Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Palladium catalyzed Br/D exchange of arenes: Selective deuterium incorporation with versatile functional group tolerance and high efficiency

Hong-Hai Zhang, Peter V. Bonnesen, and Kunlun Hong*

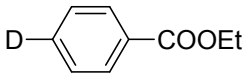
Center for Nanophase Materials Sciences, Oak Ridge National laboratory, Oak Ridge, Tennessee, TN 37831

hongkq@ornl.gov

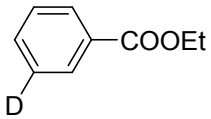
Supporting Information

General: Proton and carbon NMR spectra for all compounds were recorded in $CDCl_3$ on Varian VNMRS 500 MHz NMR spectrometer, operating at 499.717 MHz for proton. Chemical shifts were determined relative to residual $CHCl_3$ (7.26 ppm for ^{1}H-NMR and 77.2 ppm for ^{13}C-NMR). All yields reported refer to isolated yields unless otherwise indicated. GC-MS experiments were carried out using an Agilent 6890 series GC and a 5973 Mass Selective Detector System. All the solvents were degassed by purging with dry nitrogen for 2 h before use. All the reagents were purchased from commercial sources and used as received.

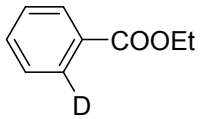
General Procedure for Br/D exchange with $Pd_2(dba)_3$/*t*-Bu_3P as catalyst and DCOONa as deuterium source: In an argon glovebox, to an 8 mL vial containing $Pd_2(dba)_3$ (18.3 mg, 0.02 mmol), *t*-Bu_3P (12 mg, 0.06 mmol), DCOONa (138 mg, 2 mmol), and aryl bromide (1 mmol) was added DMSO (1 mL). Then the sealed vial was brought out of the glovebox and put into an oil bath with pre-set to the reaction temperature. The reaction was performed at 80 ^{o}C until the GC/MS showed the reaction was completed. The reaction was quenched with saturated NH_4Cl solution. The product was extracted with dichloromethane (3 x 15 mL). The combined organic layer was washed with brine and dried over Na_2SO_4. After removal of solvents under vacuum, the crude product was purified via column chromatography (silica gel) using the appropriate binary solvent system (vol/vol).



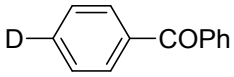
2a[1]: Purified by column chromatography (hexane/dichloromethane = 6:1, Rf = 0.5), Yield: 95% colorless oil. ^{1}H NMR: δ 8.02 (d, *J* = 10.2 Hz, 2 H), 7.41 (d, *J* = 10.2 Hz, 2 H), 4.36 (d, *J* = 8.4 Hz, 2 H), 1.38 (t, *J* = 7.8 Hz, 3 H); ^{13}C NMR: δ 166.6, 132.5 (t, *J* = 23.75 Hz), 130.5, 129.5, 128.2, 60.9, 14.3;



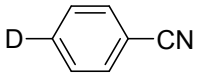
2b[1]: Purified by column chromatography (hexane/dichloromethane = 6:1, Rf = 0.5), Yield: 91% colorless oil. ^{1}H NMR: δ 8.02 - 8.04 (m, 2 H), 7.53 (d, *J* = 9.0 Hz, 1 H), 7.41 (dd, *J* = 9.0 Hz, *J* = 9.6 Hz, 3 H), 4.36 (d, *J* = 8.4 Hz, 2 H), 1.38 (t, *J* = 7.8 Hz, 3 H); ^{13}C NMR: δ 166.6, 132.7, 130.5, 129.5, 129.4, 128.3, 128.0 (t, *J* = 23.7 Hz), 60.9, 14.3;



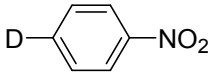
2c[2]: Purified by column chromatography (hexane/dichloromethane = 6:1, Rf = 0.5), Yield: 90% colorless oil. ^{1}H NMR: δ 7.41 (t, *J* = 8.4 Hz, 1 H), 7.00 (m, 2 H), 6.94 (s, 1 H), 3.84 (s, 3 H); ^{13}C NMR: δ 166.6, 132.8, 130.4, 129.5, 129.2 (t, *J* = 23.7 Hz), 128.3, 128.2, 60.9, 14.3



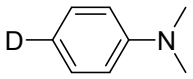
2d[3]: Purified by column chromatography (hexane/dichloromethane = 6:1, Rf = 0.5), Yield: 90% colorless oil. ^{1}H NMR: δ 7.78 - 7.80 (m, 4 H), 7.57 (t, *J* = 9.0 Hz, 1 H), 7.45 - 7.48 (m, 4 H); ^{13}C NMR: δ 196.8, 137.7, 132.5, 132.2 (t, *J* = 25.0 Hz), 130.1, 128.4, 128.2;



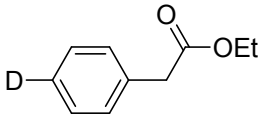
2e[1]: Purified by column chromatography (hexane/dichloromethane = 6:1, Rf = 0.5), Yield: 82% colorless oil. ^{1}H NMR: δ 7.64 (d, *J* = 9.6 Hz, 2 H), 7.46 (d, *J* = 9.6 Hz, 2 H); ^{13}C NMR: δ 132.5 (t, *J* = 25.0 Hz), 132.2, 129.0, 118.9, 112.4;



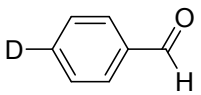
2f[4]: Purified by column chromatography (hexane/dichloromethane = 6:1, Rf = 0.5), Yield: 94% colorless oil. ^{1}H NMR: δ 8.21 (d, *J* = 0.2 Hz, 2 H), 7.53 (d, *J* = 9.6 Hz, 2 H); ^{13}C NMR: δ 148.4, 134.5 (t, *J* = 25.0 Hz), 129.4, 123.6;



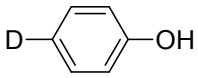
2g[4]: Purified by column chromatography (hexane/dichloromethane = 2:1, Rf = 0.4), Yield: 80% colorless oil. ^{1}H NMR: δ 7.30 (d, *J* = 9.6 Hz, 2 H), 6.81 (d, *J* = 10.8 Hz, 2 H), 3.00 (s, 6 H); ^{13}C NMR: δ 150.8, 129.1, 116.6 (t, *J* = 25.0 Hz), 112.9, 40.8;



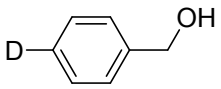
2h: Purified by column chromatography (hexane/dichloromethane = 10:1, Rf = 0.5), Yield: 93% white solid. ^{1}H NMR: δ 7.28 (dd, *J* = 10.2 Hz, *J* = 18.6 Hz, 4 H), 4.13 (q, *J* = 9.0 Hz, 2 H), 3.59 (s, 2 H), 1.23 (t, *J* = 8.4 Hz, 3 H); ^{13}C NMR: δ 171.6, 134.1, 129.2, 128.4, 126.7 (t, *J* = 25.0 Hz), 60.8, 41.4, 14.1; HRMS (ESI): calc. for $C_{10}H_{11}DO_2$ $[M]^+$ 165.0895; found 165.0894.



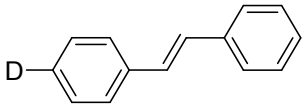
2i[4]: Purified by column chromatography (hexane/dichloromethane = 10:1, Rf = 0.5), Yield: 87% colorless oil. ^{1}H NMR: δ 9.96 (s, 1 H), 7.82 (d, *J* = 9.6 Hz, 2 H), 7.47 (d, *J* = 9.0 Hz, 2 H); ^{13}C NMR: δ 192.3, 136.4, 134.1 (t, *J* = 25.0 Hz), 129.7, 128.8;



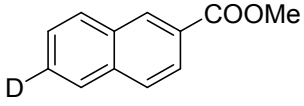
2j[5]: Purified by column chromatography (hexane/ethyl acetate = 10:1, Rf = 0.4), Yield: 82% colorless oil. ^{1}H NMR: δ 9.02 (d, *J* = 6.6 Hz, 1 H), 7.81 (d, *J* = 9.0 Hz, 1 H), 7.73 (d, *J* = 9.6 Hz, 1 H), 7.43 ~ 7.46 (m, 2 H); ^{13}C NMR: δ 155.4, 129.6, 120.6 (t, *J* = 25.0 Hz), 115.3;



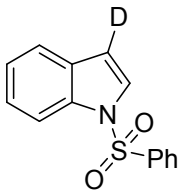
2k[6]: Purified by column chromatography (hexane/ethyl acetate = 10:1, Rf = 0.4), Yield: 94% colorless oil. ^{1}H NMR: δ 7.35 (s, 4 H), 4.67 (s, 2 H); ^{13}C NMR: δ 140.9, 128.6, 127.5 (t, *J* = 25.0 Hz), 127.1, 65.5;



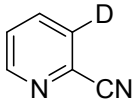
2l: Purified by column chromatography (hexane/dichloromethane = 40:1, Rf = 0.7), Yield: 89% colorless oil. ^{1}H NMR: δ 7.50 (d, *J* = 9.6 Hz, 4 H), 7.33 - 7.36 (m, 4 H), 7.20 ~ 7.26 (m, 1 H), 7.10 (s, 2 H); ^{13}C NMR: δ 137.4, 128.7, 128.6, 127.7, 127.4 (t, *J* = 25.0 Hz), 126.6; HRMS (ESI): calc. for $C_{14}H_{11}D$ $[M]^+$ 181.1002; found 181.0998.



2m: Purified by column chromatography (hexane/dichloromethane = 6:1, Rf = 0.5), Yield: 97% white solid. ^{1}H NMR: δ 8.59 (s, 1 H), 8.04 (d, *J* = 12.0 Hz, 1 H), 7.91 (d, *J* = 12.0 Hz, 1 H), 7.53 (d, *J* = 9.6 Hz, 2 H), 7.83 - 7.85 (m, 2 H), 7.50 (d, *J* = 9.0 Hz, 1 H); ^{13}C NMR: δ 167.4, 135.6, 132.6, 131.2, 129.5, 128.3, 128.0 (t, *J* = 25.0 Hz), 127.8, 127.5, 125.6, 125.3, 52.3; HRMS (ESI): calc. for $C_{12}H_9DO_2$ $[M]^+$ 187.0744; found 187.0961.



