

Electronic Supplementary Information

Chemoenzymatic Synthesis of Biotin-Appended Analogues of Gangliosides GM2, GM1, GD1a and GalNAc-GD1a for Solid-Phase Applications and Improved ELISA Tests

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Includes ¹H- and ¹³C- NMR spectra of the synthesized compounds.

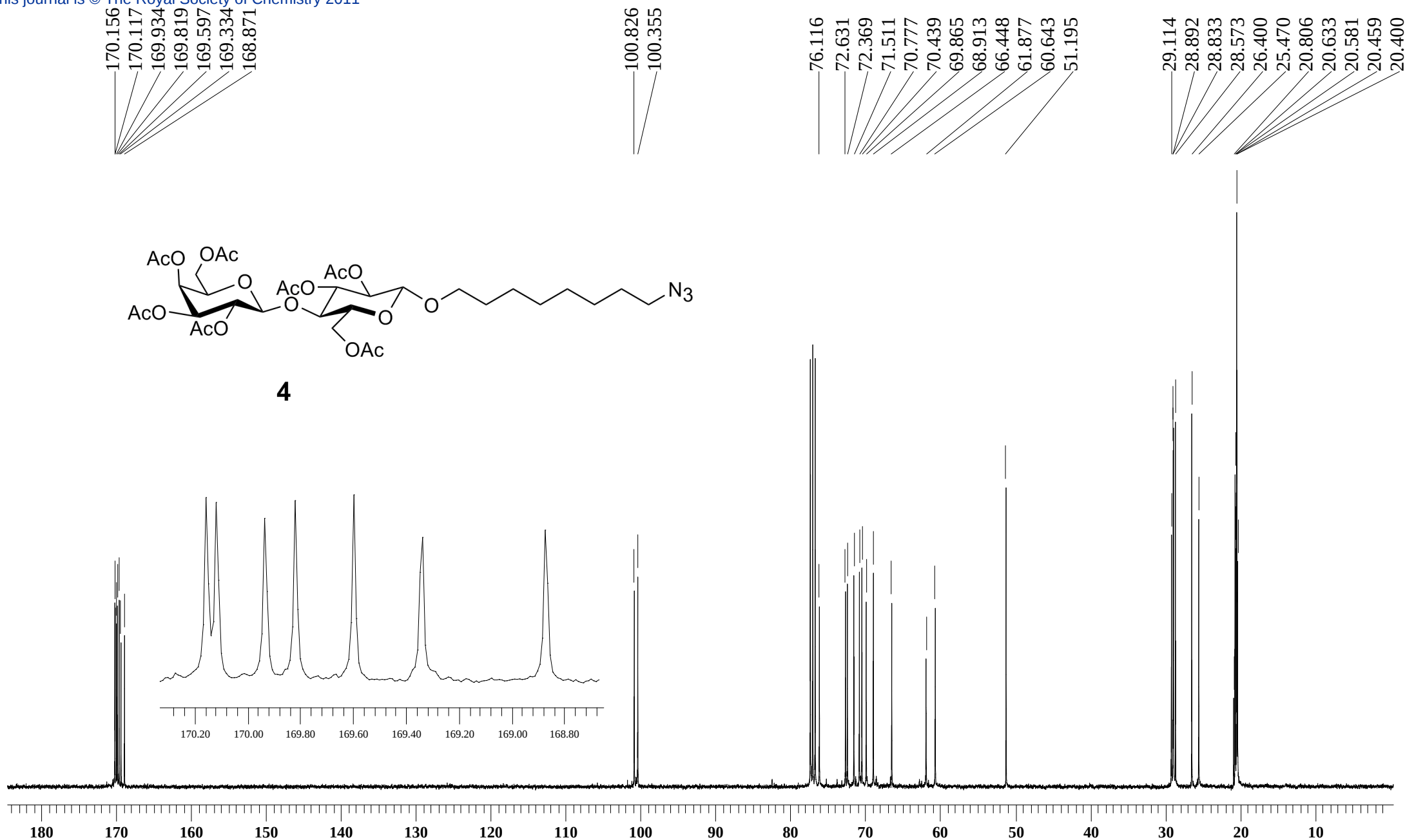
NMR spectra were recorded on a Bruker DPX 400, Bruker Avance 400 or Bruker Avance 900 (for the compound **11**) spectrometer.



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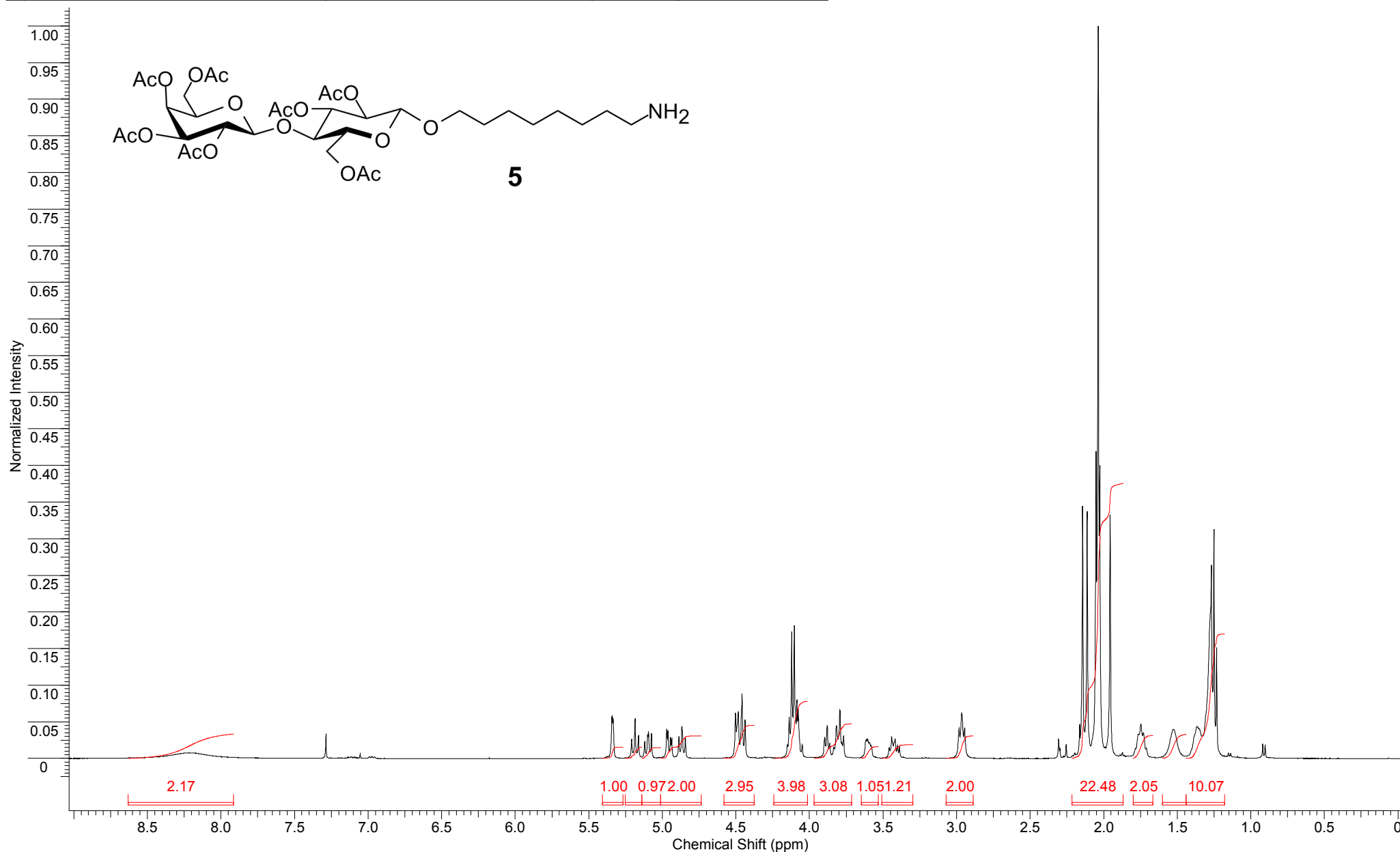
1D NMR plot parameters
CX                23.00 cm
F1P               8.000 ppm
F1               3201.04 Hz
F2P              -0.200 ppm
F2              -80.03 Hz
PPMCM            0.35652 ppm/cm
HZCM            142.65504 Hz/cm

