

## Lead Optimization of 5jc21 (CG13250), a Quinolin-2(1*H*)-one-based Inhibitor of the BRD4 member of the Bromodomain and Extraterminal (BET) Family of Proteins

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### ***Supporting Information***

*<sup>1</sup>H & <sup>13</sup>C NMR Spectra of Lead Compound 5jc21 (CG13250, 6)*

*<sup>1</sup>H NMR Spectra of all target molecules*

*HRMS Spectra of all target molecules*

new experiment

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Nov 14 2013

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

OBSERVE H1, 399.7531794 MHz

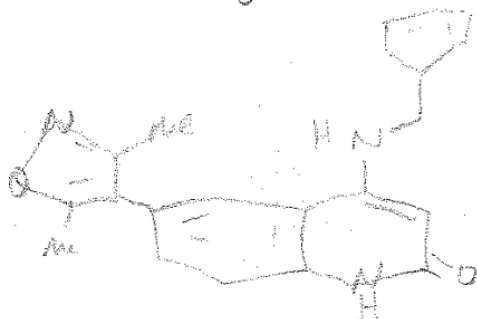
DATA PROCESSING

Line broadening 0.5 Hz

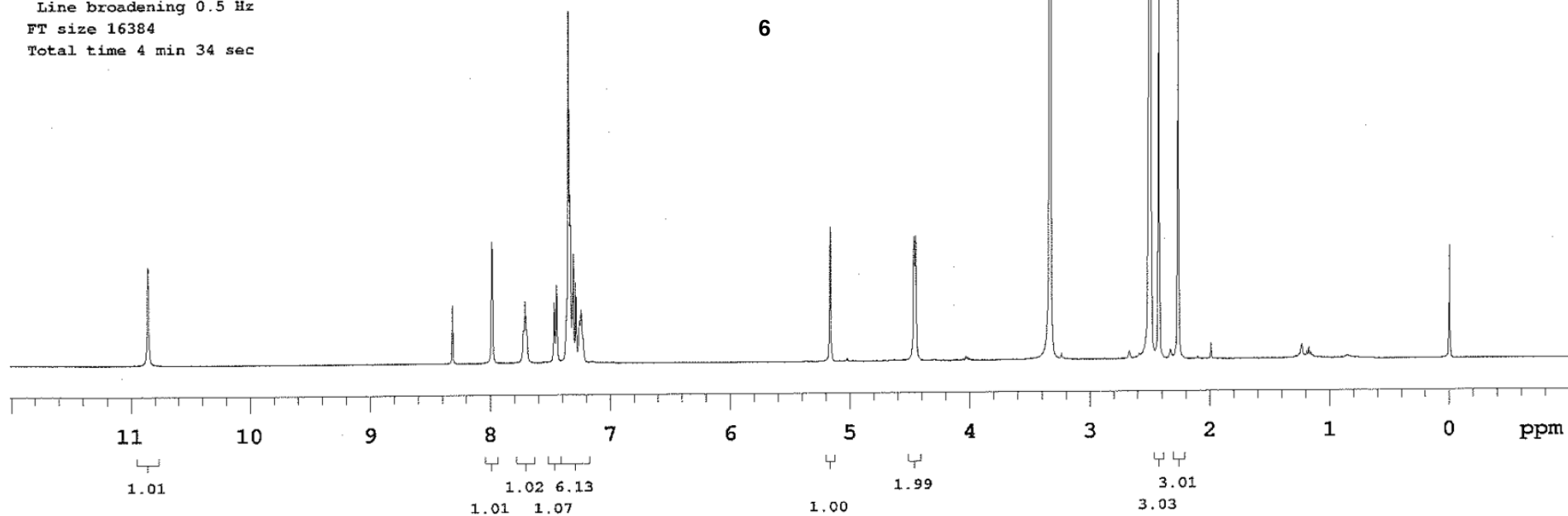
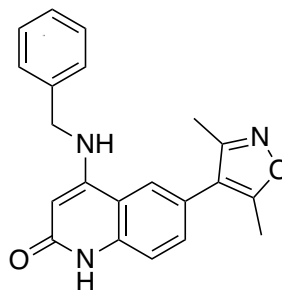
FT size 16384

Total time 4 min 34 sec

Sjc 21



  
VARIAN



5jc21

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc21-Carbon-4-26-2016

Pulse Sequence: CARBON (s2pul)

Solvent: dms0

Data collected on: Apr 26 2016

Operator: work

Relax. delay 1.000 sec

Pulse 58.1 degrees

Acq. time 0.813 sec

Width 24509.8 Hz

232 repetitions

OBSERVE C13, 100.5180605 MHz

DECOUPLE H1, 399.7551914 MHz

Power 39 dB

continuously on

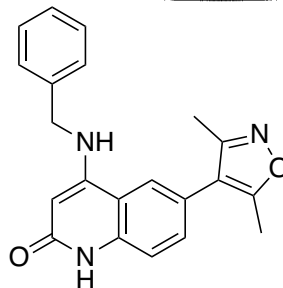
WALTZ-16 modulated

DATA PROCESSING

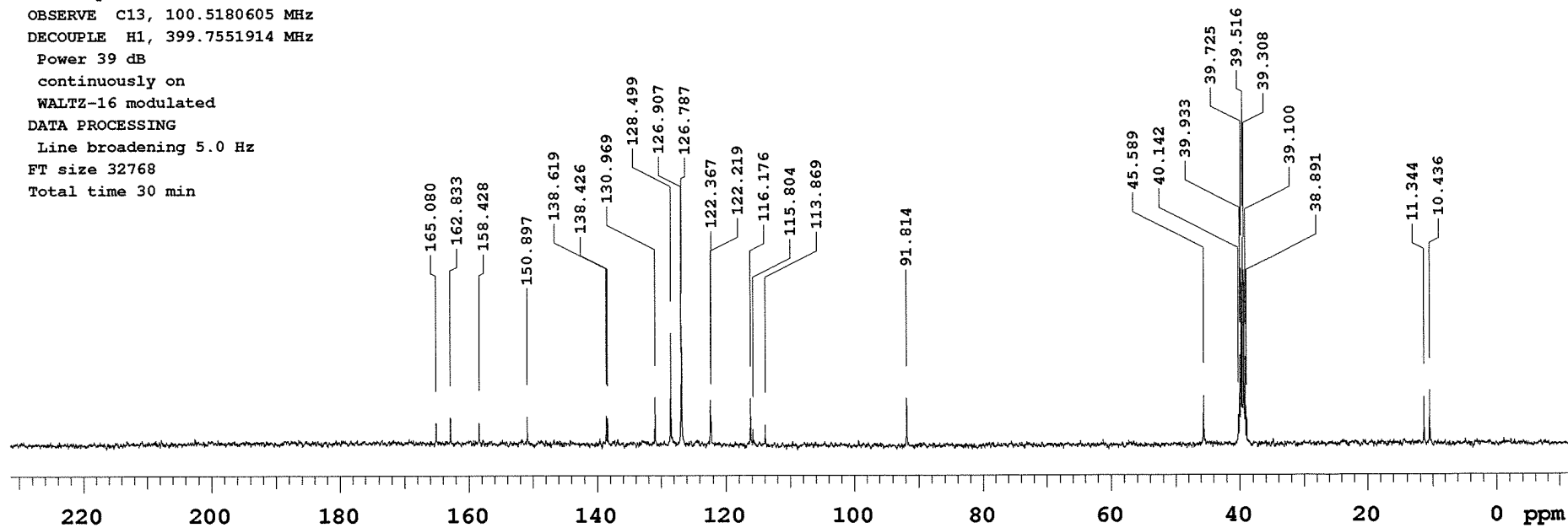
Line broadening 5.0 Hz

FT size 32768

Total time 30 min



6



MR\_22

Sample Name:

MR\_22

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: MR\_22

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Oct 31 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 5.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

32 repetitions

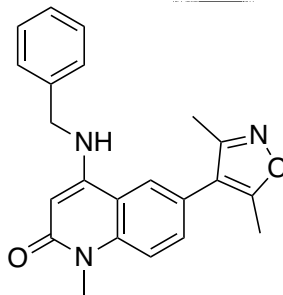
OBSERVE H1, 399.7531790 MHz

DATA PROCESSING

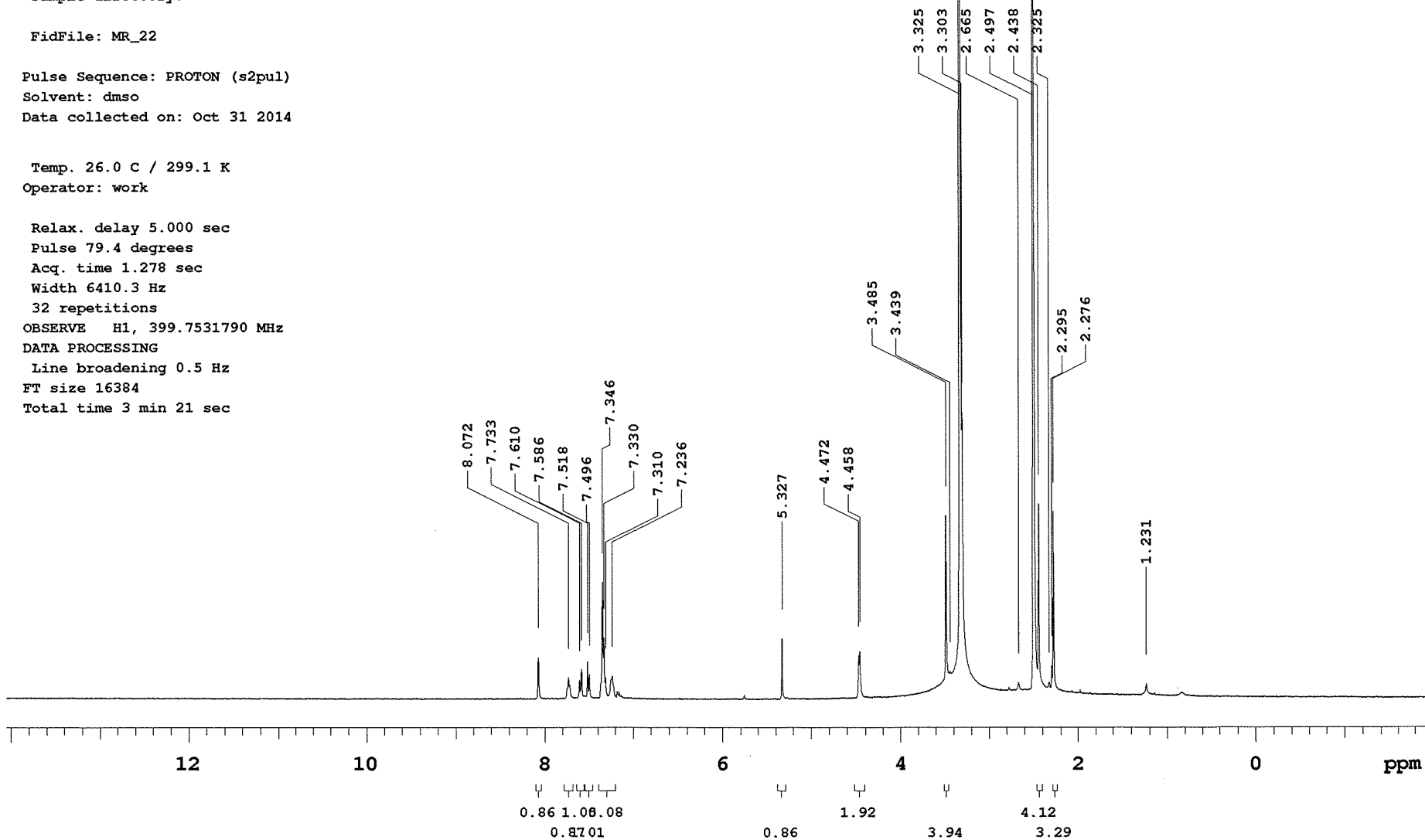
Line broadening 0.5 Hz

FT size 16384

Total time 3 min 21 sec

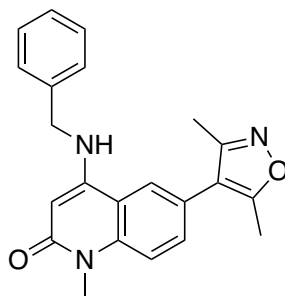


13a



MR\_22

Sample Name:  
MR\_22  
Data Collected on:  
400mr-vnmrs400  
Archive directory:  
Sample directory:



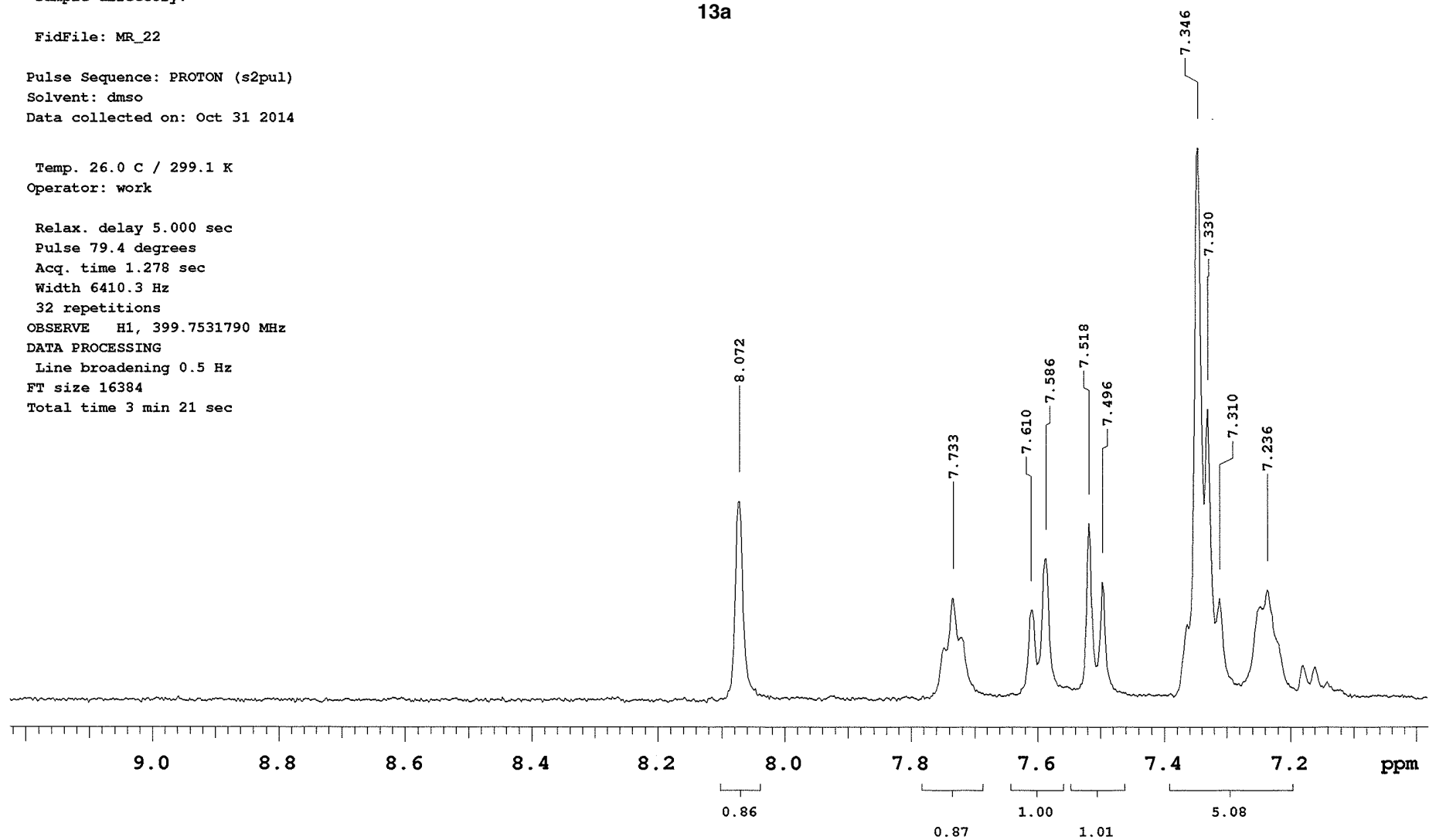
13a

FidFile: MR\_22

Pulse Sequence: PROTON (s2pul)  
Solvent: dms  
Data collected on: Oct 31 2014

Temp. 26.0 C / 299.1 K  
Operator: work

Relax. delay 5.000 sec  
Pulse 79.4 degrees  
Acq. time 1.278 sec  
Width 6410.3 Hz  
32 repetitions  
OBSERVE H1, 399.7531790 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 16384  
Total time 3 min 21 sec



5jc86-1

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc86-1-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Sep 4 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

