Supporting Information

Highly Efficient One-pot Access to Functionalised Arylboronic Acids via Non-cryogenic Bromine/Magnesium Exchanges

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General

All NMR spectra were recorded on a Bruker ARX 400 (400 MHz) spectrometer. Beside ^{1}H and ^{13}C experiments, ^{11}B and ^{19}F spectra were recorded. The chemical shifts are given in ppm downfield of TMS, although the solvents actually served as internal standard. The multiplicity is given by the following symbols: s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet). The coupling constant *J* is given in Hz.

General Procedure A

A dry and argon-flushed Schlenk-flask, equipped with a magnetic stirrer and a septum, is charged with magnesium turnings (122.0 mg, 5.0 mmol). LiCl (5.0 ml, 0.5 M in THF, 2.5 mmol) is added and the magnesium is activated with DIBAL-H (20.0 µl, 1M in toluene, 0.02 mmol). After 5 min of stirring the aryl bromide (2.0 mmol) is added in one portion at room temperature. The reaction mixture is stirred for the indicated time before trimethylborate (448.0 µl, 4.0 mmol) is added at 0 °C. The mixture is then quenched with 0.1 N HCl and extracted with EtOAc. The extract is dried over Na_2SO_4 and concentrated. The residue is purified by crystallisation.

General Procedure B

A dry and argon-flushed Schlenk-flask, equipped with a magnetic stirrer and a septum, is charged with the aryl bromide (5.0 mmol) and THF (5 ml). The solution is cooled to 0 °C and *i*-PrMgCl·LiCl (6.0 ml, 1M in THF, 6.0 mmol) is added drop-wise. The reaction mixture is stirred for the indicated time before trimethylborate (1.12 ml, 10.0 mmol) is added at 0 °C. The mixture is then quenched with 0.1 N HCl and extracted with EtOAc. The extract is dried over Na_2SO_4 and concentrated. The residue is purified by crystallisation.

4-Methoxyphenylboronic acid (1)

4-Methoxyphenylboronic acid is prepared using Procedure A. After the addition of 4-bromoanisole the reaction mixture is stirred at room temperature for 15 h before trimethylborate (448.0 µl, 4.0 mmol) is added at 0 °C. The mixture is then quenched with 0.1 N HCl and extracted with EtOAc. The extract is dried over Na_2SO_4 and concentrated. The residue is recrystallised from H_2O. ^{1}H-NMR (DMSO-d_6, 400 MHz): δ [ppm] = 3.76 (s, 3H), 6.89 (d, *J* = 8.6 Hz, 2H), 7.75 (d, *J* = 8.6 Hz, 2H), 7.83 (bs, 2H); ^{13}C-NMR (DMSO-d_6, 100 MHz): δ [ppm] = 54.8, 112.9, 135.9, 160.95; ^{11}B-NMR (DMSO-d_6, 128 MHz): δ [ppm] = 26.3.

4-(Dimethylamino)phenylboronic acid (2)

4-(Dimethylamino)phenylboronic acid is prepared using Procedure A. After the addition of 4-bromo-N,N-dimethylaniline the reaction mixture is stirred at room temperature for 15 h before trimethylborate (448.0 µl, 4.0 mmol) is added at 0 °C. The mixture is then quenched with 0.1 N HCl and extracted with EtOAc. The extract is dried over Na_2SO_4 and concentrated. The residue is recrystallised from H_2O/CH_3CN. ^{1}H-NMR (DMSO-d_6, 400 MHz): δ [ppm] = 2.91 (s, 6H), 6.65 (d, *J* = 8.9 Hz, 2H), 7.57 (s, 2H), 7.63 (d, *J* = 8.9 Hz, 2H) ; ^{13}C-NMR (DMSO-d_6, 100 MHz): δ [ppm] = 39.7, 111.0, 135.4, 151.7; ^{11}B-NMR (DMSO-d_6, 128 MHz): δ [ppm] = 27.1.

4-Trifluoromethylboronic acid (3)

4-Trifluoromethylboronic acid is prepared using Procedure A. After the addition of 4-(trifluoromethyl)-bromobenzene the reaction mixture is stirred at 0 °C for 30 min. before trimethylborate (448.0 µl, 4.0 mmol) is added at 0 °C. The mixture is then quenched with 0.1 N HCl and extracted with EtOAc. The extract is dried over Na_2SO_4 and concentrated. The residue is recrystallised from H_2O. ^{1}H-NMR (DMSO-d_6, 400 MHz): δ [ppm] = 7.68 (d, *J* = 8.1 Hz, 2H), 8.00 (d, *J* = 8.1 Hz, 2H), 8.31 (bs, 2H); ^{13}C-NMR (DMSO-d_6, 100 MHz): δ [ppm] = 123.9 (q, *J* = 3.7 Hz), 124.4 (q, *J* = 269.6 Hz), 130.2 (q, *J* = 30.9 Hz), 134.7; ^{11}B-NMR (DMSO-d_6, 128 MHz): δ [ppm] = 26.3; ^{19}F-NMR (DMSO-d_6, 376 MHz): δ [ppm] = -61.80.

4-Chloroyphenylboronic acid (4)

4-Chlorophenylboronic acid is prepared using Procedure A. After the addition of 1-bromo-4-chlorobenzene the reaction mixture is stirred at room temperature for 10 min. before trimethylborate (448.0 µl, 4.0 mmol) is added at 0 °C. The mixture is then quenched with 0.1 N HCl and extracted with EtOAc. The extract is dried over Na_2SO_4 and concentrated. The residue is recrystallised from H_2O/CH_3CN. ^{1}H-NMR (DMSO-d_6, 400 MHz): δ [ppm] = 7.39 (d, J = 8.6 Hz, 2H), 7.80 (d, J = 8.6 Hz, 2H), 8.14 (bs, 2H); ^{13}C-NMR (DMSO-d_6, 100 MHz): δ [ppm] = 127.4, 135.1, 136.0; ^{11}B-NMR (DMSO-d_6, 128 MHz): δ [ppm] = 26.6.

4-Cyanophenylboronic acid (5)

4-Cynaophenylboronic acid is prepared using Procedure B. After the addition of *i*-PrMgCl·LiCl the reaction mixture is stirred at 0 °C for 2 h before trimethylborate (1.12 ml, 10.0 mmol) is added at 0 °C. The mixture is then quenched with 0.1 N HCl and extracted with EtOAc. The extract is dried over Na_2SO_4 and concentrated. The residue is recrystallised from H_2O. ^{1}H-NMR (DMSO-d_6, 400 MHz): δ [ppm] = 7.78 (d, J = 8.1 Hz, 2H), 7.93 (d, J = 8.1 Hz, 2H), 8.35 (bs, 2H); ^{13}C-NMR (DMSO-d_6, 100 MHz): δ [ppm] = 112.4, 119.0, 131.0, 134.6; ^{11}B-NMR (DMSO-d_6, 128 MHz): δ [ppm] = 26.4.

3-Fluorophenylboronic acid (6)

3-Fluorophenylboronic acid is prepared using Procedure A. After the addition of 3-bromofluorobenzene the reaction mixture is stirred at room temperature for 15 h before trimethylborate (448.0 µl, 4.0 mmol) is added at 0 °C. The mixture is then quenched with 0.1 N HCl and extracted with EtOAc. The extract is dried over Na_2SO_4 and concentrated. The residue is recrystallised from H_2O. ^{1}H-NMR (DMSO-d_6, 400 MHz): δ [ppm] = 7.20 (m, 1H), 7.38 (m, 1H), 7.63 (m, 2H), 8.21 (bs, 2H); ^{13}C-NMR (DMSO-d_6, 100 MHz): δ [ppm] = 116.8 (d, J = 21.7 Hz), 120.0 (d, J = 19.2 Hz), 129.6 (d, J = 7.2 Hz), 130.1 (d, J = 2.6 Hz), 162.1 (d, J = 242.0 Hz); ^{11}B-NMR (DMSO-d_6, 128 MHz): δ [ppm] = 28.0; ^{19}F-NMR (DMSO-d_6, 376 MHz): δ [ppm] = -114.91;

3-Trifluoromethoxyphenylboronic acid (7)

3-Trifluoromethoxyphenylboronic acid is prepared using Procedure A. After the addition of 3-bromo-(trifluoro-methoxy)benzene the reaction mixture is stirred at room temperature for 15 h before trimethylborate (448.0 µl, 4.0 mmol) is added at 0 °C. The mixture is then quenched with 0.1 N HCl and extracted with EtOAc. The extract is dried over Na_2SO_4 and concentrated. The residue is recrystallised from H_2O. ^{1}H-NMR (DMSO-d_6, 400 MHz): δ [ppm] = 7.37 (d, J = 8.1 Hz, 1H), 7.50 (m, 1H), 7.71 (bs, 1H), 7.82 (m, J = 7.1 Hz, 1H), 8.27 (bs, 2H); ^{13}C-NMR (DMSO-d_6, 100 MHz): δ [ppm] = 120.2 (q, J = 255.9 Hz), 122.6, 125.8, 129.5, 133.1, 148.2; ^{11}B-NMR (DMSO-d_6, 128 MHz): δ [ppm] = 28.4; ^{19}F-NMR (DMSO-d_6, 376 MHz): δ [ppm] = -57.09.

2-Biphenylboronic acid (8)

2-Biphenylboronic acid is prepared using Procedure A. After the addition of 2-bromobiphenyl the reaction mixture is stirred at room temperature for 1 h before trimethylborate (448.0 µl, 4.0 mmol) is added at 0 °C. The mixture is then quenched with 0.1 N HCl and extracted with EtOAc. The extract is dried over Na_2SO_4 and concentrated. The residue is recrystallised from H_2O/CH_3CN. ^{1}H-NMR (DMSO-d_6, 400 MHz): δ [ppm] = 7.35 (m, 2H), 7.44 (m, 4H), 7.49 (m, 3H), 7.96 (s, 2H); ^{13}C-NMR (DMSO-d_6, 100 MHz): δ [ppm] = 126.1, 126.8, 128.2, 128.3, 128.3, 132.3, 143.3, 144.2; ^{11}B-NMR (DMSO-d_6, 128 MHz): δ [ppm] = 29.9.

1-Naphthaleneboronic acid (9)

1-Naphthaleneboronic acid is prepared using Procedure A. After the addition of 1-bromonaphthalene the reaction mixture is stirred at room temperature for 15 h before trimethylborate (448.0 µl, 4.0 mmol) is added at 0 °C. The mixture is then quenched with 0.1 N HCl and extracted with EtOAc. The extract is dried over Na_2SO_4 and concentrated. The residue is recrystallised from H_2O. ^{1}H-NMR (DMSO-d_6, 400 MHz): δ [ppm] = 7.48 (m, 3H), 7.75 (d, J = 6.6 Hz, 1H), 7.88 (ψt, J = 8.3 Hz, 2H), 8.39 (d, J = 8.1 Hz, 1H), 8.43 (bs, 2H); ^{13}C-NMR (DMSO-d_6, 100 MHz): δ [ppm] = 125.6, 125.9, 126.1, 128.7, 129.0, 129.7, 132.6, 133.3, 136.0; ^{11}B-NMR (DMSO-d_6, 128 MHz): δ [ppm] = 28.6.

2,4,6-Trimethylphenylboronic acid (10)

2,4,6-Trimethylphenylboronic acid is prepared using Procedure A. After the addition of 2,4,6-trimethylbromobenzene the reaction mixture is stirred at room temperature for 15 h before trimethylborate (448.0 µl, 4.0 mmol) is added at 0 °C. The mixture is then quenched with 0.1 N HCl and extracted with EtOAc. The extract is dried over Na_2SO_4 and concentrated. The residue is recrystallised from H_2O/CH_3CN. ^{1}H-NMR (DMSO-d_6, 400 MHz): δ [ppm] = 2.21 (s, 3H), 2.24 (s, 6H), 6.75 (s, 2H), 8.03 (s, 2H); ^{13}C-NMR (DMSO-d_6, 100 MHz): δ [ppm] = 20.8, 21.9, 126.4, 136.1, 138.5; ^{11}B-NMR (DMSO-d_6, 128 MHz): δ [ppm] = 30.3.

(4-{[(4-Methylphenyl)sulfonyl]oxy}phenyl)boronic acid (11)

(4-{[(4-methylphenyl)sulfonyl]oxy}phenyl)boronic acid is prepared using Procedure A. After the addition of 4-bromophenyl 4-methylbenzenesulfonate the reaction mixture is stirred at 0 °C for 2 h before trimethylborate (448.0 µl, 4.0 mmol) is added at 0 °C. The mixture is then quenched with 0.1 N HCl and extracted with EtOAc. The extract is dried over Na_2SO_4 and concentrated. The residue is recrystallised from H_2O/CH_3CN. ^{1}H-NMR (DMSO-d_6, 400 MHz): δ [ppm] = 2.41 (s, 3H), 7.00 (d, J = 8.6 Hz, 2H), 7.46 (d, J = 8.2 Hz, 2H), 7.73 (d, J = 8.2 Hz, 2H), 7.78 (d, J = 8.6 Hz, 2H), 8.15 (bs, 2H); ^{13}C-NMR (DMSO-d_6, 100 MHz): δ [ppm] = 21.2, 120.9, 128.2, 130.2, 131.5, 135.8, 145.7, 150.6; ^{11}B-NMR (DMSO-d_6, 128 MHz): δ [ppm] = 25.0.

3-Thienylboronic acid (12)

3-thienylboronic acid is prepared using Procedure B. After the addition of *i*-PrMgCl·LiCl the reaction mixture is stirred at room temperature for 30 min. before trimethylborate (1.12 ml, 10.0 mmol) is added at 0 °C. The mixture is then quenched with 0.1 N HCl and extracted with EtOAc. The extract is dried over Na_2SO_4 and concentrated. The residue is recrystallised from H_2O/CH_3CN. ^{1}H-NMR (DMSO-d_6, 400 MHz): δ [ppm] = 7.42 (dd, J = 1.0 and 4.8 Hz, 1H), 7.45 (dd, J = 2.7 and 4.8 Hz, 1H), 7.96 (dd, J = 1.0 and 2.7 Hz, 1H), 8.07 (bs, 2H); ^{13}C-NMR (DMSO-d_6, 100 MHz): δ [ppm] = 125.5, 132.8, 135.3; ^{11}B-NMR (DMSO-d_6, 128 MHz): δ [ppm] = 25.6.

(2-Methoxypyridin-3-yl)boronic acid (13)

(2-methoxypyridin-3-yl)boronic acid is prepared using Procedure A. After the addition of 3-bromo-2-methoxypyridine the reaction mixture is stirred at room temperature for 30 min. before trimethylborate (448.0 µl, 4.0 mmol) is added at 0 °C. The mixture is then quenched with 0.1 N HCl and extracted with EtOAc. The extract is dried over Na_2SO_4 and concentrated. The residue is recrystallised from H_2O/CH_3CN. ^{1}H-NMR (DMSO-d_6, 400 MHz): δ [ppm] = 3.88 (s, 3H), 6.97 (dd, J = 5.0 and 7.1 Hz, 1H), 7.86 (bs, 2H), 7.89 (dd, J = 2.2 and 7.1 Hz, 1H), 8.19 (dd, J = 2.2 and 5.0 Hz, 1H); ^{13}C-NMR (DMSO-d_6, 100 MHz): δ [ppm] = 53.0, 116.9, 144.7, 148.3, 166.3; ^{11}B-NMR (DMSO-d_6, 128 MHz): δ [ppm] = 27.9.

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23.02.2011 10:46:00

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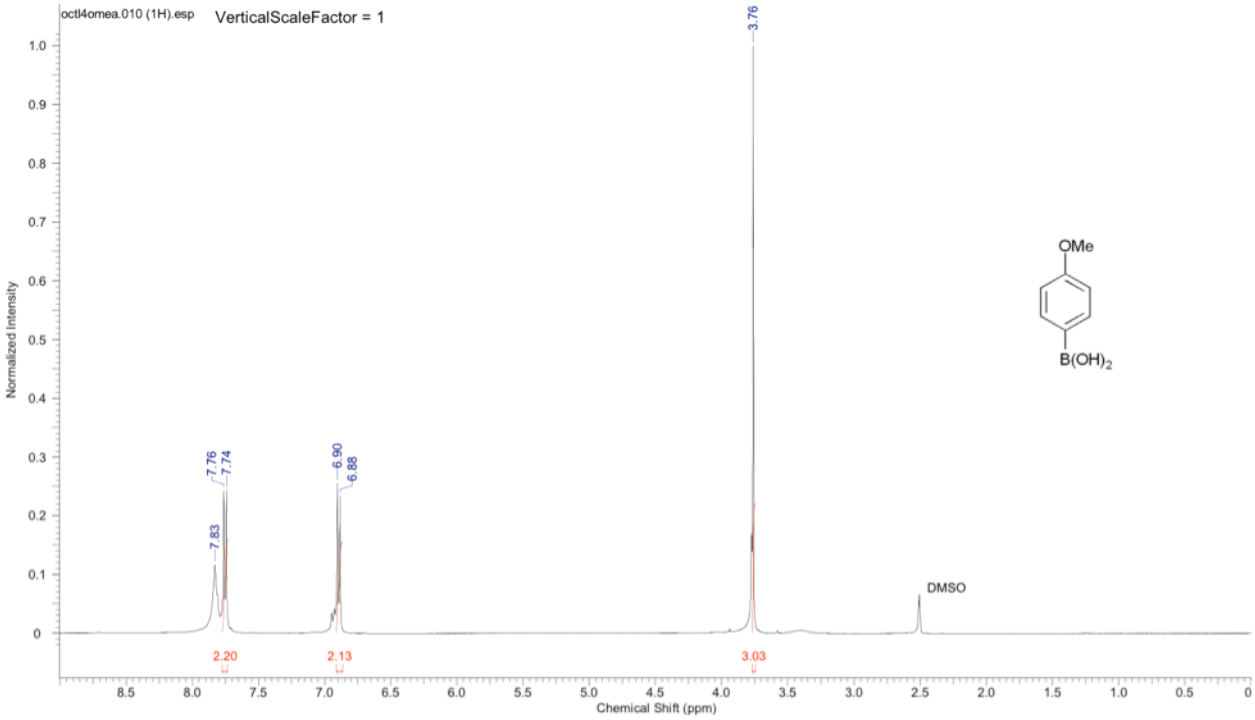

