Supporting information

Dehydrative condensation of carbonyls with non-acidic methylenes enabled by light: synthesis of benzofurans

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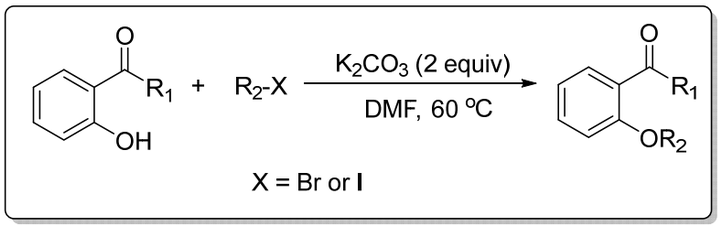
1: General comments and materials

Solvents and reagents were purchased from Sigma-Aldrich chemical company and were used without further purification unless otherwise specified. ^{1}H NMR and ^{13}C NMR spectra were recorded on Varian 300 MHz, 400 MHz, or 500 MHz spectrometers. All signals are reported in ppm with the internal reference of 7.26 ppm or 77.0 ppm for chloroform as standard. Data are reported as follows: multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet), coupling constant (*J*/Hz) and integration. All NMR spectra were recorded at room temperature (23 °C) unless otherwise indicated. High-resolution mass spectrometry was conducted using atmospheric pressure chemical ionization (APCI) or electro-spraying ionization (ESI), and was performed by McGill University on a Thermo-Scientific Exactive Orbitrap. Protonated molecular ions $[M+H]^+$ or sodium adducts $[M+Na]^+$, were used for empirical formula confirmation. All preparative chromatography was performed either through using gradient elution (hexanes and ethyl acetate) on a Biotage Isolera™ One automated chromatography system with SNAP ultra-silica2 gel cartridges and sample cartridges or through using preparative TLC plate bought from SILICYCLE company. The UV lamp employed in this investigation was purchased at Atlas Specialty Lighting

2: General protocol for the preparation of alkoxybenzopheone

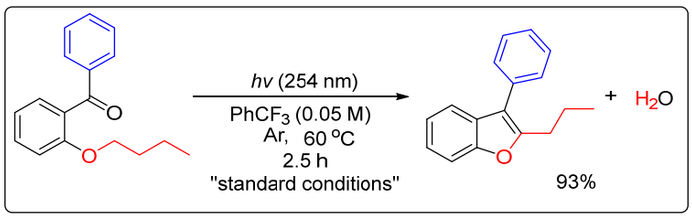


R_2X (2 equiv) was added to a solution of *ortho*-hydroxyphenone (2 mmol, 1 equiv) in 20 mL DMF. Then K_2CO_3 (552 mg, 4 mmol, 2 equiv) was added into the above solution to get a slurry, which was heated to 60 °C for 12 h. Following this, the solid was filtered away and 200 mL H_2O was added into the solution, which was extracted by EtOAc (50 mL X 3). The combined EtOAc was dried over Na_2SO_4. After the removal of Na_2SO_4, the organic solvent was concentrated by using a rotary evaporator. The residue was purified by using hexanes/EtOAc as the eluent via flash column chromatography on silica gel.

3: General procedure for the photoreaction

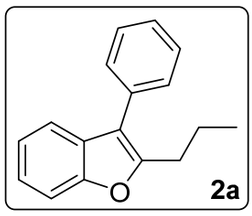
Alkoxyphenone (0.1 mmol) was added into a 10 mL quartz tube with a Teflon-coated magnetic stir bar, which was followed by the addition of 2 mL $PhCF_3$. The tube was sealed by using a septum. Through using frozen-pump-thaw protocol, the solution was degassed and recharged with argon gas for three times. Then the quartz tube was put into a pre-heated 60 °C water bath. Subsequently, the UV lamp was turned on and irradiated the quartz tube for 2.5 h. Finally, the reaction was stopped and the solvent was removed directly on rota-vap. The product was purified by using preparative TLC to get the desired benzofuran product.

4: The full screening list



Entry	Variations from Standard Conditions	Yield
1	Benzene instead of $PhCF_3$	40%
2	MeOH instead of $PhCF_3$	62%
3	Cyclohexane instead of $PhCF_3$	22%
4	DMF instead of $PhCF_3$	Trace
5	DMSO instead of $PhCF_3$	Trace
6	Acetone instead of $PhCF_3$	Trace
7	THF instead of $PhCF_3$	Trace
8	1,2-dichloroethane instead of $PhCF_3$	49%
9	*t*-BuOH instead of $PhCF_3$	78%
10	Chloroform instead of $PhCF_3$	0%
11	H_2O instead of $PhCF_3$	18%
12	CH_3CN instead of $PhCF_3$	37%
13	Toluene instead of $PhCF_3$	52%
14	80 ^{0}C instead of 60 ^{0}C (2.5 h)	94%
15	50 ^{0}C instead of 60 ^{0}C (2.5 h)	65%
16	50 ^{0}C instead of 60 ^{0}C (6 h)	82%
14	With 0.1 equiv HCl at r.t	0%
15	With 0.1 equiv $TiCl_4$ at r.t	0%
16	Air instead of argon	70%
17	O_2 instead of argon	<5%
18	NO hv	0%
20	6 h instead of 2.5 h	91%
23	0.2 M instead of 0.05 M	71%
24	0.02 M instead of 0.05 M	70%

5: Characterization data for the compounds

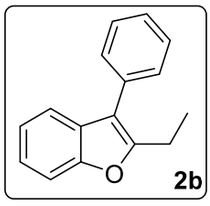


3-phenyl-2-propylbenzofuran.[1]

Rf value: 0.80 (EtOAc: Hexane=1:10)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.58 (d, *J* = 7.48 Hz, 1H), 7.54-7.46 (m, 5H), 7.43-7.36 (m, 1H), 7.32-7.21 (m, 2H), 2.86 (t, *J* = 7.41 Hz, 2H), 1.84 (sext, *J* = 7.46 Hz, 2H), 1.00 (t, *J* = 7.38 Hz, 3H);

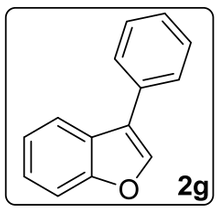
^{13}CNMR (125 MHz, $CDCl_3$): 155.1, 154.0, 132.9, 129.1, 128.9, 128.7, 127.0, 123.5, 122.5, 119.4, 116.9, 110.8, 28.7, 21.7, 13.9.



2-ethyl-3-phenylbenzofuran.[2]

Rf value: 0.77 (EtOAc: Hexane=1:10)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.61 (d, *J* = 7.70 Hz, 1H), 7.56-7.49 (m, 5H), 7.44-7.38 (m, 1H), 7.34-7.23 (m, 2H), 2.93 (q, *J* = 7.72 Hz, 2H), 1.40 (t, *J* = 7.42 Hz, 3H); **^{13}CNMR (125 MHz, $CDCl_3$):** 156.2, 154.0, 132.9, 129.1, 128.9, 128.7, 127.0, 123.6, 122.6, 119.5, 116.2, 110.8, 20.3, 13.0.

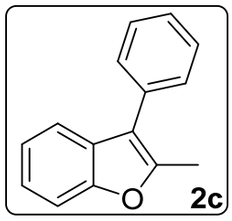


3-phenylbenzofuran.[3]

Rf value: 0.71 (EtOAc: Hexane=1:10)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.88 (dd, J_1 = 7.6 Hz, J_2 = 1.7 Hz, 1H), 7.83 (s, 1H), 7.64 (d, *J* = 7.3 Hz, 2H), 7.54 (dd, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.44-7.32 (m, 3H);

^{13}CNMR (125 MHz, $CDCl_3$): 155.8, 141.3, 132.0, 128.9, 127.5, 127.4, 126.4, 124.5, 122.9, 122.2, 120.4, 111.7.



2-methyl-3-phenylbenzofuran.[4]

Rf value: 0.77 (EtOAc: Hexane=1:10)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.61 (d, J_1 = 7.1 Hz, 1H), 7.57-7.47 (m, 5H), 7.42-7.37 (m, 1H), 7.32-7.23 (m, 3H), 2.57 (s, 3H);

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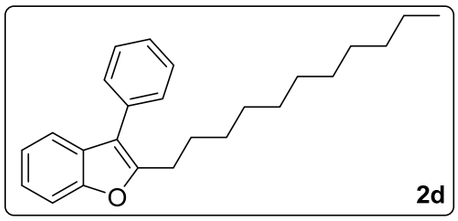
[1] A. Katritzky, Y. Ji, Y. Fang, and I. Prakash, *J. Org. Chem.*, **2001**, 66, 5613.
[2] A. Carrer, D. Brinet, J.-C. Florent, P. Rousselle, and E. Bertounesque, *J. Org. Chem.*, **2012**, 77, 1316.
[3] I. Kim, S.-H. Lee, and S. Lee, *Tetrahedron Lett.*, **2008**, 49, 6579.
[4] S.-C. Yin, Q. Zhou, X.-Y. Zhao, and L.-X. Shao, *J. Org. Chem.*, **2015**, 80, 8916.

^{13}CNMR (100 MHz, $CDCl_3$): 154.0, 151.3, 132.8, 128.9, 128.7, 126.9, 123.5, 122.6, 119.3, 116.9, 110.7, 12.8.



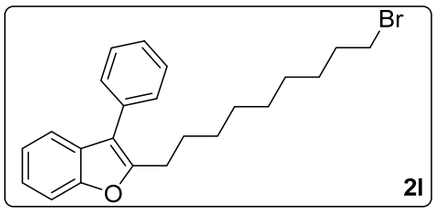
3-phenyl-2-undecylbenzofuran.

Rf value: 0.81 (EtOAc: Hexane=1:10)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.66 (d, J_1 = 7.32 Hz, 1H), 7.62-7.54 (m, 5H), 7.48-7.43 (m, 1H), 7.38-7.28 (m, 2H), 2.96 (t, J = 7.67 Hz, 3H), 1.89 (quintet, 7.46 Hz, 2H), 1.49-1.31 (m, 16H), 1.00 (t, J = 7.04 Hz, 3H);

^{13}CNMR (125 MHz, $CDCl_3$): 155.4, 154.1, 133.0, 129.1, 128.9, 128.7, 127.0, 123.5, 122.6, 119.5, 116.8, 110.9, 32.0, 31.7, 29.7, 29.7, 29.6, 29.4, 29.4, 28.4, 26.8, 22.7, 14.2.

HRMS (ESI): $(M+Na)^+$ $C_{25}H_{32}ONa$, calculated: 371.2345, found: 371.2348.



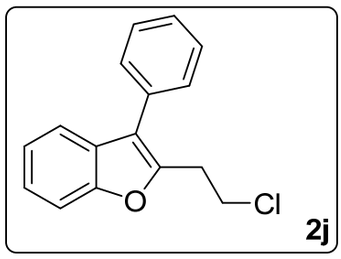
2-(9-bromononyl)-3-phenylbenzofuran.

Rf value: 0.67 (EtOAc: Hexane=1:10)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.61 (d, J = 7.48 Hz, 1H), 7.55-7.49 (m, 5H), 7.45-7.39 (m, 1H), 7.34-7.24 (m, 2H), 3.43 (t, J = 6.90 Hz, 2H), 2.91 (t, J = 7.67 Hz, 2H), 1.93-1.78 (m, 4H), 1.49-1.27 (m, 10H);

^{13}CNMR (125 MHz, $CDCl_3$): 155.2, 154.0, 132.9, 129.1, 128.9, 128.7, 127.0, 123.5, 122.6, 119.4, 116.8, 110.8, 34.0, 32.8, 29.3, 29.2, 29.2, 28.7, 28.3, 28.1, 26.7.

HRMS (ESI): $(M+H)^+$ $C_{23}H_{28}BrO$, calculated: 399.1318, found: 399.1318.



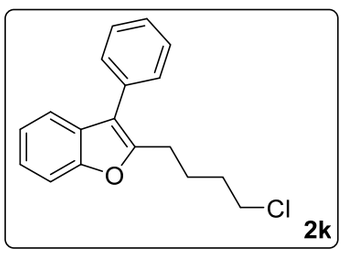
2-(2-chloroethyl)-3-phenylbenzofuran.

Rf value: 0.67 (EtOAc: Hexane=1:10)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.56 (d, J = 7.07 Hz, 1H), 7.55-7.46 (m, 5H), 7.43-7.38 (m, 1H), 7.32 (dt, J_1 = 7.41 Hz, J_2 = 1.03 Hz, 1H), 7.27-7.24 (m, 1H), 3.90 (t, J = 7.18 Hz, 2H), 3.34 (t, J = 7.23 Hz, 2H);

^{13}CNMR (125 MHz, $CDCl_3$): 154.2, 150.1, 132.0, 129.1, 128.9, 128.5, 127.4, 124.2, 122.8, 119.8, 119.2, 111.0, 41.6, 30.4.

HRMS (ESI): $(M+Na)^+$ $C_{16}H_{13}ClNaO$, calculated: 279.0547, found: 279.0533.



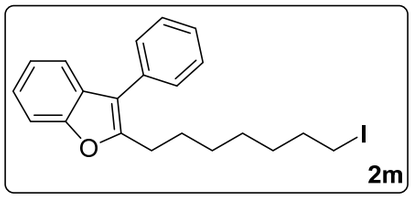
2-(4-chlorobutyl)-3-phenylbenzofuran.

Rf value: 0.54 (EtOAc: Hexane=1:10)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.61 (d, *J* = 7.41 Hz, 1H), 7.56-7.50 (m, 5H), 7.46-7.39 (m, 1H), 7.35-7.24 (m, 2H), 3.54 (t, *J* = 6.50 Hz, 2H), 2.94 (t, *J* = 7.52 Hz, 2H), 2.04-1.93 (m, 2H), 1.91-1.83 (m, 2H);

^{13}CNMR (125 MHz, $CDCl_3$): 154.2, 154.1, 132.6, 129.1, 128.8, 128.8, 127.2, 123.8, 122.7, 119.6, 117.3, 110.9, 44.5, 32.0, 25.9, 25.6.

HRMS (ESI): $(M+H)^+$ $C_{18}H_{18}ClO$, calculated: 285.1041, found: 285.1028.



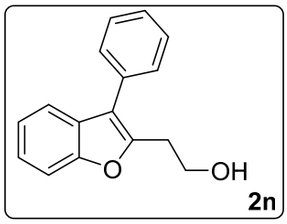
2-(7-iodoheptyl)-3-phenylbenzofuran.

Rf value: 0.67 (EtOAc: Hexane=1:10)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 7.81 Hz, 1H), 7.52-7.45 (m, 5H), 7.41-7.35 (m, 1H), 7.30-7.20 (m, 2H), 3.16 (t, *J* = 7.02 Hz, 2H), 2.87 (t, *J* = 7.68 Hz, 2H), 1.84-1.74 (m, 4H), 1.42-1.25 (m, 6H);

^{13}CNMR (125 MHz, $CDCl_3$): 155.0, 154.0, 132.8, 129.1, 128.8, 128.7, 127.0, 123.5, 122.5, 119.4, 116.9, 110.8, 44.5, 33.4, 30.3, 28.9, 28.2, 28.1, 26.6, 7.1.

HRMS (ESI): $(M+H)^+$ $C_{21}H_{24}IO$, calculated: 419.0866, found: 419.0860.



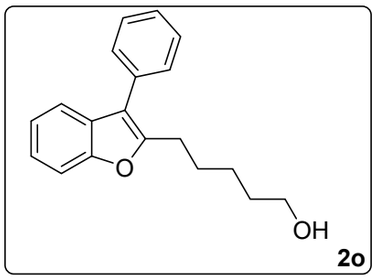
2-(3-phenylbenzofuran-2-yl)ethan-1-ol.

Rf value: 0.11 (EtOAc: Hexane=1:5)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.64-7.44 (m, 6H), 7.43-7.35 (m, 1H), 7.34-7.21 (m, 2H), 4.04 (t, *J* = 6.13 Hz, 2H), 3.15 (t, *J* = 6.27 Hz, 2H), 1.91-1.78 (br, 1H);

^{13}CNMR (125 MHz, $CDCl_3$): 154.2, 151.2, 132.2, 129.1, 128.8, 128.6, 127.3, 124.0, 122.8, 119.7, 118.8, 111.0, 61.1, 30.3.

HRMS (ESI): $(M+Na)^+$ $C_{16}H_{14}O_2Na$, calculated: 261.0886, found: 261.0882.



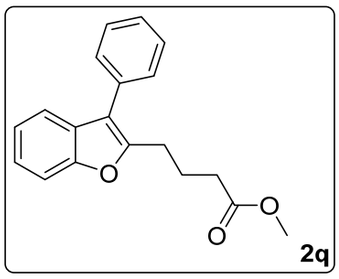
5-(3-phenylbenzofuran-2-yl)pentan-1-ol.

Rf value: 0.07 (EtOAc: Hexane=1:5)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 7.43 Hz, 1H), 7.51-7.45 (m, 5H), 7.41-7.35 (m, 1H), 7.30-7.20 (m, 2H), 3.61 (t, *J* = 6.49 Hz, 2H), 2.89 (t, *J* = 7.68 Hz, 2H), 1.82 (quintet, J = 7.64 Hz, 2H), 1.57 (quintet, J = 7.82 Hz, 2H), 1.48-1.39 (m, 2H);

^{13}CNMR (125 MHz, $CDCl_3$): 154.9, 154.0, 132.8, 129.1, 128.8, 128.7, 127.0, 123.6, 122.5, 119.4, 116.9, 110.8, 62.8, 32.4, 28.1, 26.69, 25.43.

HRMS (ESI): $(M+Na)^+$ $C_{19}H_{20}O_2Na$, calculated: 303.1356, found: 303.1344.



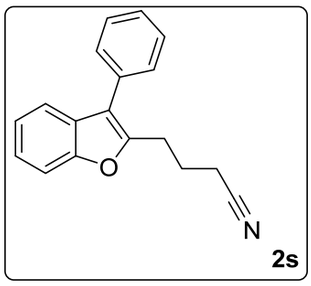
methyl 4-(3-phenylbenzofuran-2-yl)butanoate.

Rf value: 0.34 (EtOAc: Hexane=1:5)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.60 (d, *J* = 7.70 Hz, 1H), 7.55-7.48 (m, 5H), 7.45-7.38 (m, 1H), 7.35-7.23 (m, 2H), 3.64 (s, 3H), 2.97 (t, *J* = 7.46 Hz, 2H), 2.42 (t, *J* = 7.35 Hz, 2H), 2.16 (quintet, J = 7.31 Hz, 2H);

^{13}CNMR (125 MHz, $CDCl_3$): 173.51, 154.12, 153.80, 132.57, 129.12, 128.81, 128.75, 127.18, 123.82, 122.69, 119.59, 117.63, 110.94, 51.52, 33.26, 25.98, 23.58.

HRMS (ESI): $(M+Na)^+$ $C_{19}H_{18}O_3Na$, calculated: 317.1151, found: 317.1148.



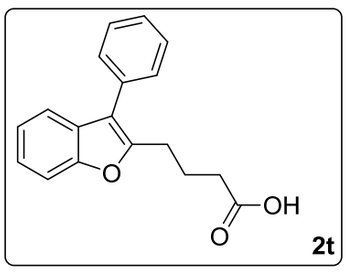
4-(3-phenylbenzofuran-2-yl)butanenitrile.

Rf value: 0.22 (EtOAc: Hexane=1:5)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.58 (d, *J* = 7.80 Hz, 1H), 7.55-7.45 (m, 5H), 7.44-7.39 (m, 1H), 7.35-7.23 (m, 2H), 3.05 (t, *J* = 7.30 Hz, 2H), 2.41 (t, *J* = 7.22 Hz, 2H), 2.15 (quintet, *J* = 7.21 Hz, 2H);

^{13}CNMR (125 MHz, $CDCl_3$): 154.13, 152.08, 132.10, 129.06, 128.99, 128.58, 127.51, 124.20, 122.93, 119.78, 119.15, 118.36, 111.02, 25.59, 24.22, 16.71.

HRMS (ESI): $(M+Na)^+$ $C_{18}H_{15}ONNa$, calculated: 284.1046, found: 284.1052.



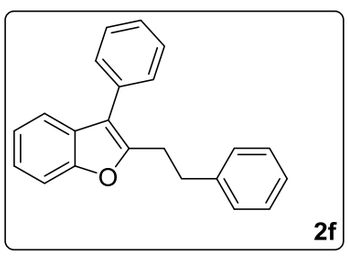
4-(3-phenylbenzofuran-2-yl)butanoic acid.

Rf value: 0.46 (EtOAc: Hexane=1:5)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.58 (d, *J* = 7.58 Hz, 1H), 7.50-7.45 (m, 5H), 7.40-7.34 (m, 1H), 7.31-7.20 (m, 2H), 2.95 (t, *J* = 7.46 Hz, 2H), 2.43 (t, *J* = 7.40 Hz, 2H), 2.12 (quintet, *J* = 7.35 Hz, 2H);

^{13}CNMR (125 MHz, $CDCl_3$): 178.51, 154.10, 153.60, 132.48, 129.09, 128.81, 128.70, 127.20, 123.85, 122.69, 119.61, 117.67, 110.95, 33.08, 25.91, 23.29.

HRMS (ESI): $(M+Na)^+$ $C_{18}H_{16}O_3Na$, calculated: 303.0992, found: 303.0984.



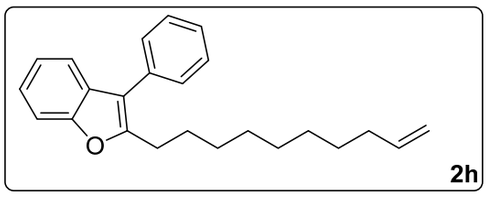
2-phenethyl-3-phenylbenzofuran.

Rf value: 0.67 (EtOAc: Hexane=1:10)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.56-7.48 (m, 2H), 7.45-7.39 (m, 2H), 7.37-7.13 (m, 10H), 3.19-3.08 (m, 4H);

^{13}CNMR (125 MHz, $CDCl_3$): 154.08, 153.79, 140.91, 132.53, 129.02, 128.83, 128.67, 128.45, 127.06, 126.19, 123.73, 122.62, 119.58, 117.52, 110.88, 34.44, 28.97.

HRMS (APCI): $(M+H)^+$ calculated: 299.14304, found: 299.14283.



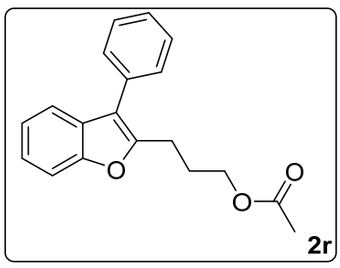
2-(dec-9-en-1-yl)-3-phenylbenzofuran.

Rf value: 0.79 (EtOAc: Hexane=1:10)

^{1}HNMR (500 MHz, $CDCl_3$): δ 7.58 (d, *J* = 7.47 Hz, 1H), 7.54-7.47 (m, 5H), 7.42-7.37 (m, 1H), 7.31-7.22 (m, 2H), 5.88-5.78 (m, 1H), 5.04-4.92 (m, 2H), 2.88 (t, *J* = 7.7 Hz, 2H), 2.08-2.02 (m, 2H), 1.80 (quintet, *J* = 7.52 Hz, 2H), 1.41-1.35 (m, 4H), 1.32-1.26 (m, 6H);

^{13}CNMR (125 MHz, $CDCl_3$): 155.32, 154.02, 139.21, 132.91, 129.09, 128.90, 128.71, 126.98, 123.51, 122.52, 119.42, 116.78, 114,21, 110.82, 33.78, 29.33, 29.27, 29.24, 29.06, 28.89, 28.36.

HRMS (APCI): $(M+H)^+$ $C_{24}H_{29}O$, calculated: 333.22129, found: 333.22112.



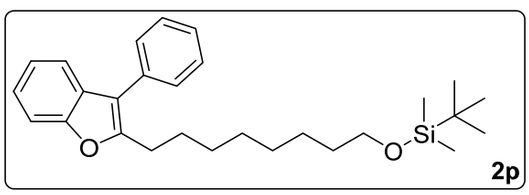
3-(3-phenylbenzofuran-2-yl)propyl acetate.

Rf value: 0.34 (EtOAc: Hexane=1:5)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.55 (d, *J* = 7.93 Hz, 1H), 7.52-7.44 (m, 5H), 7.42-7.34 (m, 1H), 7.33-7.20 (m, 2H), 4.09 (t, *J* = 6.31 Hz, 2H), 2.97 (t, *J* = 7.58 Hz, 2H), 2.12 (quintet, *J* = 7.11 Hz, 2H);

^{13}CNMR (125 MHz, $CDCl_3$): 171.01, 154.10, 153.49, 132.56, 129.08, 128.79, 128.71, 127.17, 123.83, 122.70, 119.57, 117.59, 110.89, 63.46, 27.18, 23.29, 20.77.

HRMS (ESI): $(M+Na)^+$ C19H18O3Na, calculated: 317.11482, found: 317.11446.



