Electronic Supplementary Material (ESI) for ChemComm.

Manganese-Catalysed Transfer Hydrogenation of Esters

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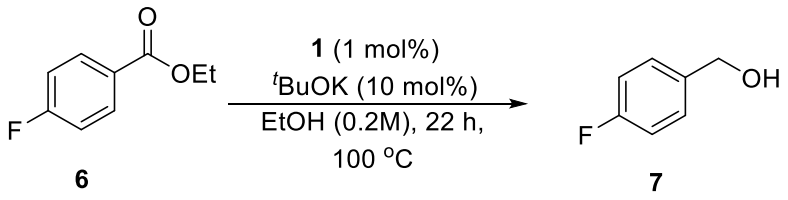
Contents

General Information:

The preparation of solutions for the use in catalytic reactions were carried out under either argon or nitrogen atmospheres. All glassware was used oven dried or flame dried and cooled under vacuum before use. When the term 'backfilled' is used it refers to filling a flask previously under vacuum with N_2/Ar by use of a Schlenk line. Unless otherwise stated, all chemicals were purchased from Sigma-Aldrich, Acros, Alfa Aesar, Strem or TCI and used as received. Substrates were not dried before use in catalysis reactions. Unless otherwise stated, solvents used were 'Extra Dry, AcroSeal™, ACROS Organics' purchased from Fisher Scientific. Room temperature refers to the temperature range 15-25 ^{o}C. Catalysts **1**-**3** were stored under dry N_2 and weighed in air. Heating the reaction mixtures was done with either an oil bath or a Drysyn heating block. Reported temperature is the oil bath or heating block temperature and not internal temperature. *In vacuo* refers to either the use of a Heidolph Laborota 4001 rotary evaporator or the use of a high-vacuum line. Analytical thin layer chromatography (TLC) was carried out on pre-coated plastic plates (Kieselgel 60 F254 silica). TLC visualization was carried out using a UV lamp (254nm) or using a 1% potassium permanganate aqueous solution. Flash silica chromatography was performed using Kieselgel 60 silica.^{1}H, ^{13}C, NMR was carried out using either a Bruker Avance II 400 (400 MHz ^{1}H, 100 MHz ^{13}C, 161 MHz ^{31}P or a Bruker Ultrashield 500 (500 MHz ^{1}H, 125 MHz ^{13}C). NMR analyses were carried out at room temperature in deuterated solvent. The chemical shifts are quoted as parts per million (ppm). Coupling constants, J, are quoted in Hz. Multiplicities are indicated by: s (singlet), d (doublet), t (triplet), q (quartet), qu (quintet), sex (sextet) and m (multiplet). The abbreviation "b" is used to denote broad peak shape. HPLC analysis has been determined using a Varian Prostar operated by Galaxie workstation PC software. For chromatograms where peak baselines were not fully resolved the lowest point between the two peaks were chosen as the cut-off point.

Dark Vs Not Dark Conditions

Table 1 Comparison of dark and not dark conditions[a]



6 **7**

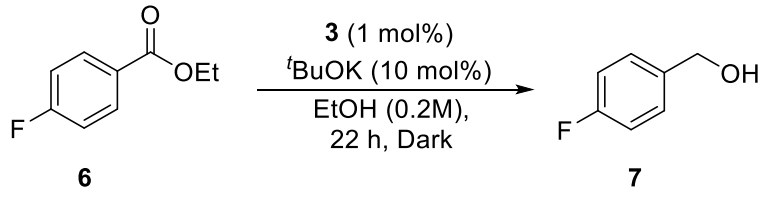
Entry	Catalyst	Conc. (M)	Not Dark/ Dark	Conversion of **6** (%)[b]	**7** (%)[b]
1	**1**	0.2	Not Dark	28	19
2	**1**	0.2	Dark[c]	59	37

[a] Conditions: **6** (0.5 mmol), 1-methylnapthalene (0.15 mmol), ^{t}BuOK (0.05 mmol) and **1** (0.005 mmol) in dry EtOH under constant flow of N_2 at 100 °C for 22h. [b] determined by ^{1}H NMR using 1-methylnapthalene as internal standard. Remainder of mass balance is unidentified products. [c] Foil covered Schlenk tube

Investigation of Catalyst **3** at Lower Temperature

As eluded to in the main text **3** is believed to have lower thermal stability so optimisation experiments were conducted at lower Temperatures.

Table 2 Catalyst **3** Temperature investiagtions[a]

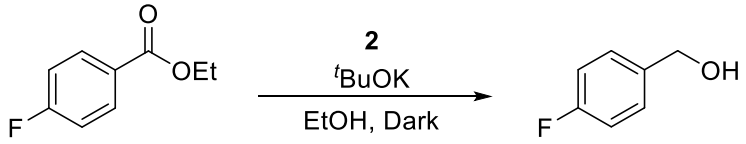


6 **7**

Entry	Conc. (M)	T (°C)	Conversion of **6** (%)[b]	**7** (%)[b]
1	0.2	80	13	13
2	0.2	90	32	17
3	0.2	100	38	22

[a] Conditions: **6** (0.5 mmol), 1-methylnapthalene (0.15 mmol), ^{t}BuOK (0.05 mmol) and **1** (0.005 mmol) in dry EtOH under N_2 for 22h. [b] determined by ^{1}H NMR using 1-methylnapthalene as internal standard. Remainder of mass balance is unidentified products.

Table 3 Further Optimisation of Conditions Using **2** as Catalyst[a]



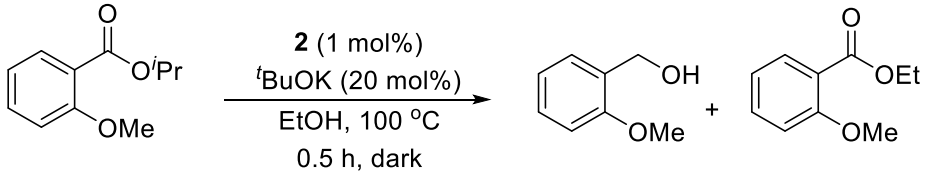
6 **7**

Entry	**2** loading (mol%)	Conc. (M)	KO^{t}Bu loading (mol %)	T (°C)	Time (h)	Conversion of **6** (%)[b]	**7** (%)[b]
1	1	0.25	20	100	22	46	43
2	1	0.5	20	100	22	66	53
3	1	0.5	20	110	22	61	47
4	1	0.75	20	100	22	82	72
5	1	1	20	100	22	84	76
6	1	1.25	20	100	22	86	77
7	1	1.5	20	100	22	89	77
8	1	2	20	100	22	90	76
9	1	2.5	20	100	22	89	75
10	1	1.5	10	100	52	71	65
11	1	2.5	30	100	22	91	52
12	1	2.5	35	100	22	93	41
13	1	2.5	10	100	68	82	62
14	0.5	2	20	100	22	85	65
15	0.5	2	40	100	22	89	33
16	0.1	2	20	100	22	74	48

[a] Conditions: **6** (0.5 mmol), 1-methylnapthalene (0.15 mmol), ^{t}BuOK and **2** in dry EtOH under N_2. [b] determined by ^{1}H NMR using 1-methylnapthalene as internal standard.

Transesterification Investigation

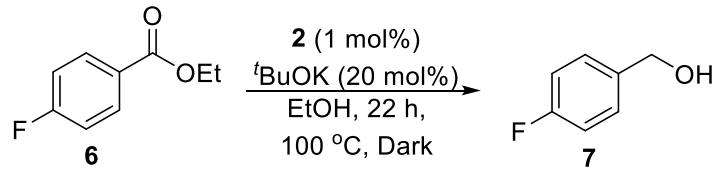
Scheme 1 Ratio of Species Present after 0.5 h Reaction with ^{i}Pr Ester[a]

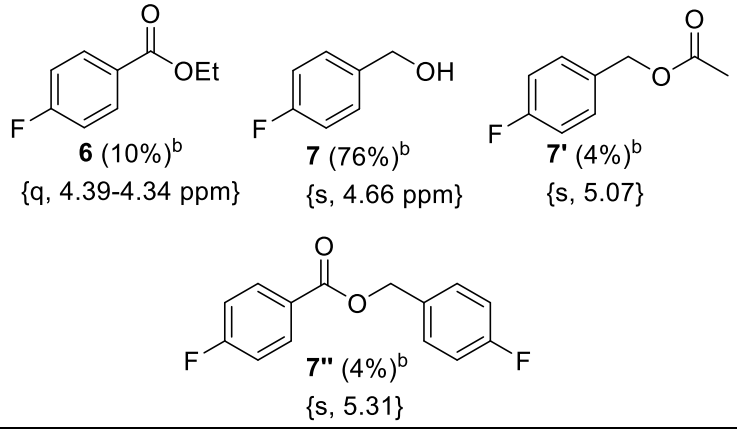


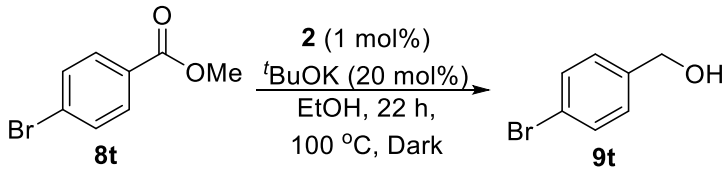
8x (7%)[b] **9f** (43%)[b] **8f** (45%)[b]

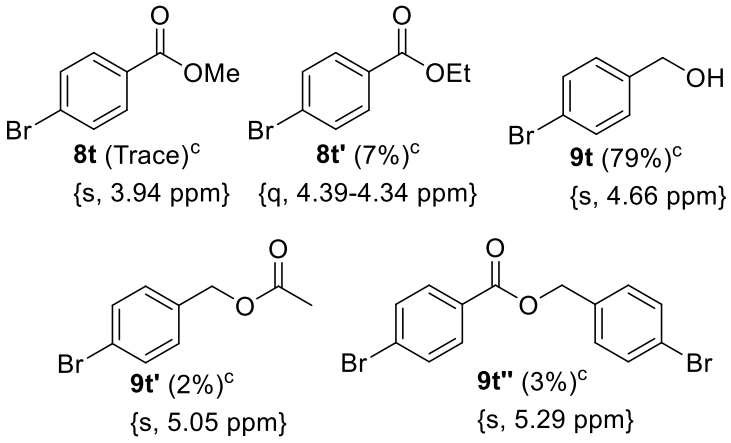
[a] Conditions: **10e** (0.5 mmol), 1-methylnapthalene (0.15 mmol), ^{t}BuOK (0.10 mmol) and **2** (0.005 mmol) in dry EtOH (0.25 mL) under N_2 at 100 °C. [b] determined by ^{1}H NMR using 1-methylnapthalene as internal standard. Remainder of mass balance is unidentified products.

Table 4 ^{1}H NMR Investigation of Species Present Following Ester Transfer Hydrogenation Reactions Catalysed by **2**[a]

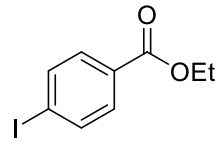
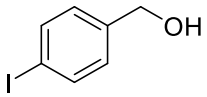
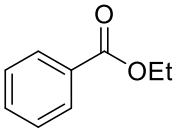
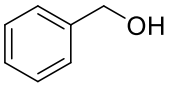
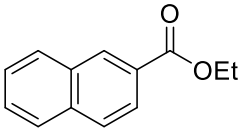
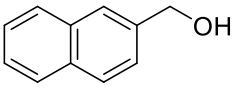
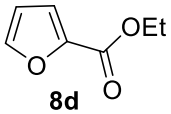
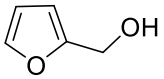
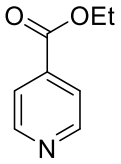
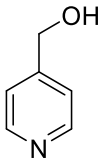
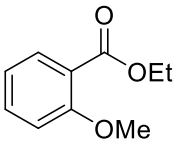
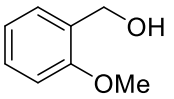
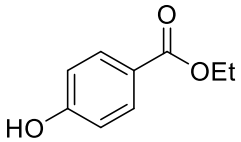
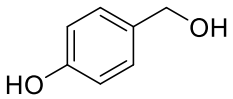
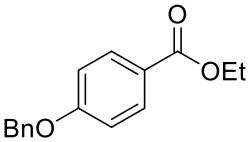
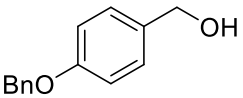
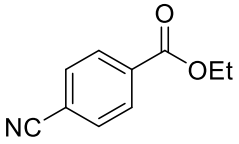
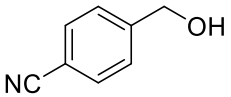


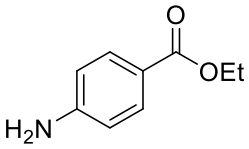
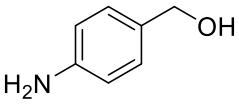
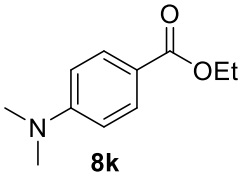
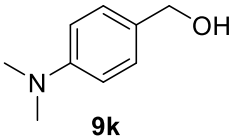
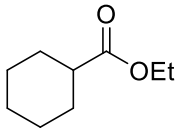
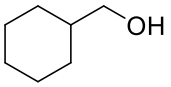
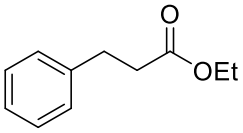
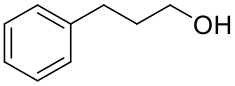
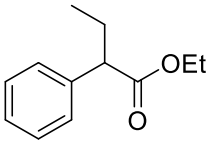
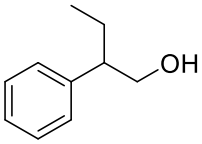
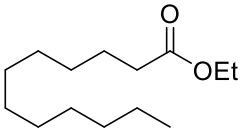
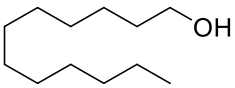
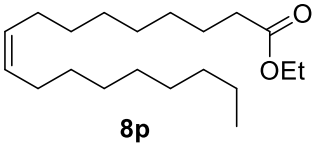
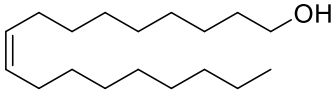
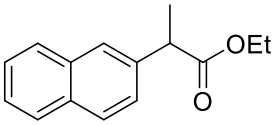
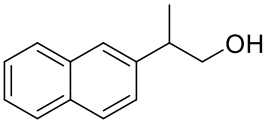
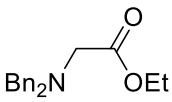
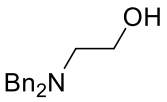
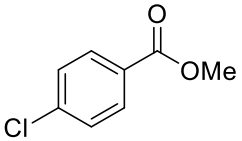
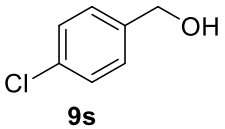


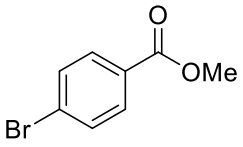
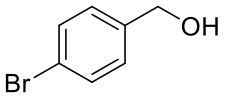
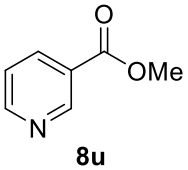
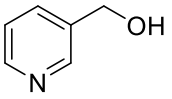
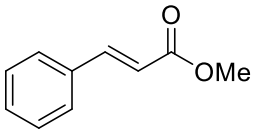
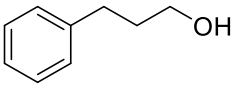
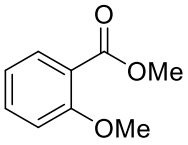
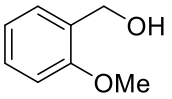
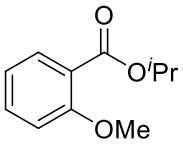
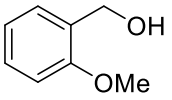




[a] Conditions: ester substrate (0.5 mmol), (1-methylnapthalene (0.15 mmol)), ^{t}BuOK (0.10 mmol) and **2** (0.005 mmol) in dry EtOH (0.25 mL) under N_2 at 100 °C. [b] determined by ^{1}H NMR using 1-methylnapthalene as internal standard. [c] determined by ^{1}H NMR using 1,4-dimethoxybenzene as internal standard. The characteristic resonances integrated to obtain values are given in { } brackets. Products were identified by comparison with literature: **7'**,[1] **7''**,[2] **9t'**,[3] **9t''**.[4]

Table 5 Substrate Scope Table Including Conversion of Ester Starting Material[a,b]				
Entry	Ester Substrate	Alcohol Product	Conversion of SM (%)[c]	Yield (%)
1	 **8a**	 **9a**	95	(81)
2	 **8b**	 **9b**	84	(69)
3	 **8c**	 **9c**	>99	(87)
4	 **8d**	 **9d**	>99	(82)
5	 **8e**	 **9e**	>99	(83)
6	 **8f**	 **9f**	>99	(76)
7	 **8g**	 **9g**	15	10[b]
8	 **8h**	 **9h**	63	(48)
9	 **8i**	 **9i**	Trace	Trace[b]

10	 **8j**	 **9j**	Trace	Trace
11	 **8k**	 **9k**	20	10[b]
12	 **8l**	 **9l**	98	(78)
13	 **8m**	 **9m**	93	(82)
14	 **8n**	 **9n**	90	(71)
15	 **8o**	 **9o**	86	(77)
16	 **8p**	 **9p**	92	(76)
17	 **8q**	 **9q**	>99	(82)
18	 **8r**	 **9r**	85	(63)
19	 **8s**	 **9s**	97	(79)

20	 **8t**	 **9t**	93	(79)
21	 **8u**	 **9u**	>99	(84)
22	 **8v**	 **9m**	95	(74)
23	 **8w**	 **9f**	>99	(82)
24	 **8x**	 **9f**	>99	(77)

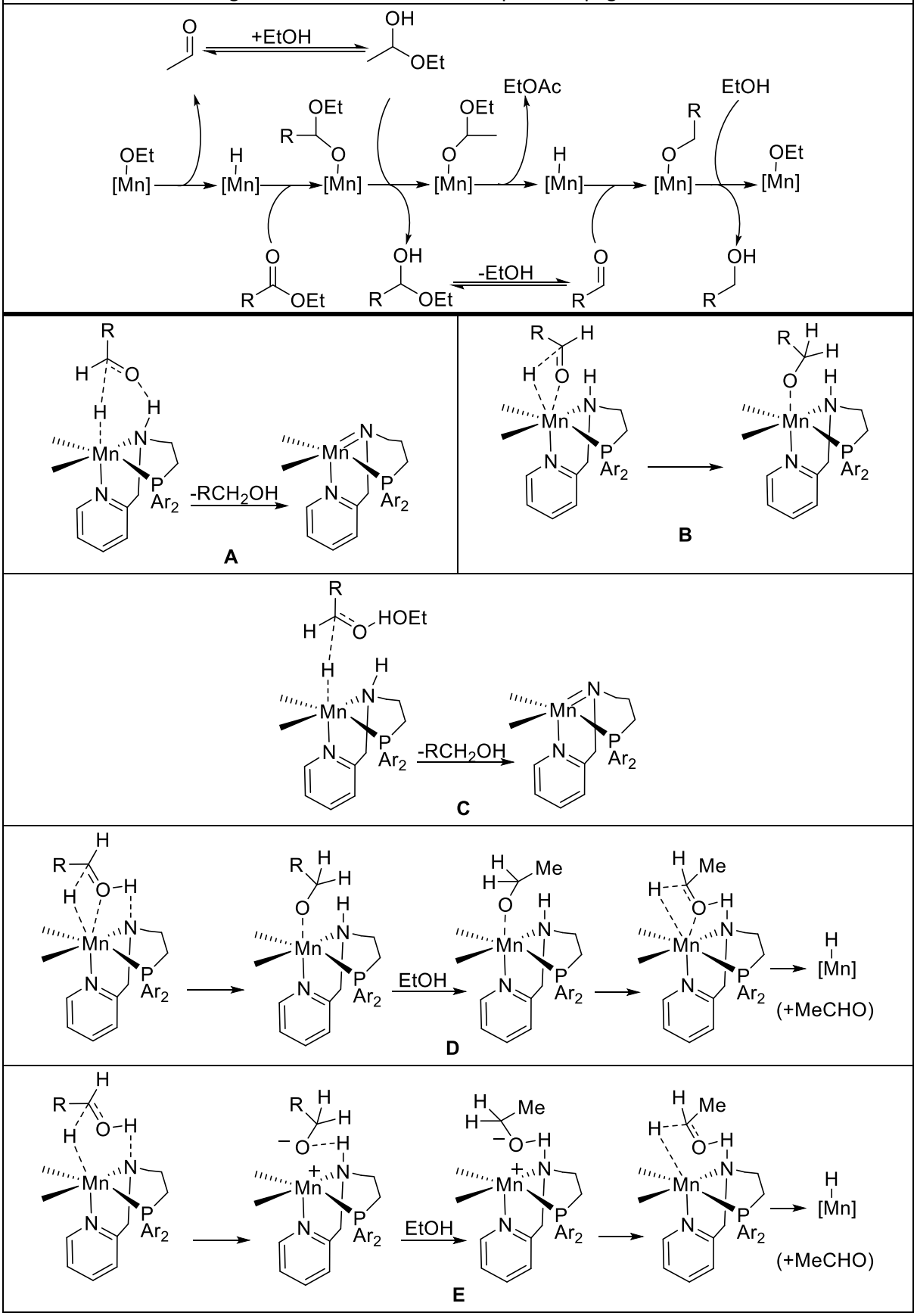
[a] Conditions: ester substrate (0.5 mmol), 1-methylnapthalene (0.15 mmol), ^{t}BuOK (0.10 mmol) and **2** (0.005 mmol) in dry EtOH (0.25 mL) under N_2 at 100 °C. [b] ester substrate (0.5 mmol), ^{t}BuOK (0.1 mmol) and **2** (0.005 mmol) in dry EtOH (0.25 mL) under N_2 atmosphere at 100 °C for 22h. [c] determined by ^{1}H NMR using 1-methylnapthalene/ 1,4-dimethoxybenzene as internal standard.

Comment on the details of the mechanism of Mn-catalysed hydrogen transfer.

Scheme 2 in the paper (reproduced and expanded upon overleaf) gives a simplified mechanism that we propose for this reaction.

The [Mn]…OEt species represented in this scheme shows an interaction of alkoxide with the manganese complex, [Mn] (i.e. either the metal itself or a ligand). A reviewer expressed interest in the details of the hydrogen transfer, so in case this is of interest to a reader, we enlarge on the options for this here. The first thing to note from the large amount of literature on hydrogen transfer processes using metal complexes with NH-amino ligands is that there are a variety of mechanisms at a detailed level. The main options discussed from the literature on ruthenium have been transposed onto the catalyst discussed in this paper. Some of these mechanisms represent initial plausible ideas from authors from papers that are not dealing with mechanistic evidence, through to others put forward as a result of experimental and computational mechanistic studies. It can also be seen that even details elucidated by kinetic evidence, detection of relevant intermediates, and DFT calculations have sometimes been revised after DFT calculations at a higher level (See P. Dub, J. C. Gordon, *Dalton Trans.*, 2016, **45**, 4756)[5] The methodology used to conduct DFT calculations on the same system can then lead to a change in the favoured scenario from the five main possibilities outlined for this Mn catalyst in the scheme below. This points to the differences being energetically subtle, and some of these distinct mechanisms can be viewed as having a closer resemblance to each other than is generally presented. Mechanisms D and E, which we would tentatively propose as being more likely than A-C, could be presented as being very distinct: one is inner sphere and one is outer sphere. However, you could also consider them as two extremes of a continuum between covalent bonding and ionic bonding (with the latter stabilised by NH functions). Metal to ligand bonds to anions can have both these characters, with the type of interaction favoured being dependent on the exact structure of the catalysts used and possibility the reaction conditions (solvent choice etc.). This probably explains the difficulty elucidating these fine details correctly. For this catalytic cycle, we would propose the ethoxide ligand needs some close contact with the overall metal complex in order to transfer a hydride, and close contact is most easily accomplished by either an attractive interaction with an NH function or the metal centre. Further mechanistic study of the details of the cycle, including quantifying the energetic differences for this specific *P,N,N*/ Mn relative to other complexes would be welcome.

Table 6 Schemes relating to mechanistic comment on previous page



Catalysts/ Ligands **1-5** were prepared using previously published syntheses[6–8]

General Procedure for the Synthesis of Ethyl Ester Substrates from Carboxylic Acids-Procedure A
To a 100 mL round bottom flask with condenser attached is added carboxylic acid which is dissolved in (not 'Extra Dry') EtOH (0.3 M) and H_2SO_4 (~1 mol%) is added. The reaction is stirred at reflux for 8 h, cooled and solvent removed *in vacuo*. The crude material is diluted in CH_2Cl_2 (1 mL/ mmol carboxylic acid used) and washed with sat. $NaHCO_3$ solution (3 mL/ mmol carboxylic acid used). The aqueous phase was extracted 2x with CH_2Cl_2 (1 mL/ mmol carboxylic acid used) and the combined organic layers washed with brine. The organic layer was then dried over Na_2SO_4, filtered and solvent removed *in vacuo*.

General Procedure for the Mn Catalysed Transfer Hydrogenation of Esters-Liquid Ester- Procedure B
Dry EtOH, ester substrate and 1-methylnapthelene were added to separate flame dried microwave vials (5 mL) equipped with a crimp cap and placed under a nitrogen atmosphere. These were degassed by sparging with either N_2 or Ar for 30 minutes. A flame dried Schlenk tube was equipped with a rubber septum, and placed under a N_2 atmosphere, prior to being briefly opened to allow the addition of Mn Cat. **2** (4.2 mg, 0.005 mmol, 0.01 eq.), and then wrapped in aluminium foil. The tube was placed under vacuum while waiting for the liquids to be sparged with inert gas. The Schlenk tube was placed under a N_2 atmosphere, prior to the addition of EtOH (0.25 mL, 2M), ester substrate (0.5 mmol, 1 eq.) and 1-methylnapthalene (20 µL, 0.15 mmol) *via* syringe. A small aliquot was then taken to determine internal standard to ester substrate ratio by ^{1}H NMR. A 1M soln of KO^{t}Bu in ^{t}BuOH (0.1 mmol, 0.2 eq.) was finally added *via* syringe and the reaction stirred in a pre-heated oil bath set at 100 ° for 22 h. Upon which time reaction was cooled and a ^{1}H NMR was taken to determine conversion using 1-methylnapthalene as internal standard. The products were isolated as described next to the analytical data.

General Procedure for the Mn Catalysed Transfer Hydrogenation of Esters-Solid Ester- Procedure C
Dry EtOH, was added to a flame dried microwave vials (5 mL) equipped with a crimp cap and placed under a nitrogen atmosphere. And was degassed by sparging with either N_2 or Ar for 30. A flame dried Schlenk tube was equipped with a rubber septum, and placed under a N_2 atmosphere, prior to being briefly opened to allow the addition of Mn Cat. **2** (4.2 mg, 0.005 mmol, 0.01 eq.) and ester substrate (0.5 mmol, 1 eq.) and then wrapped in aluminium foil. The tube was placed under vacuum while waiting for the liquids to be sparged with inert gas. The Schlenk tube was placed under a N_2 atmosphere, prior to the addition of EtOH (0.25 mL, 2M) *via* syringe. A 1M soln of KO^{t}Bu in ^{t}BuOH (0.1 mmol, 0.2 eq.) was finally added *via* syringe and the reaction stirred in a pre-heated oil bath set at 100 ° for 22 h. Upon which time reaction was cooled and a ^{1}H NMR was taken to determine conversion using 1,4-dimethoxybenzene as internal standard. The products were isolated as described next to the analytical data.

Procedure for the Mn Catalysed Transfer Hydrogenation of Esters-with *in situ* Generation of **2**-Procedure D
Dry EtOH, 4-fluorobenzoate and 1-methylnapthelene were added to separate flame dried microwave vials (5 mL) equipped with a crimp cap and placed under a nitrogen atmosphere. These were degassed by sparging with either N_2 or Ar for 30 minutes. A flame dried Schlenk tube was equipped with a rubber septum, and placed under a N_2 atmosphere, prior to being briefly opened to allow the addition of $Mn(CO)_5Br$ (1.4 mg, 0.005 mmol, 0.01 eq.) and Ligand **4** (3.1 mg, 0.005 mmol, 0.01 eq.) and then wrapped in aluminium foil. The tube was placed under vacuum while waiting for the liquids to be sparged with inert gas. The Schlenk tube was placed under a N_2 atmosphere, prior

to the addition of EtOH (0.25 mL, 2M) *via* syringe and the reaction stirred in a pre-heated oil bath set at 100 °C for 2 h. Ethyl 4-fluorobenzoate (0.5 mmol, 1 eq.) and 1-methylnapthalene (20 µL, 0.15 mmol) were then added *via* syringe to the Schlenk tube. A small aliquot was then taken to determine internal standard to ester substrate ratio by ^{1}H NMR. A 1M soln of KO^{t}Bu in ^{t}BuOH (0.1 mmol, 0.2 eq.) was finally added *via* syringe and the reaction stirred in a pre-heated oil bath set at 100 °C for 24 h. Upon which time reaction was cooled and a ^{1}H NMR was taken to determine conversion using 1-methylnapthalene as internal standard. The products were isolated as described next to the analytical data.

General Procedure for the One Pot Esterification/Transfer Hydrogenation using Mn Cat **2**- Procedure E

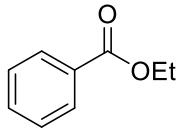
Dry EtOH, was added to a flame dried microwave vial (5 mL) equipped with a crimp cap and placed under a nitrogen atmosphere. And was degassed by sparging with either N_2 or Ar for 30 minutes. A flame dried Schlenk tube was equipped with a rubber septum, and placed under a N_2 atmosphere, prior to being briefly opened to allow the addition of Carboxylic acid substrate (0.5 mmol, 1 eq.) and DMAP (6.1 mg, 0.05 mmol, 0.1 eq.) and then wrapped in aluminium foil. The tube was placed under vacuum while waiting for the solvent to be sparged with inert gas. The Schlenk tube was placed under a N_2 atmosphere and cooled to 0 °C, prior to the addition of EtOH (0.25 mL, 2M) *via* syringe. DIC (90 µL, 0.575 mmol, 1.15 eq.) was added and the reaction was stirred at 0 °C for 10 minutes before being warmed to rt and stirred for a further 2 h. The rubber septum was briefly opened again to allow addition of Mn Cat. **2** (4.2 mg, 0.005 mmol, 0.01 eq.) before a 1M soln of KO^{t}Bu in ^{t}BuOH (0.1 mmol, 0.2 eq.) was finally added *via* syringe and the reaction stirred in a pre-heated oil bath set at 100 °C for 22 h. Upon which time reaction was cooled and a ^{1}H NMR was taken to determine conversion using 1,4-dimethoxybenzene as internal standard. The products were isolated as described next to the analytical data.

