

Supplementary data

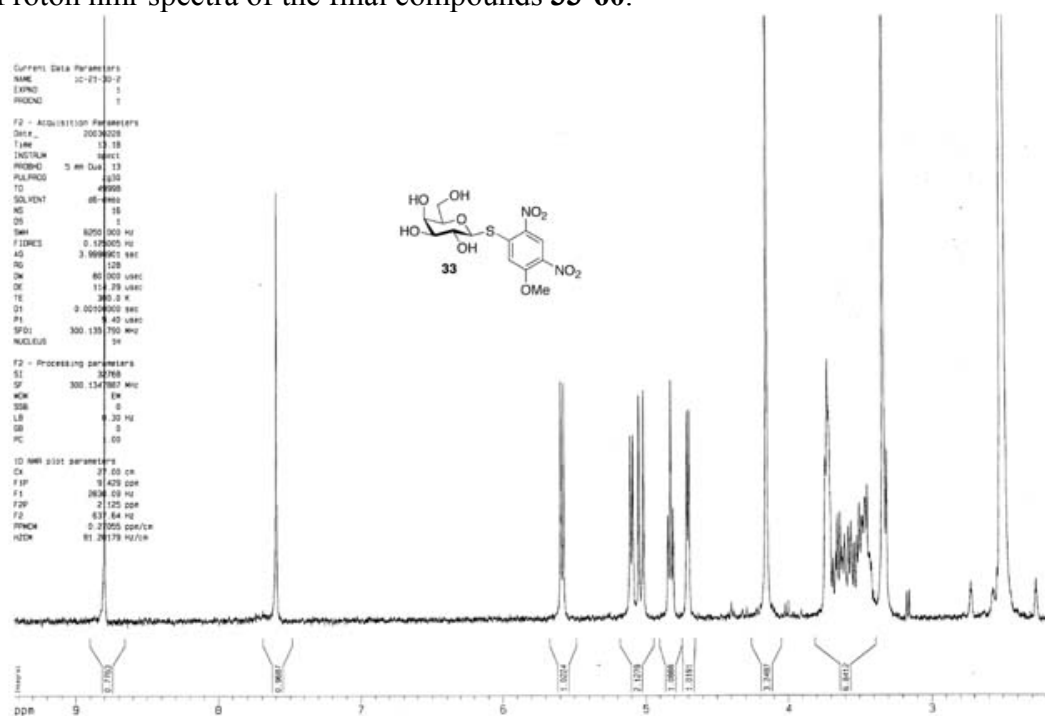
Synthesis of a phenyl thio- β -D-galactopyranoside library from 1,5-difluoro-2,4-dinitrobenzene: Discovery of efficient and selective monosaccharide inhibitors of galectin-7

Ian Cumpstey^a, Susanne Carlsson^b, Hakon Leffler^b, and Ulf J. Nilsson^{a*}

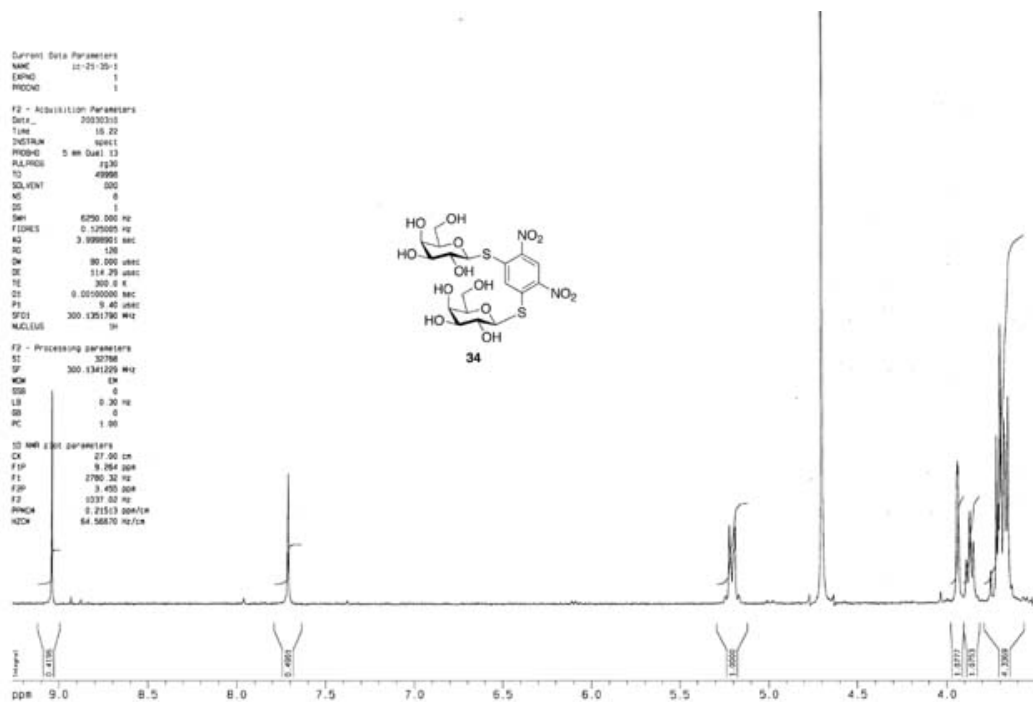
^a Organic Chemistry, Lund University, Box 124, SE-221 00, Lund, SWEDEN. Fax: +46 46 2228218; Tel: +46 46 2228209; E-mail: ulf.nilsson@organic.lu.se

^b Section MIG, Department of Laboratory Medicine, Lund University, Solvegatan 23, SE-223 62, Lund, SWEDEN

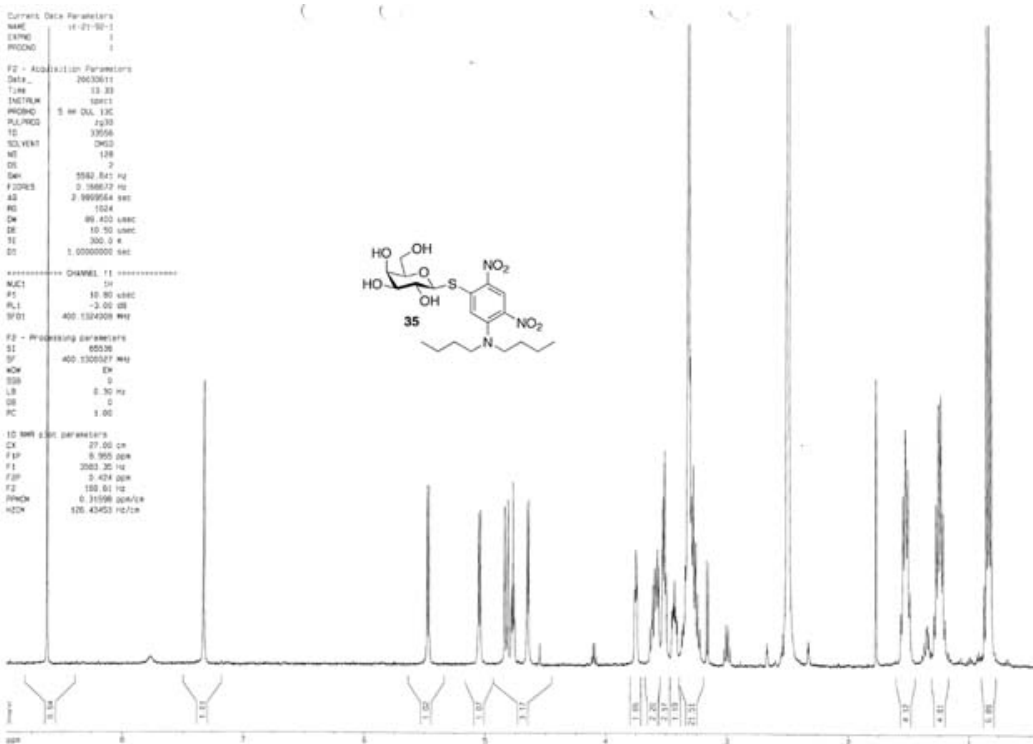
Proton nmr spectra of the final compounds **33-60**.