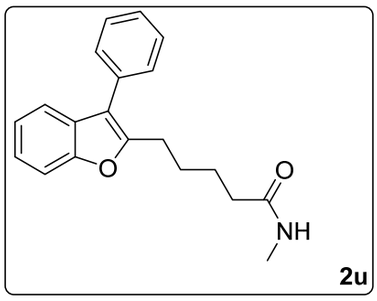
tert-butyldimethyl((8-(3-phenylbenzofuran-2-yl)octyl)oxy)silane.

Rf value: 0.66 (EtOAc: Hexane=1:10)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.55 (d, *J* = 7.58 Hz, 1H), 7.51-7.45 (m, 5H), 7.40-7.34 (m, 1H), 7.29-7.18 (m, 2H), 3.58 (t, *J* = 6.64 Hz, 2H), 2.85 (t, *J* = 7.74 Hz, 2H), 1.78 (quintet, *J* = 7.65 Hz, 2H), 1.53-1.44 (m, 2H), 1.37-1.26 (m, 8H), 0.89 (s, 9H), 0.04 (s, 6H);

^{13}CNMR (125 MHz, $CDCl_3$): 155.31, 154.02, 132.91, 129.09, 128.90, 128.71, 126.98, 123.50, 122.52, 119.42, 116.78, 110.82, 63.31, 32.86, 29.31, 29.30, 29.26, 28.37, 26.75, 25.99, 25.77, 18.38, -5.24.

HRMS (APCI): $(M+H)^+$ $C_{28}H_{41}O_2Si$, calculated: 437.28703, found: 437.28651.



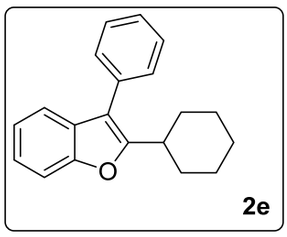
N-methyl-5-(3-phenylbenzofuran-2-yl)pentanamide.

Rf value: 0.33 (EtOAc: Hexane=1:0)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.55 (d, *J* = 7.59 Hz, 1H), 7.51-7.44 (m, 5H), 7.40-7.34 (m, 1H), 7.29-7.19 (m, 2H), 5.40 (br, 1H), 2.89 (t, *J* = 7.58 Hz, 2H), 2.75 (t, J = 4.80 Hz, 2H), 2.13 (t, J = 7.47 Hz, 2H), 1.81 (quintet, *J* = 7.32 Hz, 2H), 1.68 (quintet, *J* = 8.23 Hz, 2H);

^{13}CNMR (125 MHz, $CDCl_3$): 173.25, 154.53, 154.02, 132.73, 129.08, 128.81, 128.77, 127.12, 123.69, 122.64, 119.50, 117.13, 110.85, 36.25, 27.88, 26.35, 26.25, 25.26.

HRMS (ESI): $(M+Na)^+$ $C_{20}H_{21}NO_2Na$, calculated: 330.14645, found: 330.14510.



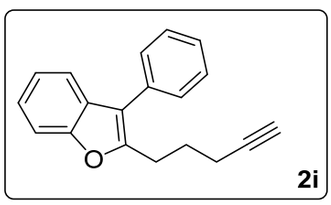
2-cyclohexyl-3-phenylbenzofuran

Rf value: 0.76 (EtOAc: Hexane=1:10)

^{1}HNMR (500 MHz, $CDCl_3$): δ 7.61 (d, *J* = 7.62 Hz, 1H), 7.59-7.52 (m, 5H), 7.48-7.42 (m, 1H), 7.36-7.25 (m, 2H), 3.07-2.97 (m, 1H), 2.01-1.85 (m, 6H), 1.84-1.76 (m, 1H), 1.49-1.35 (m, 3H);

^{13}CNMR (125 MHz, $CDCl_3$): 159.11, 153.92, 133.07, 129.29, 129.04, 128.79, 127.02, 123.51, 122.52, 119.52, 115.34, 110.93, 36.34, 31.76, 26.33, 25.92.

HRMS (ESI): $(M+Na)^+$ $C_{20}H_{21}O$, calculated: 277.1587, found: 277.1578.



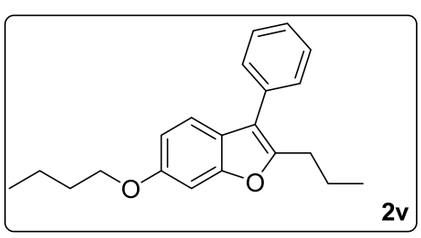
2-(pent-4-yn-1-yl)-3-phenylbenzofuran

Rf value: 0.63 (EtOAc: Hexane=1:10)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 7.74 Hz, 1H), 7.54-7.44 (m, 5H), 7.41-7.34 (m, 1H), 7.32-7.20 (m, 2H), 3.00 (t, *J* = 7.62 Hz, 2H), 2.28 (dt, J_1 = 6.94 Hz, J_2 = 2.65 Hz, 2H), 2.03 (quintet, *J* = 7.37 Hz, 2H), 1.94 (t, *J* = 2.71 Hz, 1H);

^{13}CNMR (100 MHz, $CDCl_3$): 154.08, 153.95, 132.60, 129.12, 128.75, 127.11, 123.75, 122.64, 119.56, 117.49, 110.89, 83.60, 68.92, 27.16, 25.75, 18.11;

HRMS (ESI): $(M+H)^+$ $C_{19}H_{17}O$, calculated: 261.1274, found: 261.1265.



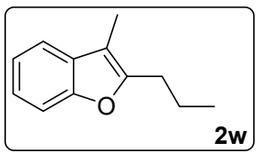
6-butoxy-3-phenyl-2-propylbenzofuran

Rf value: 0.87 (EtOAc: Hexane = 1:10)

^{1}HNMR (500 MHz, $CDCl_3$): δ 7.52-7.47 (m, 4H), 7.42 (d, *J* = 8.47 Hz, 1H), 7.40-7.35 (m, 1H), 7.04 (d, *J* = 2.15 Hz, 1H), 6.88 (dd, J_1 = 2.14 Hz, J_2 = 8.46 Hz, 1H), 4.04 (t, *J* = 7.68 Hz, 2H), 1.86-1.77 (m, 4H), 1.59-1.51 (m, 2H), 1.02 (t, *J* = 7.37 Hz,3H), 1.00 (t, *J* = 7.47 Hz,3H);

^{13}CNMR (125 MHz, $CDCl_3$): 157.0, 154.9, 153.9, 133.1, 129.0, 128.6, 126.8, 122.1, 119.4, 116.6, 111.7, 96.6, 68.3, 31.3, 28.7, 21.8, 19.2, 13.9, 13.8;

HRMS (ESI): $(M+H)^+$ $C_{21}H_{25}O_2$, calculated: 309.1849, found: 309.1845.



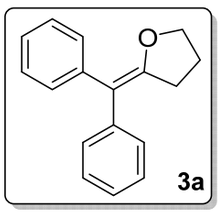
3-methyl-2-propylbenzofuran

Rf value: 0.84 (EtOAc: Hexane = 1:10)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.47-7.42 (m, 1H), 7.41-7.37 (m, 1H), 7.25-7.18 (m, 2H), 2.73 (t, *J* = 7.28 Hz, 2H), 2.19 (s, 3H), 1.77 (sextet, *J* = 7.31 Hz, 2H), 0.99 (t, *J* = 7.42 Hz,3H);

^{13}CNMR (100 MHz, $CDCl_3$): 154.3, 153.8, 130.4, 122.9, 121.8, 118.5, 110.4, 109.6, 28.2, 21.6, 19.2, 13.7, 7.8;

HRMS (ESI): $(M+H)^+$ $C_{12}H_{15}O$, calculated: 175.1117, found: 175.1112.



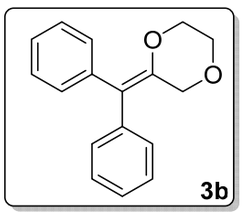
2-(diphenylmethylene)tetrahydrofuran

Rf value: 0.38 (EtOAc: Hexane = 1:10)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.45-7.39 (m, 2H), 7.37-7.32 (m, 2H), 7.31-7.20 (m, 5H), 7.17-7.11 (m, 1H), 4.30 (t, *J* = 6.80 Hz, 2H), 2.64 (t, *J* = 7.52 Hz, 3H), 2.05 (quintet, *J* = 7.14 Hz, 2H);

^{13}CNMR (100 MHz, $CDCl_3$): 155.3, 142.1, 139.9, 130.5, 128.9, 128.2, 127.7, 126.0, 125.2, 110.6, 71.3, 30.2, 24.9;

HRMS (ESI): $[M+H]^+$ $C_{17}H_{17}O$, calculated: 237.12739, found: 237.12803.



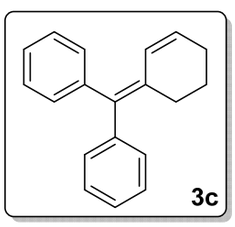
2-(diphenylmethylene)-1,4-dioxane

Rf value: 0.56 (EtOAc: Hexane = 1:5)

^{1}HNMR (400 MHz, $CDCl_3$): δ 7.36-7.28 (m, 6H), 7.27-7.22 (m, 4H), 5.71 (d, *J* = 0.95 Hz, 1H), 4.72 (s, 1H), 4.15-4.10 (m, 2H), 4.08-4.05 (m, 2H);

^{13}CNMR (100 MHz, $CDCl_3$): 141.0, 138.8, 129.0, 128.9, 128.3, 128.1, 126.6, 126.3, 126.1, 64.7, 63.9, 52.8;

HRMS (ESI): $[M+H]^+$ $C_{17}H_{17}O_2$, calculated: 253.12231, found: 253.12208.



(cyclohex-2-en-1-ylidenemethylene)dibenzene[5]

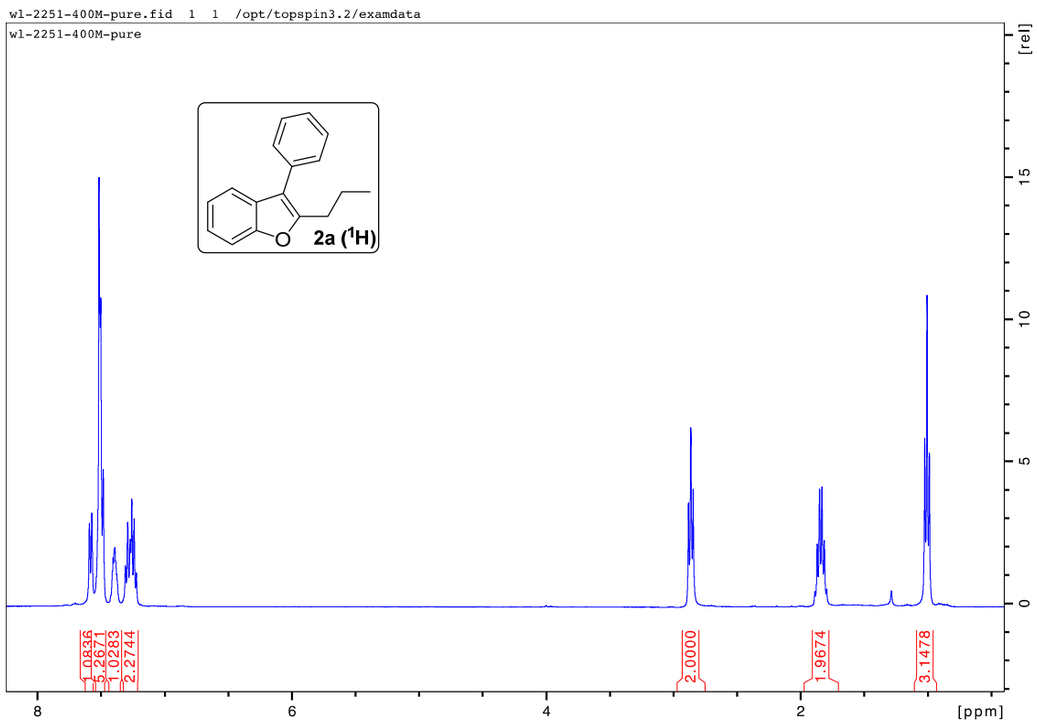
Rf value: 0.79 (EtOAc: Hexane = 1:10)

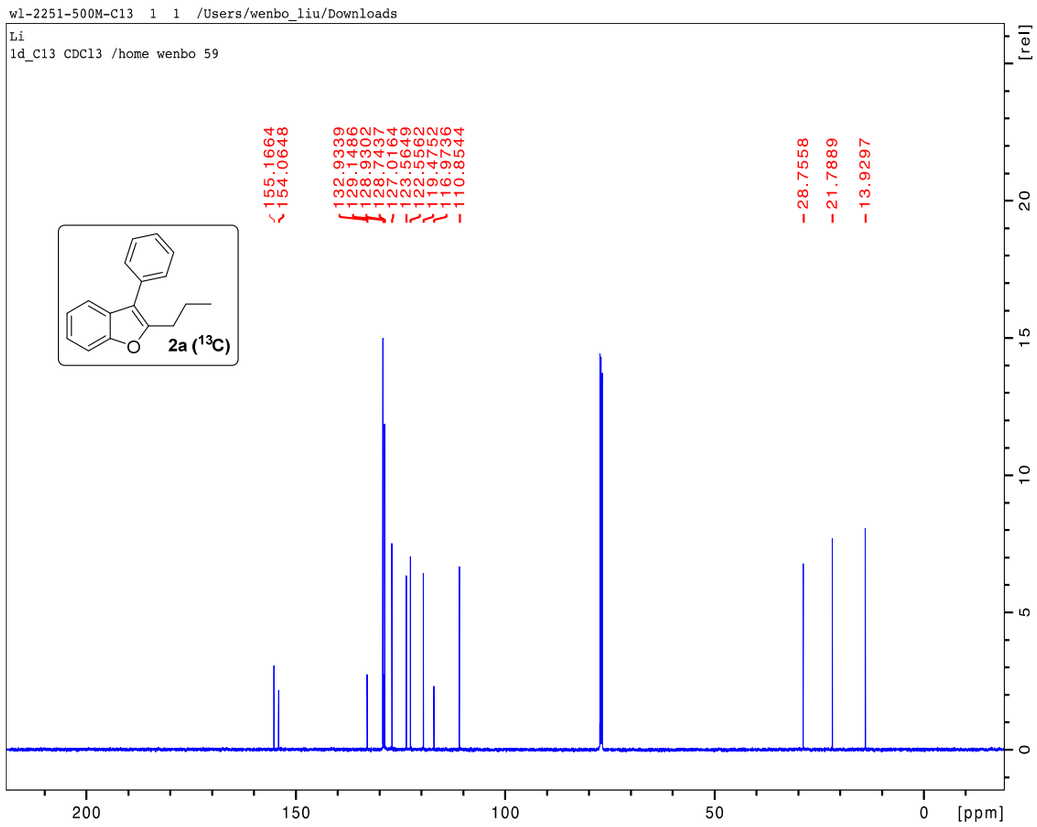
^{1}HNMR (500 MHz, $CDCl_3$): δ 7.33-7.27 (m, 4H), 7.27-7.19 (m, 2H), 7.19-7.14 (m, 4H), 6.27 (d, *J* = 10.23 Hz, 1H), 5.85 (dt, J_1 = 10.18 Hz, J_2 = 3.96 Hz, 1H), 2.48 (t, *J* = 6.23 Hz, 2H), 2.24-2.16 (m, 2H), 1.76 (quintet, *J* = 6.06 Hz, 2H);

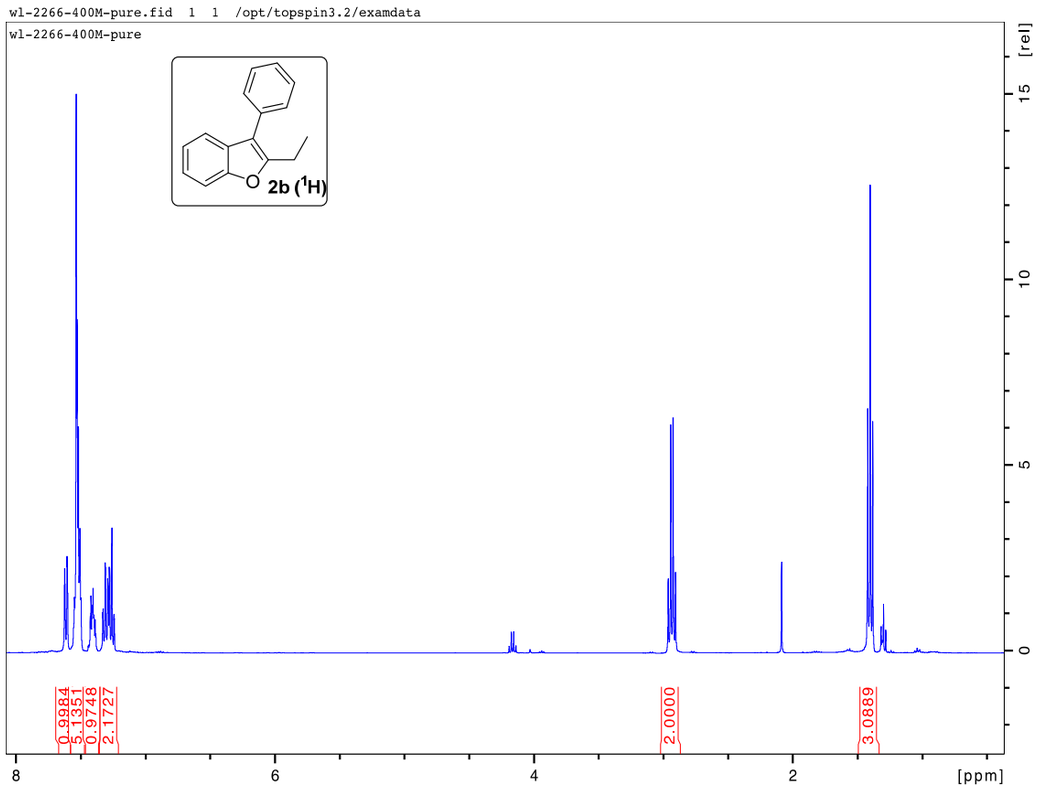
^{13}CNMR (125 MHz, $CDCl_3$): 142.4, 142.2, 136.8, 133.0, 130.8, 130.5, 130.3, 128.2, 127.74, 127.71, 126.4, 126.3, 29.0, 26.0, 23.3;

[5] K. Wang, S. Chen, H. Zhang, S. Xu, F. Ye, Y. Zhang and J. Wang, *Org. Biomol. Chem.* **2016**, 14, 3809.