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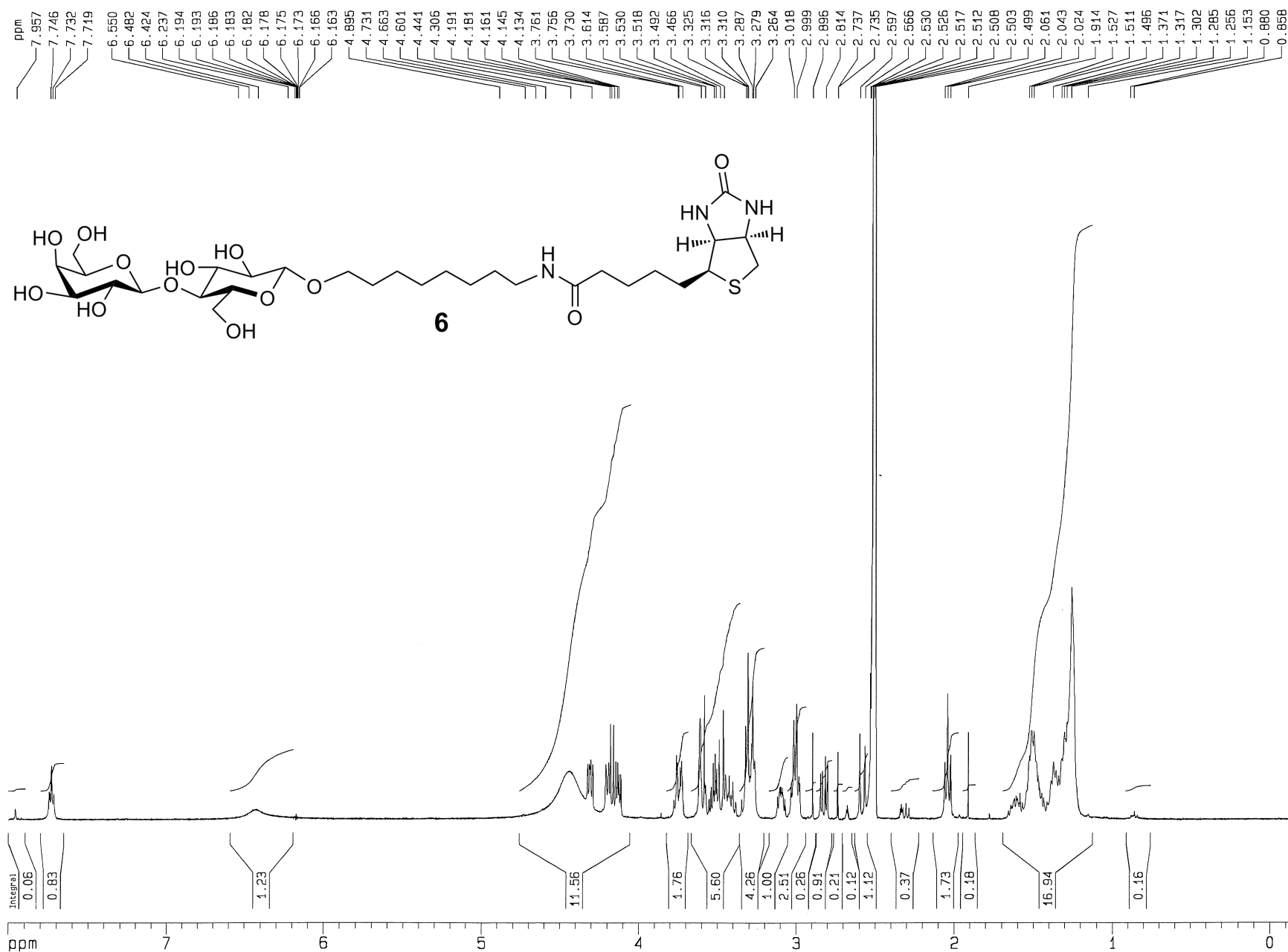


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Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	12710.3887	Sweep Width (Hz)	31846.16	Temperature (degree C)	27.000

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Points Count	16384	Pulse Sequence	zg30	Receiver Gain	90.50	Owner	veldhuis
Spectrum Offset (Hz)	2471.0088	Sweep Width (Hz)	8223.18	Temperature (degree C)	27.000	SW(cyclical) (Hz)	8223.68
		Solvent	CHLOROFORM-d				