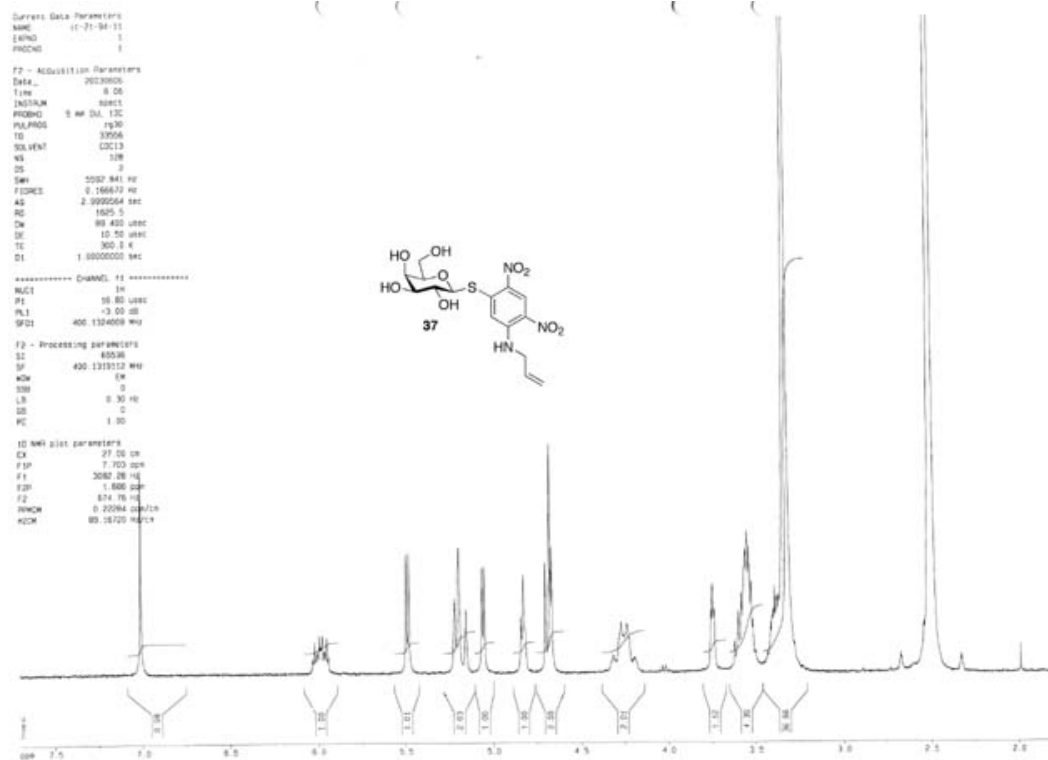


10 test circuit parameters	
CK	27.00 cm
F1P	9.264 GHz
F1	2760.32 Hz
F2P	9.450 GHz
F2	1037.02 Hz
FWHM	0.21513 GHz/cm
QTCW	64.56870 Hz/cm



10 mm size parameters	
CX	27.00 cm
FIP	0.995 g/cm
F1	2083.30 Hz
F2F	0.424 g/cm
F2	188.61 Hz
FWHM	0.31596 g/cm/cm
H2CM	126.43453 Hz/cm





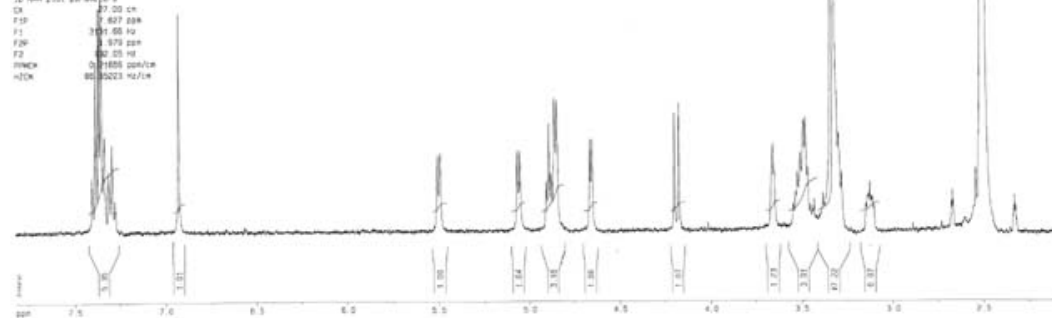
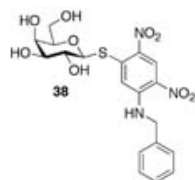
Current Data Parameters
NAME 11-21-09-11
EXNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030606
Time 7.34
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 128
DS 2
SWH 10062.841 Hz
FIDRES 0.166670 Hz
AQ 2.9999564 sec
RG 1632.5
CW 86.400 uHz
DE 16.50 uHz
TE 300.0 K
DT 1.0000000 sec

===== CHANNEL f1 =====
NUC1 13
P1 10.00 uHz
PL1 -3.00 dB
SFO1 400.1304008 MHz

F2 - Processing Parameters
SI 65536
SF 400.1315112 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR data parameters
CA 27.00 cm
F1P 7.627 dB
F1 100.00 Hz
F2P 0.970 dB
F2 100.00 Hz
NUC1 13
NUC2 1H
AQ 0.0000000 sec
PC 1.00

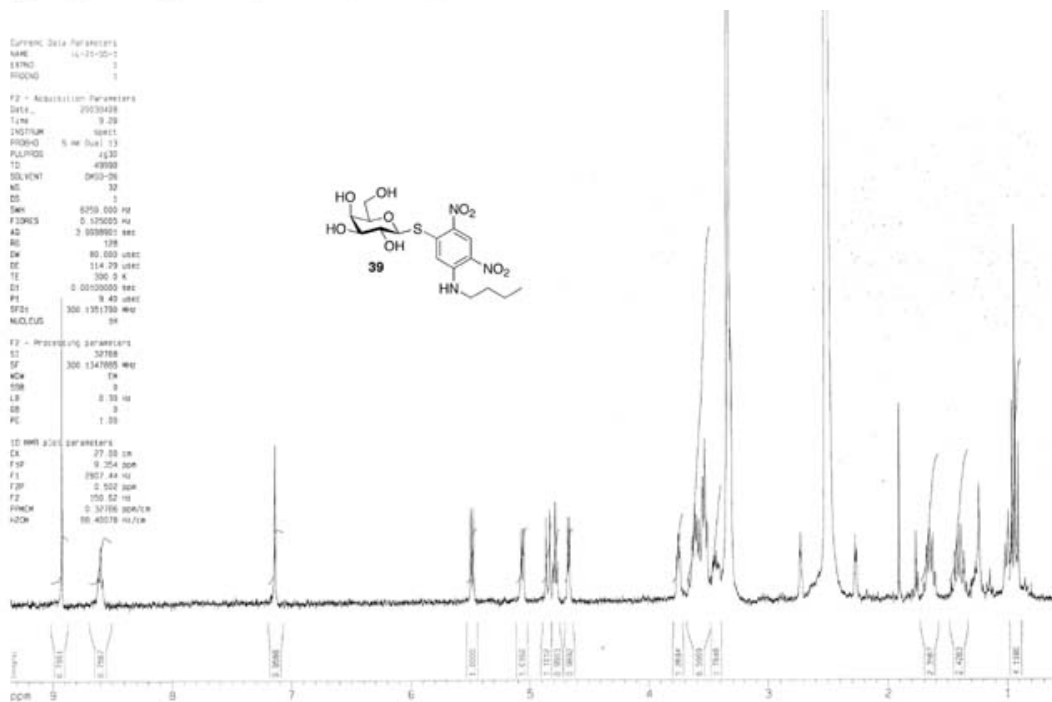
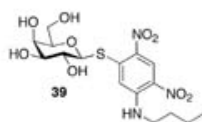