6: Copies of spectra of all the compounds



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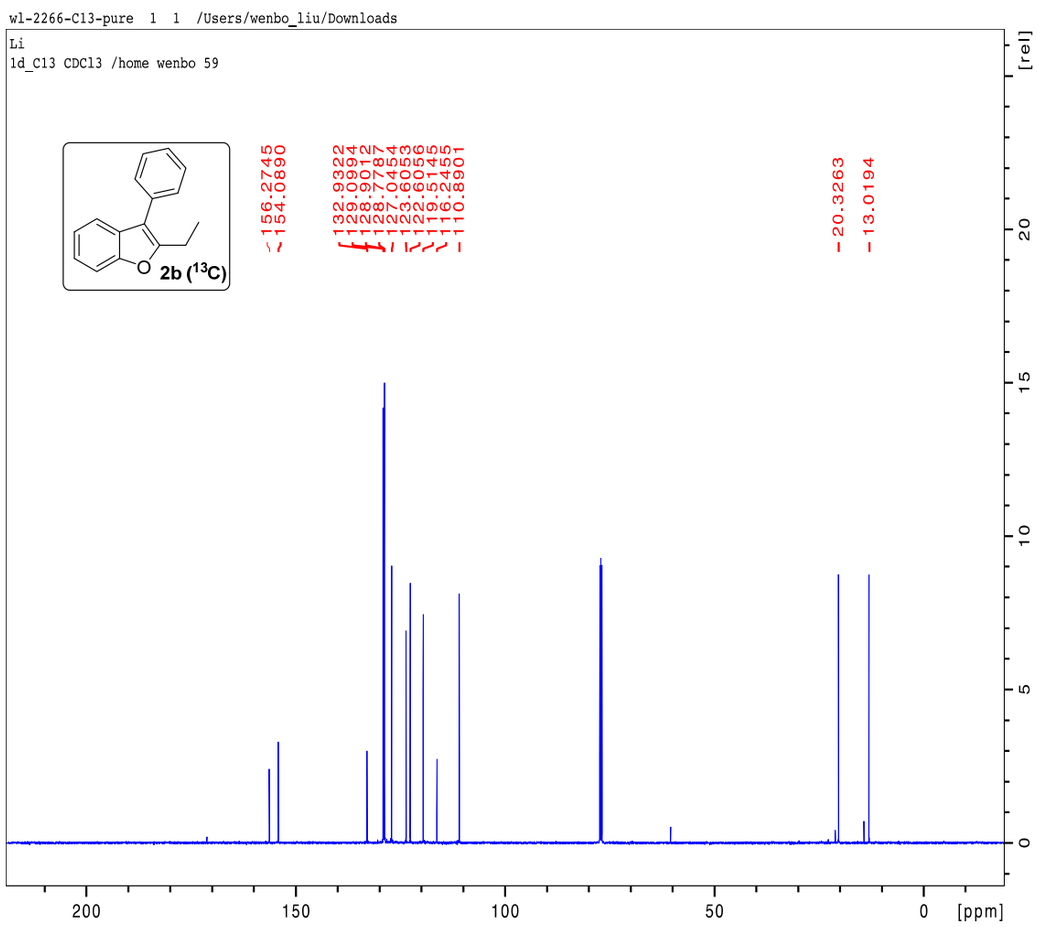
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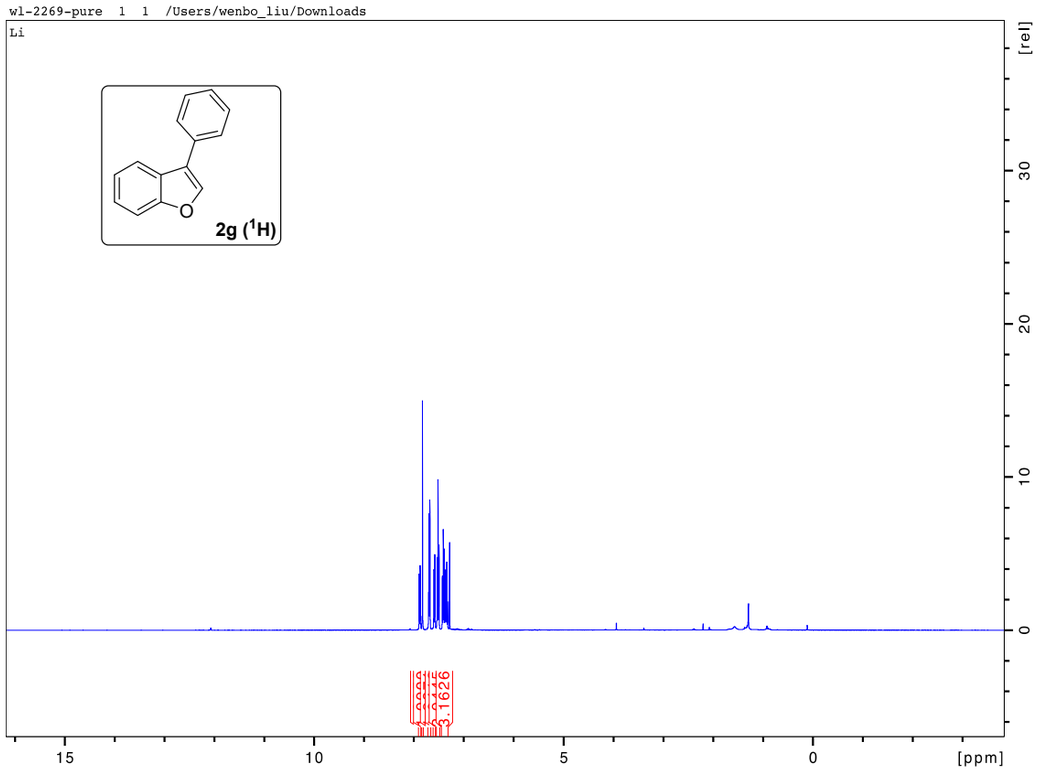
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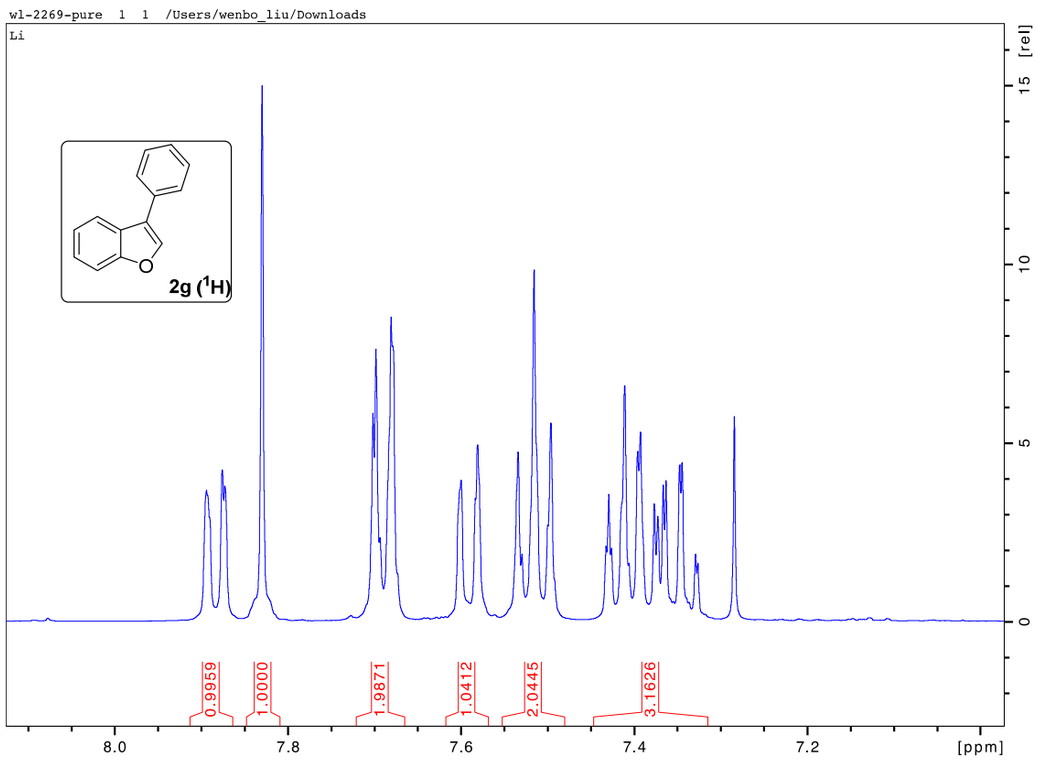
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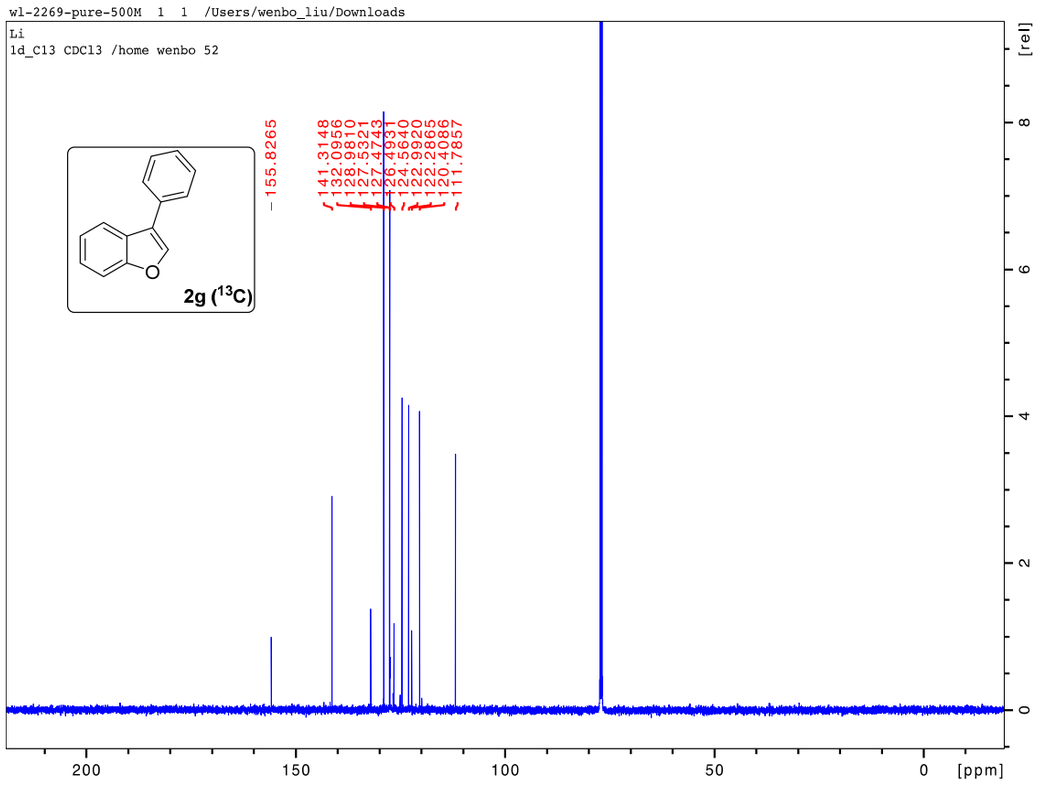
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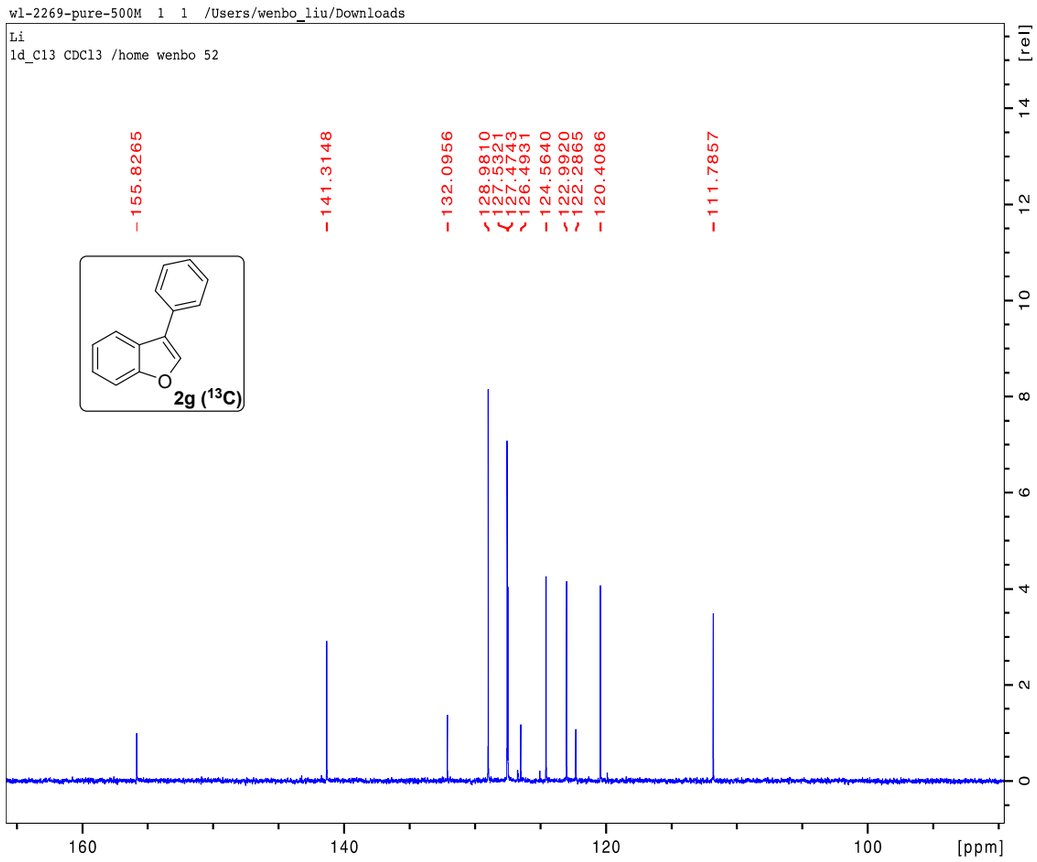
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1d_C13 CDCl3 /home wenbo 52
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141.3148
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127.5321
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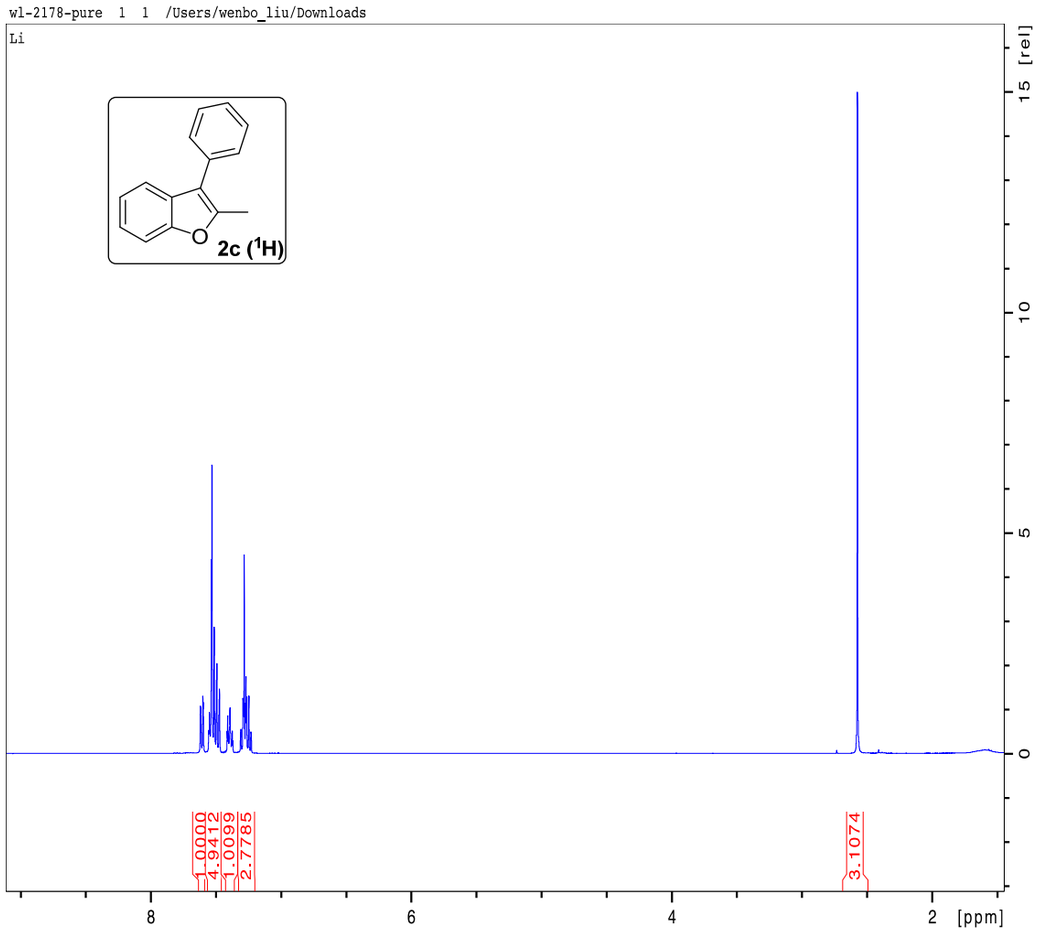
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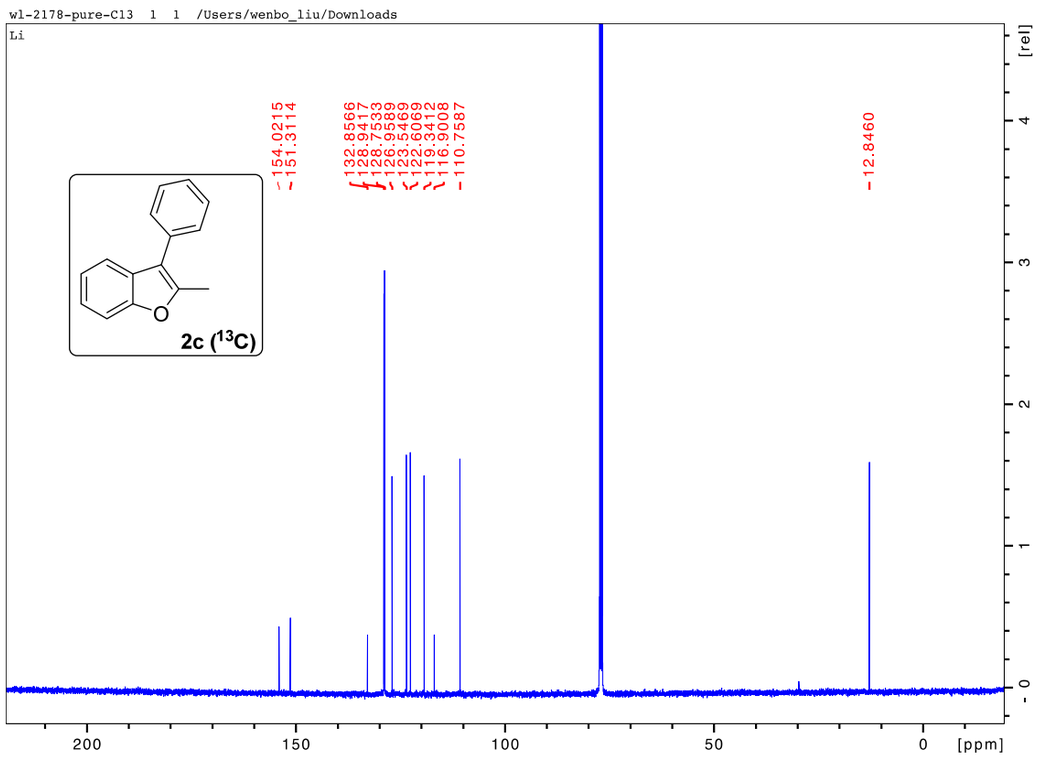
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1
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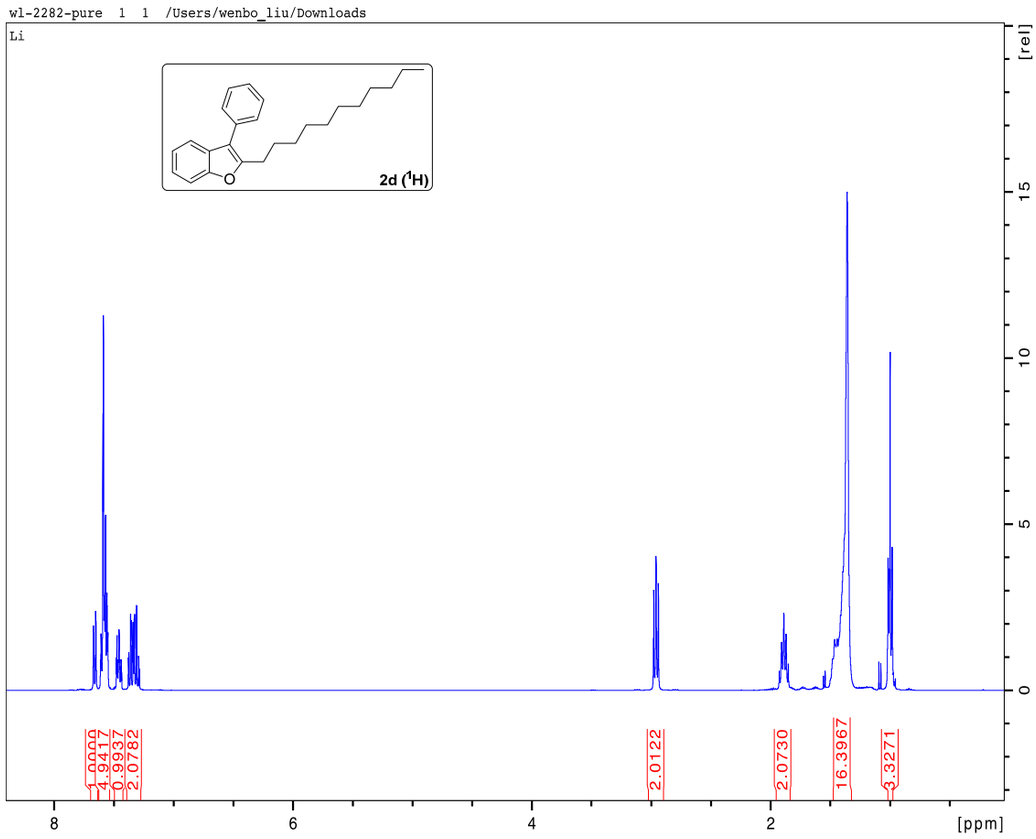
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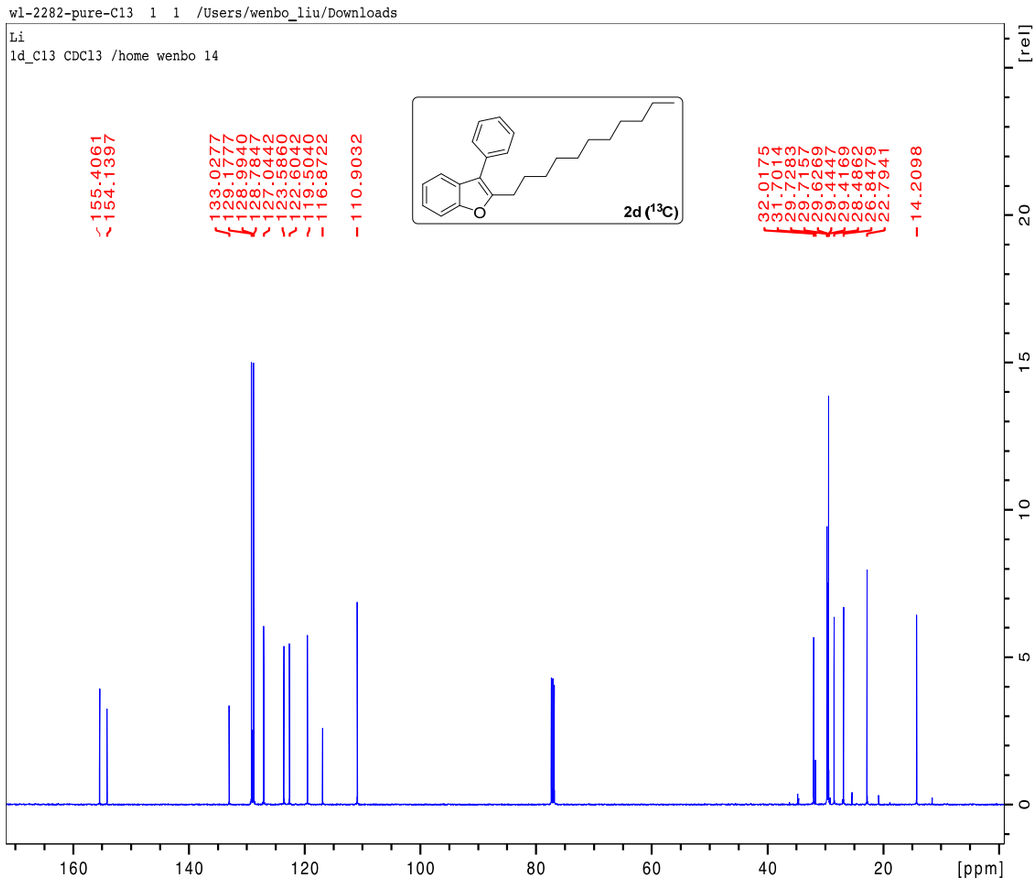
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32.0175
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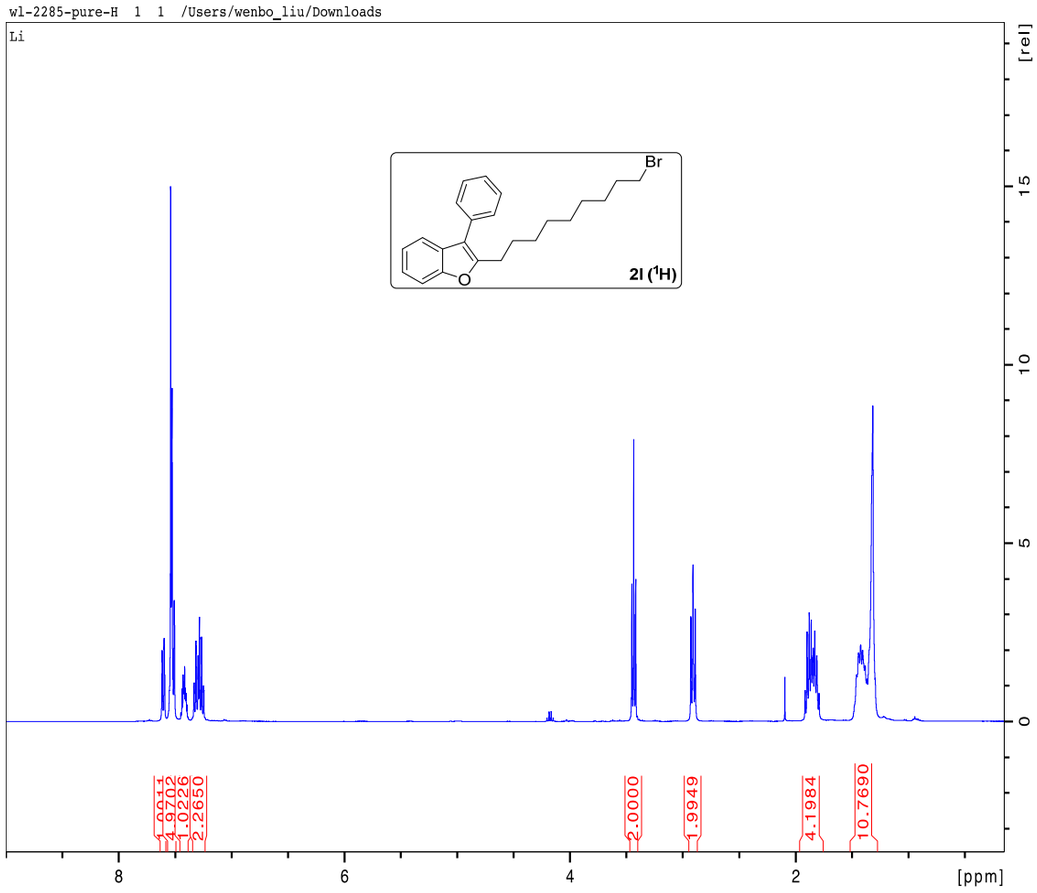
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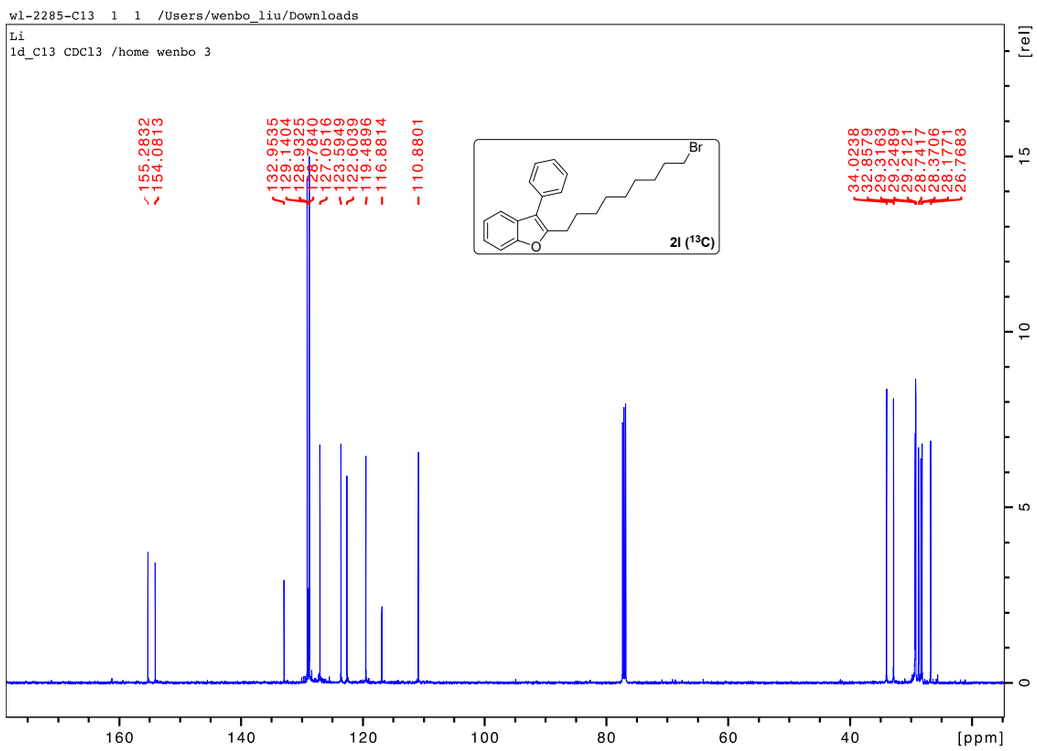
[rel]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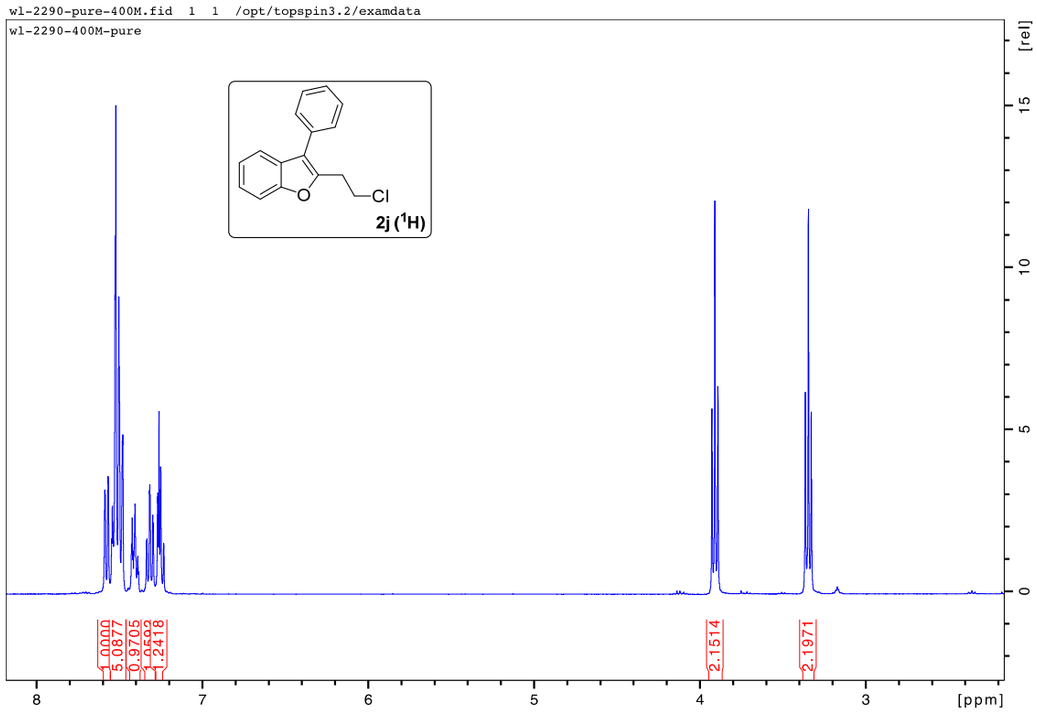
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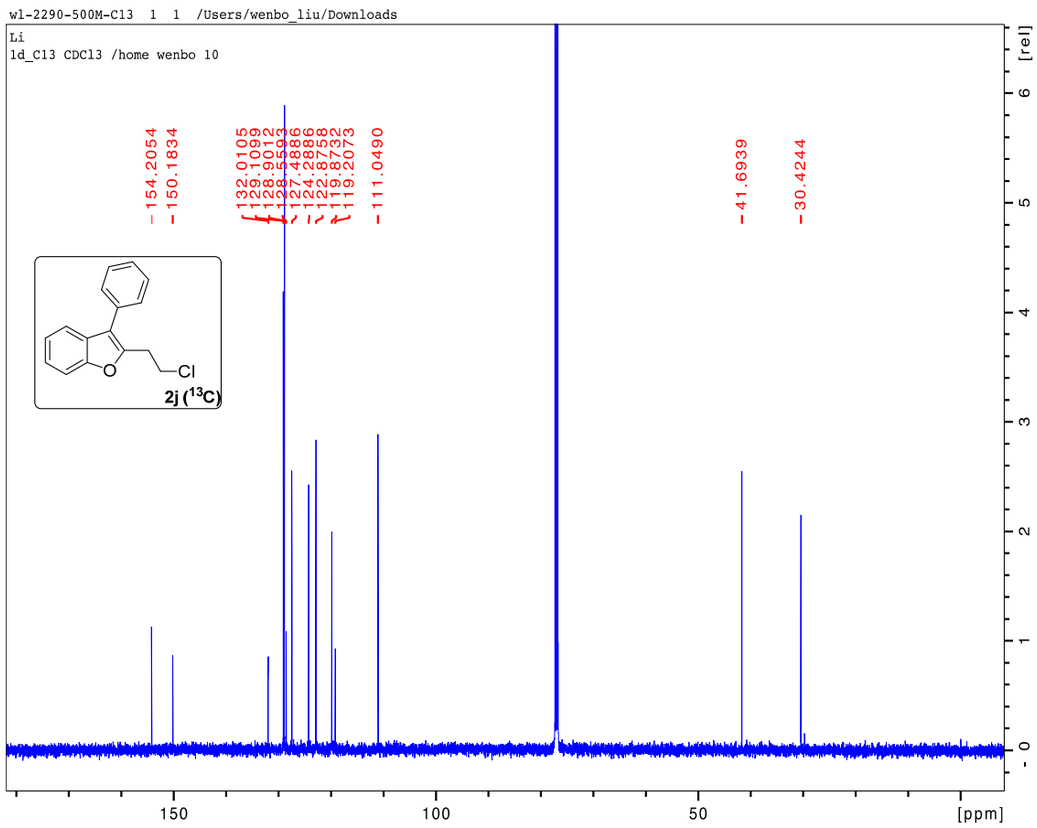
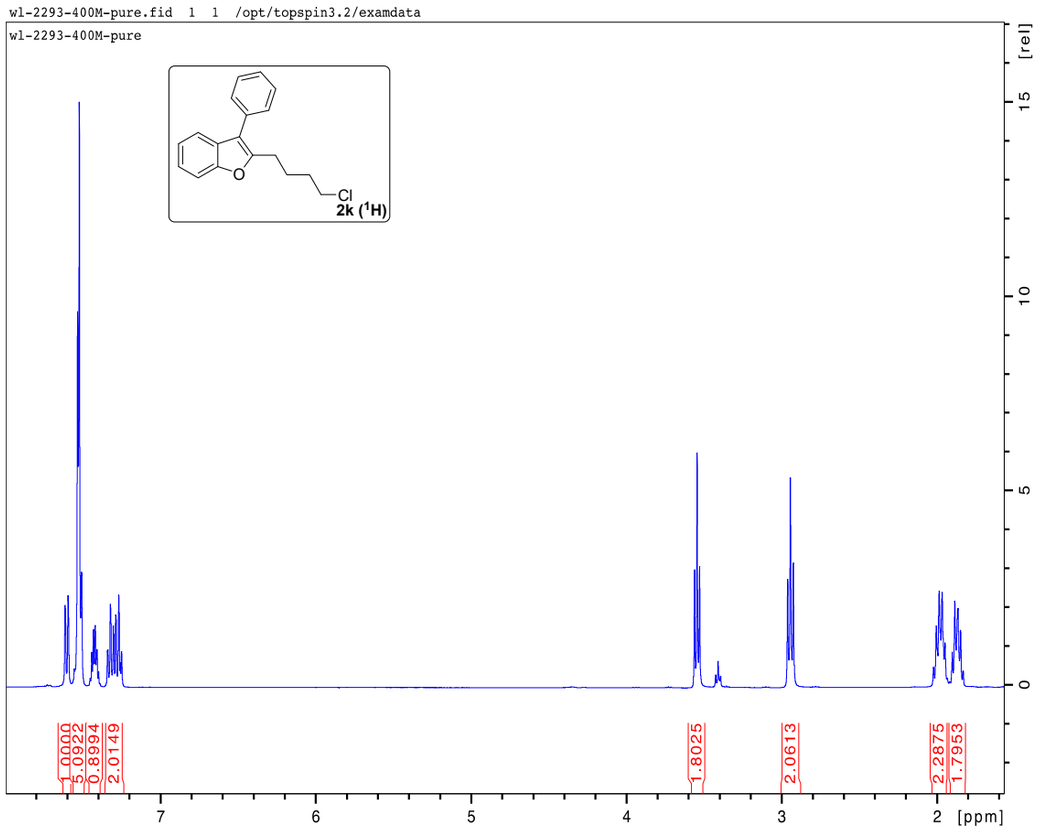
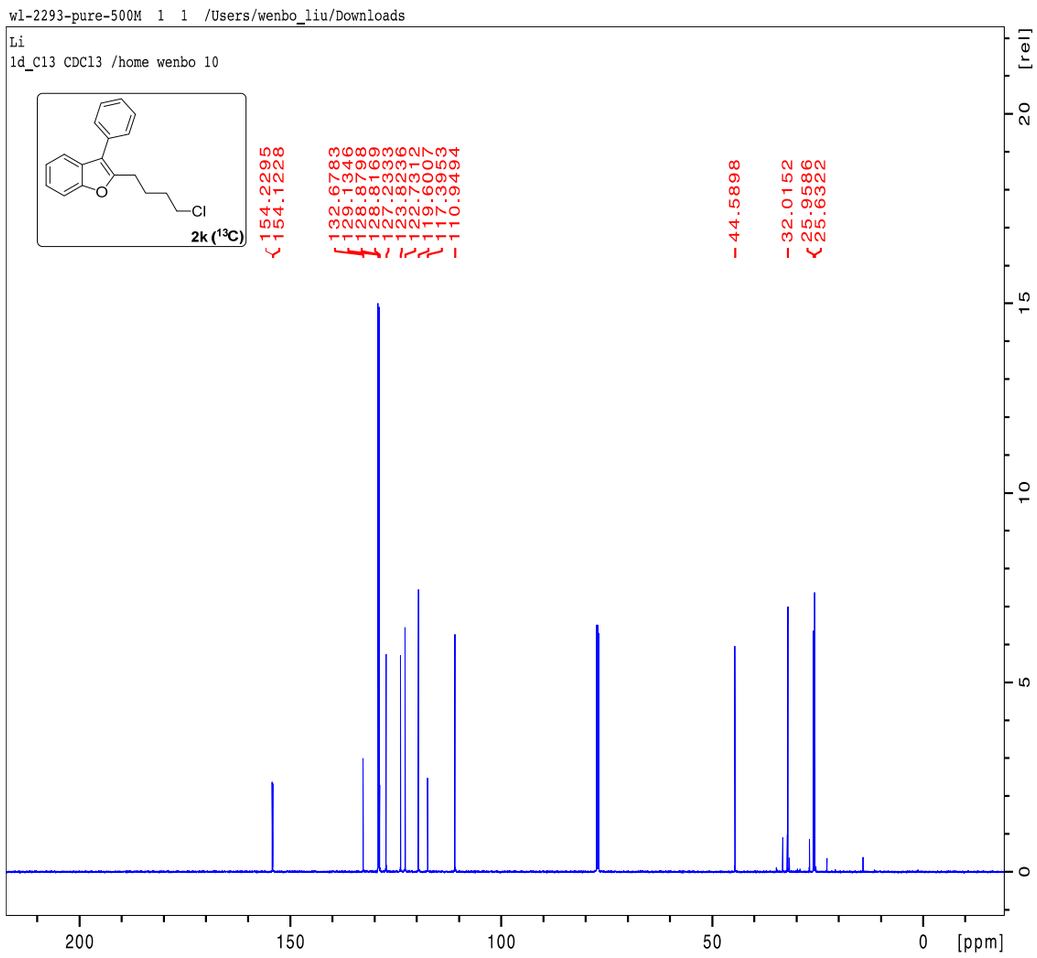
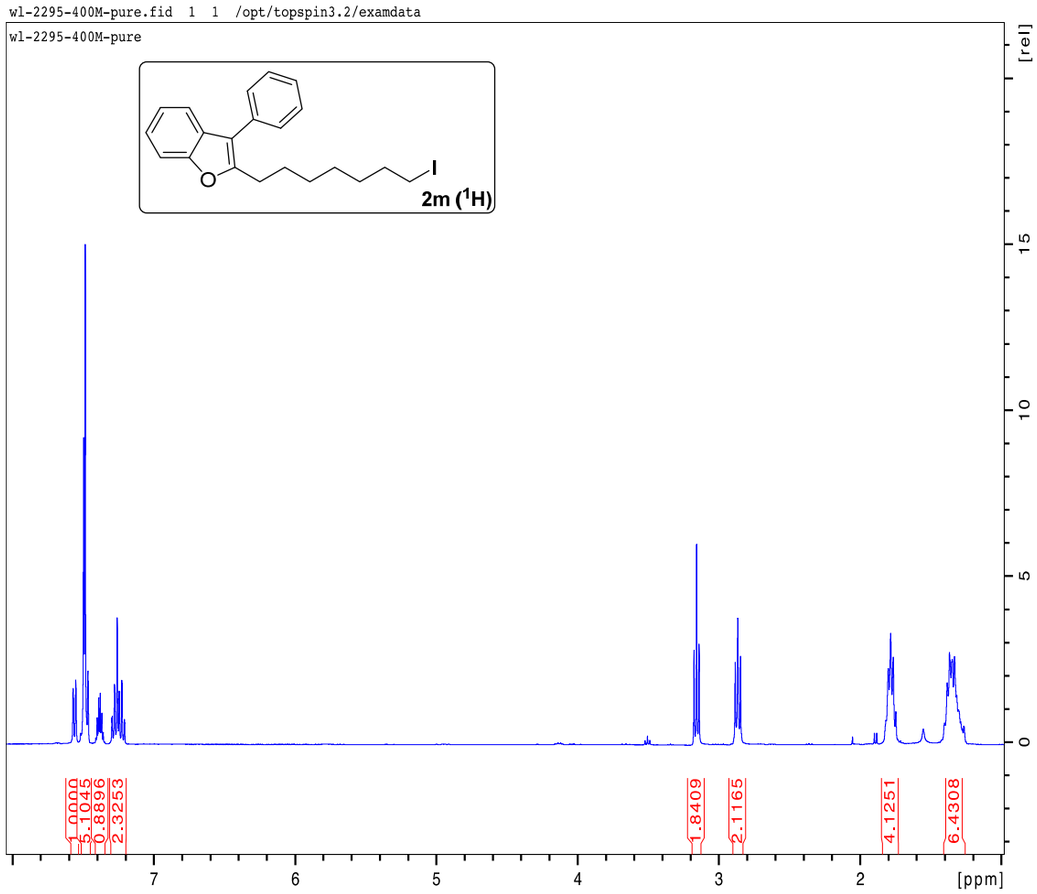
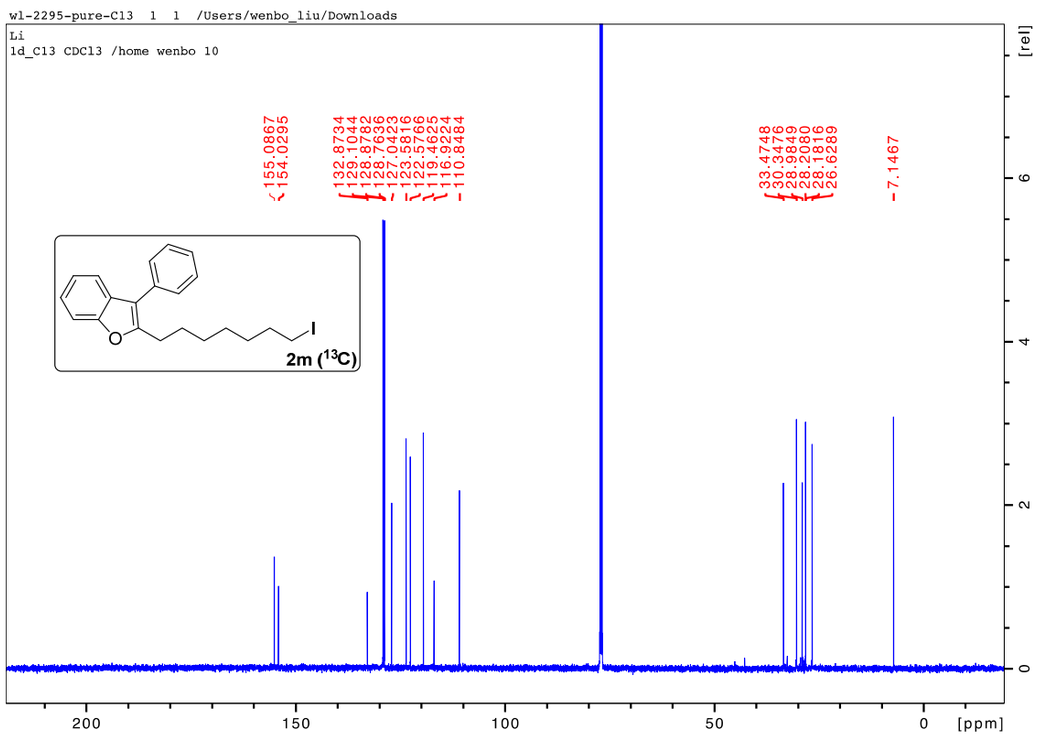
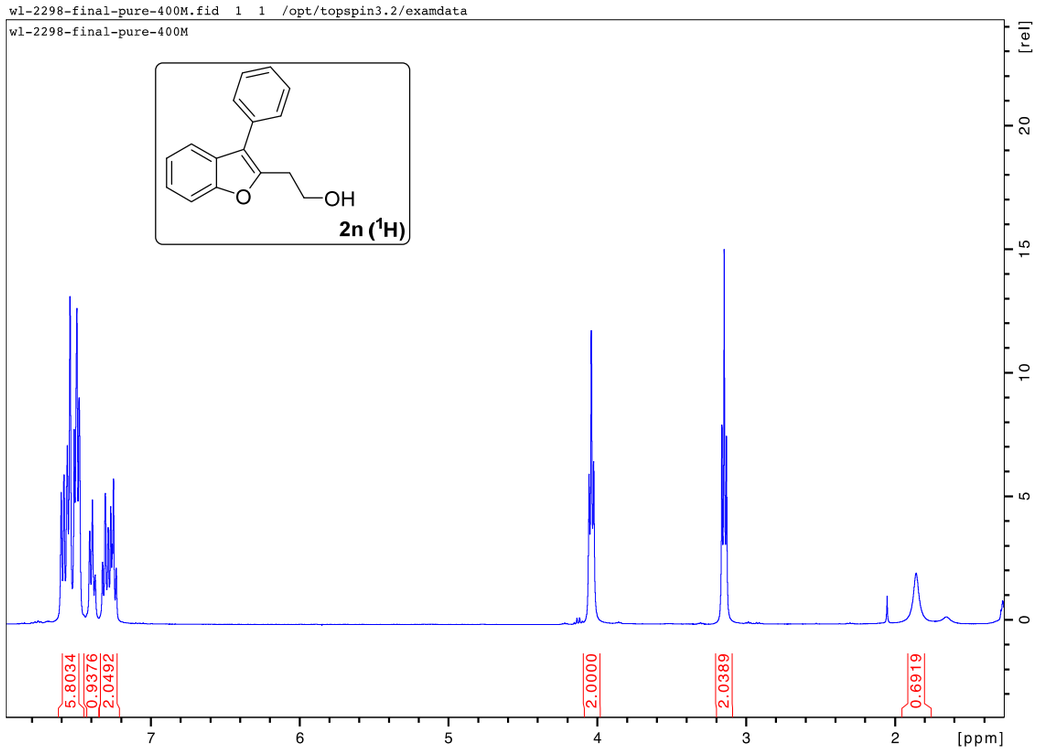

