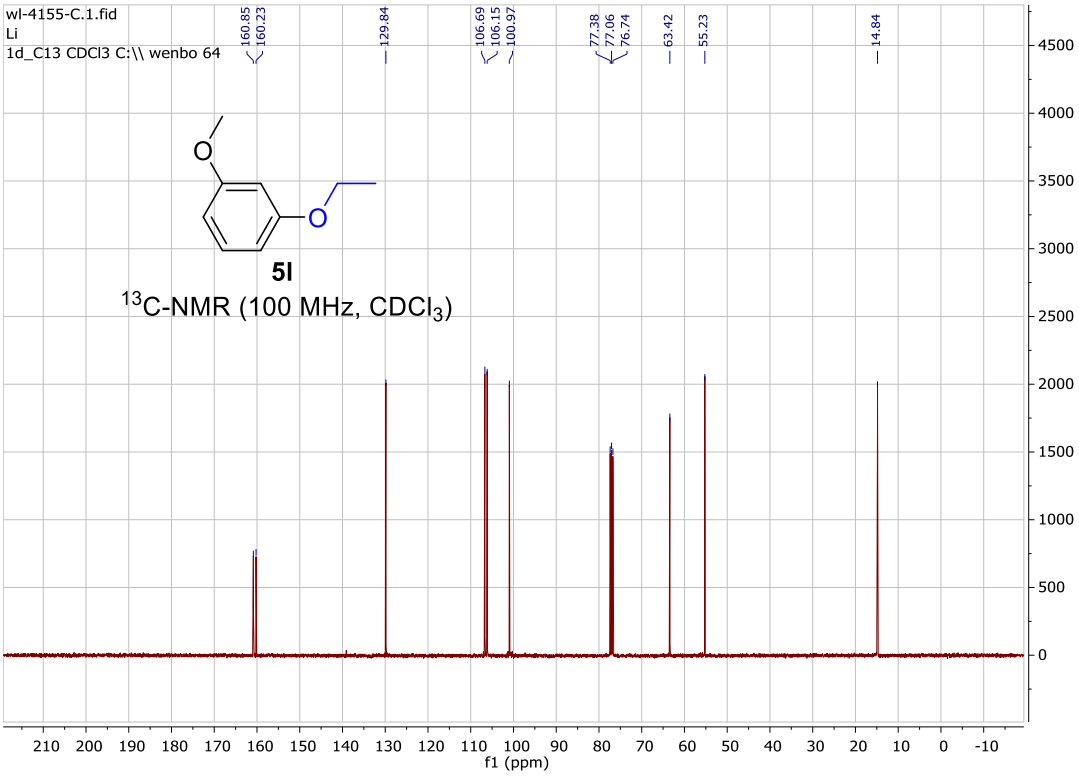

wl-4146-C.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 65
156.57
142.04
127.03
113.64
77.35
77.03
76.71
63.28
57.05
37.94
32.34
31.79
31.71
14.95
5j
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

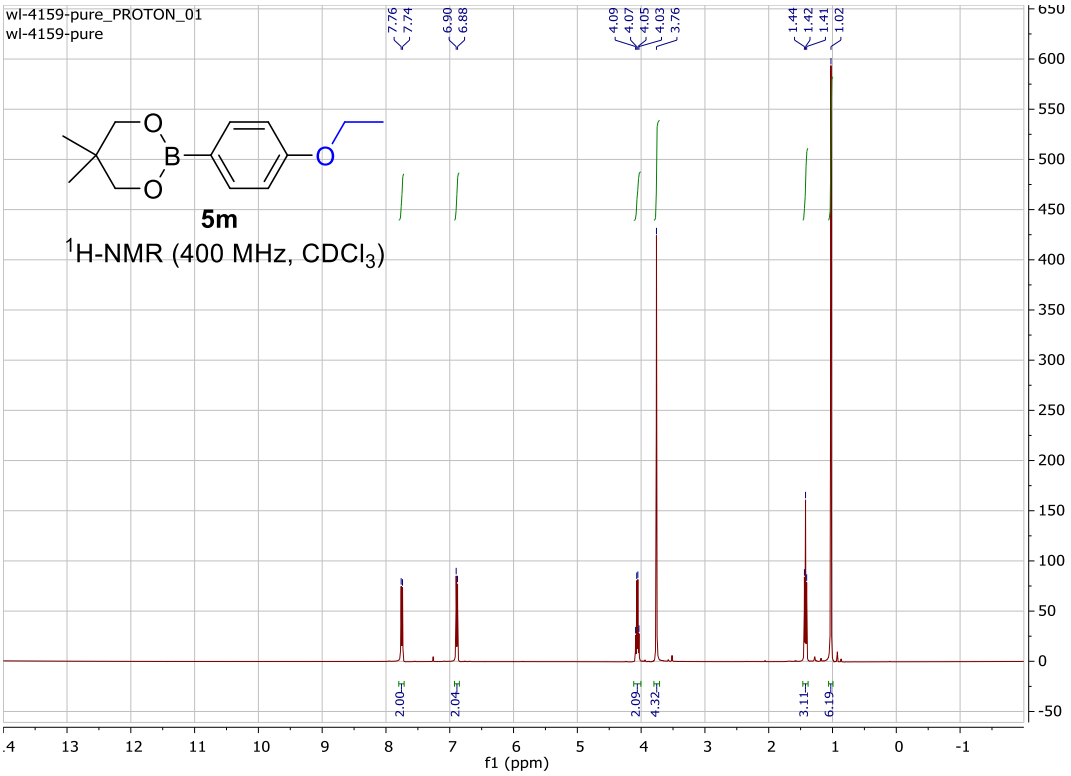

wl-4150-H_PROTON_01
wl-4150-H
7.39
7.37
7.35
7.20
7.18
7.12
7.07
7.05
4.09
4.07
4.05
4.04
1.45
1.43
1.42
F3C
O
5k
1H-NMR (400 MHz, CDCl3)
1.00
0.97
0.94
0.92
2.07
3.09
f1 (ppm)

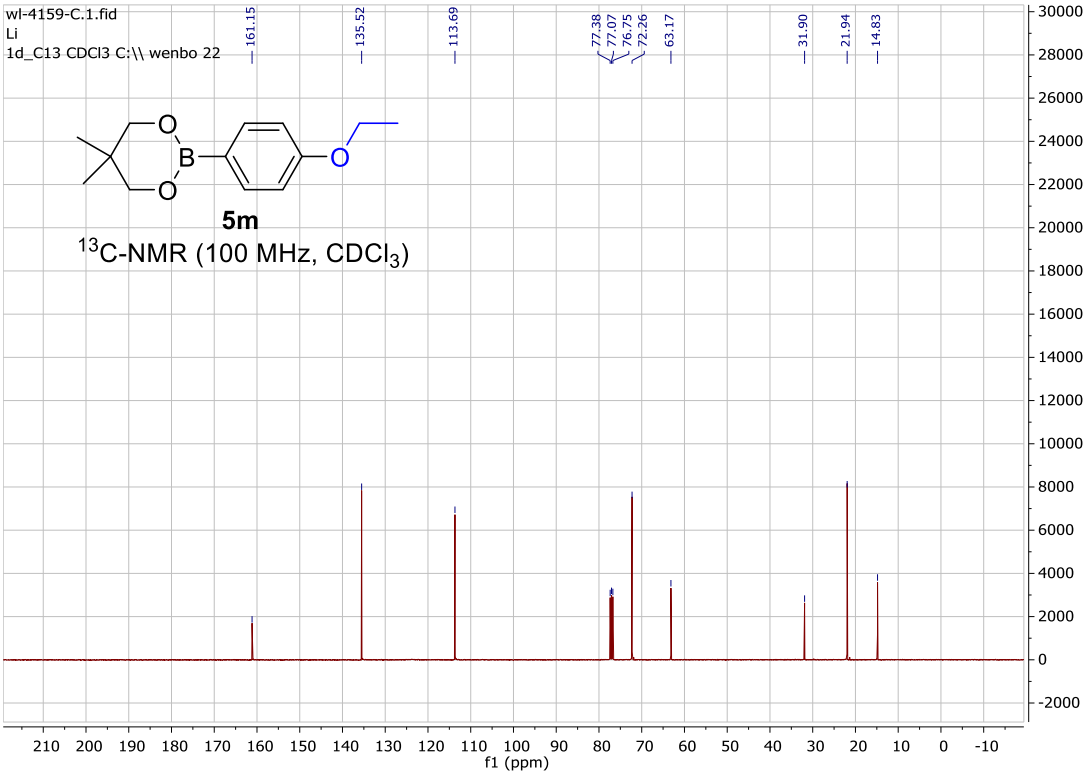

wl-4150-400M.2.fid
Li
1d_C13 CDCl3 C:\\ wenbo 55
159.07
132.22
131.95
131.63
131.31
129.88
128.07
125.37
122.66
119.96
117.99
117.98
117.23
117.19
117.15
117.11
111.26
111.22
111.18
111.14
63.76
14.66
F3C
O
5k
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

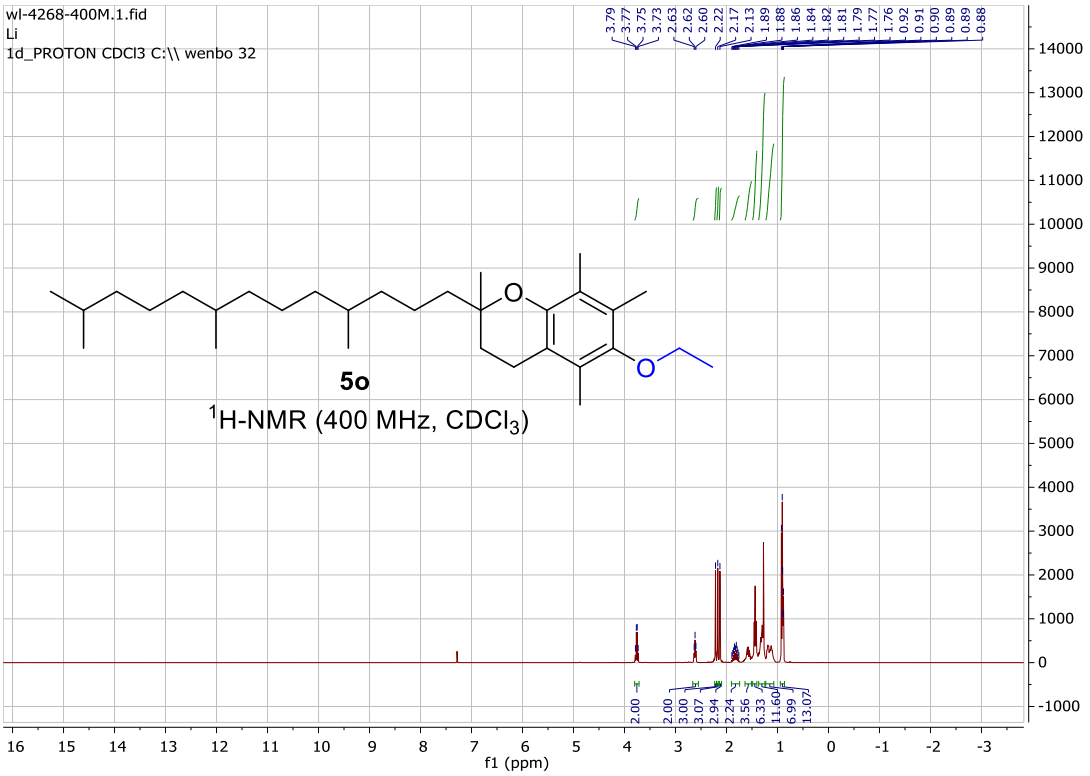

wl-4150-400M.1.fid
Li
1d_F19CPD CDCl3 C:\\ wenbo 55
-62.76
F3C
O
5k
19F-NMR (376 MHz, CDCl3)
f1 (ppm)

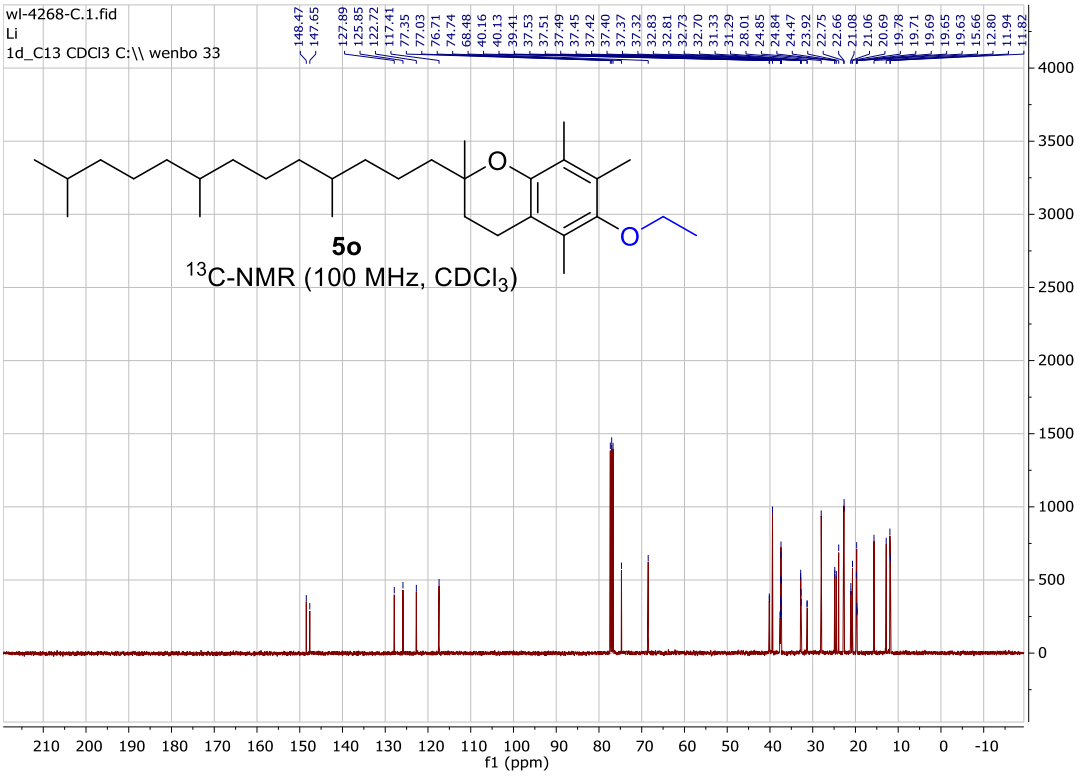

wl-4155-pure_PROTON_01
wl-4155-pure
7.20
7.18
7.16
6.52
6.52
6.50
6.50
6.48
6.48
6.47
4.05
4.03
4.01
4.00
3.79
1.44
1.42
1.40
O
O
5l
1H-NMR (400 MHz, CDCl3)
1.00
3.04
2.23
3.37
3.25
f1 (ppm)

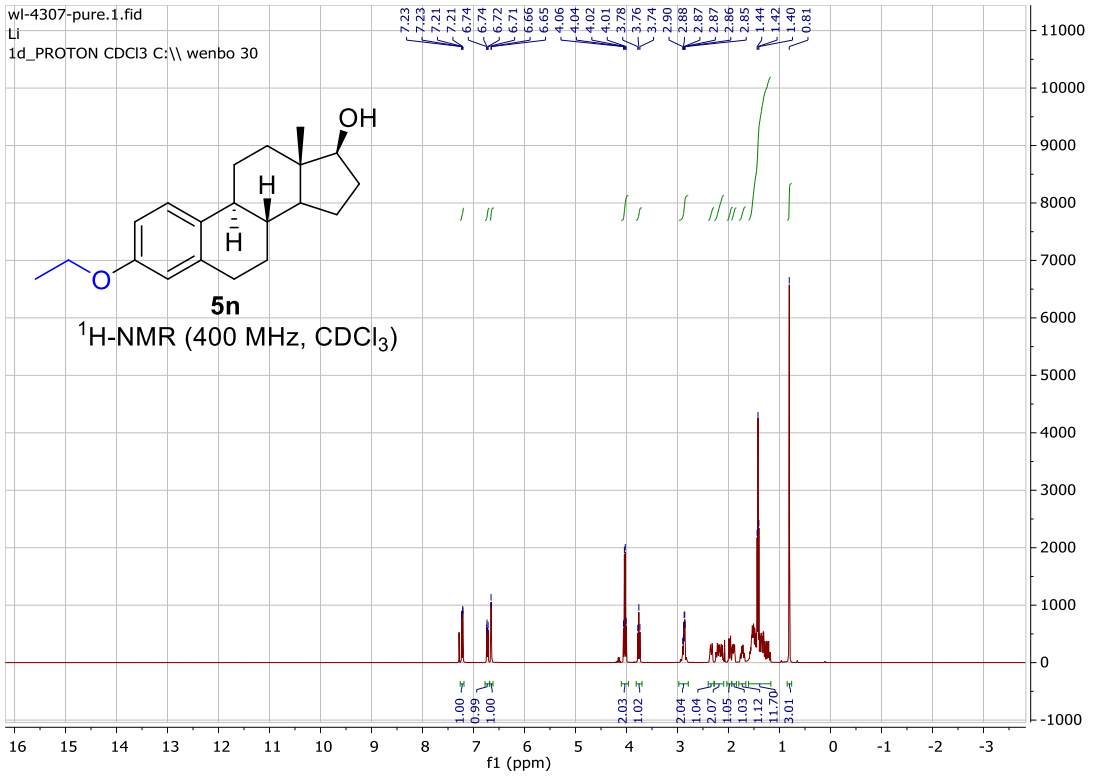

wl-4155-C.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 64
160.85
160.23
129.84
106.69
106.15
100.97
77.38
77.06
76.74
63.42
55.23
14.84
O
O
5l
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

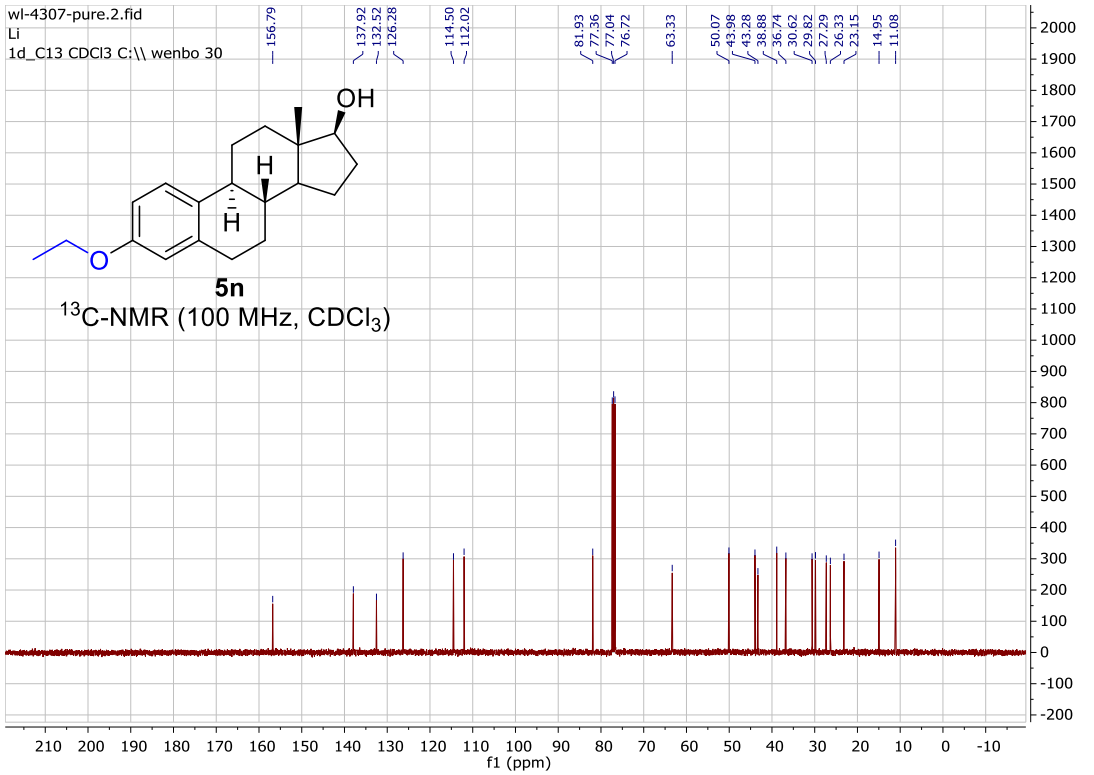

wl-4159-pure_PROTON_01
wl-4159-pure
7.76
7.74
6.90
6.88
4.09
4.07
4.05
4.03
3.76
1.44
1.42
1.41
1.02
O
B
O
O
5m
1H-NMR (400 MHz, CDCl3)
2.00
2.04
2.09
4.32
3.11
6.19
f1 (ppm)

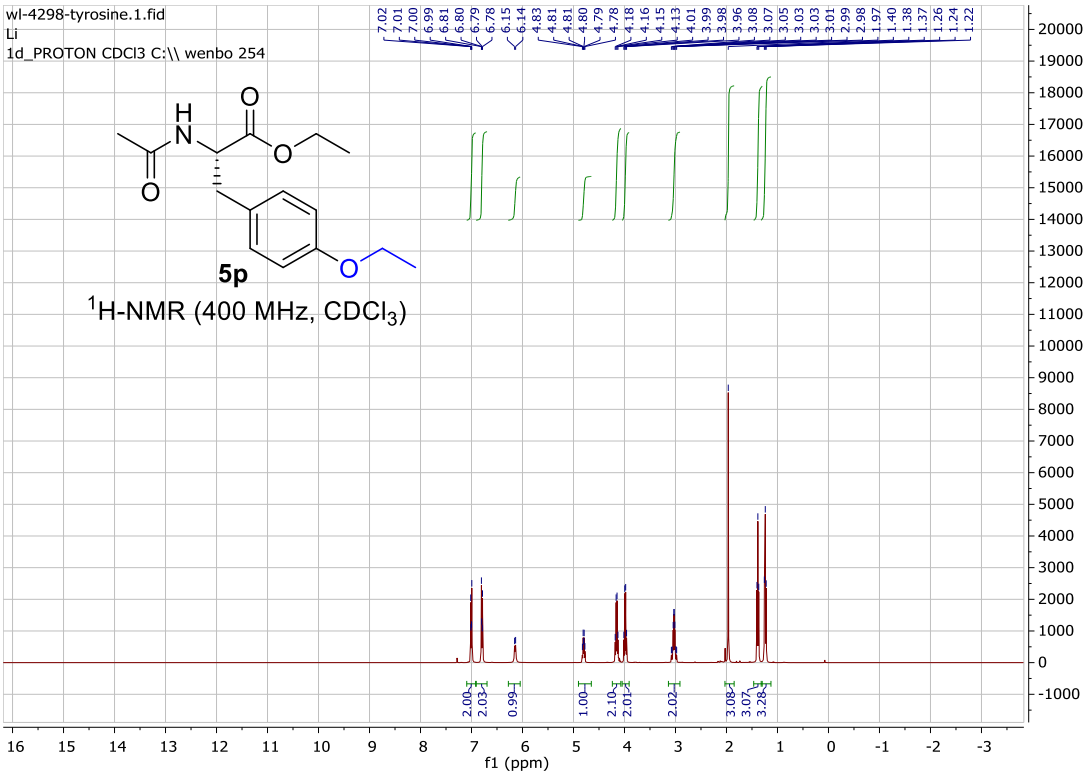

wl-4159-C.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 22
161.15
135.52
113.69
77.38
77.07
76.75
72.26
63.17
31.90
21.94
14.83
O
B
O
O
5m
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

