Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Material (ESI) for Chemical Communications

*Supporting Information*

# Methanol as Hydrogen Source: Transfer Hydrogenation of Aromatic Aldehydes with a Rhodacycle

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## 1. General information

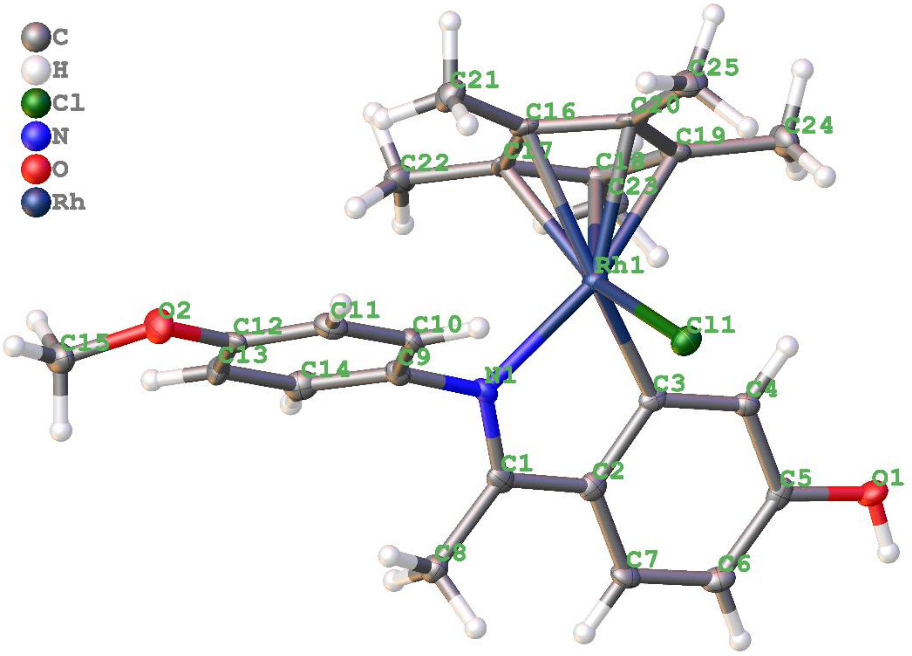
Unless otherwise specified, all reactions were carried out under an open atmosphere using standard techniques, all chemicals were purchased commercially and used as received without further purification, and methanol was HPLC grade. All columns were run using a mixture of hexane/ethyl acetate and silica gel 60 Å (230-400 mesh). $^1$H and $^{13}$C NMR spectra were recorded on a Bruker 400 MHz spectrometer using $CDCl_3$ with TMS as the internal standard at 289 K, unless stated otherwise.

## 2. Crystal structure determination of complex 2

Single-crystal X-ray diffraction data for **2** were collected on a suitable sample mounted on a Rigaku AFC-12K goniometer using a Rigaku Saturn 724+ are detector and 007HF Molybdenum rotating anode source. Samples were mounted under inert oil using a 10 um MiTeGen tip at 100 K. Data were integrated using SAINT[1] and scaled using SADABS.[2] Structural solution was by direct methods using SHELXT[3] implemented in Olex2[4] and refined on $F_o^2$ by full-matrix least squares refinement via SHELXL-2013.[5] CCDC 1851386 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

## 3. Crystal data and structure refinement for complex 2

$C_{25}H_{29}ClNO_2Rh$ ($M$ =513.85 g/mol): monoclinic, space group $P2_1/n$ (no. 14), $a$ = 8.6375(3) Å, $b$ = 13.8673(4) Å, $c$ = 18.4717(6) Å, $\beta$ = 103.076(3)°, $V$ = 2155.15(12) Å$^3$, $Z$ = 4, $T$ = 100 K, $\mu$(MoK$\alpha$) = 0.939 mm$^{-1}$, *Dcalc* = 1.584 g/cm$^3$, 34723 reflections measured ($3.7° \leq 2\Theta \leq 52.74°$), 4406 unique ($R_{int}$ = 0.1371, $R_{sigma}$ = 0.0711) which were used in all calculations. The final $R_1$ was 0.0477 (>2sigma(I)) and $wR_2$ was 0.0868 (all data).



**SI Figure 1.** X-ray crystallographic structure of complex **2**

**SI Table 1. Crystal data and structure refinement for complex 2**

| | |
|---|---|
| Identification code | **2** |
| Empirical formula | $C_{25}H_{29}ClNO_2Rh$ |
| Formula weight | 513.85 |
| Temperature/K | 100 |
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| a/Å | 8.6375(3) |
| b/Å | 13.8673(4) |
| c/Å | 18.4717(6) |
| α/° | 90.00 |
| β/° | 103.076(3) |
| γ/° | 90.00 |
| Volume/Å$^3$ | 2155.15(12) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.584 |
| μ/mm$^{-1}$ | 0.939 |
| F(000) | 1056.0 |
| Crystal size/mm$^3$ | 0.03 × 0.02 × 0.005 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 3.7 to 52.74 |
| Index ranges | $-10 \leq h \leq 10$, $-17 \leq k \leq 17$, $-22 \leq l \leq 23$ |
| Reflections collected | 34723 |
| Independent reflections | 4406 [$R_{int}$ = 0.1371, $R_{sigma}$ = 0.0711] |
| Data/restraints/parameters | 4406/0/279 |
| Goodness-of-fit on F$^2$ | 1.063 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0477, $wR_2$ = 0.0794 |
| Final R indexes [all data] | $R_1$ = 0.0673, $wR_2$ = 0.0868 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.59/-0.62 |

## 4. General procedure for the preparation of imine ligands

Imine ligands were prepared according to the literature.[6] In a 250 mL round bottomed flask, ketone (5.0 mmol), amine (5.5 mmol) and $NaHCO_3$ (420 mg, 5 mmol) were dissolved in toluene (80 mL). 4Å molecular sieves (1.2 g) were introduced. The resulting mixture was fitted with a Dean-Stark condenser and heated to reflux for 24 h. Hot filtration, to remove solid residues, followed by removal of solvent *in vacuo,* gave the crude products which were crystallised using hexane/DCM.

## 5. General procedure for the preparation of rhodium complexes

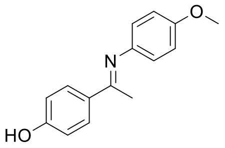
A Radleys tube was charged with $[Cp^*RhCl_2]_2$ dimer (100 mg, 0.16 mmol) ($Cp^* = C_5Me_5$), imine ligand (2.2 eqv.) and NaOAc (10 eqv.). DCM (10 mL) was then added under a nitrogen atmosphere and the reaction stirred overnight at room temperature. The resulting mixture was then filtered through Celite® to remove insoluble materials, dried over $MgSO_4$, and filtered, and the solvent removed *in vacuo.* The crude solid product was then washed with diethyl ether/hexane to afford an orange air and moisture stable pure compound.[6,7]

## 6. Aldehyde reduction procedure

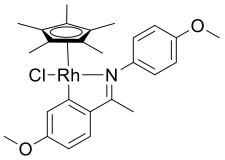
Aldehyde (0.25 mmol), catalyst (0.0025 mmol) and $Cs_2CO_3$ (0.5 eqv.) were placed in a Radleys tube followed by the addition of MeOH (1.5 mL). The reaction mixture was then heated to reflux at 90 °C for 1 hour. After completion, the resulting mixture was cooled to room temperature, washed with $H_2O$, extracted with ethyl acetate, dried over $MgSO_4$, and filtered, and the solvent removed *in vacuo.* The crude product was purified by flash chromatography (hexane:ethyl acetate).

## 7. Analytical data of rhodium complexes and alcohol products

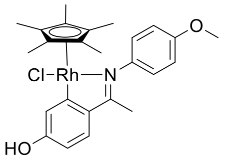
### 7.1 Data of ligands and complexes



**4-Methoxy-N-(1-(4-hydroxyphenyl)ethylidene)aniline:** White solid ; m.p. = 120-122 °C; $^{1}$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.83 (d, J = 8.8 Hz, 2H), 6.90 (d, J = 8.8 Hz, 2H), 6.81 (d, J = 8.8 Hz, 2H), 6.75 (d, J = 8.8 Hz, 2.4 Hz, 2H), 3.81 (s, 3H), 2.22 (s, 3H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 165.90, 158.15, 156.08, 144.68, 132.32, 129.15, 121.19, 115.32, 114.40, 55.64, 17.55; HRMS for $C_{15}H_{15}NO_2$ $[M + H]^+$: m/z calc.: 242.1176; Found: 242.1173.

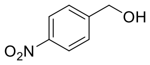


**Rhodium complex formed from 4-methoxy-N-(1-(4-methoxyphenyl)ethylidene)aniline (1):**[8] Orange solid; m.p. = 227-229 °C; $^{1}$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.41 (d, J = 8.5 Hz, 1H), 7.37 (d, J = 2.3 Hz, 1H), 6.93 (d, J = 8.8 Hz, 2H), 6.58 (dd, J = 8.5, 2.3 Hz, 1H), 3.91 (s, 3H), 3.85 (s, 3H), 2.27 (s, 3H), 1.39 (s, 15H). Due to the fluxionality, two of the aromatic hydrogens in **1** appeared very broad and featureless at rt (see ref 8 for explanation for a similar observation); A better resolved spectrum was obatined in $CD_2Cl_2$. $^{1}$H NMR ($CD_2Cl_2$, 400 MHz, 298 K) δ (ppm): 7.50-7.25 (a br peak overlapped with two doublets, 4H), 6.96 (d, J = 8.8 Hz, 2H), 6.60 (dd, J = 8.5, 2.3 Hz, 1H), 3.92 (s, 3H), 3.84 (s, 3H), 2.26 (s, 3H), 1.37 (s, 15H); $^{1}$H NMR ($CD_2Cl_2$, 400 MHz, 213 K) δ (ppm): 7.75 (d, J = 8.8 Hz, 1H), 7.41 (d, J = 8.5 Hz, 1H), 7.24 (d, J = 2.0 Hz, 1H), 6.96 (d, J = 8.8 Hz, 1H), 6.86-6.79 (m, 2H), 6.56 (dd, J = 8.5, 2.0 Hz, 1H), 3.85 (s, 3H), 3.79 (s, 3H), 2.22 (s, 3H), 1.28 (s, 15H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 160.98, 157.63, 143.74, 140.82, 129.13, 124.48, 120.82, 108.59, 96.25, 96.19, 55.67, 55.27, 17.17, 8.94. More concentrated sample run in $CD_2Cl_2$ to resolve quaternary C's and Rh-C coupling; $^{13}$C NMR ($CD_2Cl_2$, 100 MHz, 298 K) δ (ppm): 186.86 (d, $J_{Rh-C}$ = 33 Hz)[9], 178.32, 161.42, 158.18, 144.13, 141.49, 129.31, 124.80, 121.24, 114.30, 108.72, 96.67, 96.61, 56.03, 55.67, 17.31, 9.08; HRMS for $C_{26}H_{31}ClRhNO_2$ $[M – Cl]^+$: m/z calc.: 492.1406; Found: 492.1410.

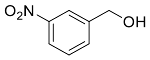


**Rhodium complex formed from 4-methoxy-N-(1-(4-hydroxyphenyl)ethylidene)aniline (2):**[8] Orange solid; m.p. = 225-229 °C; $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.26 (d, J = 8.3 Hz, 2H), 7.20 (d, J = 2.3 Hz, 1H), 6.94 (d, J = 8.3 Hz, 2H), 6.43 (dd, J = 8.3, 2.3 Hz, 1H), 3.85 (s, 3H), 2.24 (s, 3H), 1.38 (s, 15H). Due to the fluxionality, the aromatic region showed a similar feature to that observed in **1** at rt; $^1$H NMR ($CD_2Cl_2$, 400 MHz, 298 K) δ (ppm): 7.50-7.05 (br m, similar to those in **1**, 4H), 6.96 (d, J = 8.6 Hz, 1H), 6.43 (d, J = 8.2 Hz, 1H), 6.22 (br s, 1H), 3.84 (s, 3H), 2.24 (s, 3H), 1.36 (s, 15H); $^1$H NMR ($CD_2Cl_2$, 400 MHz, 213 K) δ (ppm): 7.73 (d, J = 8.6 Hz, 1H), 7.35 (br s, 1H), 7.14 (d, J = 8.2 Hz, 1H), 7.0 (s, 1H), 6.99 (d, J = 8.6 Hz, 1H), 6.86-6.80 (m, 2H), 6.2 (d, J = 8.2 Hz, 1H), 3.80 (s, 3H), 2.20 (s, 3H), 1.28 (s, 15H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 157.84, 157.62, 143.78, 140.57, 129.33, 122.91, 110.47, 100.15, 96.24, 96.18, 55.69, 17.18, 8.91. More concentrated sample run in $CD_2Cl_2$ to resolve quaternary C's and Rh-C coupling; $^{13}$C NMR ($CD_2Cl_2$, 100 MHz, 298 K) δ (ppm): 186.53 (d, $J_{Rh\text{-}C}$ = 33 Hz)[9], 178.59, 158.40, 158.15, 144.17, 141.03, 129.56, 124.86, 123.38, 114.35, 110.62, 100.58, 96.66, 96.60, 56.05, 17.31, 9.06; HRMS for $C_{25}H_{29}ClRhNO_2$ $[M - Cl]^+$: m/z calc.: 478.1248; Found: 478.1255.

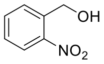
## 7.2 Data of alcohol products



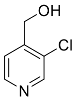
**4-Nitrophenylmethanol:**[10] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 8.22 (d, J = 8.6 Hz, 2H), 7.54 (d, J = 8.6 Hz, 2H), 4.84 (s, 2H), 1.83 (br s, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 148.22, 127.14, 123.90, 64.19; HRMS for $C_7H_7NO_3$ $[M + H]^+$: m/z calc.: 154.0499; found: 154.0503.



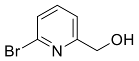
**3-Nitrophenylmethanol:**[11] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 8.23 (s, 1H), 8.14 (d, J = 8.0 Hz, 1H), 7.70 (d, J = 8.0 Hz, 1H), 7.53 (t, J = 8.0 Hz, 1H), 4.82 (s, 2H), 2.21 (br s, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 148.53, 143.00, 132.75, 129.58, 122.62, 121.63, 64.10; HRMS for $C_7H_7NO_3$ $[M + H]^+$: m/z calc.: 154.0499; found: 154.0505.



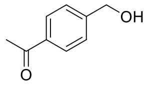
**2-Nitrophenylmethanol:**[12] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 8.11 (d, J = 8.2 Hz, 1H), 7.75 (d, J = 7.5 Hz, 1H), 7.67 (t, J = 7.5 Hz, 1H), 7.48 (t, J = 7.5 Hz, 1H), 4.98 (s, 2H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 147.83, 136.89, 134.30, 130.18, 128.68, 125.19, 62.75; HRMS for $C_7H_7NO_3$ $[(M - H_2O) + H]^+$: m/z calc.: 136.0393; found: 136.0396.



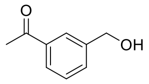
**3-Chloropyridin-4-methanol:**[13] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 8.51 (s, 1H), 8.50 (d, J = 5.6 Hz, 1H), 7.53 (d, J = 5.2 Hz, 1H), 4.83 (d, J = 5.6 Hz, 2H), 2.3 (t, J = 5.8 Hz, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 148.88, 148.22, 147.42, 129.76, 121.98, 61.36; HRMS for $C_6H_6ClNO$ $[M + H]^+$: m/z calc.: 144.0211; found: 144.021.



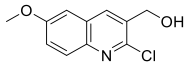
**6-Bromopyridin-2-methanol:**[14] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.55 (t, J = 7.6, 1H), 7.40 (d, J = 7.6 Hz, 1H), 7.29 (d, J = 7.6 Hz, 1H), 4.75 (s, 2H), 3.15 (br s, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 161.33, 141.54, 139.20, 126.81, 119.43, 64.34; HRMS for $C_6H_6BrNO$ $[M + H]^+$: m/z calc.: 187.9706; found: 187.9706.



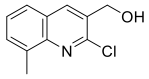
**4-Acetyl phenylmethanol:**[15] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.93 (d, J = 8.3 Hz, 2H), 7.44 (d, J = 8.3 Hz, 2H), 4.76 (s, 2H), 2.59 (s, 3H), 2.22 (br s, 1H) ; $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 198.14, 146.41, 136.40, 128.74, 126.73, 64.69, 26.78; HRMS for $C_9H_{10}O_2$ $[M + H]^+$: m/z calc.: 151.0754; found: 151.075.



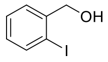
**3-Acetyl phenylmethanol:**[16] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.94 (s, 1H), 7.86 (d, J = 7.6 Hz, 1H), 7.57 (d, J = 7.6 Hz, 1H), 7.45 (t, J =7.6 Hz, 1H), 4.75 (s, 2H), 2.60 (s, 3H), 2.45 (br s, 1H) ; $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 198.50, 141.60, 137.37, 131.71, 128.90, 127.64, 126.71, 64.77, 26.82; HRMS for $C_9H_{10}O_2$ $[M + H]^+$: m/z calc.: 151.0754; found: 151.0751.



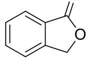
**2-Chloro-6-methoxyquinolin-3-methanol:**[17] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 8.18 (s, 1H), 7.91 (d, J = 9.2 Hz, 1H), 7.37 (dd, J = 9.2, 2.8 Hz, 1H), 7.09 (d, J = 2.8 Hz, 1H), 4.91 (d, J = 5.6 Hz, 2H), 3.93 (s, 3H), 2.23 (t, J = 5.9 Hz, 1H);$^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 158.42, 146.55, 143.05, 135.22, 132.60, 129.76, 128.64, 122.94, 105.34, 62.26, 55.76; HRMS for $C_{11}H_{10}ClNO$ $[M + H]^+$: m/z calc.: 224.0473; found: 224.0475.



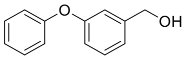
**2-Chloro-8-methylquinolin-3-methanol:**[18] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 8.24 (s,1H), 7.68 (d, J = 7.9 Hz, 1H), 7.56 (d, J = 7.2 Hz, 1H), 7.45 (t, J = 7.6 Hz, 1H), 4.93 (d, J = 6.0 Hz, 2H), 2.14 (t, J = 6.0 Hz, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 148.20, 146.41, 136.65, 136.61, 132.04, 130.47, 127.56, 127.08, 125.59, 62.34, 17.99; HRMS for $C_{11}H_{10}ClNO_2$ $[M + H]^+$: m/z calc.: 208.0524; found: 208.0524.



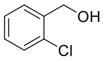
**2-Iodophenylmethanol:**[19] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.83 (d, J = 7.6 Hz, 1H), 7.46 (d, J = 7.6 Hz, 1H), 7.37 (t, J = 7.6 Hz, 1H), 7.01 (t, J = 7.6 Hz, 1H), 4.69 (d, J = 6.2 Hz, 2H), 1.99 (t, J = 6.2 Hz, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 142.75, 139.37, 129.48, 128.65, 128.64, 97.63, 69.50; HRMS for $C_7H_7IO$ $[(M – H_2O) + H]^+$: m/z calc.: 216.9509; found: 216.9514.



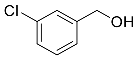
**Isobenzofuran-1(3H)-one:**[20] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.92 (d, J = 7.6 Hz, 1H), 7.69 (t, J = 7.6 Hz, 1H), 7.54 (t, J = 7.6 Hz, 1H), 7.50 (d, J = 7.6 Hz, 1H ), 5.34 (s, 2H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 171.25, 146.63, 134.14, 129.16, 125.90, 125.83, 122.22, 69.79; HRMS for $C_8H_6O_2$ $[M + H]^+$: m/z calc.: 135.0441; found: 135.0444.



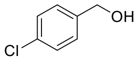
**3-Phenoxyphenylmethanol:**[21] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.36-7.26 (m, 3H), 7.13-7.04 (m, 2H), 7.00 (d, J = 7.5 Hz, 3H), 6.91 (d, J = 8.2 Hz, 1H), 4.62 (s, 2H), 2.04 (br s, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 157.72, 157.14, 143.06, 130.01, 129.91, 123.51, 121.65, 119.17, 118.04, 117.21, 65.07; HRMS for $C_{13}H_{12}O_2$ $[M + H]^+$: m/z calc.: 201.091; found: 201.0914.



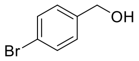
**2-Chlorophenylmethanol:**[12] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.49 (d, J = 7.2 Hz, 1H), 7.37 (d, J = 7.6 Hz, 1H), 7.28 (t, J = 7.2, Hz, 1H), 7.24 (t, J = 7.6 Hz, 1H), 4.79 (d, J = 6.3 Hz, 2H), 1.93 (t, J = 6.3 Hz, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 138.26, 132.84, 129.47, 128.97, 128.86, 127.15, 62.99; HRMS for $C_7H_7ClO$ $[(M - H_2O) + H]^+$: m/z calc.: 125.0153; found: 125.0155.



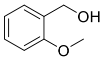
**3-Chlorophenylmethanol:**[22] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.36 (s, 1H), 7.32-7.20 (m, 3H), 4.67(s, 2H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 142.93, 134.55, 129.94, 127.83, 127.07, 124.96, 64.63; HRMS for $C_7H_7ClO$ $[(M - H_2O) + H]^+$: m/z calc.: 125.0153; found: 125.0154.



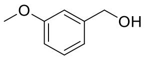
**4-Chlorophenylmethanol:**[10] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.36-7.28 (m, 4H), 4.67 (d, J = 5.2 Hz, 2H), 1.73 (br t, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 139.37, 133.50, 128.82, 128.41, 64.72; HRMS for $C_7H_7ClO$ $[(M - H_2O) + H]^+$: m/z calc.: 125.0153; found: 125.0155.



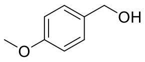
**4-Bromophenylmethanol:**[10] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.48 (d, J = 8.3 Hz, 1H), 7.23 (d, J = 8.3 Hz, 2H), 4.64 (s, 2H), 1.82 (br s, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 139.89, 131.76, 128.72, 121.59, 64.72; HRMS for $C_7H_7BrO$ $[(M - H_2O) + H]^+$: m/z calc.: 168.9647; found: 168.9646.



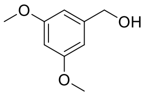
**2-Methoxyphenylmethanol:**[23] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.32-7.24 (m, 2H), 6.95 (t, J = 7.4 Hz, 1H), 6.89 (d, J = 8.2 Hz, 1H), 4.68 (s, 2H), 3.87 (s, 3H), 2.38 (br s, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 157.57, 129.12, 129.10, 128.89, 120.77, 110.31, 62.30, 55.38; HRMS for $C_8H_{10}O_2$ $[(M - H_2O) + H]^+$ : m/z calc.: 121.0648; found: 121.0651.



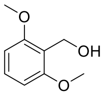
**3-Methoxyphenylmethanol:**[15] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.31-7.25 (m, 1H), 6.97-6.92 (m, 2H), 6.86-6.81 (m, 1H), 4.68 (s, 2H), 3.82 (s, 3H), 1.72 (br s, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 159.96, 142.64, 129.75, 119.23, 113.42, 112.36, 65.43, 55.37; HRMS for $C_8H_{10}O_2$ $[M + H]^+$: m/z calc.: 139.0754; found: 139.0756.



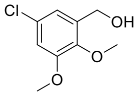
**4-Methoxyphenylmethanol:**[24] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.29 (d, J = 8.6 Hz, 2H), 6.89 (d, J = 8.6 Hz, 2H), 4.61 (s, 2H) 3.81 (s, 3H), 1.64 (br s, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 159.35, 133.25, 128.78, 114.10, 65.20, 55.44; HRMS for $C_8H_{10}O_2$ $[(M - H_2O) + H]^+$: m/z calc.: 121.0648; found: 121.0652.



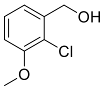
**3,5-Dimethoxyphenylmethanol:**[25] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 6.48 (d, J = 2.10 Hz, 2H), 6.35 (d, J = 2.10 Hz, 1H), 4.56 (s, 2H), 3.75 (s, 6H), 2.65 (br s, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 161.10, 143.50, 104.67, 99.76, 65.46, 55.48; HRMS for $C_9H_{12}O_3$ $[M + H]^+$: m/z calc.: 169.0859; found: 169.0863.



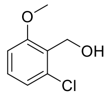
**2,6-Dimethoxyphenylmethanol:**[26] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.22 (t, J = 8.4 Hz, 1H), 6.56 (d, J = 8.4 Hz, 2H), 4.79 (d, J = 6.3 Hz, 2H), 3.84 (s, 6H), 2.49 (t, J = 6.3 Hz, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 158.53, 129.25, 117.16, 103.94, 55.86, 54.85; HRMS for $C_9H_{12}O_3$ $[(M - H_2O) + H]^+$: m/z calc.: 151.0754; found: 151.0754.



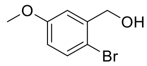
**5-Chloro-2,3-dimethoxyphenylmethanol:** $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 6.95 (s, 1H), 6.85 (s, 1H), 4.66 (s, 2H), 3.85 (br s, 6H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 153.08, 145.52, 135.74, 129.18, 120.29, 112.62, 61.09, 61.01, 56.15; HRMS for $C_9H_{11}ClO_3$ $[(M - H_2O) + H]^+$: m/z calc.: 185.0364; found: 185.0364.



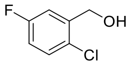
**2-Chloro-3-methoxyphenylmethanol:**[27] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.25 (t, J = 8.0 Hz, 1H), 7.10 (d, J = 8.0 Hz, 1H), 6.90 (d, J = 8.0 Hz, 1H), 4.79 (d, J = 6.2 Hz, 2H), 3.91(s, 3H), 2.02 (t, J = 6.2 Hz, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 155.18, 139.91, 127.52, 120.96, 120.54, 111.31, 63.19, 56.42; HRMS for $C_8H_9ClO_2$ $[(M - H_2O) + H]^+$: m/z calc.: 155.0258; found: 155.0263.



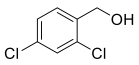
**2-Chloro-6-methoxyphenylmethanol:** $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.23 (d, J = 7.6 Hz, 1H), 7.13 (t, J = 7.6 Hz, 1H), 7.09 (d, J = 7.6 Hz, 1H), 4.83 (s, 2H), 2.46 (s, 3H), 1.93 (br s, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 139.75, 136.05, 134.97, 129.35, 129.17, 127.44, 59.77, 19.82; HRMS for $C_8H_9ClO_2$ [(M – Cl) + H]$^+$ : m/z calc.: 139.0309; found: 139.0309.



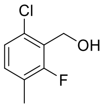
**2-Bromo-5-methoxyphenylmethanol:**[28] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.40 (d, J = 8.7 Hz, 1H), 7.05 (d, J = 3.1 Hz, 1H), 6.71 (dd, J = 8.7, 3.1 Hz, 1H), 4.69 (s, 2H), 3.79 (s, 3H), 2.25 (br s, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 159.37, 140.85, 133.26, 114.89, 114.35, 112.62, 65.13, 55.64; HRMS for $C_8H_9BrO_2$ [(M – $H_2O$) + H]$^+$: m/z calc.: 198.9753; found; 198.976.



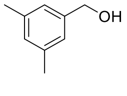
**2-Chloro-5-fluorophenylmethanol:** $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.30 (dd, J = 8.7, 5.0 Hz, 1H), 7.26 (dd, J = 8.7, 3.1 Hz, 1H), 6.94 (td, J = 8.7, 3.1 Hz, 1H), 4.76 (d, J = 4.2 Hz, 2H), 2.08 (br t, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 161.77 (d, $J_{C-F}$ = 246.4 Hz), 140.54 (d, $J_{C-F}$ = 7.3 Hz), 130.57 (d, $J_{C-F}$ = 8.2 Hz), 126.98 (d, $J_{C-F}$ = 3.2 Hz), 115.58 (d, $J_{C-F}$ = 18.6 Hz), 115.34 (d, $J_{C-F}$ = 19.6 Hz), 62.42 (d, $J_{C-F}$ = 1.2 Hz); HRMS for $C_7H_6ClFO$ [(M – $H_2O$) + H]$^+$: m/z calc.: 143.0058; found: 143.0063.



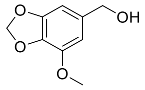
**2,4-Dichlorophenylmethanol:**[29] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.44 (d, J = 8.2 Hz, 1H), 7.38 (s, 1H), 7.27 (d, J = 8.2 Hz, 1H), 4.75 (s, 2H), 1.99 (br s, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 136.89, 133.97, 133.32, 129.56, 129.27, 127.42, 62.35; HRMS for $C_7H_6Cl_2O$ [(M – $H_2O$) + H]$^+$: m/z calc.: 158.9763; found: 158.977.



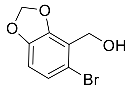
**6-Chloro-2-fluoro-3-methylphenyl-methanol:** $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.11-7.04 (m, 2H), 4.83 (d, J = 4.0 Hz, 2H), 2.25 (d, J = 2.2 Hz, 3H), 2.13 (br t, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 160.03 (d, $J_{C-F}$ = 248.5 Hz), 132.44 (d, $J_{C-F}$ = 5.3 Hz), 131.49 (d, $J_{C-F}$ = 6.5 Hz), 125.56 (d, $J_{C-F}$ = 18.9 Hz), 124.83 (d, $J_{C-F}$ = 4.0 Hz), 124.16 (d, $J_{C-F}$ = 18.9 Hz), 56.52 (d, $J_{C-F}$ = 5.3 Hz), 14.51 (d, $J_{C-F}$ = 4.0 Hz); HRMS for $C_8H_6ClFO$ [(M – $H_2O$) + H]$^+$: m/z calc.: 157.0215; found: 157.0218.