lactose-biotin



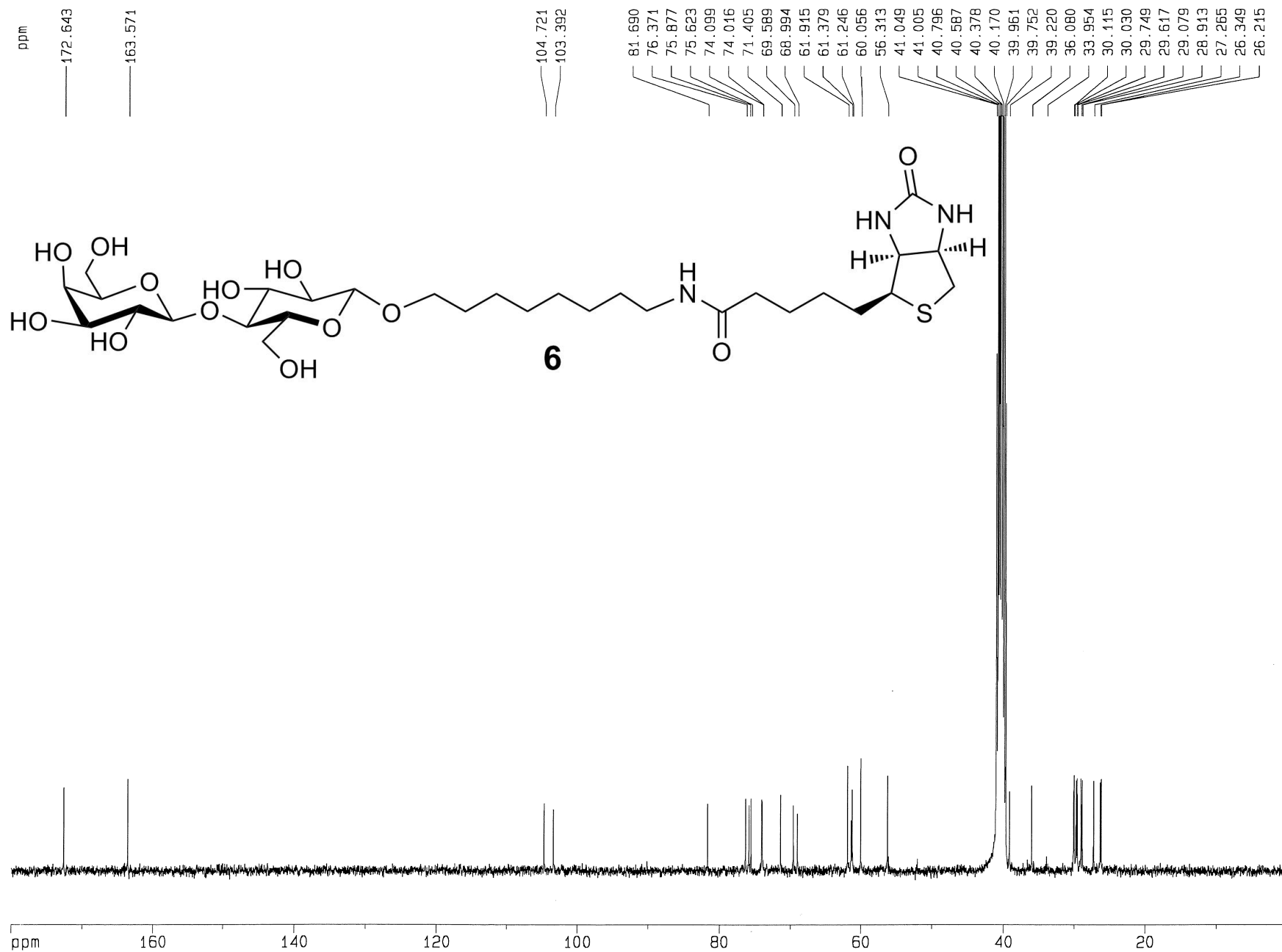
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PULPROG zg30
TD 32768
SOLVENT DMSO
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 203.2
DW 60.800 usec
DE 9.00 usec
TE 300.0 K
D1 1.00000000 sec

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NUC1 1H
P1 9.50 usec
PL1 -6.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB -0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 23.00 cm
F1P 9.000 ppm
F1 3201.04 Hz
F2P -0.200 ppm
F2 -80.03 Hz
PPMCM 0.35652 ppm/cm
HZCM 142.65504 Hz/cm



Current Data Parameters

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EXPNO 186
PROCNO 1

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Time 12.57
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PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 3689
DS 8
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 32768
DW 15.700 usec
DE 9.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

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NUC1 13C
P1 6.70 usec
PL1 -6.00 dB
SF01 100.6254358 MHz

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CPDPRG2 waltz16
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PL12 18.00 dB
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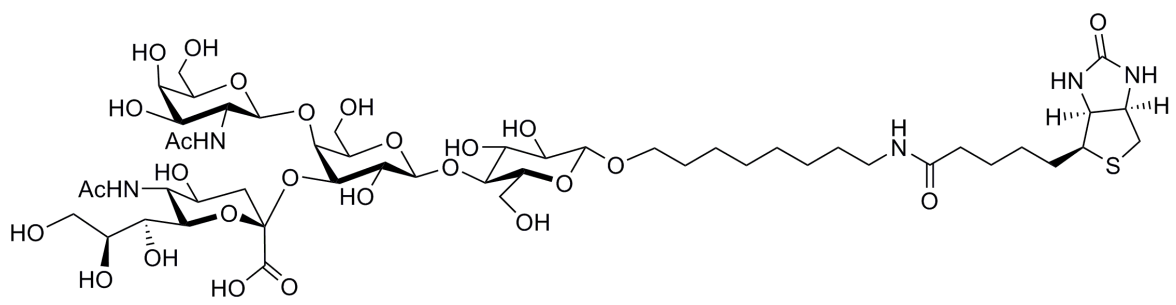
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PC 1.40