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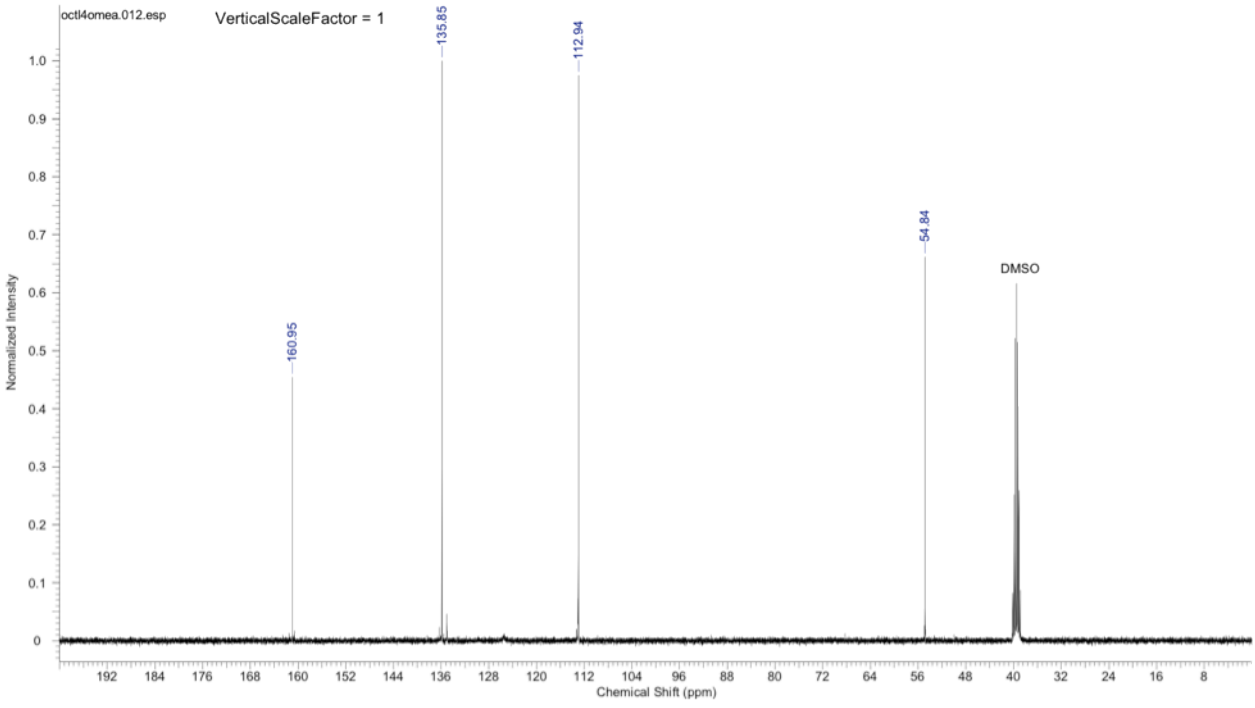

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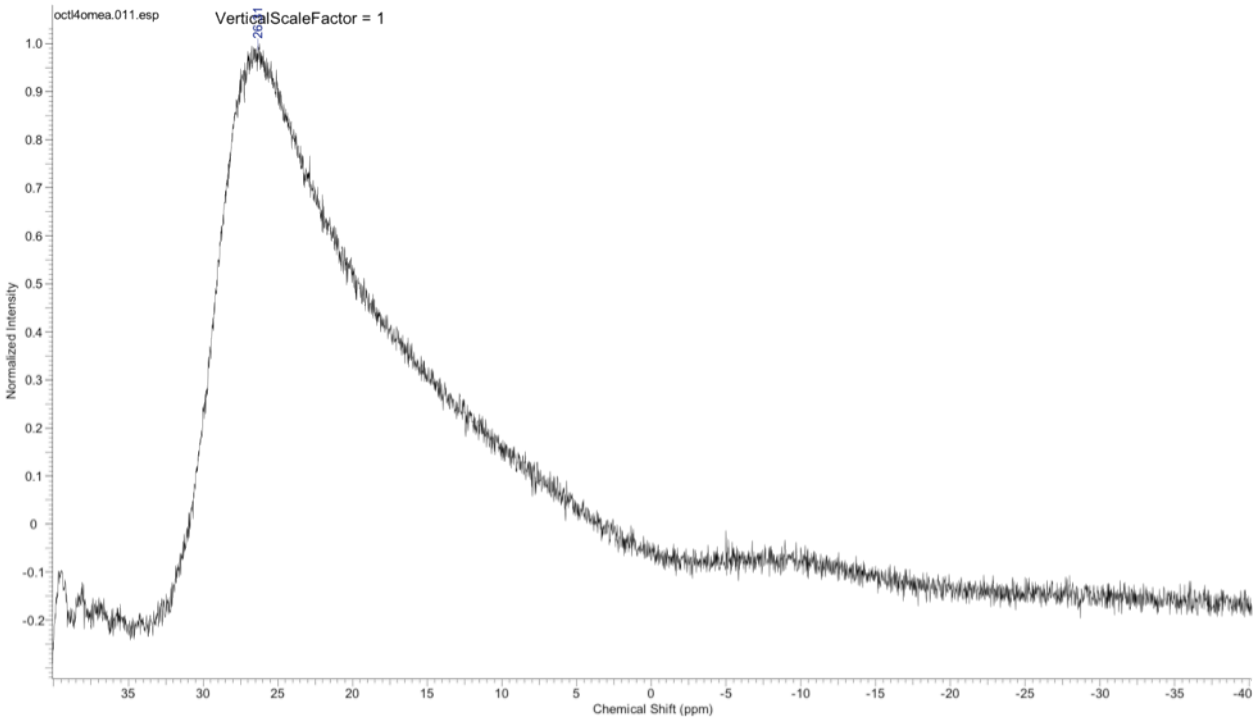

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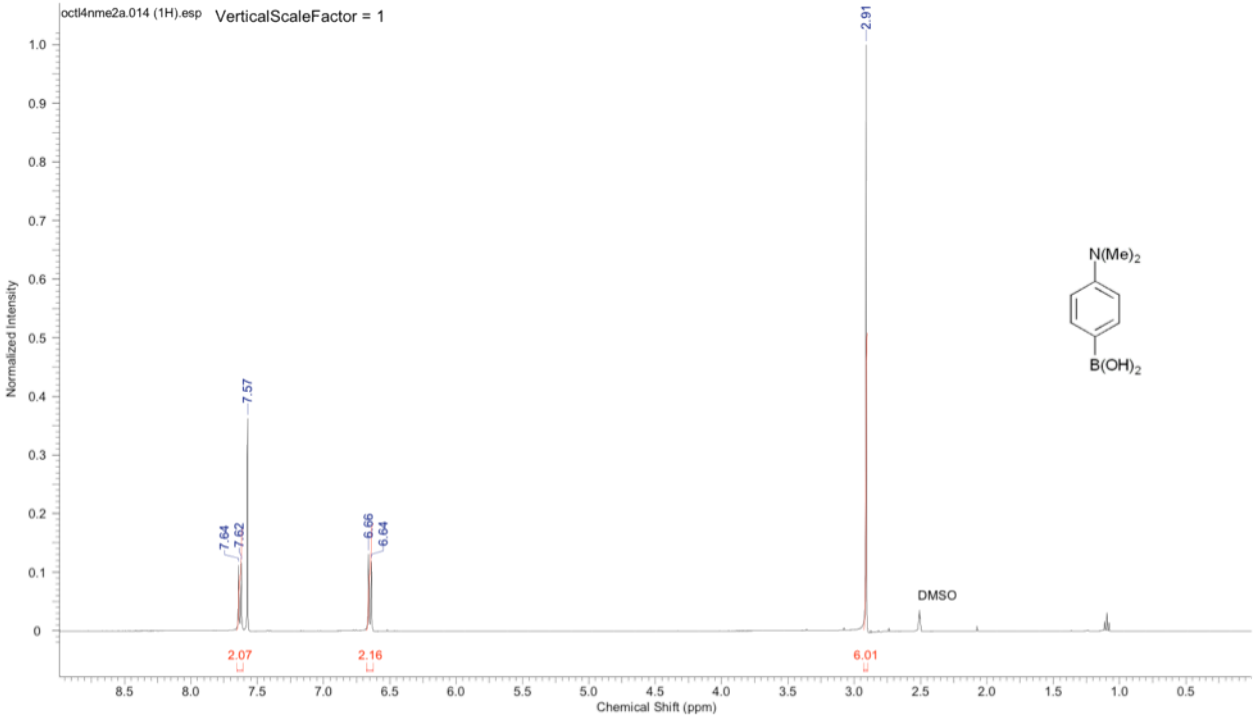

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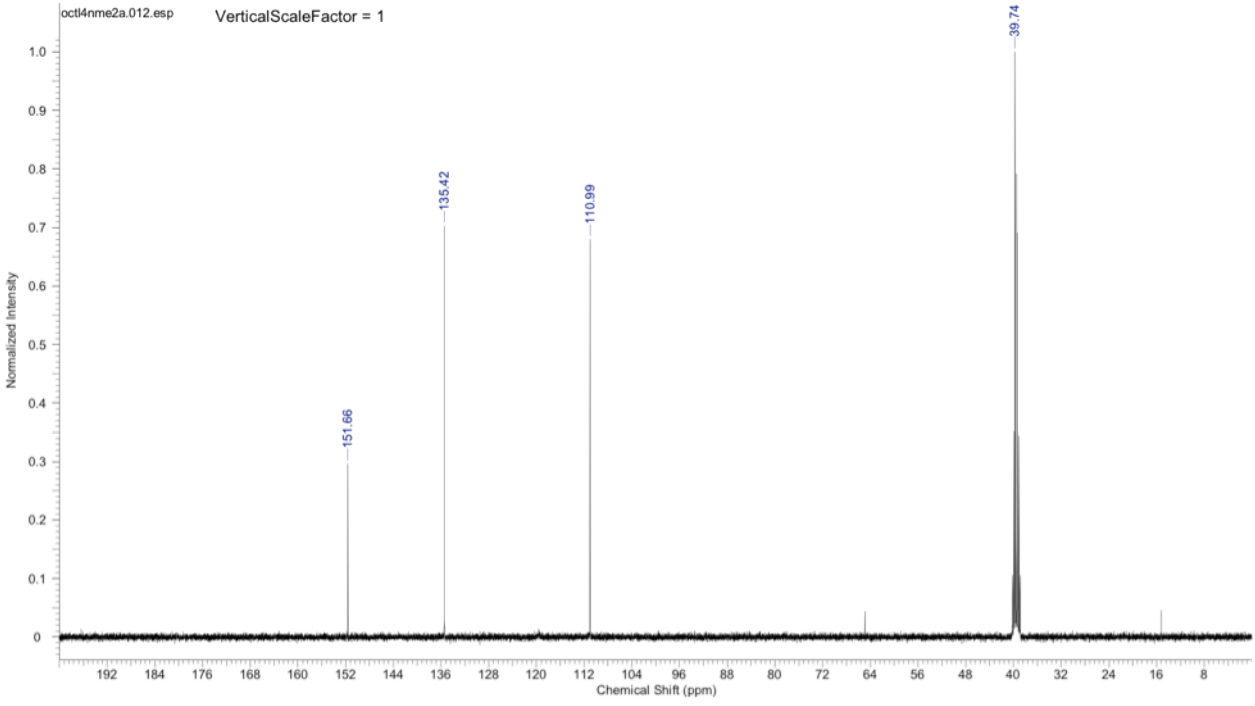

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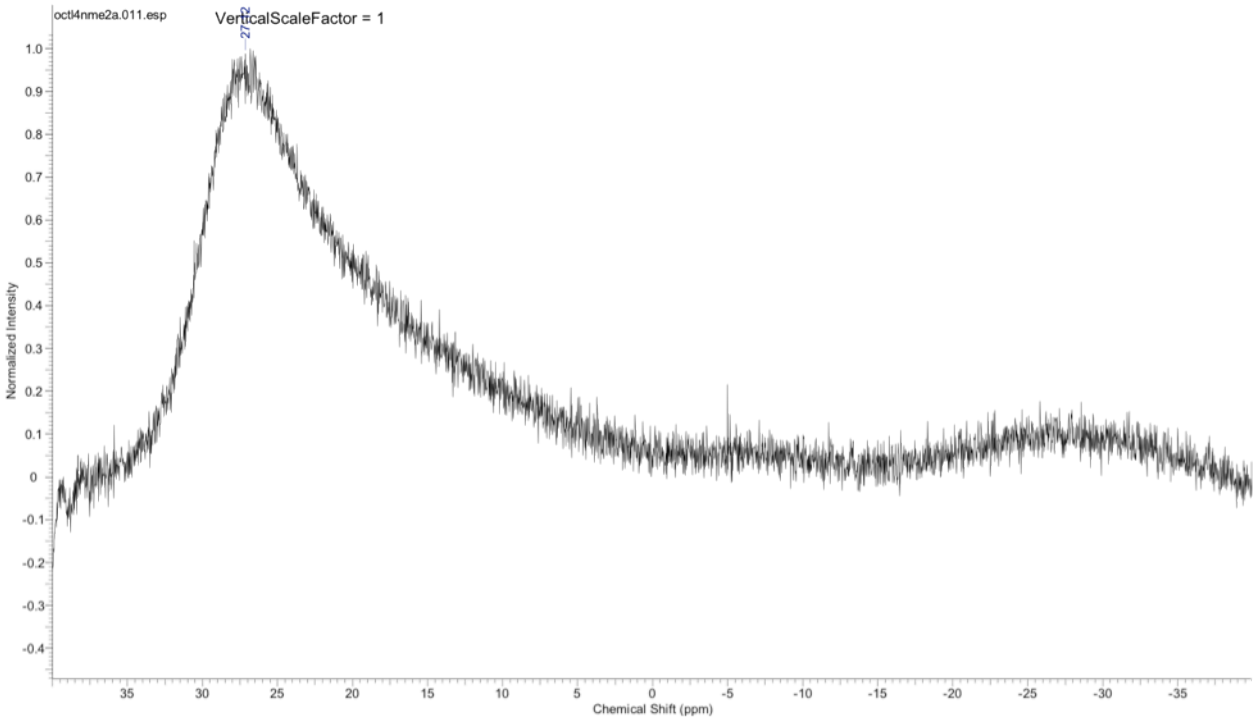

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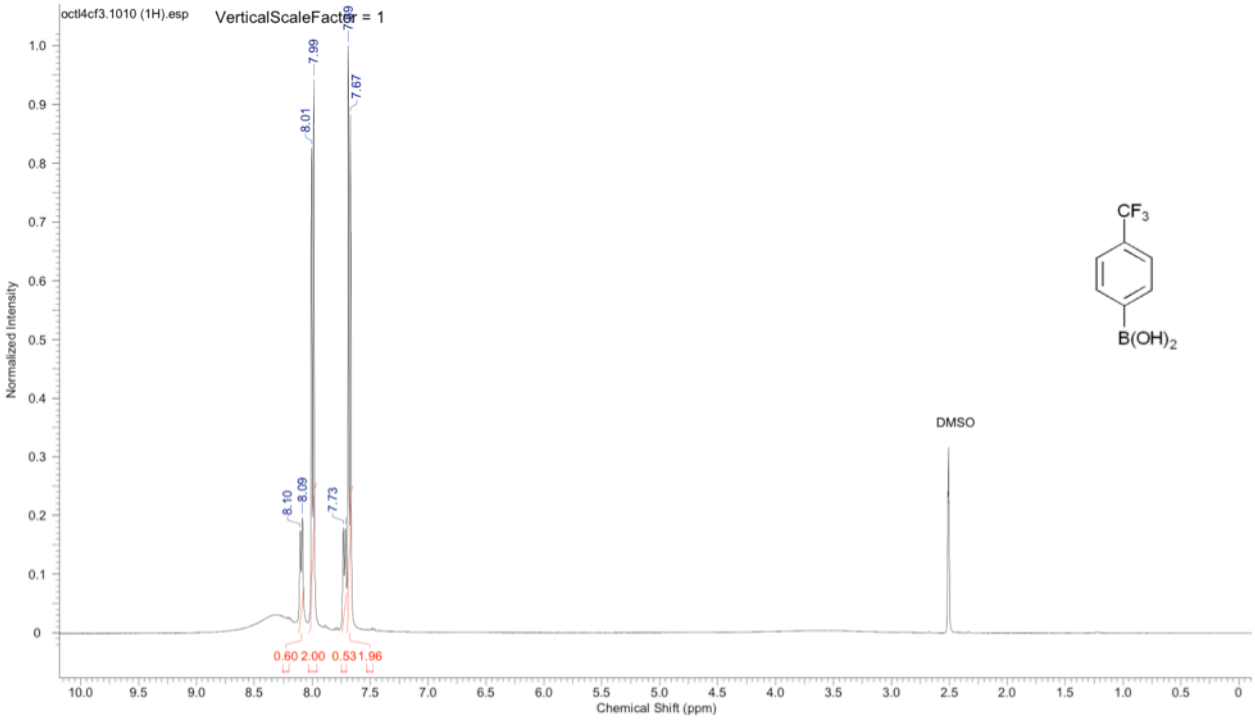

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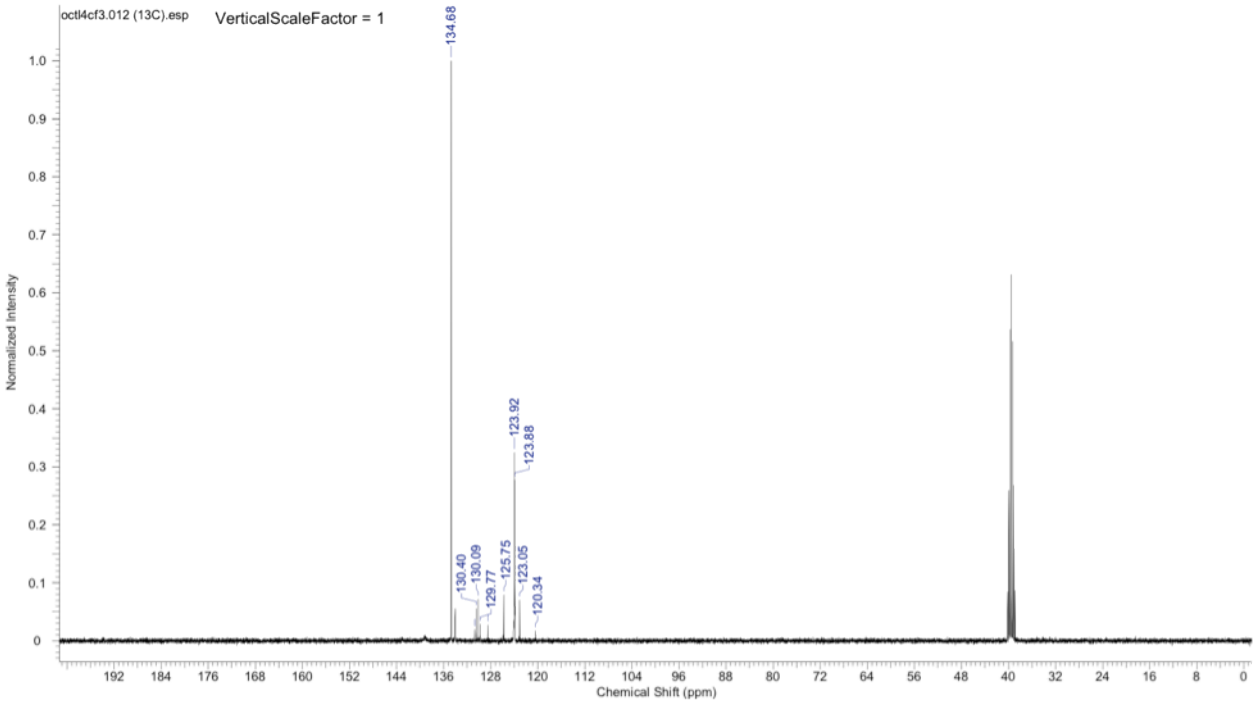

