

**Boron-based hybrids as novel scaffolds for the development of drugs with  
neuroprotective properties**

Ivana Cacciatore,<sup>a,\*</sup> Hasan Turkez,<sup>b</sup> Annalisa Di Rienzo,<sup>a</sup> Michele Ciulla,<sup>a</sup> Adil Mardinoglu,<sup>c,d</sup> and Antonio Di Stefano<sup>a</sup>

**SUPPORTING INFORMATION**

**NMR and MS spectra of compounds**

NMR Spectra (3aR)-2-(azidomethyl)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[d][1,3,2]dioxaborole (2)



Gradient Shimming

Sample Name:

Data Collected on:

m300-mercury300

Archive directory:

/export/home/chempack/vnmrsys/data

Sample directory:

Fidfile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Feb 11 2015

Operator: caccia

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.706 sec

Width 4803.1 Hz

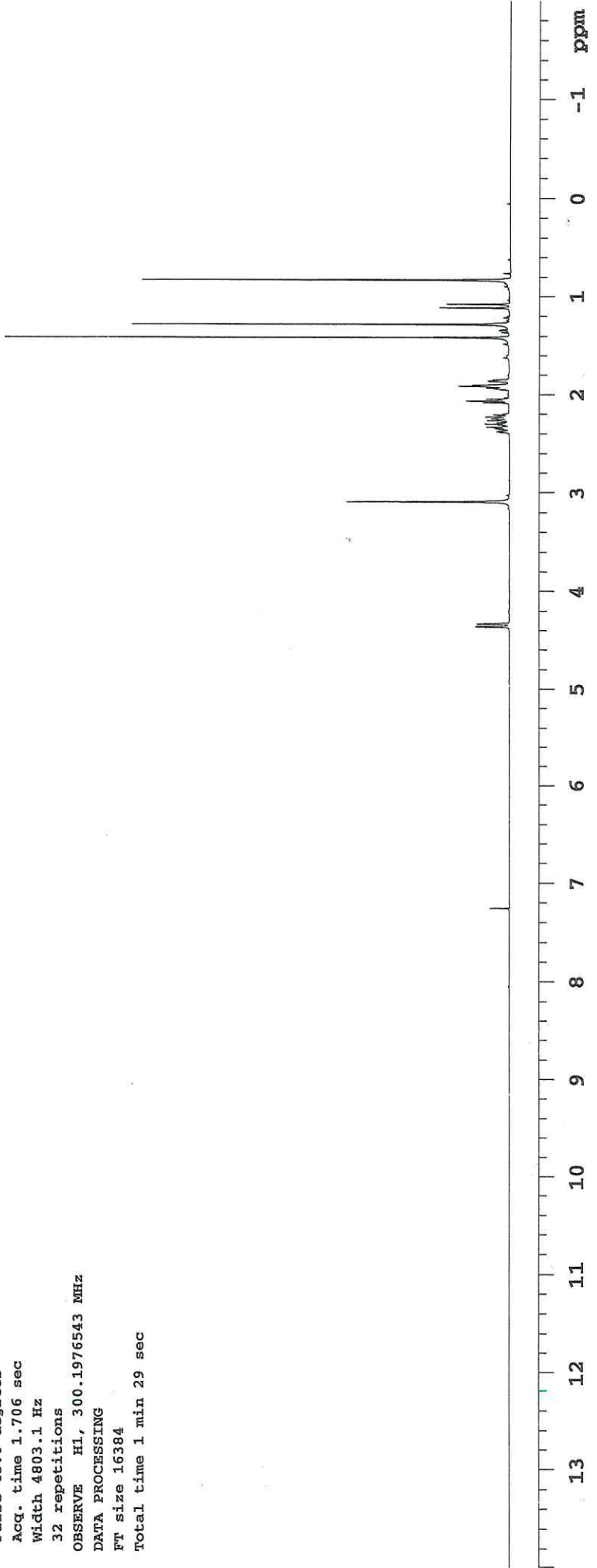
32 repetitions

OBSERVE H1, 300.1976543 MHz

DATA PROCESSING

FT size 16384

Total time 1 min 29 sec



Gradient Shimming

Sample Name:

Data Collected on:  
m300-mercury300  
Archive directory:  
/export/home/chempack/vnmrsys/data  
Sample directory:

FidFile: PROTON

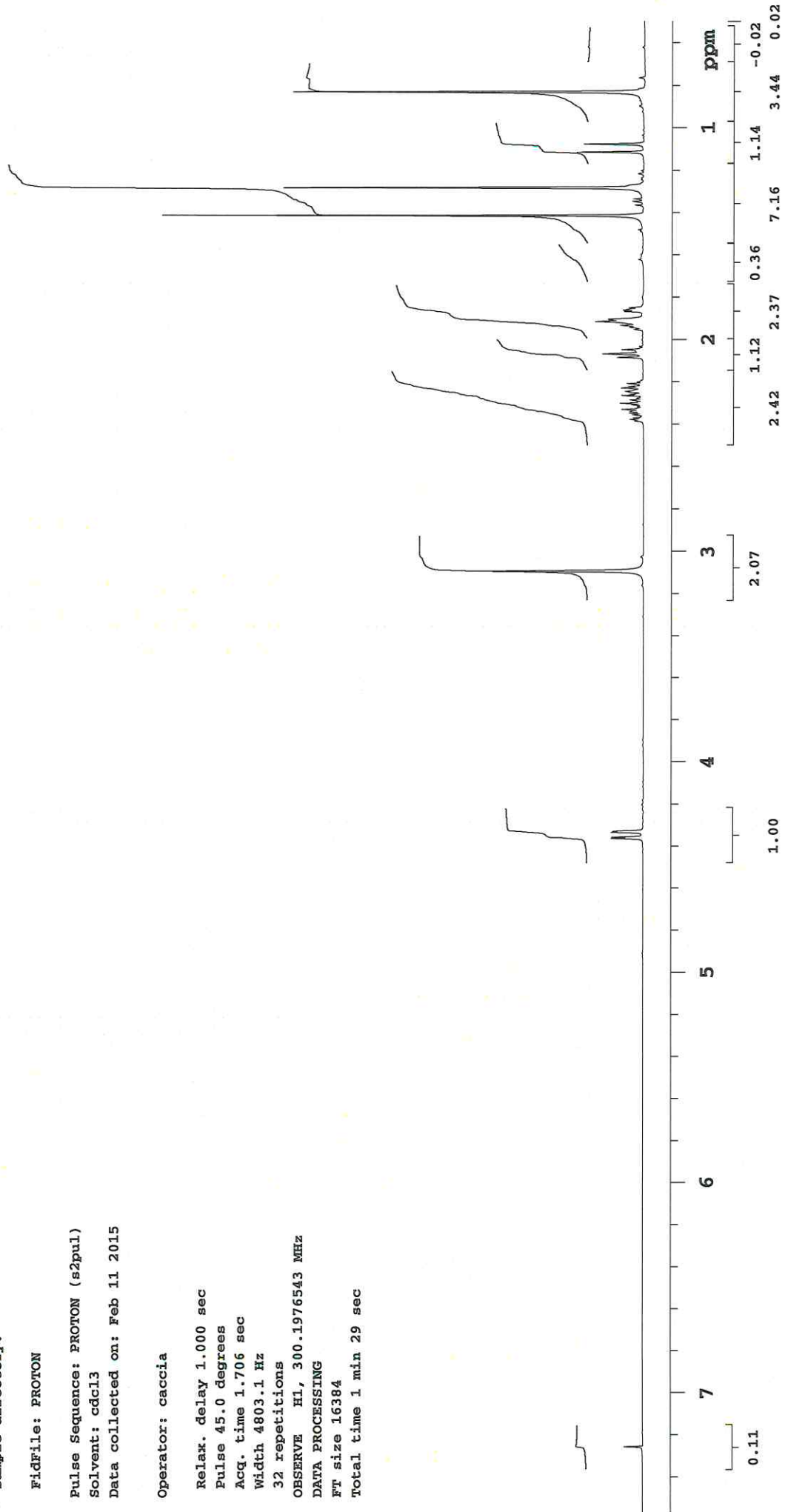
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 11 2015

Operator: caccia

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.706 sec  
Width 4803.1 Hz  
32 repetitions  
OBSERVE H1, 300.1976543 MHz  
DATA PROCESSING  
Ft size 16384  
Total time 1 min 29 sec



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Gradient Shimming

Sample Name:

Data Collected on:  
m300-mercury300  
Archive directory:  
/export/home/chempack/vnmrsys/data  
Sample directory:

FidFile: PROTON

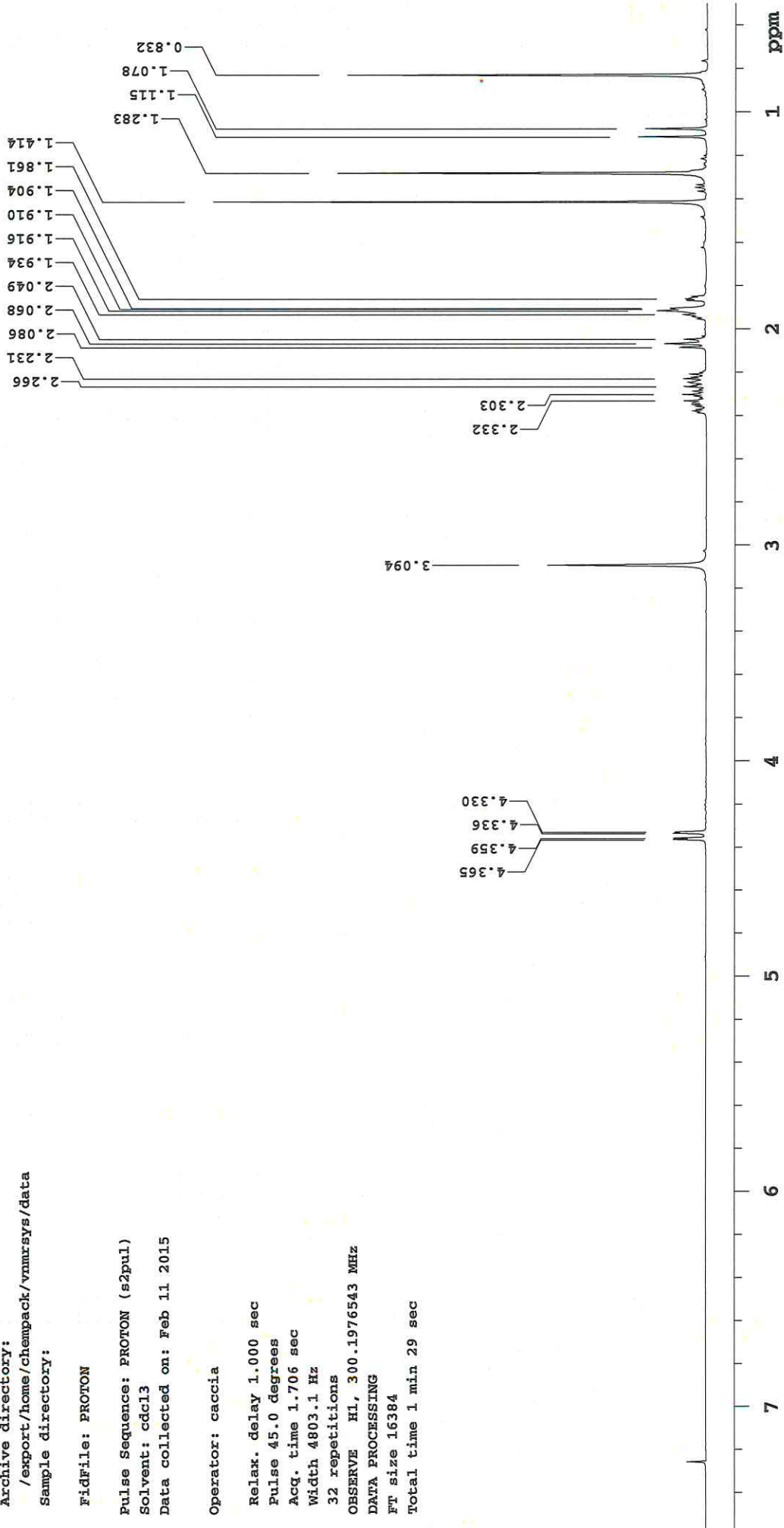
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 11 2015