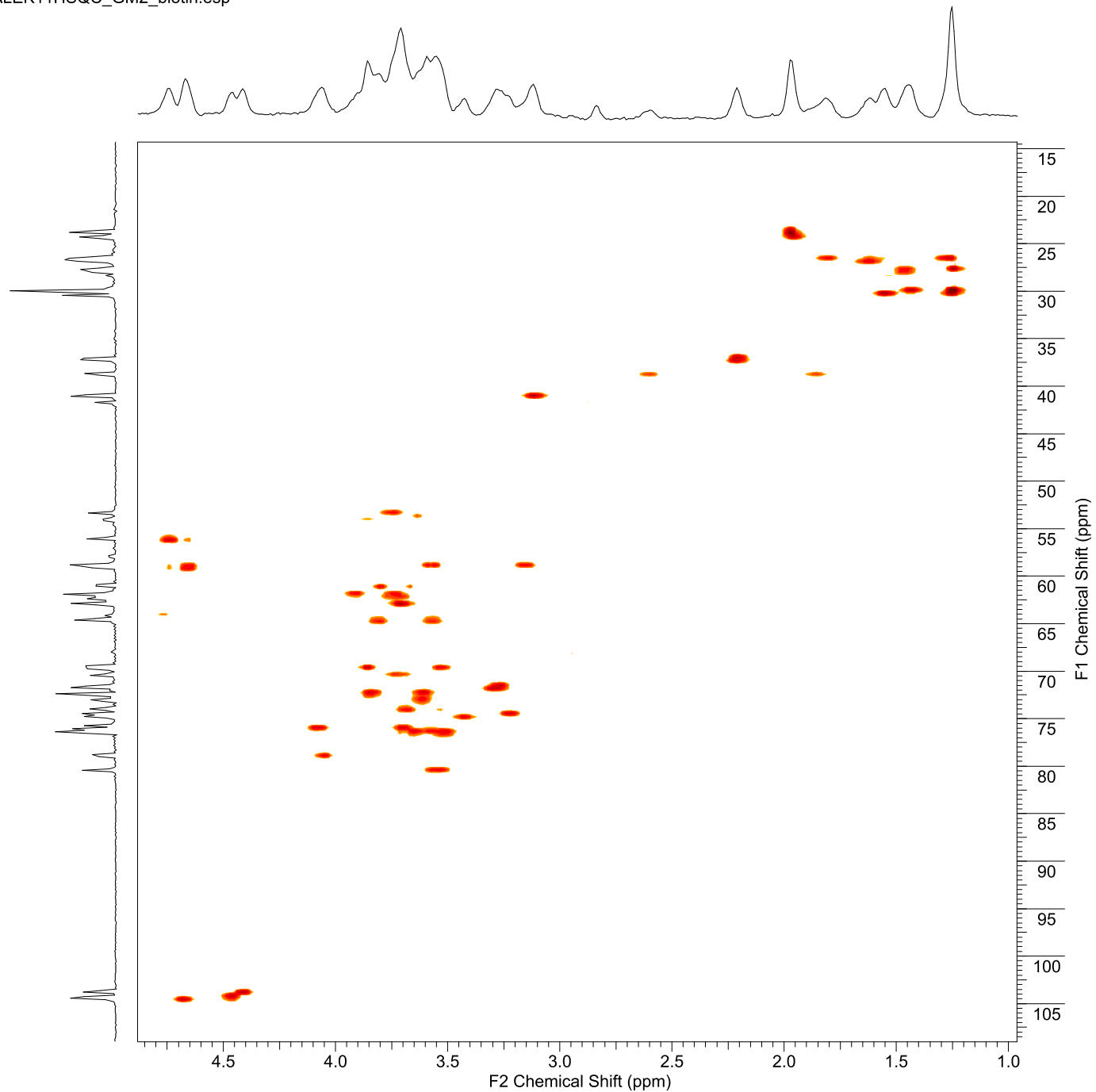
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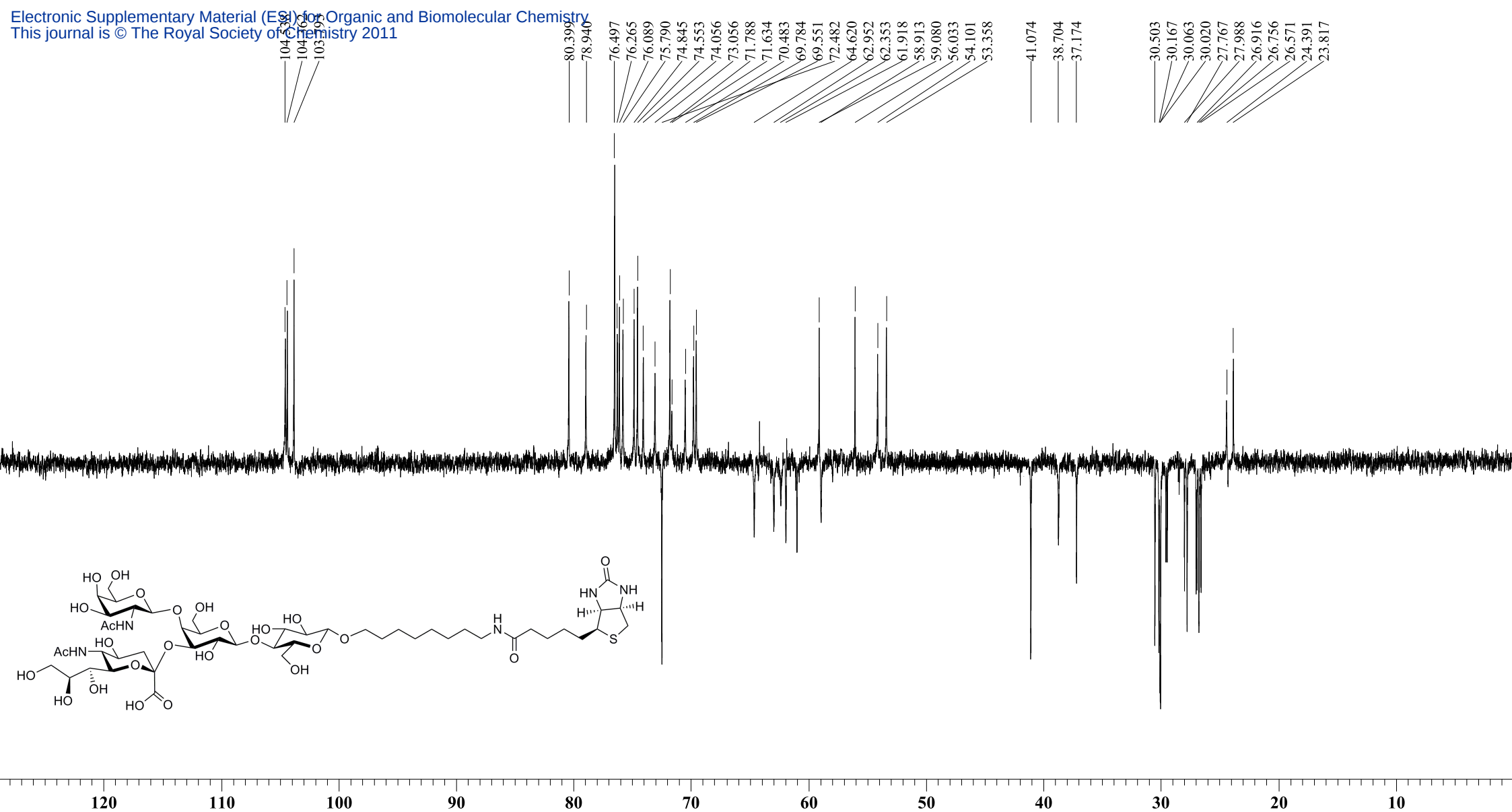
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F1 18110.29 Hz
F2P 0.000 ppm
F2 0.00 Hz
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HZCM 787.40393 Hz/cm

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Date	14 May 2011 08:59:28		
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Nucleus	(1H, 13C)	Number of Transients	46
		Origin	spect
Original Points Count	(512, 1024)	Owner	ORC
		Points Count	(1024, 1024)
Pulse Sequence	hsqcetgpsi2	Solvent	D2O
		Sweep Width (Hz)	(3605.77, 16604.09)
Temperature (degree C)	25.460	Title	GM2-biotin

