

Supporting Information

Total Synthesis of MECA-79

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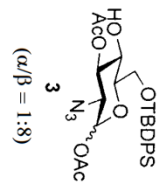
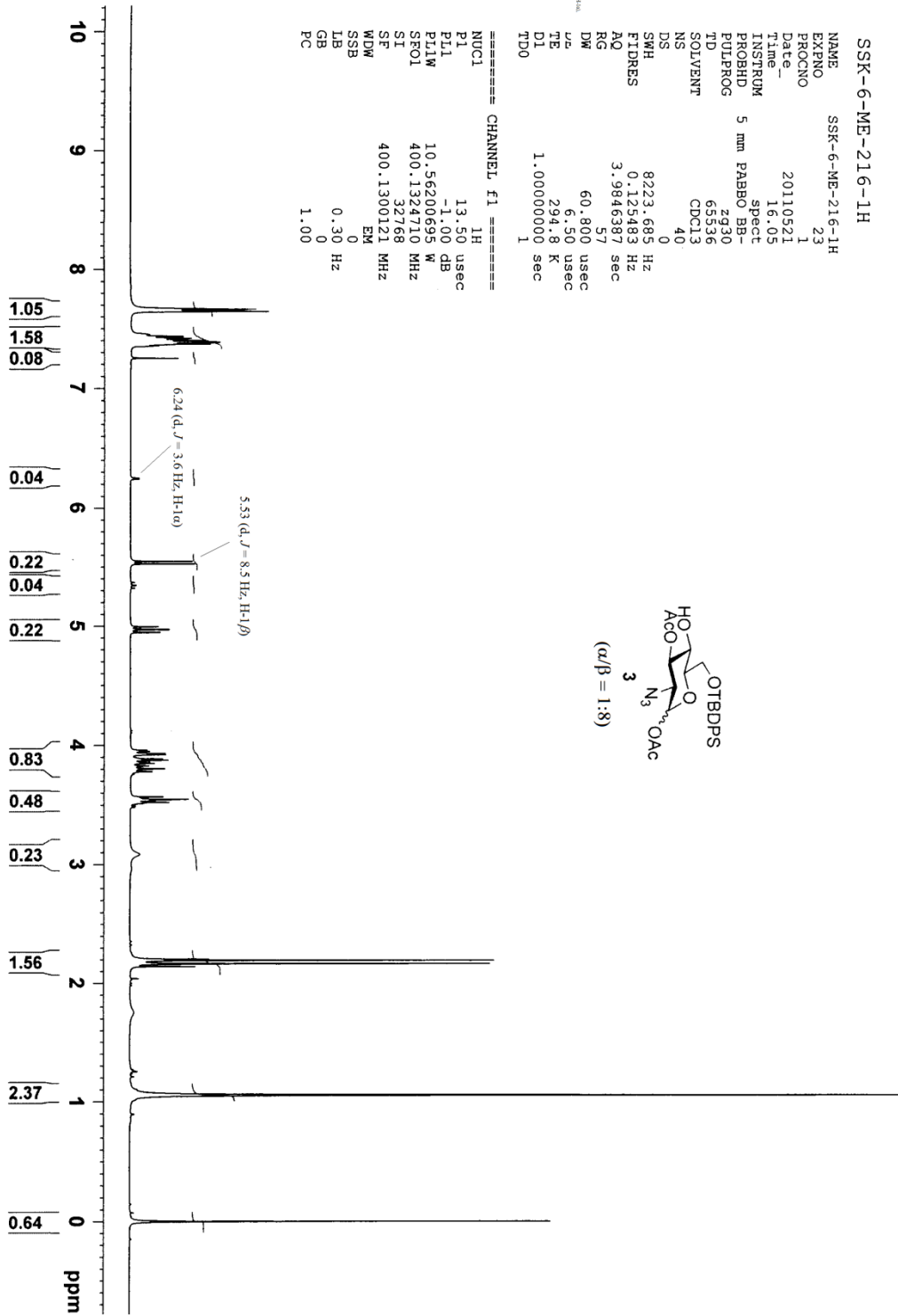
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SSK-6-ME-216-1H

NAME SSK-6-ME-216-1H
 EXPNO 23
 PROCNO 1
 Date_ 20110521
 Time_ 16.05
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 40
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.129483 Hz
 AQ 3.9846387 sec
 RG 57
 DW 60.800 usec
 DE 6.50 usec
 TE 294.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.50 usec
 PL1 -1.00 dB
 PL1W 10.56200695 W
 SFO1 400.1324710 MHz
 SI 32768
 SF 400.1300121 MHz
 WDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



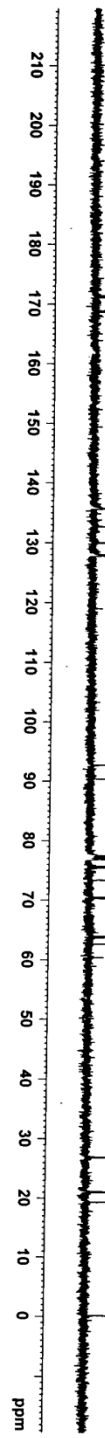
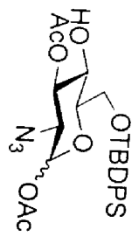
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NAME SSK-6-ME-216-13C
 EXPNO 24
 PROCNO 2
 Date_ 20110521
 Time_ 16:10
 INSTRUM spect
 PROBD 5 mm PABBO-RR-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 117
 DS 4
 SMH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 2050
 DW 20.800 usec
 DE 6.50 usec
 TE 295.5 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUCL1 13C
 P1 8.75 usec
 PL1 -2.00 dB
 PL1W 56.53121948 W
 SFO1 100.6228298 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUCL2 1H
 P2 80.00 usec
 PCPDZ -1.00 dB
 PL2 14.50 dB
 PL2W 10.5620695 W
 PL12W 0.23767781 W
 SFO2 400.1316008 MHz
 ST 100.612759 MHz
 SF 100.612759 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

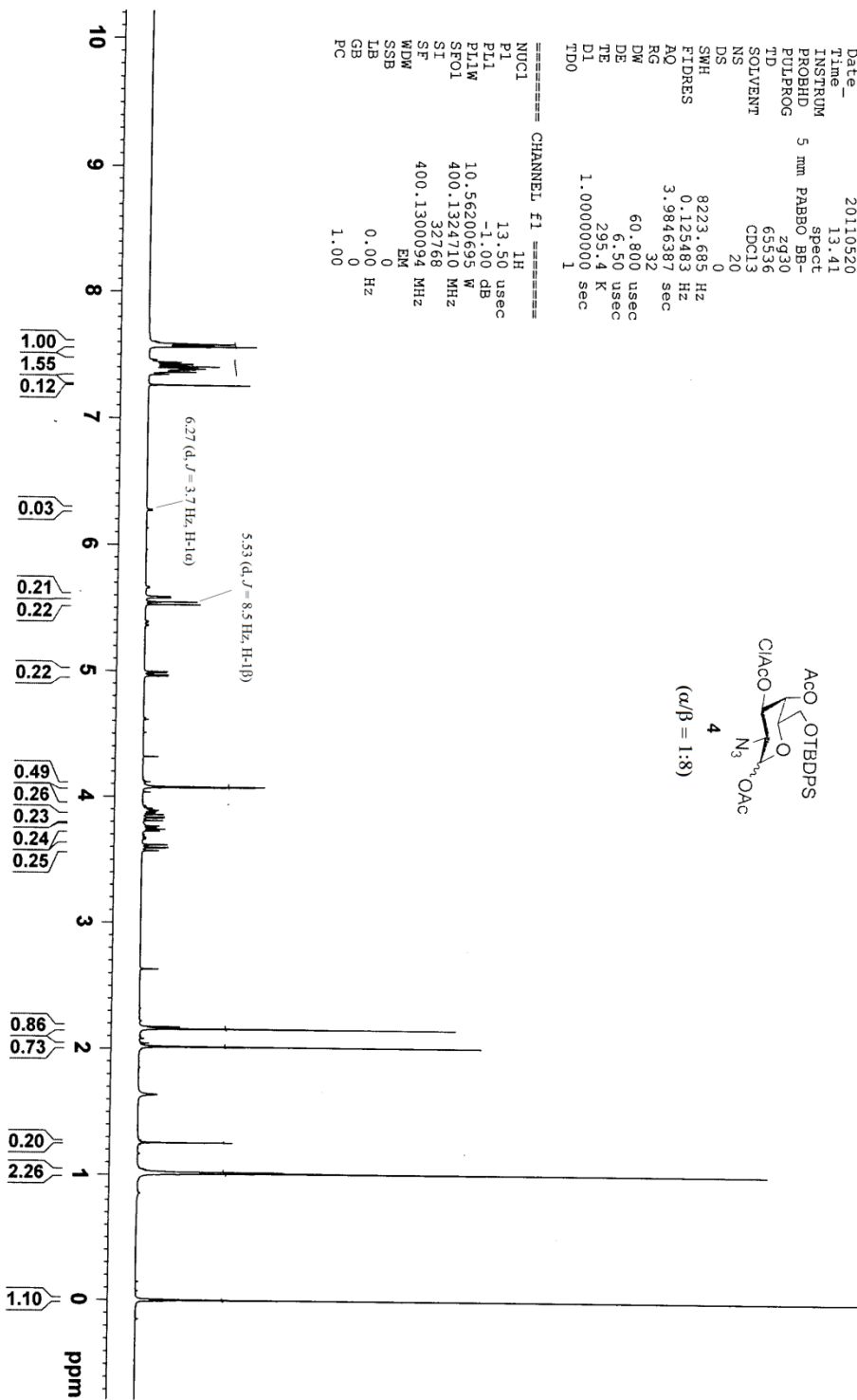
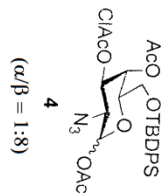
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 77.20
 76.88
 75.75
 75.53
 73.45
 70.55
 64.05
 62.75
 26.96
 21.11
 21.04
 19.38
 0.15



SSK-6-ME-278-1H

NAME SSK-6-ME-278-1H
 EXNO 22
 PROCNO 1
 Date 20110520
 Time 13.41
 INSTRUM 5 mm PABBO BB-
 PROBHD spect
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 20
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 32
 DM 60.800 usec
 DE 6.50 usec
 TE 295.4 K
 D1 1.00000000 sec
 TD0 1

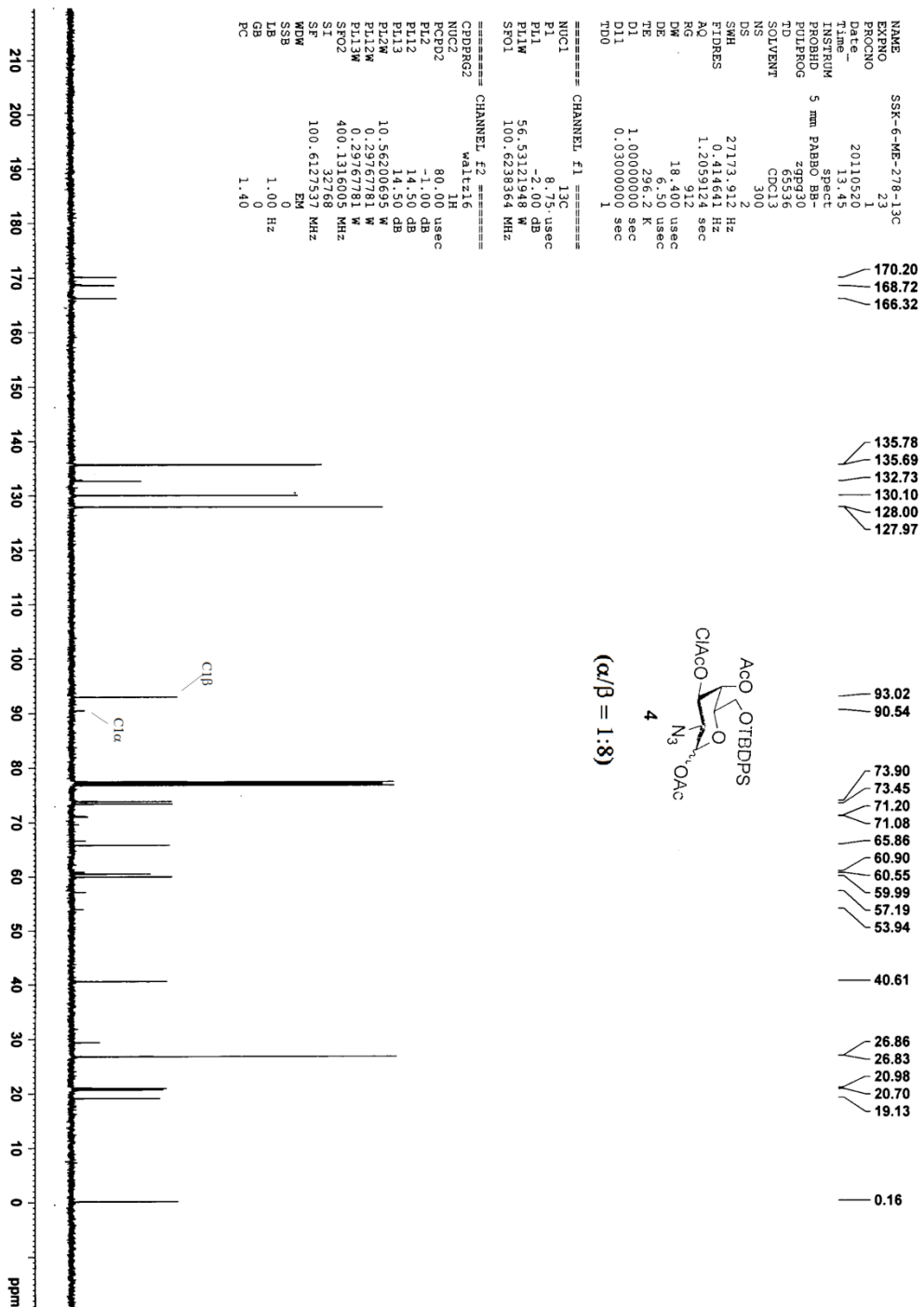
===== CHANNEL f1 =====
 NUCL 1H
 P1 13.50 usec
 PL1 -1.00 dB
 PL1W 10.56200695 W
 SF01 400.1324710 MHz
 SI 32768
 SF 400.1300094 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