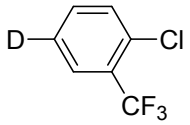
2n: Purified by column chromatography (hexane/dichloromethane = 2:1, Rf = 0.5), Yield: 95% white solid. ^{1}H NMR: δ 7.98 (d, *J* = 9.6 Hz, 1 H), 7.86 (d, *J* = 8.4 Hz, 2 H), 7.55 (s, 1 H), 7.51 (t, *J* = 9.0 Hz, 2 H), 7.41 (t, *J* = 9.0 Hz, 2 H), 7.30 (t, *J* = 9.6 Hz, 1 H), 7.21 (t, *J* = 9.0 Hz, 1 H); ^{13}C NMR: δ 138.5, 135.0, 134.0, 130.8, 129.4, 126.9, 126.4, 124.8, 123.6, 121.6, 113.7, 109.2 (t, *J* = 25.0 Hz); HRMS (ESI): calc. for $C_{14}H_{11}DNO_2S$ $[M+H]^+$ 259.0646; found 259.0640.



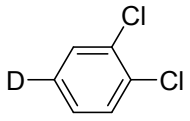
2o: Purified by column chromatography (hexane/dichloromethane = 1:1, Rf = 0.4), Yield: 80% white solid. ^{1}H NMR: δ 8.70 - 8.72 (m, 1 H), 7.82 (d, *J* = 9.6 Hz, 1 H), 7.51 (dd, *J* = 6.0 Hz, *J* = 9.0 Hz, 1 H); ^{13}C NMR: δ 151.4, 137.1, 134.2, 128.4 (t, *J* = 25.0 Hz), 127.1, 117.3;

General Procedure for synthesis of deuterium-labeled aryl chloride with DCOONa as

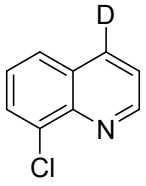
deuterium source: In an argon glovebox, to an 8 mL vial containing $Pd_2(dba)_3$ (18.3 mg, 0.02 mmol), *t*-Bu_3P (12 mg, 0.06 mmol), DCOONa (138 mg, 2 mmol), and aryl bromide (1 mmol) was added DMSO (1 mL). Then the sealed vial was brought out of the glovebox and put into an oil bath with pre-setting temperature. The reaction was performed at 80 °C until the GC/MS showed the reaction was completed. The reaction was quenched with saturated NH_4Cl solution. The product was extracted with dichloromethane (3 x 15 mL). The combined organic layer was washed with brine and dried over Na_2SO_4. After removal of solvents under vacuum, the crude product was purified via column chromatography (silica gel).



3a: Purified by column chromatography (hexane/dichloromethane = 20:1, Rf = 0.5), Yield: 73% colorless oil. ^{1}H NMR: δ 7.68 (s, 1 H), 7.45 ~ 7.50 (m, 2 H); ^{13}C NMR: δ 132.9, 132.5, 131.6, 128.6 (q, *J* = 30.4 Hz), 127.6 (q, *J* = 4.8 Hz), 126.6 (t, *J* = 25.0 Hz), 124.1, 121.9;

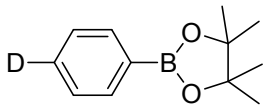


3b: Purified by column chromatography (hexane/dichloromethane = 40:1, Rf = 0.7), Yield: 81% colorless oil. ^{1}H NMR: δ 7.42 ~ 7.43 (m, 2 H), 7.18 (d, *J* = 9.6 Hz, 1 H); ^{13}C NMR: δ 132.5, 130.5, 130.4, 127.6, 127.4 (t, *J* = 25.0 Hz);

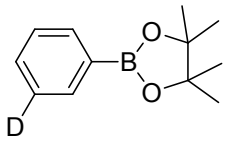


3c: Purified by column chromatography (hexane/dichloromethane = 1:1, Rf = 0.5), Yield: 92% white solid. ^{1}H NMR: δ 7.25 (d, *J* = 9.0 Hz, 2 H), 6.84 (d, *J* = 10.2 Hz, 2 H), 4.91 (s, 1H); ^{13}C NMR: δ 151.1, 144.5, 136.4 (t, *J* = 25.0 Hz), 133.5, 129.8, 129.6, 127.0, 126.7, 121.9; HRMS (ESI): calc. for C_9H_6DClN $[M+H]^+$ 165.0324; found 165.0323.

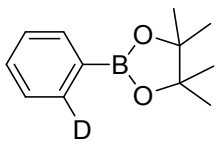
General Procedure for synthesis of deuterium-labeled aryl boronic acid ester with $NaBD_4$ as deuterium source: In an argon glovebox, to 8 mL vial containing $Pd_2(dba)_3$ (18.3 mg, 0.02 mmol), *t*-Bu_3P (12 mg, 0.06 mmol), $NaBD_4$ (80 mg, 2 mmol), and aryl bromide (1 mmol) was added DMSO (2 mL). The reaction was performed at 80 °C until the GC-MS showed the reaction was completed. The reaction was quenched with saturated NH_4Cl solution. The product was extracted with dichloromethane (3 x 15 mL). The combined organic layer was washed with brine and dried over Na_2SO_4. After removal of solvents under vacuum, the crude product was purified via column chromatography (silica gel).



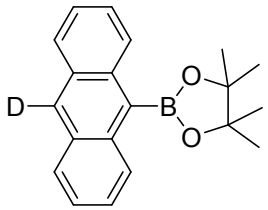
3d: Purified by column chromatography (hexane/dichloromethane = 6:1, Rf = 0.5), Yield: 74% colorless oil. ^1H NMR: δ 7.79 (d, *J* = 7.8 Hz, 2 H), 7.34 (d, *J* = 9.0 Hz, 2 H), 1.33 (s, 12 H); ^{13}C NMR: δ 134.8, 131.2 (t, *J* = 25.0 Hz), 127.7, 83.9, 25.0; HRMS (ESI): calc. for $C_{12}H_6DBO_2$ $[M]^+$ 205.1379; found 205.1382.



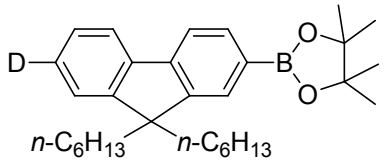
3e: Purified by column chromatography (hexane/dichloromethane = 6:1, Rf = 0.5), Yield: 88% colorless oil. ^1H NMR: δ 7.79 ~ 7.80 (m, 2 H), 7.44 (d, *J* = 9.0 Hz, 1 H), 7.35 (t, *J* = 9.0 Hz, 1 H), 1.33 (s, 12 H); ^{13}C NMR: δ 134.8, 134.7, 131.2, 127.8, 127.5 (t, *J* = 25.0 Hz), 83.9, 25.0; HRMS (ESI): calc. for $C_{12}H_6DBO_2$ $[M]^+$ 205.1379; found 205.1380.



3f: Purified by column chromatography (hexane/dichloromethane = 6:1, Rf = 0.5), Yield: 76% colorless oil. ^1H NMR: δ 7.79 (d, *J* = 7.8 Hz, 1 H), 7.44 (t, *J* = 9.0 Hz, 1 H), 7.35 (t, *J* = 7.8 Hz, 2 H), 1.33 (s, 12 H); ^{13}C NMR: δ 134.8, 134.6 (t, *J* = 25.0 Hz), 131.4, 127.8, 127.7, 83.9, 25.0; HRMS (ESI): calc. for $C_{12}H_6DBO_2$ $[M]^+$ 205.1379; found 205.1374.

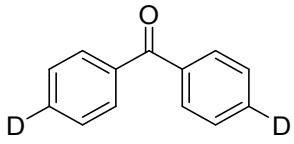


3g: Purified by column chromatography (hexane/dichloromethane = 6:1, Rf = 0.5), Yield: 90% white solid. ^1H NMR ($CDCl_3$, ppm): δ 8.43 (d, *J* = 9.6 Hz, 2 H), 7.97 (d, *J* = 9.0 Hz, 2 H), 7.41 ~ 7.48 (m, 4 H), 1.57 (s, 12 H); ^{13}C NMR ($CDCl_3$, ppm): δ 136.0, 131.1, 129.2 (t, *J* = 25.0 Hz), 128.8, 128.4, 125.9, 124.9, 84.4, 25.2; HRMS (ESI): cald. For $C_{20}H_{21}DBO_2$ $[M+H]^+$ 306.1770; found 306.1778

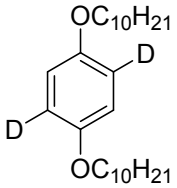


3h: Purified by column chromatography (hexane/dichloromethane = 4:1, Rf = 0.4), Yield: 95% white solid. ^{1}H NMR: δ 8.00 (d, *J* = 9.6 Hz, 1 H), 7.74 (s, 1 H), 7.00 (dd, *J* = 10.2 Hz, *J* = 12.6 Hz, 2 H), 7.32 (s, 1 H), 7.30 (d, *J* = 9.6 Hz, 1 H), 1.94 ~ 1.99 (m, 4 H), 1.38 (s, 12 H), 0.98 ~ 1.10 (m, 12 H), 0.74 (t, *J* = 9.0 Hz, 6 H), 0.55 ~ 0.59 (m, 4 H); ^{13}C NMR: δ 151.4, 150.0, 144.2, 141.0, 133.8, 128.9, 127.4 (t, *J* = 25.0 Hz), 126.7, 122.9, 120.2, 119.1, 55.2, 40.3, 31.6, 30.4, 29.8, 25.0, 23.8, 22.7, 14.1; HRMS (ESI): calc. for $C_{31}H_{45}DBO_2$ $[M+H]^+$ 462.3648; found 462.3653.