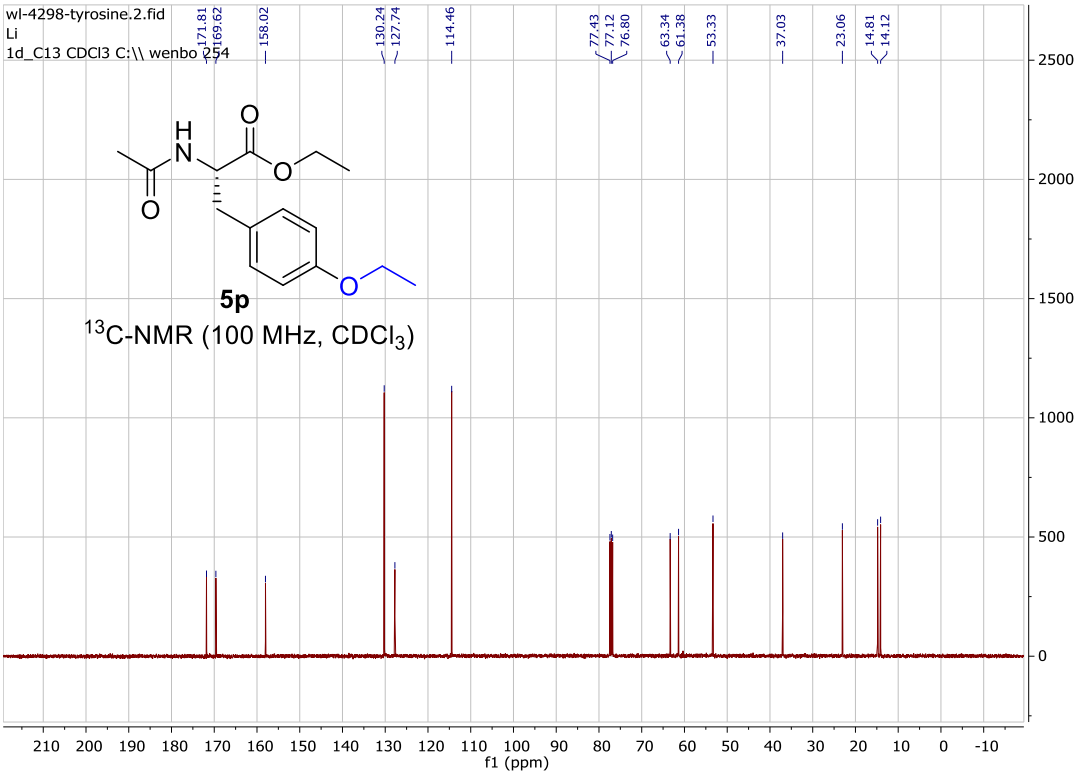

wl-4268-400M.1.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 32
O
O
5o
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

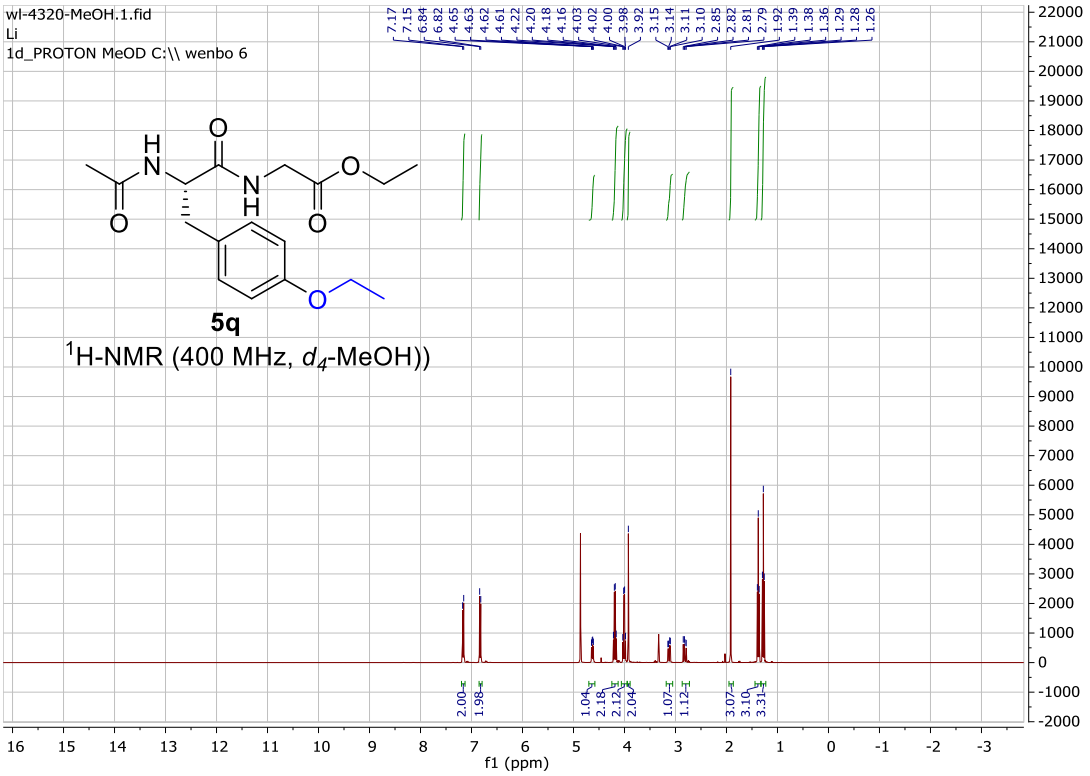

wl-4268-C.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 33
O
O
5o
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

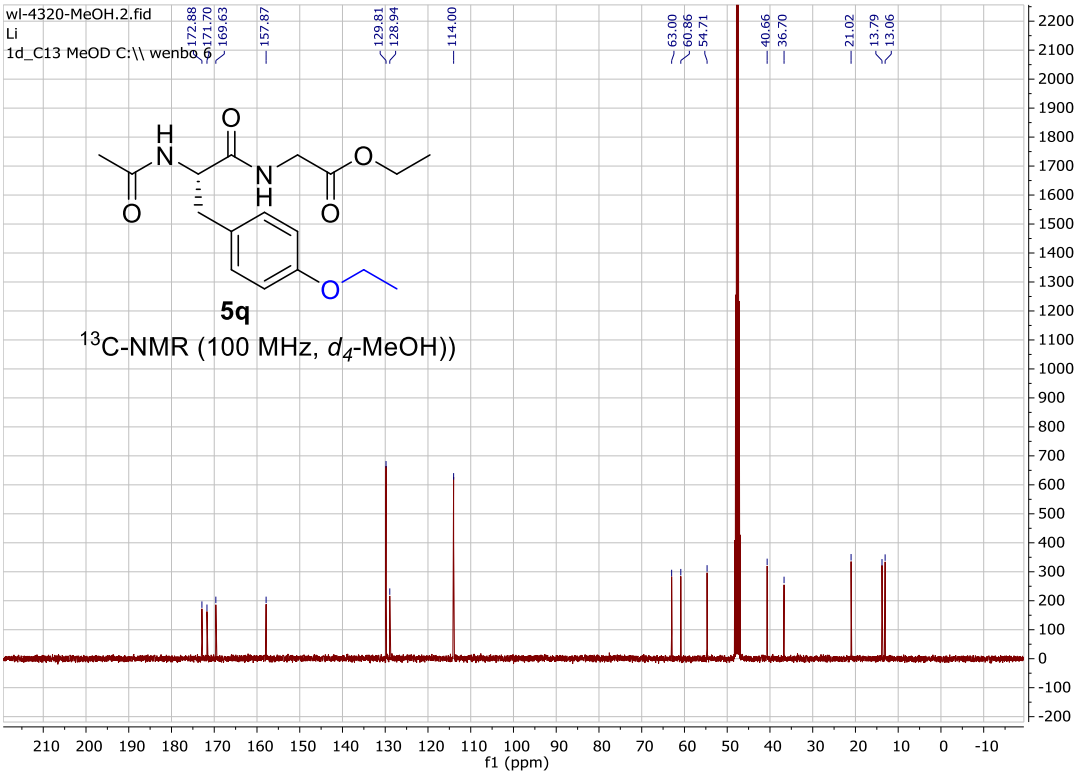

wl-4307-pure.1.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 30
OH
H
H
O
5n
^{1}H-NMR (400 MHz, $CDCl_3$)
f1 (ppm)

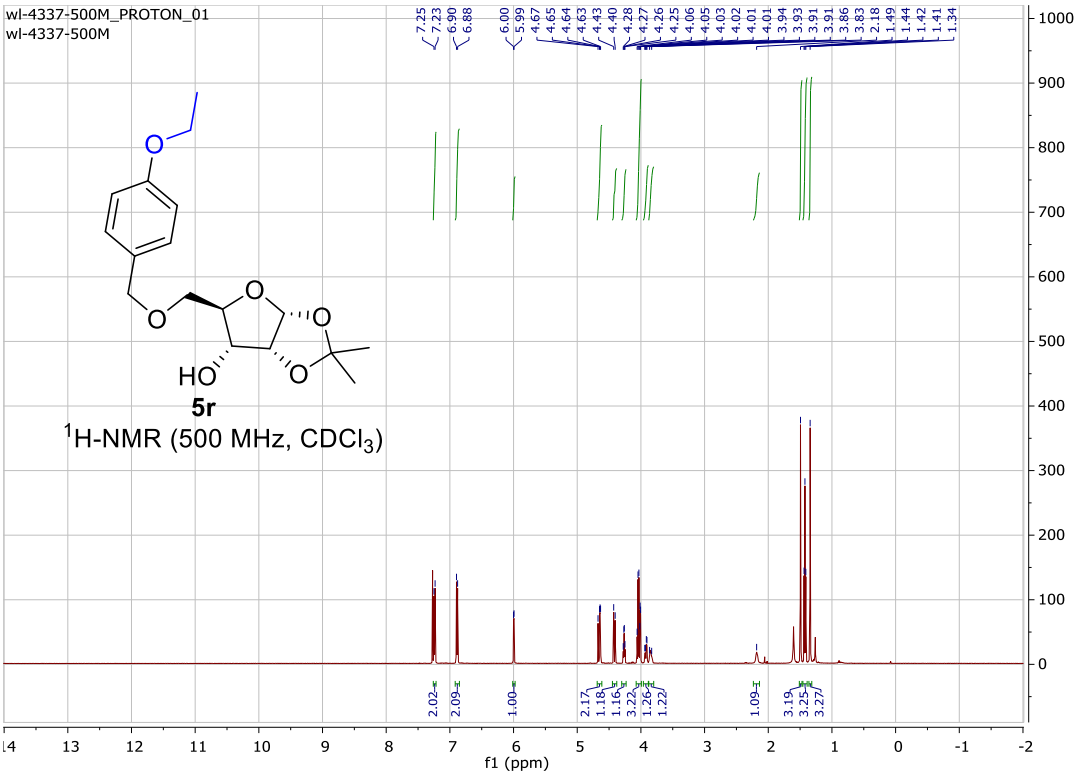

wl-4307-pure.2.fid
Li
1d_C13 CDCl3 C:\\ wenbo 30
OH
H
H
O
5n
^{13}C-NMR (100 MHz, $CDCl_3$)
f1 (ppm)

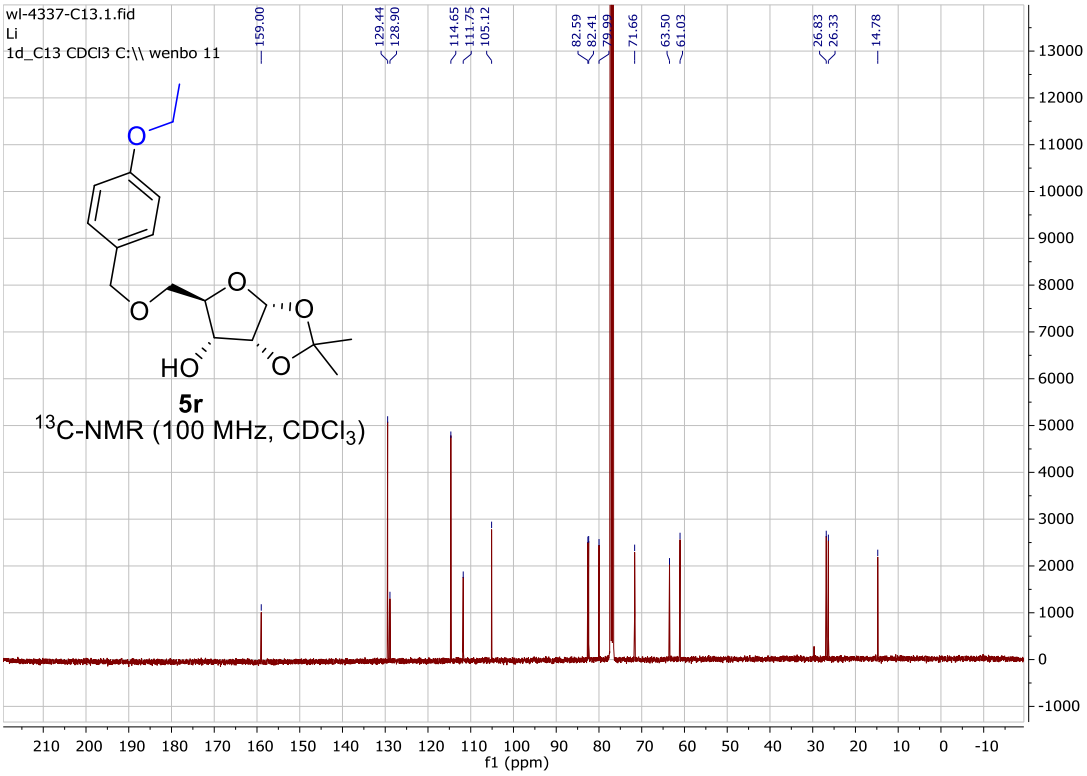

wl-4298-tyrosine.1.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 254
5p
^{1}H-NMR (400 MHz, $CDCl_3$)
f1 (ppm)

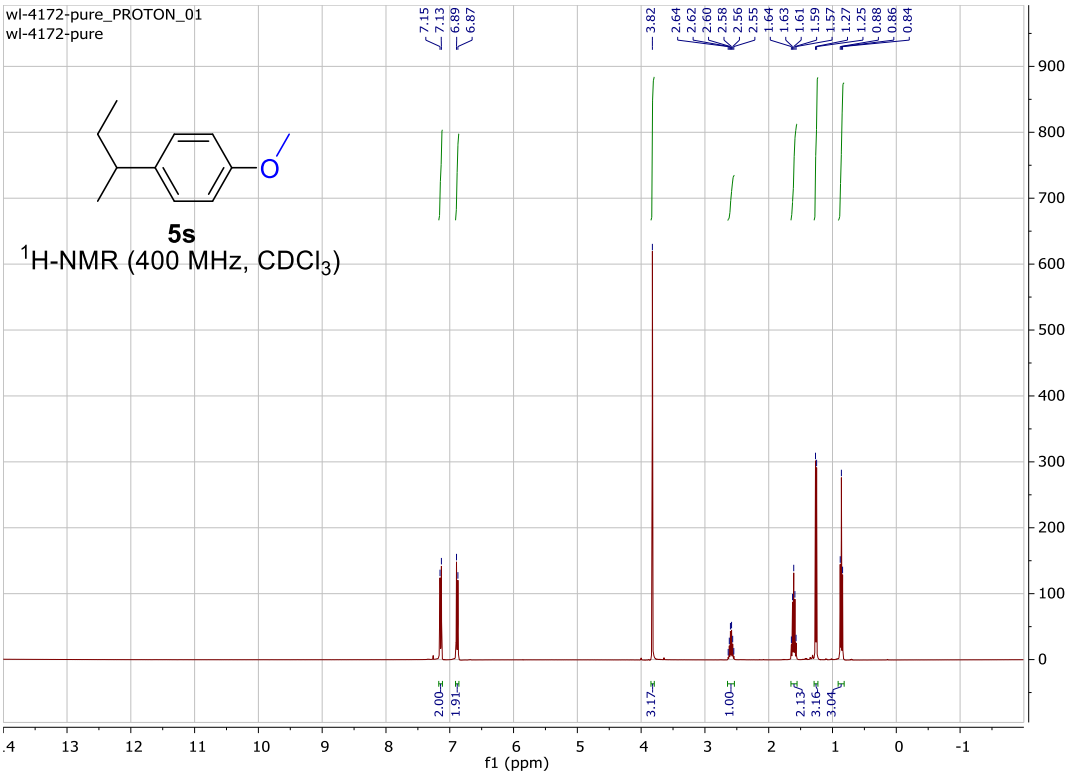

wl-4298-tyrosine.2.fid
Li
1d_C13 CDCl3 C:\\ wenbo 254
5p
^{13}C-NMR (100 MHz, $CDCl_3$)
f1 (ppm)

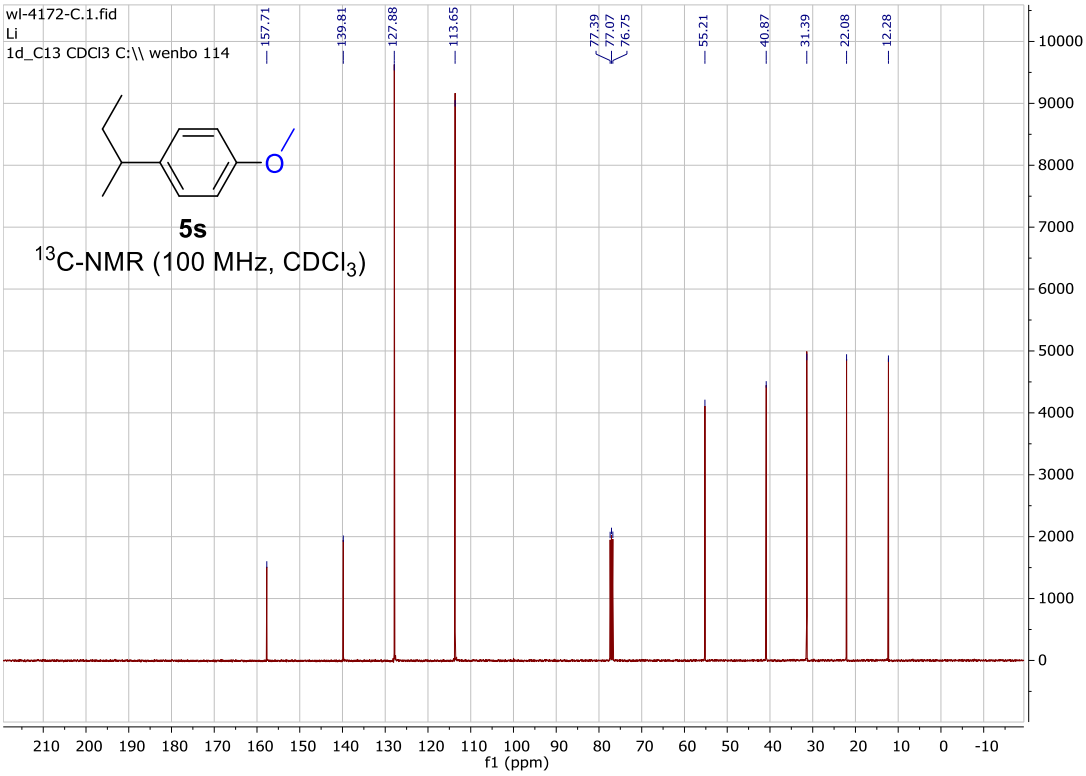

wl-4320-MeOH.1.fid
Li
1d_PROTON MeOD C:\\ wenbo 6
5q
1H-NMR (400 MHz, d4-MeOH))
f1 (ppm)

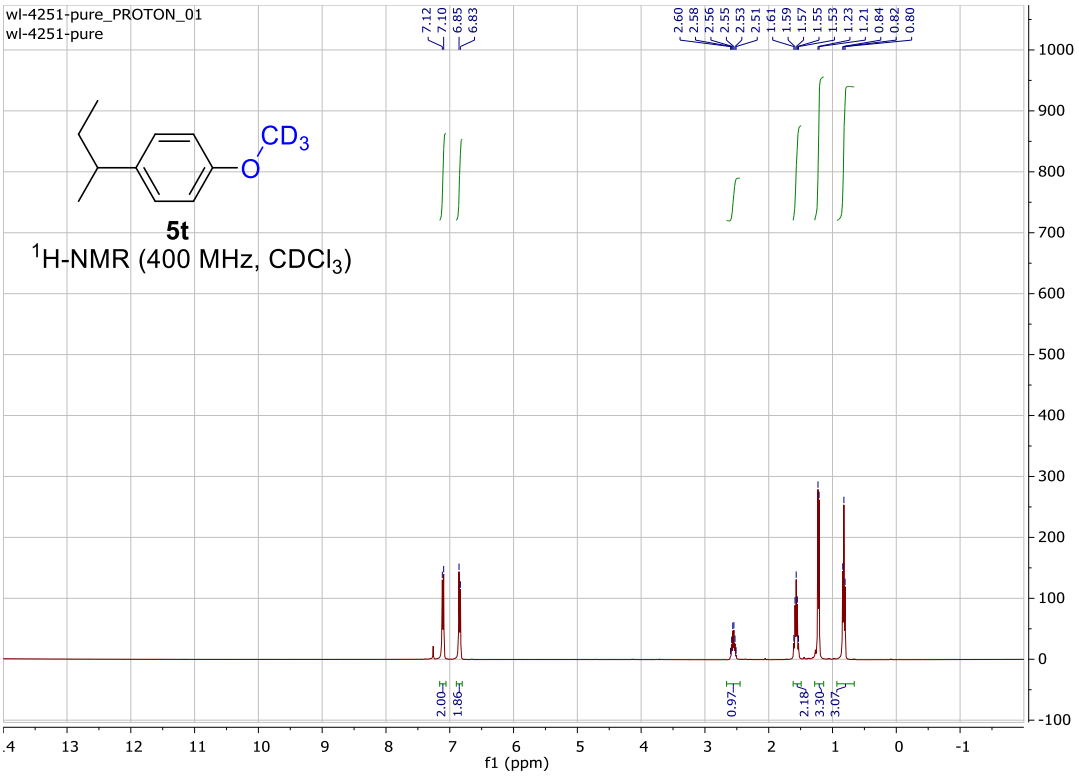

wl-4320-MeOH.2.fid
Li
1d_C13 MeOD C:\\ wenbo 6
5q
13C-NMR (100 MHz, d4-MeOH))
f1 (ppm)