General Procedure for the Mn Catalysed Transfer Hydrogenation of Esters NMR Species Determination Experiments - Procedure F

Dry EtOH, ester substrate and 1-methylnapthelene were added to separate flame dried microwave vials (5 mL) equipped with a crimp cap and placed under a nitrogen atmosphere. These were degassed by sparging with either N_2 or Ar for 30 minutes. A flame dried Schlenk tube was equipped with a rubber septum, and placed under a N_2 atmosphere, prior to being briefly opened to allow the addition of Mn Cat. **2** (4.2 mg, 0.005 mmol, 0.01 eq.), and then wrapped in aluminium foil. The tube was placed under vacuum while waiting for the liquids to be sparged with inert gas. The Schlenk tube was placed under a N_2 atmosphere, prior to the addition of EtOH (0.25 mL, 2M), ester substrate (0.5 mmol, 1 eq.) and 1-methylnapthalene (20 µL, 0.15 mmol) *via* syringe. A small aliquot was then taken to determine internal standard to ester substrate ratio by ^{1}H NMR. A 1M soln of KO^{t}Bu in ^{t}BuOH (0.1 mmol, 0.2 eq.) was finally added *via* syringe and the reaction stirred in a pre-heated oil bath set at 100 ° for 22 h. Upon which time reaction was cooled and a ^{1}H NMR was taken to determine conversion, product and side product proportions using 1-methylnapthalene as internal standard.

Characterisation:

Ethyl Benzoate-**8b**

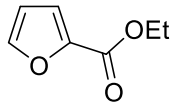


Synthesised by procedure A

Yield (16.8 mmol scale): 2.09 g (85%) of colourless oil

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.58 – 7.51 (m, 1H), 7.47 – 7.41 (m, 2H), 4.38 (q, *J* = 7.1 Hz, 2H), 1.40 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.7 (C), 132.8 (Ar-H), 130.5 (Ar-H), 129.6 (Ar-H), 128.3 (Ar-H), 61.0 (CH_2), 14.4 (CH_3). Fits with previously published data.[9]

Ethyl 2-furoate- **8d**

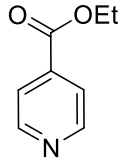


Synthesised by procedure A

Yield (25 mmol scale): 2.95 g (84%) of colourless oil

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (dt, *J* = 2.0, 1.0 Hz, 1H), 7.17 (ddd, *J* = 3.5, 1.4, 0.8 Hz, 1H), 6.50 (dd, *J* = 3.5, 1.7 Hz, 1H), 4.37 (q, *J* = 7.2, 2H), 1.38 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 158.9 (Ar-C), 146.3 (Ar-H), 117.9 (Ar-H), 112.0 (Ar-H), 59.9 (CH_2), 14.5 (CH_3). Fits with previously published data.[9]

Ethyl Isonicotinate- **8e**

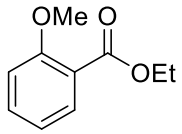


Synthesised by procedure A

Yield (24.4 mmol scale): 3.04 g (82%) of yellow oil

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 – 8.75 (m, 2H), 8.12 – 7.66 (m, 2H), 4.40 (q, *J* = 7.2 Hz, 2H), 1.39 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.1 (C=O), 150.5 (Ar-H), 137.7 (C), 122.9 (Ar-H), 61.8 (CH_2), 14.2 (CH_3). Fits with previously published data.[10]

Ethyl 2-methoxybenzoate-**8f**

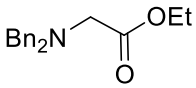


Synthesised by procedure A

Yield (19.7 mmol scale): 3.23 g (91%) of Colourless oil

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (dd, *J* = 7.9, 1.8 Hz, 1H), 7.48 (ddd, *J* = 8.4, 7.4, 1.8 Hz, 1H), 7.00 (dddd, *J* = 7.8, 4.2, 3.4, 1.0 Hz, 2H), 4.38 (q, *J* = 7.1 Hz, 2H), 3.92 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.2 (C), 159.1 (C), 133.3 (Ar-H), 131.5 (Ar-H), 120.4 (Ar), 120.1 (Ar-H), 112.0 (Ar-H), 60.8 (CH_3), 56.0 (CH_2), 14.3 (CH_3). Fits with previously published data.[9]

N,N-Dibenzylglycine Ethyl Ester- **8r**

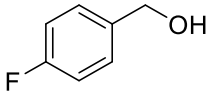


Synthesised by procedure A

Yield (1.96 mmol scale): 0.45 g (81 %) of white solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.18 (m, 10H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.81 (s, 4H), 3.29 (s, 2H), 1.26 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 171.7 (C=O), 139.2 (Ar-C), 129.1 (Ar-H), 128.5 (Ar-H), 127.3 (Ar-H), 60.4 (CH_2), 57.9 (CH_2), 53.8 (CH_2), 14.4 (CH_3). Fits with previously published data.[11]

4-Fluorobenzyl Alcohol-**7**



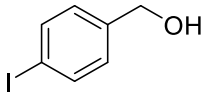
Synthesised by procedure B

Purified by flash column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 / MeOH 95:5 as eluent)

Yield (0.5 mmol scale): 46.8 mg (74%) pale yellow oil

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.30 (m, 2H), 7.10 – 7.00 (m, 2H), 4.66 (s, 2H), 1.76 (bs, OH). ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.4 (d, *J* = 245.5 Hz) (Ar-F), 136.7 (d, *J* = 3.2 Hz) (Ar-C), 128.9 (d, *J* = 8.2 Hz) (Ar-H), 115.5 (d, *J* = 21.4 Hz) (Ar-H), 64.7 (CH_2). Fits with previously published data.[12]

4-Iodobenzyl Alcohol-**9a**



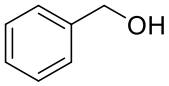
Synthesised by Procedure C

Purified by flash column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 /MeOH 95:5 as eluent)

Yield (0.5 mmol scale): 98.1 mg (81%) of white crystalline solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.67 (m, 2H), 7.14 – 7.10 (m, 2H), 4.65 (s, 2H), 1.71 (bs, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.5 (C), 137.61 (Ar-H), 128.8 (Ar-H), 93.01 (C), 64.7 (CH_2). Fits with previously published data.[13]

Benzyl Alcohol- **9b**



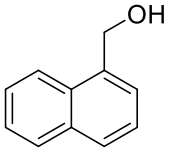
Synthesised by Procedure B

Purified by silica gel flash column chromatography (CH_2Cl_2 then CH_2Cl_2 / MeOH 97:3 then 95:5 as eluent)

Yield (1 mmol scale): 74.9 mg (69%) as a colourless oil

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.35 (m, 4H), 7.34 – 7.27 (m, 1H), 4.70 (s, 2H), 1.72 (bs, O-H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.0 (C), 128.7 (Ar-H), 127.8 (Ar-H), 127.1 (Ar-H), 65.6 (CH_2). Fits with previously published data.[13]

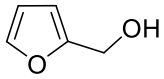
1-naphthylmethanol-**9c**



Synthesised by Procedure B

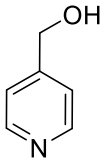
Purified by flash column chromatography using CH_2Cl_2 / MeOH (95:5) as eluent
Yield (1 mmol scale): 137.7 mg (87%) of pale yellow oil
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.2 Hz, 1H), 8.01 – 7.75 (m, 2H), 7.62 – 7.51 (m, 3H), 7.48 (t, *J* = 7.5 Hz, 1H), 5.19 (s, 2H), 1.70 (bs, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.4 (Ar-C), 133.9 (Ar-C), 131.3 (Ar-C), 128.8 (Ar-H), 128.7 (Ar-H), 126.5 (Ar-H), 126.0 (Ar-H), 125.5 (Ar-H), 125.5 (Ar-H), 123.8 (Ar-H), 63.8 (CH_2). Fits with previously published data.[14]

Furfuryl Alcohol- **9d**



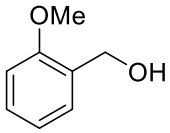
Synthesised by Procedure C
Purified by flash column chromatography on silica gel (CH_2Cl_2 the CH_2Cl_2 /MeOH 95:5 as eluent)
Yield (0.5 mmol scale): 40.2 mg (82%) of yellow oil
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (dd, *J* = 1.9, 0.8 Hz, 1H), 6.34 (dd, *J* = 3.2, 1.8 Hz, 1H), 6.29 (d, *J* = 3.2 Hz, 1H), 4.61 (s, 2H), 1.88 (bs, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.1 (Ar-C), 142.7 (Ar-H), 110.5 (Ar-H), 107.9 (Ar-H), 57.6 (CH_2). Fits with previously published data.[12]

4-Pyridinemethanol-**9e**



Synthesised by Procedure B
Purified by flash column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 /MeOH 95:5 as eluent)
Yield (1 mmol scale): 90.4 mg (83%) as an off-white solid
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, 2H), 7.30 (d, *J* = 5.1 Hz, 2H), 4.75 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.37 (Ar-C), 149.6 (Ar-H), 121.2 (Ar-H), 63.3 (CH_2).
Fits with previously published data.[15]

2-methoxybenzyl Alcohol- **9f**



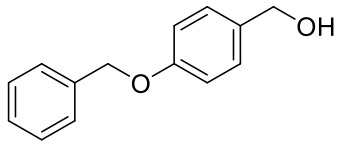
Synthesised by Procedure B- From **8f**
Purified by flash column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 /MeOH 95:5 as eluent)
Yield (0.5 mmol scale): 52.3 mg (76%)
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.26 (m, 2H), 6.98-6.92 (m, 1H), 6.91 – 6.87 (m, 1H), 4.69 (s, 2H), 3.87 (s, 3H), 2.36 (bs, O-H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.6 (Ar-C), 129.2 (Ar-C), 129.1 (Ar-H), 128.9 (Ar-H), 120.8 (Ar-H), 110.4 (Ar-H), 62.3 (CH_2), 55.4 (CH_3). Fits with previously published data.[14]

Synthesised by Procedure B- From **8w**
Purified by flash column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 /MeOH 95:5 as eluent)
Yield (0.5 mmol scale): 56.7 mg (82%)
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.23 (m, 2H), 6.98 – 6.91 (m, 1H), 6.91 – 6.86 (m, 1H), 4.68 (s, 2H), 3.85 (s, 3H), 2.55 (bs, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.5 (Ar-C), 129.1 (Ar-C), 129.0 (Ar-H), 128.8 (Ar-H), 120.7 (Ar-H), 110.3 (Ar-H), 62.1 (CH_2), 55.3 (CH_3). Fits with previously published data.[14]

Synthesised by Procedure B- From **8x**
Purified by flash column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 /MeOH 95:5 as eluent)
Yield (0.5 mmol scale): 53.3 mg (77%)
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.25 (m, 2H), 6.99 – 6.92 (m, 1H), 6.91 – 6.86 (m, 1H), 4.69 (s, 2H), 3.86 (s, 3H), 2.53 (bs, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.5 (Ar-C), 129.1 (Ar-C), 129.0 (Ar-H), 128.8 (Ar-H), 120.7 (Ar-H), 110.3 (Ar-H), 62.1 (CH_2), 55.3 (CH_3). Fits with previously published data.[14]

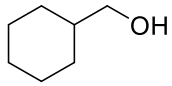
Synthesised by Procedure E- From **10a**
Purified by flash column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 / MeOH 99:1 then 98:2 as eluent) followed by washing with 15 mL HCl (1M), extracting with 3x 10 mL CH_2Cl_2, washing with 15 mL Brine, drying over Na_2SO_4, filtering and drying *in vacuo.*
Yield (0.5 mmol scale): 50.2 mg (73%)
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.26 (m, 2H), 6.98 – 6.92 (m, 1H), 6.91 – 6.87 (m, 1H), 4.69 (s, 2H), 3.87 (s, 3H), 2.38 (bs, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.6, 129.2, 129.1, 128.9, 120.8, 110.3, 62.3, 55.4. Fits with previously published data.[14]

4-Benzyloxybenzyl Alcohol-**9h**



Synthesised by Procedure C- using 2 mol% **2**
Purified by flash column chromatography on silica gel using CH_2Cl_2 then CH_2Cl_2 / MeOH (95:5) as eluent.
Yield (0.5 mmol scale): 51.6 mg (48%)
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.27 (m, 7H), 7.01 – 6.95 (m, 2H), 5.08 (s, 2H), 4.61 (s, 2H), 1.97 (bs, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.4 (Ar-C), 137.0 (Ar-C), 133.5 (Ar-C), 128.7 (Ar-H), 128.7 (Ar-H), 128.1 (Ar-H), 127.5 (Ar-H), 115.0 (Ar-H), 70.1 (CH_2), 65.0 (CH_2). Fits with previously published data.[16]

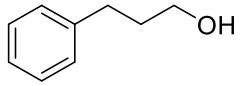
Cyclohexanemethanol- **9l**



Synthesised by Procedure B
Purified by flash column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 / MeOH 95:5 as eluent)
Yield (0.5 mmol scale): 44.6 mg (78%) of Yellow oil
^{1}H NMR (400 MHz, $CDCl_3$) δ 3.44 (d, *J* = 6.4 Hz, 2H), 1.80 – 1.64 (m, 5H), 1.48 (dddd, *J* = 12.7, 11.5, 6.4, 3.2 Hz, 1H), 1.33 – 1.08 (m, 3H), 0.93 (qd, *J* = 13.8, 12.9, 3.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 68.9 (CH_2), 40.6 (CH), 29.7 (CH_2), 26.7 (CH_2), 26.0 (CH_2). Fits with previously published data.[14]

Synthesised by Procedure E
Purified by flash column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 / MeOH 99:1 then 98:2 as eluent) followed by washing with 15 mL HCl (1M), extracting with 3x 10 mL CH_2Cl_2, washing with 15 mL Brine, drying over Na_2SO_4, filtering and drying *in vacuo*
Yield (0.5 mmol scale): 42.5 mg (74%) of Yellow oil
^{1}H NMR (400 MHz, $CDCl_3$) δ 3.43 (d, *J* = 6.4 Hz, 2H), 1.85 – 1.60 (m, 5H), 1.48 (tt, *J* = 12.7, 11.4, 6.5, 3.2 Hz, 1H), 1.37 – 1.08 (m, 3H), 0.92 (qd, *J* = 13.3, 12.6, 3.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 68.9 (CH_2), 40.6 (CH), 29.7 (CH_2), 26.7 (CH_2), 26.0 (CH_2). Fits with previously published data.[14]

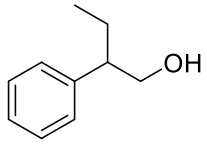
3-Phenylpropan-1-ol- **9m**



Synthesised by Procedure B from **8m**
Purified by flash column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 /MeOH 95:5 as eluent)
Yield (0.5 mmol Scale): 56.1 mg (82%) of yellow oil
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.27 (m, 2H), 7.23 – 7.16 (m, 3H), 3.69 (t, *J* = 6.4 Hz, 2H), 2.72 (t, *J* = 7.7 Hz, 2H), 1.93 (p, *J* = 6.1 Hz, 2H), 1.69 (s, O-H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.6 (Ar-C), 128.3 (Ar-H), 128.2 (Ar-H), 125.7 (Ar-H), 62.1 (CH_2), 34.1 (CH_2), 31.9 (CH_2). Fits with previously published data.[12]

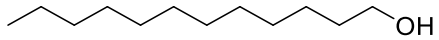
Synthesised by Procedure C from **8v**
Purified by flash column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 /MeOH 95:5 as eluent)
Yield (0.5 mmol Scale): 50.2 mg (74%) of yellow oil
^{1}H NMR (400 MHz, $CDCL_3$) δ 7.33 – 7.27 (m, 2H), 7.24 – 7.17 (m, 3H), 3.68 (t, *J* = 6.4 Hz, 2H), 2.72 (t, *J* = 7.8 Hz, 2H), 1.96 – 1.85 (m, 2H), 1.54 (bs, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.9 (Ar-C), 128.5 (Ar-H), 128.5 (Ar-H), 126.0 (Ar-H), 62.4 (CH_2), 34.3 (CH_2), 32.2 (CH_2). Fits with previously published data.[12]

2-Phenylbutan-1-ol- **9n**



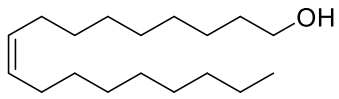
Synthesised by Procedure B- using 1.5 mol% **2**
Purified by flash column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 /MeOH 95:5 as eluent)
Yield (0.5 mmol scale): 53.5 mg (71%) of yellow oil
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.33 (m, 2H), 7.30 – 7.21 (m, 3H), 3.86 – 3.71 (m, 2H), 2.72 (m, 1H), 1.86 – 1.72 (m, 1H), 1.69 – 1.54 (m, 1H), 0.86 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.4 (Ar-C), 128.7 (Ar-H), 128.2 (Ar-H), 126.8 (Ar-H), 67.5 (CH_2), 50.6 (CH), 25.1 (CH_2), 12.1 (CH_3). Fits with previously published data.[17]

Lauryl Alcohol-**9o**



Synthesised by Procedure B – Using 1.5 mol% **2**
Purified by column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 /MeOH 95:5 as eluent)
Yield (0.5 mmol Scale): 71.8 mg (77%) of off white solid
^{1}H NMR (500 MHz, $CDCl_3$) δ 3.64 (t, *J* = 6.6 Hz, 2H), 1.56 (p, *J* = 6.6 Hz, 2H), 1.45 – 1.16 (m, 18H), 0.88 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 63.3 (CH_2), 33.0 (CH_2), 32.1 (CH_2), 29.8 (CH_2), 29.8 (CH_2), 29.8 (CH_2), 29.7 (CH_2), 29.6 (CH_2), 29.5 (CH_2), 25.9 (CH_2), 22.8 (CH_2), 14.25 (CH_3). Fits with previously published data.[12]

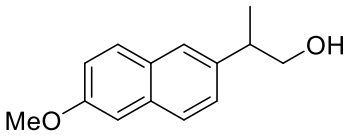
Oleyl Alcohol- **9p**



Synthesised by Procedure B- Using 1.5 mol% **2**
Purified by column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 / MeOH 95:5 as eluent)
Yield (0.5 mmol scale): 101.5 mg (76%) of pale yellow oil
^{1}H NMR (400 MHz, $CDCl_3$) δ 5.38 – 5.29 (m, 2H), 3.63 (t, *J* = 6.6 Hz, 2H), 2.15 (s, OH), 2.01 (q, *J* = 6.4 Hz, 4H), 1.56 (p, *J* = 6.6 Hz, 2H), 1.36 – 1.26 (m, 22H), 0.87 (t, J= 6.8 Hz, 3H). ^{13}C NMR (101 MHz,

$CDCl_3$) δ 130.1 (CH), 129.9 (CH), 63.2 (CH_2), 32.9 (CH_2), 32.0 (CH_2), 29.9 (CH_2), 29.9 (CH_2), 29.7 (CH_2), 29.6 (CH_2), 29.5 (CH_2), 29.5 (CH_2), 29.4 (CH_2), 29.3 (CH_2), 27.3 (CH_2), 27.3 (CH_2), 25.9 (CH_2), 22.8 (CH_2), 14.2 (CH_3). Fits with previously published data.[12]

(rac)-Naproxol-**9q**



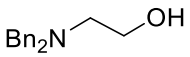
Synthesised by Procedure C

Purified by flash column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 / MeOH (95:5) as eluent)

Yield (0.5 mmol scale): 88.9 mg (82%) of white solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (dd, *J* = 8.6, 6.1 Hz, 2H), 7.63 – 7.58 (m, 1H), 7.34 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.19 – 7.10 (m, 2H), 3.92 (s, 3H), 3.77 (d, *J* = 6.7 Hz, 2H), 3.08 (sex, *J* = 6.8 Hz, 1H), 1.98 (s, OH), 1.35 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.5 (Ar-OMe), 138.8 (Ar-C), 133.6 (Ar-C), 129.2 (Ar-H), 129.1 (Ar-C), 127.3 (Ar-H), 126.4 (Ar-H), 126.0 (Ar-H), 119.0 (Ar-H), 105.7 (Ar-H), 68.7 (CH_2), 55.4 (CH_3), 42.5 (CH), 17.8 (CH_3). Chiral analysis was performed using a Chiralcel OD-H column using n-hexane / isopropanol (96/4) mobile phase, flow 1.0 mL/min; tR (S-enantiomer): 17.5 min; tR (R-enantiomer): 18.4 min. Racemic. Fits with previously published data.[18]

N,N-Dibenzylethanolamine- **9r**



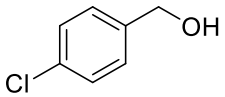
Synthesised by Procedure C

Purified by flash column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 / MeOH 99:1 then 98:2 as eluent)

Yield (0.5 mmol scale): 76.0 mg (63 %) of brown oil

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.24 (m, 10H), 3.67 (s, 4H), 3.62 (t, *J* = 5.4 Hz, 2H), 2.71 (t, *J* = 5.4 Hz, 2H), 2.59 (bs, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.9 (Ar-C), 129.1 (Ar-H), 128.5 (Ar-H), 127.3 (Ar-H), 58.7 (CH_2), 58.3 (CH_2), 54.9 (CH_2). Fits with previously published data.[19]

4-Chlorobenzyl Alcohol- **9s**



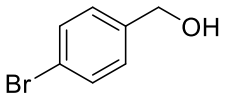
Synthesised by Procedure C

Purified by flash column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 / MeOH 95:5)

Yield (0.5 mmol scale): 56.5 mg (79%) of white crystalline solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.25 (m, 4H), 4.65 (s, 2H), 2.00 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.4 (Ar-Cl), 133.5 (Ar-C), 128.79 (Ar-H), 128.4 (Ar-H), 64.6 (CH_2). Fits with previously published data.[13]

4-Bromobenzyl Alcohol- **9t**



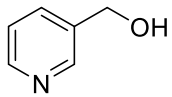
Synthesised by Procedure C

Purified by flash column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 / MeOH 95:5)

Yield (0.5 mmol Scale): 73.5 mg (79%) of White Crystalline Solid

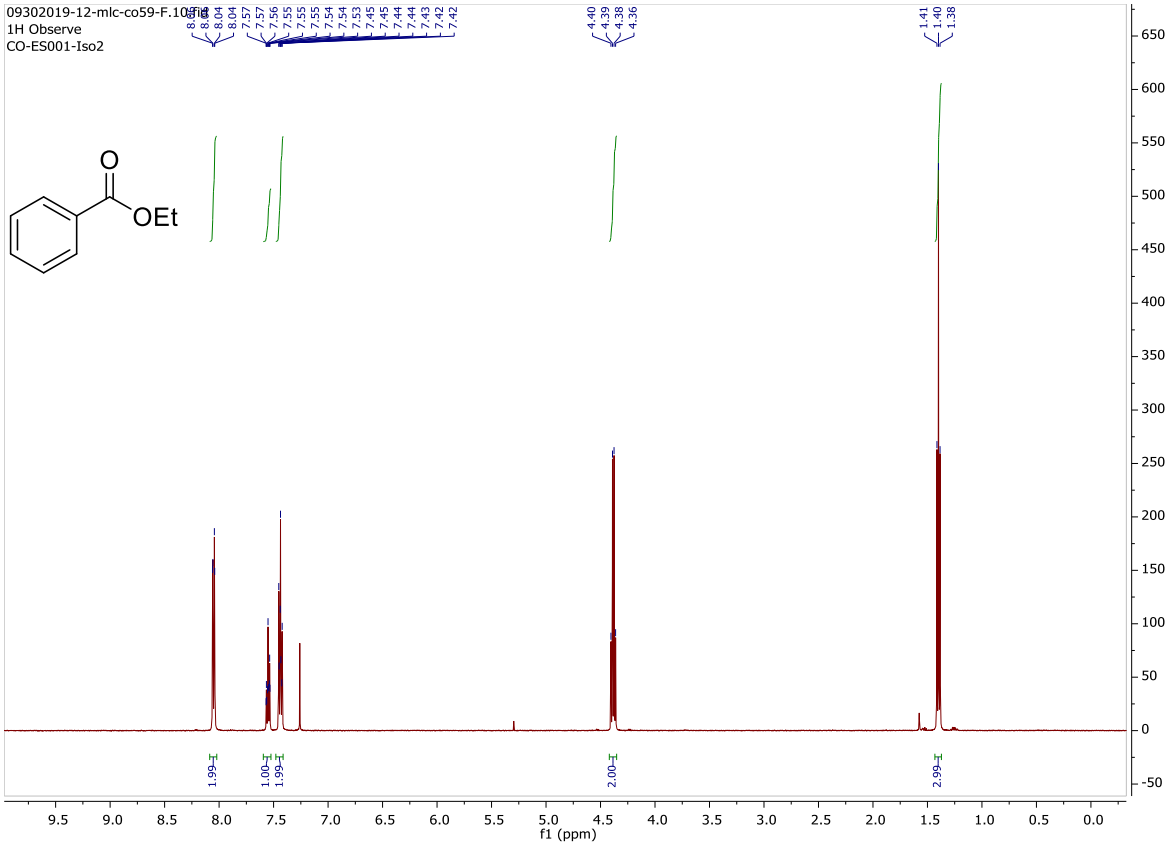
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.45 (m, 2H), 7.24 – 7.19 (m, 2H), 4.62 (s, 2H), 2.07 (bs, OH). ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.9 (Ar-C), 131.7 (Ar-H), 128.7 (Ar-H), 121.6 (Ar-Br), 64.6 (CH_2). Fits with previously published data.[13]

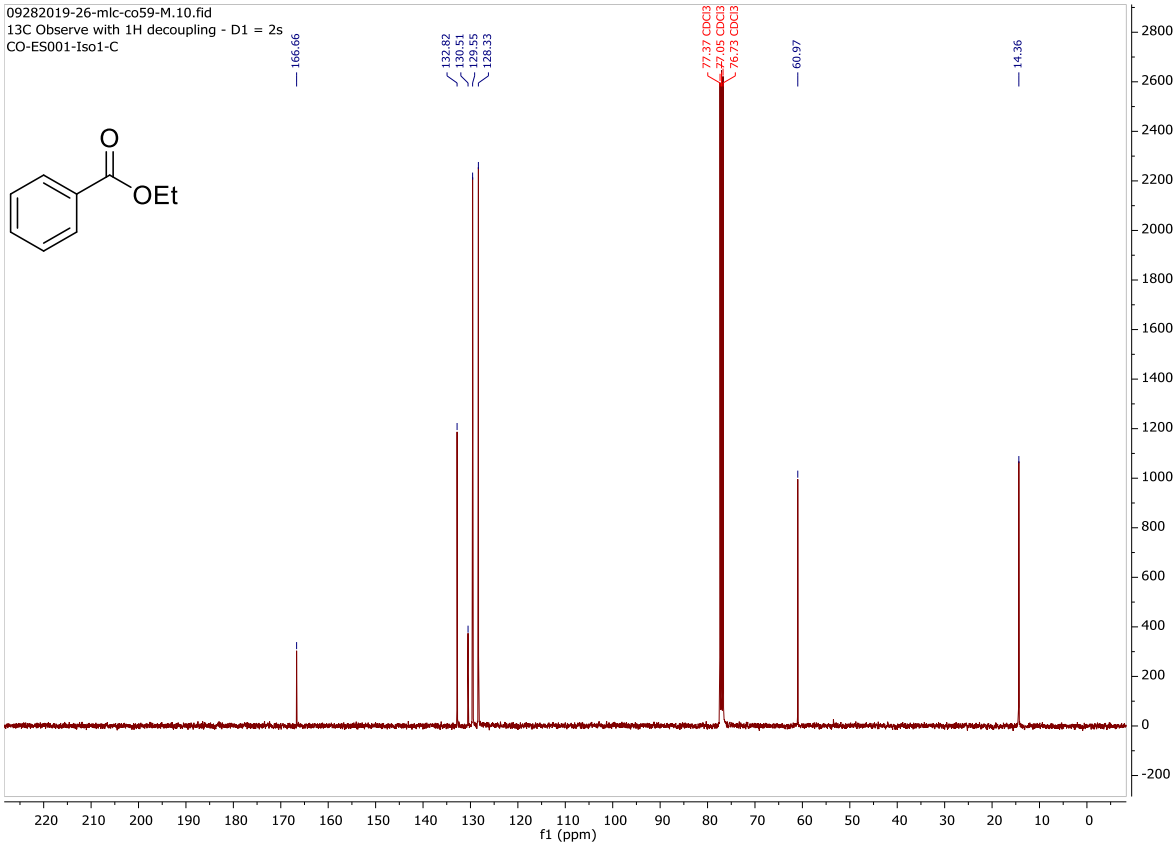
3-Pyridinemethanol-**9u**

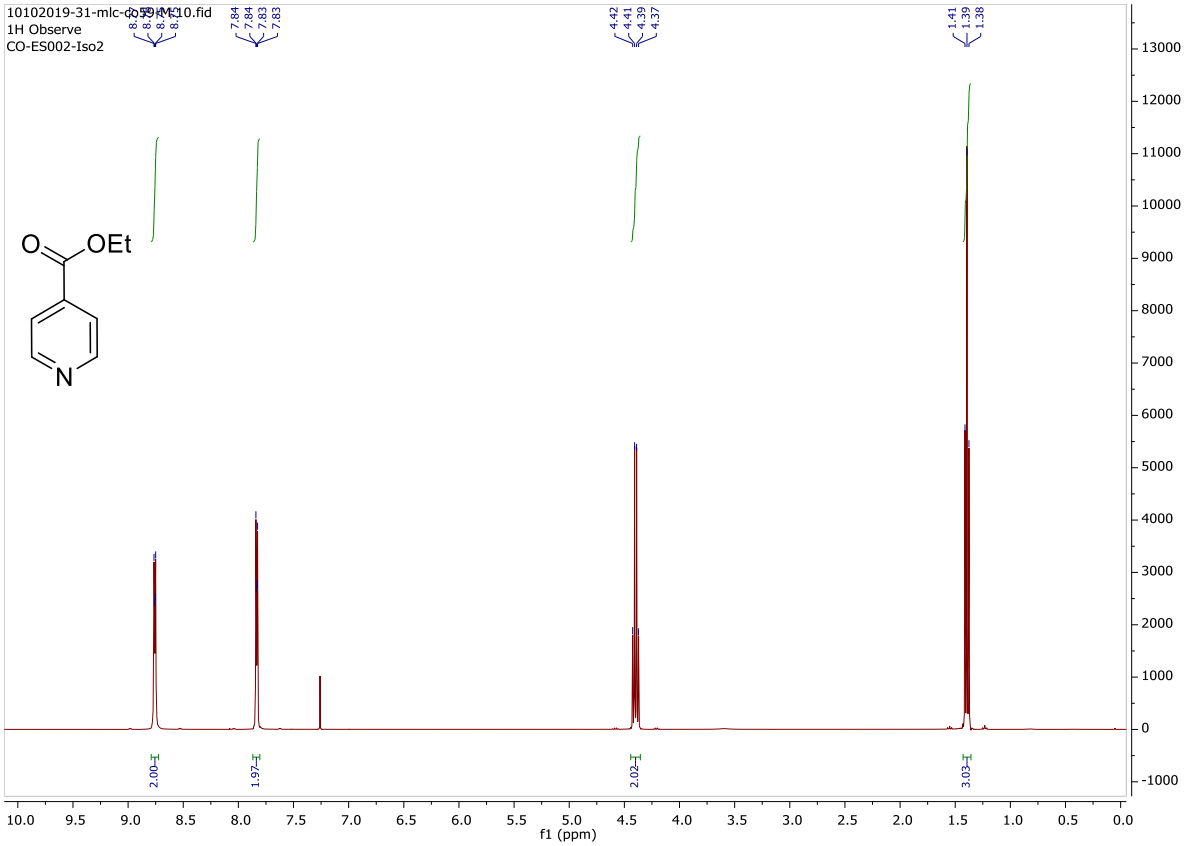


Synthesised by Procedure C
Purified by flash column chromatography on silica gel (CH_2Cl_2 then CH_2Cl_2 / MeOH 95:5 then 90:10)
Yield (0.5 mmol Scale): 45.9 mg (84%) of Yellow oil
^{1}H NMR (500 MHz, MeOD) δ 8.65 – 8.35 (m, 2H), 7.90 – 7.78 (m, 1H), 7.51 – 7.34 (m, 1H), 4.66 (s, 2H). ^{13}C NMR (126 MHz, MeOD) δ 148.8 (Ar-C), 139.2 (Ar-H) 136.9 (Ar-H), 125.2 (Ar-H), 62.5 (CH_2). Fits with previously published data.[20]

