Supplementary Information

Controlling chlorination versus cyclosulfonation of cis-diols using ionic liquid solvents

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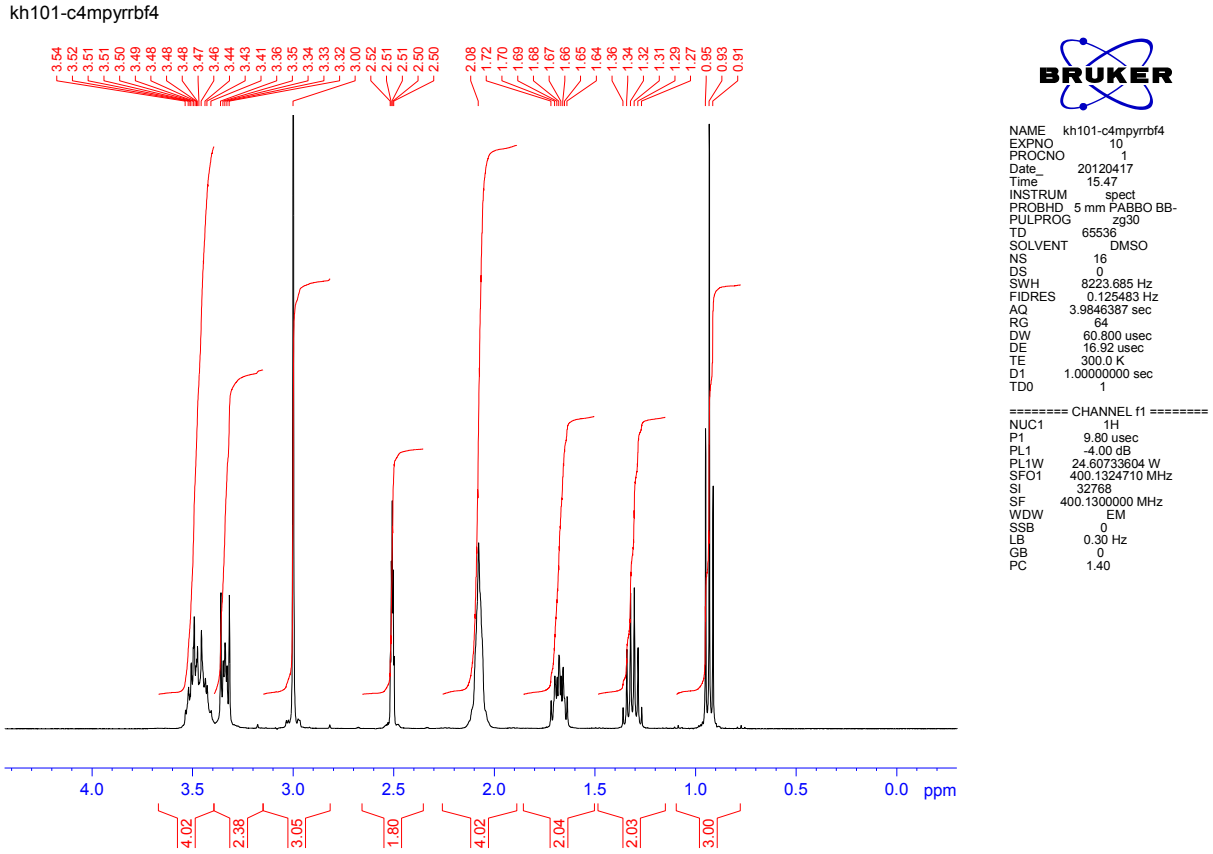
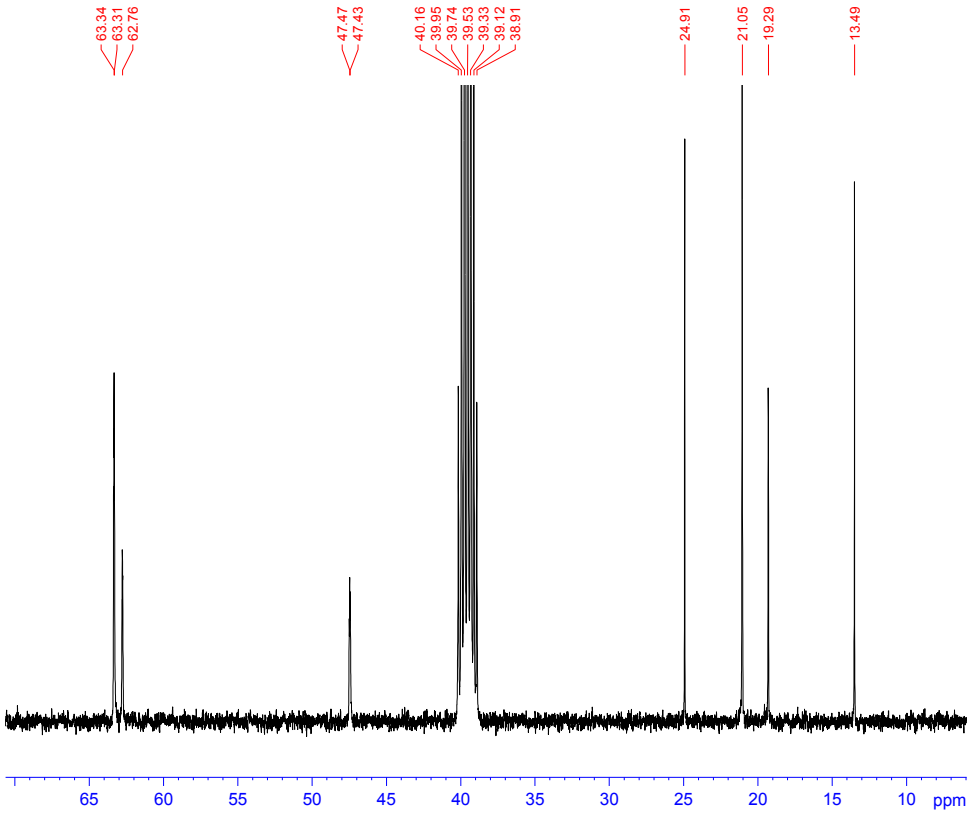
Figure S1 ^{1}H [C_4mpyrr][BF_4] ionic liquid

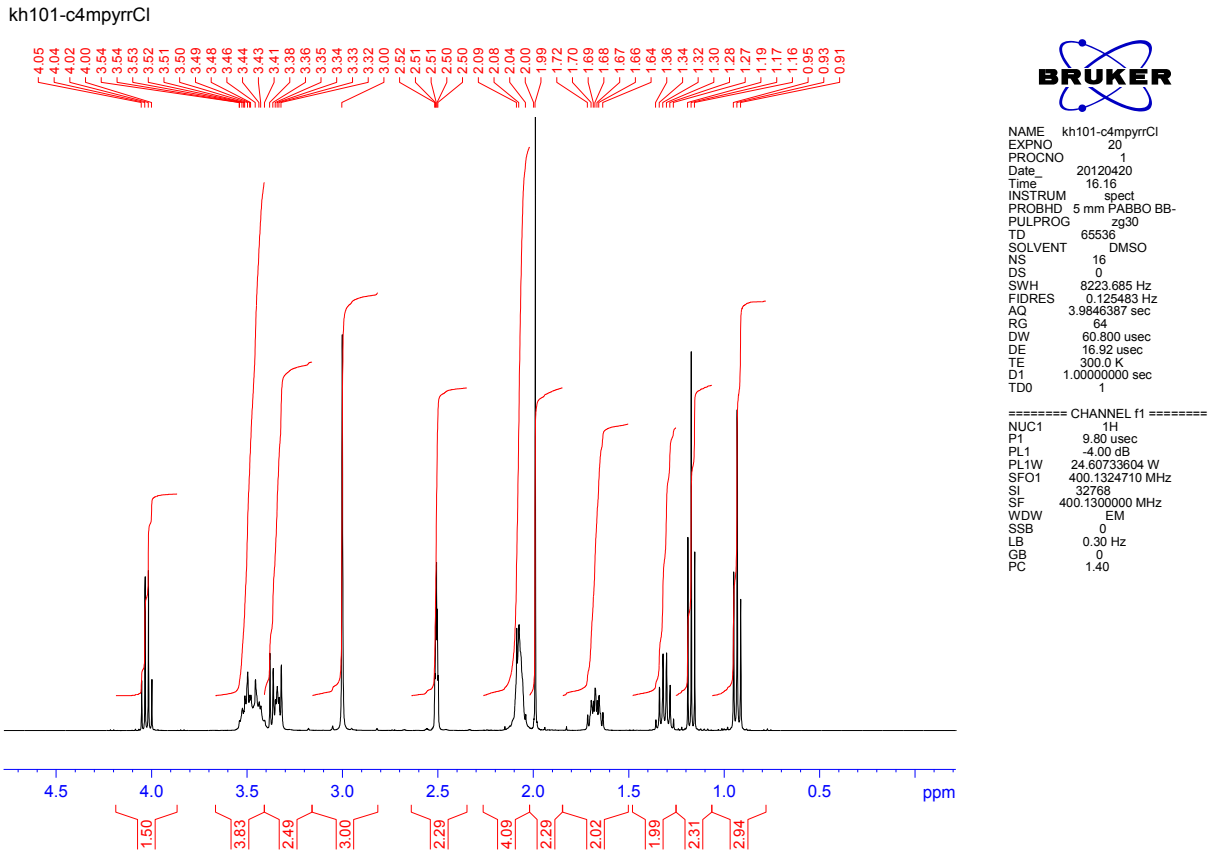


S2 ^{13}C [C_4mpyrr][BF_4] ionic liquid

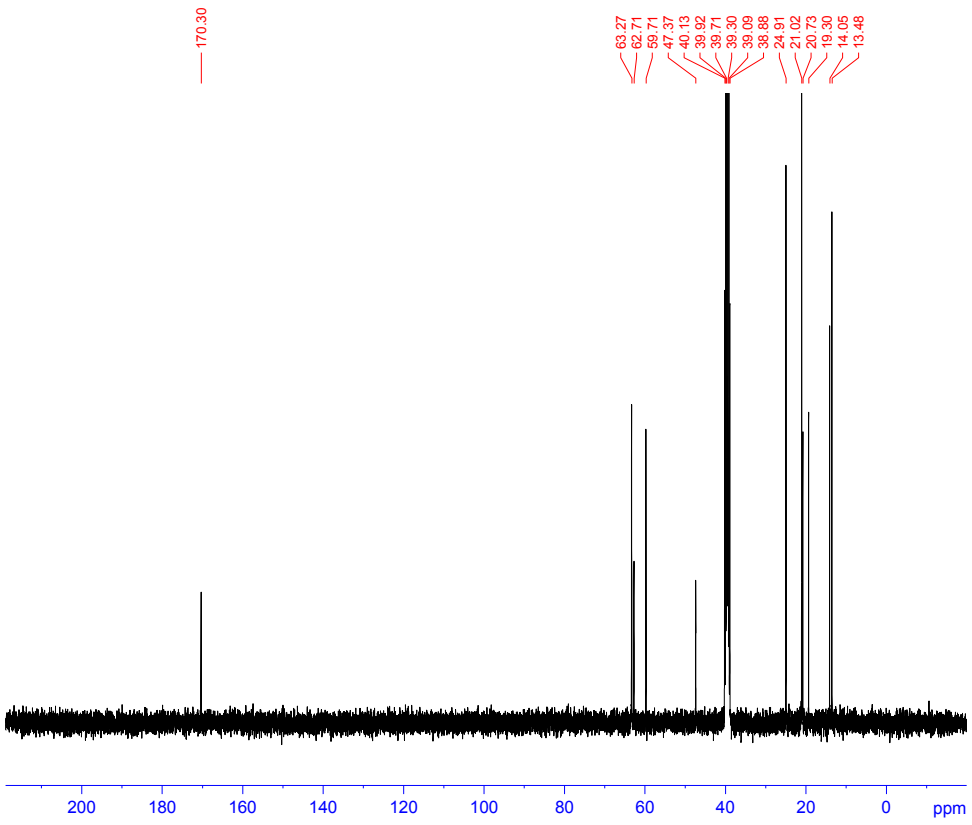



```
NAME     kh101-c4mpyrrbf4
EXPNO            11
PROCNO            1
Date_         20120417
Time              19.35
INSTRUM           spect
PROBHD    5 mm PABBO BB-
PULPROG         zgpg30
TD              65536
SOLVENT           DMSO
NS                512
DS                  4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                2050
DW              20.800 usec
DE              10.04 usec
TE              300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                 1

======== CHANNEL f1 ========
NUC1              13C
P1              7.80 usec
PL1             -3.60 dB
PL1W         82.86334991 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2              1H
PCPD2           80.00 usec
PL2             -4.00 dB
PL12            14.24 dB
PL13            14.24 dB
PL2W         24.60733604 W
PL12W         0.36903250 W
PL13W         0.36903250 W
SFO2        400.1316005 MHz
SI              65536
SF          100.6128193 MHz
WDW               EM
SSB               0
LB              1.00 Hz
GB                0
PC              1.40
```

S3 ^{1}H [C_4mpyrr][Cl] ionic liquid



S4 ^{13}C [C_4mpyrr][Cl] ionic liquid



BRUKER

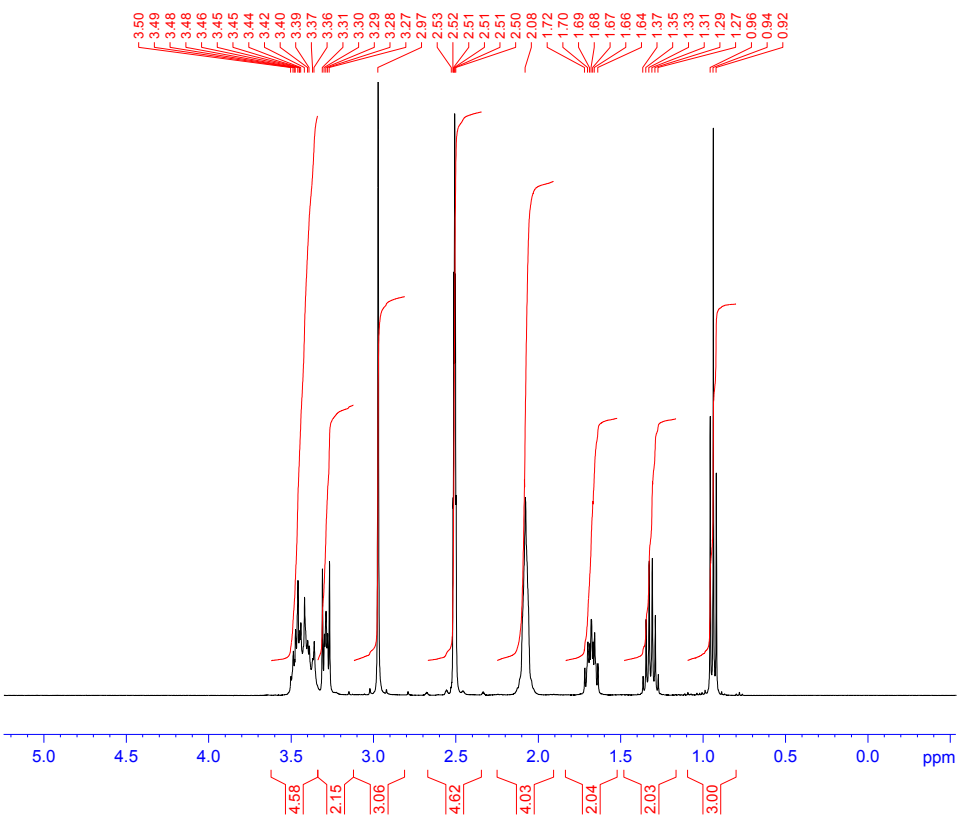
NAME kh101-c4mpyrrCl
EXPNO 21
PROCNO 1
Date_ 20120421
Time 11.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 10.04 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.80 usec
PL1 -3.60 dB
PL1W 82.86334991 W
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.24 dB
PL13 14.24 dB
PL2W 24.60733604 W
PL12W 0.36903250 W
PL13W 0.36903250 W
SFO2 400.1316005 MHz
SI 65536
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S5 ^{1}H [C_4mpyrr][FAP] ionic liquid

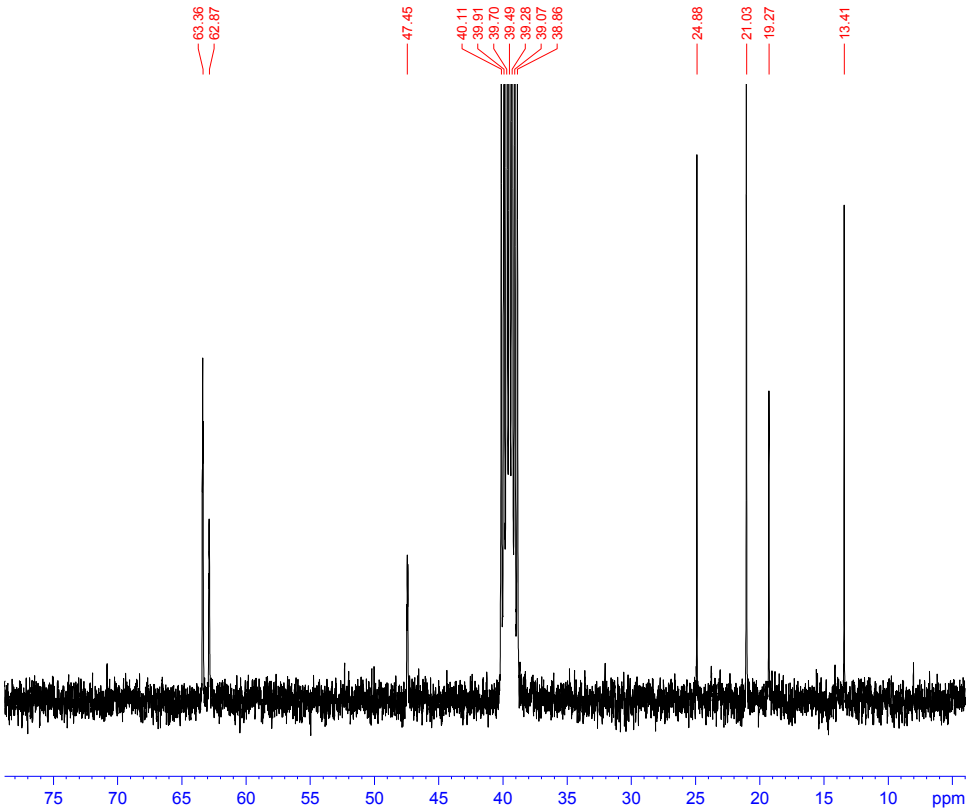
KH101-c4mpyrrFAP



NAME kh101-c4mpyrrFAP
EXPNO 10
PROCNO 1
Date_ 20120416
Time 19.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 16.92 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.80 usec
PL1 -4.00 dB
PL1W 24.60733604 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

S6 ^{13}C [C_4mpyrr][FAP] ionic liquid



BRUKER

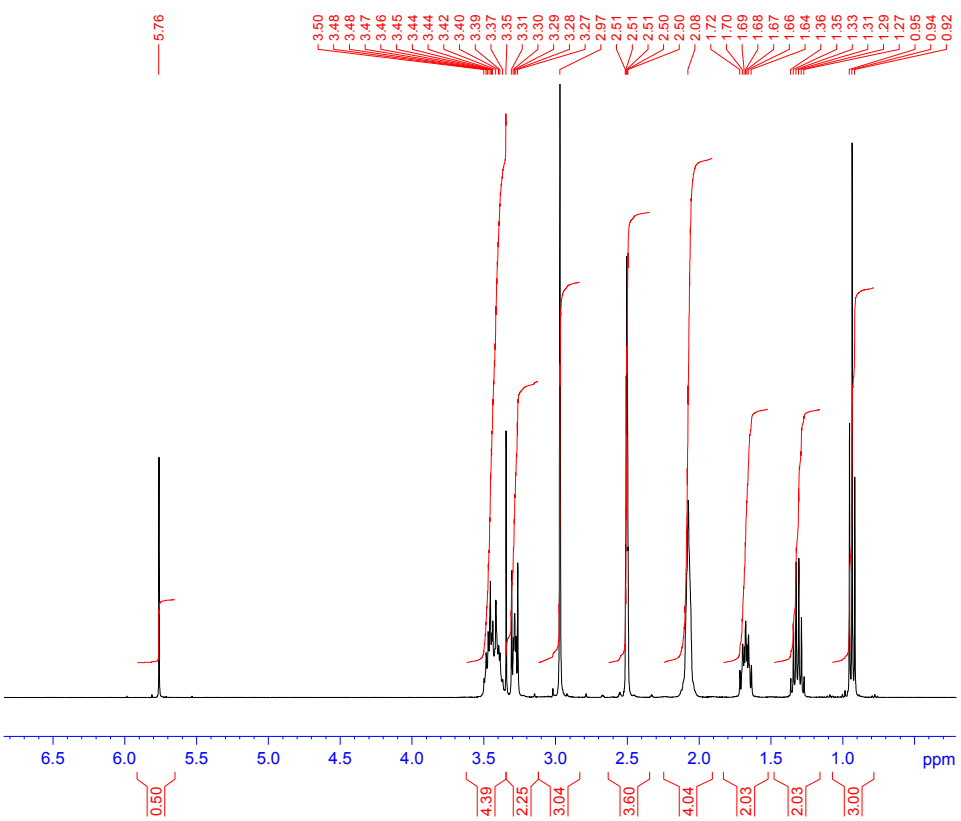
NAME kh101-c4mpyrrFAP
EXPNO 11
PROCNO 1
Date_ 20120416
Time 20.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 10.04 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.80 usec
PL1 -3.60 dB
PL1W 82.86334991 W
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.24 dB
PL13 14.24 dB
PL2W 24.60733604 W
PL12W 0.36903250 W
PL13W 0.36903250 W
SFO2 400.1316005 MHz
SI 65536
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S7 ^{1}H [C_4mpyrr][NTf_2] ionic liquid