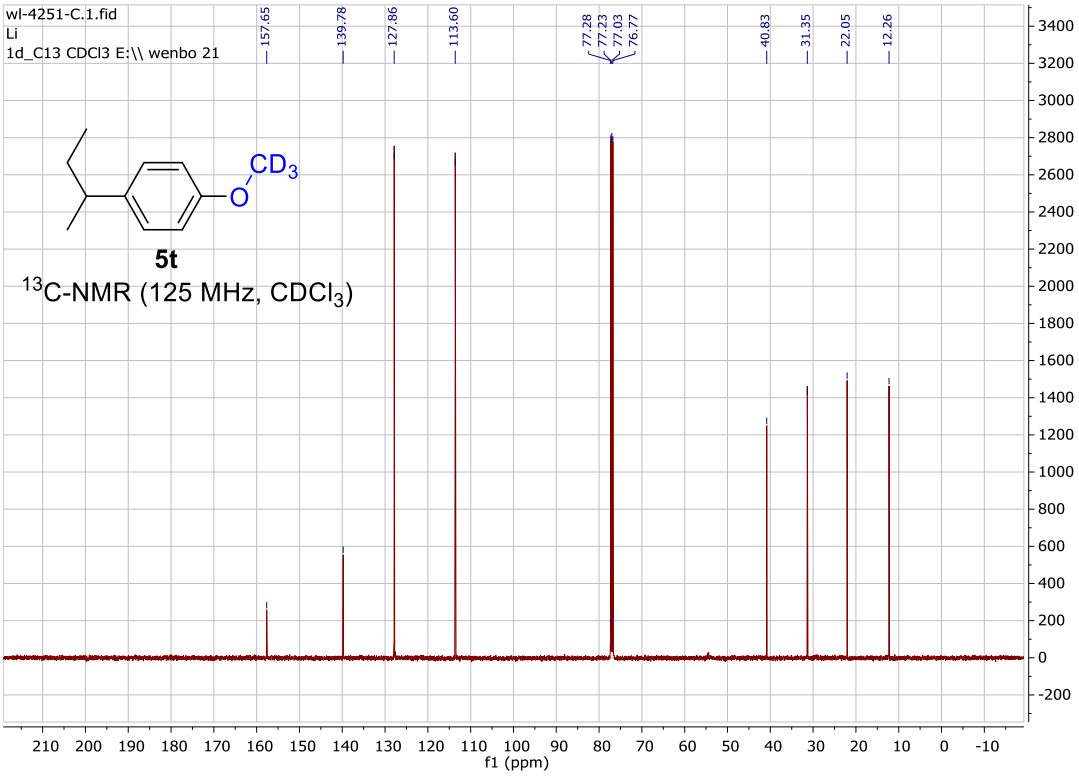

wl-4337-500M_PROTON_01
wl-4337-500M
5r
1H-NMR (500 MHz, CDCl3)
f1 (ppm)

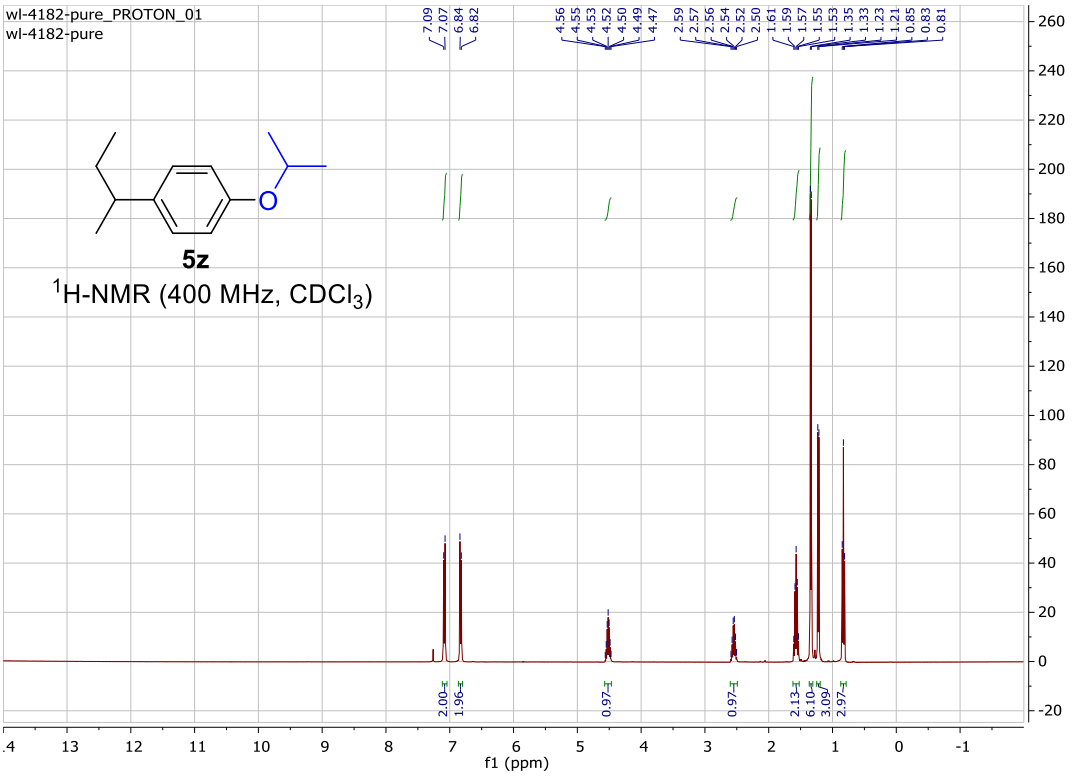

wl-4337-C13.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 11
5r
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

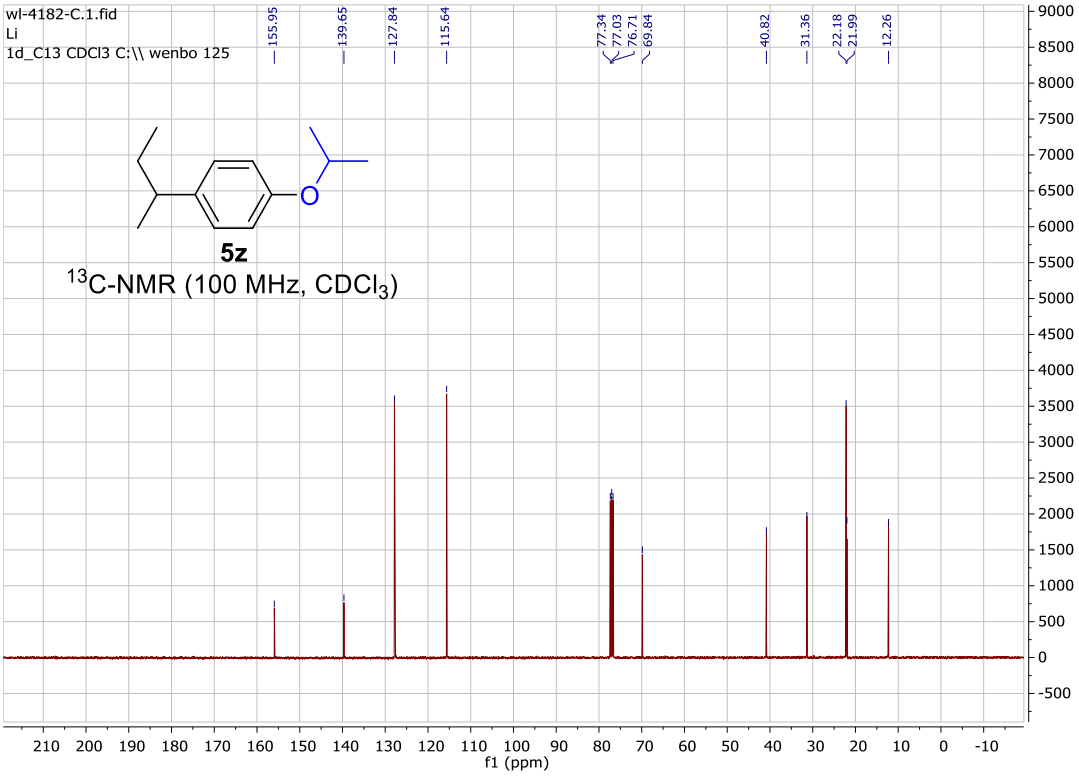

wl-4172-pure_PROTON_01
wl-4172-pure
7.15
7.13
6.89
6.87
3.82
2.64
2.62
2.60
2.58
2.56
2.55
1.64
1.63
1.61
1.59
1.57
1.27
1.25
0.88
0.86
0.84
5s
1H-NMR (400 MHz, CDCl3)
2.00
1.91
3.17
1.00
2.13
3.16
3.04
f1 (ppm)

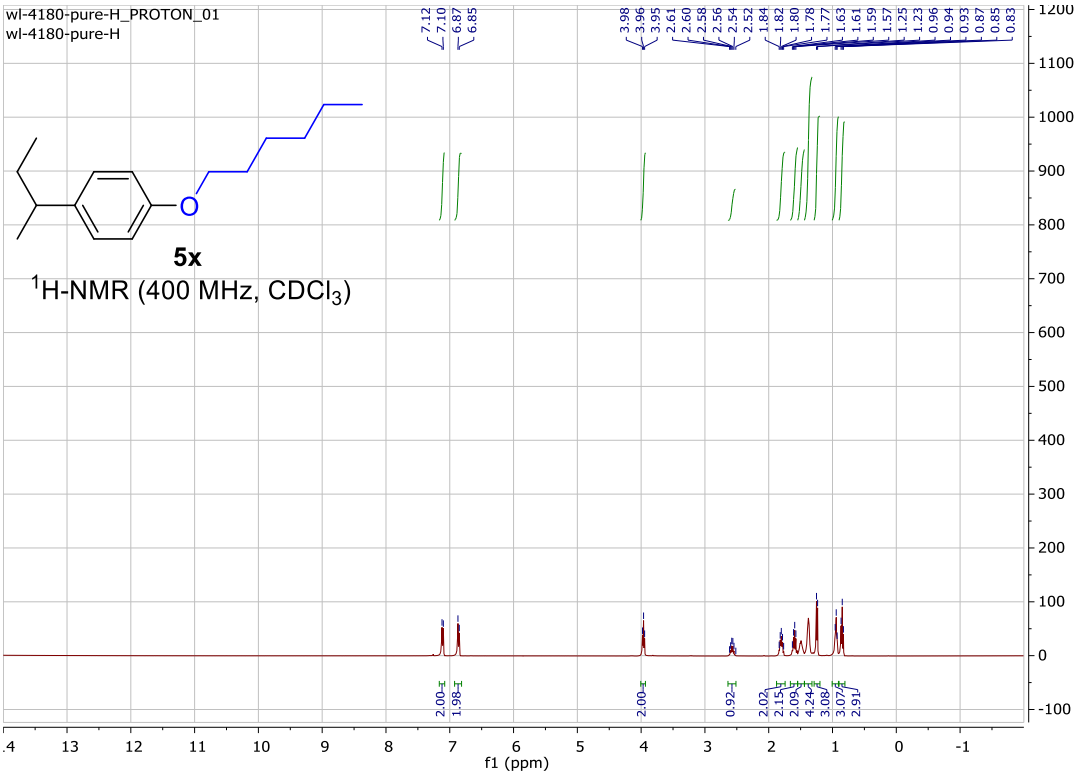

wl-4172-C.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 114
157.71
139.81
127.88
113.65
77.39
77.07
76.75
55.21
40.87
31.39
22.08
12.28
5s
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

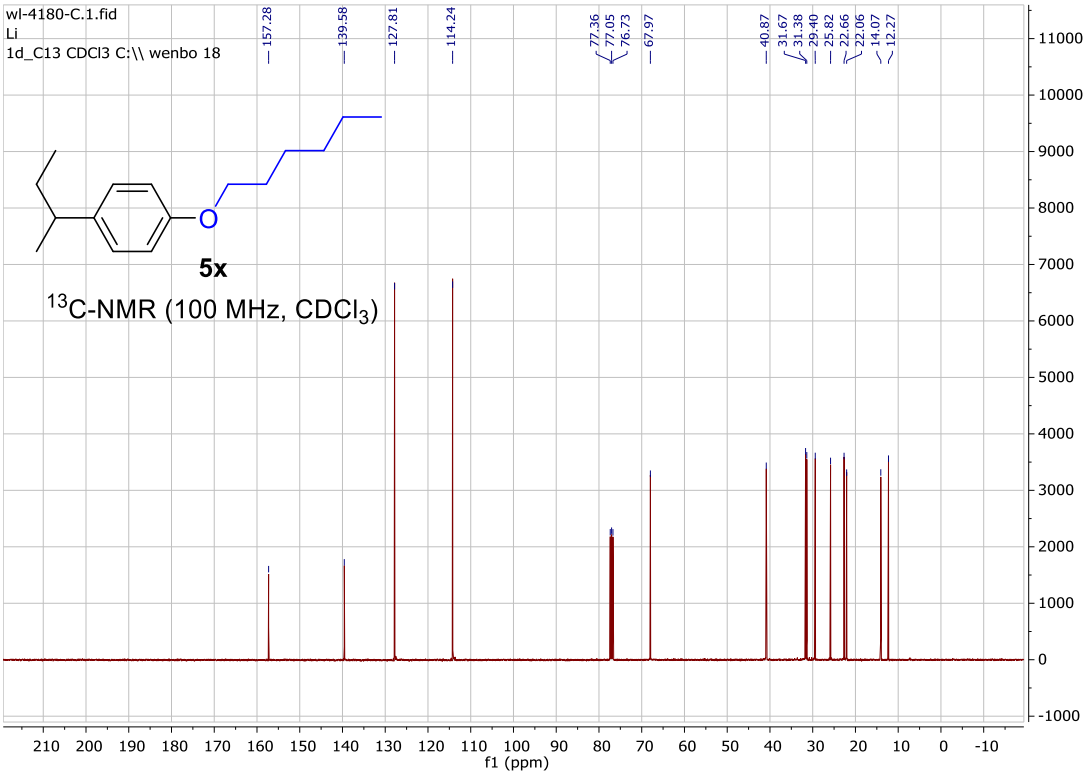

wl-4251-pure_PROTON_01
wl-4251-pure
7.12
7.10
6.85
6.83
2.60
2.58
2.56
2.55
2.53
2.51
1.61
1.59
1.57
1.55
1.53
1.23
1.21
0.84
0.82
0.80
CD3
O
5t
1H-NMR (400 MHz, CDCl3)
2.00
1.86
0.97
2.18
3.30
3.07
f1 (ppm)

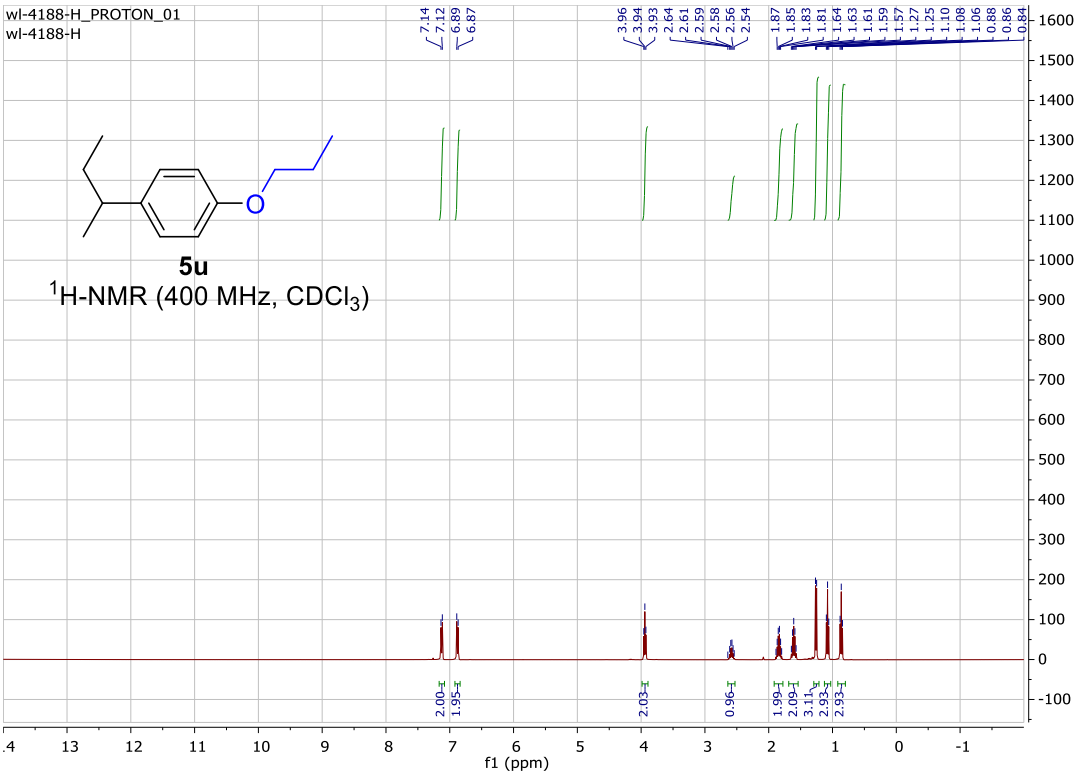

wl-4251-C.1.fid
Li
1d_C13 CDCl3 E:\\ wenbo 21
157.65
139.78
127.86
113.60
77.28
77.23
77.03
76.77
40.83
31.35
22.05
12.26
CD3
O
5t
13C-NMR (125 MHz, CDCl3)
f1 (ppm)

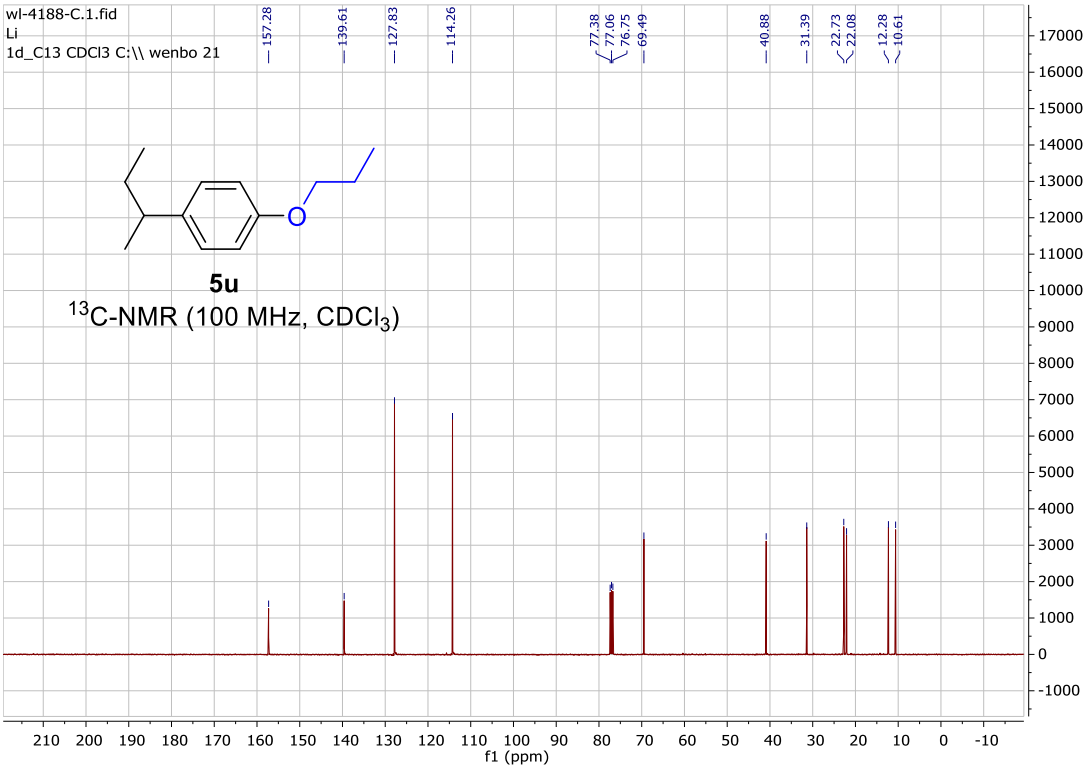

wl-4182-pure_PROTON_01
wl-4182-pure
5z
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

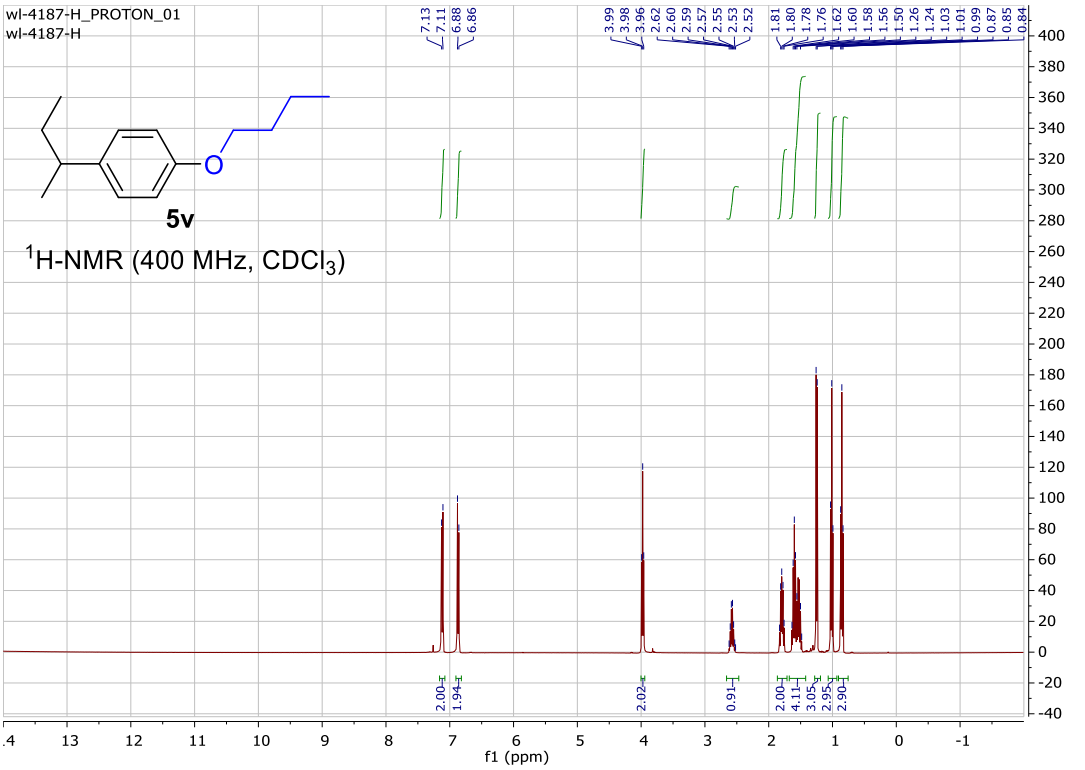

wl-4182-C.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 125
5z
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

