

Supporting Information

Discovery of Potent Dual Binding Site Acetylcholinesterase Inhibitors via Homo- and Heterodimerization of Coumarin-Based Moieties

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Saverio Cellamare,^[a] and Cosimo D. Altomare^[a]

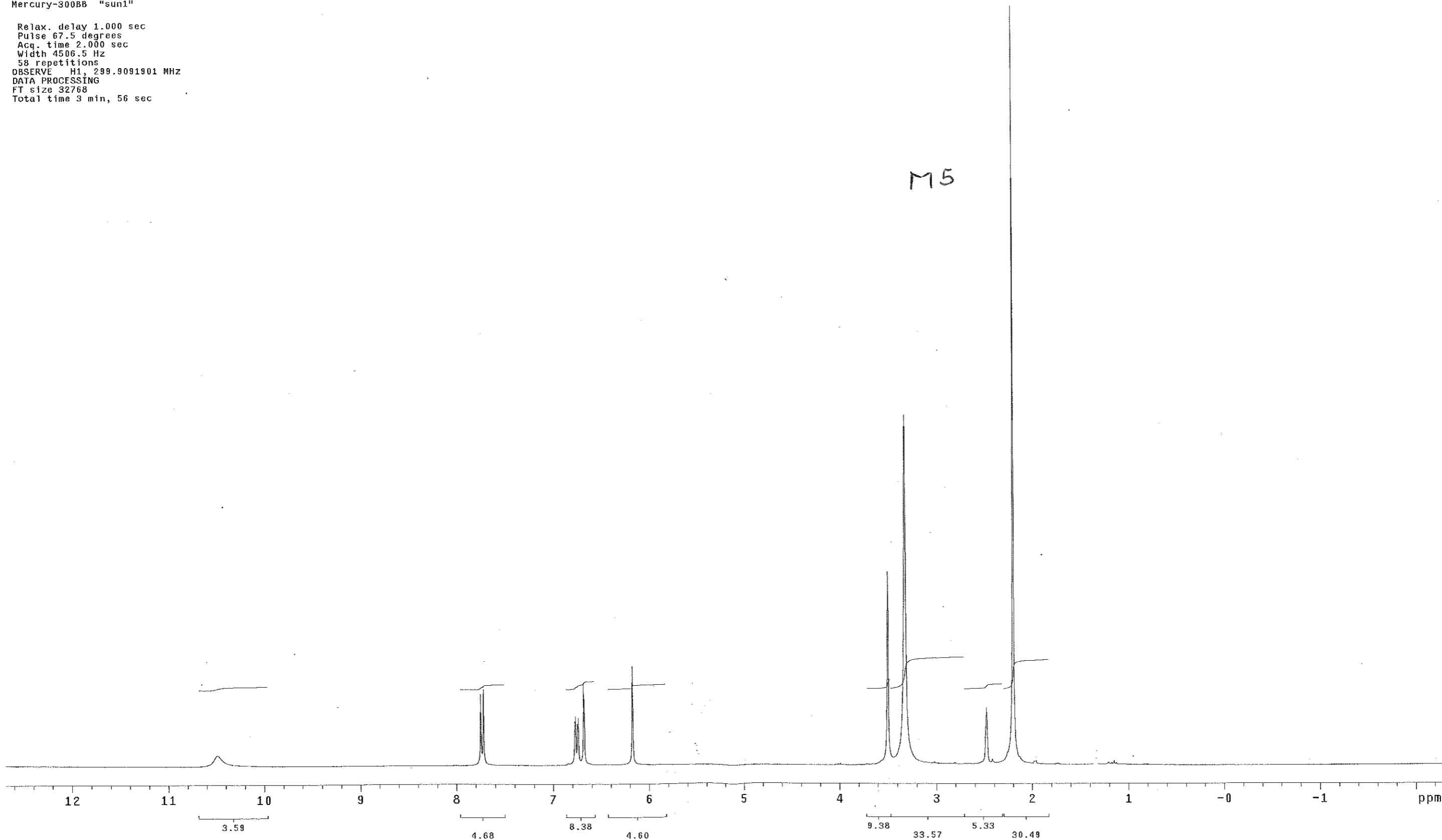
cmdc_201700282_sm_miscellaneous_information.pdf

STANDARD 1H OBSERVE

Pulse Sequence: s2pu1

Solvent: DMSO
Ambient temperature
Mercury-300BB "sun1"

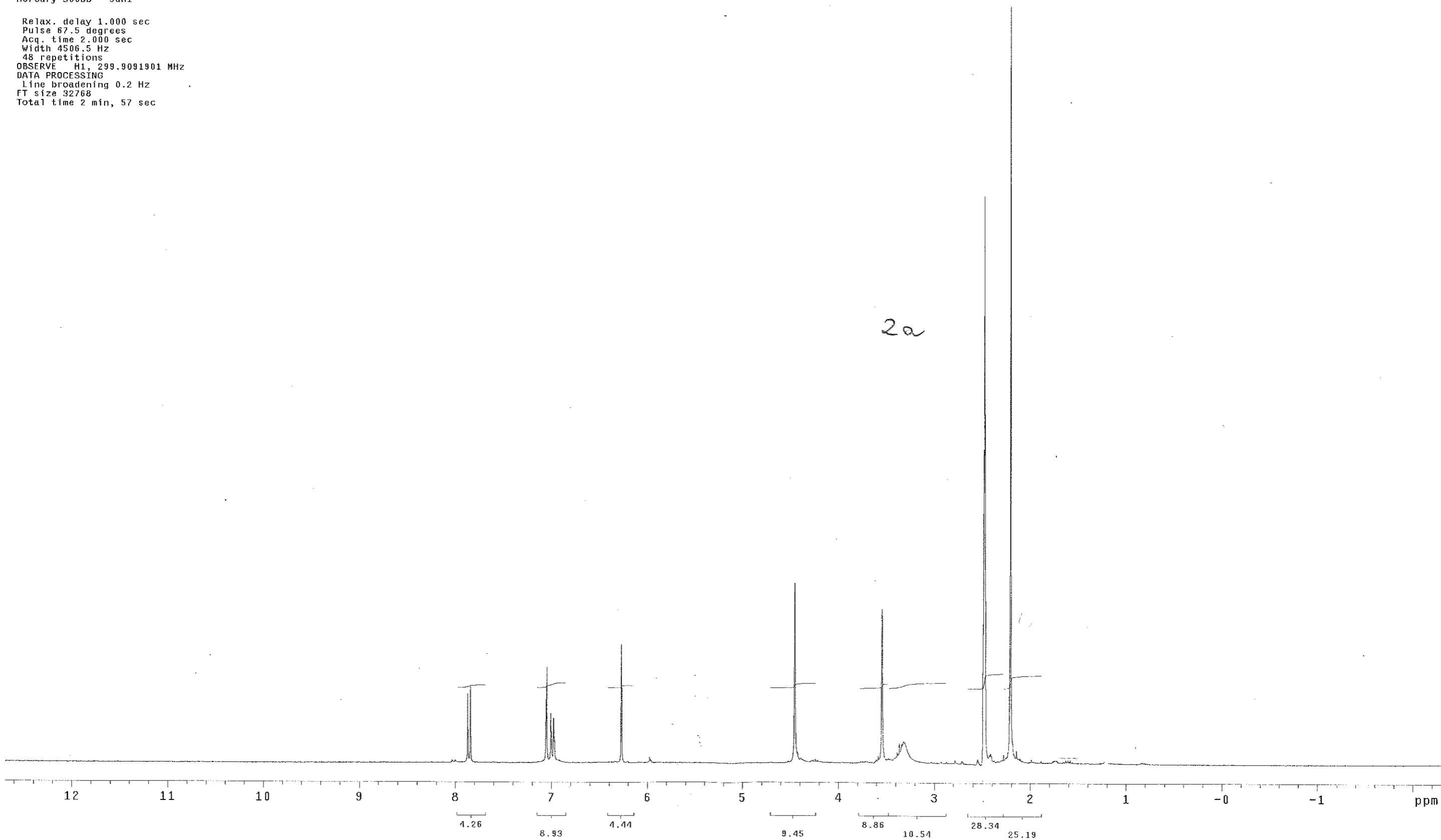
Relax. delay 1.000 sec
Pulse 67.5 degrees
Acq. time 2.000 sec
Width 4506.5 Hz
58 repetitions
OBSERVE H1, 299.9091901 MHz
DATA PROCESSING
FT size 32768
Total time 3 min, 56 sec



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300BB "sun1"

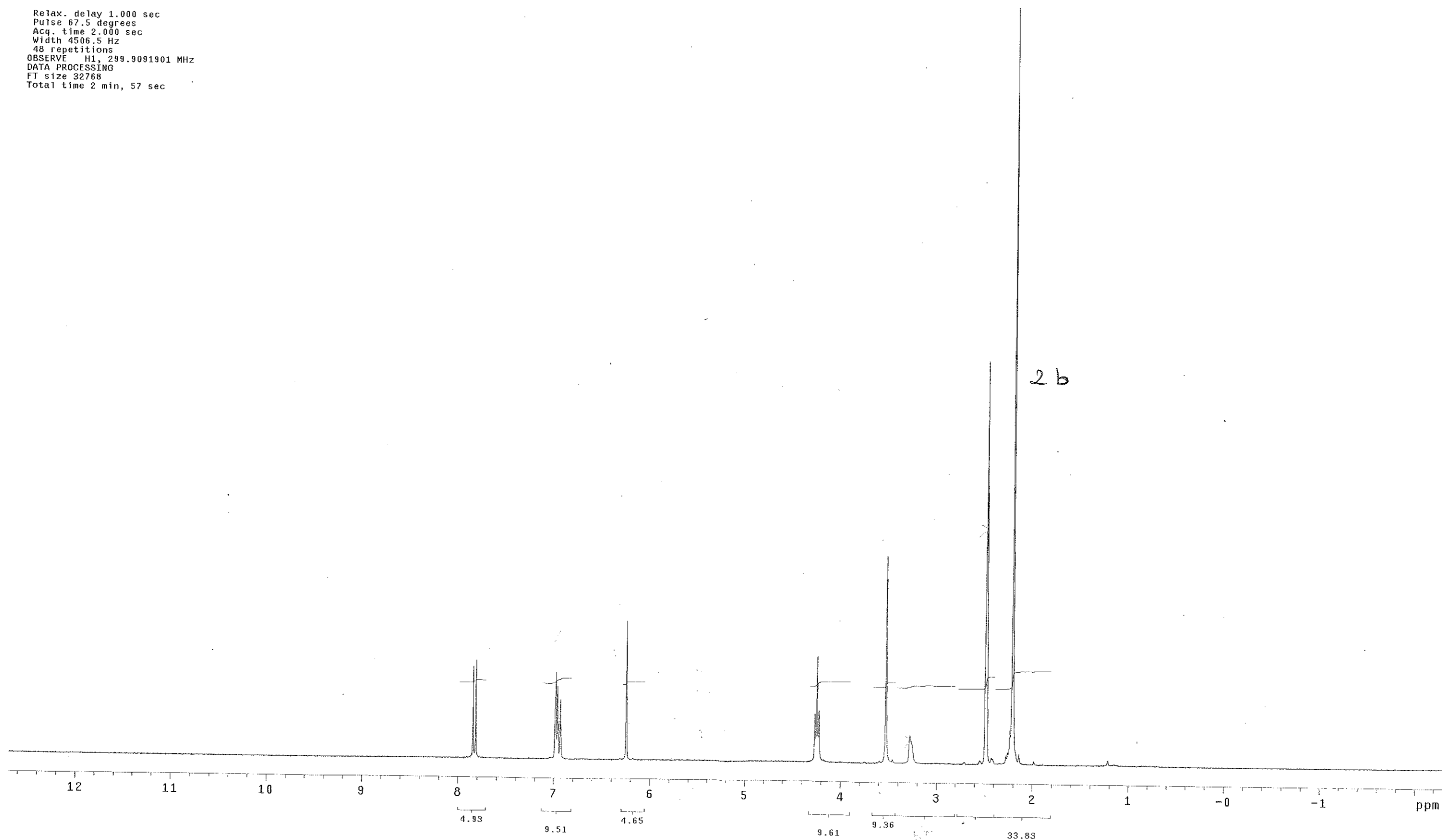
Relax. delay 1.000 sec
Pulse 67.5 degrees
Acq. time 2.000 sec
Width 4506.5 Hz
48 repetitions
OBSERVE H1, 299.9091901 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 2 min, 57 sec



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300BB "sun1"

Relax. delay 1.000 sec
Pulse 67.5 degrees
Acq. time 2.000 sec
Width 4506.5 Hz
48 repetitions
OBSERVE H1, 299.9091901 MHz
DATA PROCESSING
FT size 32768
Total time 2 min, 57 sec