Spectra


09302019-12-mlc-co59-F.10.fid
1H Observe
CO-ES001-Iso2
8.08
8.06
8.04
8.04
7.57
7.57
7.56
7.56
7.55
7.55
7.55
7.54
7.54
7.53
7.45
7.45
7.44
7.44
7.43
7.42
7.42
4.40
4.39
4.38
4.36
1.41
1.40
1.38
O
OEt
1.99
1.00
1.99
2.00
2.99
f1 (ppm)


09282019-26-mlc-co59-M.10.fid
13C Observe with 1H decoupling - D1 = 2s
CO-ES001-Iso1-C
166.66
132.82
130.51
129.55
128.33
77.37 CDCl3
77.05 CDCl3
76.73 CDCl3
60.97
14.36
O
OEt
f1 (ppm)


10102019-31-mlc-co59-M.10.fid
1H Observe
CO-ES002-Iso2
8.79
8.78
8.77
8.76
7.84
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7.83
7.83
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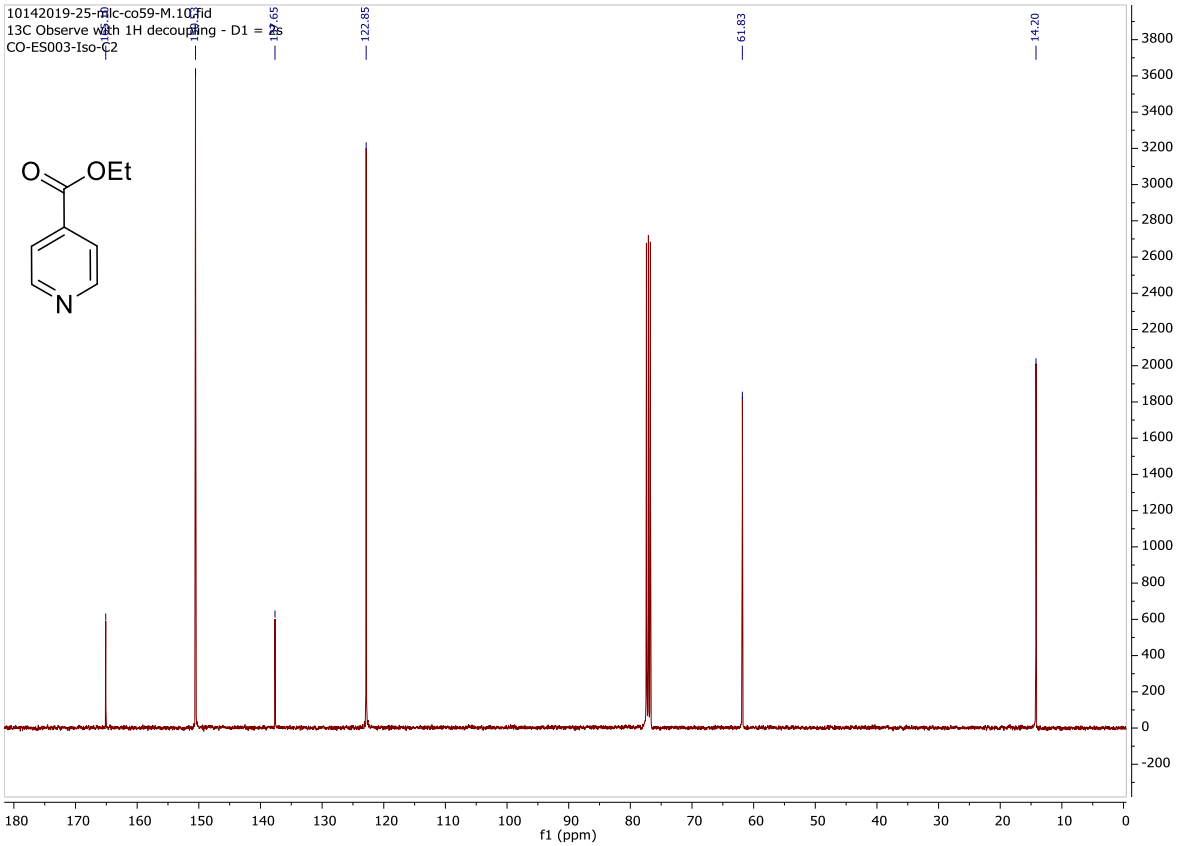
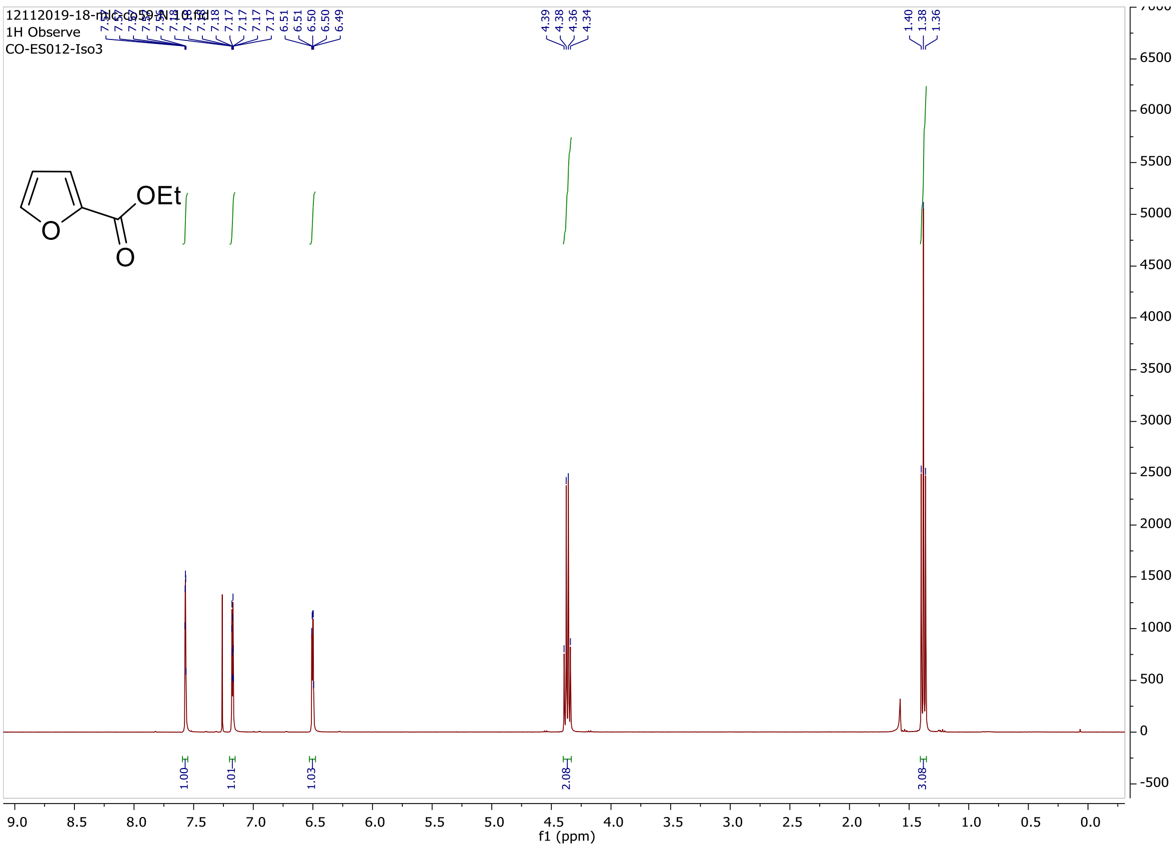
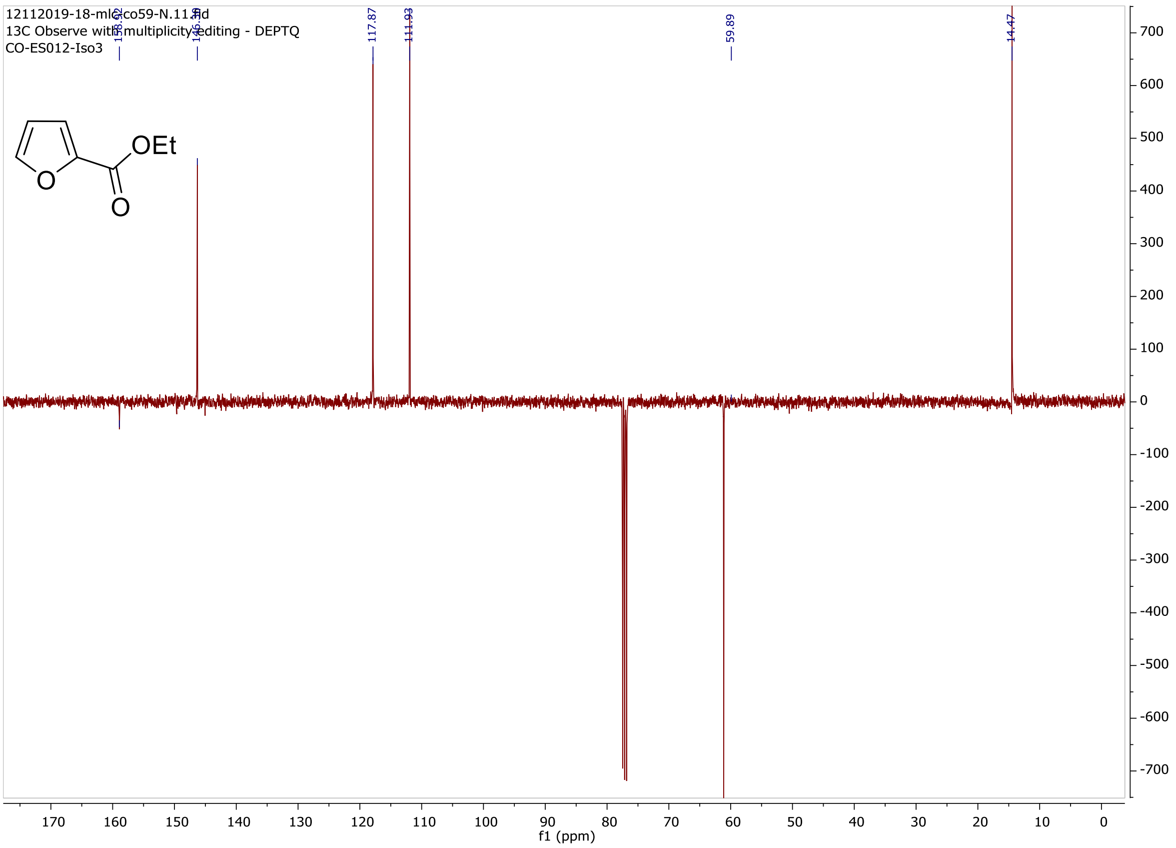
4.41
4.39
4.37
1.41
1.39
1.38
O
OEt
N
2.00
1.97
2.02
3.03
f1 (ppm)

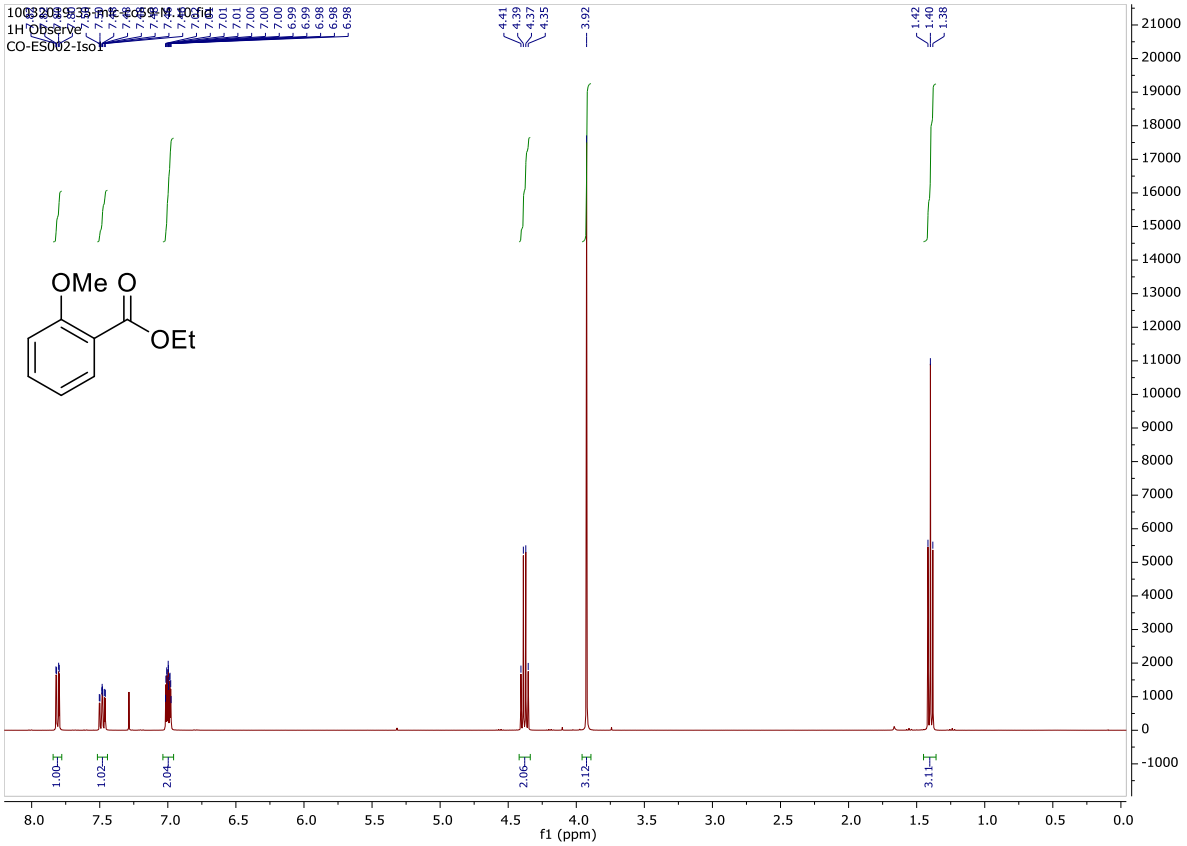

10142019-25-mlc-co59-M.10.fid
13C Observe with 1H decoupling - D1 = 2s
CO-ES003-Iso-C2
150.48
142.27
127.65
122.85
61.83
14.20
O
OEt
N
f1 (ppm)

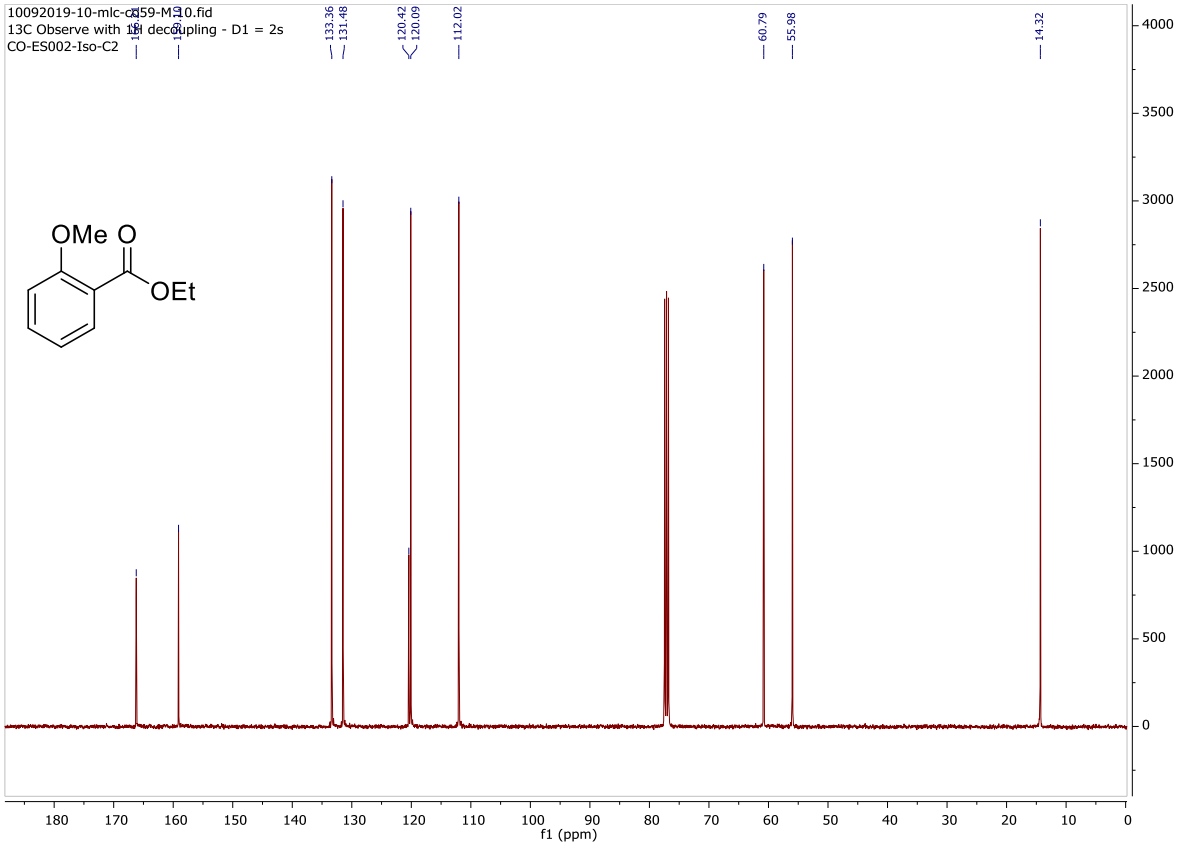


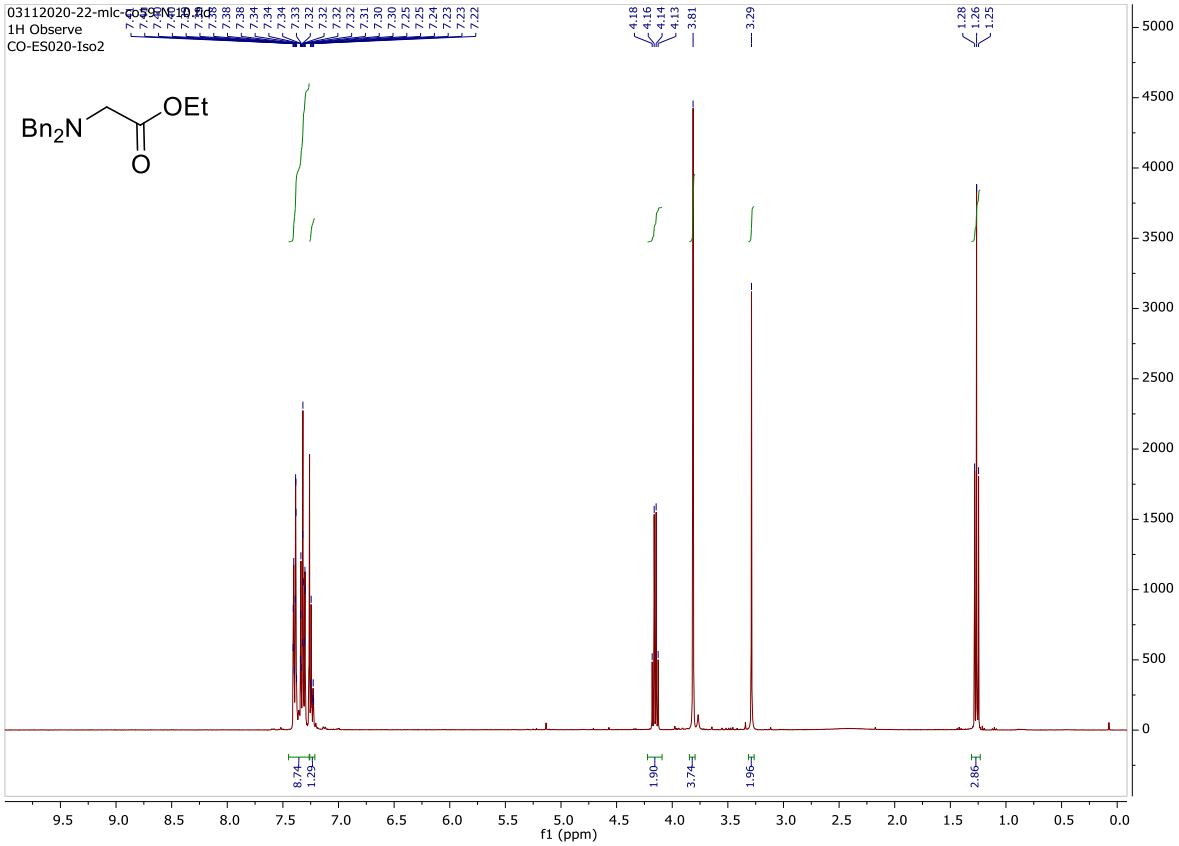
12112019-18-mlc-co59-N.10.fid
1H Observe
CO-ES012-Iso3
OEt
O
O
1.00
1.01
1.03
2.08
3.08
f1 (ppm)

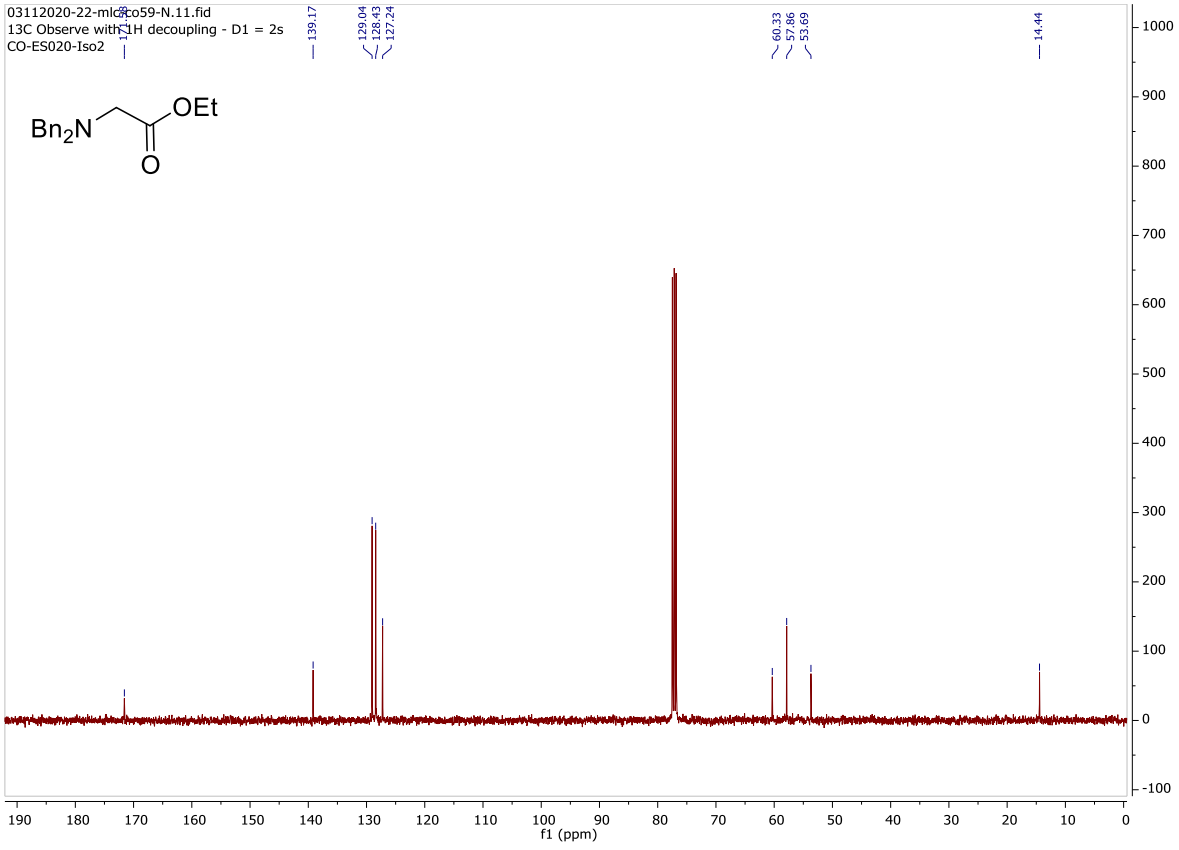


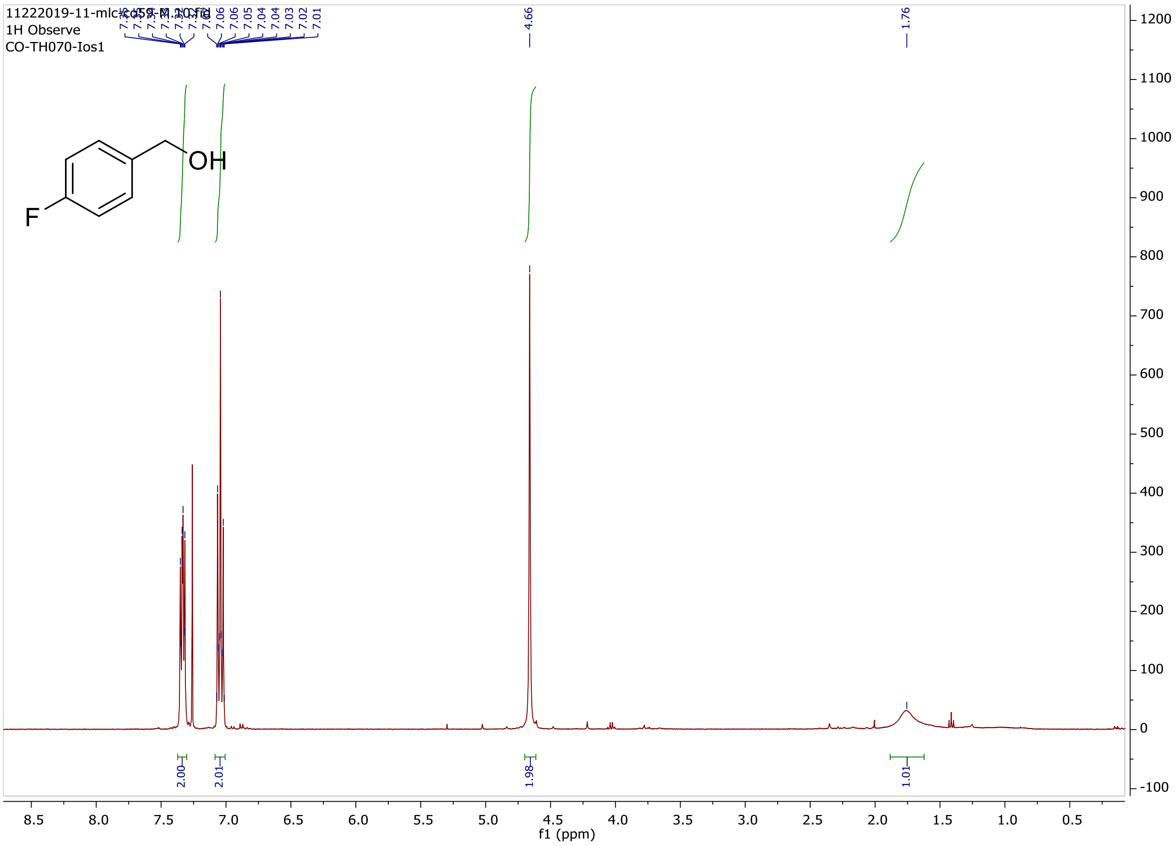
12112019-18-mlc-co59-N.11.fid
13C Observe with multiplicity editing - DEPTQ
CO-ES012-Iso3
117.87
111.93
59.89
14.47
OEt
O
O
f1 (ppm)

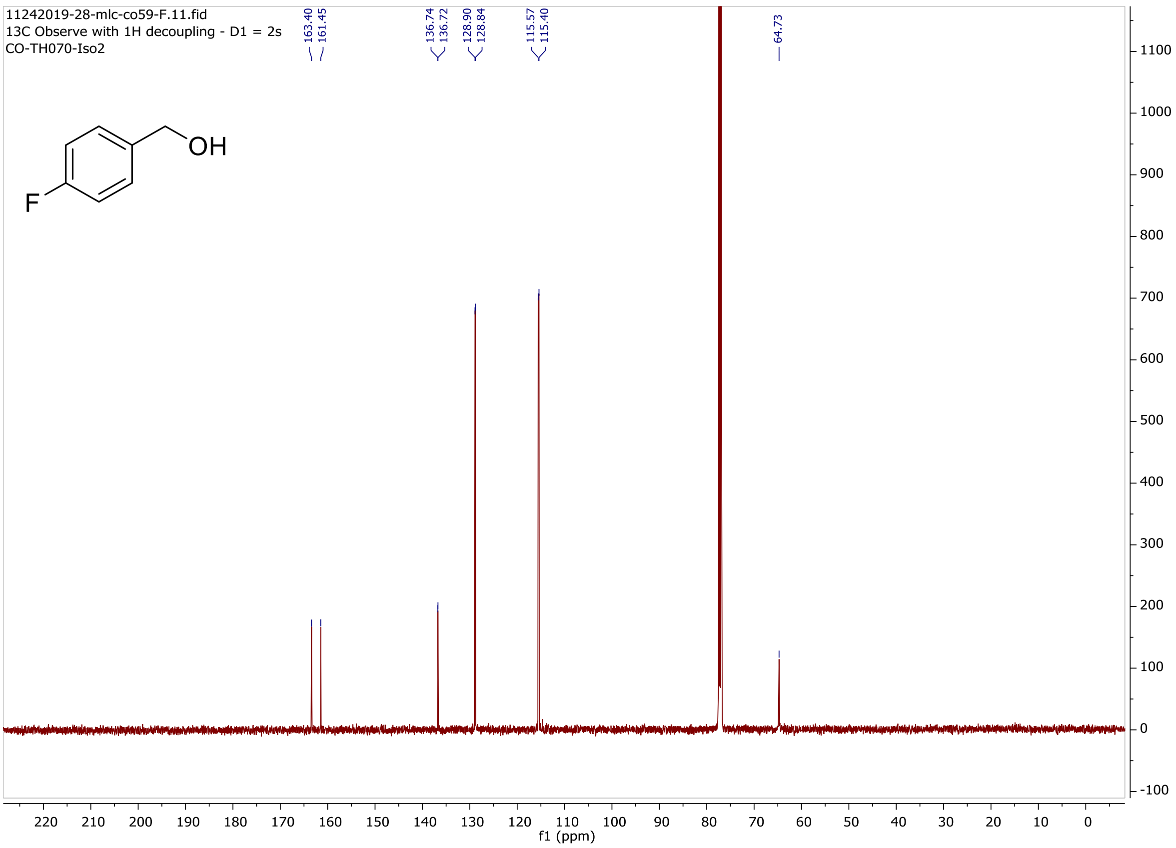

1H Observe
CO-ES002-Iso1
OMe O
OEt
f1 (ppm)