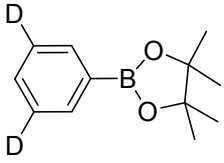
General Procedure for synthesis of perdeuterium-labeled aryl compounds: In an argon glovebox, to 8 mL vial containing $Pd_2(dba)_3$ (18.3 mg, 0.02 mmol), *t*-Bu_3P (12 mg, 0.06 mmol), DCOONa or $NaBD_4$ (2 equivalent to bromide), and aryl bromide (1 mmol) was added DMSO (1 mL). The reaction was performed at 80 °C until the GC-MS showed the reaction was completed. The reaction was quenched with saturated NH_4Cl solution. The product was extracted with dichloromethane (3 x 15 mL). The combined organic layer was washed with brine and dried over Na_2SO_4. After removal of solvents under vacuum, the crude product was purified via column chromatography (silica gel).



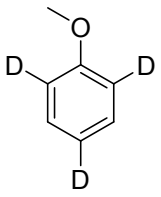
4a: Purified by column chromatography (hexane/dichloromethane = 6:1, Rf = 0.5), Yield: 95% colorless oil. ^{1}H NMR: δ 7.79 (d, *J* = 10.2 Hz, 4 H), 7.46 (d, *J* = 9.6 Hz, 4 H); ^{13}C NMR: δ 197.0, 137.8, 132.3 (t, *J* = 25.0 Hz), 128.4; HRMS (ESI): calc. for $C_{13}H_8D_2O$ $[M]^+$ 184.0852; found 184.0859.



4b: Purified by column chromatography (hexane/dichloromethane = 6:1, Rf = 0.4), Yield: 95% white solid. ^{1}H NMR: δ 6.80 (s, 2 H), 3.87 (t, *J* = 7.8 Hz, 4 H), 1.70 ~ 1.76 (m, 4 H), 1.39 ~ 1.43 (m, 4 H), 1.25 ~ 1.33 (m, 24 H), 0.86 (t, *J* = 9.0 Hz, 6 H); ^{13}C NMR: δ 153.3, 115.5, 115.3 (t, *J* = 25.0 Hz), 68.8, 32.1, 29.8, 29.7, 29.6, 29.6, 29.5, 26.2, 22.9, 14.3; HRMS (ESI): calc. for $C_{26}H_{25}D_2O_2$ $[M+H]^+$ 393.3696; found 393.3704.



4c: Purified by column chromatography (hexane/dichloromethane = 5:1, Rf = 0.5), Yield: 74% colorless oil. ^{1}H NMR: δ 7.79 (s, 2 H), 7.43 (s, 1 H), 1.32 (s, 12 H); ^{13}C NMR: δ 134.6, 131.0, 127.4 (t, *J* = 25.0 Hz), 83.7, 24.8; HRMS (ESI): calc. for $C_{12}H_5D_2BO_2$ $[M]^+$ 206.1442; found 206.1437.

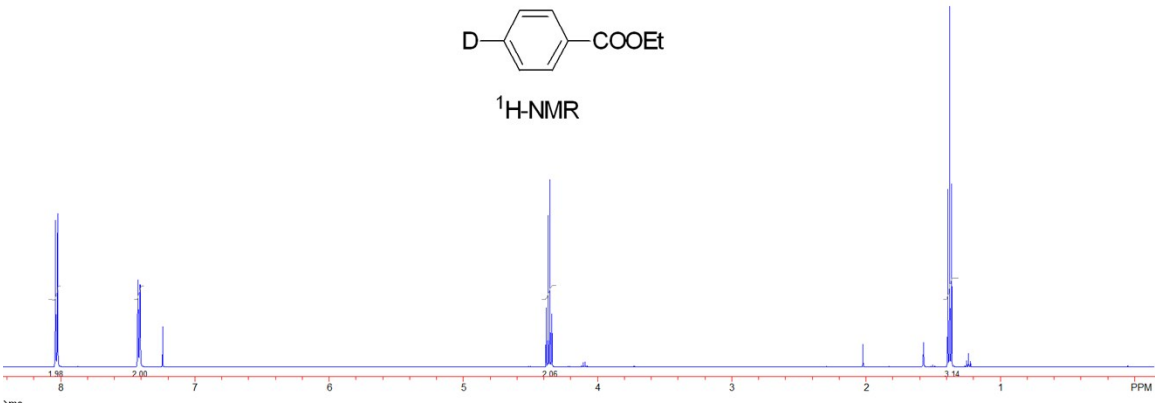


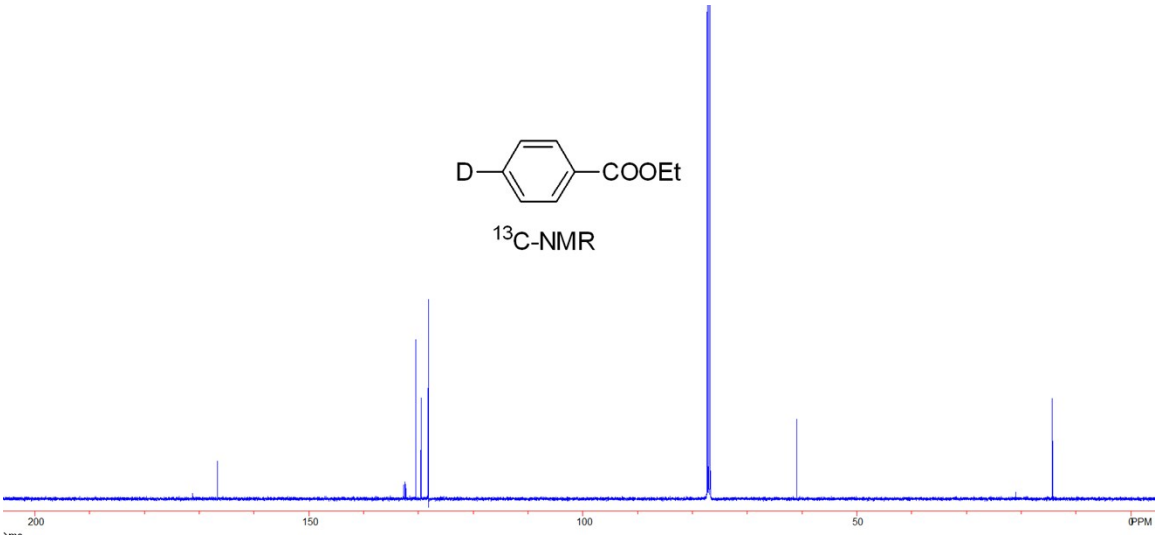
4d: Purified by column chromatography (hexane/dichloromethane = 10:1, Rf = 0.6), Yield: 65% colorless oil. ^{1}H NMR: δ 7.29 (s, 2 H), 3.80 (s, 3 H); ^{13}C NMR: δ 159.4, 129.2, 120.3 (t, *J* = 25.0 Hz), 113.6 (t, *J* = 25.0 Hz), 55.1;

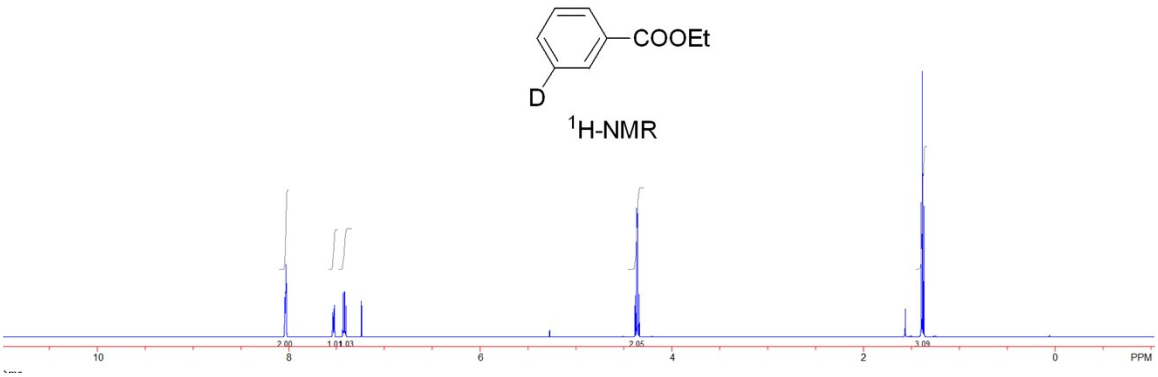
References cited:

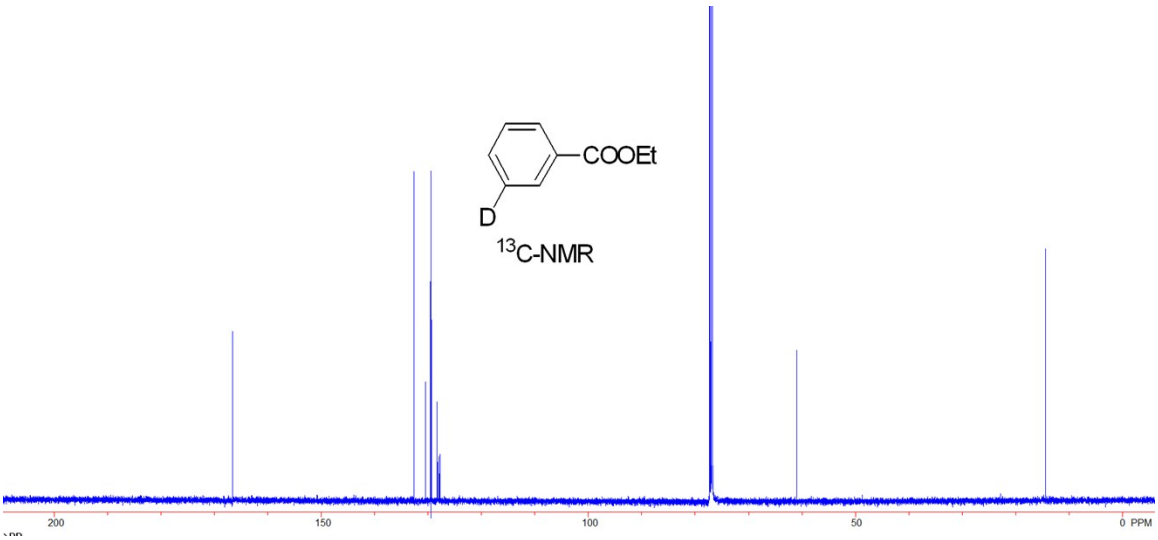
1. S. W. Landvatter, D. J. Schauer, K. T. Garnes, J. F. Mack and L. B. Killmer Jr., *J. Labelled Cpd. Radiopharm.* 2001, **44**, 1025-1033;
2. Q. Liu, Y. Lan, J. Liu, G. Li, Y. D. Wu and A. Lei, *J. Am. Chem. Soc*. 2009, **131**, 10201-10210;
3. F. Labre, Y. Gimbert, P. Bannwarth, S. Olivero, E. Dunach and P. Y. Chavant, *Org. Lett.* 2014, **16**, 2366;
4. M. Linden, J. Borsboom, F. Kaspersen and G. Kemperman, *Eur. J. Org. Chem.* 2008, 2989-2997;
5. C. Y. Lee, S. J. Ahn and C. H. Cheon, *J. Org. Chem.* 2013, **78**, 12154-12160;
6. T. Furuyama, M. Yonehara, S. Arimoto, M. Kobayashi, Y. Matsumoto and M. Uchiyama, *Chem. Eur. J.* 2008, **14**, 10348-10356;