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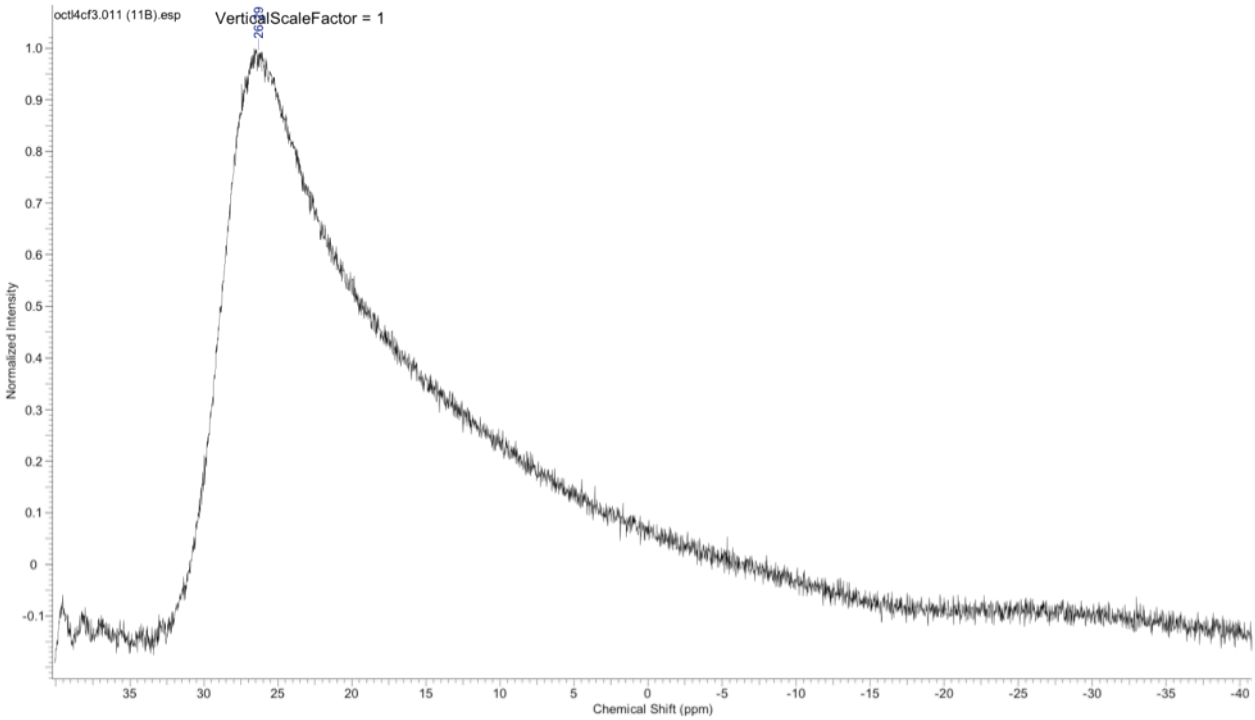

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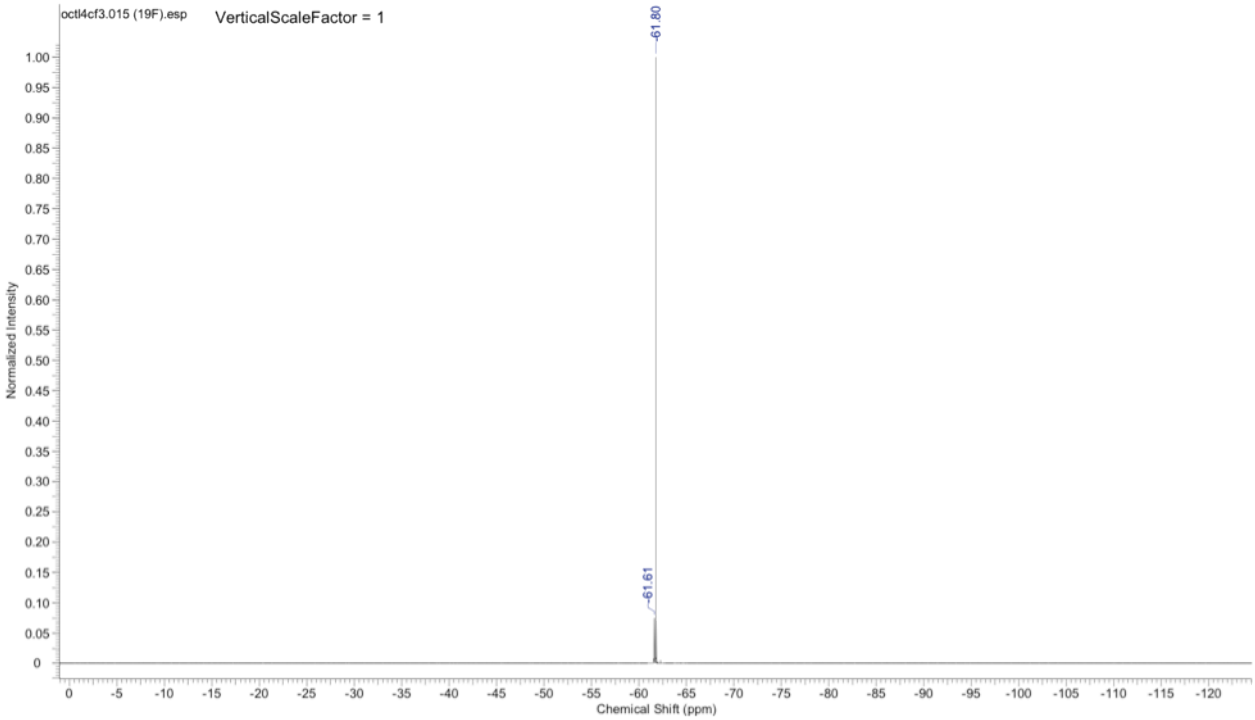
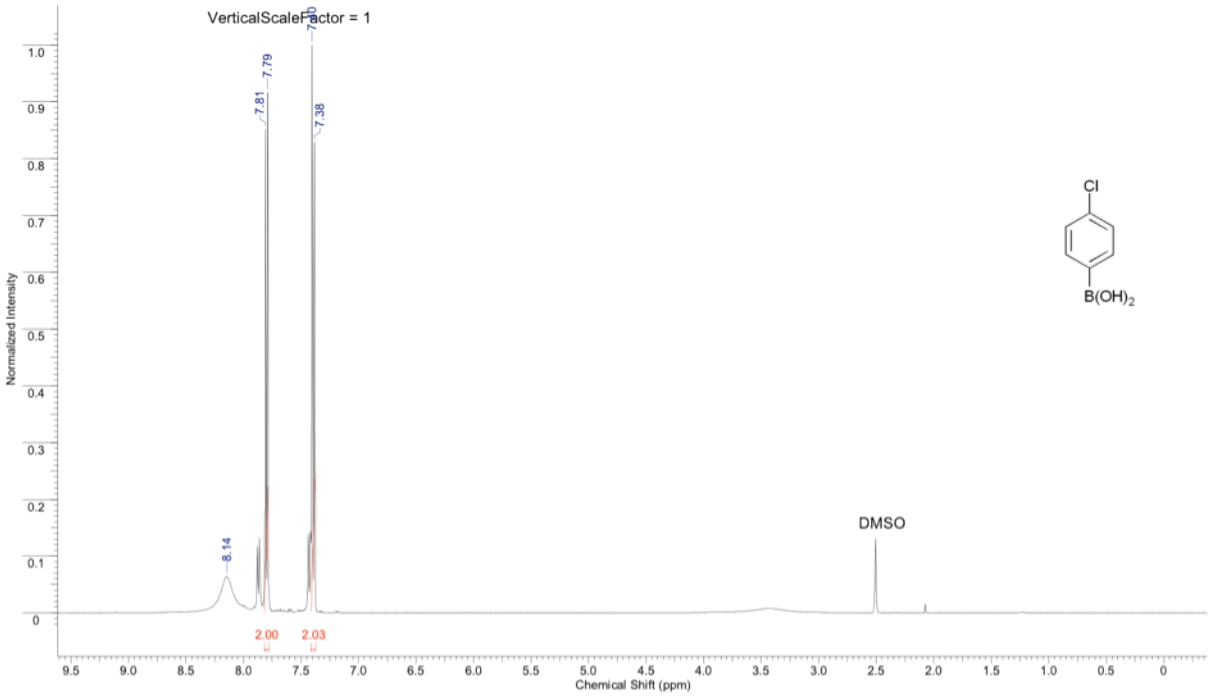
Nucleus	19F	***Number of Transients***	32	***Origin***	spect	***Original Points Count***	65491	***Owner***	nmr400
Points Count	65536	***Pulse Sequence***	zgfhigqn30	***Receiver Gain***	512.00	***SW(cyclical) (Hz)***	75187.97	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	-35919.2852	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	75186.82	***Temperature (degree C)***	27.000		



Compound 4:

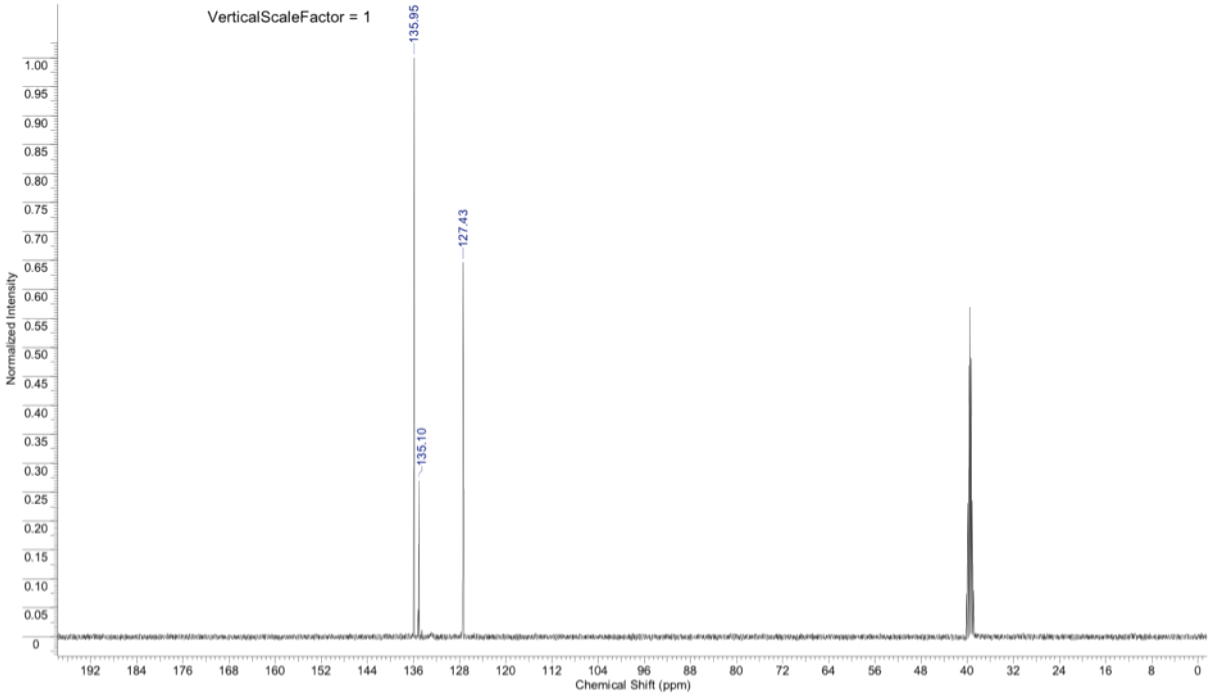
09.05.2011 11:39

Acquisition Time (sec)	1.9793	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	27 Apr 2011 19:54:40
File Name	\\VBOXSVR\vbshare\ECPM Strasbourg\Boronic acids - Strasbourg\octl4cl1\octl4cl1_1010000fid					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	16384
Owner	nmr400	***Points Count***	16384	***Pulse Sequence***	zg30	***Receiver Gain***	181.00
SW(cyclical) (Hz)	8278.15	***Solvent***	DMSO-D6	***Spectrum Offset (Hz)***	2471.0115	***Sweep Width (Hz)***	8277.64
Temperature (degree C)	27.000						



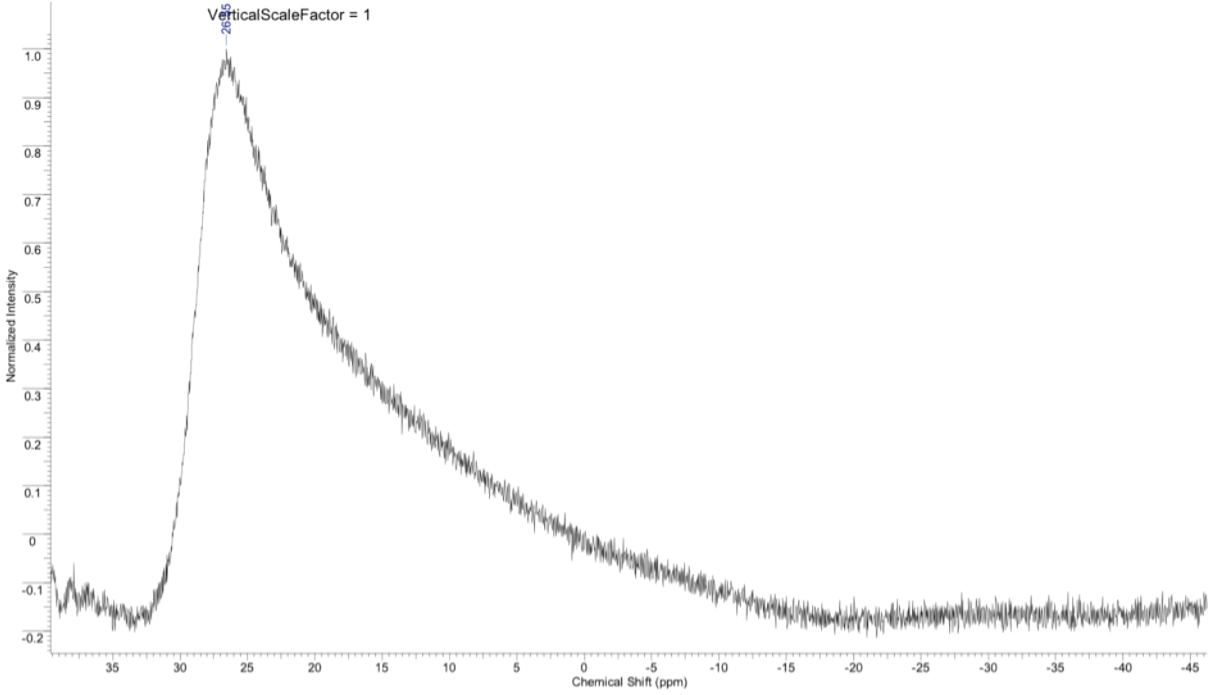
09.05.2011 11:43

Acquisition Time (sec)	1.3665	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	28 Apr 2011 16:17:04
File Name	\\VBOXSVR\vbshare\ECPM Strasbourg\Boronic acids - Strasbourg\octl4cl1\octl4cl1_020000fid					***Frequency (MHz)***	100.62
Nucleus	13C	***Number of Transients***	1024	***Origin***	spect	***Original Points Count***	32768
Owner	nmr400	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	16384.00
SW(cyclical) (Hz)	23980.81	***Solvent***	DMSO-D6	***Spectrum Offset (Hz)***	10015.1631	***Sweep Width (Hz)***	23980.08
Temperature (degree C)	27.000						



09.05.2011 11:44

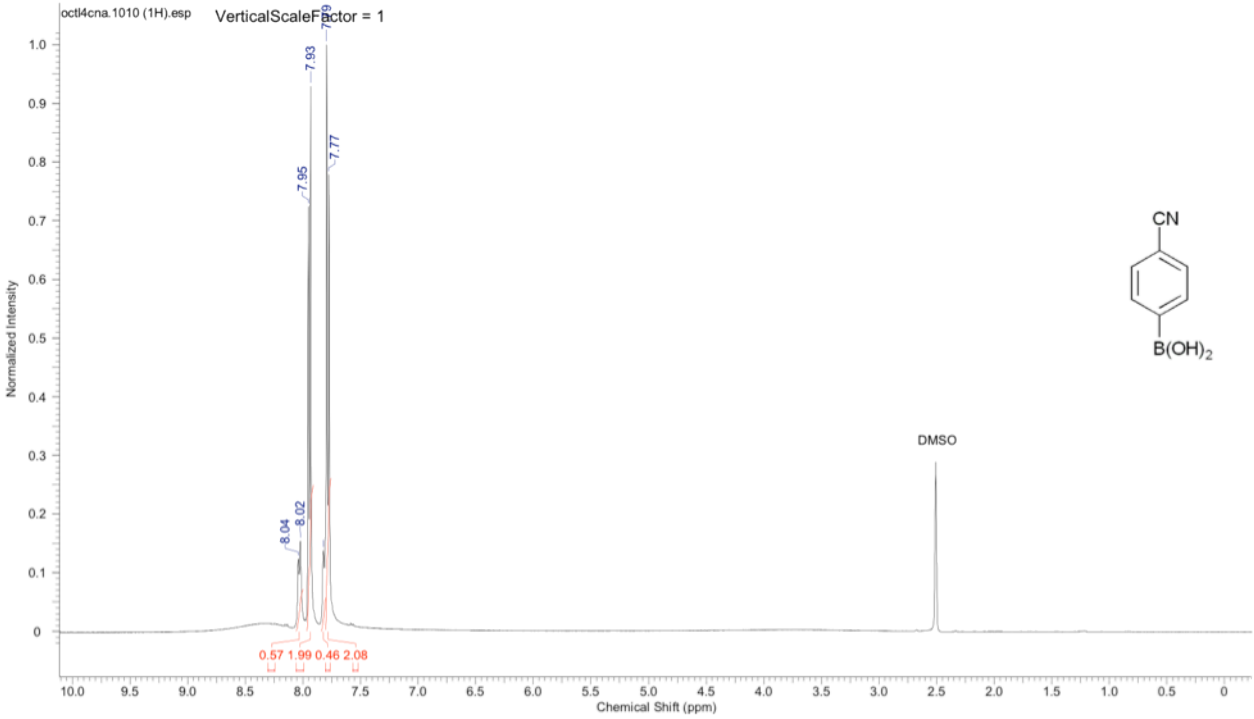
Acquisition Time (sec)	0.3479	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	27 Apr 2011 20:01:04
File Name	\\VBOXSVR\vbshare\ECPM Strasbourg\Boronic acids - Strasbourg\octl4cl1\octl4cl1_011000fid					***Frequency (MHz)***	128.38
Nucleus	11B	***Number of Transients***	128	***Origin***	spect	***Original Points Count***	4026
Owner	nmr400	***Points Count***	4096	***Pulse Sequence***	zgpg	***Receiver Gain***	574.70
SW(cyclical) (Hz)	11574.07	***Solvent***	DMSO-D6	***Spectrum Offset (Hz)***	-641.9142	***Sweep Width (Hz)***	11571.25
Temperature (degree C)	27.100						