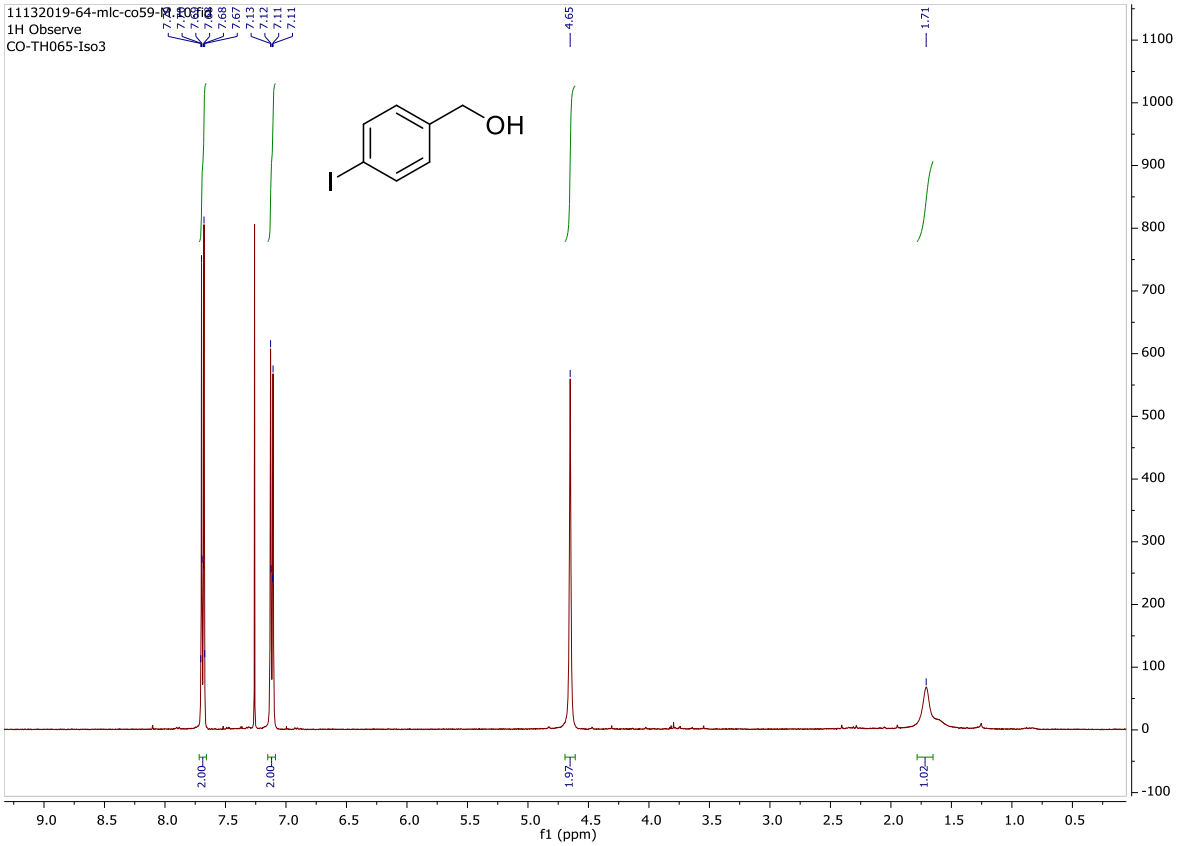

13C Observe with 1H decoupling - D1 = 2s
CO-ES002-Iso-C2
OMe O
OEt
f1 (ppm)

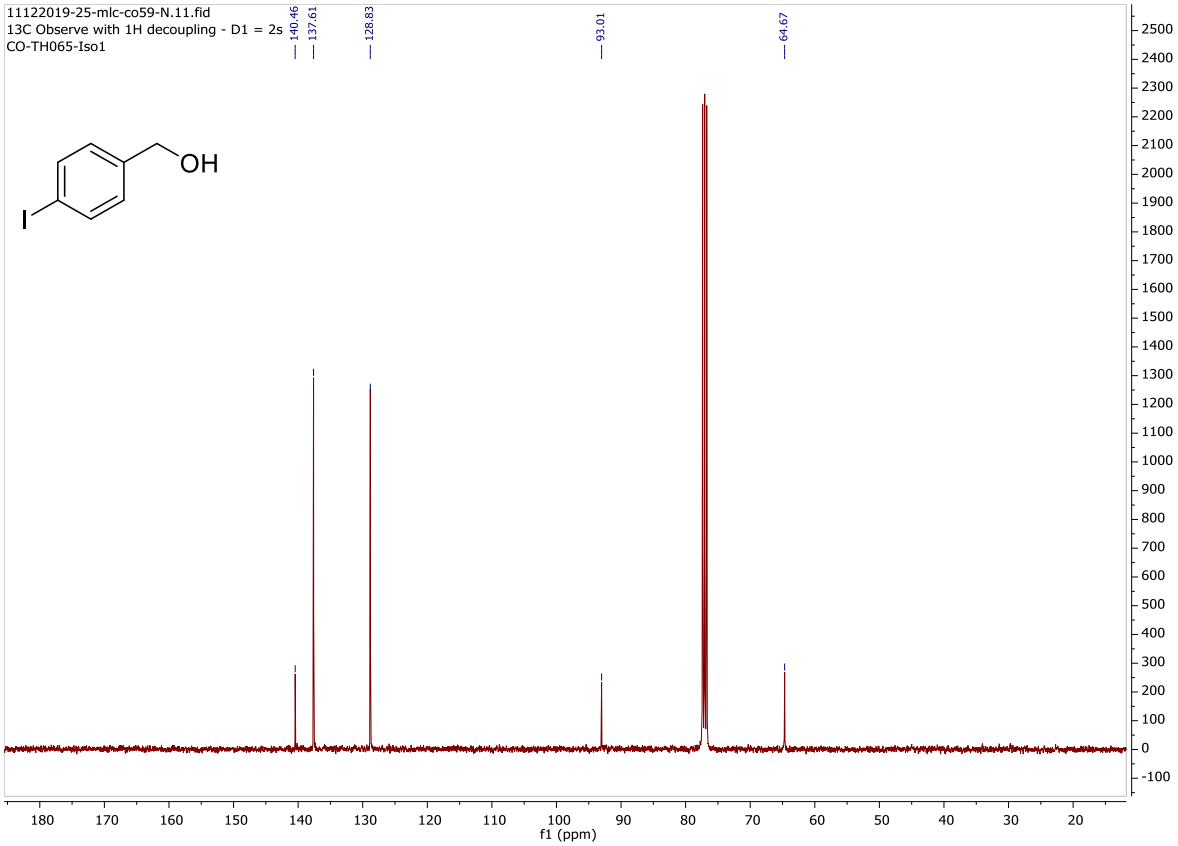

1H Observe
CO-ES020-Iso2
Bn2N
OEt
O
4.18
4.16
4.14
4.13
3.81
3.29
1.28
1.26
1.25
8.74
1.29
1.90
3.74
1.96
2.86
f1 (ppm)

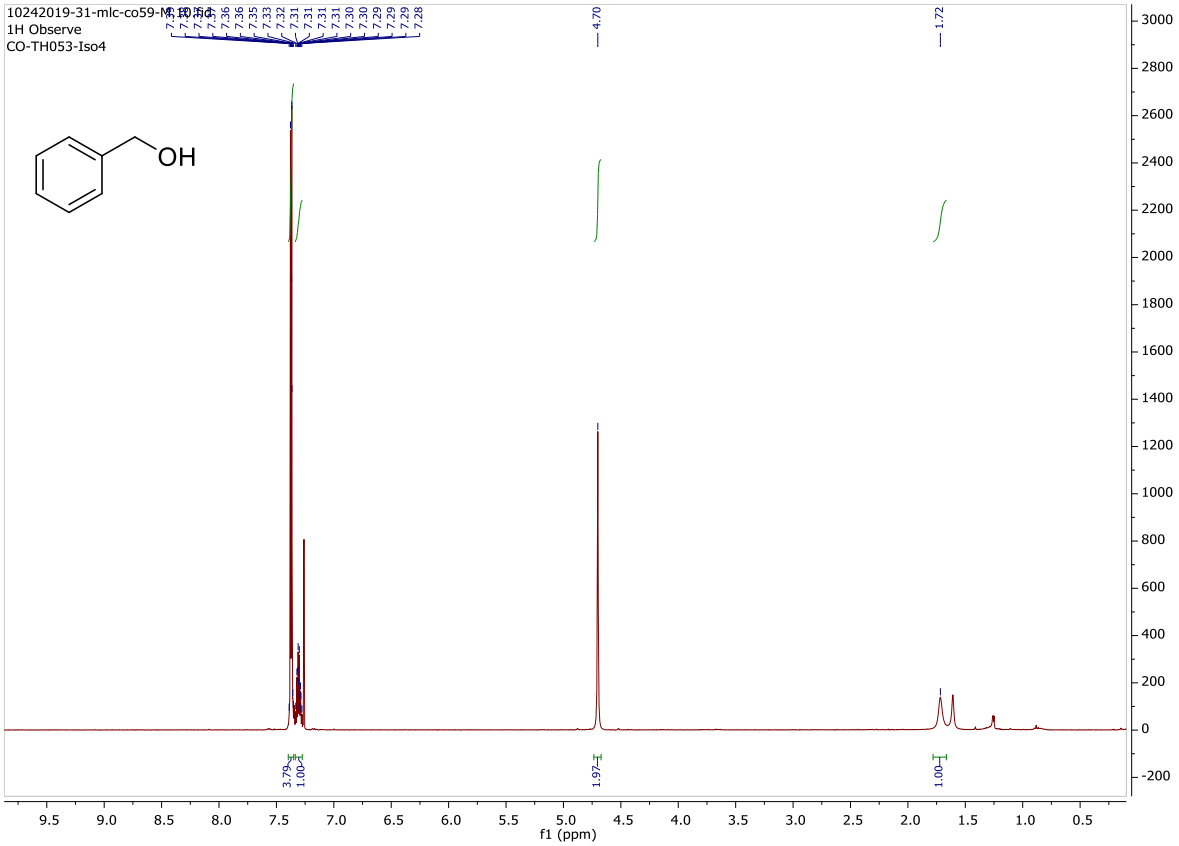

13C Observe with 1H decoupling - D1 = 2s
CO-ES020-Iso2
Bn2N
OEt
O
139.17
129.04
128.43
127.24
60.33
57.86
53.69
14.44
f1 (ppm)

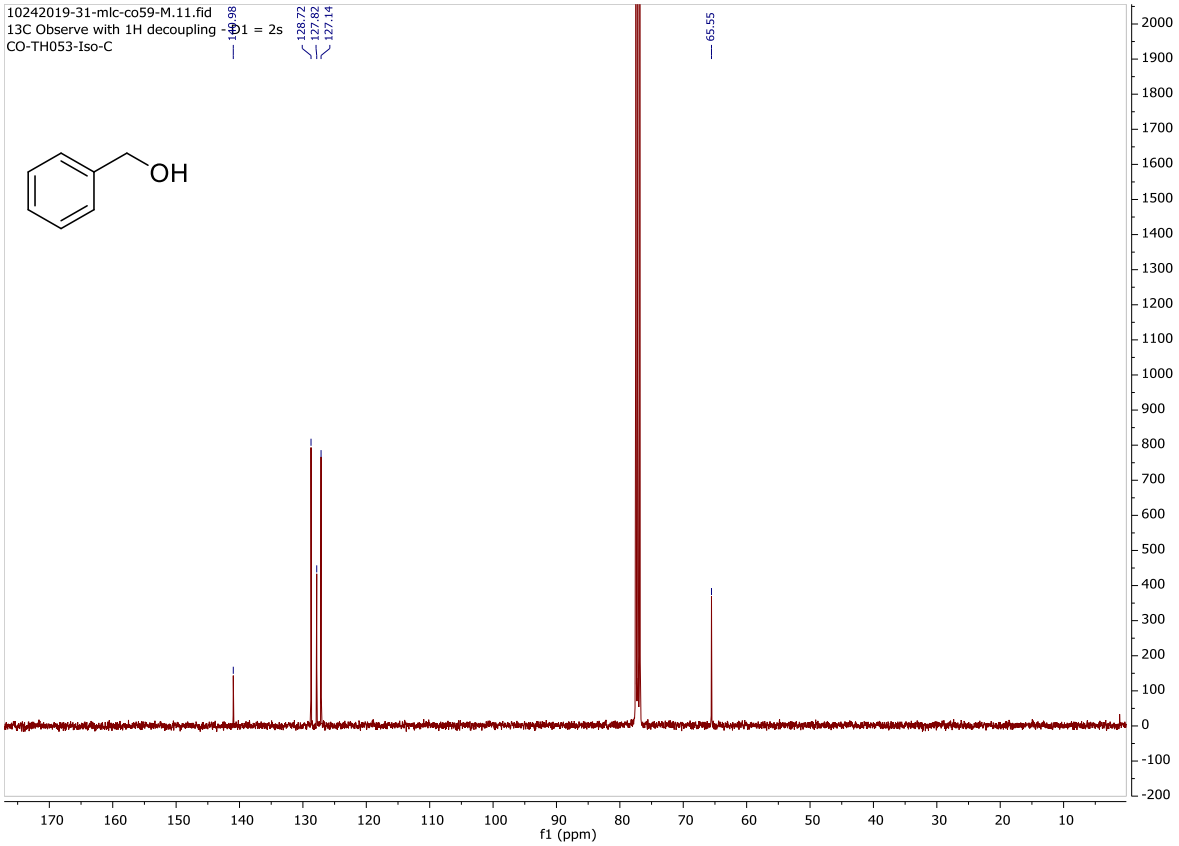

11222019-11-mlc-co59-M.10.fid
1H Observe
CO-TH070-Ios1
OH
F
4.66
1.76
2.00
2.01
1.98
1.01
f1 (ppm)

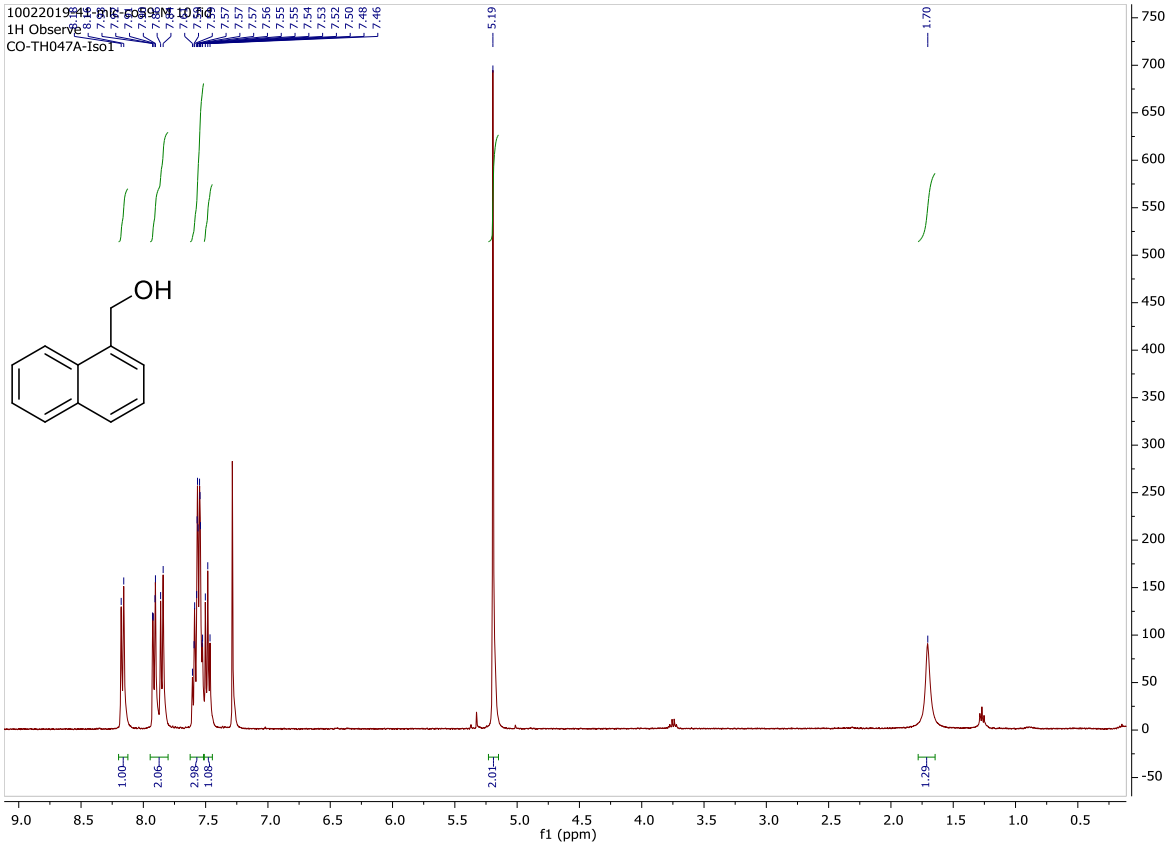

11242019-28-mlc-co59-F.11.fid
13C Observe with 1H decoupling - D1 = 2s
CO-TH070-Iso2
163.40
161.45
136.74
136.72
128.90
128.84
115.57
115.40
64.73
OH
F
f1 (ppm)

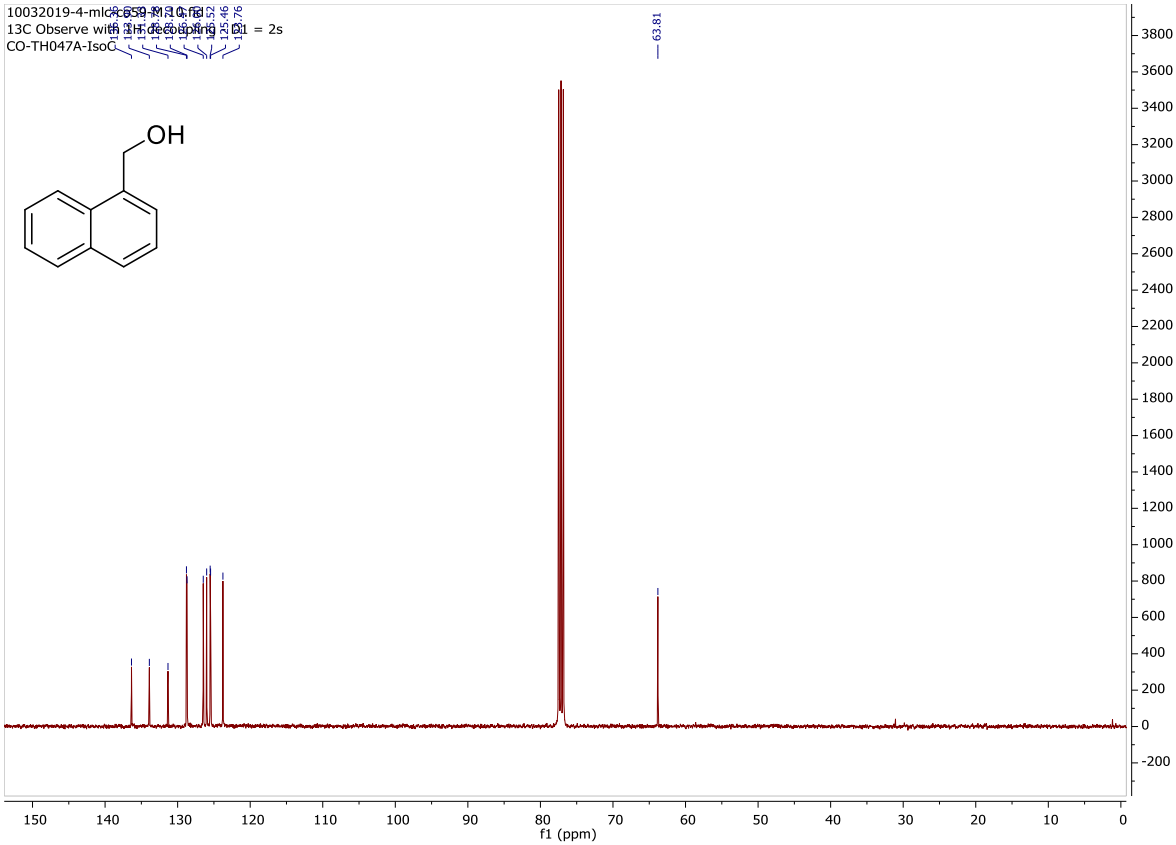

11132019-64-mlc-co59-N.10.fid
1H Observe
CO-TH065-Iso3
7.71
7.70
7.68
7.67
7.13
7.12
7.11
7.11
4.65
1.71
OH
I
2.00
2.00
1.97
1.02
f1 (ppm)

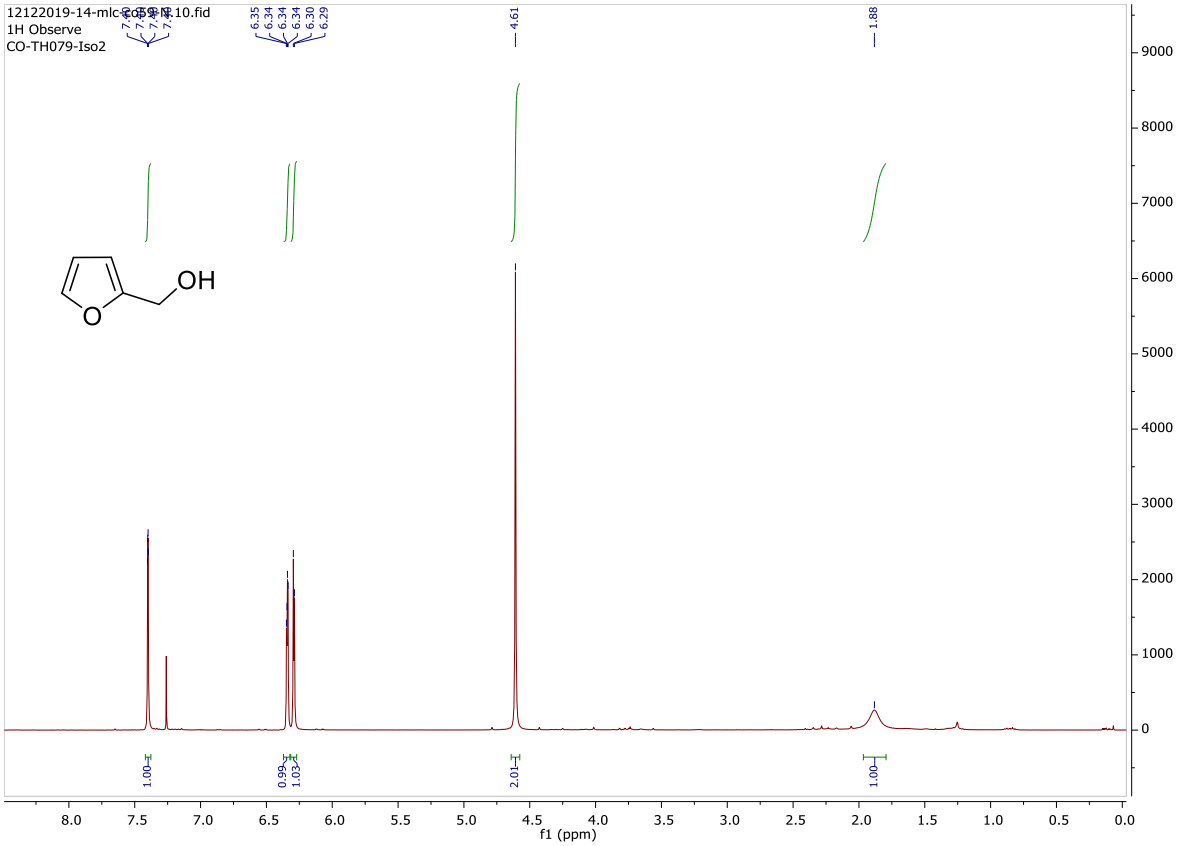

11122019-25-mlc-co59-N.11.fid
13C Observe with 1H decoupling - D1 = 2s
CO-TH065-Iso1
140.46
137.61
128.83
93.01
64.67
OH
I
f1 (ppm)

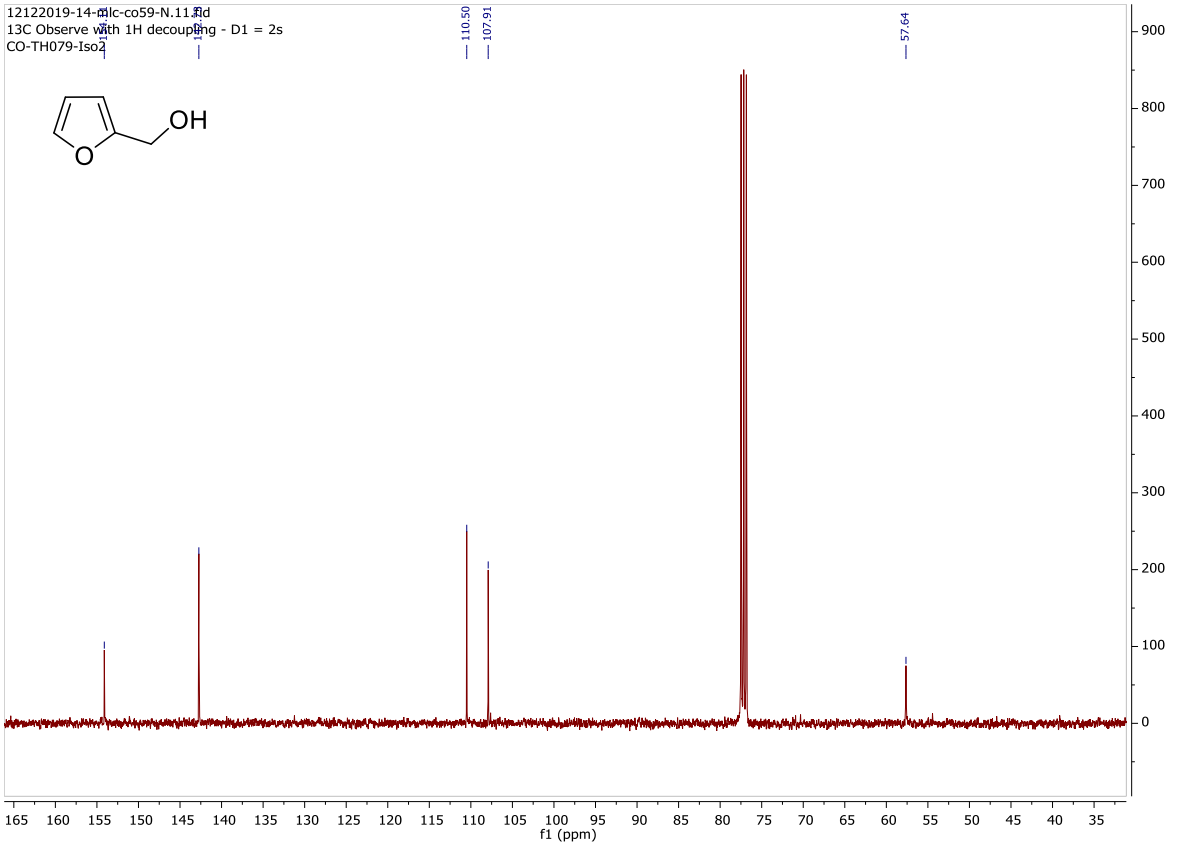

10242019-31-mlc-co59-M.10.fid
1H Observe
CO-TH053-Iso4
OH
4.70
1.72
3.79
1.00
1.97
1.00
f1 (ppm)

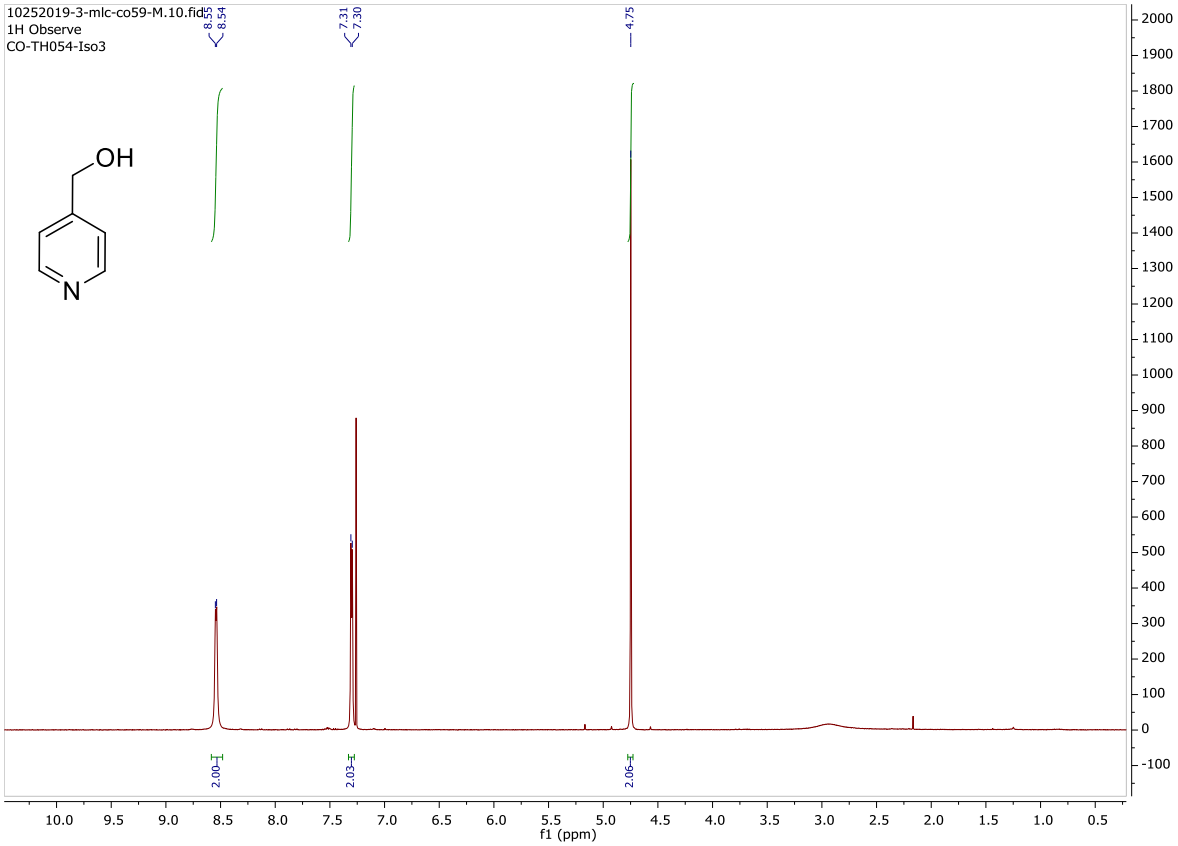

10242019-31-mlc-co59-M.11.fid
13C Observe with 1H decoupling - D1 = 2s
CO-TH053-Iso-C
OH
140.98
128.72
127.82
127.14
65.55
f1 (ppm)