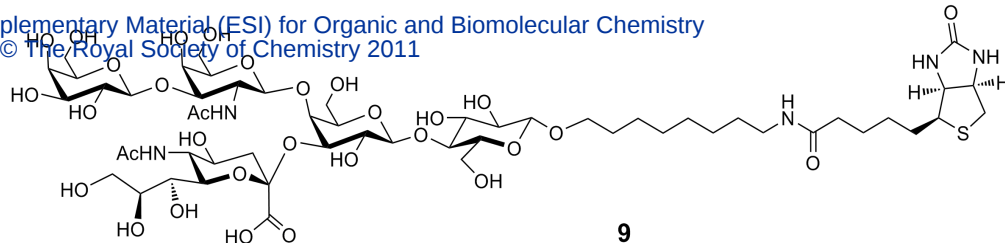


ALEK11HSQC_GM2_biotin.esp

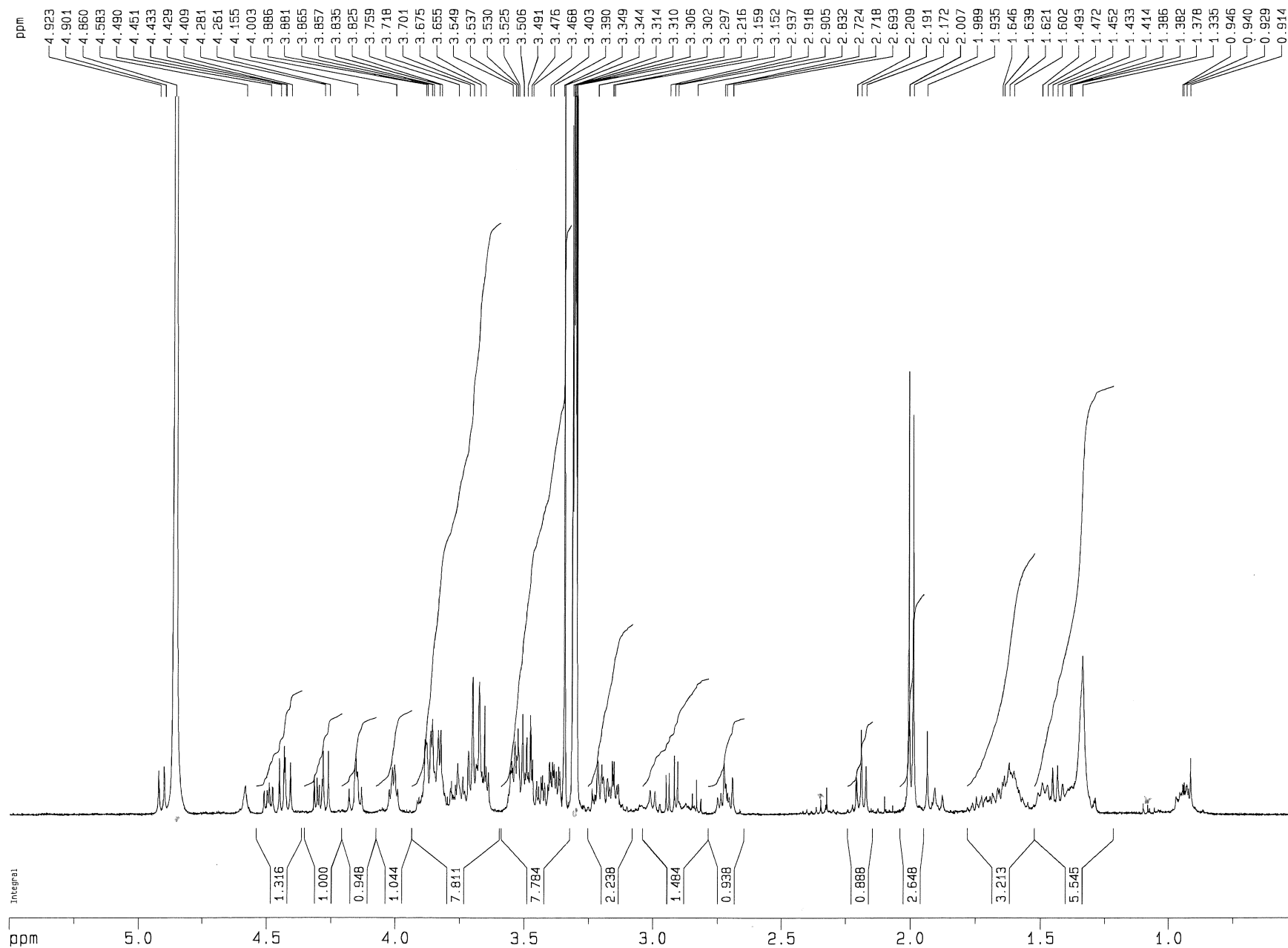




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Frequency (MHz)	100.63	Nucleus	13C	Number of Transients	30720	Origin spect
Original Points Count	32768	Owner	Orc	Points Count	32768	Pulse Sequence jmod
Receiver Gain	2050.00	SW(cyclical) (Hz)	24038.46	Solvent	DEUTERIUM OXIDE	
Spectrum Offset (Hz)	10064.0225	Sweep Width (Hz)	24037.73	Temperature (degree C)	19.760	



GM1-Gating, CHELEX only



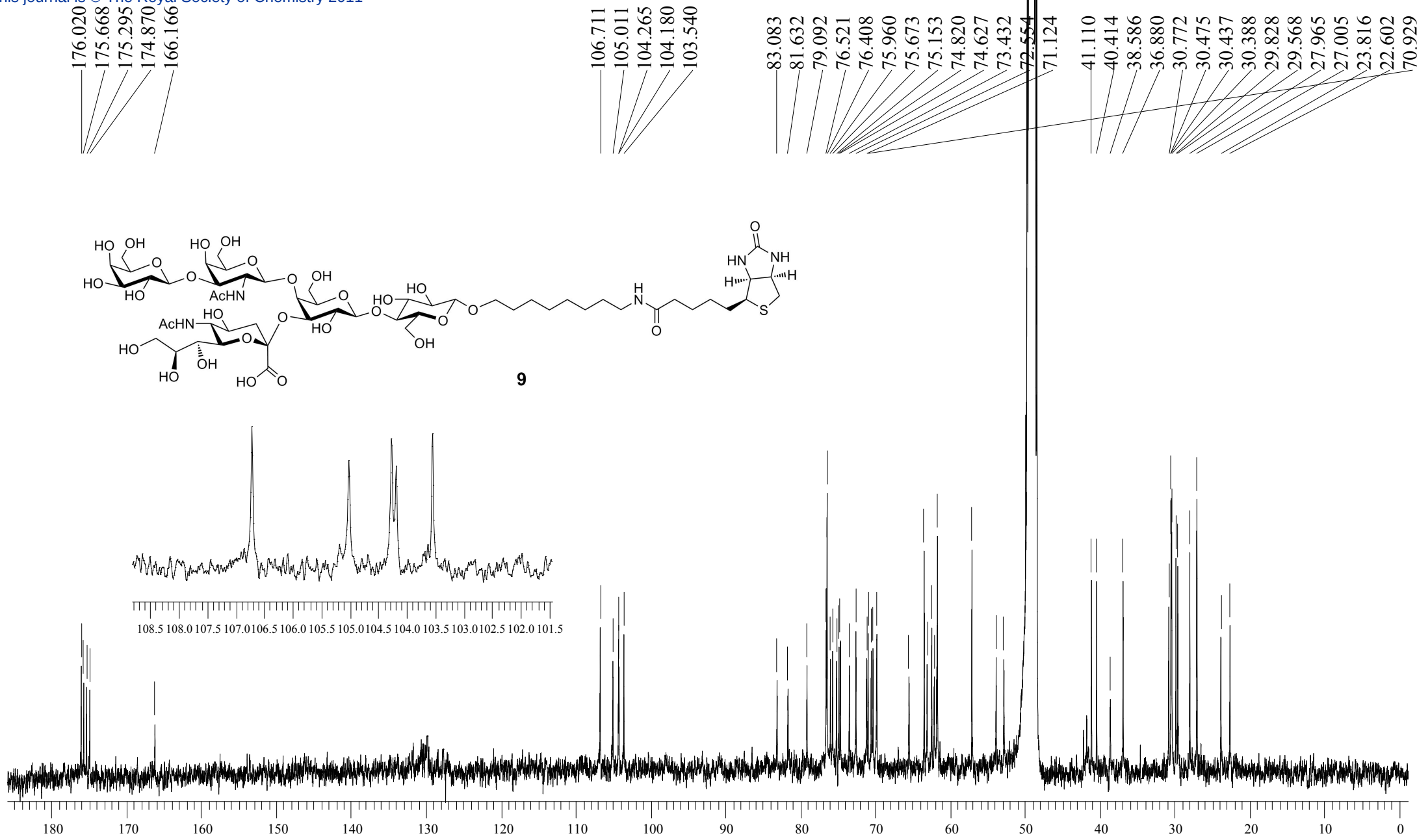
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PROCNO 1