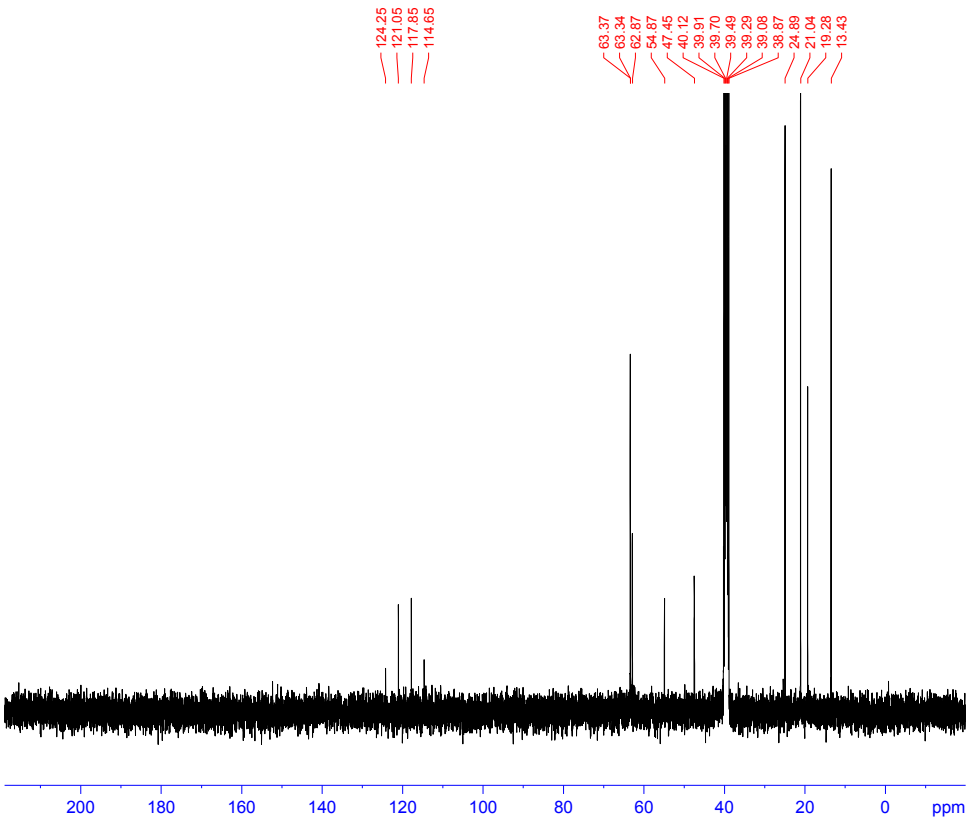
kh101-c4mpyrrntf2



NAME kh101-C4mpyrrntf2
EXPNO 20
PROCNO 1
Date_ 20120416
Time 15.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 114
DW 60.800 usec
DE 16.92 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.80 usec
PL1 -4.00 dB
PL1W 24.60733604 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

S8 ^{13}C [C_4mpyrr][NTf_2] ionic liquid



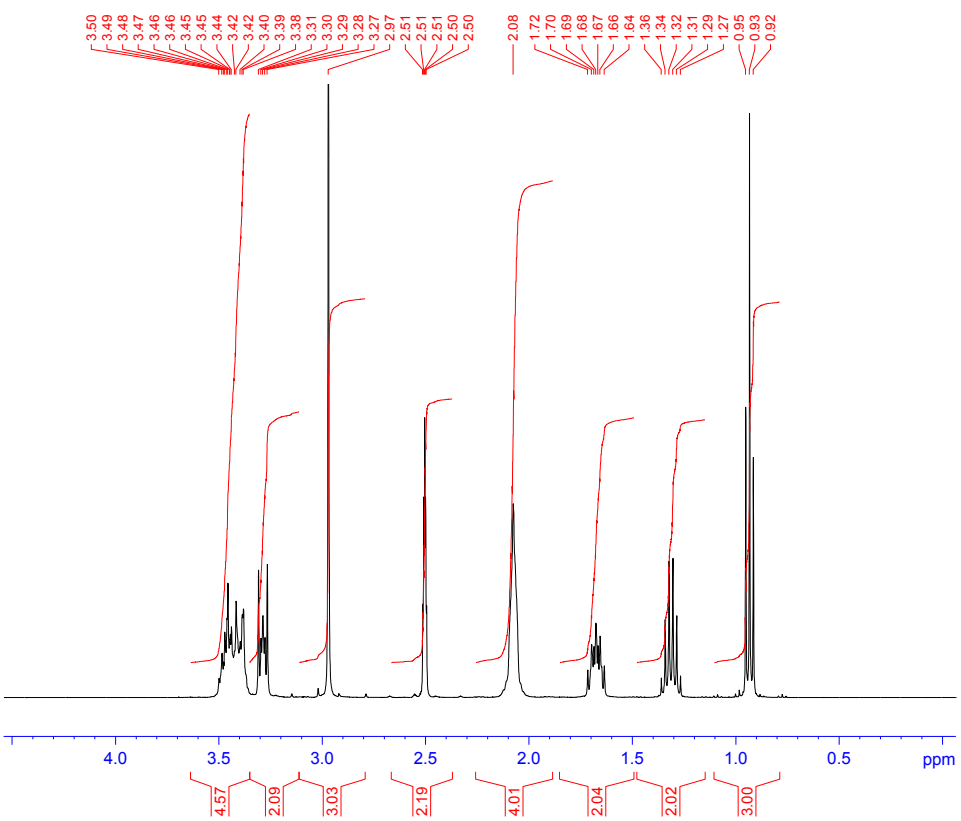
NAME kh101-C4mpyrrntf2
EXPNO 21
PROCNO 1
Date_ 20120416
Time 21.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 10.04 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.80 usec
PL1 -3.60 dB
PL1W 82.86334991 W
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.24 dB
PL13 14.24 dB
PL2W 24.60733604 W
PL12W 0.36903250 W
PL13W 0.36903250 W
SFO2 400.1316005 MHz
SI 65536
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S9 ^{1}H [C_4mpyrr][OTf] ionic liquid

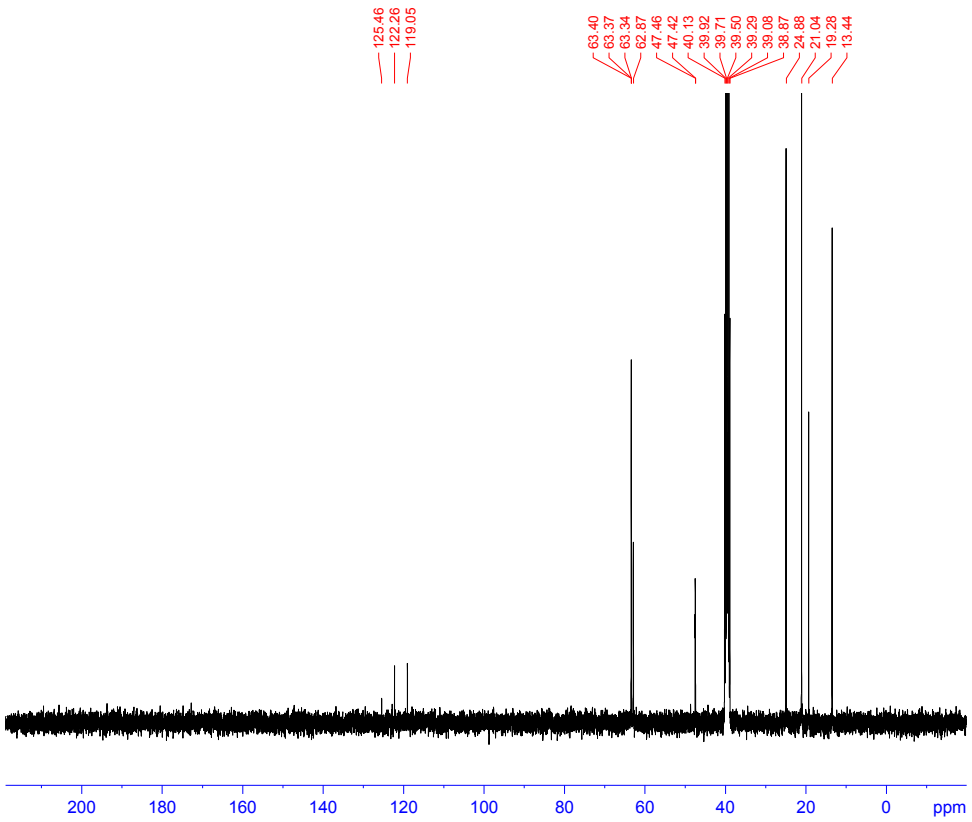
kh101-c4mpyrrOTf



NAME kh101-c4mpyrrOTf
EXPNO 10
PROCNO 1
Date_ 20120416
Time 18.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 80.6
DW 60.800 usec
DE 16.92 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.80 usec
PL1 -4.00 dB
PL1W 24.60733604 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

S10 $^{13}C[C_4mpyrr][OTf]$ ionic liquid



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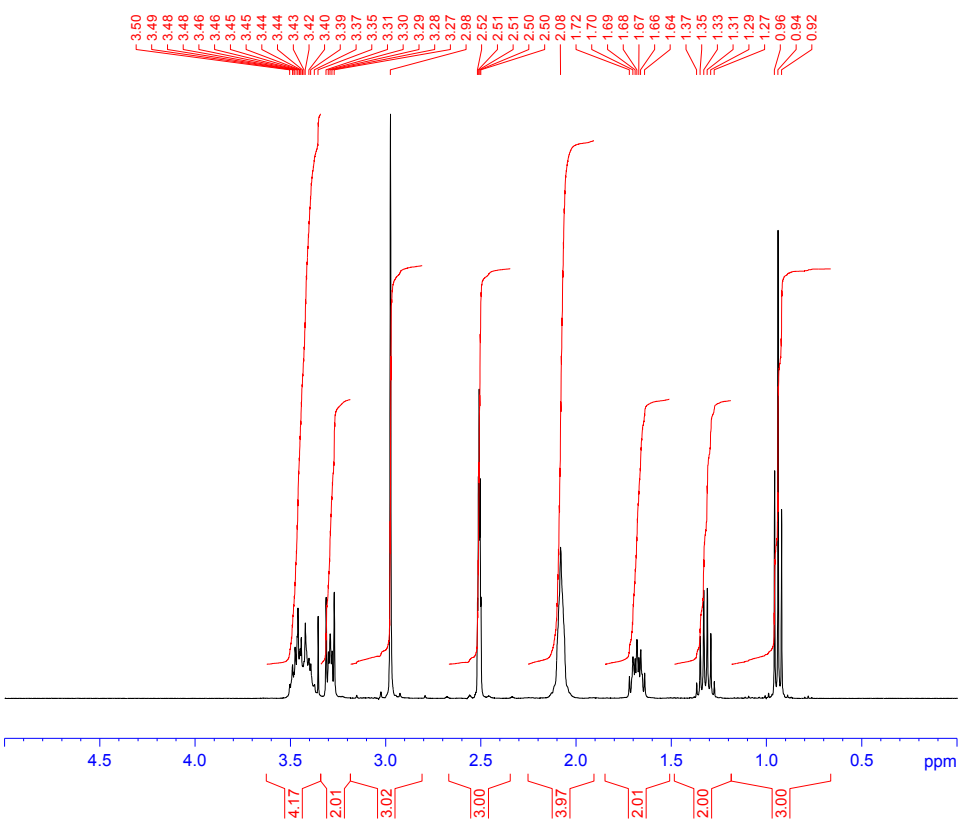
NAME kh101-c4mpyrrOTf
EXPNO 11
PROCNO 1
Date_ 20120416
Time 19.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 10.04 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.80 usec
PL1 -3.60 dB
PL1W 82.86334991 W
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.24 dB
PL13 14.24 dB
PL2W 24.60733604 W
PL12W 0.36903250 W
PL13W 0.36903250 W
SFO2 400.1316005 MHz
SI 65536
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S11 ^{1}H of [C$_4$mpyrr][FAP] following reaction and extraction of products

kh101-c4mpyrrFAP after reaction

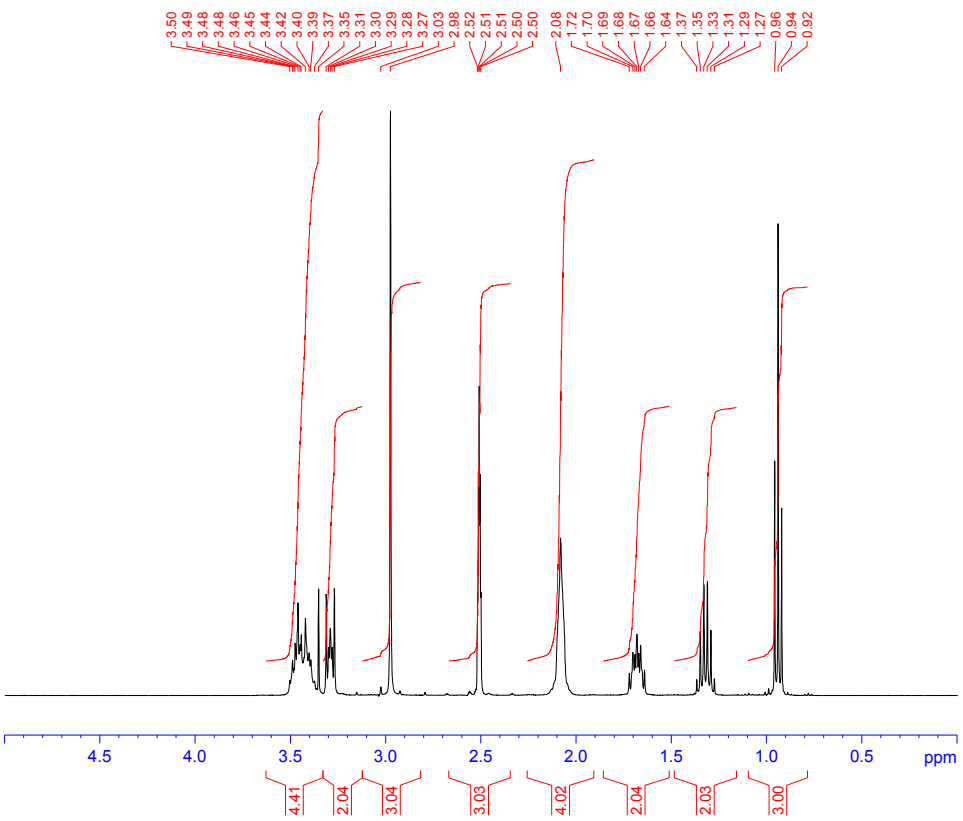


NAME kh101-c4mpyrrFAP after reaction
EXPNO 20
PROCNO 1
Date_ 20120503
Time 16.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 101
DW 60.800 usec
DE 16.92 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.80 usec
PL1 -4.00 dB
PL1W 24.60733604 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

S12 ^{1}H of [C_4mpyrr][NTf_2] following reaction and extraction of products

kh101-c4mpyrrntf2 after reaction

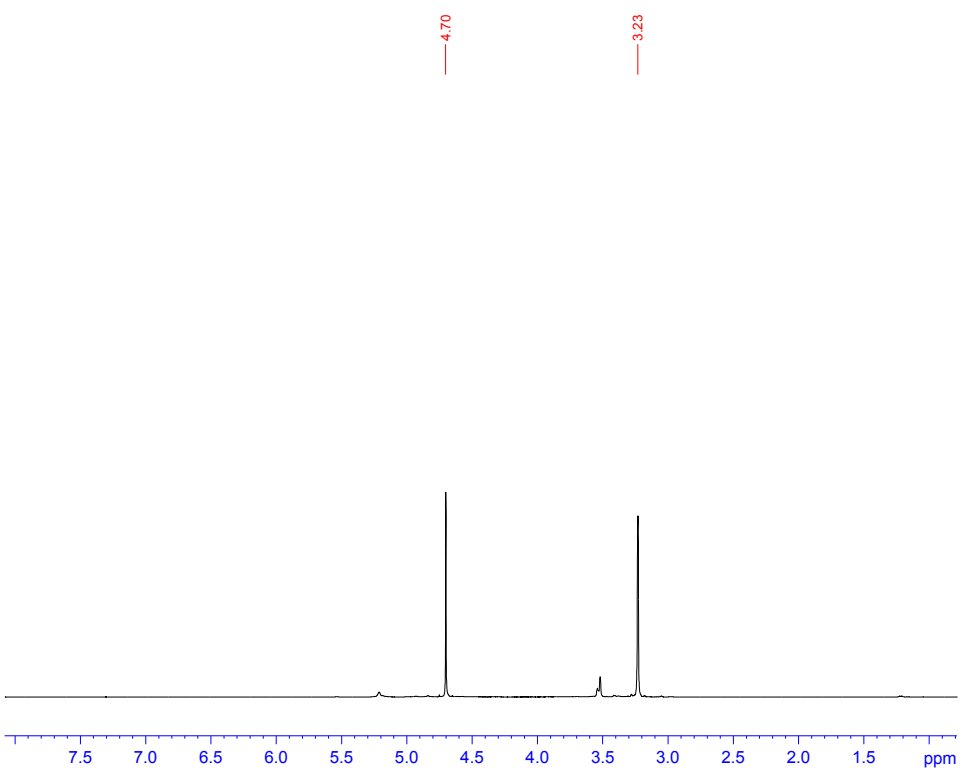


NAME kh101-c4mpyrrntf2 after reaction
EXPNO 20
PROCNO 1
Date_ 20120503
Time 16.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.98466387 sec
RG 90.5
DW 60.800 usec
DE 16.92 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.80 usec
PL1 -4.00 dB
PL1W 24.60733604 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

S13 ^{1}H of ethylene glycol-d2

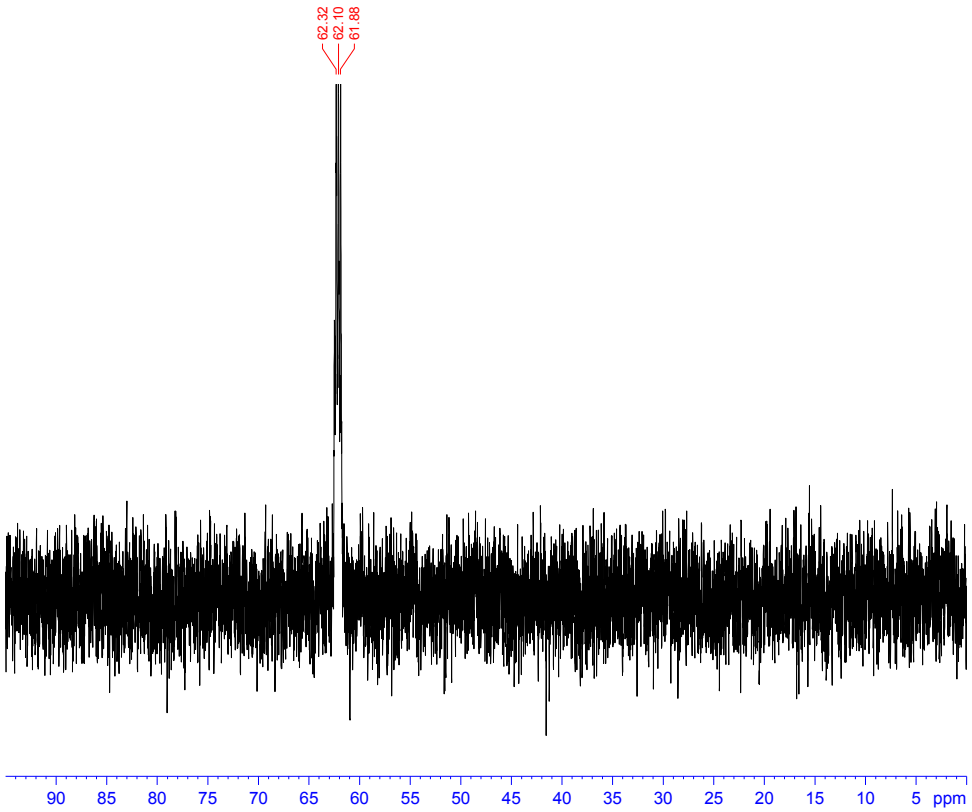
kh101-ethandiol



NAME kh101-ethanediol
EXPNO 10
PROCNO 1
Date_ 20120417
Time 15.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT D2O
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 101
DW 60.800 usec
DE 16.92 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.80 usec
PL1 -4.00 dB
PL1W 24.60733604 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

S14 ^{13}C of ethylene glycol-d2



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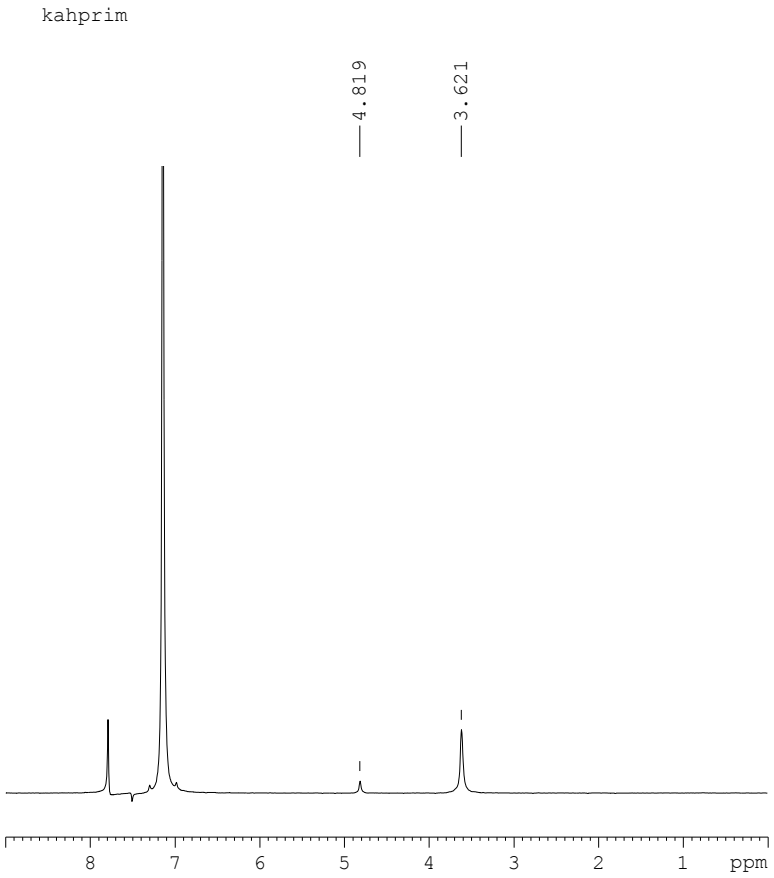
NAME kh101-prim
EXPNO 10
PROCNO 1
Date_ 20120511
Time 16.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 10.04 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.80 usec
PL1 -3.60 dB
PL1W 82.86334991 W
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.24 dB
PL13 14.24 dB
PL2W 24.60733604 W
PL12W 0.36903250 W
PL13W 0.36903250 W
SFO2 400.1316005 MHz
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