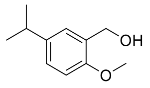
**3,5-Dimethylphenylmethanol:**[30] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 6.97 (s, 2H), 6.93 (s, 1H), 4.61 (s, 2H), 2.32 (s, 6H), 1.70 (br s, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 140.94, 138.31, 129.39, 124.97, 65.56, 21.38; HRMS for $C_9H_{12}O$ $[(M - H_2O) + H]^+$: m/z calc.: 119.0855; found: 119.0855.



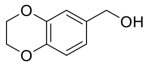
**7-Methoxybenzo[d][1,3]dioxol-5-methanol:**[31] $^1H$ NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 6.54 (s, 1H), 6.53 (s, 1H), 5.95 (s, 2H), 4.56 (s, 2H), 3.89 (s, 3H), 1.90 (br s, 1H); $^{13}C$ NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 149.03, 143.76, 135.69, 134.72, 106.56, 101.57, 101.43, 65.46, 56.66; HRMS for $C_9H_{10}O_4$ $[(M - H_2O) + H]^+$: m/z calc.: 165.0546; found: 165.0547.



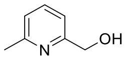
**5-Bromobenzo[d][1,3]dioxol-4-methanol:**[32] $^1H$ NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.02 (d, J = 8.3 Hz, 1H), 6.64 (d, J = 8.3 Hz, 1H), 6.00 (s, 2H), 4.74 (s, 2H), 2.26 (br s, 1H); $^{13}C$ NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 147.29, 147.25, 125.40, 121.78, 115.14, 109.30, 102.00, 59.64; HRMS for $C_8H_7BrO_3$ $[(M - H_2O) + H]^+$: m/z calc.: 212.9546; found: 202.9547.



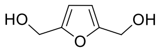
**5-Isopropyl-2-methoxyphenylmethanol:**[33] $^1H$ NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.12 (m, 2H), 6.81 (d, J = 8.0 Hz, 1H), 4.67 (d, J = 5.0 Hz, 2H), 3.84 (s, 3H), 2.86 (septet, J = 6.9 Hz, 1H), 2.38 (t, J = 5.0 Hz, 1H), 1.22 (d, J = 6.9 Hz, 6H); $^{13}C$ NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 155.72, 141.25, 128.86, 127.14, 126.59, 110.25, 62.60, 55.49, 33.46, 24.34; HRMS for $C_{11}H_{16}O_2$ $[(M - H_2O) + H]^+$: m/z calc.: 163.1117; found: 163.1123.



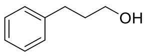
**2,3-Dihydrobenzo[b][1,4]dioxin-6-methanol:**[34] $^1H$ NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 6.89-6.78 (m, 3H), 4.53 (s, 2H), 4.23 (s, 4H), 2.02 (br s, 1H); $^{13}C$ NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 143.60, 143.19, 134.46, 120.39, 117.41, 116.32, 65.05, 64.47; HRMS for $C_9H_{10}O_3$ $[(M - H_2O) + H]^+$: m/z calc.: 149.0597; found: 149.0598.



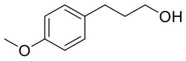
**(6-Methylpyridin-2-yl)methanol:**[35] $^1H$ NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.56 (t, J = 7.8 Hz, 1H), 7.15 (d, J = 7.8 Hz, 1H), 7.09 (d, J= 7.8 Hz, 1H), 4.72 (s, 2H), 3.77 (br s, 1H), 2.54 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 158.42, 157.49, 137.09, 121.90, 117.59, 64.10, 24.26; HRMS for $C_7H_9NO$ $[M - H]^+$: m/z calc.: 122.0684; found: 122.100.



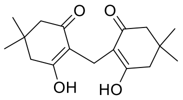
**Furan-2,5-diyldimethanol:**[36] $^1H$ NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 6.20 (s, 2H), 4.54 (s, 4H), 2.87 (br s, 2H). $^{13}C$ NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 154.13, 108.63, 57.39; HRMS for $C_6H_8O_3$ $[(M - H_2O) + H]^+$: m/z calc.: 111.0441; found: 111.0445.



**3-Phenylpropan-1-ol:**[37] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.32-7.16 (m, 5H), 3.67 (t, J = 6.3 Hz, 2H), 2.70 (t, J = 7.6 Hz, 2H), 1.94-1.84 (m, 2H), 1.47 (br s, 1H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 141.94, 128.54, 128.52, 125.98, 62.39, 34.34, 32.20; HRMS for $C_9H_{12}O$ $[(M - H_2O) + H]^+$: m/z calc.: 119.0855; found: 119.0859.



**3-(4-Methoxyphenyl)propan-1-ol:**[38] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 7.11 (d, J = 8.6 Hz, 2H), 6.83 (d, J = 8.6 Hz, 2H), 3.78 (s, 3H), 3.66 (t, J = 6.4 Hz, 2H), 2.65 (t, J = 7.5 Hz, 2H), 1.86 (pent, J = 6.4 Hz, 2H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 157.92, 133.97, 129.41, 113.95, 62.38, 55.39, 34.56, 31.27; HRMS for $C_{10}H_{14}O_2$ $[M + NH_4]^+$: m/z calc.: 184.1332; Found: 184.1339.



**2,2’-Methylenebis(3-hydroxy-5,5-dimethylcyclohex-2-en-1-one:**[39] $^1$H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm): 11.57 (br s, 2H), 3.16 (s, 2H), 2.29 (s, 4H), 2.28 (s, 4H), 1.05 (s, 12H); $^{13}$C NMR ($CDCl_3$, 100 MHz, 298 K) δ (ppm): 189.68, 113.63, 46.15, 31.94, 29.66, 27.24, 16.10.

## 8. References

1 SAINT v7.68A (Bruker, 2009).

2 SADABS-2008/4 (Bruker, 2010).

3 G. M. Sheldrick, *Acta. Cryst.*, 2015, **A71**, 3.

4 O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Cryst.*, 2009, **42**, 339.

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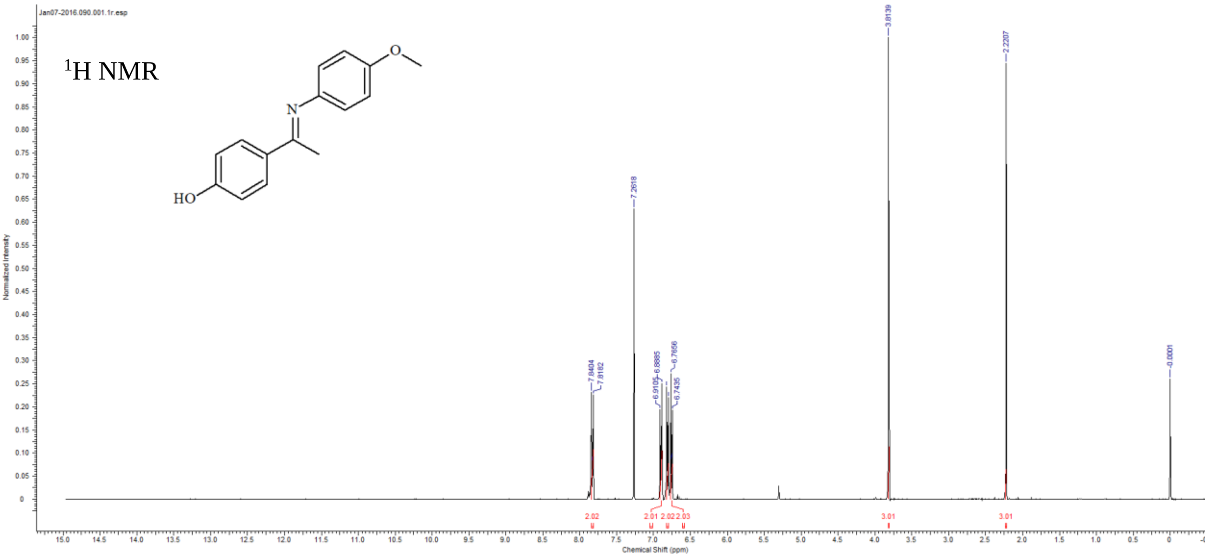
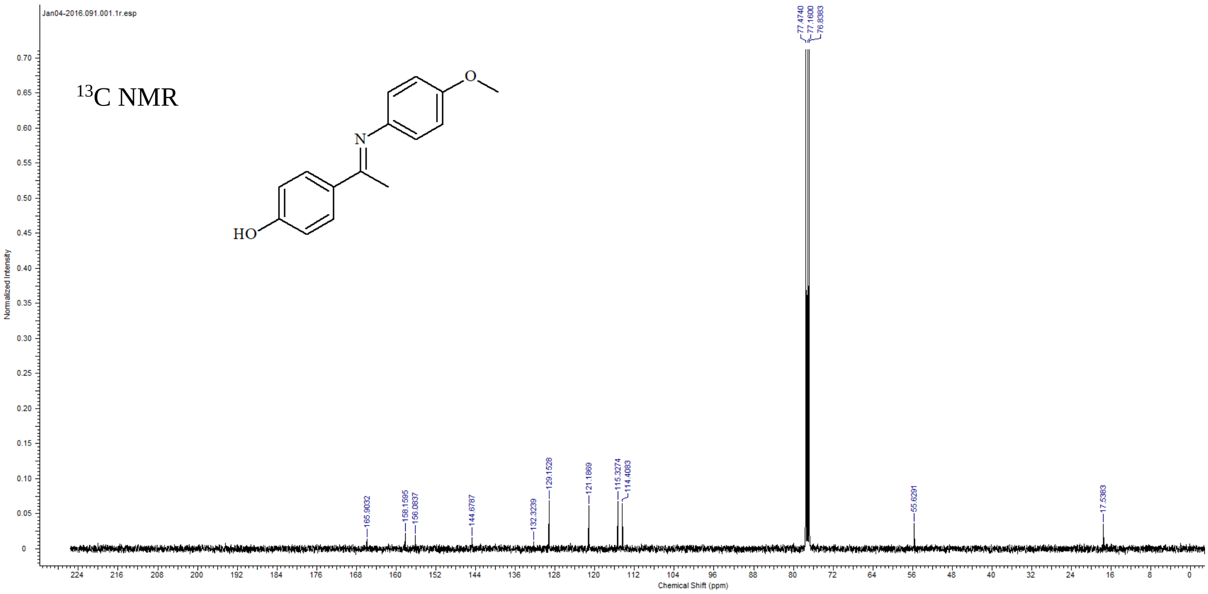
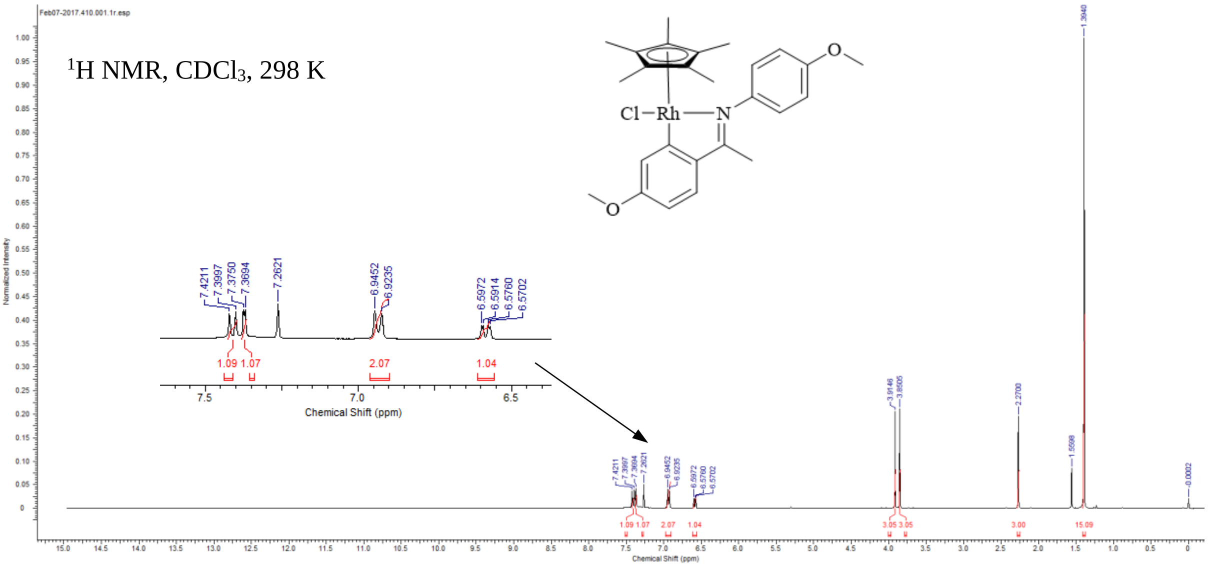
# 9. Copies of NMR Spectra



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Cl
Rh
N
O
O
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7.4211
7.3997
7.3750
7.3694
7.2621
6.9452
6.9235
6.5972
6.5914
6.5760
6.5702
1.09
1.07
2.07
1.04
Chemical Shift (ppm)
3.9146
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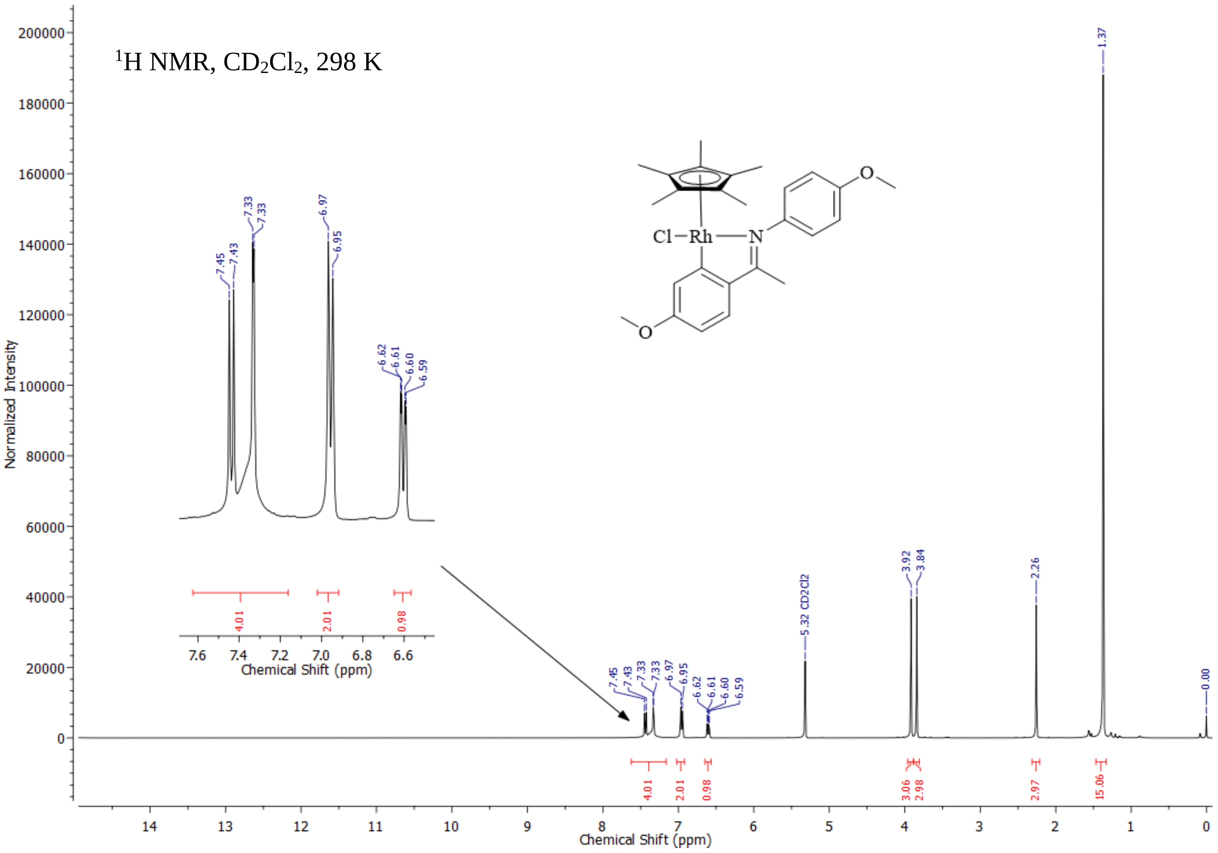
2.2700
1.5598
1.3940
0.0002
3.05
3.05
3.00
15.09
Chemical Shift (ppm)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Cl
Rh
N
O
O
Normalized Intensity
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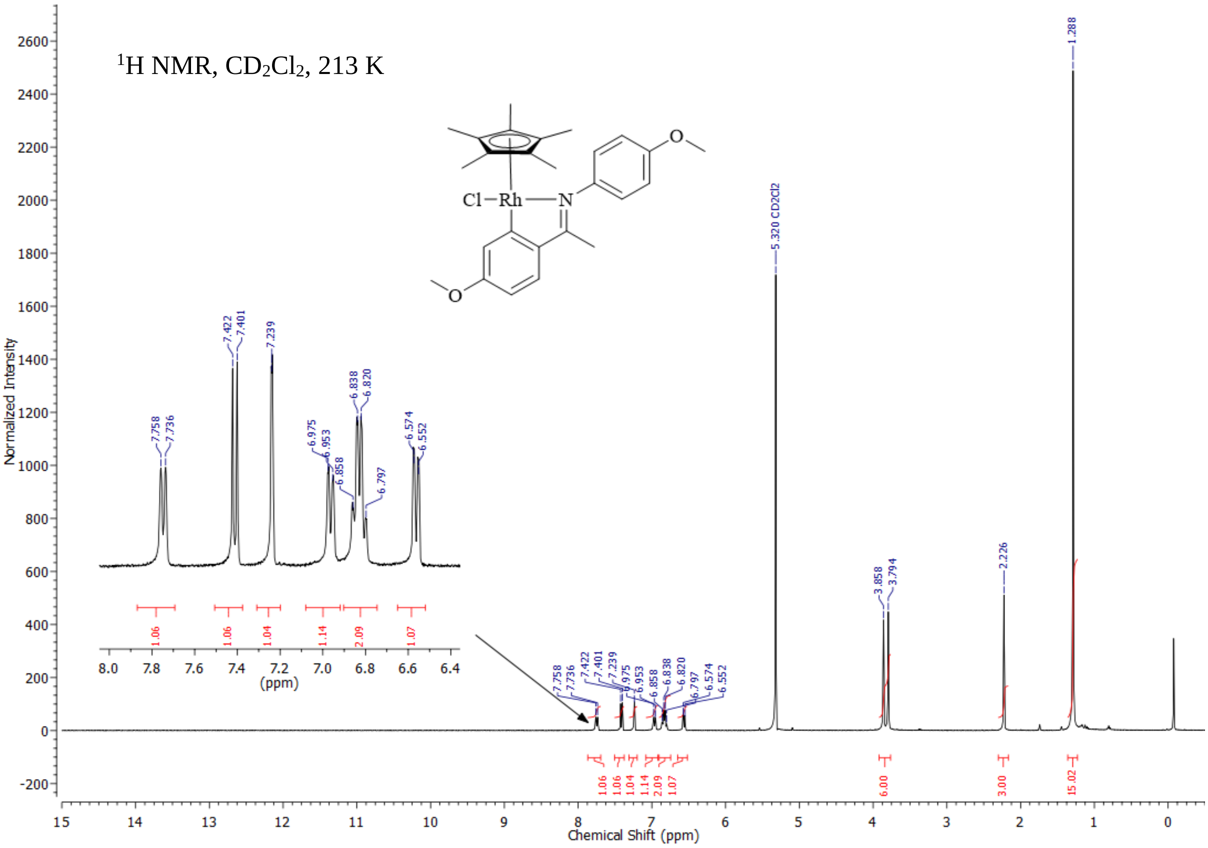
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
7.45
7.43
7.33
7.33
6.97
6.95
6.62
6.61
6.60
6.59
4.01
2.01
0.98
7.6
7.4
7.2
7.0
6.8
6.6
Chemical Shift (ppm)
5.32 CD2Cl2
3.92
3.84
2.26
1.37
0.00
3.06
2.98
2.97
15.06
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)



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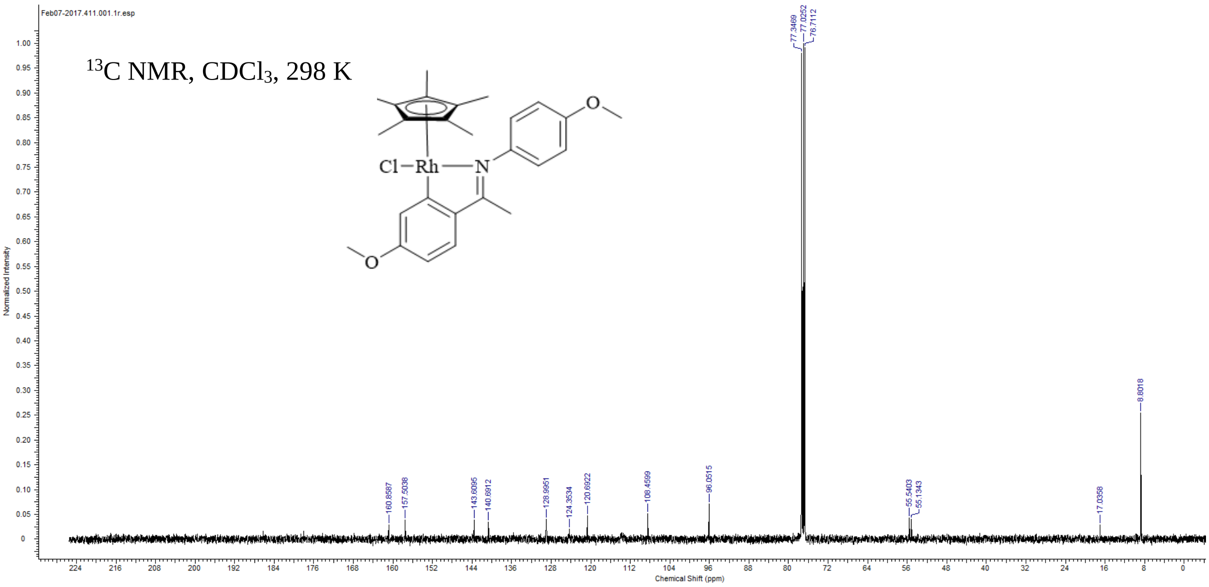