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INSTRUM dpx_400
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PULPROG zg30
TO 32768
SOLVENT MeOH
NS 512
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 456.1
DW 60.800 usec
DE 9.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 -6.00 dB
SF01 400.1324710 MHz

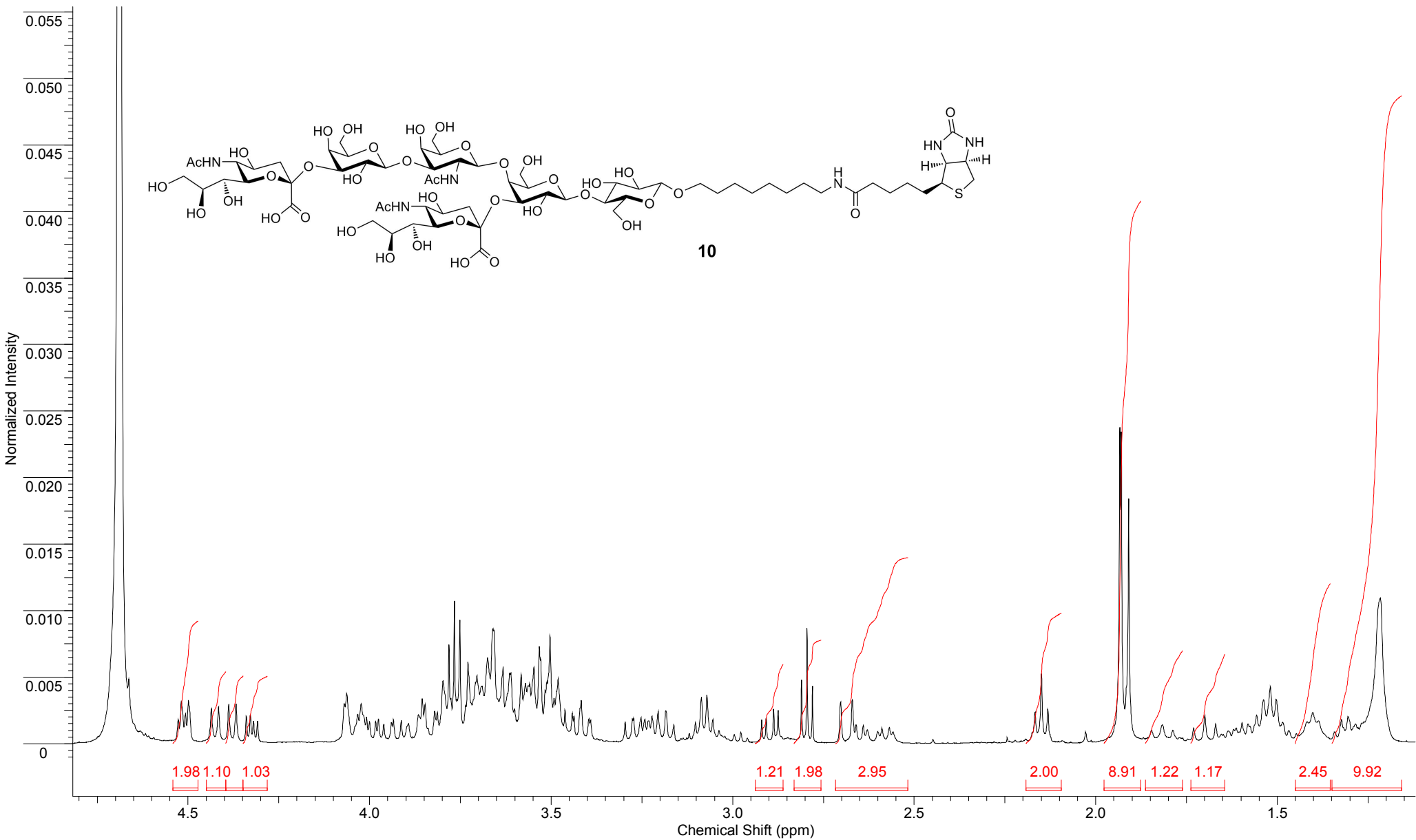
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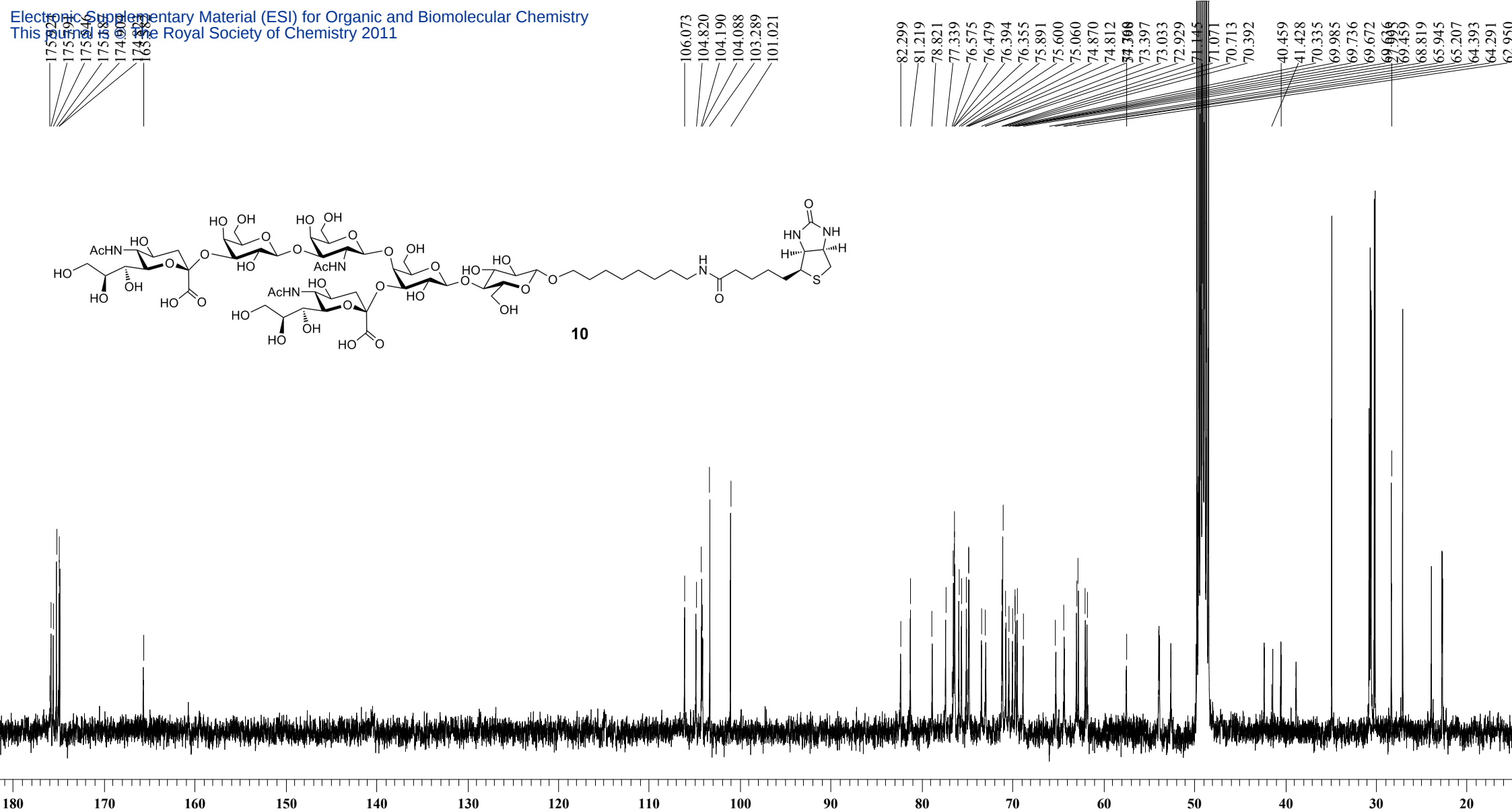
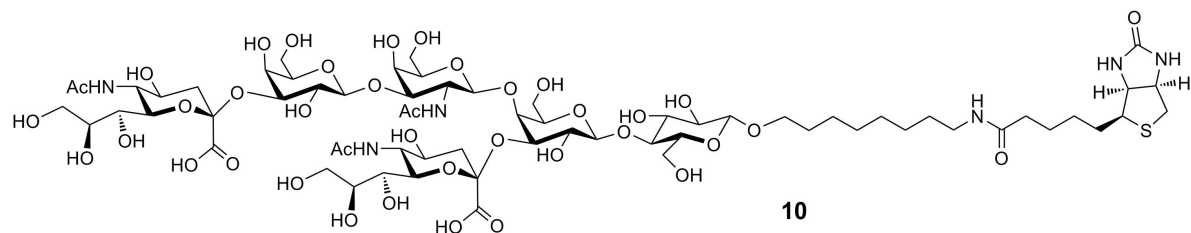
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F1 2200.72 Hz
F2P 0.500 ppm
F2 200.07 Hz
PPMCM 0.21739 ppm/cm
HZCM 86.98479 Hz/cm