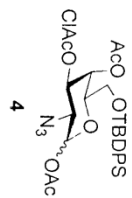
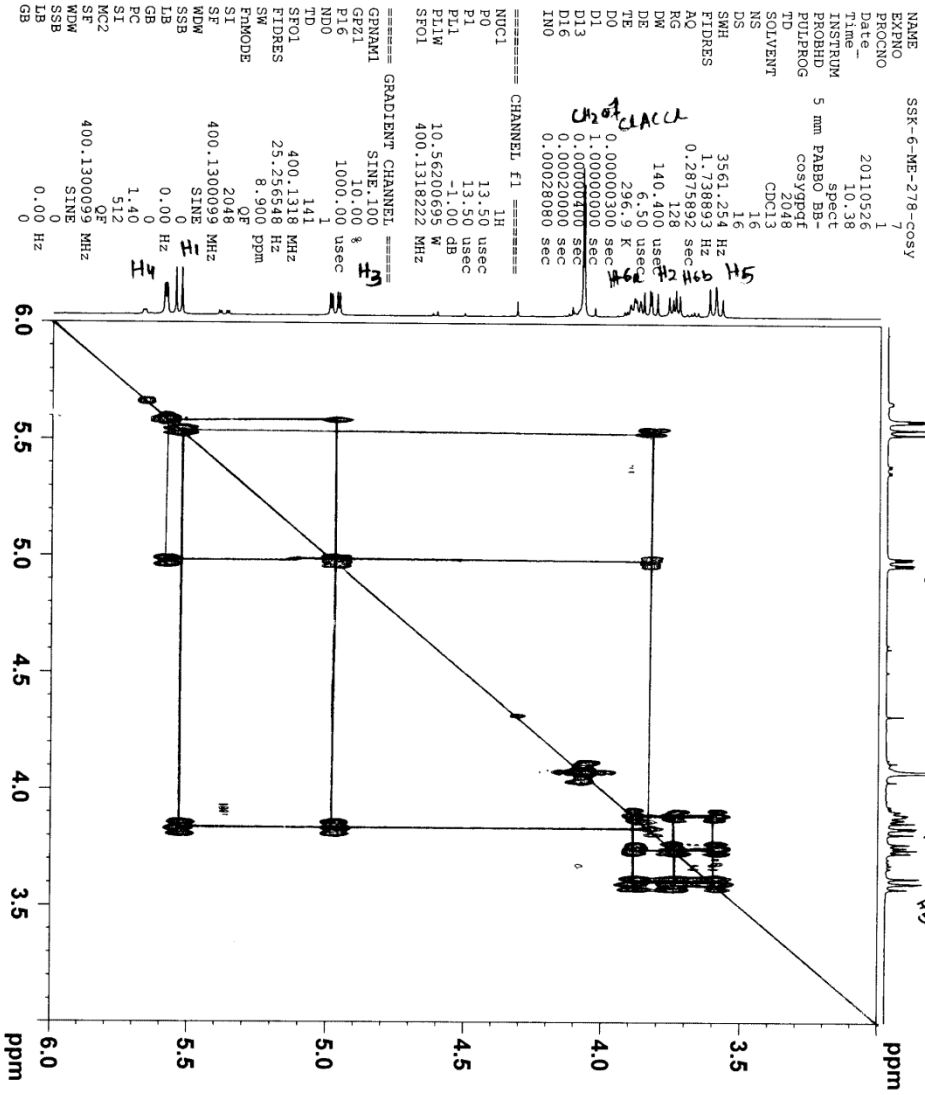
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NAME SSK-6-ME-278-13C
 EXPNO 23
 PROCNO 1
 Date_ 20110520
 Time 13.45
 INSTRUM Spect
 PULPROG 5 mm PABBO
 TD 4096
 SOLVENT DMSO
 NS 300
 DS 2
 SWH 27173.912 Hz
 FIDRES 0.414641 Hz
 AQ 1.2059124 sec
 RG 912
 DM 18.400 usec
 DE 6.50 usec
 TE 296.2 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.75 usec
 PL1 -2.00 dB
 PL1W 56.53121948 W
 SFO1 100.6238364 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 14.50 dB
 PL13 14.50 dB
 PL14 14.50 dB
 PL15 10.56200695 W
 PL16 0.2667781 W
 PL17 0.2667781 W
 SFO2 400.1316001 MHz
 SF 100.6127537 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



SSK-6-ME-278-COSY

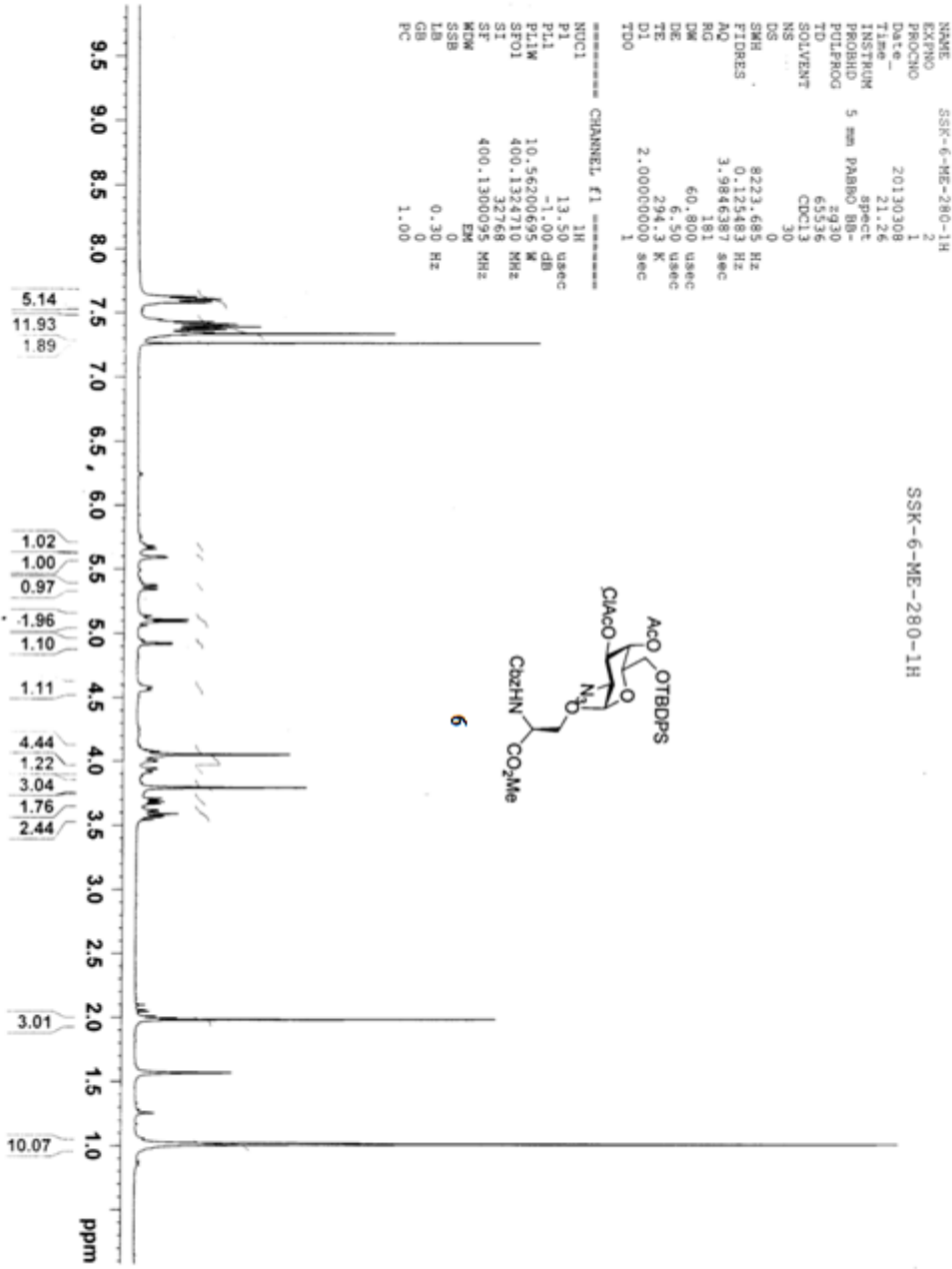


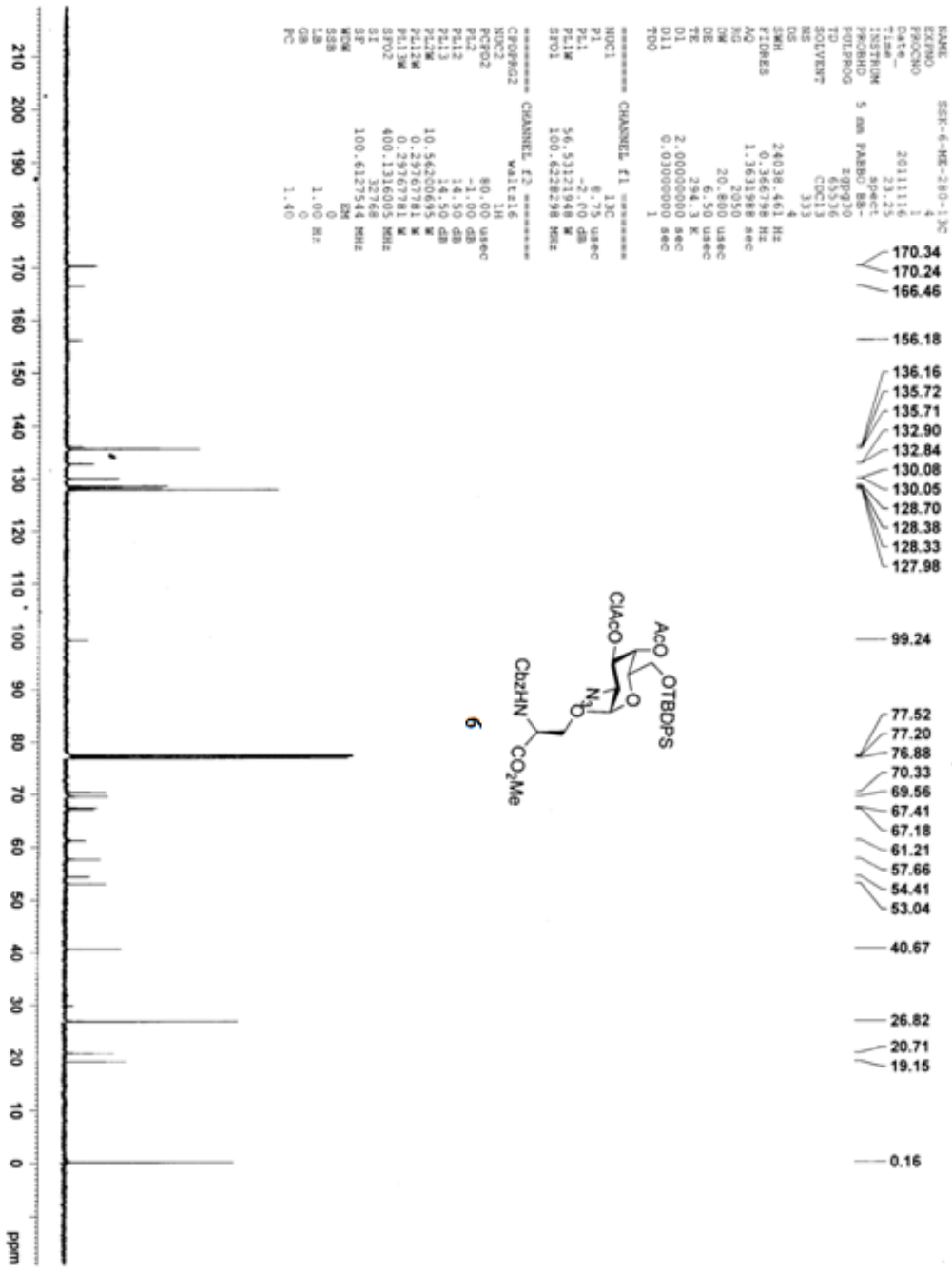
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NAME SSK-6-ME-278-cosy
EXPNO 1
PROCNO 1
Date_ 20110526
Time 10:38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygprf4
TD 42048
SOLVENT CDCl3
NS 16
DS 16
SWH 3561.254 Hz
FIDRES 1.739893 Hz
AQ 0.2879892 sec
RG 140.128
DM 140.400 usec
DE 26.50 K
TE 0.0000300 sec
D0 1.00000000 sec
D1 0.00000400 sec
D12 0.00020000 sec
D16 0.00028080 sec
IN0 0.00028080 sec