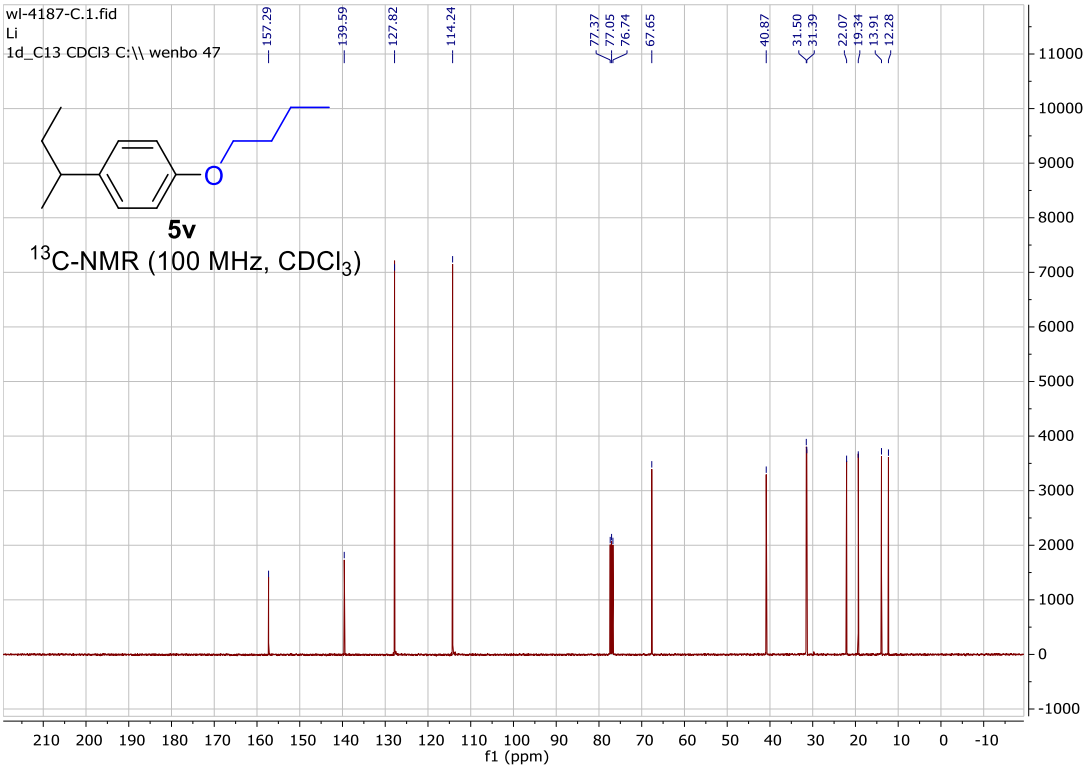

wl-4180-pure-H_PROTON_01
wl-4180-pure-H
7.12
7.10
6.87
6.85
3.98
3.96
3.95
2.61
2.60
2.58
2.56
2.54
2.52
1.84
1.82
1.80
1.78
1.77
1.63
1.61
1.59
1.57
1.25
1.23
0.96
0.94
0.93
0.87
0.85
0.83
O
5x
1H-NMR (400 MHz, CDCl3)
2.00
1.98
2.00
0.92
2.02
2.15
2.09
4.24
3.08
3.07
2.91
f1 (ppm)

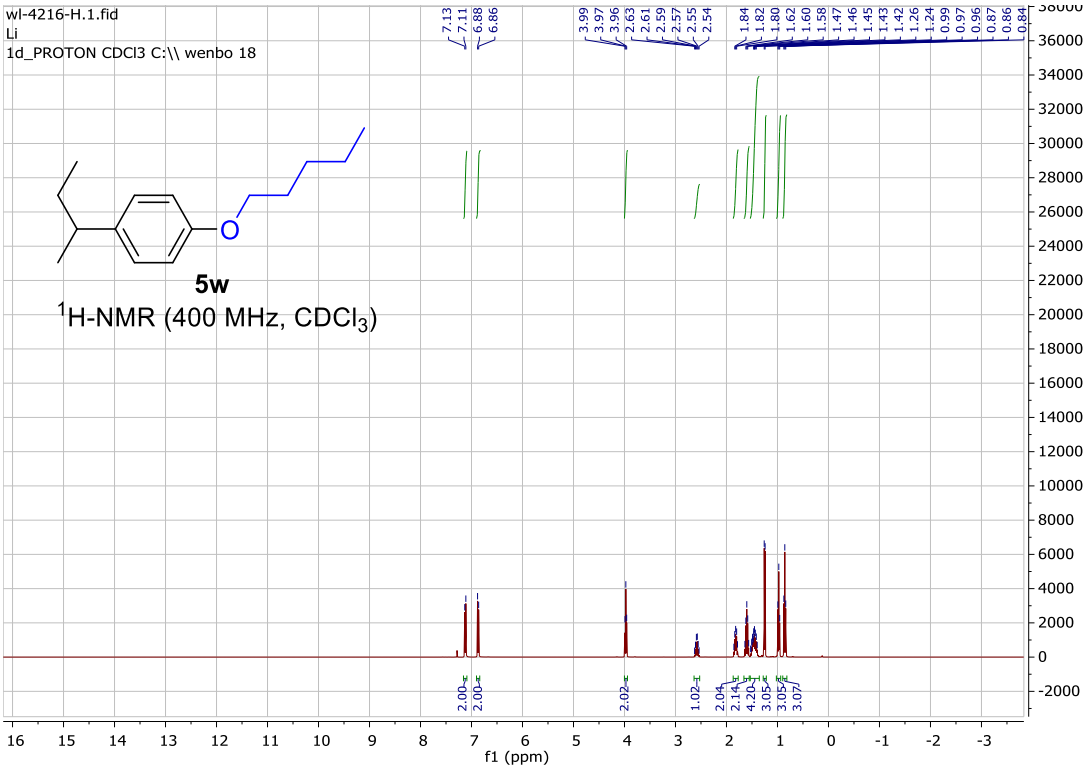

wl-4180-C.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 18
157.28
139.58
127.81
114.24
77.36
77.05
76.73
67.97
40.87
31.67
31.38
29.40
25.82
22.66
22.06
14.07
12.27
O
5x
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

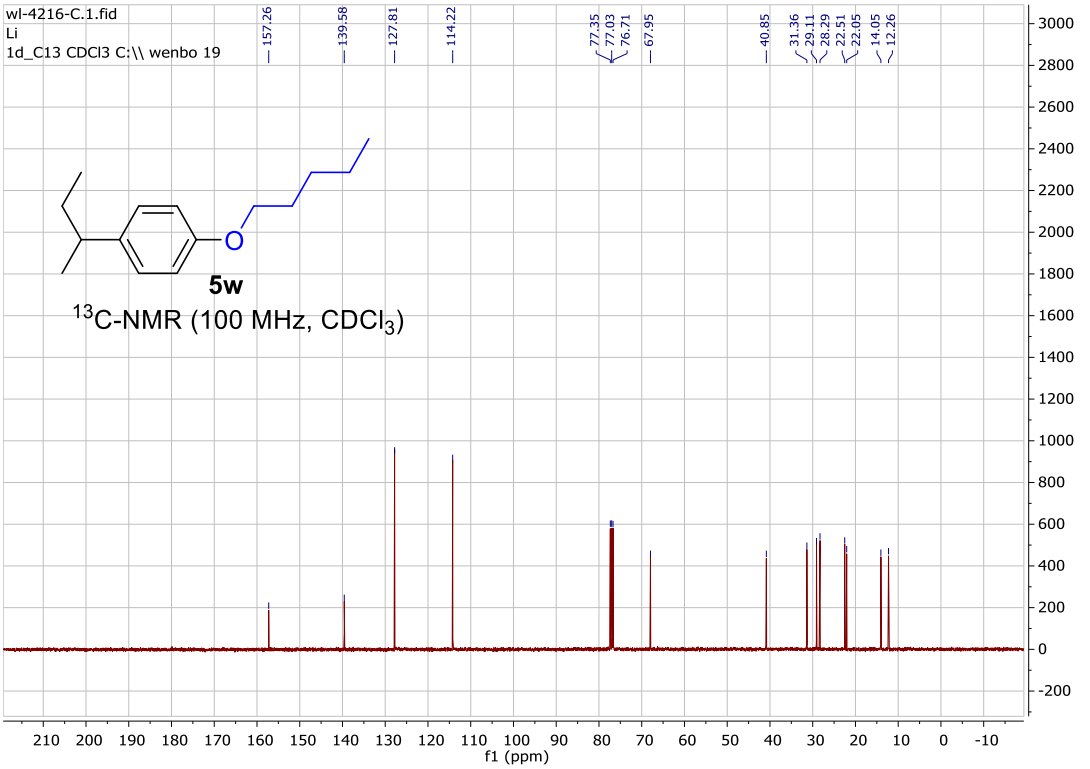

wl-4188-H_PROTON_01
wl-4188-H
7.14
7.12
6.89
6.87
3.96
3.94
3.93
2.64
2.61
2.59
2.58
2.56
2.54
1.87
1.85
1.83
1.81
1.64
1.63
1.61
1.59
1.57
1.27
1.25
1.10
1.08
1.06
0.88
0.86
0.84
O
5u
1H-NMR (400 MHz, CDCl3)
2.00
1.95
2.03
0.96
1.99
2.09
3.11
2.93
2.93
f1 (ppm)

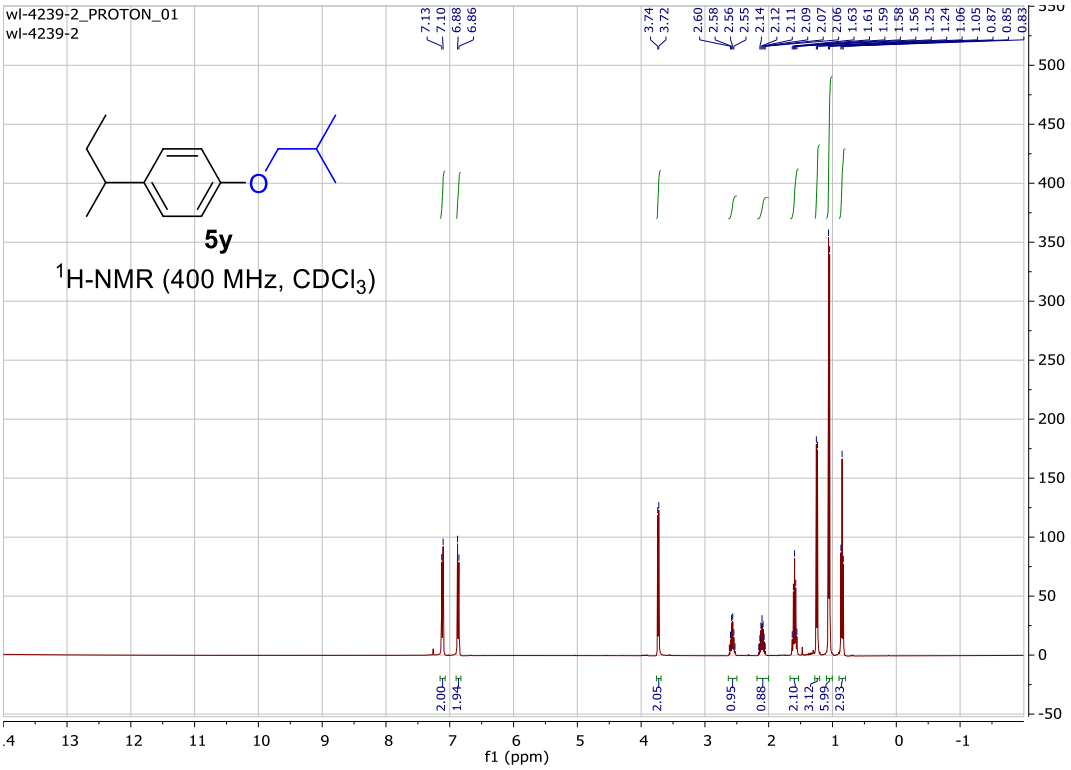

wl-4188-C.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 21
157.28
139.61
127.83
114.26
77.38
77.06
76.75
69.49
40.88
31.39
22.73
22.08
12.28
10.61
O
5u
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

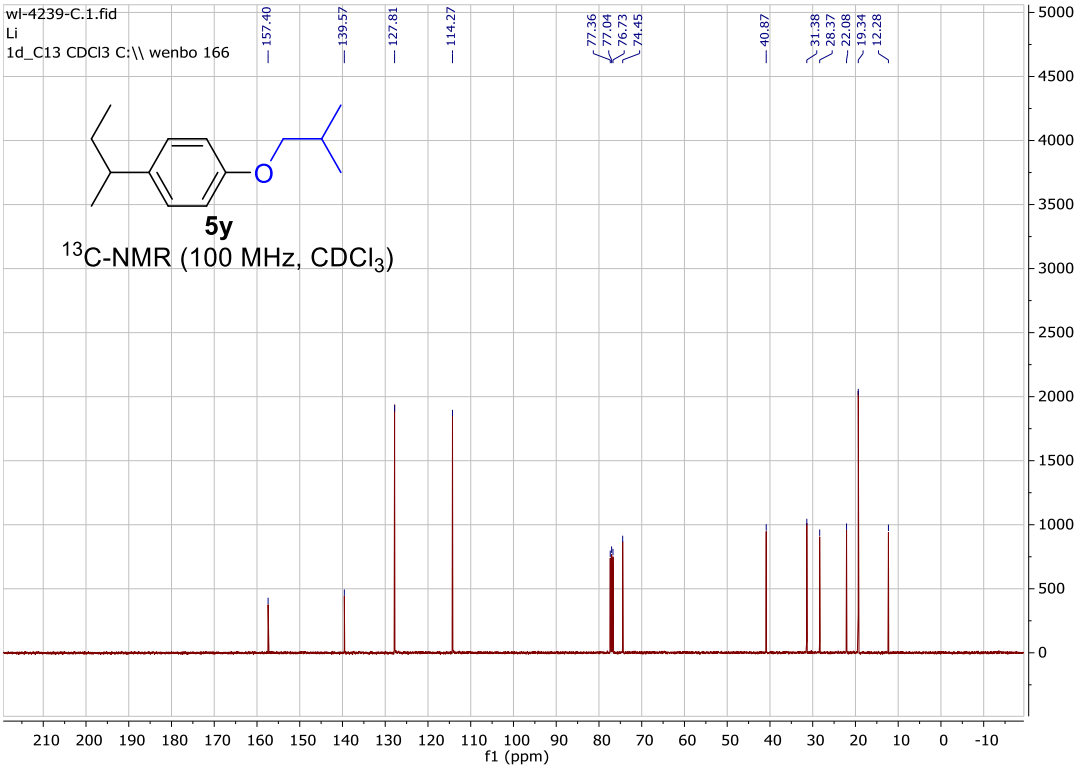

wl-4187-H_PROTON_01
wl-4187-H
5v
^{1}H-NMR (400 MHz, $CDCl_3$)
f1 (ppm)

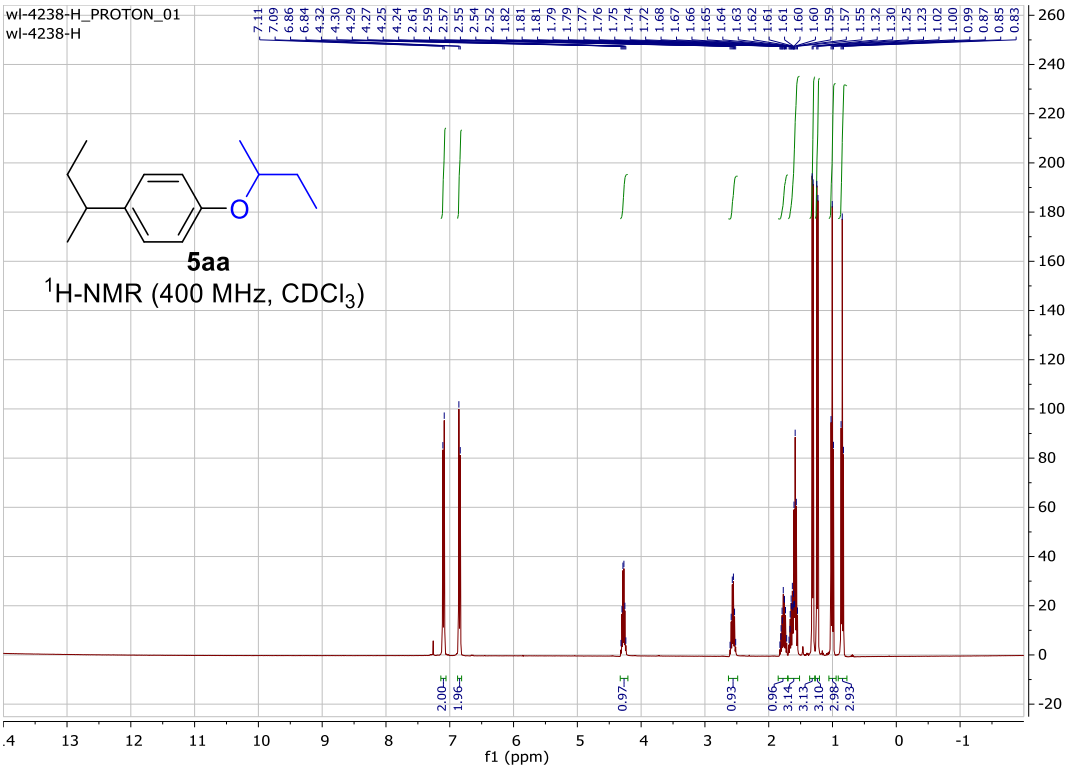

wl-4187-C.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 47
5v
^{13}C-NMR (100 MHz, $CDCl_3$)
f1 (ppm)

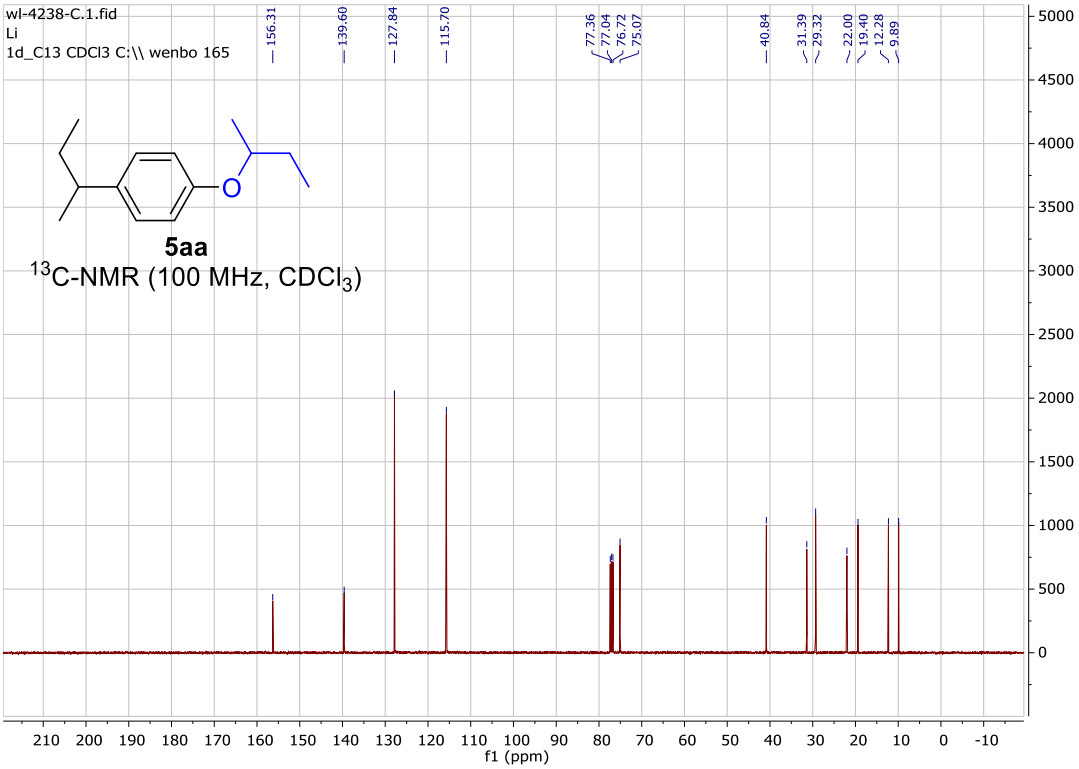

wl-4216-H.1.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 18
5w
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