Acquisition Time (sec)	1.0289	Comment	5 mm Dual 13C/1H	Date	09 Sep 09:01:52
Date Stamp	09 Sep 09:01:52	File Name	D:\NF\014000fid		
Frequency (MHz)	100.63	Nucleus	13C	Number of Transients	76800
Original Points Count	32768	Owner	veldhuis	Points Count	32768
Receiver Gain	32768.00	SW (cyclical) (Hz)	31847.13	Solvent	CD3OD
Spectrum Offset (Hz)	12897.4619	Sweep Width (Hz)	31846.16	Temperature (degree C)	27.000

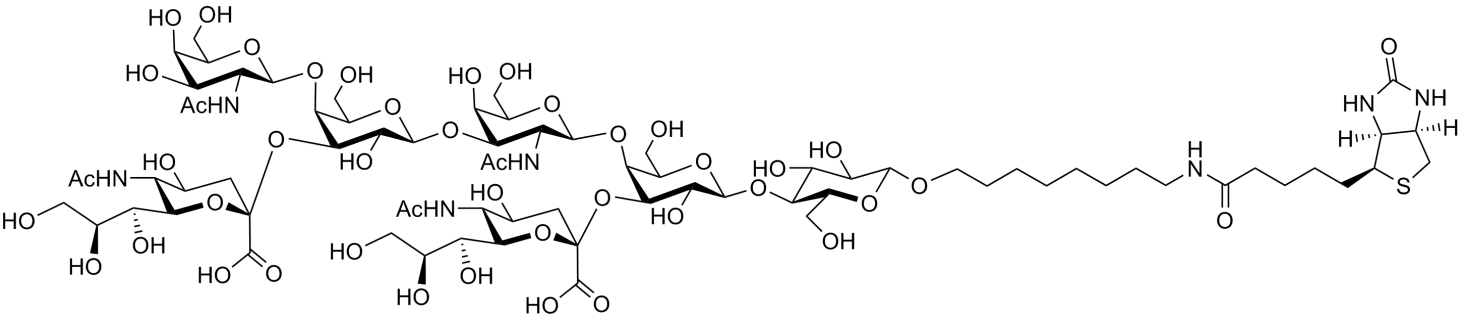
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Original Points Count	16384	Owner	veldhuis	Points Count	16384	Pulse Sequence zg30
Receiver Gain	71.80	SW(cyclical) (Hz)	4789.27	Solvent	DEUTERIUM OXIDE	
Spectrum Offset (Hz)	1996.2163	Sweep Width (Hz)	4788.98	Temperature (degree C)	27.000	