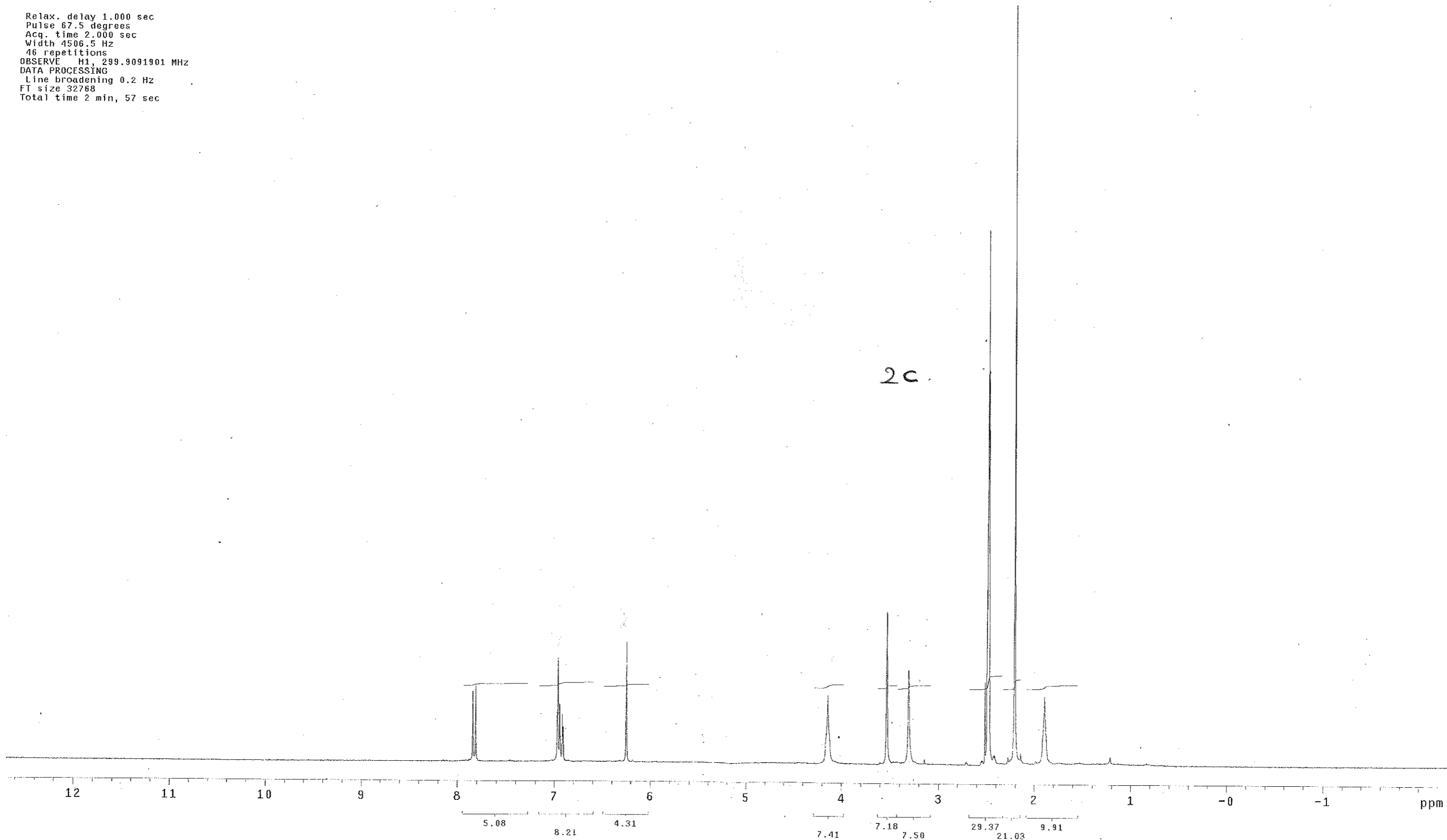


STANDARD 1H OBSERVE

Pulse Sequence: s2pu1

Solvent: DMSO
Ambient temperature
Mercury-300BB "sun1"

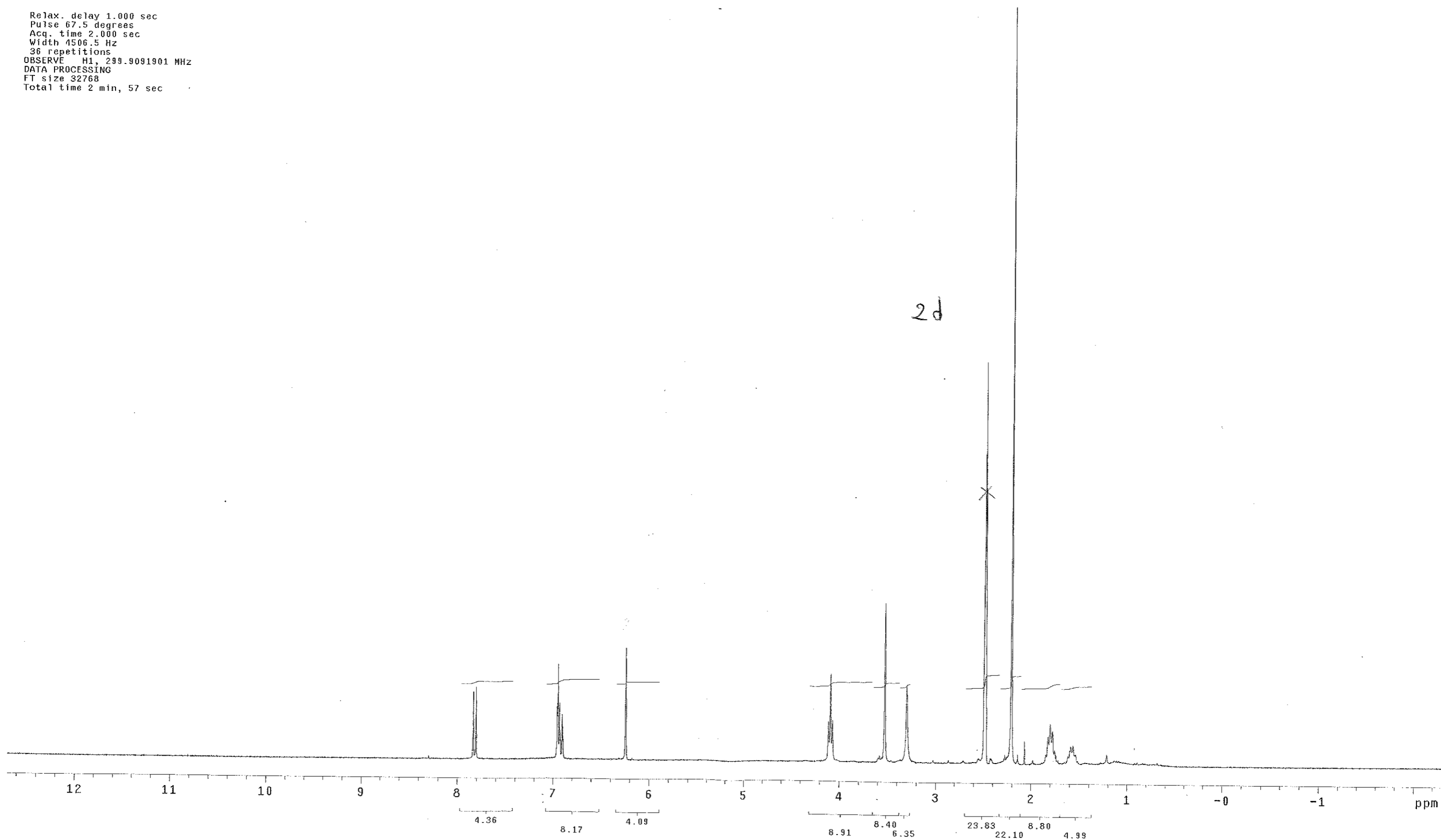
Relax. delay 1.000 sec
Pulse 67.5 degrees
Acq. time 2.000 sec
Width 4506.5 Hz
46 repetitions
OBSERVE H1, 299.9091901 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 2 min, 57 sec



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300BB "sun1"

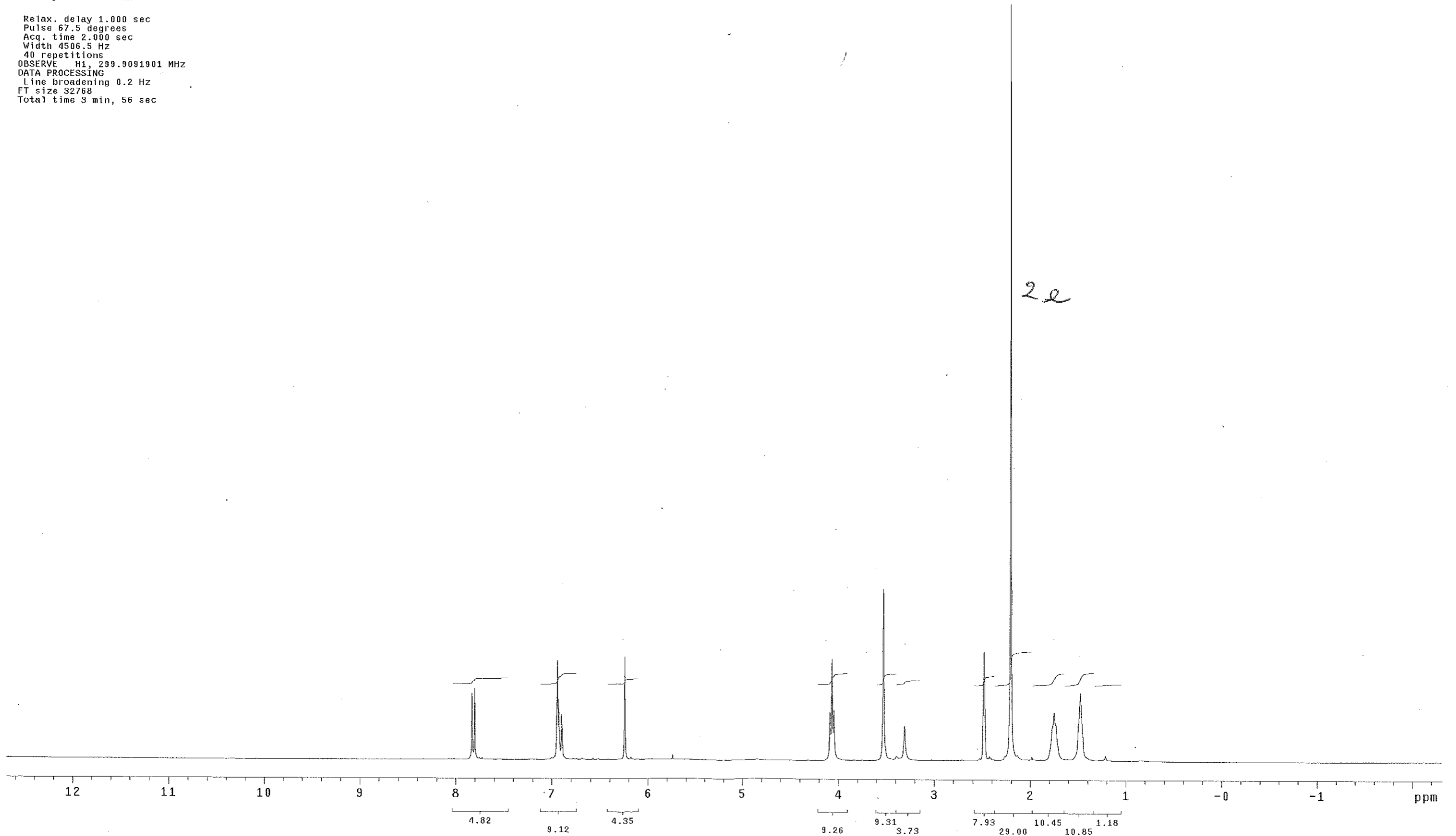
Relax. delay 1.000 sec
Pulse 67.5 degrees
Acq. time 2.000 sec
Width 4506.5 Hz
36 repetitions
OBSERVE H1, 299.9091901 MHz
DATA PROCESSING
FT size 32768
Total time 2 min, 57 sec



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300BB "sun1"

Relax. delay 1.000 sec
Pulse 67.5 degrees
Acq. time 2.000 sec
Width 4506.5 Hz
40 repetitions
OBSERVE H1, 299.9091901 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 3 min, 56 sec