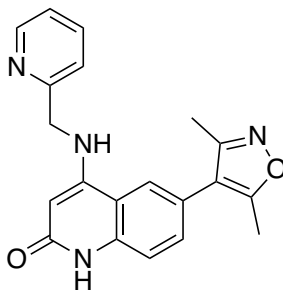
OBSERVE H1, 399.7531801 MHz

DATA PROCESSING

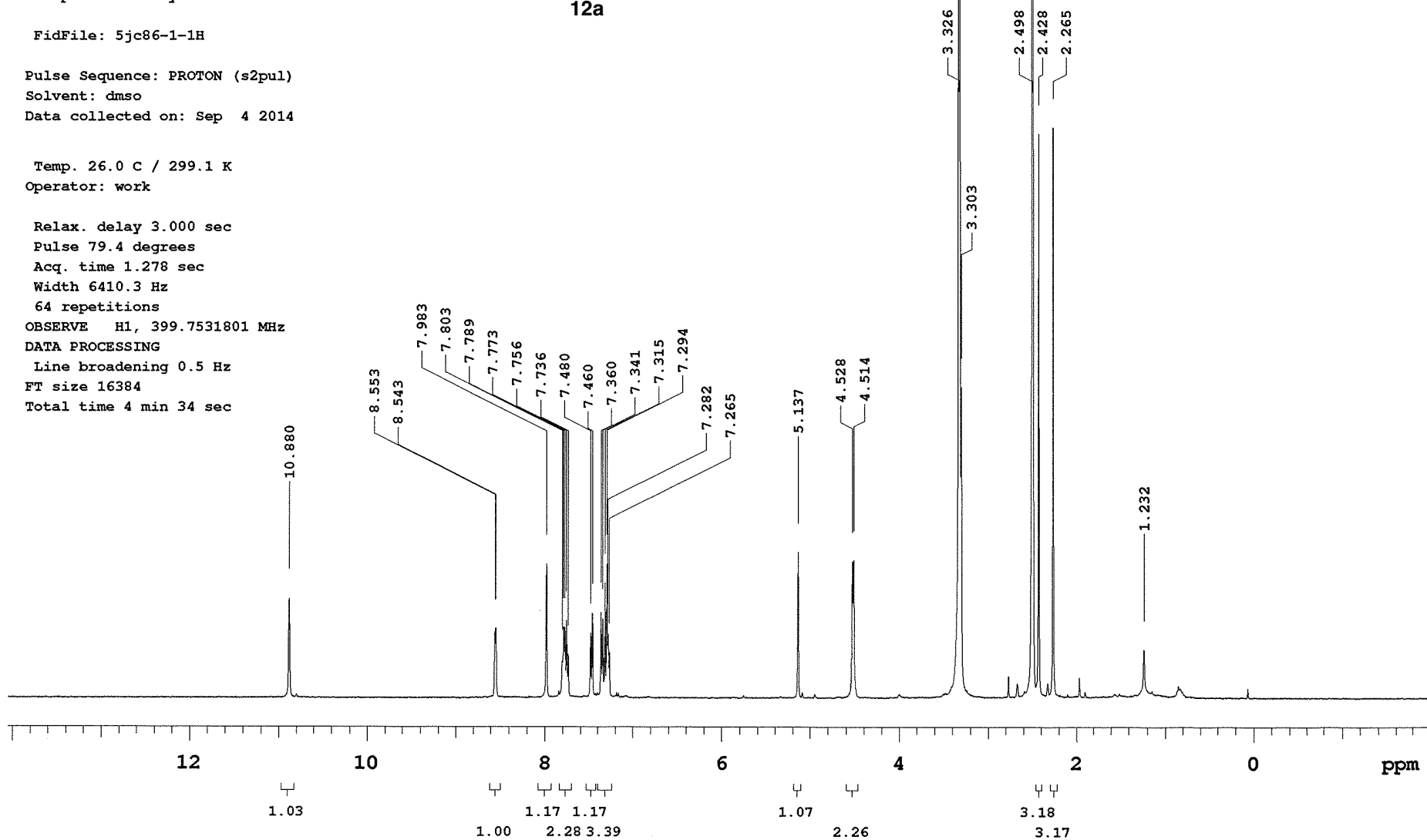
Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



12a



5jc86-2

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc86-2-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Aug 29 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

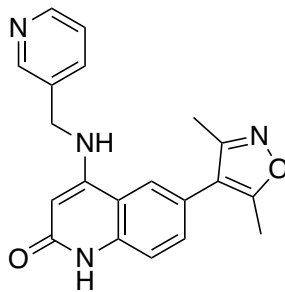
OBSERVE H1, 399.7531777 MHz

DATA PROCESSING

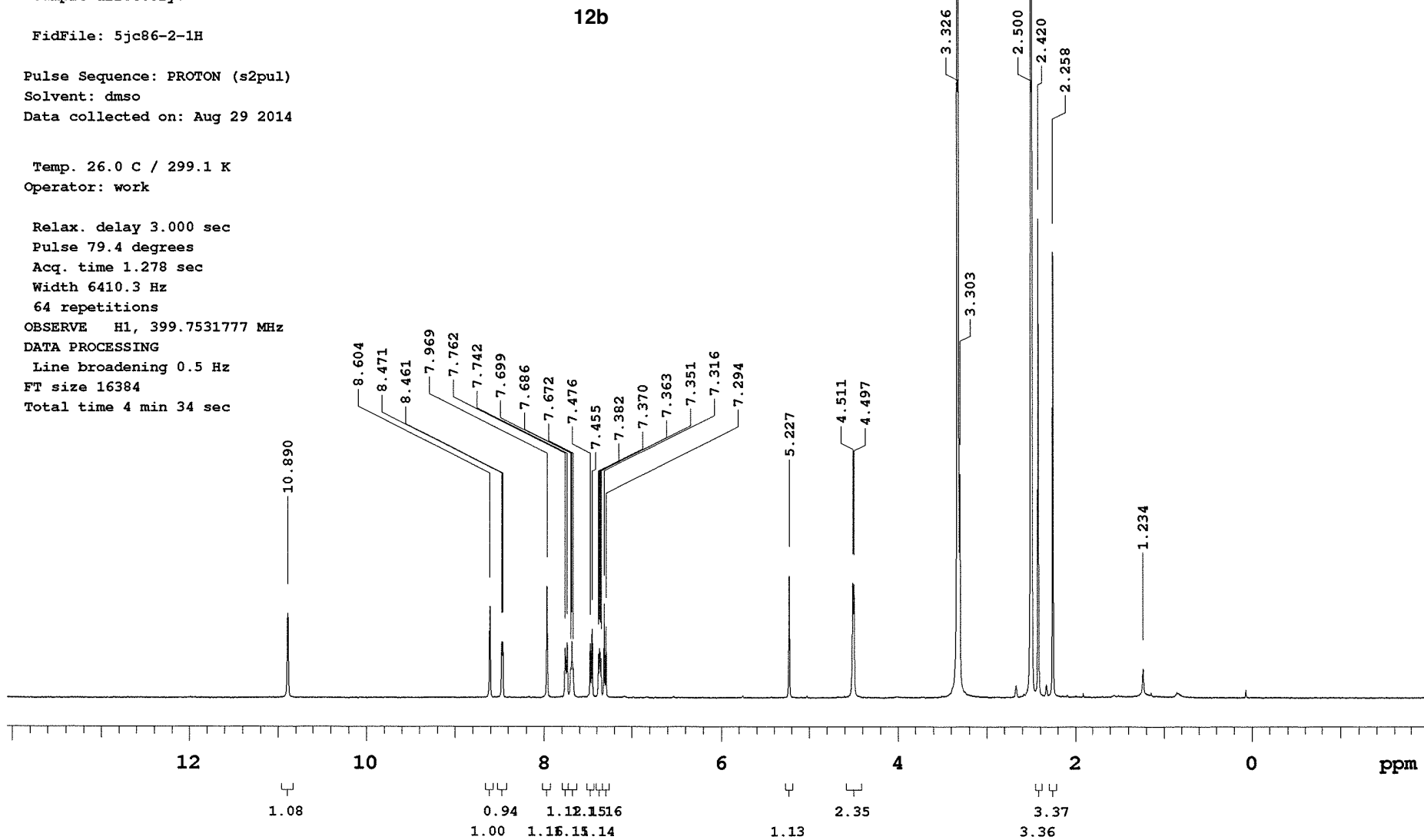
Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



12b



5jc86-2

Sample Name:

Data Collected on:  
400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc86-2-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Aug 29 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

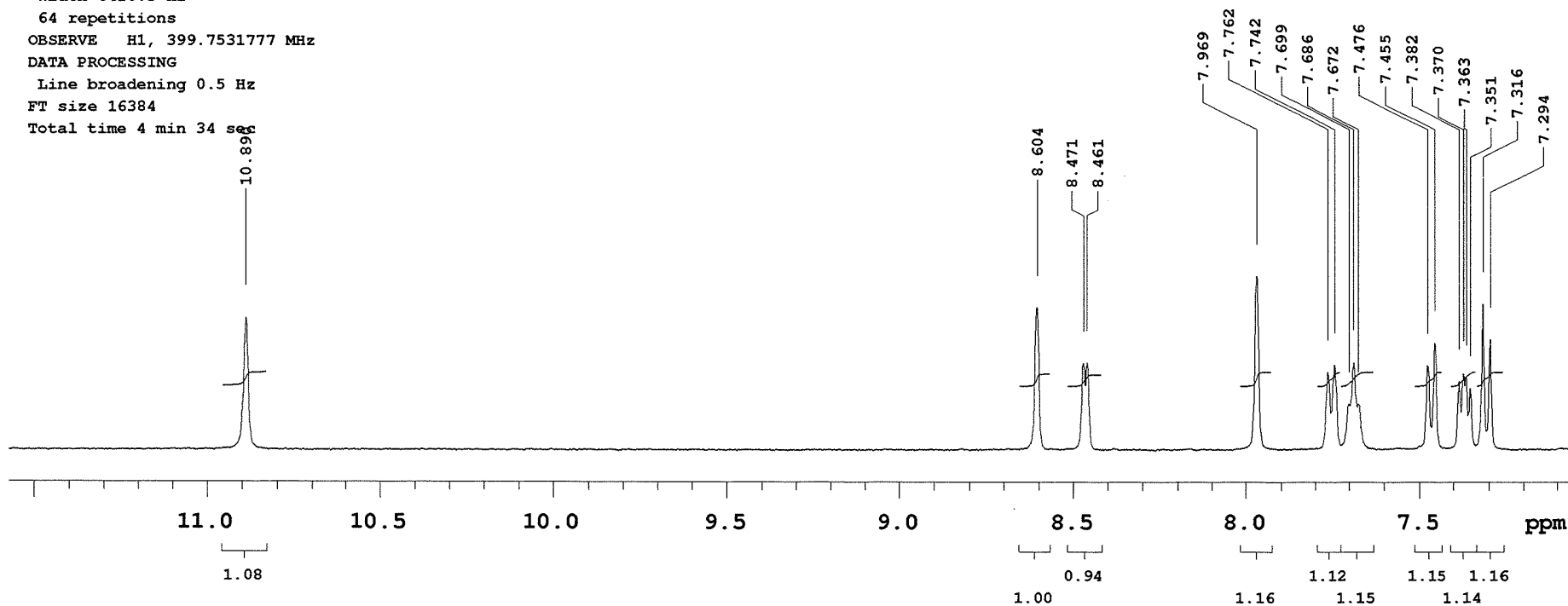
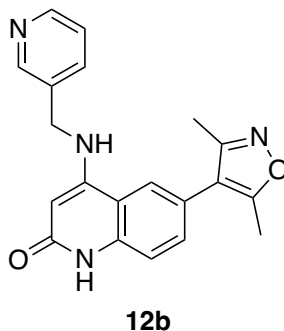
OBSERVE H1, 399.7531777 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



MR67

Sample Name:  
MR67

Data Collected on:  
400mr-vnmrs400

Archive directory:

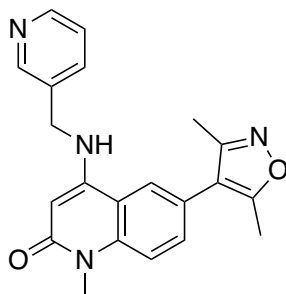
Sample directory:

FidFile: MR67

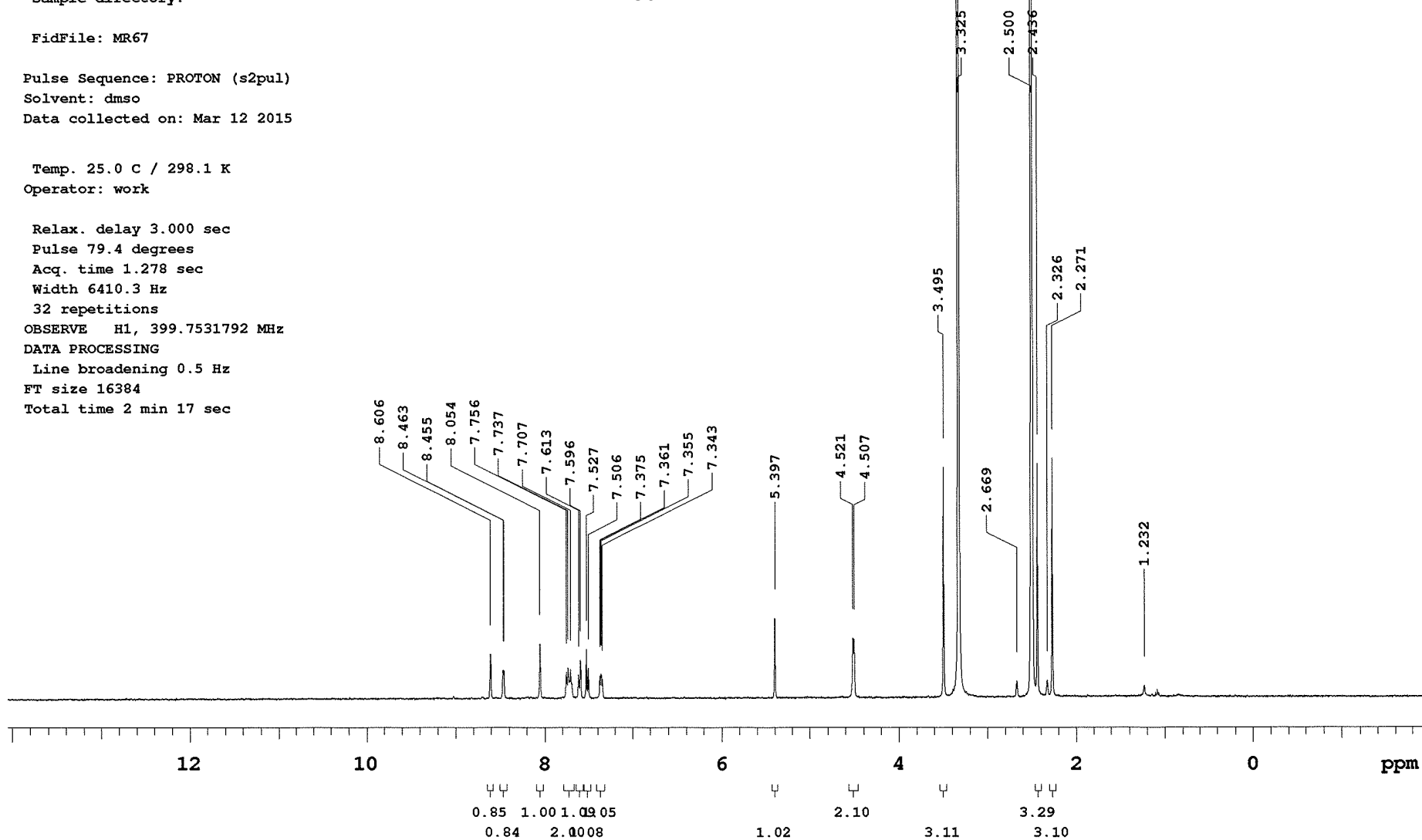
Pulse Sequence: PROTON (s2pul)  
Solvent: dms0  
Data collected on: Mar 12 2015

Temp. 25.0 C / 298.1 K  
Operator: work

Relax. delay 3.000 sec  
Pulse 79.4 degrees  
Acq. time 1.278 sec  
Width 6410.3 Hz  
32 repetitions  
OBSERVE H1, 399.7531792 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 16384  
Total time 2 min 17 sec



13b



MR67

Sample Name:  
MR67

Data Collected on:  
400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: MR67