Current Data Parameters
NAME 11-22-09-1
EXNO 1
PROCNO 1

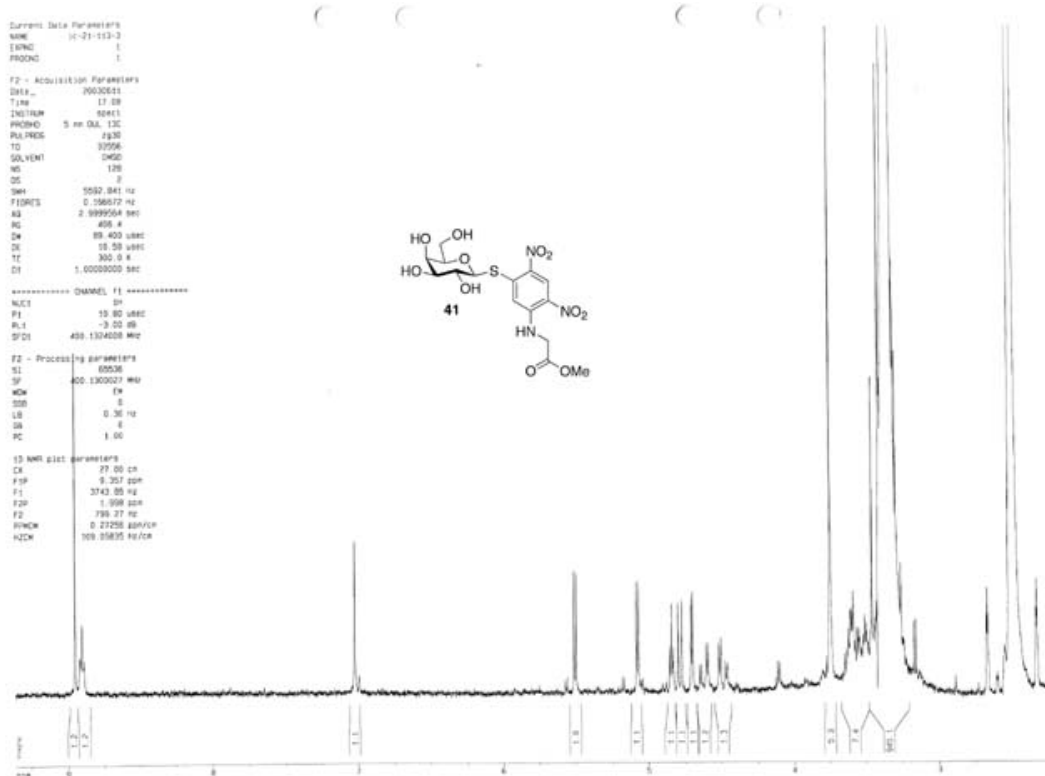
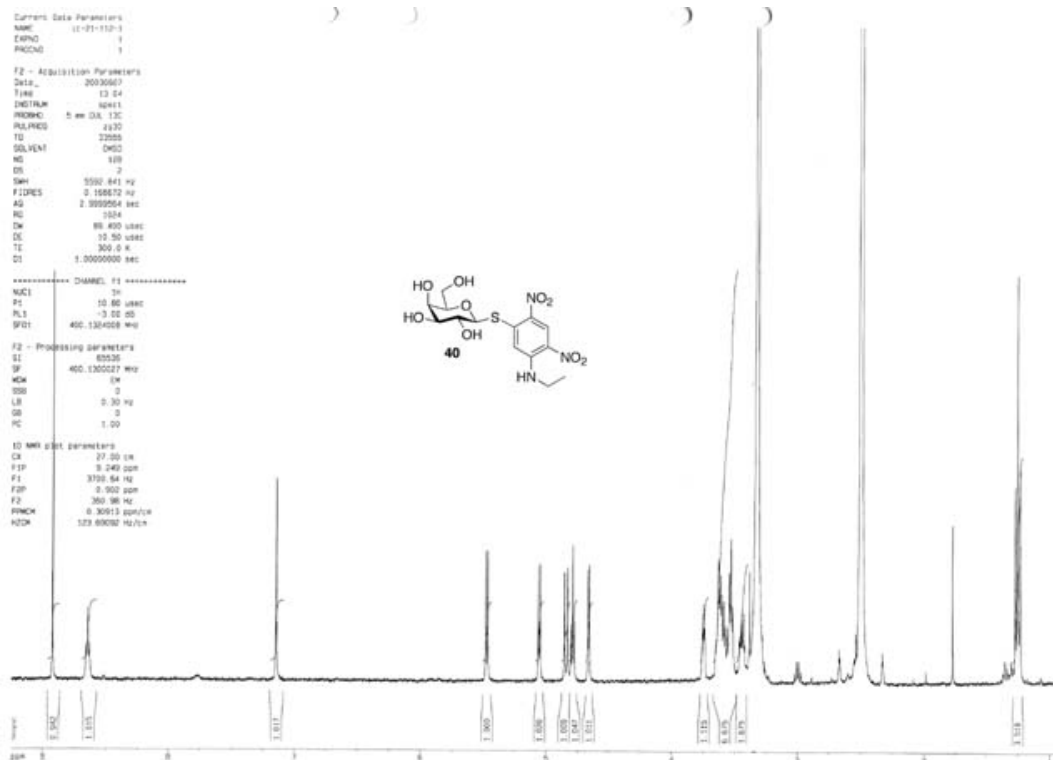
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Date_ 20030606
Time 9.29
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
SOLVENT DMSO-d6
NS 128
DS 2
SWH 10062.841 Hz
FIDRES 0.166670 Hz
AQ 2.9999564 sec
RG 1632.5
CW 86.400 uHz
DE 16.50 uHz
TE 300.0 K
DT 1.0000000 sec

F2 - Processing Parameters
SI 65536
SF 400.1315112 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR data parameters
CA 27.00 cm
F1P 7.627 dB
F1 100.00 Hz
F2P 0.970 dB
F2 100.00 Hz
NUC1 13
NUC2 1H
AQ 0.0000000 sec
PC 1.00



Supplementary data



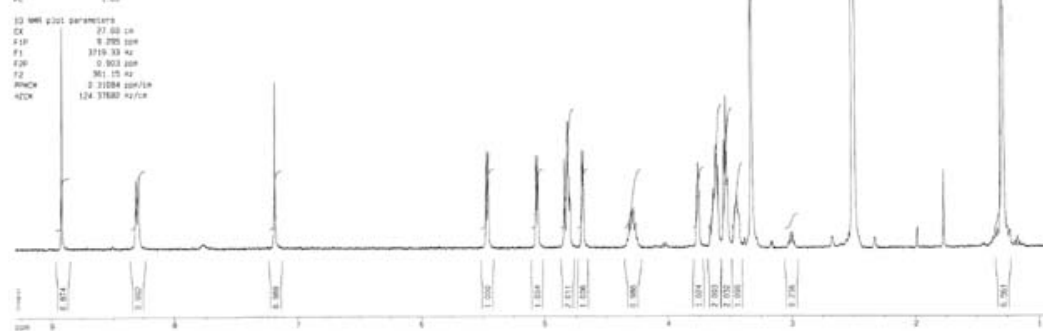
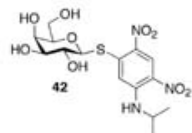
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NAME 11-21-108-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230204
Time 15:30
INSTRUM spect
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PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 64
DS 2
SWH 5502.841 Hz
FIDRES 0.166872 Hz
AQ 2.9992564 sec
RG 3274
SQ 88.400 uhrz
DC 15.50 uhrz
TE 300.2 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 uhrz
PL1 -1.00 dB
SFO1 400.1340000 MHz

F2 - Processing parameters
SI 32768
SF 400.1340000 MHz
WDW EM
SSB 0
LB 3.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 27.00 cm
F1 10.208 uhrz
F2 3719.33 Hz
F3 0.303 uhrz
F4 361.15 Hz
F5 2.1084 uhrz/cm
F6 124.37880 Hz/cm



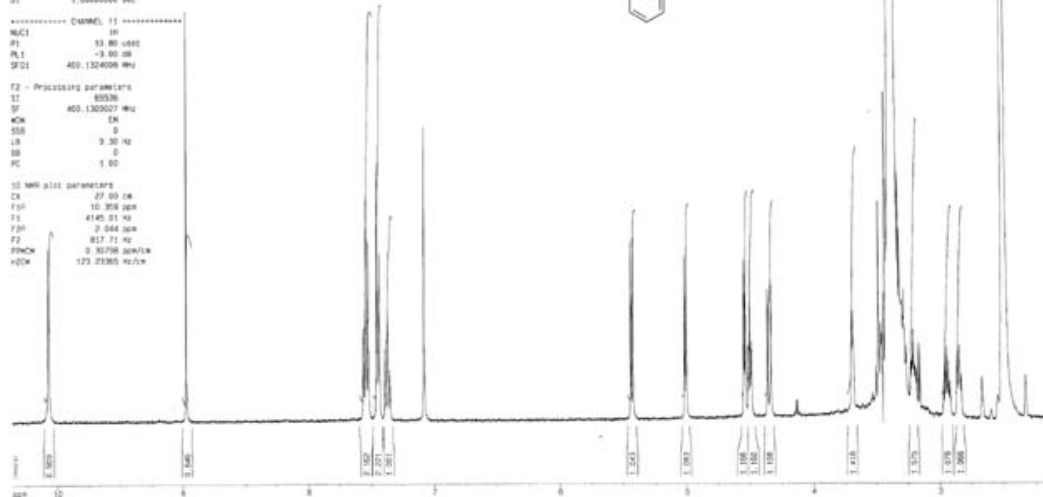
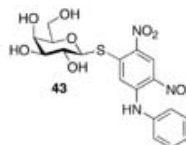
Current Data Parameters
NAME 11-21-108-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230416
Time 19:05
INSTRUM spect
PROBHD 5 mm QNP 13C
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 64
DS 2
SWH 5502.841 Hz
FIDRES 0.166872 Hz
AQ 2.9992564 sec
RG 3274
SQ 88.400 uhrz
DC 15.50 uhrz
TE 300.2 K
D1 1.00000000 sec