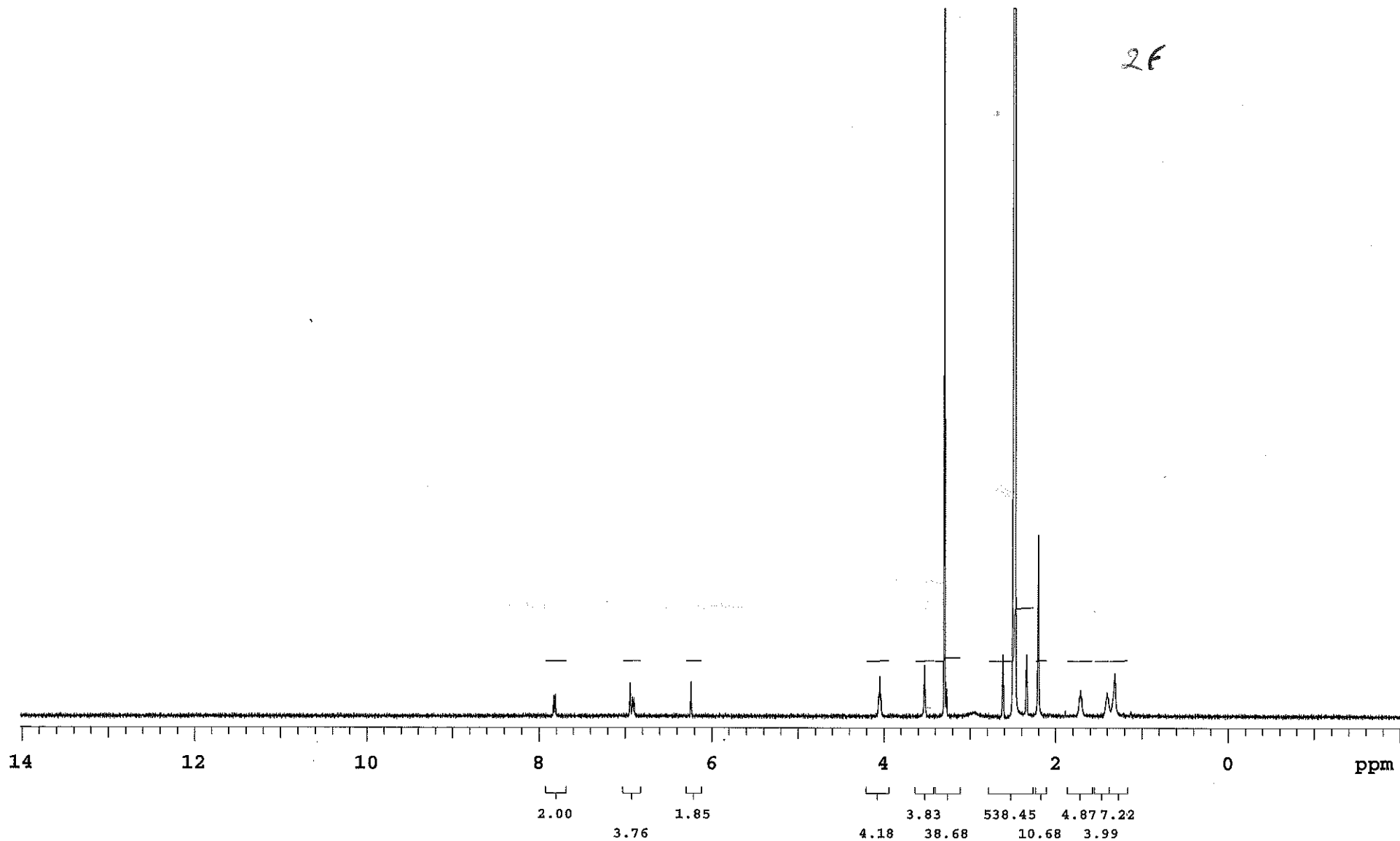
ASF23

Sample Name **ASF23**
Date collected **2017-04-27**

Pulse sequence **PROTON**
Solvent **dmso**

Temperature **25**
Spectrometer **Agilent500-vnmrs500**

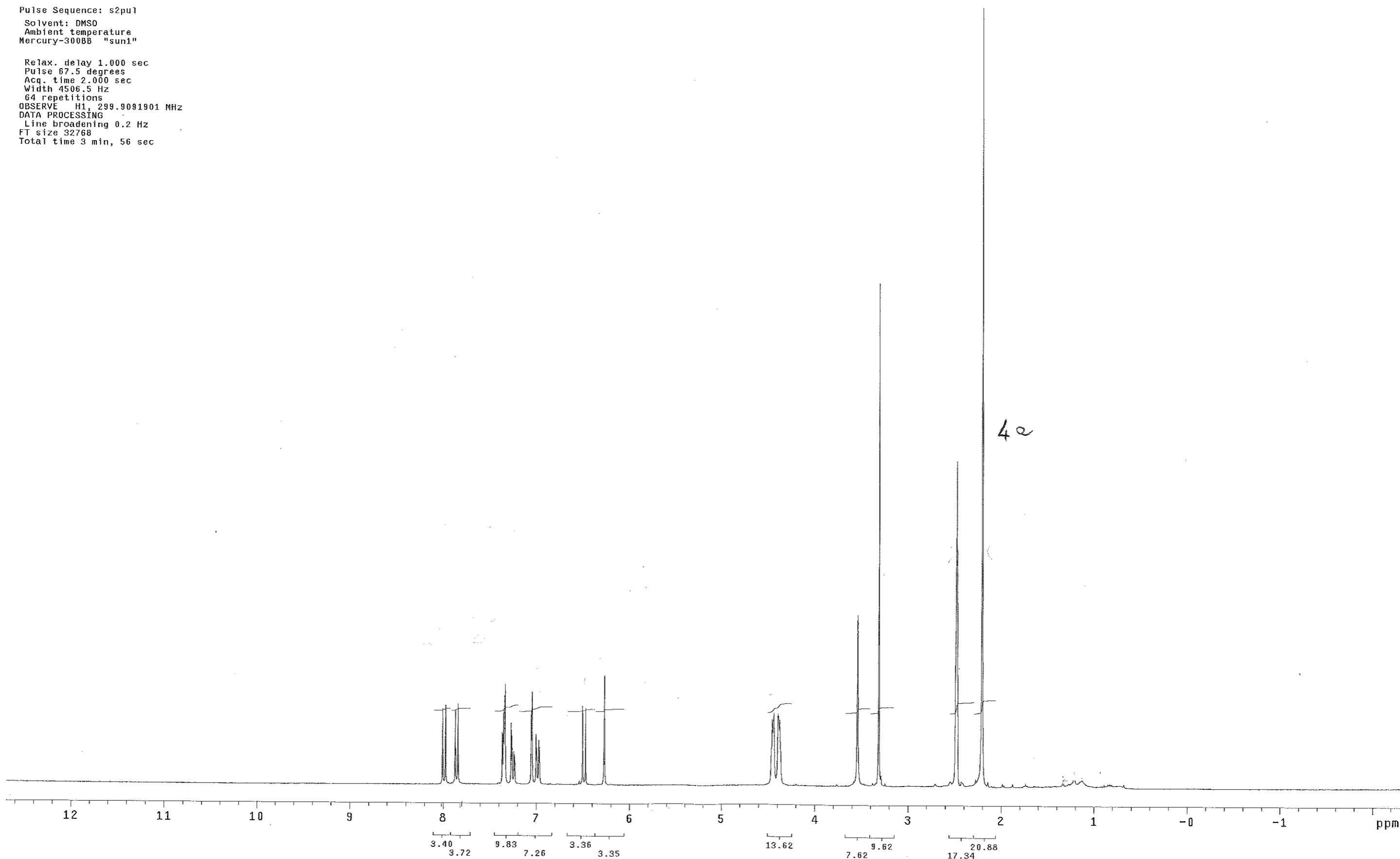
Study owner **vnmr2**
Operator **vnmr2**



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300BB "sun1"

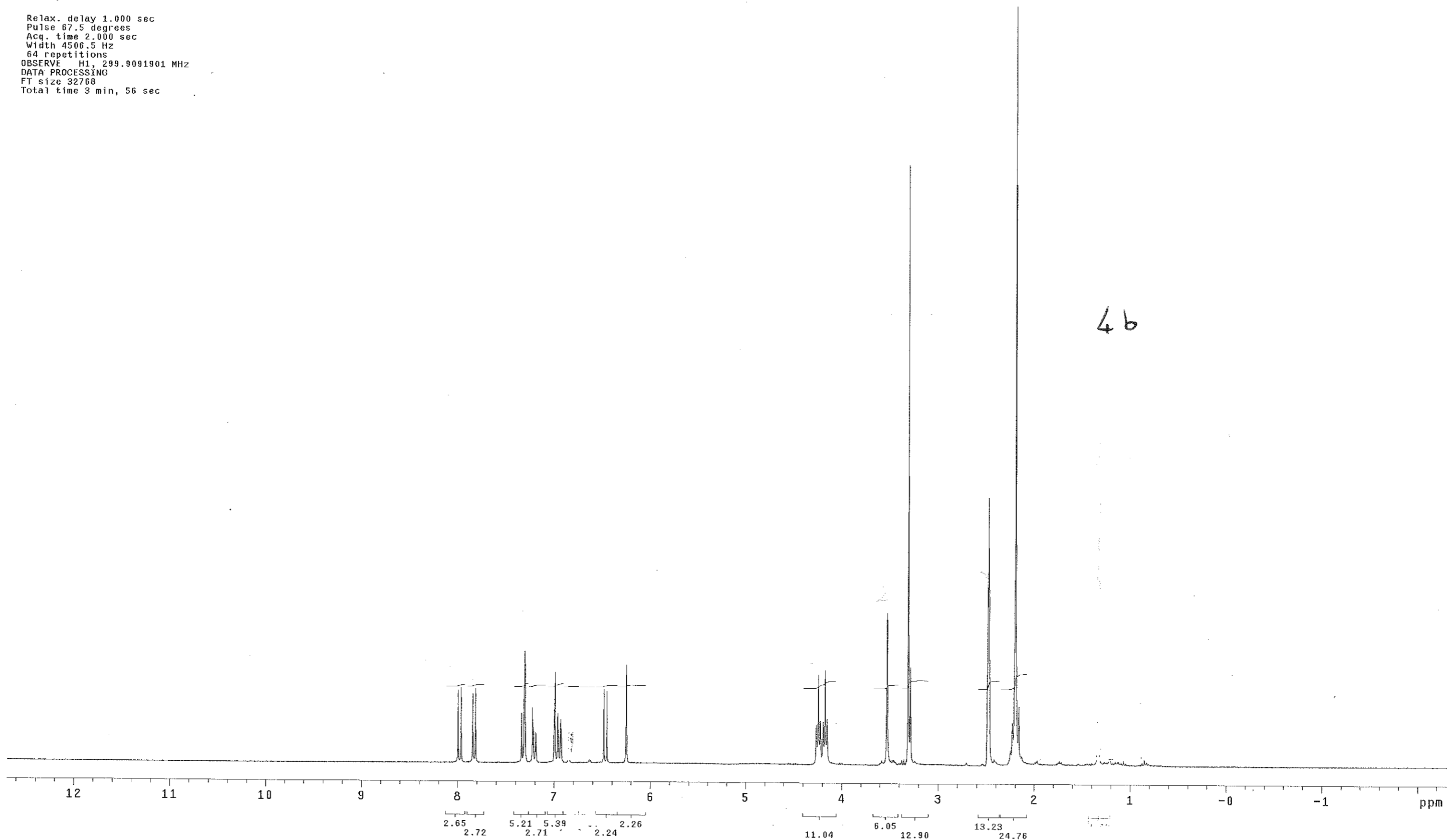
Relax. delay 1.000 sec
Pulse 67.5 degrees
Acq. time 2.000 sec
Width 4506.5 Hz
64 repetitions
OBSERVE H1, 299.9091901 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 3 min, 56 sec



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300BB "sun1"