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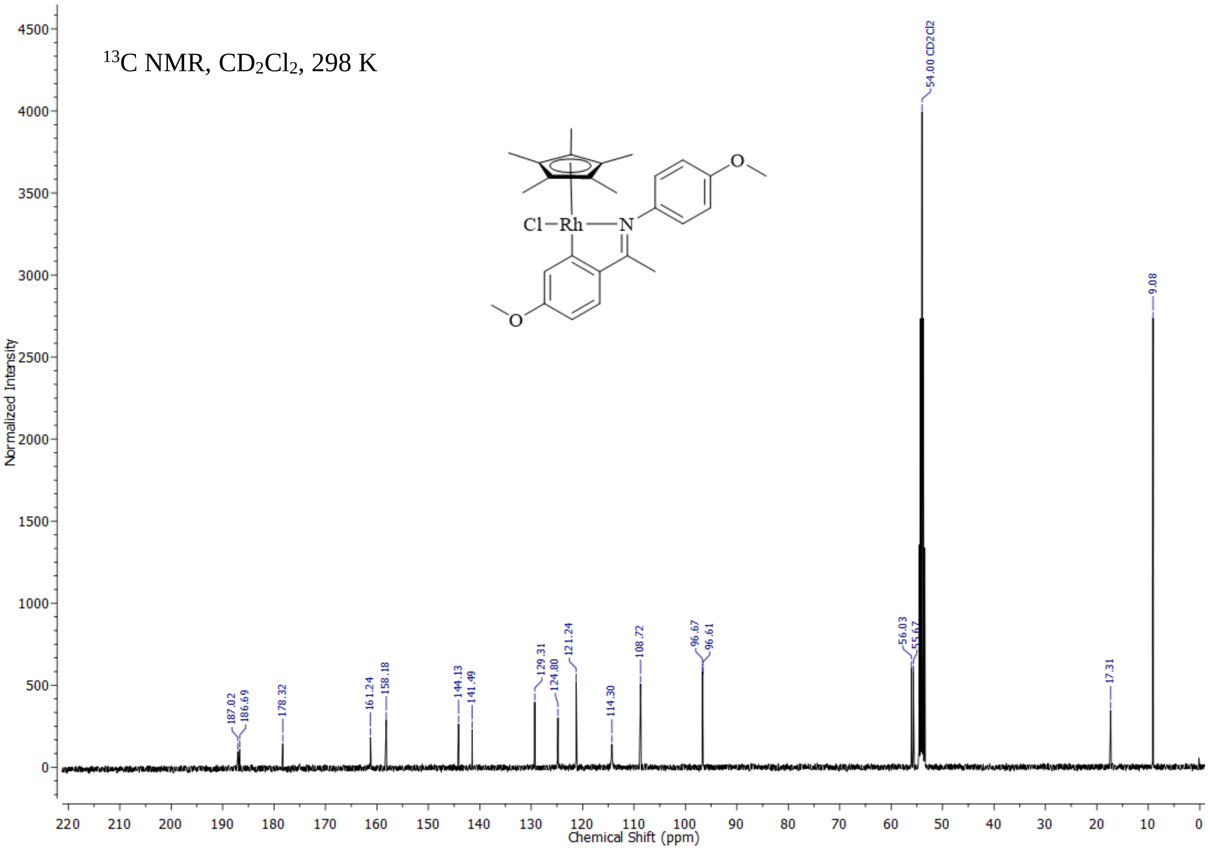
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Cl
Rh
N
O
O
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9.08
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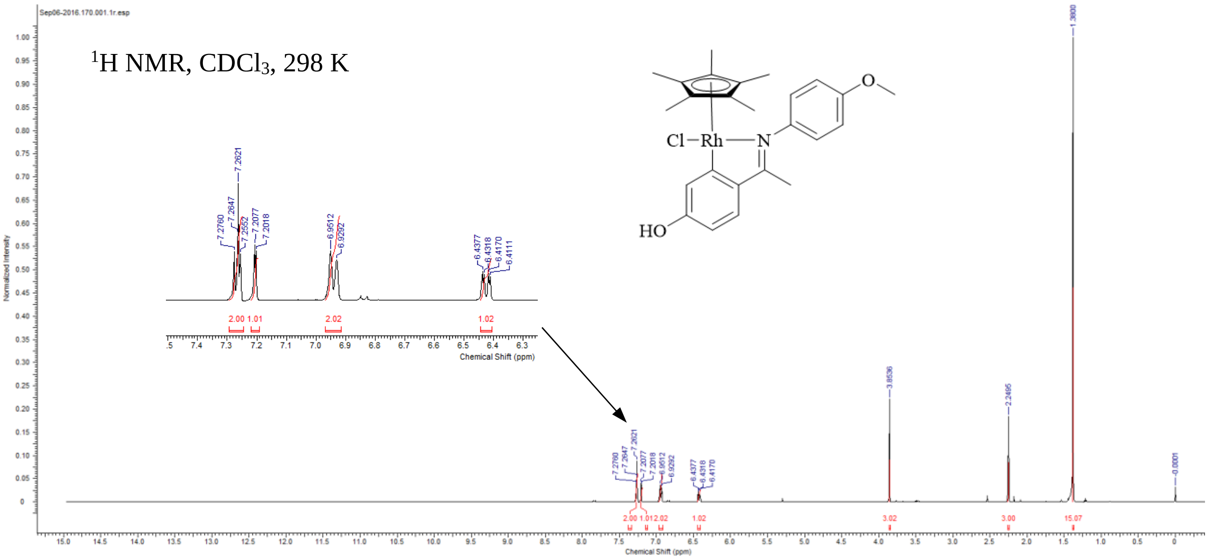
186.69
178.32
161.24
158.18
144.13
141.49
129.31
124.80
121.24
114.30
108.72
96.67
96.61
56.03
55.67
17.31
Normalized Intensity
Chemical Shift (ppm)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Rh
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O
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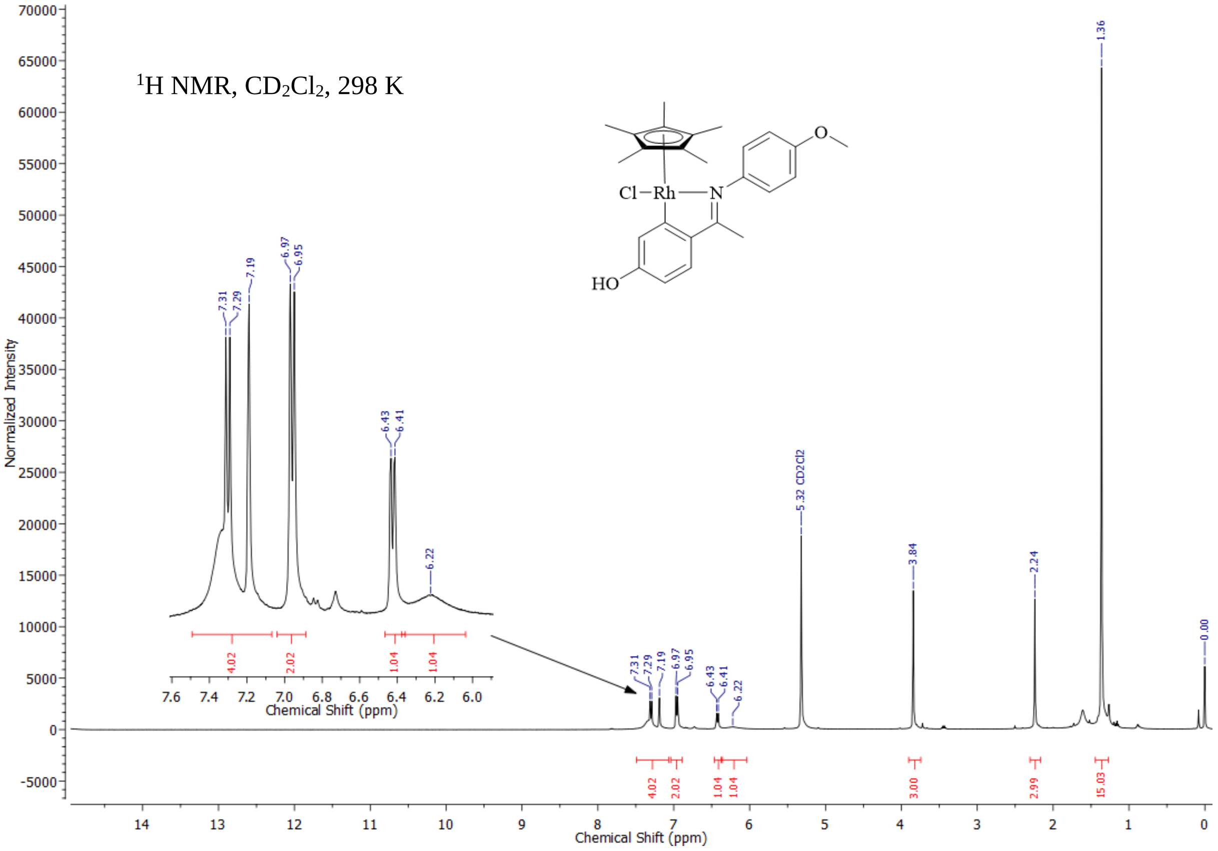
7.2552
7.2077
7.2018
6.9512
6.9292
6.4377
6.4318
6.4170
6.4111
2.00
1.01
2.02
1.02
3.8536
2.2495
1.3600
0.0001
3.02
3.00
15.07
Normalized Intensity
Chemical Shift (ppm)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Rh
N
O
HO
Normalized Intensity
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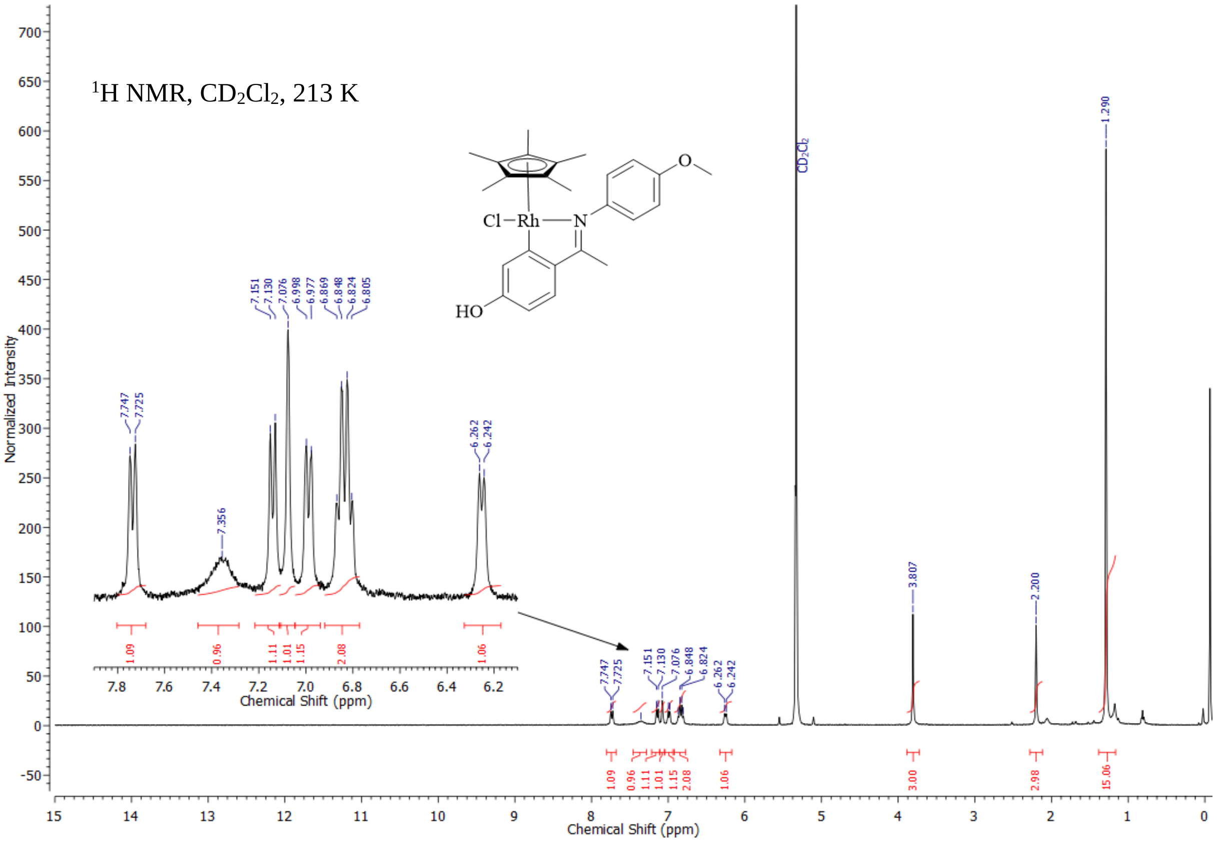
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
7.31
7.29
7.19
6.97
6.95
6.43
6.41
6.22
4.02
2.02
1.04
1.04
7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0
Chemical Shift (ppm)
5.32 CD2Cl2
3.84
2.24
1.36
0.00
3.00
2.99
15.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
Chemical Shift (ppm)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Rh
N
O
HO
Normalized Intensity
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
7.747
7.725
7.356
7.151
7.130
7.076
6.998
6.977
6.869
6.848
6.824
6.805
6.262
6.242
1.09
0.96
1.11
1.01
1.15
2.08
1.06
7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2
Chemical Shift (ppm)
CD2Cl2
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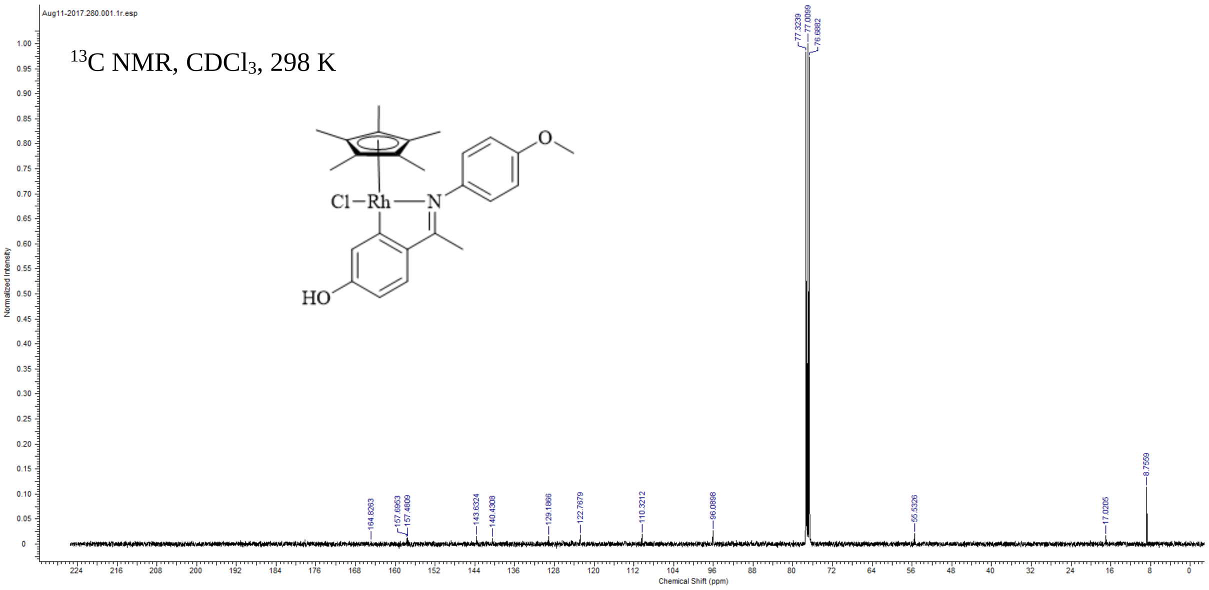
2.200
1.290
3.00
2.98
15.06
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
Chemical Shift (ppm)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Rh
N
O
HO
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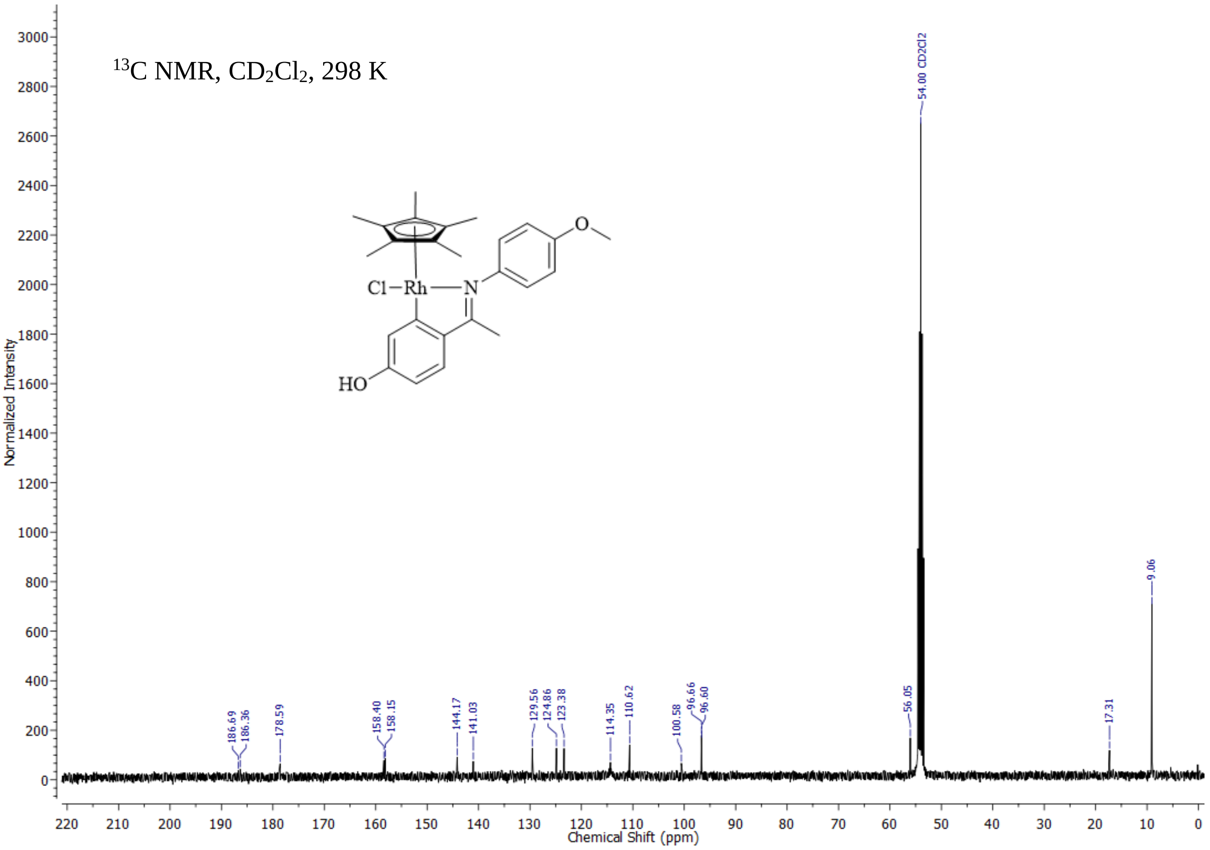
77.0099
76.6882
164.8263
157.6953
157.4809
143.6324
140.4308
129.1866
122.7679
110.3212
96.0898
55.5326
17.0205
8.7559
Normalized Intensity
Chemical Shift (ppm)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Rh
N
O
HO
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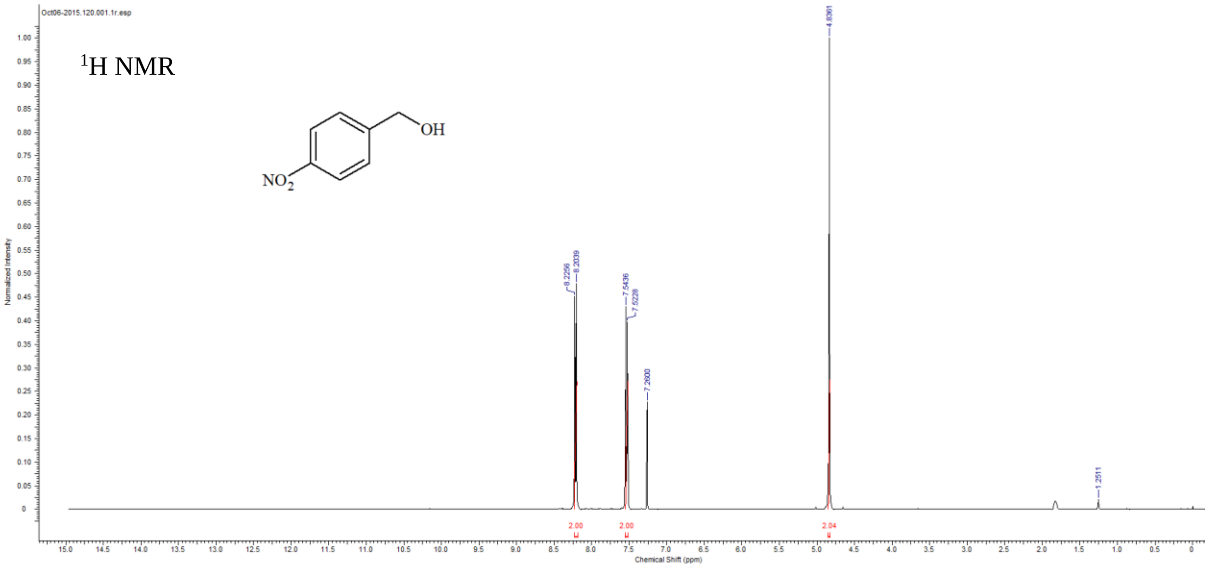
186.36
178.59
158.40
158.15
144.17
141.03
129.56
124.86
123.38
114.35
110.62
100.58
96.66
96.60
56.05
17.31
9.06
Normalized Intensity
Chemical Shift (ppm)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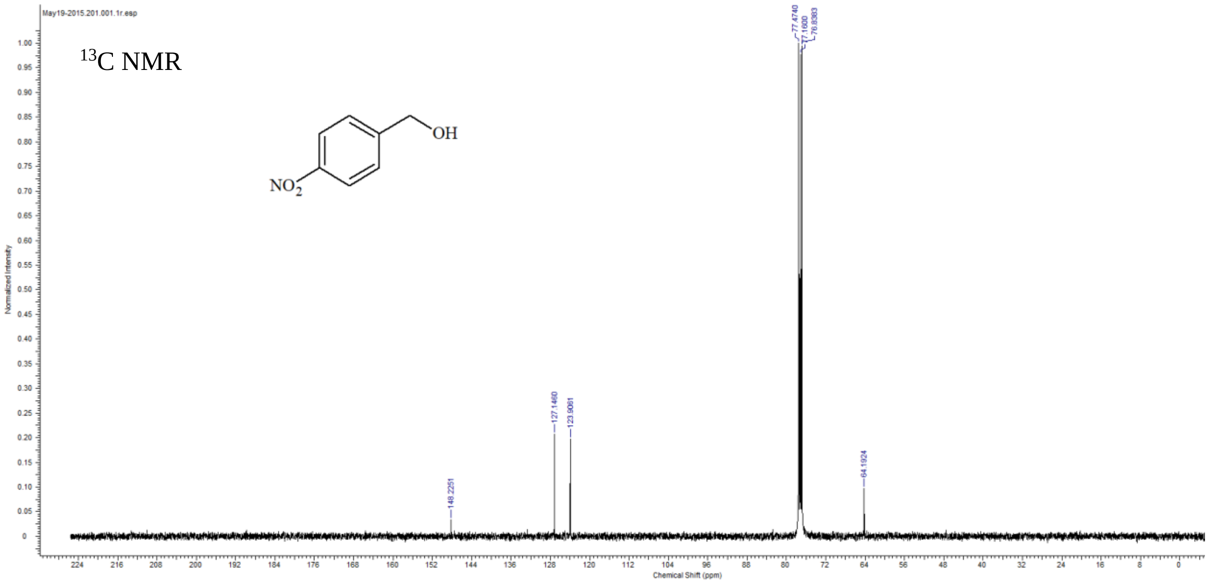
2.00
2.00
2.04
Normalized Intensity
Chemical Shift (ppm)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77.4740
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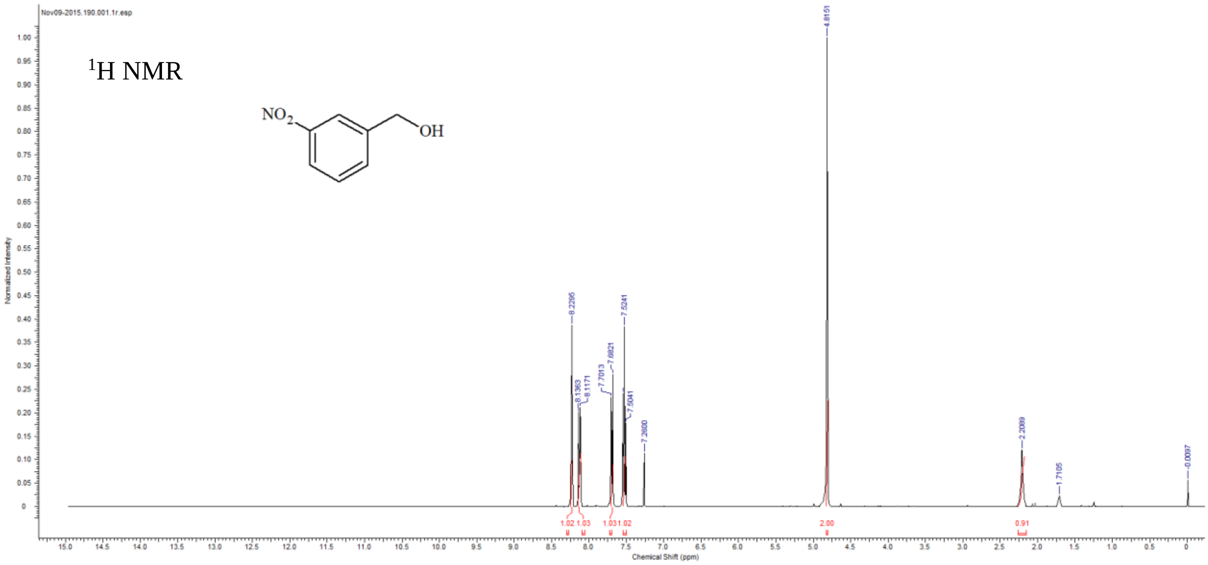
76.8383
64.1924
Normalized Intensity
Chemical Shift (ppm)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7.5241
7.5041
7.2600
4.8151
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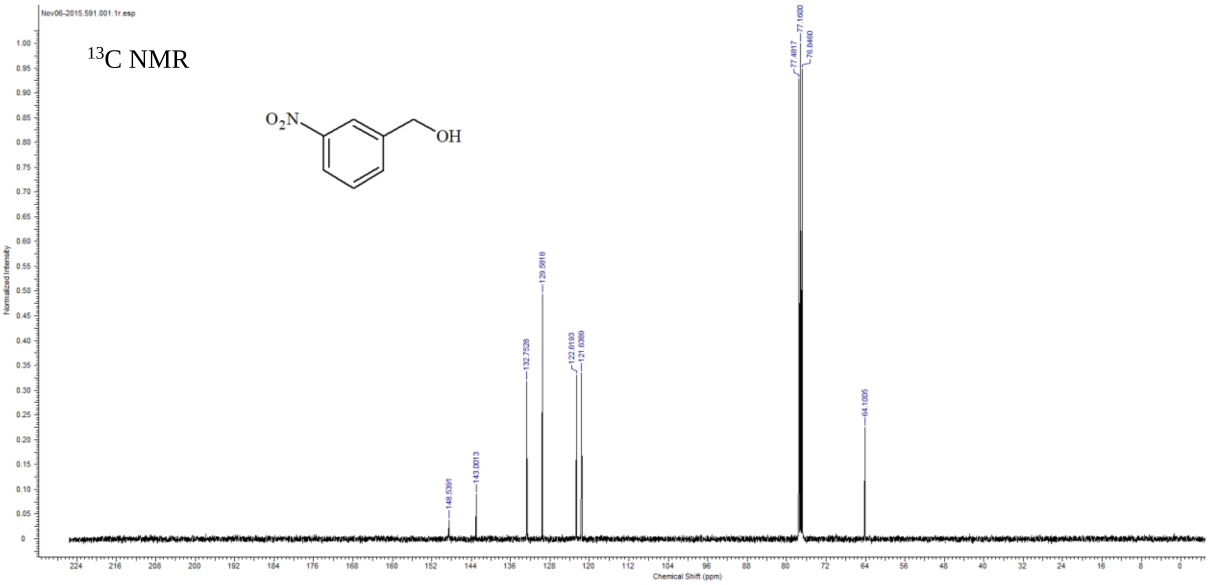
0.0097
1.02
1.03
1.03
1.02
2.00
0.91
Normalized Intensity
Chemical Shift (ppm)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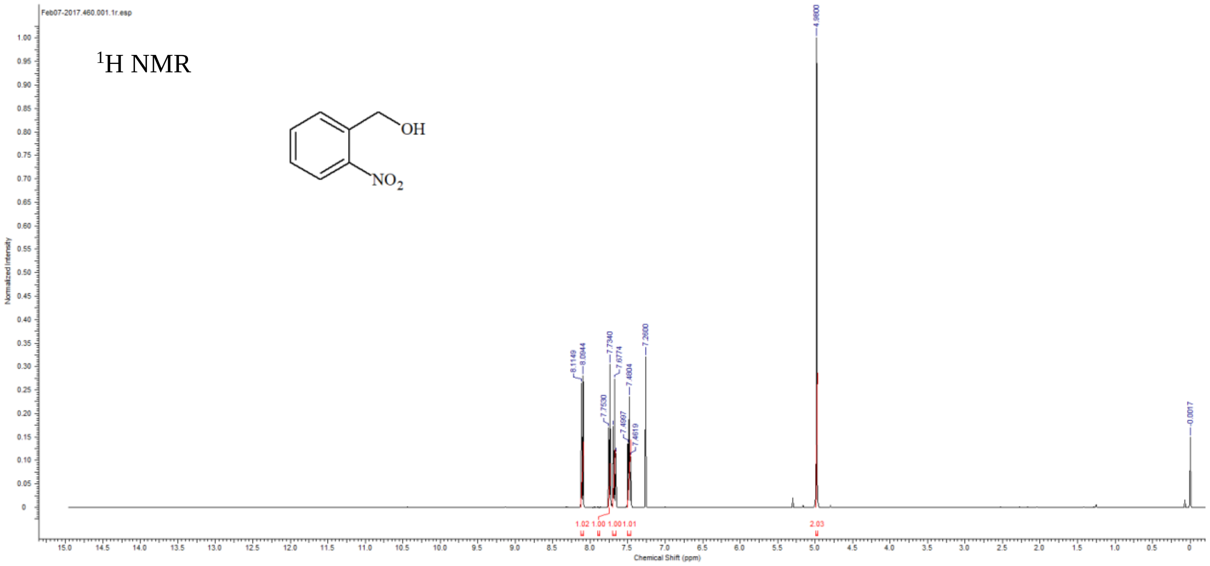
76.8460
64.1005
Normalized Intensity
Chemical Shift (ppm)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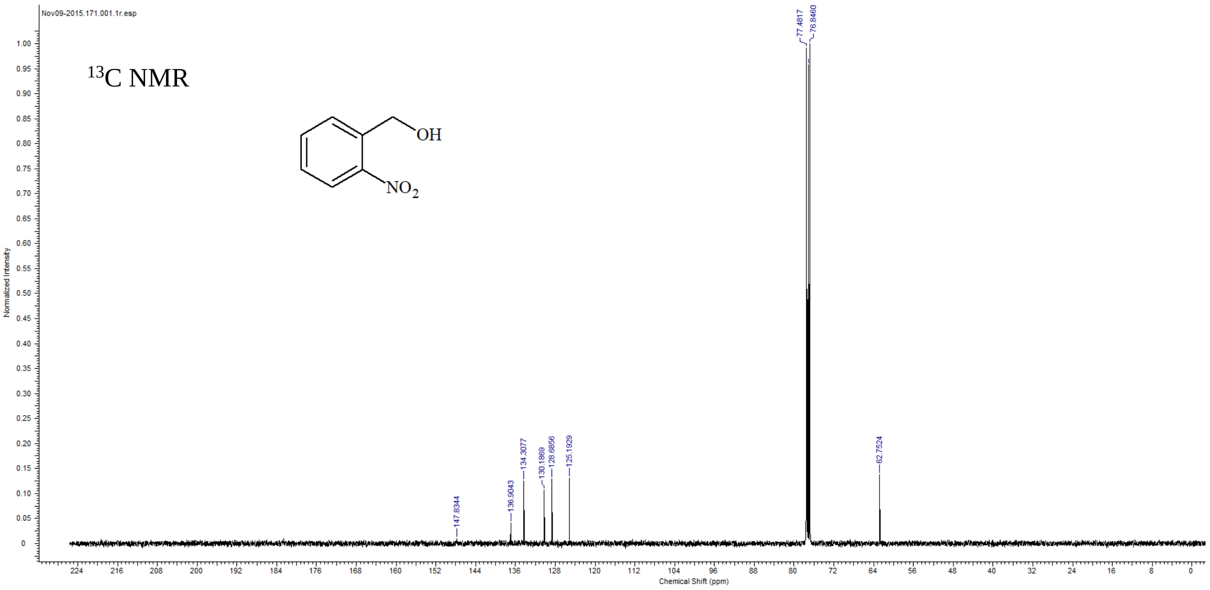
1.00
1.00
1.01
2.03
Normalized Intensity
Chemical Shift (ppm)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125.1929
77.4817
76.8460
62.7524
Normalized Intensity
Chemical Shift (ppm)