wl-2290-500M-C13 1 1 /Users/wenbo_liu/Downloads
Li
1d_C13 CDCl3 /home wenbo 10
154.2054
150.1834
132.0105
129.1099
128.9012
128.5593
127.4886
124.2886
122.8758
119.8732
119.2073
111.0490
41.6939
30.4244
Cl
2j (13C)
[rel]
[ppm]

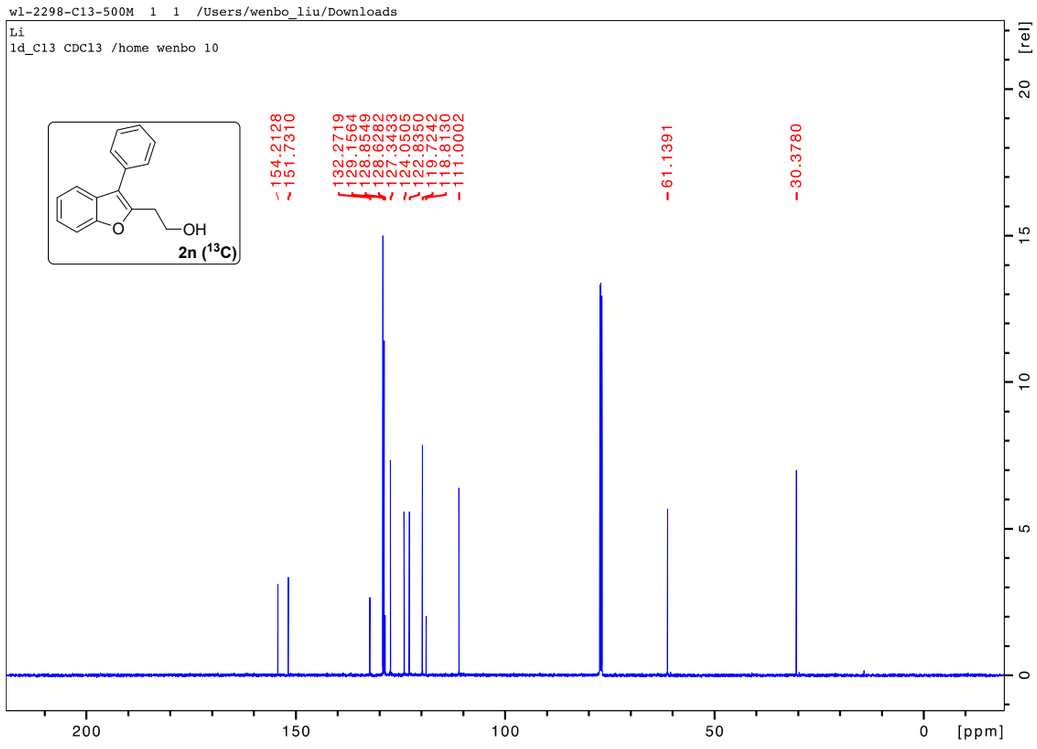

wl-2293-400M-pure.fid 1 1 /opt/topspin3.2/examdata
wl-2293-400M-pure
Cl
2k (^{1}H)
1.0000
5.0922
0.8994
2.0149
1.8025
2.0613
2.2875
1.7953
[rel]
[ppm]

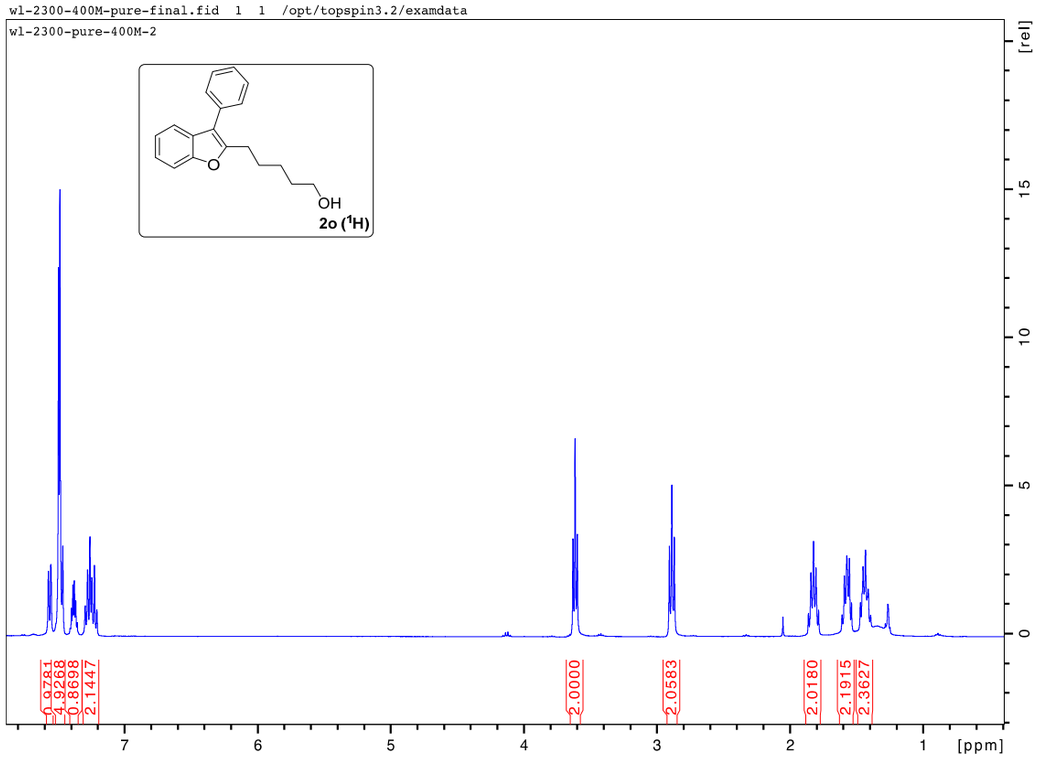

wl-2293-pure-500M 1 1 /Users/wenbo_liu/Downloads
Li
1d_C13 CDCl3 /home wenbo 10
Cl
2k (^{13}C)
154.2295
154.1228
132.6783
129.1346
128.8798
128.8169
127.2333
123.8236
123.7312
120.9907
117.3953
110.3494
44.5898
32.0152
25.9586
25.6322
[rel]
[ppm]