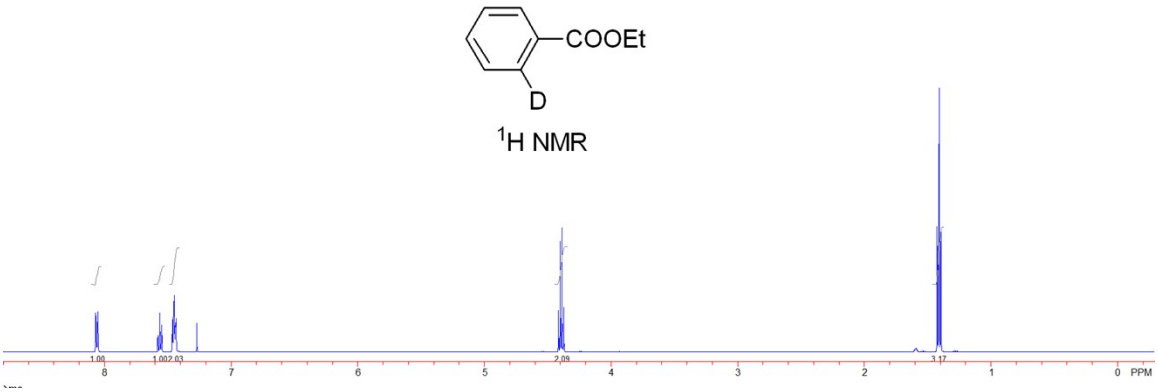
^{1}H and ^{13}C NMR Spectra:

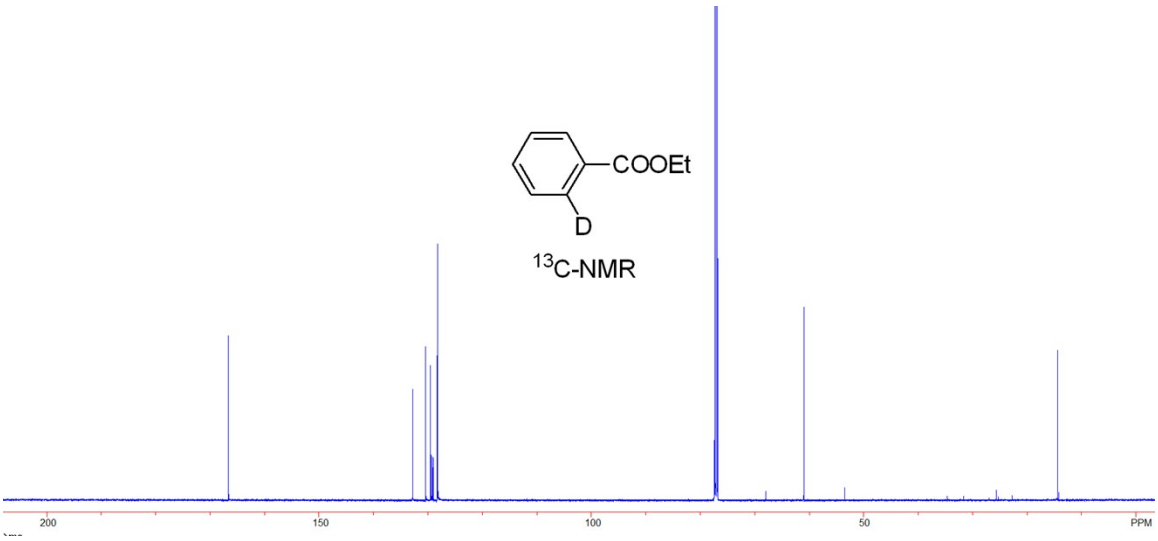


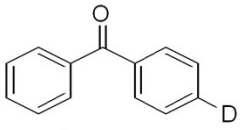



COOEt
D
1H-NMR
2.00
1.01
1.03
2.05
3.09
10
8
6
4
2
0
PPM

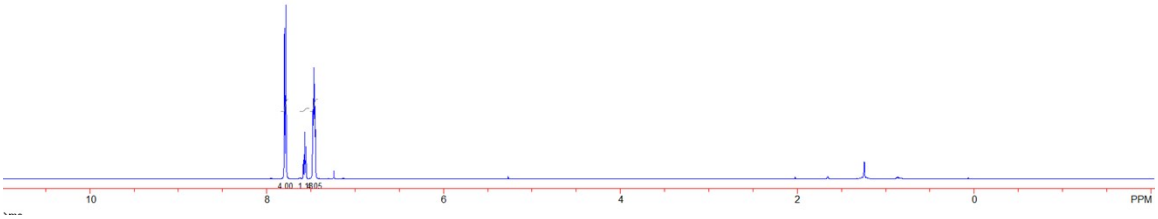

COOEt
D
13C-NMR
200
150
100
50
0 PPM

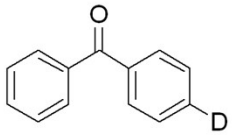

COOEt
D
1H NMR
1.00
1.00
2.03
2.09
3.17
8
7
6
5
4
3
2
1
0
PPM


COOEt
D
13C-NMR
200
150
100
50
PPM

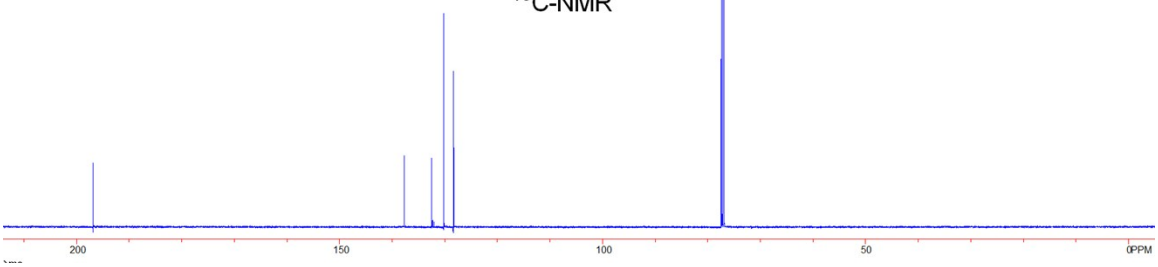


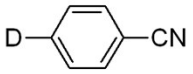
^{1}H-NMR



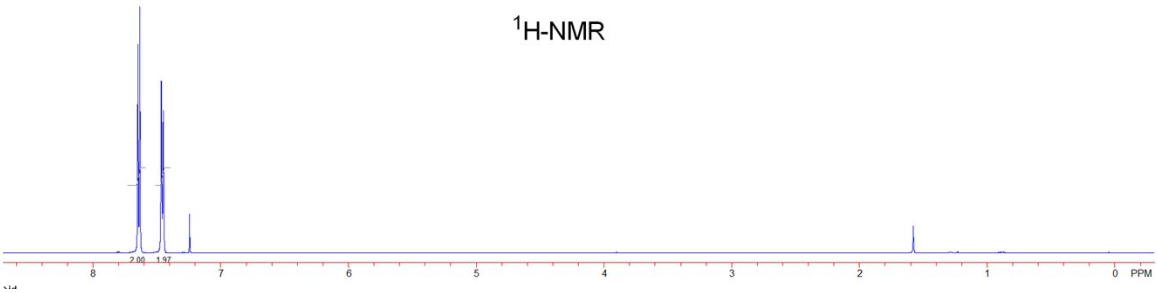


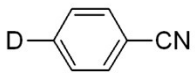
^{13}C-NMR



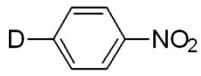


^{1}H-NMR

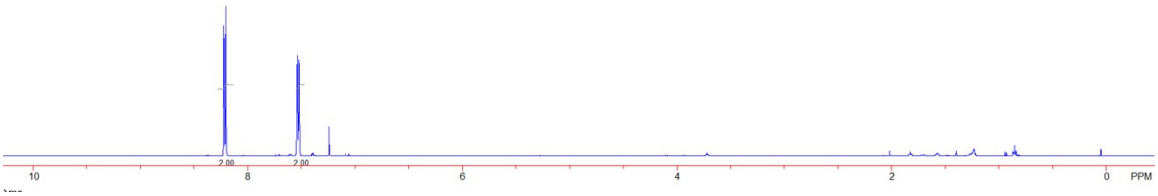


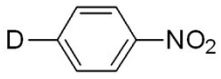


^{13}C-NMR

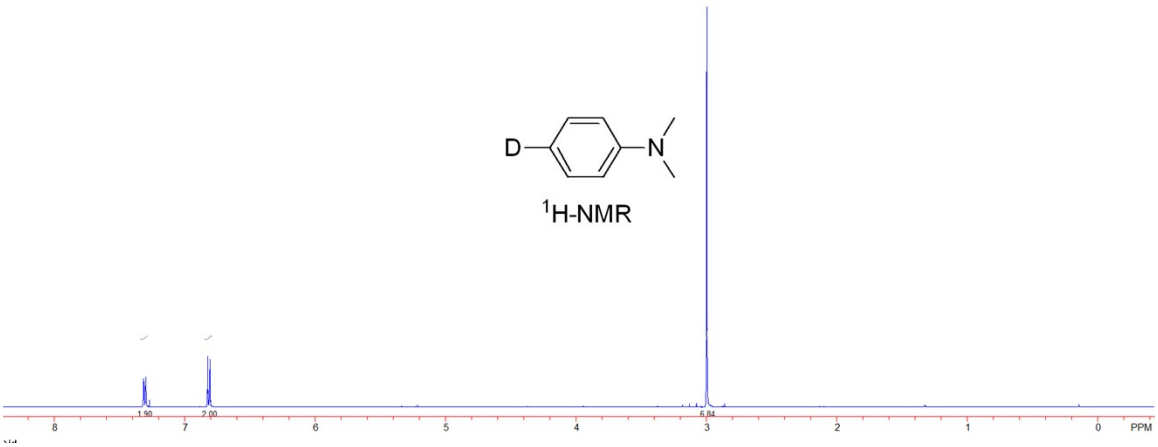


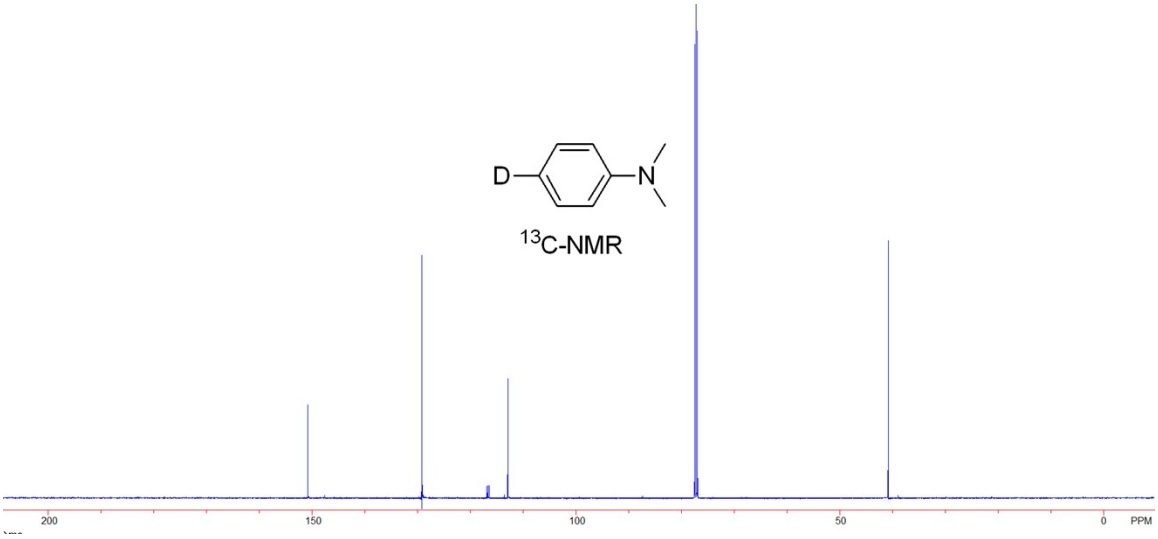
^{1}H-NMR

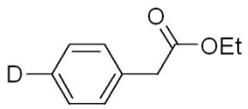




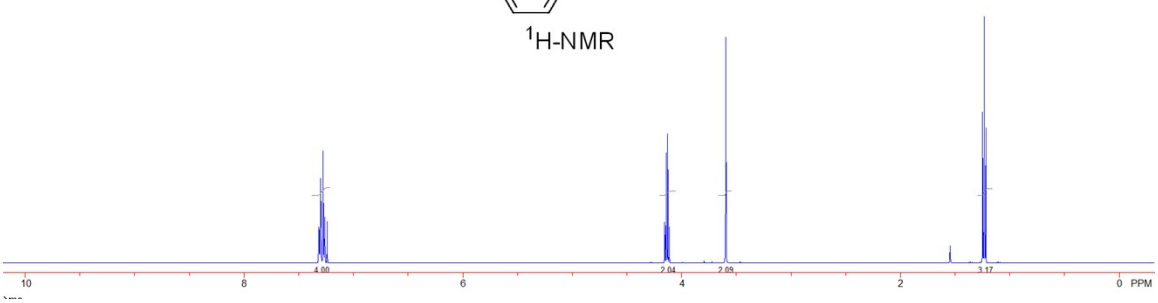
^{13}C-NMR

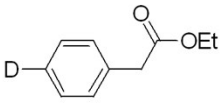

D
N
1H-NMR
1.90
2.00
6.84
8
7
6
5
4
3
2
1
0
PPM


D
N