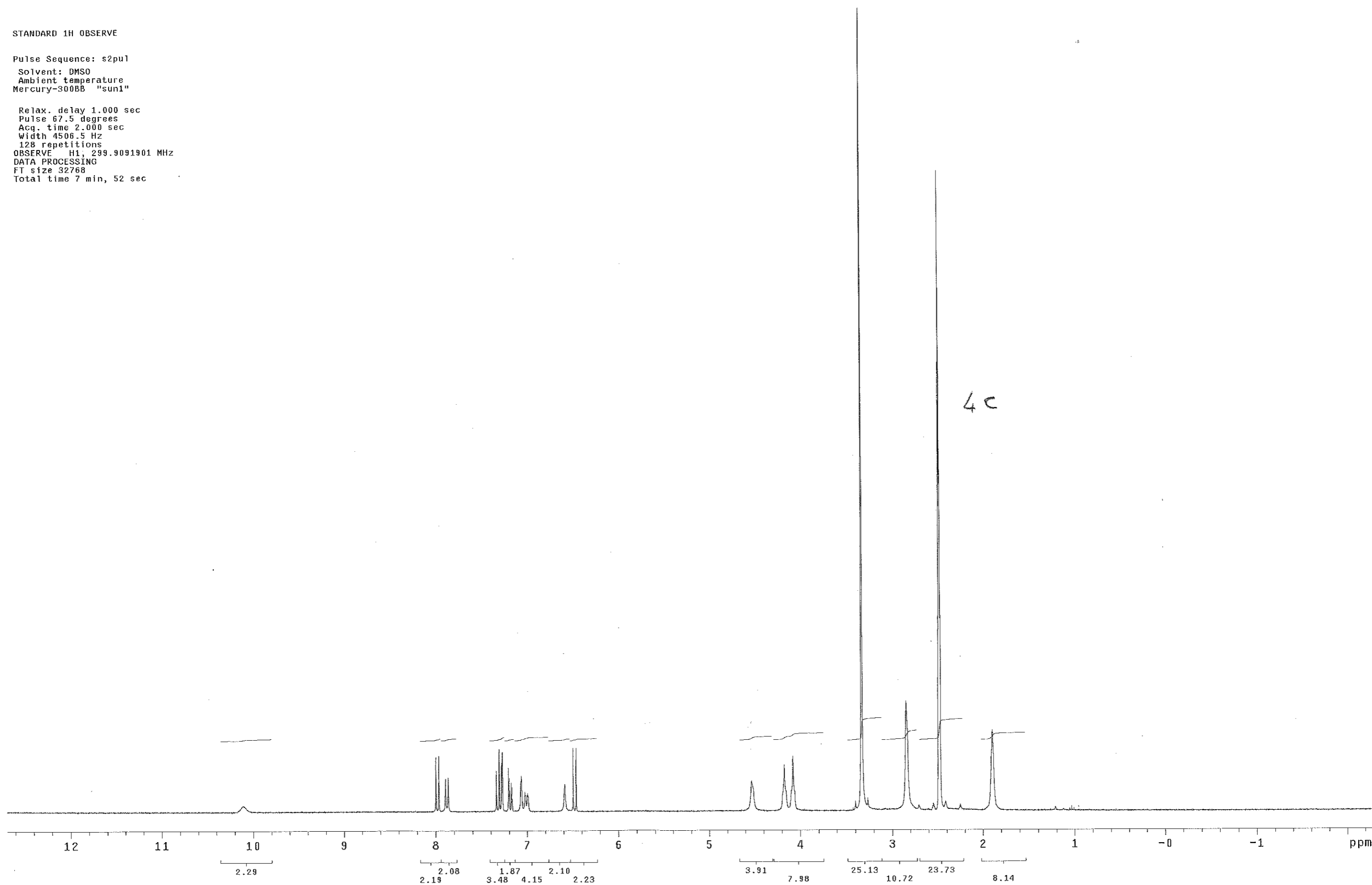
Relax. delay 1.000 sec
Pulse 67.5 degrees
Acq. time 2.000 sec
Width 4506.5 Hz
64 repetitions
OBSERVE H1, 299.9091901 MHz
DATA PROCESSING
FT size 32768
Total time 3 min, 56 sec



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300BB "sun1"

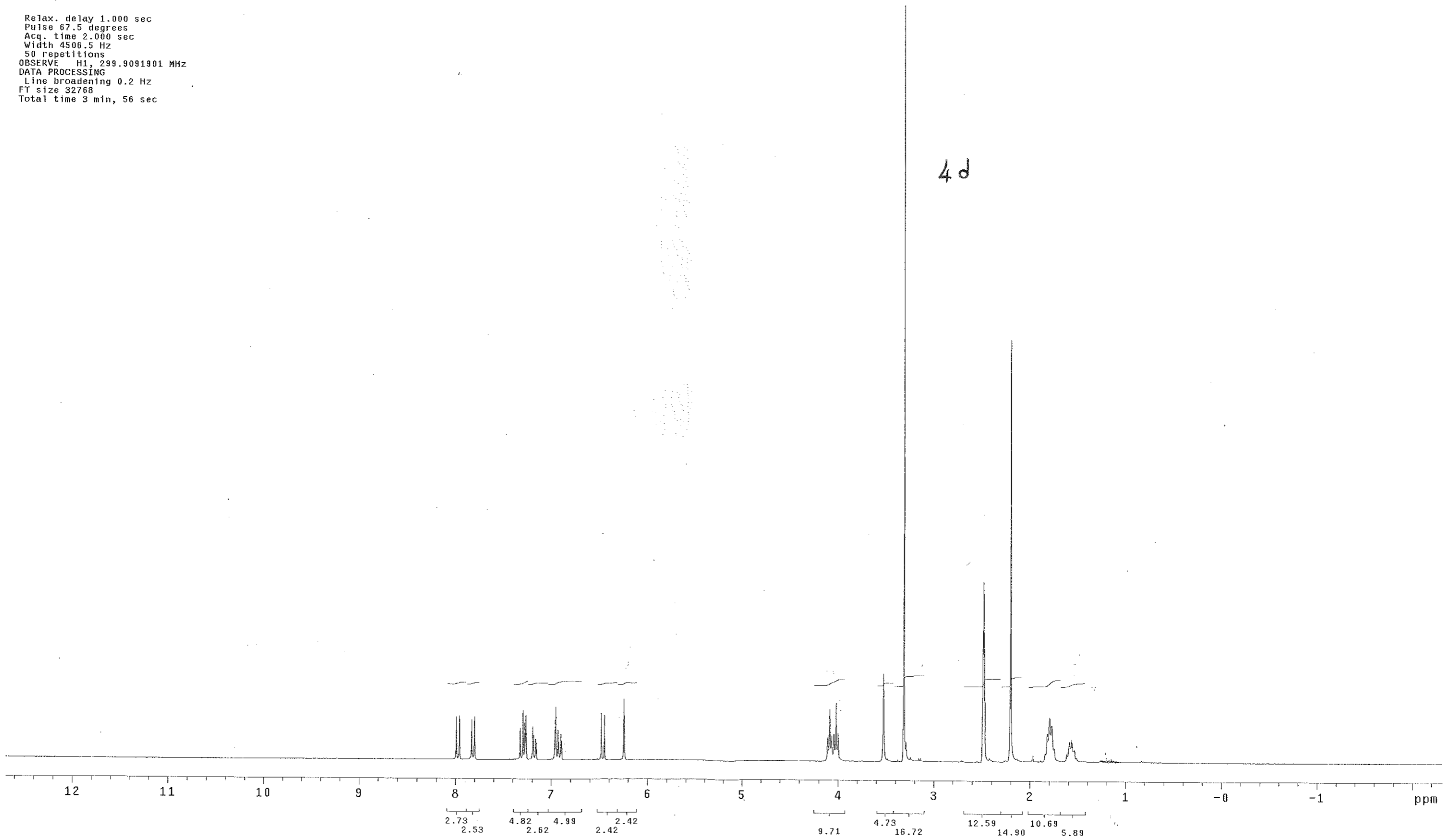
Relax. delay 1.000 sec
Pulse 67.5 degrees
Acq. time 2.000 sec
Width 4506.5 Hz
128 repetitions
OBSERVE H1, 299.9091901 MHz
DATA PROCESSING
FT size 32768
Total time 7 min, 52 sec



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300BB "sun1"

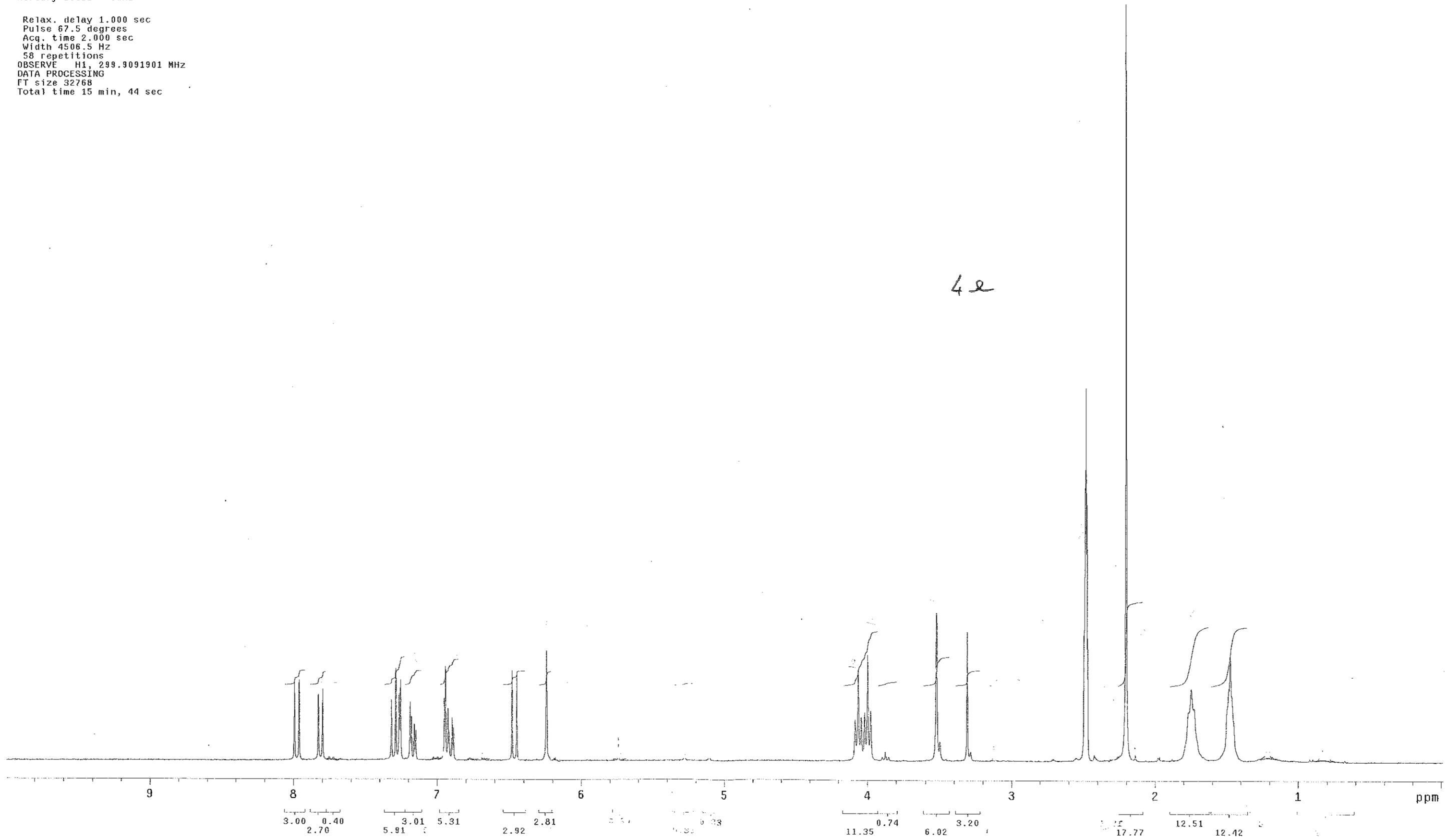
Relax. delay 1.000 sec
Pulse 67.5 degrees
Acq. time 2.000 sec
Width 4506.5 Hz
50 repetitions
OBSERVE H1, 299.9091901 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 3 min, 56 sec



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300BB "suni"

Relax. delay 1.000 sec
Pulse 67.5 degrees
Acq. time 2.000 sec
Width 4506.5 Hz
58 repetitions
OBSERVE H1, 299.9091901 MHz
DATA PROCESSING
FT size 32768
Total time 15 min, 44 sec