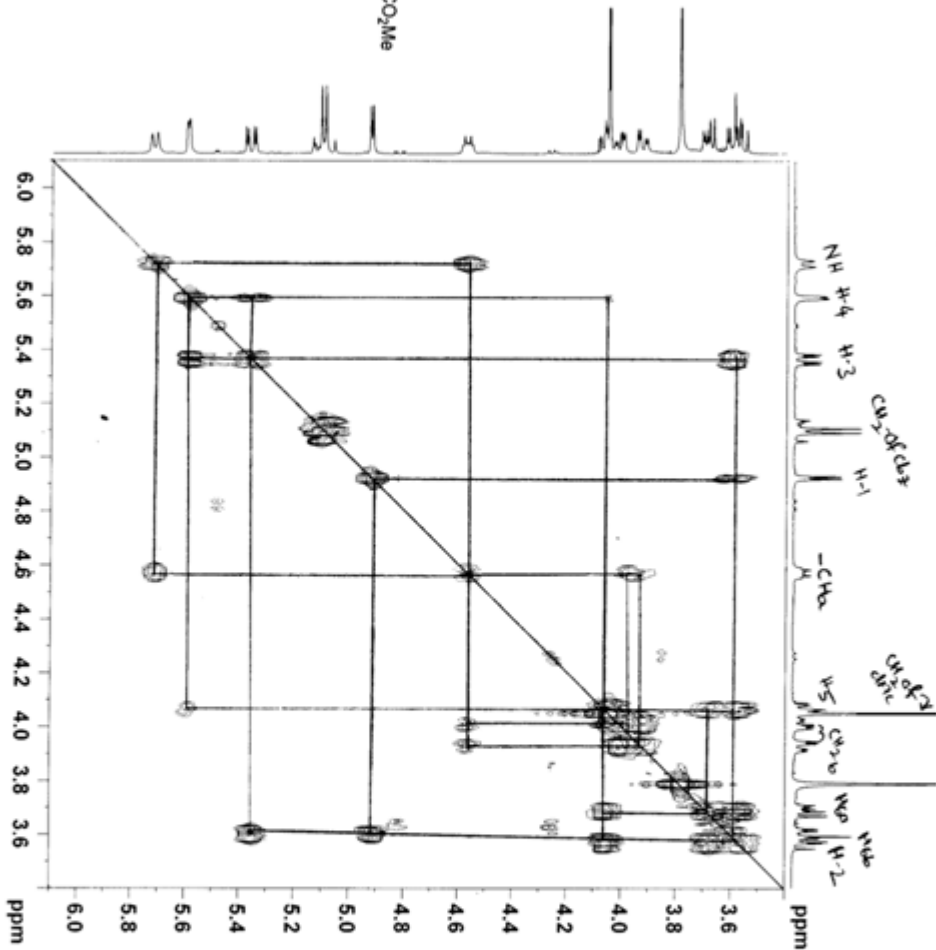
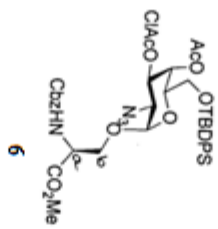
===== CHANNEL f1 =====
NUC1 1H
P1 13.50 usec
PL1 13.50 usec
PL12 1.00 dB
PL1W 10.56200695 W
SF01 400.1318222 MHz

===== GRADIENT CHANNEL =====
GENAMI SINE:100
SFZ1 10.00 %
F16 1000.00 usec
ND0 1
TD 141
SF01 400.1318 MHz
FIDRES 25.256548 Hz
SN 8.900 ppm
F2MODE QF
SI 2048
SF 400.1300099 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
FC 1.40
SI2 QF
SC 400.1300099 MHz
SHW SINE
SFB 0
GB 0.00 Hz
  
```





SSK-6-ME-280-1H FOR COSY



```

NAME          SSK-6-ME-280-1H COSY
EXPNO         64
PROCNO        2
F2          20110618
Date_         11
Time          1.47
INSTRUM       spect
PROBHD        5 mm PASAD BB-
PULPROG       coesypppgf
TD            2048
SOLVENT       CDCl3
NS            100
DS            16
SMR           3612.717 Hz
FIDRES       1.764022 Hz
AQ           0.2834932 sec
RG            203
DE           138.400 usec
TE           294.2 K
DO           0.00003100 sec
D1           1.00000000 sec
D13          0.00000400 sec
D16          0.00020000 sec
IR0           0.00027680 sec

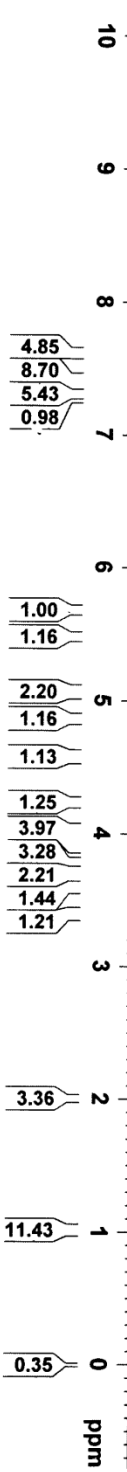
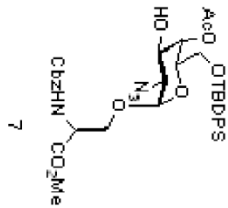
***** CHANNEL F1 *****
NUC1          13
P1            13.20 usec
PL1           -1.00 dB
P1LW         10.36200695 W
SFO1         400.1315961 MHz

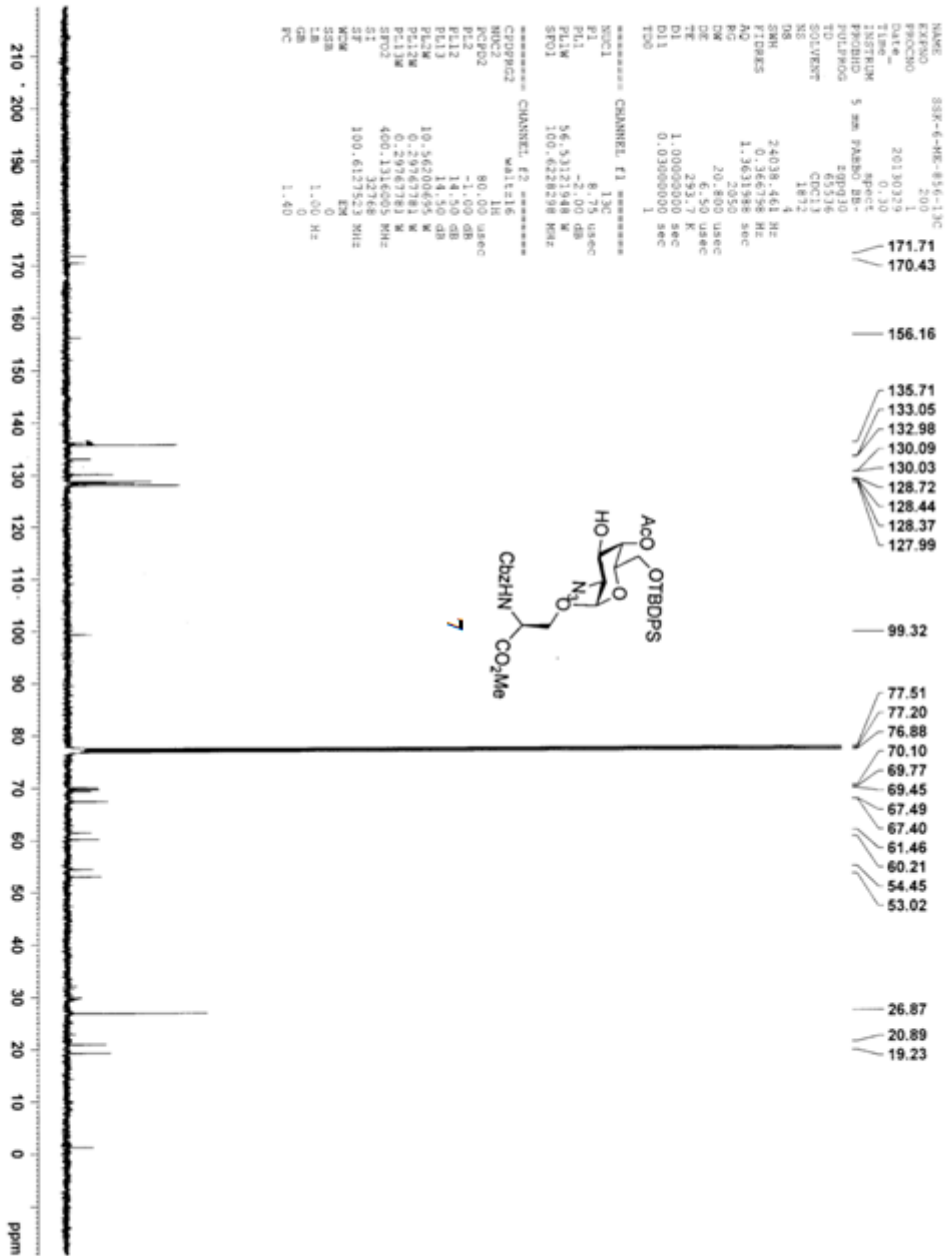
***** GRADIENT CHANNEL *****
GPRM1        SINE.100
GP21         10.00 %
P16          1000.00 usec
NCO          1
TD1          181
SFO1         400.1315 MHz
SFORS        19.319258 Hz
SFORES       9.00000000 Hz
PDMODER      SF
SF           400.1300099 MHz
SINE         SINE
SSA          0
LB           0.00 Hz
GB           0
PC           1.40
SI           0
SF2          400.1300000 MHz
SFO2         SINE
MVD          0
SDB          0
LB           0.00 Hz
GB           0
  
```

SSK-6-ME-856-1H

NAME SSK-6-ME-856-1H
 EXPNO 1
 PROCNO 1
 Date_ 20130329
 Time_ 0.10
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 30
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 128
 DW 60.800 usec
 DE 6.50 usec
 TE 293.5 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.50 usec
 PL1 -1.00 dB
 PL1W 10.56200695 W
 SFO1 400.1324710 MHz
 SI 32.768
 SF 400.1300095 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

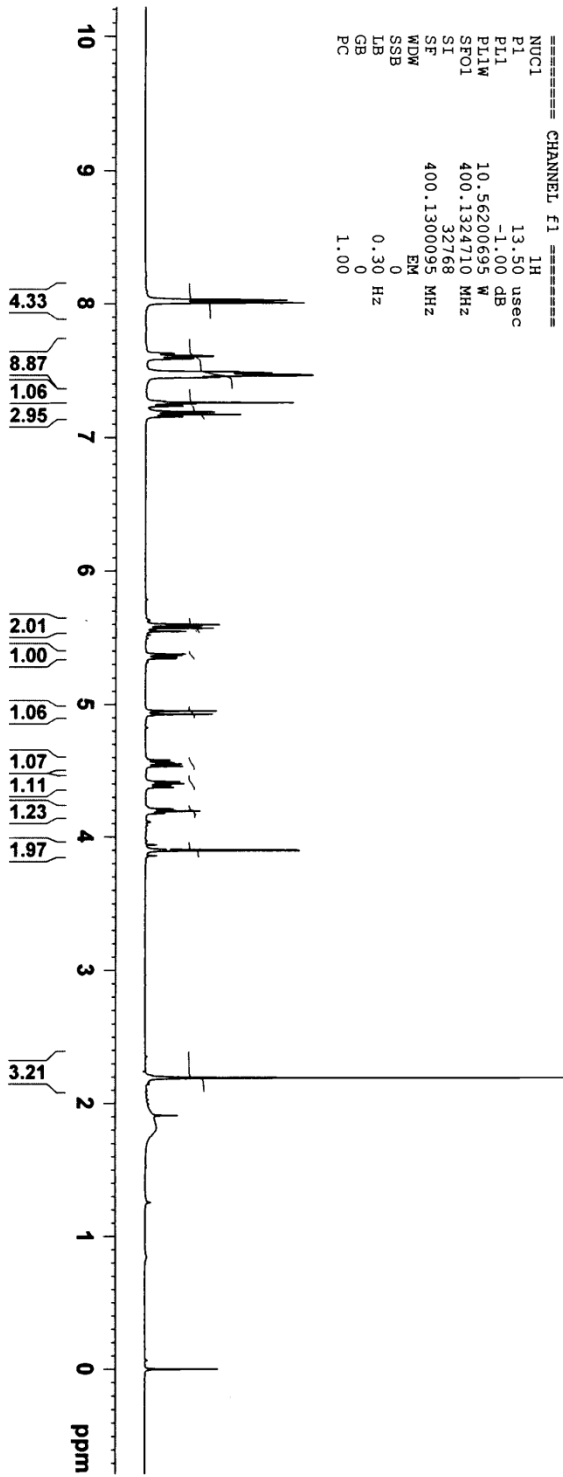


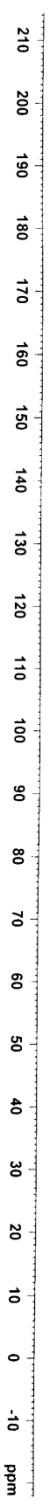


SSK-11-AMB-114-1H-

NAME SSK-11-AMB-114-1H-
EXPNO 999
PROCNO 1
Date_ 20140612
Time_ 22.17
INSTRUM spect
PROBHD 5 mm SEI 1H/D-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 21
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 90.5
DW 60.800 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.50 usec
PL1 -1.00 dB
PL1W 10.56200695 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





170.59
166.81
166.16
165.38

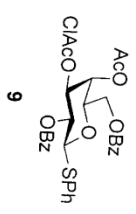
133.81
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132.64
130.08
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129.48
129.21
129.08
128.76
128.71
128.38

SSK-11-AMB-114-13C

87.23
77.45
77.20
76.95
74.77
73.92
67.81
67.58
62.34

40.51

20.88



Current Data Parameters
 NAME SSK-11-AMB-114-13C
 EXPNO 9
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140613
 Time 23.17
 INSTRUM spect
 NS14HD 5 mm PABBO
 PULPROG zgpg30
 TD 65536
 SFO1 125.770637 MHz
 SOLVENT DMSO
 NS 585
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 197.27
 DW 16.800 usec
 DE 2.79 K
 TE 300.2 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 125.770637 MHz
 NU1 13C
 P1 8.90 usec
 PLW1 103.0000000 W

==== CHANNEL f2 =====
 SFO2 500.132003 MHz
 NU2 1H
 CDDPRG12 waltz16
 PCPD2 80.00 usec
 PLW2 13.0000000 W
 PLW12 0.34327999 W
 PLW13 0.21969999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577683 MHz
 K2W EM
 SFS 0 1.00 Hz
 GB 0 1.40
 PC 1.40

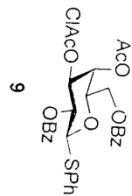
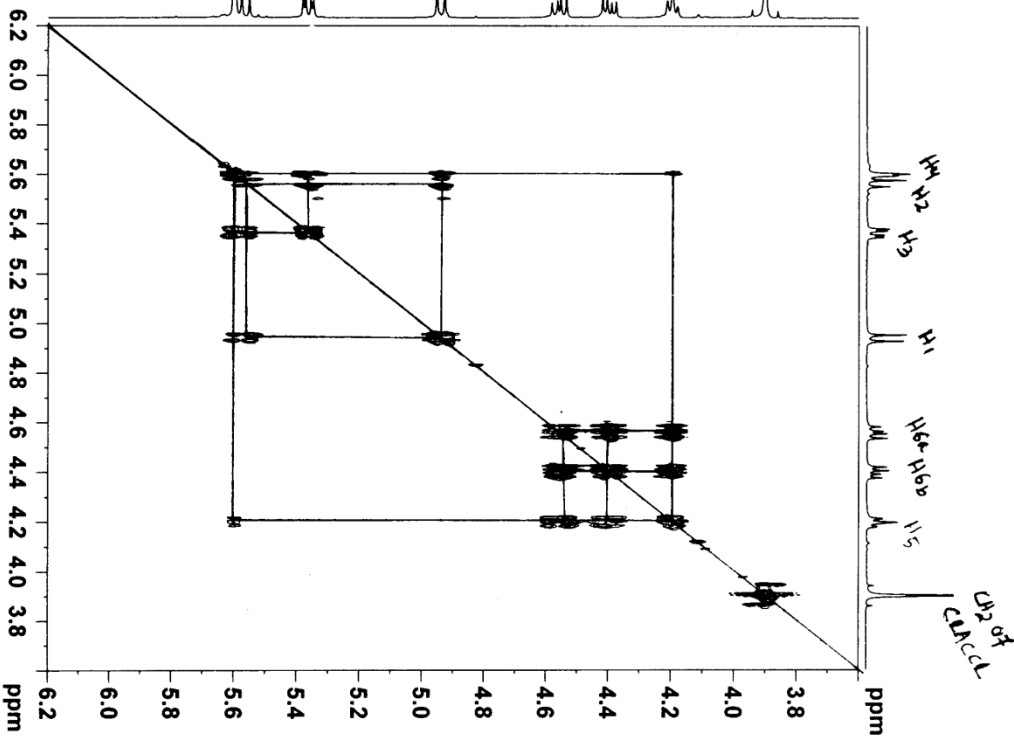
SSK-11-AMB-114-COSY