Operator: caccia

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.706 sec  
Width 4803.1 Hz  
32 repetitions  
OBSERVE H1, 300.1976543 MHz  
DATA PROCESSING  
Ft size 16384  
Total time 1 min 29 sec



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NMR Spectra of ((3aR)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[d][1,3,2]dioxaborol-2-yl)methanaminium chloride (3)

Gradient Shimming

Sample Name:

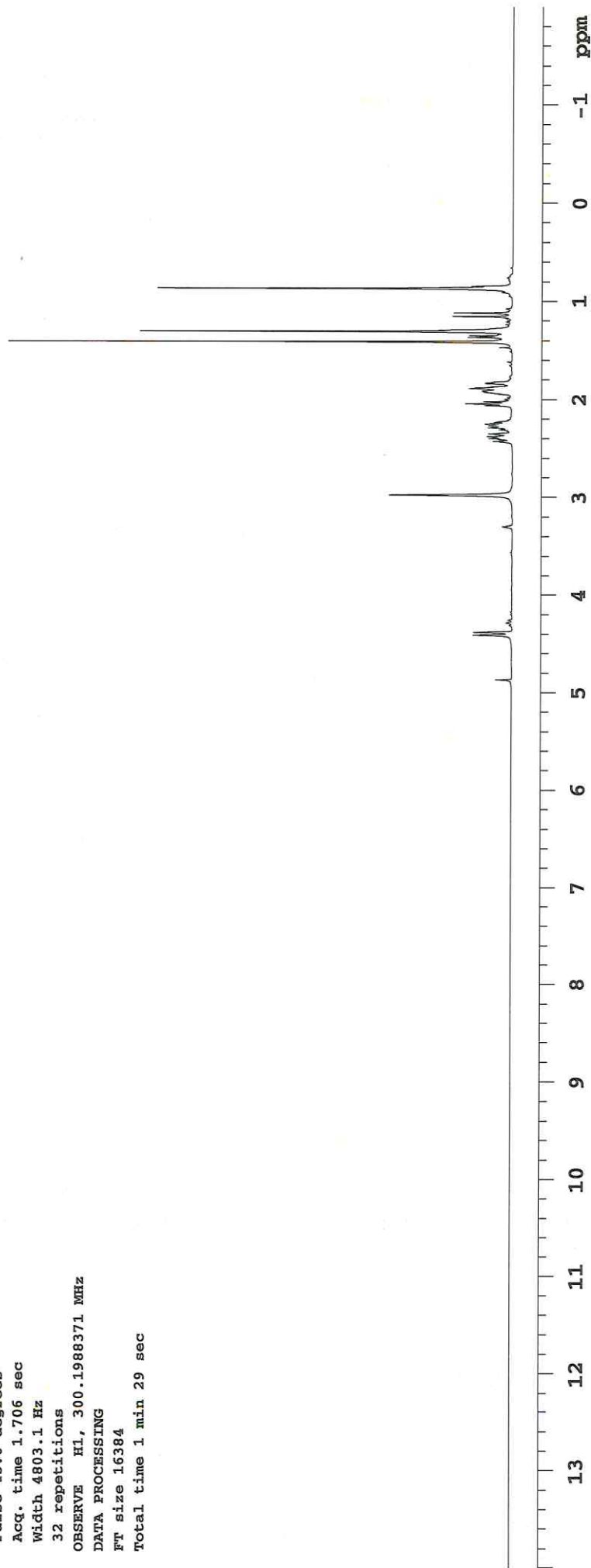
Data Collected on:  
m300-mercury300  
Archive directory:  
/export/home/chempack/vnmrsys/data  
Sample directory:

Fidfile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: cd3od  
Data collected on: Mar 18 2015

Operator: caccia

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.706 sec  
Width 4803.1 Hz  
32 repetitions  
OBSERVE H1, 300.1988371 MHz  
DATA PROCESSING  
FT size 16384  
Total time 1 min 29 sec



Gradient Shimming

Sample Name:

Data Collected on:

m300-mercury300

Archive directory:

/export/home/chempack/vnmrsys/data

Sample directory:

Fidfile: PROTON

Pulse Sequence: PROTON (s2pul1)