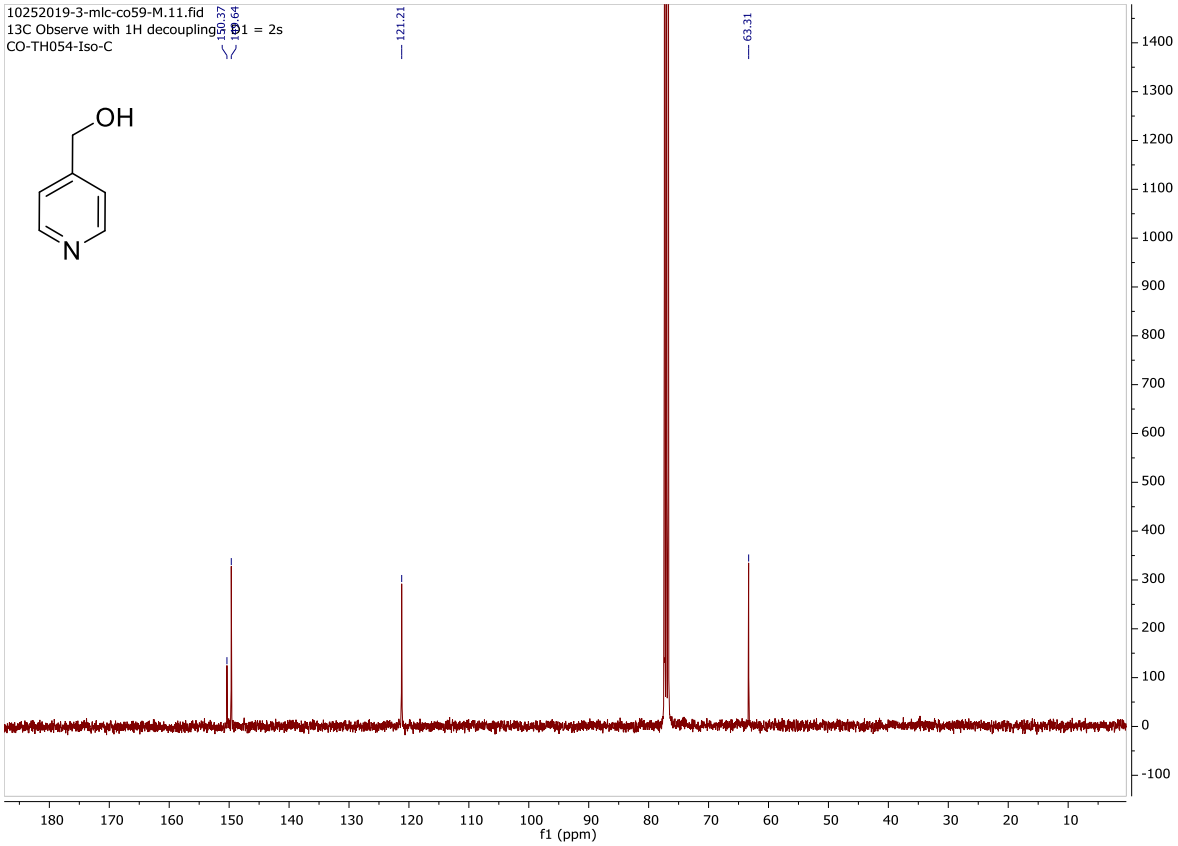

1H Observe
CO-TH047A-Iso1
OH
5.19
1.70
1.00
2.06
2.98
1.08
2.01
1.29
f1 (ppm)

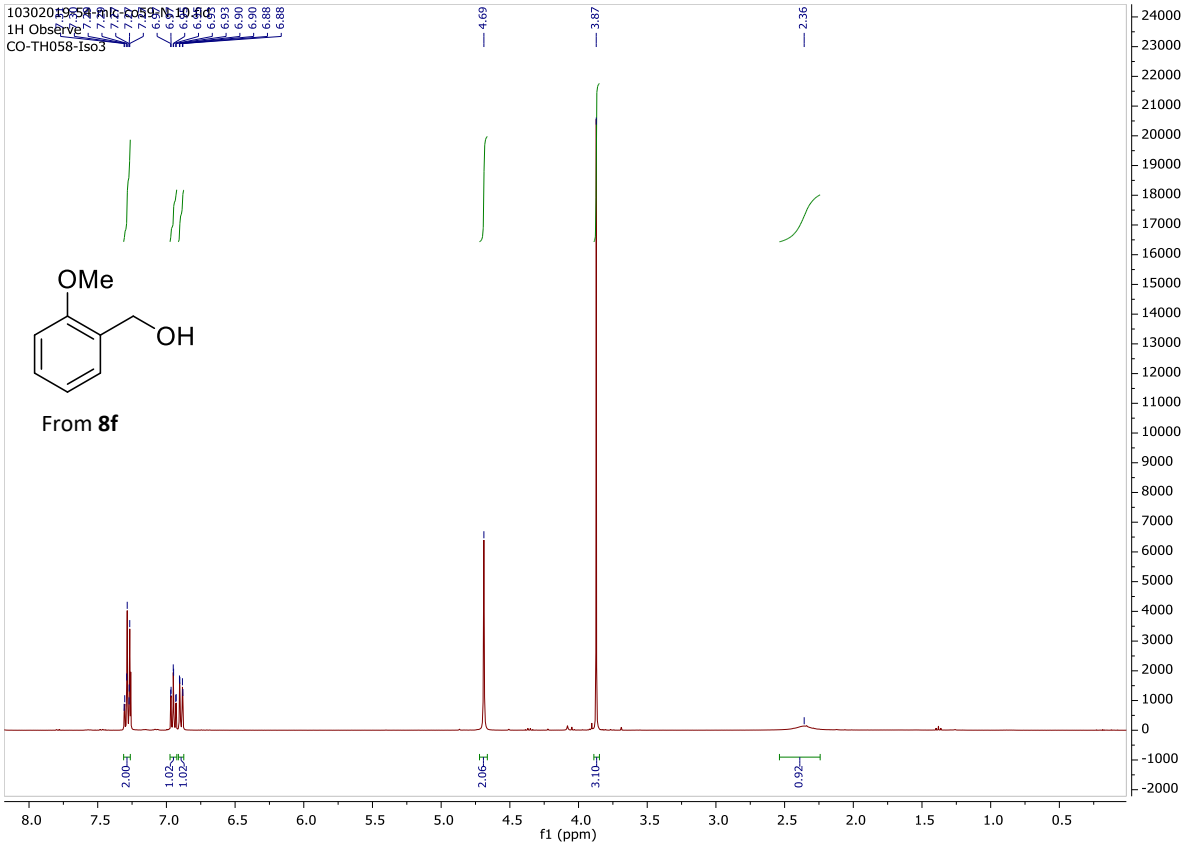

13C Observe with 1H decoupling
CO-TH047A-IsoC
OH
63.81
f1 (ppm)

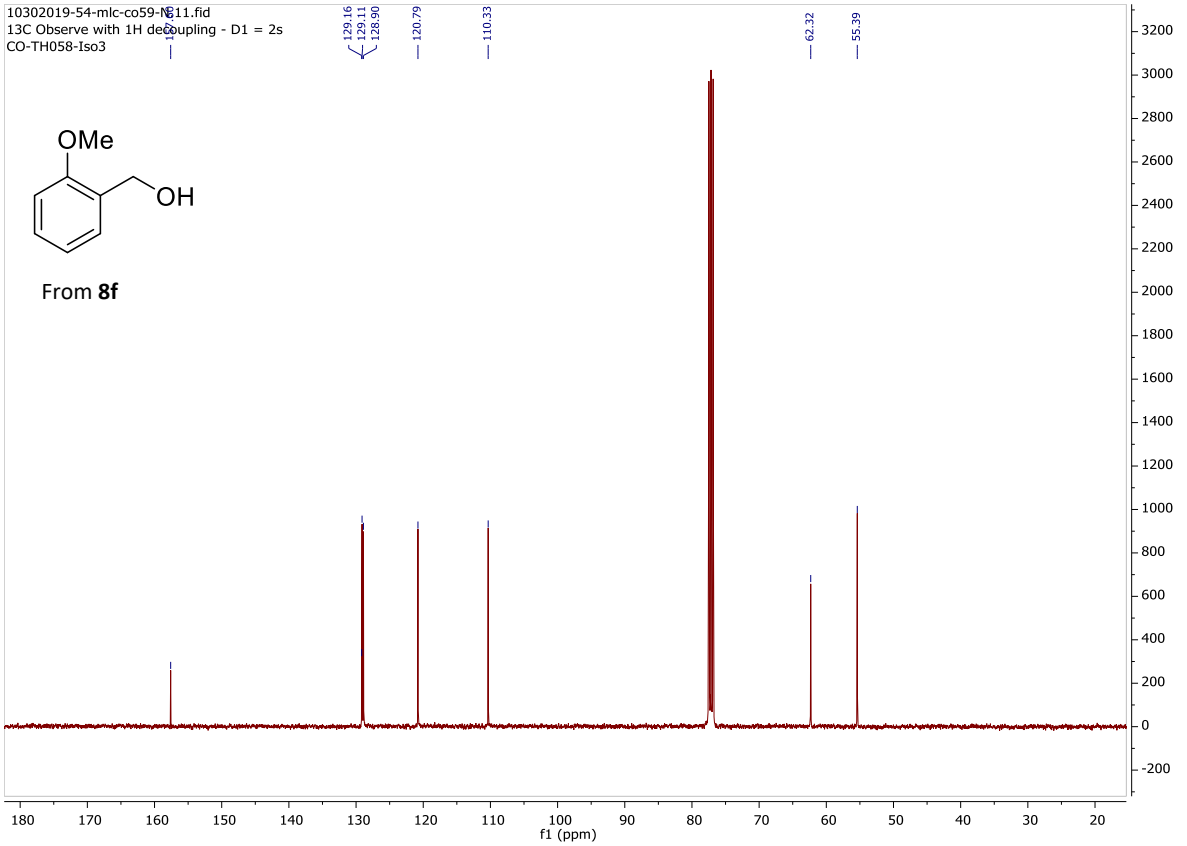

12122019-14-mlc-co59-N.10.fid
1H Observe
CO-TH079-Iso2
7.41
7.41
7.40
7.40
6.35
6.34
6.34
6.34
6.30
6.29
4.61
1.88
OH
O
1.00
0.99
1.03
2.01
1.00
f1 (ppm)

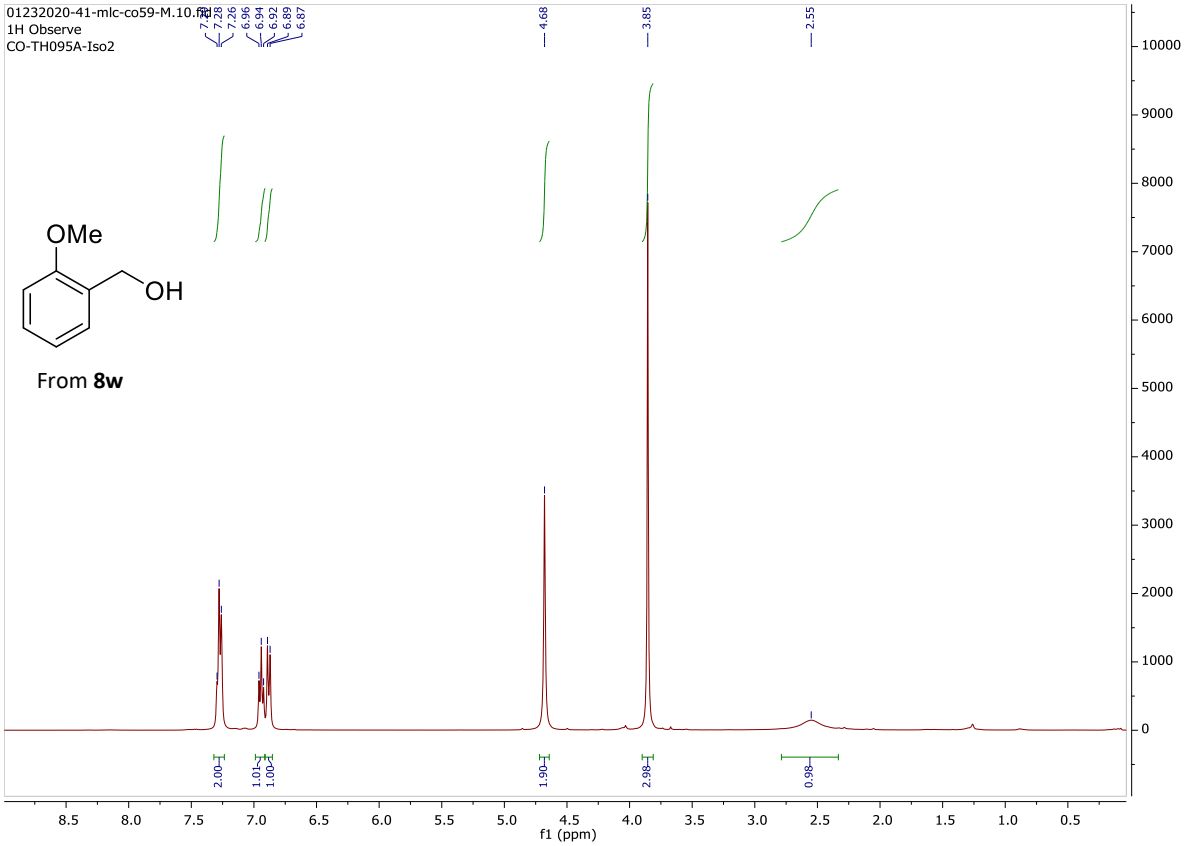

12122019-14-mlc-co59-N.11.fid
13C Observe with 1H decoupling - D1 = 2s
CO-TH079-Iso2
110.50
107.91
57.64
OH
O
f1 (ppm)

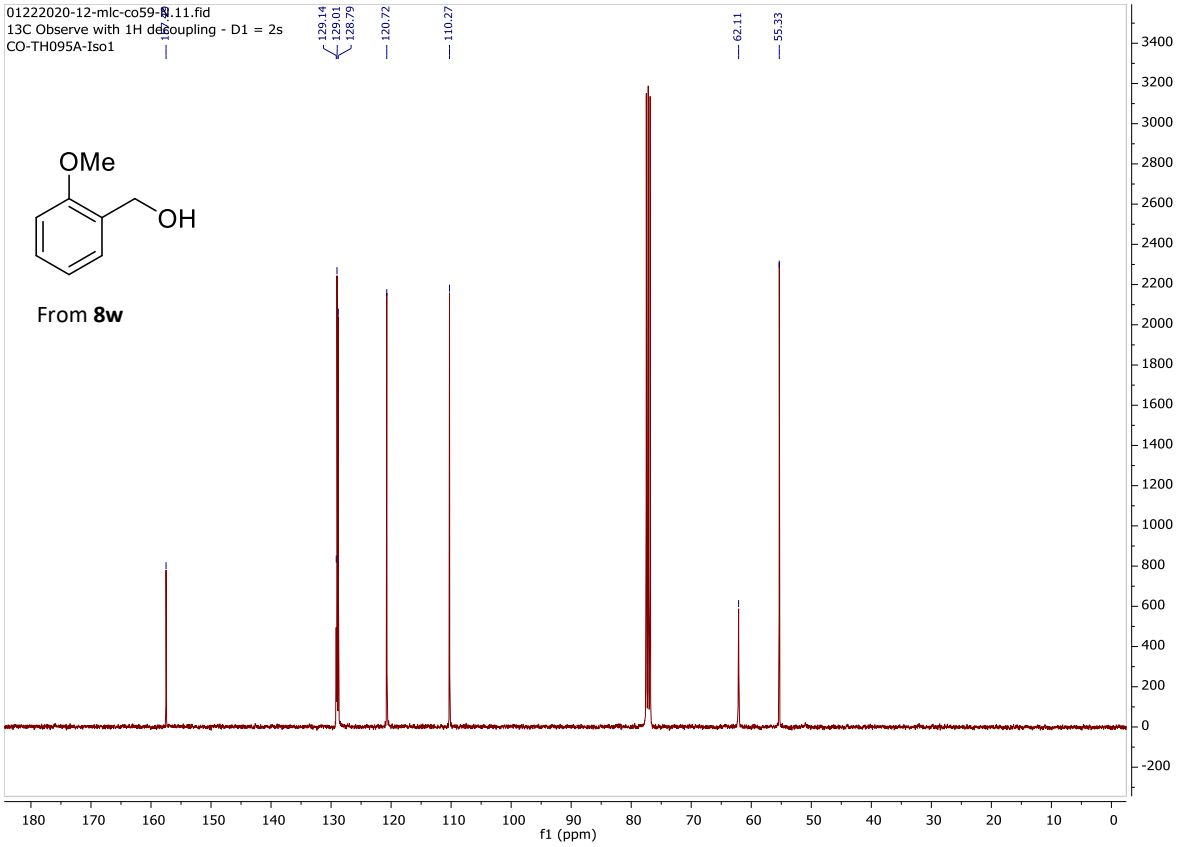

10252019-3-mlc-co59-M.10.fid
1H Observe
CO-TH054-Iso3
8.55
8.54
7.31
7.30
4.75
OH
N
2.00
2.03
2.06
f1 (ppm)

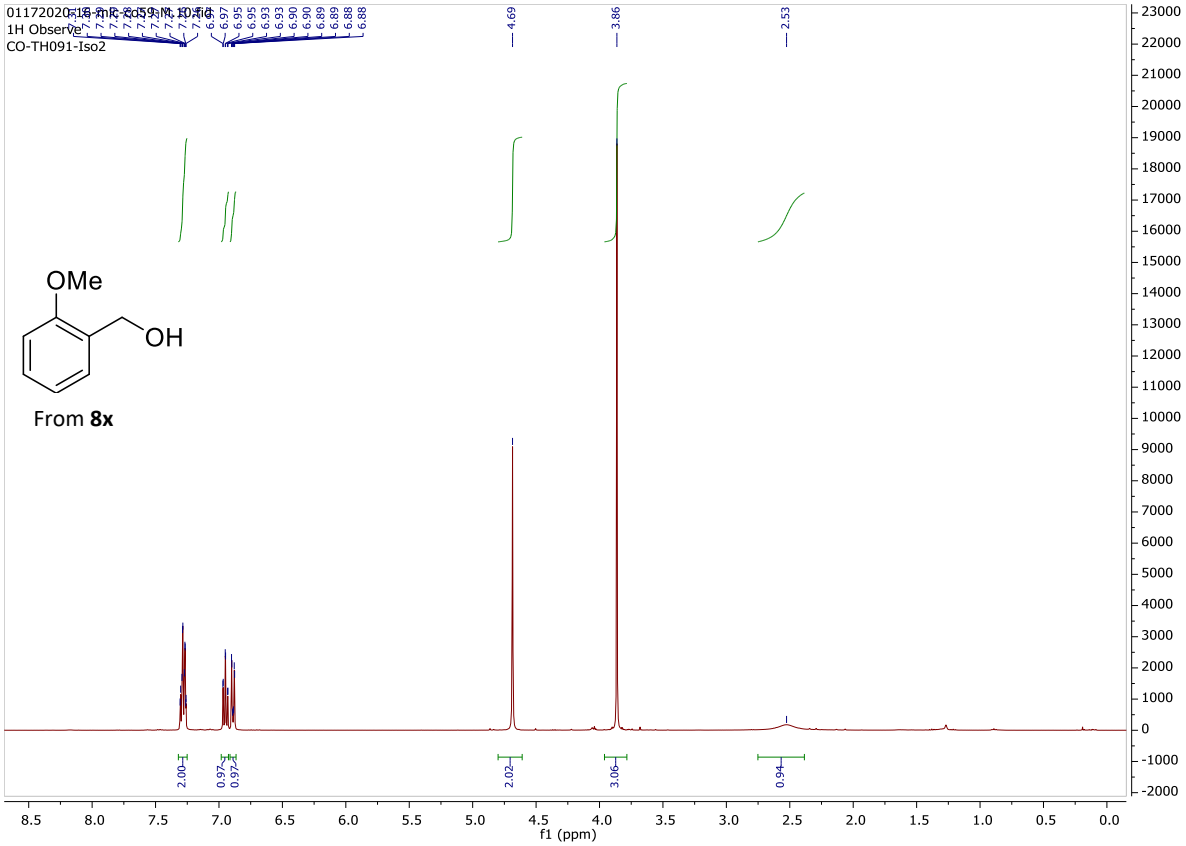

10252019-3-mlc-co59-M.11.fid
13C Observe with 1H decoupling, d1 = 2s
CO-TH054-Iso-C
150.37
149.64
121.21
63.31
OH
N
f1 (ppm)

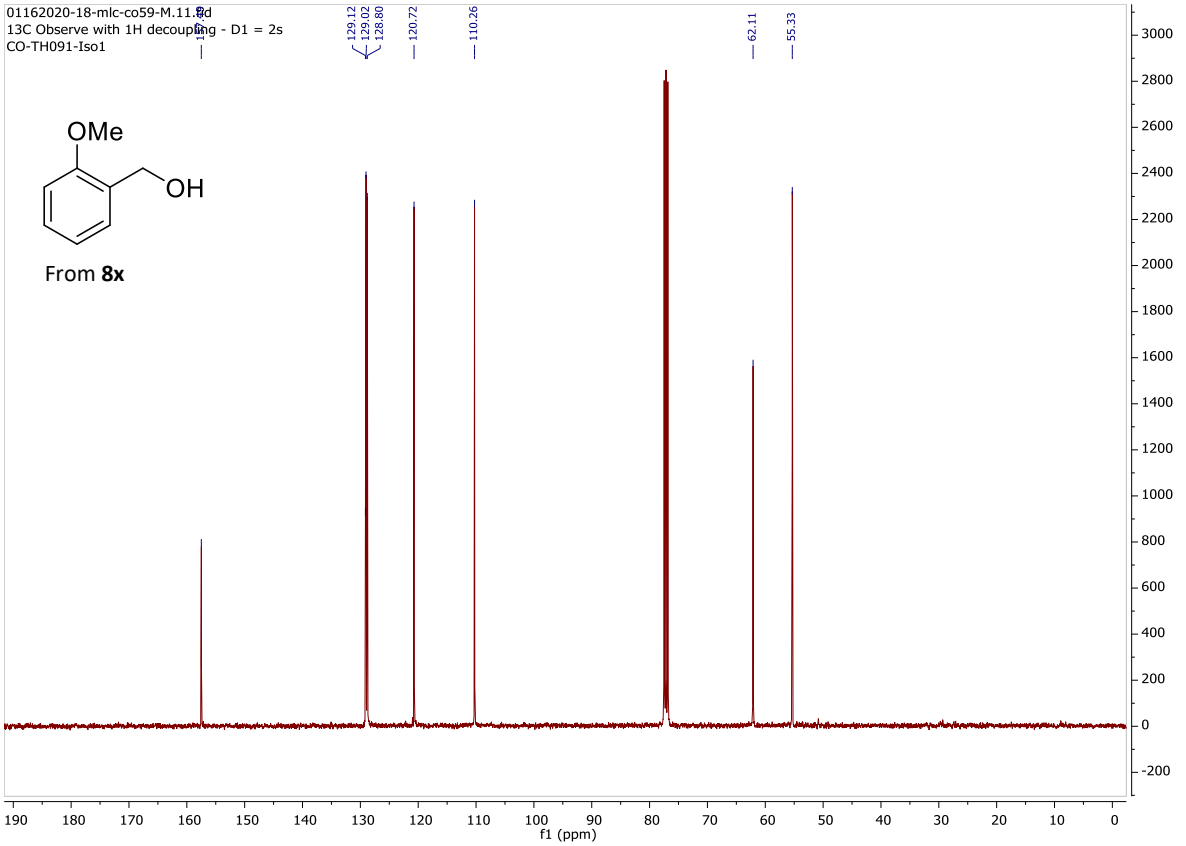

1H Observe
CO-TH058-Iso3
4.69
3.87
2.36
OMe
OH
From 8f
f1 (ppm)

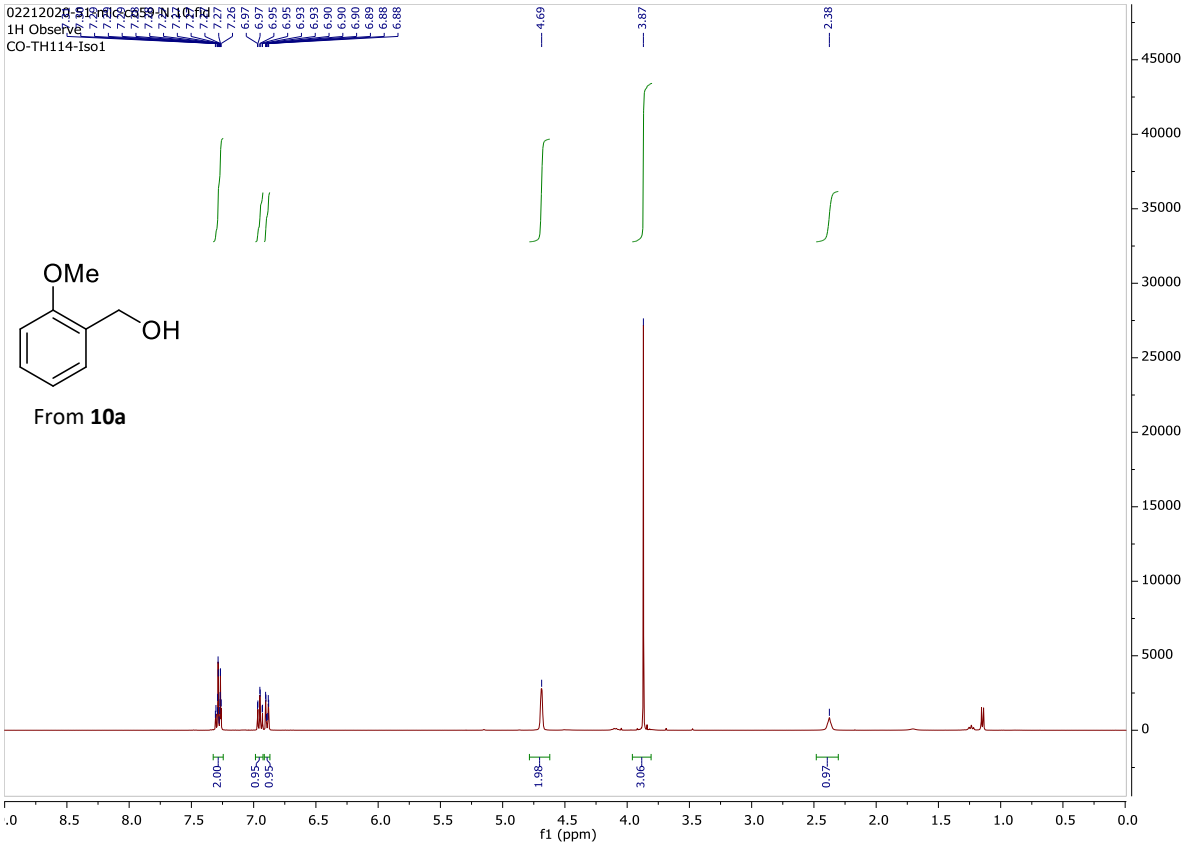

13C Observe with 1H decoupling - D1 = 2s
CO-TH058-Iso3
129.16
129.11
128.90
120.79
110.33
62.32
55.39
OMe
OH
From 8f
f1 (ppm)

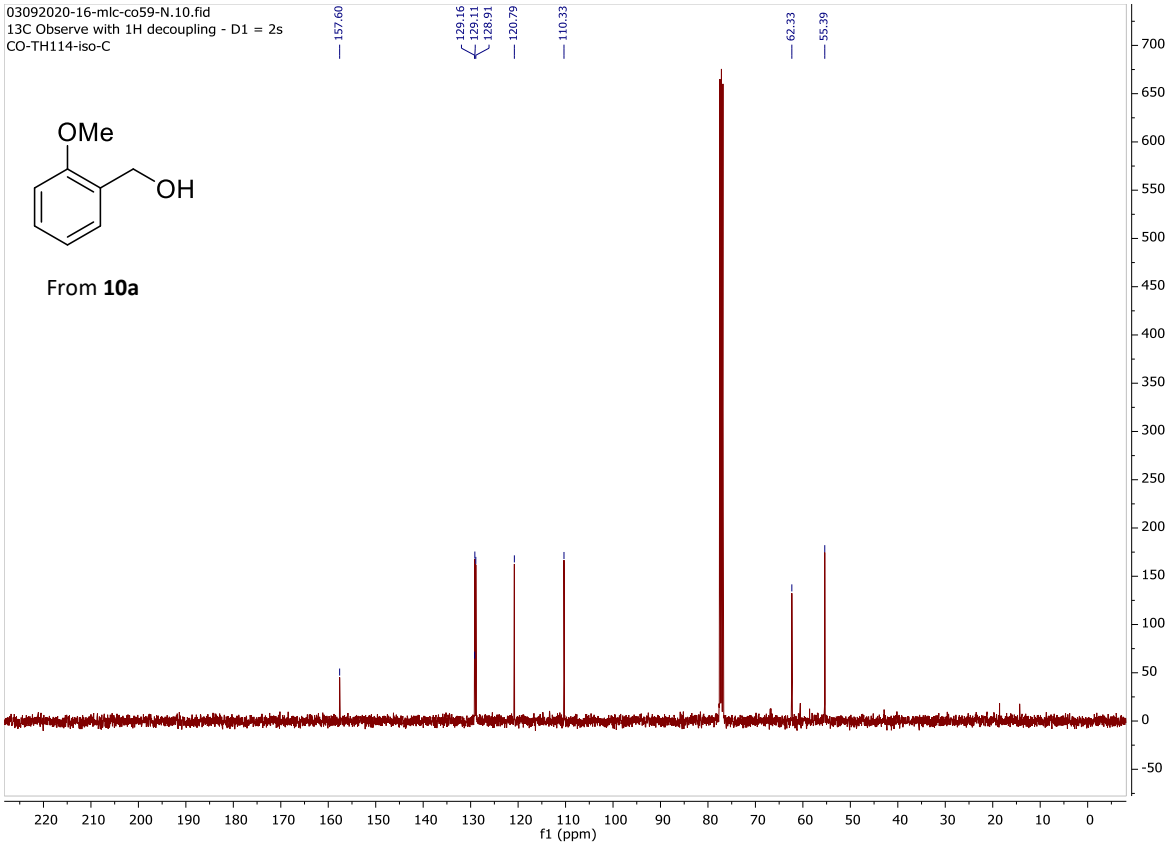

01232020-41-mlc-co59-M.10.fid
1H Observe
CO-TH095A-Iso2
7.28
7.26
6.96
6.94
6.92
6.89
6.87
4.68
3.85
2.55
OMe
OH
From 8w
2.00
1.01
1.00
1.90
2.98
0.98
f1 (ppm)