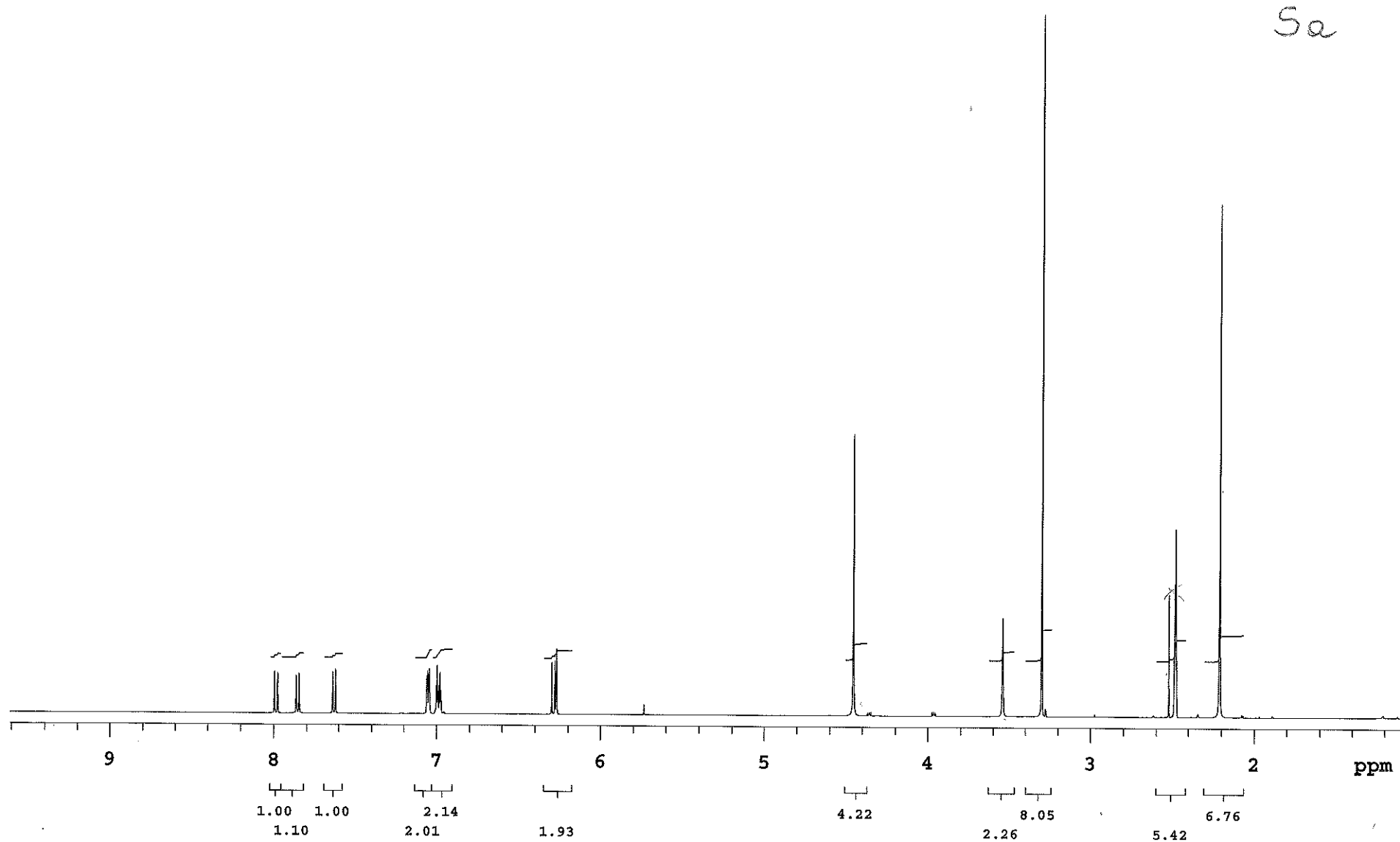
LP1305

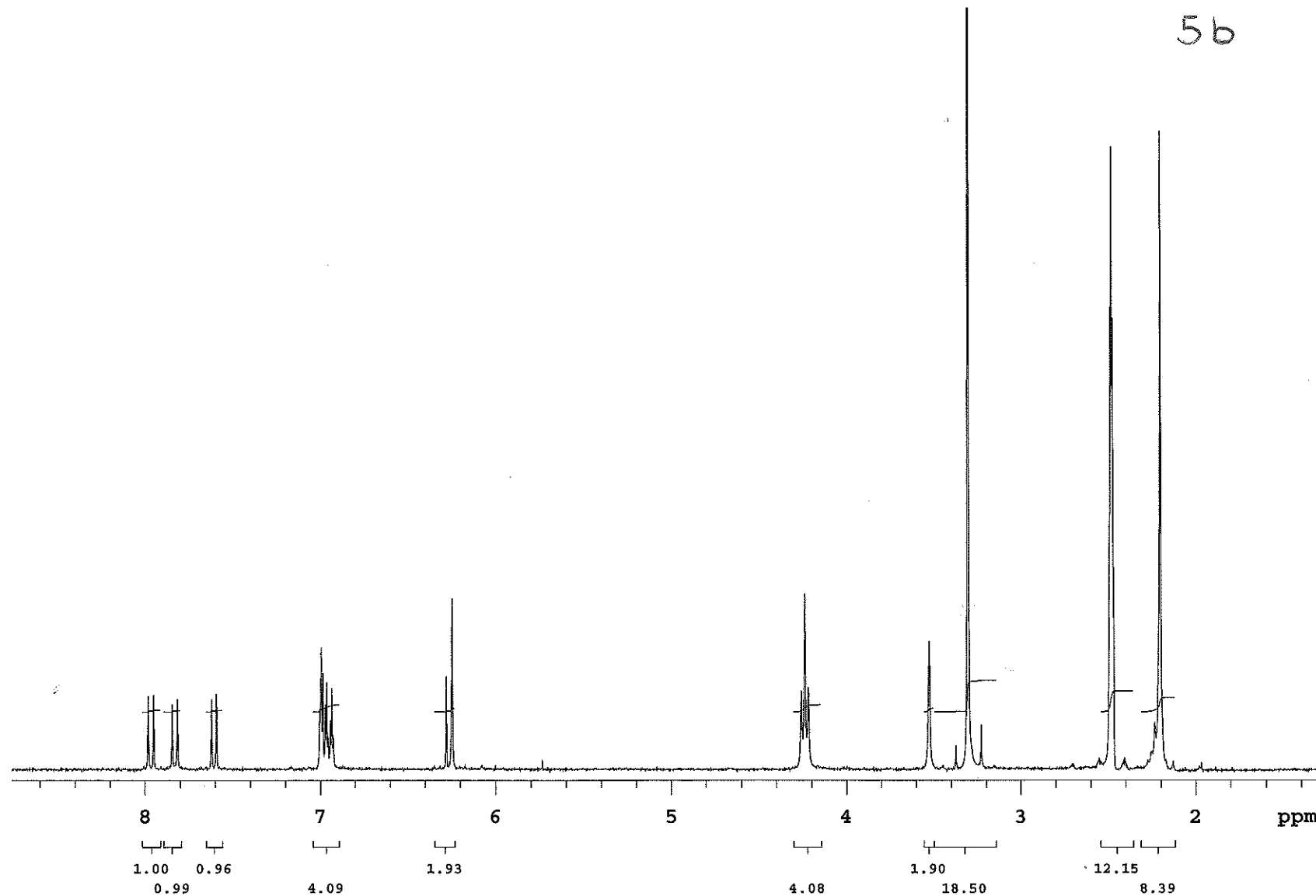
Sample Name LP1305
Date collected 2016-10-04

Pulse sequence PROTON
Solvent dmsd

Temperature 25
Spectrometer Agilent500-vnmrs500

Study owner vnmr2
Operator vnmr2





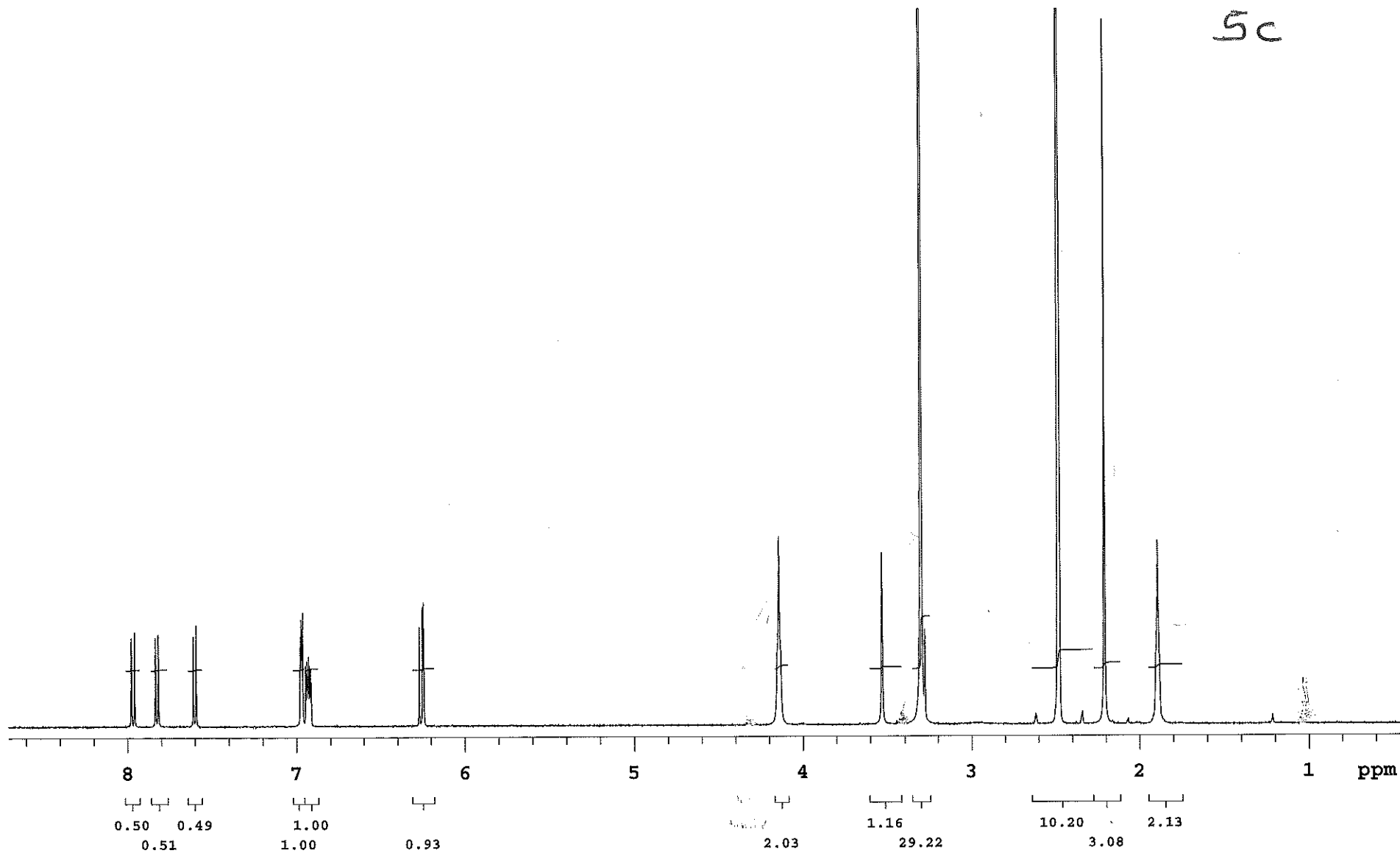
LP1283

Sample Name LP1283
Date collected 2016-05-31

Pulse sequence PROTON
Solvent dms0

Temperature 25
Spectrometer Agilent500-vnmrs500

Study owner vnmr2
Operator vnmr2

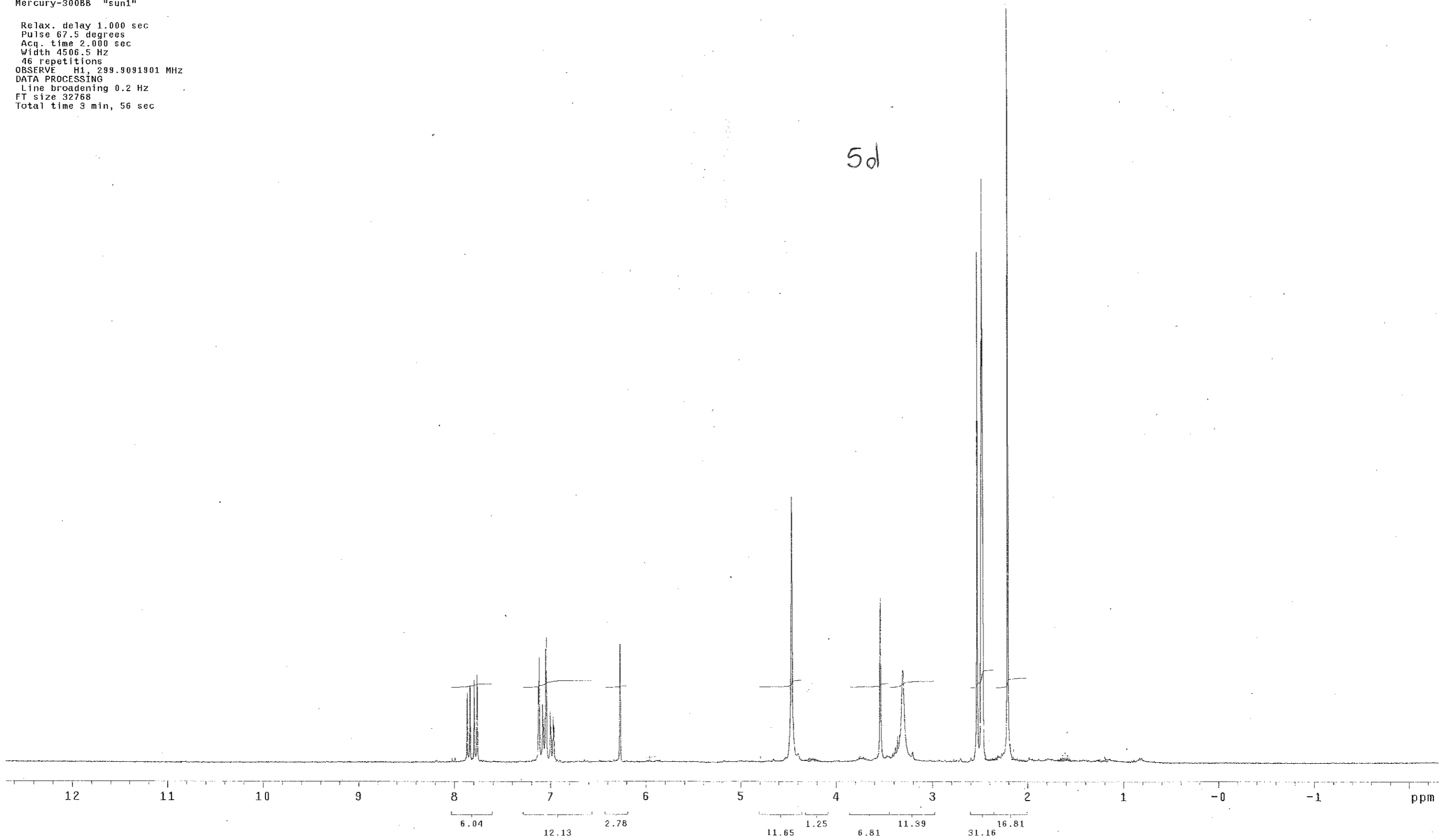


STANDARD 1H OBSERVE

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300BB "sun1"