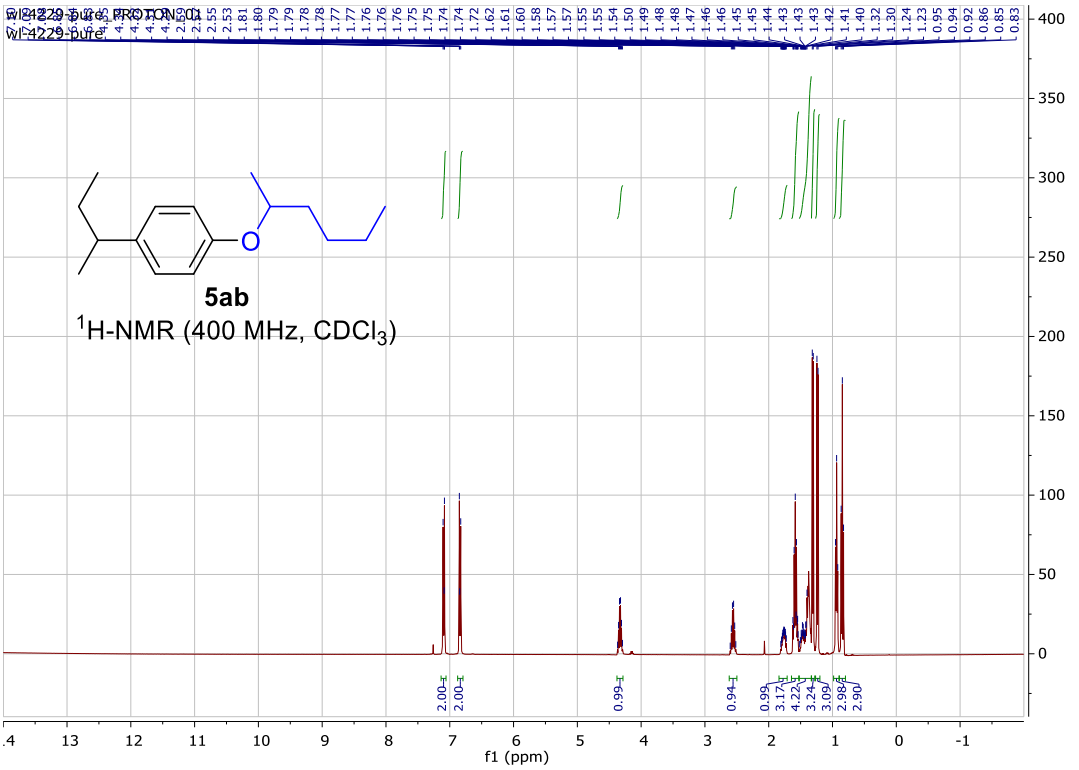

wl-4216-C.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 19
5w
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

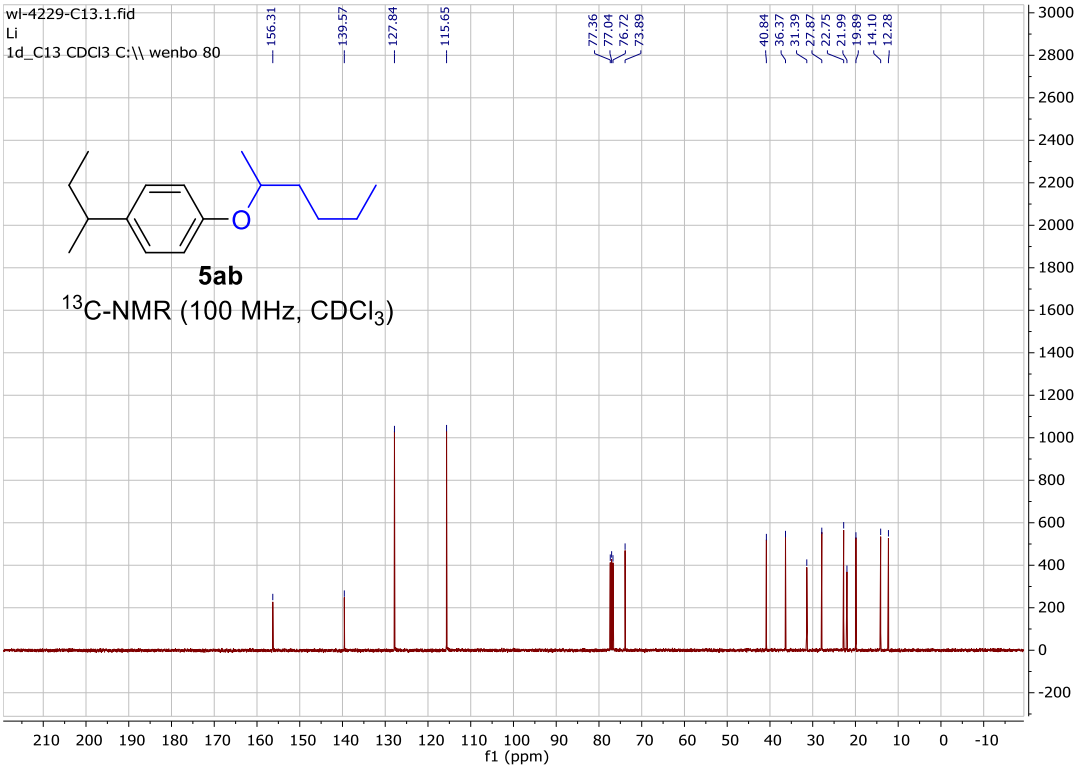

wl-4239-2_PROTON_01
wl-4239-2
5y
^{1}H-NMR (400 MHz, $CDCl_3$)
f1 (ppm)

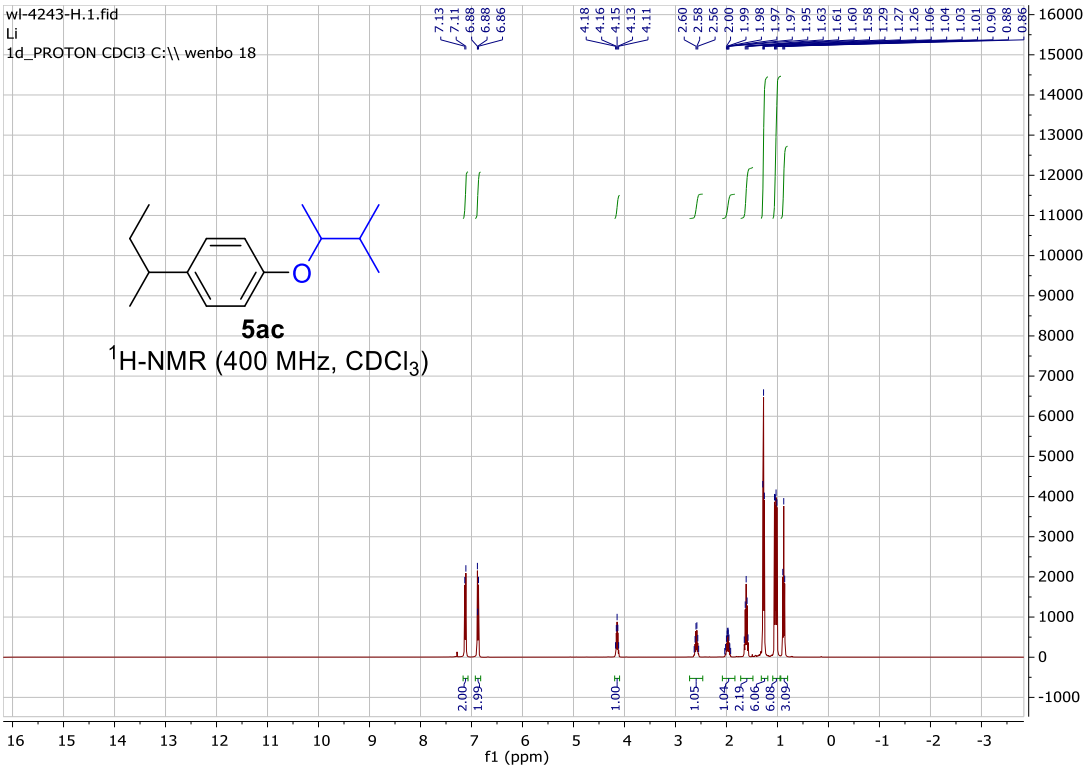

wl-4239-C.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 166
5y
^{13}C-NMR (100 MHz, $CDCl_3$)
f1 (ppm)

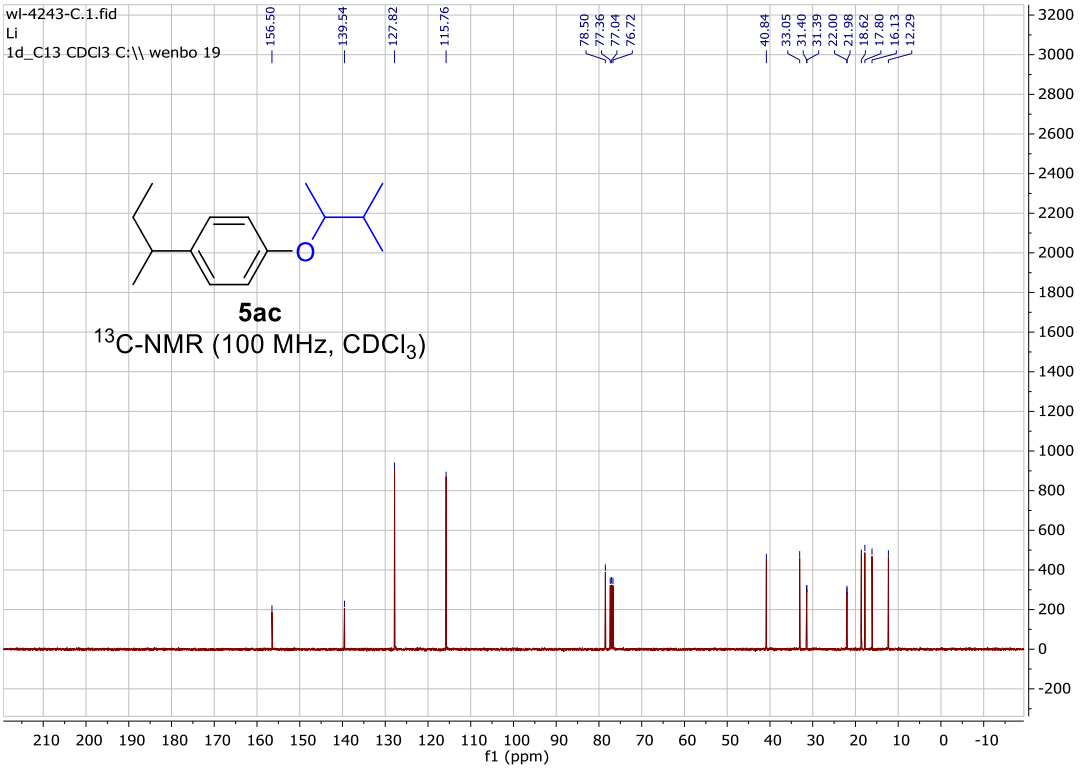

wl-4238-H_PROTON_01
wl-4238-H
5aa
^{1}H-NMR (400 MHz, $CDCl_3$)
f1 (ppm)

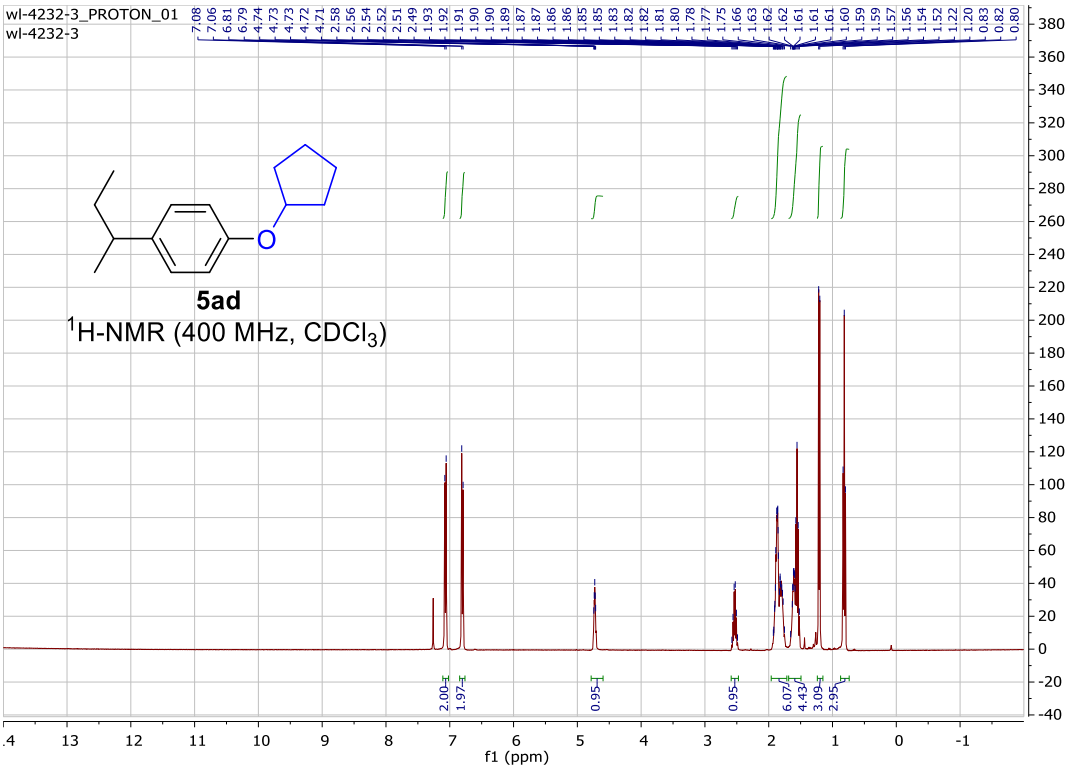

wl-4238-C.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 165
5aa
^{13}C-NMR (100 MHz, $CDCl_3$)
f1 (ppm)

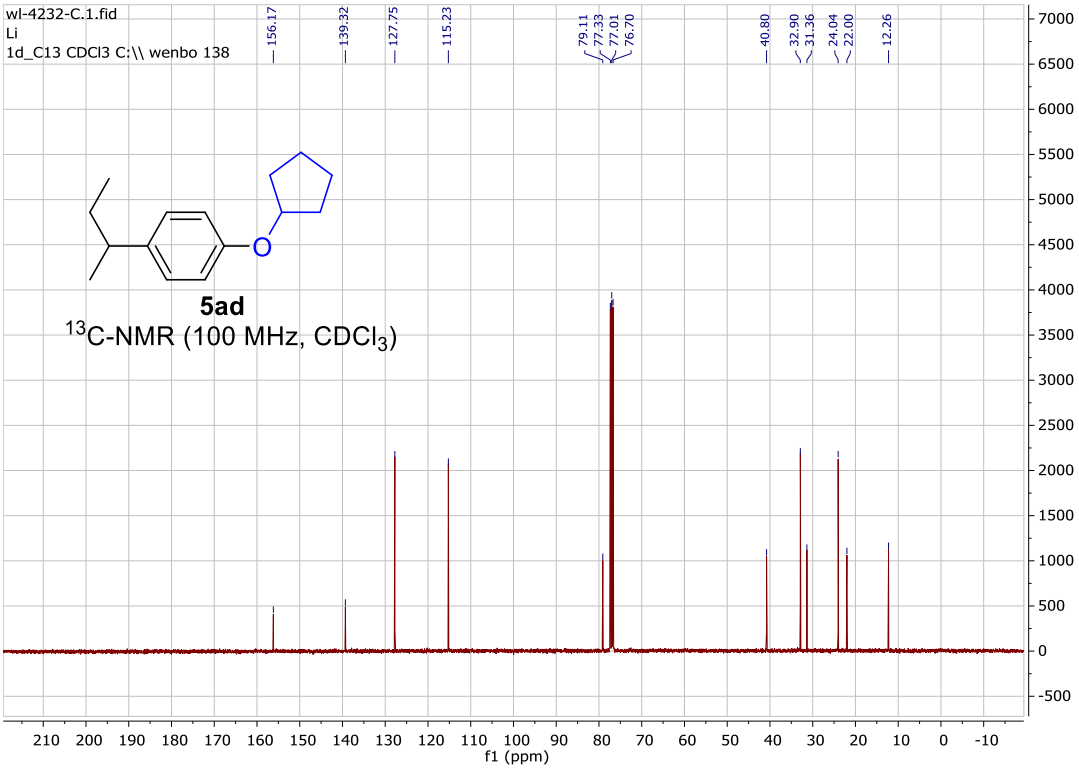

wl-4229-pure
wl-4229-pure
5ab
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

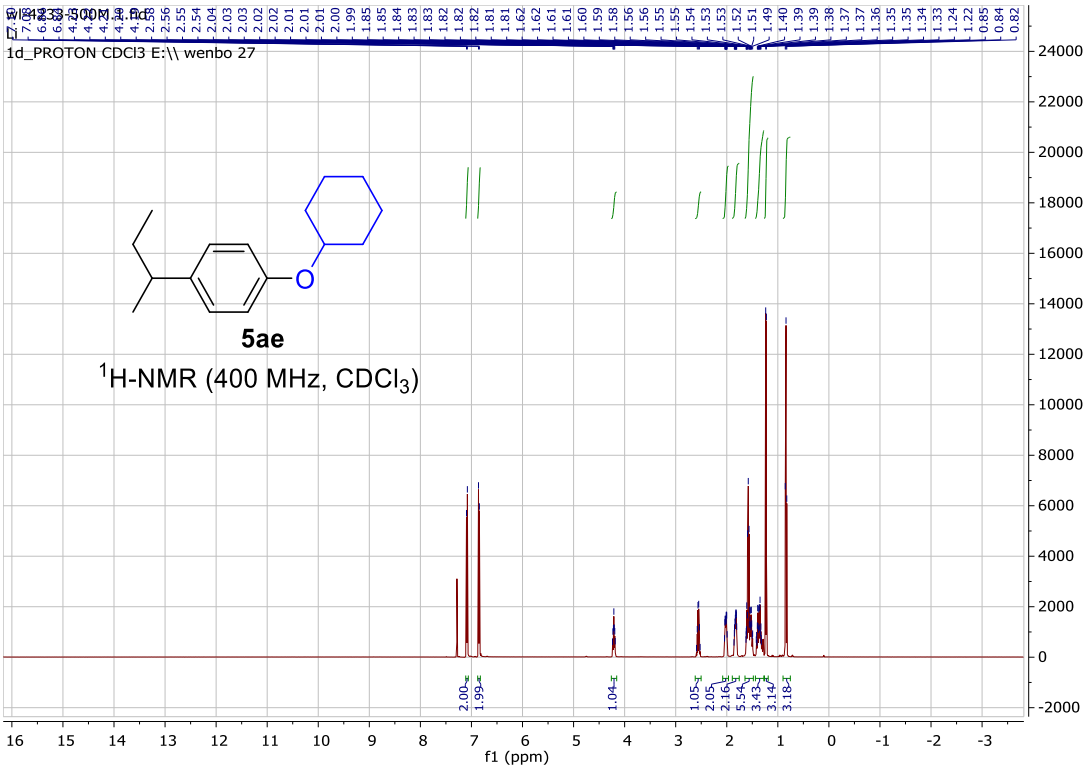

wl-4229-C13.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 80
5ab
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

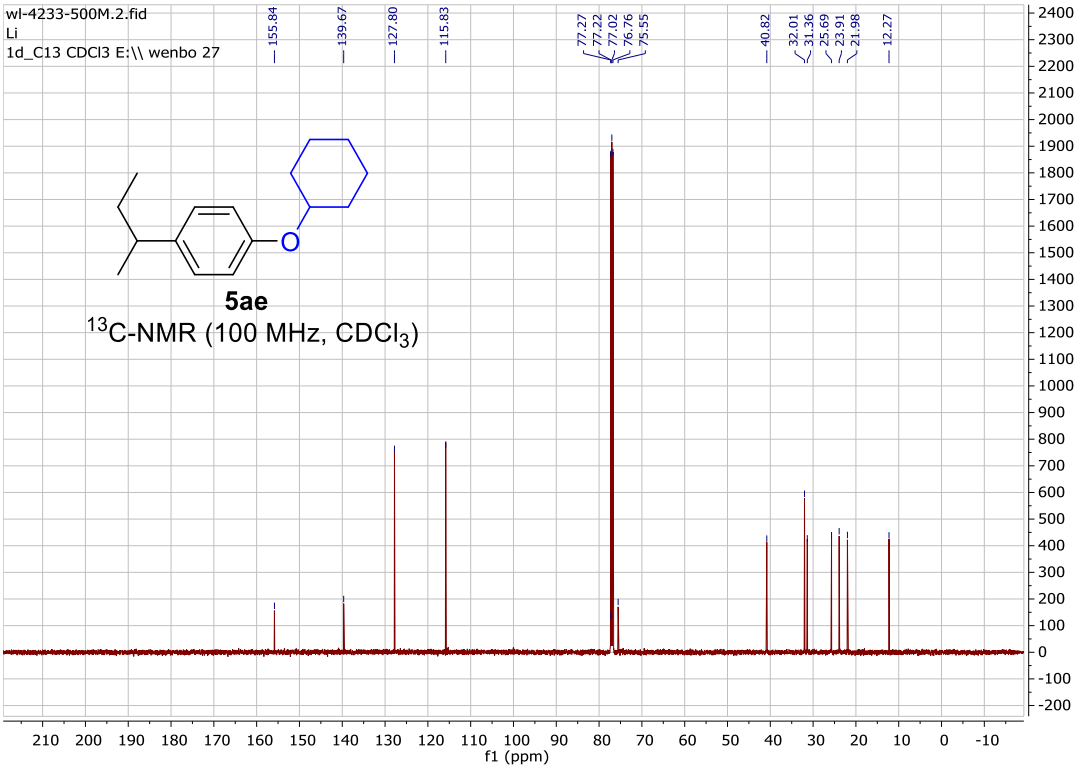

wl-4243-H.1.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 18
5ac
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

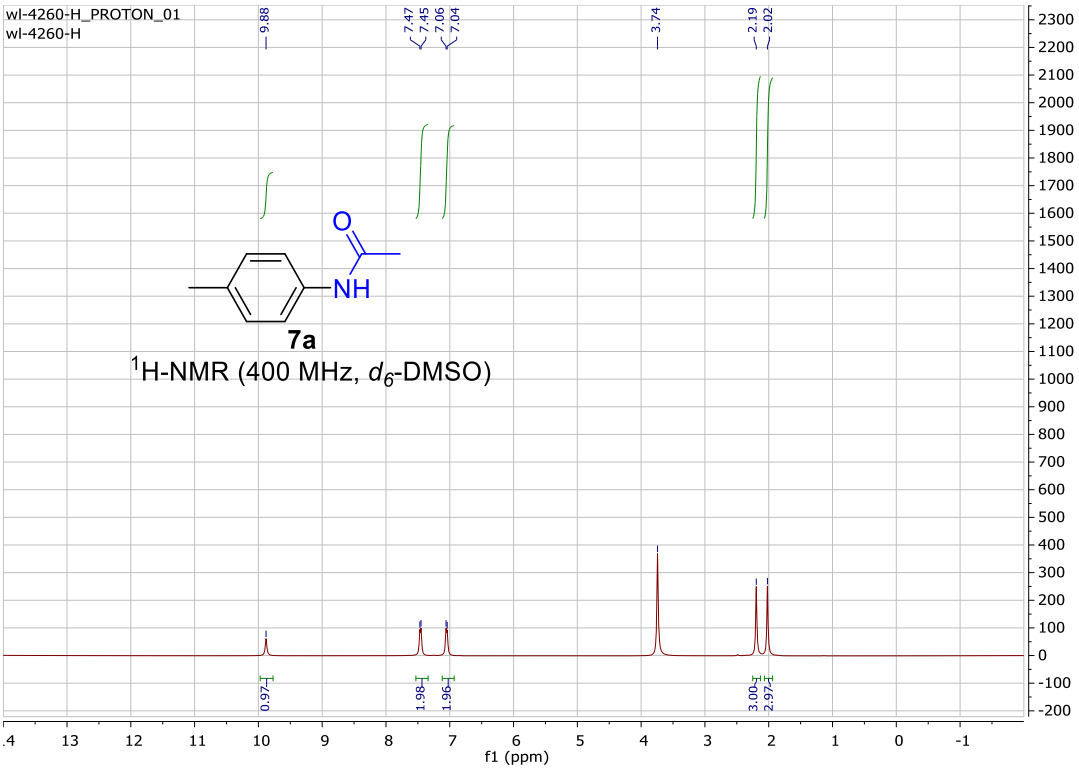

wl-4243-C.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 19
5ac
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