Compound 5:

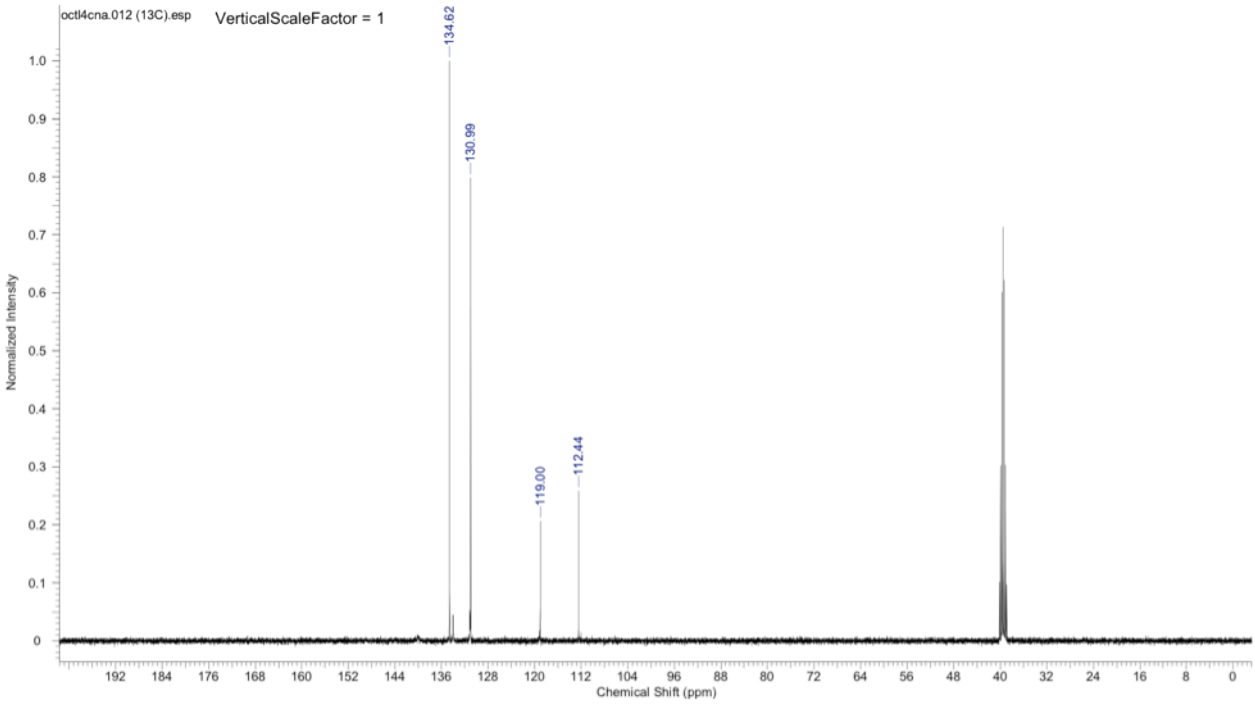
01.03.2011 17:27:25

Acquisition Time (sec)	1.9792	*Comment*	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			*Date*	18 Feb 2011 17:32:00		
Date Stamp	18 Feb 2011 17:32:00			*File Name*	\\VBOXSVR\VBShare\Timo\octl4cna\1010\fid			*Frequency (MHz)*	400.13
Nucleus	1H	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	16384	*Owner*	nmr400
Points Count	16384	*Pulse Sequence*	zg30	*Receiver Gain*	161.30	*SW(cyclical) (Hz)*	8278.15	*Solvent*	DMSO-d6
Spectrum Offset (Hz)	2470.9705	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	8277.64	*Temperature (degree C)*	27.000		



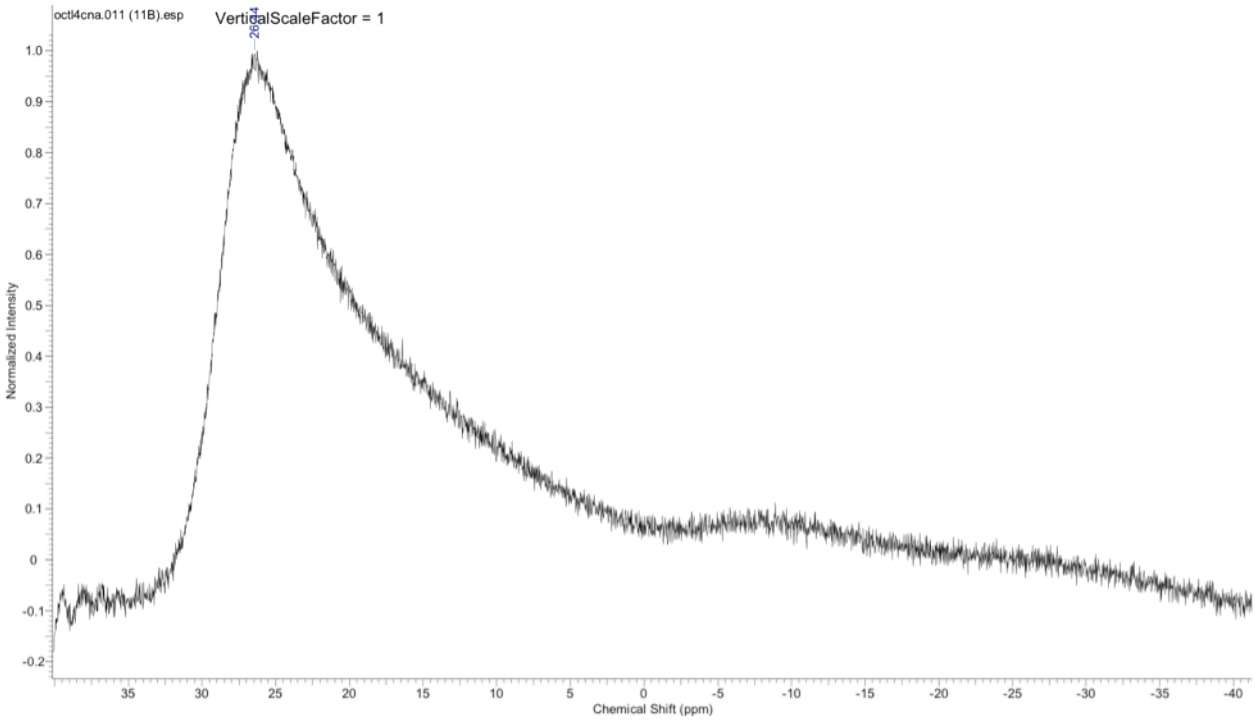
01.03.2011 17:29:21

Acquisition Time (sec)	1.3664	*Comment*	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			*Date*	18 Feb 2011 18:21:04
Date Stamp	18 Feb 2011 18:21:04			*File Name*	\\VBOXSVR\VBShare\Timo\octl4cna\12\fid		
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	1024	*Origin*	spect
Original Points Count	32768	*Owner*	nmr400	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	16384.00	*SW(cyclical) (Hz)*	23980.81	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	10014.6221
Spectrum Type	STANDARD	*Sweep Width (Hz)*	23980.08	*Temperature (degree C)*	27.000		



01.03.2011 17:30:29

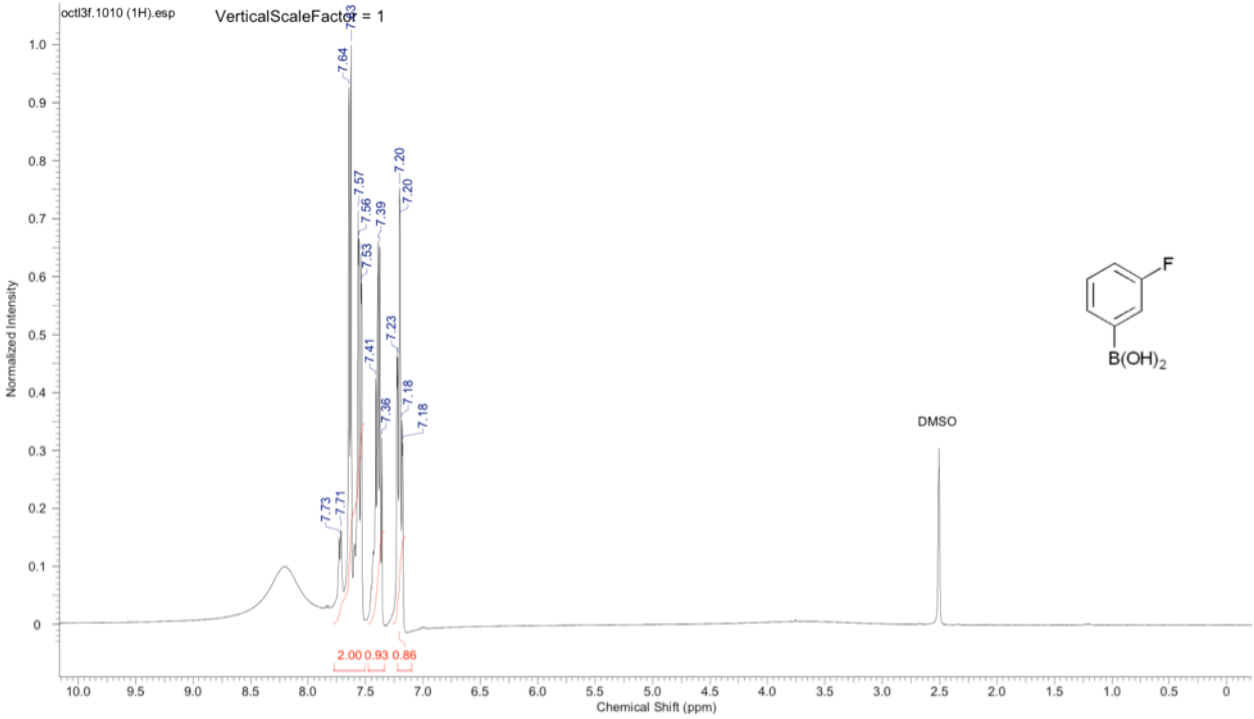
Acquisition Time (sec)	0.3478	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	18 Feb 2011 17:38:24		
Date Stamp	18 Feb 2011 17:38:24			***File Name***	\\VBOXSVR\VBShare\Timo\octl4cna\11\fid			***Frequency (MHz)***	128.38
Nucleus	11B	***Number of Transients***	128	***Origin***	spect	***Original Points Count***	4026	***Owner***	nmr400
Points Count	4096	***Pulse Sequence***	zgpg	***Receiver Gain***	574.70	***SW(cyclical) (Hz)***	11574.07	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	-641.8885	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	11571.25	***Temperature (degree C)***	27.100		



Compound 6:

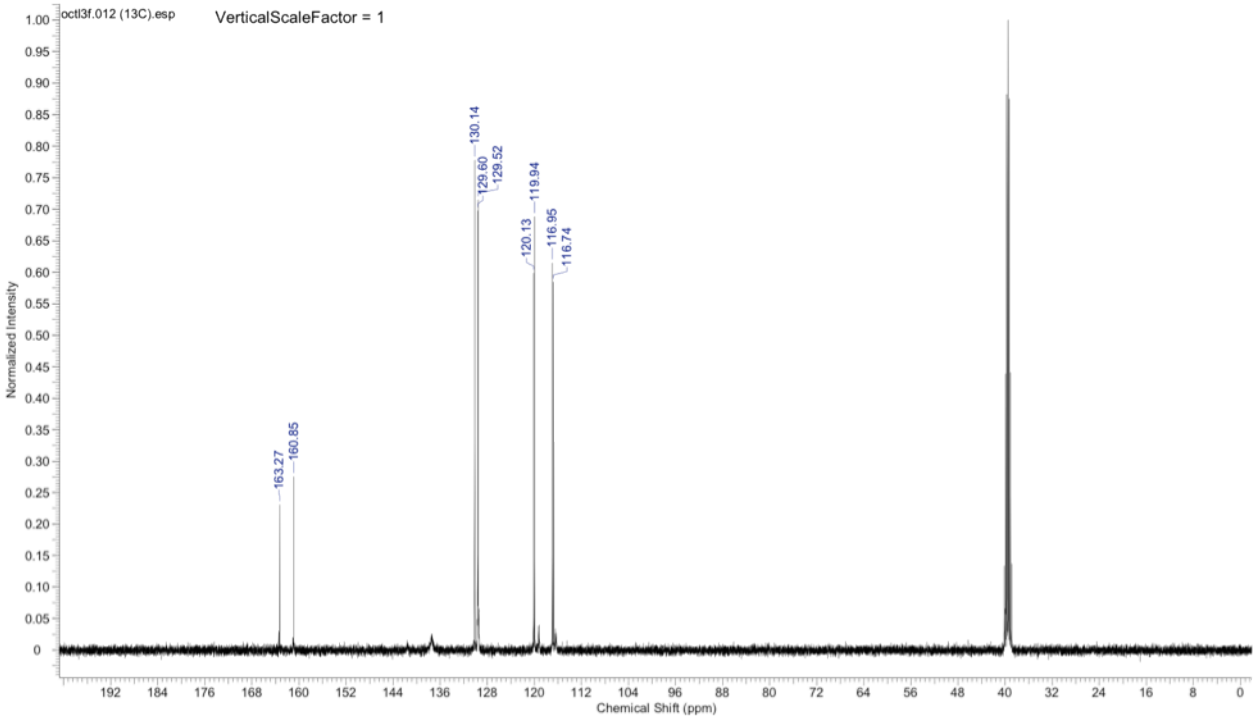
01.03.2011 17:32:15

Acquisition Time (sec)	1.9792	*Comment*	5 mm PABBO BB-1H/D Z-GRD Z863001/0017	*Date*	17 Feb 2011 00:40:48		
Date Stamp	17 Feb 2011 00:40:48			*File Name*	\\VBOXSVR\VBShare\Timo\octl3f\1010\fid	*Frequency (MHz)*	400.13
Nucleus	1H	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	16384	*Owner*	nmr400
Points Count	16384	*Pulse Sequence*	zg30	*Receiver Gain*	71.80	*SW(cyclical) (Hz)*	8278.15	*Solvent*	DMSO-d6
Spectrum Offset (Hz)	2470.9705	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	8277.64	*Temperature (degree C)*	27.000		



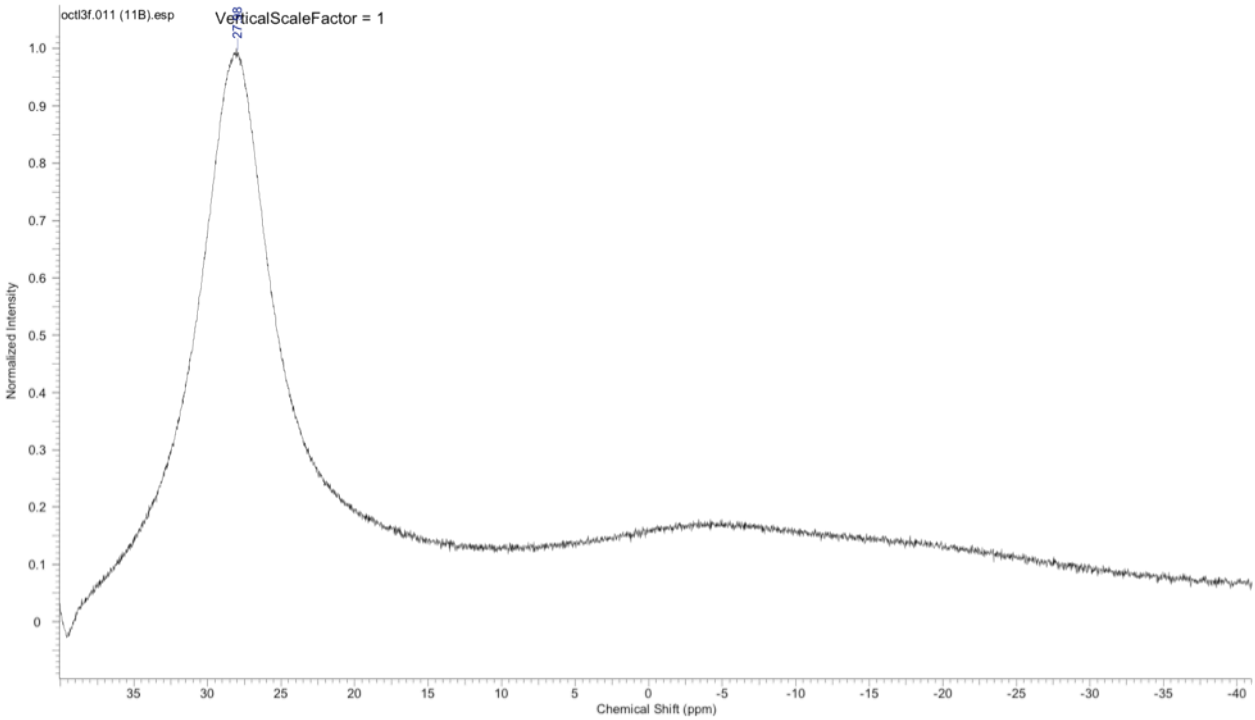
01.03.2011 17:33:46

Acquisition Time (sec)	1.3664	*Comment*	5 mm PABBO BB-1H/D Z-GRD Z863001/0017	*Date*	17 Feb 2011 01:32:00		
Date Stamp	17 Feb 2011 01:32:00			*File Name*	\\VBOXSVR\VBShare\Timo\octl3f\12\fid	*Frequency (MHz)*	100.61
Nucleus	13C	*Number of Transients*	1024	*Origin*	spect	*Original Points Count*	32768	*Owner*	nmr400
Points Count	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	16384.00	*SW(cyclical) (Hz)*	23980.81	*Solvent*	DMSO-d6
Spectrum Offset (Hz)	10022.1162	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	23980.08	*Temperature (degree C)*	27.000		