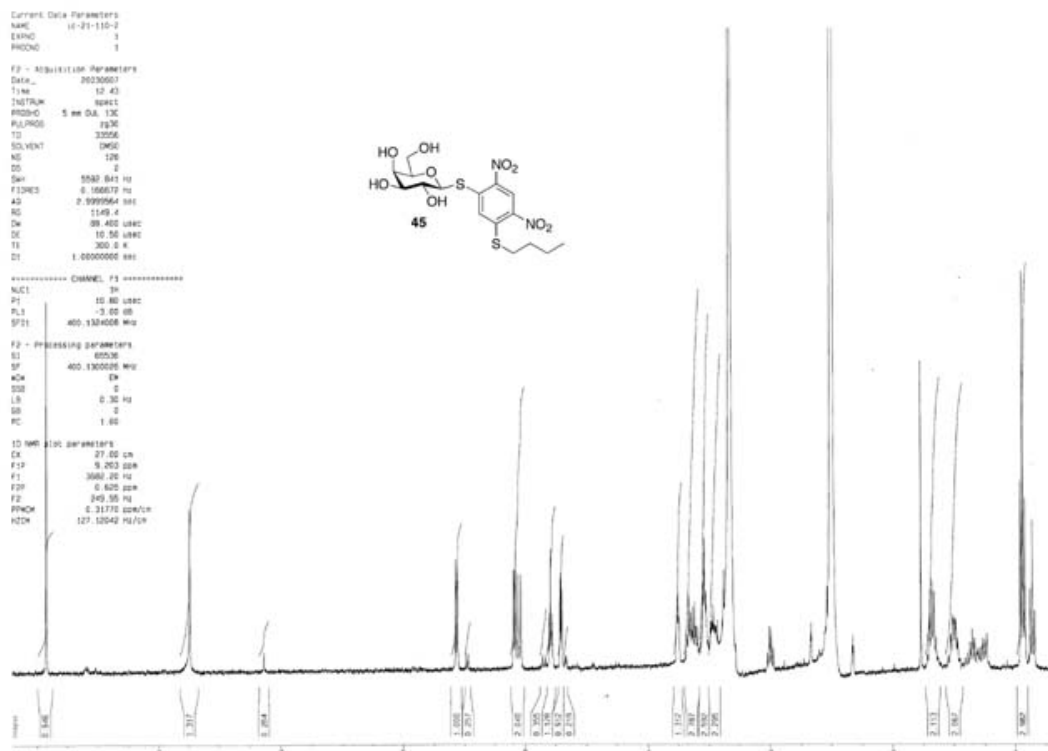
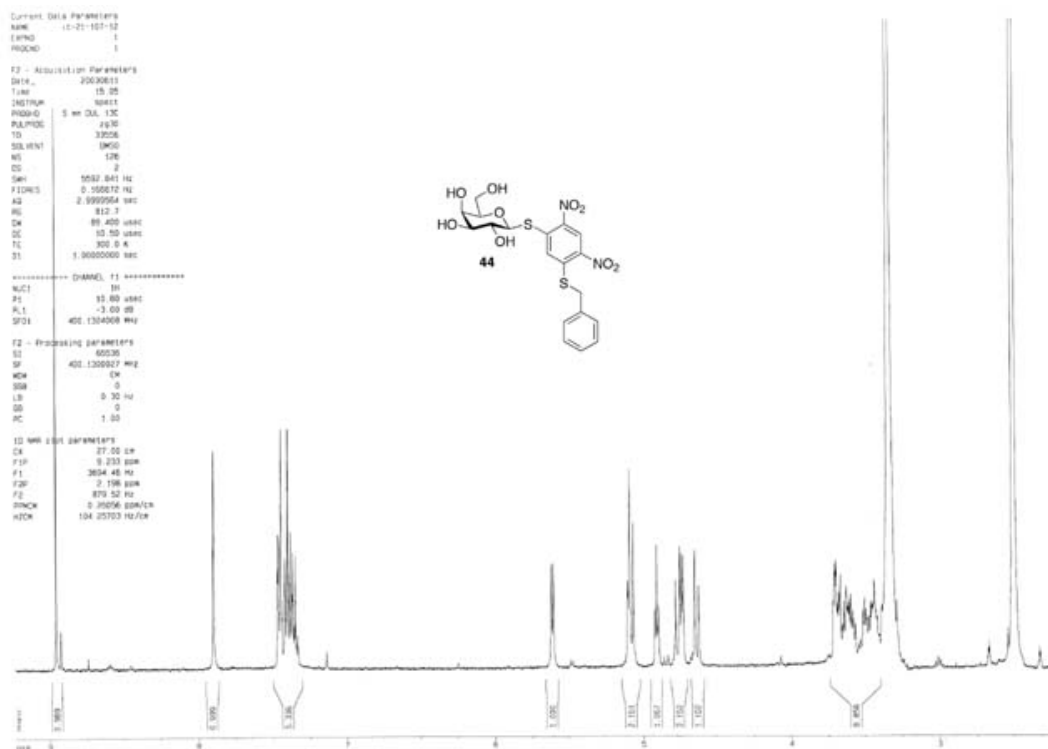
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 uhrz
PL1 -1.00 dB
SFO1 400.1340000 MHz

F2 - Processing parameters
SI 32768
SF 400.1340000 MHz
WDW EM
SSB 0
LB 3.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 27.00 cm
F1 10.208 uhrz
F2 3719.33 Hz
F3 0.303 uhrz
F4 361.15 Hz
F5 2.1084 uhrz/cm
F6 124.37880 Hz/cm



Supplementary data



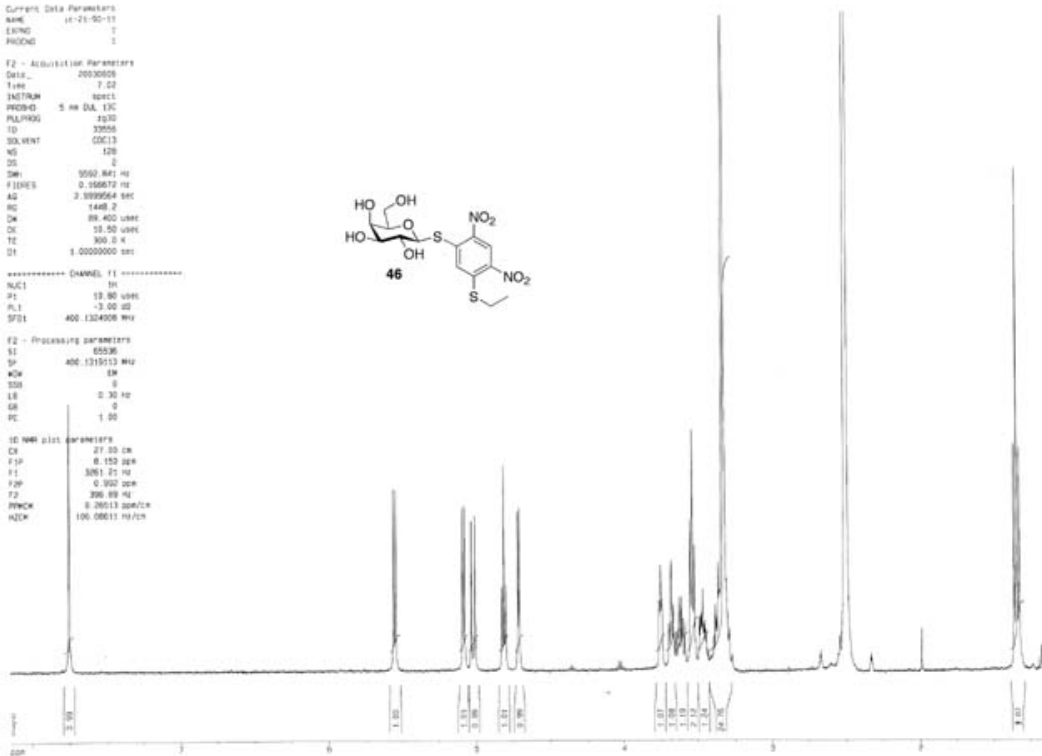
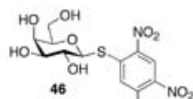
Current Data Parameters
NAME 14-21-50-11
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030809
Time 12.02
INSTRUM spect
PROBHD 5 mm DAI 13C
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 128
DS 4
SWH 9500.841 Hz
FIDRES 0.166872 Hz
AQ 3.3899564 sec
RG 1448.2
DM 88.400 usec
DE 18.50 usec
TE 300.2 K
D1 1.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 19.80 usec
PL1 -3.00 dB
SFO1 400.1324508 MHz

F2 - Processing parameters
SI 65536
SF 400.1315113 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 27.00 cm
F1P 0.153 ppm
F1 3061.21 Hz
F2P 0.930 ppm
F2 380.89 Hz
PQMC 0.26513 ppm/cm
H2CM 100.00611 Hz/cm