```

NAME          SSK-11-AMB-114-COSY
EXPNO         1
PROCNO        1
Date_         20140612
Time_        22:22:20
INSTRUM       5 mm SEI IH/D-
PROBHD        cosyprdf
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            16
DS            16
SWH           1302.083 Hz
FIDRES        0.635783 Hz
AQ            0.7864820 sec
RG            384.000 usec
DE            5.50 usec
TE            29.0 K
D0            0.00000300 sec
D1            1.00000000 sec
D12           0.00020000 sec
D13           0.00020000 sec
D16           0.00076800 sec
IN0           0.00076800 sec

===== CHANNEL f1 =====
NUC1          1H
P1            6.75 usec
PL1          -3.00 dB
PL12         16.73965454 dB
PL16         400.1318685 MHz
SF01         400.1300935 MHz

===== GRADIENT CHANNEL =====
GPRAM1       SINE_100
GPZ1         10.00 %
PLG          1000.00 usec
ND0
TD           82
SF01         400.1316 MHz
FIDRES        15.878823 Hz
SN           3.254 ppm
F2MODE       VE
SI           2048
SF           400.1300935 MHz
SFO1         400.1300935 MHz
SINE
WDW          SINE
SSB          0
LB           0.00 Hz
GB           0
EC           1.40
FC           0
SC2          512
SF           400.1300095 MHz
SFO1         400.1300095 MHz
SINE
SSB          0
LB           0.00 Hz
GB           0
  
```



SSK-11-AMB-144-1H

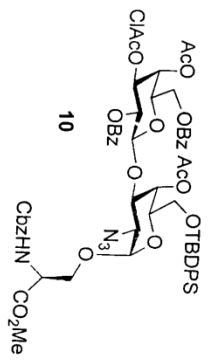
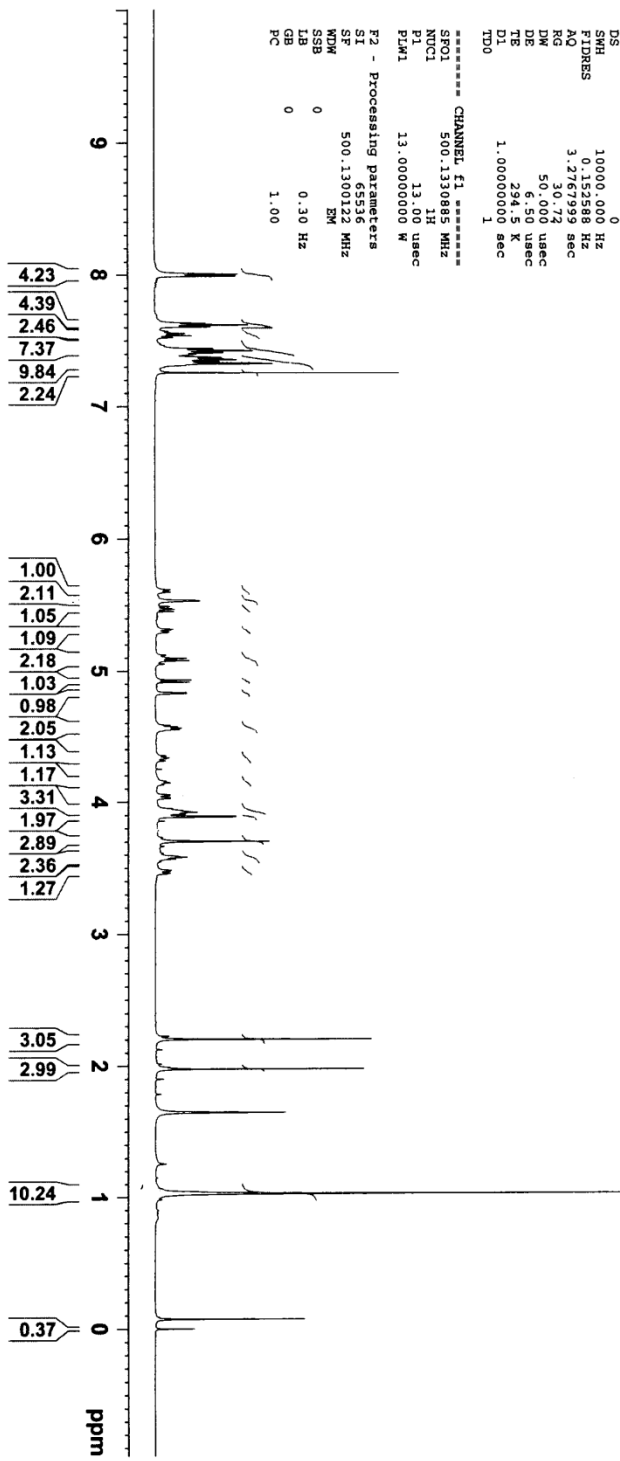
Current Data Parameters
 NAME SSK-11-AMB-144-1H
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20131110
 Time 11.43
 INSTRUM spect
 PROBD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CMC13
 NS 1
 DS 1
 SMH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 30.72
 DW 50.000 usec
 DE 6.50 usec
 TE 294.5 K
 D 1.0000000 sec
 TDO 1

***** CHANNEL f1 *****
 SFO1 500.130885 MHz
 NUC1 1H
 P1 13.00 usec
 PLM1 13.00000000 W

F2 - Processing Parameters
 SI 46536
 SF 500.1300122 MHz
 EM
 SSB 0
 LB 0 0.30 Hz
 GB 0
 PC 1.00



- SSK-11-AMB-224-13C
- 170.67
 - 170.40
 - 169.39
 - 166.82
 - 165.94
 - 165.25
 - 156.12
 - 136.11
 - 135.71
 - 135.70
 - 133.55
 - 133.54
 - 133.21
 - 133.16
 - 129.95
 - 129.87
 - 129.44
 - 129.29
 - 128.75
 - 128.67
 - 128.58
 - 128.50
 - 128.39
 - 127.88
 - 127.83
 - 101.71
 - 98.86
 - 77.45
 - 77.40
 - 77.20
 - 76.95
 - 74.39
 - 72.63
 - 70.89
 - 70.79
 - 69.44
 - 69.31
 - 68.92
 - 67.44
 - 66.86
 - 62.52
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 - 54.32
 - 52.88
 - 40.50
 - 26.84
 - 20.85
 - 20.72
 - 19.24

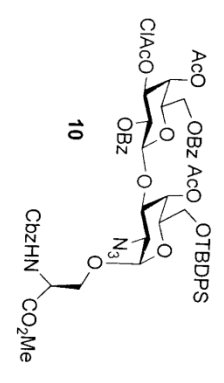
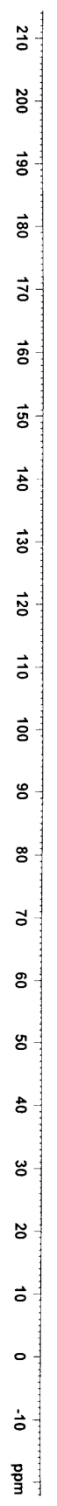
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 NAME SSK-11-AMB-224-13C
 EXPMO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140603
 Time 19:06
 INSTRUM 5 mm PABBO BBO
 PULPROG zgpg30
 TD 28516
 SOLVENT CDCl3
 NS 239
 DS 4
 SMH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 197.27
 DM 16.800 usec
 DE 8.50 usec
 TE 29.59 usec
 D1 1.0000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL F1 =====
 SFO1 125.7703637 MHz
 NUCL1 13C
 P1 8.90 usec
 FLM1 103.00000000 W

==== CHANNEL F2 =====
 SFO2 500.1320065 MHz
 NUCL2 1H
 CPDPRG2 waltz16
 BCPD2 13.00000000 W
 PLM12 0.34327999 W
 PLM13 0.21969999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577337 MHz
 MDW 0 EM
 SSB 0 1.00 Hz
 GB 0
 EC 1.40



SSK-11-AMB-227-1h

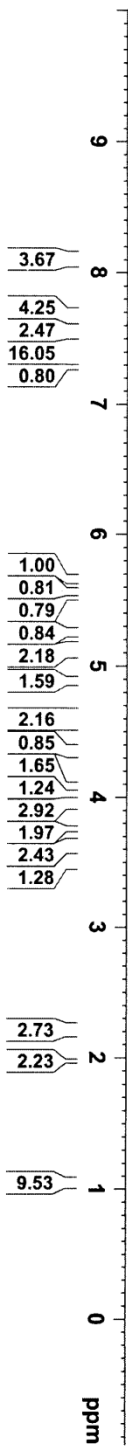
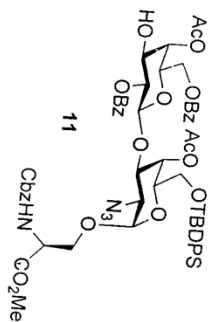
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NAME SSK-11-AMB-227-1h
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters

Date_ 20140613
Time 23.57
INSTRUM spect
PROBHD 5 mm BBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 41
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.276797 sec
RG 972
DE 50.000 usec
TE 297.8 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.130892 MHz
NUC1 13C
P1 13.00 usec
PL1 13.00000000 W

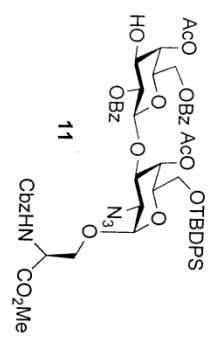