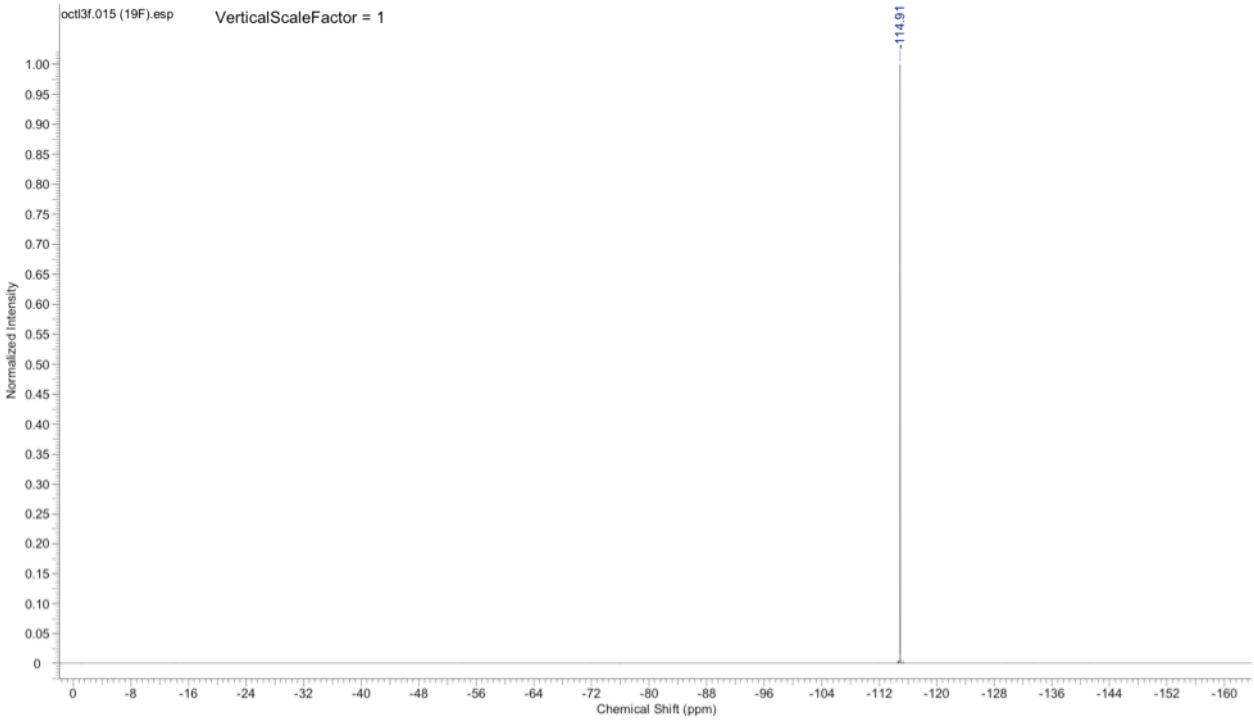
01.03.2011 17:34:55

Acquisition Time (sec)	0.3478	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	17 Feb 2011 00:47:12		
Date Stamp	17 Feb 2011 00:47:12			***File Name***	\\VBOXSVR\VBShare\Timo\octl3f\11\fid			***Frequency (MHz)***	128.38
Nucleus	11B	***Number of Transients***	128	***Origin***	spect	***Original Points Count***	4026	***Owner***	nmr400
Points Count	4096	***Pulse Sequence***	zgpg	***Receiver Gain***	362.00	***SW(cyclical) (Hz)***	11574.07	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	-641.8885	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	11571.25	***Temperature (degree C)***	27.000		



01.03.2011 17:36:03

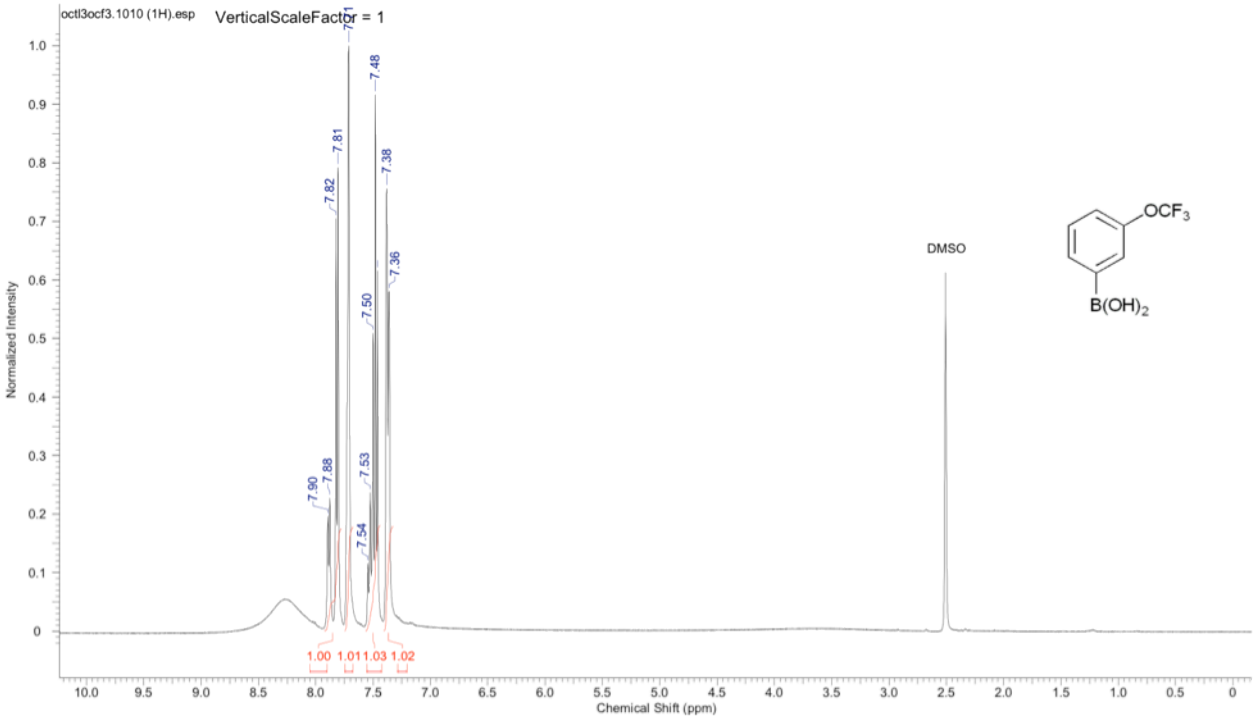
Acquisition Time (sec)	0.8710	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	17 Feb 2011 01:42:40		
Date Stamp	17 Feb 2011 01:42:40			***File Name***	\\VBOXSVR\VBShare\Timo\octl3f\15\fid			***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	32	***Origin***	spect	***Original Points Count***	65491	***Owner***	nmr400
Points Count	65536	***Pulse Sequence***	zgfhigqn30	***Receiver Gain***	645.10	***SW(cyclical) (Hz)***	75187.97	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	-35919.2852	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	75186.82	***Temperature (degree C)***	27.000		



Compound 7:

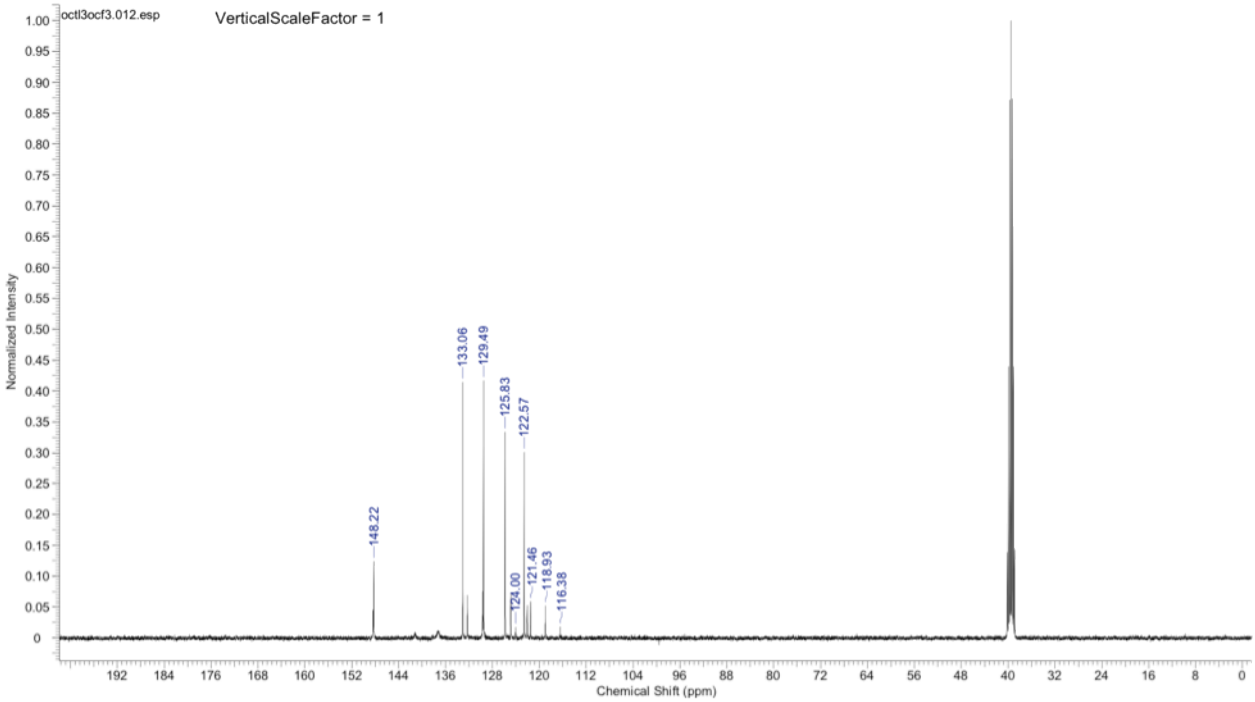
01.03.2011 17:37:21

Acquisition Time (sec)	1.9792	*Comment*	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			*Date*	16 Feb 2011 23:32:32		
Date Stamp	16 Feb 2011 23:32:32			*File Name*	\\VBOXSVR\VBShare\Timo\octl3ocf3\1010\fid			*Frequency (MHz)*	400.13
Nucleus	1H	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	16384	*Owner*	nmr400
Points Count	16384	*Pulse Sequence*	zg30	*Receiver Gain*	161.30	*SW(cyclical) (Hz)*	8278.15	*Solvent*	DMSO-d6
Spectrum Offset (Hz)	2470.9705	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	8277.64	*Temperature (degree C)*	27.000		



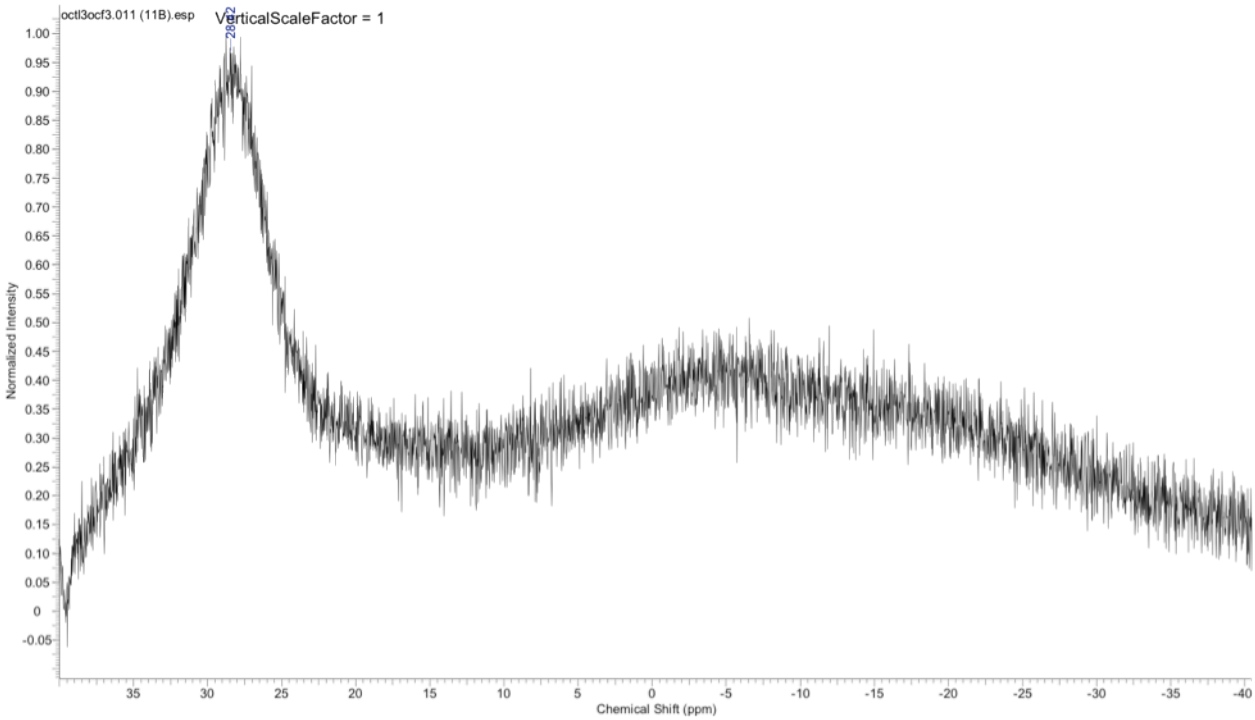
01.03.2011 17:41:57

Acquisition Time (sec)	1.3664	*Comment*	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			*Date*	17 Feb 2011 00:23:44
Date Stamp	17 Feb 2011 00:23:44			*File Name*	\\VBOXSVR\VBShare\Timo\octl3ocf3\12\fid		
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	1024	*Origin*	spect
Original Points Count	32768	*Owner*	nmr400	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	16384.00	*SW(cyclical) (Hz)*	23980.81	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	10016.2422
Spectrum Type	STANDARD	*Sweep Width (Hz)*	23980.08	*Temperature (degree C)*	27.000		



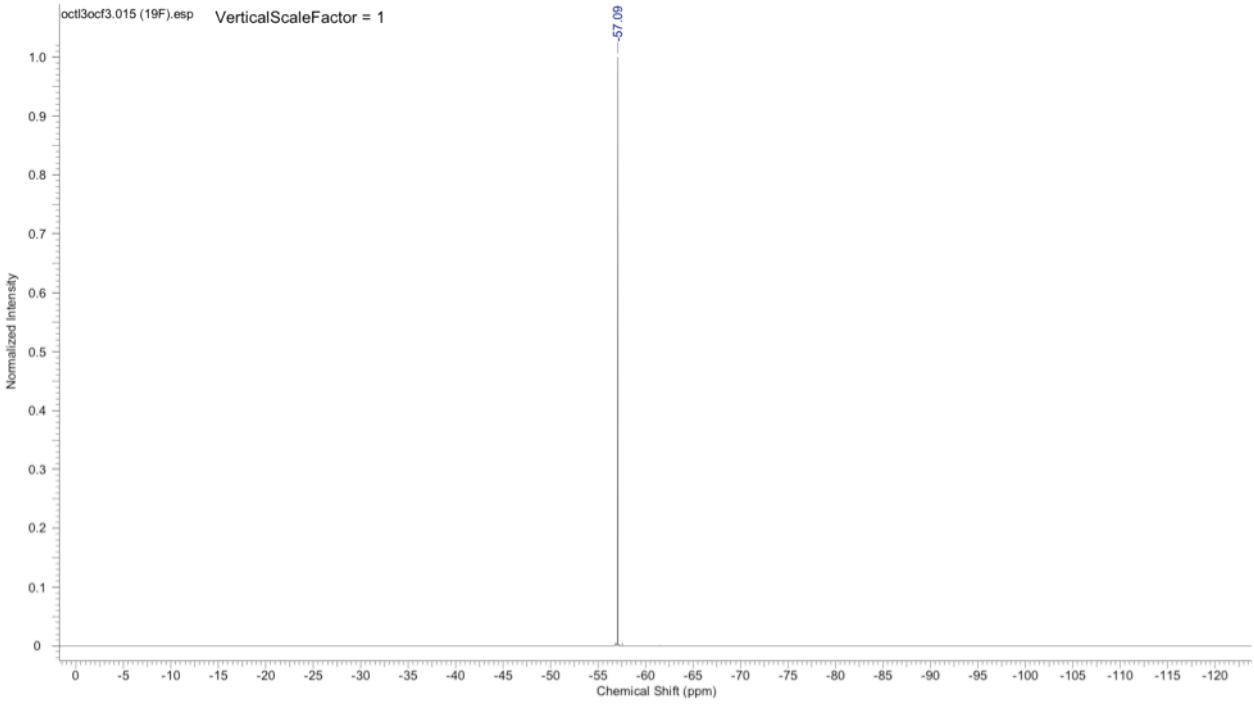
01.03.2011 17:43:39

Acquisition Time (sec)	0.3478	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	16 Feb 2011 23:38:56		
Date Stamp	16 Feb 2011 23:38:56			***File Name***	\\VBOXSVR\VBShare\Timo\octl3ocf3\11\fid			***Frequency (MHz)***	128.38
Nucleus	11B	***Number of Transients***	128	***Origin***	spect	***Original Points Count***	4026	***Owner***	nmr400
Points Count	4096	***Pulse Sequence***	zgpg	***Receiver Gain***	574.70	***SW(cyclical) (Hz)***	11574.07	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	-641.8885	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	11571.25	***Temperature (degree C)***	26.900		



01.03.2011 17:44:54

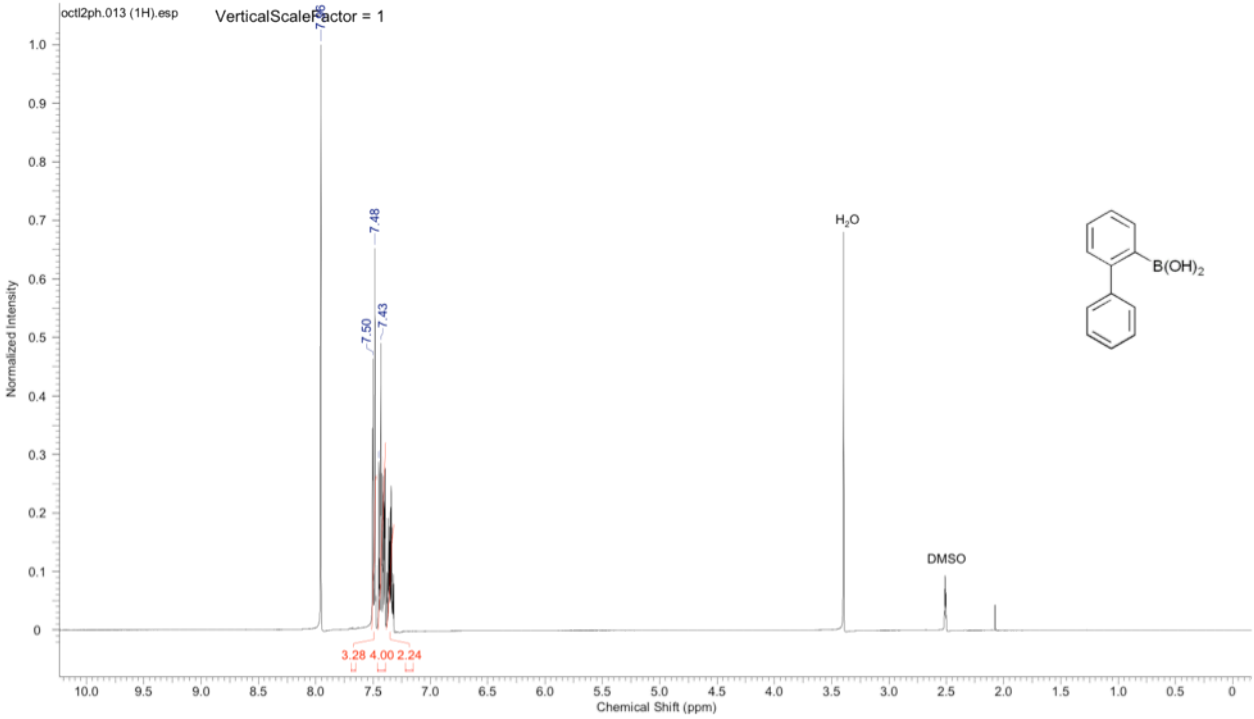
Acquisition Time (sec)	0.8710	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	17 Feb 2011 00:34:24		
Date Stamp	17 Feb 2011 00:34:24			***File Name***	\\VBOXSVR\VBShare\Timo\octl3ocf3\15\fid				
Frequency (MHz)	376.50	***Nucleus***	19F	***Number of Transients***	32	***Origin***	spect		
Original Points Count	65491	***Owner***	nmr400	***Points Count***	65536	***Pulse Sequence***	zgfhigqn30		
Receiver Gain	574.70	***SW(cyclical) (Hz)***	75187.97	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	-35919.2852		
Spectrum Type	STANDARD	***Sweep Width (Hz)***	75186.82	***Temperature (degree C)***	27.000				