Solvent: cd3od

Data collected on: Mar 18 2015

Operator: caccia

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.706 sec

Width 4803.1 Hz

32 repetitions

OBSERVE H1, 300.1988371 MHZ

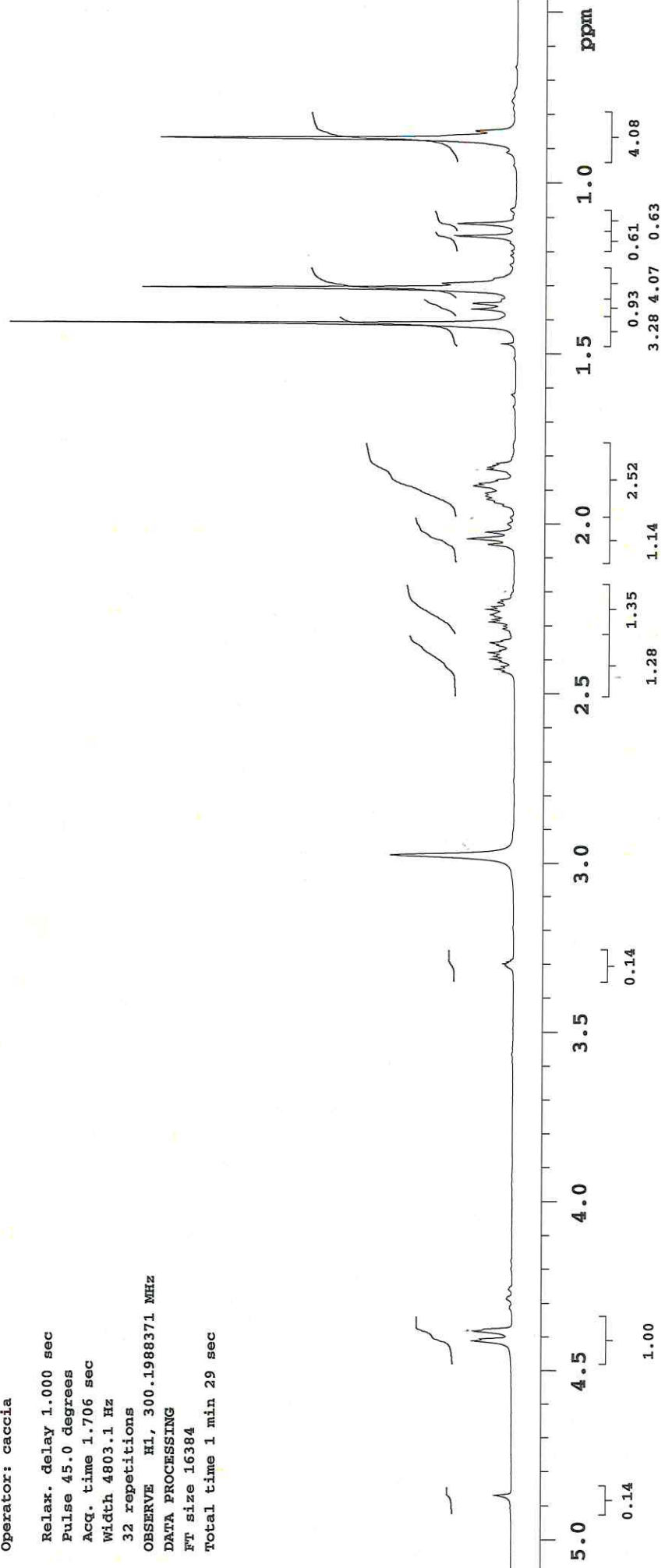
DATA PROCESSING

FT size 16384

Total time 1 min 29 sec



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Gradient Shimming

Sample Name:

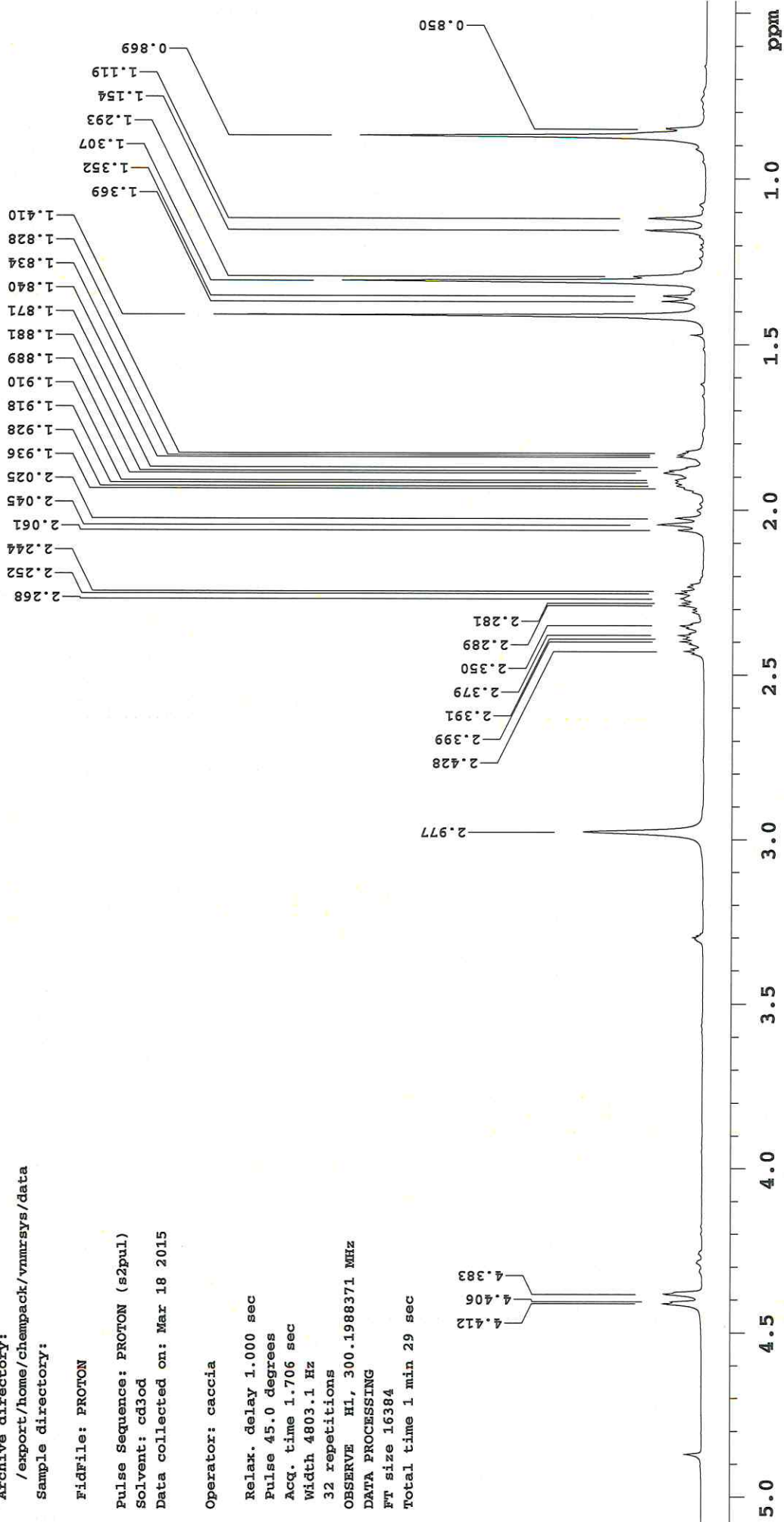
Data Collected on:  
m300-mercury300  
Archive directory:  
/export/home/chempack/vnmrsys/data  
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: cd3od  
Data collected on: Mar 18 2015

Operator: caccia

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.706 sec  
Width 4803.1 Hz  
32 repetitions  
OBSERVE H1, 300.1988371 MHz  
DATA PROCESSING  
FT size 16384  
Total time 1 min 29 sec