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Mar 12 2015

Temp. 25.0 C / 298.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

32 repetitions

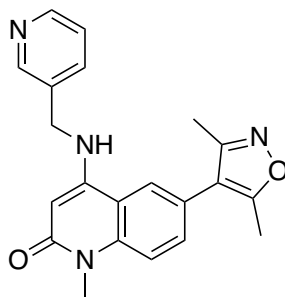
OBSERVE H1, 399.7531792 MHz

DATA PROCESSING

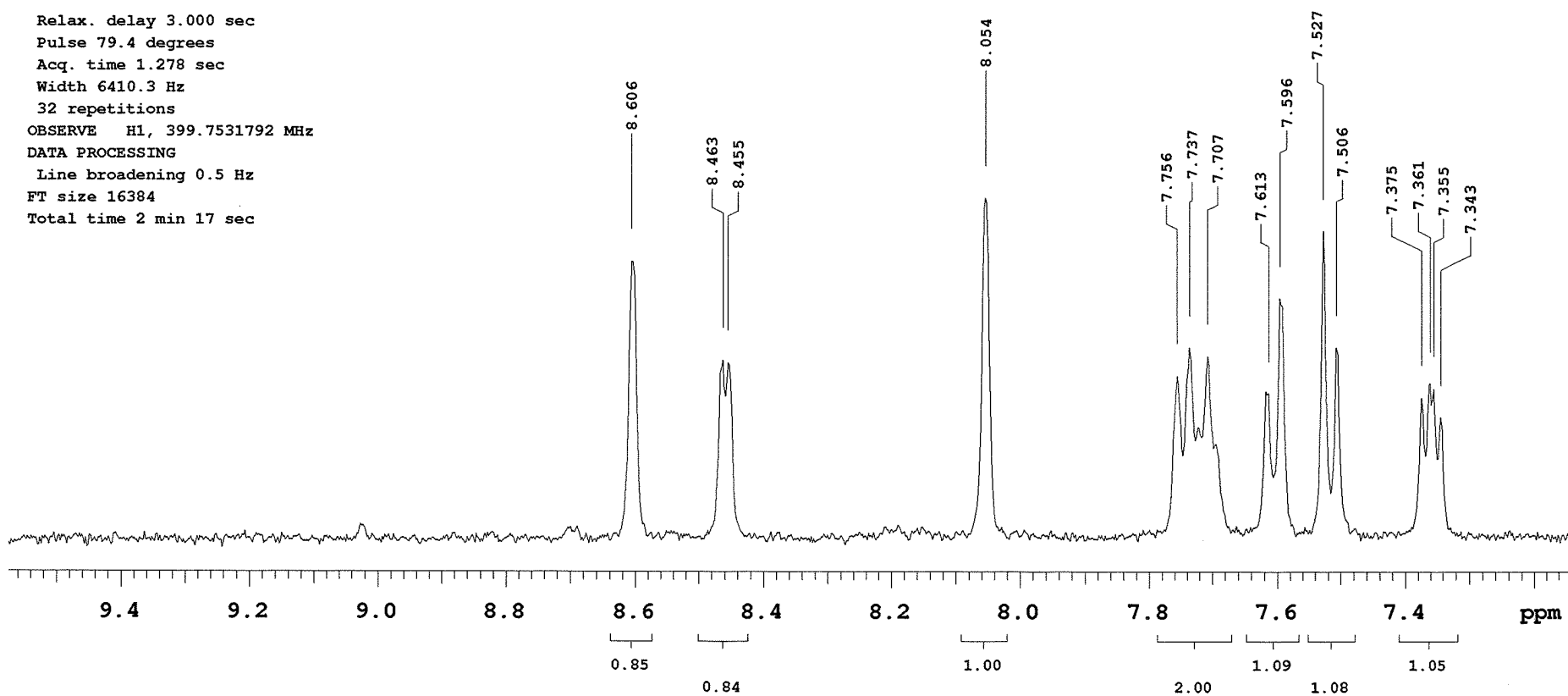
Line broadening 0.5 Hz

FT size 16384

Total time 2 min 17 sec



13b



5jc86-3

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc86-3-1H-Prep

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Sep 11 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

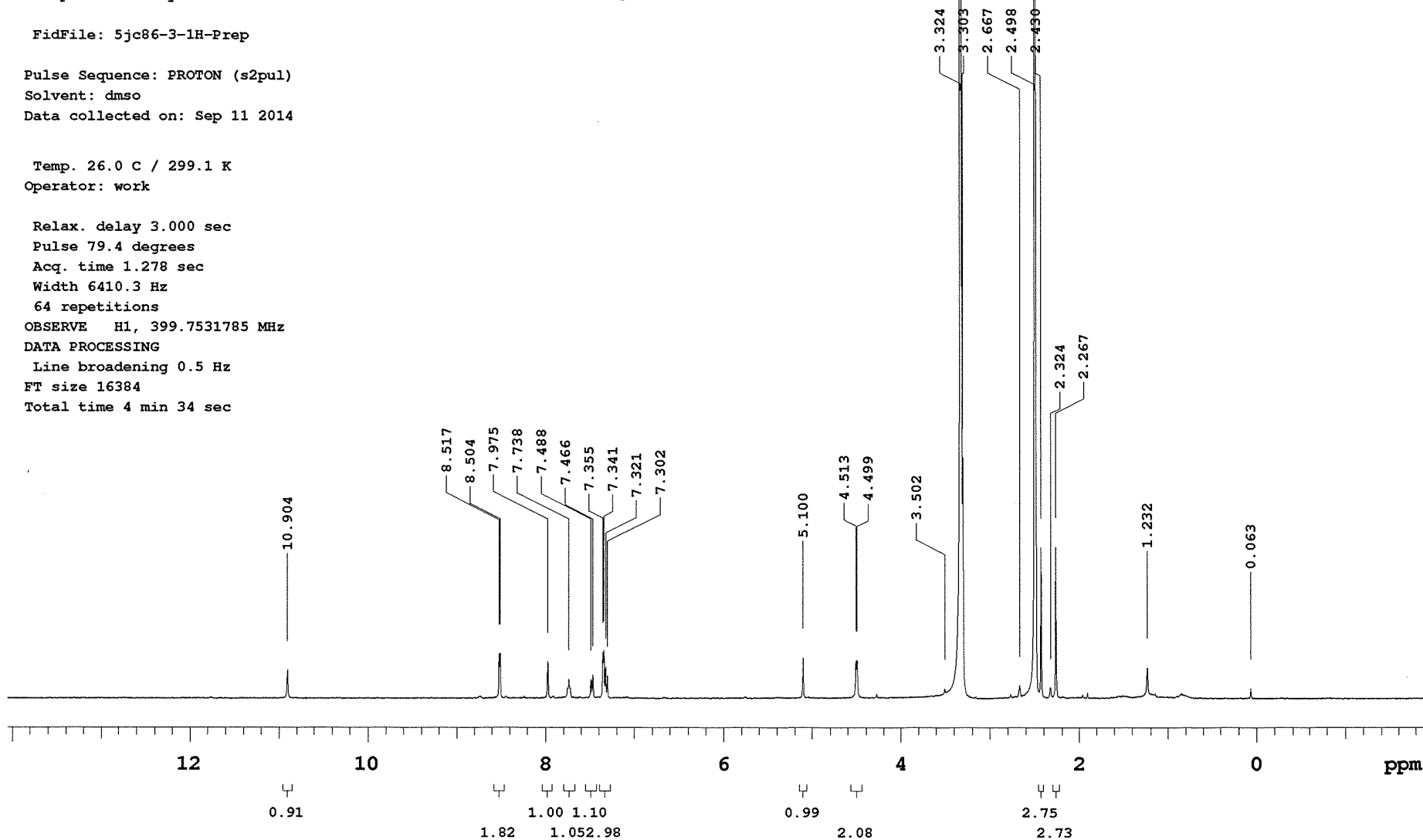
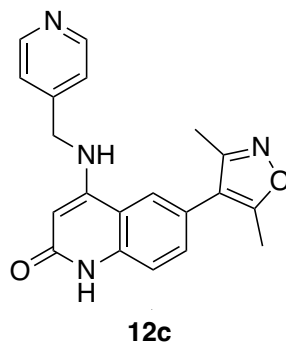
OBSERVE H1, 399.7531785 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



5jc85-2

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc85-2-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Aug 22 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

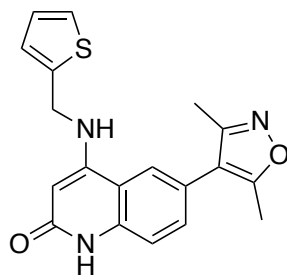
OBSERVE H1, 399.7531785 MHz

DATA PROCESSING

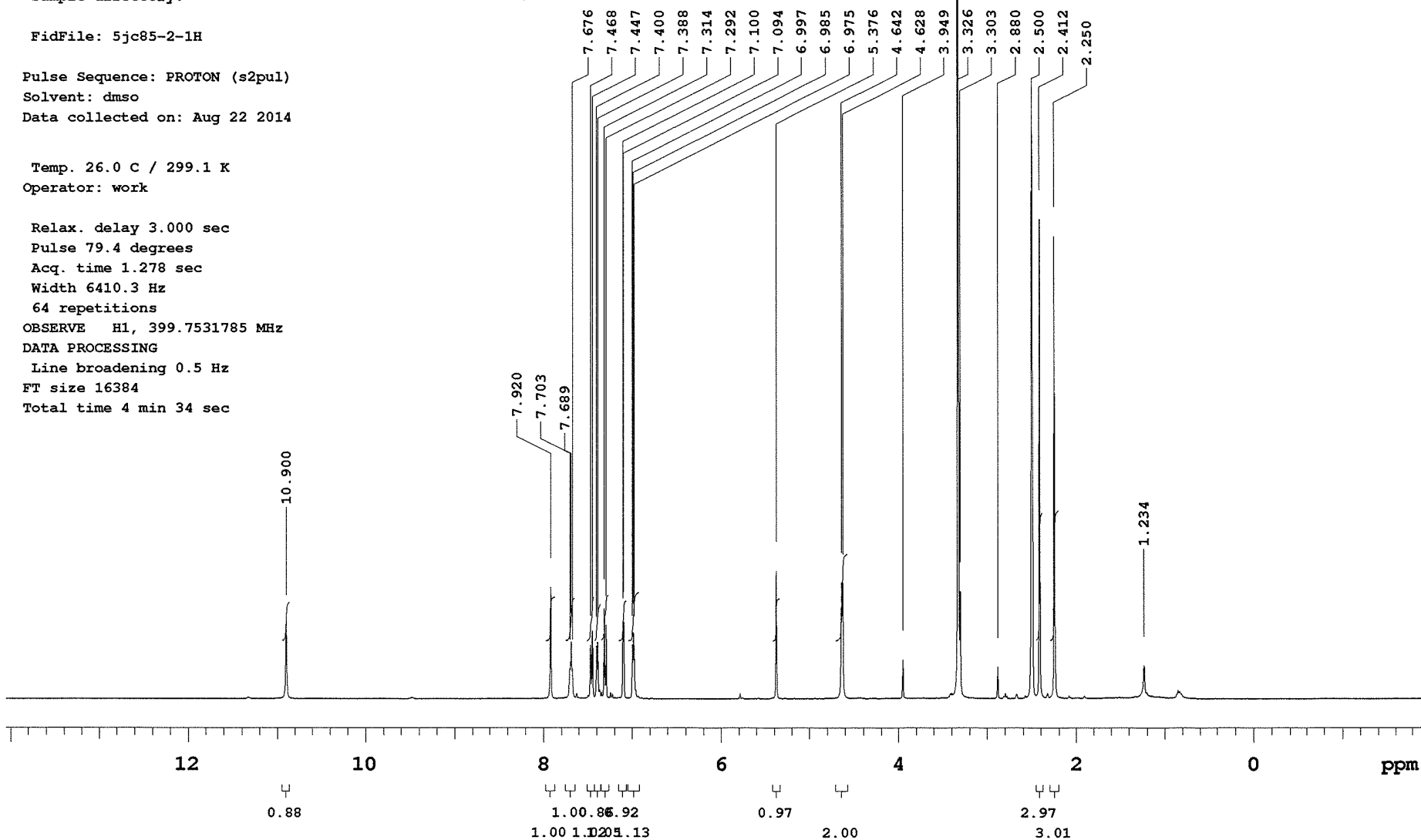
Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



12h



5jc85-2

Sample Name:

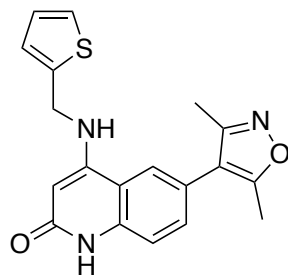
Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc85-2-1H



12h

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Aug 22 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

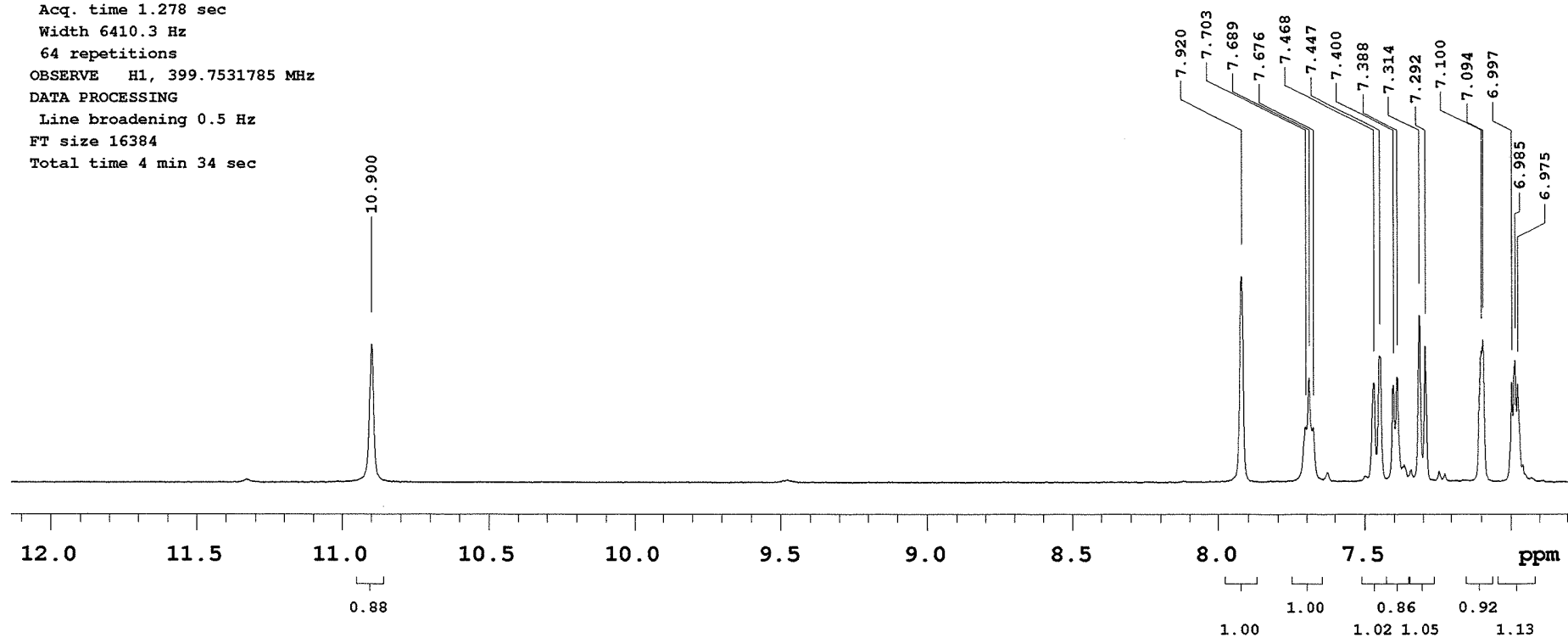
OBSERVE H1, 399.7531785 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



MR75

Sample Name:  
MR75

Data Collected on:  
400mr-vnmrs400

Archive directory:

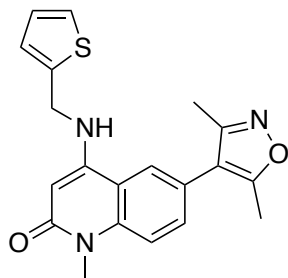
Sample directory:

FidFile: MR75

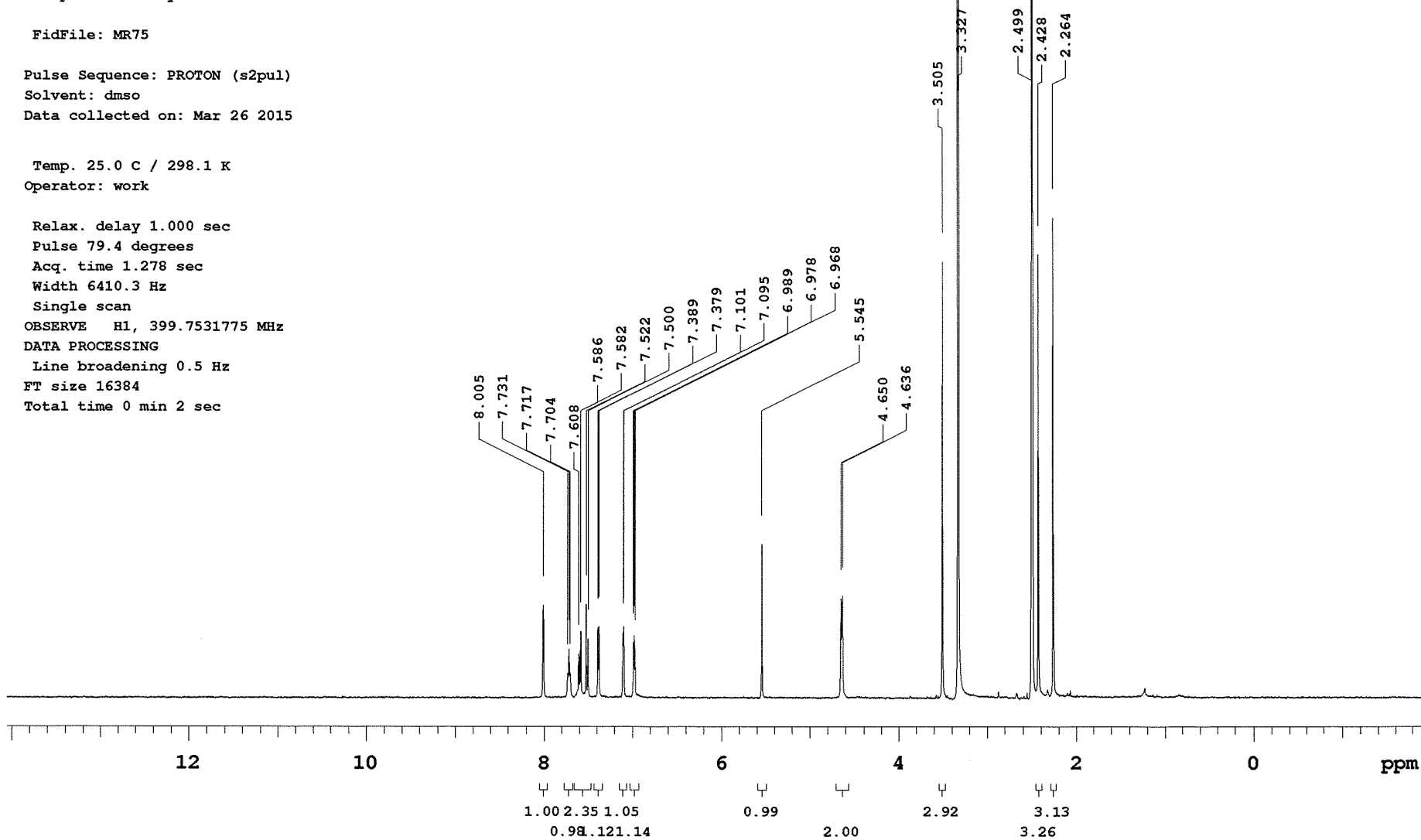
Pulse Sequence: PROTON (s2pul)  
Solvent: dmsc  
Data collected on: Mar 26 2015

Temp. 25.0 C / 298.1 K  
Operator: work

Relax. delay 1.000 sec  
Pulse 79.4 degrees  
Acq. time 1.278 sec  
Width 6410.3 Hz  
Single scan  
OBSERVE H1, 399.7531775 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 16384  
Total time 0 min 2 sec



13c



MR75

Sample Name:  
MR75

Data Collected on:  
400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: MR75

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Mar 26 2015

Temp. 25.0 C / 298.1 K

Operator: work

Relax. delay 1.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

Single scan

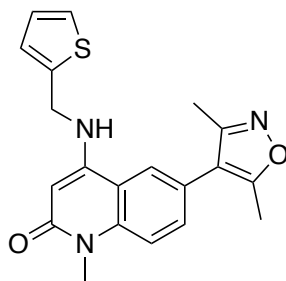
OBSERVE H1, 399.7531775 MHz

DATA PROCESSING

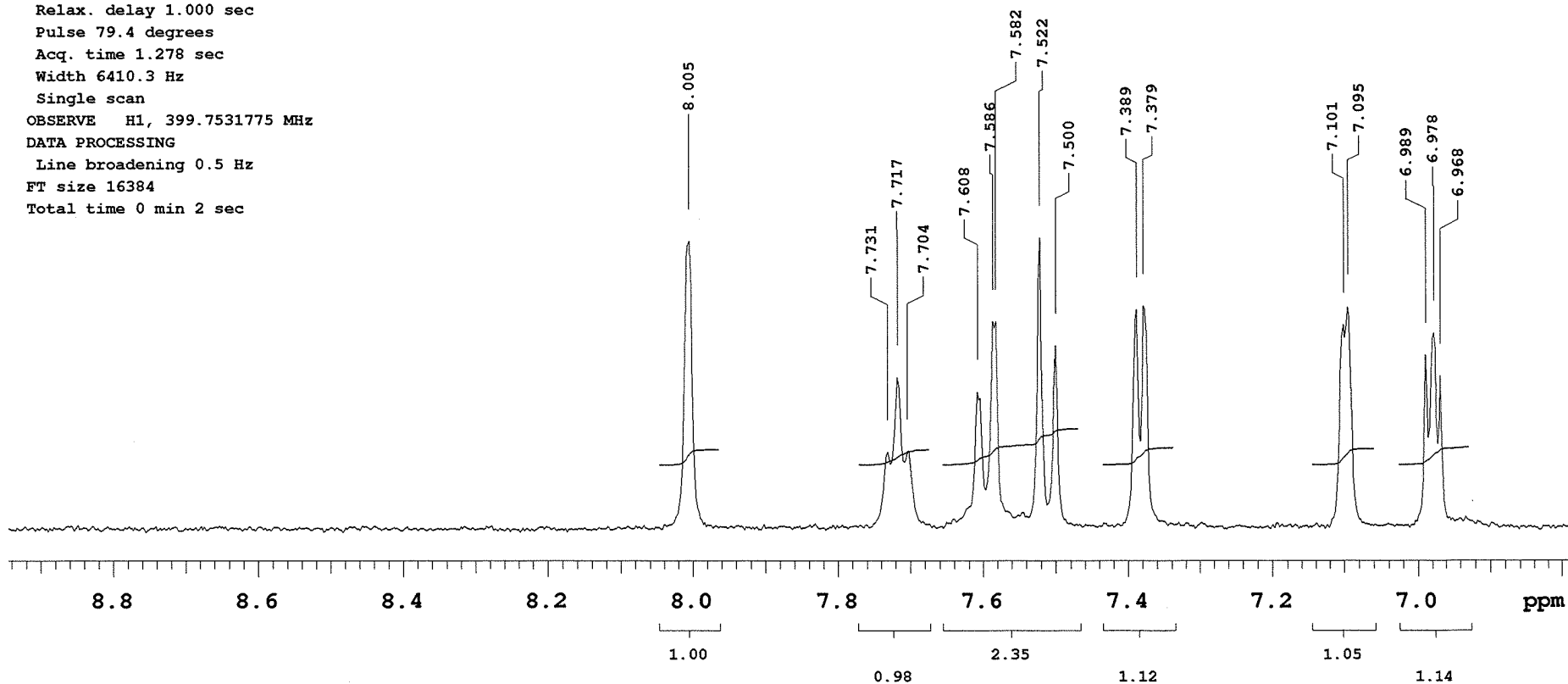
Line broadening 0.5 Hz

FT size 16384

Total time 0 min 2 sec



13c



5jc85-1

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc85-1-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Aug 22 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

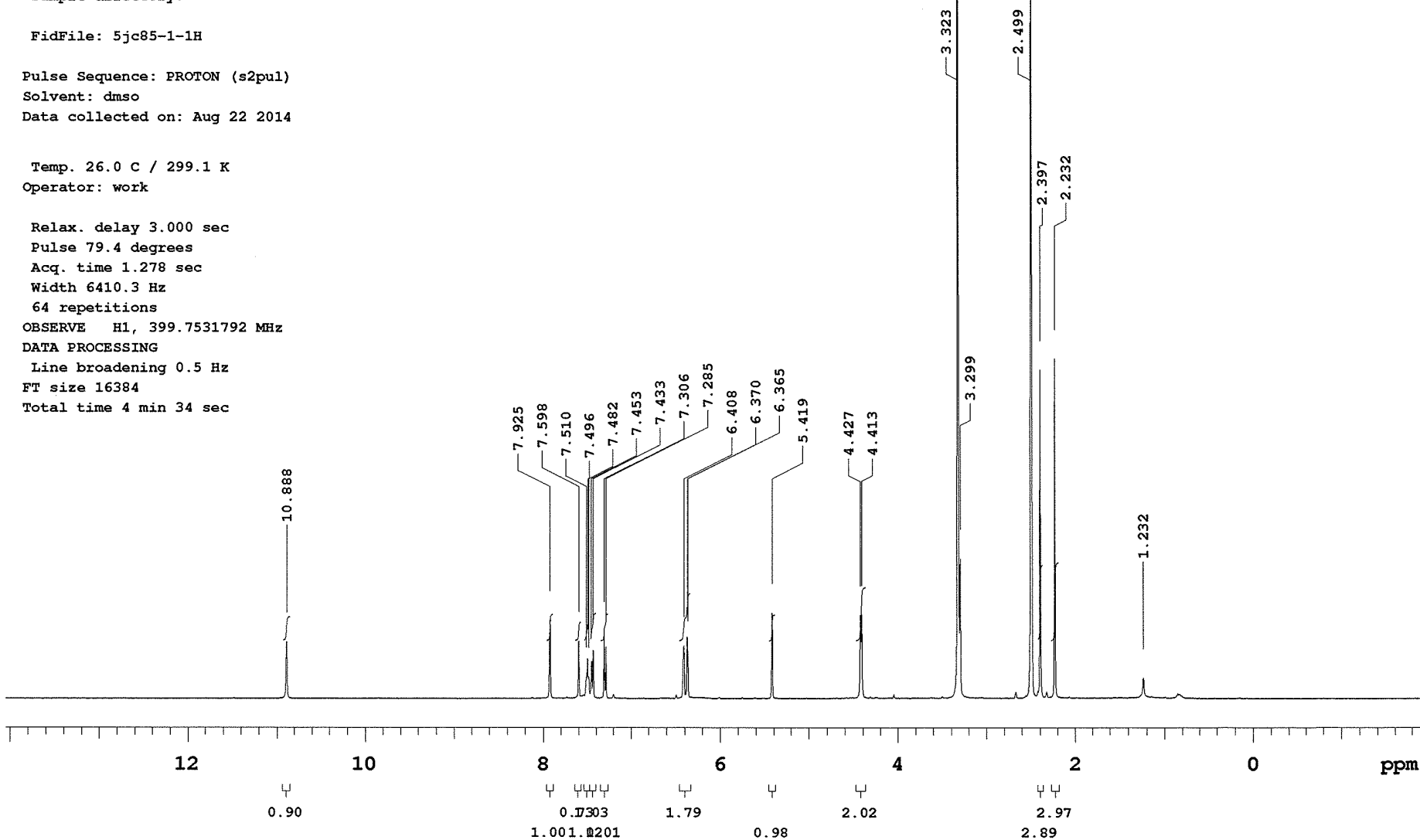
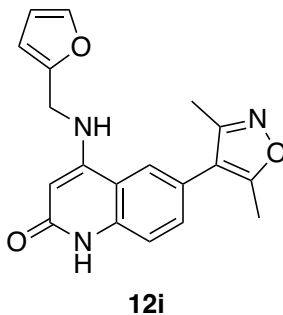
OBSERVE H1, 399.7531792 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



5jc85-1

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc85-1-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Aug 22 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

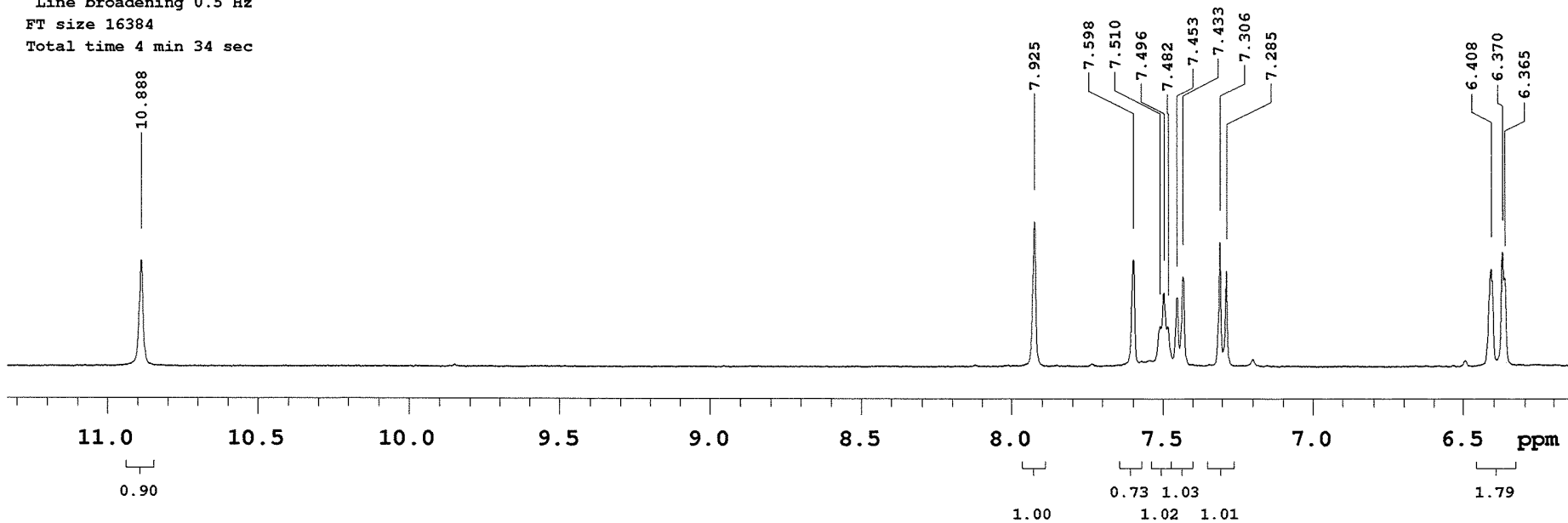
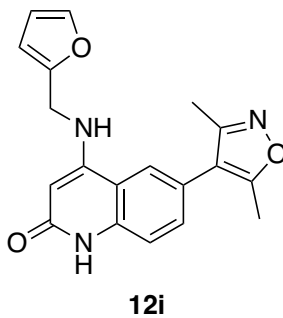
OBSERVE H1, 399.7531792 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



5jc87

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc87-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Sep 11 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

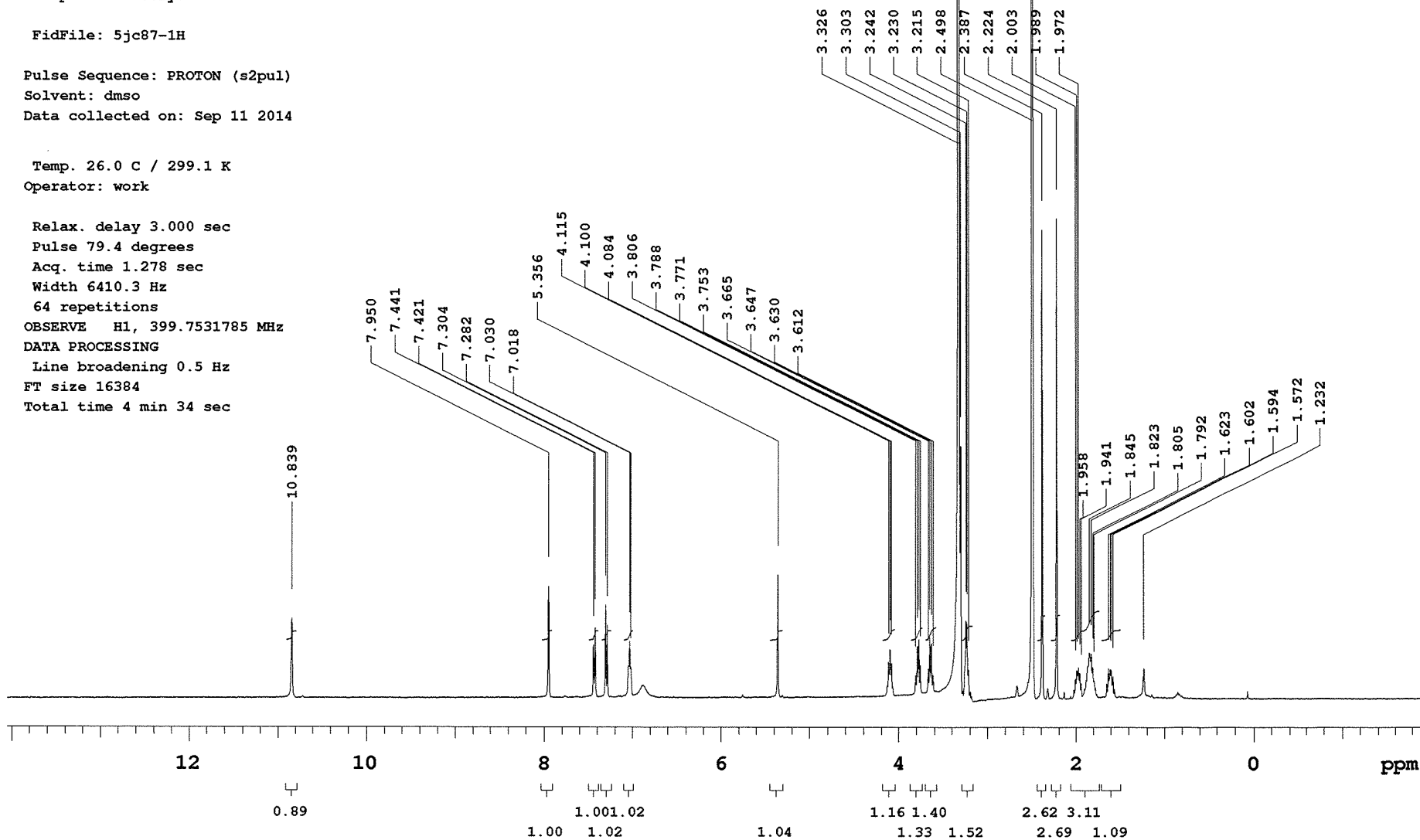
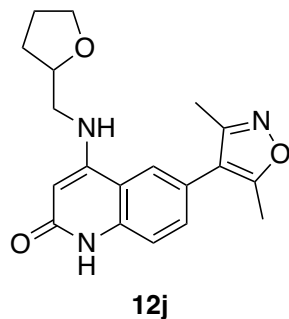
OBSERVE H1, 399.7531785 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



new experiment

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc80-2-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Jul 10 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