F2 - Processing parameters
SI 65536
SF 500.130000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



SSK-11-AMB-177-13C

171.08
170.50
170.37
169.26
166.52
166.18
165.95
165.23
156.05
135.99
135.61
135.57
133.32
133.22
133.07
132.96
129.83
129.74
129.59
129.45
128.60
128.49
128.37
128.30
128.25
128.00
127.77
127.74
127.71
101.58
98.78
77.46
77.40
77.20
76.95
74.50
73.06
72.95
72.48
71.11
70.99
70.86
69.98
69.52
68.78
67.30
67.08
62.54
61.71
59.36
54.21
52.77

26.73
20.81
20.61
19.13
19.08



Current Data Parameters
 NAME SSK-11-AMB-177-13C
 EXPNO 13
 PROCNO 1

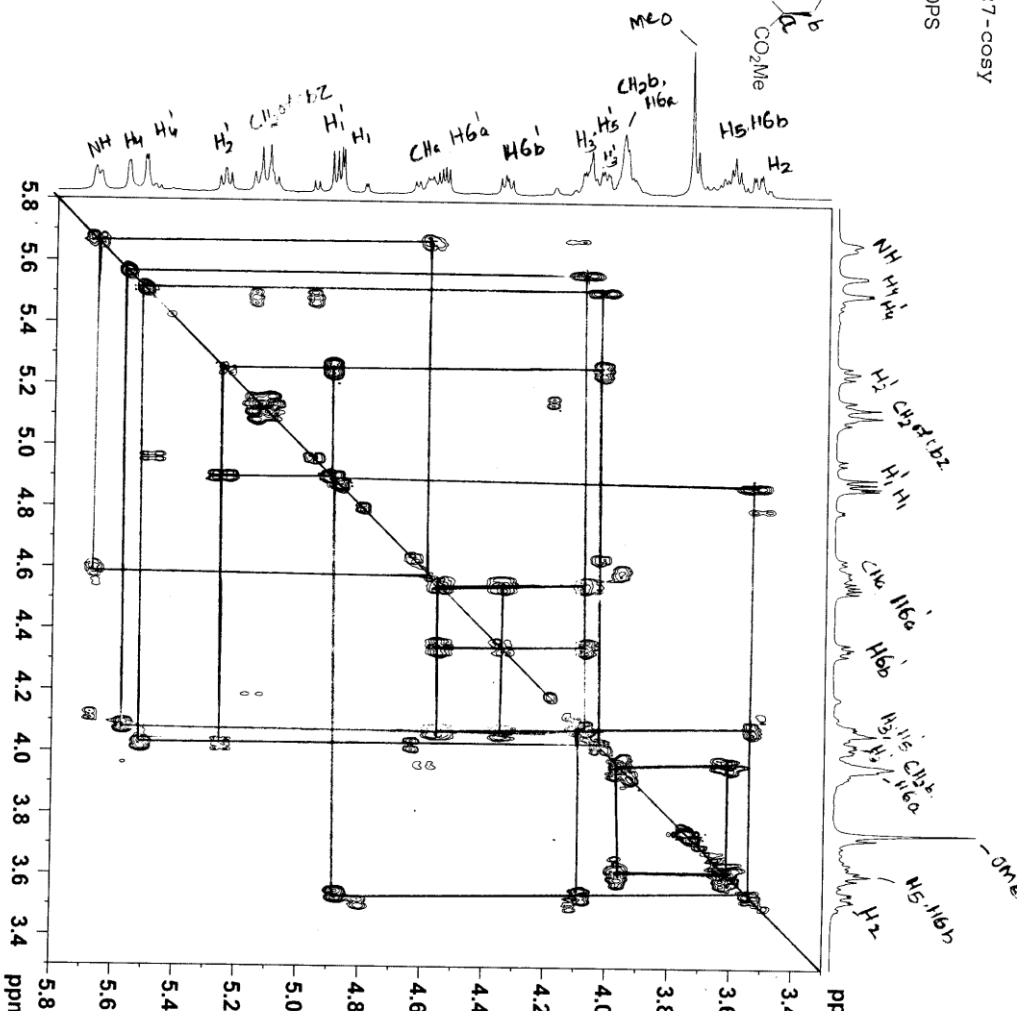
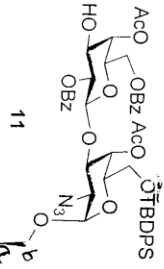
F2 - Acquisition Parameters
 Date_ 20140126
 Time 11:25
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 91
 DS 4
 SMH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 197.27
 DQ 16.890 usec
 DE 1.480 usec
 TE 293.7 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

==== CHANNEL #1 =====
 SFO1 125.7703637 MHz
 NUQ1 13C
 P1 8.99 usec
 P1A1 103.00000000 W

==== CHANNEL #2 =====
 SFO2 500.1320005 MHz
 NUQ2 1H
 CPDPRD12 waltz16
 PCPD2 80.00 usec
 PLM12 13.00000000 W
 PLM13 0.34327999 W
 PLM13 0.21969999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577928 MHz
 VM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

SSK-11-AMB-227-cosy



Current Data Parameters
 Name: SSK-11-AMB-227-cosy
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_ Time: 20120523 13:53
 INSTRUM: spect
 PROBHD: 5 mm PABBO BB/
 PULPROG: cosypppqr
 T1: 1.00
 SOLVENT: CDCl3
 NS: 4
 DS: 8
 SWH: 1490.757 Hz
 FIDRES: 0.1453446 Hz
 AQ: 0.343446 sec
 RG: 61.42
 DW: 335.400 usec
 DE: 6.50 usec
 TE: 300.2 K
 D0: 0.0000100 sec
 D1: 1.000000000 sec
 D11: 0.030000000 sec
 D12: 0.0002000 sec
 D13: 0.0000000 sec
 D16: 0.0002000 sec
 INO: 0.00067080 sec

===== CHANNEL f1 =====
 SFO1: 500.132400 MHz
 NUC1: 1H
 P0: 13.00 usec
 P1: 13.00 usec
 PL1: 2500.00 usec
 PL10: 13.0000000 usec
 PL11: 3.250000000 M

===== GRADIENT CHANNEL =====
 GPCP: SMC010.100
 GP2P: SMC010.100
 P16: 1000.00 usec

F1 - Acquisition parameters
 SFO1: 500.132400 MHz
 FIDRES: 15.21809 Hz
 SW: 2.981 ppm
 RMWDEL: QF

F2 - Processing parameters
 SI: 1024
 SF: 500.1300000 MHz
 WDM: 0 Hz
 SSB: 0 Hz
 GB: 0
 PC: 1.40

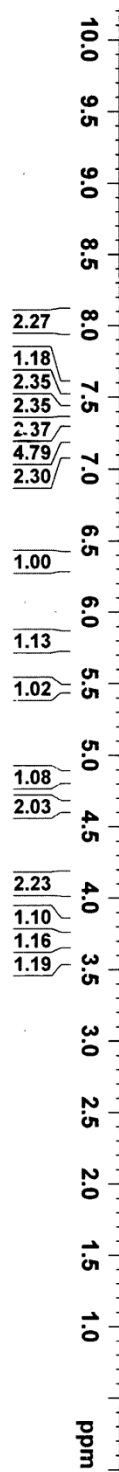
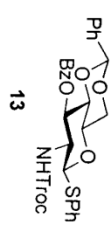
F1 - Processing parameters
 SI: 1024
 SF: 500.1300000 MHz
 WDM: 0 Hz
 SSB: 0 Hz
 GB: 0
 PC: 1.40

SSK-11-AMB-226-1H

SSK-11-AMB-226-1H

NAME SSK-11-AMB-226-1H
 EXRNO 1
 PROCNO 1
 Date_ 20140614
 Time 14.35
 INSTRUM 5 mm SEI 1H/D-
 PROBD spect
 PULPROG zg30
 TD 2930
 F2 65536
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 28.5
 DW 60.800 usec
 DE 6.50 usec
 TE 295.9 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUCL 1H
 P1 6.75 usec
 PL1 -3.00 dB
 PL1W 16.73965454 W
 SF01 400.1324710 MHz
 SI 32768
 SF 400.1300213 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



SSK-11-AMB-226-13C

167.03
154.60
136.92
133.70
132.69
132.57
130.13
129.01
128.95
128.55
128.14
128.11
125.87
100.96
95.45
88.35
87.73
77.37
77.12
76.86
74.42
73.80
70.49
68.30
55.52

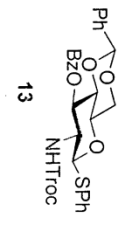
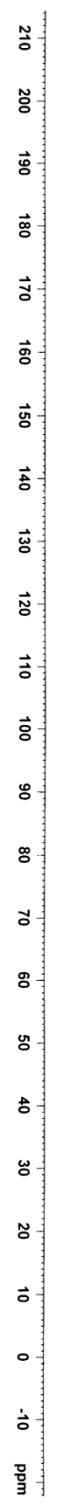
Current Data Parameters
NAME SSK-11-AMB-226-13C
EXENO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140617
Time 11:24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 396
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 197.27
DM 16.880 usec
DE 4.480 usec
TE 297.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 125.7703637 MHz
NUC1 13C
P1 8.90 usec
PL1 103.00000000 W
PLM1

==== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
PCPD12 waltz16
PCPD2 80.00 usec
PLM2 13.00000000 W
PLM12 0.34327999 W
PLM13 0.21969999 W

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



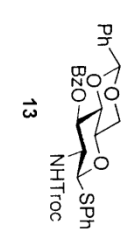
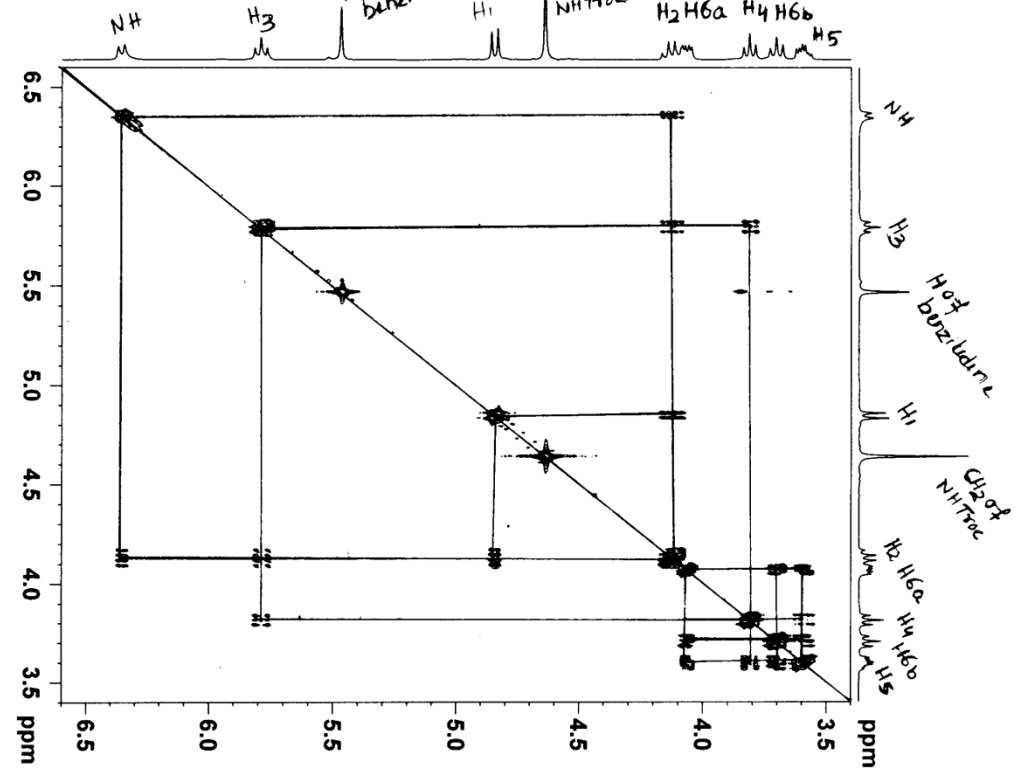
SSK-11-AMB-226-COSY