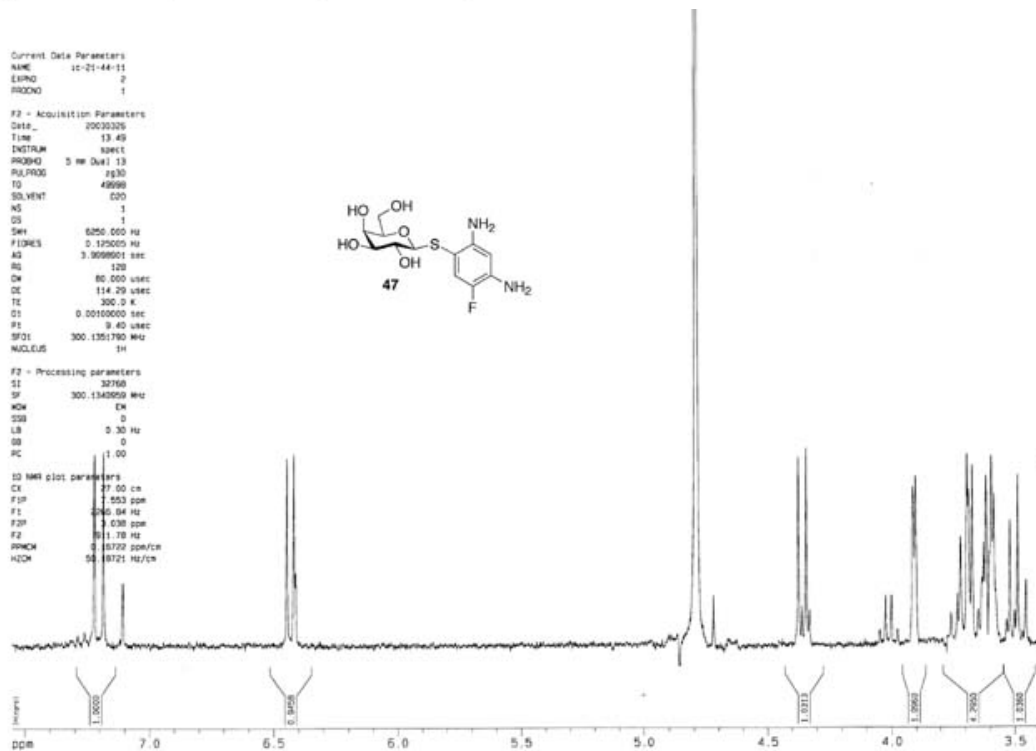
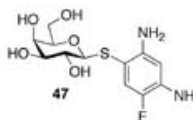


Current Data Parameters
NAME 14-21-44-11
EXPNO 2
PROCNO 1

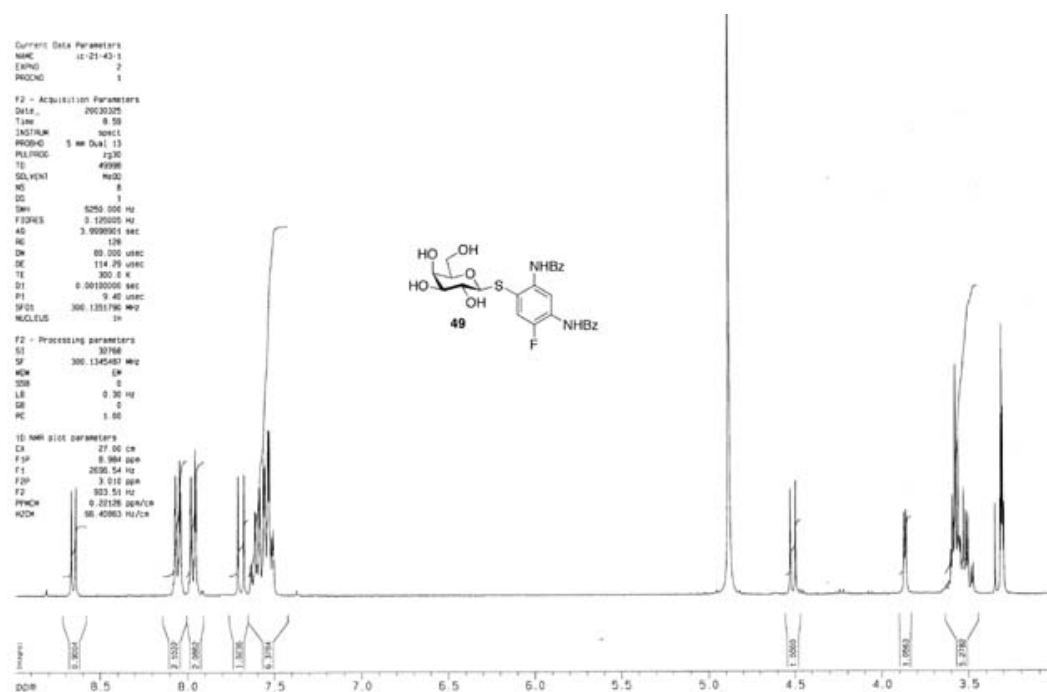
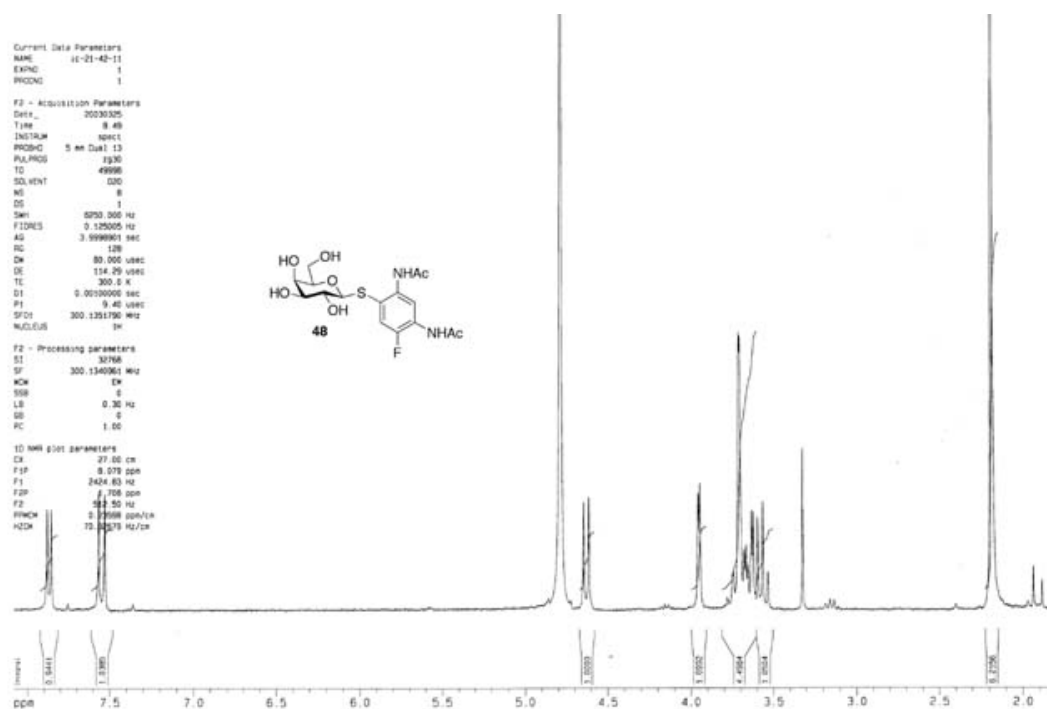
F2 - Acquisition Parameters
Date_ 20030326
Time 13.49
INSTRUM spect
PROBHD 5 mm DAI 13
PULPROG zgpg30
TD 49998
SOLVENT CDCl3
NS 1
DS 1
SWH 6250.000 Hz
FIDRES 0.170000 Hz
AQ 3.3699501 sec
RG 120
DM 80.000 usec
DE 114.29 usec
TE 300.2 K
D1 0.00100000 sec
P1 9.40 usec
SFO1 300.1351790 MHz
NUC1 1H

F2 - Processing parameters
SI 32768
SF 300.1340559 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 27.00 cm
F1P 1.553 ppm
F1 3061.04 Hz
F2P 1.030 ppm
F2 381.78 Hz
PQMC 0.16722 ppm/cm
H2CM 98.18721 Hz/cm