Compound 8:

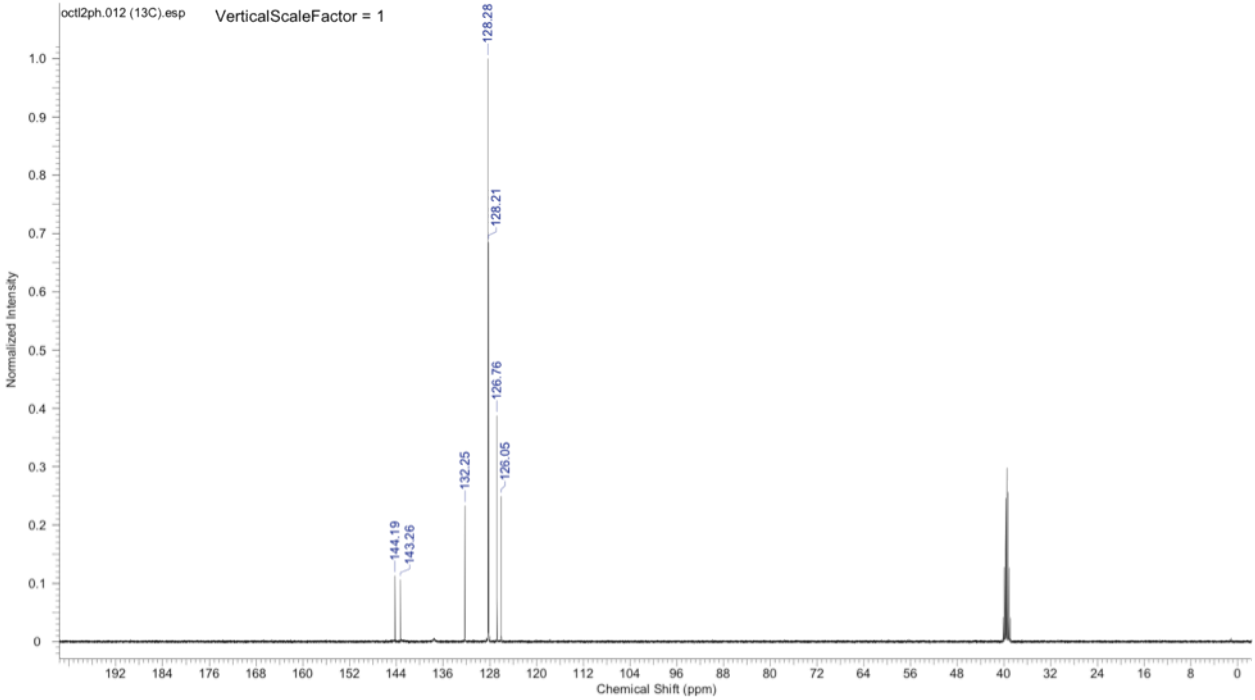
01.03.2011 17:46:23

Acquisition Time (sec)	3.9584	*Comment*	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			*Date*	17 Feb 2011 22:17:52		
Date Stamp	17 Feb 2011 22:17:52			*File Name*	\\VBOXSVR\VBShare\Timo\octl2ph\13\fid			*Frequency (MHz)*	400.13
Nucleus	1H	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	32768	*Owner*	nmr400
Points Count	32768	*Pulse Sequence*	zgig30	*Receiver Gain*	71.80	*SW(cyclical) (Hz)*	8278.15	*Solvent*	DMSO-d6
Spectrum Offset (Hz)	2470.9590	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	8277.89	*Temperature (degree C)*	27.300		



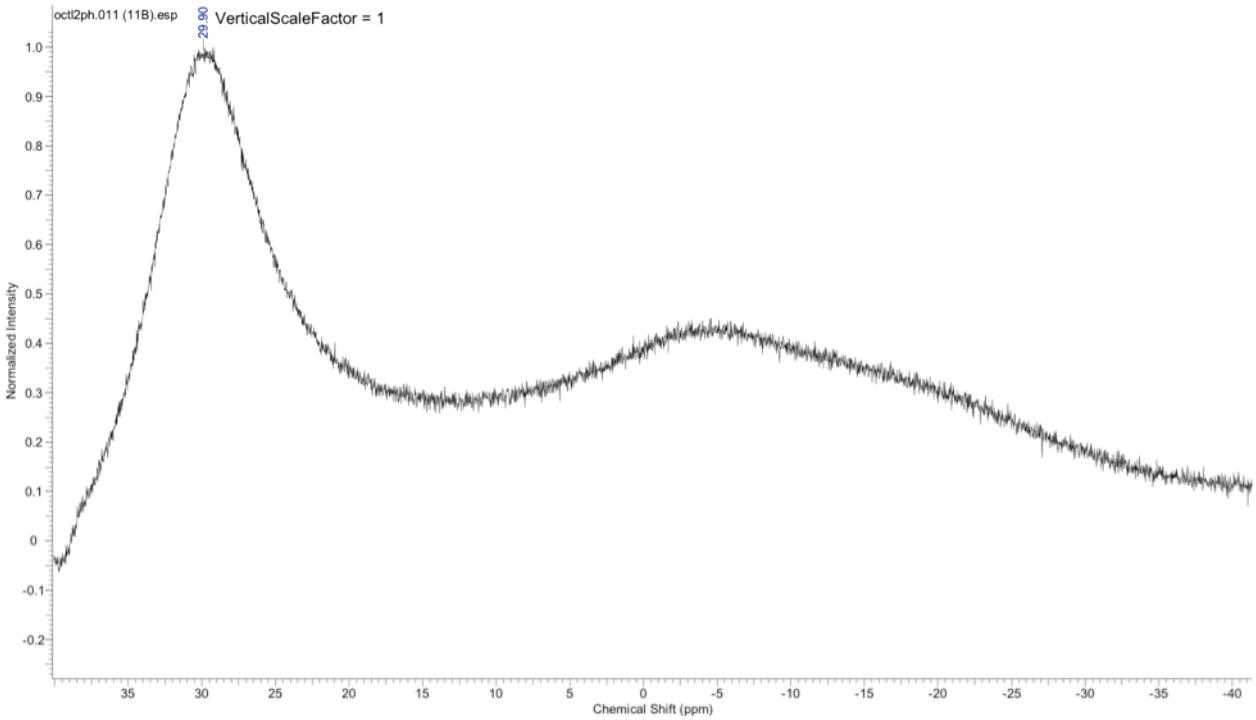
01.03.2011 17:49:01

Acquisition Time (sec)	1.3664	*Comment*	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			*Date*	17 Feb 2011 22:13:36
Date Stamp	17 Feb 2011 22:13:36			*File Name*	\\VBOXSVR\VBShare\Timo\octl2ph\12\fid		
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	1024	*Origin*	spect
Original Points Count	32768	*Owner*	nmr400	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	16384.00	*SW(cyclical) (Hz)*	23980.81	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	10014.6113
Spectrum Type	STANDARD	*Sweep Width (Hz)*	23980.08	*Temperature (degree C)*	27.000		



01.03.2011 17:50:03

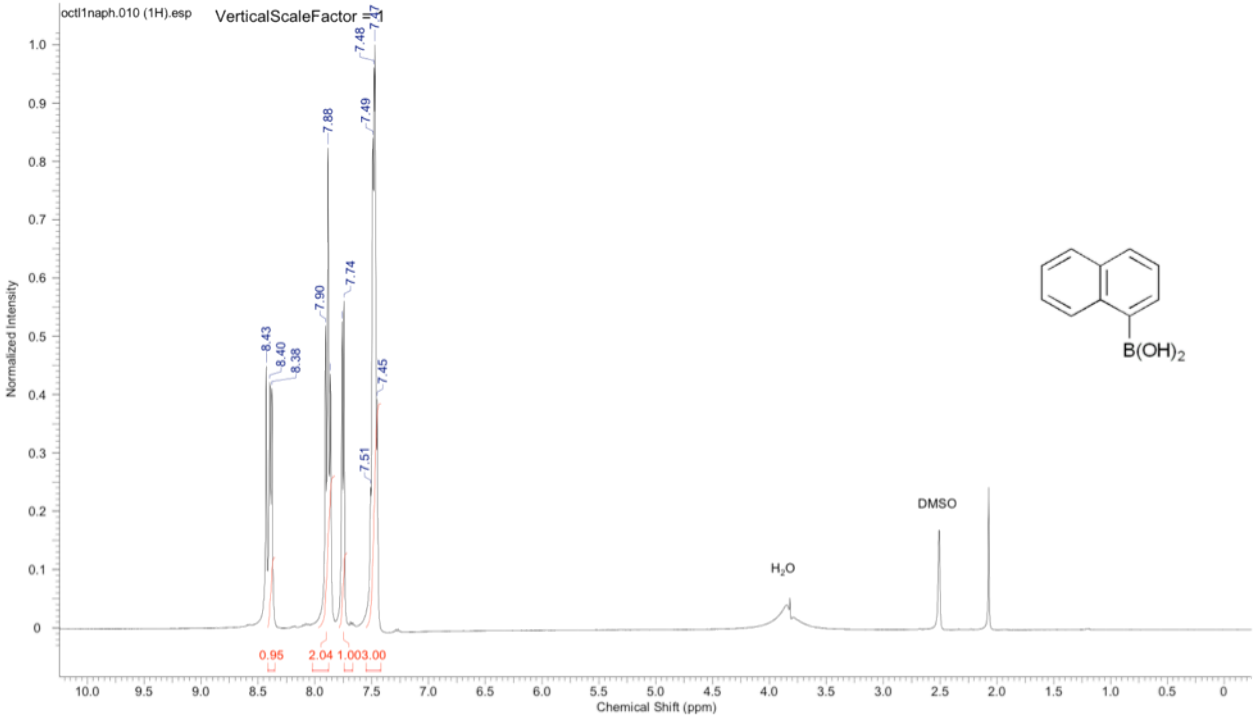
Acquisition Time (sec)	0.3478	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	17 Feb 2011 21:28:48		
Date Stamp	17 Feb 2011 21:28:48			***File Name***	\\VBOXSVR\VBShare\Timo\octl2ph\11\fid			***Frequency (MHz)***	128.38
Nucleus	11B	***Number of Transients***	128	***Origin***	spect	***Original Points Count***	4026	***Owner***	nmr400
Points Count	4096	***Pulse Sequence***	zgpg	***Receiver Gain***	574.70	***SW(cyclical) (Hz)***	11574.07	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	-641.8885	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	11571.25	***Temperature (degree C)***	27.100		



Compound 9:

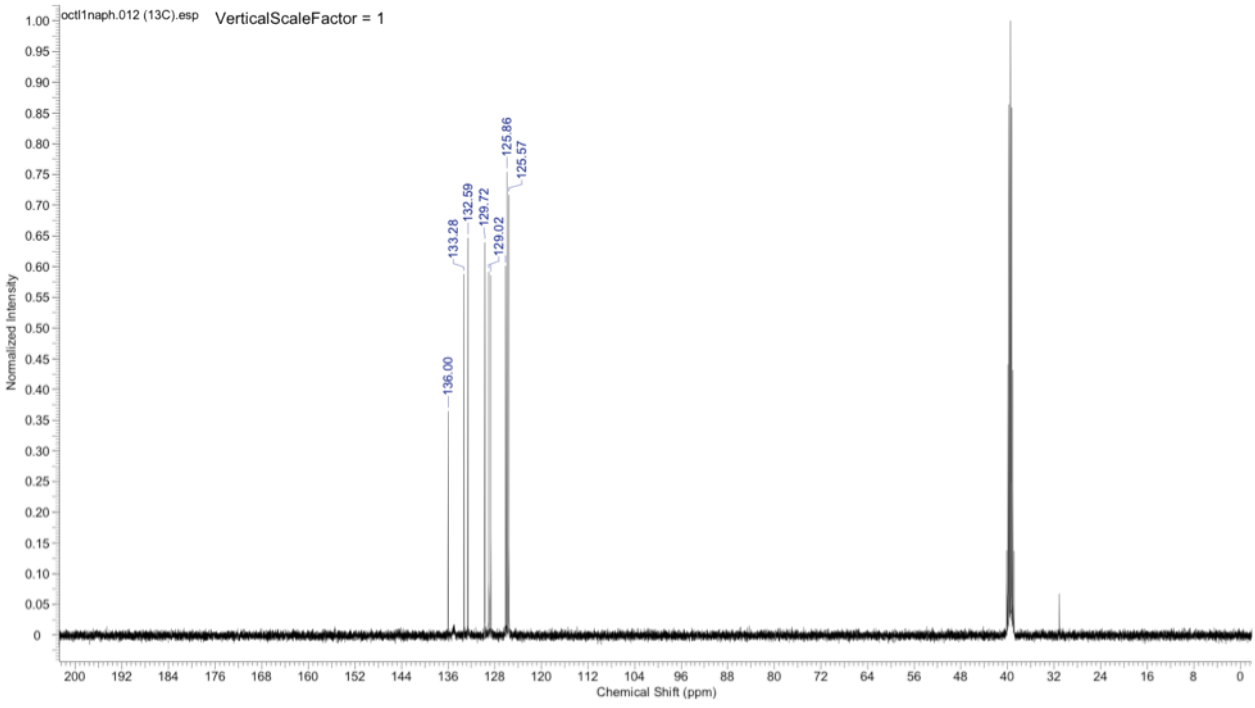
01.03.2011 17:51:29

Acquisition Time (sec)	1.9792	*Comment*	5 mm PABBO BB-1H/D Z-GRD Z863001/0017	*Date*	18 Feb 2011 16:32:16		
Date Stamp	18 Feb 2011 16:32:16			*File Name*	\\VBOXSVR\VBShare\Timo\octl1naph\10\fid	*Frequency (MHz)*	400.13
Nucleus	1H	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	16384	*Owner*	nmr400
Points Count	16384	*Pulse Sequence*	zgcppr	*Receiver Gain*	90.50	*SW(cyclical) (Hz)*	8278.15	*Solvent*	DMSO-d6
Spectrum Offset (Hz)	1528.0964	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	8277.64	*Temperature (degree C)*	27.000		



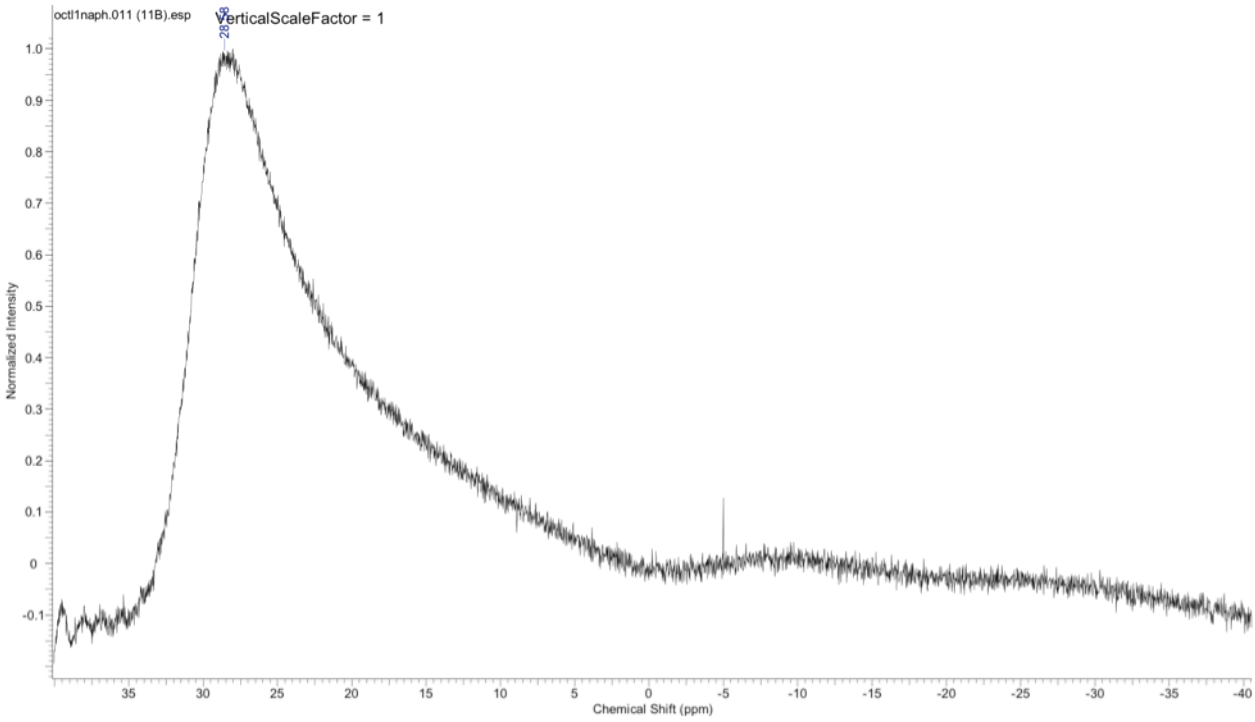
01.03.2011 17:53:56

Acquisition Time (sec)	1.3664	*Comment*	5 mm PABBO BB-1H/D Z-GRD Z863001/0017	*Date*	18 Feb 2011 17:21:20		
Date Stamp	18 Feb 2011 17:21:20			*File Name*	\\VBOXSVR\VBShare\Timo\octl1naph\12\fid		
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	1024	*Origin*	spect
Original Points Count	32768	*Owner*	nmr400	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	16384.00	*SW(cyclical) (Hz)*	23980.81	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	10061.6484
Spectrum Type	STANDARD	*Sweep Width (Hz)*	23980.08	*Temperature (degree C)*	27.000		