```

NAME          SSK-11-AMB-226-COSY
EXPNO         1
PROCNO        1
Date_         20140614
Time          14.59
INSTRUM       spect
PROBHD        5 mm SEI 1H/D-
PULPROG       cosygpgf
TD            2048
SOLVENT       CDCl3
NS            16
DS            16
SMH           1393.534 Hz
FIDRES        0.680437 Hz
AQ            0.7348724 sec
RG            22.6
DM            358.800 usec
DE            6.50 usec
TE            296.0 K
D0            0.00000300 sec
D1            1.00000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00071815 sec

===== CHANNEL f1 =====
NUC1          1H
P0            13.50 usec
P1            13.50 usec
PL1           -1.00 dB
PL1W          10.56200695 W
SFO1          400.1320005 MHz

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPZ1          10.00 %
P16           1000.00 usec
ND0           1
TD            232
SFO1          400.132 MHz
FIDRES        6.001980 Hz
SW            3.480 ppm
FnmODE        QF
SI            2048
SF            400.1300213 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
  
```



SSK-11-AMB-222B-1H

Current Data Parameters
 NAME SSK-11-AMB-222B-1H
 EXPNO 8
 PROCNO 1

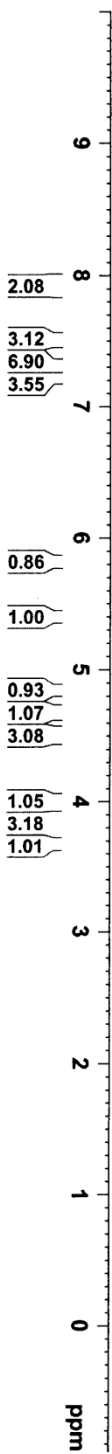
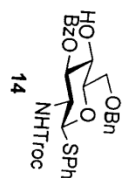
F2 - Acquisition Parameters

Date_ 20140620
 Time 23.41
 INSTRUM 5 mm PABBO-BB
 PULPROG zgpg30
 FIDPROC 65536
 TD 65536
 SOLVENT CDCl3
 NS 7
 DS 2

SMH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 30.72
 DR 50.000 usec
 DE 6.50 usec
 TE 297.7 K
 D1 1.00000000 sec
 TD0 1

***** CHANNEL F1 *****
 SFO1 500.1330885 MHz
 P1 13.00 usec
 P2 13.00 usec
 PLM1 13.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300262 MHz
 WDM 0 EM
 SSB 0
 GB 0 0.30 Hz
 RB 0
 PC 1.00

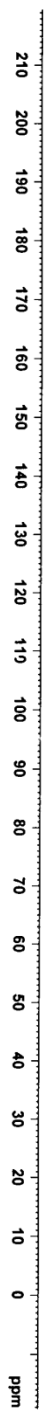
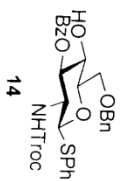


NAME SSK-11-AMB-222-13C
 EXPNO 9
 PROCNO 1
 Date_ 20140612
 Time_ 21.23
 INSTRUM spect
 PROBHD 5 mm SEI 1H/D-
 PULPROG zgpg30
 TD 65336
 SOLVENT CDCl3
 NS 549
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 181
 DW 20.800 usec
 DE 6.50 usec
 TE 296.1 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

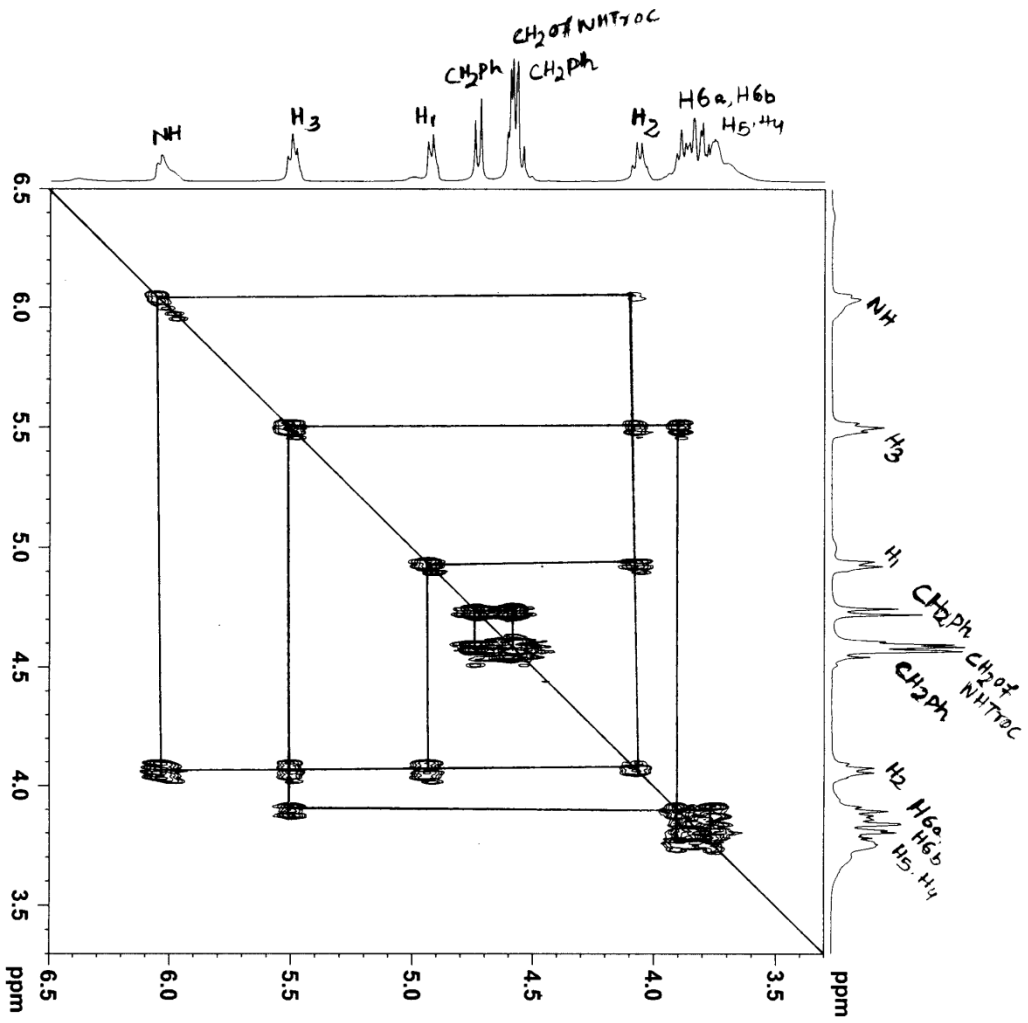
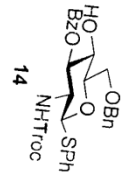
==== CHANNEL f1 =====
 NUCl 13C
 P1 8.75 usec
 P11 -2.00 dB
 P11W 56.53121948 W
 SFO1 100.628298 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUCC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 14.50 dB
 PL13 14.50 dB
 PL2W 10.56200695 W
 PL12W 0.29767781 W
 PL13W 0.29767781 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6127686 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

- 167.42
- 154.48
- 137.89
- 133.77
- 133.56
- 133.16
- 132.15
- 131.93
- 130.11
- 129.17
- 129.03
- 128.86
- 128.67
- 128.35
- 127.94
- 127.63
- 95.46
- 86.94
- 78.61
- 77.52
- 77.20
- 76.88
- 74.33
- 73.67
- 70.46
- 69.90
- 55.07
- 54.70



SSK-11-AMB-222-COSY



SSK-11-AMB-156-1H

Current Data Parameters
 NAME SSK-11-AMB-156-1H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters

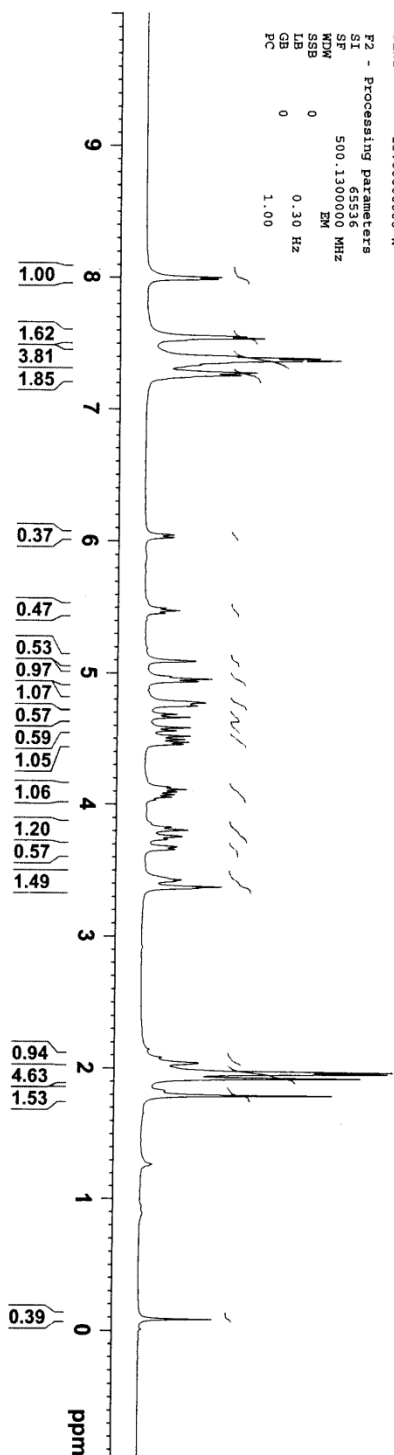
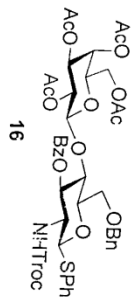
Date_ 2013.09
 Time_ 13.49
 INSTRUM spect
 PROBRD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CMC13
 NS 19
 DS 2
 SFO1 10000.000 Hz
 FIDRES 0.145418 Hz
 AQ 3.276799 sec
 RG 15.73
 DW 50.000 usec
 DE 6.50 usec
 TE 295.2 K
 D1 1.00000000 sec
 TDO 1

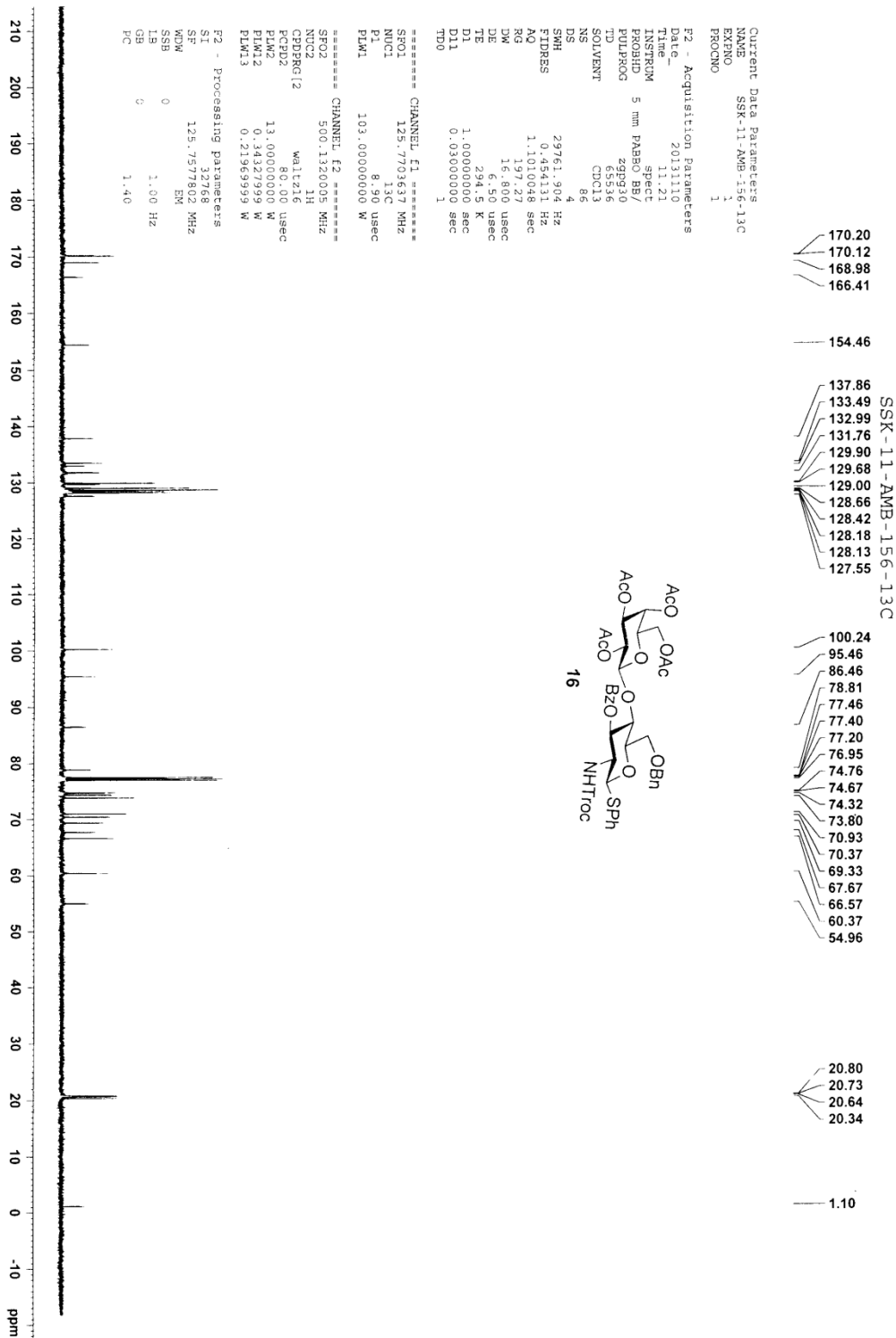
==== CHANNEL f1 =====

SFO1 500.1330885 MHz
 NUC1 1H
 P1 13.00 usec
 PL1 13.00000000 W

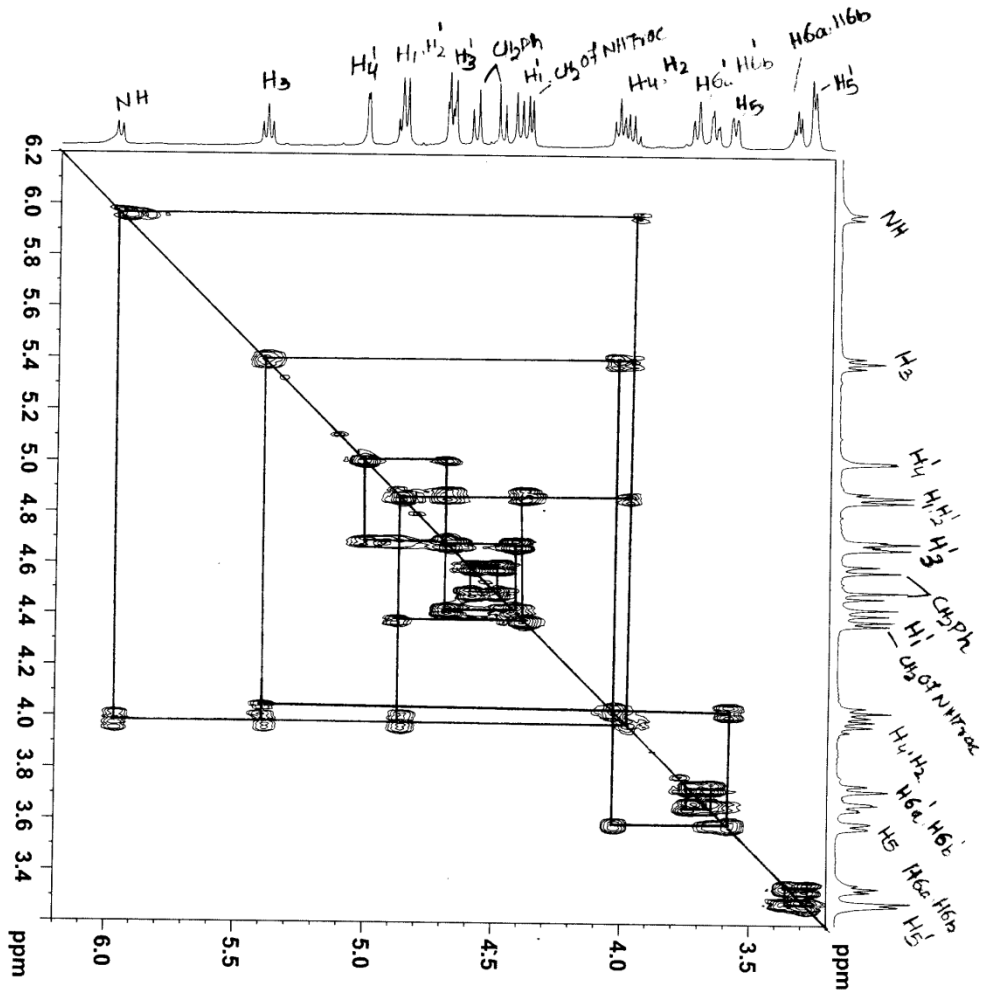
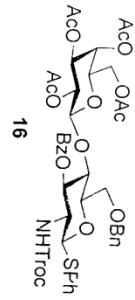
F2 - Processing parameters

SF 65536
 KW 500.1300000 MHz
 SSB 0
 LB 0
 GB 0
 PC 1.00





SSK-11-AMB-156-COSY



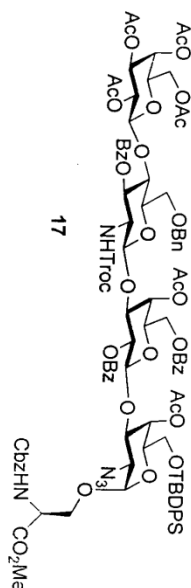
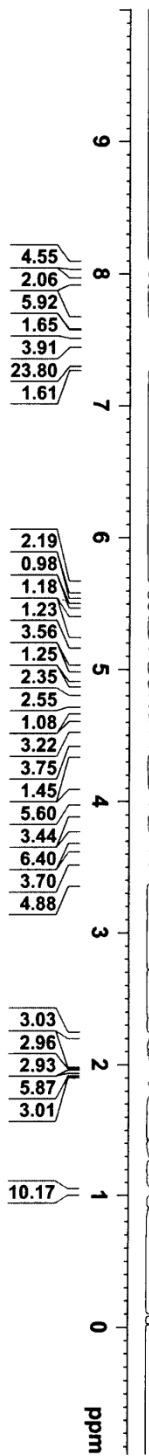
ssk-11-amb-158-1h

Current Data Parameters
 NAME ssk-11-amb-158-1h
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 2013114
 Time 22.42
 INSTRUM spect
 PROBD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 3