NMR AND MS SPECTRA of 5-((S)-1,2-dithiolan-3-yl)-N-(((3aR)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[d][1,3,2]dioxaborol-2-yl)methyl)pentanamide  
(BLA)

BIA

Gradient Shimming



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Sample Name:

Data Collected on:

m300-mercury300

Archive directory:

/export/home/chempack/vnmrsys/data

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 27 2015

Operator: caccia

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.706 sec

Width 4803.1 Hz

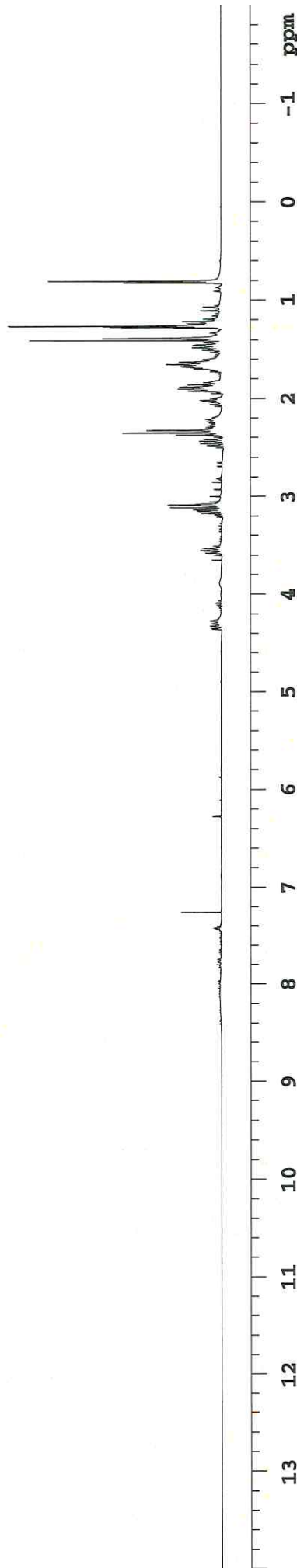
8 repetitions

OBSERVE H1, 300.1976543 MHz

DATA PROCESSING

FT size 16384

Total time 0 min 23 sec



Gradient Shimming

Sample Name:

Data Collected on:  
m300-mercury300  
Archive directory:  
/export/home/chempack/vnmrsys/data  
Sample directory:

FidFile: PROTON

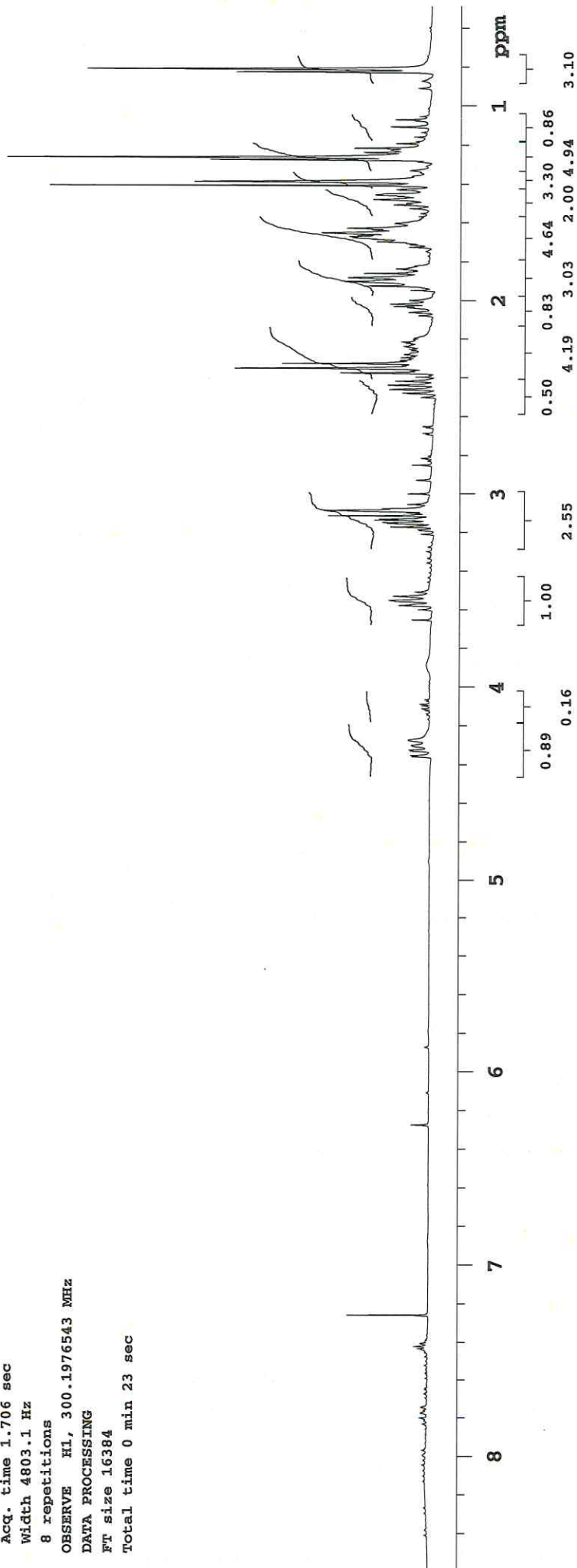
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Mar 27 2015

Operator: caccia

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.706 sec  
Width 4803.1 Hz  
8 repetitions  
OBSERVE H1, 300.1976543 MHZ  
DATA PROCESSING  
Ft size 16384  
Total time 0 min 23 sec



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Gradient Shimmining

Sample Name:

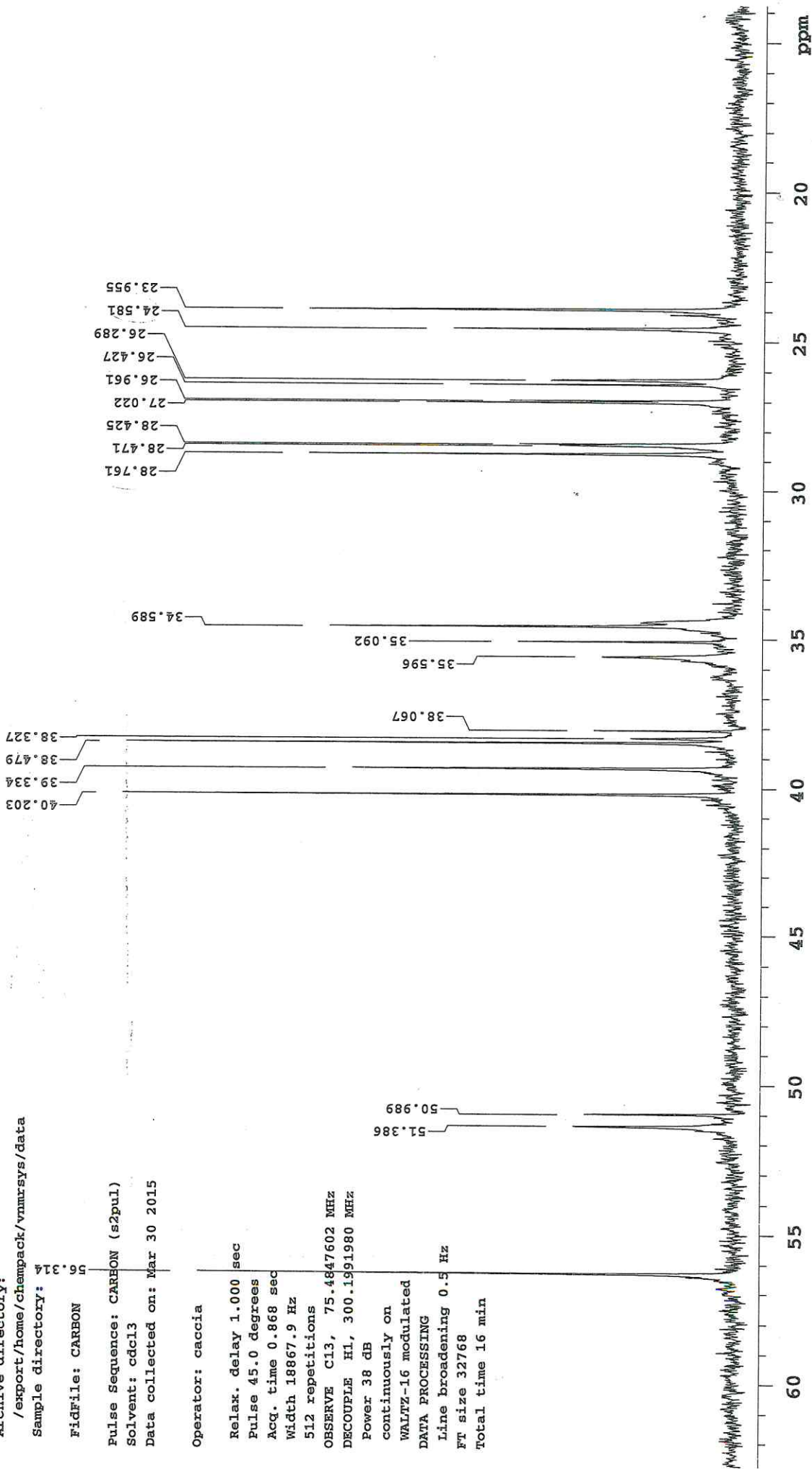
Data Collected on:  
 m300-mercury300  
 Archive directory:  
 /export/home/chempack/vnmrsys/data  
 Sample directory: 4  
 3  
 4

FidFile: CARBON

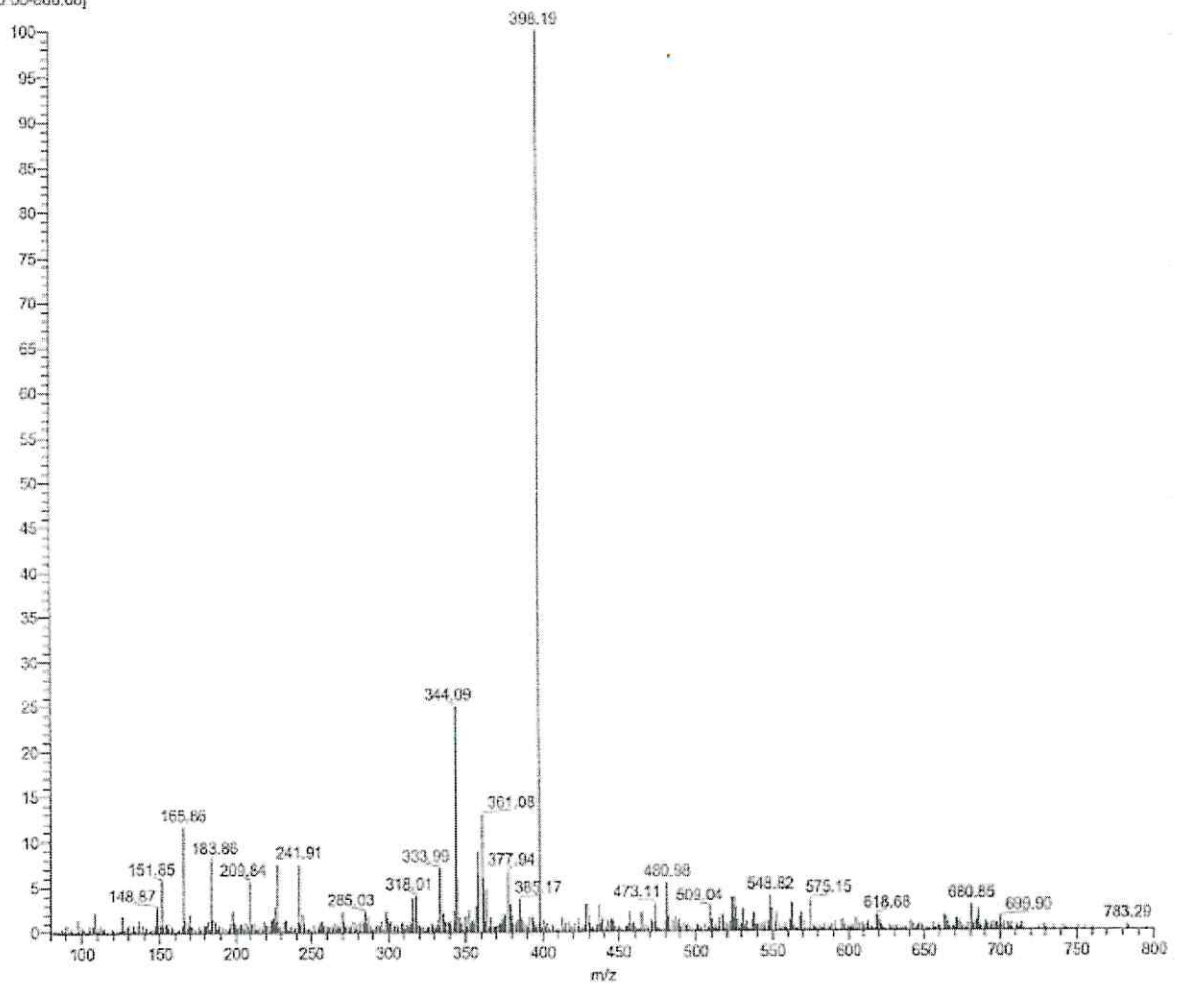
Pulse Sequence: CARBON (s2pul)  
 Solvent: cdc13  
 Data collected on: Mar 30 2015