01.03.2011 17:54:59

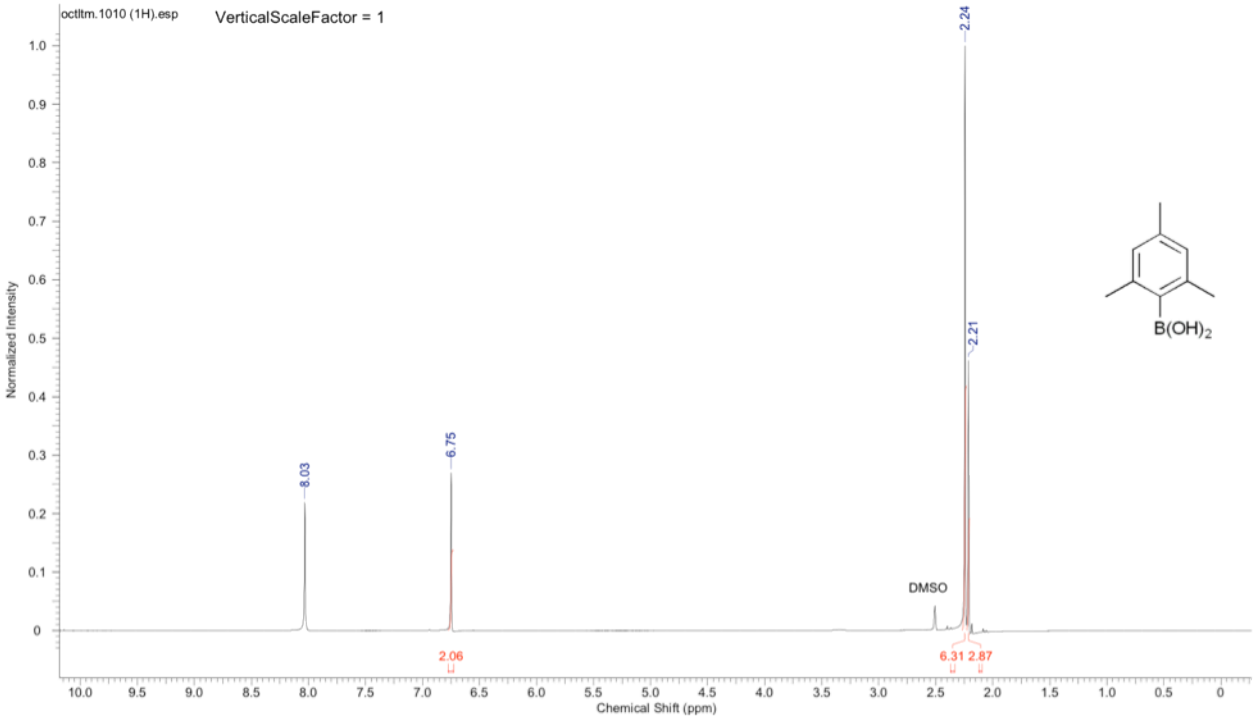
Acquisition Time (sec)	0.3478	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	18 Feb 2011 16:36:32		
Date Stamp	18 Feb 2011 16:36:32			***File Name***	\\VBOXSVR\VBShare\Timo\octl1naph\11\fid			***Frequency (MHz)***	128.38
Nucleus	11B	***Number of Transients***	128	***Origin***	spect	***Original Points Count***	4026	***Owner***	nmr400
Points Count	4096	***Pulse Sequence***	zgpg	***Receiver Gain***	574.70	***SW(cyclical) (Hz)***	11574.07	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	-641.8885	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	11571.25	***Temperature (degree C)***	27.100		



Compound 10:

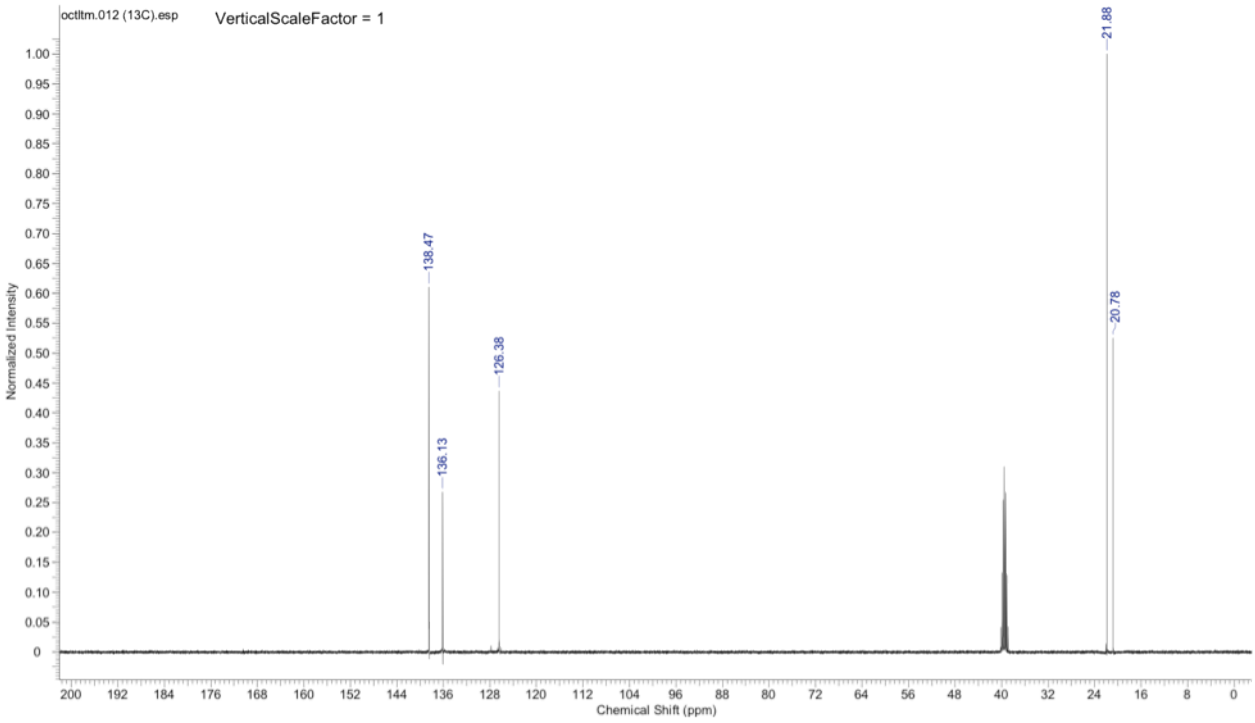
01.03.2011 17:56:12

Acquisition Time (sec)	1.9792	*Comment*	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			*Date*	17 Feb 2011 23:24:00		
Date Stamp	17 Feb 2011 23:24:00			*File Name*	\\VBOXSVR\VBShare\Timo\octltm\1010\fid			*Frequency (MHz)*	400.13
Nucleus	1H	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	16384	*Owner*	nmr400
Points Count	16384	*Pulse Sequence*	zg30	*Receiver Gain*	90.50	*SW(cyclical) (Hz)*	8278.15	*Solvent*	DMSO-d6
Spectrum Offset (Hz)	2470.9705	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	8277.64	*Temperature (degree C)*	27.000		



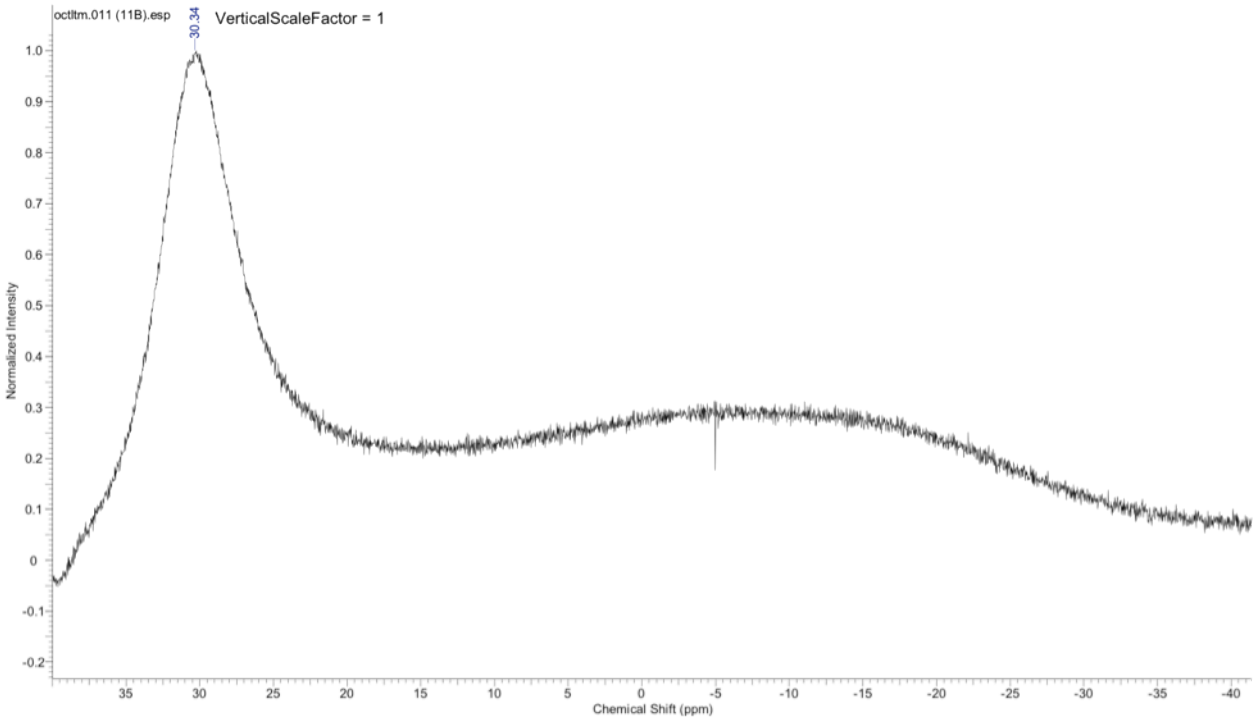
01.03.2011 17:57:59

Acquisition Time (sec)	1.3664	*Comment*	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			*Date*	18 Feb 2011 00:15:12		
Date Stamp	18 Feb 2011 00:15:12			*File Name*	\\VBOXSVR\VBShare\Timo\octltm\12\fid			*Frequency (MHz)*	100.61
Nucleus	13C	*Number of Transients*	1024	*Origin*	spect	*Original Points Count*	32768	*Owner*	nmr400
Points Count	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	16384.00	*SW(cyclical) (Hz)*	23980.81	*Solvent*	DMSO-d6
Spectrum Offset (Hz)	10013.0830	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	23980.08	*Temperature (degree C)*	27.000		



01.03.2011 17:59:16

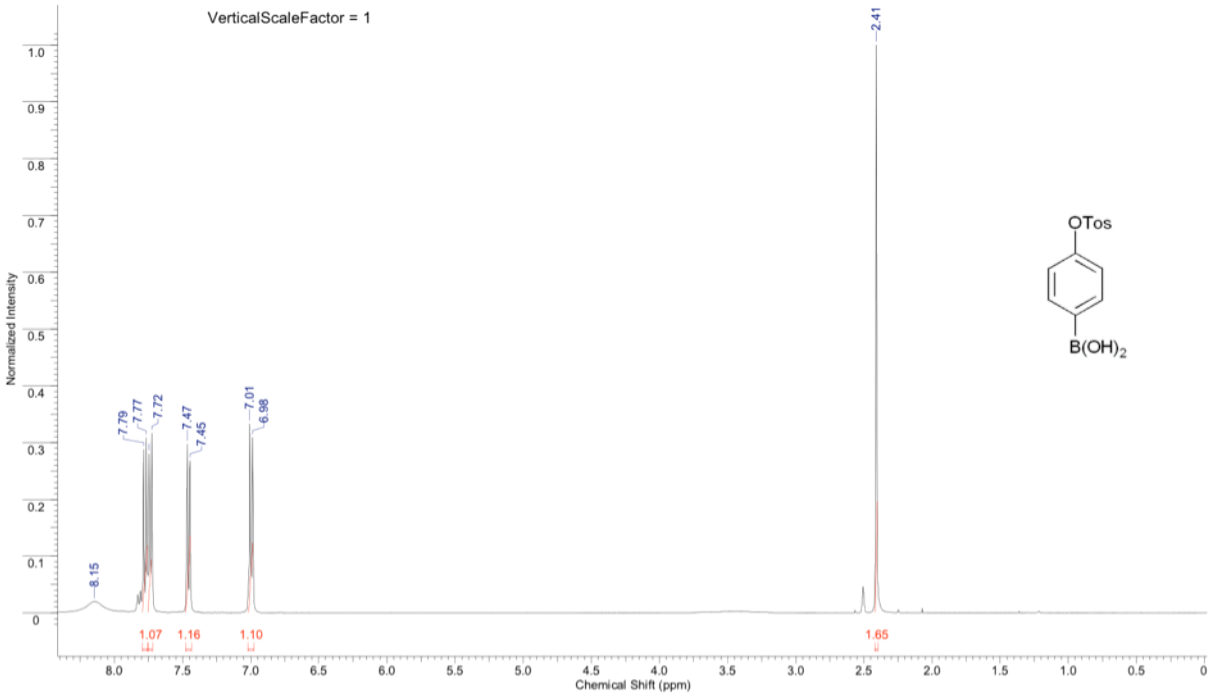
Acquisition Time (sec)	0.3478	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	17 Feb 2011 23:30:24		
Date Stamp	17 Feb 2011 23:30:24			***File Name***	\\VBOXSVR\VBShare\Timo\octltm\11\fid			***Frequency (MHz)***	128.38
Nucleus	11B	***Number of Transients***	128	***Origin***	spect	***Original Points Count***	4026	***Owner***	nmr400
Points Count	4096	***Pulse Sequence***	zgpg	***Receiver Gain***	574.70	***SW(cyclical) (Hz)***	11574.07	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	-641.8885	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	11571.25	***Temperature (degree C)***	27.100		



Compound 11:

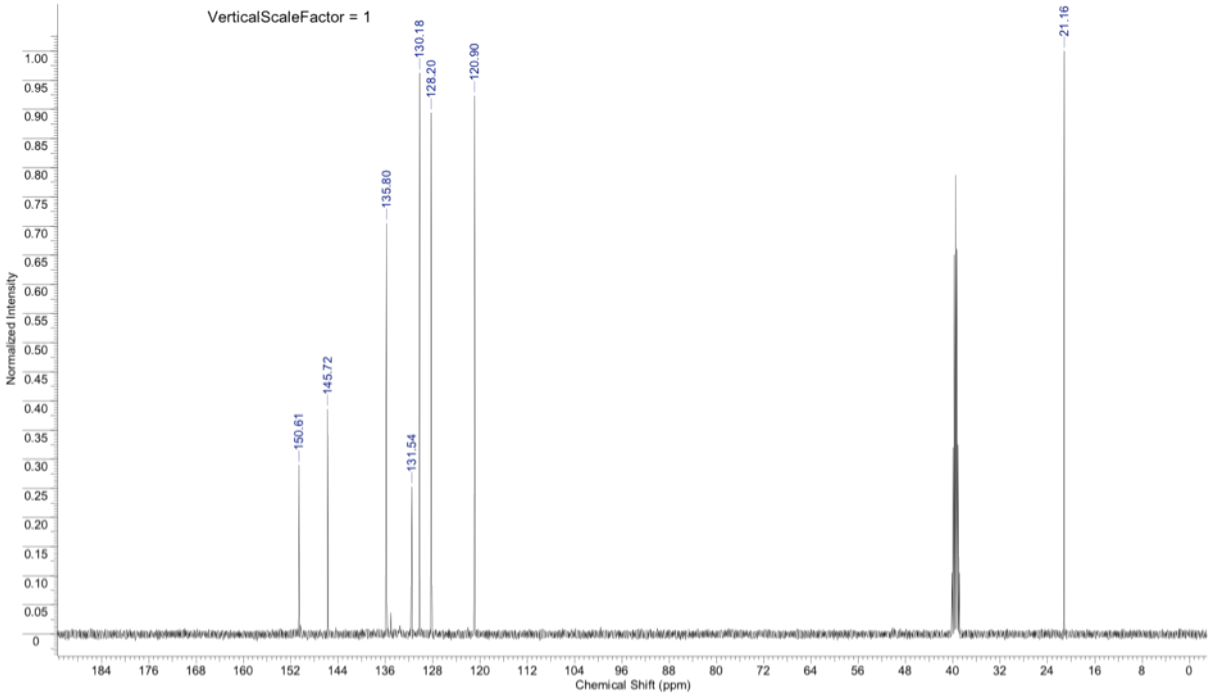
09.05.2011 11:47

Acquisition Time (sec)	3.9585	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	28 Apr 2011 16:23:28
File Name	\\VBOXSVR\vbshare\ECPM Strasbourg\Boronic acids - Strasbourg\octl4otos\octl4otos_010000fid					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768
Owner	nmr400	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	71.80
SW(cyclical) (Hz)	8278.15	***Solvent***	DMSO-D6	***Spectrum Offset (Hz)***	2471.0076	***Sweep Width (Hz)***	8277.89
Temperature (degree C)	27.000						



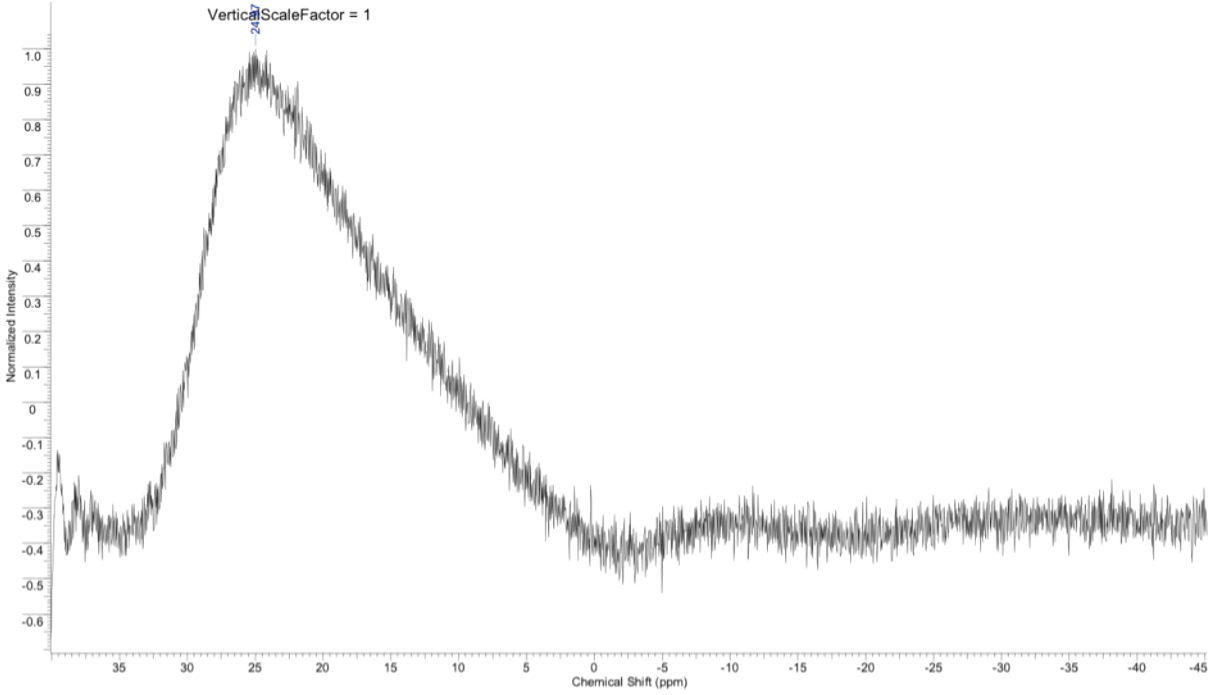
09.05.2011 11:49

Acquisition Time (sec)	1.3665	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	28 Apr 2011 17:18:56
File Name	\\VBOXSVR\vbshare\ECPM Strasbourg\Boronic acids - Strasbourg\octl4otos\octl4otos_014000fid					***Frequency (MHz)***	100.62
Nucleus	13C	***Number of Transients***	1024	***Origin***	spect	***Original Points Count***	32768
Owner	nmr400	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	16384.00
SW(cyclical) (Hz)	23980.81	***Solvent***	DMSO-D6	***Spectrum Offset (Hz)***	10015.1523	***Sweep Width (Hz)***	23980.08
Temperature (degree C)	27.000						