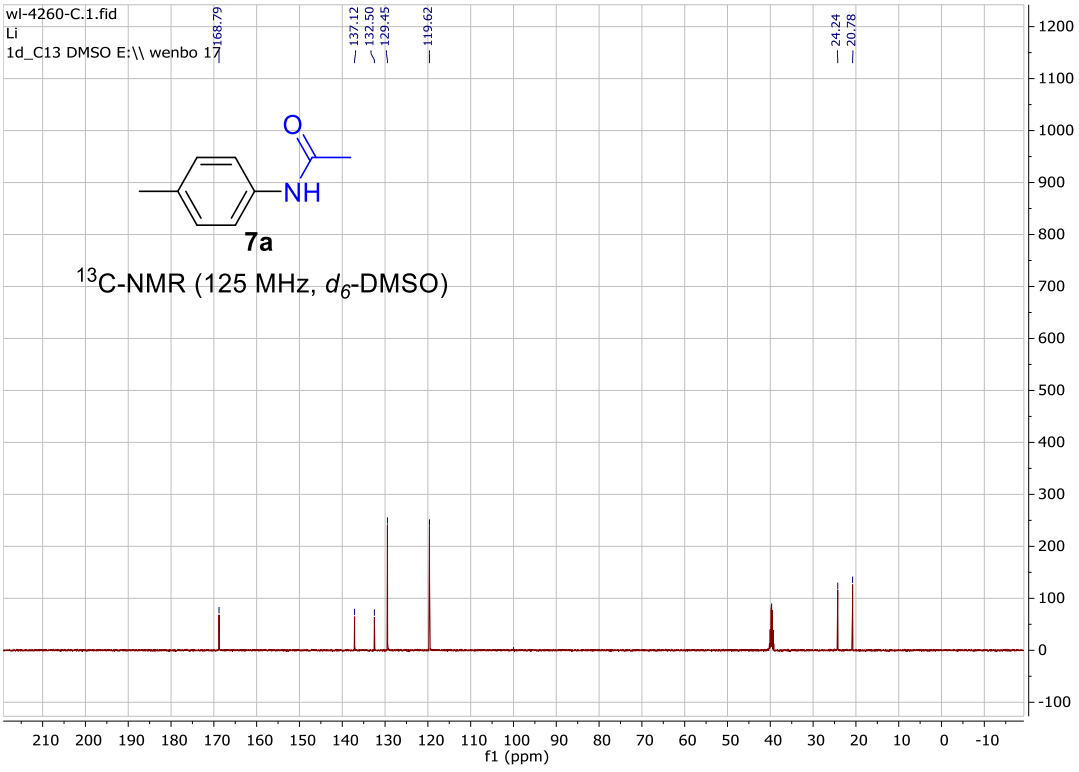

wl-4232-3_PROTON_01
wl-4232-3
5ad
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

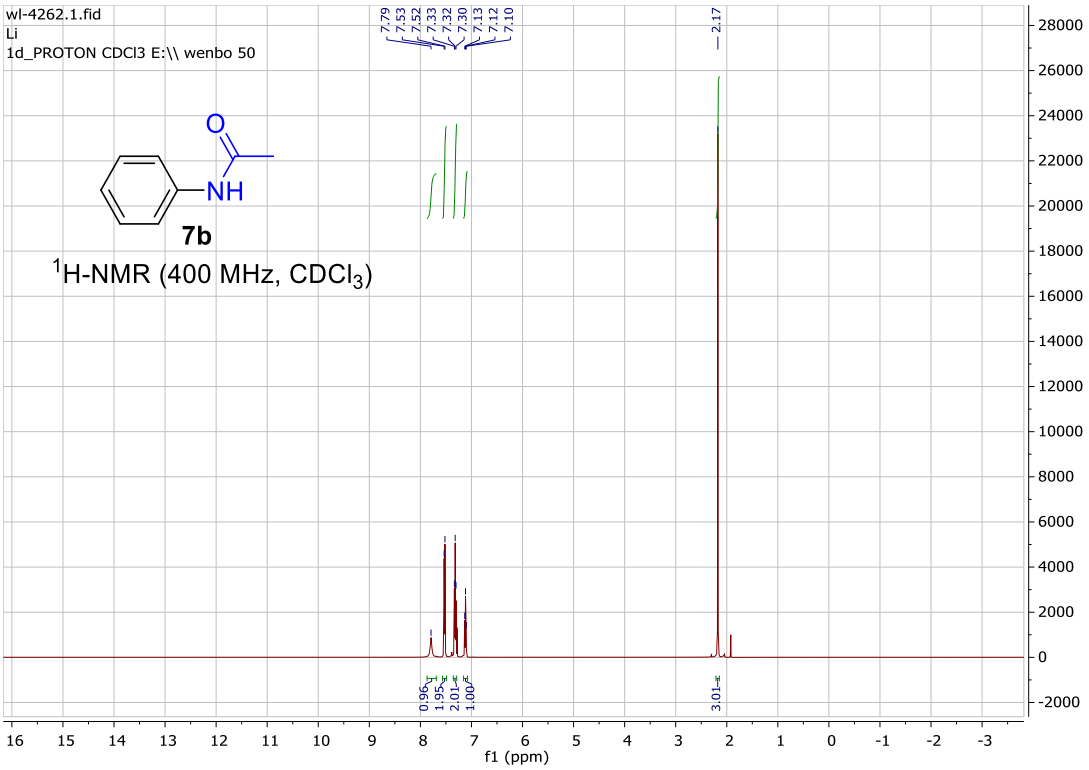

wl-4232-C.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 138
5ad
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

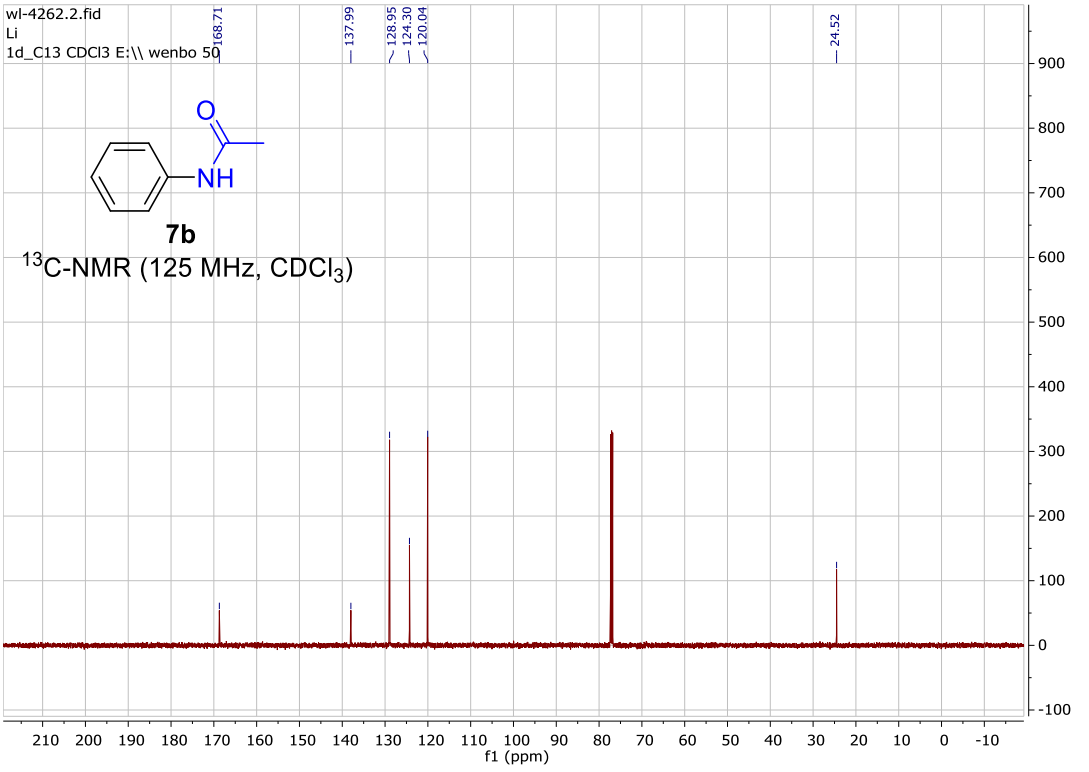

1d_PROTON CDCl3 E:\\ wenbo 27
5ae
1H-NMR (400 MHz, CDCl3)
f1 (ppm)

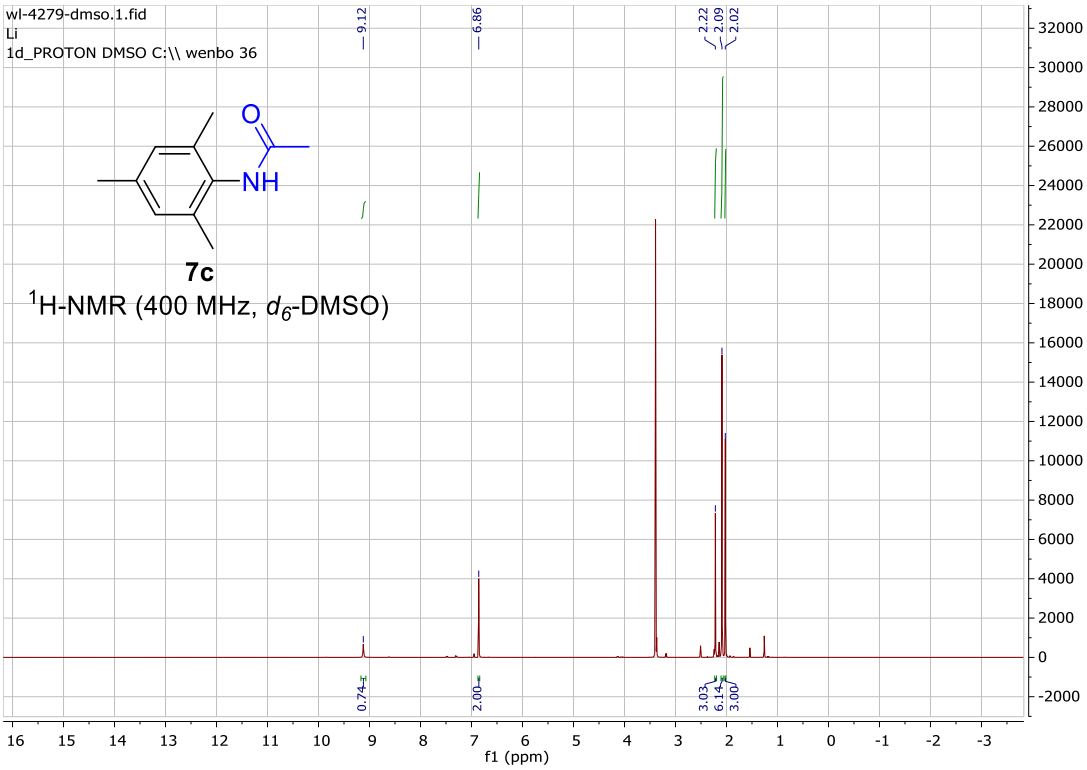

wl-4233-500M.2.fid
Li
1d_C13 CDCl3 E:\\ wenbo 27
5ae
13C-NMR (100 MHz, CDCl3)
f1 (ppm)

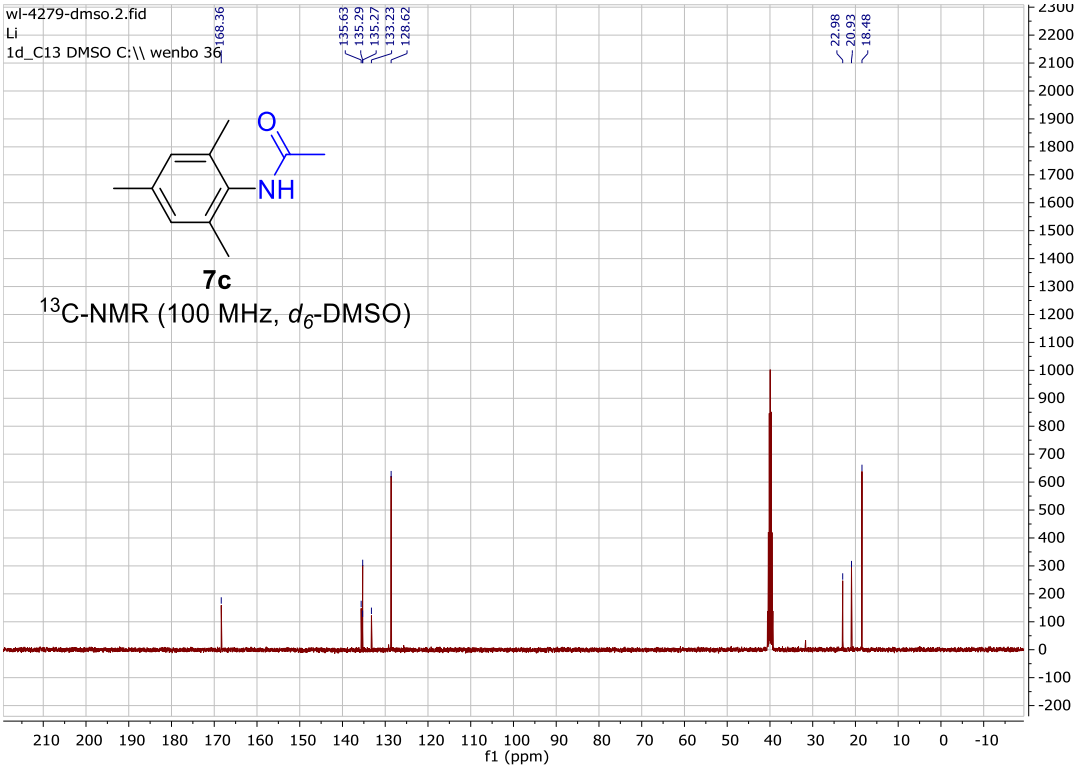

wl-4260-H_PROTON_01
wl-4260-H
9.88
7.47
7.45
7.06
7.04
3.74
2.19
2.02
O
NH
7a
1H-NMR (400 MHz, d6-DMSO)
0.97
1.98
1.96
3.00
2.97
f1 (ppm)

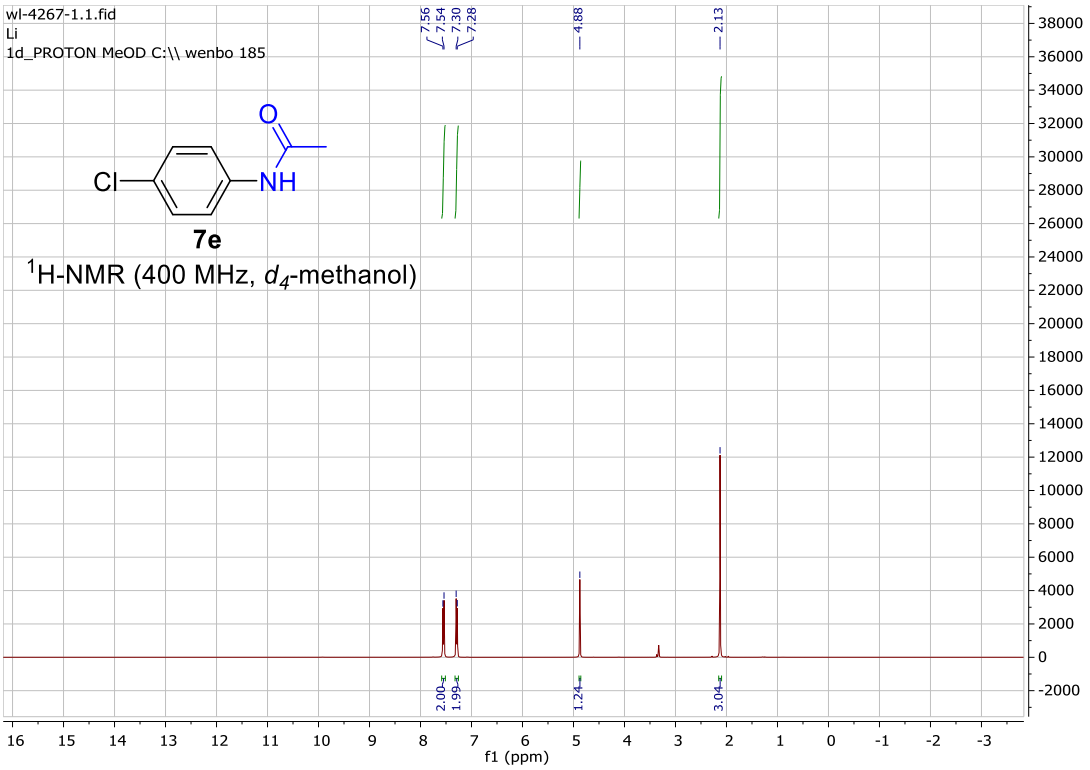

wl-4260-C.1.fid
Li
1d_C13 DMSO E:\\ wenbo 17
168.79
137.12
132.50
129.45
119.62
24.24
20.78
O
NH
7a
13C-NMR (125 MHz, d6-DMSO)
f1 (ppm)

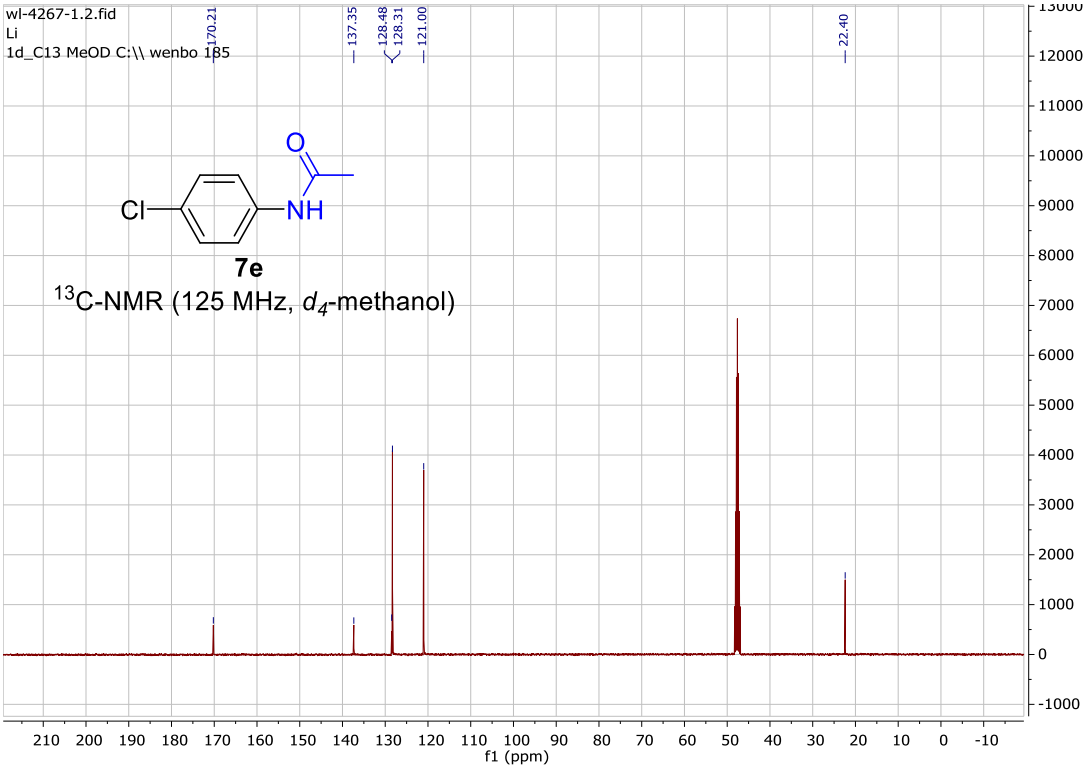

wl-4262.1.fid
Li
1d_PROTON CDCl3 E:\\ wenbo 50
7.79
7.53
7.52
7.33
7.32
7.30
7.13
7.12
7.10
2.17
O
NH
7b
1H-NMR (400 MHz, CDCl3)
0.96
1.95
2.01
1.00
3.01
f1 (ppm)

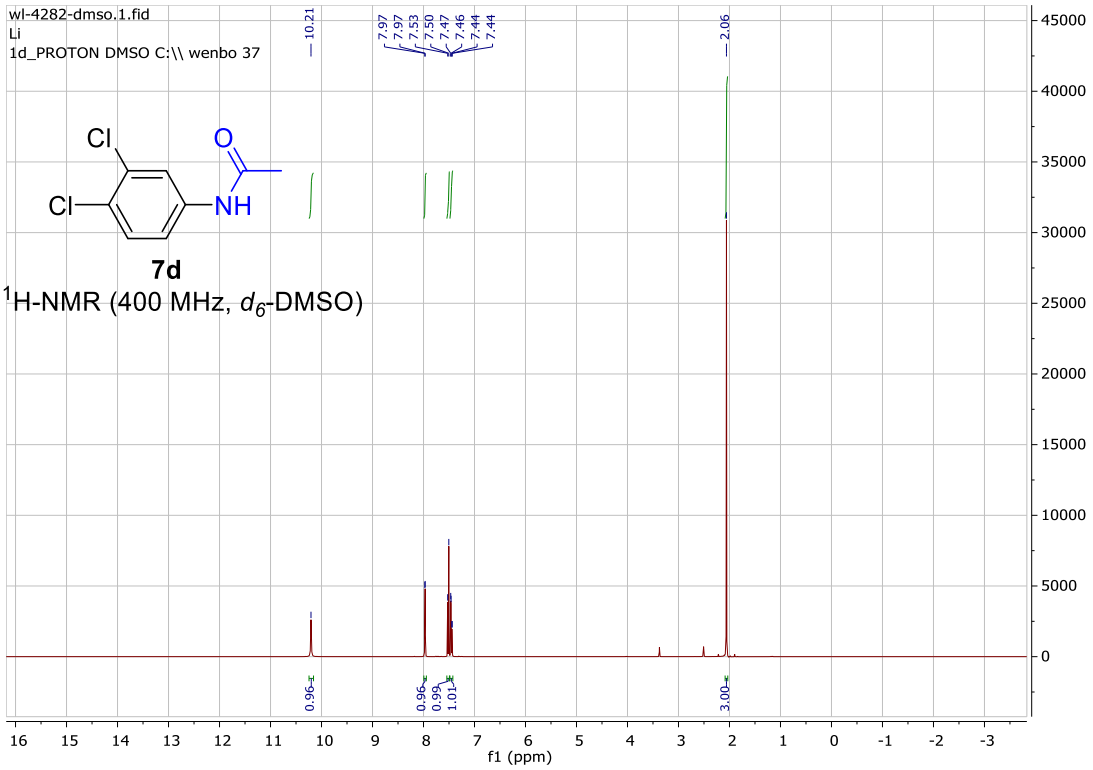

wl-4262.2.fid
Li
1d_C13 CDCl3 E:\\ wenbo 50
168.71
137.99
128.95
124.30
120.04
24.52
O
NH
7b
13C-NMR (125 MHz, CDCl3)
f1 (ppm)