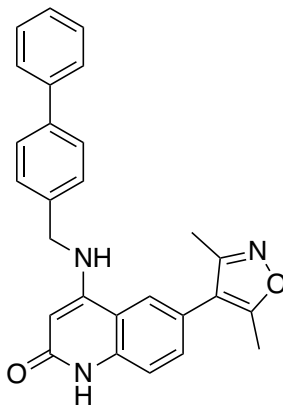
OBSERVE H1, 399.7531797 MHz

DATA PROCESSING

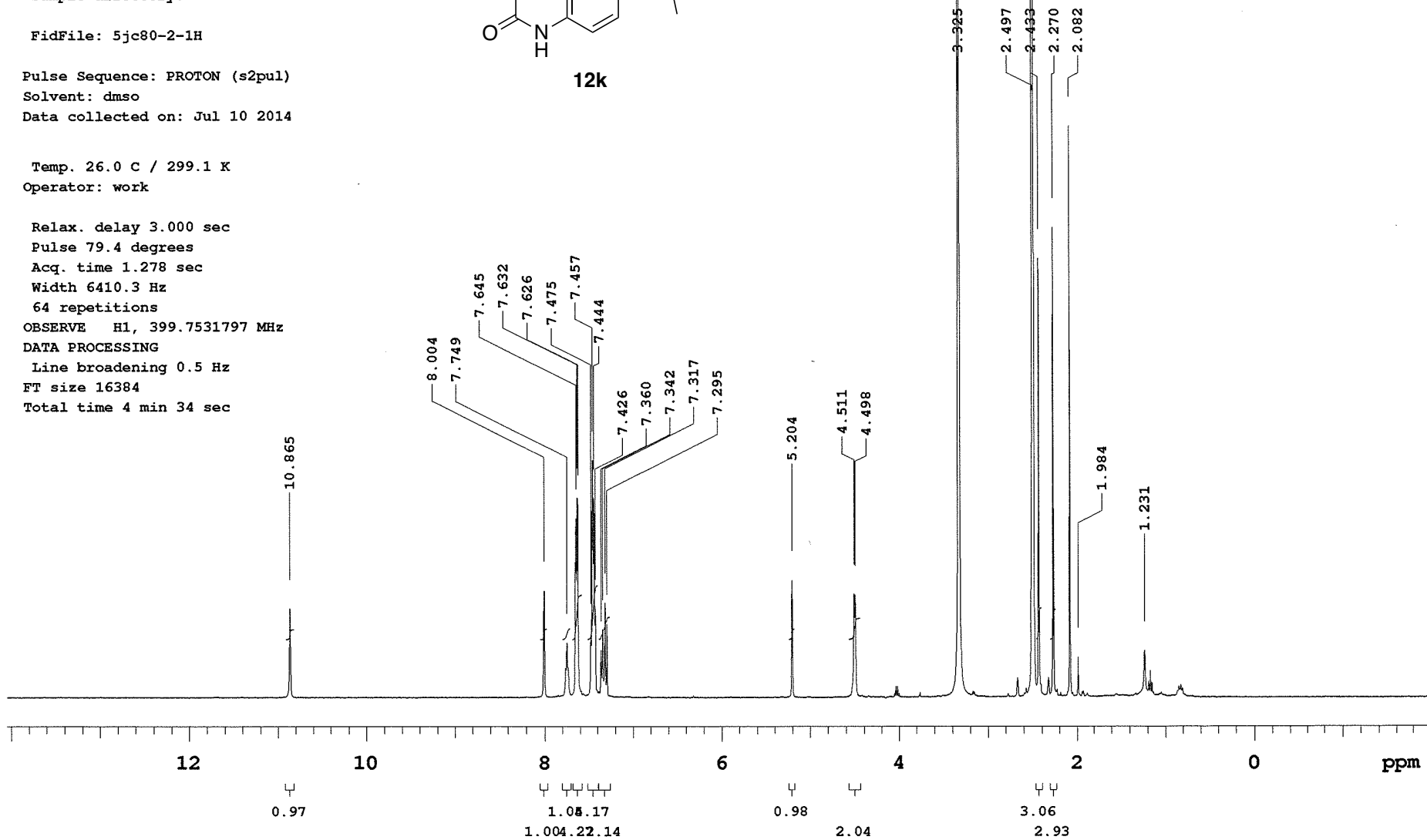
Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



12k



new experiment

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

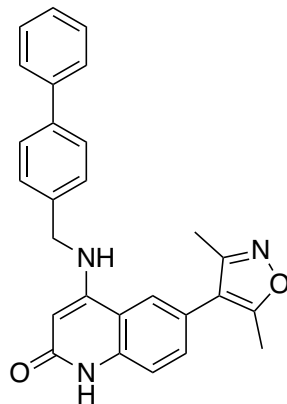
Sample directory:

FidFile: 5jc80-2-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dmso

Data collected on: Jul 10 2014



12k

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

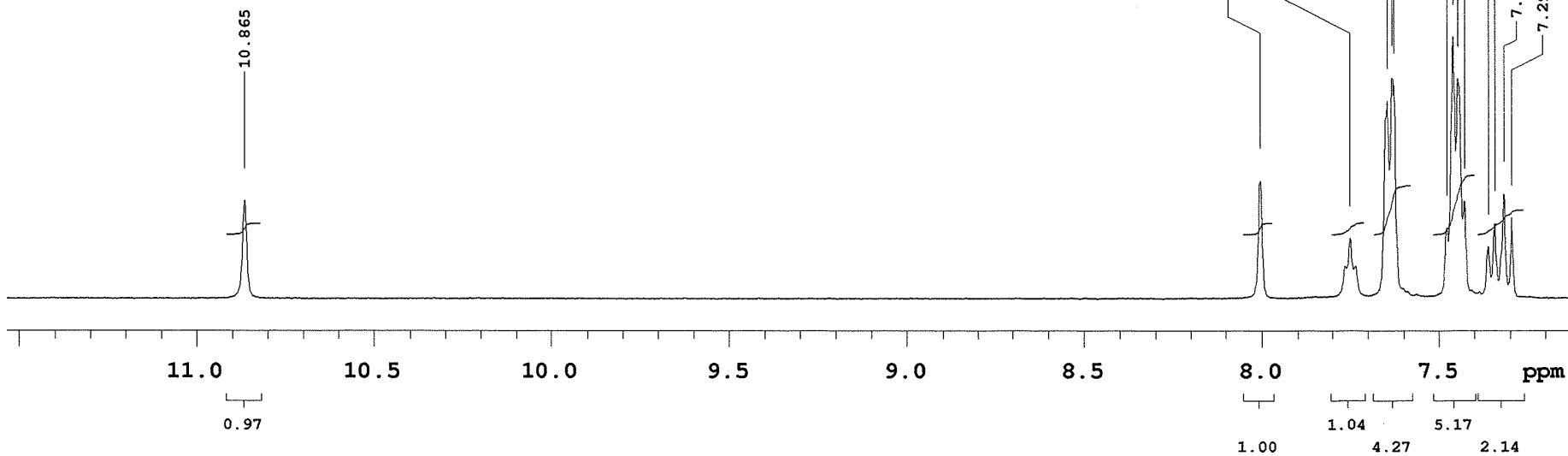
OBSERVE H1, 399.7531797 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



5jc88

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc88-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Sep 19 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

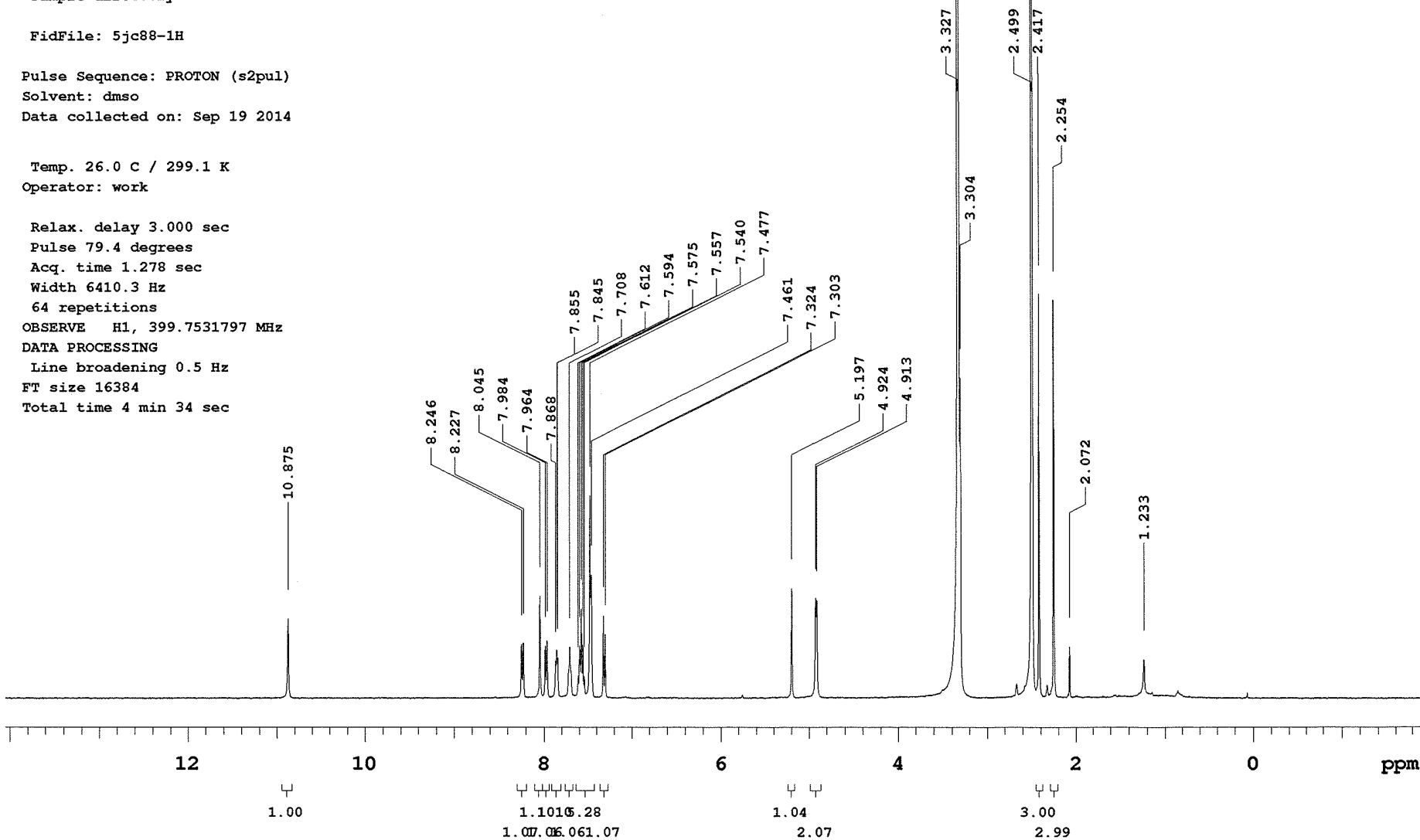
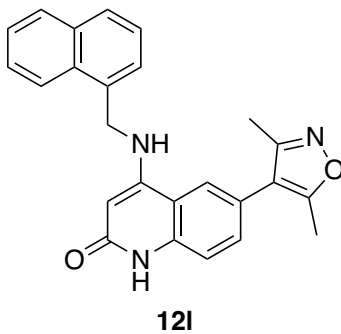
OBSERVE H1, 399.7531797 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



5jc88

Sample Name:

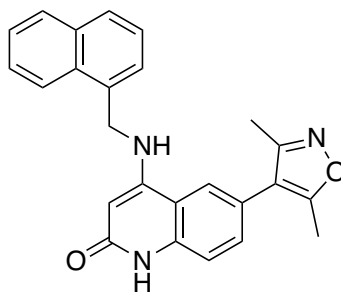
Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc88-1H



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Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Sep 19 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

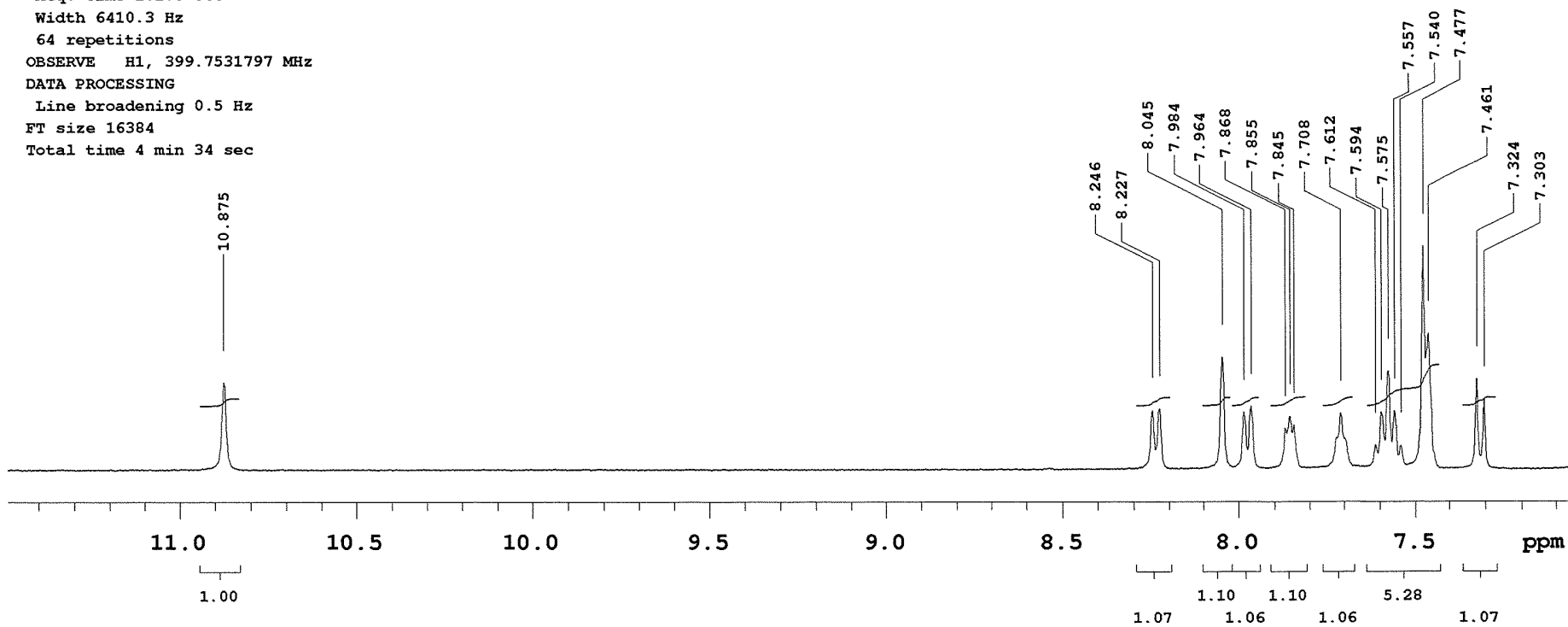
OBSERVE H1, 399.7531797 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



5jc89

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc89-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Sep 19 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