13C-NMR
200
150
100
50
0
PPM

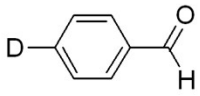


^{1}H-NMR

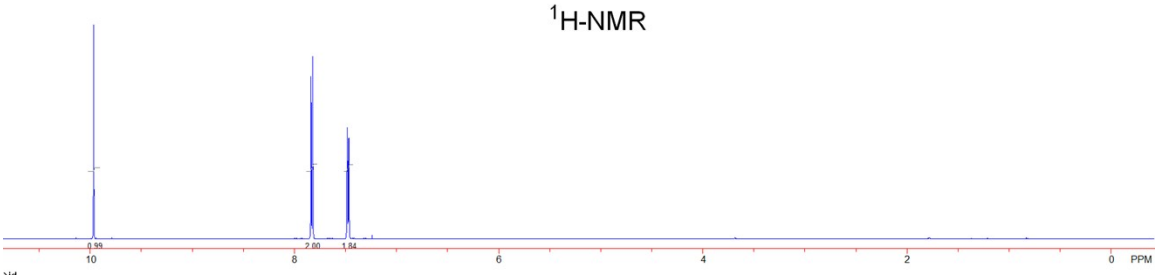


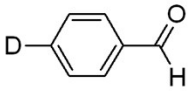


^{13}C-NMR

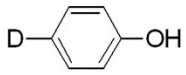


^{1}H-NMR

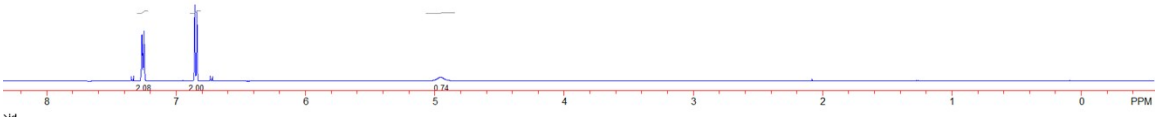


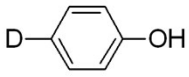


^{13}C-NMR

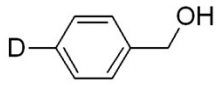


^{1}H-NMR

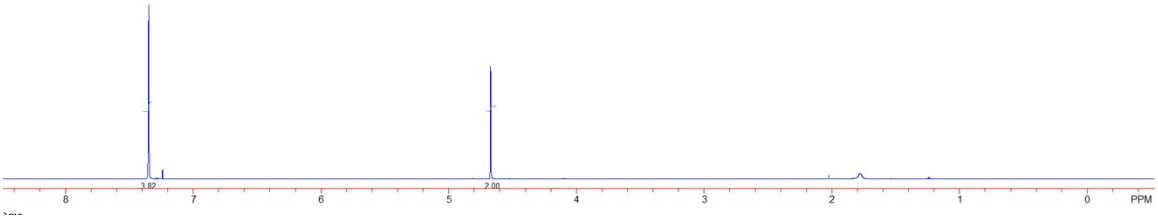


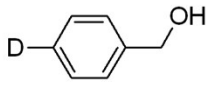


^{13}C-NMR

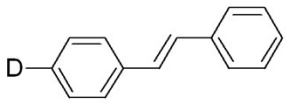


^{1}H-NMR

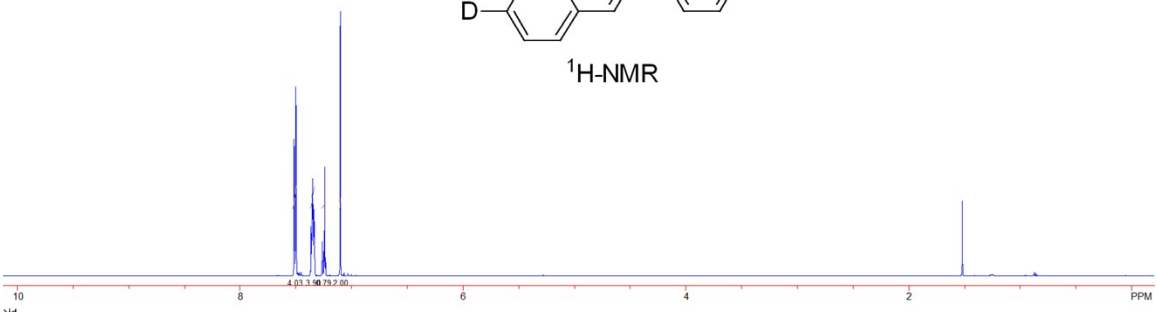


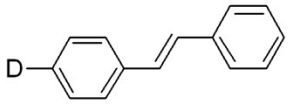


^{13}C-NMR

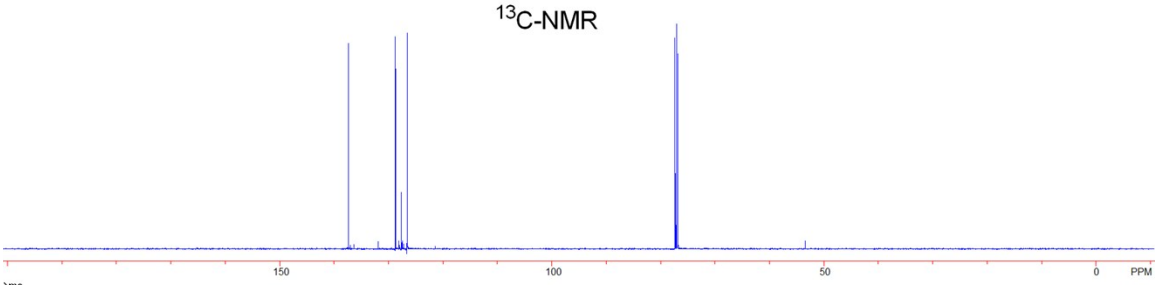


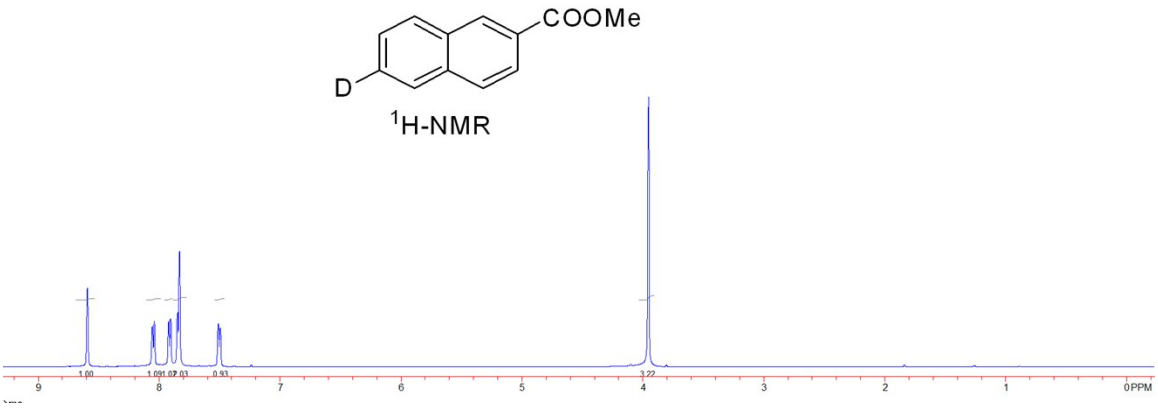
^{1}H-NMR

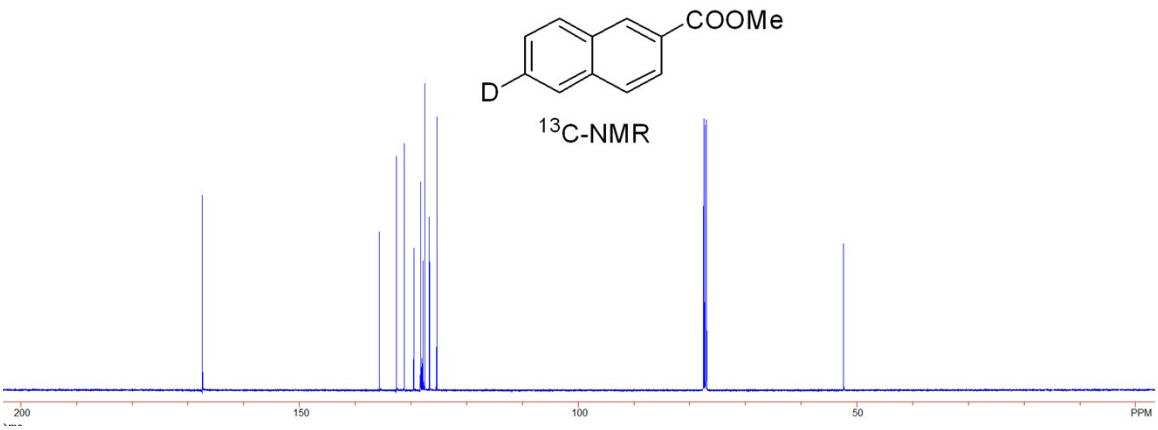


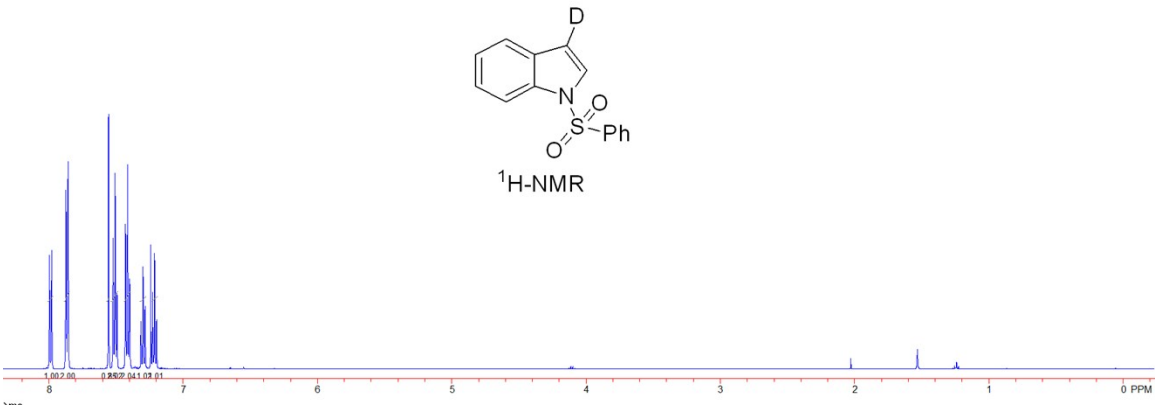


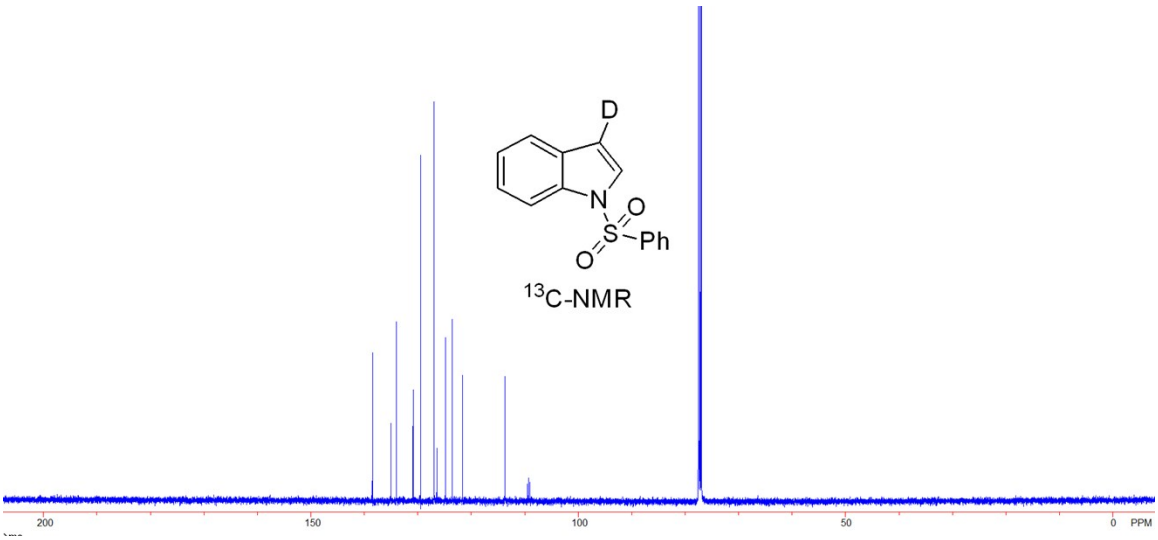
^{13}C-NMR

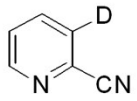



COOMe
D
1H-NMR
9
8
7
6
5
4
3
2
1
0PPM

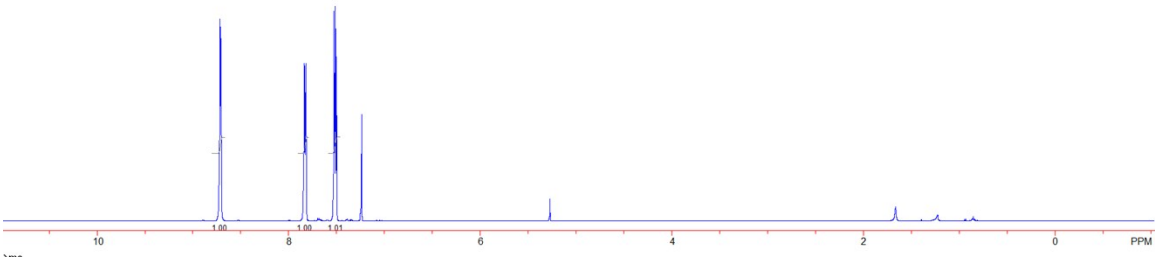

COOMe
D