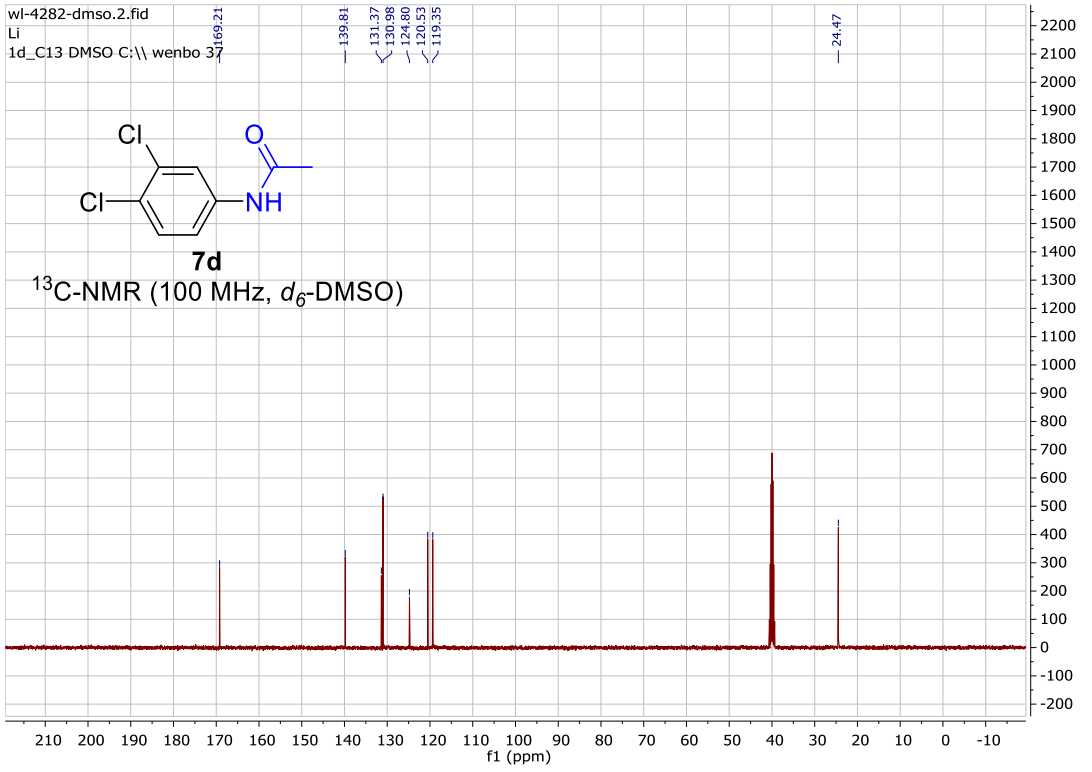

wl-4279-dmso.1.fid
Li
1d_PROTON DMSO C:\\ wenbo 36
9.12
6.86
2.22
2.09
2.02
O
NH
7c
1H-NMR (400 MHz, d6-DMSO)
0.74
2.00
3.03
6.14
3.00
f1 (ppm)

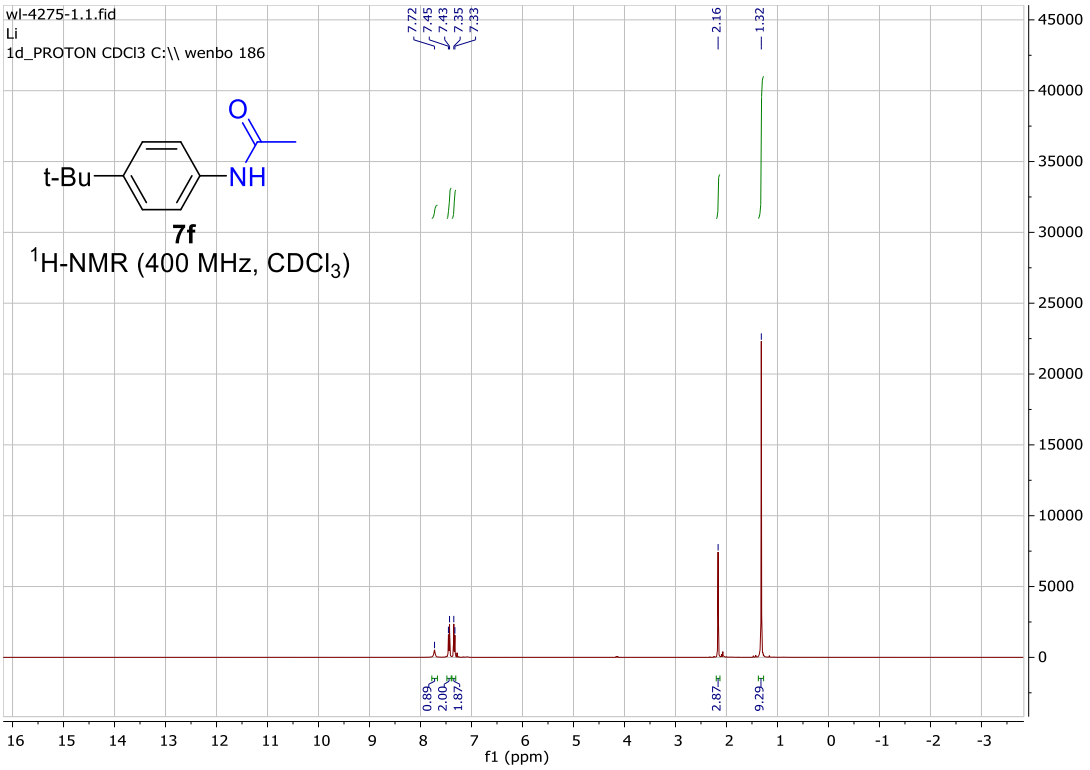

wl-4279-dmso.2.fid
Li
1d_C13 DMSO C:\\ wenbo 36
168.36
135.63
135.29
135.27
133.23
128.62
22.98
20.93
18.48
O
NH
7c
13C-NMR (100 MHz, d6-DMSO)
f1 (ppm)

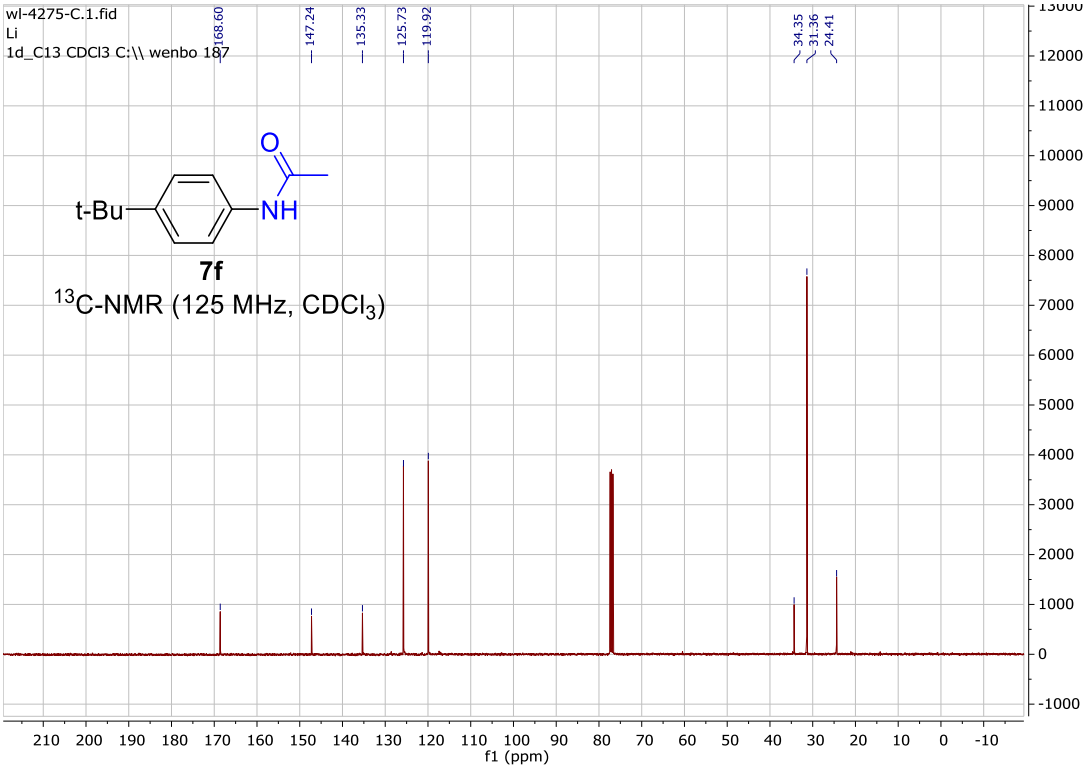

wl-4267-1.1.fid
Li
1d_PROTON MeOD C:\\ wenbo 185
7.56
7.54
7.30
7.28
4.88
2.13
Cl
NH
O
7e
1H-NMR (400 MHz, d4-methanol)
2.00
1.99
1.24
3.04
f1 (ppm)

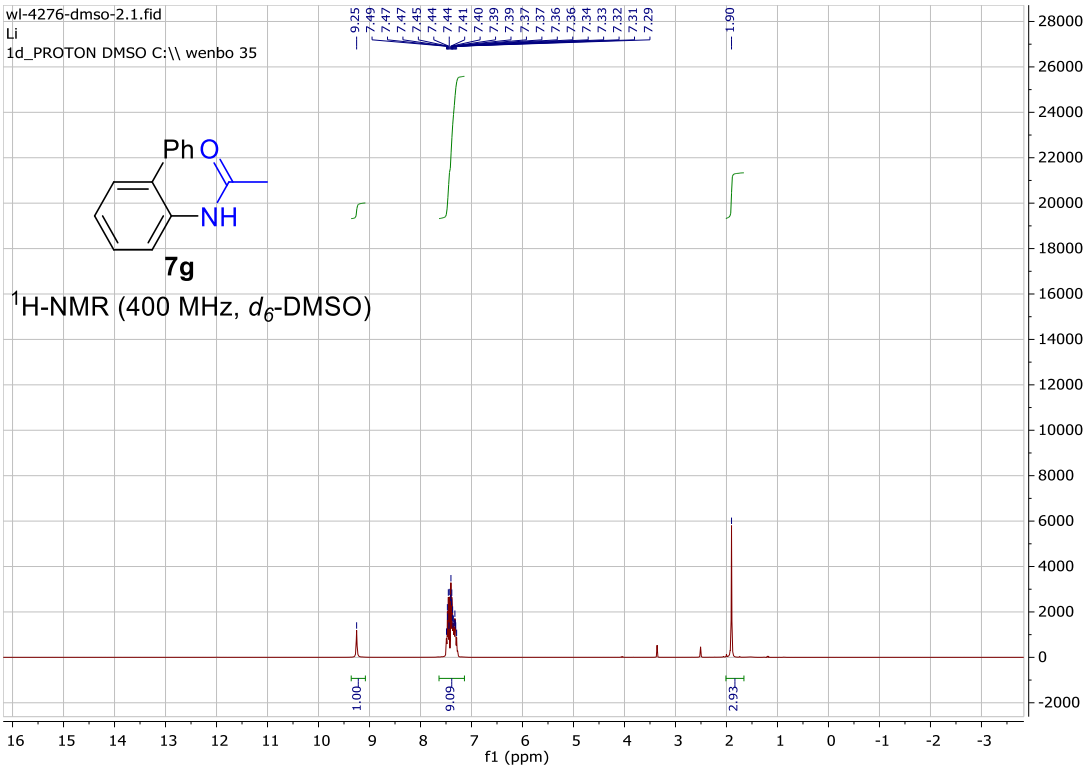

wl-4267-1.2.fid
Li
1d_C13 MeOD C:\\ wenbo 185
170.21
137.35
128.48
128.31
121.00
22.40
Cl
NH
O
7e
13C-NMR (125 MHz, d4-methanol)
f1 (ppm)

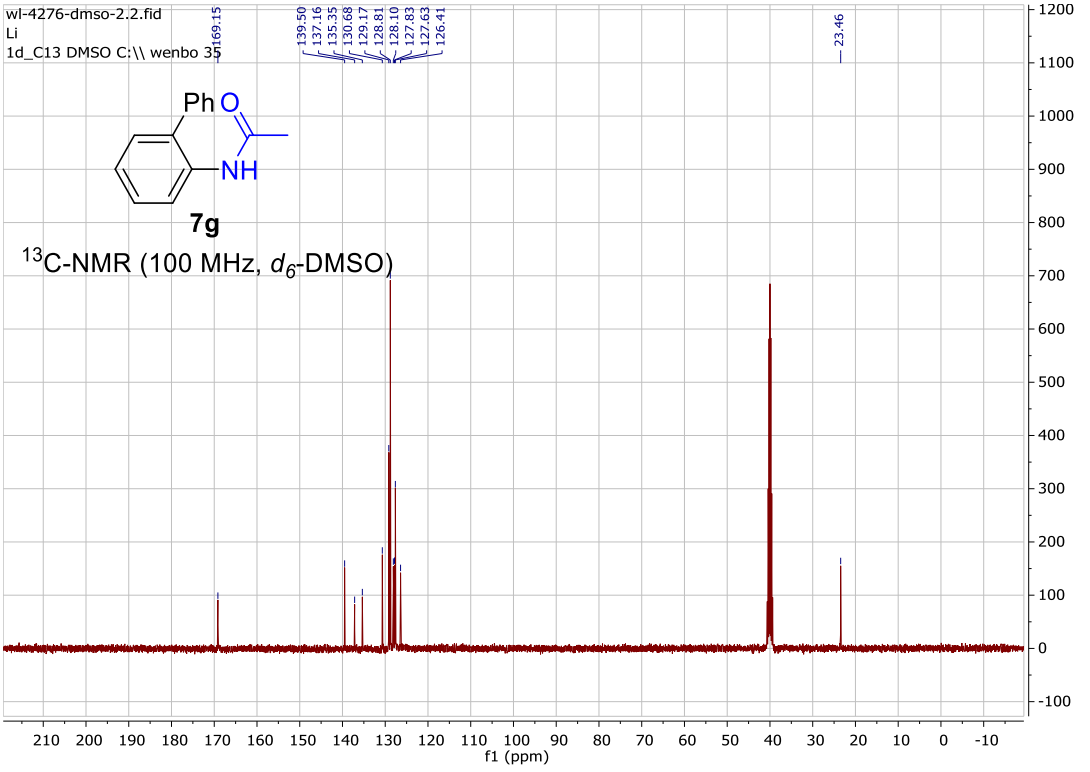

wl-4282-dmso.1.fid
Li
1d_PROTON DMSO C:\\ wenbo 37
10.21
7.97
7.97
7.53
7.50
7.47
7.46
7.44
7.44
2.06
Cl
Cl
O
NH
7d
1H-NMR (400 MHz, d6-DMSO)
0.96
0.96
0.99
1.01
3.00
f1 (ppm)

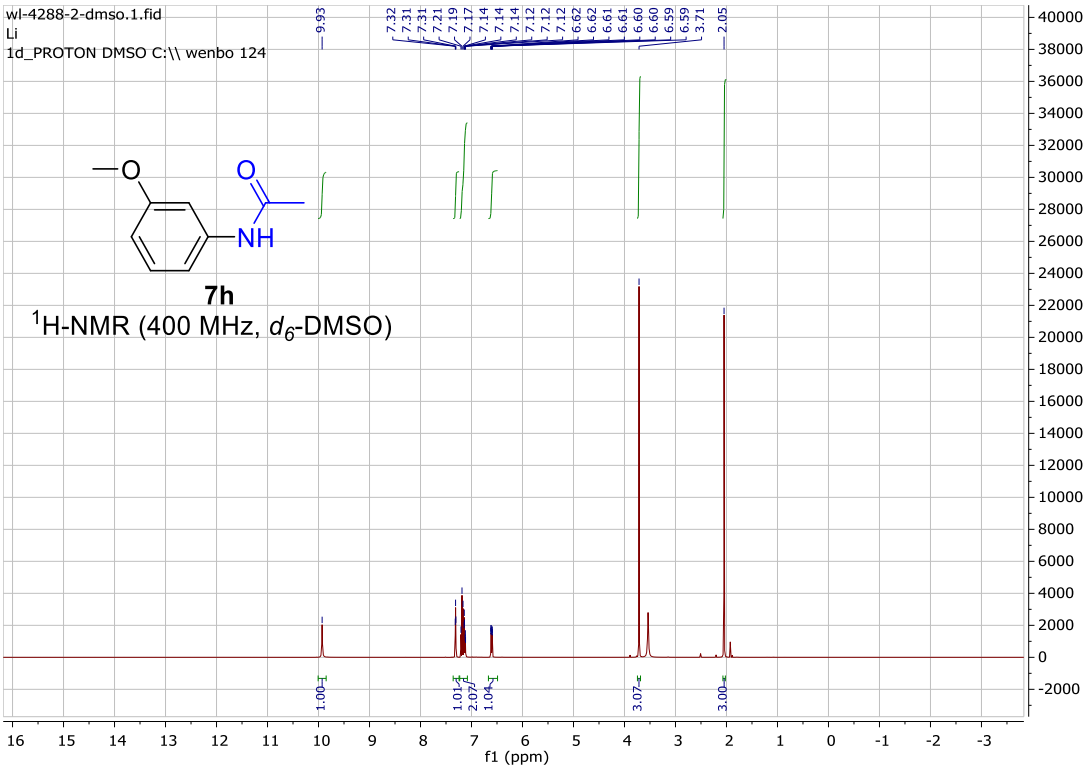

wl-4282-dmso.2.fid
Li
1d_C13 DMSO C:\\ wenbo 37
169.21
139.81
131.37
130.98
124.80
120.53
119.35
24.47
Cl
Cl
O
NH
7d
13C-NMR (100 MHz, d6-DMSO)
f1 (ppm)

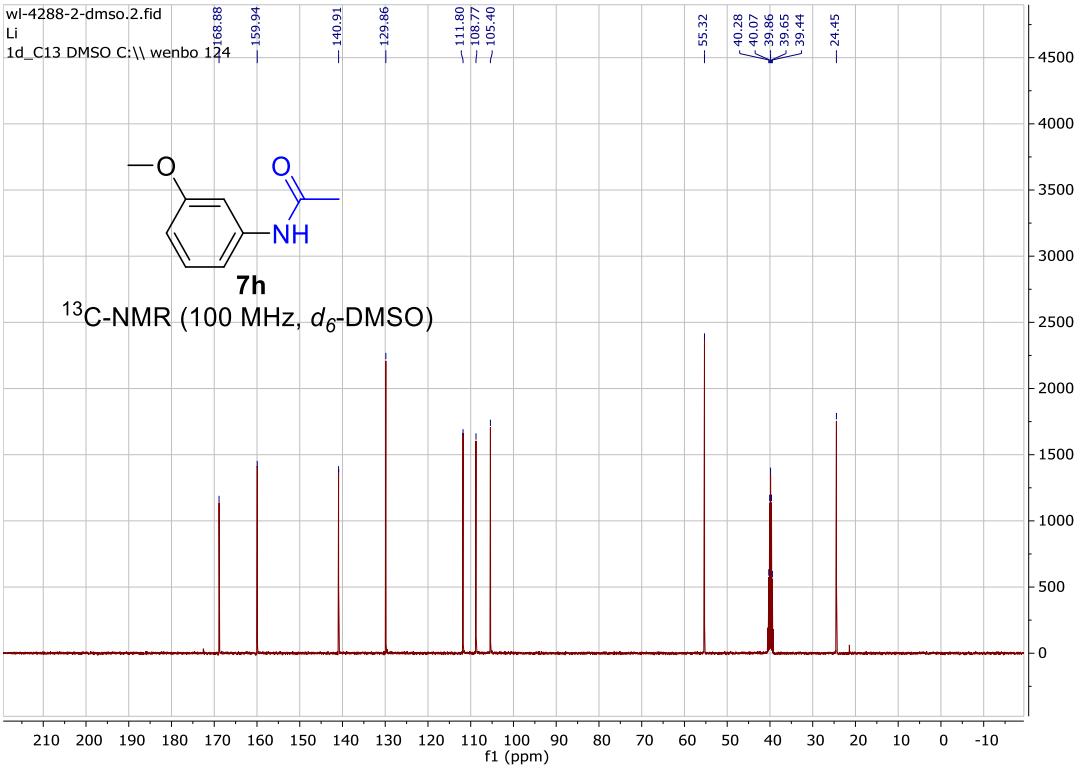

wl-4275-1.1.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 186
7.72
7.45
7.43
7.35
7.33
2.16
1.32
t-Bu
NH
O
7f
1H-NMR (400 MHz, CDCl3)
0.89
2.00
1.87
2.87
9.29
f1 (ppm)