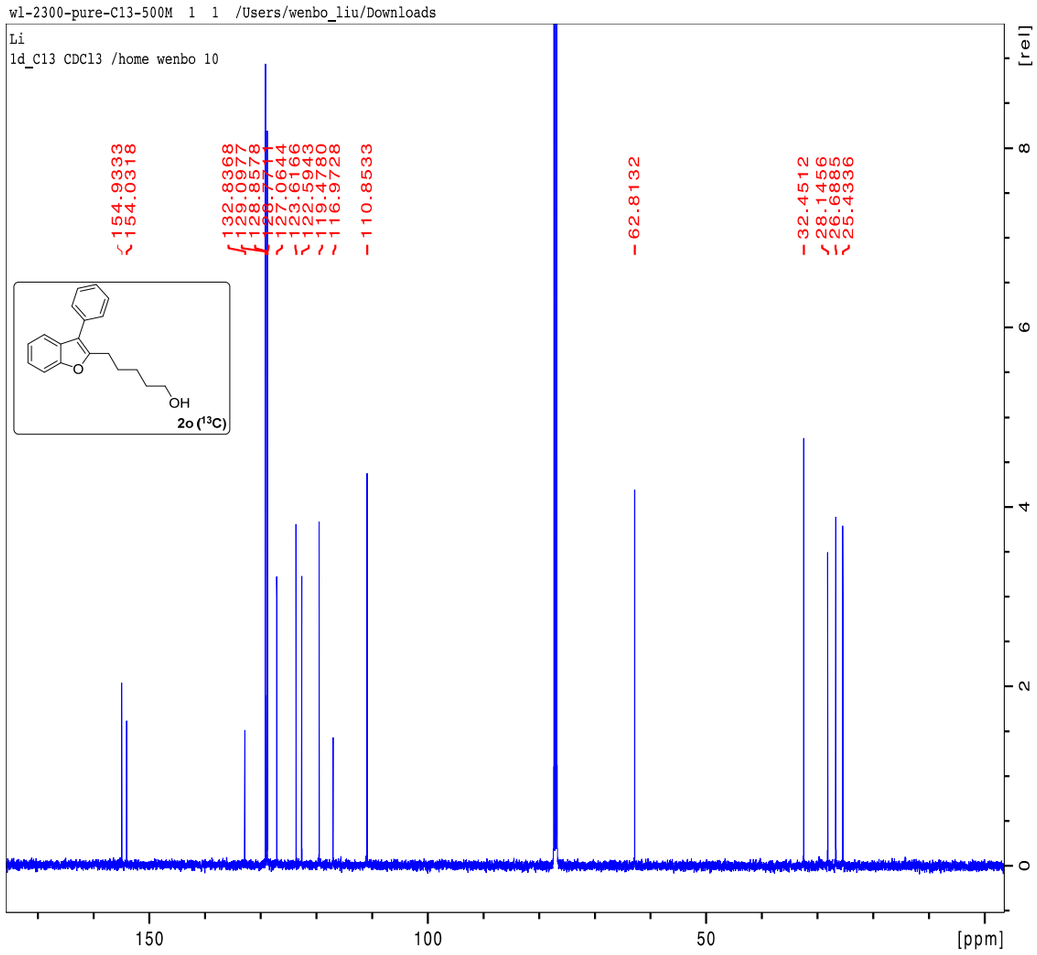

wl-2295-400M-pure.fid 1 1 /opt/topspin3.2/examdata
wl-2295-400M-pure
2m (^{1}H)
[rel]
1.0000
5.1045
0.8896
2.3253
1.8409
2.1165
4.1251
6.4308
[ppm]

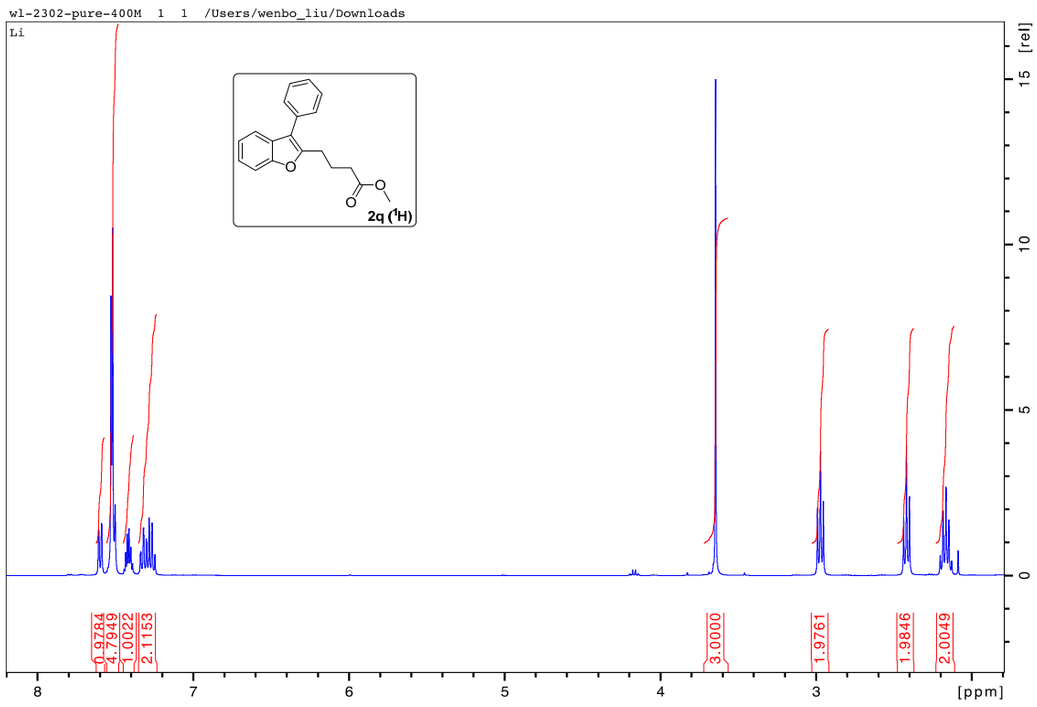

wl-2295-pure-C13 1 1 /Users/wenbo_liu/Downloads
Li
1d_C13 CDCl3 /home wenbo 10
155.0867
154.0295
132.8734
129.1044
128.8782
128.7636
127.0423
123.5816
122.5766
119.4625
116.9224
110.8484
33.4748
30.3476
28.2049
28.2000
28.1816
26.6289
7.1467
2m (^{13}C)
[rel]
[ppm]

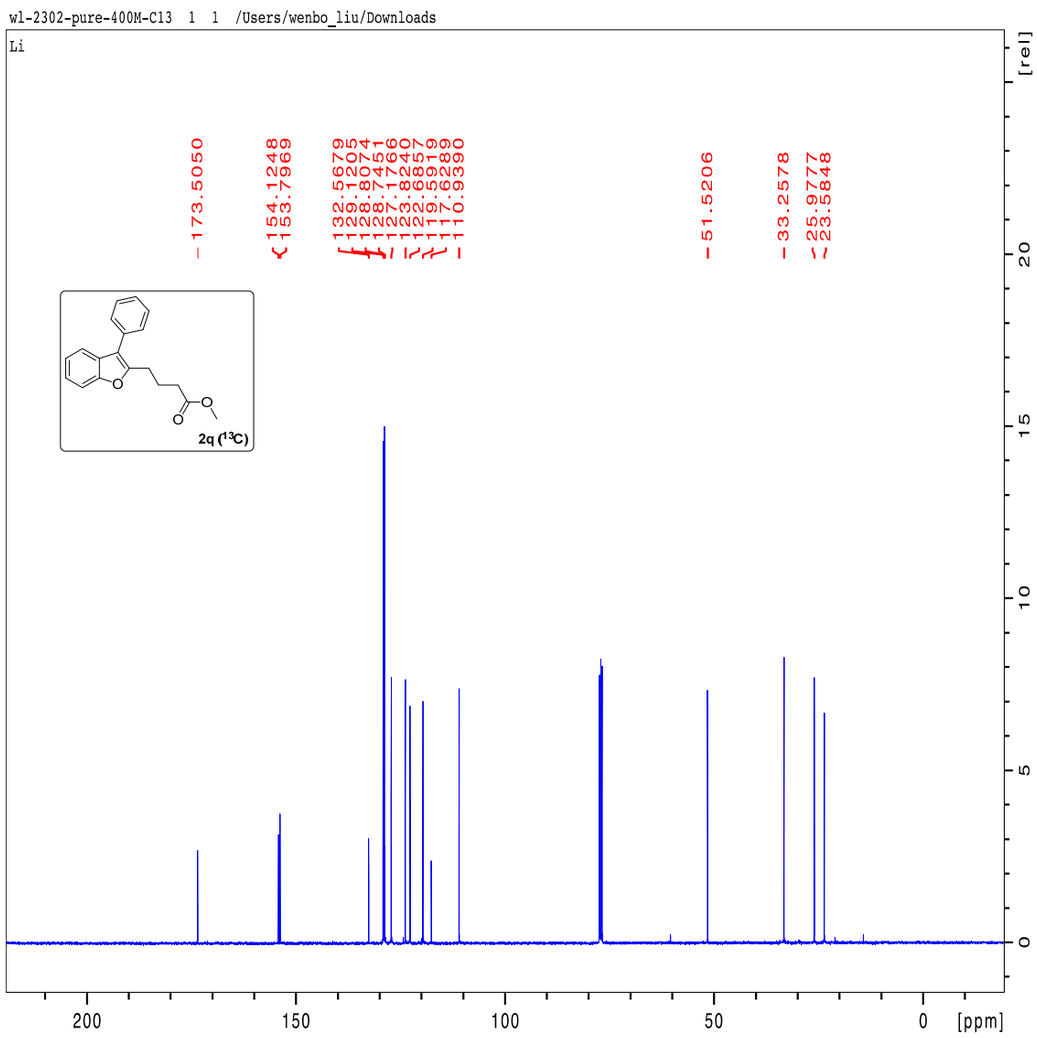

wl-2298-final-pure-400M.fid 1 1 /opt/topspin3.2/examdata
wl-2298-final-pure-400M
OH
2n (1H)
[rel]
5.8034
0.9376
2.0492
2.0000
2.0389
0.6919
[ppm]

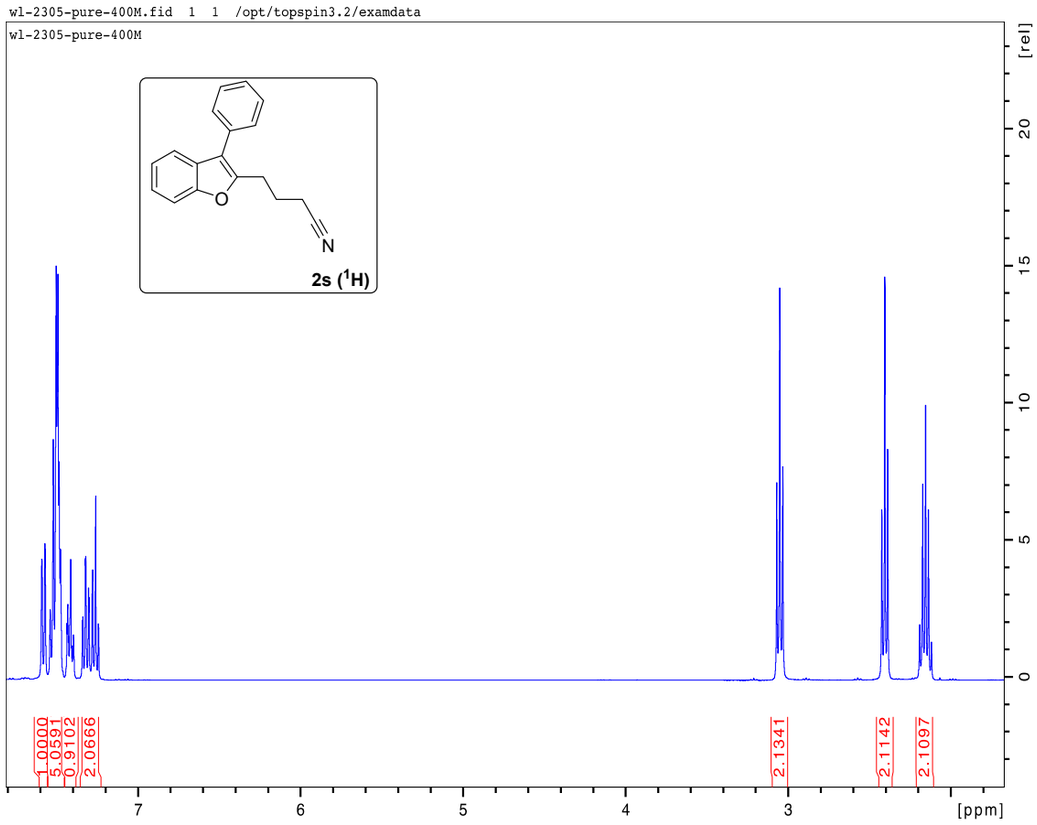

wl-2298-C13-500M 1 1 /Users/wenbo_liu/Downloads
Li
1d_C13 CDCl3 /home wenbo 10
OH
2n (13C)
154.2128
151.7310
132.2719
129.1564
128.8549
128.6282
127.3433
124.0505
122.8350
119.7242
118.8130
111.0002
61.1391
30.3780
[rel]
[ppm]

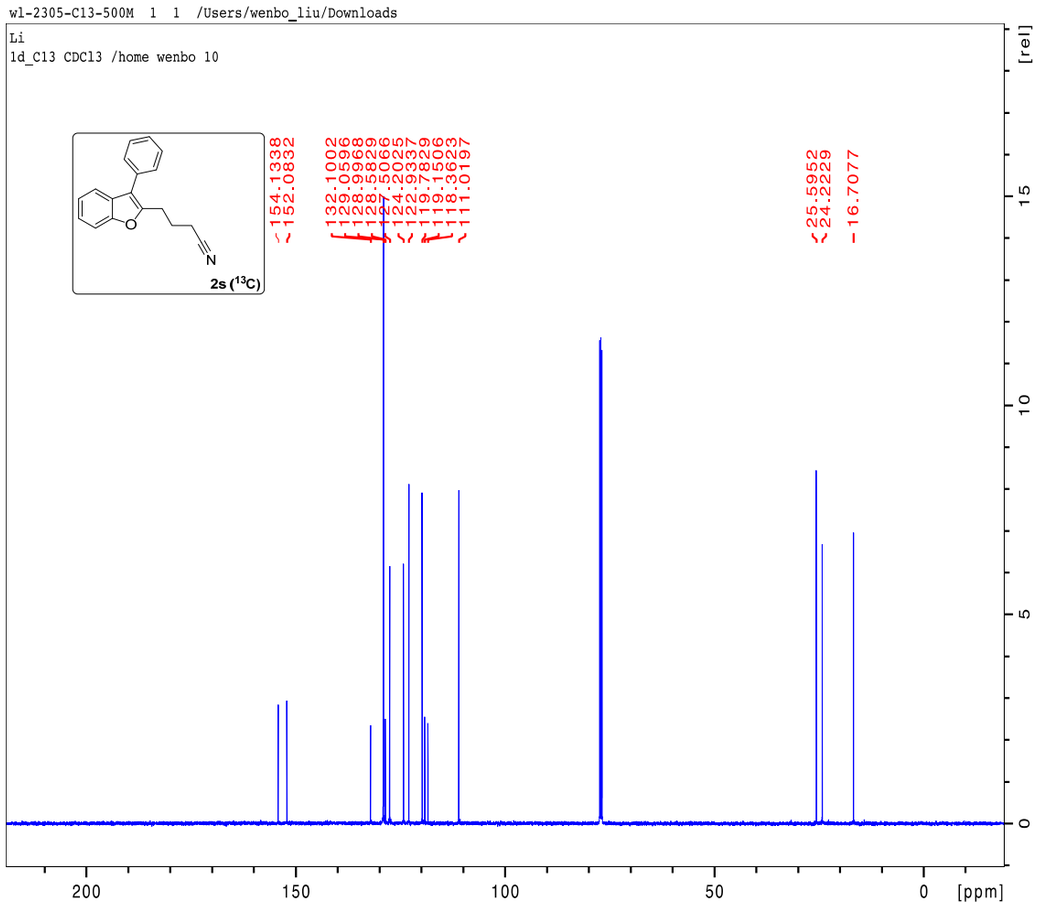

wl-2300-400M-pure-final.fid 1 1 /opt/topspin3.2/examdata
wl-2300-pure-400M-2
OH
2o (1H)
[rel]
0.9281
4.9268
0.8698
2.1447
2.0000
2.0583
2.0180
2.1915
2.3627
[ppm]

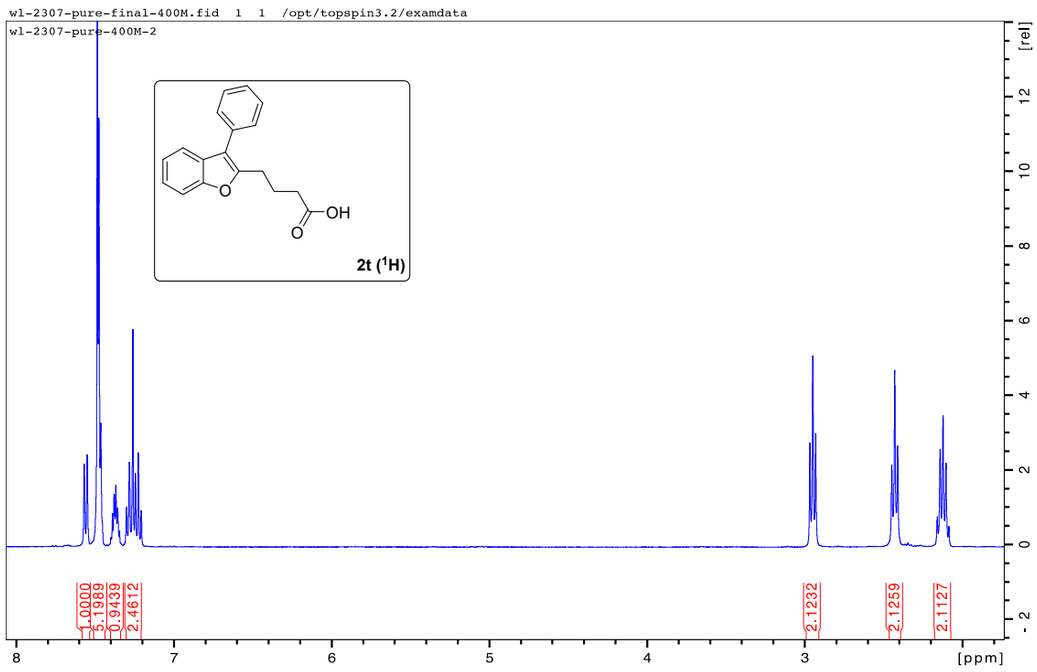

wl-2300-pure-C13-500M 1 1 /Users/wenbo_liu/Downloads
Li
1d_C13 CDCl3 /home wenbo 10
154.9333
154.0318
132.8368
129.0977
128.8578
127.0644
123.6166
122.5943
119.4780
116.9728
110.8533
62.8132
32.4512
28.1456
26.6885
25.4336
OH
2o (13C)
[rel]
[ppm]

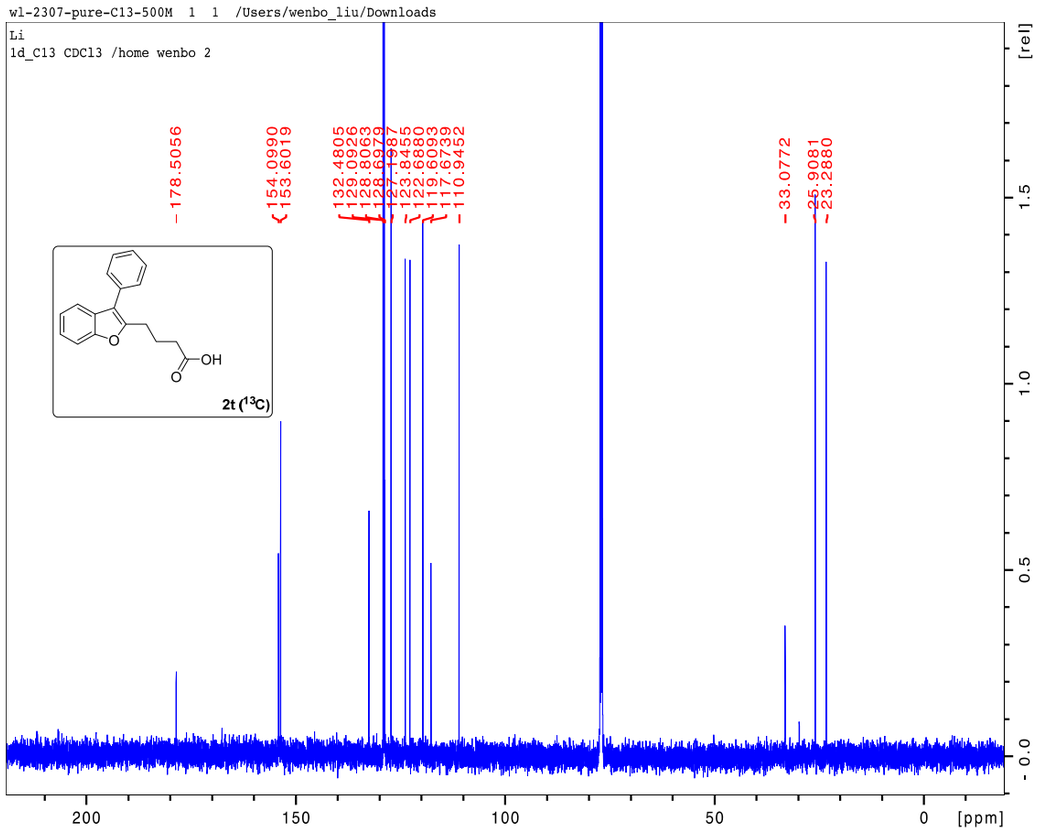

wl-2302-pure-400M 1 1 /Users/wenbo_liu/Downloads
Li
2q (1H)
0.9784
4.7949
1.0022
2.1153
3.0000
1.9761
1.9846
2.0049
[rel]
[ppm]

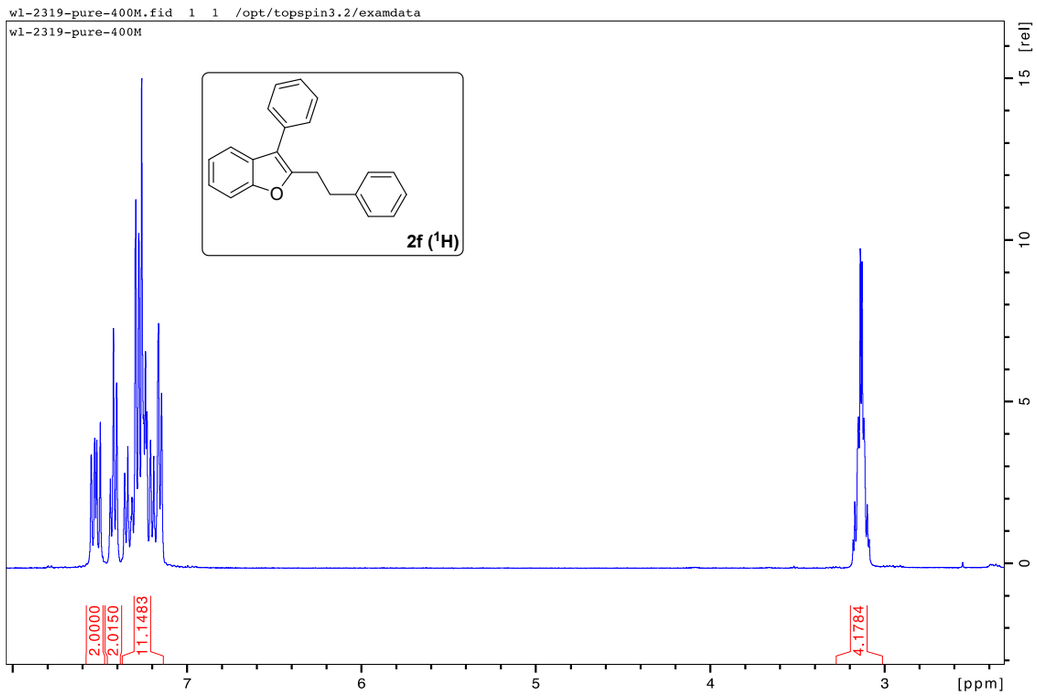

wl-2302-pure-400M-C13 1 1 /Users/wenbo_liu/Downloads
Li
173.5050
154.1248
153.7969
132.5679
129.1205
128.8074
128.7451
127.1766
123.8240
122.6857
119.5919
117.6289
110.9390
51.5206
33.2578
25.9777
23.5848
2q (13C)
[rel]
[ppm]