13C-NMR
200
150
100
50
PPM

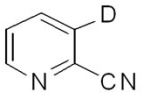

D
N
O
S
Ph
O
1H-NMR
8
7
6
5
4
3
2
1
0 PPM


D
N
O
S
Ph
O
13C-NMR
200
150
100
50
0 PPM

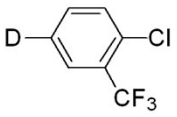


^{1}H-NMR

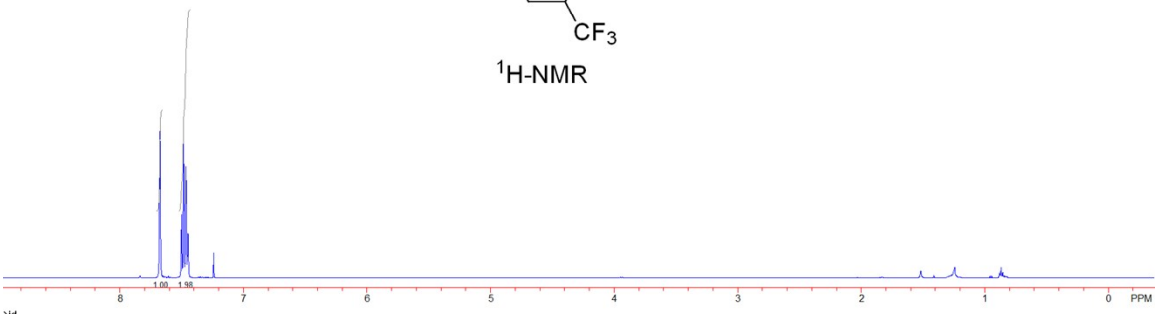


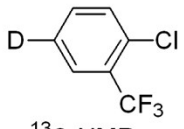


^{13}C-NMR

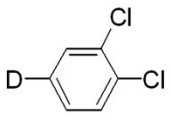


^{1}H-NMR

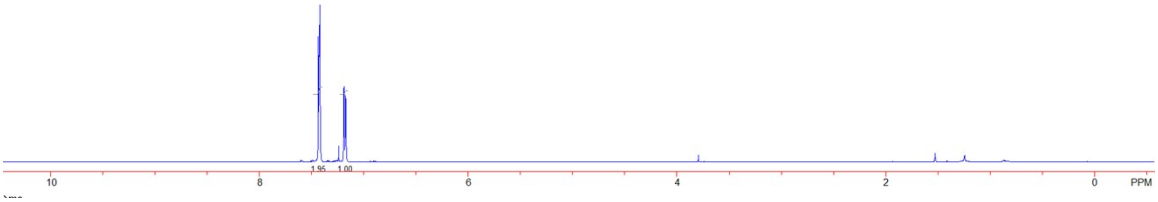


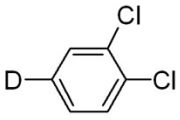


^{13}C-NMR

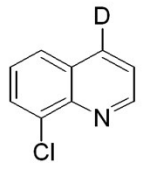


^{1}H-NMR

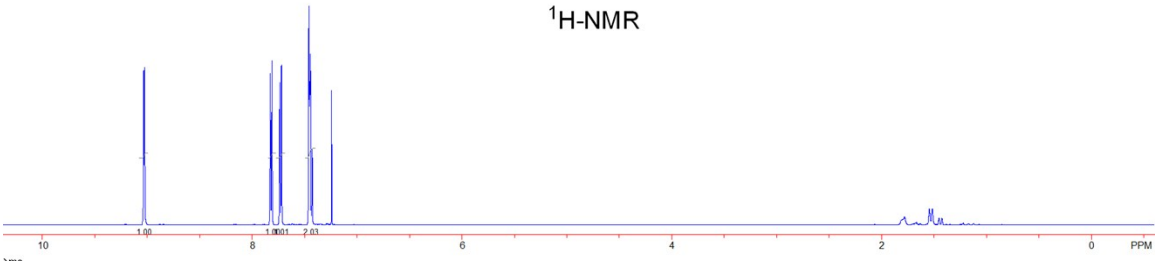


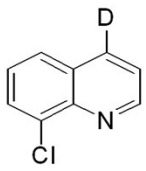


^{13}C-NMR

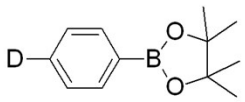


^{1}H-NMR

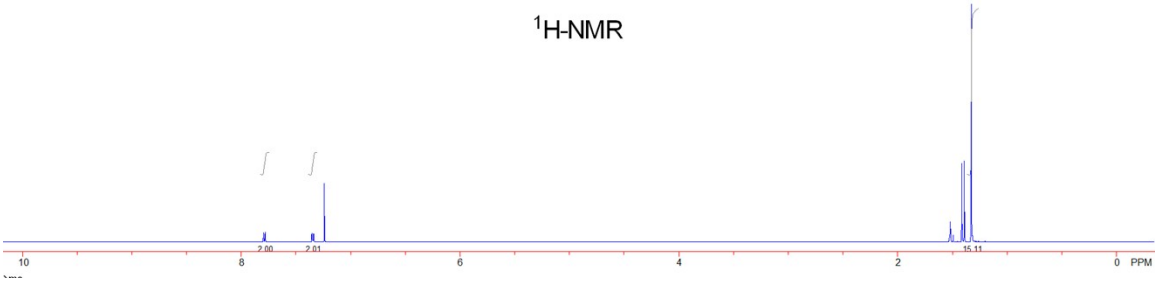


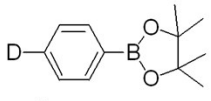


^{13}C-NMR

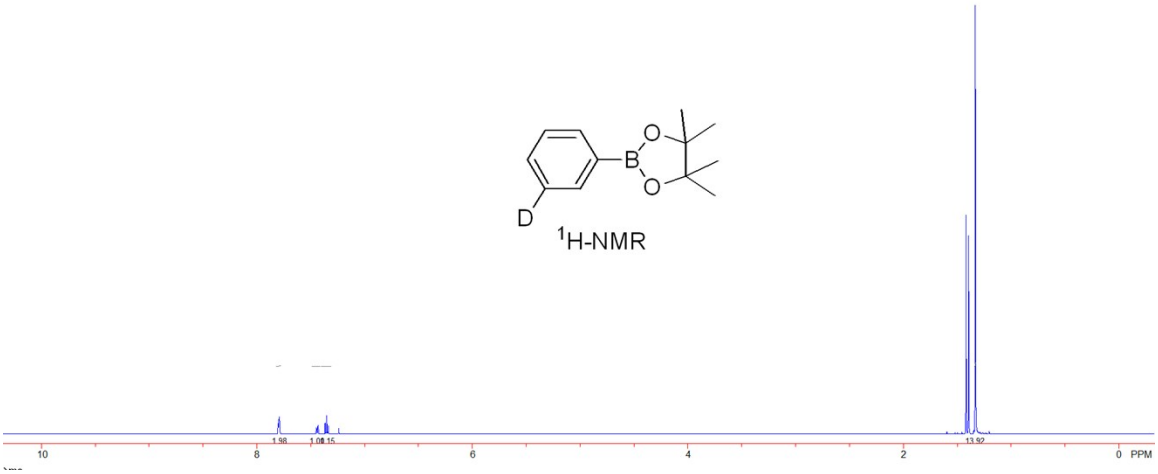


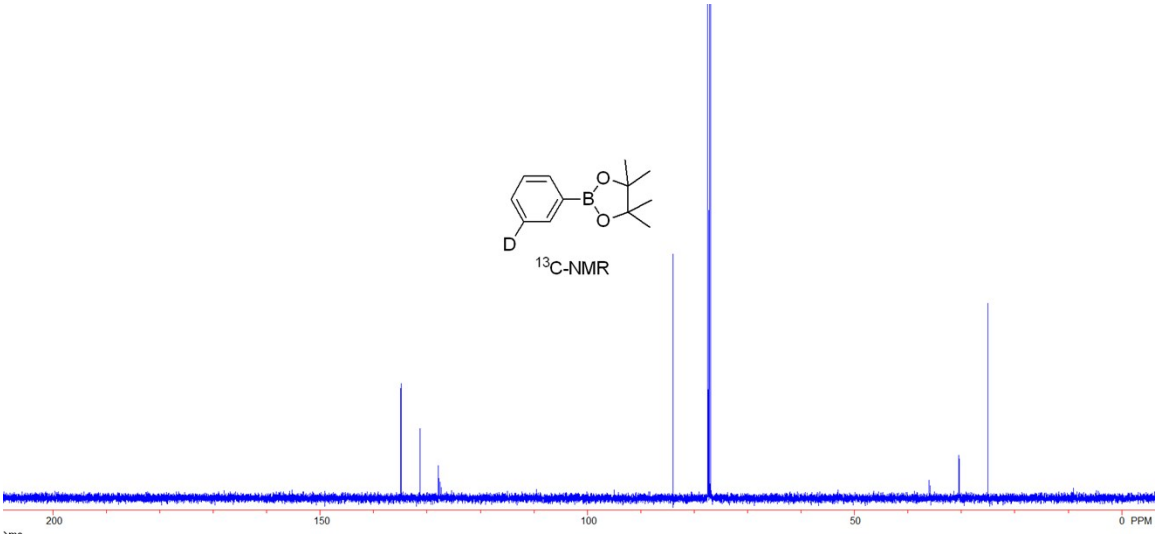
^{1}H-NMR

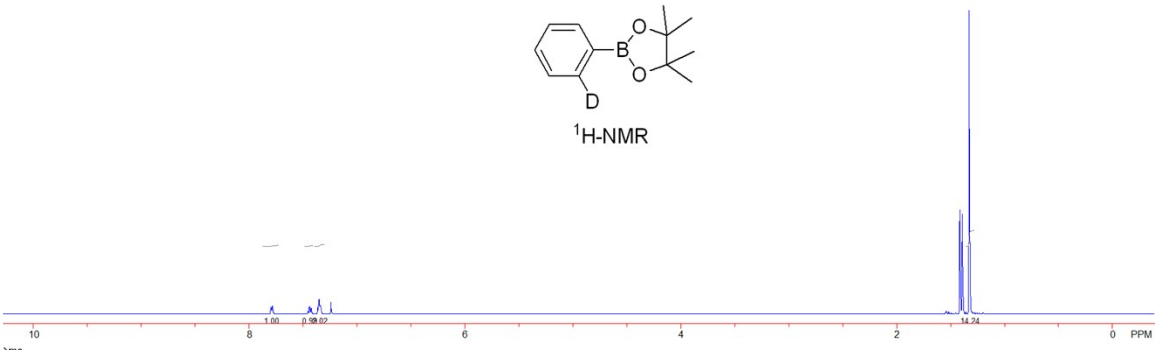




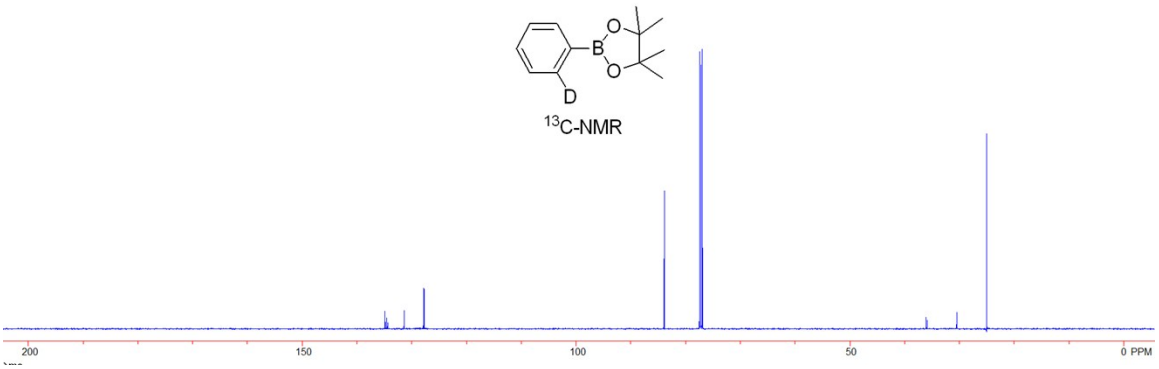
^{13}C-NMR


D
B
O
O
1H-NMR
1.98
1.08
1.15
13.92
10
8
6
4