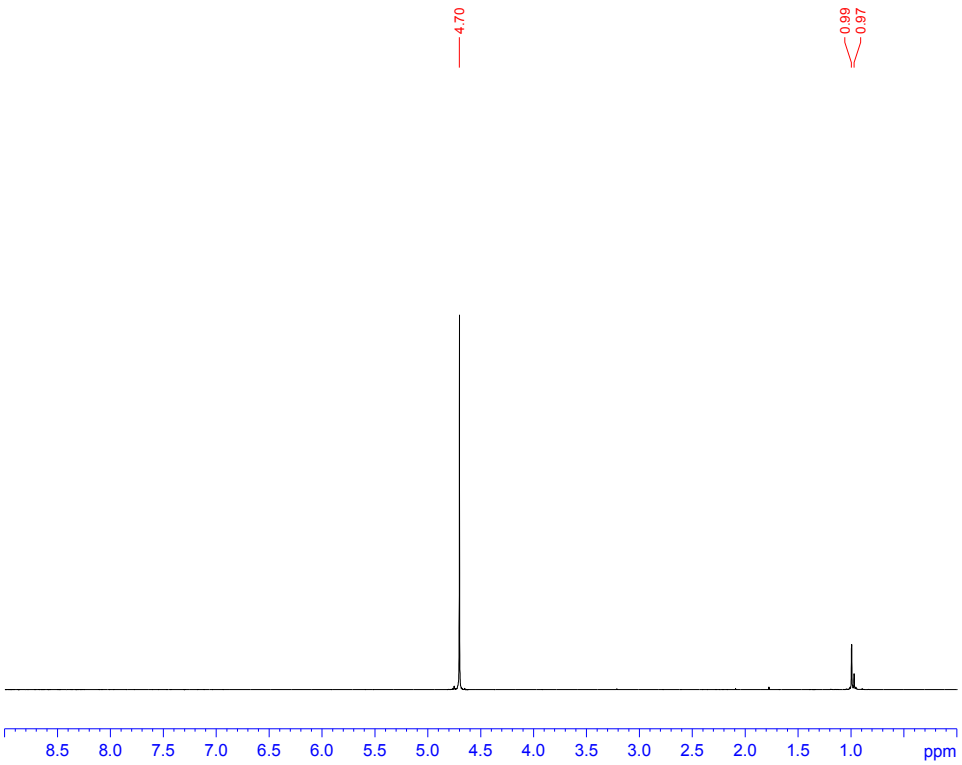
S15 ^{2}H of ethylene glycol-d2



NAME	kahprim
EXPNO	20
PROCNO	1
Date_	20070515
Time	15.14
INSTRUM	spect
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	4096
SOLVENT	C6D6
NS	128
DS	8
SWH	1531.863 Hz
FIDRES	0.373990 Hz
AQ	1.3369844 sec
RG	500
DW	326.400 usec
DE	7.11 usec
TE	293.2 K
D1	0.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	2H
P1	400.00 usec
PL1	5.00 dB
SFO1	76.7735374 MHz
SI	4096
SF	76.7729606 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

S16 ^{1}H of 2,3-butanediol-d2

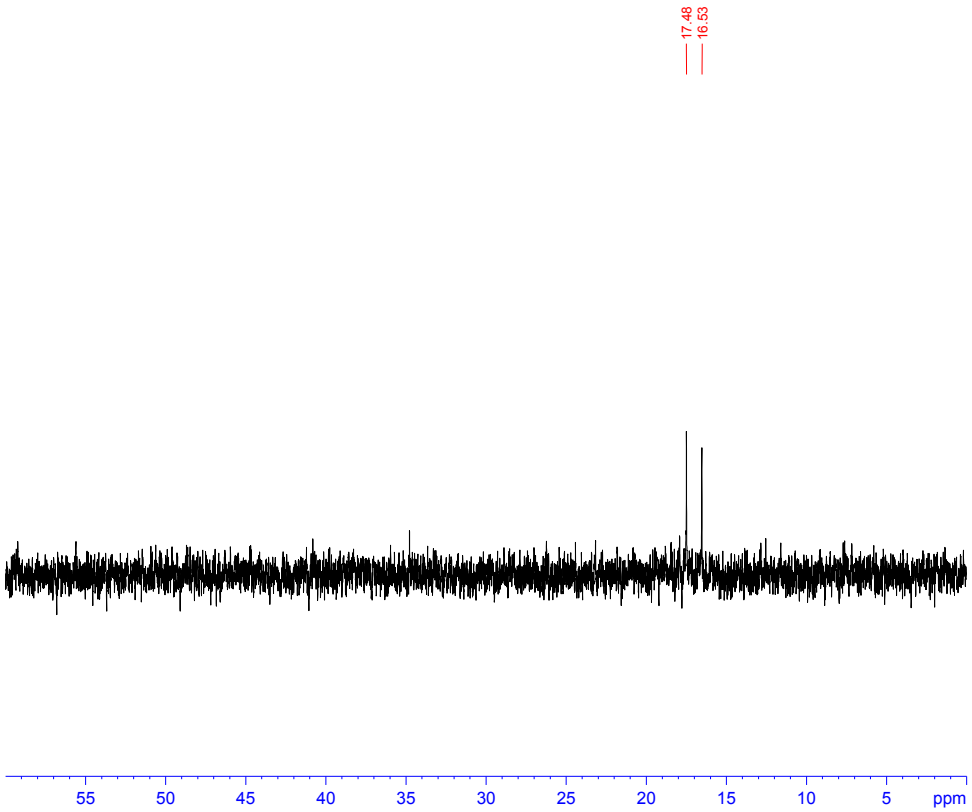
kh101-2,3butanediol



NAME kh101-2,3butanediol
EXPNO 20
PROCNO 1
Date_ 20120417
Time 15.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT D2O
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 181
DW 60.800 usec
DE 16.92 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.80 usec
PL1 -4.00 dB
PL1W 24.60733604 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

S17 ^{13}C of 2,3-butanediol-d2



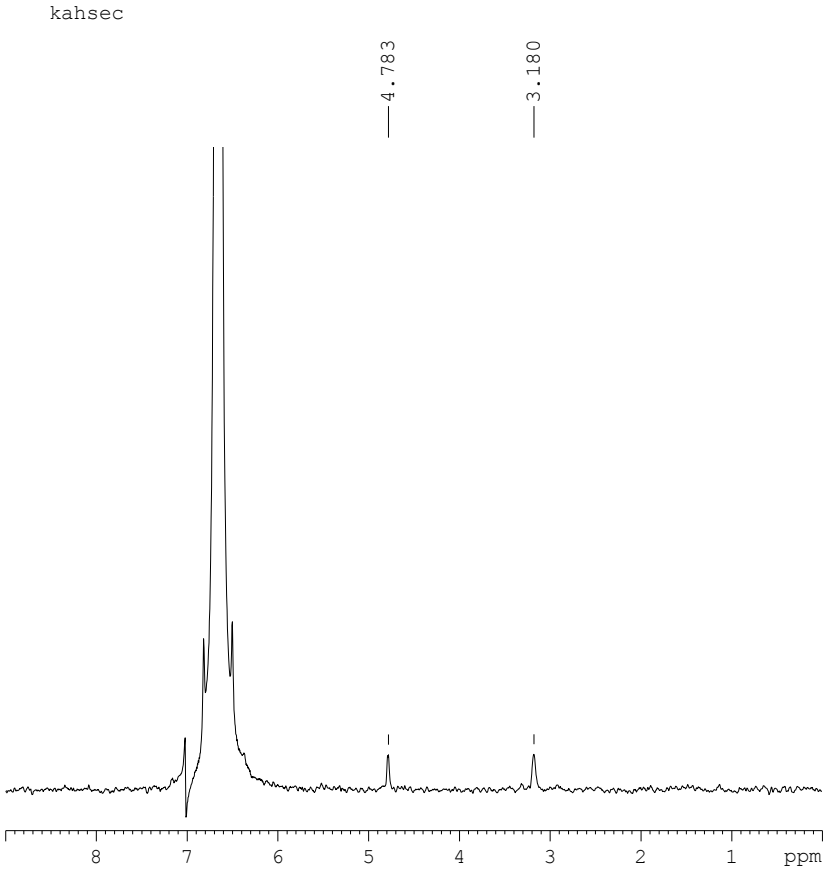
BRUKER

NAME kh101-2,3butanediol
EXPNO 21
PROCNO 1
Date_ 20120417
Time 20.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 10.04 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.80 usec
PL1 -3.60 dB
PL1W 82.86334991 W
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.24 dB
PL13 14.24 dB
PL2W 24.60733604 W
PL12W 0.36903250 W
PL13W 0.36903250 W
SFO2 400.1316005 MHz
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

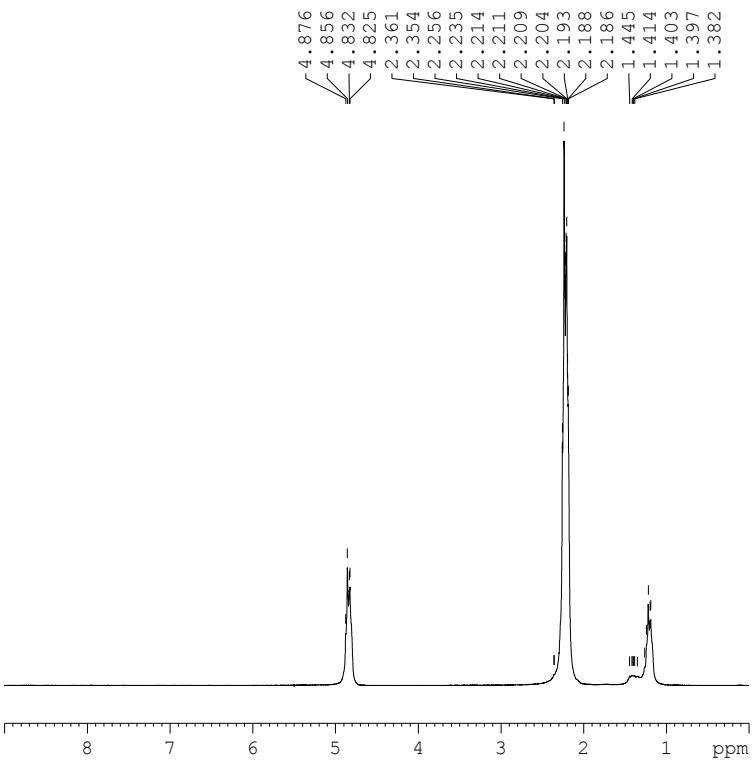
S18 ^{2}H of 2,3-butanediol-d2



NAME	KAHS6CDOM
EXPNO	10
PROCNO	1
Date_	20061109
Time	10.23
INSTRUM	spect
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	4096
SOLVENT	C6D6
NS	128
DS	4
SWH	1531.863 Hz
FIDRES	0.373990 Hz
AQ	1.3369844 sec
RG	500
DW	326.400 usec
DE	7.11 usec
TE	293.2 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	2H
P1	400.00 usec
PL1	5.00 dB
SFO1	76.7735374 MHz
SI	4096
SF	76.7729984 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

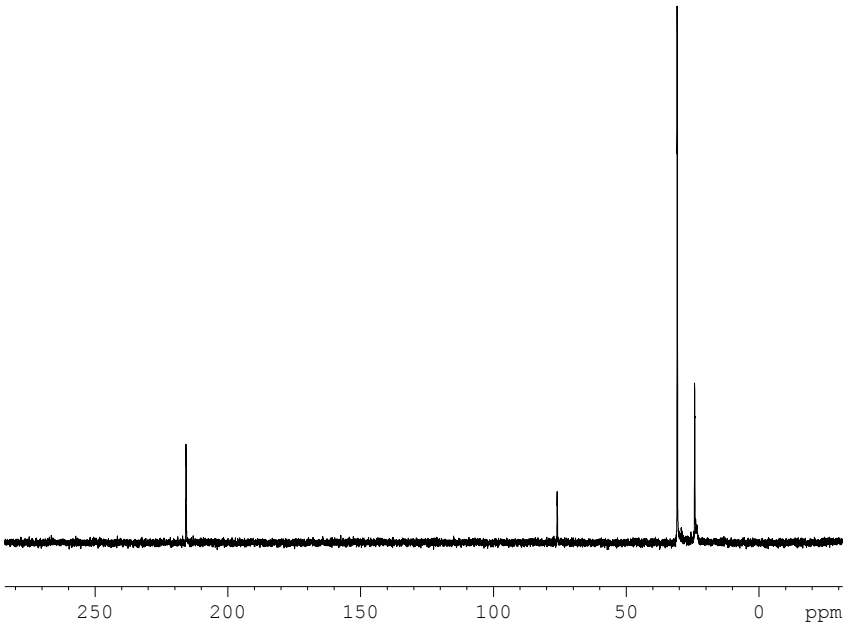
S19 ^{1}H of 2,3- pinacol-d6

kahtert



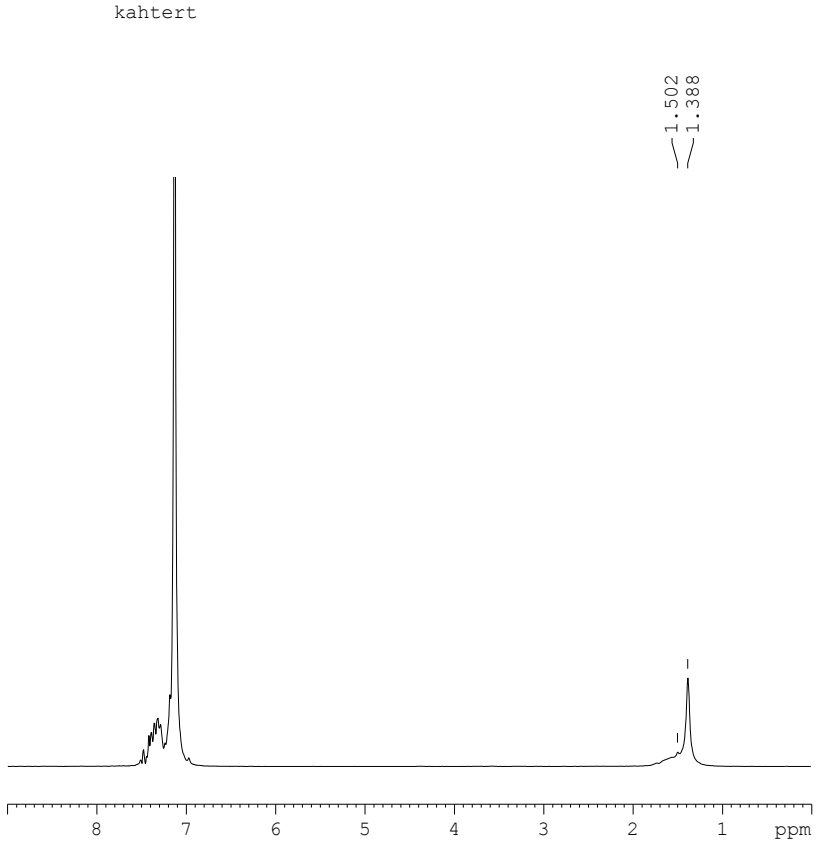
NAME	KAHtert
EXPNO	30
PROCNO	1
Date_	20071030
Time	16.57
INSTRUM	spect
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	65536
SOLVENT	D2O
NS	16
DS	4
SWH	7507.507 Hz
FIDRES	0.114555 Hz
AQ	4.3647475 sec
RG	80.6
DW	66.600 usec
DE	7.11 usec
TE	0.0 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	6.00 usec
PL1	-3.00 dB
SFO1	500.1327507 MHz
SI	32768
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

S20 ^{13}C of pinacol-d6



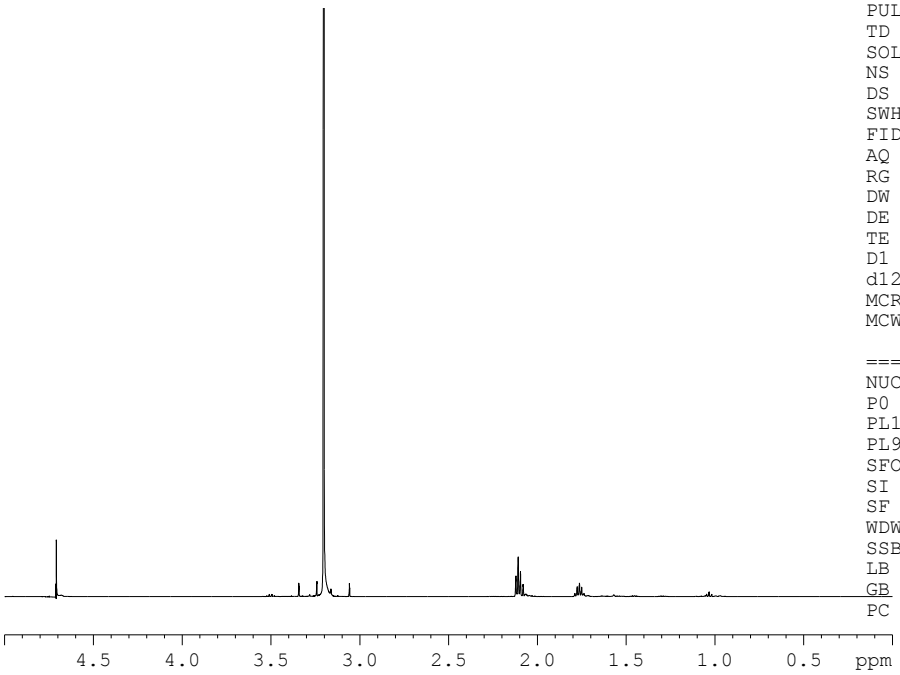
NAME	KAHtert
EXPNO	32
PROCNO	1
Date_	20071030
Time	17.45
INSTRUM	spect
PROBHD	5 mm Multinucl
PULPROG	zgpg
TD	65536
SOLVENT	D2O
NS	1024
DS	4
SWH	39682.539 Hz
FIDRES	0.605507 Hz
AQ	0.8258036 sec
RG	1448.2
DW	12.600 usec
DE	5.50 usec
TE	0.0 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	13C
P1	7.00 usec
PL1	0.00 dB
SFO1	125.7736214 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	120.00 dB
PL12	14.00 dB
PL13	20.00 dB
SFO2	500.1320005 MHz

S21 ^{2}H of pinacol-d6



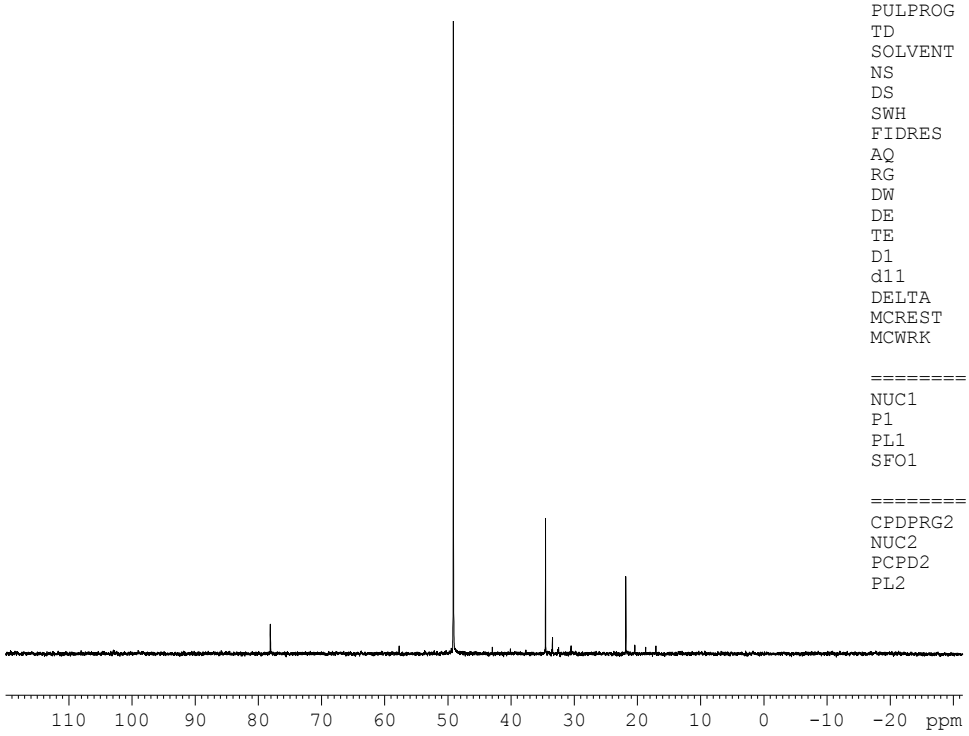
NAME	KAHtert
EXPNO	11
PROCNO	1
Date_	20070404
Time	14.21
INSTRUM	spect
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	4096
SOLVENT	D2O
NS	128
DS	4
SWH	1531.863 Hz
FIDRES	0.373990 Hz
AQ	1.3369844 sec
RG	500
DW	326.400 usec
DE	7.11 usec
TE	0.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	2H
P1	400.00 usec
PL1	5.00 dB
SFO1	76.7735374 MHz
SI	4096
SF	76.7729617 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

S22 ^{1}H of 1,2-cyclohexanediol-d2



NAME	KAHcyc
EXPNO	21
PROCNO	1
Date_	20071030
Time	3.54
INSTRUM	spect
PROBHD	5 mm Multinucl
PULPROG	zg0pr
TD	65536
SOLVENT	D2O
NS	128
DS	4
SWH	7507.507 Hz
FIDRES	0.114555 Hz
AQ	4.3647475 sec
RG	57
DW	66.600 usec
DE	7.11 usec
TE	0.0 K
D1	1.00000000 sec
d12	0.00002000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	1H
P0	10.00 usec
PL1	-3.00 dB
PL9	55.00 dB
SFO1	500.1323539 MHz
SI	32768
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

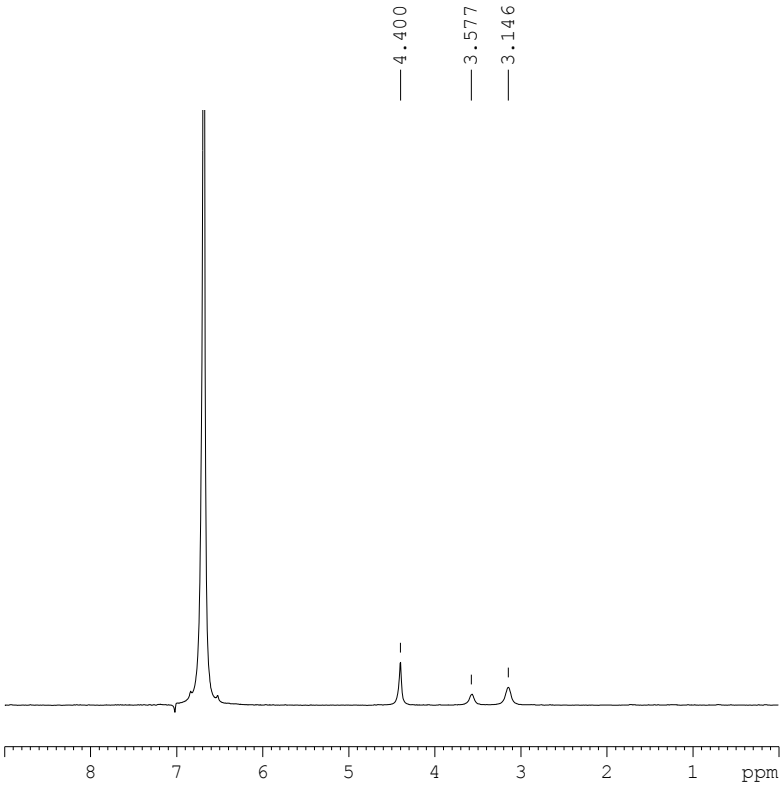
S23 ^{13}C of 1,2-cyclohexanediol-d2



NAME	KAHcyc
EXPNO	22
PROCNO	1
Date_	20071030
Time	5.33
INSTRUM	spect
PROBHD	5 mm Multinucl
PULPROG	zgpg
TD	65536
SOLVENT	D2O
NS	2048
DS	4
SWH	39682.539 Hz
FIDRES	0.605507 Hz
AQ	0.8258036 sec
RG	5160.6
DW	12.600 usec
DE	5.50 usec
TE	0.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	13C
P1	7.00 usec
PL1	0.00 dB
SFO1	125.7736214 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	120.00 dB