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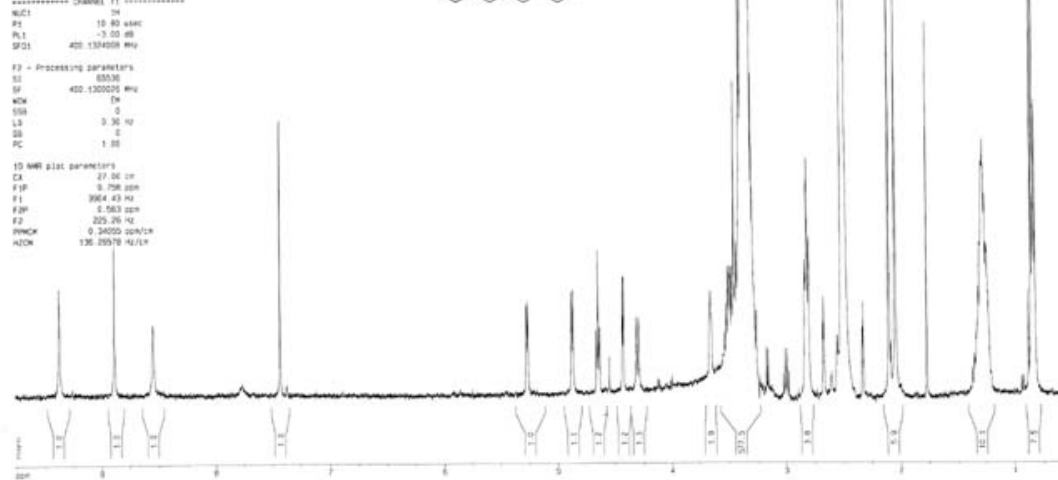
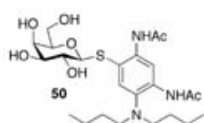


Current Data Parameters
NAME 10-21-10-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030611
Time 05:40
INSTRUM spect
PROBHD 5 mm QNP 13C
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 128
DS 2
SWH 5092.841 Hz
FIDRES 0.166672 Hz
AQ 2.999964 sec
RG 429.4
DM 88.400 usec
DE 19.50 usec
TE 300.2 K
SI 1.5000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 19.80 usec
PL1 -3.00 dB
SFO1 400.134000 MHz
F2 - Processing parameters
SI 65536
SF 400.130000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CA 27.00 cm
FAP 9.708 ppm
FI 3984.43 Hz
F2 0.503 ppm
F3 225.26 Hz
PUNCH 0.34000 sec/Hz
H2O 136.25578 Hz/Hz

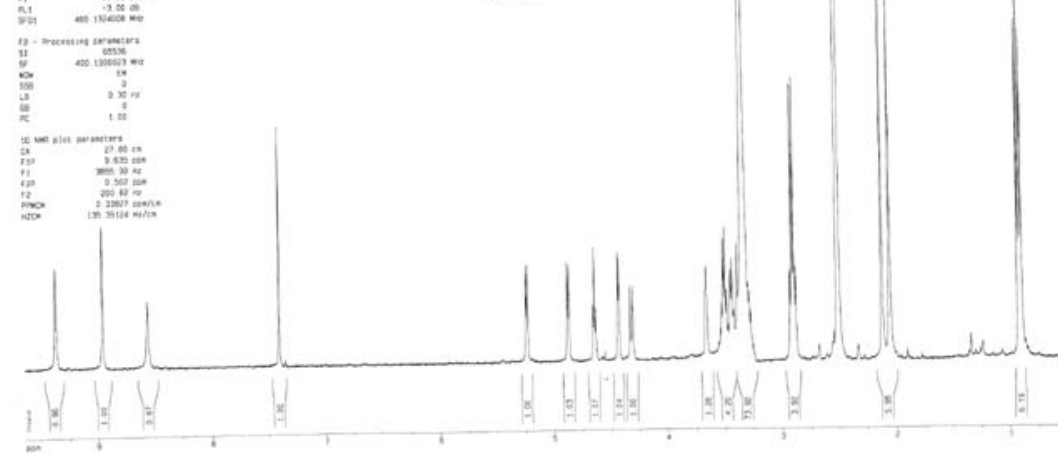
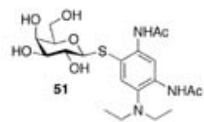


Current Data Parameters
NAME 10-21-10-1
EXPNO 1
PROCNO 1

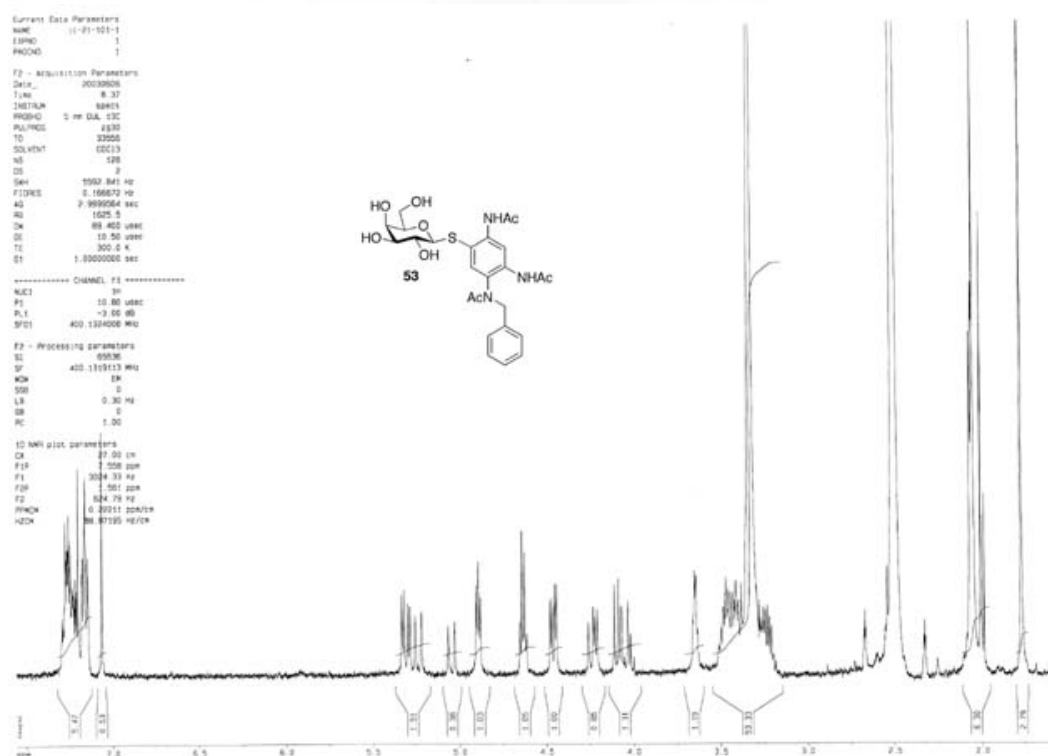
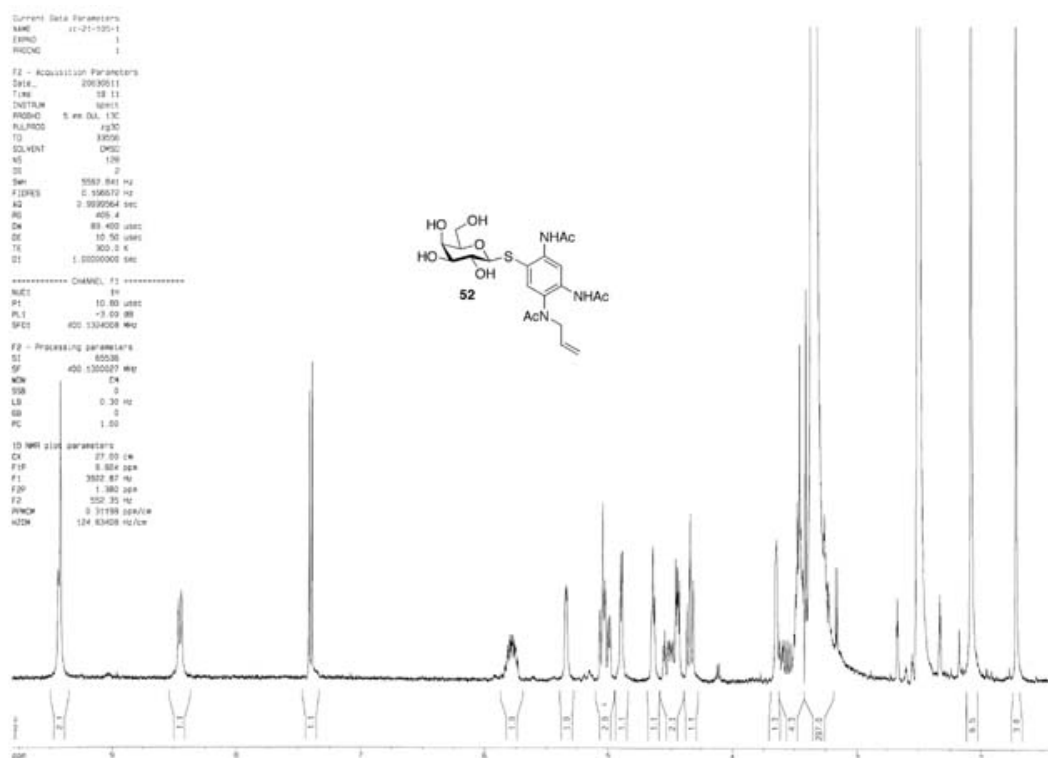
F2 - Acquisition Parameters
Date_ 20030611
Time 13:01
INSTRUM spect
PROBHD 5 mm QNP 13C
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 128
DS 2
SWH 5092.841 Hz
FIDRES 0.166672 Hz
AQ 2.999964 sec
RG 429.4
DM 88.400 usec
DE 19.50 usec
TE 300.2 K
SI 1.5000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 19.80 usec
PL1 -3.00 dB
SFO1 400.134000 MHz
F2 - Processing parameters
SI 65536
SF 400.130000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CA 27.00 cm
FAP 9.708 ppm
FI 3984.43 Hz
F2 0.503 ppm
F3 225.26 Hz
PUNCH 0.34000 sec/Hz
H2O 136.25578 Hz/Hz