2
0 PPM

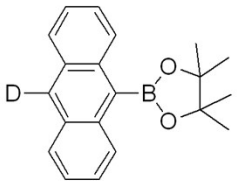

D
B
O
O
13C-NMR
200
150
100
50
0 PPM



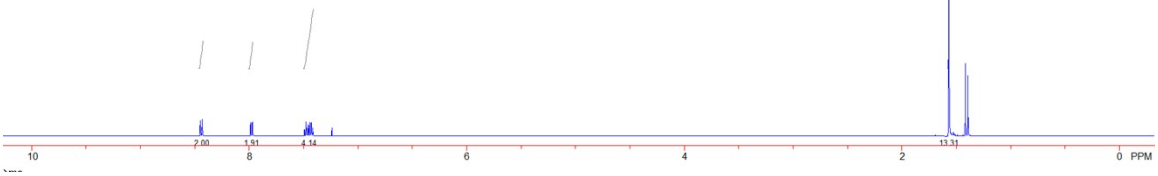
^{1}H-NMR

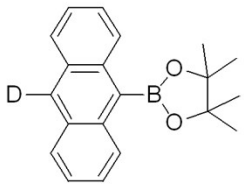


^{13}C-NMR

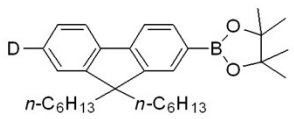


^{1}H-NMR

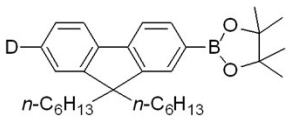




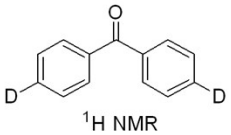
^{13}C-NMR



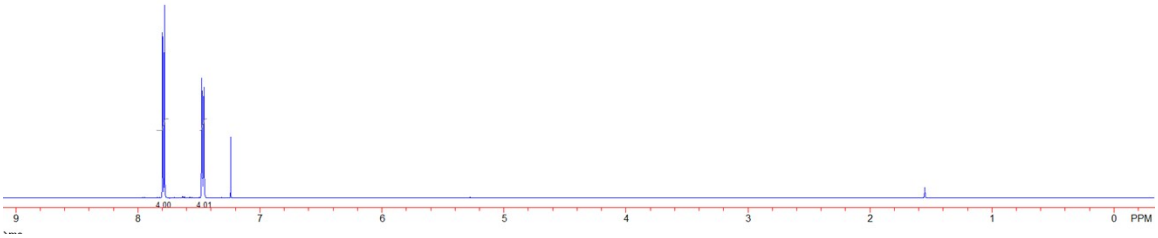
^{1}H NMR

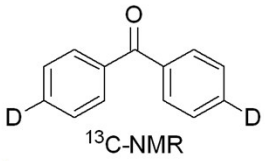


^{13}C-NMR

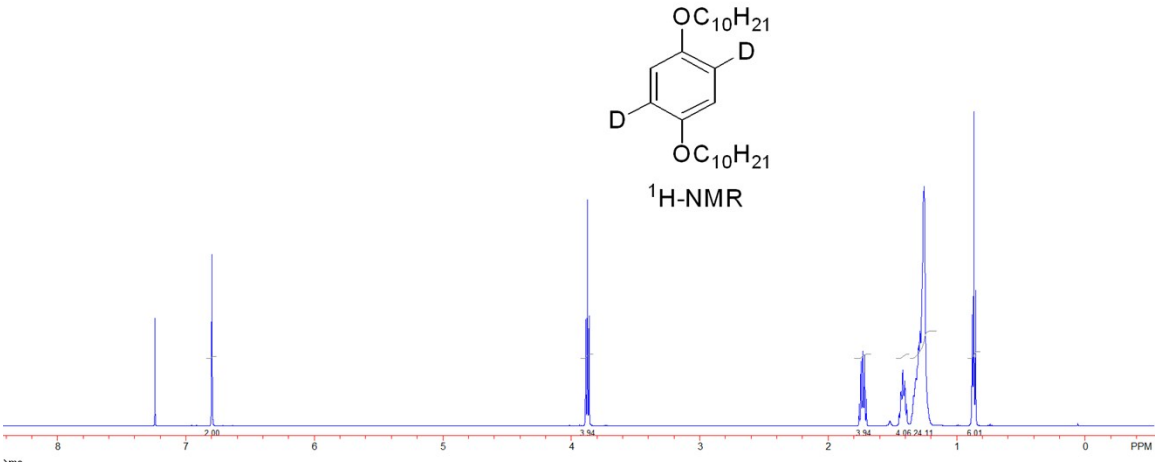


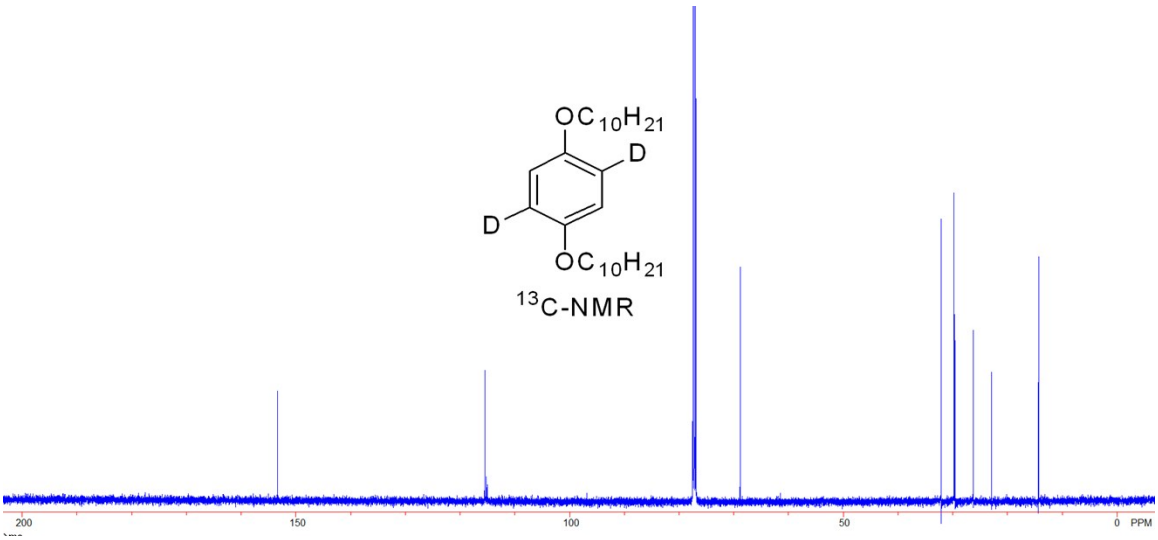
^{1}H NMR

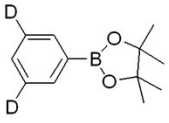




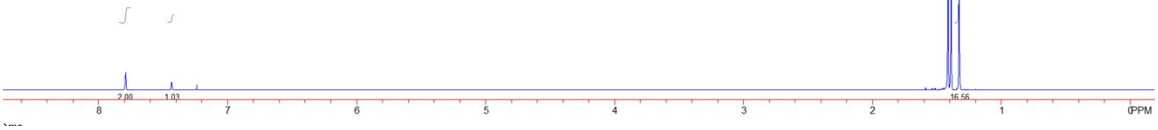
^{13}C-NMR

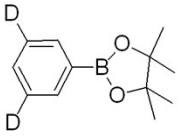

OC10H21
D
D
OC10H21
1H-NMR
2.00
3.94
3.94
4.06
24.11
6.01
8
7
6
5
4
3
2
1
0
PPM


OC10H21
D
D
OC10H21
13C-NMR
200
150
100
50
0
PPM

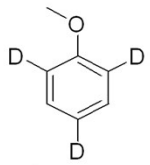


^{1}H NMR

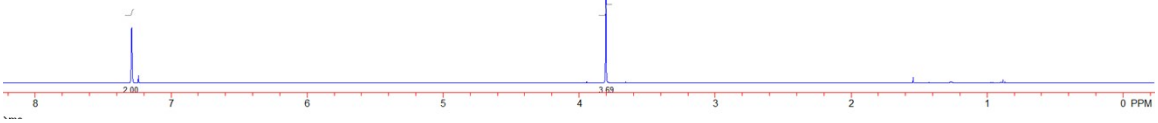


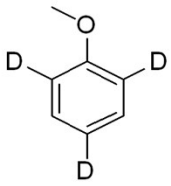


^{13}C-NMR



^{1}H NMR





^{13}C-NMR