Relax. delay 1.000 sec
Pulse 67.5 degrees
Acq. time 2.000 sec
Width 4506.5 Hz
46 repetitions
OBSERVE H1, 299.9091901 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 3 min, 56 sec

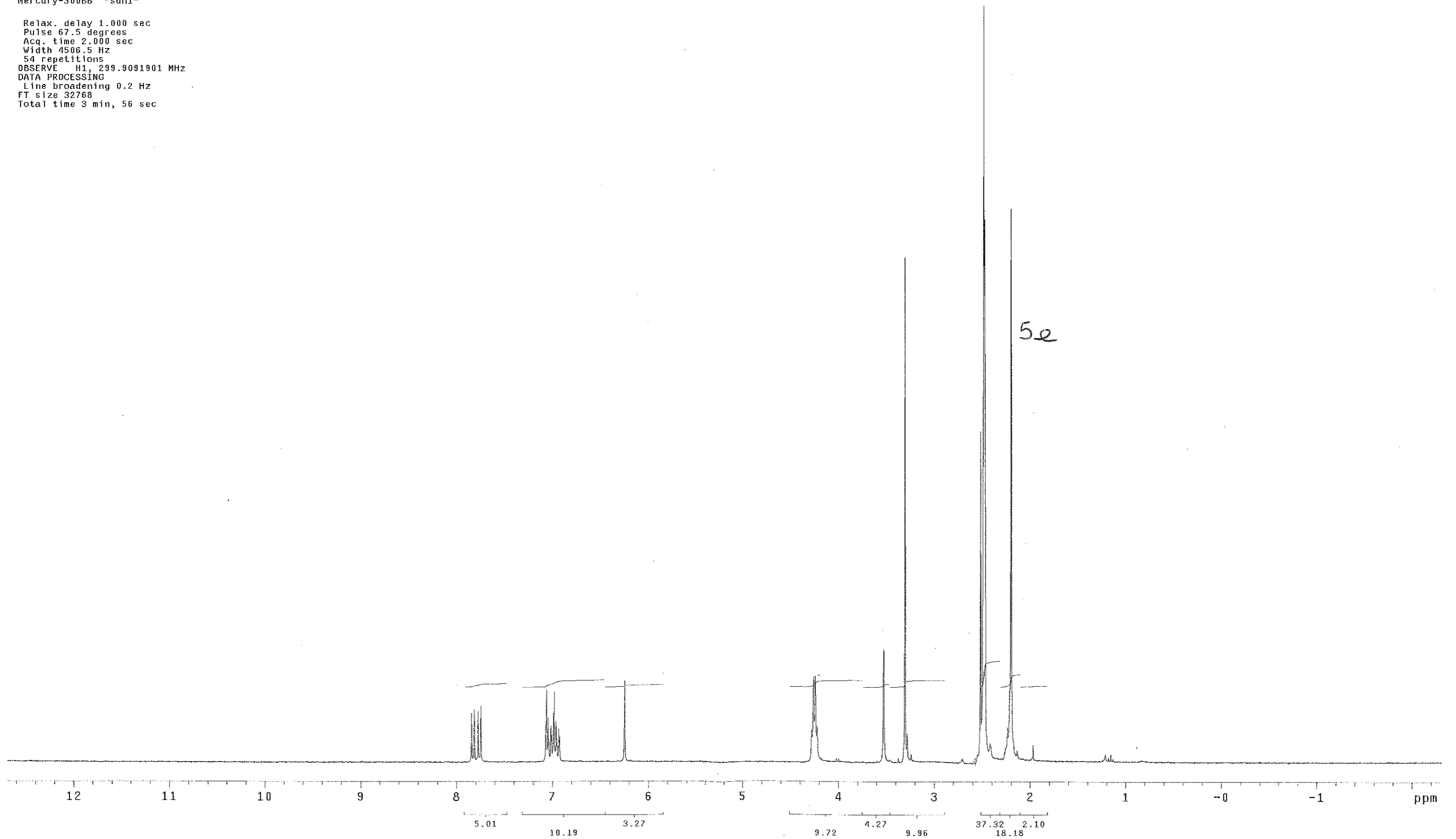
5d



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300BB "sun1"

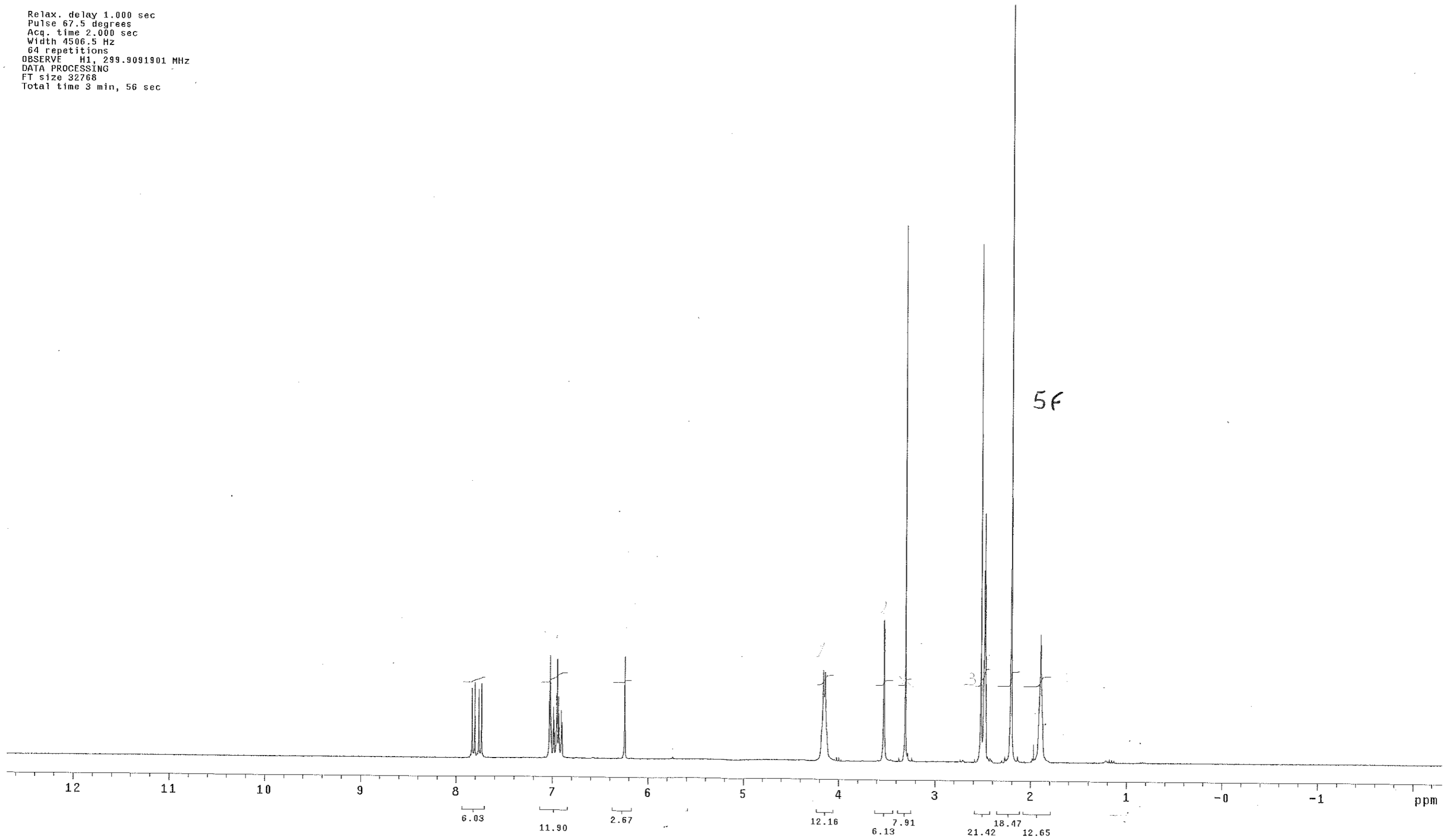
Relax. delay 1.000 sec
Pulse 67.5 degrees
Acq. time 2.000 sec
Width 4506.5 Hz
54 repetitions
OBSERVE H1, 299.9091901 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 3 min, 56 sec



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300BB "sun1"

Relax. delay 1.000 sec
Pulse 67.5 degrees
Acq. time 2.000 sec
Width 4506.5 Hz
64 repetitions
OBSERVE H1, 299.9091901 MHz
DATA PROCESSING
FT size 32768
Total time 3 min, 56 sec

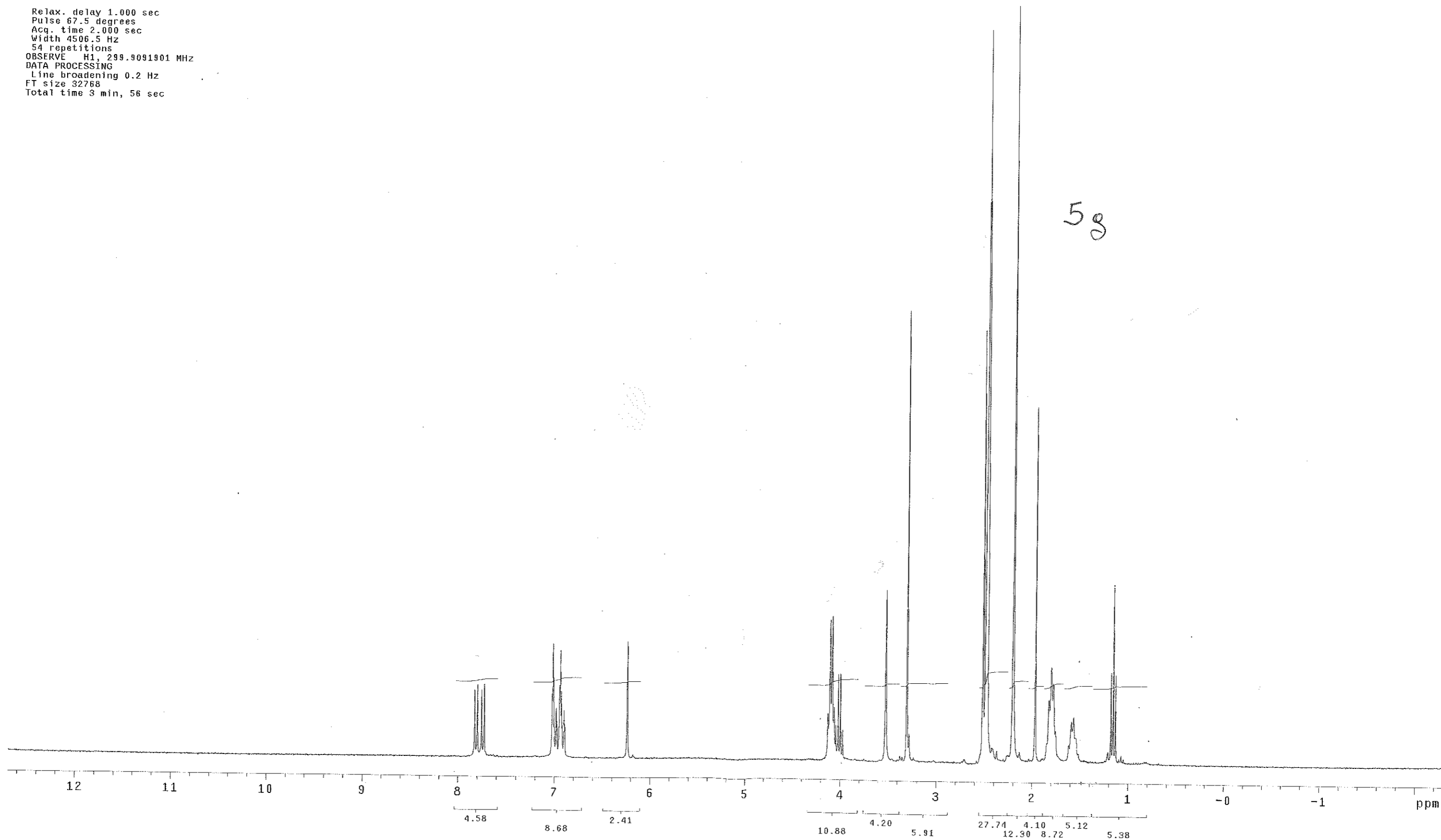


STANDARD 1H OBSERVE

Pulse Sequence: s2pu1

Solvent: DMSO
Ambient temperature
Mercury-30088 "sun1"