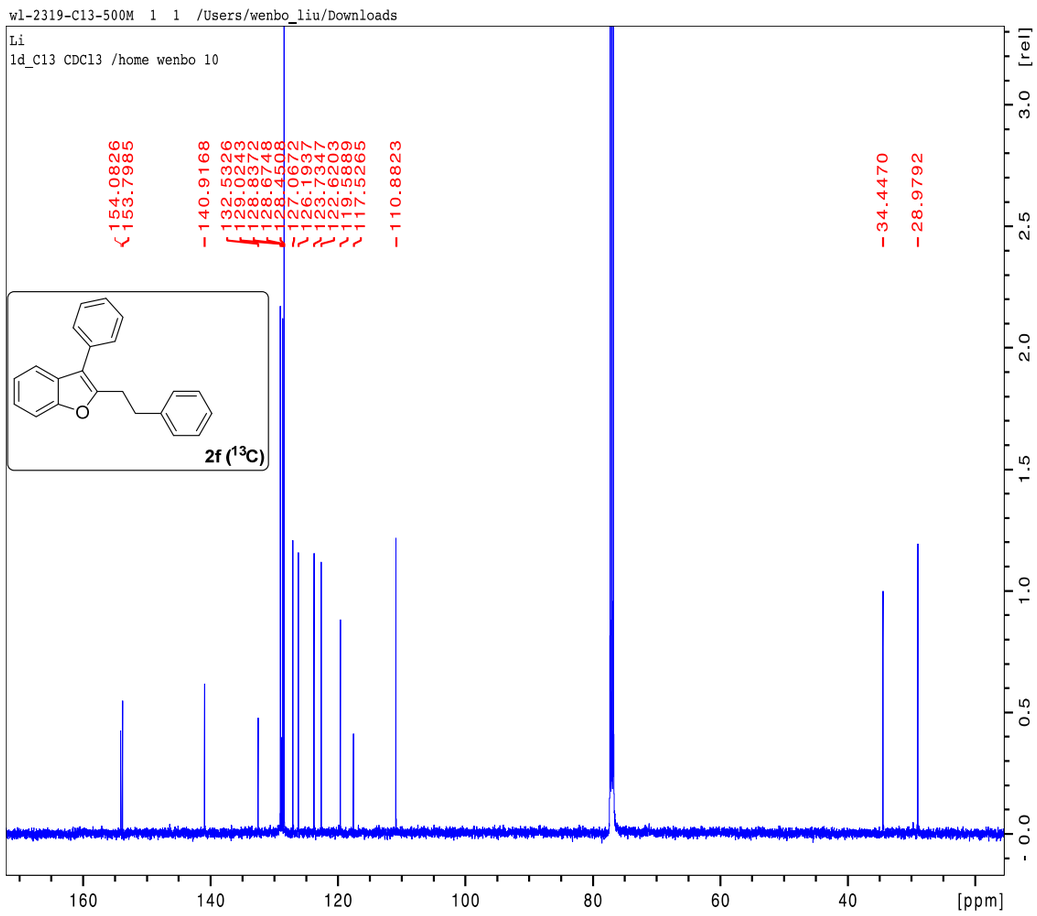

wl-2305-pure-400M.fid 1 1 /opt/topspin3.2/examdata
wl-2305-pure-400M
2s (^{1}H)
1.0000
5.0591
0.9102
2.0666
2.1341
2.1142
2.1097
[rel]
[ppm]

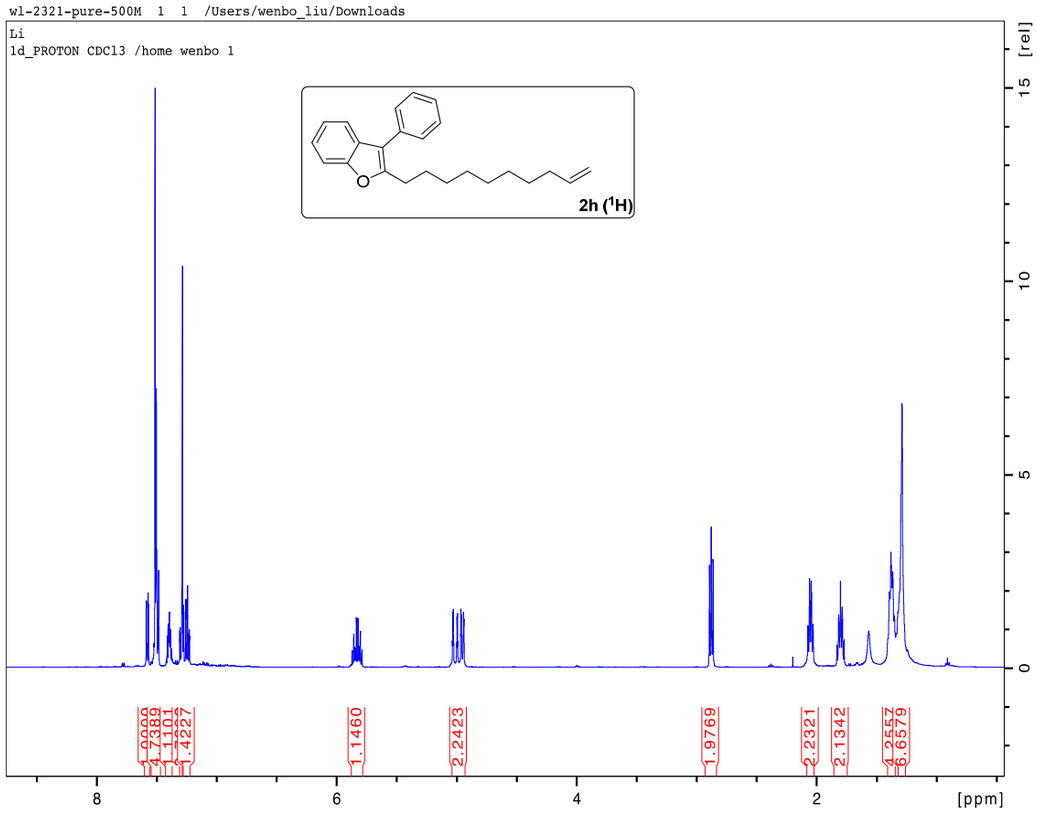

wl-2305-C13-500M 1 1 /Users/wenbo_liu/Downloads
Li
1d_C13 CDCl3 /home wenbo 10
2s (^{13}C)
154.1338
152.0832
132.1002
129.0596
128.3868
127.5066
124.2025
122.9337
119.7829
119.1506
118.3623
111.0197
25.5952
24.2229
16.7077
[rel]
[ppm]

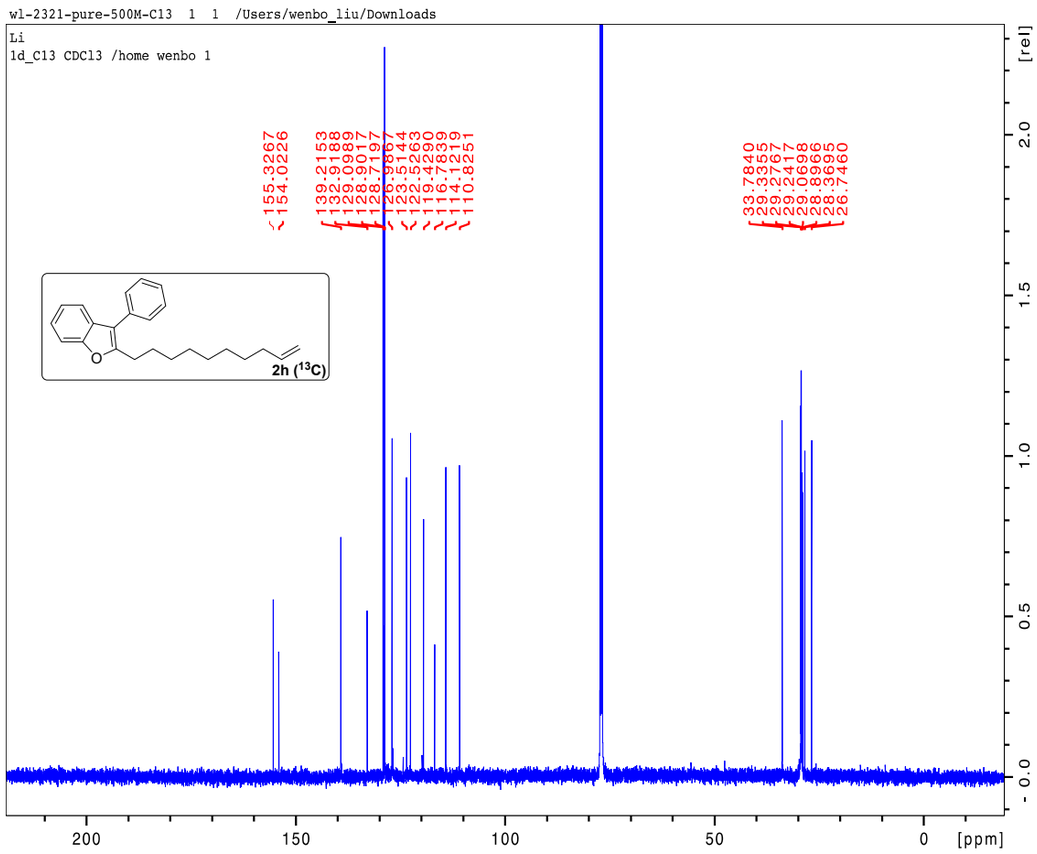

wl-2307-pure-final-400M.fid 1 1 /opt/topspin3.2/examdata
wl-2307-pure-400M-2
OH
O
O
2t (^{1}H)
1.0000
3.1989
0.9439
2.4612
2.1232
2.1259
2.1127
[rel]
[ppm]

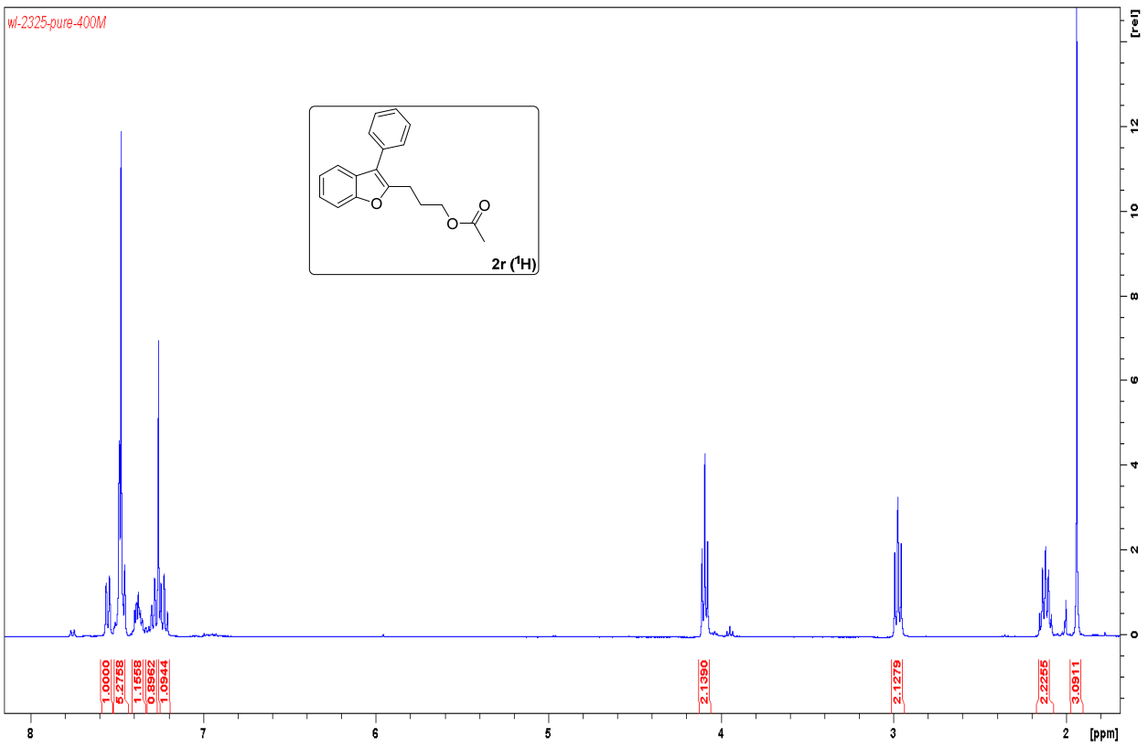

wl-2307-pure-C13-500M 1 1 /Users/wenbo_liu/Downloads
Li
1d_C13 CDCl3 /home wenbo 2
178.5056
154.0990
153.6019
132.4805
129.0926
128.8063
128.6979
127.1087
123.8455
122.6880
119.6093
117.6739
110.9452
33.0772
25.9081
23.2880
OH
O
O
2t (^{13}C)
[rel]
[ppm]

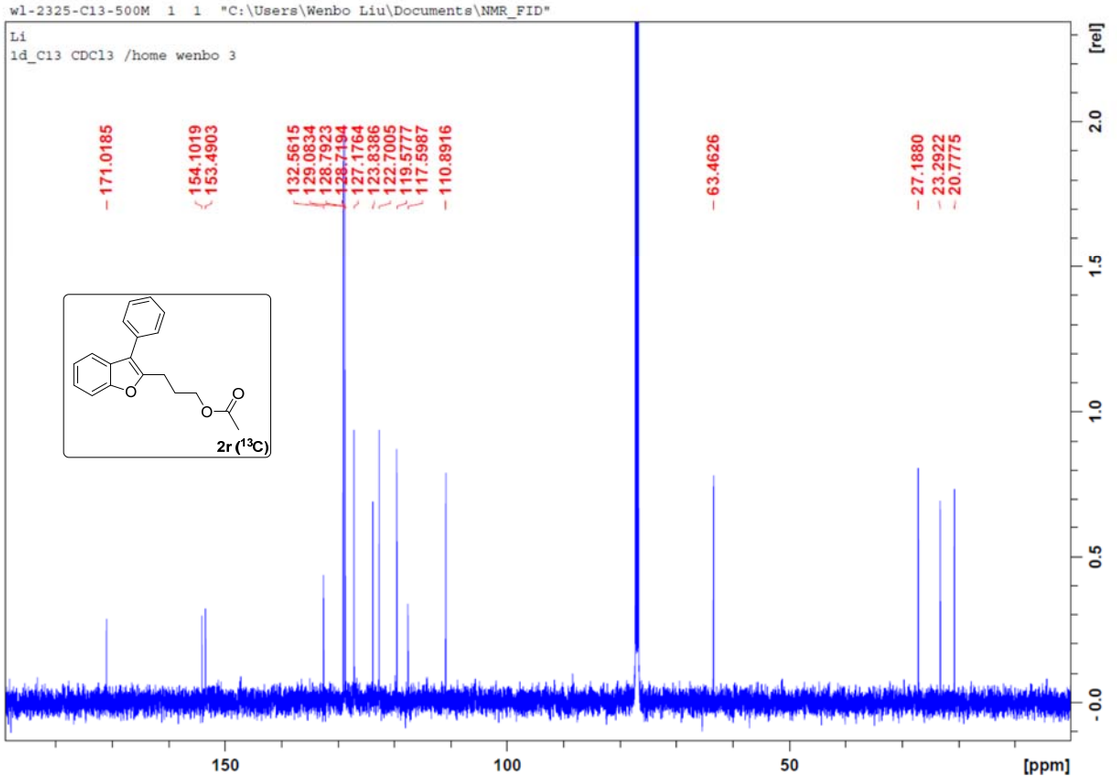

wl-2319-pure-400M.fid 1 1 /opt/topspin3.2/examdata
wl-2319-pure-400M
2f (^{1}H)
2.0000
2.0150
11.1483
4.1784
[ppm]
[rel]

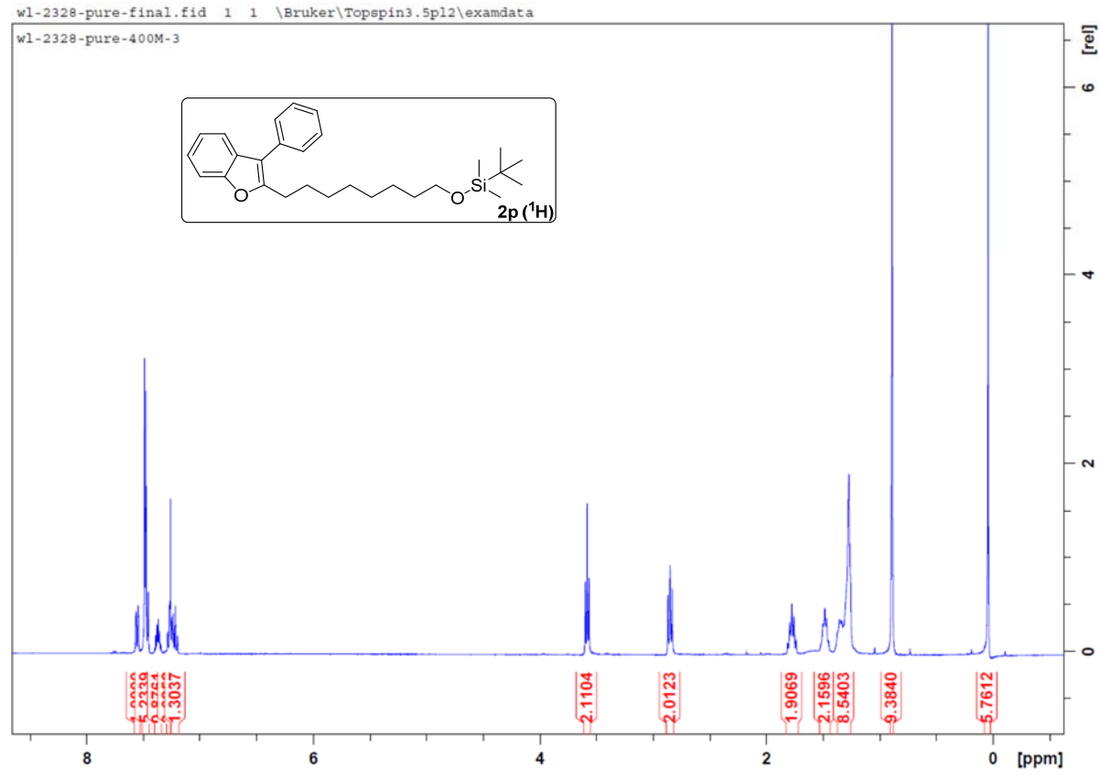

wl-2319-C13-500M 1 1 /Users/wenbo_liu/Downloads
Li
1d_C13 CDCl3 /home wenbo 10
154.0826
153.7985
140.9168
132.5326
129.0243
128.8372
128.6748
128.4508
127.0672
126.1937
123.7347
122.6203
119.5889
117.5265
110.8823
34.4470
28.9792
2f (^{13}C)
[ppm]
[rel]

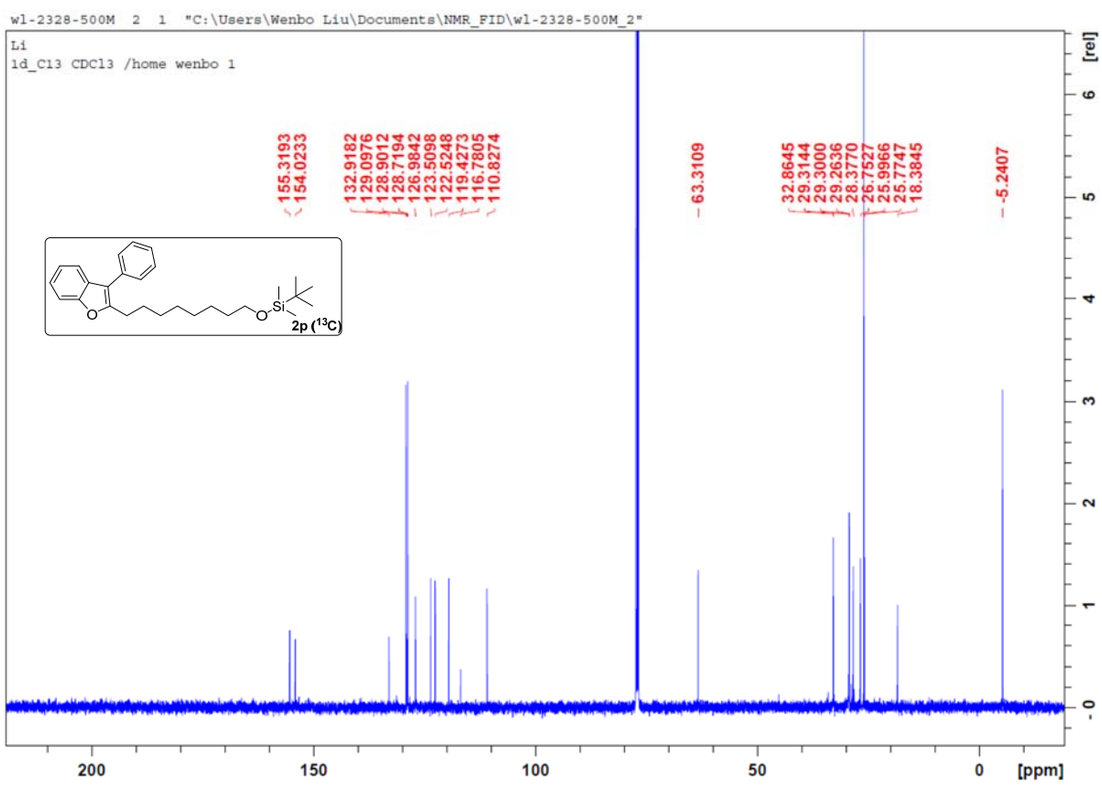

wl-2321-pure-500M 1 1 /Users/wenbo_liu/Downloads
Li
1d_PROTON CDCl3 /home wenbo 1
2h (^{1}H)
1.0000
4.7389
1.1101
1.4227
1.1460
2.2423
1.9769
2.2321
2.1342
4.2557
6.6579
8
6
4
2
[ppm]
15
10
5
0
[rel]

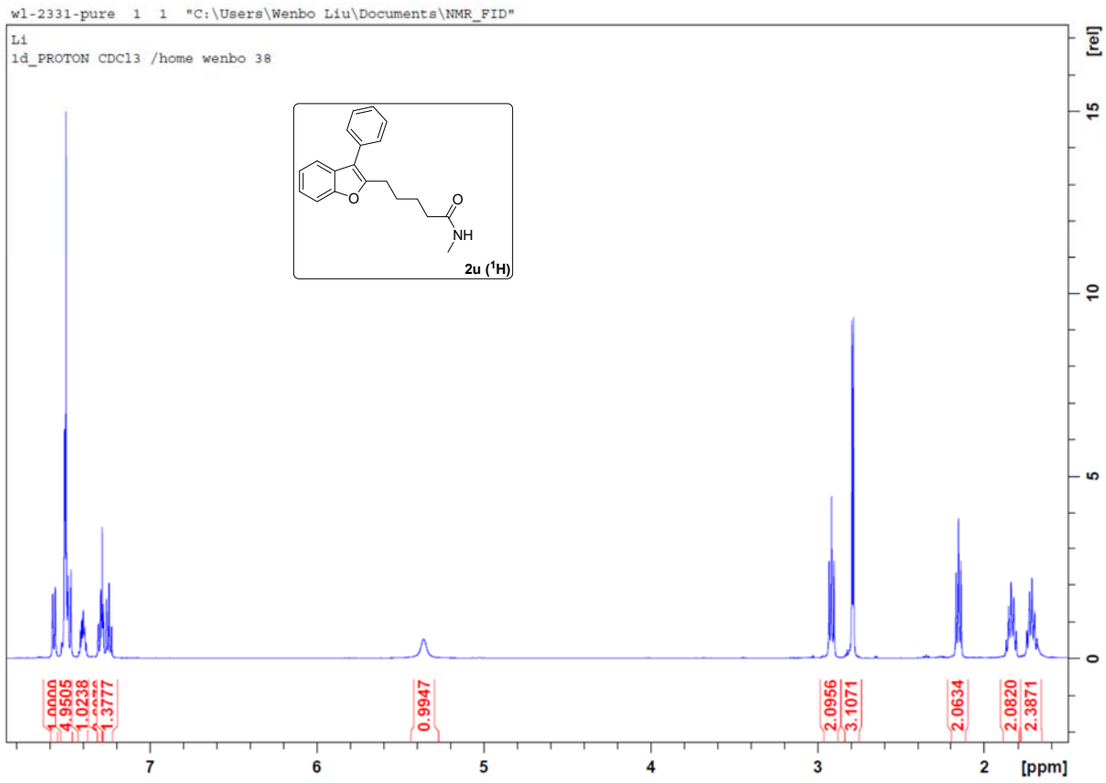

wl-2321-pure-500M-C13 1 1 /Users/wenbo_liu/Downloads
Li
1d_C13 CDCl3 /home wenbo 1
2h (^{13}C)
155.3267
154.0226
139.2153
132.9188
129.0989
128.9017
128.7197
126.9867
123.5144
122.5263
119.4290
116.7239
114.1219
110.8251
33.7840
29.3355
29.2767
29.2417
29.0698
28.8966
28.3695
26.7460
200
150
100
50
0
[ppm]
2.0
1.5
1.0
0.5
- 0.0
[rel]