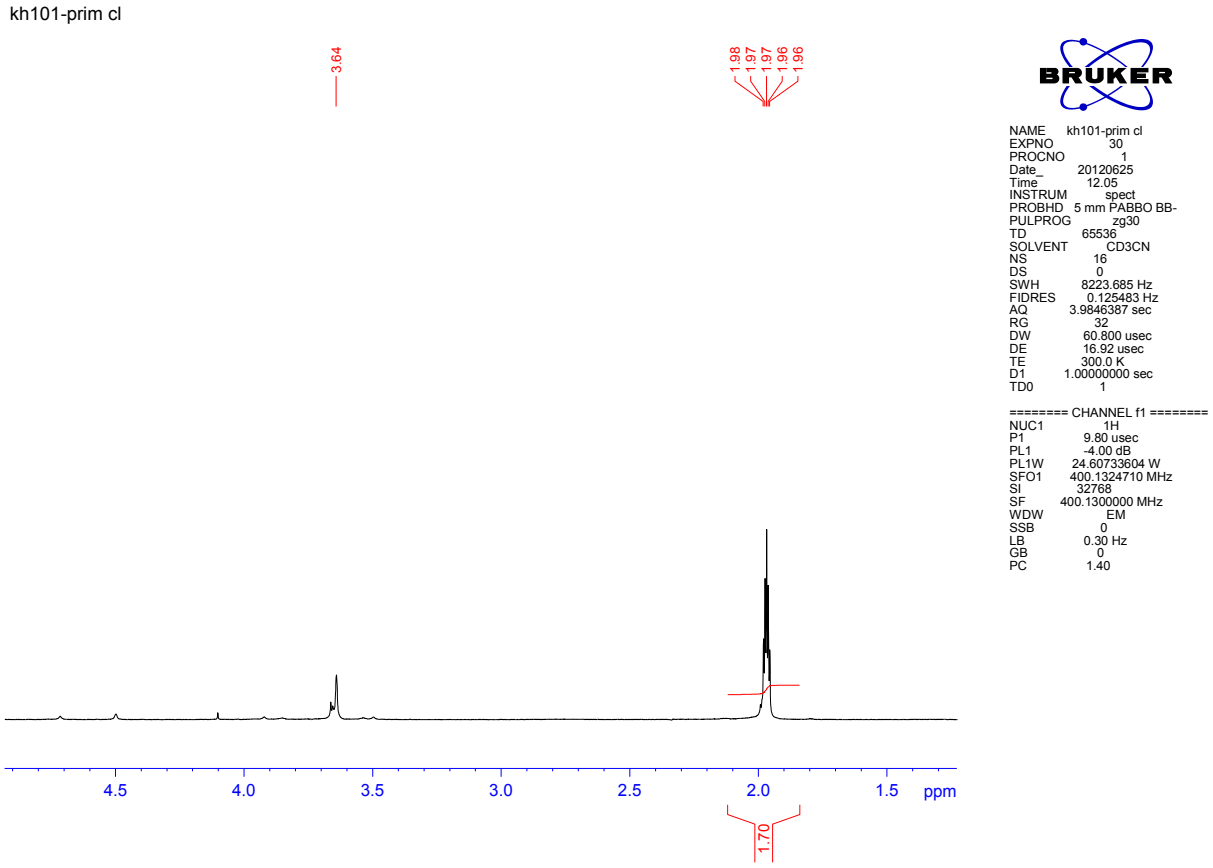
S24 ^{2}H of 1,2-cyclohexanediol-d2

kahcyclic



NAME	KAHCYCH2O
EXPNO	10
PROCNO	1
Date_	20061109
Time	12.28
INSTRUM	spect
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	4096
SOLVENT	C6D6
NS	128
DS	4
SWH	1531.863 Hz
FIDRES	0.373990 Hz
AQ	1.3369844 sec
RG	500
DW	326.400 usec
DE	7.11 usec
TE	293.4 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	2H
P1	400.00 usec
PL1	5.00 dB
SFO1	76.7735374 MHz
SI	4096
SF	76.7729984 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

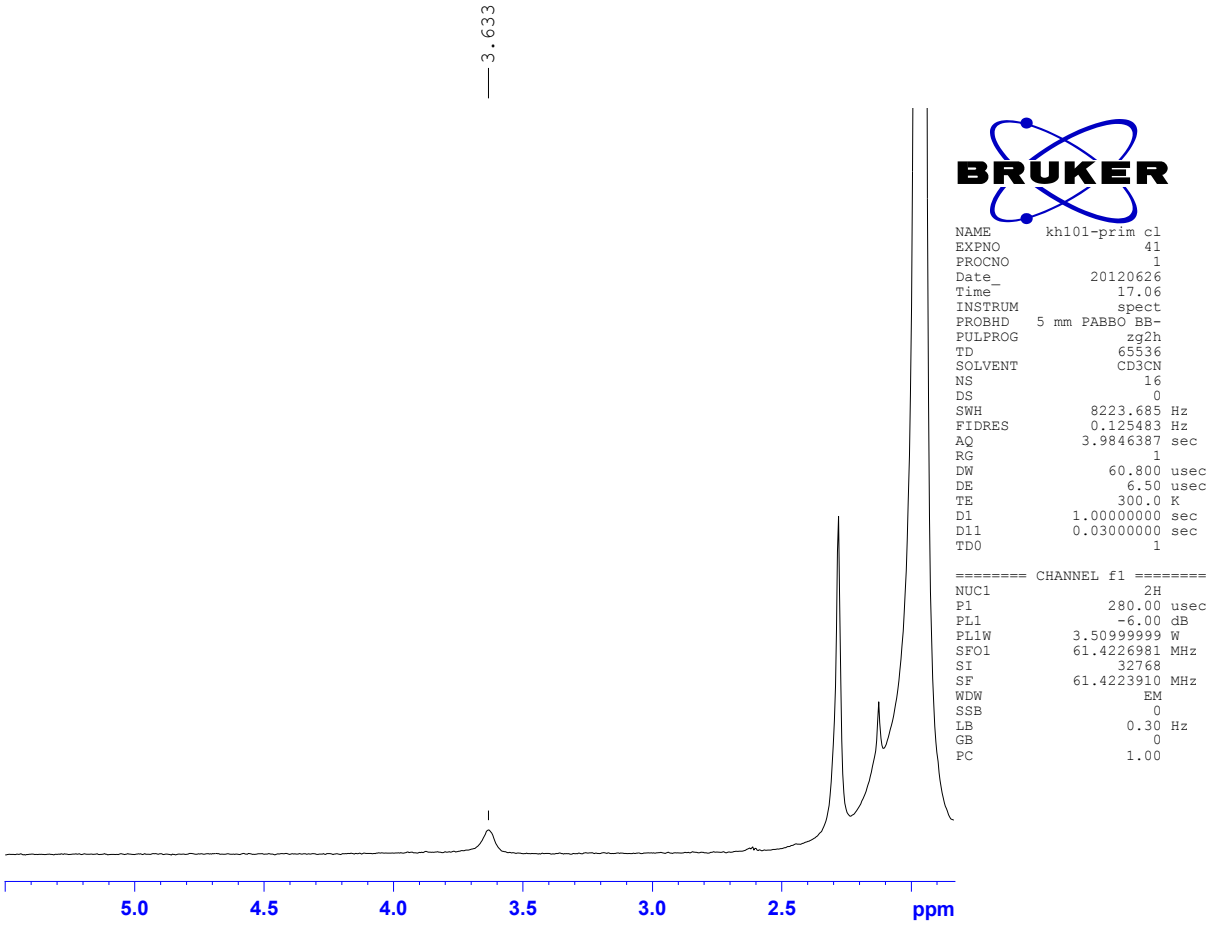
S25 ^{1}H dichloroethane-d2



NAME kh101-prim cl
EXPNO 30
PROCNO 1
Date_ 20120625
Time 12.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CD3CN
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 32
DW 60.800 usec
DE 16.92 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

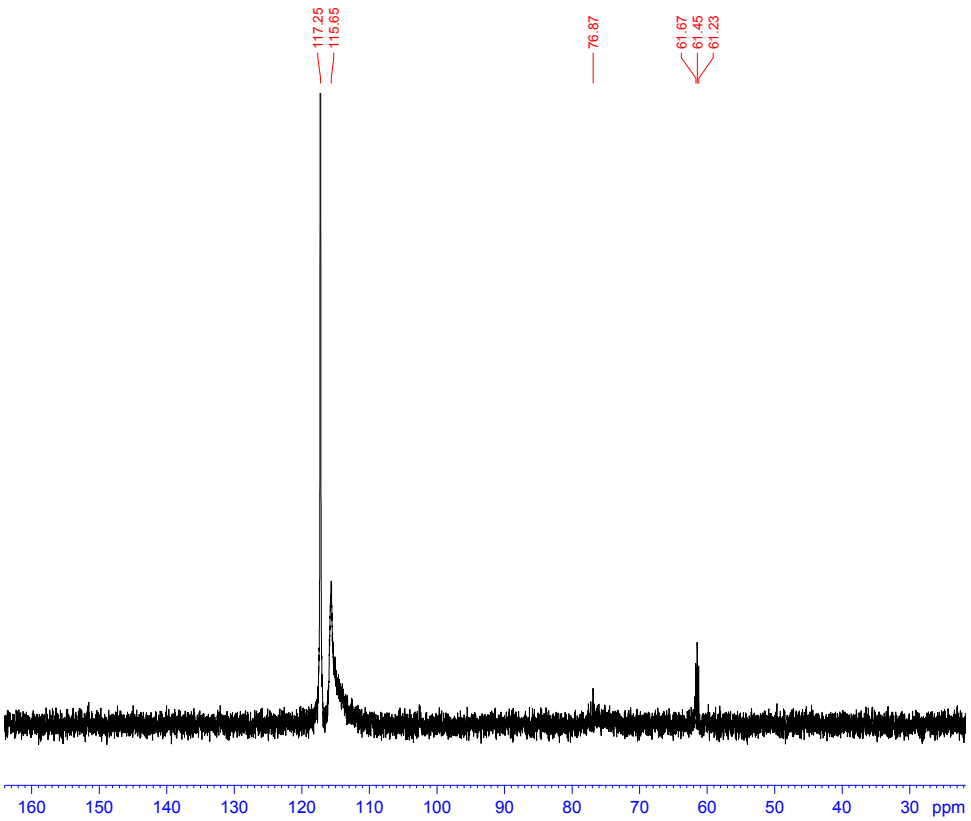
======== CHANNEL f1 ========
NUC1 1H
P1 9.80 usec
PL1 -4.00 dB
PL1W 24.60733604 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

S26 ^{2}H dichloroethane-d2




```
NAME          kh101-prim cl
EXPNO                   41
PROCNO                   1
Date_             20120626
Time                 17.06
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg2h
TD                  65536
SOLVENT             CD3CN
NS                     16
DS                      0
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                      1
DW                 60.800 usec
DE                  6.50 usec
TE                 300.0 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   2H
P1                280.00 usec
PL1                -6.00 dB
PL1W           3.50999999 W
SFO1           61.4226981 MHz
SI                  32768
SF             61.4223910 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

S27 ^{13}C dichloroethane-d2



BRUKER

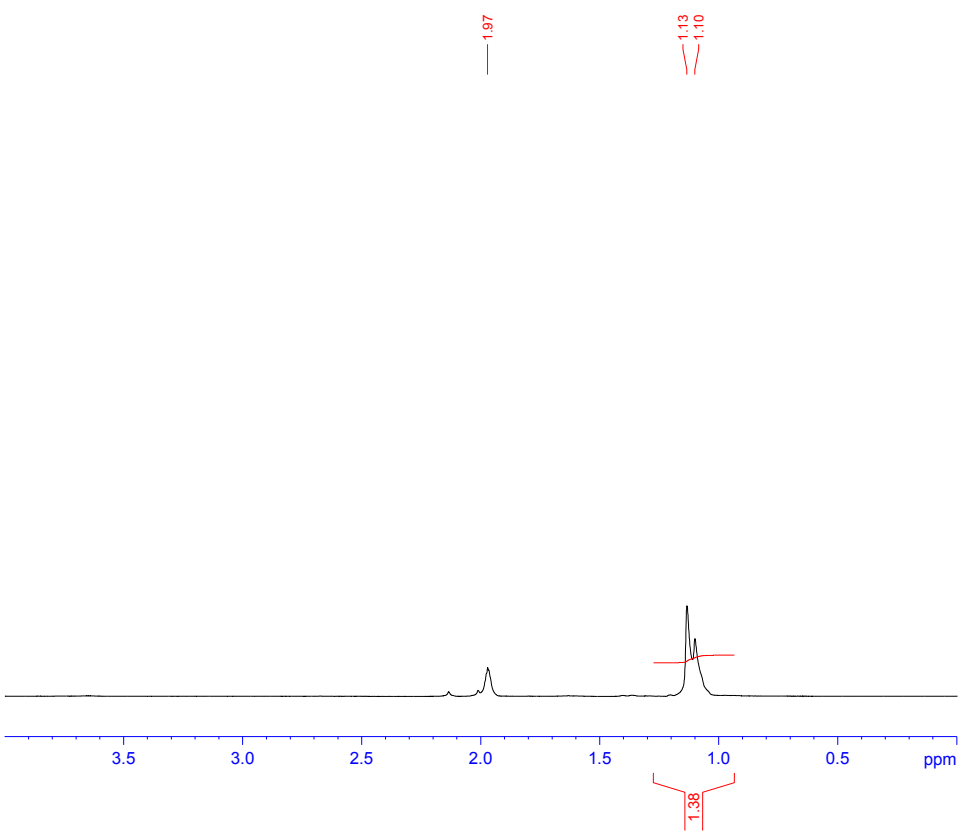
NAME kh101-prim cl
EXPNO 50
PROCNO 1
Date_ 20120626
Time 18.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CD3CN
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 10.04 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.80 usec
PL1 -3.60 dB
PL1W 82.86334991 W
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.24 dB
PL13 14.24 dB
PL2W 24.60733604 W
PL12W 0.36903250 W
PL13W 0.36903250 W
SFO2 400.1316005 MHz
SI 65536
SF 100.6128570 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S28 ^{1}H 2,3-dichlorobutane-d2

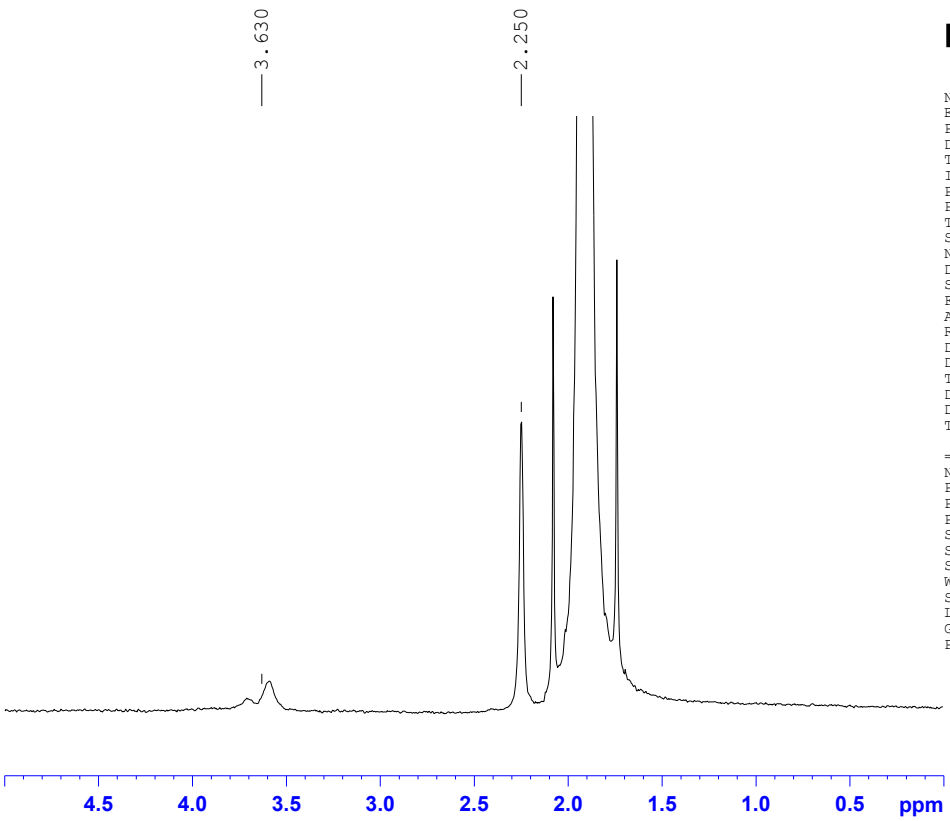
kh101-sec cl



NAME kh101-sec cl
EXPNO 30
PROCNO 1
Date_ 20120625
Time 15.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CD3CN
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 11.3
DW 60.800 usec
DE 16.92 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

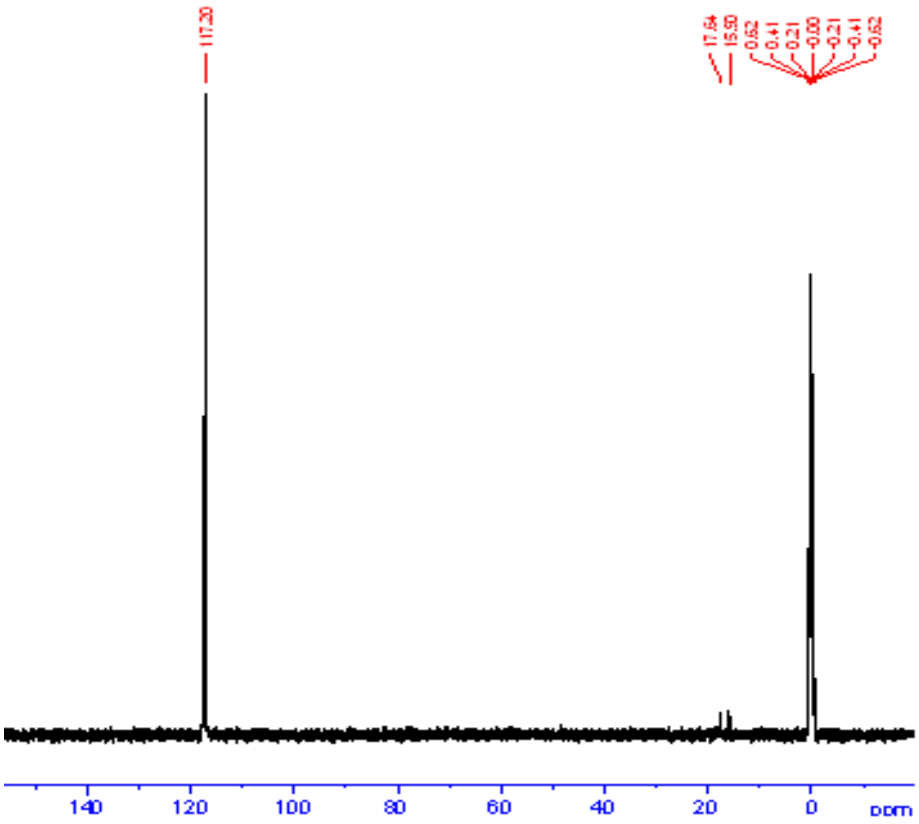
======== CHANNEL f1 ========
NUC1 1H
P1 9.80 usec
PL1 -4.00 dB
PL1W 24.60733604 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

S29 ^{2}H 2,3dichlorobutane-d2

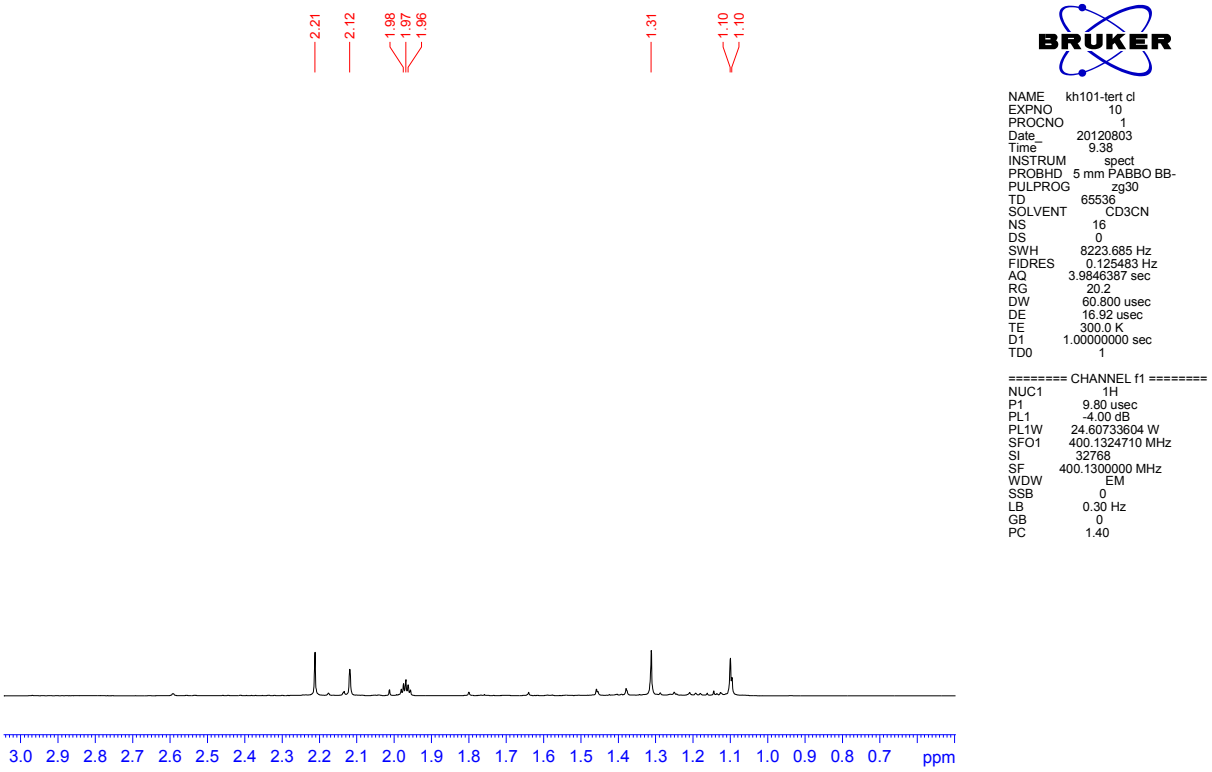


NAME	kh101-sec cl
EXPNO	32
PROCNO	1
Date_	20120626
Time	17.14
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg2h
TD	65536
SOLVENT	CD3CN
NS	16
DS	0
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	1
DW	60.800 usec
DE	6.50 usec
TE	300.0 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	2H
P1	280.00 usec
PL1	-6.00 dB
PL1W	3.50999999 W
SFO1	61.4226981 MHz
SI	32768
SF	61.4223910 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

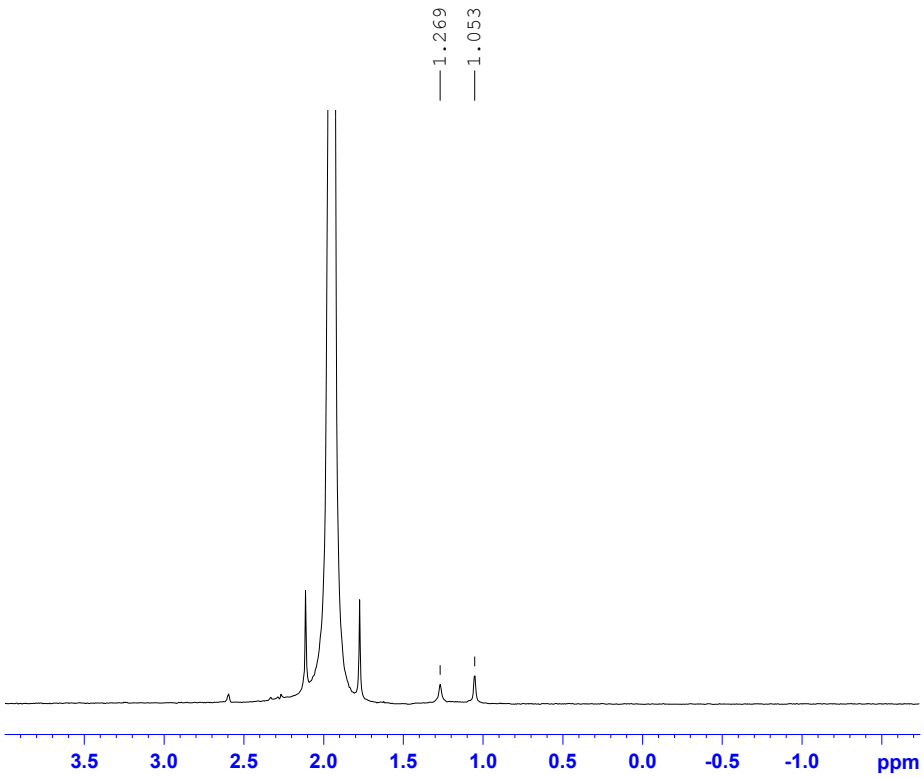
S30 ^{13}C 2,3-dichlorobutane-d2



S31 attempt to prepare ^{1}H 2,3-dichloro-2,3-dimethylbutane-d6 by direct HCl chlorination led to the pinacolic rearrangement deuteriated products (see ^{13}C NMR below) δ 2.15ppm and 1.2ppm according to Aldrich)

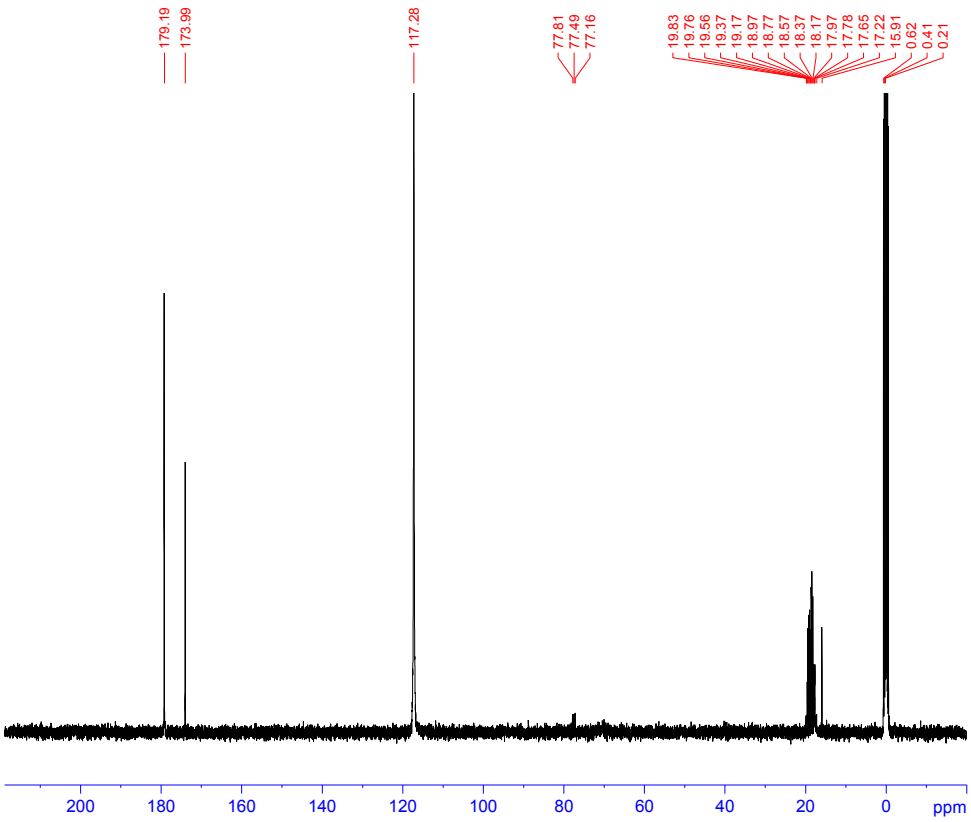


S32 ^{2}H 2,3-dichloro-2,3-dimethylbutane-d6