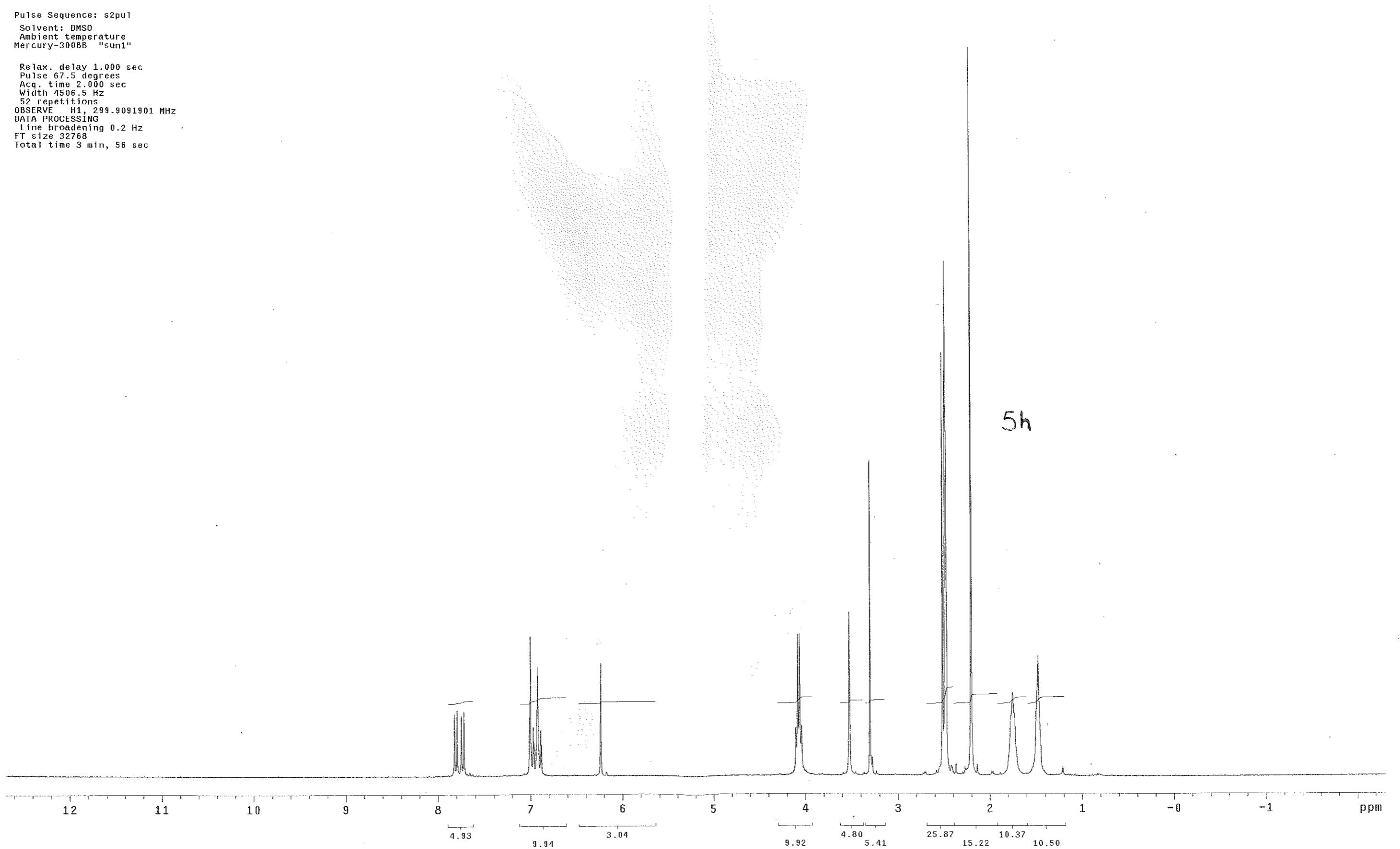
Relax. delay 1.000 sec
Pulse 67.5 degrees
Acq. time 2.000 sec
Width 4506.5 Hz
54 repetitions
OBSERVE H1, 299.9091901 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 3 min, 56 sec



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300BB "sun1"

Relax. delay 1.000 sec
Pulse 67.5 degrees
Acq. time 2.000 sec
Width 4506.5 Hz
52 repetitions
OBSERVE H1, 299.9091901 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 3 min, 56 sec



10

LP1302

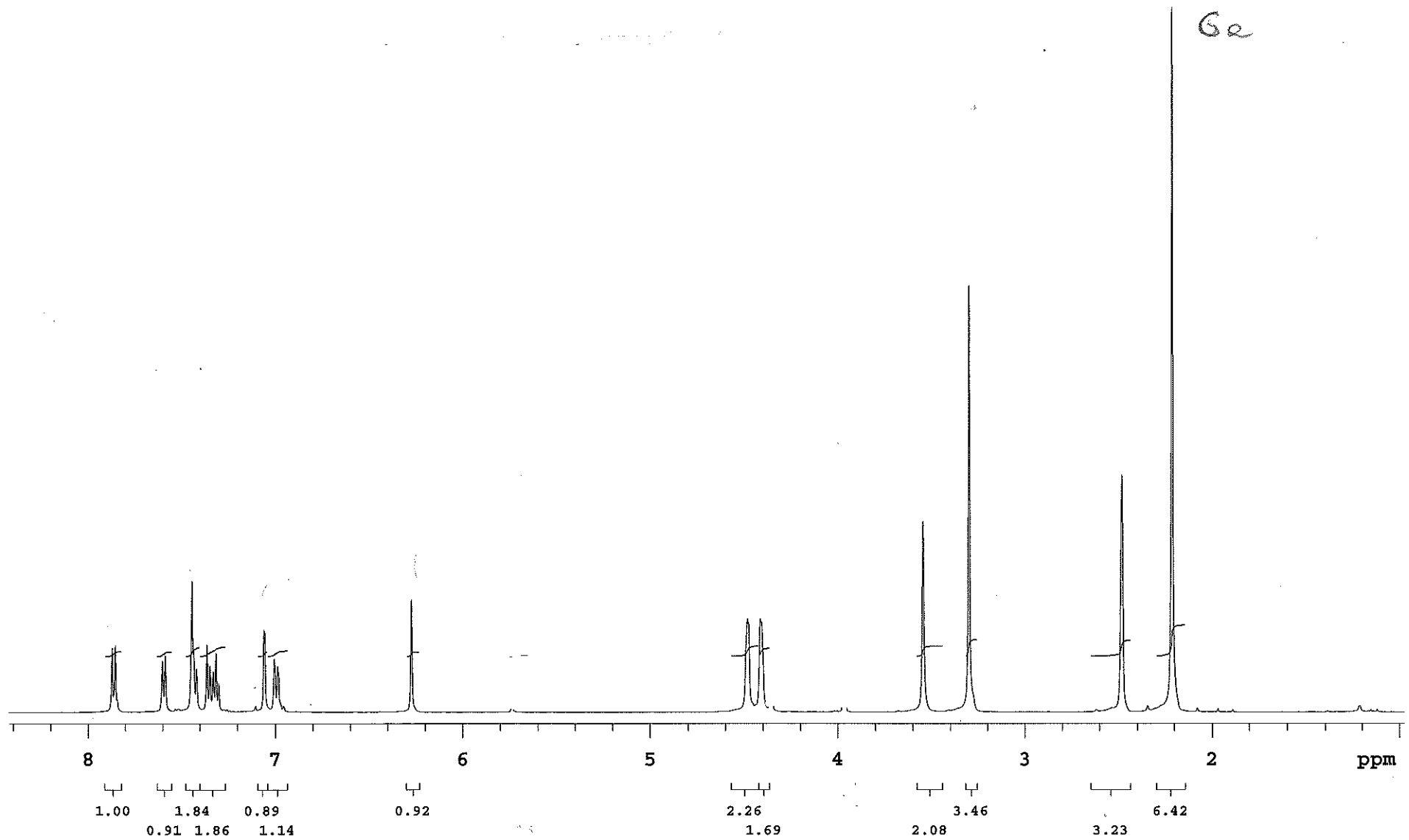
B26

Sample Name **LP1302**
Date collected **2016-10-03**

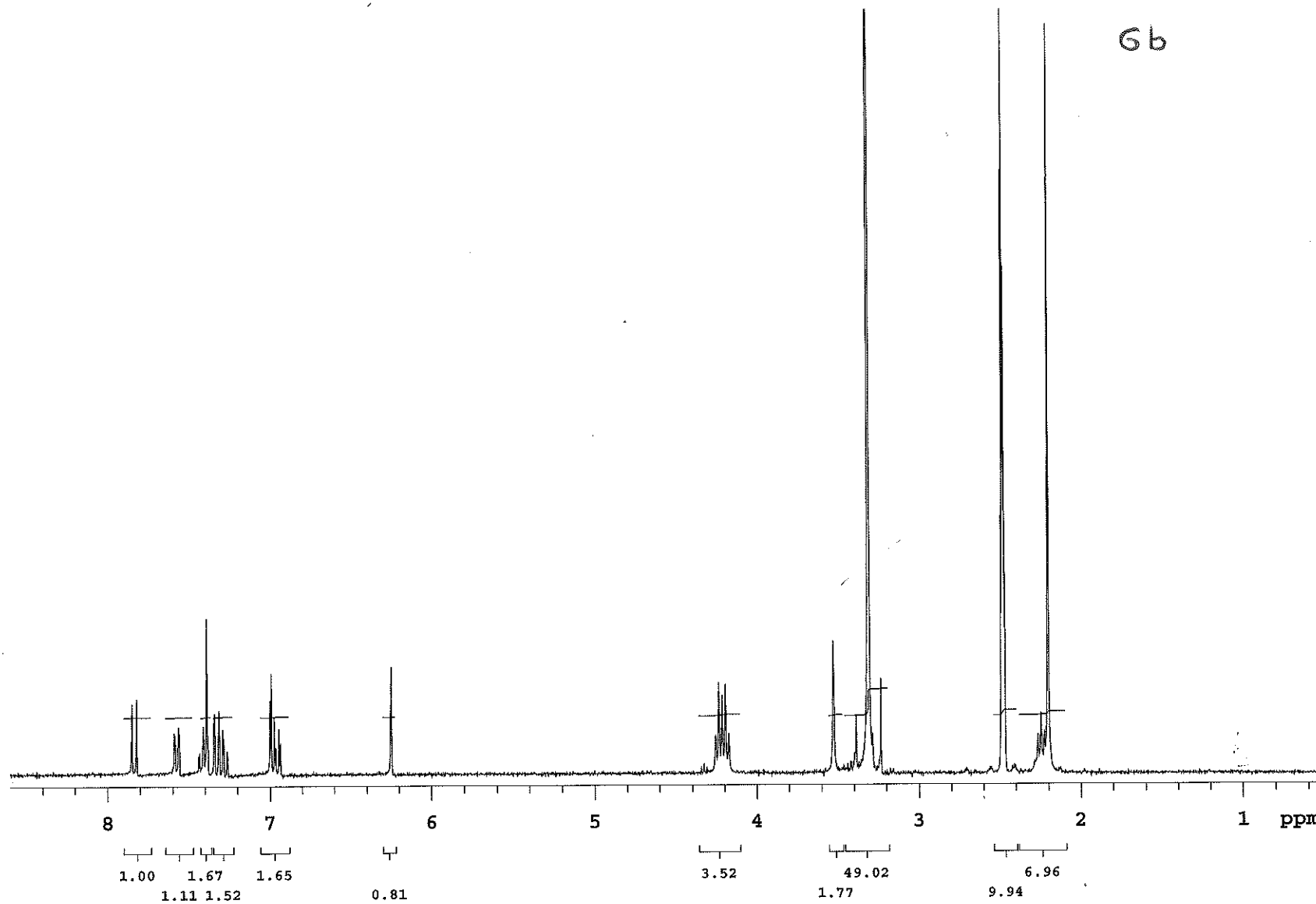
Pulse sequence **PROTON**
Solvent **dmsd**