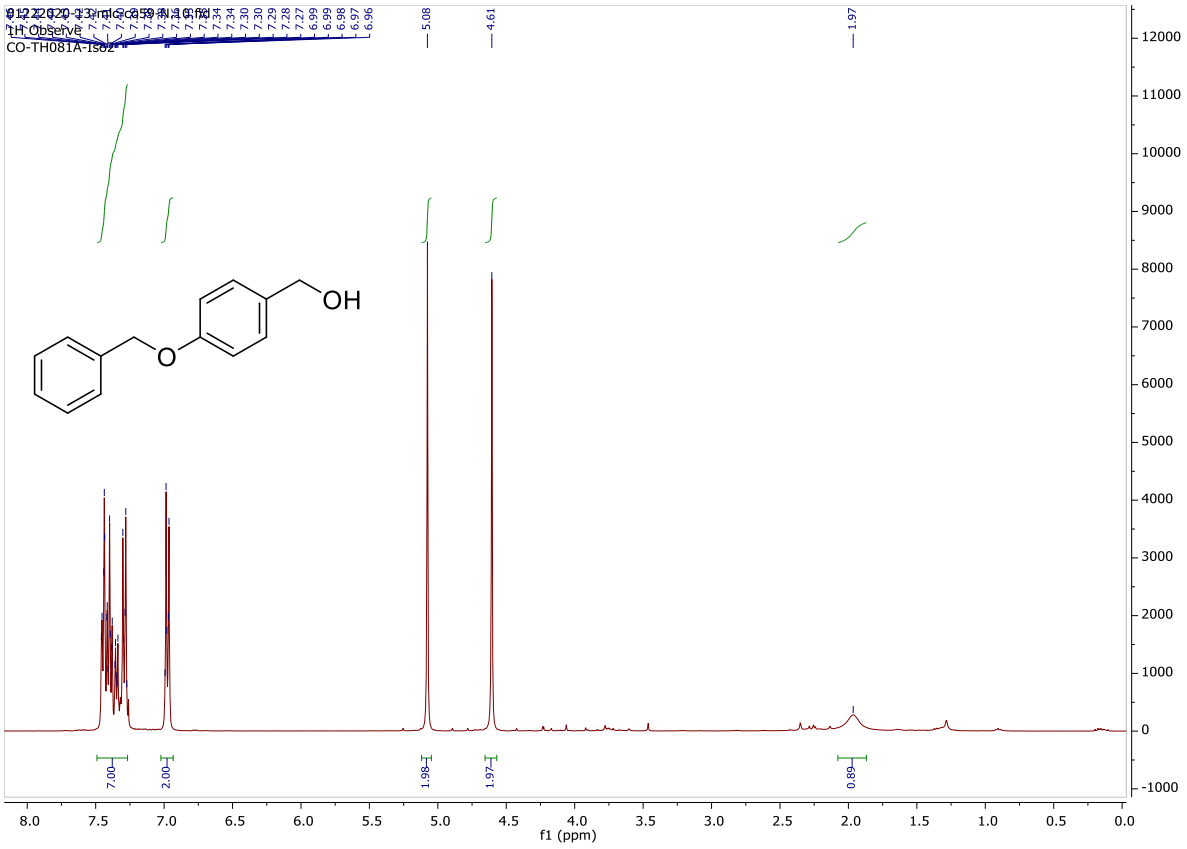

01222020-12-mlc-co59-M.11.fid
13C Observe with 1H decoupling - D1 = 2s
CO-TH095A-Iso1
129.14
129.01
128.79
120.72
110.27
62.11
55.33
OMe
OH
From 8w
f1 (ppm)

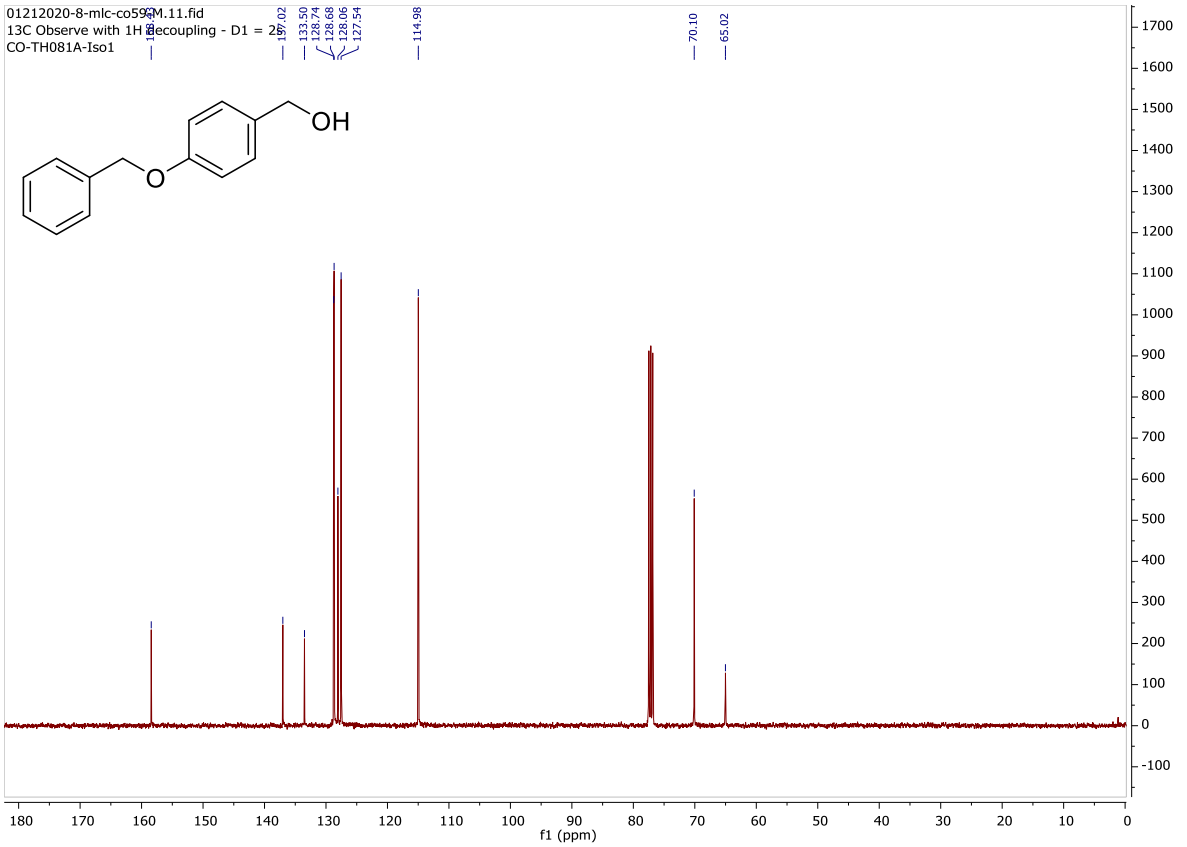

1H Observe
CO-TH091-Iso2
4.69
3.86
2.53
OMe
OH
From 8x
2.00
0.97
0.97
2.02
3.06
0.94
f1 (ppm)

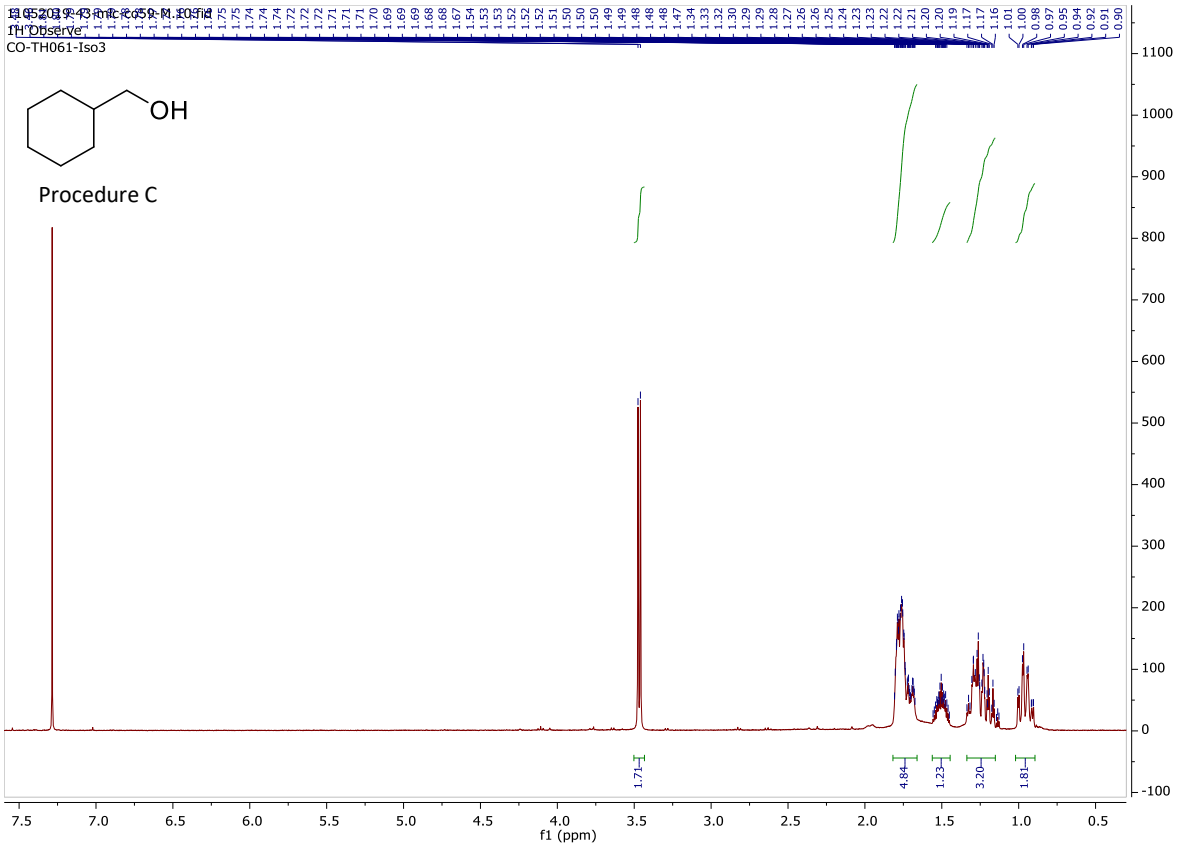

13C Observe with 1H decoupling - D1 = 2s
CO-TH091-Iso1
129.12
129.02
128.80
120.72
110.26
62.11
55.33
OMe
OH
From 8x
f1 (ppm)

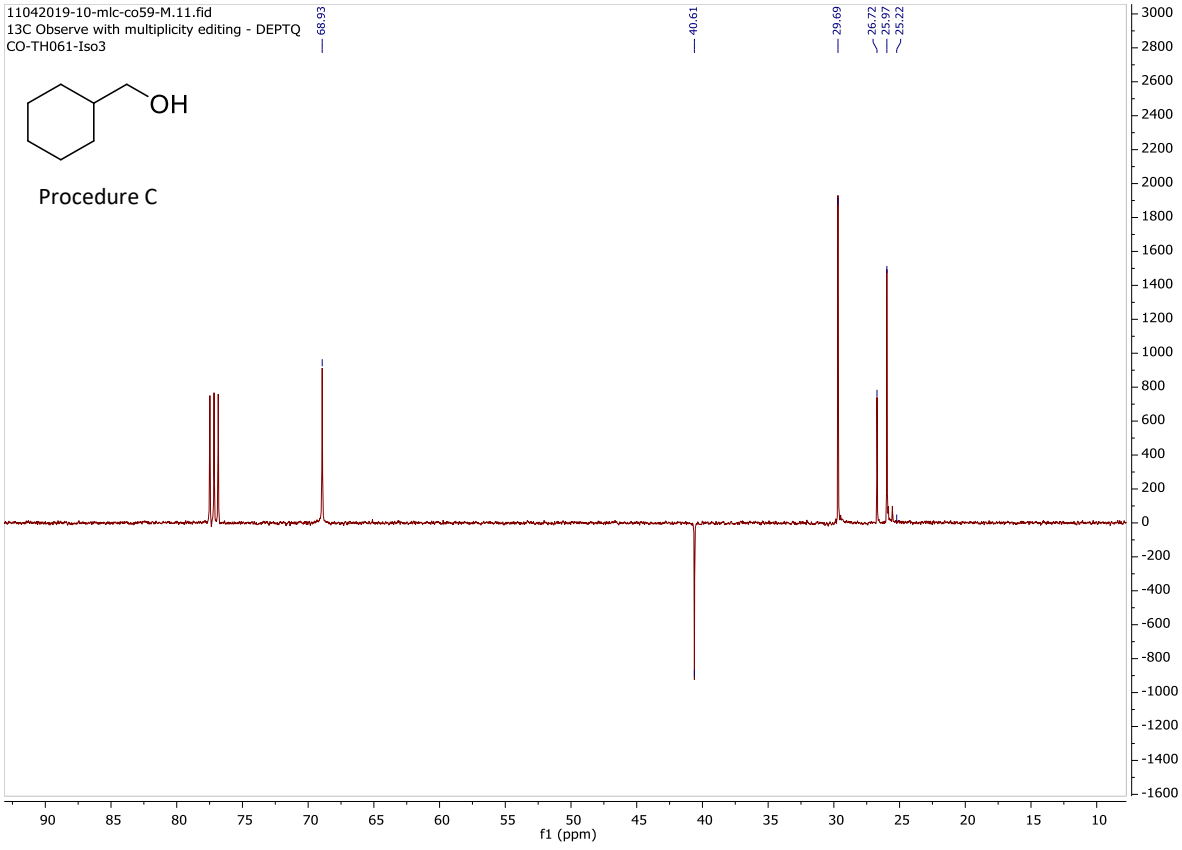

1H Observe
CO-TH114-Iso1
4.69
3.87
2.38
OMe
OH
From **10a**
f1 (ppm)

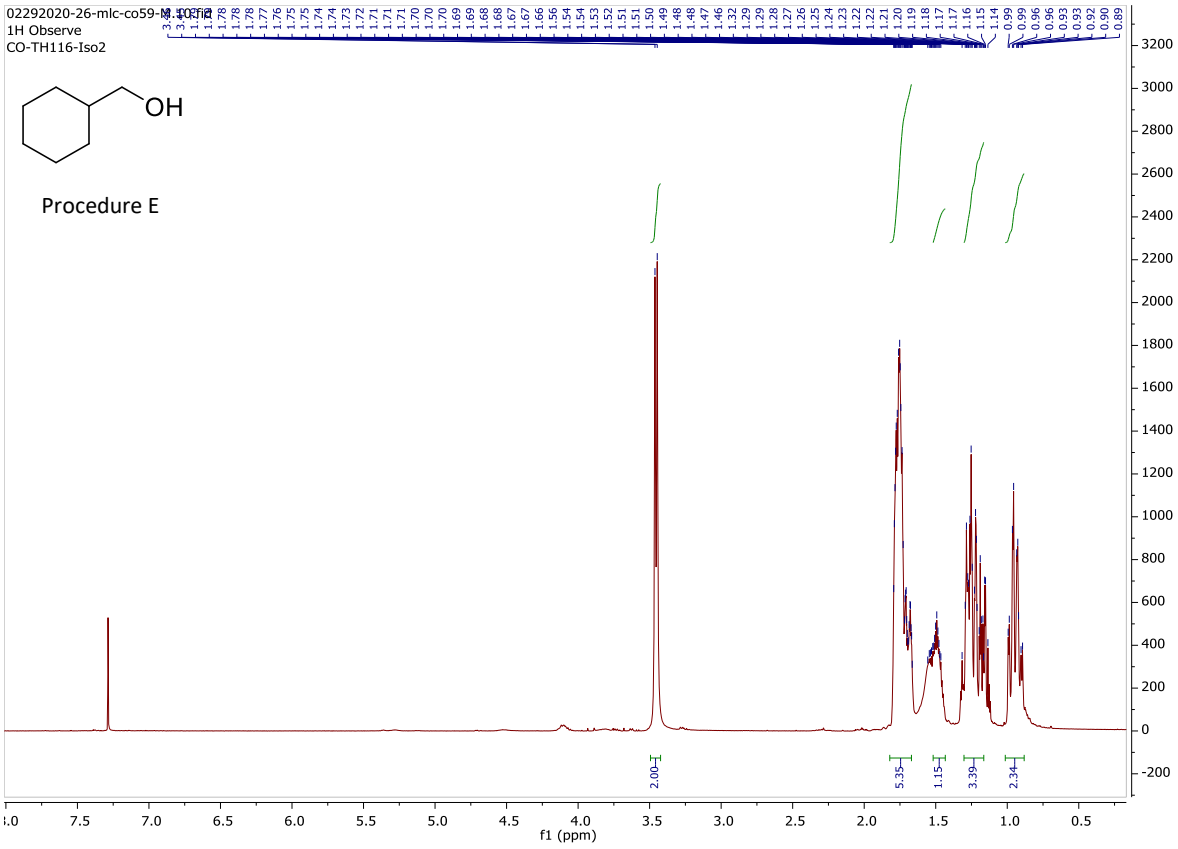

03092020-16-mlc-co59-N.10.fid
13C Observe with 1H decoupling - D1 = 2s
CO-TH114-iso-C
157.60
129.16
129.11
128.91
120.79
110.33
62.33
55.39
OMe
OH
From **10a**
f1 (ppm)

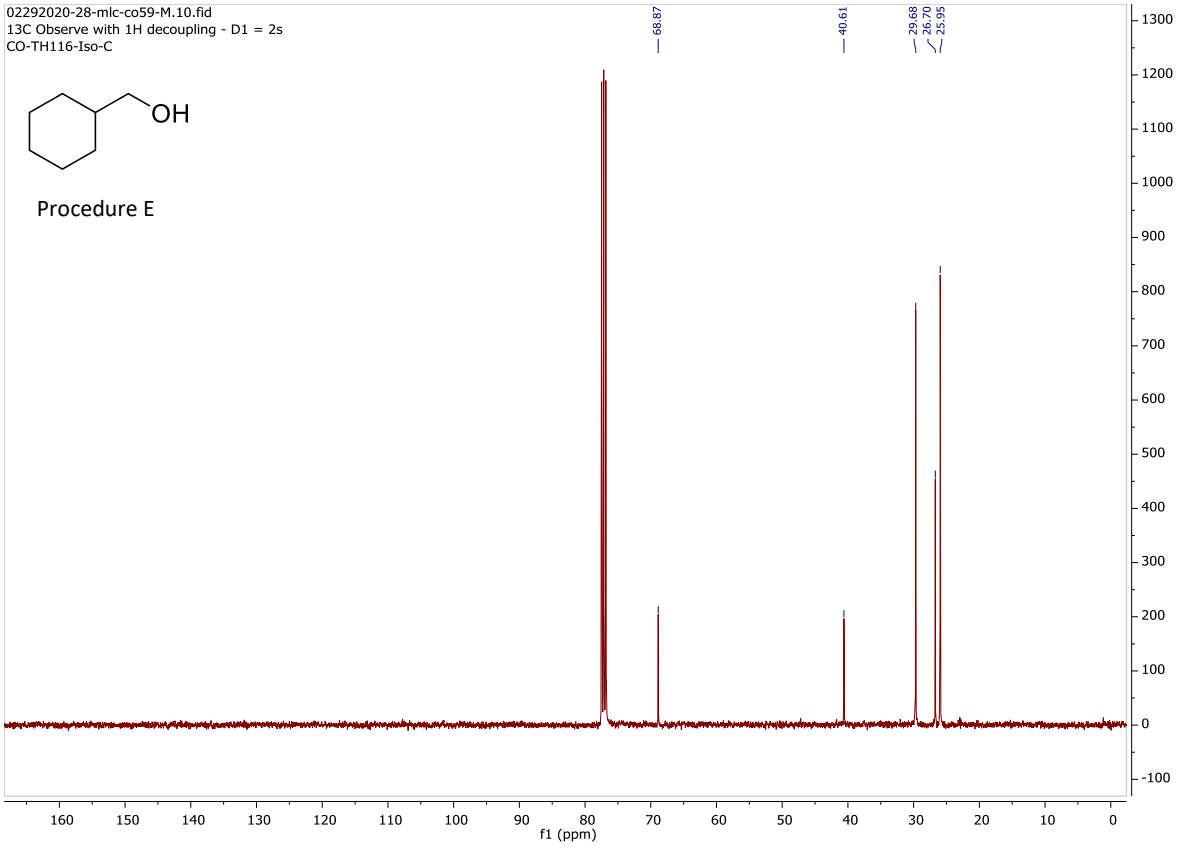

1H Observe
CO-TH081A-Iso2
5.08
4.61
1.97
OH
O
7.00
2.00
1.98
1.97
0.89
f1 (ppm)

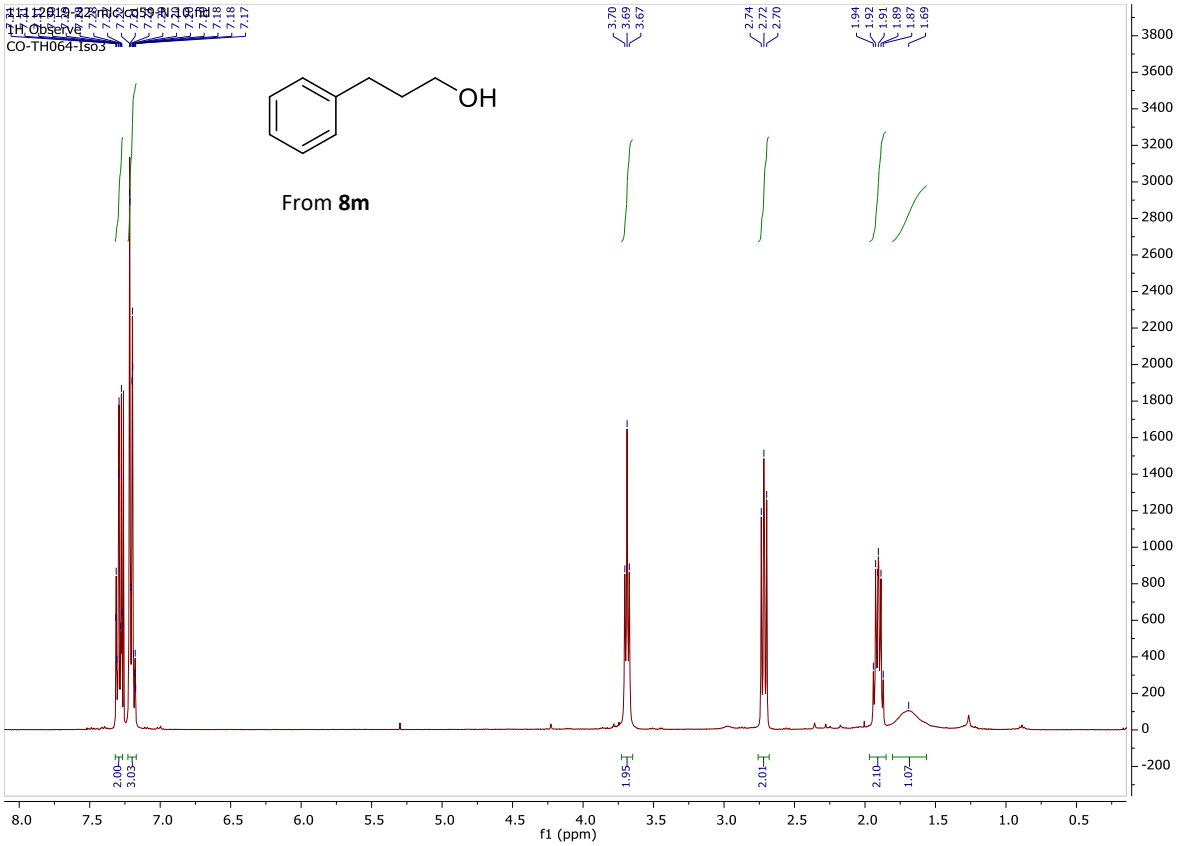

01212020-8-mlc-co594M.11.fid
13C Observe with 1H decoupling - D1 = 2s
CO-TH081A-Iso1
159.02
133.50
129.74
128.68
128.06
127.54
114.98
70.10
65.02
OH
O
f1 (ppm)

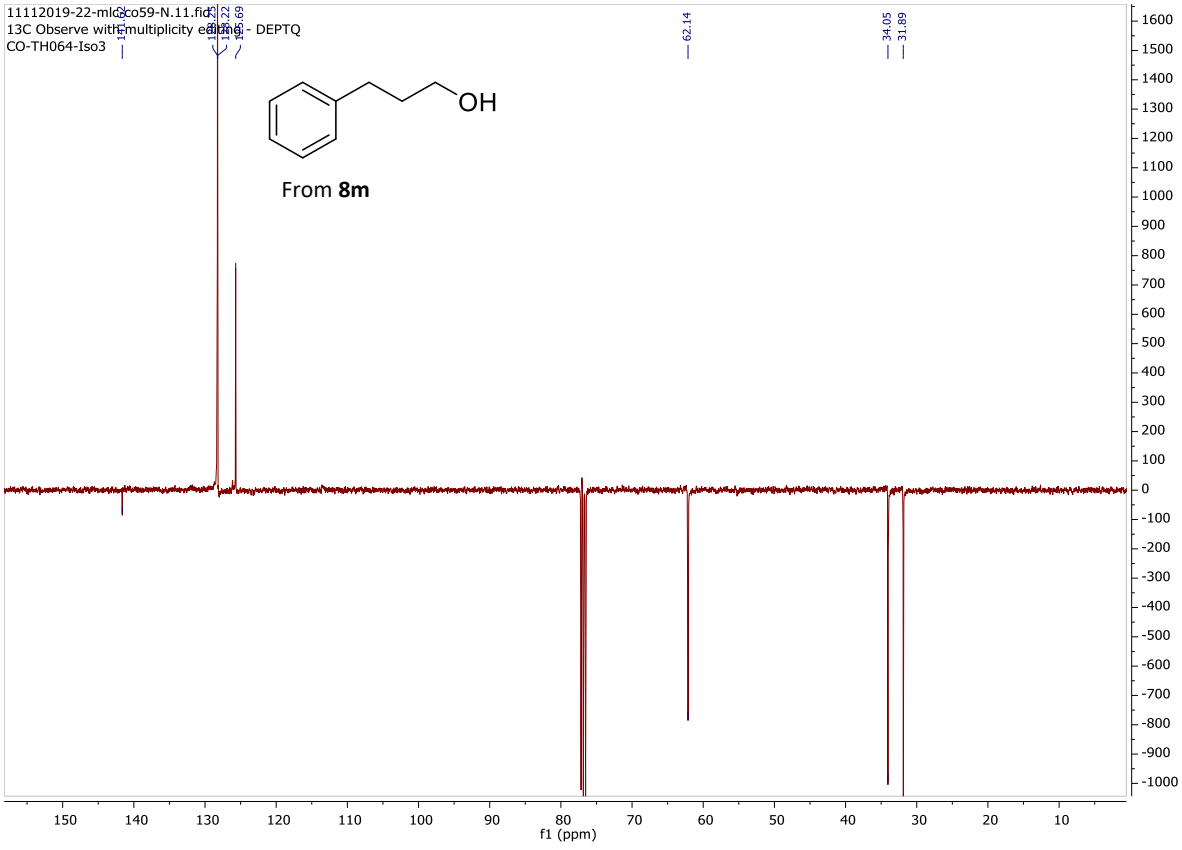

1H Observe
CO-TH061-Iso3
OH
Procedure C
1.71
4.84
1.23
3.20
1.81
f1 (ppm)

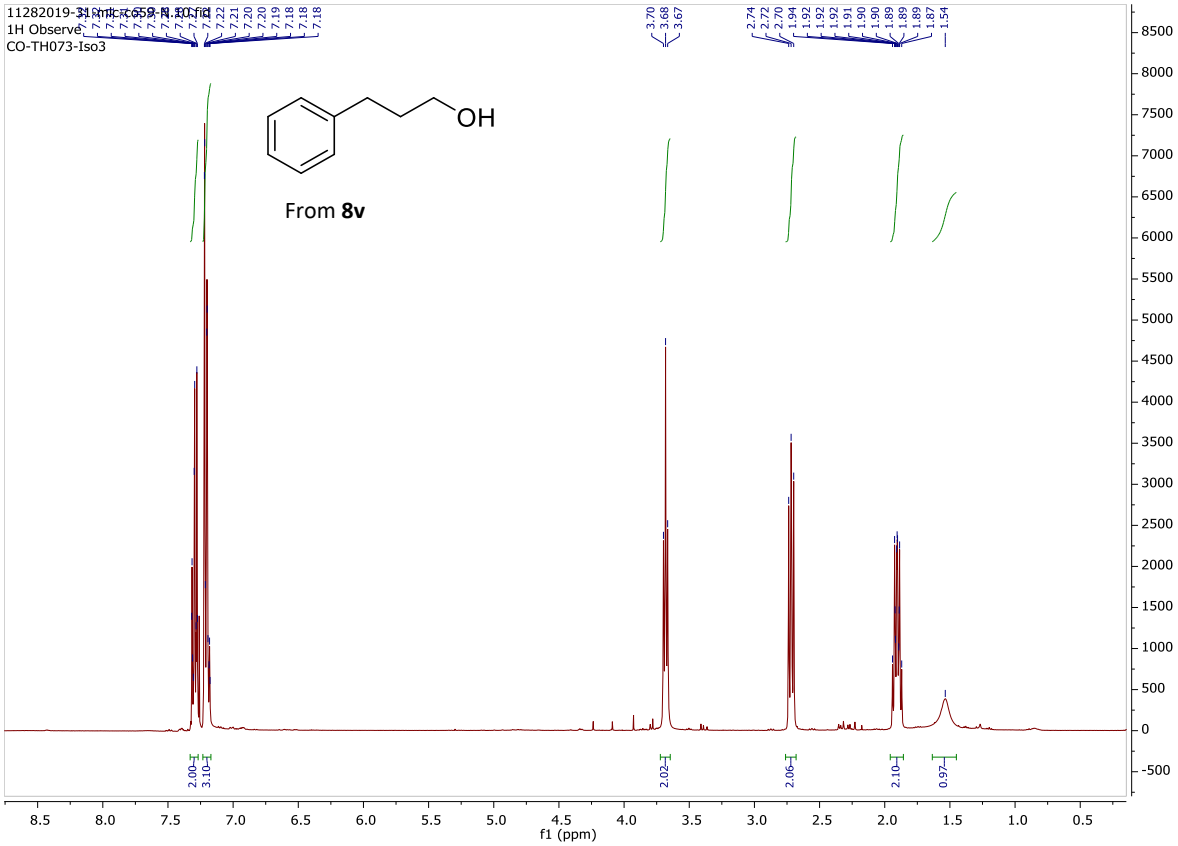

11042019-10-mlc-co59-M.11.fid
13C Observe with multiplicity editing - DEPTQ
CO-TH061-Iso3
68.93
40.61
29.69
26.72
25.97
25.22
OH
Procedure C
f1 (ppm)