```
NAME          kh101-tert cl
EXPNO                   11
PROCNO                   1
Date_             20120803
Time                 9.43
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg2h
TD                  65536
SOLVENT             CD3CN
NS                     16
DS                      0
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                      1
DW                 60.800 usec
DE                  6.50 usec
TE                 300.0 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   2H
P1                280.00 usec
PL1                -6.00 dB
PL1W           3.50999999 W
SFO1           61.4226981 MHz
SI                  32768
SF             61.4223910 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

S33 ^{13}C 2,3-dichloro-2,3-dimethylbutane-d6 (+ pinacolic rearrangement product)



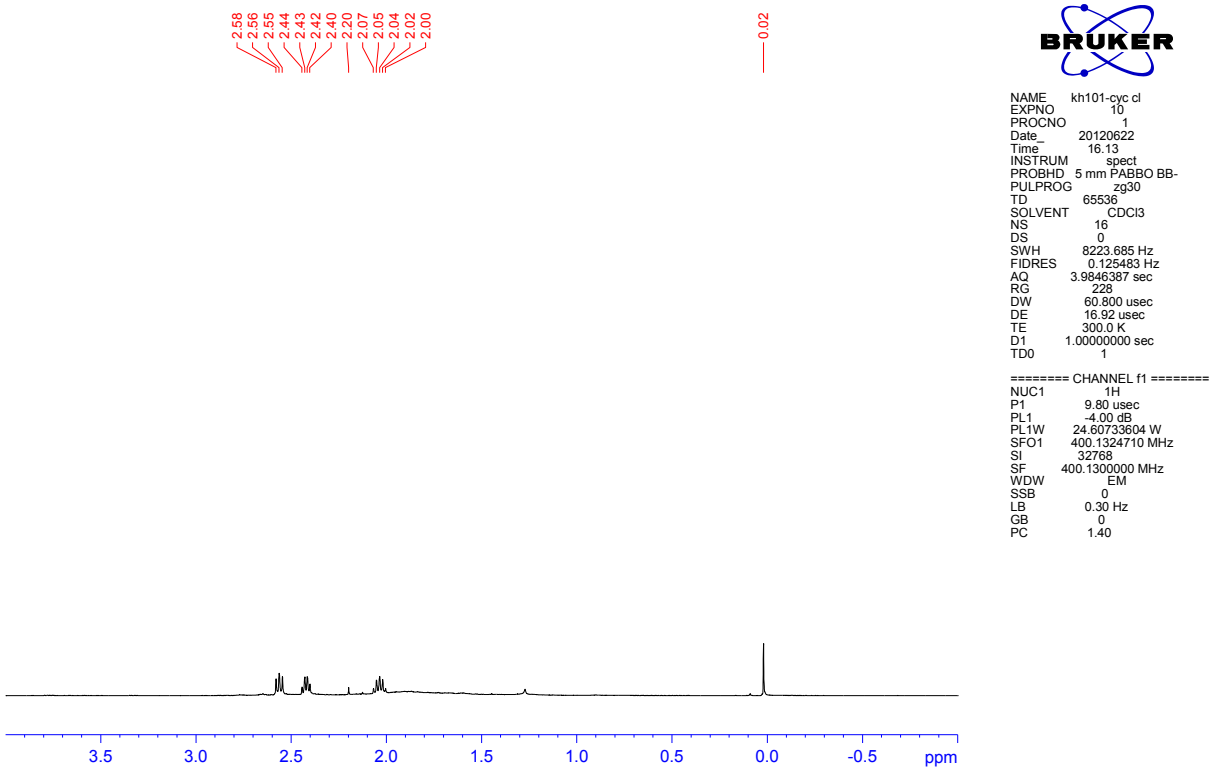
BRUKER

NAME KH-101-sec cl-CH3CN
EXPNO 20
PROCNO 1
Date_ 20120709
Time 18.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CD3CN
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 10.04 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

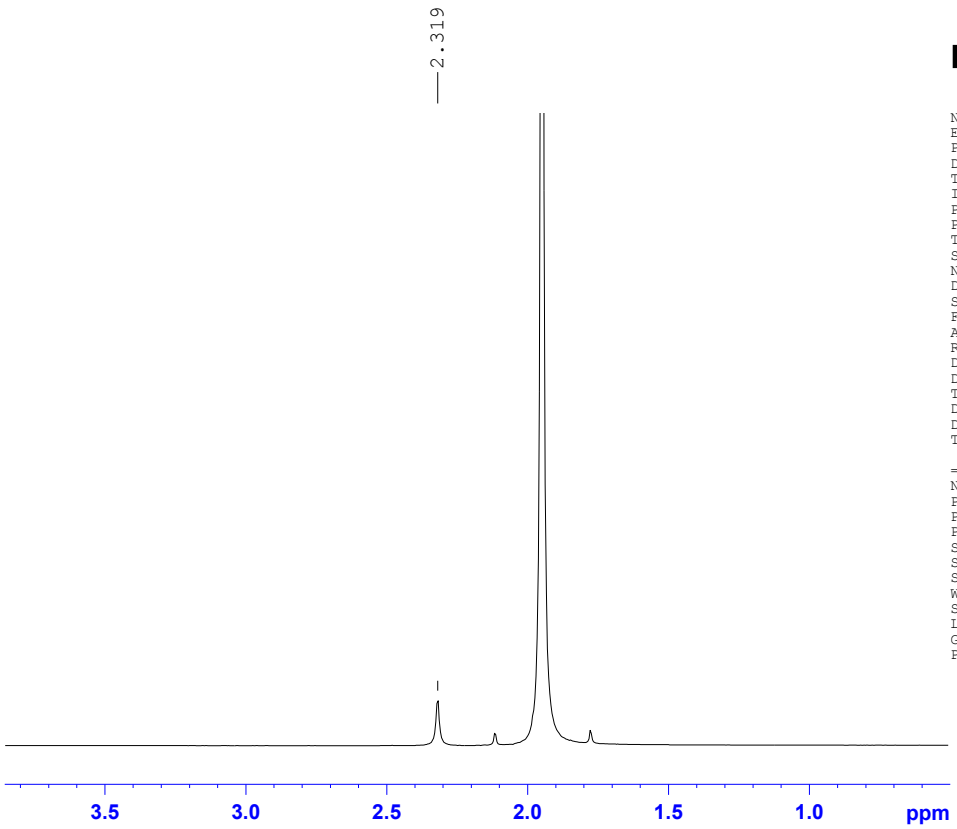
======== CHANNEL f1 ========
NUC1 13C
P1 7.80 usec
PL1 -3.60 dB
PL1W 82.86334991 W
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.24 dB
PL13 14.24 dB
PL2W 24.60733604 W
PL12W 0.36903250 W
PL13W 0.36903250 W
SFO2 400.1316005 MHz
SI 65536
SF 100.6128258 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S34 ^{1}H 1,2-dichlorocyclohexane-d2

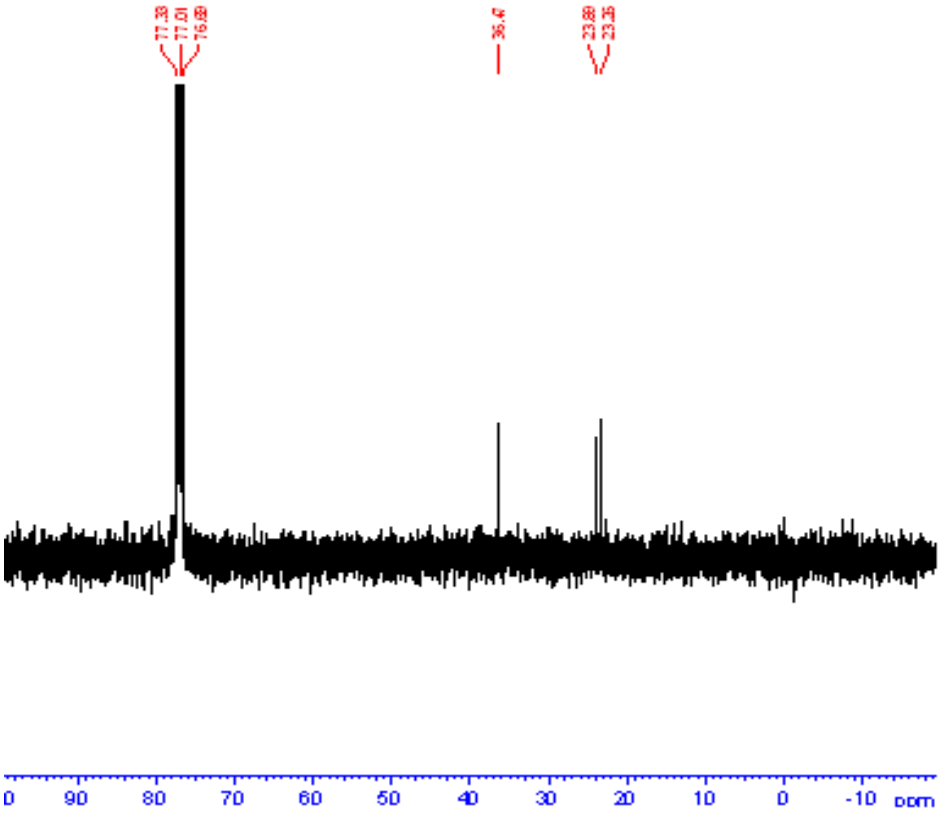


S35 ^{2}H 1,2-dichlorocyclohexane-d2



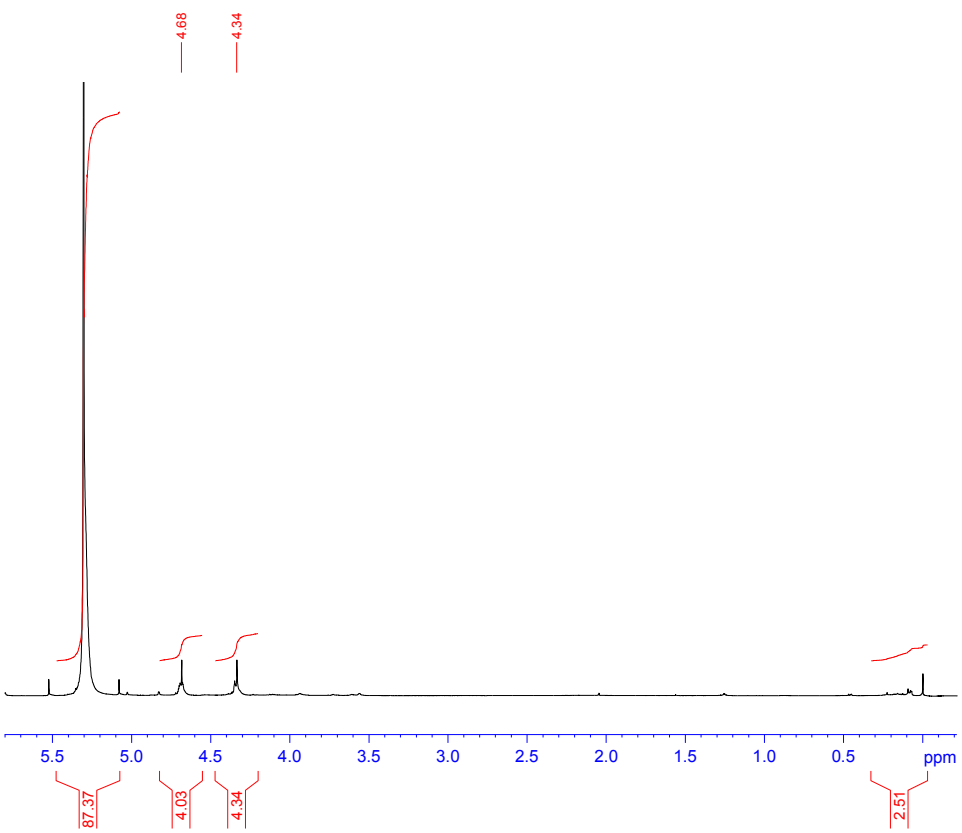

```
NAME          kh101-cyc cl
EXPNO                   32
PROCNO                   1
Date_             20120626
Time                 17.24
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg2h
TD                   65536
SOLVENT              CD3CN
NS                      16
DS                       0
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                       1
DW                  60.800 usec
DE                   6.50 usec
TE                  300.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    2H
P1                  280.00 usec
PL1                  -6.00 dB
PL1W           3.50999999 W
SFO1           61.4226981 MHz
SI                   32768
SF             61.4223910 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

S36 ^{13}C 1,2-dichlorocyclohexane-d2



S37 ^{1}H -ethylene glycol sulfite-d2

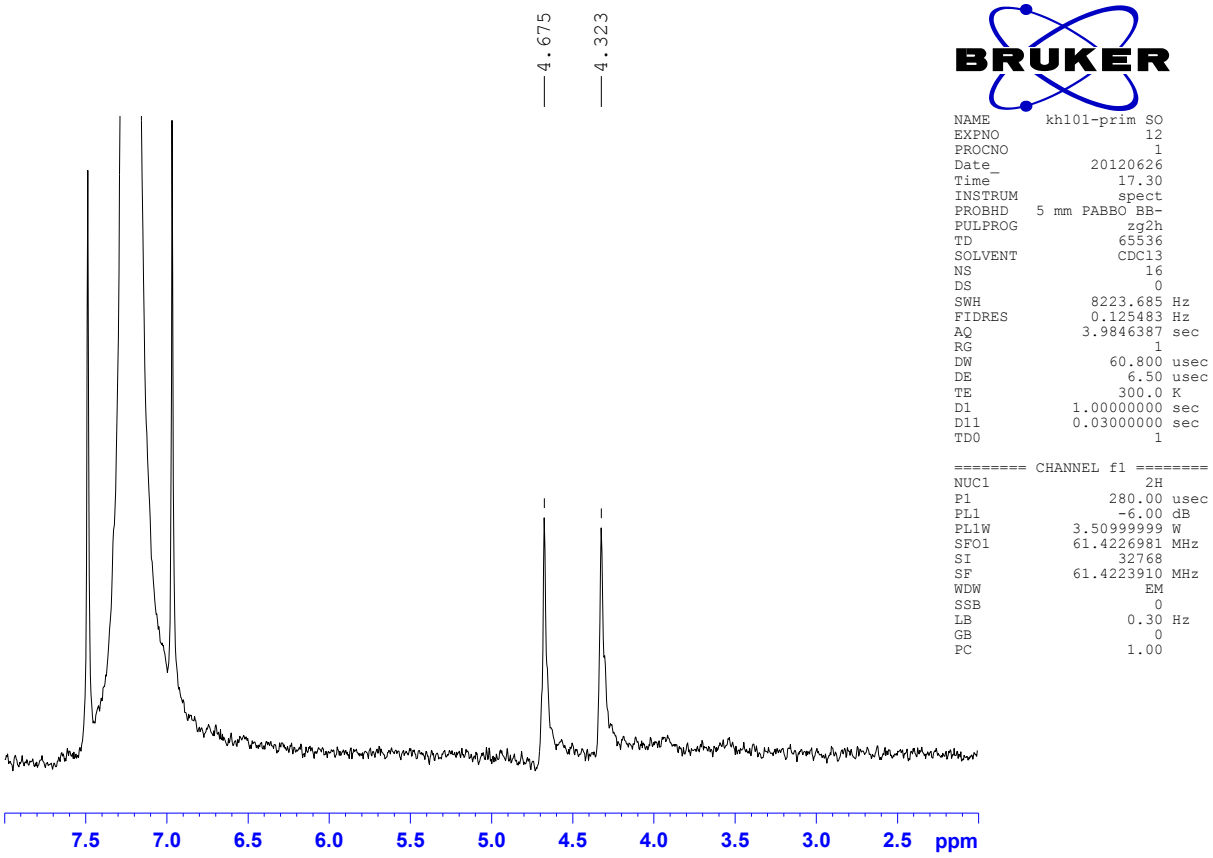
kh101-prim SO



NAME kh101-prim SO
EXPNO 10
PROCNO 1
Date_ 20120625
Time 17.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 80.6
DW 60.800 usec
DE 16.92 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

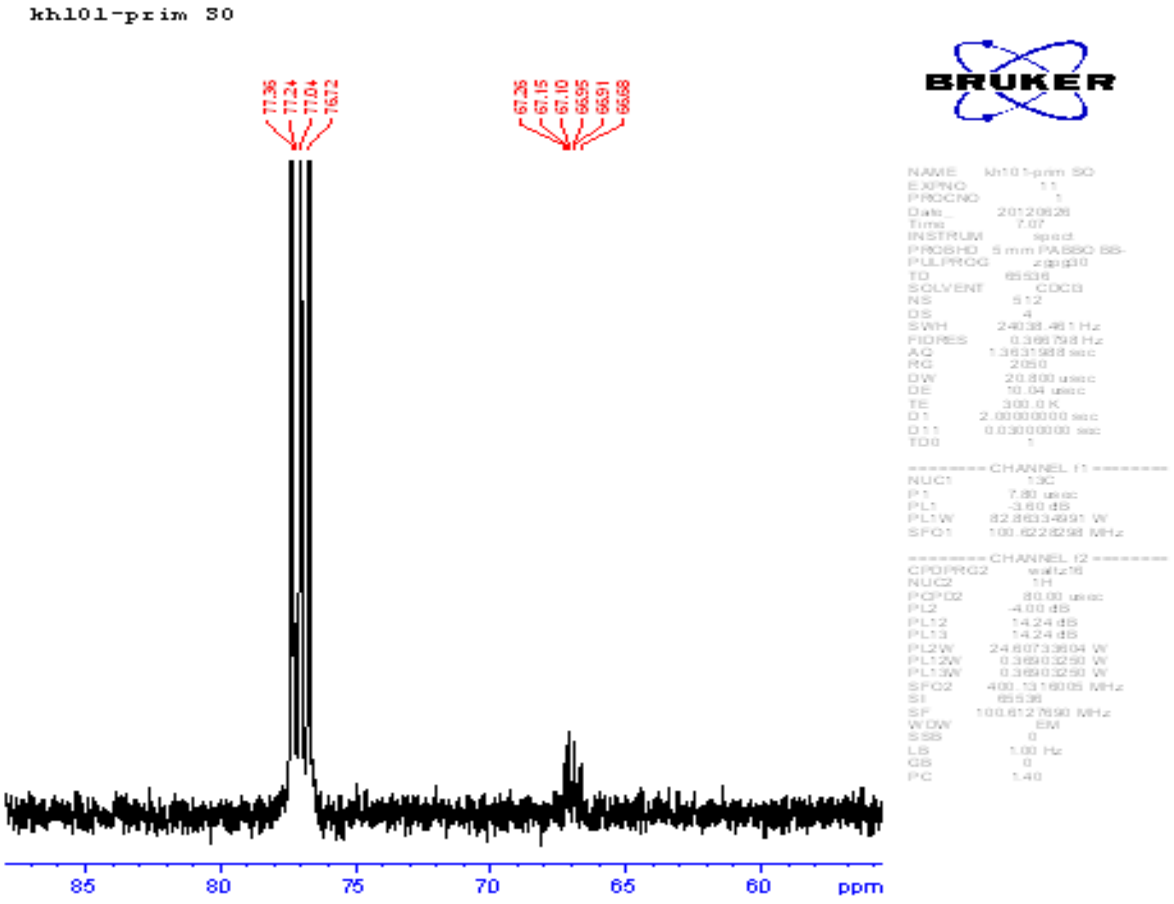
======== CHANNEL f1 ========
NUC1 1H
P1 9.80 usec
PL1 -4.00 dB
PL1W 24.60733604 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300069 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

S38 ^{2}H -ethylene glycol sulfite-d2



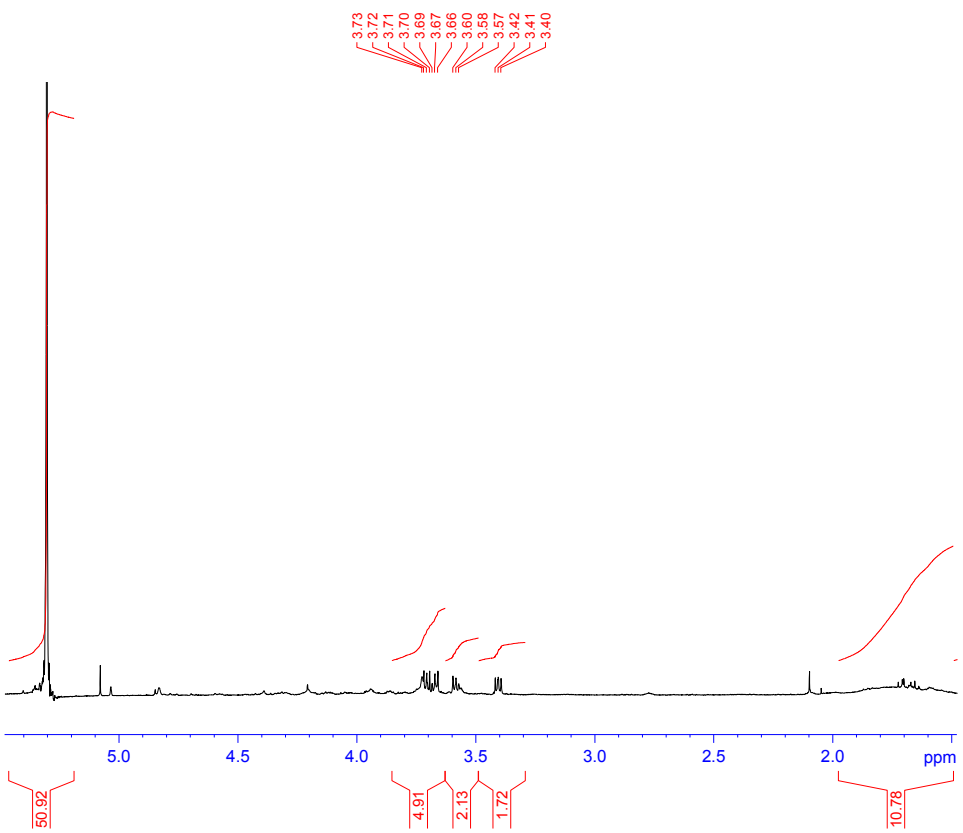