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OH
Cl
N
8.5135
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7.5360
7.5236
7.2600
4.8315
4.8176
2.3054
2.3201
2.2908
1.6261
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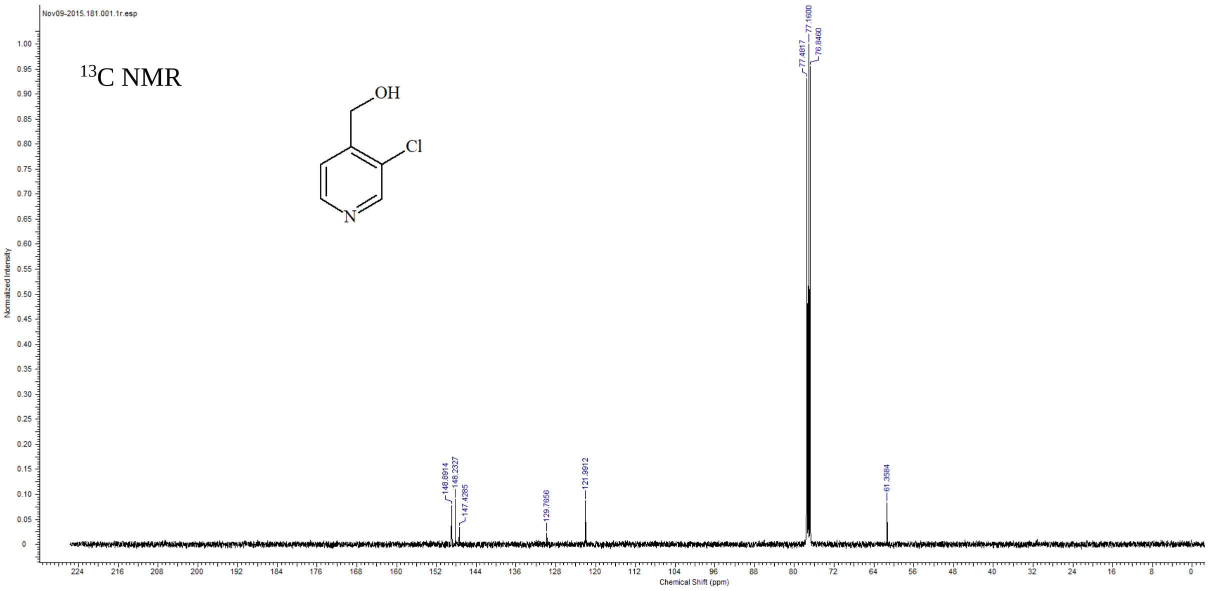
2.00
1.03
2.02
1.03
Normalized Intensity
Chemical Shift (ppm)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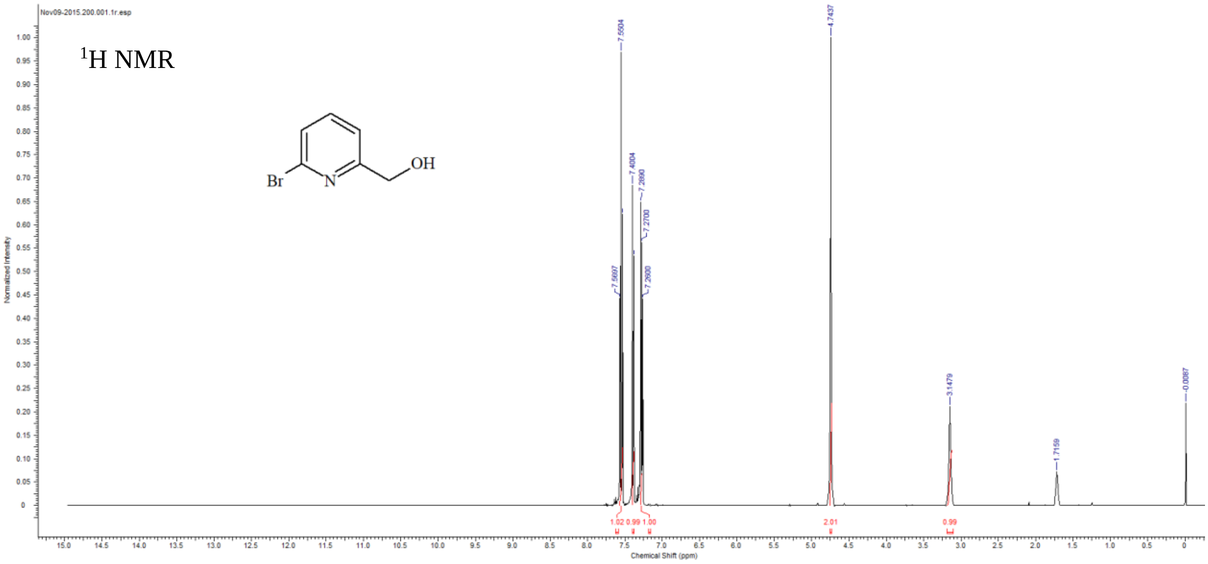
77.1600
76.8460
61.3584
Normalized Intensity
Chemical Shift (ppm)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N
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7.2600
4.7437
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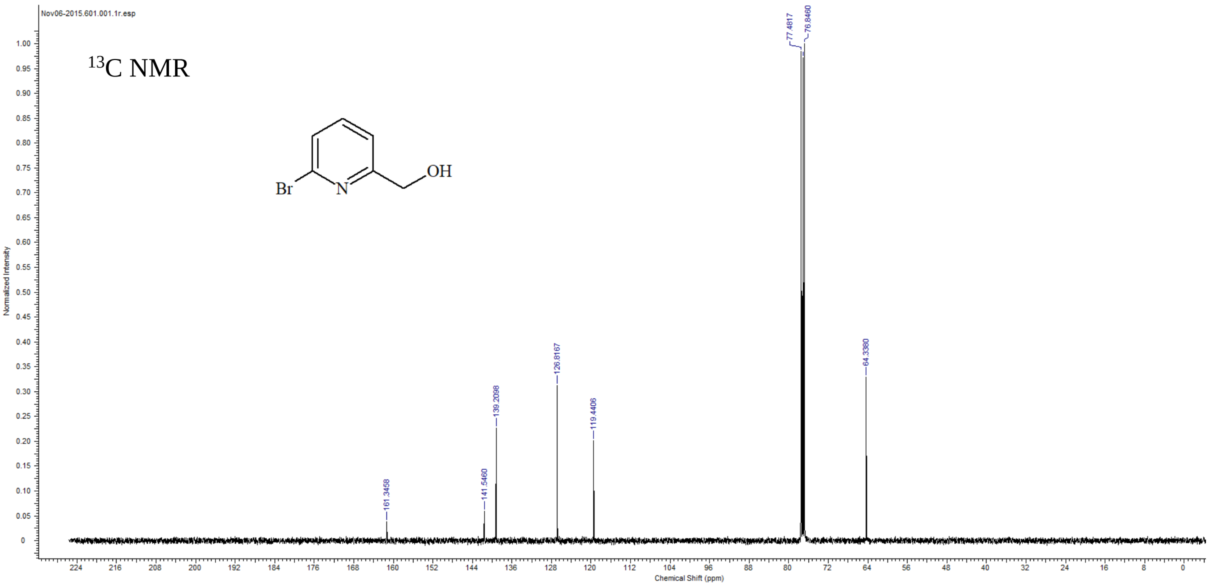
1.00
2.01
0.99
Normalized Intensity
Chemical Shift (ppm)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N
OH
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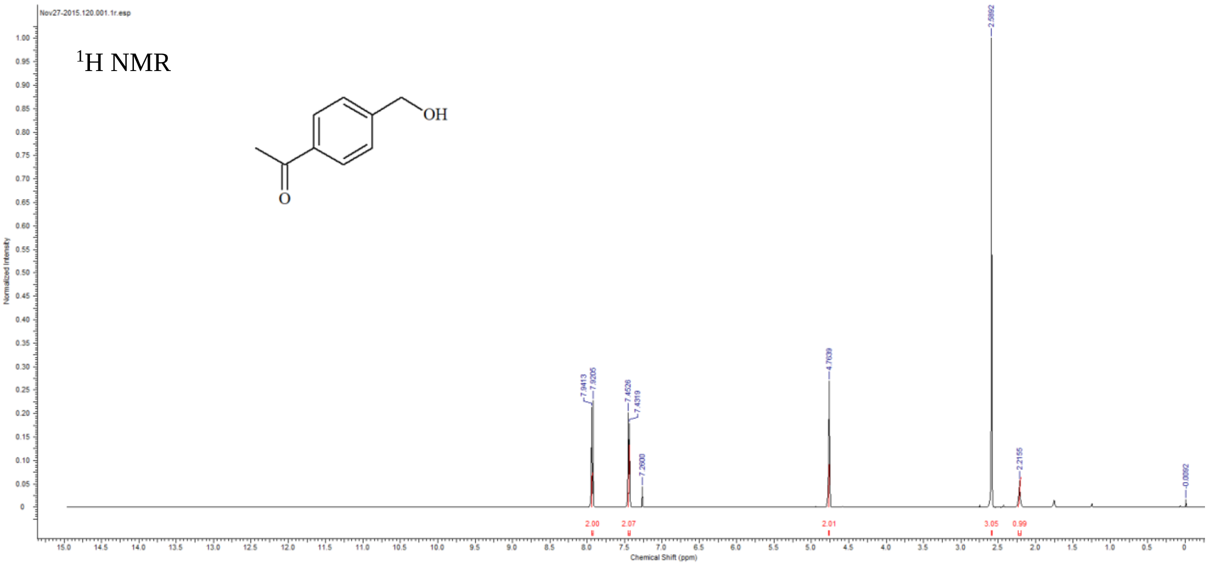
64.3380
Normalized Intensity
Chemical Shift (ppm)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2.07
2.01
3.05
0.99
Normalized Intensity
Chemical Shift (ppm)


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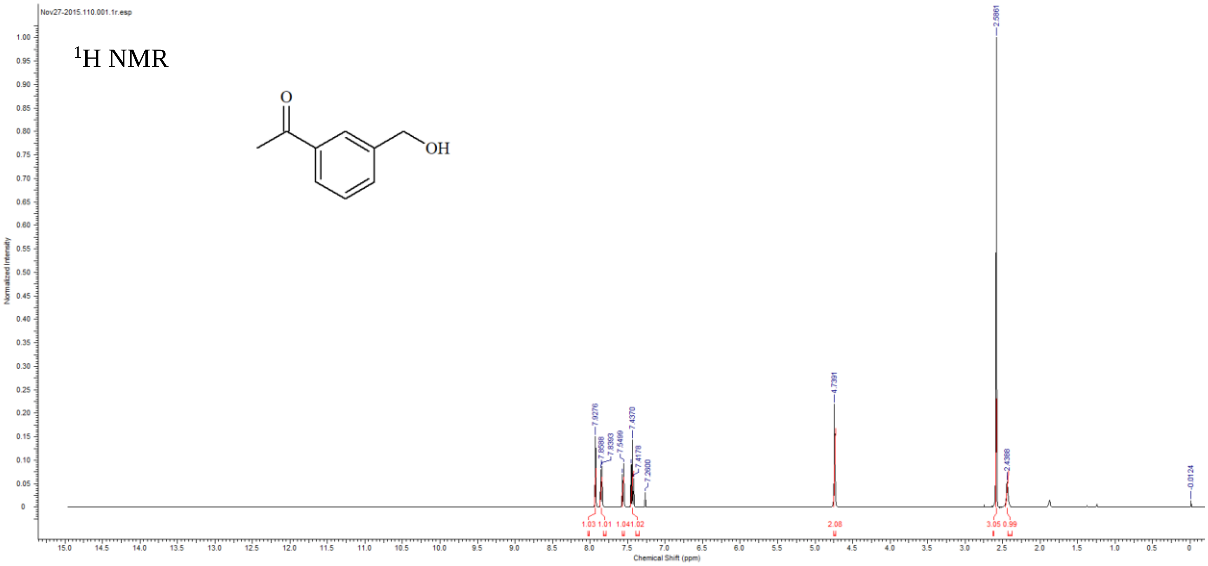
26.7757
Normalized Intensity
Chemical Shift (ppm)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2.4388
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1.03
1.01
1.04
1.02
2.08
3.05
0.99
Normalized Intensity
Chemical Shift (ppm)


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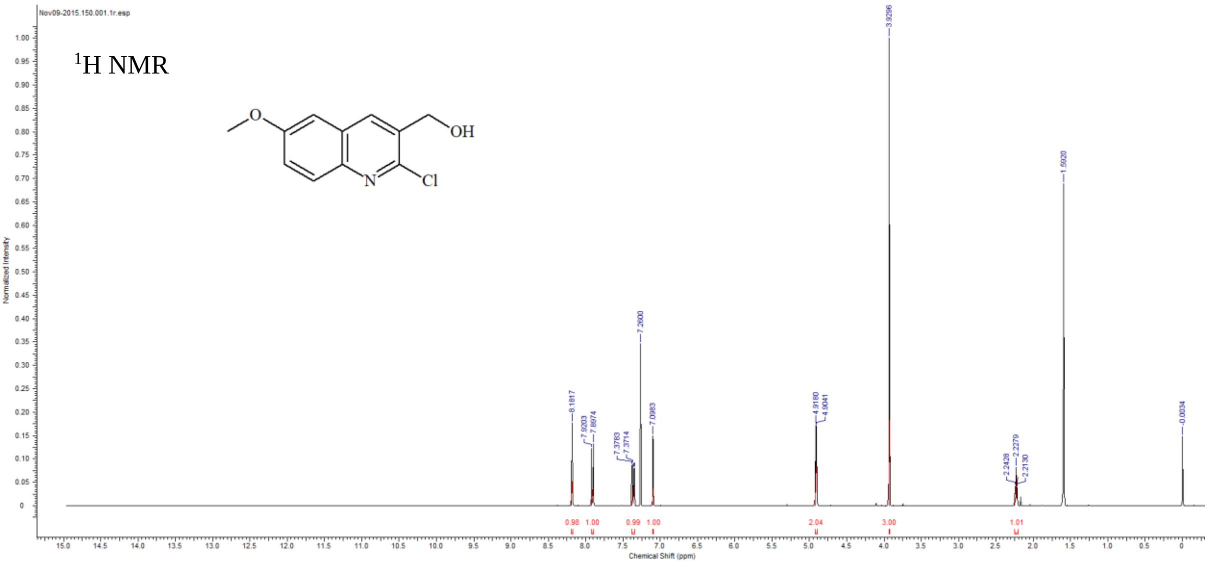
Normalized Intensity
Chemical Shift (ppm)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3.00
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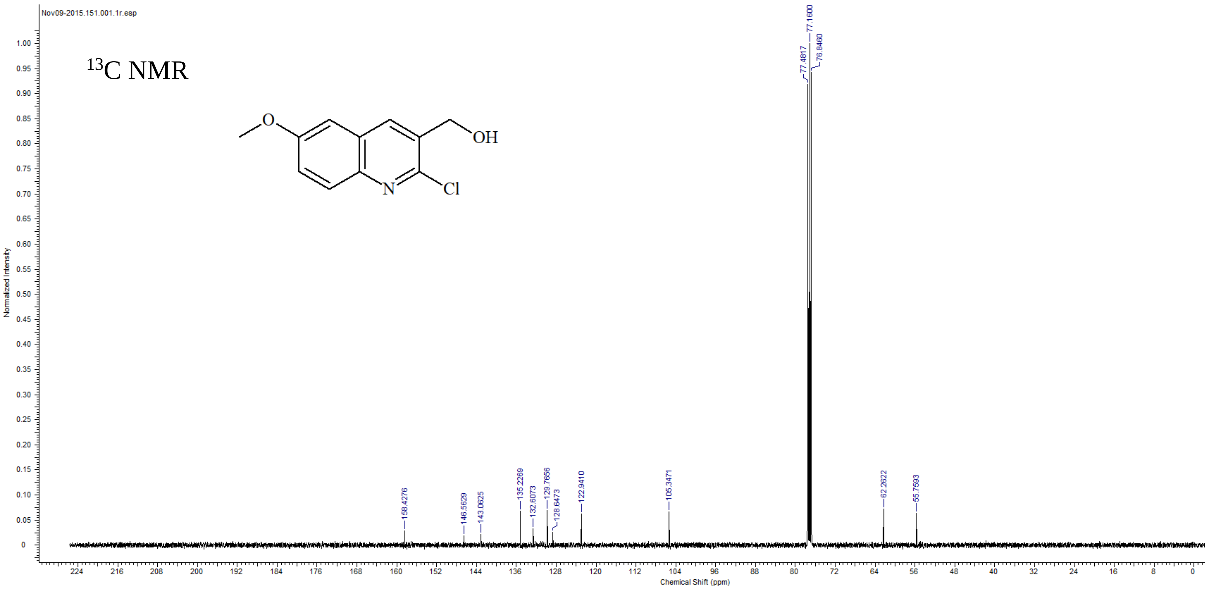
Normalized Intensity
Chemical Shift (ppm)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135.2269
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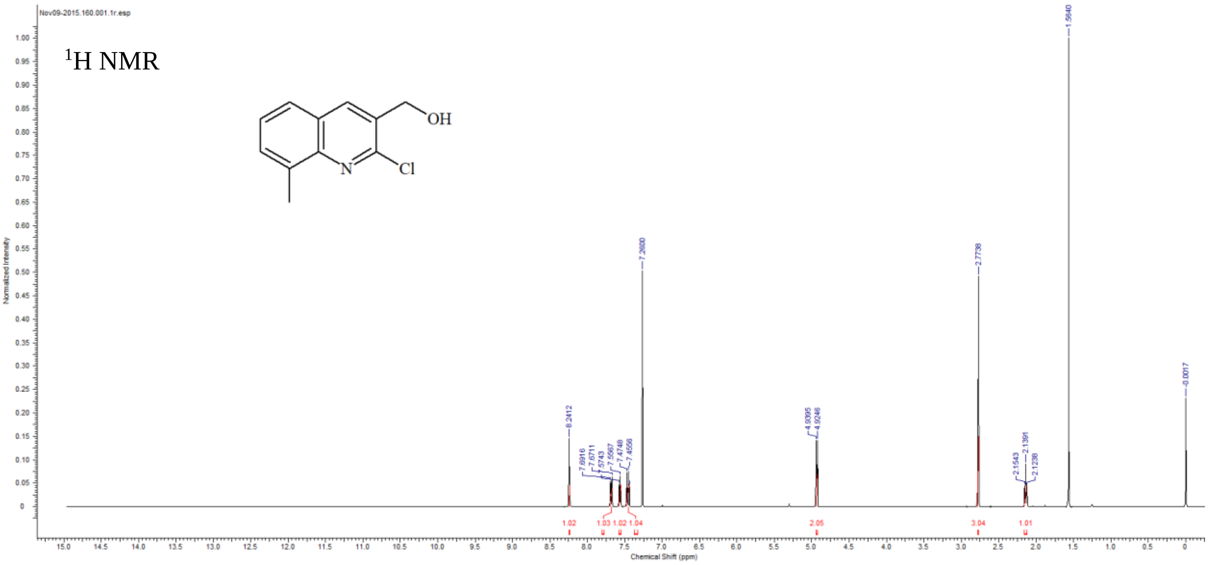
Normalized Intensity
Chemical Shift (ppm)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1.01
Normalized Intensity
Chemical Shift (ppm)


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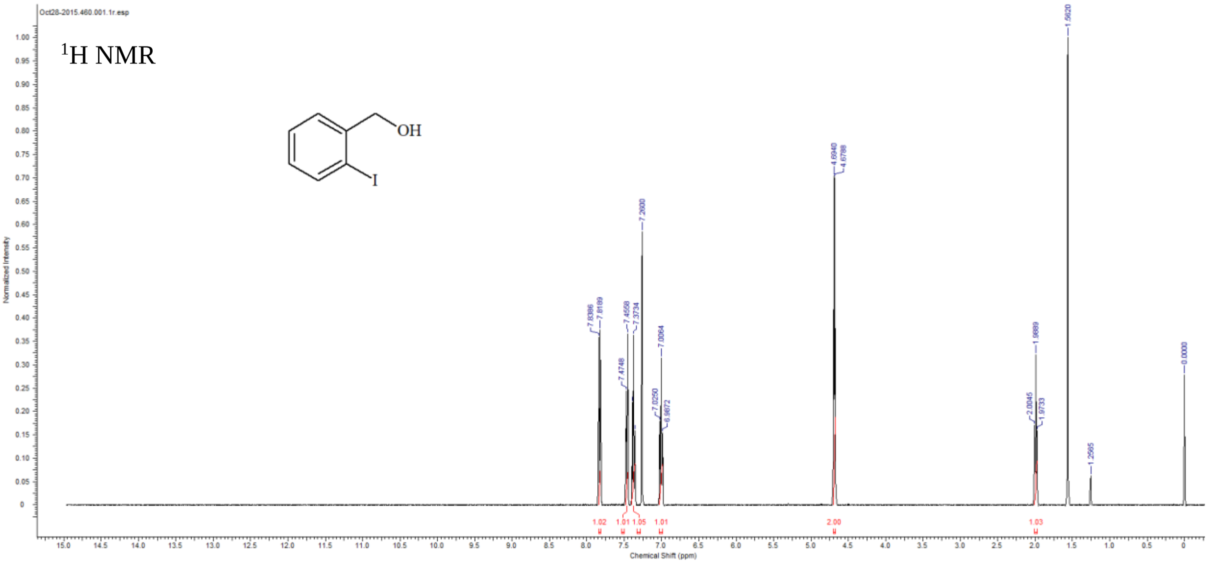
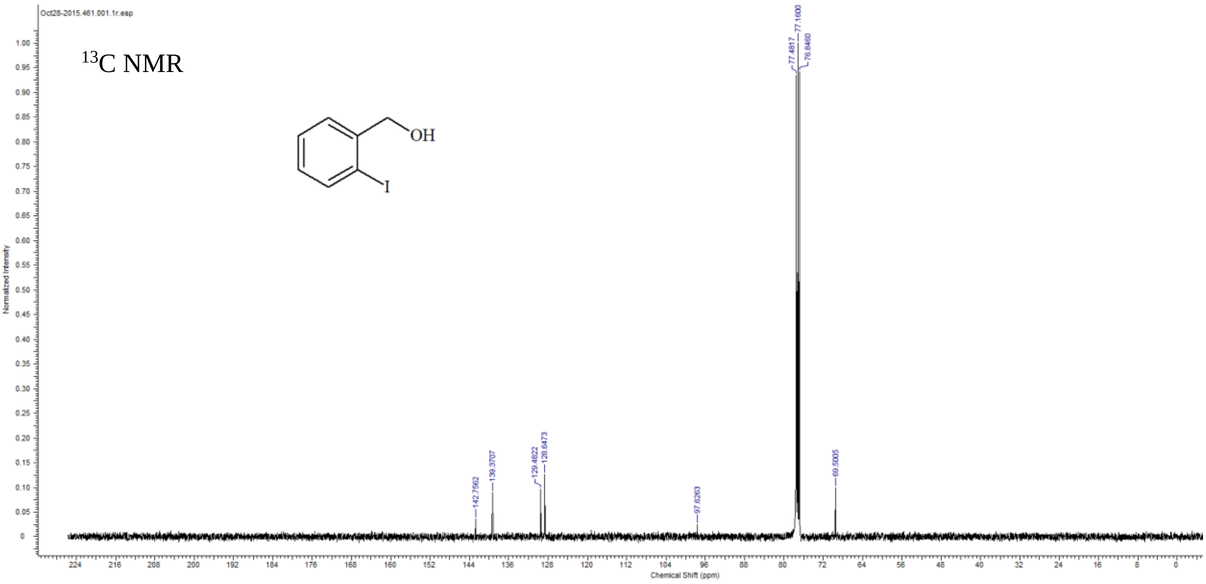
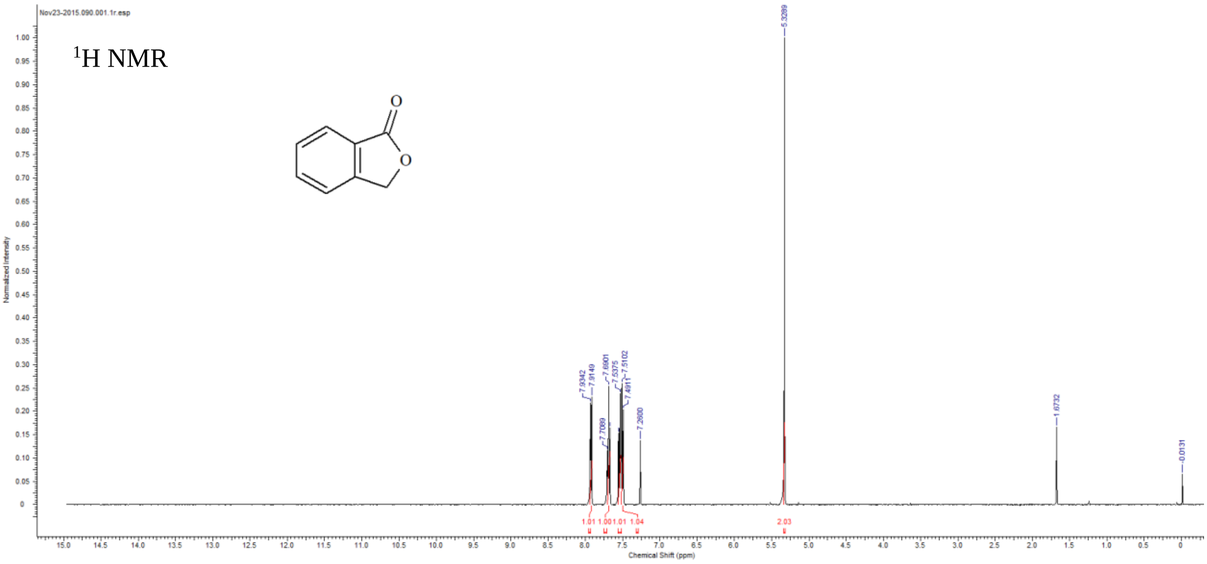
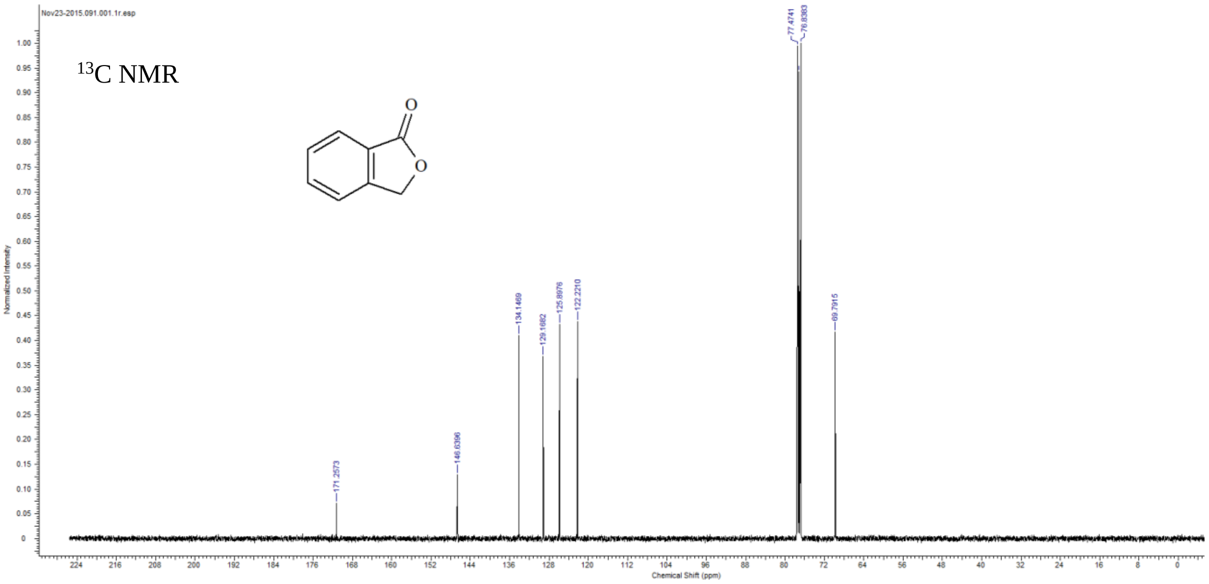
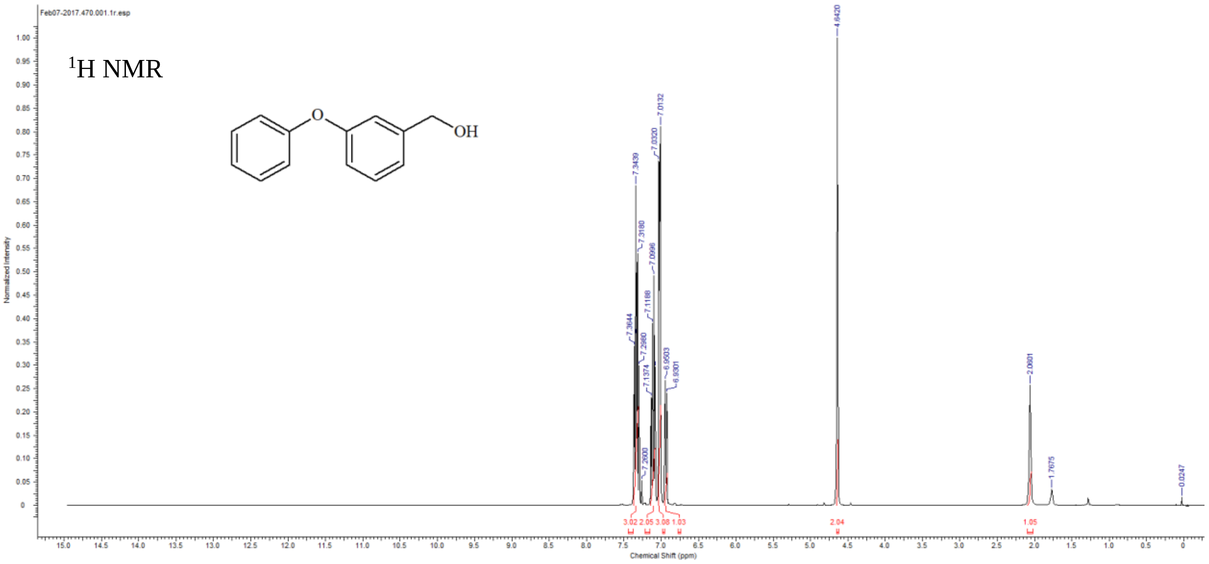
76.8460
148.2021
146.4174
136.6592
132.0405
130.4780
127.5673
127.0848
125.5988
62.3388
17.9825
Normalized Intensity
Chemical Shift (ppm)

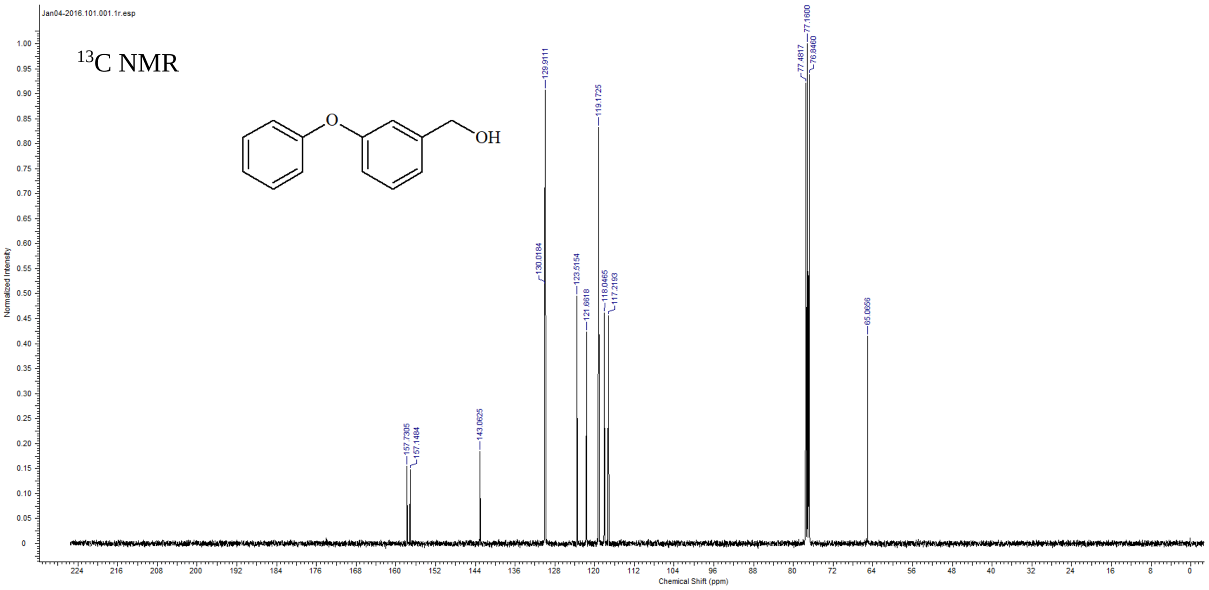

Oct28-2015.460.001.1r.esp
$^1$H NMR
OH
I
7.8386
7.8189
7.4748
7.4558
7.3734
7.2600
7.0250
7.0064
6.9872
4.6940
4.6788
2.0045
1.9889
1.9733
1.5620
1.2595
0.0000
1.02
1.01
1.05
1.01
2.00
1.03
Normalized Intensity
Chemical Shift (ppm)