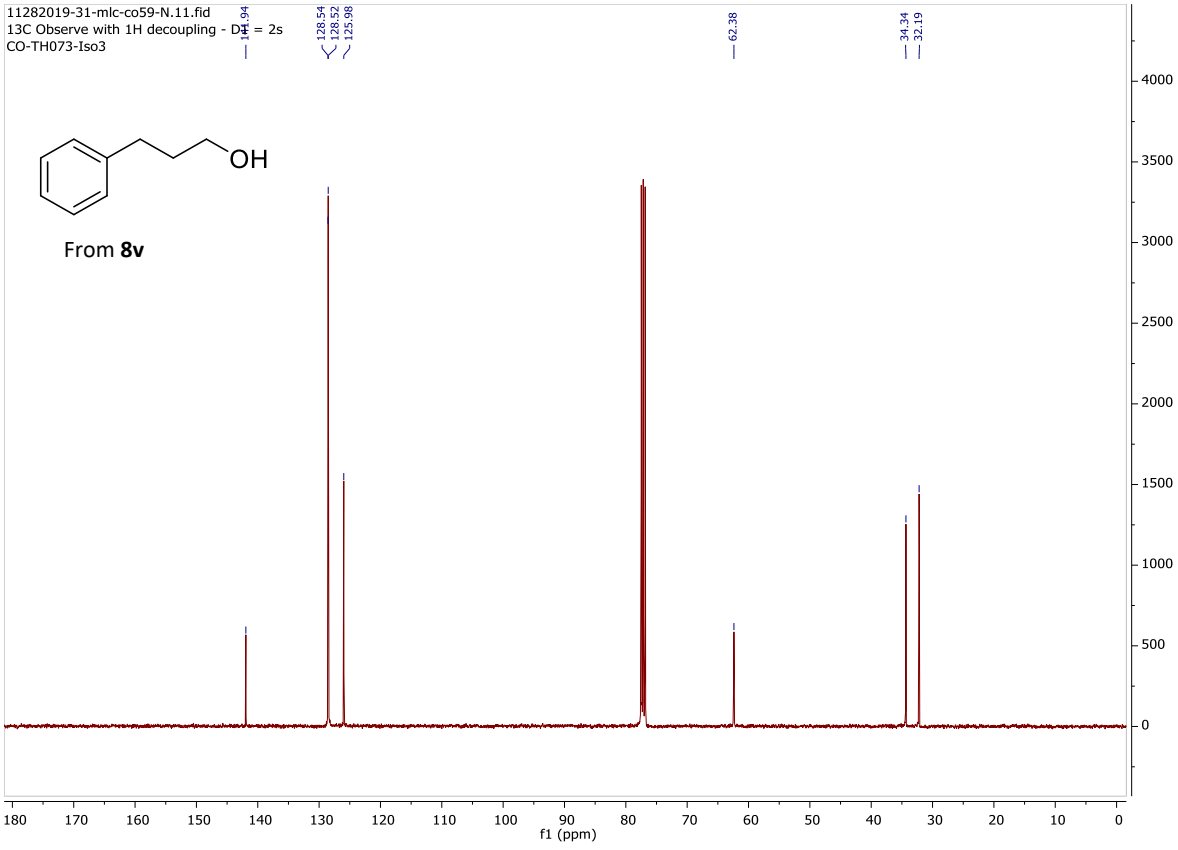

02292020-26-mlc-co59-M.10.fid
1H Observe
CO-TH116-Iso2
OH
Procedure E
2.00
5.35
1.15
3.39
2.34
f1 (ppm)

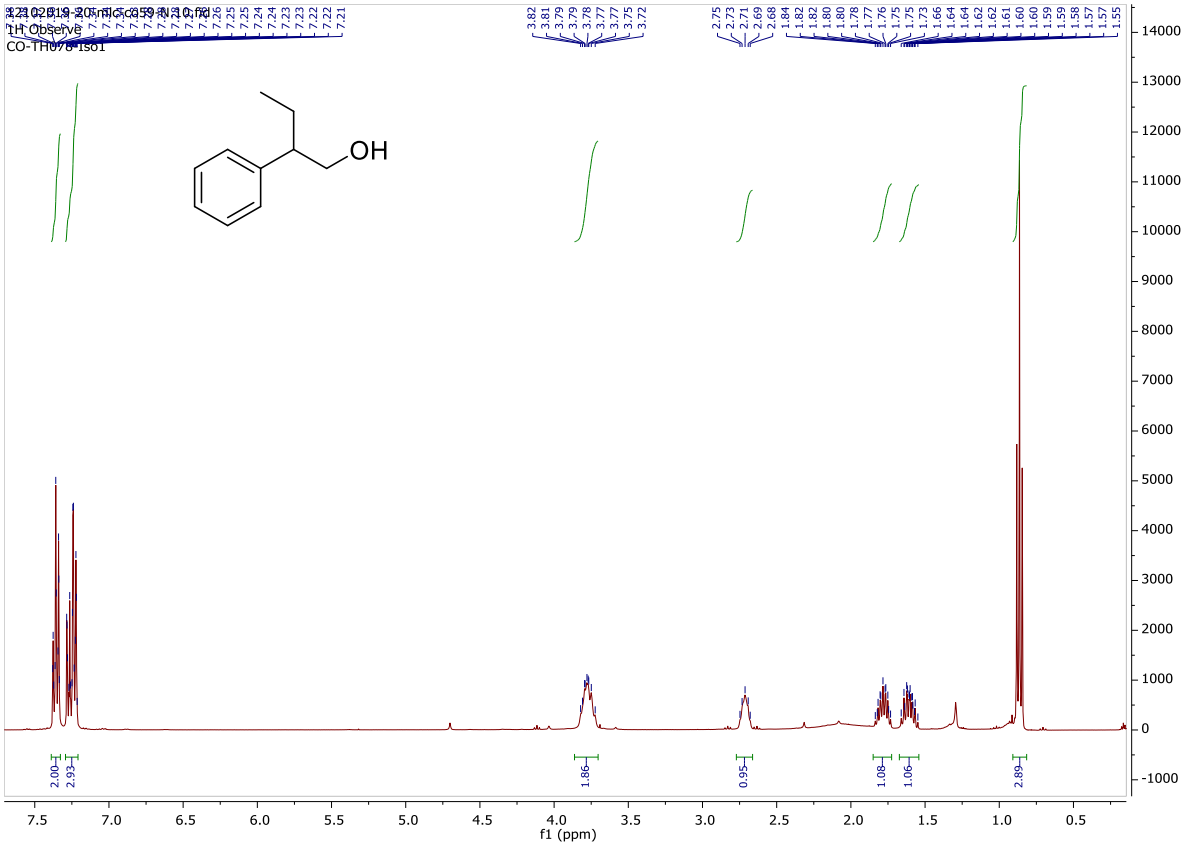

02292020-28-mlc-co59-M.10.fid
13C Observe with 1H decoupling - D1 = 2s
CO-TH116-Iso-C
68.87
40.61
29.68
26.70
25.95
OH
Procedure E
f1 (ppm)

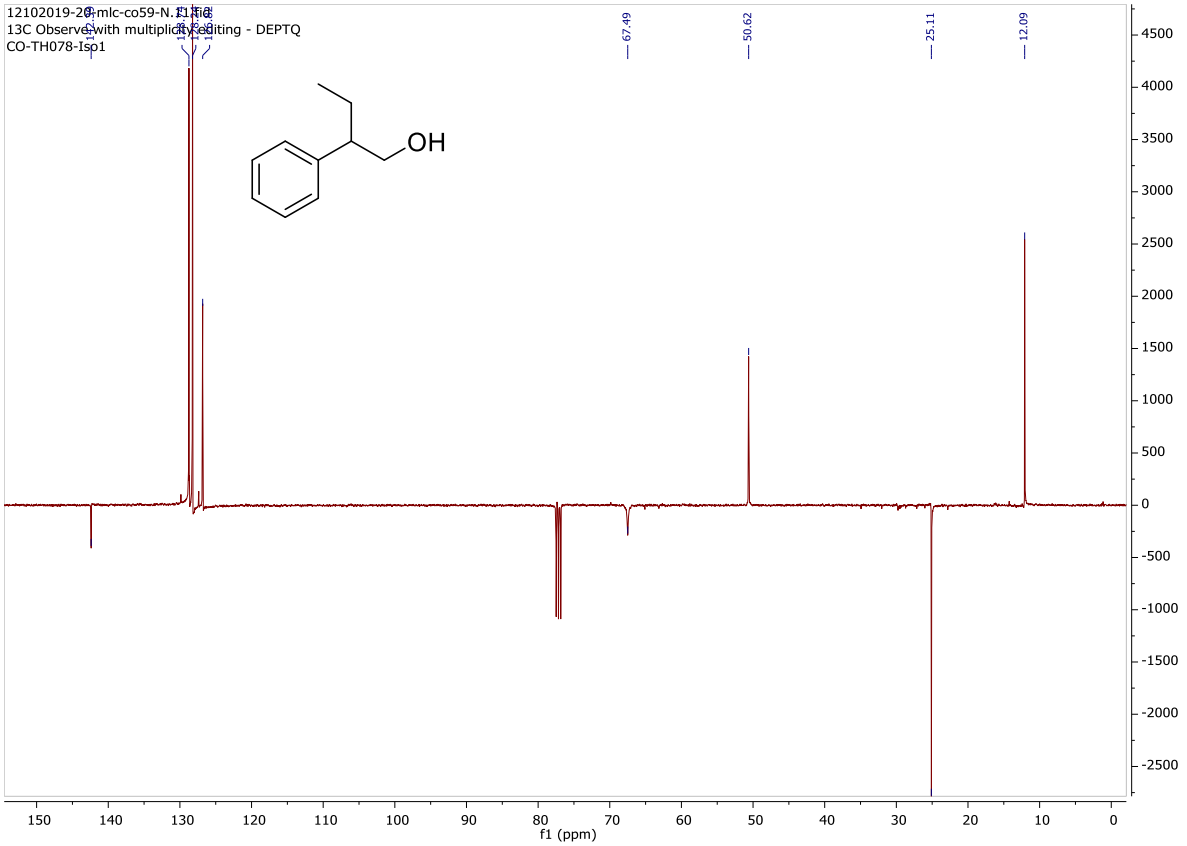

11112019-22-mlc-co59-N.10.fid
1H Observe
CO-TH064-Iso3
OH
From **8m**
f1 (ppm)

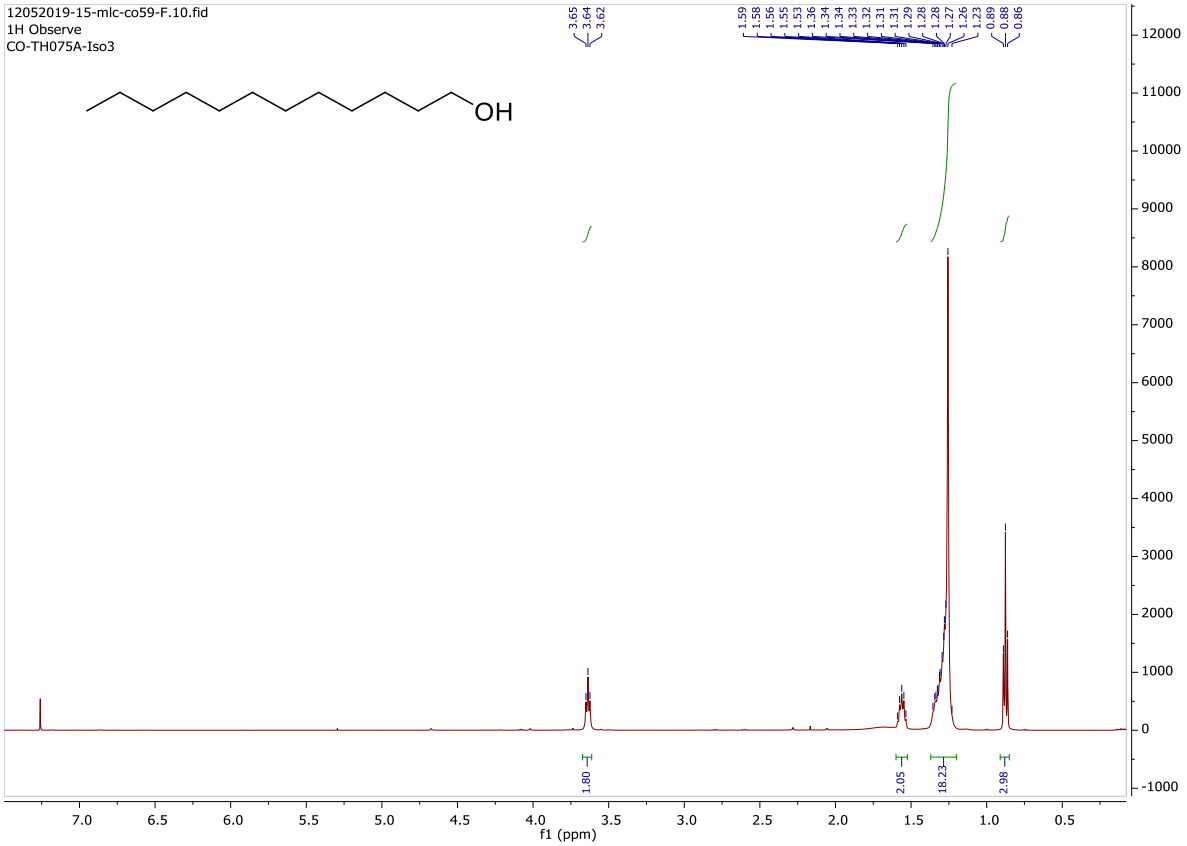

11112019-22-mlc-co59-N.11.fid
13C Observe with multiplicity editing - DEPTQ
CO-TH064-Iso3
OH
From **8m**
f1 (ppm)

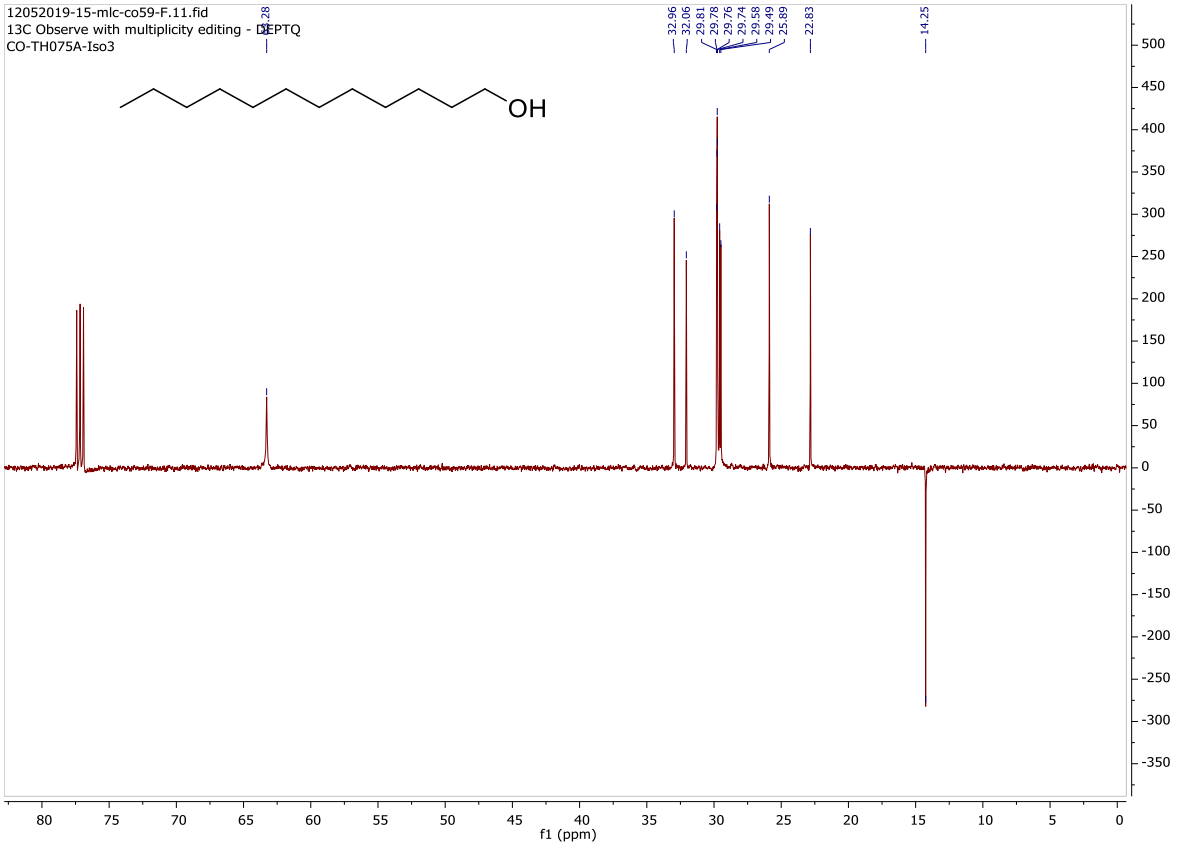

11282019-31-mlc-co59-N.10.fid
1H Observe
CO-TH073-Iso3
OH
From 8v
f1 (ppm)

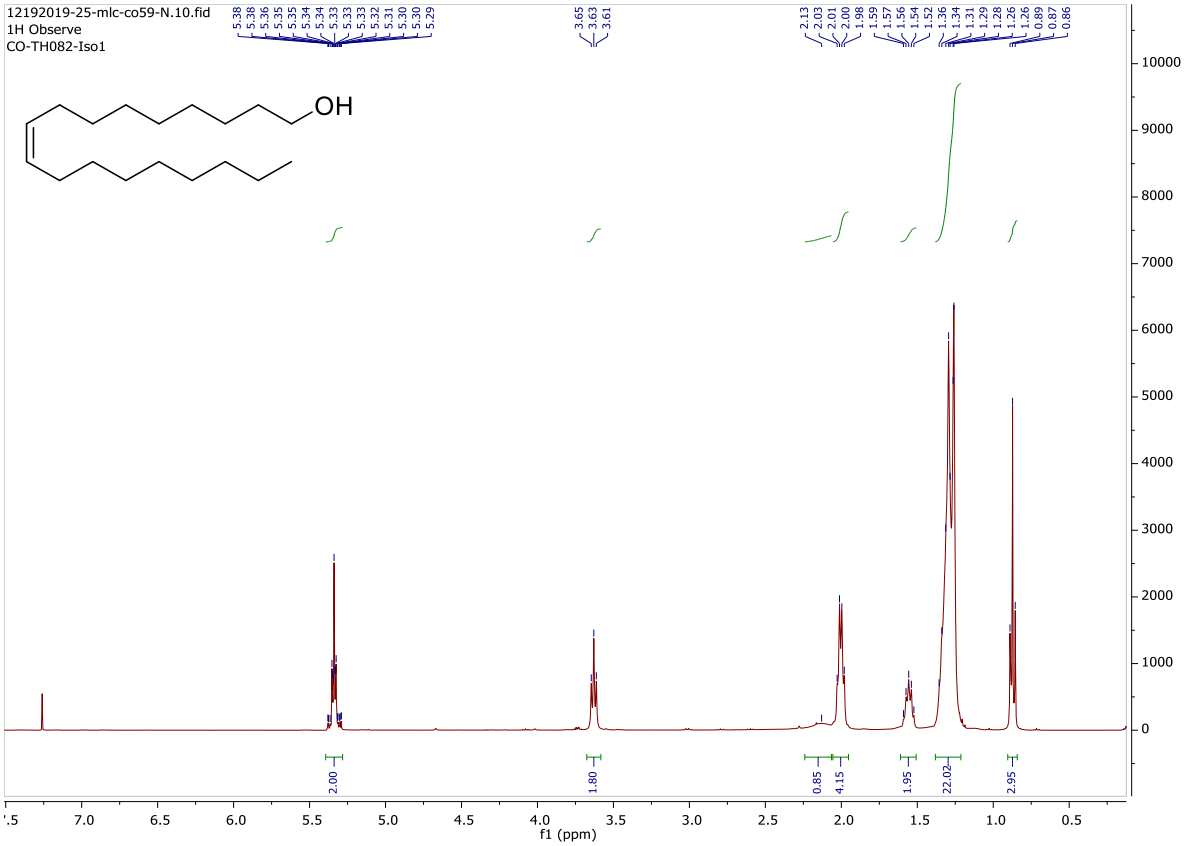

11282019-31-mlc-co59-N.11.fid
13C Observe with 1H decoupling - D1 = 2s
CO-TH073-Iso3
OH
From 8v
f1 (ppm)

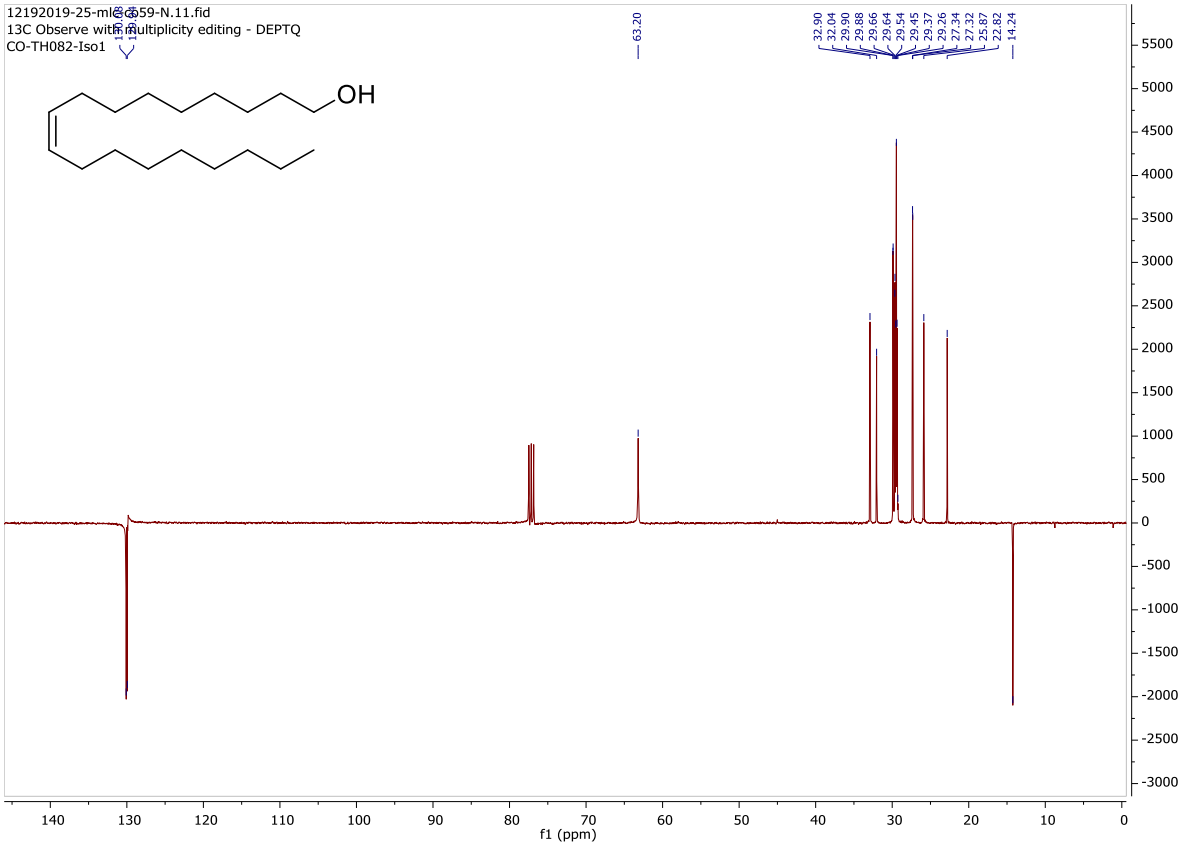

1H Observe
CO-TH078-Iso1
OH
f1 (ppm)

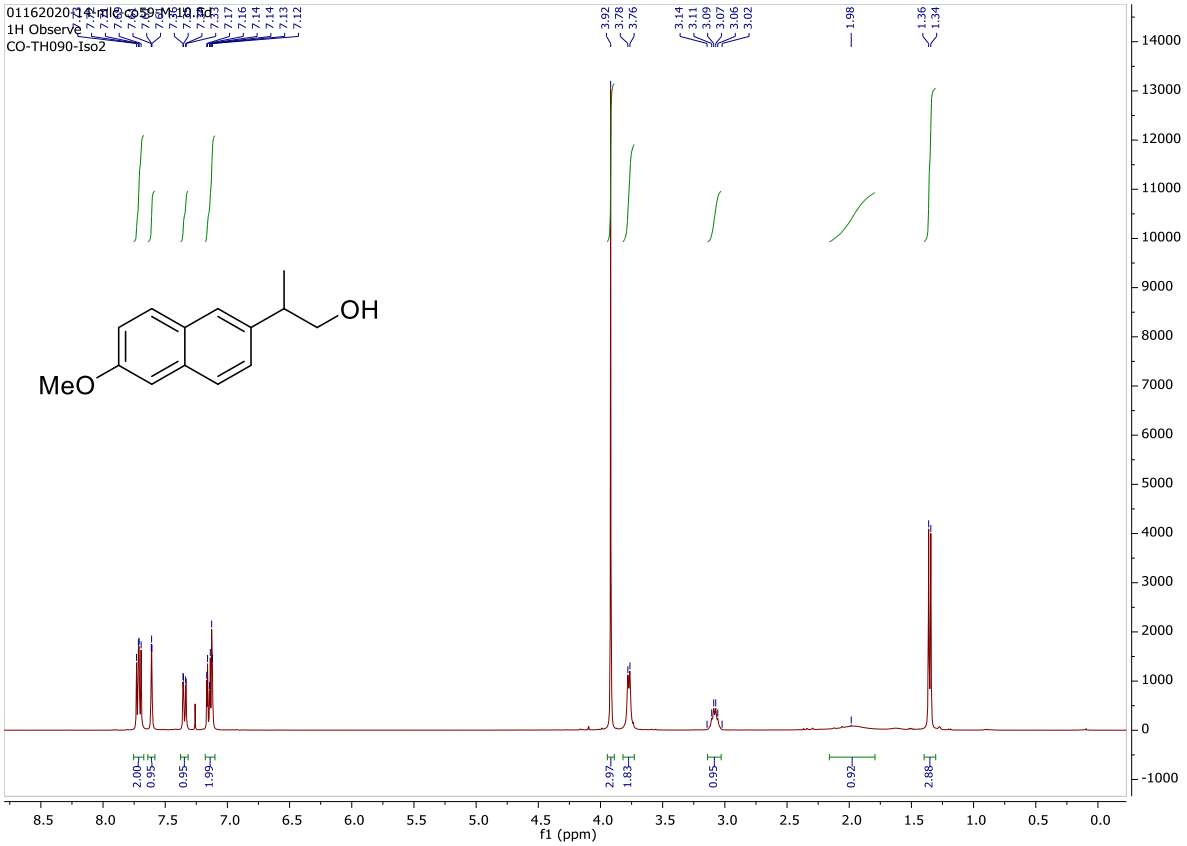

13C Observe with multiplicity editing - DEPTQ
CO-TH078-Iso1
67.49
50.62
25.11
12.09
OH
f1 (ppm)

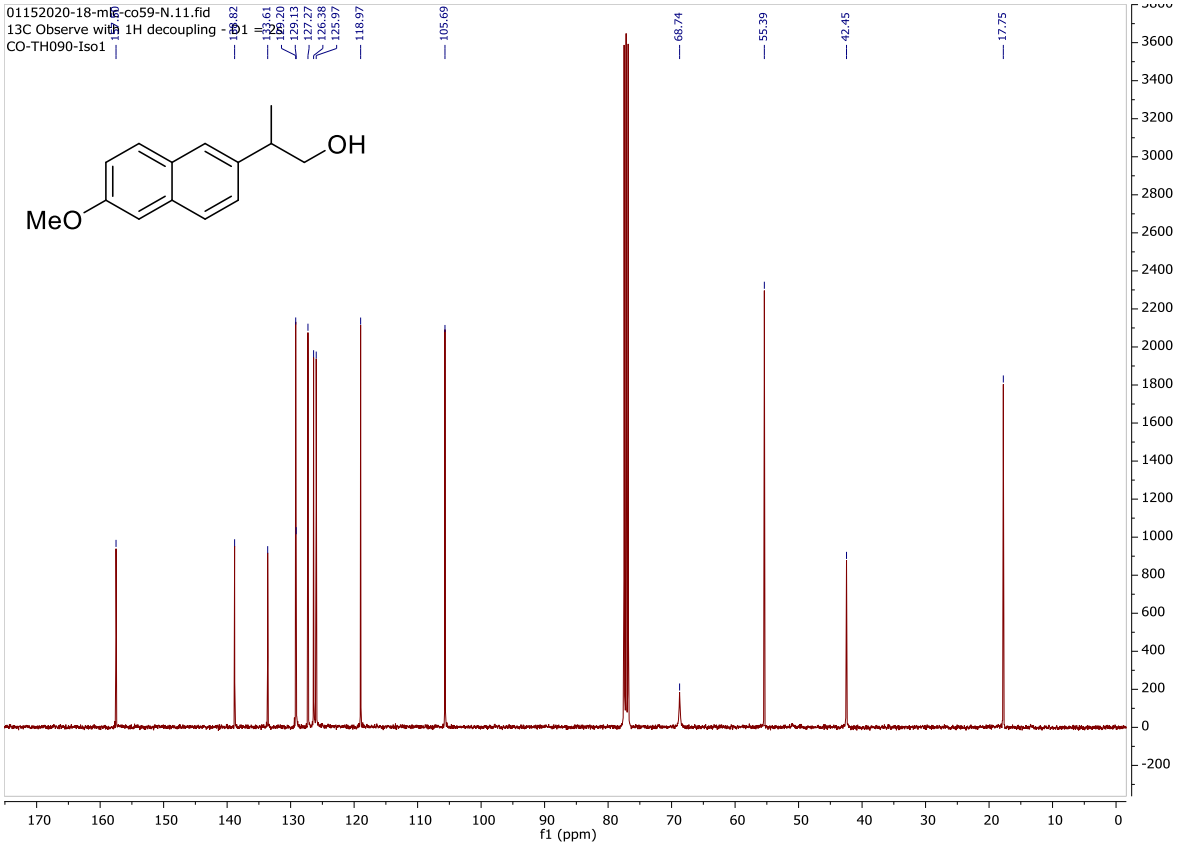

12052019-15-mlc-co59-F.10.fid
1H Observe
CO-TH075A-Iso3
OH
f1 (ppm)