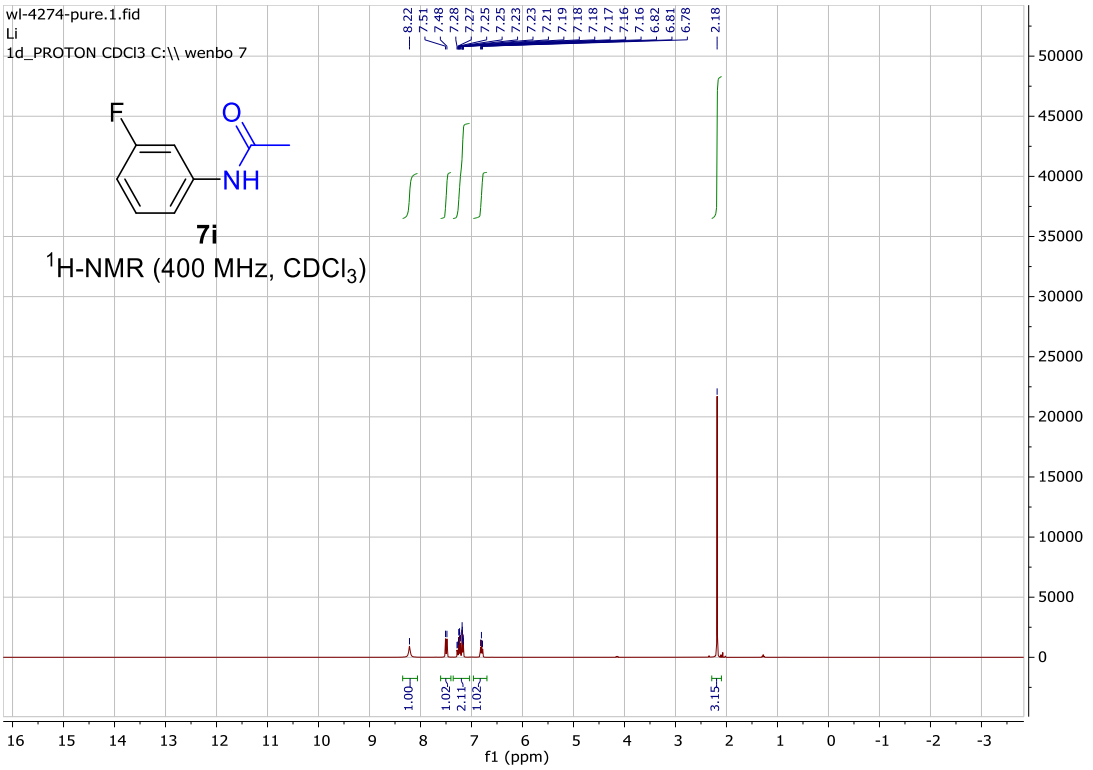

wl-4275-C.1.fid
Li
1d_C13 CDCl3 C:\\ wenbo 187
168.60
147.24
135.33
125.73
119.92
34.35
31.36
24.41
t-Bu
NH
O
7f
13C-NMR (125 MHz, CDCl3)
f1 (ppm)

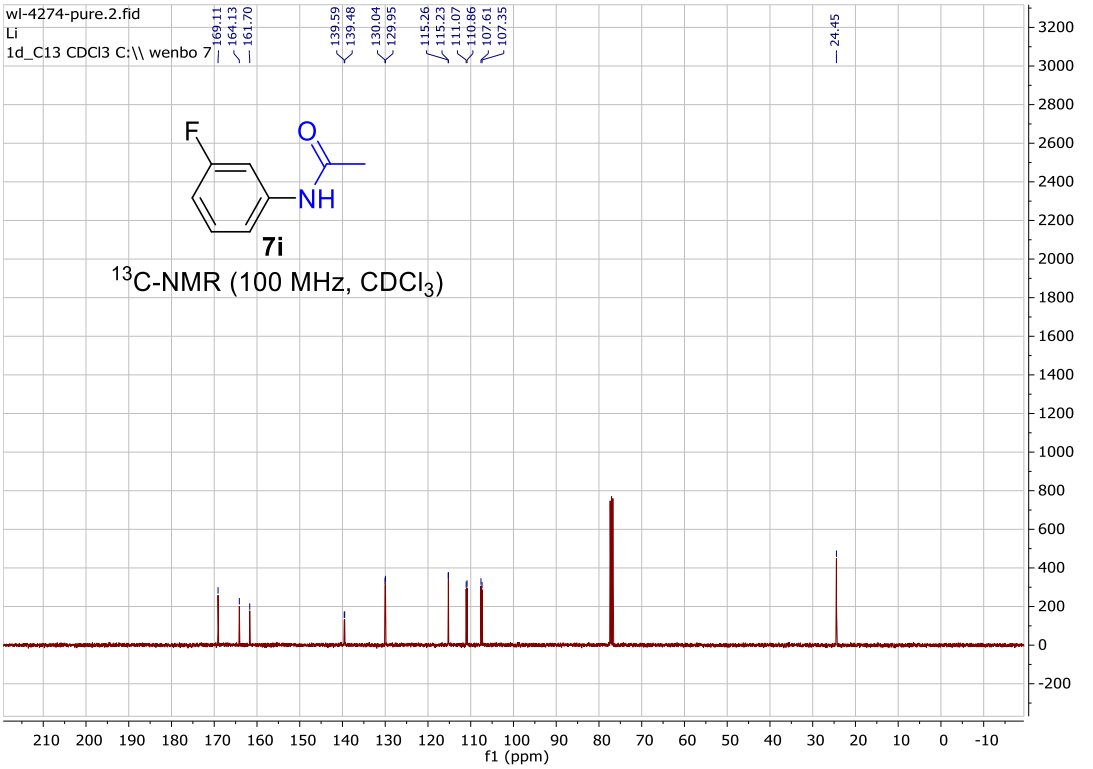

wl-4276-dmso-2.1.fid
Li
1d_PROTON DMSO C:\\ wenbo 35
9.25
7.49
7.47
7.47
7.45
7.44
7.44
7.41
7.40
7.39
7.39
7.37
7.37
7.36
7.36
7.34
7.33
7.32
7.31
7.29
1.90
Ph
O
NH
7g
1H-NMR (400 MHz, d6-DMSO)
1.00
9.09
2.93
f1 (ppm)

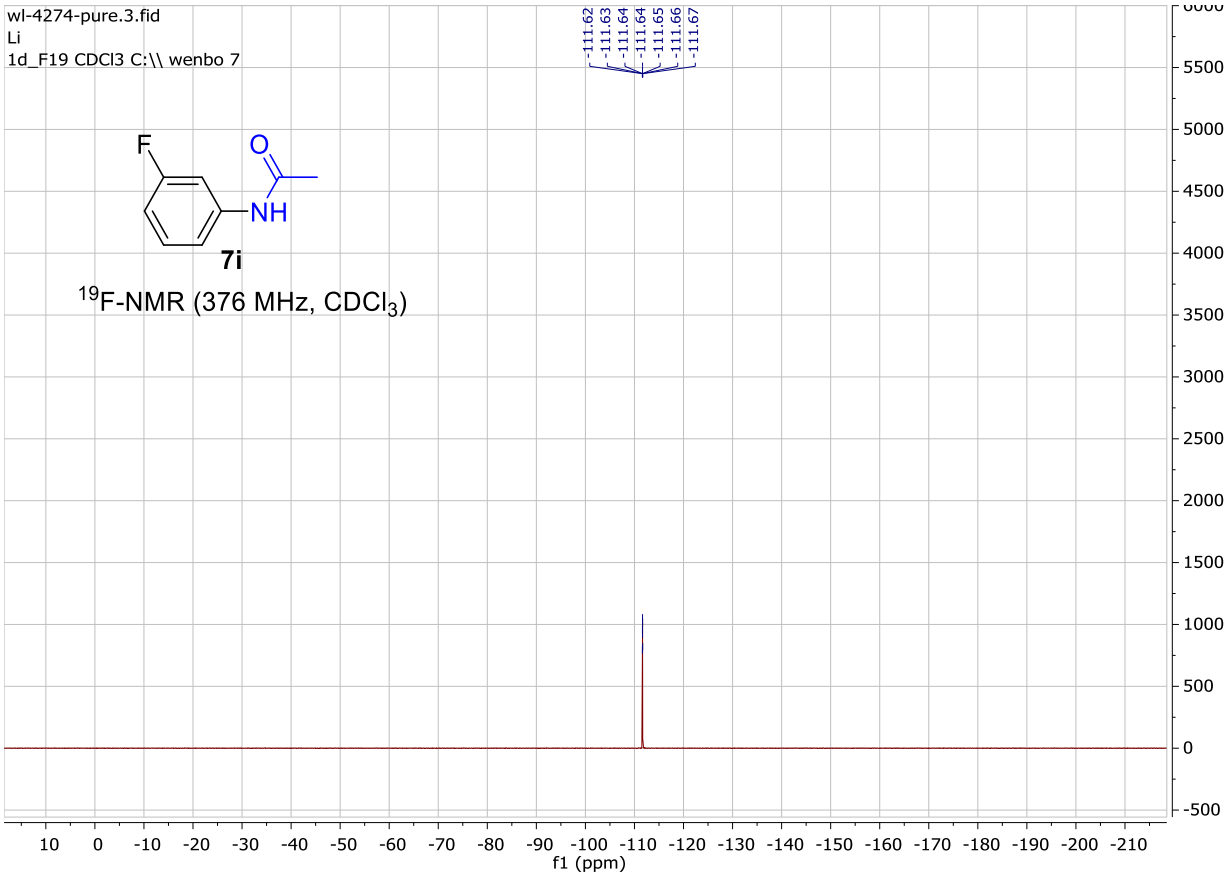

wl-4276-dmso-2.2.fid
Li
1d_C13 DMSO C:\\ wenbo 35
169.15
139.50
137.16
135.35
130.68
129.17
128.81
128.10
127.83
127.63
126.41
23.46
Ph
O
NH
7g
13C-NMR (100 MHz, d6-DMSO)
f1 (ppm)

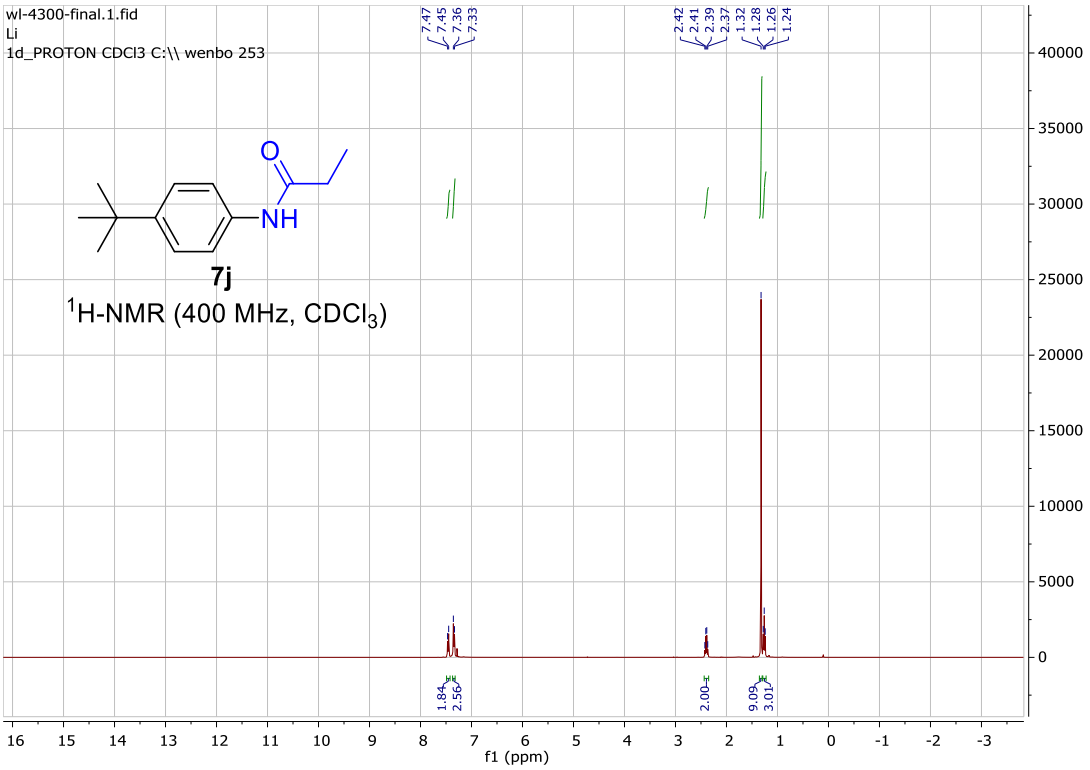

wl-4288-2-dmso.1.fid
Li
1d_PROTON DMSO C:\\ wenbo 124
9.93
7.32
7.31
7.31
7.21
7.19
7.17
7.14
7.14
7.14
7.12
7.12
7.12
6.62
6.62
6.61
6.61
6.60
6.60
6.59
6.59
3.71
2.05
O
O
NH
7h
1H-NMR (400 MHz, d6-DMSO)
1.00
1.01
2.07
1.04
3.07
3.00
f1 (ppm)

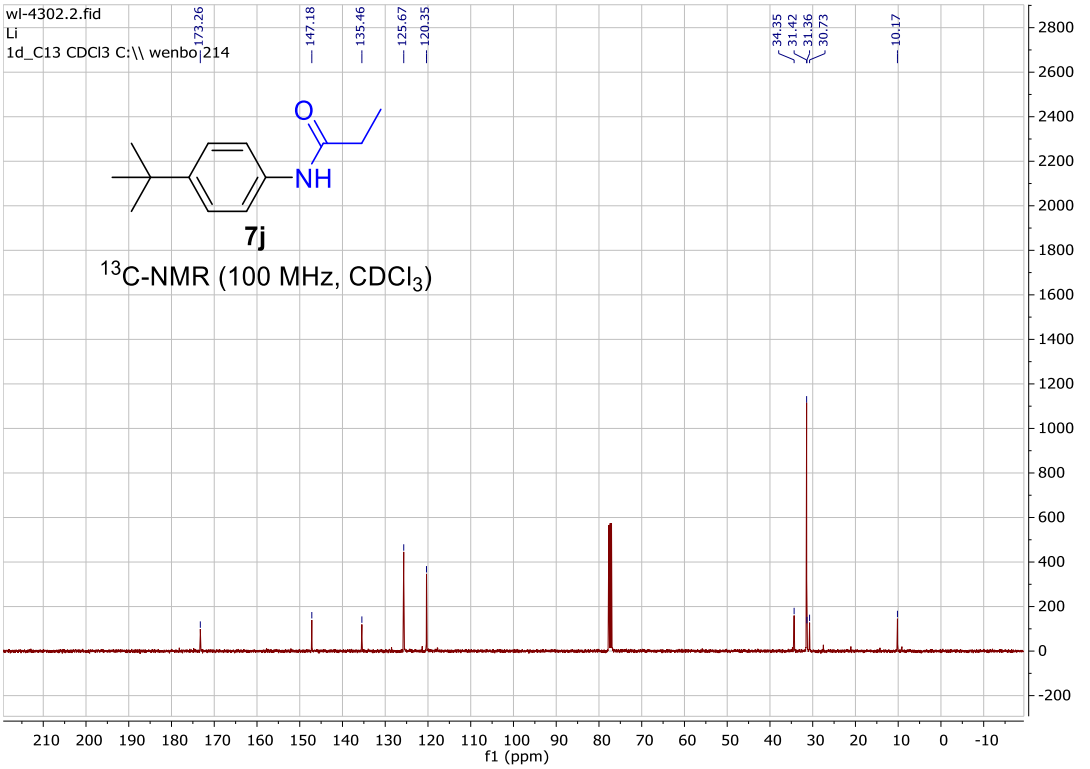

wl-4288-2-dmso.2.fid
Li
1d_C13 DMSO C:\\ wenbo 124
168.88
159.94
140.91
129.86
111.80
108.77
105.40
55.32
40.28
40.07
39.86
39.65
39.44
24.45
O
O
NH
7h
13C-NMR (100 MHz, d6-DMSO)
f1 (ppm)

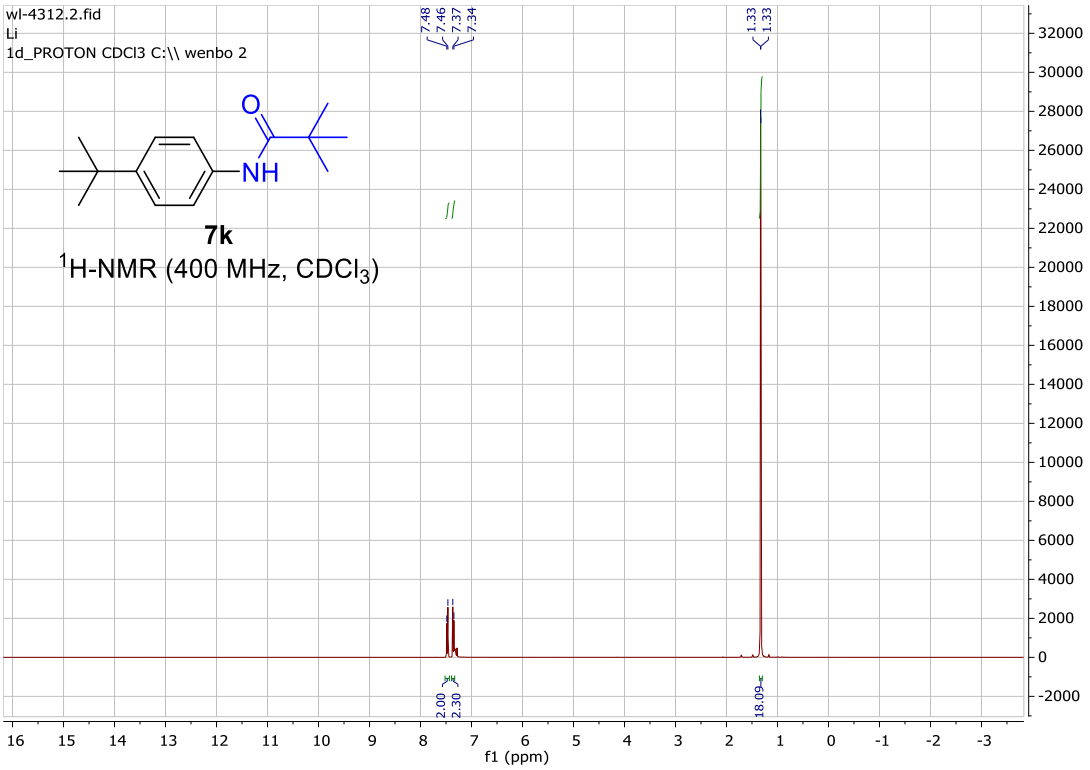

wl-4274-pure.1.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 7
8.22
7.51
7.48
7.28
7.27
7.25
7.25
7.23
7.23
7.21
7.19
7.18
7.18
7.17
7.16
7.16
6.82
6.81
6.78
2.18
F
O
NH
7i
1H-NMR (400 MHz, CDCl3)
1.00
1.02
2.11
1.02
3.15
f1 (ppm)

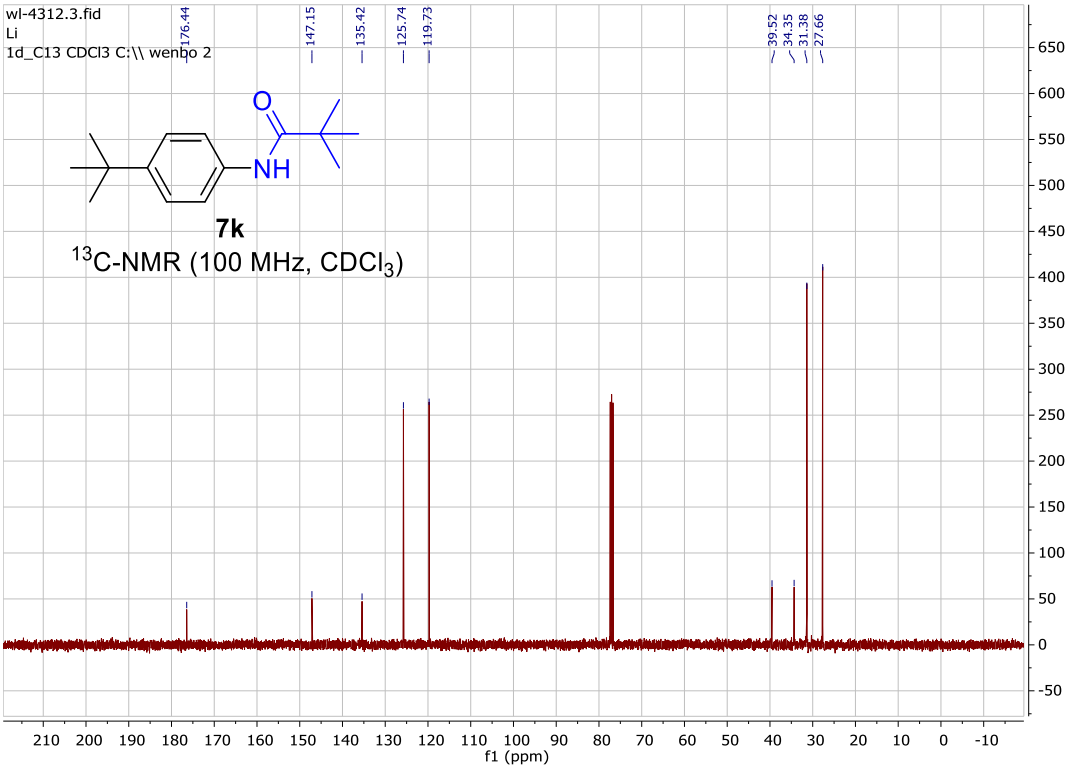

wl-4274-pure.2.fid
Li
1d_C13 CDCl3 C:\\ wenbo 7
169.11
164.13
161.70
139.59
139.48
130.04
129.95
115.26
115.23
111.07
110.86
107.61
107.35
24.45
F
O
NH
7i
13C-NMR (100 MHz, CDCl3)
f1 (ppm)


wl-4274-pure.3.fid
Li
1d_F19 CDCl3 C:\\ wenbo 7
-111.62
-111.63
-111.64
-111.64
-111.65
-111.66
-111.67
F
O
NH
7i
19F-NMR (376 MHz, CDCl3)
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


wl-4300-final.1.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 253
7.47
7.45
7.36
7.33
2.42
2.41
2.39
2.37
1.32
1.28
1.26
1.24
O
NH
7j
1H-NMR (400 MHz, CDCl3)
1.84
2.56
2.00
9.09
3.01
f1 (ppm)


wl-4302.2.fid
Li
1d_C13 CDCl3 C:\\ wenbo 214
173.26
147.18
135.46
125.67
120.35
34.35
31.42
31.36
30.73
10.17
O
NH
7j
13C-NMR (100 MHz, CDCl3)
f1 (ppm)


wl-4312.2.fid
Li
1d_PROTON CDCl3 C:\\ wenbo 2
7.48
7.46
7.37
7.34
1.33
1.33
O
NH
7k
1H-NMR (400 MHz, CDCl3)
2.00
2.30
18.09
f1 (ppm)


wl-4312.3.fid
Li
1d_C13 CDCl3 C:\\ wenbo 2
176.44
147.15
135.42
125.74
119.73
39.52
34.35
31.38
27.66
O
NH
7k
13C-NMR (100 MHz, CDCl3)
f1 (ppm)