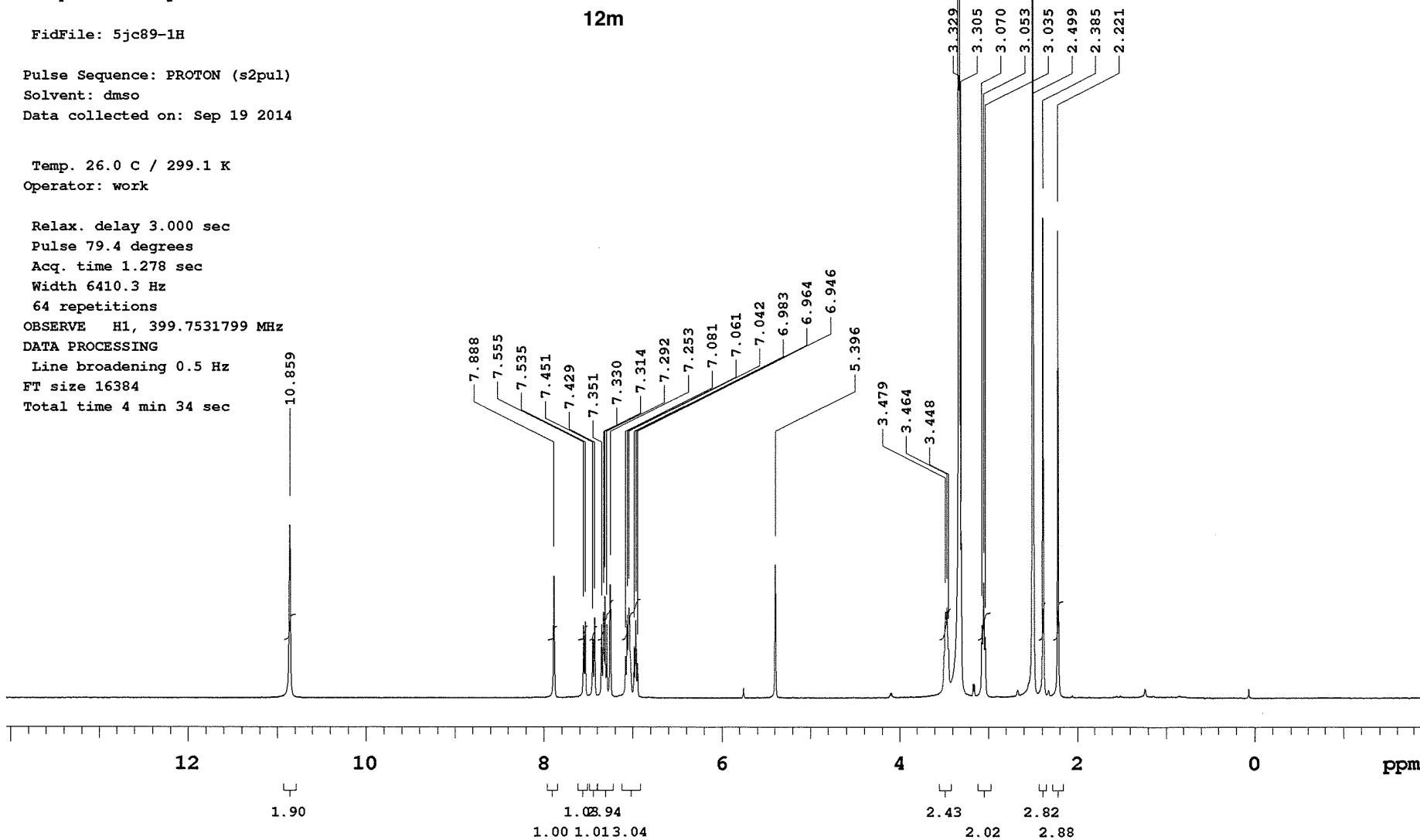
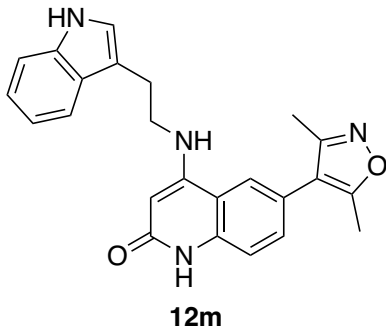
OBSERVE H1, 399.7531799 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



5jc89

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc89-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Sep 19 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

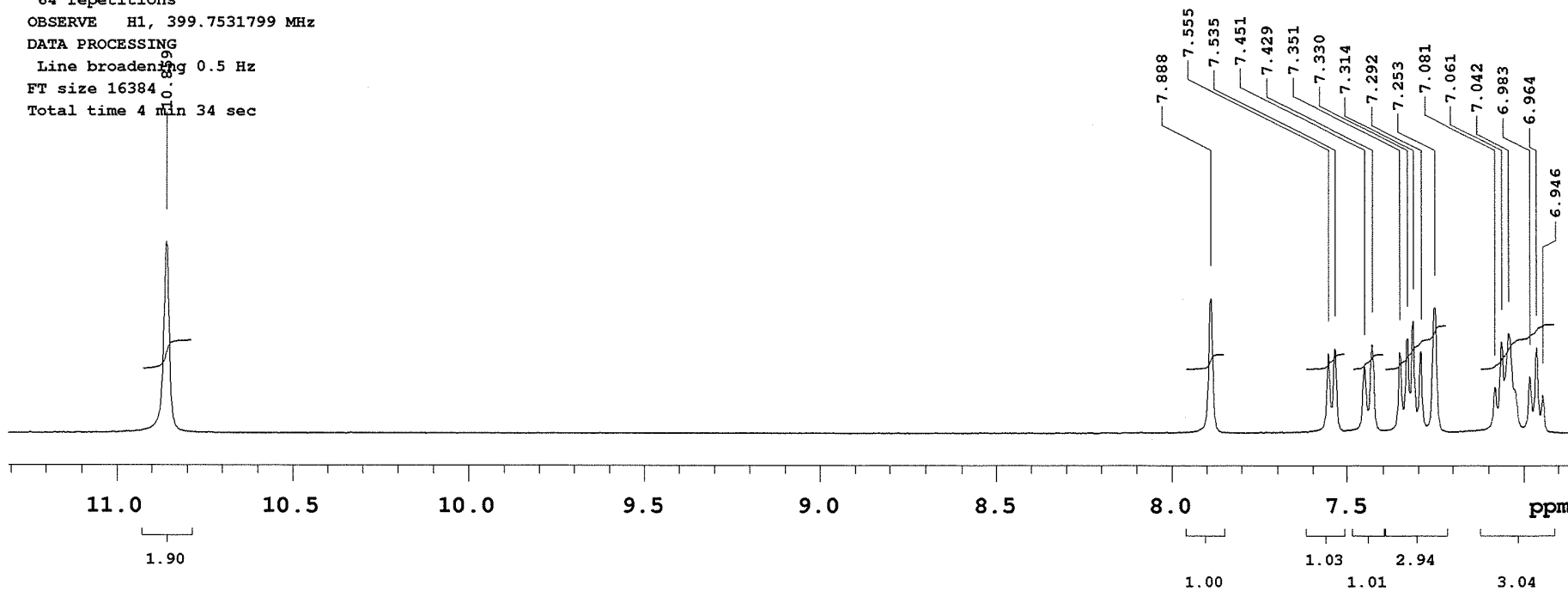
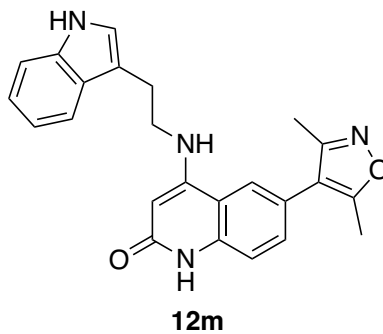
OBSERVE H1, 399.7531799 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



5jc83-1

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc83-1-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Aug 22 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

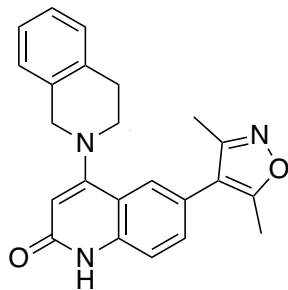
OBSERVE H1, 399.7531792 MHz

DATA PROCESSING

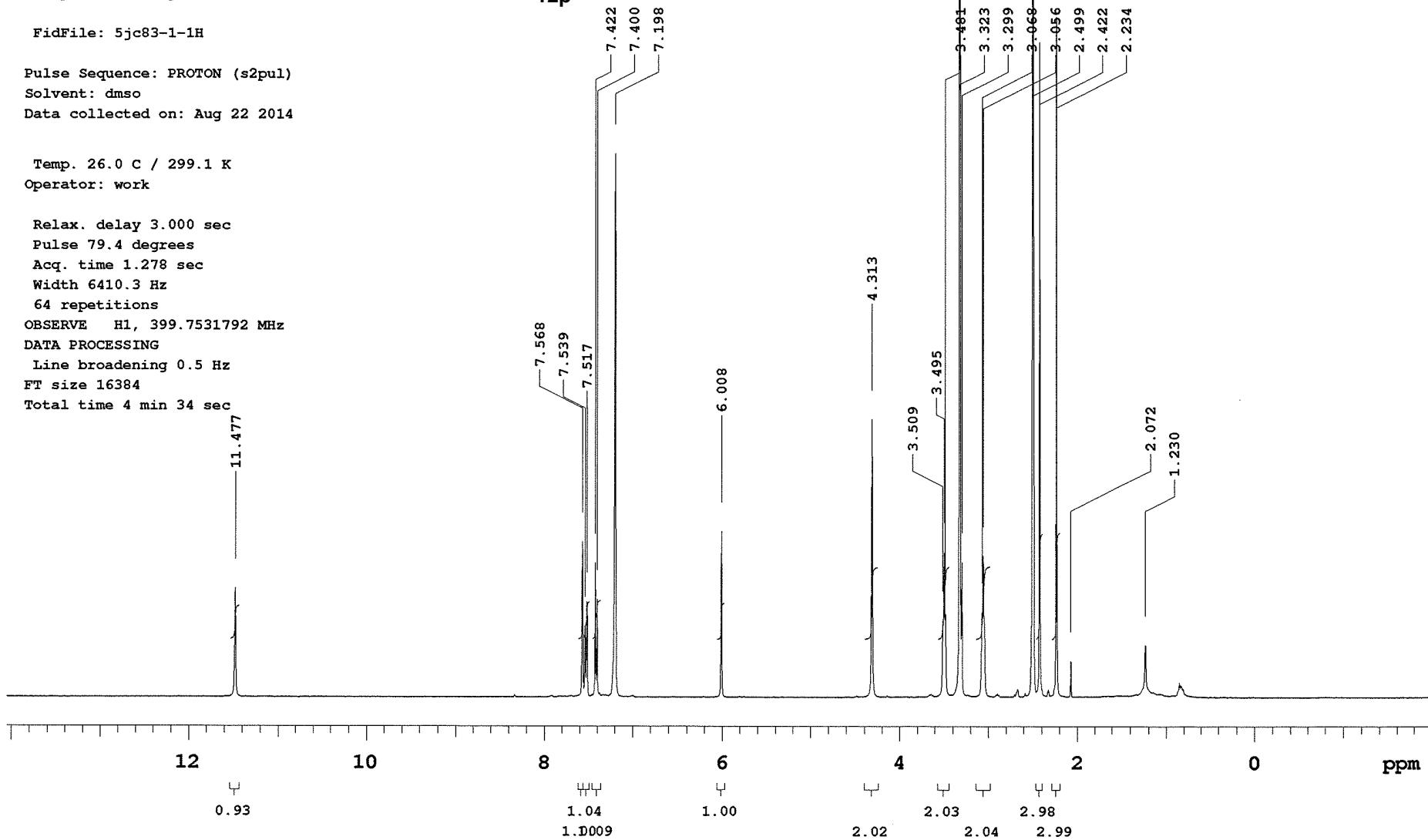
Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



12p



5jc83-1

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc83-1-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Aug 22 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

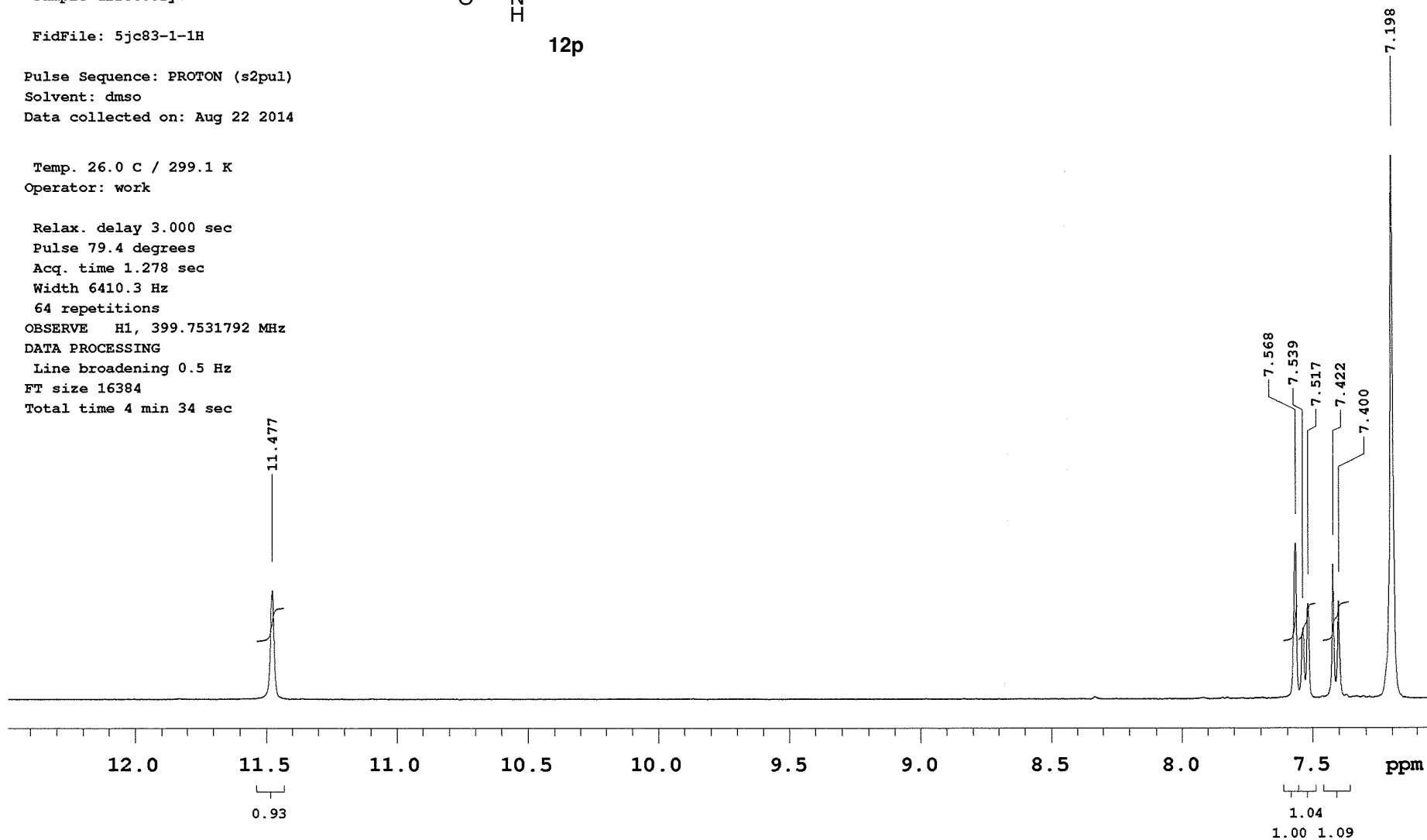
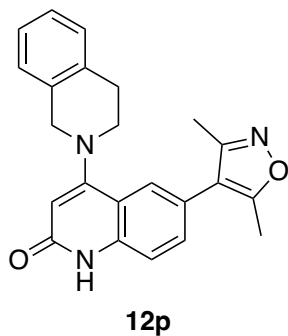
OBSERVE H1, 399.7531792 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



5jc77

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc77-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Jun 26 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

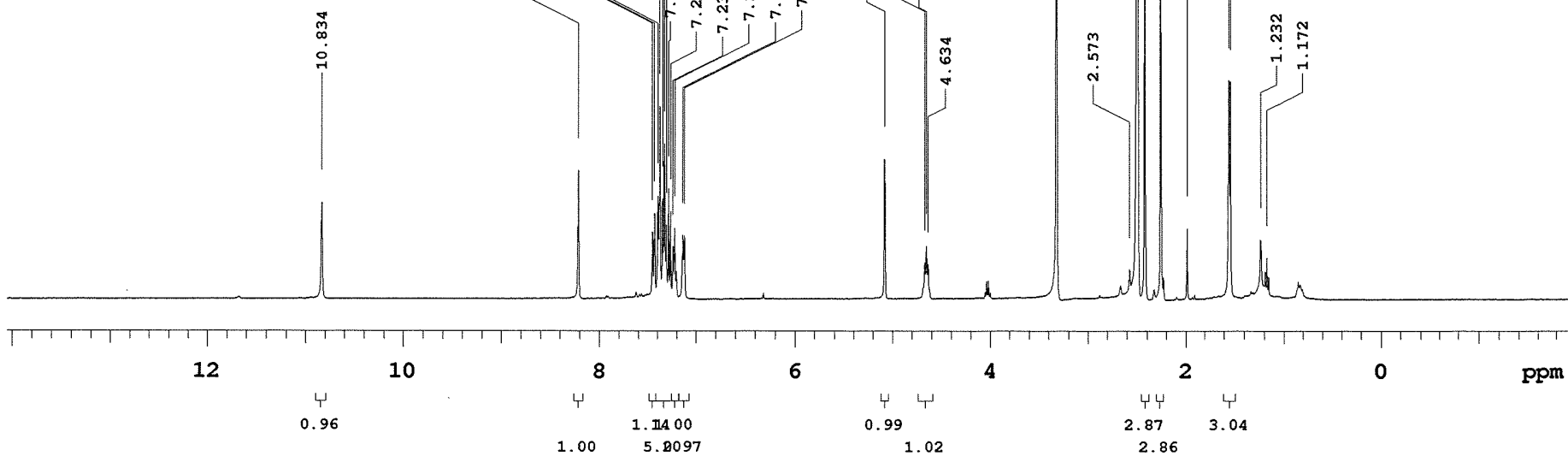
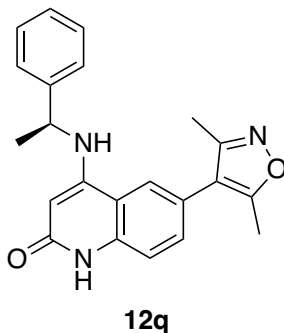
OBSERVE H1, 399.7531799 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