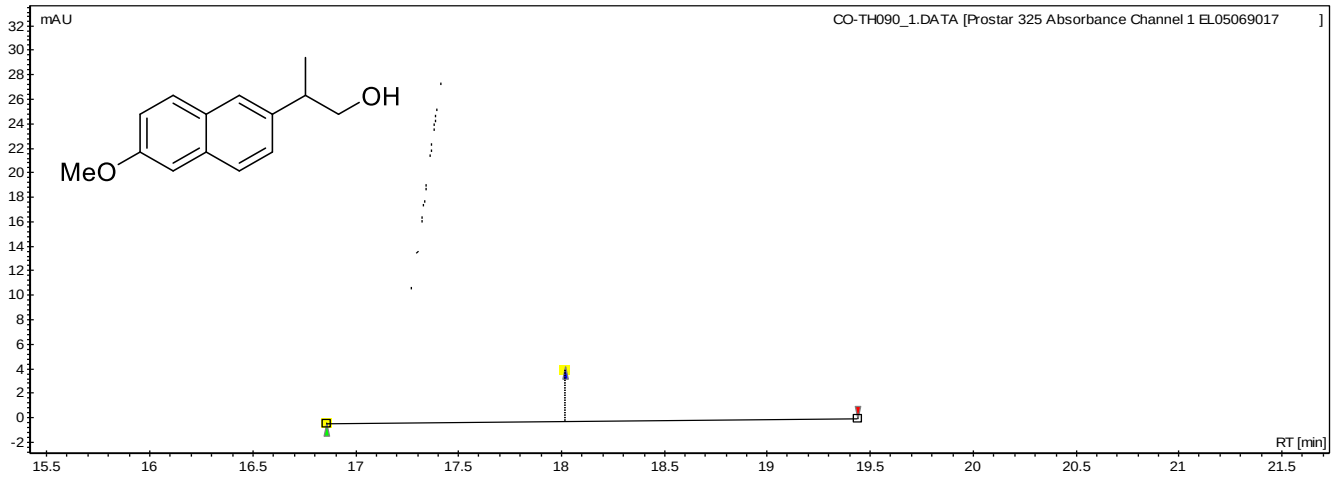

12052019-15-mlc-co59-F.11.fid
13C Observe with multiplicity editing - DEPTQ
CO-TH075A-Iso3
OH
f1 (ppm)

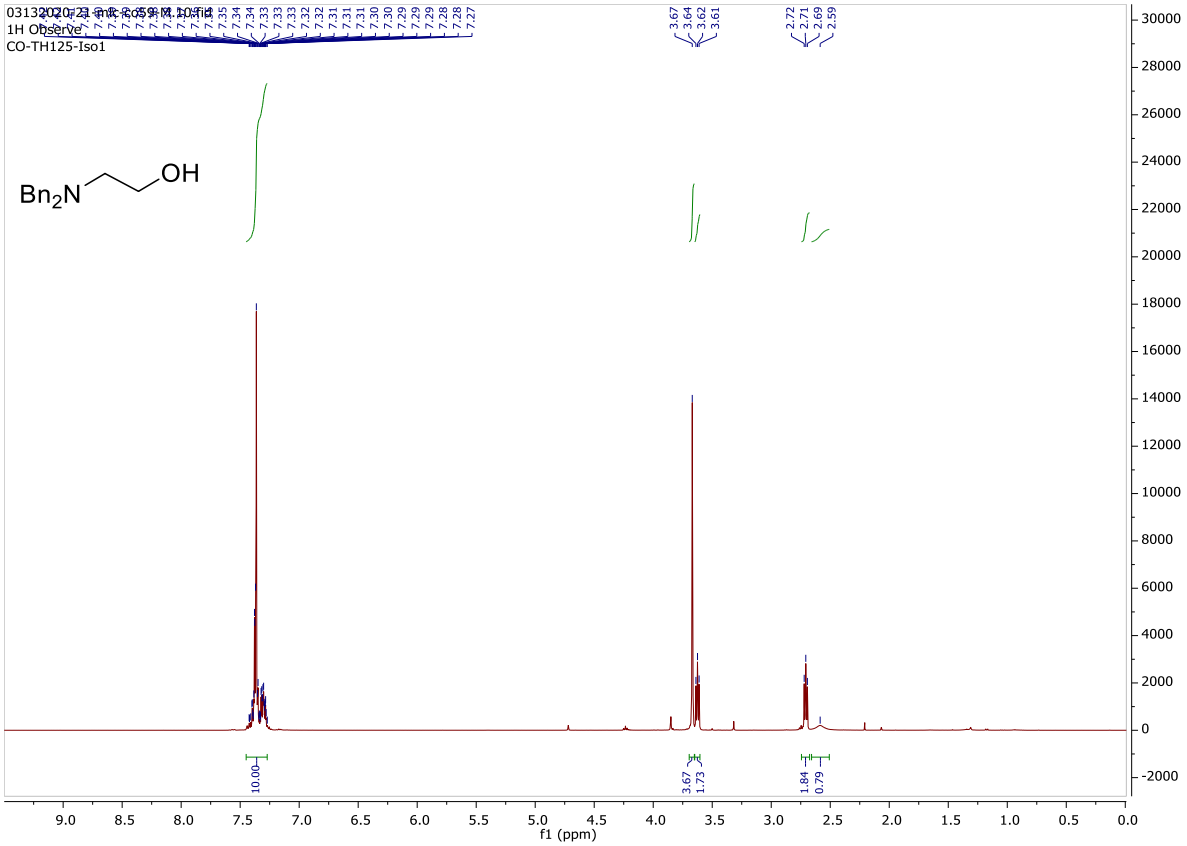

12192019-25-mlc-co59-N.10.fid
1H Observe
CO-TH082-Iso1
OH
f1 (ppm)

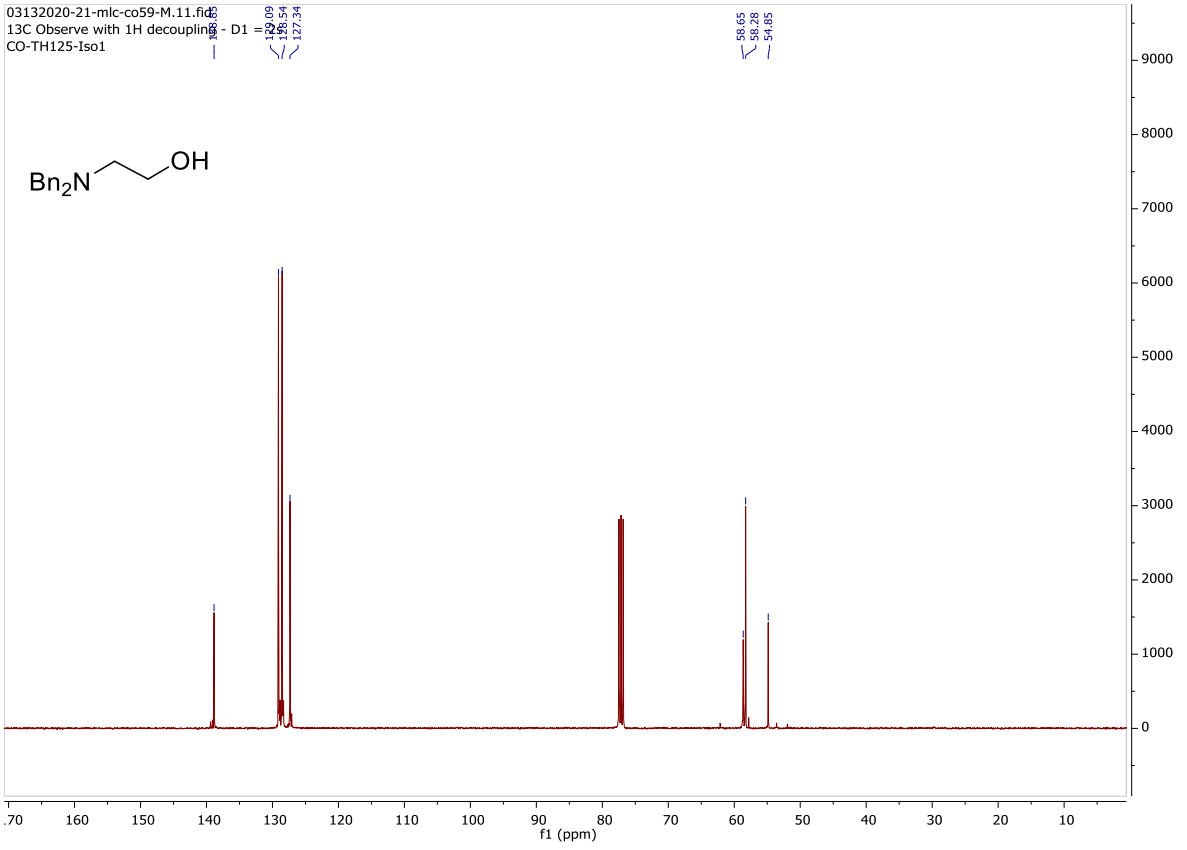

12192019-25-mlc-co59-N.11.fid
13C Observe with multiplicity editing - DEPTQ
CO-TH082-Iso1
OH
f1 (ppm)

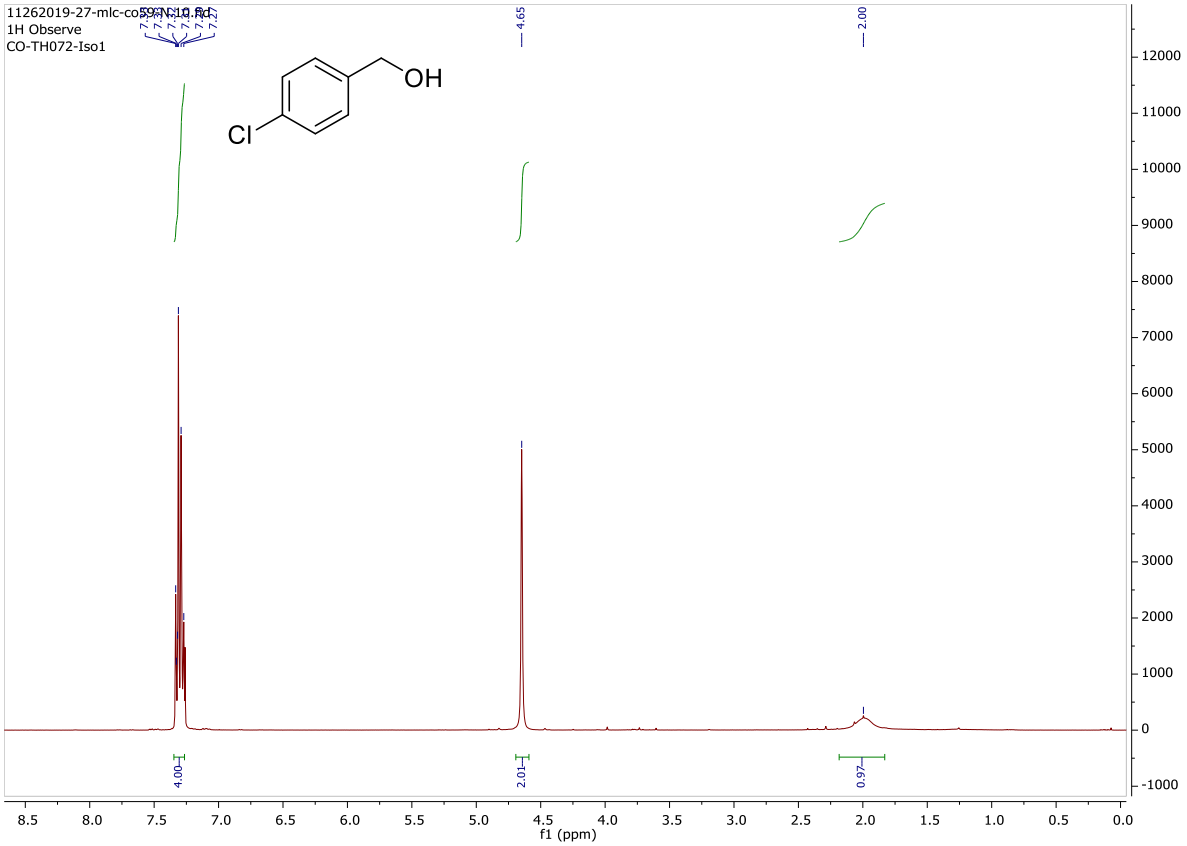

1H Observe
CO-TH090-Iso2
3.92
3.78
3.76
3.14
3.11
3.09
3.07
3.06
3.02
1.98
1.36
1.34
OH
MeO
2.00
0.95
0.95
1.99
2.97
1.83
0.95
0.92
2.88
f1 (ppm)

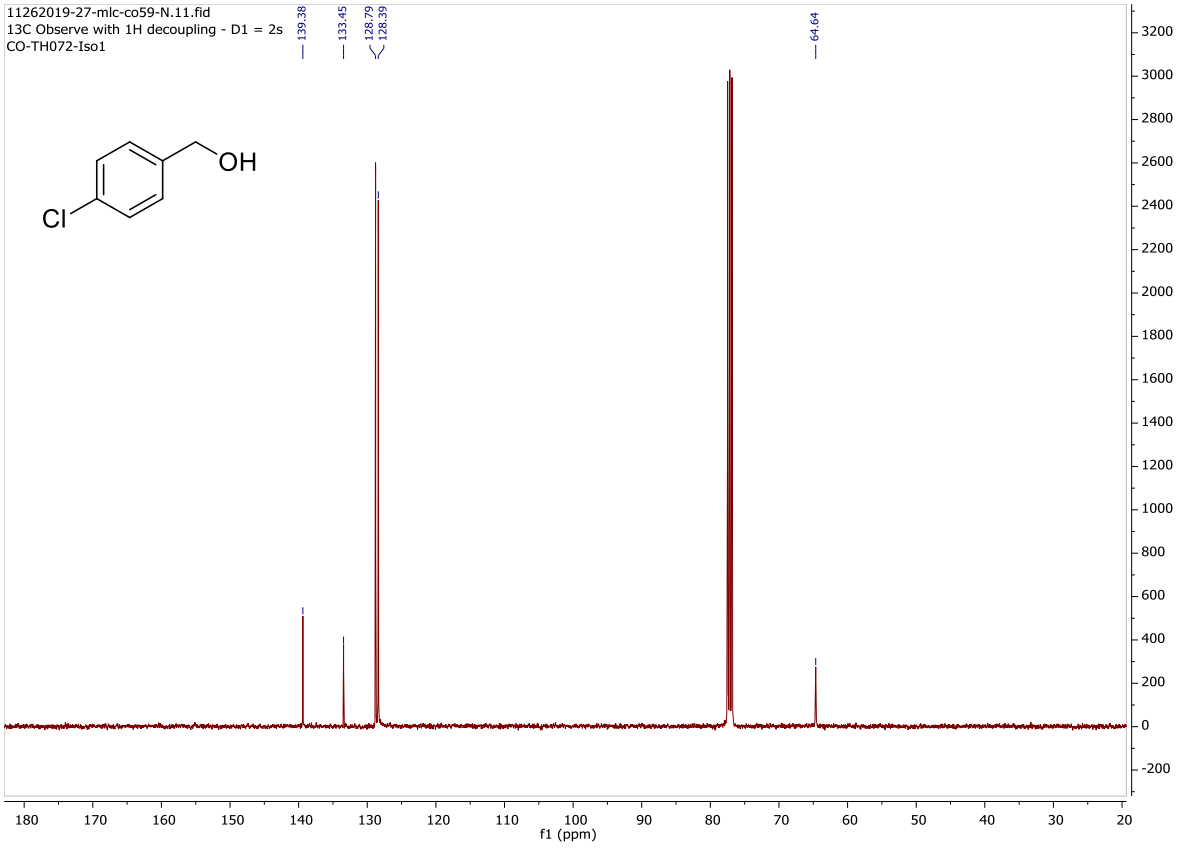

13C Observe with 1H decoupling
CO-TH090-Iso1
159.82
143.61
129.20
129.13
127.27
126.38
125.97
118.97
105.69
68.74
55.39
42.45
17.75
OH
MeO
f1 (ppm)

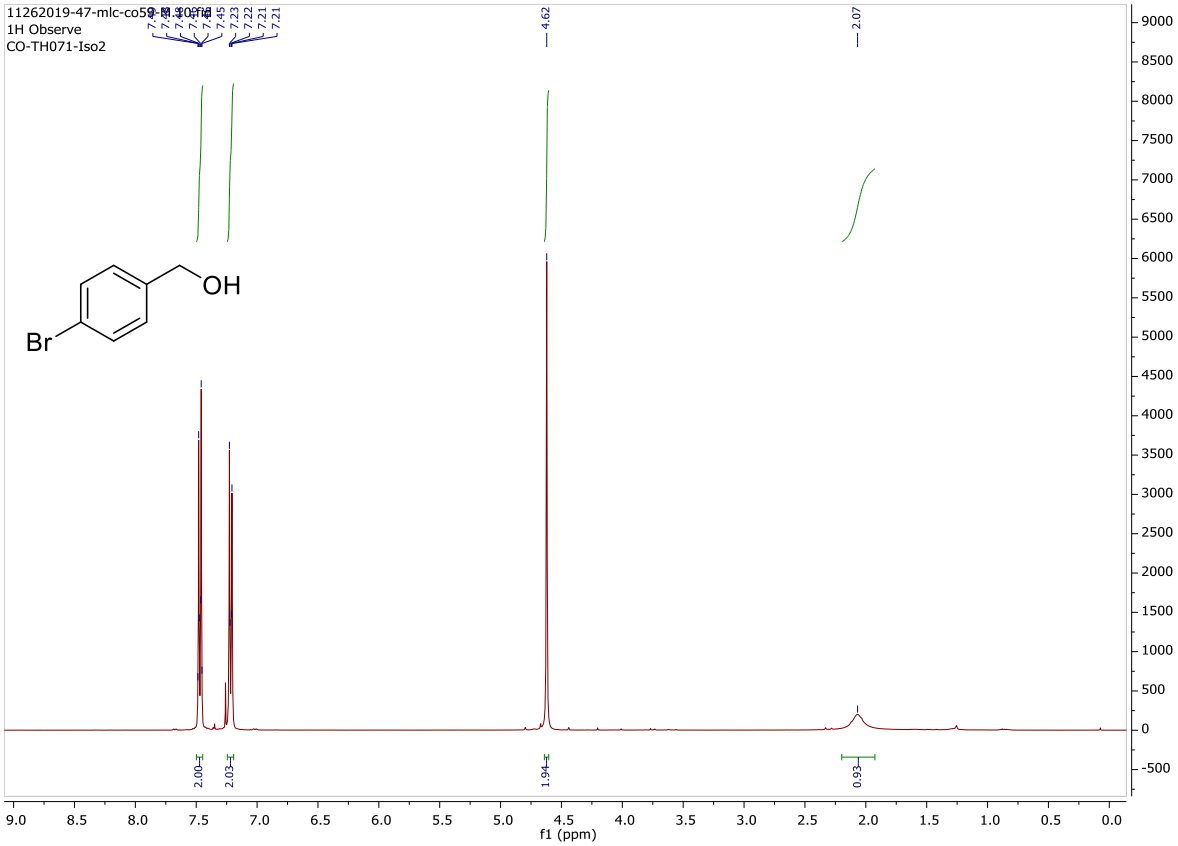

mAU
CO-TH090_1.DATA [Prostar 325 Absorbance Channel 1 EL05069017]
32
30
28
26
24
22
20
18
16
14
12
10
8
6
4
2
0
-2
OH
MeO
15.5
16
16.5
17
17.5
18
18.5
19
19.5
20
20.5
21
21.5
RT [min]

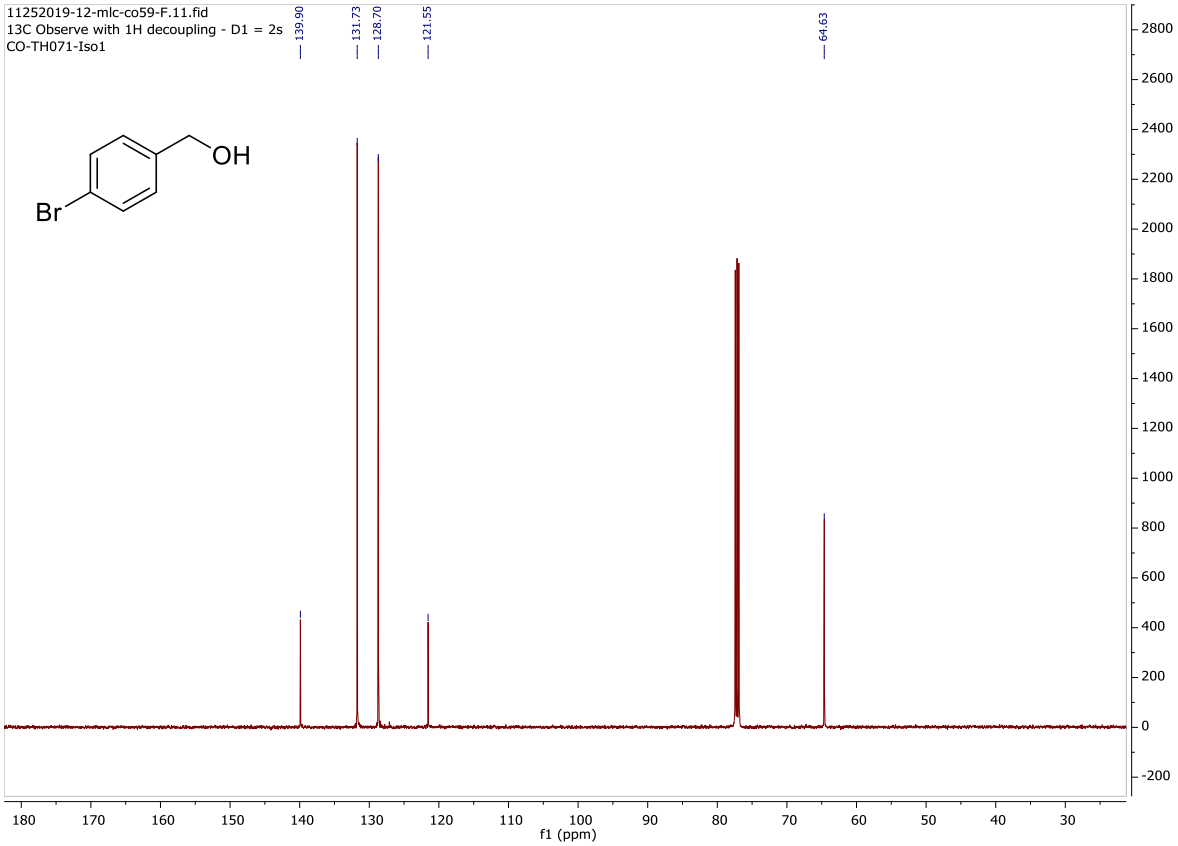

1H Observe
CO-TH125-Iso1
Bn2N
OH
f1 (ppm)

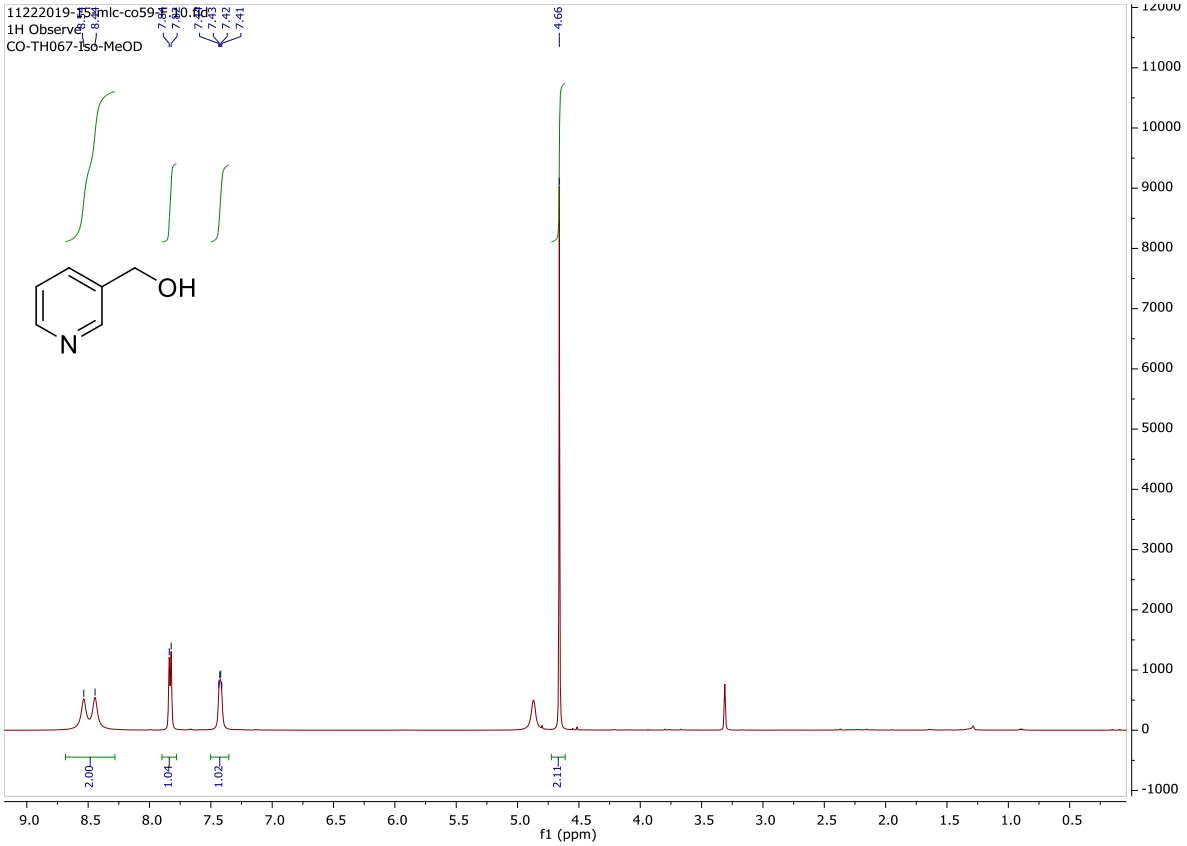

13C Observe with 1H decoupling - D1 =
CO-TH125-Iso1
Bn2N
OH
f1 (ppm)

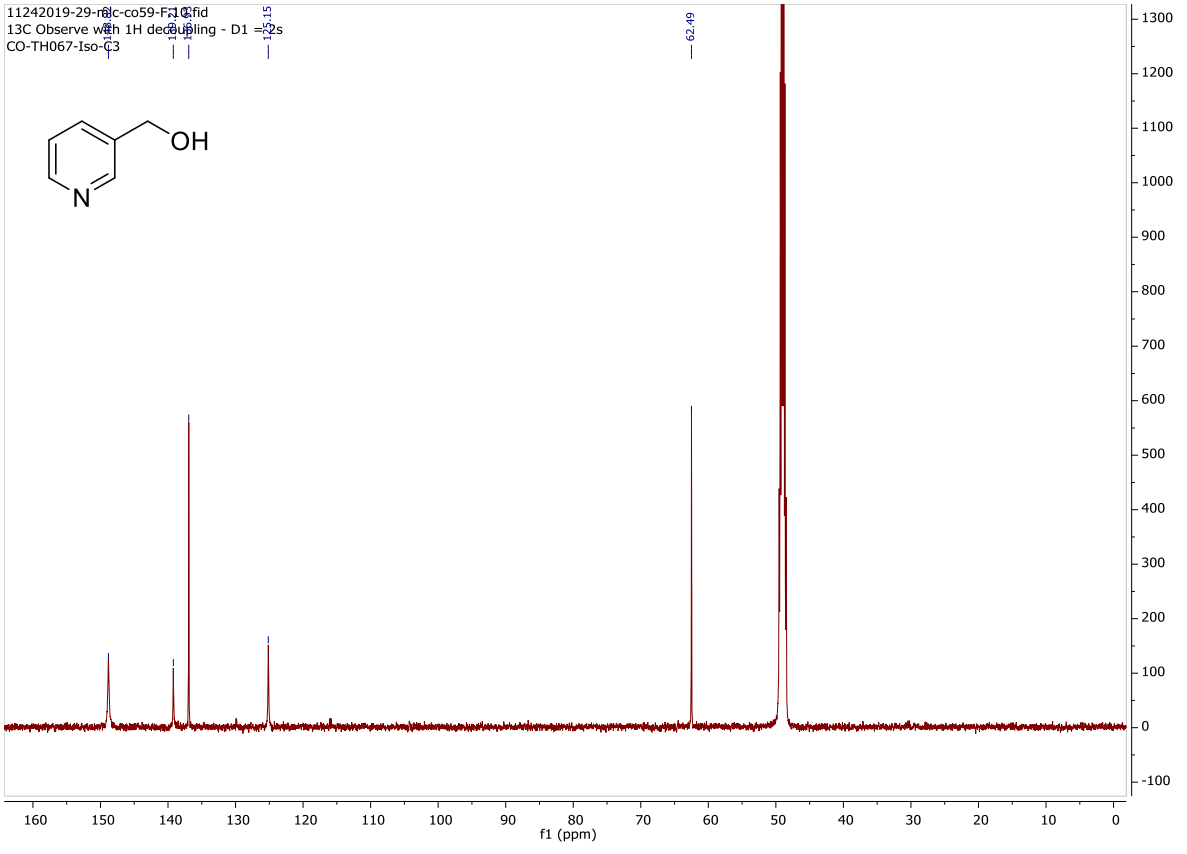

11262019-27-mlc-co59-N.10.fid
1H Observe
CO-TH072-Iso1
OH
Cl
4.65
2.00
4.00
2.01
0.97
f1 (ppm)


11262019-27-mlc-co59-N.11.fid
13C Observe with 1H decoupling - D1 = 2s
CO-TH072-Iso1
139.38
133.45
128.79
128.39
64.64
OH
Cl
f1 (ppm)


11262019-47-mlc-co59-M.10.fid
1H Observe
CO-TH071-Iso2
7.45
7.23
7.22
7.21
7.21
4.62
2.07
OH
Br
2.00
2.03
1.94
0.93
f1 (ppm)


11252019-12-mlc-co59-F.11.fid
13C Observe with 1H decoupling - D1 = 2s
CO-TH071-Iso1
139.90
131.73
128.70
121.55
64.63
OH
Br
f1 (ppm)


11222019-15-mlc-co59-H-10.fid
1H Observe
CO-TH067-Iso-MeOD
8.54
8.53
7.84
7.83
7.42
7.41
4.66
OH
N
2.00
1.04
1.02
2.11
f1 (ppm)


11242019-29-mlc-co59-F-13C.fid
13C Observe with 1H decoupling - D1 = 2s
CO-TH067-Iso-C13
62.49
OH
N
f1 (ppm)

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