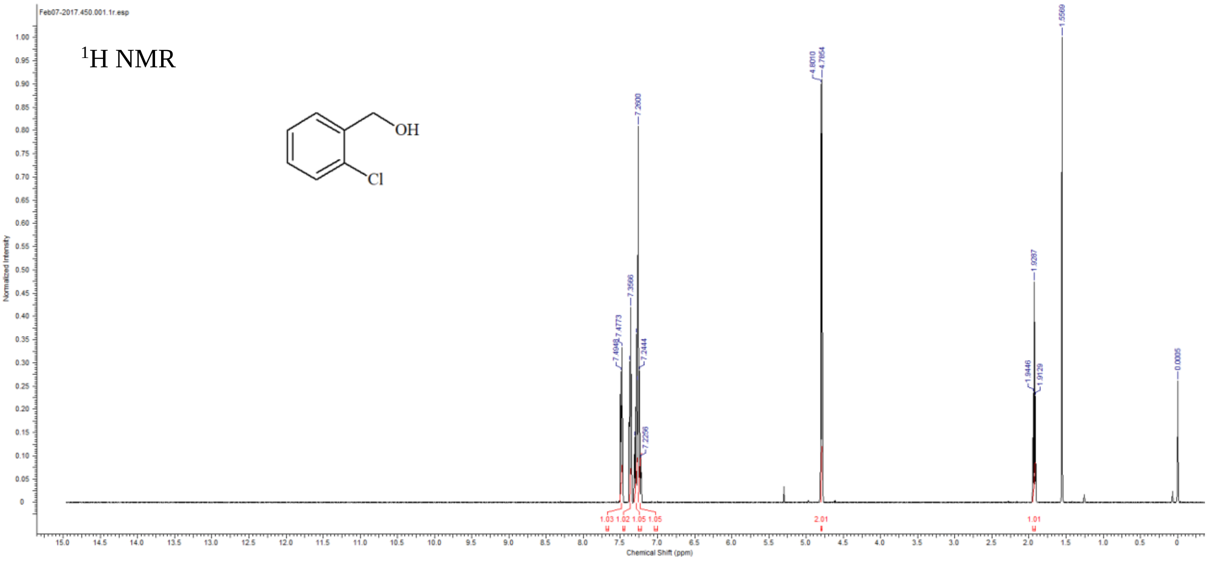

Oct28-2015.461.001.1r.esp
$^{13}$C NMR
OH
I
142.7562
139.3707
129.4622
128.6473
97.6263
77.4817
77.1600
76.8460
69.5005
Normalized Intensity
Chemical Shift (ppm)

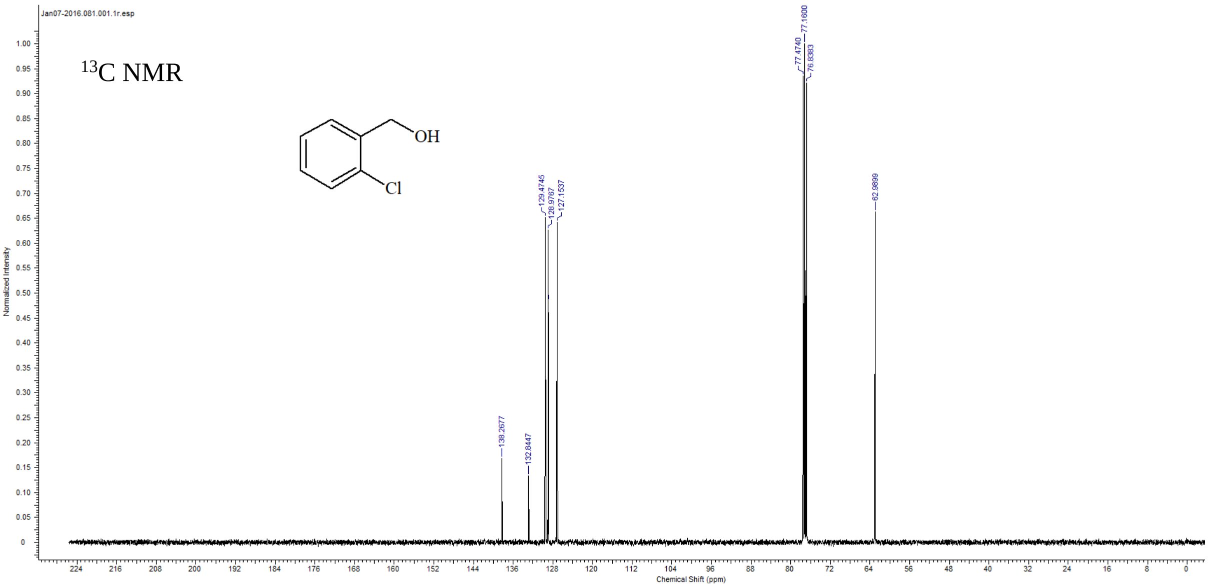

Nov23-2015.090.001.1r.esp
$^1$H NMR
O
O
7.9342
7.9149
7.7089
7.6901
7.5375
7.5102
7.4911
7.2600
5.3289
1.6732
0.0131
1.01
1.00
1.01
1.04
2.03
Normalized Intensity
Chemical Shift (ppm)

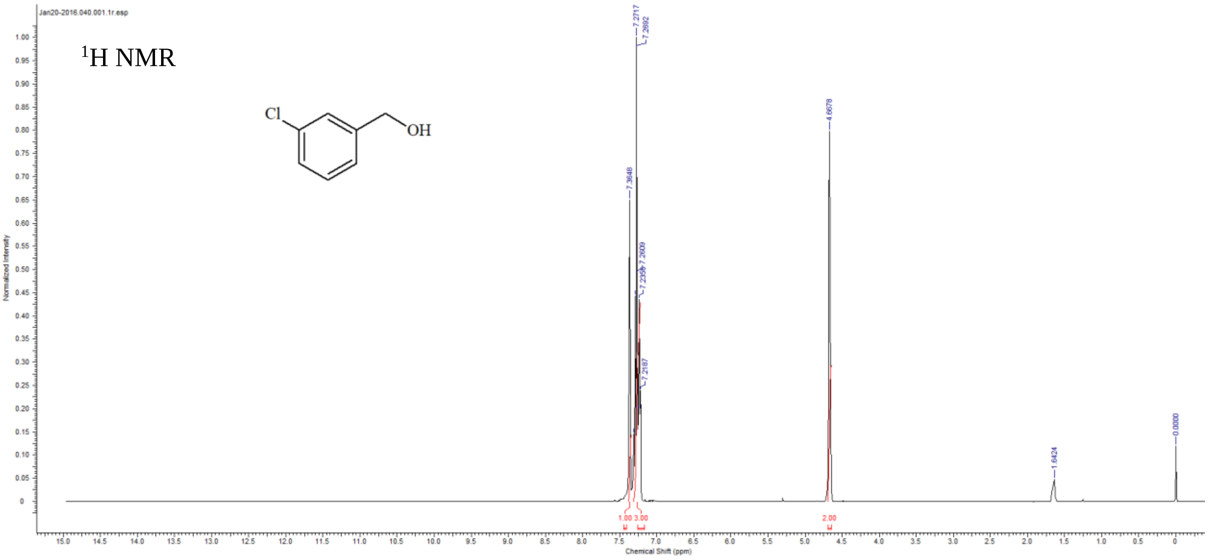

Nov23-2015.091.001.1r.esp
13C NMR
O
O
171.2573
146.6396
134.1469
129.1682
125.8976
122.2210
77.4741
76.8383
69.7915
Normalized Intensity
Chemical Shift (ppm)

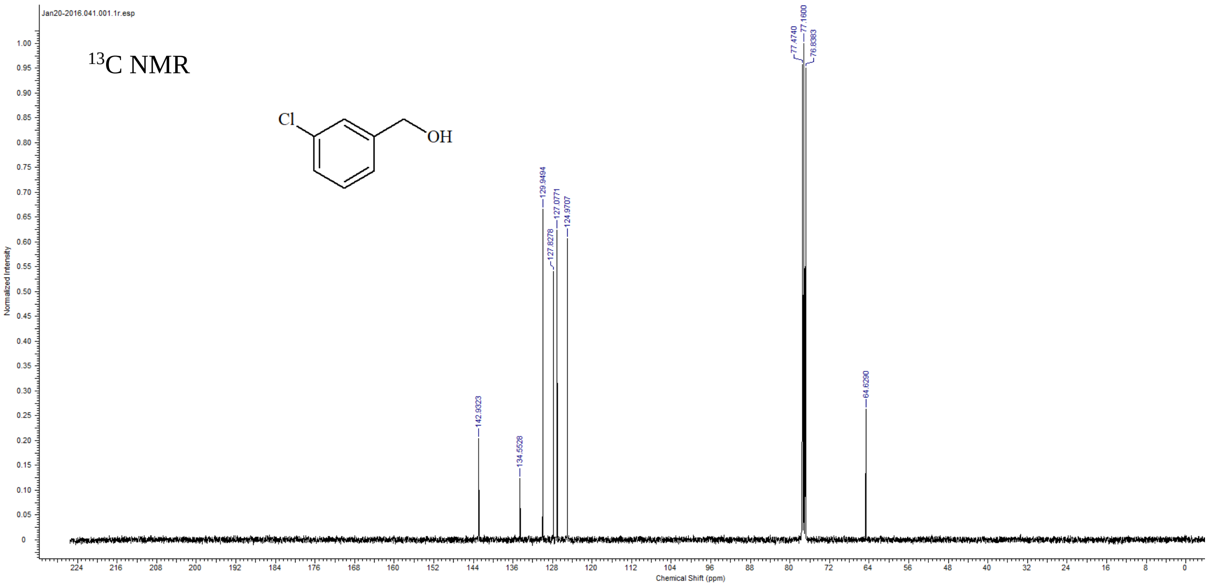

Feb07-2017.470.001.1r.esp
1H NMR
O
OH
7.3644
7.3439
7.3180
7.2980
7.2603
7.1374
7.1188
7.0996
7.0320
7.0132
6.9503
6.9301
4.6420
2.0601
1.7675
0.0247
3.02
2.05
3.08
1.03
2.04
1.05
Normalized Intensity
Chemical Shift (ppm)

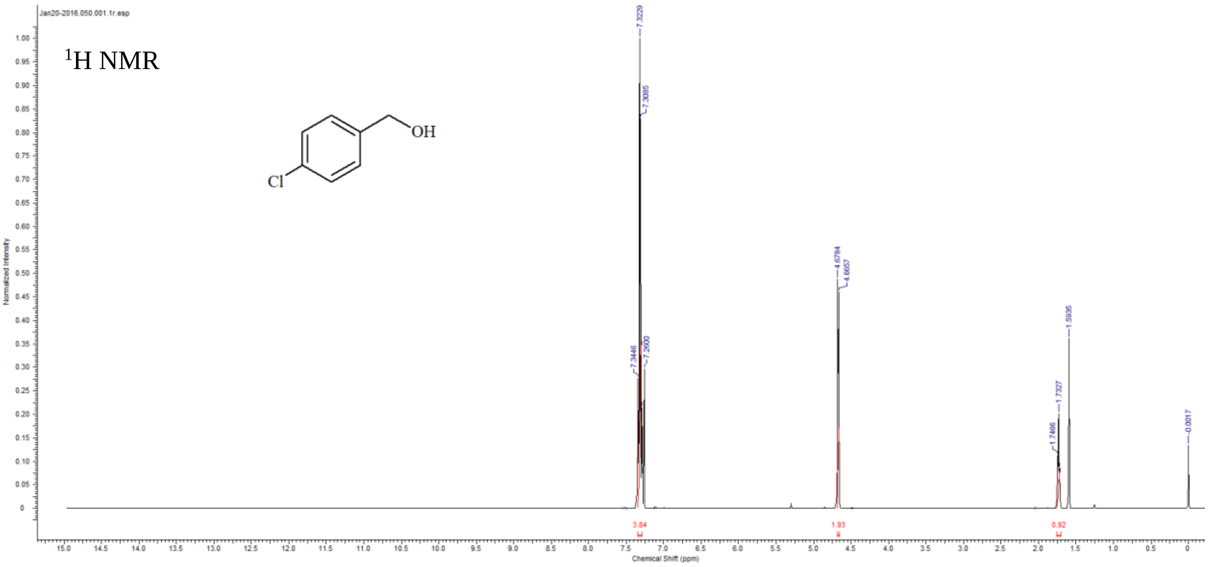

Jan04-2016.101.001.1r.esp
13C NMR
O
OH
157.7305
157.1484
143.0625
130.0184
129.9111
123.5154
121.6618
119.1725
118.0465
117.2193
77.4817
77.1600
76.8460
65.0656
Normalized Intensity
Chemical Shift (ppm)

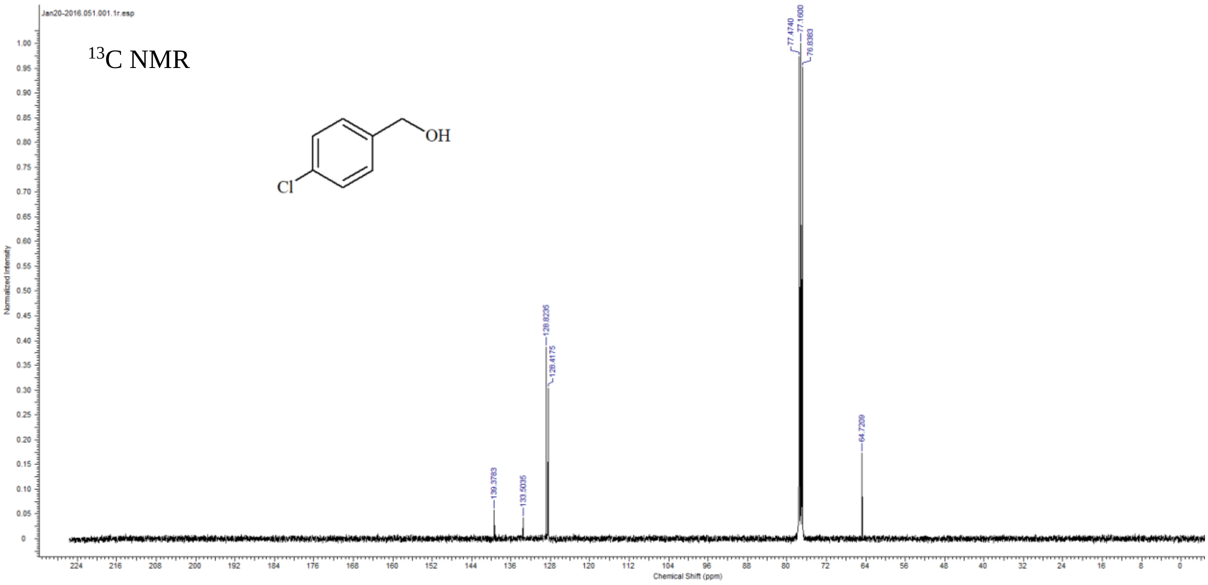

Feb07-2017.450.001.1r.esp
$^1$H NMR
OH
Cl
7.4948
7.4773
7.3566
7.2600
7.2444
7.2256
4.8010
4.7864
1.9446
1.9287
1.9129
1.5569
0.0005
1.03
1.02
1.05
1.05
2.01
1.01
Normalized Intensity
Chemical Shift (ppm)

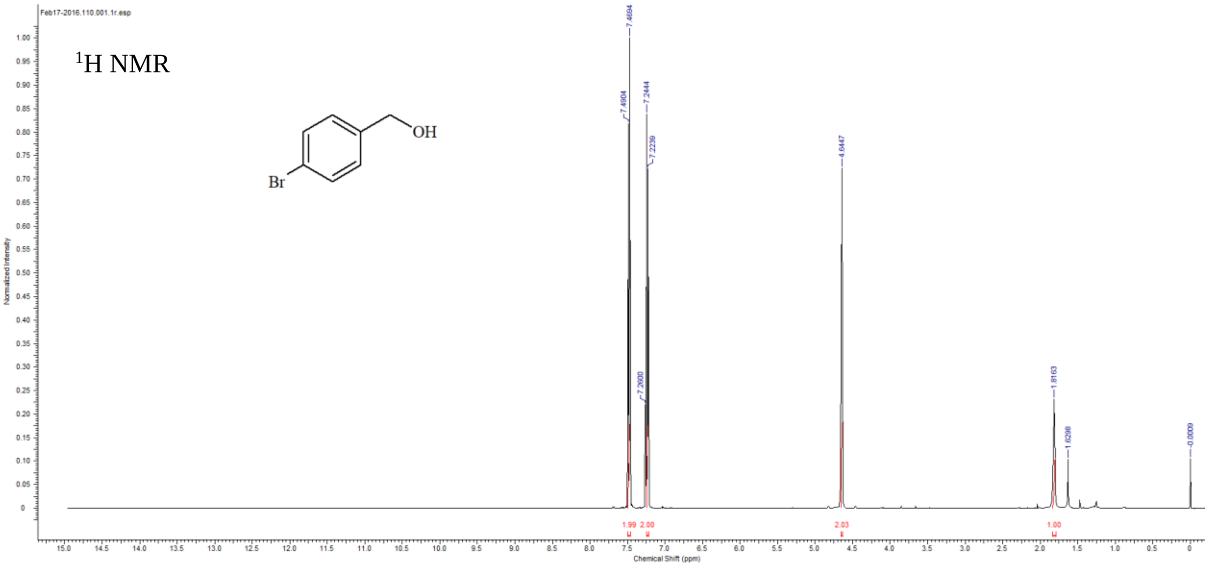

Jan07-2016.081.001.1r.esp
$^{13}$C NMR
OH
Cl
138.2677
132.8447
129.4745
128.9767
127.1537
77.4740
77.1600
76.8383
62.9899
Normalized Intensity
Chemical Shift (ppm)


Jan20-2016.040.001.1r.esp
$^1$H NMR
Cl
OH
7.3648
7.2717
7.2692
7.2609
7.2356
7.2187
4.6678
1.6424
0.0000
1.00
3.00
2.00
Normalized Intensity
Chemical Shift (ppm)

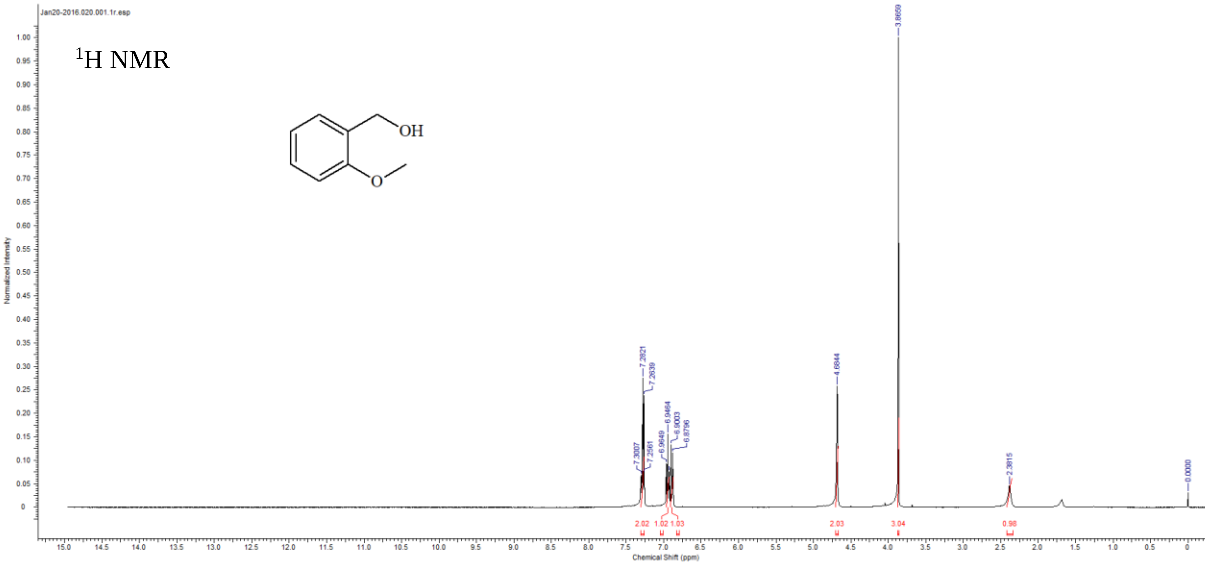

Jan20-2016.041.001.1r.esp
$^{13}$C NMR
Cl
OH
142.9323
134.5528
129.9494
127.8278
127.0771
124.9707
77.4740
77.1600
76.8383
64.6290
Normalized Intensity
Chemical Shift (ppm)

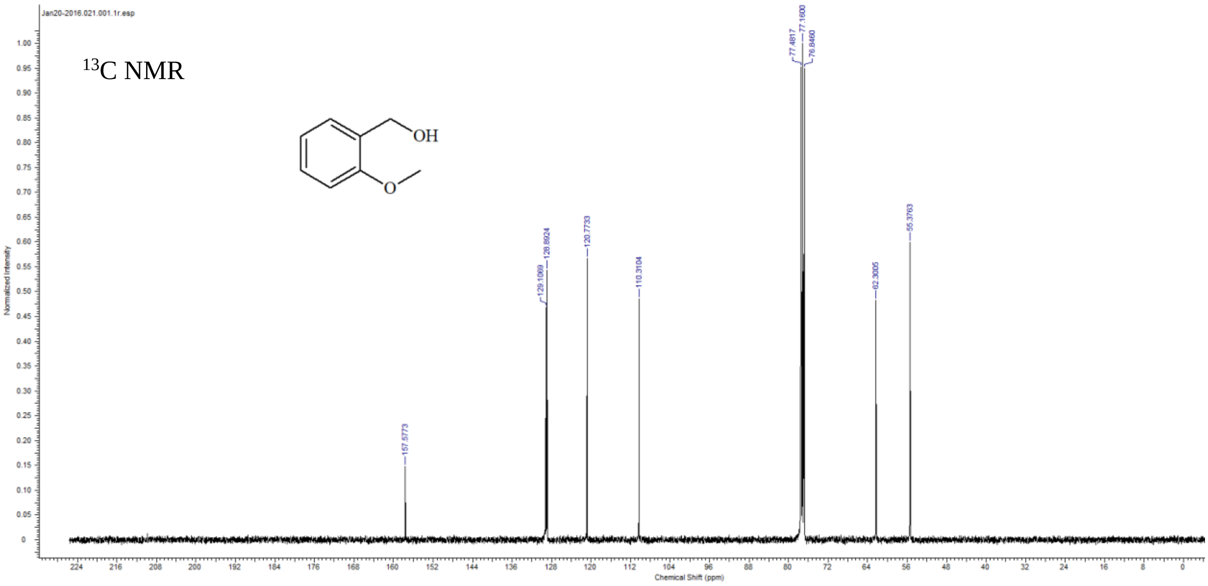

Jan20-2016.050.001.1r.esp
$^{1}$H NMR
OH
Cl
7.3229
7.3085
7.3446
7.2600
4.6784
4.6657
1.5935
1.7327
1.7466
-0.0017
3.84
1.93
0.92
Normalized Intensity
Chemical Shift (ppm)

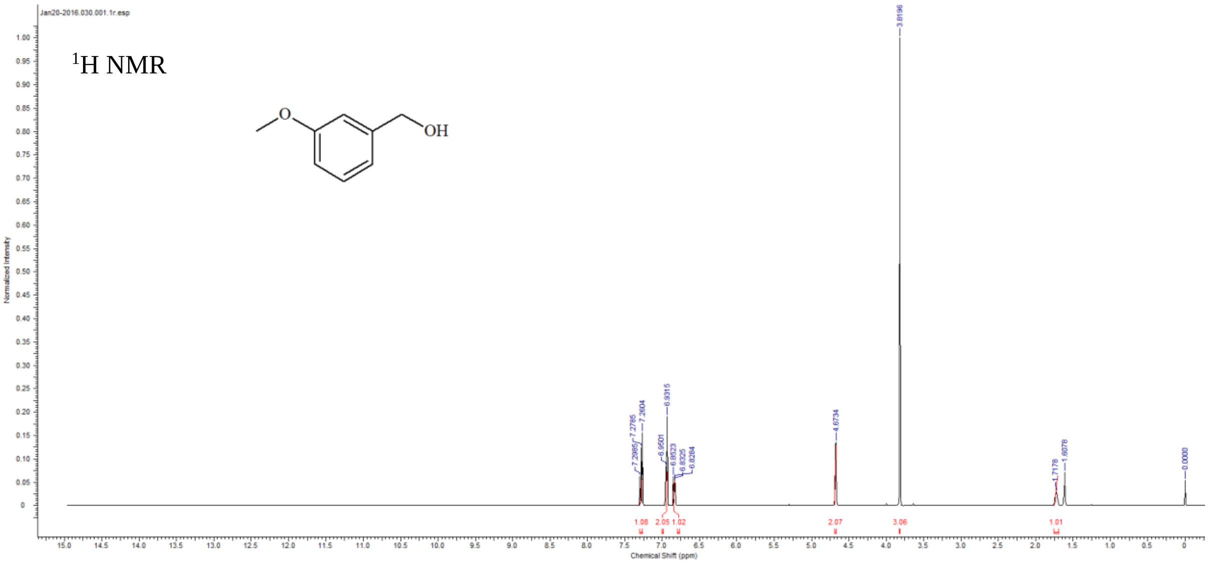

Jan20-2016.051.001.1r.esp
$^{13}$C NMR
OH
Cl
139.3783
133.5035
128.8236
128.4175
77.4740
77.1600
76.8383
64.7209
Normalized Intensity
Chemical Shift (ppm)

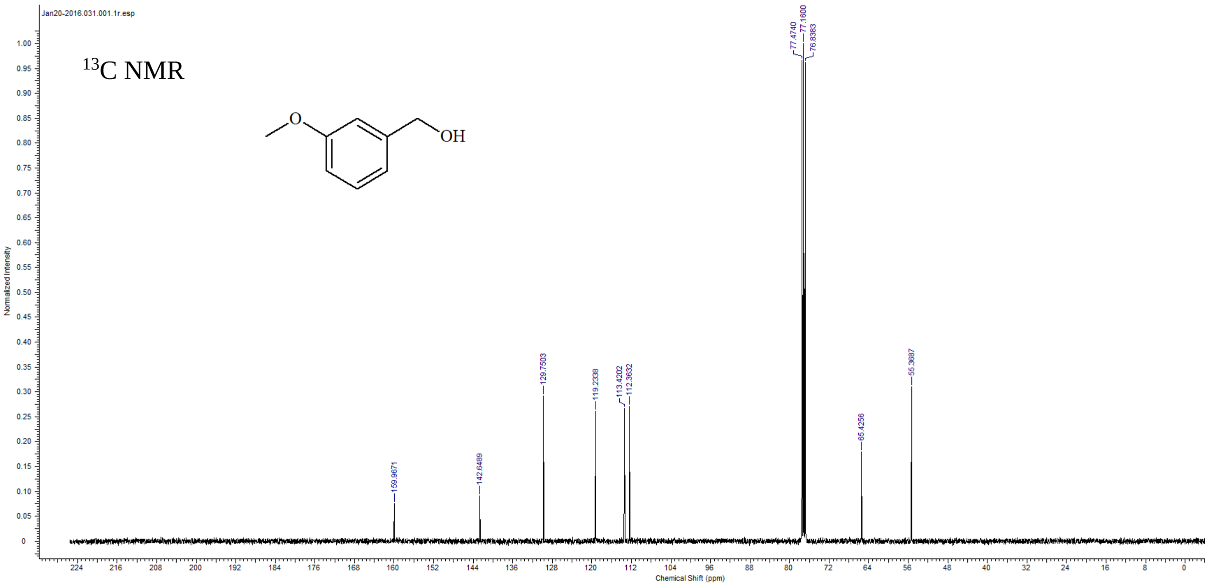

Feb17-2016.110.001.1r.esp
$^1$H NMR
OH
Br
7.4904
7.4694
7.2444
7.2239
7.2600
4.6447
1.8163
1.6298
-0.0009
1.99
2.00
2.03
1.00
Normalized Intensity
Chemical Shift (ppm)