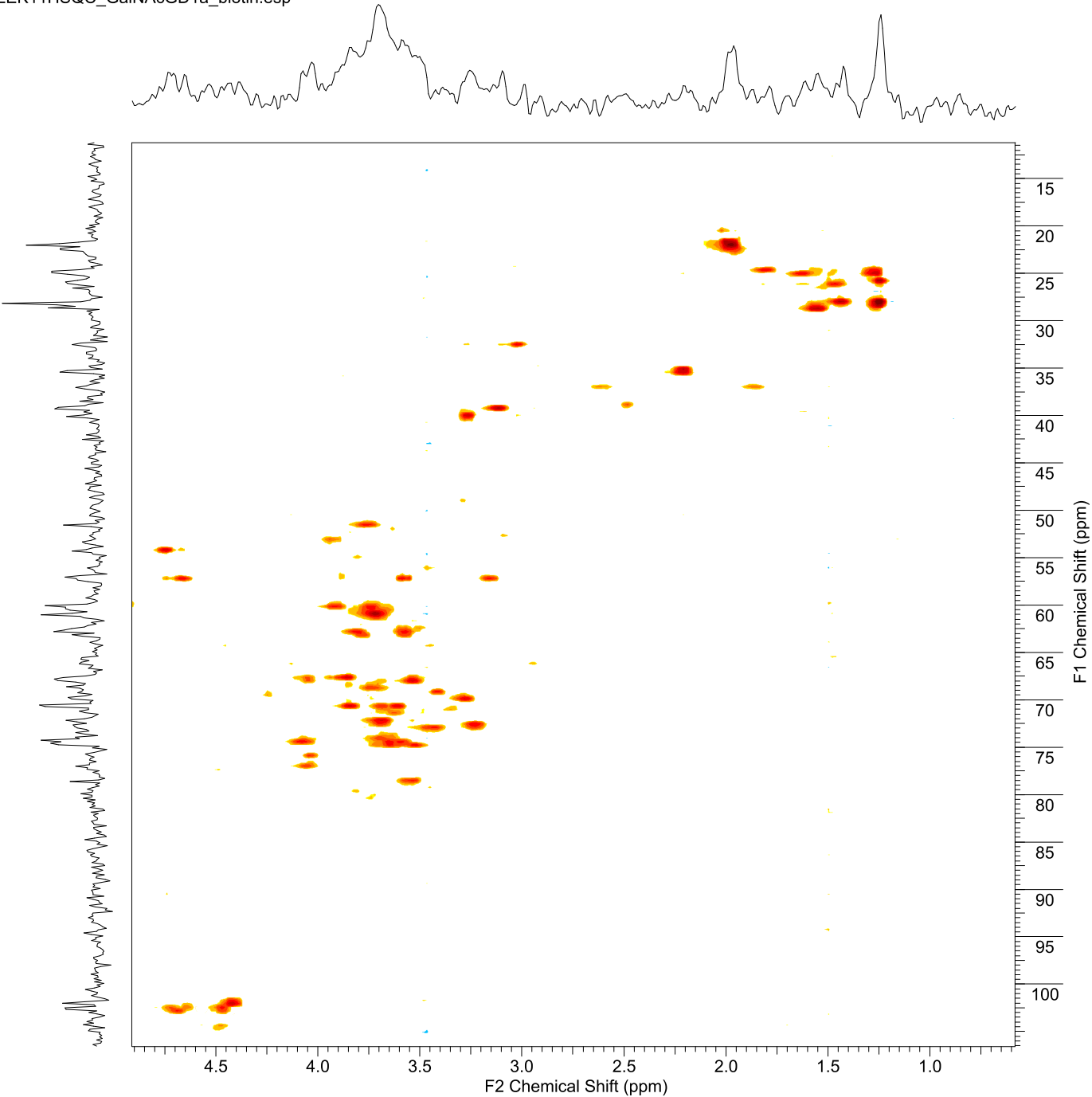


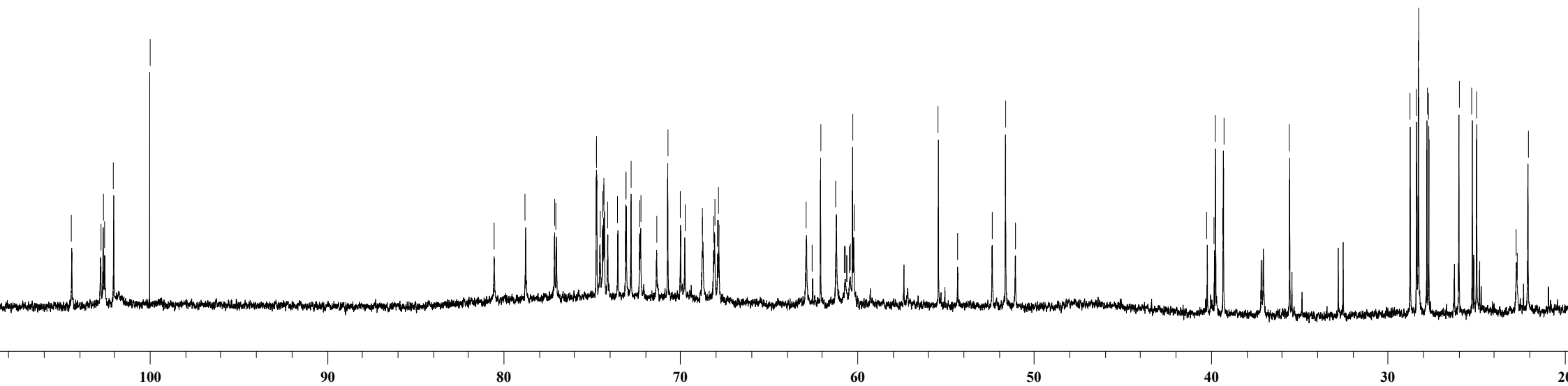
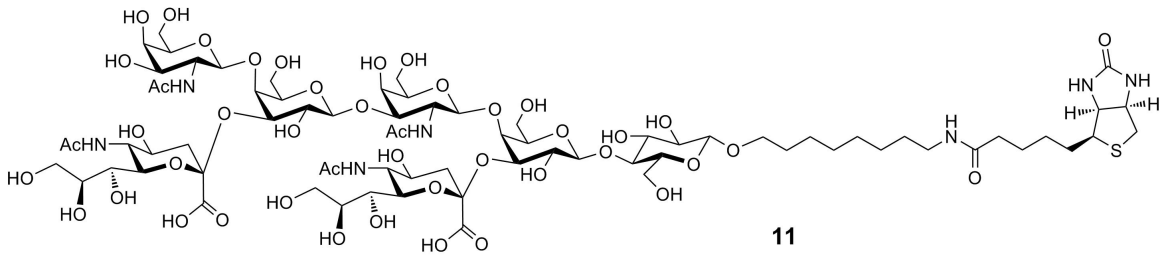
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Origin	spect	Original Points Count	32768	Owner	Orc	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	181.00	SW(cyclical) (Hz)	24038.46	Solvent	MeOD	Spectrum Offset (Hz)	10206.9521	Sweep Width (Hz)	24037.73
Temperature (degree C)	25.160								

Acquisition Time (sec)	(0.1420, 0.0617)	Comment	5 mm PABBI 1H/D-BB Z-GRD Z820201/0172
Date	14 May 2011 09:34:50		
File Name	D:\OBC\ALEK11HSQC\2\pdata\1\2rr	Frequency (MHz)	(400.17, 100.63)
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		Origin	spect
Original Points Count	(512, 1024)	Owner	ORC
		Points Count	(1024, 1024)
Pulse Sequence	hsqcetgpsi2	Solvent	D2O
		Sweep Width (Hz)	(3605.77, 16604.09)
Temperature (degree C)	25.360	Title	GalNAC-GD1a-biotin



ALEK11HSQC_GalNAcGD1a_biotin.esp





Acquisition Time (sec)	0.3604	Comment	1D 13C, 298K	Date	10 Jun 11:22:40	
Date Stamp	10 Jun 11:22:40			File Name	D:\NF\data900\LSF_Han_150408\LSF_Han_150408_008000fid	
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Owner	psm	Points Count	16384	Pulse Sequence	zgpg30	Receiver Gain 8192.00
Solvent				Spectrum Offset (Hz)	22637.5723	Sweep Width (Hz) 45451.77
						Original Points Count
						SW(cyclical) (Hz)
						Temperature (degree C)