Temperature **25**
Spectrometer **Agilent500-vnmrs500**

Study owner **vnmr2**
Operator **vnmr2**



Ge



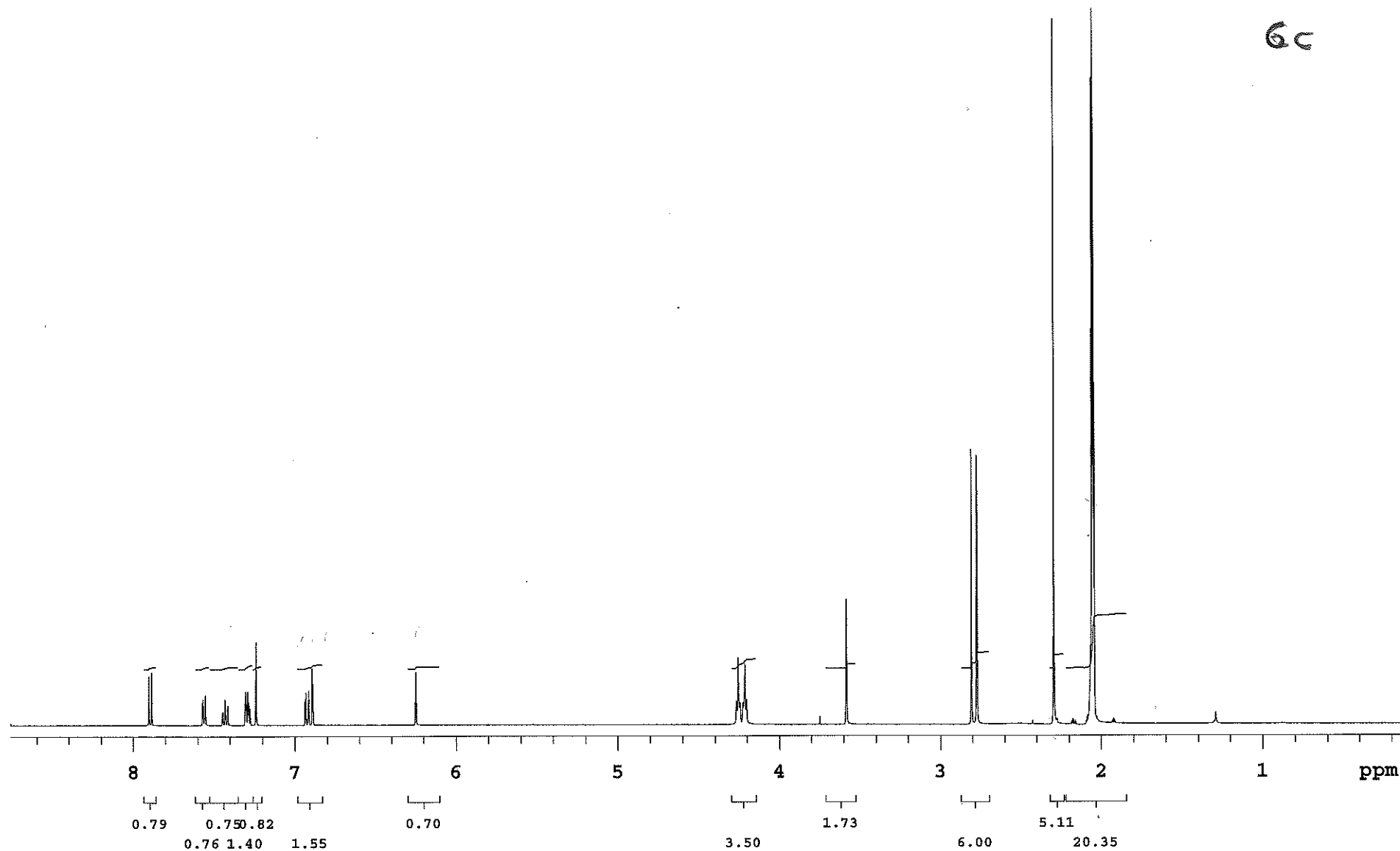
LP1280

Sample Name LP1280
Date collected 2016-05-20

Pulse sequence PROTON
Solvent acetone

Temperature 25
Spectrometer Agilent500-vnmrs500

Study owner vnmr2
Operator vnmr2



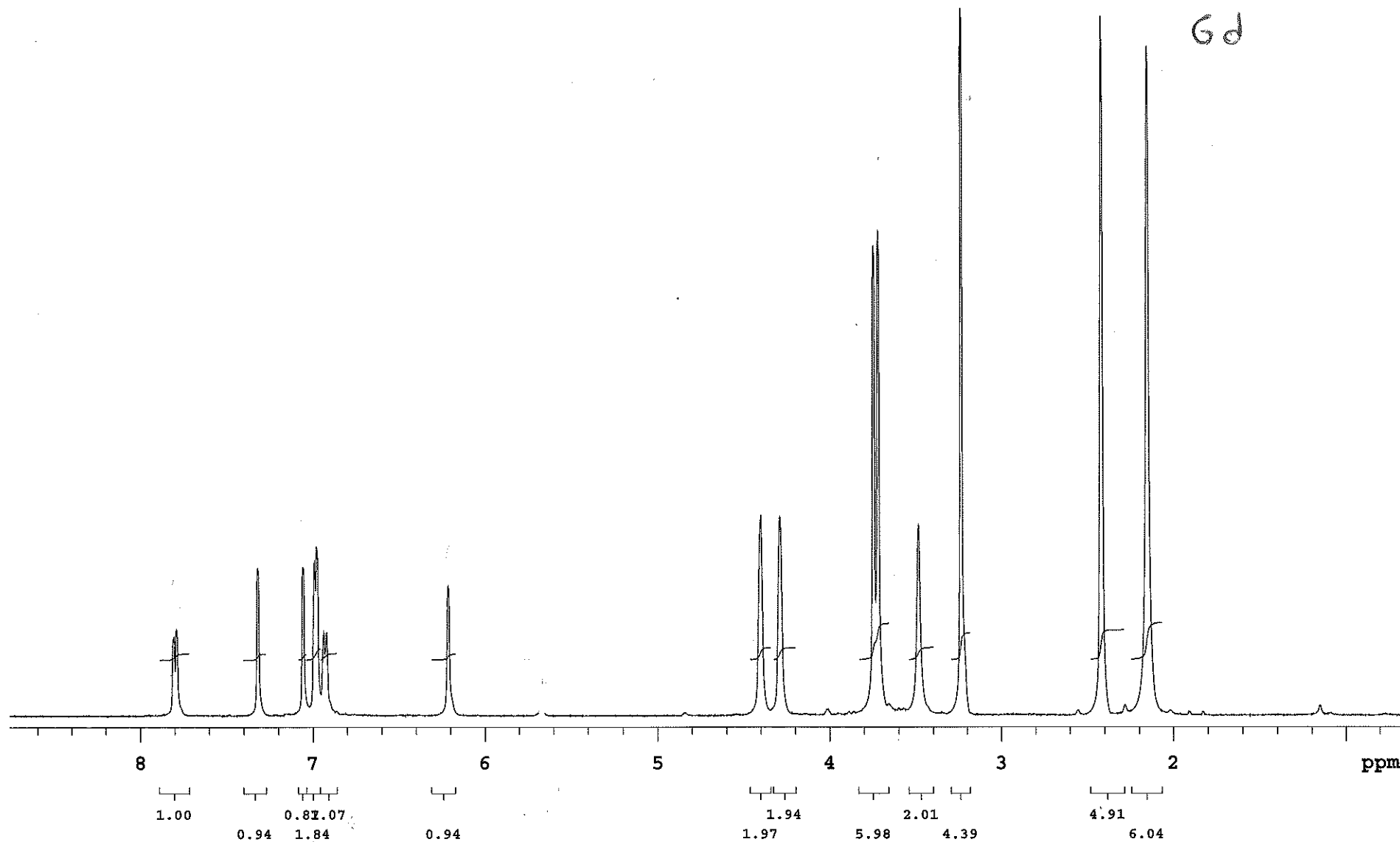
LP1306

Sample Name LP1306
Date collected 2016-10-04

Pulse sequence PROTON
Solvent ~~cdcl3~~ DMSO-d₆

Temperature 25
Spectrometer Agilent500-vnmrs500

Study owner vnmr2
Operator vnmr2



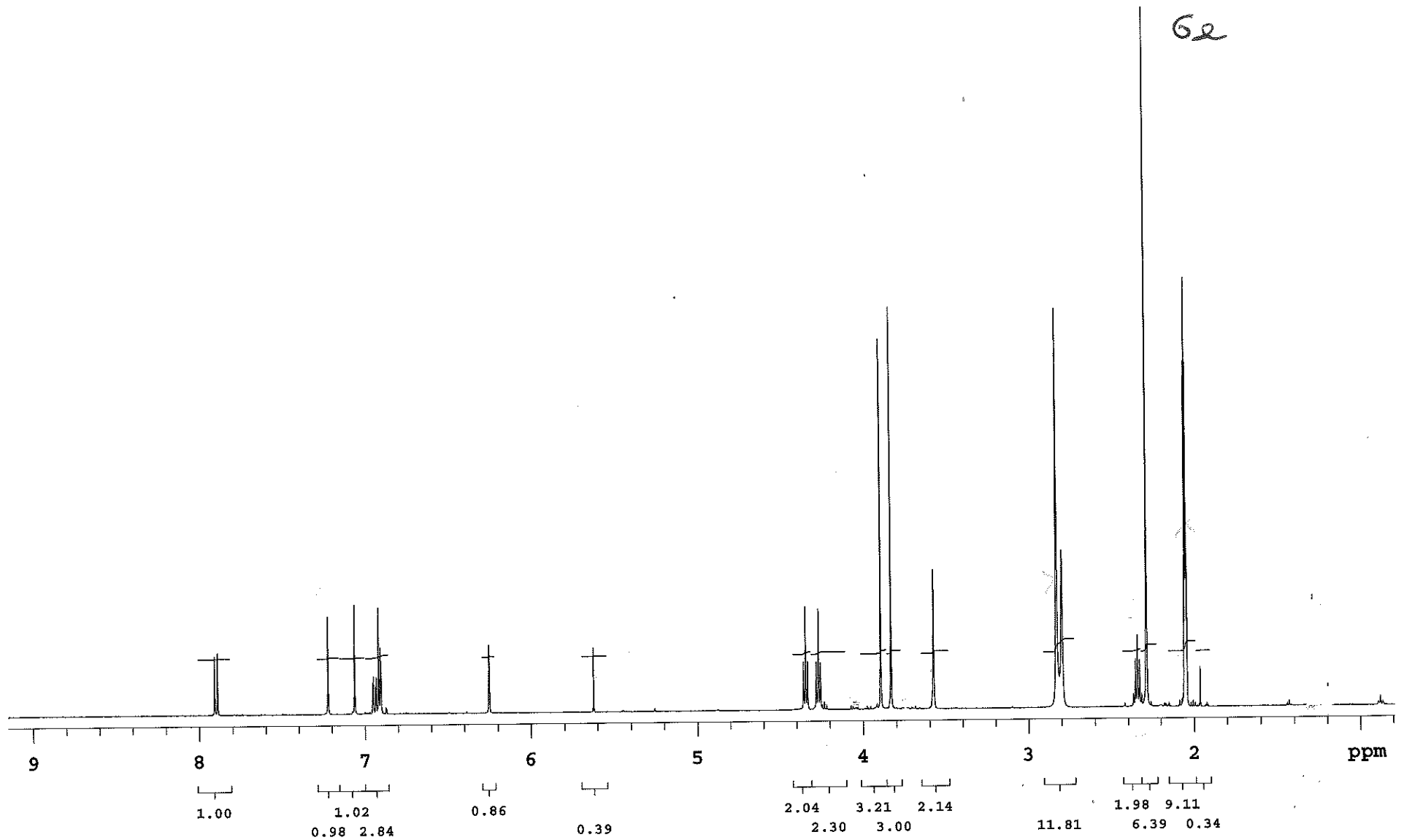
LP1292

Sample Name LP1292
Date collected 2016-06-29

Pulse sequence PROTON
Solvent acetone

Temperature 22
Spectrometer Agilent500-vnmrs500

Study owner vnmr2
Operator vnmr2



Lp1291

Sample Name Lp1291
Date collected 2016-06-30

Pulse sequence PROTON
Solvent acetone

Temperature 22
Spectrometer Agilent500-vnmrs500

Study owner vnmr2
Operator vnmr2