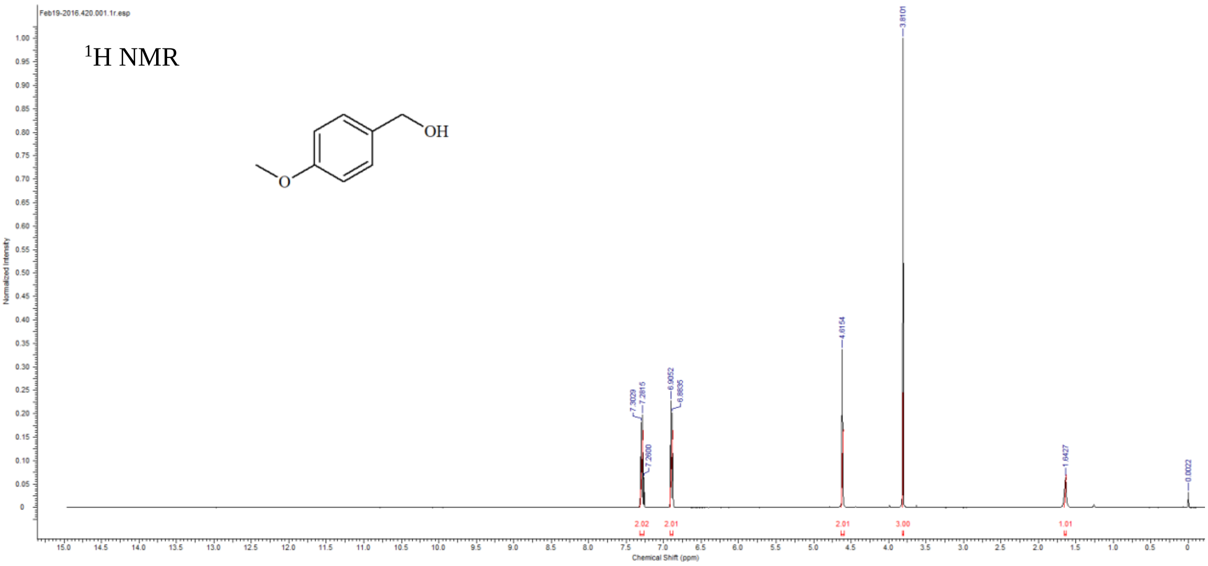

Feb17-2016.111.001.1r.esp
$^{13}$C NMR
OH
Br
139.9068
131.7724
128.7239
121.5929
77.4817
76.8460
64.7209
Normalized Intensity
Chemical Shift (ppm)

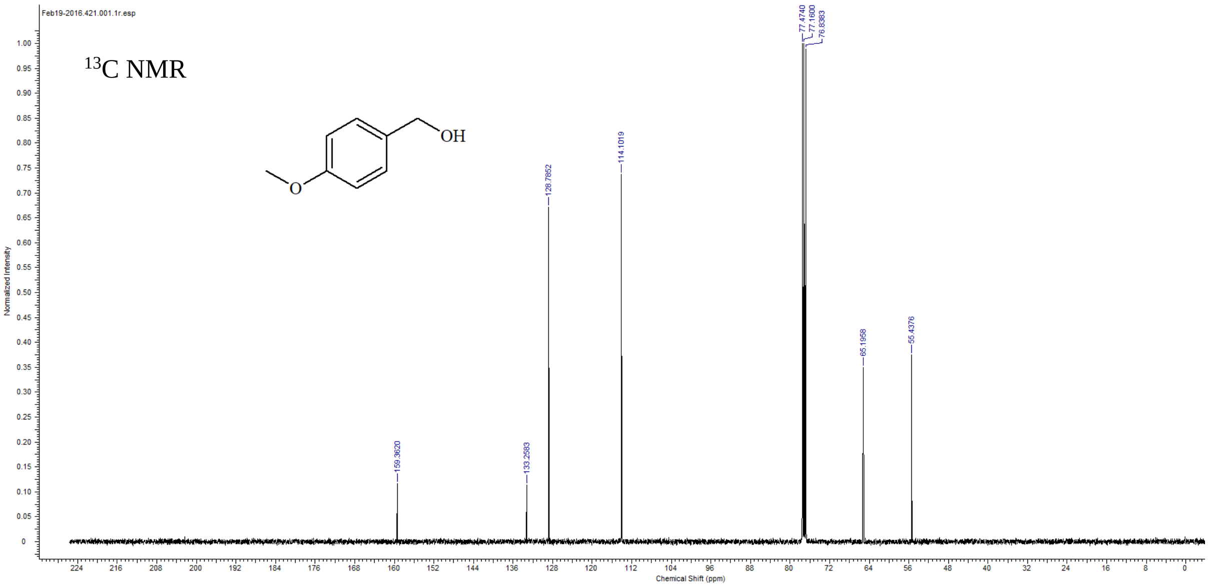

Jan20-2016.020.001.1r.esp
$^1$H NMR
OH
O
7.3007
7.2821
7.2639
7.2561
6.9649
6.9464
6.9003
6.8796
4.6844
3.8659
2.3815
0.0000
2.02
1.02
1.03
2.03
3.04
0.98
Normalized Intensity
Chemical Shift (ppm)

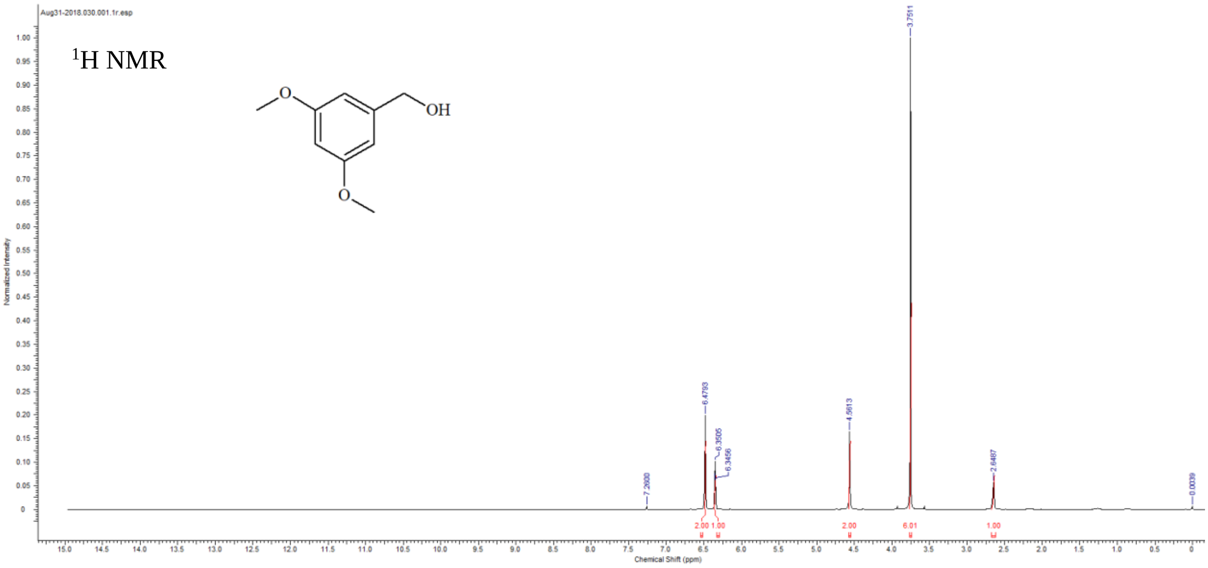

Jan20-2016.021.001.1r.esp
$^{13}$C NMR
OH
O
77.4817
77.1600
76.8460
157.5773
129.1069
128.6924
120.7733
110.3104
62.3005
55.3763
Normalized Intensity
Chemical Shift (ppm)

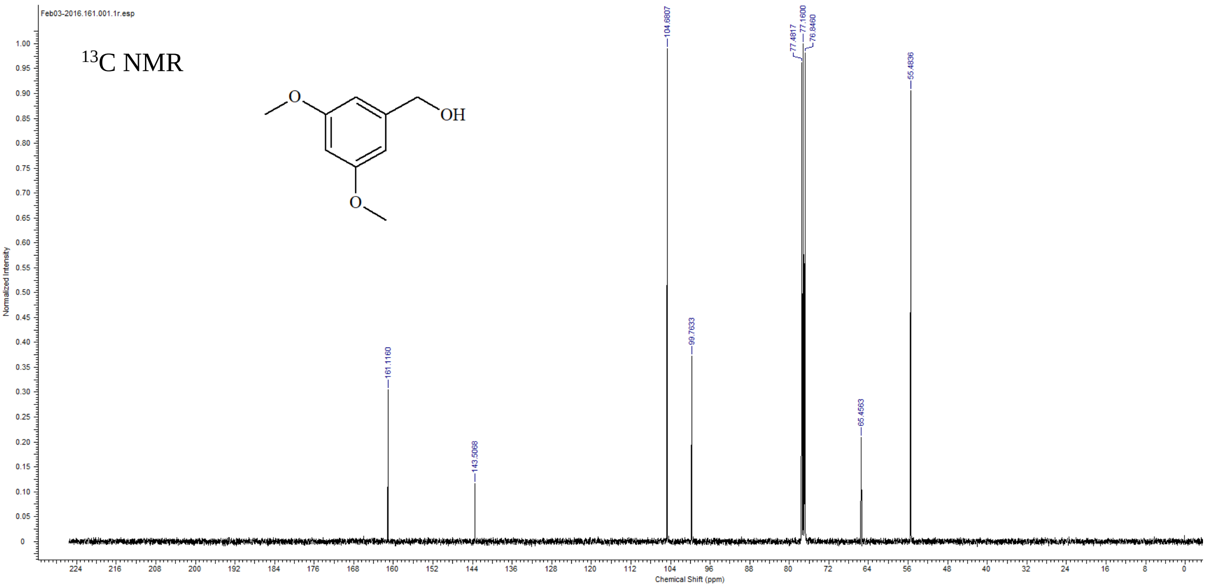

Jan20-2016.030.001.1r.esp
$^{1}$H NMR
O
OH
7.2985
7.2785
7.2604
6.9501
6.9315
6.8523
6.8325
6.8284
4.6734
3.8196
1.7178
1.6678
0.0000
1.08
2.05
1.02
2.07
3.06
1.01
Normalized Intensity
Chemical Shift (ppm)

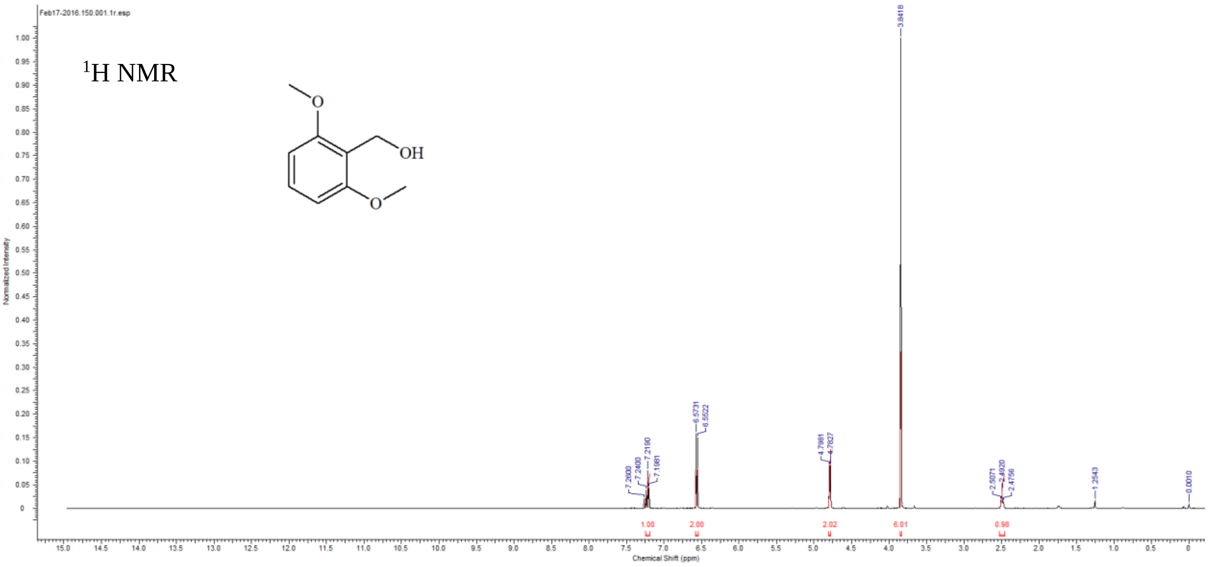

Jan20-2016.031.001.1r.esp
$^{13}$C NMR
O
OH
77.4740
77.1600
76.8383
159.9671
142.6489
129.7503
119.2338
113.4202
112.3632
65.4256
55.3687
Normalized Intensity
Chemical Shift (ppm)


Feb19-2016.420.001.1r.esp
$^1$H NMR
OH
O
7.3029
7.2815
7.2600
6.9052
6.8835
4.6154
3.8101
1.6427
0.0022
2.02
2.01
2.01
3.00
1.01
Normalized Intensity
Chemical Shift (ppm)

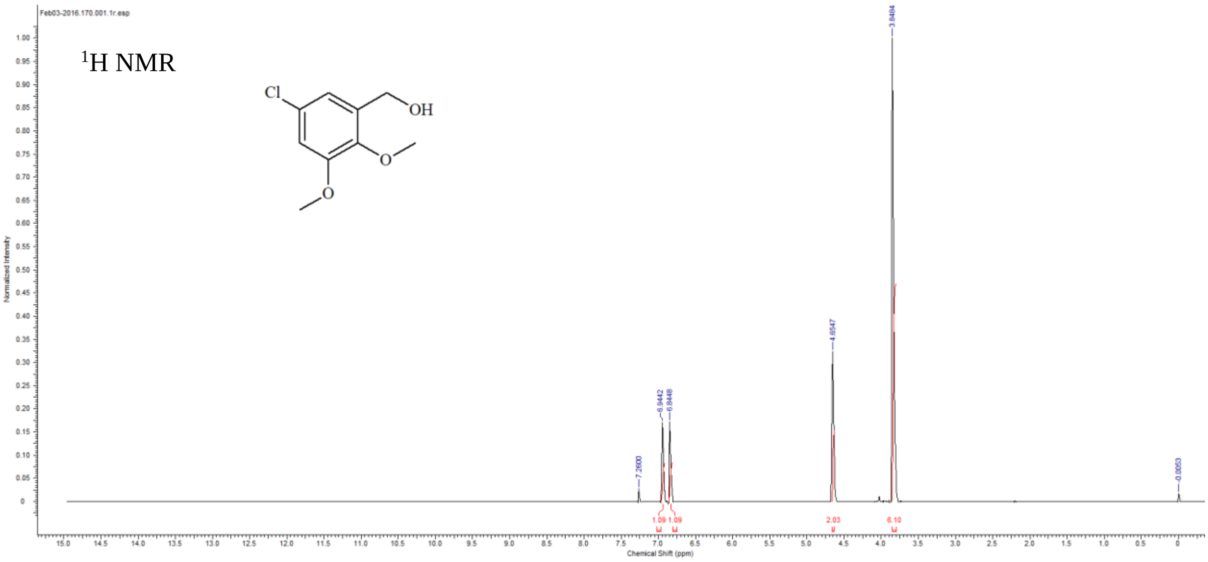

Feb19-2016.421.001.1r.esp
$^{13}$C NMR
OH
O
159.3620
133.2583
128.7862
114.1019
77.4740
77.1600
76.8383
65.1958
55.4376
Normalized Intensity
Chemical Shift (ppm)

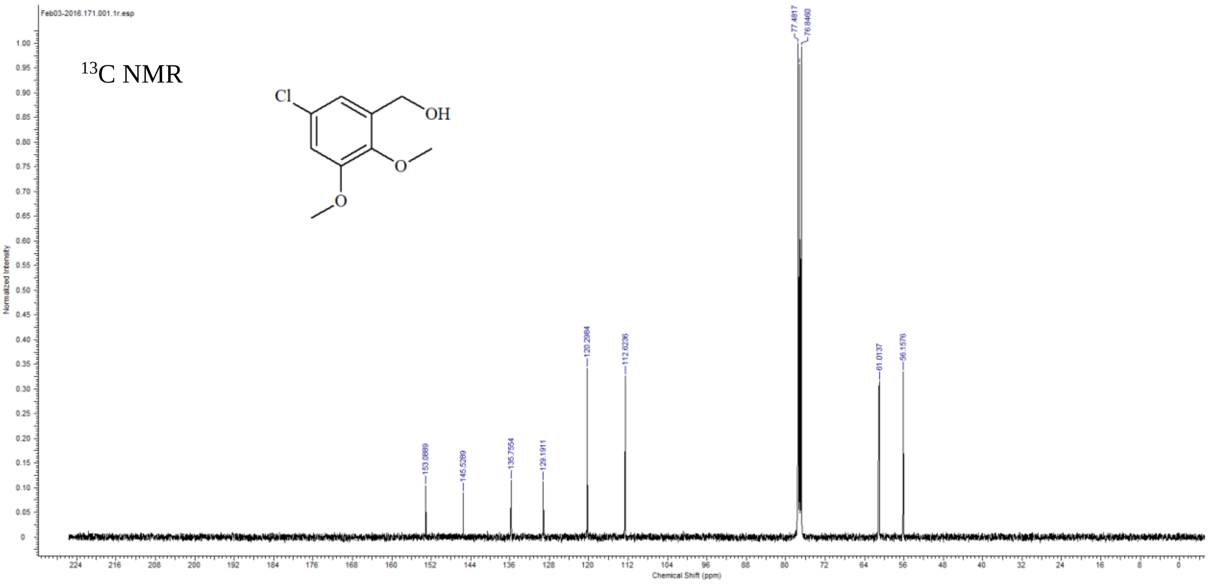

Aug31-2018.030.001.1r.esp
$^1$H NMR
O
OH
O
7.2600
6.4793
6.3505
6.3456
4.5613
3.7511
2.6467
0.0039
2.00
1.00
2.00
6.01
1.00
Normalized Intensity
Chemical Shift (ppm)

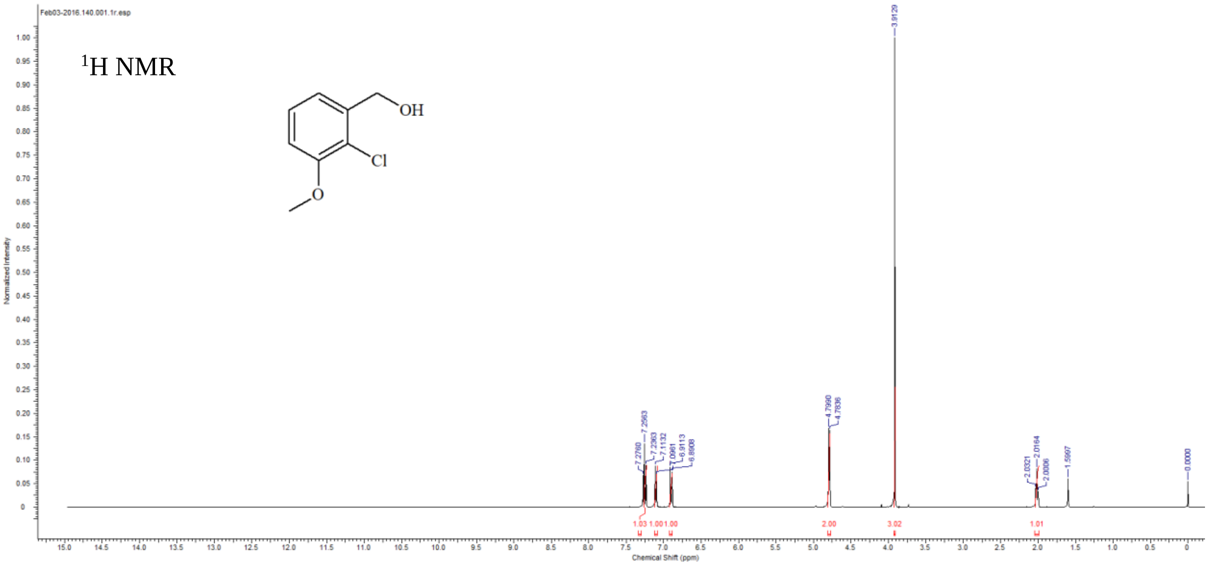

Feb03-2016.161.001.1r.esp
$^{13}$C NMR
O
OH
O
161.1160
143.5068
104.6807
99.7633
77.4817
77.1600
76.8460
65.4563
55.4836
Normalized Intensity
Chemical Shift (ppm)

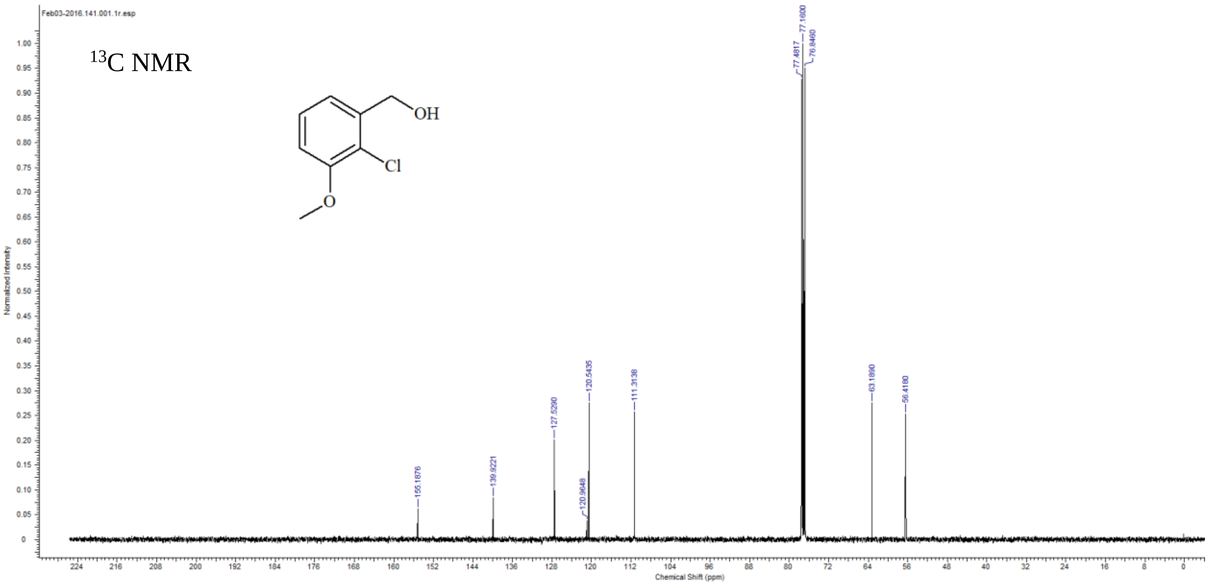

Feb17-2016.150.001.1r.esp
$^{1}$H NMR
O
OH
O
7.2600
7.2400
7.2190
7.1981
6.5731
6.5522
4.7981
4.7827
3.8418
2.5071
2.4920
2.4756
1.2543
0.0010
1.00
2.00
2.02
6.01
0.98
Normalized Intensity
Chemical Shift (ppm)

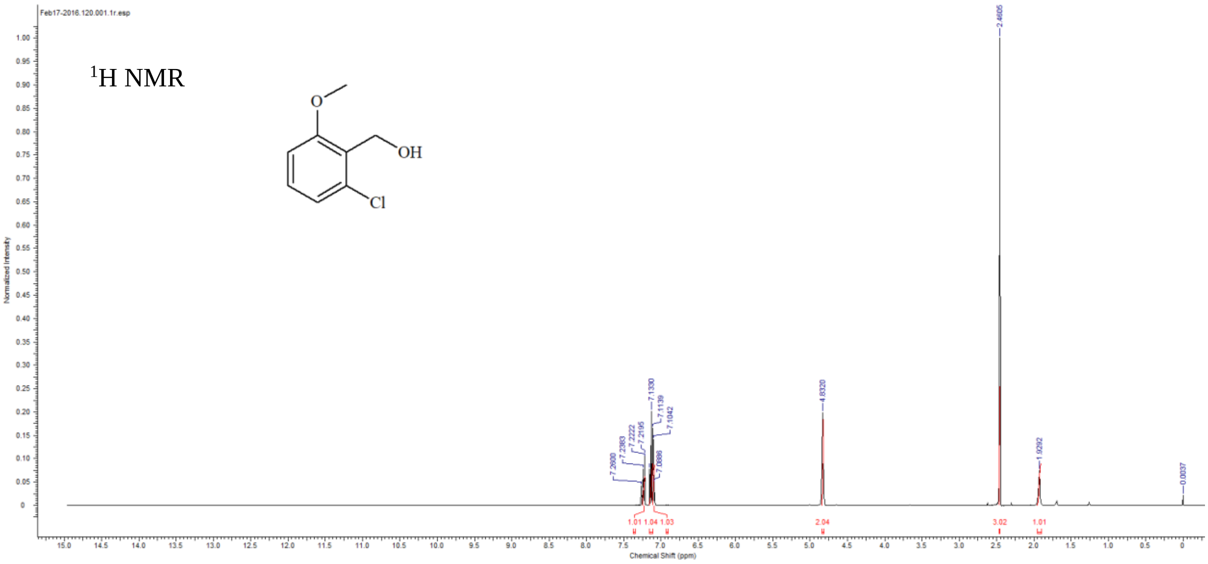

Feb17-2016.151.001.1r.esp
$^{13}$C NMR
O
OH
O
158.5348
129.2601
117.1657
103.9454
77.4817
77.1600
76.8460
55.8589
54.8478
29.8165
Normalized Intensity
Chemical Shift (ppm)

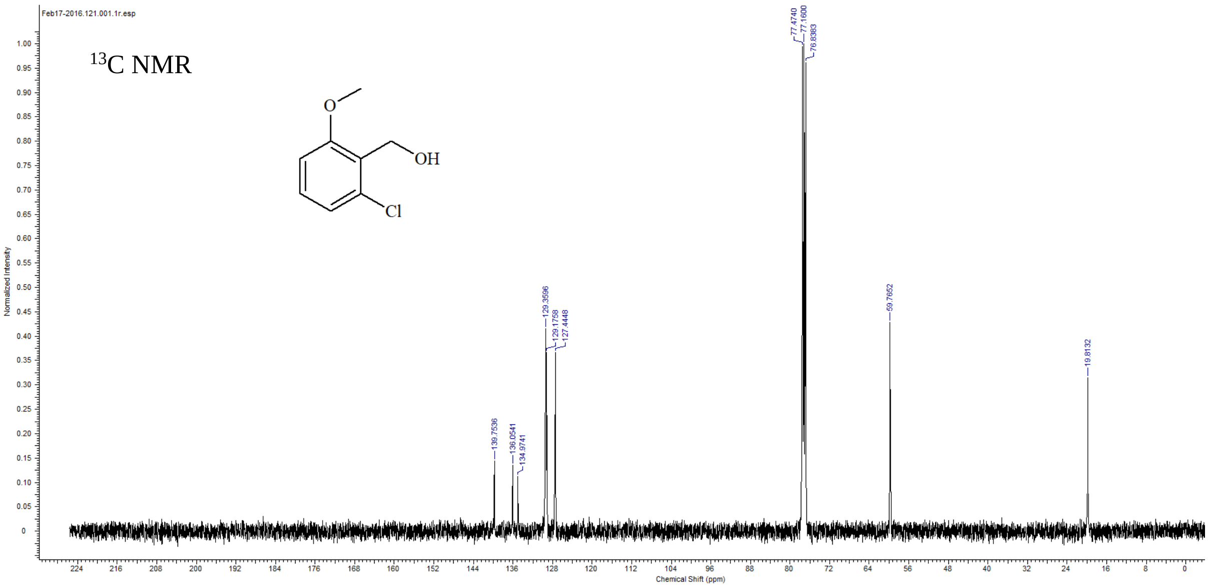

Feb03-2016.170.001.1r.esp
$^1$H NMR
Cl
OH
O
O
Normalized Intensity
3.8484
4.6547
6.9442
6.8448
7.2600
-0.0053
1.09
1.09
2.03
6.10
Chemical Shift (ppm)

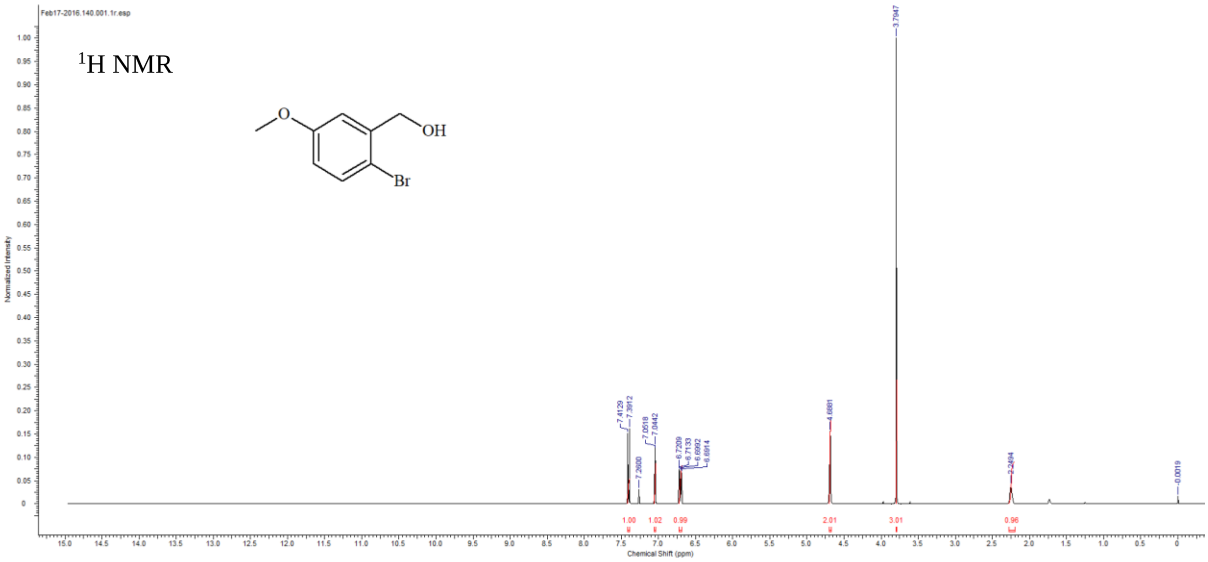

Feb03-2016.171.001.1r.esp
$^{13}$C NMR
Cl
OH
O
O
Normalized Intensity
77.4817
76.8460
120.2984
112.6236
61.0137
56.1576
153.0889
145.5289
135.7554
129.1911
Chemical Shift (ppm)