```
NAME          kh101-prim SO
EXPNO                   12
PROCNO                   1
Date_             20120626
Time                 17.30
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg2h
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      0
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                      1
DW                 60.800 usec
DE                  6.50 usec
TE                 300.0 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   2H
P1                280.00 usec
PL1                -6.00 dB
PL1W           3.50999999 W
SFO1           61.4226981 MHz
SI                  32768
SF             61.4223910 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

S39 ^{13}C -ethylene glycol sulfite-d2



S40 ^{1}H-ethylene glycol sulfate-d2

kh101-prim-SO2

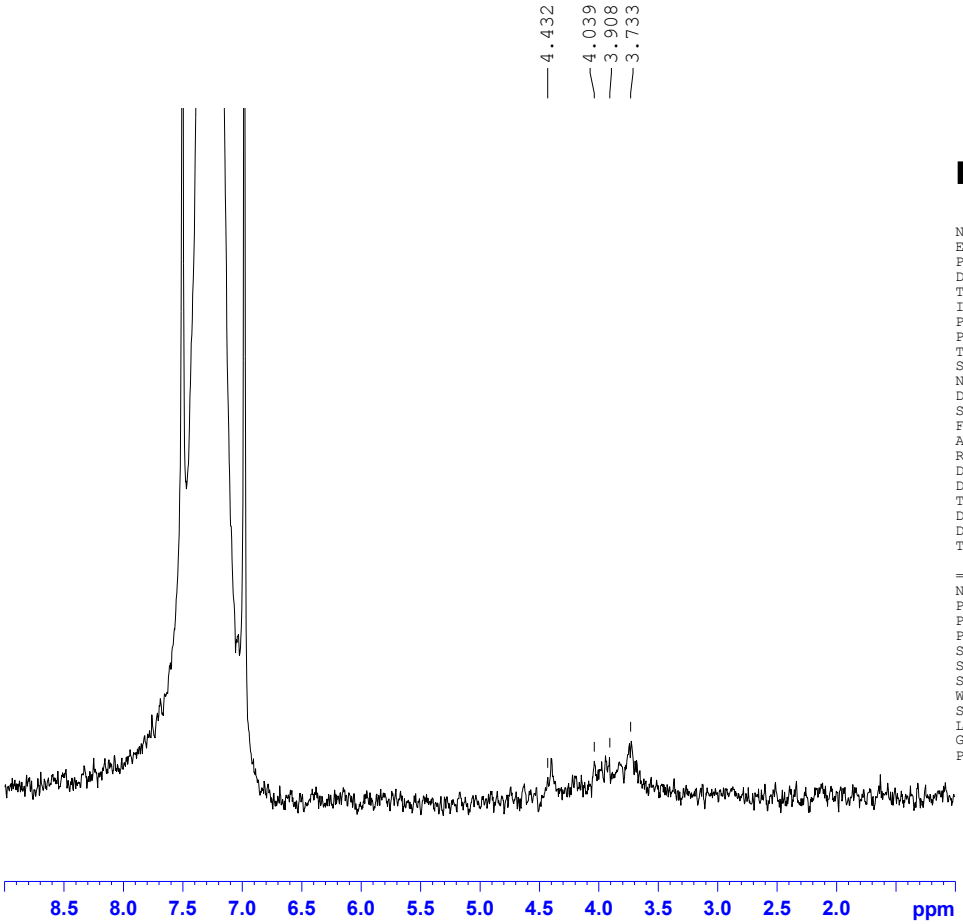


BRUKER

NAME kh101-prim-SO2
EXPNO 10
PROCNO 1
Date_ 20120626
Time 16.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 16.92 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

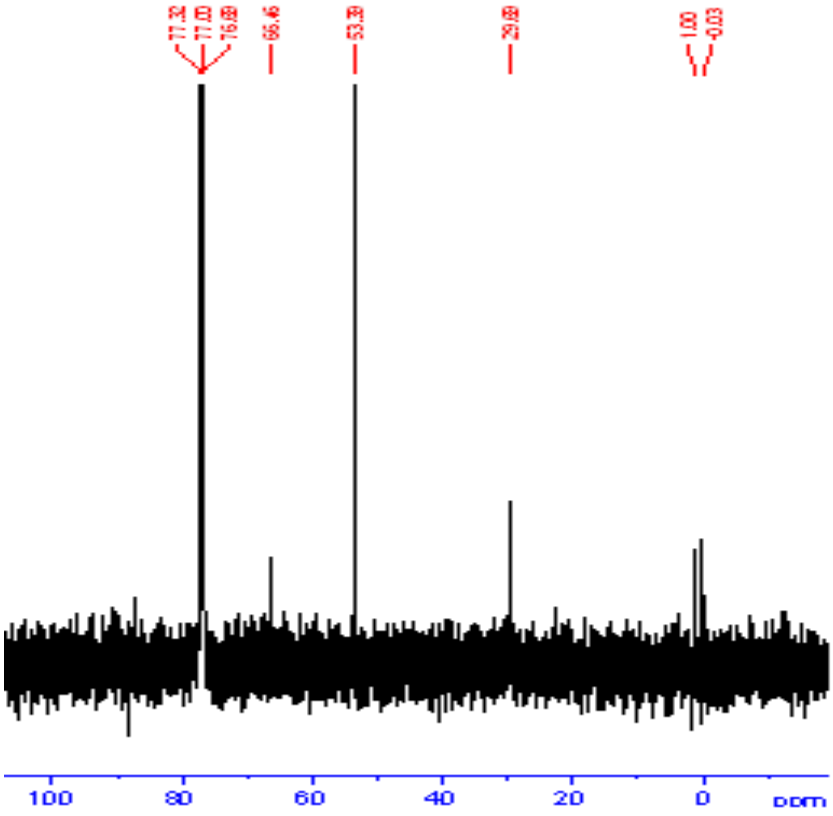
======== CHANNEL f1 ========
NUC1 1H
P1 9.80 usec
PL1 -4.00 dB
PL1W 24.60733604 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300082 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

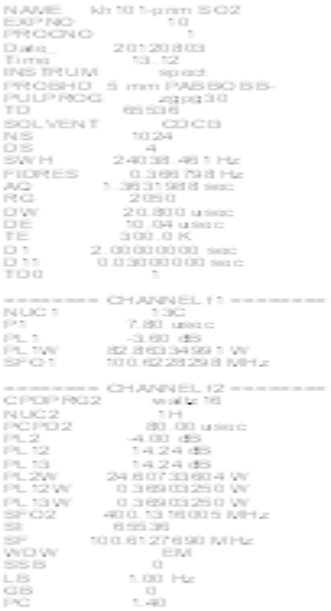
S41 ^{2}H-ethylene glycol sulfate-d2




```
NAME          kh101-prim-SO2
EXPNO                     21
PROCNO                     1
Date_               20120725
Time                   13.23
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zg2h
TD                     65536
SOLVENT                CDCl3
NS                        32
DS                         0
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                3.9846387 sec
RG                         1
DW                    60.800 usec
DE                     6.50 usec
TE                    300.0 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      2H
P1                   280.00 usec
PL1                   -6.00 dB
PL1W              3.50999999 W
SFO1              61.4226981 MHz
SI                     32768
SF                61.4223910 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

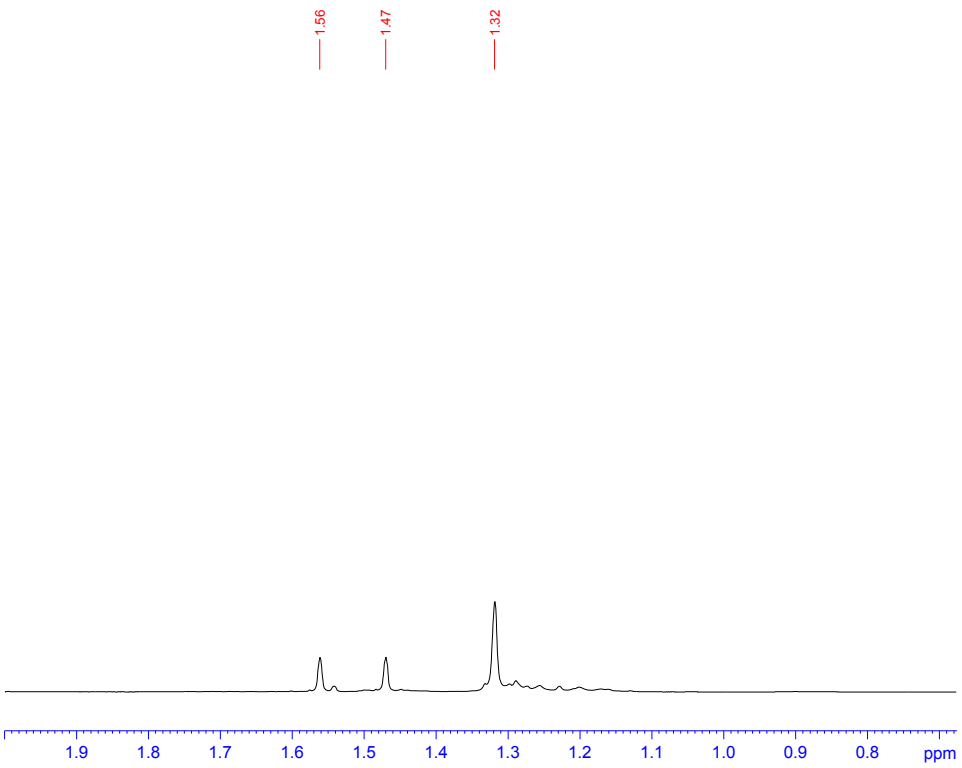
S42 ^{13}C-ethylene glycol sulfate-d2





S43 ^{1}H- 2,3-butanediol sulfite-d_2

kh101-sec SO

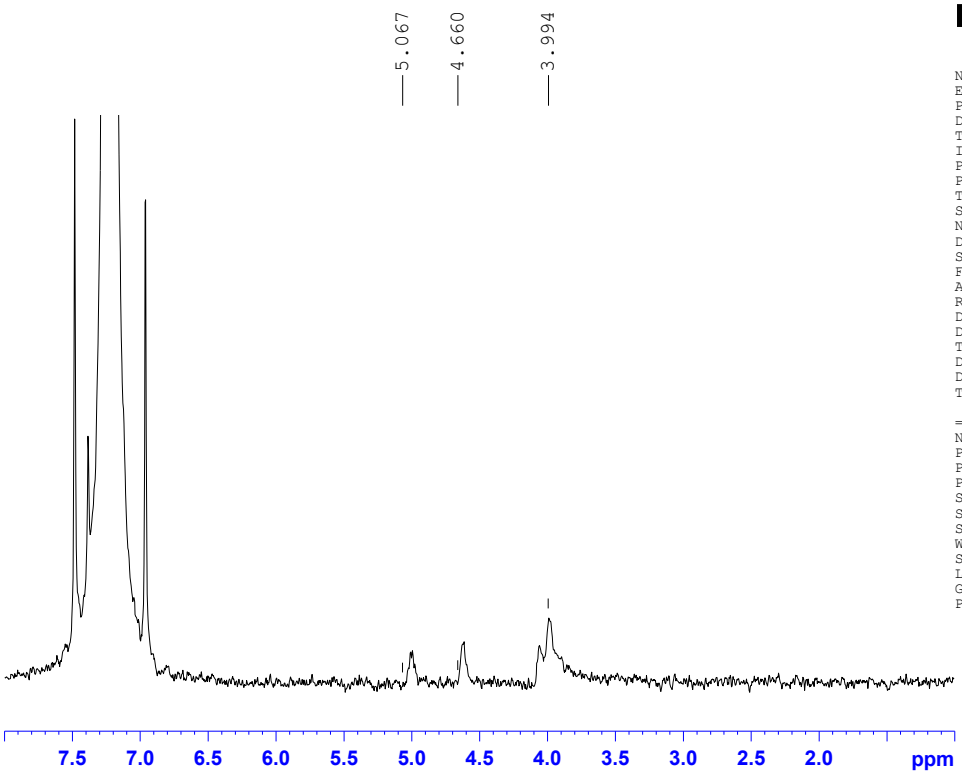


BRUKER

NAME kh101-sec SO
EXPNO 12
PROCNO 1
Date_ 20120626
Time 17.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 32
DW 60.800 usec
DE 16.92 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.80 usec
PL1 -4.00 dB
PL1W 24.60733604 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

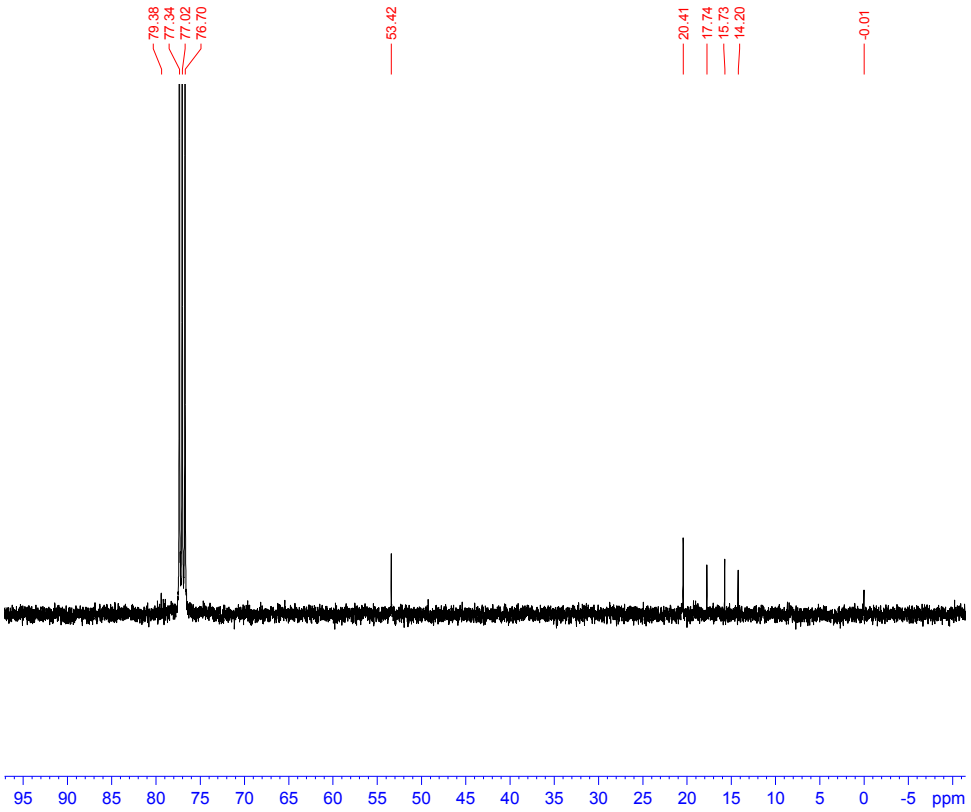
S44 ^{2}H- 2,3-butanediol sulfite-d$_2$



BRUKER

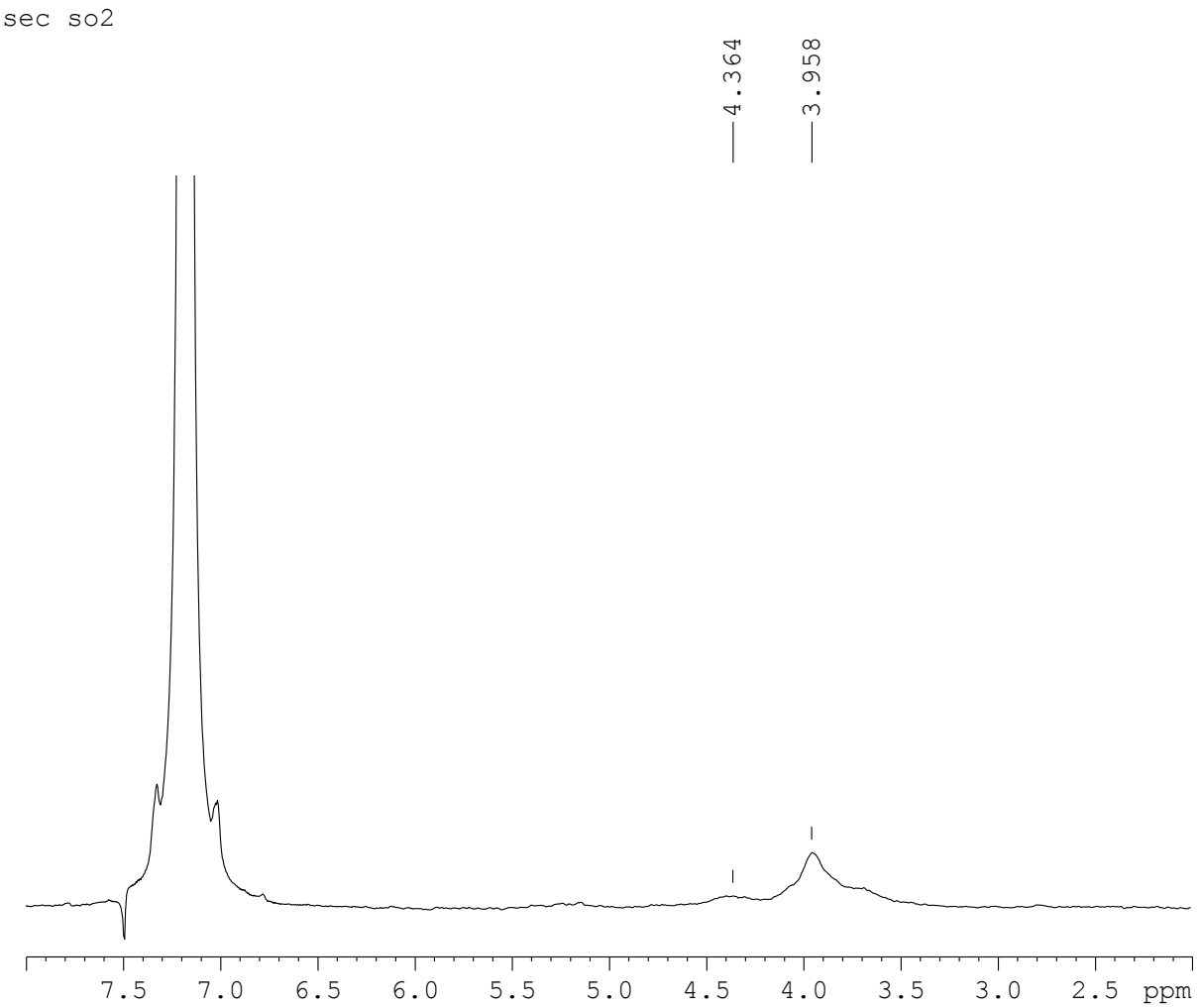
NAME	kh101-sec SO
EXPNO	13
PROCNO	1
Date_	20120626
Time	17.54
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg2h
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	1
DW	60.800 usec
DE	6.50 usec
TE	300.0 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	2H
P1	280.00 usec
PL1	-6.00 dB
PL1W	3.50999999 W
SFO1	61.4226981 MHz
SI	32768
SF	61.4223910 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

S45 ^{13}C- 2,3-butanediol sulfite-d_2

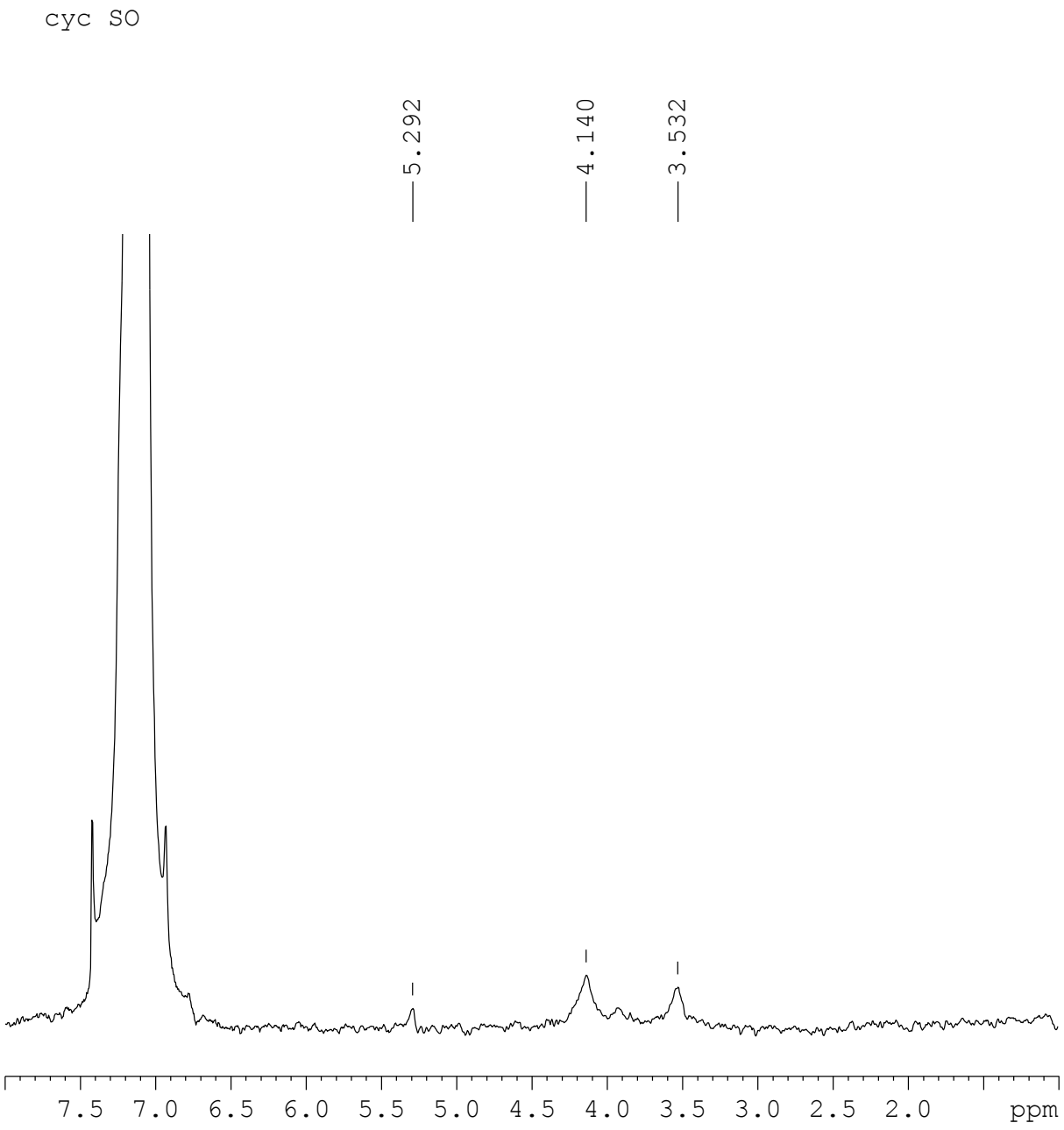