09.05.2011 11:50

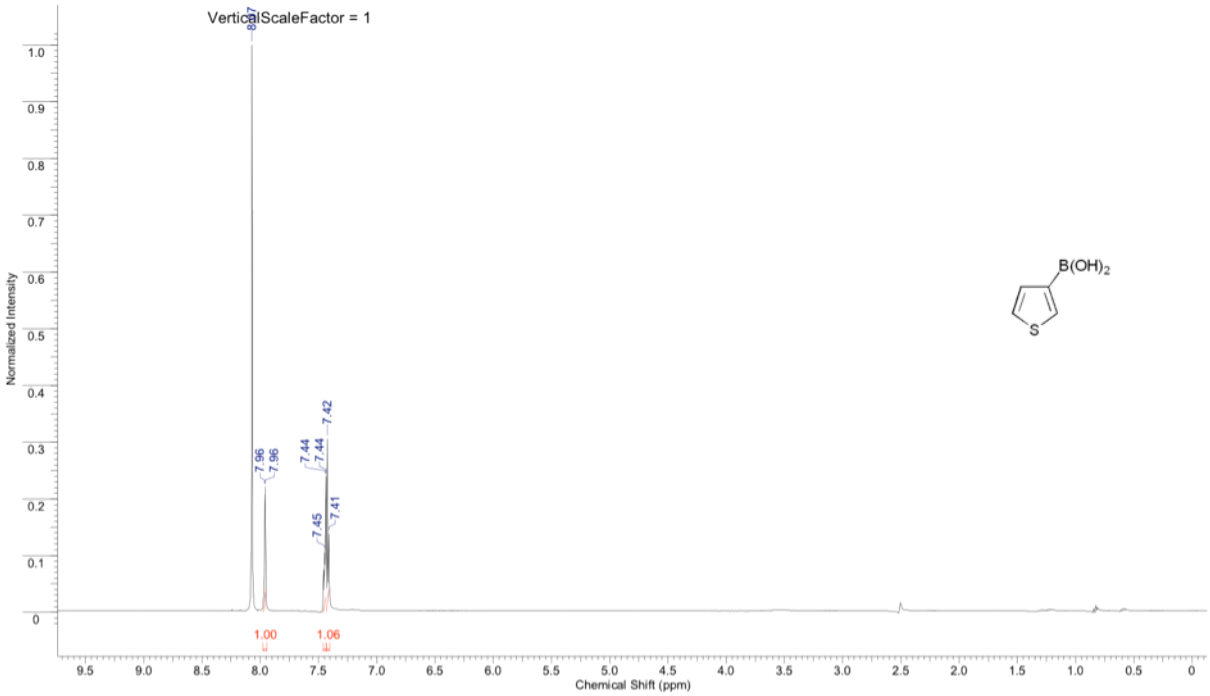
Acquisition Time (sec)	0.3479	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	28 Apr 2011 16:27:44
File Name	\\VBOXSVR\vbshare\ECPM Strasbourg\Boronic acids - Strasbourg\octl4otos\octl4otos_011000fid					***Frequency (MHz)***	128.38
Nucleus	11B	***Number of Transients***	128	***Origin***	spect	***Original Points Count***	4026
Owner	nmr400	***Points Count***	4096	***Pulse Sequence***	zgpg	***Receiver Gain***	574.70
SW(cyclical) (Hz)	11574.07	***Solvent***	DMSO-D6	***Spectrum Offset (Hz)***	-641.9142	***Sweep Width (Hz)***	11571.25
Temperature (degree C)	27.100						



Compound 12:

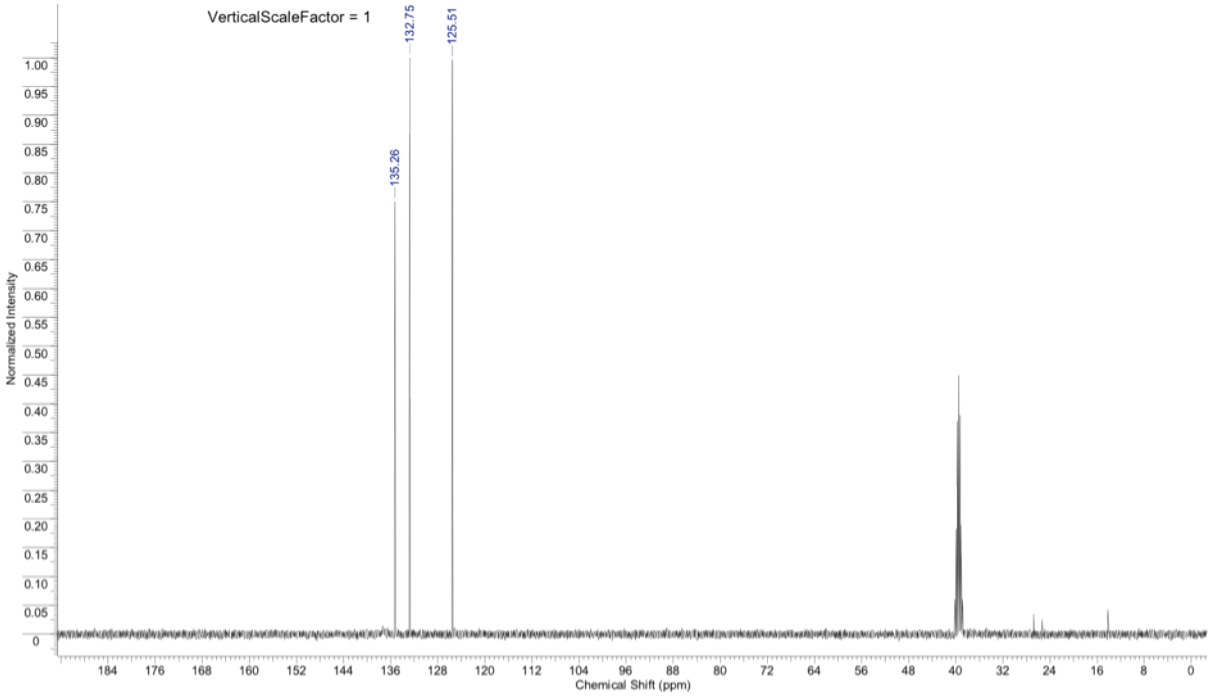
09.05.2011 11:52

Acquisition Time (sec)	3.9585	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	19 Apr 2011 10:05:52
File Name	\\VBOXSVR\vbshare\ECPM Strasbourg\Boronic acids - Strasbourg\octlth3\octlth3_010000fid					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768
Owner	nmr400	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	35.90
SW(cyclical) (Hz)	8278.15	***Solvent***	DMSO-D6	***Spectrum Offset (Hz)***	2471.0076	***Sweep Width (Hz)***	8277.89
Temperature (degree C)	27.000						



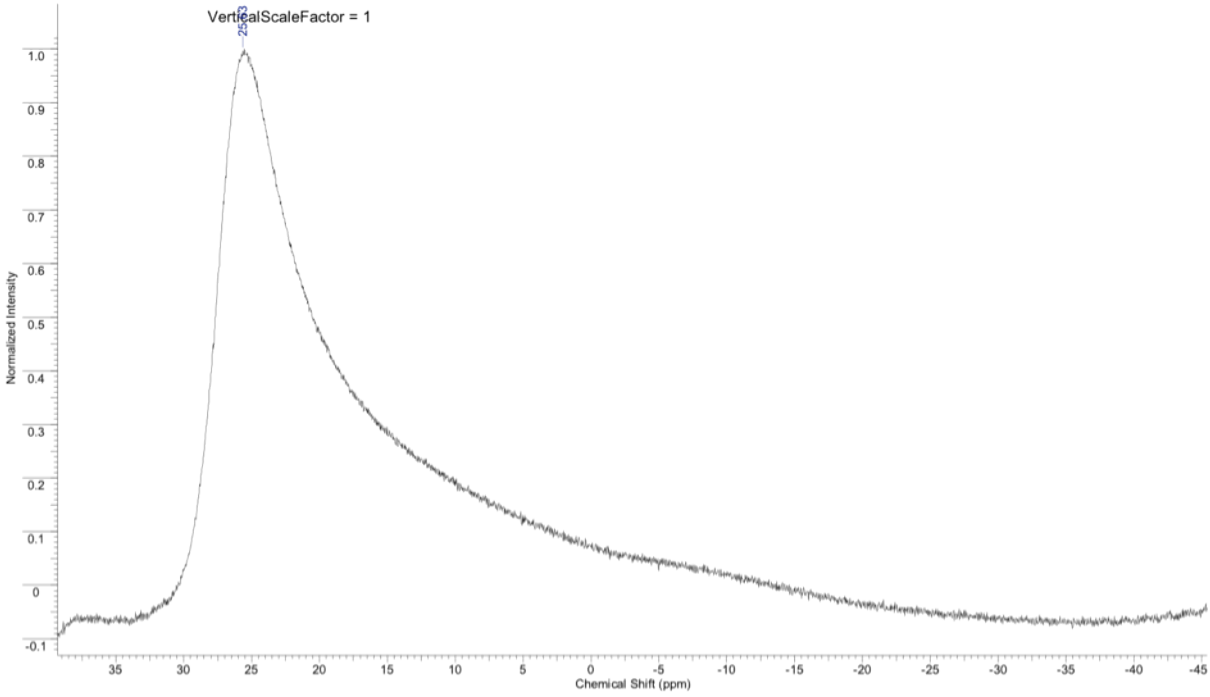
09.05.2011 11:56

Acquisition Time (sec)	1.3665	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	19 Apr 2011 10:31:28
File Name	\\VBOXSVR\vbshare\ECPM Strasbourg\Boronic acids - Strasbourg\octlth3\octlth3_014000fid					***Frequency (MHz)***	100.62
Nucleus	13C	***Number of Transients***	256	***Origin***	spect	***Original Points Count***	32768
Owner	nmr400	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	16384.00
SW(cyclical) (Hz)	23980.81	***Solvent***	DMSO-D6	***Spectrum Offset (Hz)***	10048.0771	***Sweep Width (Hz)***	23980.08
Temperature (degree C)	27.000						



09.05.2011 11:58

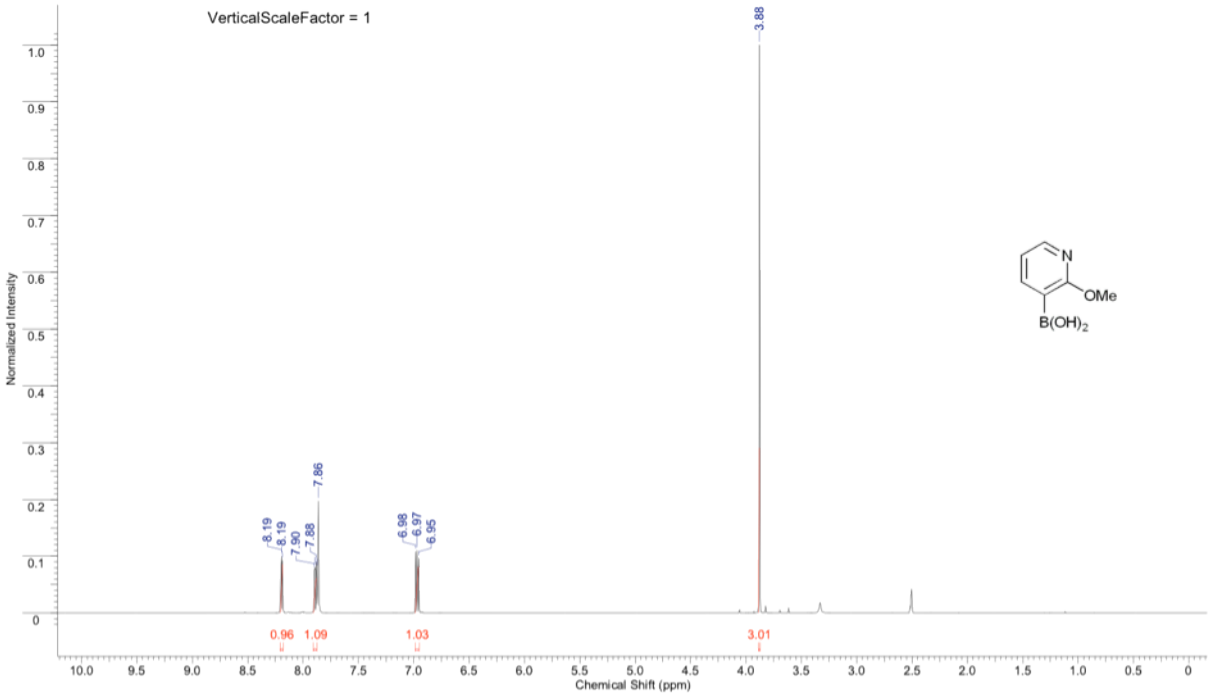
Acquisition Time (sec)	0.3488	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	19 Apr 2011 10:14:24
File Name	\\VBOXSVR\vbshare\ECPM Strasbourg\Boronic acids - Strasbourg\octlth3\octlth3_012000fid					***Frequency (MHz)***	128.38
Nucleus	11B	***Number of Transients***	128	***Origin***	spect	***Original Points Count***	4036
Owner	nmr400	***Points Count***	4096	***Pulse Sequence***	zg	***Receiver Gain***	362.00
SW(cyclical) (Hz)	11574.07	***Solvent***	DMSO-D6	***Spectrum Offset (Hz)***	-641.9142	***Sweep Width (Hz)***	11571.25
Temperature (degree C)	27.000						



Compound 13:

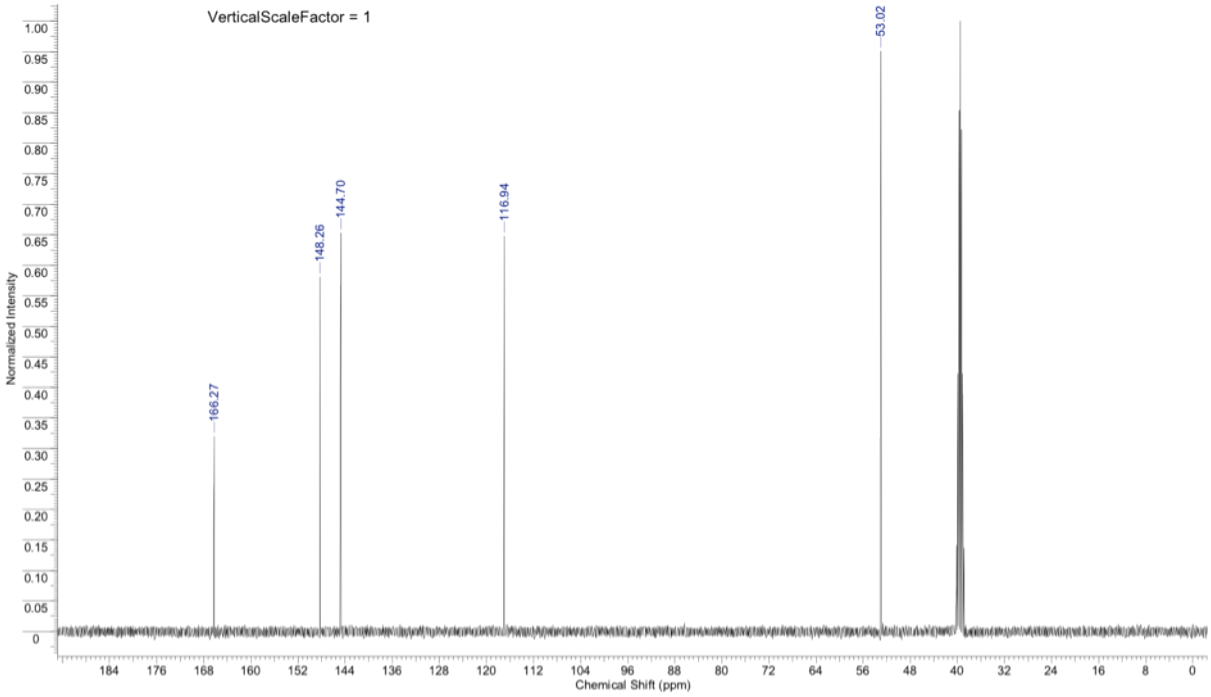
09.05.2011 11:59

Acquisition Time (sec)	3.9585	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	28 Apr 2011 17:27:28
File Name	\\VBOXSVR\vbshare\ECPM Strasbourg\Boronic acids - Strasbourg\octl2ome3py\octl2ome3py_010000fid					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768
Owner	nmr400	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	256.00
SW(cyclical) (Hz)	8278.15	***Solvent***	DMSO-D6	***Spectrum Offset (Hz)***	2471.0076	***Sweep Width (Hz)***	8277.89
Temperature (degree C)	27.000						



09.05.2011 12:00

Acquisition Time (sec)	1.3665	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	28 Apr 2011 18:22:56
File Name	\\VBOXSVR\vbshare\ECPM Strasbourg\Boronic acids - Strasbourg\octl2ome3py\octl2ome3py_014000fid					***Frequency (MHz)***	100.62
Nucleus	13C	***Number of Transients***	1024	***Origin***	spect	***Original Points Count***	32768
Owner	nmr400	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	16384.00
SW(cyclical) (Hz)	23980.81	***Solvent***	DMSO-D6	***Spectrum Offset (Hz)***	10012.8271	***Sweep Width (Hz)***	23980.08
Temperature (degree C)	27.000						



09.05.2011 12:01

Acquisition Time (sec)	0.3488	***Comment***	5 mm PABBO BB-1H/D Z-GRD Z863001/0017			***Date***	28 Apr 2011 17:33:52
File Name	\\VBOXSVR\vbshare\ECPM Strasbourg\Boronic acids - Strasbourg\octl2ome3py\octl2ome3py_012000fid					***Frequency (MHz)***	128.38
Nucleus	11B	***Number of Transients***	128	***Origin***	spect	***Original Points Count***	4036
Owner	nmr400	***Points Count***	4096	***Pulse Sequence***	zg	***Receiver Gain***	574.70
SW(cyclical) (Hz)	11574.07	***Solvent***	DMSO-D6	***Spectrum Offset (Hz)***	-641.9142	***Sweep Width (Hz)***	11571.25
Temperature (degree C)	27.000