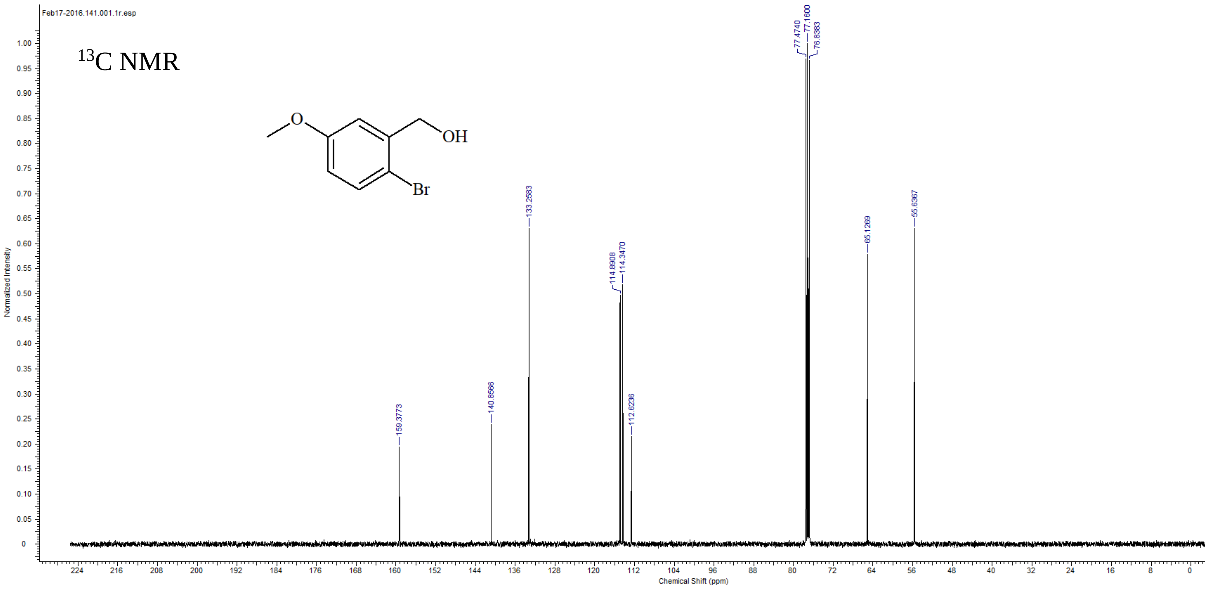

Feb03-2016.140.001.1r.esp
$^1$H NMR
OH
Cl
O
Normalized Intensity
3.9129
4.7990
4.7836
7.2760
7.2563
7.2363
7.1132
7.0961
6.9113
6.8908
2.0321
2.0164
2.0006
1.5997
0.0000
1.03
1.00
1.00
2.00
3.02
1.01
Chemical Shift (ppm)

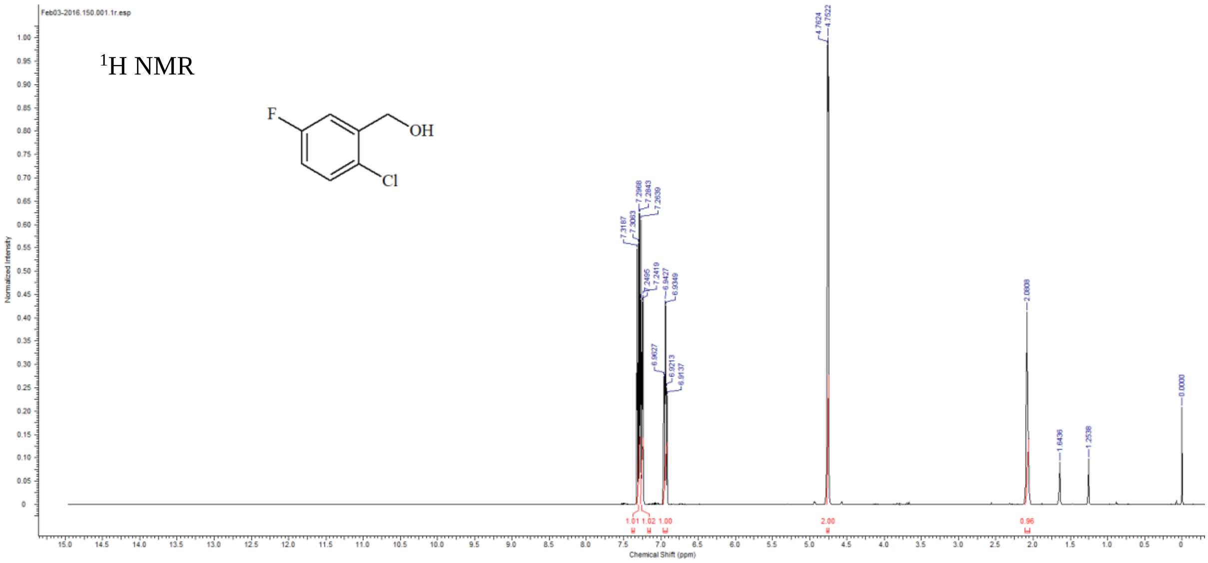

Feb03-2016.141.001.1r.esp
$^{13}$C NMR
OH
Cl
O
155.1876
139.9221
127.5290
120.9648
120.5435
111.3138
77.4817
77.1600
76.8460
63.1890
56.4180
Normalized Intensity
Chemical Shift (ppm)

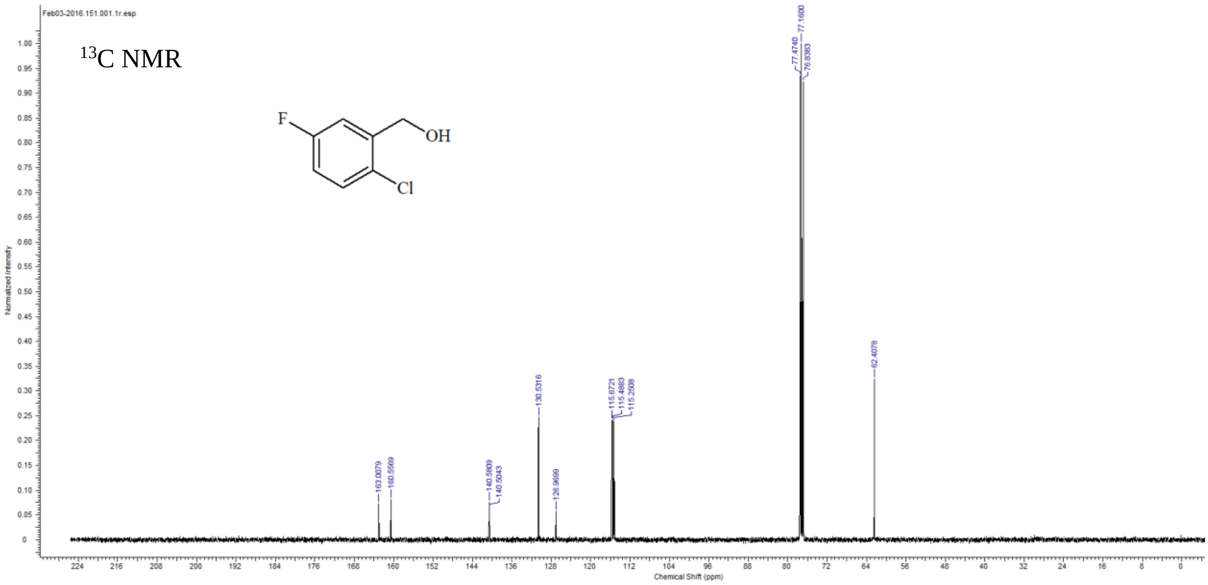

Feb17-2016.120.001.1r.esp
$^{1}$H NMR
O
OH
Cl
7.2600
7.2383
7.2222
7.2195
7.1330
7.1139
7.1042
7.0886
4.8320
2.4605
1.9292
0.0037
1.01 1.04 1.03
2.04
3.02
1.01
Normalized Intensity
Chemical Shift (ppm)


Feb17-2016.121.001.1r.esp
$^{13}$C NMR
O
OH
Cl
139.7536
136.0541
134.9741
129.3596
129.1758
127.4448
77.4740
77.1600
76.8383
59.7652
19.8132
Normalized Intensity
Chemical Shift (ppm)

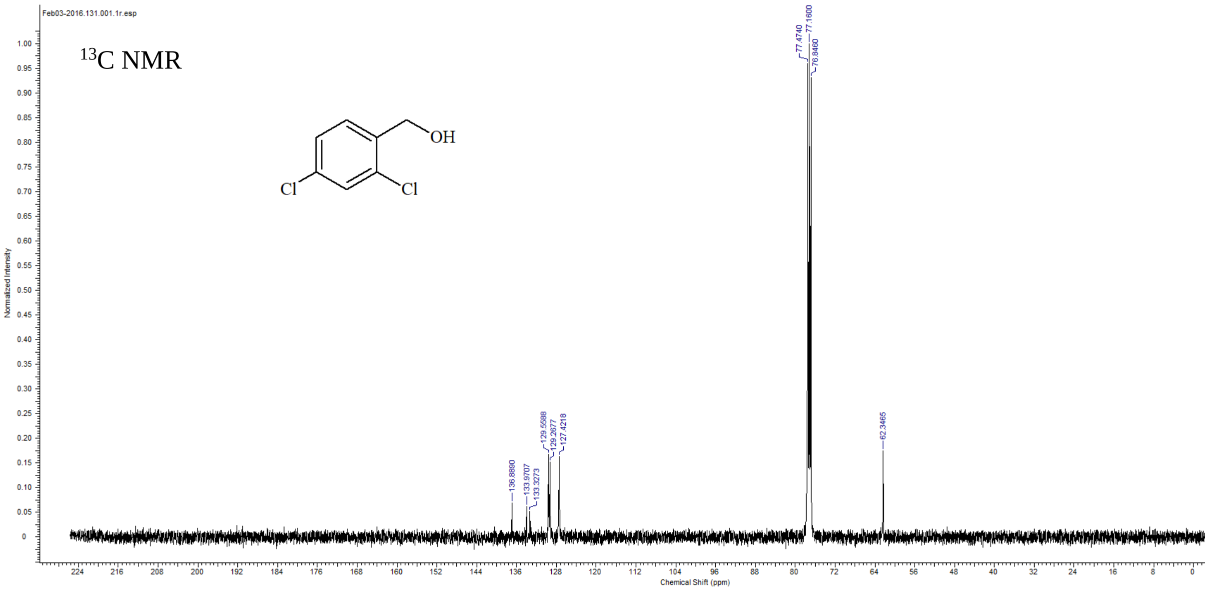

Feb17-2016.140.001.1r.esp
1H NMR
O
OH
Br
Normalized Intensity
7.4129
7.3912
7.2600
7.0518
7.0442
6.7209
6.7133
6.6992
6.6914
4.6881
3.7947
2.2494
0.0019
1.00
1.02
0.99
2.01
3.01
0.96
Chemical Shift (ppm)

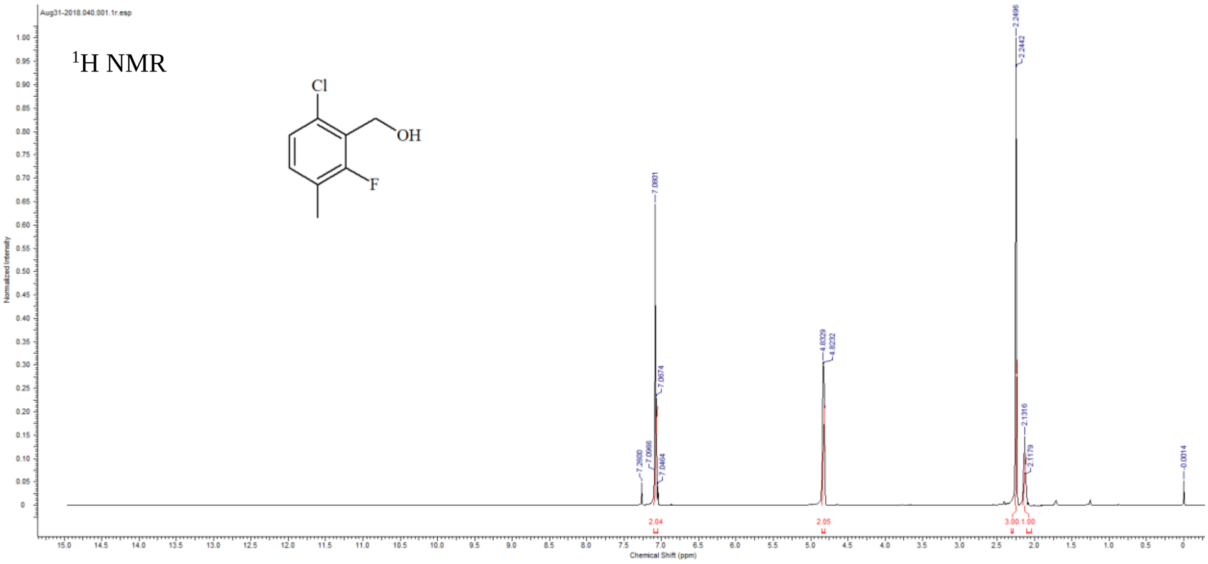

Feb17-2016.141.001.1r.esp
13C NMR
O
OH
Br
Normalized Intensity
159.3773
140.8566
133.2583
114.8908
114.3470
112.6236
77.4740
77.1600
76.8383
65.1269
55.6367
Chemical Shift (ppm)

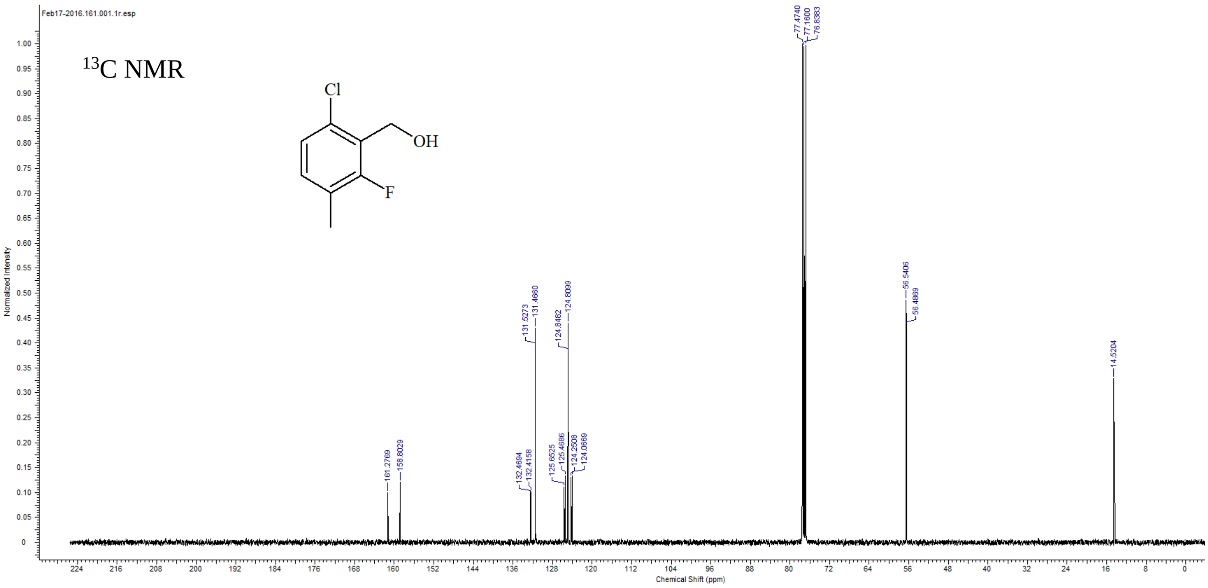

Feb03-2016.150.001.1r.esp
1H NMR
F
OH
Cl
Normalized Intensity
7.3187
7.3063
7.2968
7.2843
7.2639
7.2495
7.2419
6.9427
6.9349
6.9627
6.9213
6.9137
4.7624
4.7522
2.0809
1.6436
1.2538
0.0000
1.01
1.02
1.00
2.00
0.96
Chemical Shift (ppm)

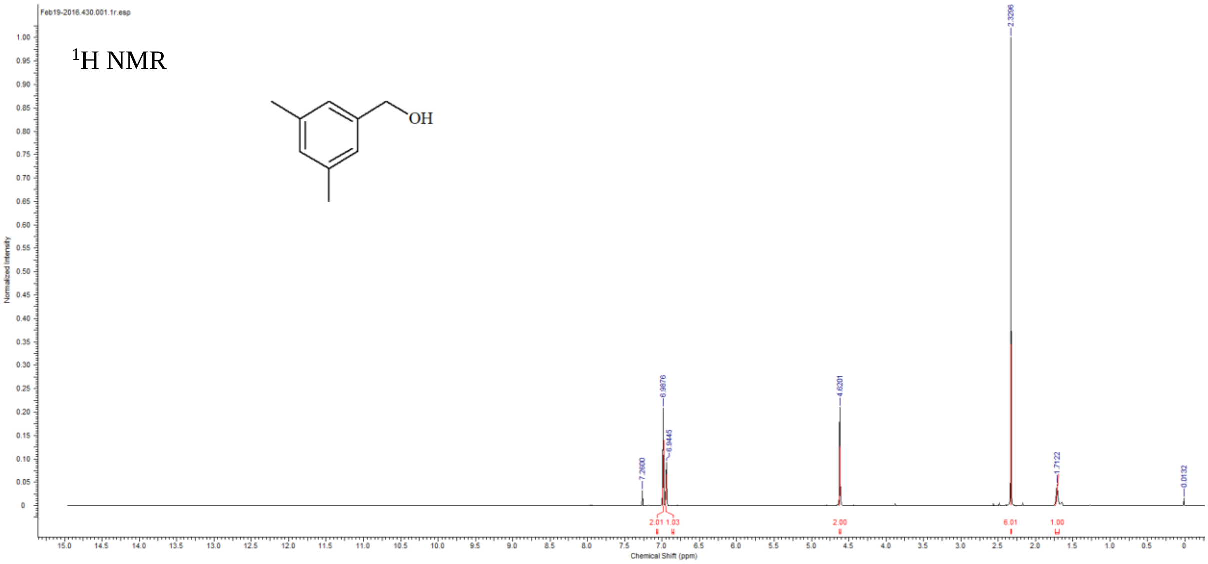

Feb03-2016.151.001.1r.esp
$^{13}$C NMR
F
OH
Cl
Normalized Intensity
163.0079
160.5569
140.5809
140.5043
130.5316
128.9699
115.6721
115.4883
115.2508
77.4740
77.1600
76.8383
62.4078
Chemical Shift (ppm)

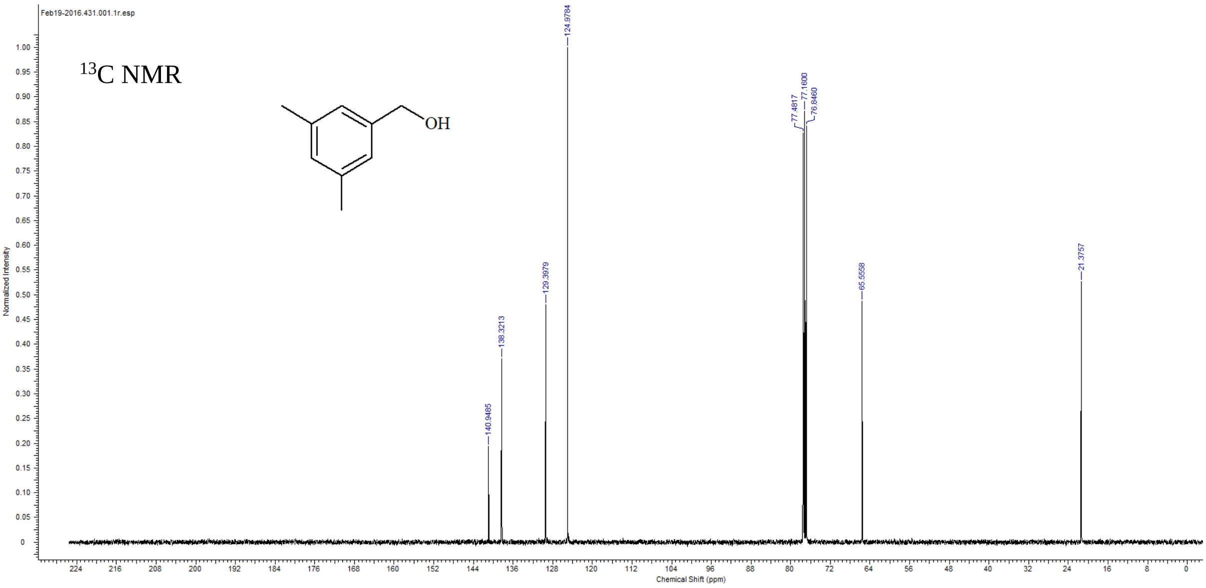

Feb03-2016.130.001.1r.esp
$^{1}$H NMR
OH
Cl
Cl
Normalized Intensity
7.4470
7.4262
7.3772
7.2621
4.7456
1.9987
1.5976
0.0000
1.00
1.00
1.01
2.02
1.01
Chemical Shift (ppm)

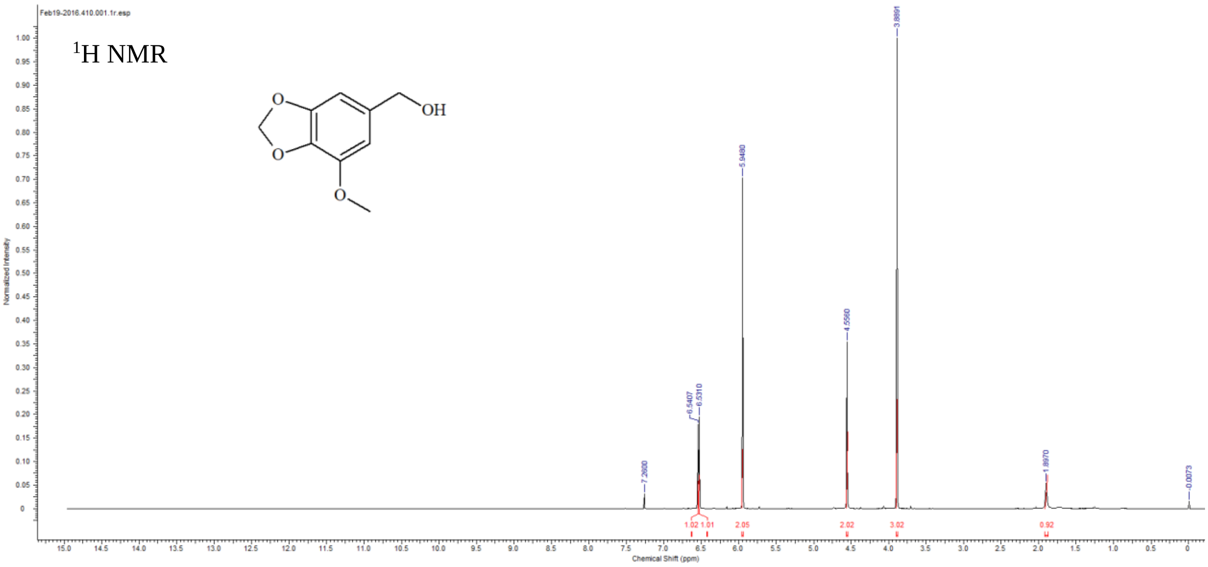

Feb03-2016.131.001.1r.esp
$^{13}$C NMR
OH
Cl
Cl
Normalized Intensity
136.8890
133.9707
133.3273
129.5588
129.2677
127.4218
77.4740
77.1600
76.8460
62.3465
Chemical Shift (ppm)

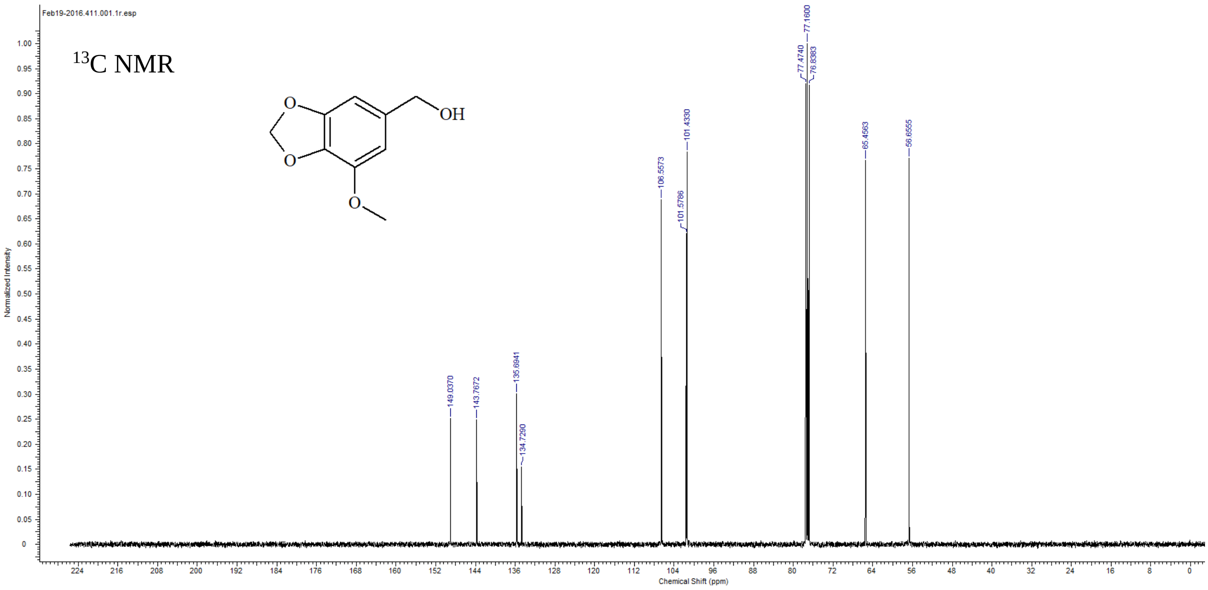

Aug31-2018.040.001.1r.esp
¹H NMR
Cl
OH
F
Normalized Intensity
7.2600
7.0966
7.0801
7.0674
7.0464
4.8329
4.8232
2.2496
2.2442
2.1316
2.1179
-0.0014
2.04
2.05
3.00
1.00
Chemical Shift (ppm)

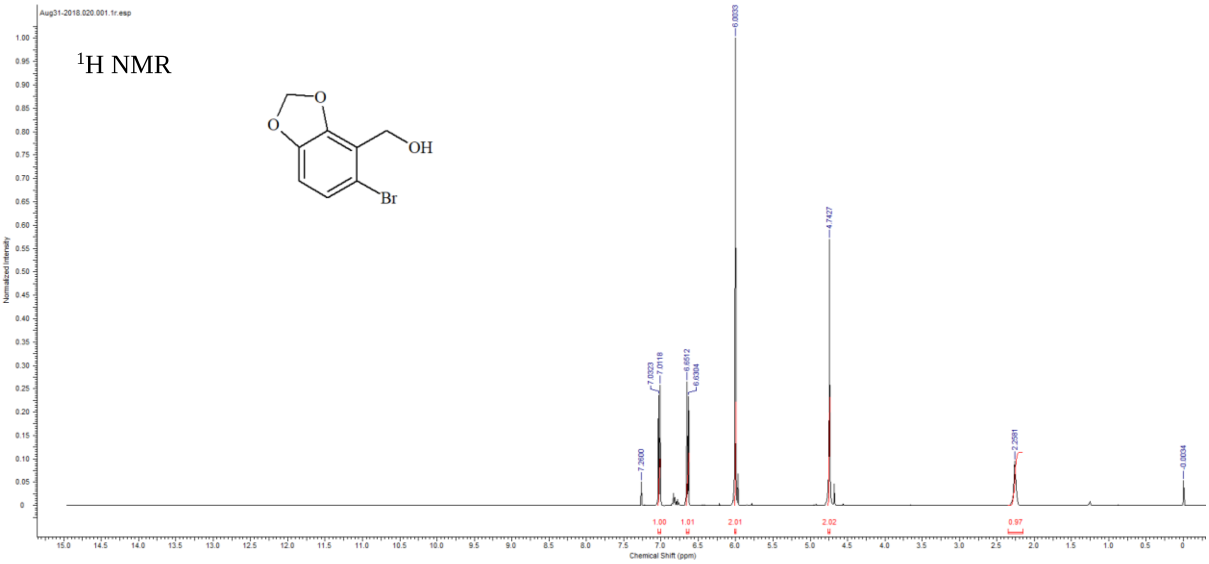

Feb17-2016.161.001.1r.esp
¹³C NMR
Cl
OH
F
Normalized Intensity
161.2769
158.8029
132.4694
132.4158
131.5273
131.4660
125.6525
125.4686
124.8482
124.8099
124.2508
124.0669
77.4740
77.1600
76.8383
56.5406
56.4869
14.5204
Chemical Shift (ppm)