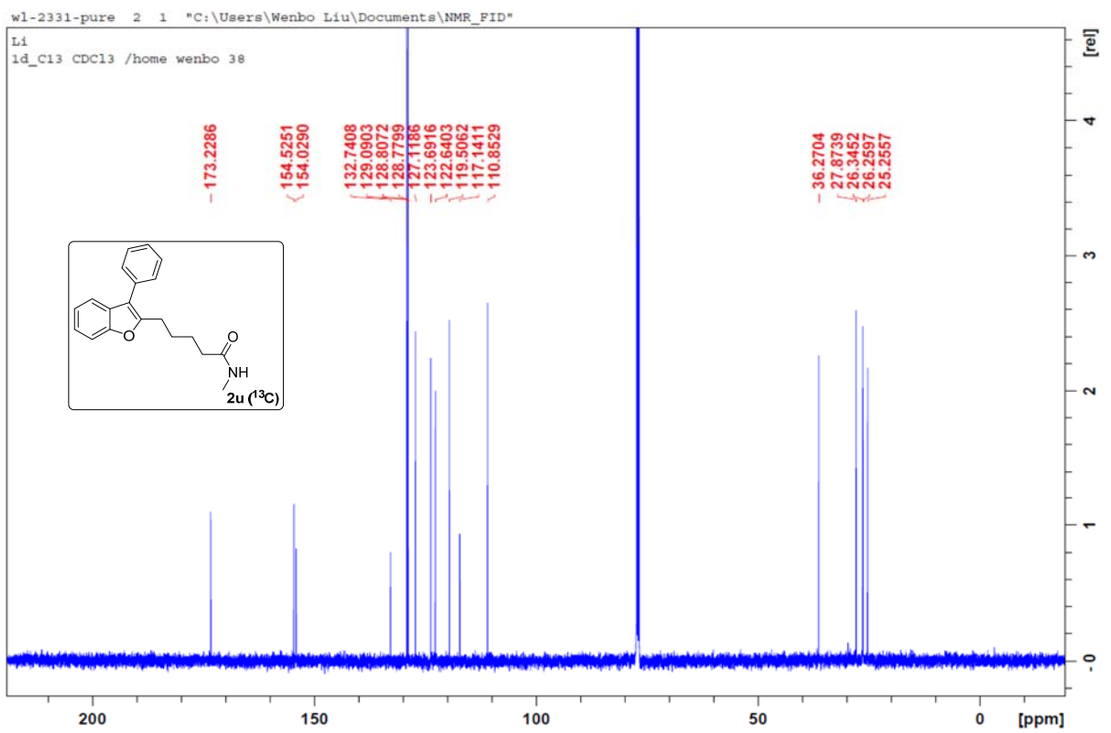

wl-2325-pure-400M
2r (^{1}H)
1.0000
5.2768
1.1668
0.8962
1.0944
2.1390
2.1279
2.2265
3.0911
[ppm]
[rel]

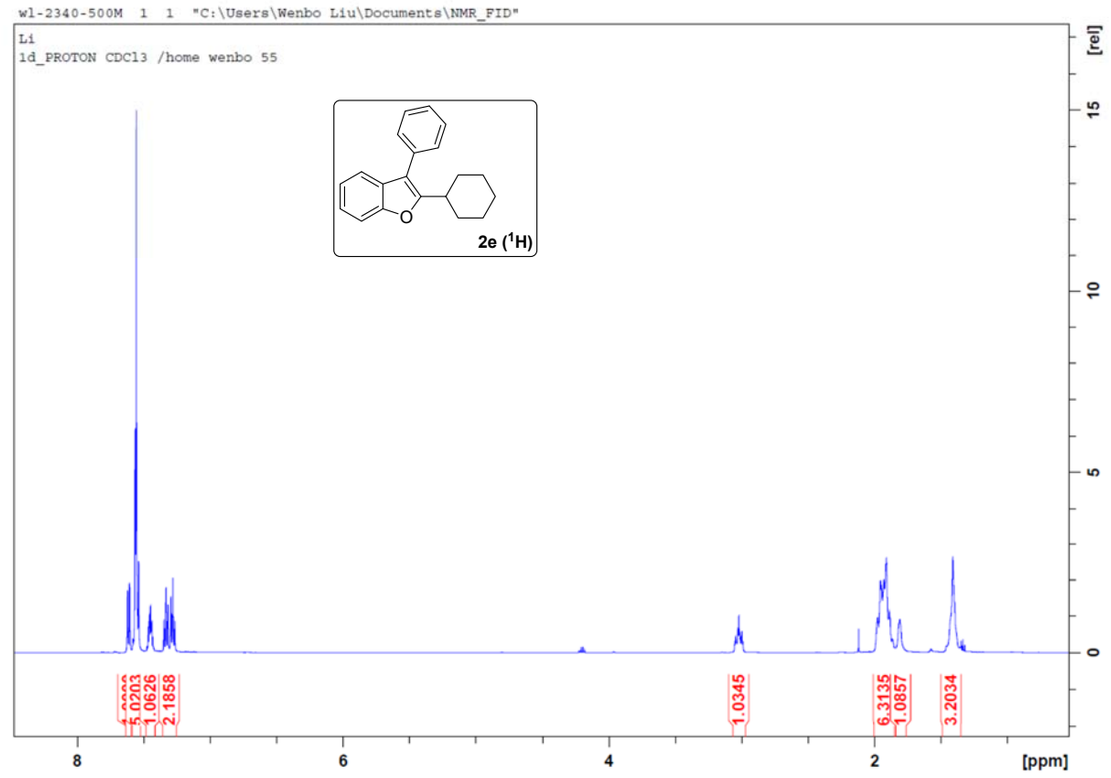

wl-2325-C13-500M 1 1 "C:\Users\Wenbo Liu\Documents\NMR_FID"
Li
1d_C13 CDCl3 /home wenbo 3
171.0185
154.1019
153.4903
132.5615
129.0834
128.7923
128.7194
127.1764
123.8386
122.7005
119.5777
117.5987
110.8916
63.4626
27.1880
23.2922
20.7775
2r (^{13}C)
[ppm]
[rel]

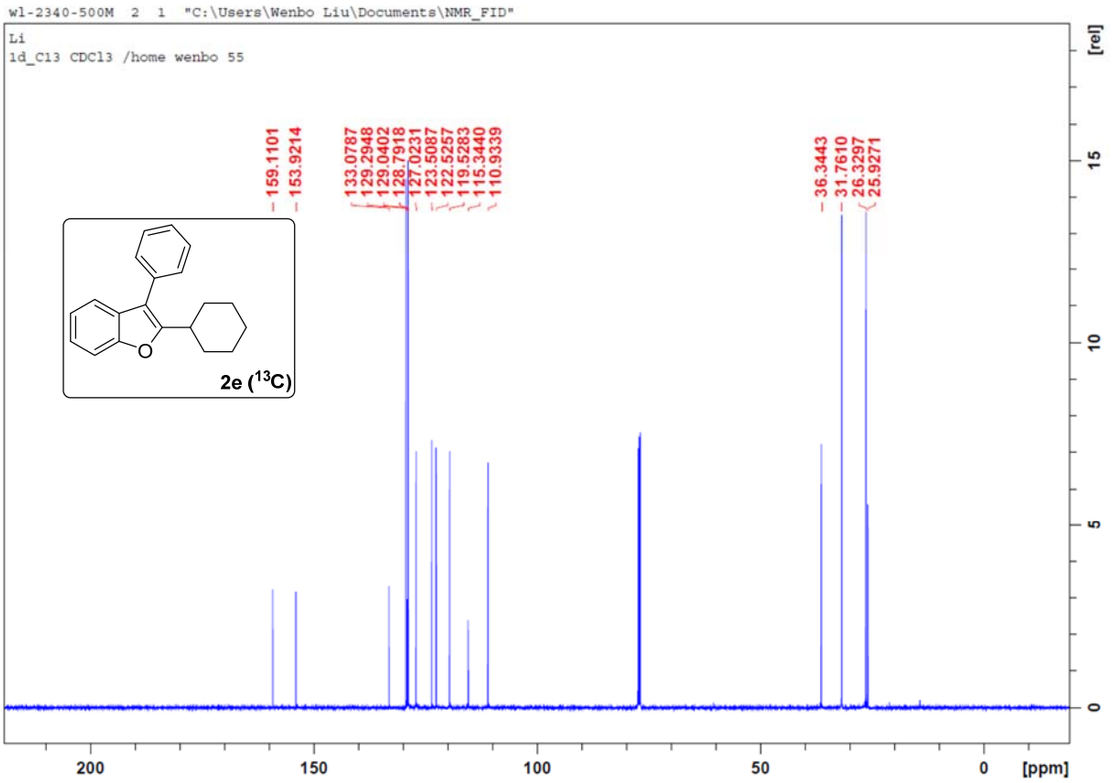

wl-2328-pure-final.fid 1 1 \Bruker\Topspin3.5pl2\examdata
wl-2328-pure-400M-3
2p (1H)
[rel]
[ppm]
1.3037
2.1104
2.0123
1.9069
2.1596
8.5403
9.3840
5.7612

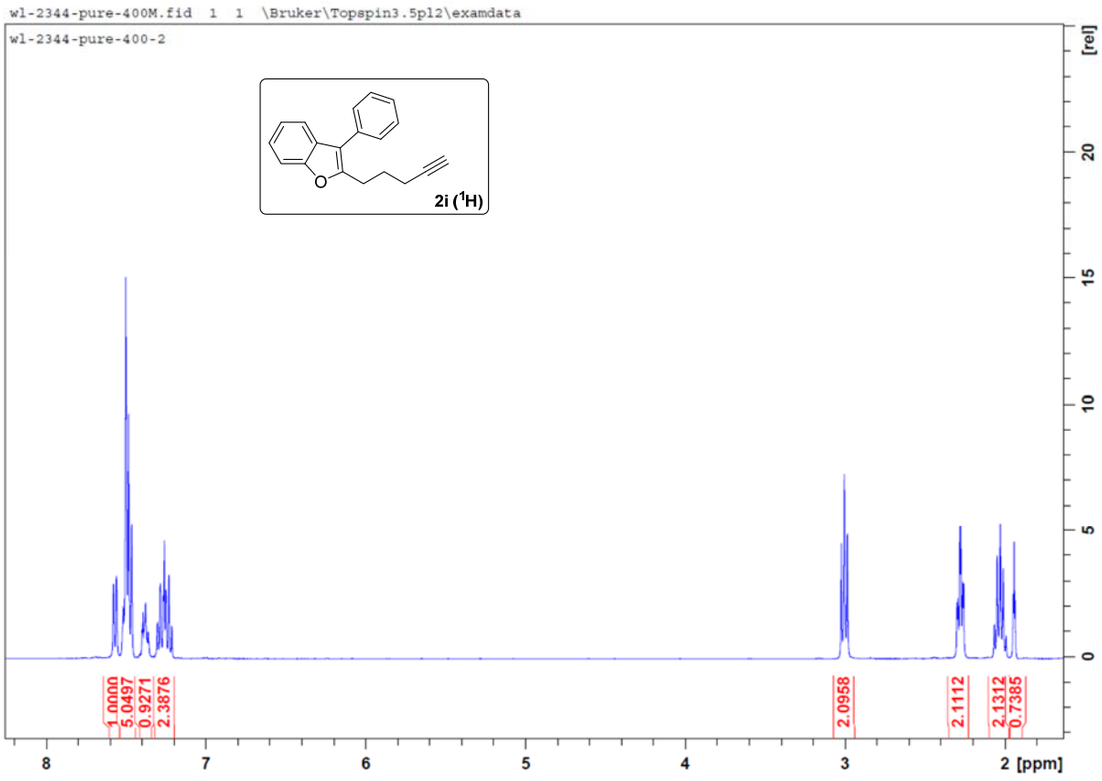

wl-2328-500M 2 1 "C:\Users\Wenbo Liu\Documents\NMR_FID\wl-2328-500M_2"
Li
1d_C13 CDCl3 /home wenbo 1
155.3193
154.0233
132.9182
129.0976
128.9012
128.7194
126.9842
123.5098
122.5248
119.4273
116.7805
110.8274
63.3109
32.8645
29.3144
29.3000
29.2636
28.3770
26.7527
25.9966
25.7747
18.3845
-5.2407
2p (13C)
[rel]
[ppm]

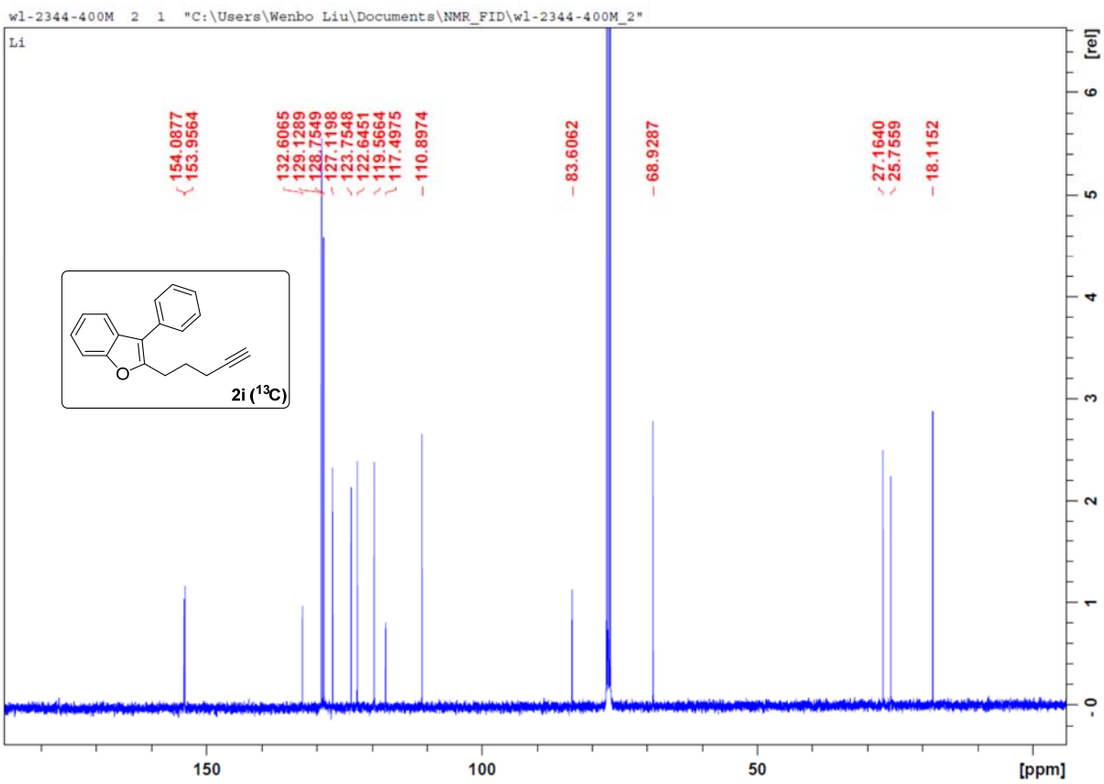

wl-2331-pure 1 1 "C:\Users\Wenbo Liu\Documents\NMR_FID"
Li
1d_PROTON CDCl3 /home wenbo 38
2u (^{1}H)
1.0000
4.9505
1.0238
1.3777
0.9947
2.0956
3.1071
2.0634
2.0820
2.3871
[ppm]
[rel]

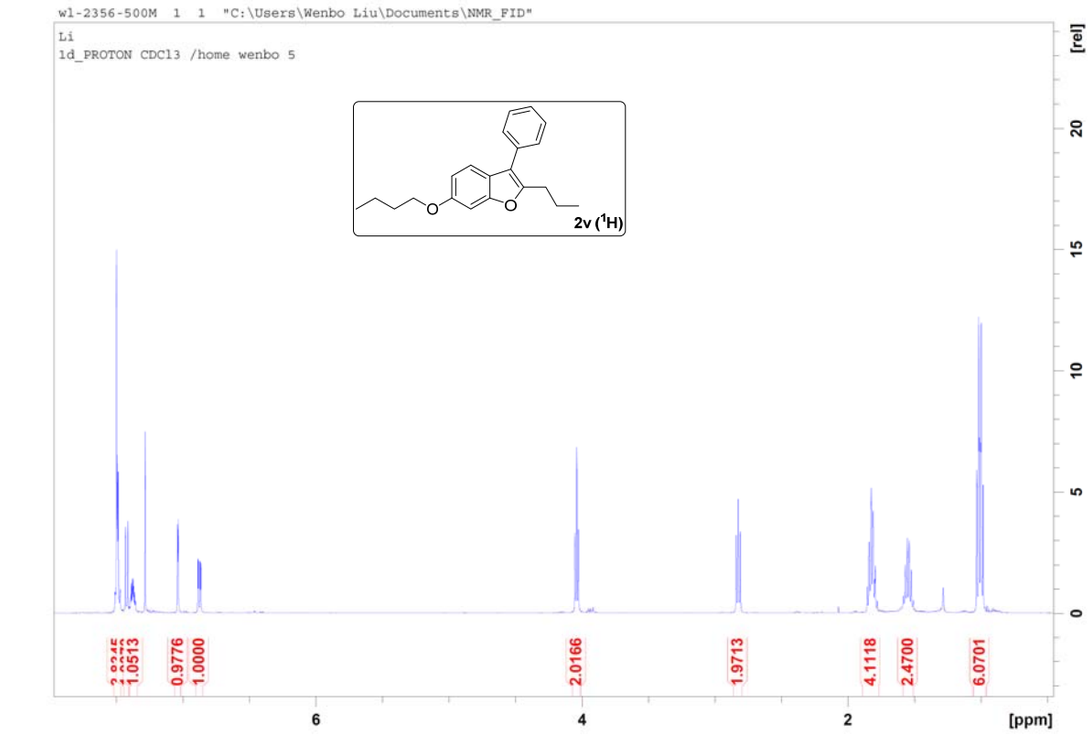

wl-2331-pure 2 1 "C:\Users\Wenbo Liu\Documents\NMR_FID"
Li
1d_C13 CDCl3 /home wenbo 38
173.2286
154.5251
154.0290
132.7408
129.0903
128.8072
128.7799
127.1186
123.6916
122.6403
119.5062
117.1411
110.8529
36.2704
27.8739
26.3452
26.2597
25.2557
2u (^{13}C)
[ppm]
[rel]

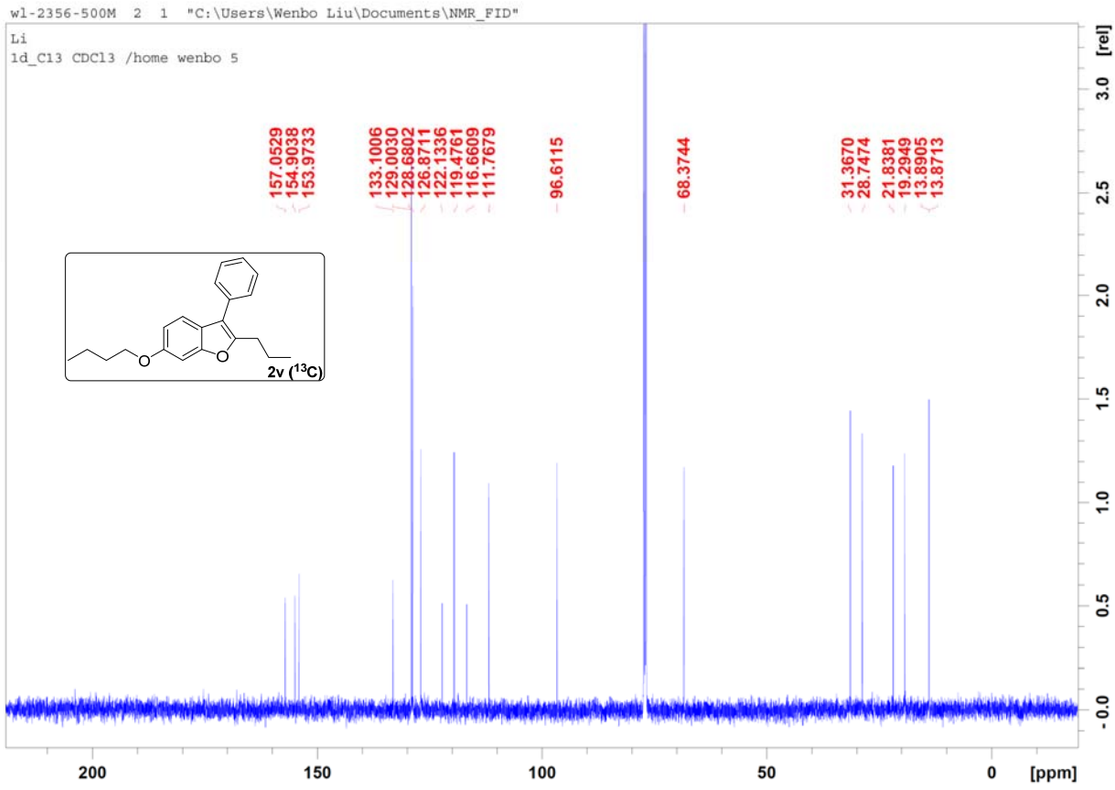

wl-2340-500M 1 1 "C:\Users\Wenbo Liu\Documents\NMR_FID"
Li
1d_PROTON CDCl3 /home wenbo 55
2e (^{1}H)
1.0626
2.1858
1.0345
6.3135
1.0857
3.2034
[rel]
[ppm]

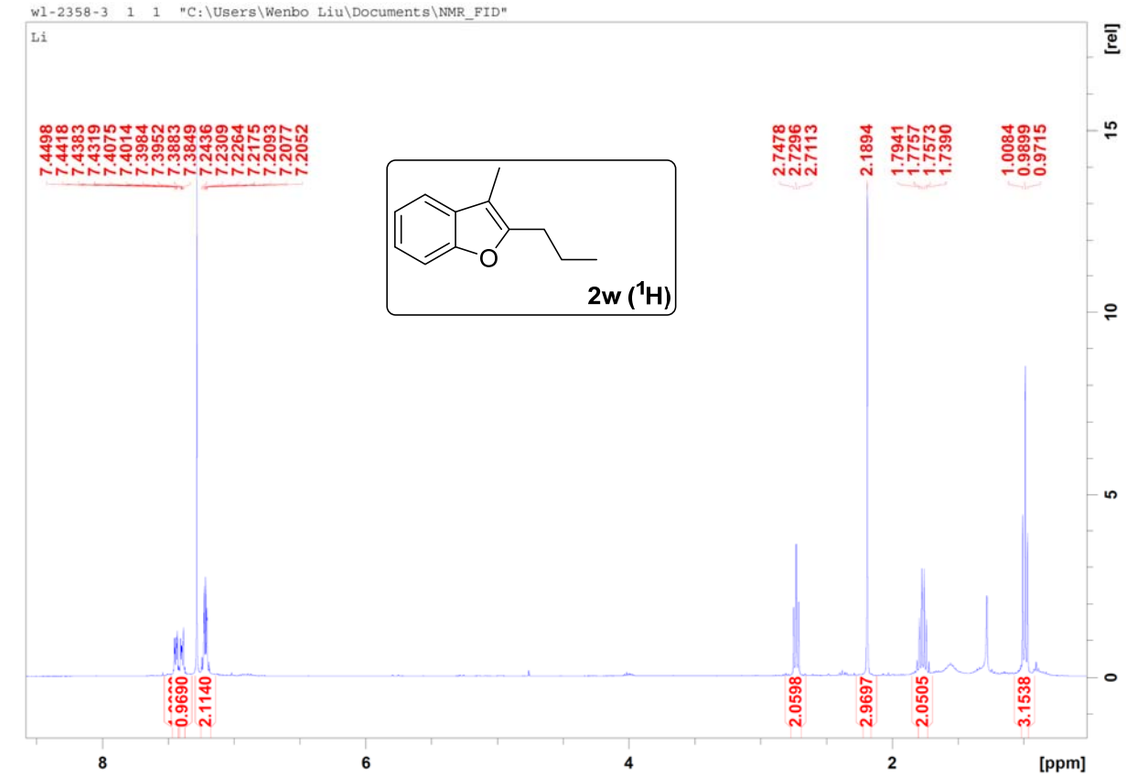

wl-2340-500M 2 1 "C:\Users\Wenbo Liu\Documents\NMR_FID"
Li
1d_C13 CDCl3 /home wenbo 55
159.1101
153.9214
133.0787
129.2948
129.0402
128.7918
127.0231
123.5087
122.5257
119.5283
115.3440
110.9339
36.3443
31.7610
26.3297
25.9271
2e (^{13}C)
[rel]
[ppm]