Operator: caccia

Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 0.868 sec  
 Width 18867.9 Hz  
 512 repetitions  
 OBSERVE C13, 75.4847602 MHz  
 DECOUPLE H1, 300.1991980 MHz  
 Power 38 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 32768  
 Total time 16 min



BLA File 121112346 #118 RT: 1.61 AV: 1 NL: 1.99E7 T: +c ESI Full ms  
[90.00-800.00]



## Gradient Shimming

Sample Name:  
Acidolipoico-Gly  
Data Collected on:  
m300-mercury300  
Archive directory:  
/export/home/chempack/vnmrsys/data  
Sample directory:

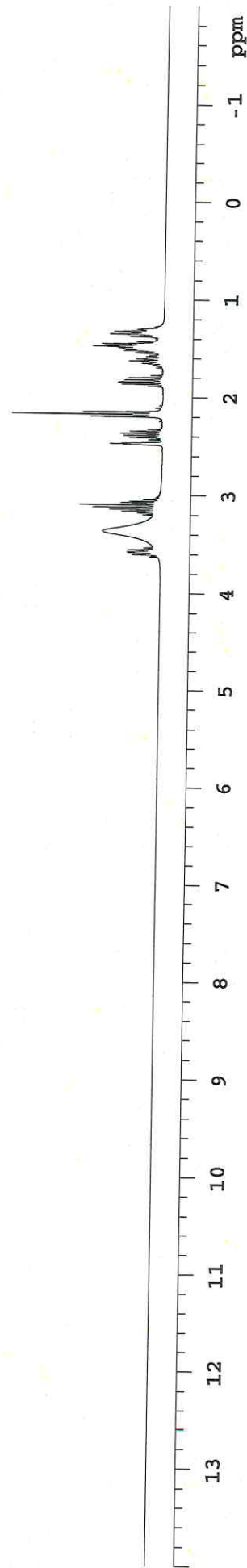
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: dms0  
Data collected on: Mar 9 2021

Operator: caccia

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.706 sec  
Width 4803.1 Hz  
32 repetitions

OBSERVE H1, 300.1990802 MHz  
DATA PROCESSING  
Ft size 16384  
Total time 1 min 29 sec





Gradient Shimming

Sample Name:  
Acidolipoico-Gly  
Data Collected on:  
m300-mercury300  
Archive directory:  
/export/home/chempack/vnmrsys/data  
Sample directory:

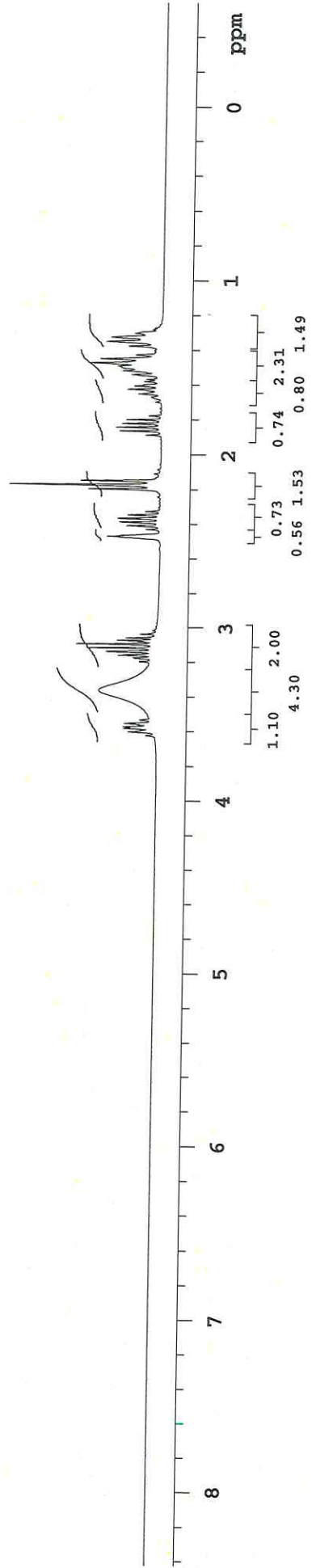
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: dmso  
Data collected on: Mar 9 2021

Operator: caccia

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.706 sec  
Width 4803.1 Hz  
32 repetitions

OBSERVE H1, 300.1990802 MHZ  
DATA PROCESSING  
Ft size 16384  
Total time 1 min 29 sec