Supplementary data



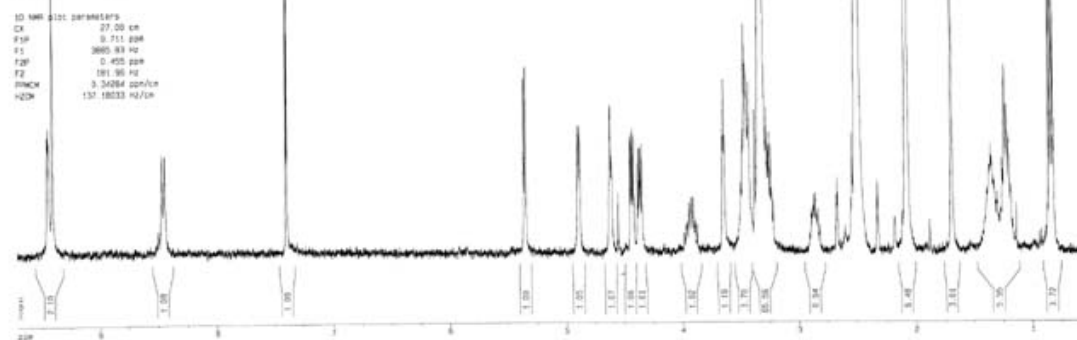
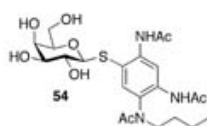
Current Data Parameters
NAME 117-103-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030811
Time 14.33
INSTRUM spect
PROBHD 5 mm QNP 1H/13C
PULPROG zgpg30
TD 32768
SOLVENT DMSO
AQ 128
DS 2
SWH 500.841 Hz
FIDRES 0.166872 Hz
AQ 2.5999564 sec
RG 1149.4
CW 89.400 usec
DE 10.50 usec
TE 300.0 K
DT 1.0000000 sec

***** CHANNEL f1 *****
NUC1 13
P1 10.00 usec
PL1 -2.00 dB
SFO1 400.1304008 MHz

F2 - Processing parameters
SI 65536
SF 400.1300077 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 27.00 cm
F1P 9.711 ppm
F1 3995.93 Hz
F2P 0.455 ppm
F2 181.96 Hz
PWCW 0.34284 ppm/cm
H2CW 137.18033 Hz/cm



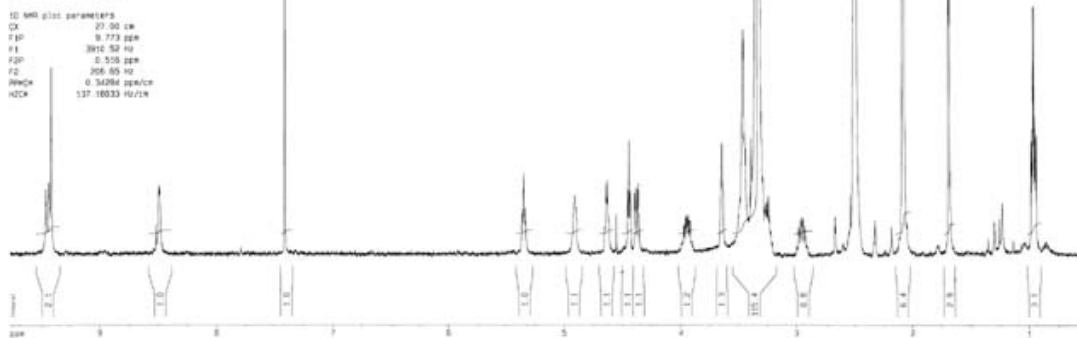
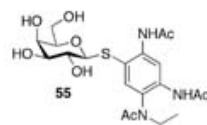
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EXPNO 1
PROCNO 1

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TD 32768
SOLVENT DMSO
AQ 128
DS 2
SWH 500.841 Hz
FIDRES 0.166872 Hz
AQ 2.5999564 sec
RG 1149.4
CW 89.400 usec
DE 10.50 usec
TE 300.0 K
DT 1.0000000 sec

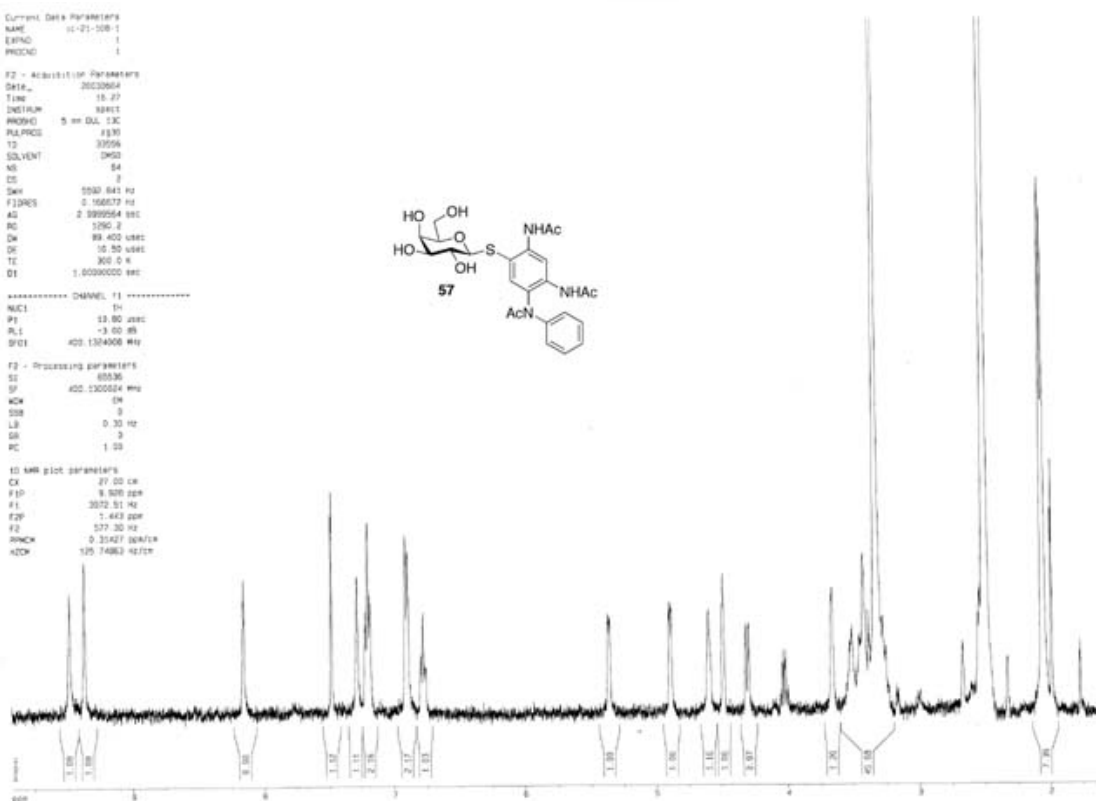
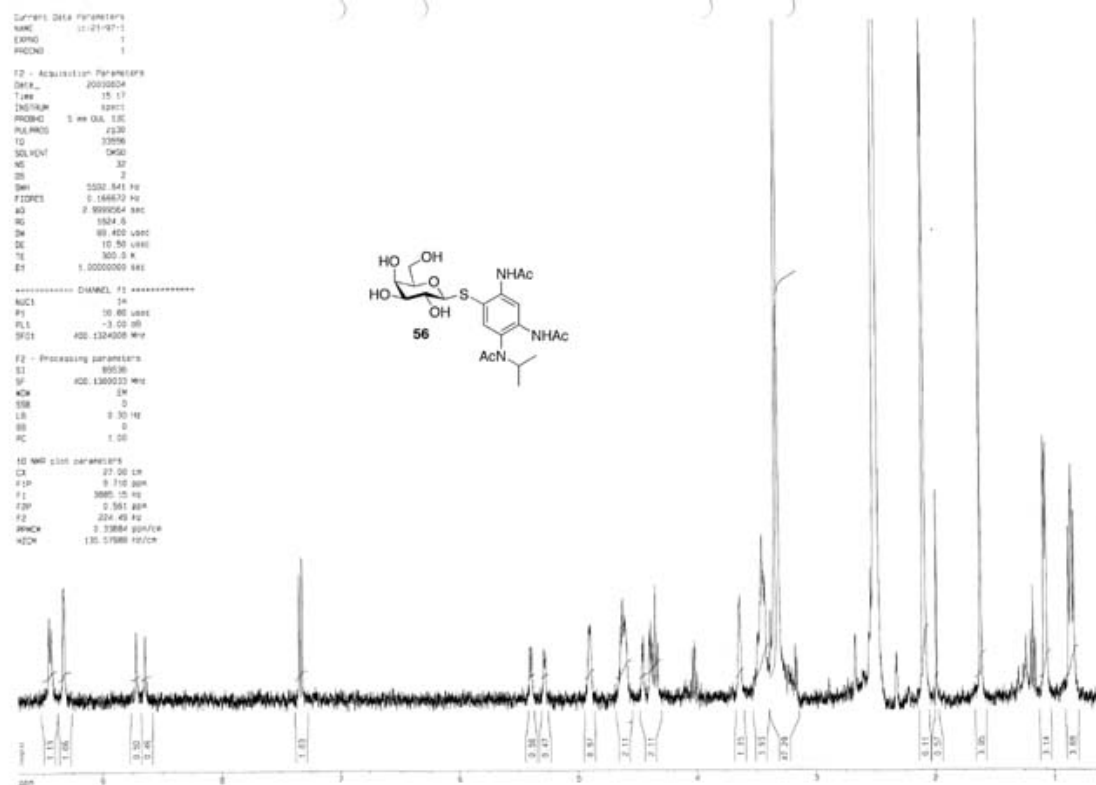
***** CHANNEL f1 *****
NUC1 13
P1 10.00 usec
PL1 -2.00 dB
SFO1 400.1304008 MHz