```
NAME        kh101-sec SO
EXPNO               20
PROCNO               1
Date_         20120626
Time             20.07
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                 2050
DW               20.800 usec
DE               10.04 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                7.80 usec
PL1               -3.60 dB
PL1W         82.86334991 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               -4.00 dB
PL12              14.24 dB
PL13              14.24 dB
PL2W         24.60733604 W
PL12W         0.36903250 W
PL13W         0.36903250 W
SFO2         400.1316005 MHz
SI                65536
SF           100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

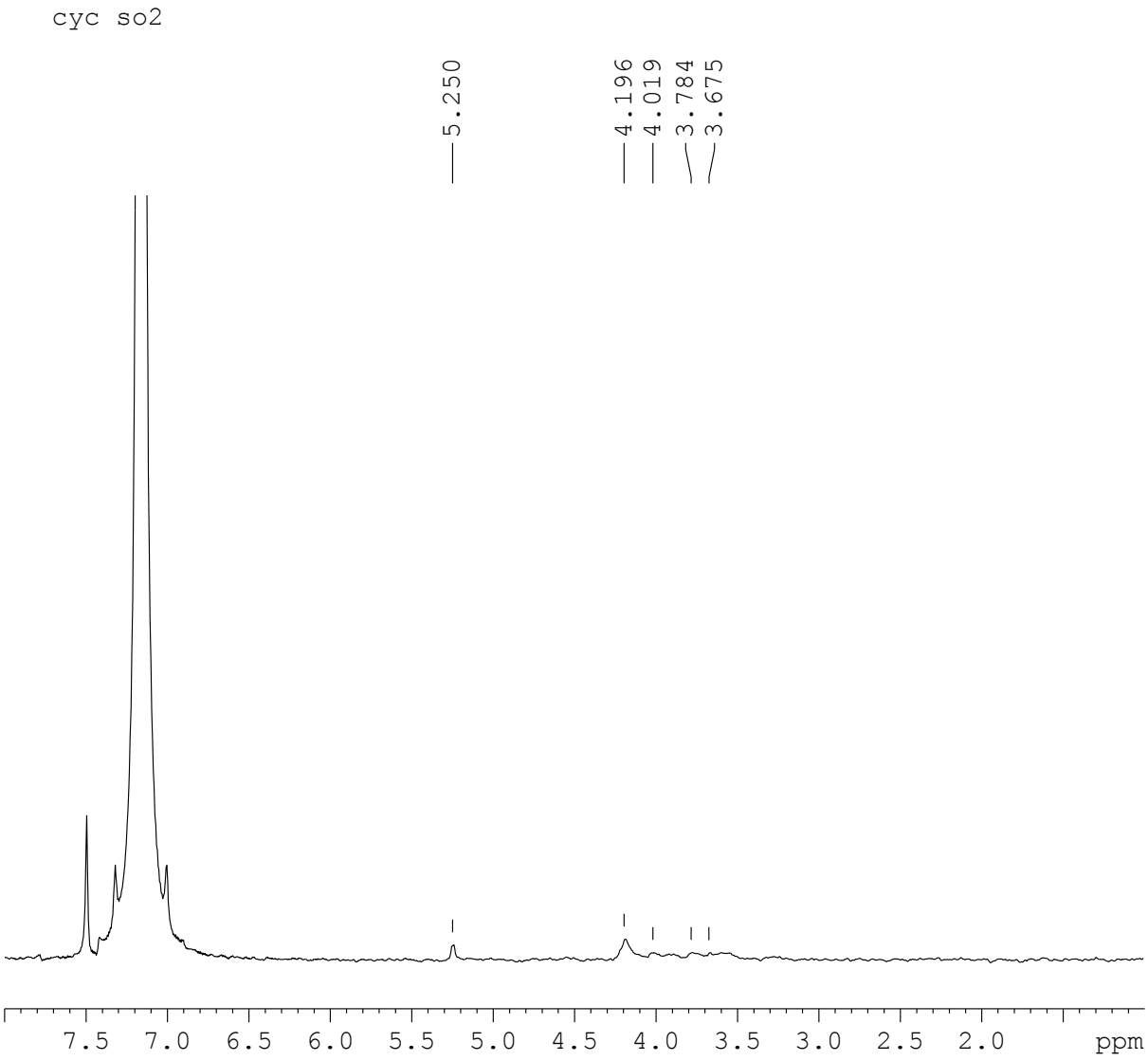
S46 ^{2}H- 2,3-butanediol sulfate-d_2



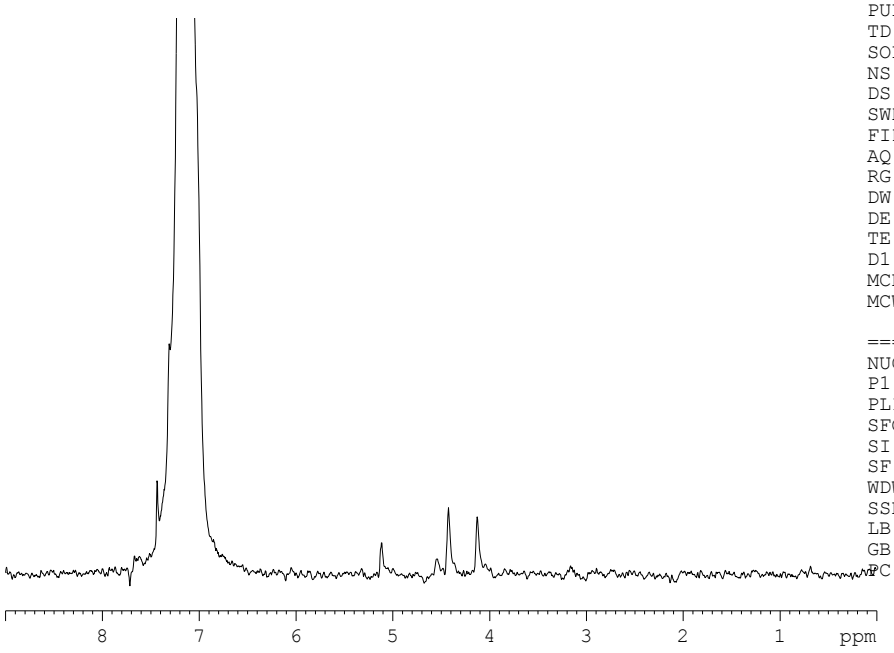
S47 ^{2}H Cyclohexanediol sulfite d2



S48 ^{2}H Cyclohexandiol sulfate-d_2



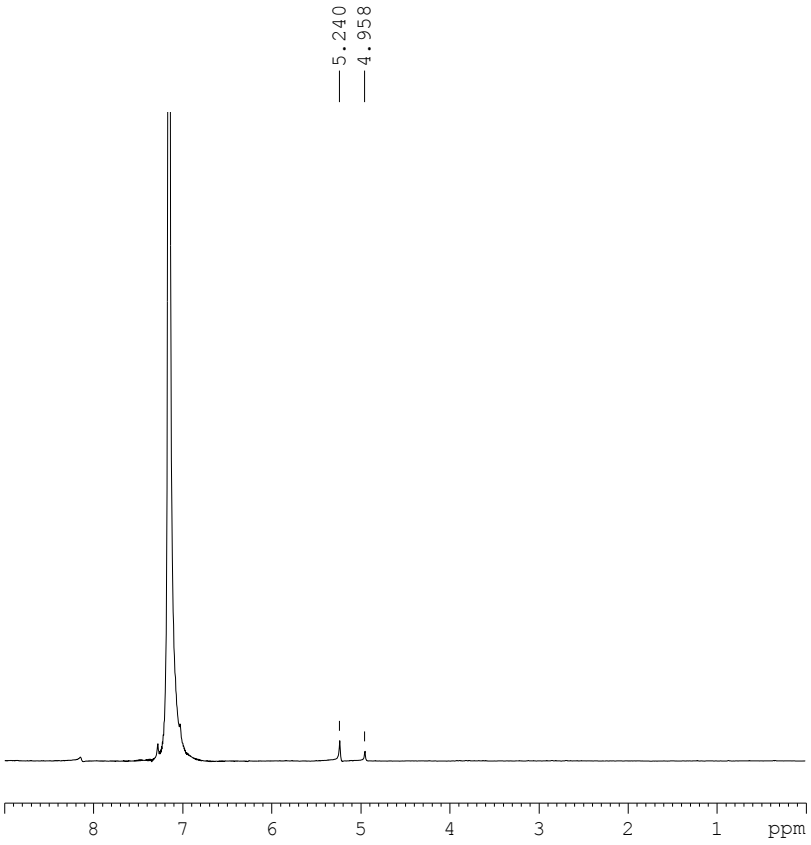
S49 ^{2}H ethylene glycol-d2 reaction with $SOCl_2$ in IL2



NAME	kah299b
EXPNO	11
PROCNO	1
Date_	20070424
Time	10.03
INSTRUM	spect
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	4096
SOLVENT	D2O
NS	128
DS	4
SWH	1531.863 Hz
FIDRES	0.373990 Hz
AQ	1.3369844 sec
RG	500
DW	326.400 usec
DE	7.11 usec
TE	300.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	2H
P1	400.00 usec
PL1	5.00 dB
SFO1	76.7735374 MHz
SI	4096
SF	76.7729664 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

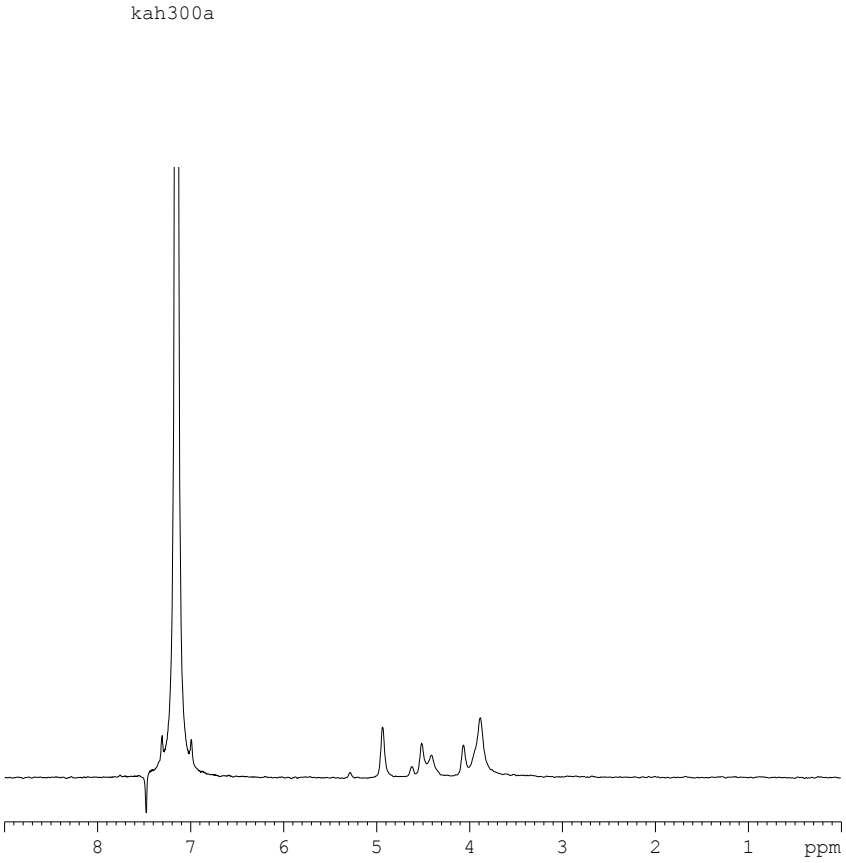
S50 ^{2}H ethylene glycol-d2 reaction with $SOCl_2$ and base in IL2

kah314b



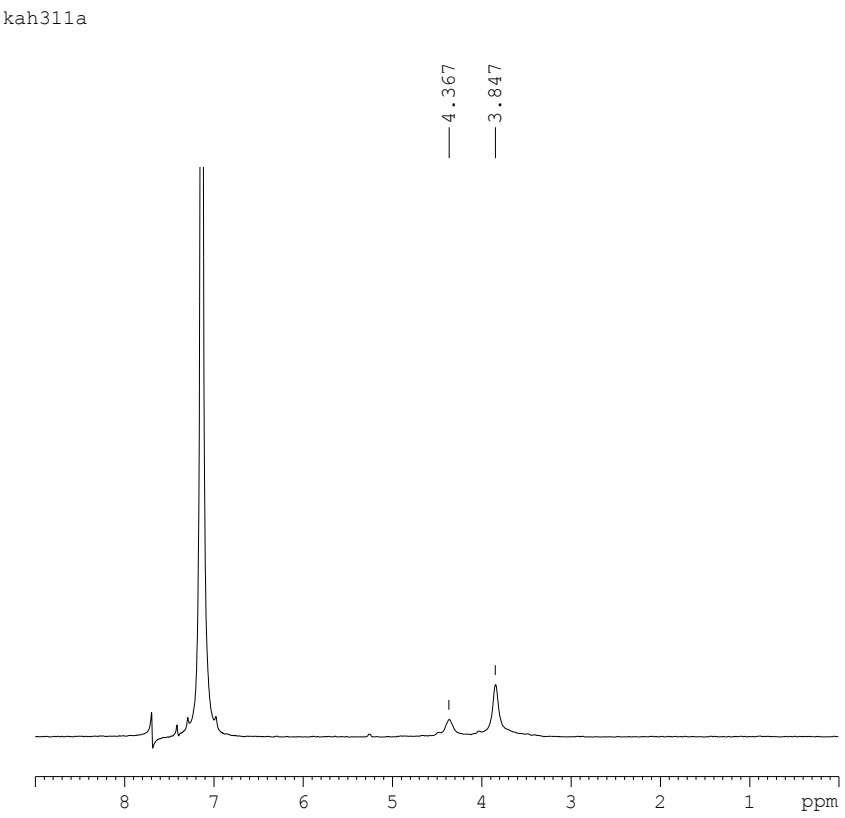

```
NAME              kah314b
EXPNO                  11
PROCNO                  1
Date_            20070503
Time                10.29
INSTRUM             spect
PROBHD    5 mm TXI 13C Z
PULPROG              zg30
TD                   4096
SOLVENT              C6D6
NS                    128
DS                      8
SWH             1531.863 Hz
FIDRES          0.373990 Hz
AQ             1.3369844 sec
RG                   500
DW               326.400 usec
DE                 7.11 usec
TE                300.0 K
D1           0.50000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                   2H
P1                400.00 usec
PL1                 5.00 dB
SFO1          76.7735374 MHz
SI                   4096
SF            76.7731569 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.00
```

S51 ^{2}H 2,3-butanediol-d2 reaction with $SOCl_2$ in IL1



NAME	kah300a
EXPNO	11
PROCNO	1
Date_	20070424
Time	12.15
INSTRUM	spect
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	4096
SOLVENT	D2O
NS	128
DS	4
SWH	1531.863 Hz
FIDRES	0.373990 Hz
AQ	1.3369844 sec
RG	500
DW	326.400 usec
DE	7.11 usec
TE	300.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	2H
P1	400.00 usec
PL1	5.00 dB
SFO1	76.7735374 MHz
SI	4096
SF	76.7729632 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

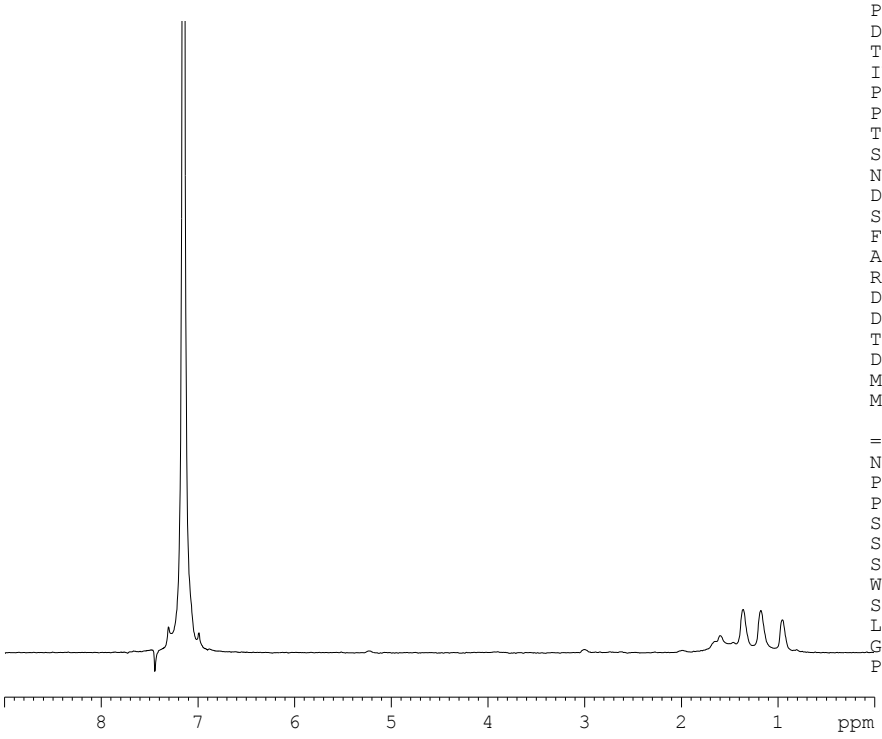
S52 ^{2}H 2,3-butanediol-d2 reaction with $SOCl_2$ and base in IL1



NAME	KAH311a
EXPNO	21
PROCNO	1
Date_	20070504
Time	18.04
INSTRUM	spect
PROBHD	5 mm TXI 13C Z
PULPROG	zg30
TD	4096
SOLVENT	C6D6
NS	128
DS	8
SWH	1531.863 Hz
FIDRES	0.373990 Hz
AQ	1.3369844 sec
RG	500
DW	326.400 usec
DE	7.11 usec
TE	300.0 K
D1	0.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	2H
P1	400.00 usec
PL1	5.00 dB
SFO1	76.7735374 MHz
SI	4096
SF	76.7729682 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