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 53.37
 DW 50.000 usec
 DE 6.50 usec
 TE 295.6 K
 TD 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 SF01 500.130885 MHz
 NUC1 1H
 P1 13.00 usec
 PLM1 13.00000000 W

F2 - Processing parameters
 SI 4096
 SF 500.130000 MHz
 MDW 0 EM
 SSB 0
 LB 0 0.30 Hz
 GB 0
 PC 1.00



- 170.44
170.37
170.24
170.20
170.18
169.40
169.18
166.19
165.91
164.90
156.13
154.04
138.15
136.16
135.75
135.70
133.59
133.53
133.36
133.24
129.93
129.84
129.77
129.57
128.74
128.69
128.55
128.47
128.40
128.05
127.88
127.81
102.24
101.80
100.36
98.94
95.48
77.45
77.20
76.95
74.09
74.03
73.96
72.61
71.49
71.26
71.00
70.55
69.66
69.37
69.16
68.87
67.65
67.42
66.62
62.74
62.35
60.51
59.55
56.39
54.34
52.88
26.86
21.03
20.83
20.80
20.73
20.67
20.57
19.26

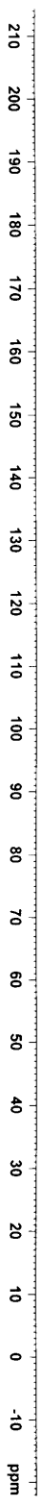
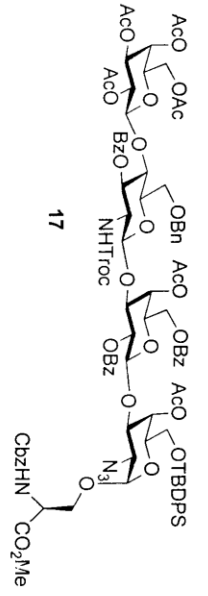
skk-11-amb-158-13c

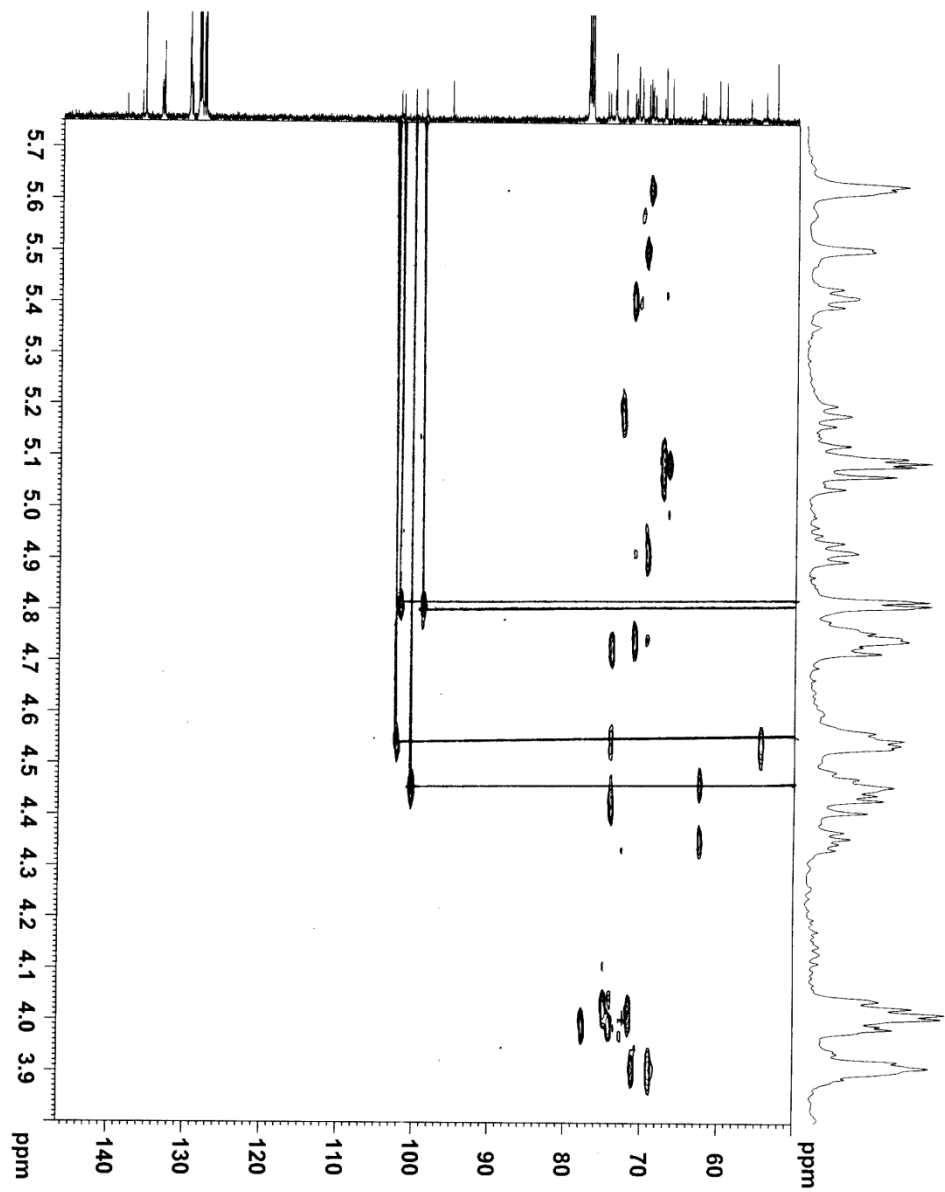
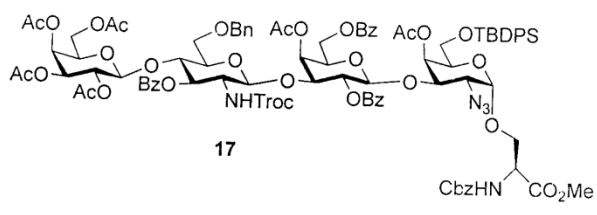
Current Data Parameters
 NAME skk-11-amb-11
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20131111
 Time 22.4
 PROBHD 5 mm F401P1
 PULPROG zgpg30
 TD 6553
 SOLVENT CDCl3
 NS 92
 DS 2
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 197.27
 DW 16.800 usec
 DE 2.50 usec
 TE 300.2 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TDO 1

==== CHANNEL f1 =====
 SF01 125.7703637 MHz
 NUC1 13C
 P1 8.90 usec
 PLW1 103.00000000 W

==== CHANNEL f2 =====
 SF02 500.1320005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 13.00000000 W
 PLM2 0.34327999 W
 PLM3 0.21969999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577706 MHz
 WDW 0
 SSB 0
 GB 0
 PC 1.40





SSK-11-AMB-181-1H

Current Data Parameters
 EXPNO 1
 PROCNO 1

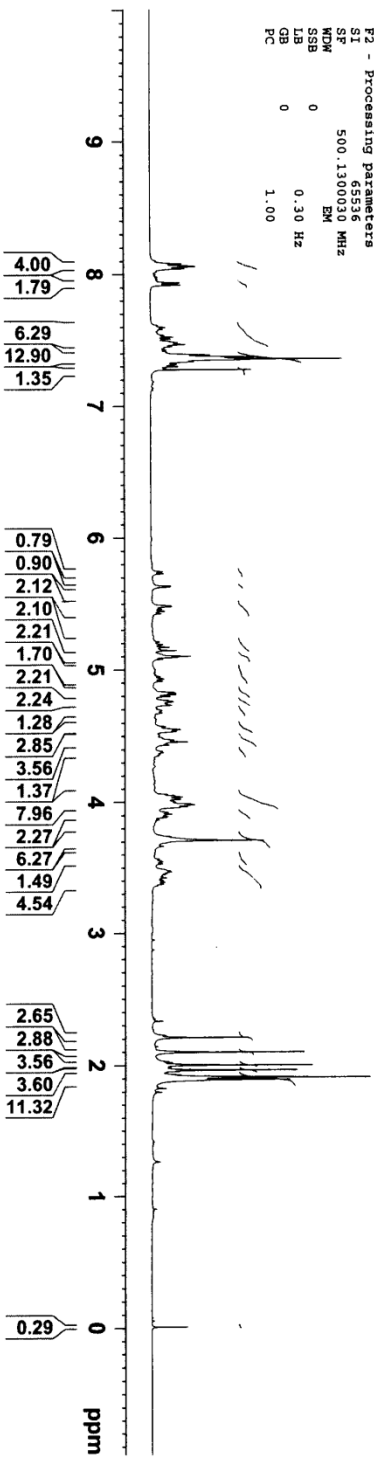
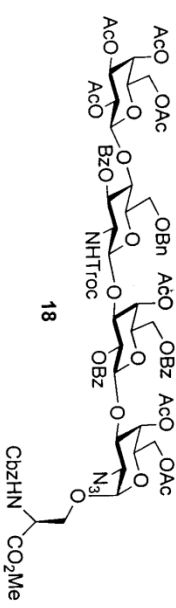
F2 - Acquisition Parameters
 Date_ 20140202
 Time 10.39

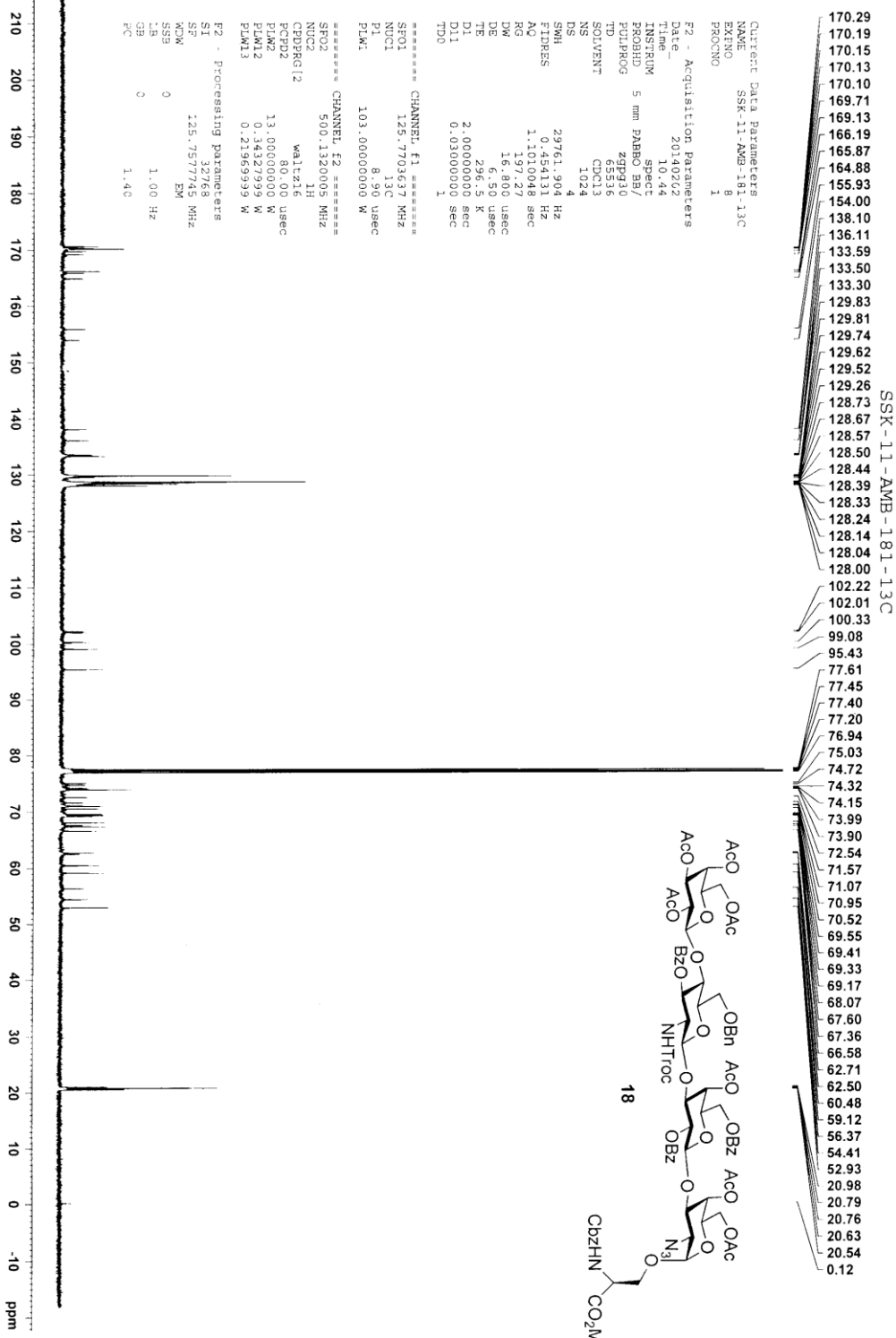
INSTRUM spect
 PROBRD 5 mm PABBO B9/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 40
 DS 2

SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 30.72
 DM 50.000 usec
 DE 1.000 usec
 TE 295.9 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 500.130885 MHz
 NUC1 1H
 P1 13.00 usec
 PL1 13.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.130030 MHz
 MDM EM
 SSB 0
 LB 0 0.30 Hz
 GB 1.00



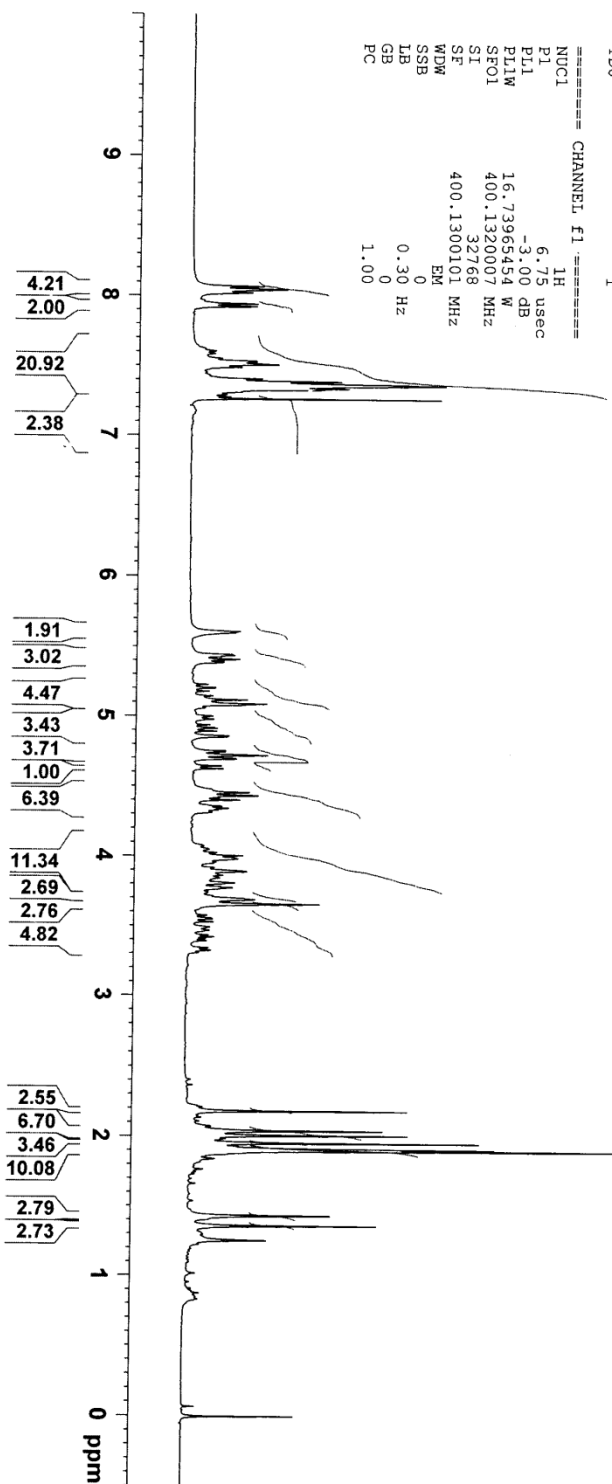
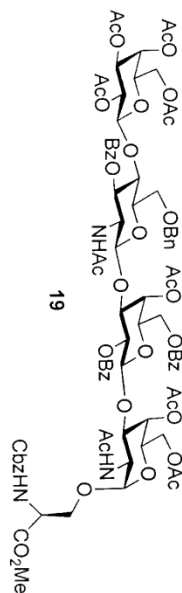


SSK-11-AMB-185-1H

SSK-11-AMB-185-1H

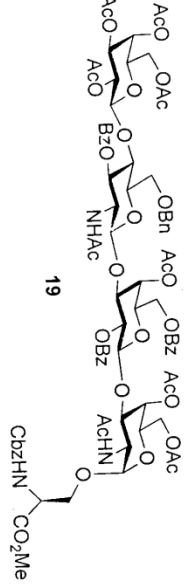
NAME SSK-11-AMB-185-1H
EXPNO 1
PROCNO 1
Date_ 20140212
Time_ 22.06
INSTRUM spect
PROBHD 5 mm SEI 1H/D-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 68
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 71.8
DW 60.800 usec
DE 6.50 usec
TE 295.8 K
D1 1.0000000 sec
TD0 1

===== CHANNEL F1 =====
NUC1 1H
P1 6.75 usec
PL1 -3.00 dB
PL1W 16.73965454 W
SFO1 400.1320007 MHz
SI 32768
SE 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



- 170.64
- 170.56
- 170.32
- 170.26
- 170.20
- 170.16
- 170.09
- 169.27
- 166.35
- 166.14
- 164.86
- 155.92
- 138.18
- 136.07
- 134.14
- 133.54
- 133.38
- 129.89
- 129.84
- 129.64
- 129.41
- 129.21
- 128.80
- 128.67
- 128.63
- 128.60
- 128.54
- 128.50
- 128.12
- 128.03
- 128.00
- 102.02
- 100.84
- 100.38
- 98.57
- 77.45
- 77.20
- 76.94
- 71.83
- 70.97
- 70.54
- 69.39
- 69.28
- 69.21
- 68.40
- 67.92
- 67.79
- 67.49
- 66.60
- 63.03
- 62.62
- 60.43
- 54.64
- 54.47
- 52.77
- 49.04
- 22.75
- 22.57
- 20.96
- 20.84
- 20.78
- 20.65
- 20.59

SSK-11-AMB-185-13C



Current Data Parameters
 NAME SSK-11-AMB-185-13C
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Param
 Date_ 20140717
 Time_ 18:40:00
 INSTRUM spect
 PROBRH 5 mm PABRO BB
 PULPROG zgpg31
 TD 65531
 SOLVENT CDCl3
 NS 296
 DS 4
 SMH 34722.223 Hz
 FIDRES 0.5229819 Hz
 AQ 0.9437184 sec
 DQ 1.471700 usec
 DE 6.150 usec
 TE 296.2 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

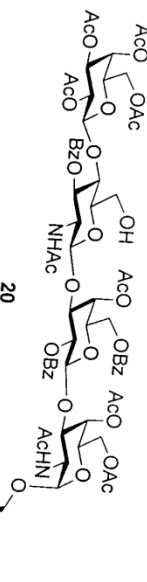
==== CHANNEL f1 =====
 SFO1 125.7721254 MHz
 NUQ1 13C