F2 - Processing parameters
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WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

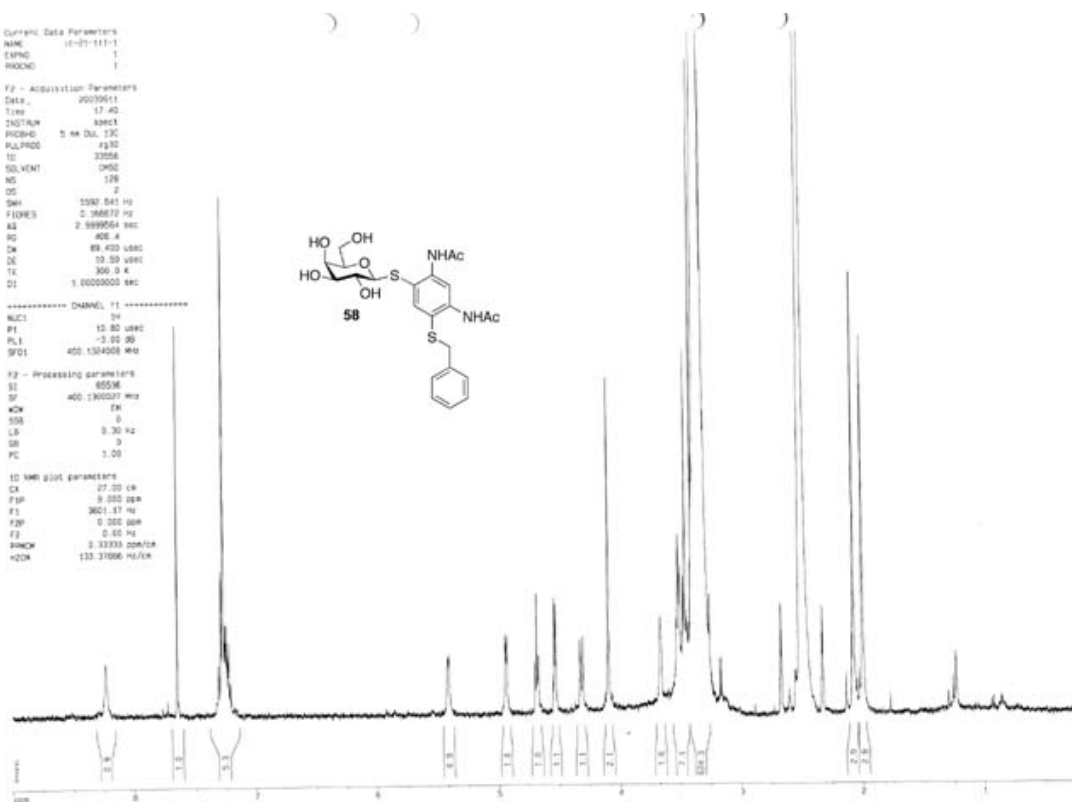
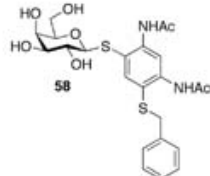
1D NMR plot parameters
CX 27.00 cm
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F1 3910.52 Hz
F2P 0.515 ppm
F2 206.65 Hz
PWCW 0.34284 ppm/cm
H2CW 137.18033 Hz/cm



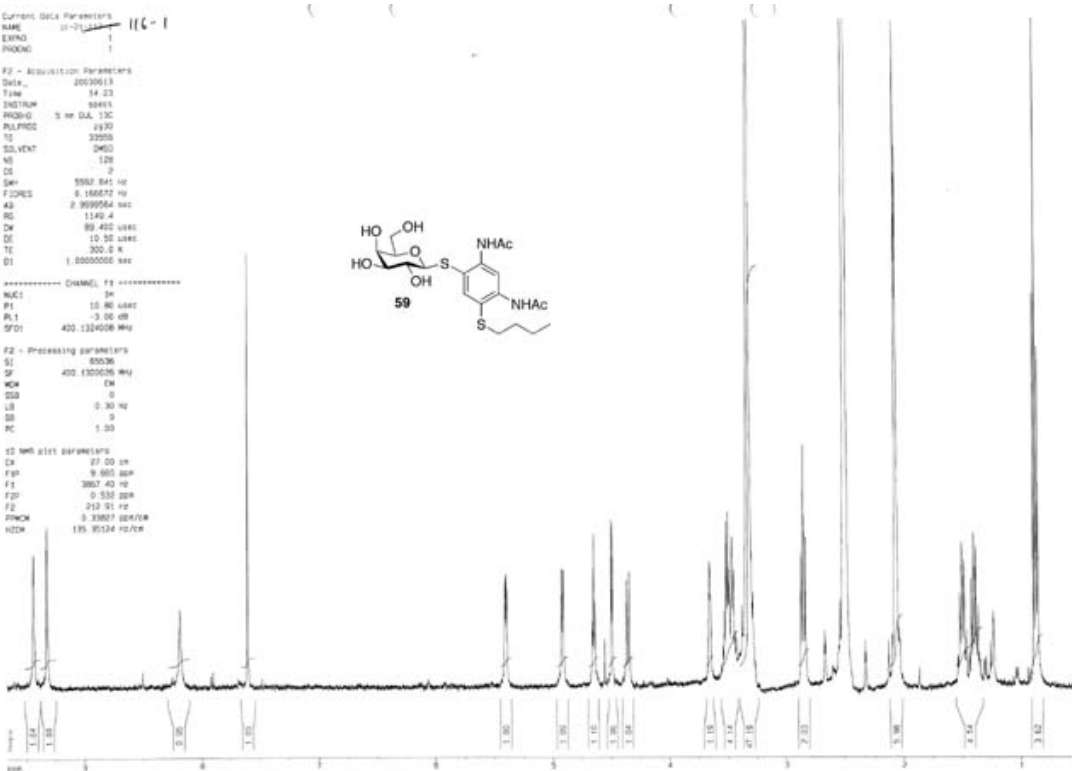
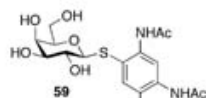
Supplementary data



10 km/s plot parameters	
CA	27.00 km
F1P	9.000 dB
F1	3601.17 Hz
F2P	0.000 dB
F2	0.00 Hz
SNRICH	0.33333 dB
H20M	133.37006 Hz



SD with six parameters	
CM	27.00 cm
F ₉₅	9.605 g/g
F ₁	3867.40 Hz
F ₂₀	0.532 g/g
F ₂	212.91 Hz
FWHM	0.33627 g/g
WDM	135.85124 Hz/g



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