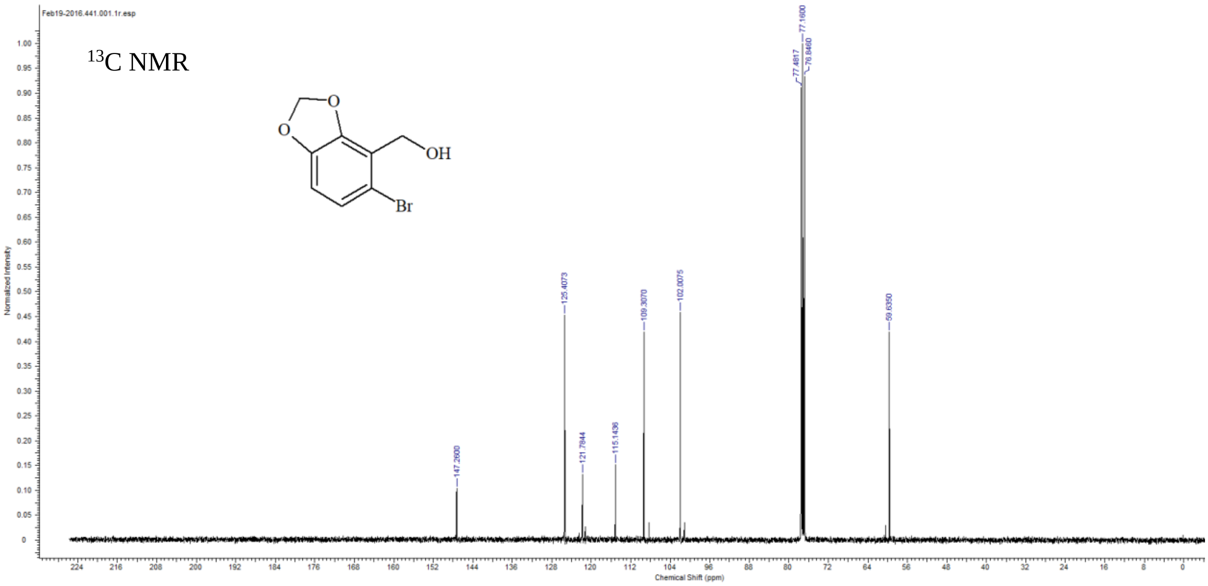

Feb19-2016.430.001.1r.esp
¹H NMR
OH
Normalized Intensity
7.2600
6.9876
6.9445
4.6201
2.3296
1.7122
0.0132
2.01
1.03
2.00
6.01
1.00
Chemical Shift (ppm)

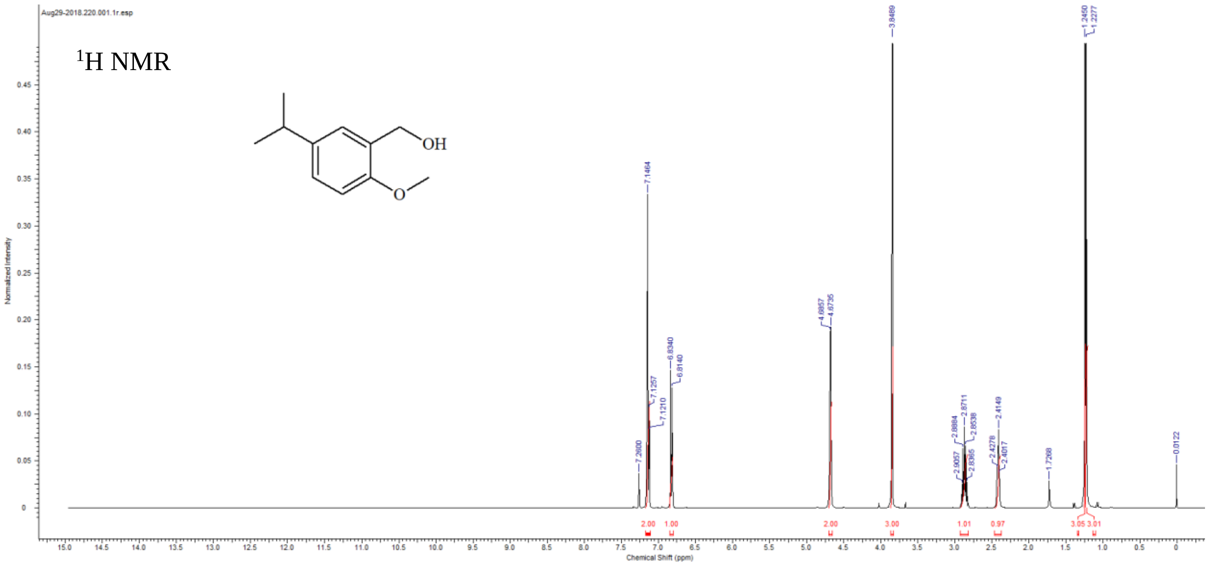

Feb19-2016.431.001.1r.esp
$^{13}$C NMR
OH
140.9495
138.3213
129.3979
124.9784
77.4817
77.1600
76.8460
65.5558
21.3757
Normalized Intensity
Chemical Shift (ppm)

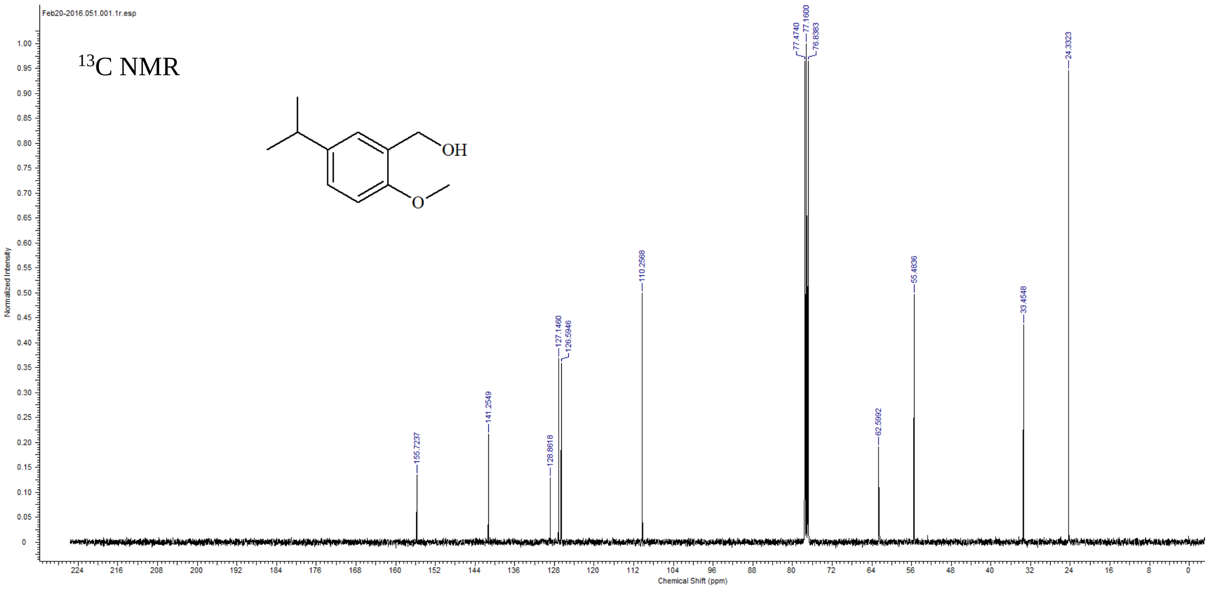

Feb19-2016.410.001.1r.esp
$^{1}$H NMR
O
O
OH
O
7.2600
6.5407
6.5310
5.9480
4.5560
3.8891
1.8970
0.0073
1.02
1.01
2.05
2.02
3.02
0.92
Normalized Intensity
Chemical Shift (ppm)

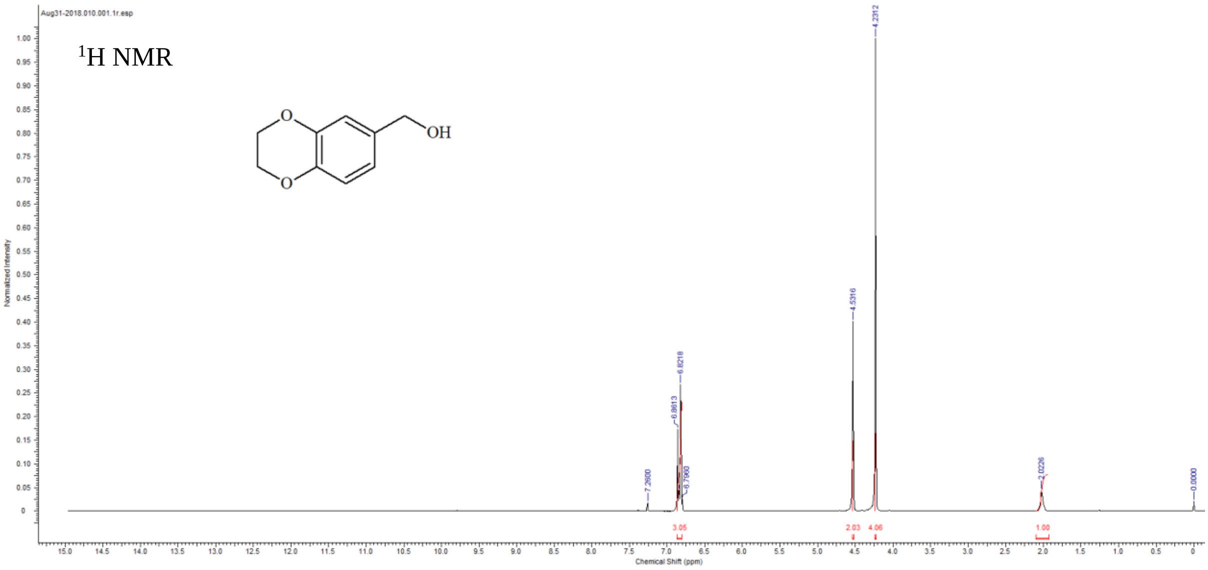

Feb19-2016.411.001.1r.esp
$^{13}$C NMR
O
O
OH
O
149.0370
143.7672
135.6941
134.7290
106.5573
101.5786
101.4330
77.4740
77.1600
76.8383
65.4563
56.6555
Normalized Intensity
Chemical Shift (ppm)

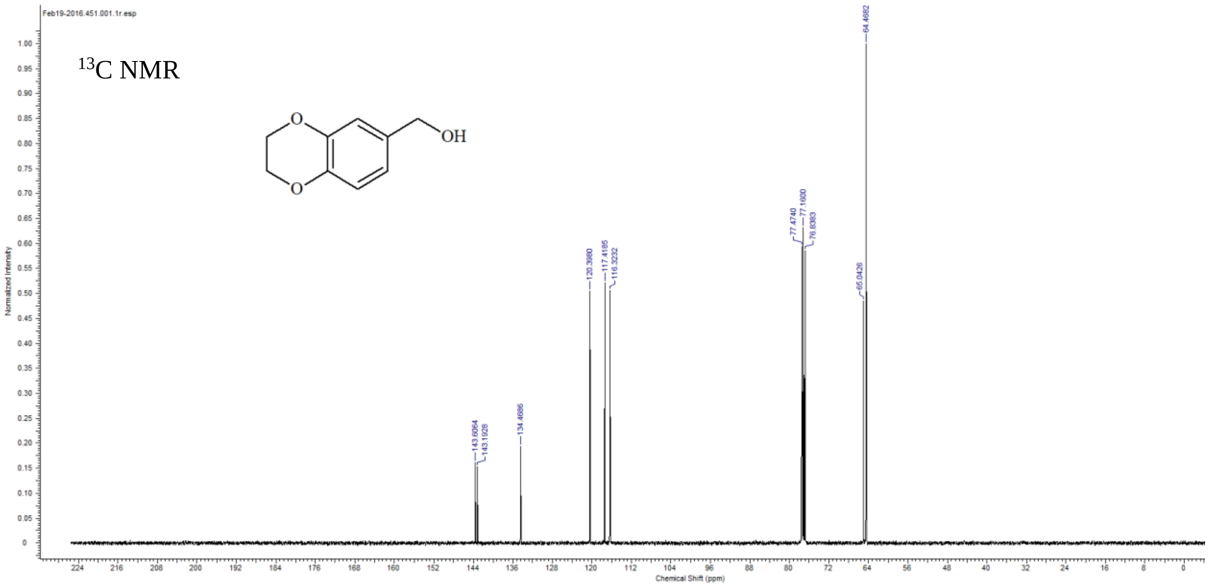

Aug31-2018.020.001.1r.esp
$^1$H NMR
O
O
OH
Br
6.0033
4.7427
7.0323
7.0118
6.6512
6.6304
7.2600
2.2581
-0.0034
1.00
1.01
2.01
2.02
0.97
Normalized Intensity
Chemical Shift (ppm)

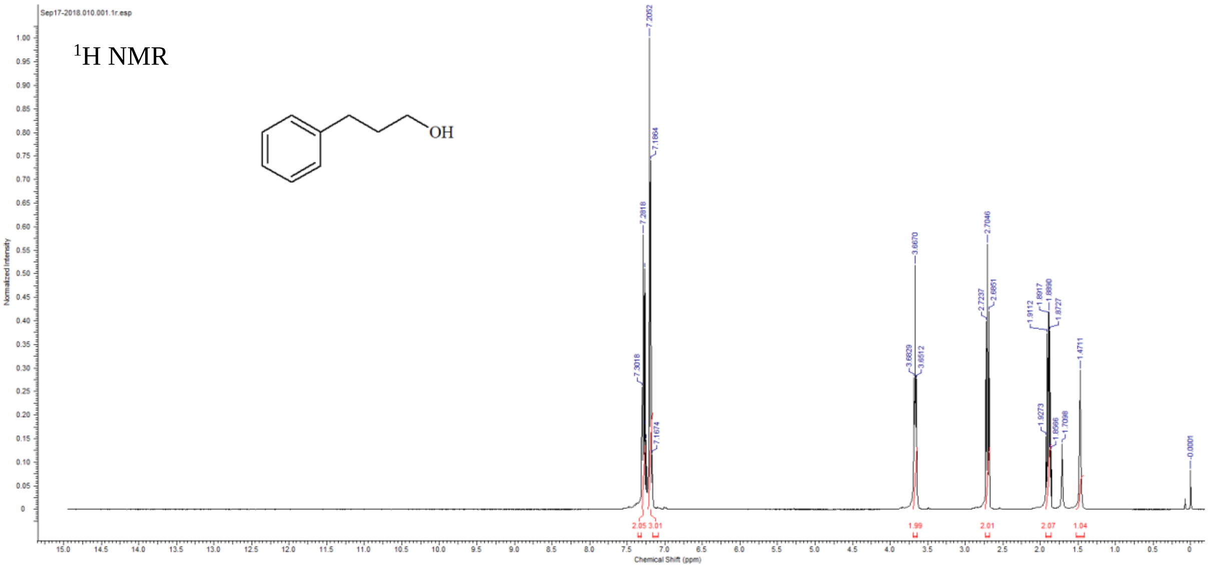

Feb19-2016.441.001.1r.esp
$^{13}$C NMR
O
O
OH
Br
77.4817
77.1600
76.8460
125.4073
109.3070
102.0075
59.6350
147.2600
121.7844
115.1436
Normalized Intensity
Chemical Shift (ppm)

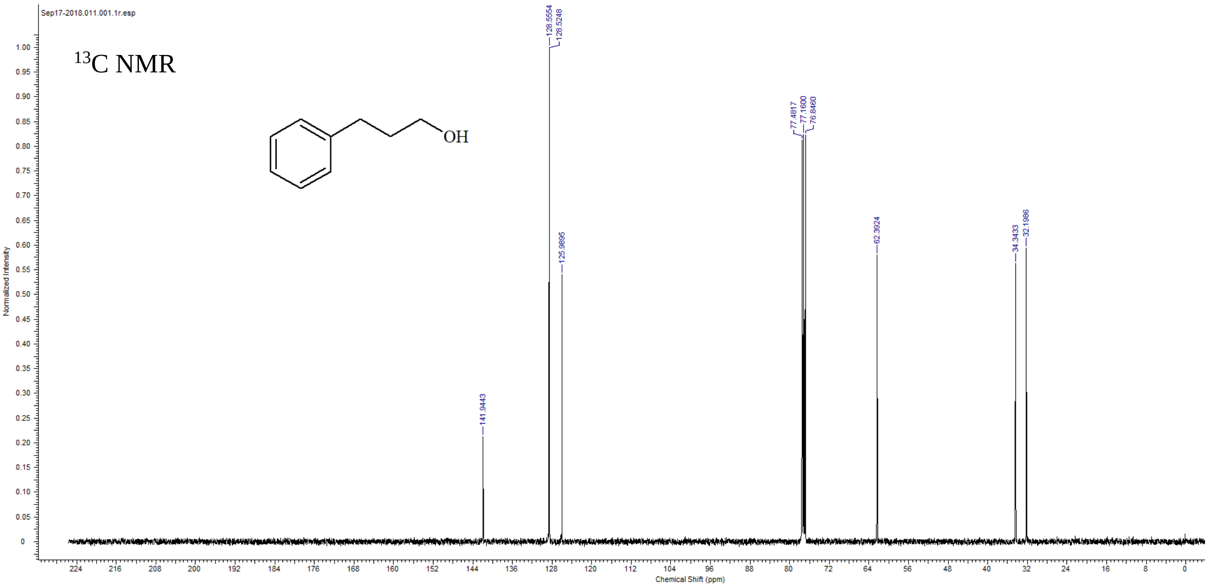

Aug29-2018.220.001.1r.esp
$^1$H NMR
OH
O
3.8469
1.2450
1.2277
7.1464
4.6857
4.6735
6.8340
6.8140
7.1257
7.1210
2.8884
2.8711
2.8538
2.9057
2.8365
2.4149
2.4278
2.4017
7.2600
1.7288
0.0122
2.00
1.00
2.00
3.00
1.01
0.97
3.05
3.01
Normalized Intensity
Chemical Shift (ppm)

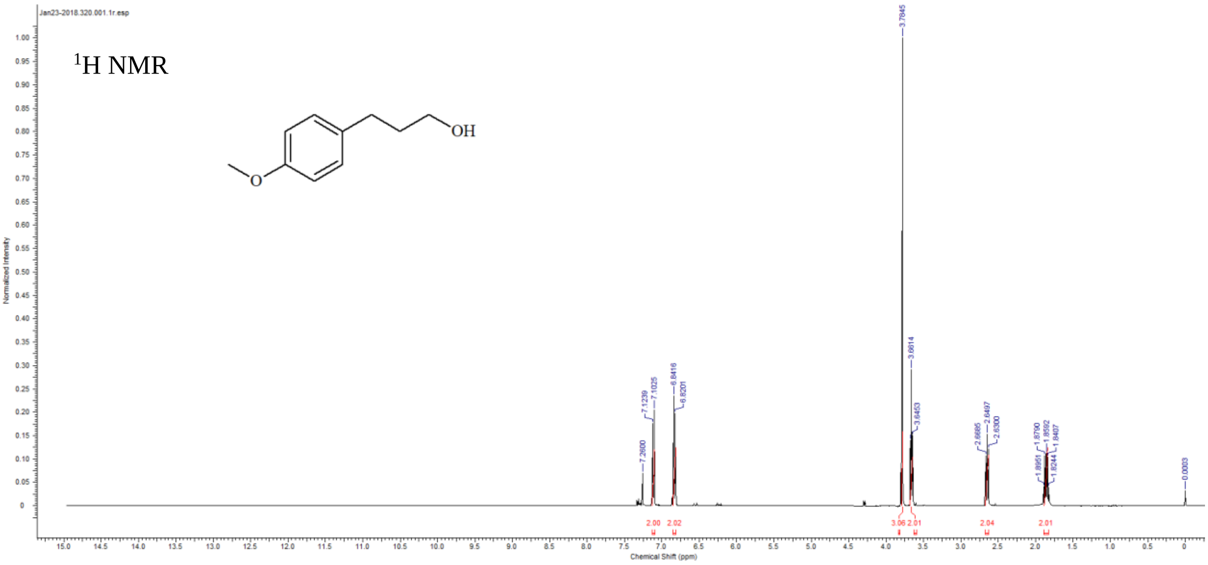

Feb20-2016.051.001.1r.esp
$^{13}$C NMR
OH
O
155.7237
141.2549
128.8818
127.1460
126.5946
110.2568
77.4740
77.1600
76.8383
62.5992
55.4836
33.4548
24.3323
Normalized Intensity
Chemical Shift (ppm)

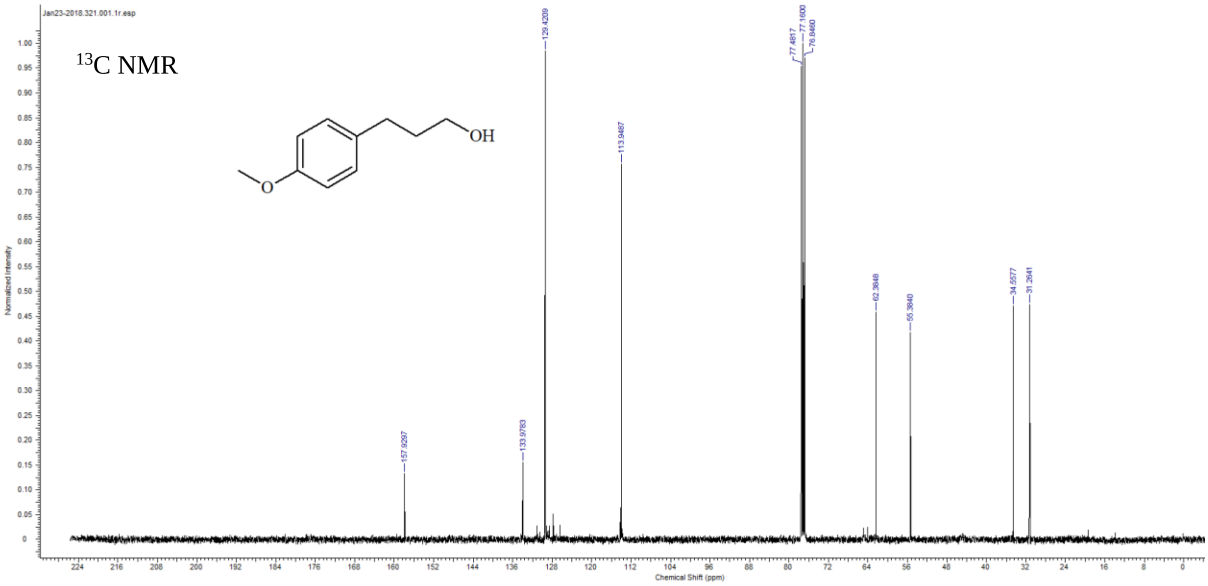

Aug31-2018.010.001.1r.esp
$^{1}$H NMR
O
O
OH
7.2600
6.8613
6.8218
6.7990
4.5316
4.2312
2.0226
0.0000
3.05
2.03
4.06
1.00
Normalized Intensity
Chemical Shift (ppm)


Feb19-2016.451.001.1r.esp
$^{13}$C NMR
O
O
OH
143.6064
143.1928
134.4686
120.3980
117.4185
116.3232
77.4740
77.1600
76.8383
65.0426
64.4682
Normalized Intensity
Chemical Shift (ppm)

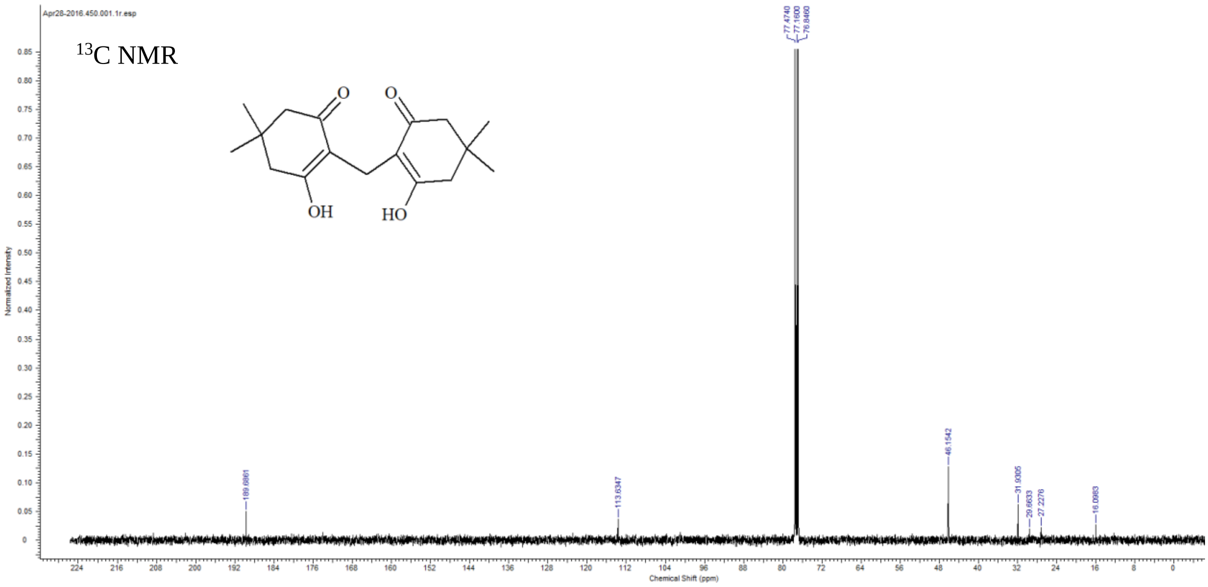

Sep17-2018.010.001.1r.esp
$^{1}$H NMR
OH
7.2052
7.1864
7.2818
7.3018
7.1674
3.6670
3.6829
3.6512
2.7046
2.7237
2.6851
1.9112
1.8917
1.8890
1.8727
1.4711
0.0001
2.05
3.01
1.99
2.01
2.07
1.04
Normalized Intensity
Chemical Shift (ppm)

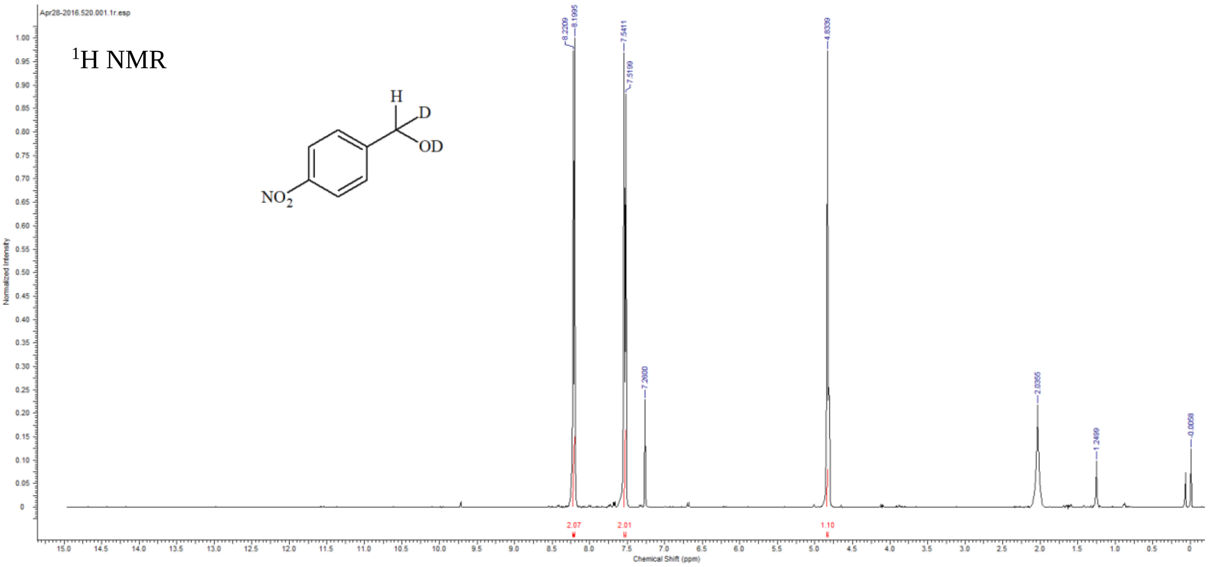

Sep17-2018.011.001.1r.esp
$^{13}$C NMR
OH
141.9443
128.5554
128.5248
125.9695
77.4817
77.1600
76.8460
62.3924
34.3433
32.1986
Normalized Intensity
Chemical Shift (ppm)


Jan23-2018.320.001.1r.esp
$^{1}$H NMR
OH
O
3.7845
3.6614
3.6453
7.2600
7.1239
7.1025
6.8416
6.8201
2.6685
2.6497
2.6300
1.8951
1.8790
1.8592
1.8407
1.8244
0.0003
2.00
2.02
3.06
2.01
2.04
2.01
Normalized Intensity
Chemical Shift (ppm)


Jan23-2018.321.001.1r.esp
$^{13}$C NMR
OH
O
157.9297
133.9783
129.4209
113.9487
77.4817
77.1600
76.8460
62.3848
55.3840
34.5577
31.2641
Normalized Intensity
Chemical Shift (ppm)


Apr27-2016.300.001.1r.esp
$^{1}$H NMR
O
O
OH
HO
11.5699
7.2600
3.1586
2.2932
2.2813
1.5581
1.0500
-0.0012
2.00
2.03
8.03
2.04
12.06
Normalized Intensity
Chemical Shift (ppm)


Apr28-2016.450.001.1r.esp
$^{13}$C NMR
O
O
OH
HO
189.6861
113.6347
77.4740
77.1600
76.8460
46.1542
31.9305
29.8633
27.2276
16.0983
Normalized Intensity
Chemical Shift (ppm)


Apr28-2016.520.001.1r.esp
$^1$H NMR
H
D
OD
NO$_2$
8.2209
8.1995
7.5411
7.5199
7.2600
4.8339
2.0355
1.2499
-0.0058
2.07
2.01
1.10
Normalized Intensity
Chemical Shift (ppm)
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0
15.0
14.5
14.0
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0