Gradient Shimming



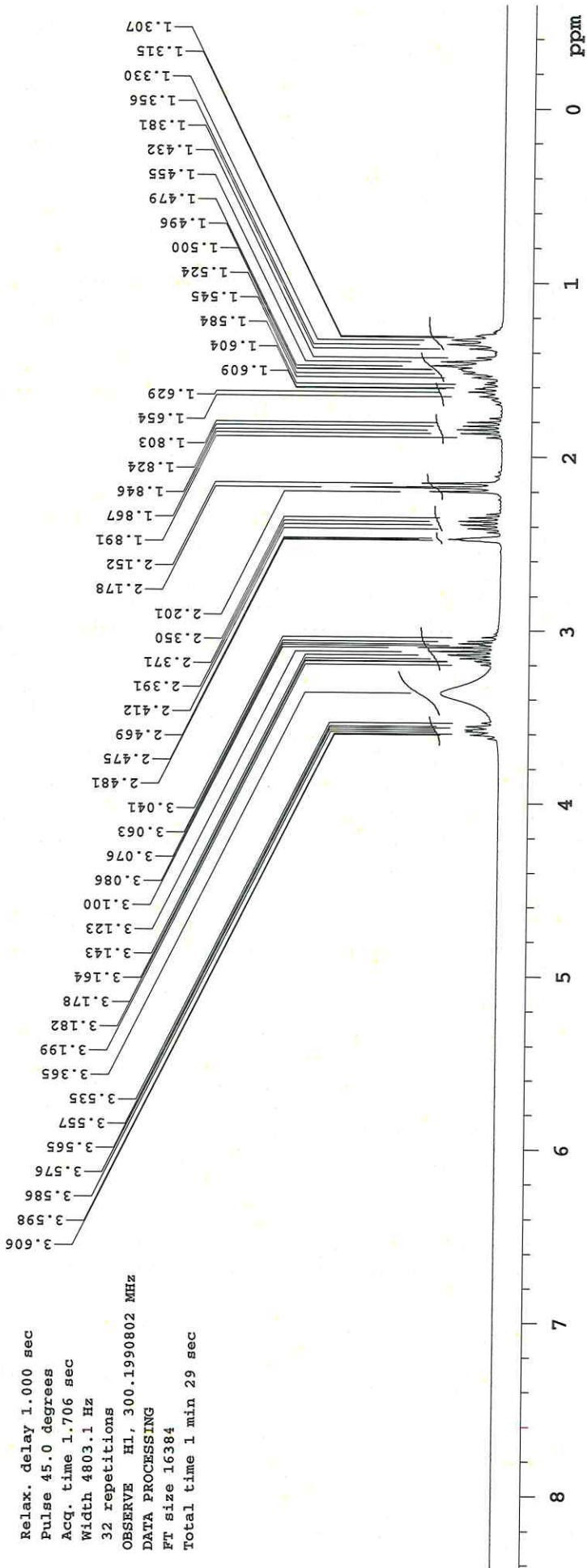
Sample Name:  
Acidolipoico-Gly  
Data Collected on:  
m300-mercury300  
Archive directory:  
/export/home/chempack/vnmrsys/data  
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: dmsd  
Data collected on: Mar 9 2021

Operator: caccia

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.706 sec  
Width 4803.1 Hz  
32 repetitions  
OBSERVE H1, 300.1990802 MHz  
DATA PROCESSING  
Ft size 16384  
Total time 1 min 29 sec



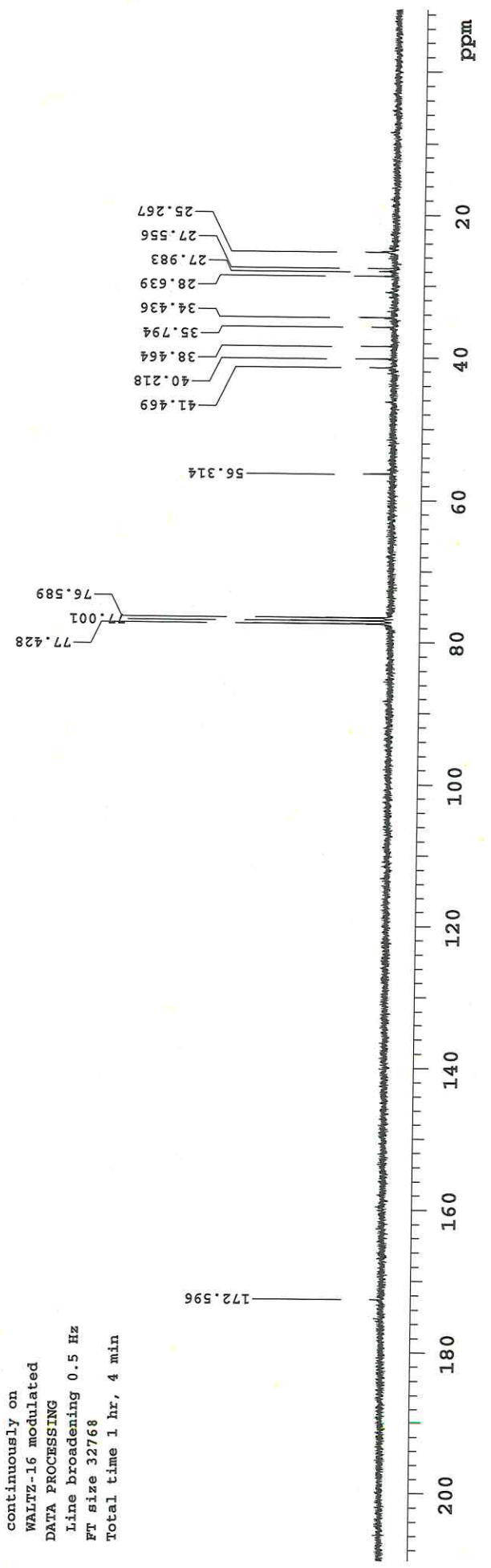


Sample Name:  
Gly-Ia  
Data Collected on:  
m300-mercury300  
Archive directory:  
/home/caccia/vnmrSYS/data  
Sample directory:  
AutoSW\_calib\_20210712\_02  
F1GFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Jul 13 2021

Operator: caccia

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
2000 repetitions  
OBSERVE CH3, 75.4847602 MHz  
DECOUPLE H1, 300.1991980 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 1 hr, 4 min



BLA\_1\_File\_121112349\_#118\_RT: 1.61\_AV: 1\_NL: 1.09E7\_T: + e ESI Full ms  
[60.00-800.00]