 P1 8.30 usec
 P1M1 103.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUQ2 1H
 CDDPR12 Waltz16
 PCPDP2 13.00000000 W
 PLW12 0.34327999 W
 PLW13 0.21969999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577658 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



SSK-11-AMB-187-1H

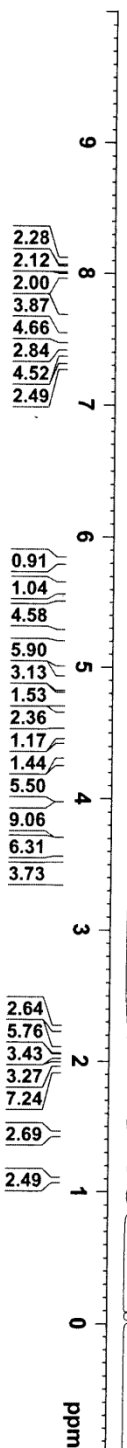


Current Data Parameters
 NAME SSK-11-AMB-187-1H
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140214
 Time 23.05
 INSTRUM spect
 PROBRD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 2
 DS 15
 SWH 10000.002 Hz
 FIDRRS 0.152588 Hz
 AQ 3.276799 sec
 RG 106.54
 DW 50.000 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.00000000 sec
 D10 1

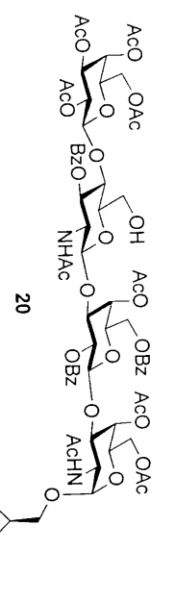
===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 13.00 usec
 PLM1 13.00000000 W

F2 - Processing parameters
 SI 32768
 SF 500.130000 MHz
 MDW 500.130000 MHz
 SSB 0
 LB 0 0.30 Hz
 GB 0
 PC 1.00



SKK-11-amb-170-13C

- 171.14
- 170.65
- 170.39
- 170.26
- 170.17
- 170.07
- 169.69
- 166.22
- 165.96
- 164.84
- 165.95
- 134.02
- 133.71
- 133.60
- 133.50
- 130.23
- 129.92
- 129.82
- 129.71
- 129.50
- 129.43
- 129.13
- 128.84
- 128.74
- 128.67
- 128.53
- 101.84
- 101.29
- 100.92
- 98.59
- 77.48
- 77.23
- 76.98
- 71.30
- 71.07
- 70.60
- 69.62
- 69.47
- 69.33
- 68.39
- 67.91
- 67.53
- 66.52
- 63.04
- 61.52
- 60.14
- 55.39
- 54.49
- 52.80
- 49.06
- 22.55
- 22.36
- 21.31
- 20.89
- 20.84
- 20.73
- 20.70
- 20.67



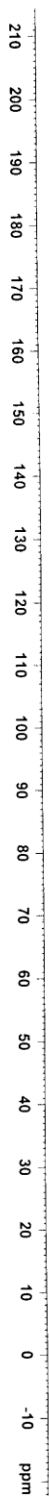
Current Data Parameters
 NAME skk-11-amb-170-13c
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131213
 Time 22.32
 INSTRUM spect
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1920
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 1971.27
 DM 16.800 usec
 DE 4.50 usec
 TE 298.3 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TDO 1

==== CHANNEL f1 =====
 SF01 125.7703637 MHz
 NUC1 13C
 P1 8.90 usec
 PL1 103.0000000 W

==== CHANNEL f2 =====
 SF02 500.1320005 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 80.00 usec
 PLW2 13.0000000 W
 PLM12 0.34327999 W
 PLM13 0.21969999 W

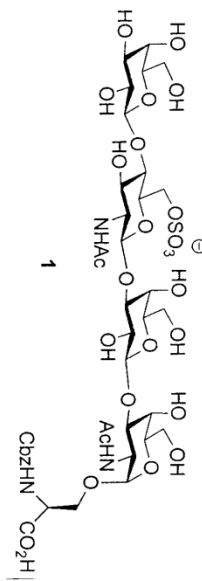
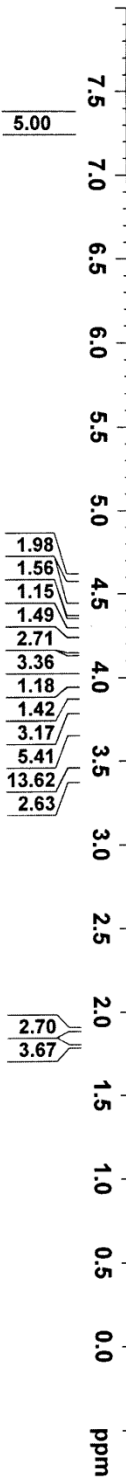
F2 - Processing parameters
 SI 32768
 SF 125.7577635 MHz
 WDM 0
 ZSR 2.00 Hz
 GB 0
 PC 1.40



SSK-11-AMB-213-1H

NAME SSK-11-AMB-213-1H
 EXPNO 2
 PROCNO 1
 Date_ 20140426
 Time_ 16.31
 INSTRUM spect
 PROBHID 5 mm SEI 1H/D-
 PULPROG zg30
 TD 65536
 SOLVENT D2O
 NS 173
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 161
 DM 60.800 usec
 DE 6.50 usec
 TE 295.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.75 usec
 PL1 -3.00 dB
 PL1W 16.73965454 W
 SFO1 400.1324710 MHz
 SI 32768
 SF 400.1300107 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



SKK-11-AMB-213-13C

Current Data Parameters
 NAME SKK-11-AMB-213-13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20140530
 Time_ 11:11
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 SOLVENT d2o
 NS 6326
 DS 16079
 SFO1 207.1804 MHz
 SF 207.1804 MHz
 AQ 0.45413 sec
 RG 1.010048 sec
 DM 1.97127 sec
 DE 16.800 usec
 TE 295.7 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 1.00000000 sec
 D13 1.00000000 sec

==== CHANNEL f1 =====

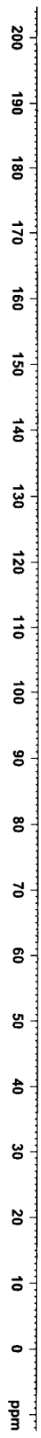
SFO1 125.770357 MHz
 SF 125.770357 MHz
 PC1 8.90 usec
 PL1 103.0000000 W
 PLM1

==== CHANNEL f2 =====

SFO2 500.1320005 MHz
 SF 500.1320005 MHz
 NI 1H
 NUC2 1H
 CPDPRG12 waltz16
 SFO3 125.770357 MHz
 SF 125.770357 MHz
 PC2 13.00000000 usec
 PLM2 0.34327999 W
 PLM3 0.21959999 W
 PLM13

F2 - Processing parameters

SI 32768
 SF 125.757890 MHz
 WDM 0 EX
 AS 0
 DS 0
 IB 2.00 Hz
 GB 0
 PC 1.40



- 182.54
- 181.55
- 174.95
- 174.68
- 157.78
- 136.52
- 128.89
- 128.76
- 128.48
- 127.86
- 127.74
- 104.70
- 102.70
- 98.00
- 82.33
- 77.76
- 75.43
- 74.69
- 72.61
- 72.51
- 72.27
- 71.08
- 70.83
- 69.74
- 68.81
- 68.71
- 68.62
- 68.44
- 67.11
- 66.62
- 61.11
- 55.29
- 48.57
- 23.37
- 22.30
- 22.21
- 20.17