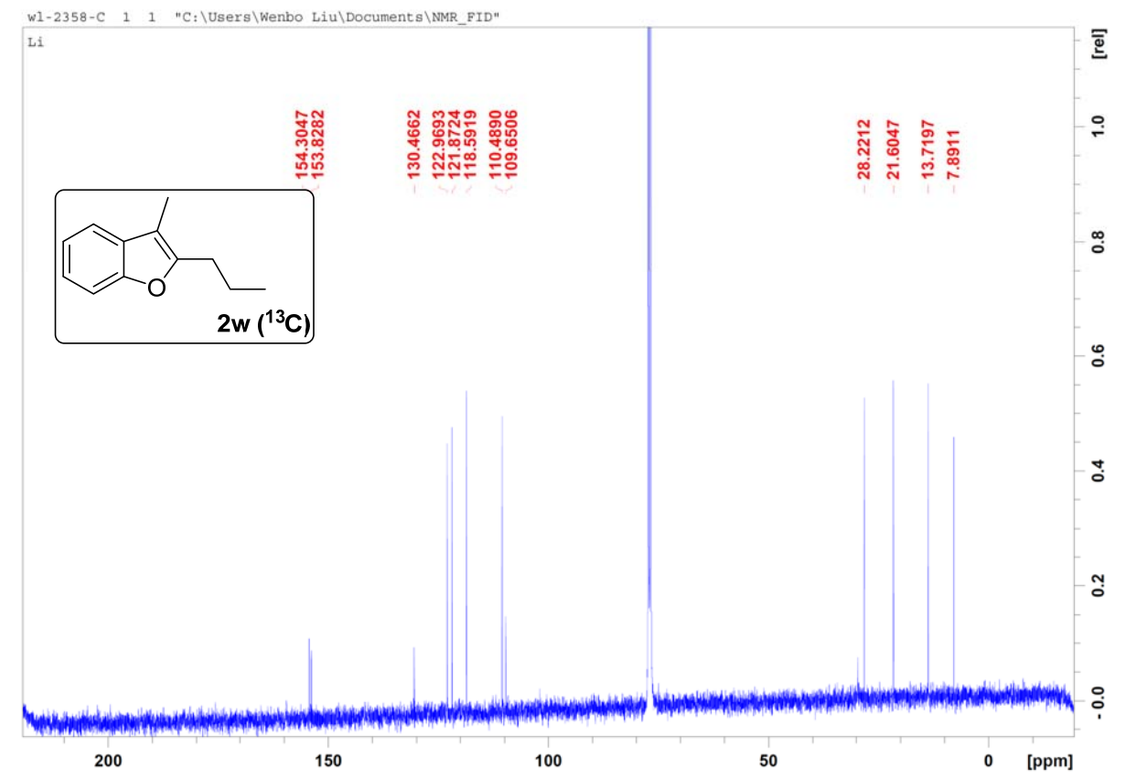

wl-2344-pure-400M.fid 1 1 \Bruker\Topspin3.5pl2\examdata
wl-2344-pure-400-2
2i (^{1}H)
1.0000
5.0497
0.9271
2.3876
2.0958
2.1112
2.1312
0.7385
8
7
6
5
4
3
2 [ppm]
[rel]

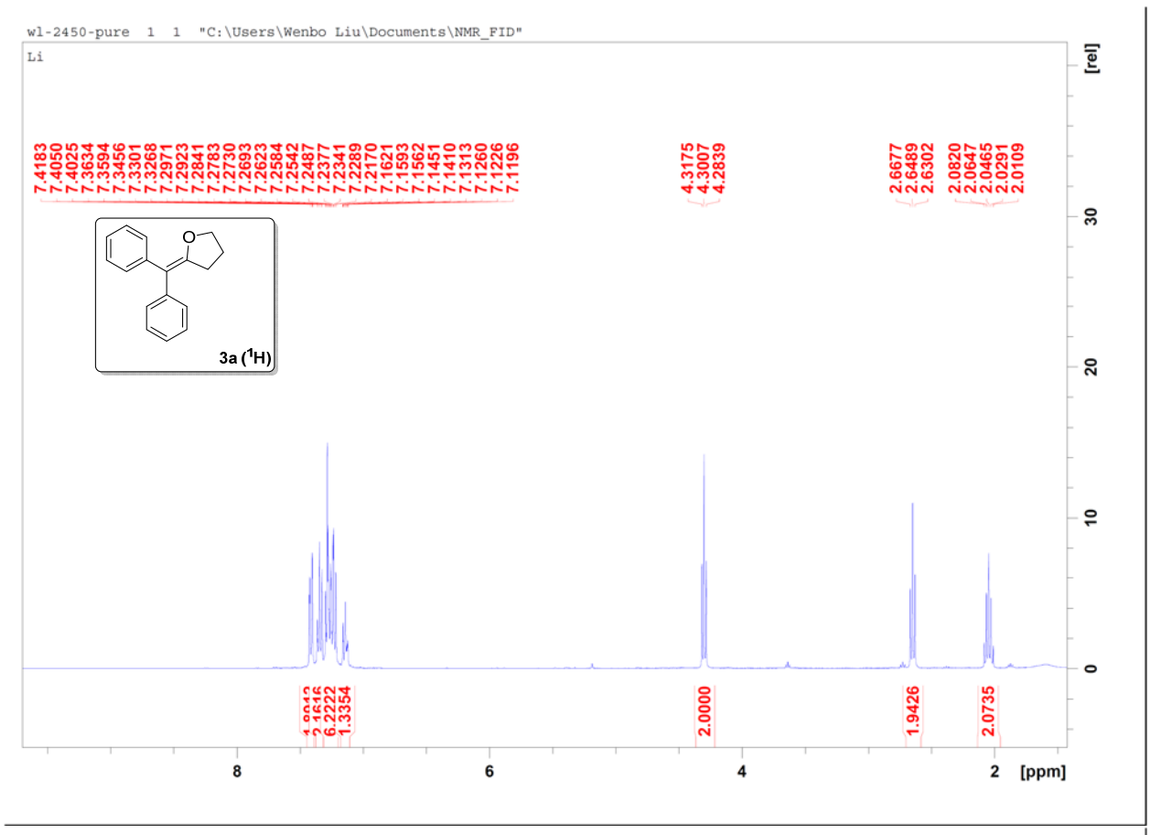

wl-2344-400M 2 1 "C:\Users\Wenbo Liu\Documents\NMR_FID\wl-2344-400M_2"
Li
2i (^{13}C)
154.0877
153.9564
132.6065
129.1289
128.7549
127.1198
123.7548
122.6451
119.5664
117.4975
110.8974
83.6062
68.9287
27.1640
25.7559
18.1152
150
100
50
[ppm]
[rel]

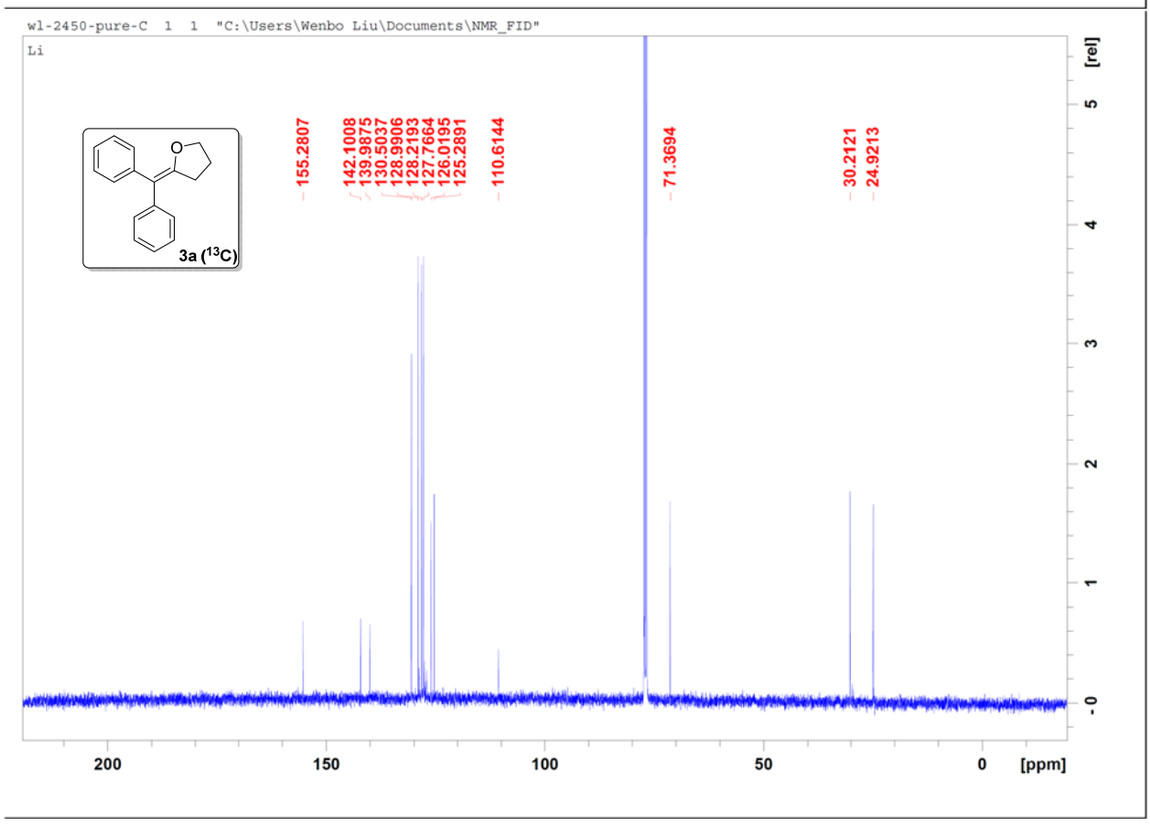

wl-2356-500M 1 1 "C:\Users\Wenbo Liu\Documents\NMR_FID"
Li
1d_PROTON CDCl3 /home wenbo 5
2v (^{1}H)
1.0513
0.9776
1.0000
2.0166
1.9713
4.1118
2.4700
6.0701
[rel]
[ppm]

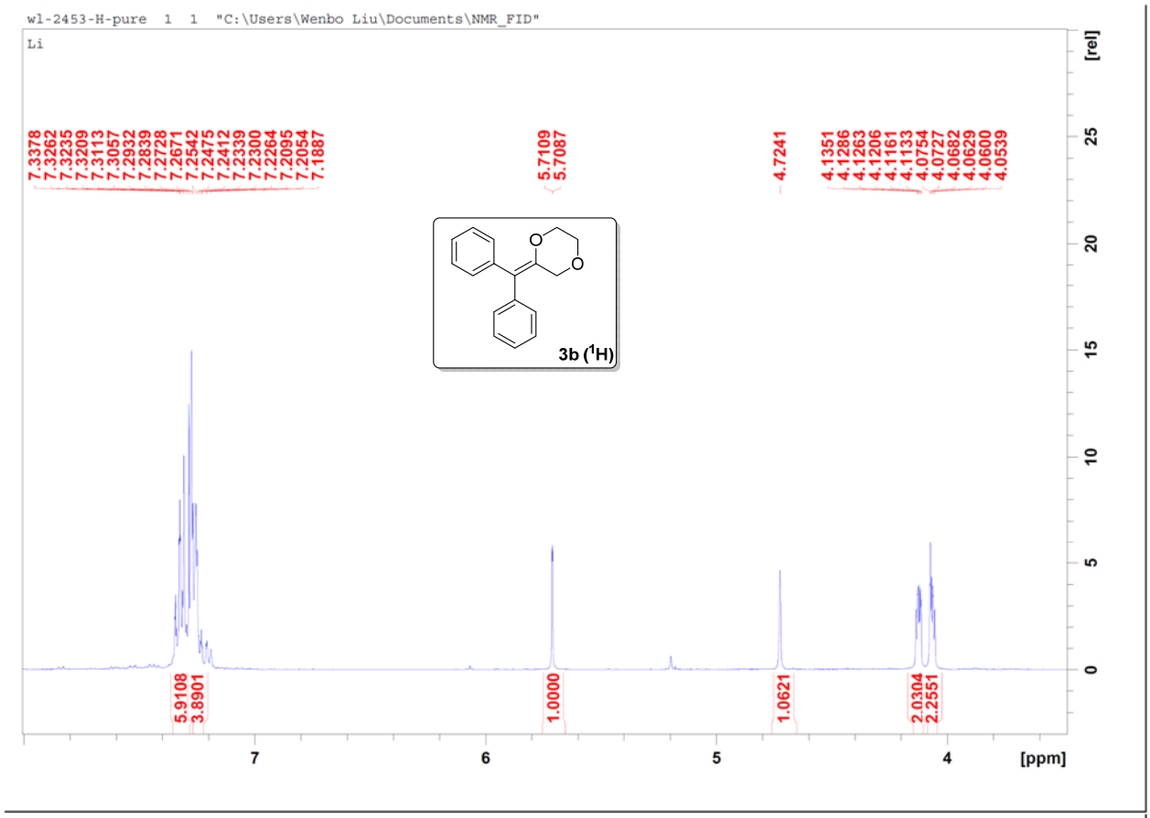

wl-2356-500M 2 1 "C:\Users\Wenbo Liu\Documents\NMR_FID"
Li
1d_C13 CDCl3 /home wenbo 5
157.0529
154.9038
153.9733
133.1006
129.0030
128.6802
126.8711
122.1336
119.4761
116.6609
111.7679
96.6115
68.3744
31.3670
28.7474
21.8381
19.2949
13.8905
13.8713
2v (^{13}C)
[rel]
[ppm]

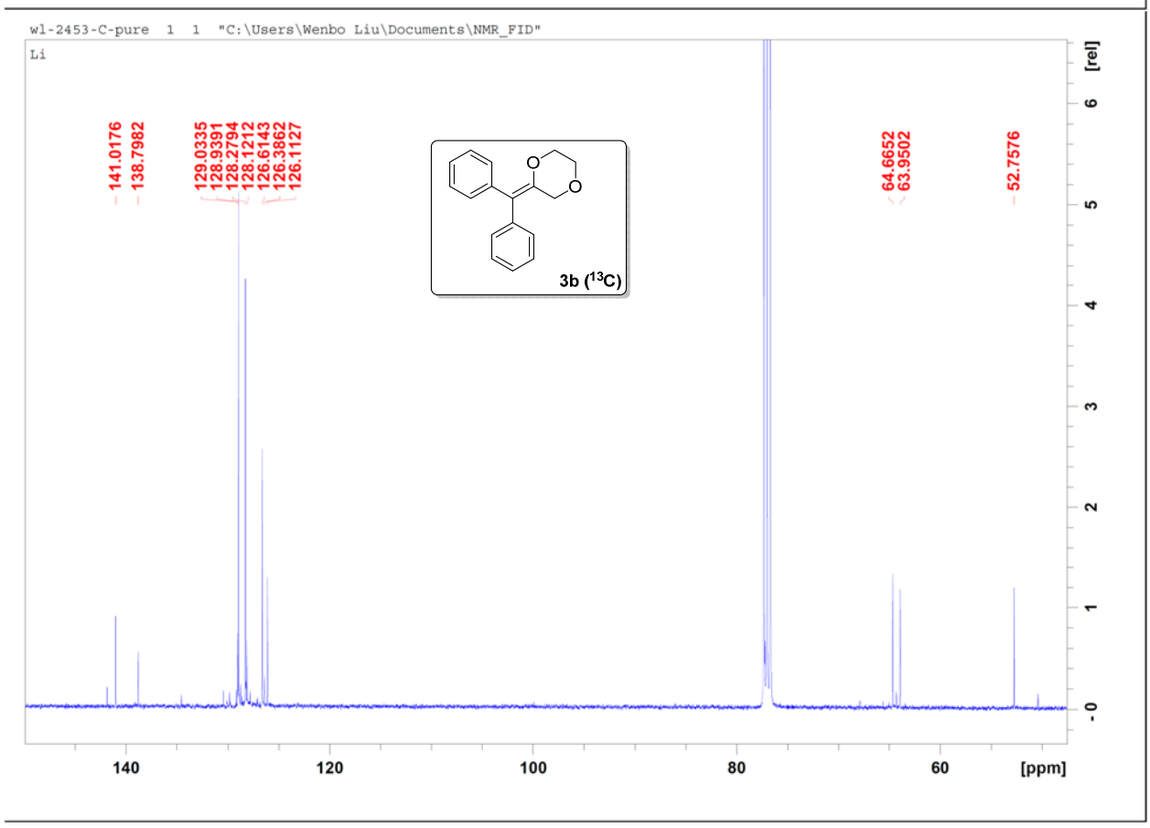

wl-2358-3 1 1 "C:\Users\Wenbo Liu\Documents\NMR_FID"
Li
7.4498
7.4418
7.4383
7.4319
7.4075
7.4014
7.3984
7.3952
7.3883
7.3849
7.2436
7.2309
7.2264
7.2175
7.2093
7.2077
7.2052
2.7478
2.7296
2.7113
2.1894
1.7941
1.7757
1.7573
1.7390
1.0084
0.9899
0.9715
0.9690
2.1140
2.0598
2.9697
2.0505
3.1538
2w (1H)
[rel]
[ppm]

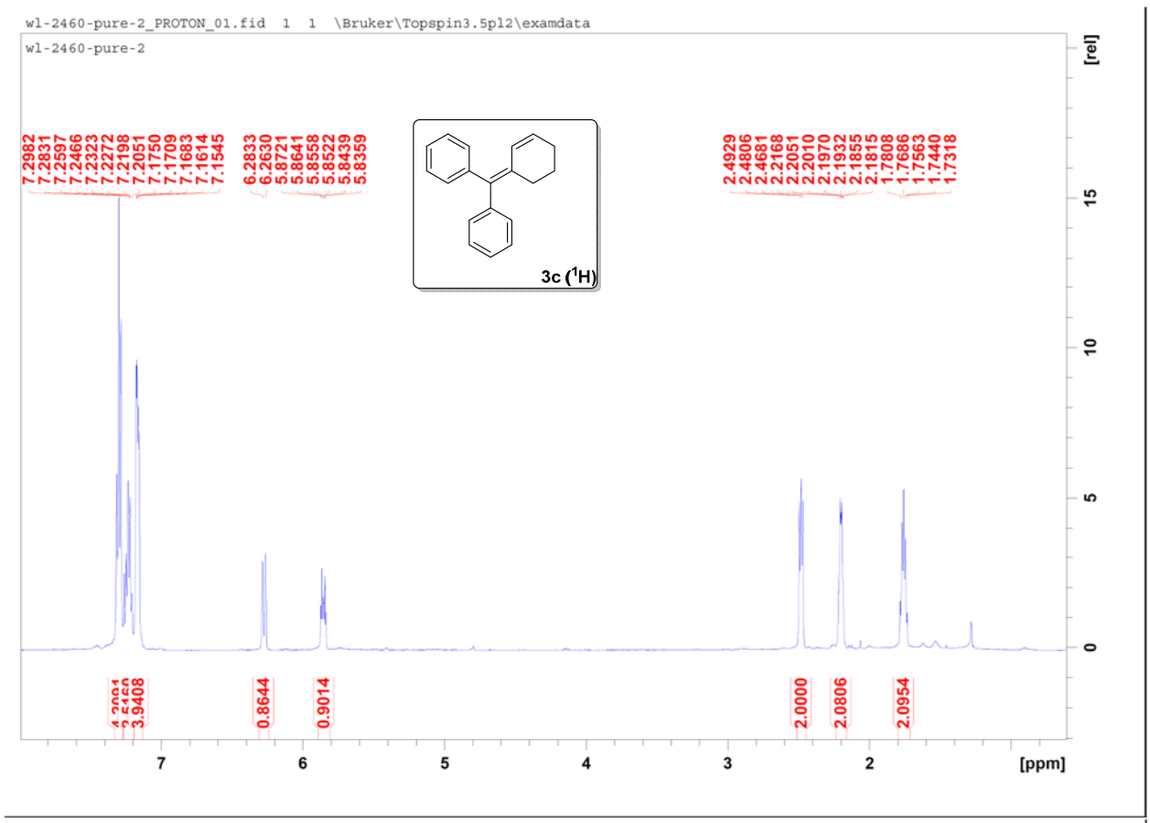

wl-2358-C 1 1 "C:\Users\Wenbo Liu\Documents\NMR_FID"
Li
154.3047
153.8282
130.4662
122.9693
121.8724
118.5919
110.4890
109.6506
28.2212
21.6047
13.7197
7.8911
2w (13C)
[rel]
[ppm]

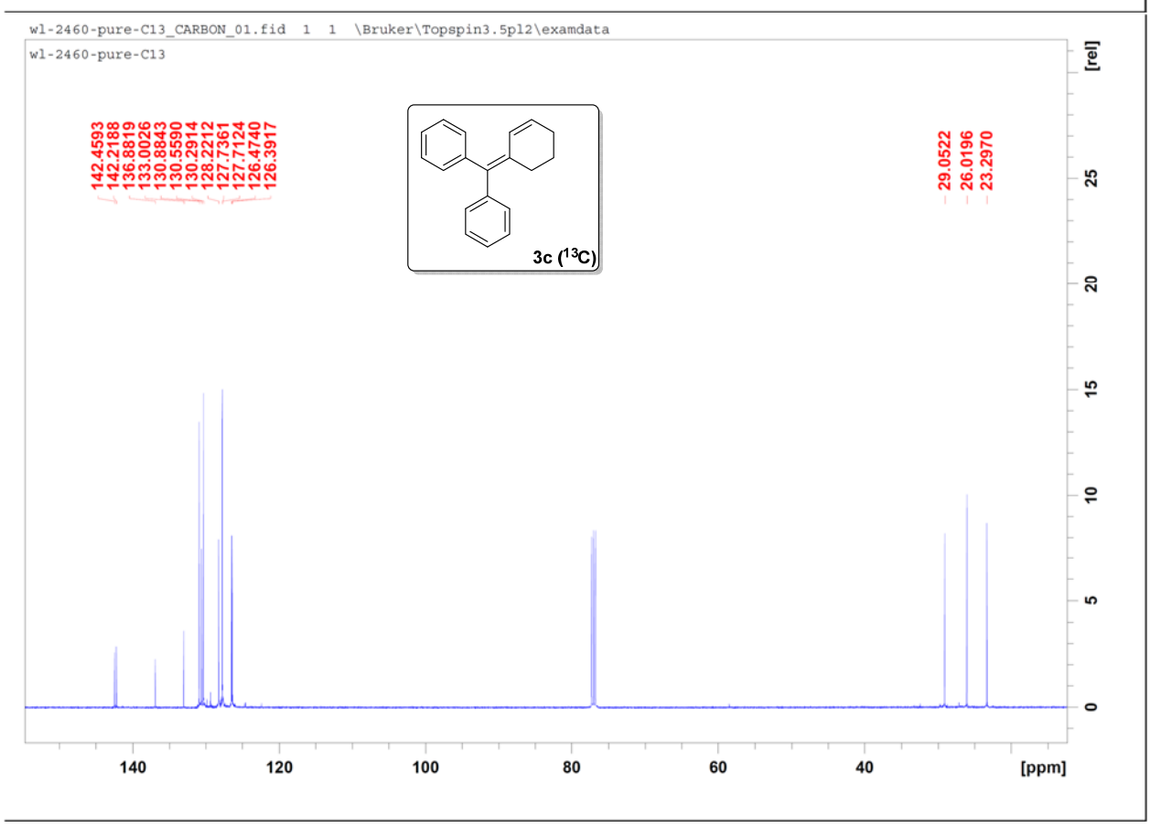

wl-2450-pure 1 1 "C:\Users\Wenbo Liu\Documents\NMR_FID"
Li
7.4183
7.4050
7.4025
7.3634
7.3594
7.3456
7.3301
7.3268
7.2971
7.2923
7.2841
7.2783
7.2730
7.2693
7.2623
7.2584
7.2542
7.2487
7.2377
7.2341
7.2289
7.2170
7.1621
7.1593
7.1562
7.1451
7.1410
7.1313
7.1260
7.1226
7.1196
4.3175
4.3007
4.2839
2.6677
2.6489
2.6302
2.0820
2.0647
2.0465
2.0291
2.0109
3a (1H)
2.0000
1.9426
2.0735
[rel]
[ppm]


wl-2450-pure-C 1 1 "C:\Users\Wenbo Liu\Documents\NMR_FID"
Li
155.2807
142.1008
139.9875
130.5037
128.9906
128.2193
127.7664
126.0195
125.2891
110.6144
71.3694
30.2121
24.9213
3a (13C)
[rel]
[ppm]


wl-2453-H-pure 1 1 "C:\Users\Wenbo Liu\Documents\NMR_FID"
Li
7.3378
7.3262
7.3235
7.3209
7.3113
7.3057
7.2932
7.2839
7.2728
7.2671
7.2542
7.2475
7.2412
7.2339
7.2300
7.2264
7.2095
7.2054
7.1887
5.7109
5.7087
4.7241
4.1351
4.1286
4.1263
4.1206
4.1161
4.1133
4.0754
4.0727
4.0682
4.0629
4.0600
4.0539
3b (1H)
5.9108
3.8901
1.0000
1.0621
2.0304
2.2551
[rel]
[ppm]


wl-2453-C-pure 1 1 "C:\Users\Wenbo Liu\Documents\NMR_FID"
Li
141.0176
138.7982
129.0335
128.9391
128.2794
128.1212
126.6143
126.3862
126.1127
64.6652
63.9502
52.7576
3b (13C)
[rel]
[ppm]


wl-2460-pure-2_PROTON_01.fid 1 1 \Bruker\Topspin3.5pl2\examdata
wl-2460-pure-2
7.2982
7.2831
7.2597
7.2466
7.2323
7.2272
7.2198
7.2051
7.1750
7.1709
7.1683
7.1614
7.1545
6.2833
6.2630
5.8721
5.8641
5.8558
5.8522
5.8439
5.8359
2.4929
2.4806
2.4681
2.2168
2.2051
2.2010
2.1970
2.1932
2.1855
2.1815
1.7808
1.7686
1.7563
1.7440
1.7318
3c (1H)
3.9408
0.8644
0.9014
2.0000
2.0806
2.0954
[rel]
[ppm]


wl-2460-pure-C13_CARBON_01.fid 1 1 \Bruker\Topspin3.5pl2\examdata
wl-2460-pure-C13
142.4593
142.2188
136.8819
133.0026
130.8843
130.5590
130.2914
128.2212
127.7361
127.7124
126.4740
126.3917
29.0522
26.0196
23.2970
3c (13C)
[rel]
[ppm]