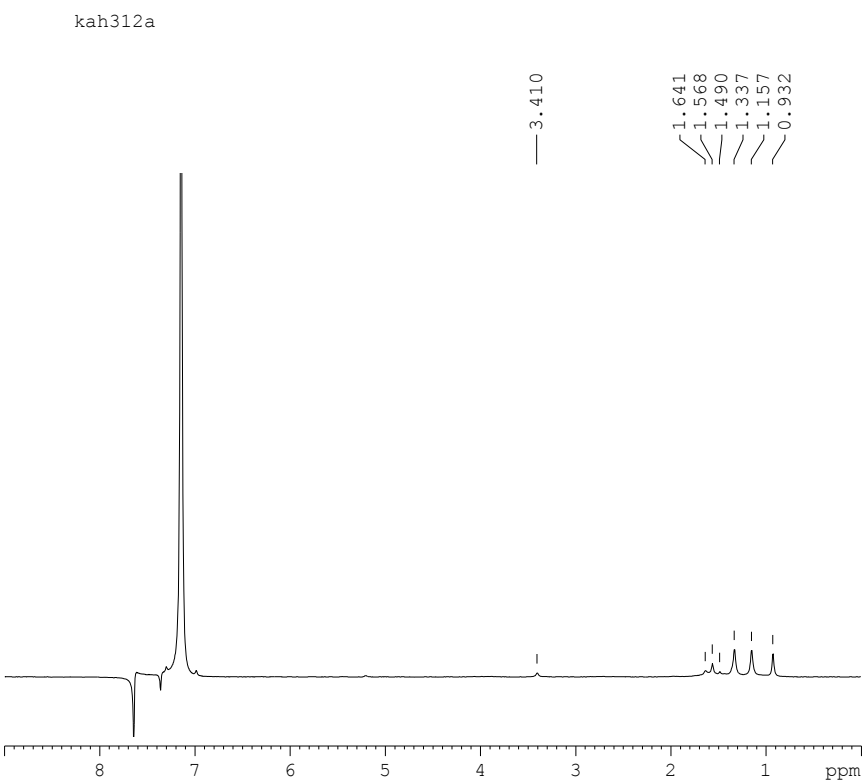
S53 ^{2}H pinacol-d6 reaction with $SOCl_2$ in IL1

kah301a



NAME	KAH301a
EXPNO	11
PROCNO	1
Date_	20070424
Time	14.26
INSTRUM	spect
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	4096
SOLVENT	C6D6
NS	128
DS	4
SWH	1531.863 Hz
FIDRES	0.373990 Hz
AQ	1.3369844 sec
RG	500
DW	326.400 usec
DE	7.11 usec
TE	300.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	2H
P1	400.00 usec
PL1	5.00 dB
SFO1	76.7735374 MHz
SI	4096
SF	76.7729656 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

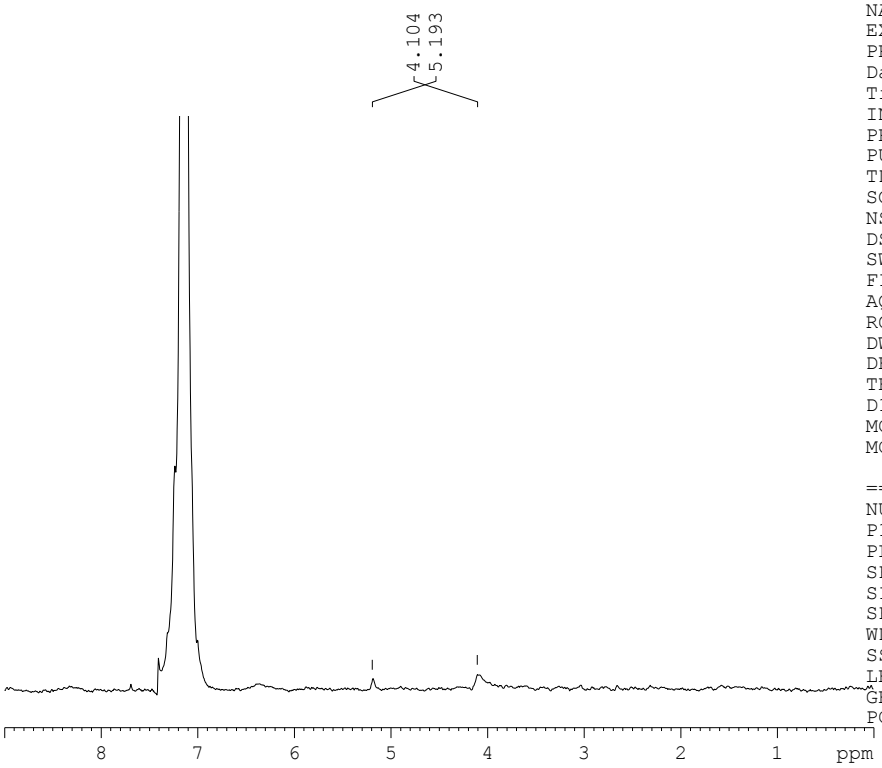
S54 ^{2}H pinacol-d6 reaction with $SOCl_2$ and base in IL1



NAME	KAH312a
EXPNO	11
PROCNO	1
Date_	20070502
Time	12.34
INSTRUM	spect
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	4096
SOLVENT	C6D6
NS	128
DS	8
SWH	1531.863 Hz
FIDRES	0.373990 Hz
AQ	1.3369844 sec
RG	500
DW	326.400 usec
DE	7.11 usec
TE	510.3 K
D1	0.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	2H
P1	400.00 usec
PL1	5.00 dB
SFO1	76.7735374 MHz
SI	4096
SF	76.7729719 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

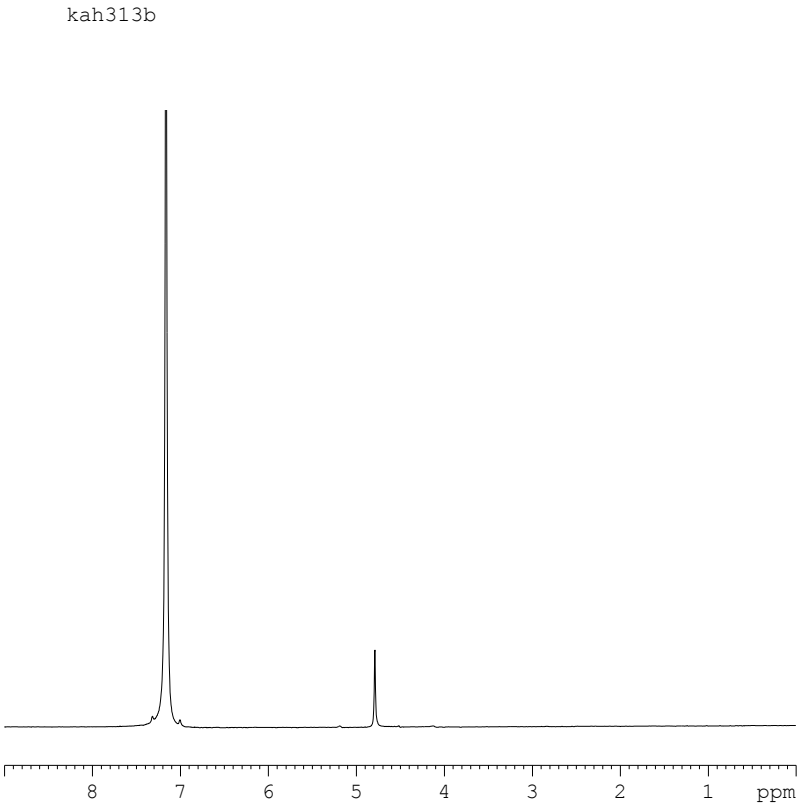
S55 ^{2}H 1,2-cyclohexanediol-d2 reaction with $SOCl_2$ in IL2

kah306a



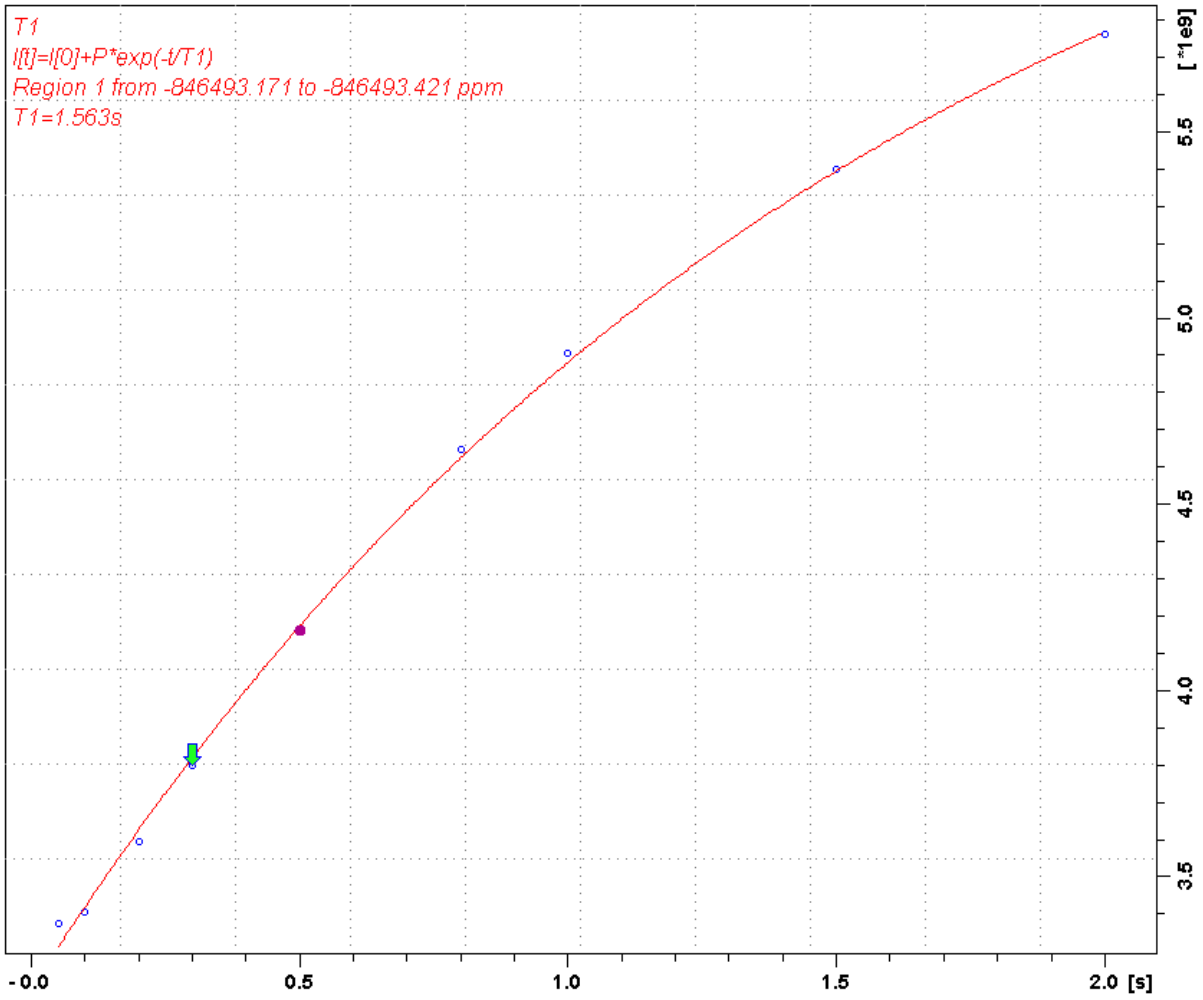
NAME	kah306a
EXPNO	11
PROCNO	1
Date_	20070425
Time	15.39
INSTRUM	spect
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	4096
SOLVENT	D2O
NS	128
DS	4
SWH	1531.863 Hz
FIDRES	0.373990 Hz
AQ	1.3369844 sec
RG	500
DW	326.400 usec
DE	7.11 usec
TE	300.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	2H
P1	400.00 usec
PL1	5.00 dB
SFO1	76.7735374 MHz
SI	4096
SF	76.7729683 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

S56 ^{2}H 1,2-cyclohexanediol-d2 reaction with $SOCl_2$ and base in IL1

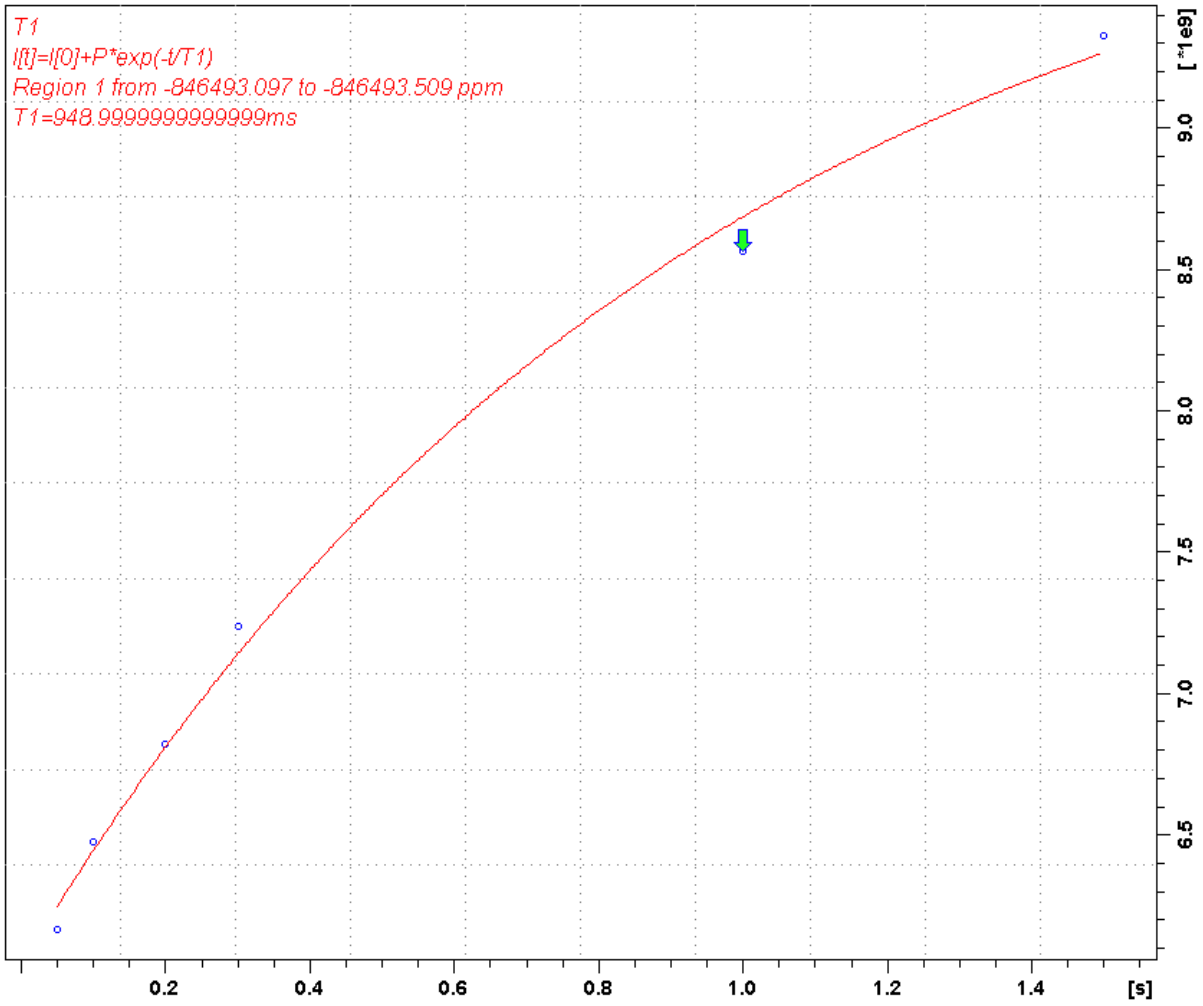


NAME	KAH313b	
EXPNO	11	
PROCNO	1	
Date_	20070502	
Time	14.10	
INSTRUM	spect	
PROBHD	5 mm Multinucl	
PULPROG	zg30	
TD	4096	
SOLVENT	C6D6	
NS	128	
DS	8	
SWH	1531.863	Hz
FIDRES	0.373990	Hz
AQ	1.3369844	sec
RG	500	
DW	326.400	usec
DE	7.11	usec
TE	510.3	K
D1	0.50000000	sec
MCREST	0.00000000	sec
MCWRK	0.01500000	sec
======== CHANNEL f1 ========		
NUC1	2H	
P1	400.00	usec
PL1	5.00	dB
SFO1	76.7735374	MHz
SI	4096	
SF	76.7731909	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.00	

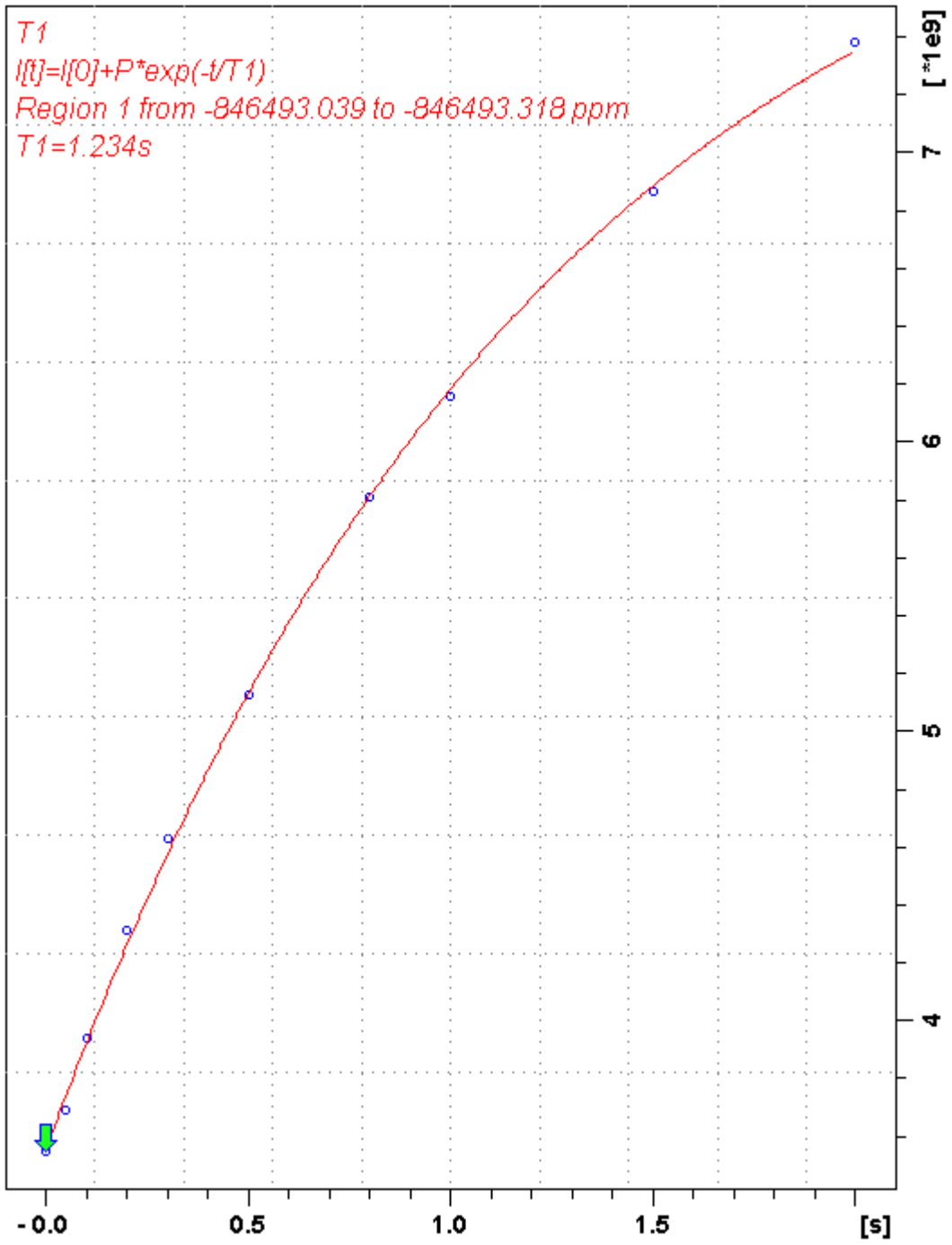
S57 T1 butanediol in NTf2



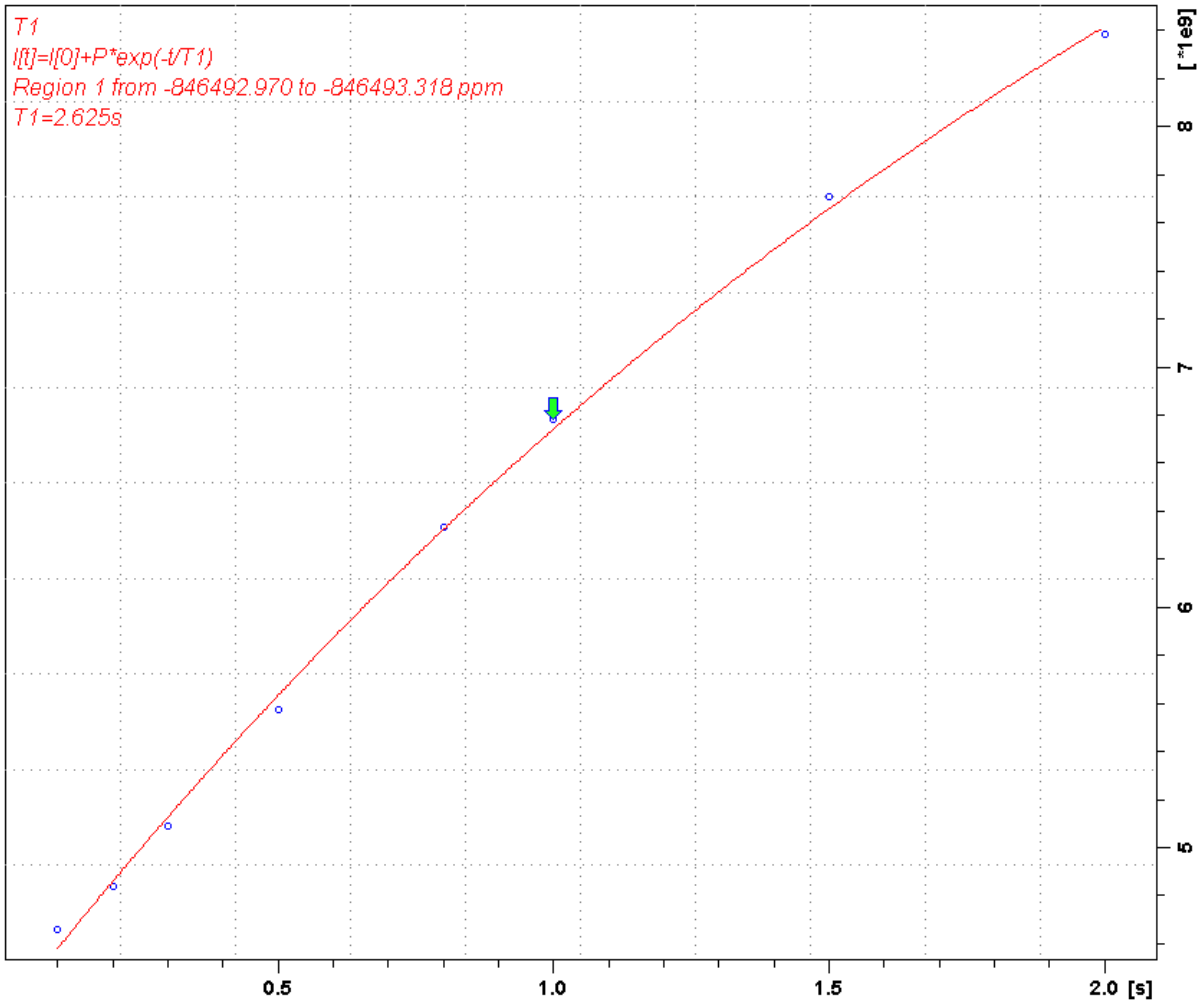
S58 T1 butanediol-d2 in FAP



S59 T1 butanediol sulfite in NTf2



S60 T1 butanediol sulfite in DCM



S61 T1 butanediol sulfite in FAP