5jc77

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc77-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Jun 26 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

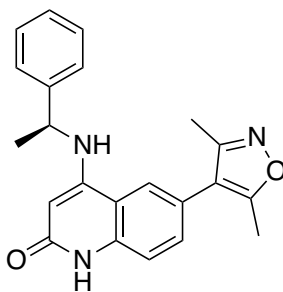
OBSERVE H1, 399.7531799 MHz

DATA PROCESSING

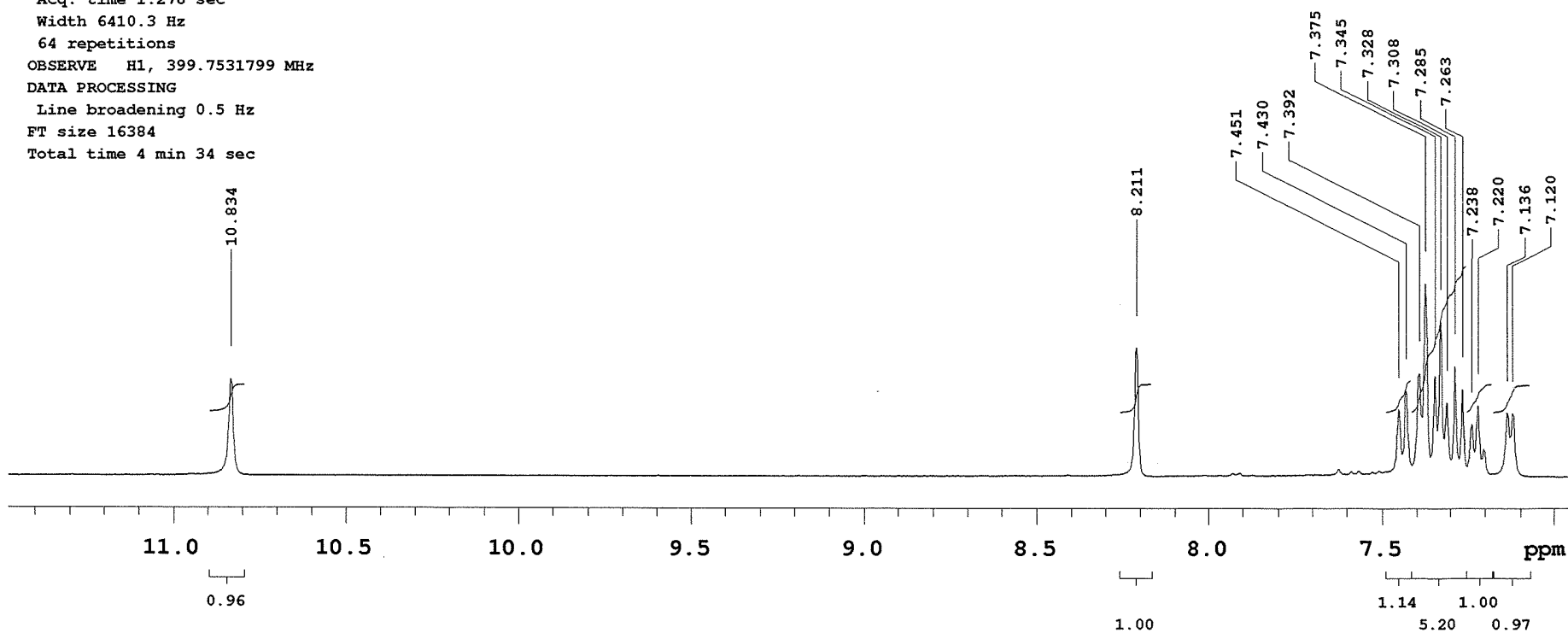
Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



12q



5jc80-1

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc80-1-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dmso

Data collected on: Jul 10 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

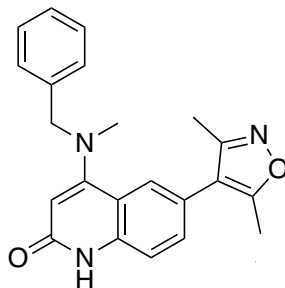
OBSERVE H1, 399.7531796 MHz

DATA PROCESSING

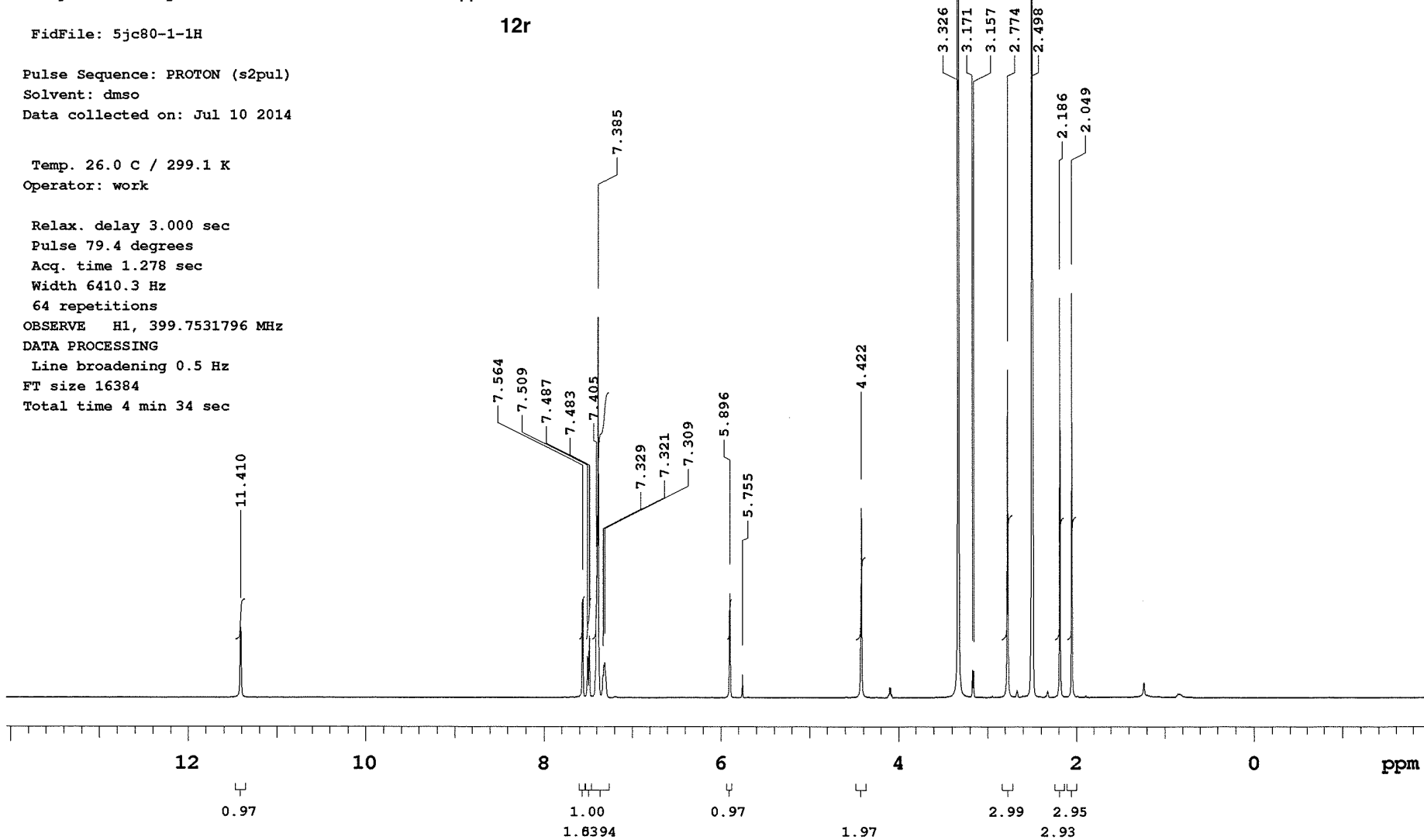
Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



12r



5jc80-1

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc80-1-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Jul 10 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

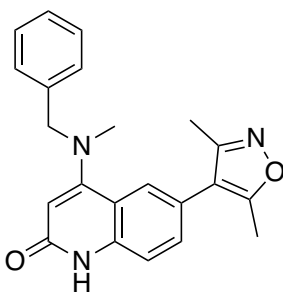
OBSERVE H1, 399.7531796 MHz

DATA PROCESSING

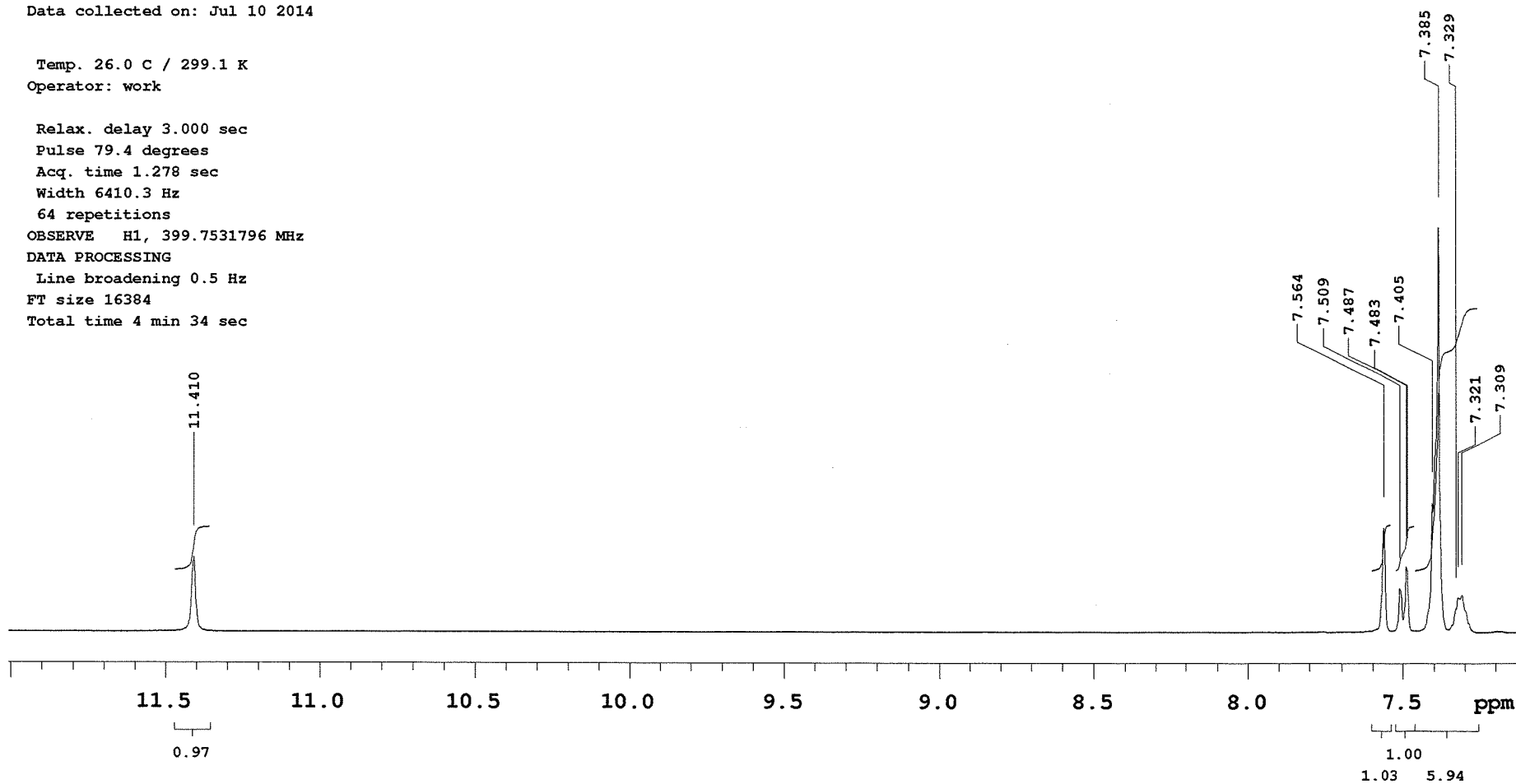
Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



12r



5jc84-1

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc84-1-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Aug 29 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

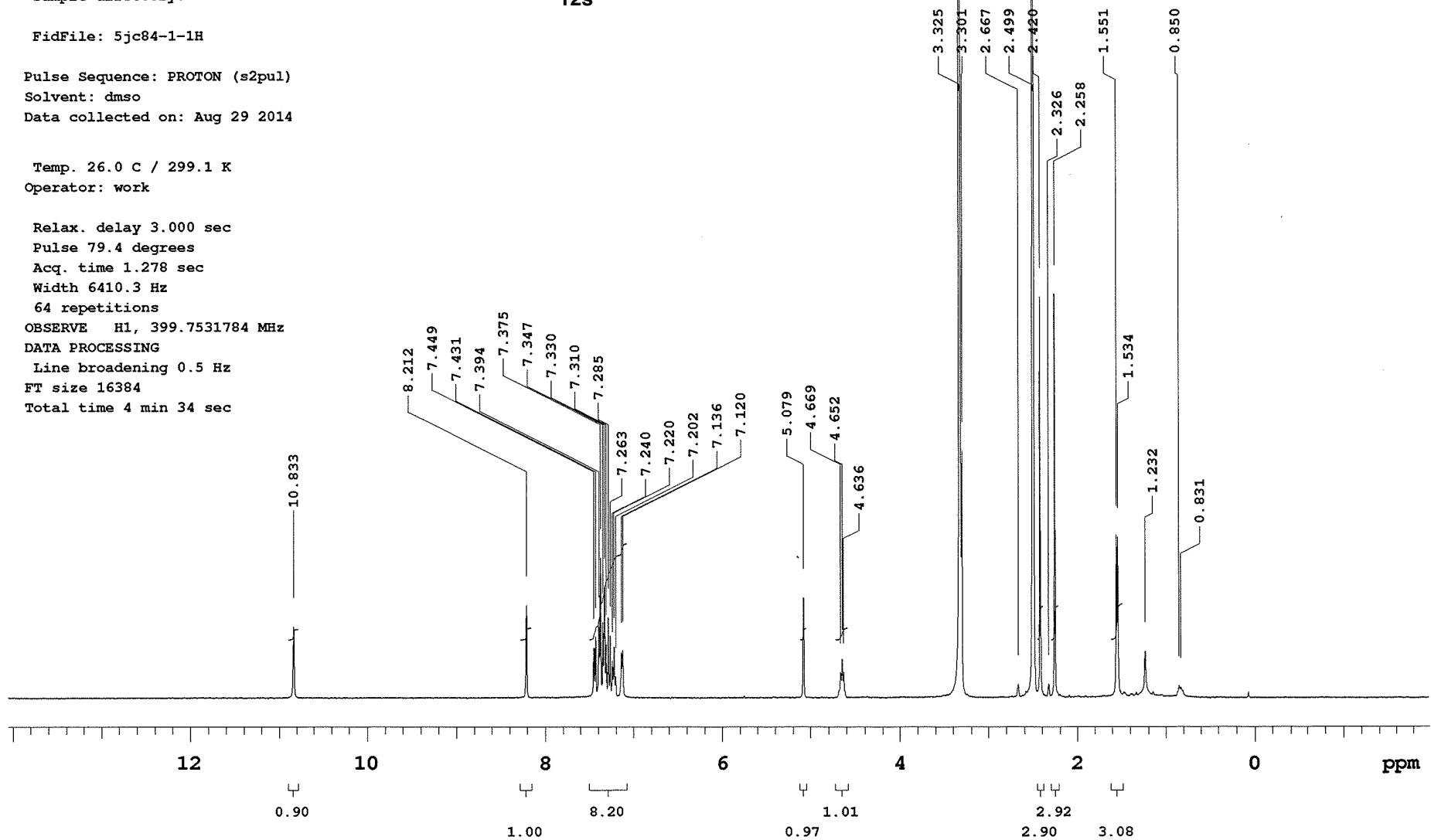
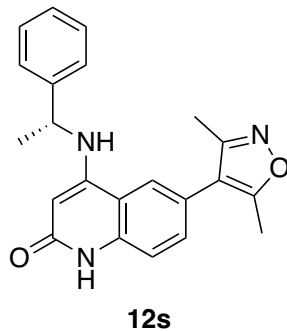
OBSERVE H1, 399.7531784 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



MR89

Sample Name:

MR89

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: MR89

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Apr 23 2015

Temp. 25.0 C / 298.1 K

Operator: work

Relax. delay 2.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

8 repetitions

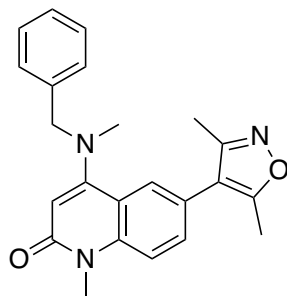
OBSERVE H1, 399.7531790 MHz

DATA PROCESSING

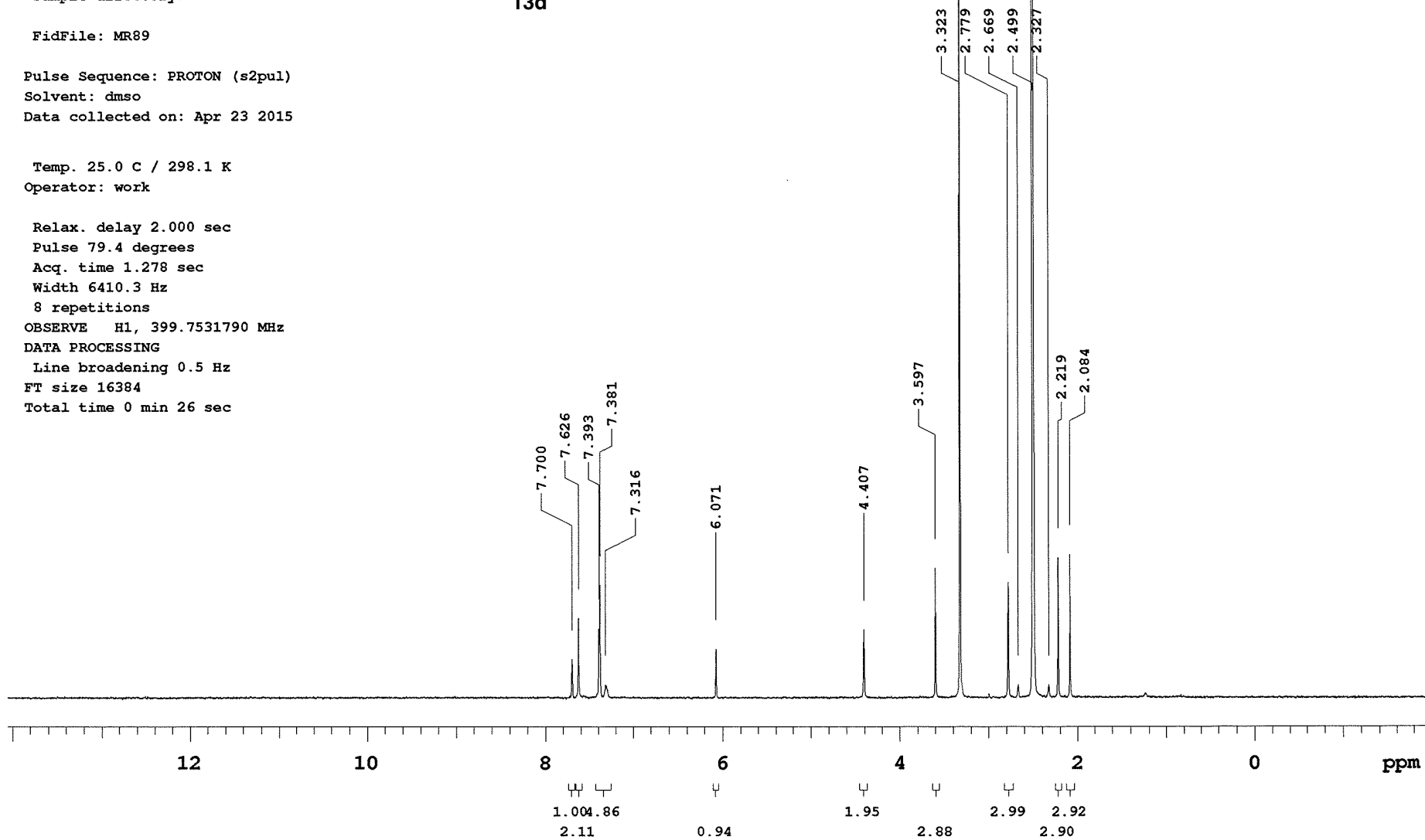
Line broadening 0.5 Hz

FT size 16384

Total time 0 min 26 sec



13d



MR\_27

Sample Name:

MR\_27

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: MR\_27

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Dec 4 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

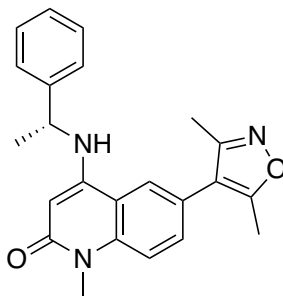
OBSERVE H1, 399.7531793 MHz

DATA PROCESSING

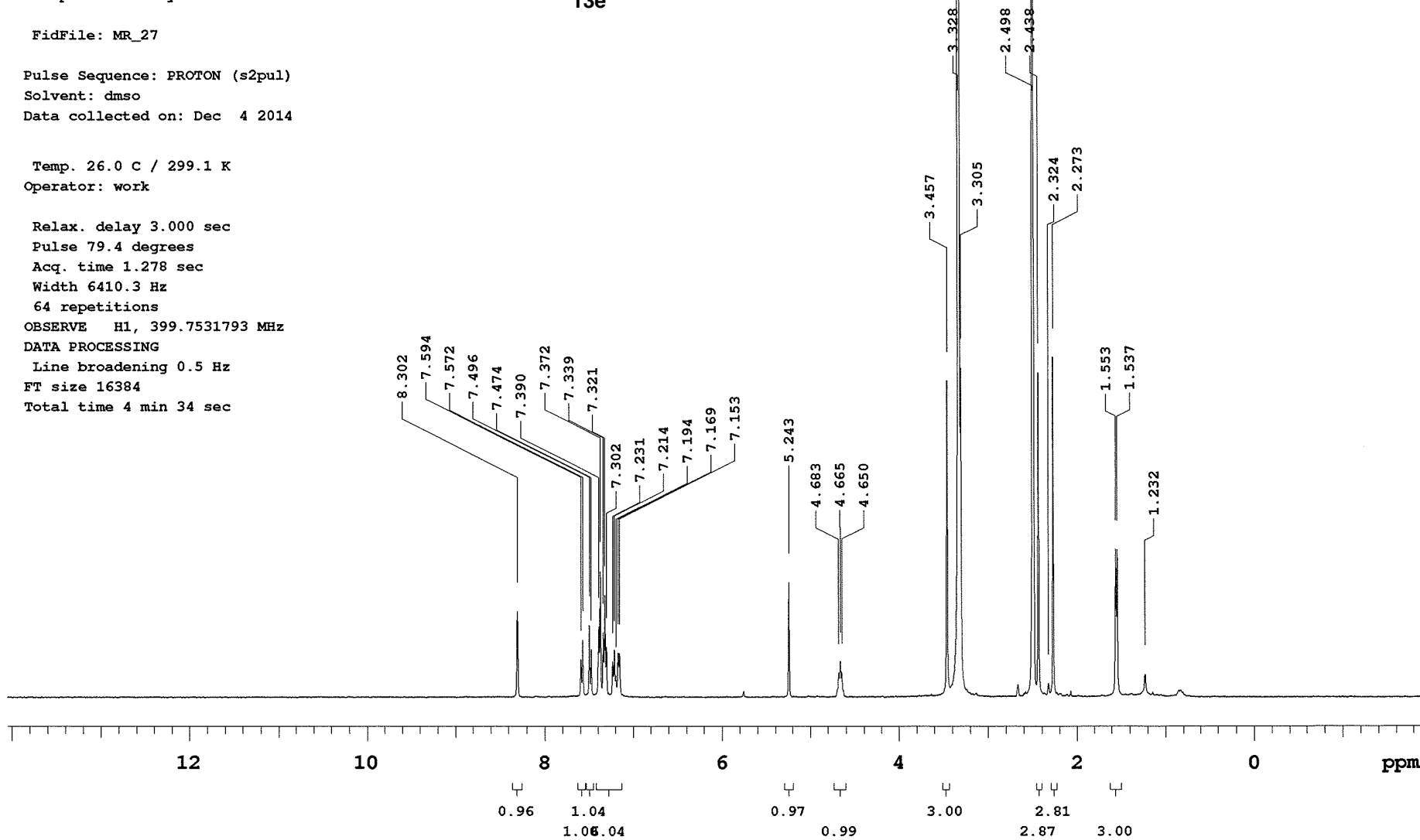
Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



13e



MR\_27

Sample Name:

MR\_27

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: MR\_27

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Dec 4 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

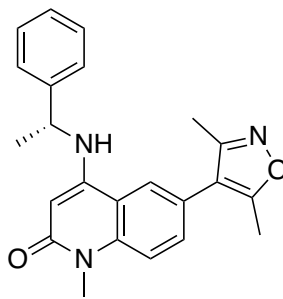
OBSERVE H1, 399.7531793 MHz

DATA PROCESSING

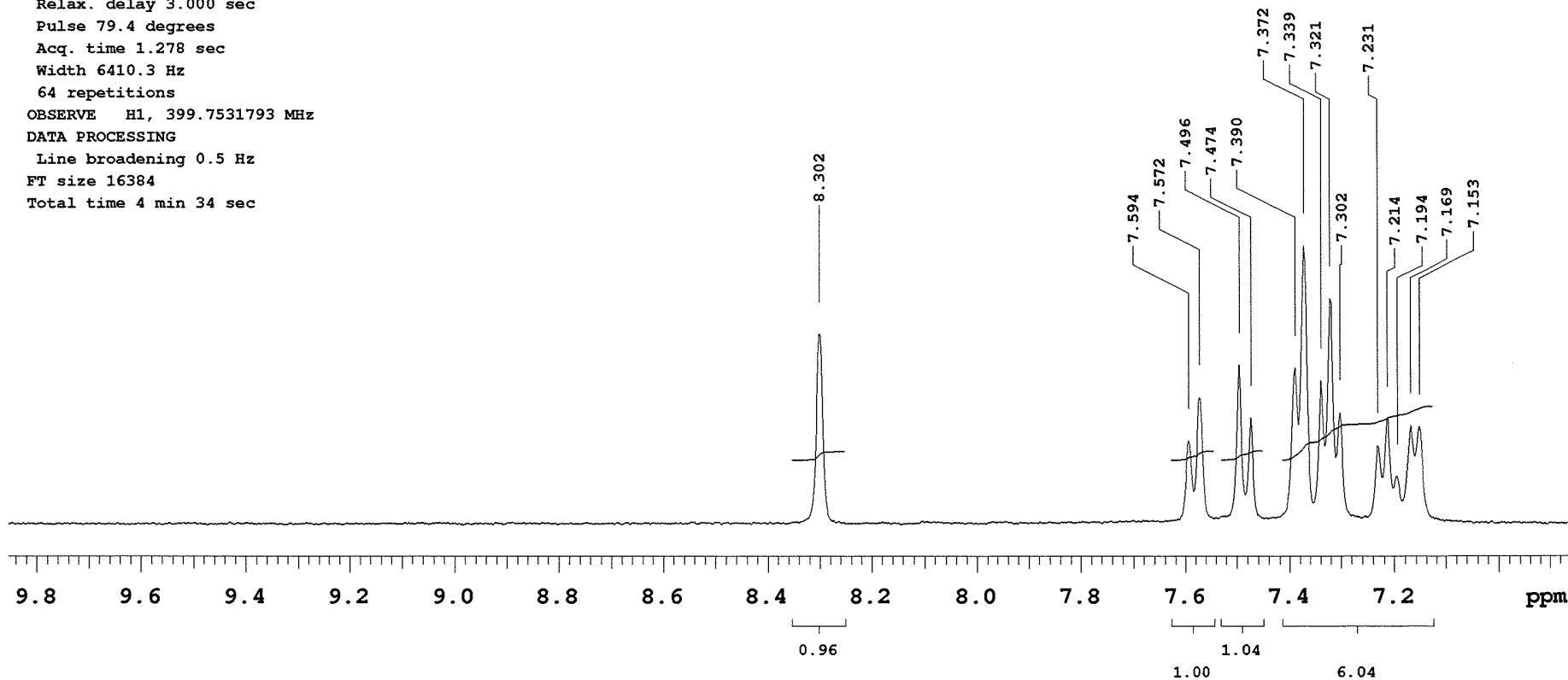
Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



13e



5jc55

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc55-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Apr 2 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

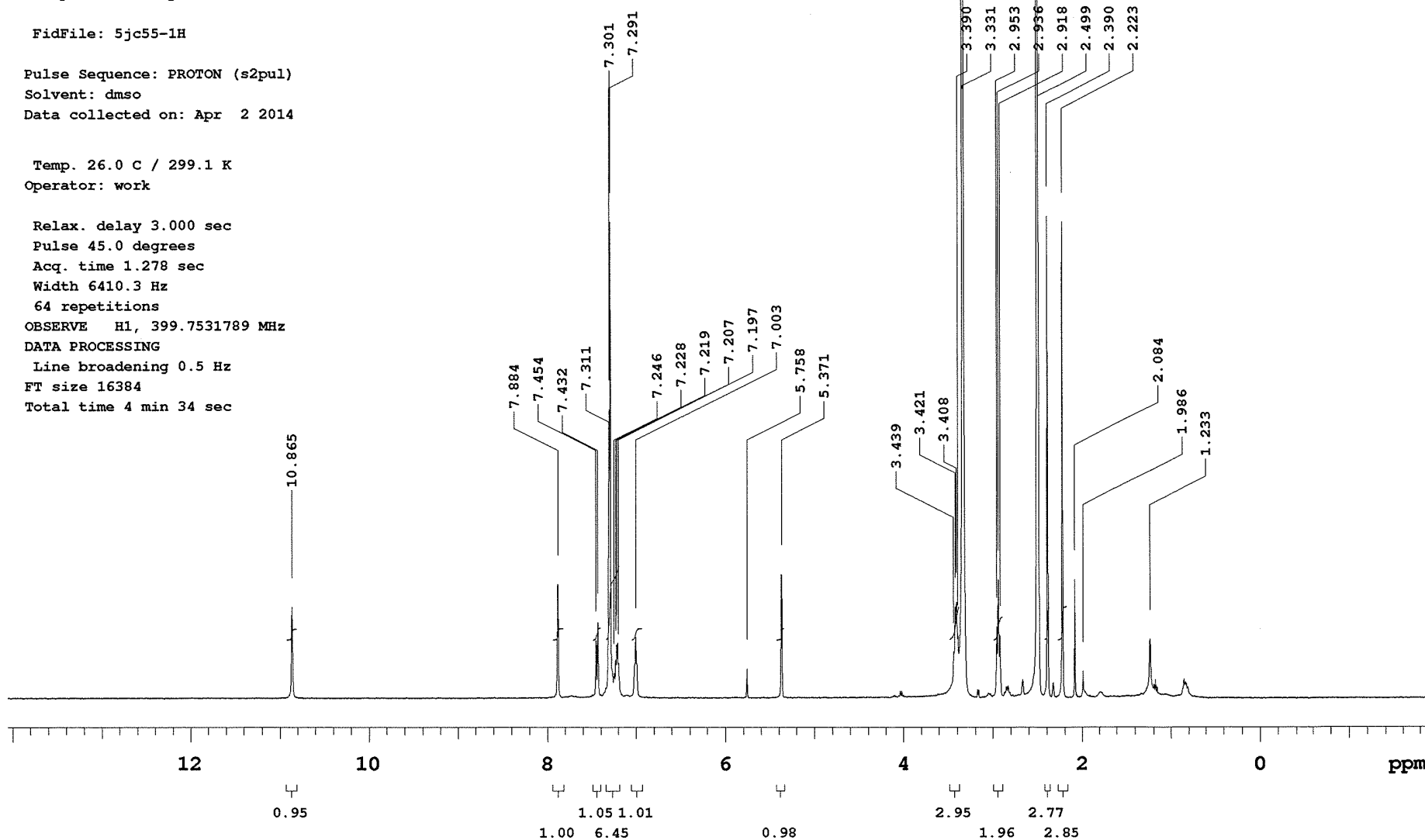
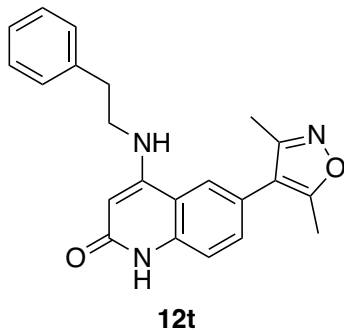
OBSERVE H1, 399.7531789 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



5jc57-1

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc57-1-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Apr 9 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

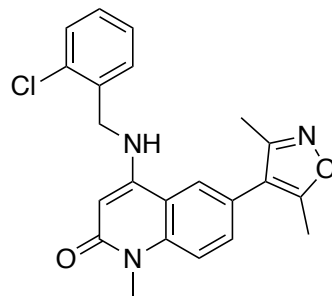
OBSERVE H1, 399.7531778 MHz

DATA PROCESSING

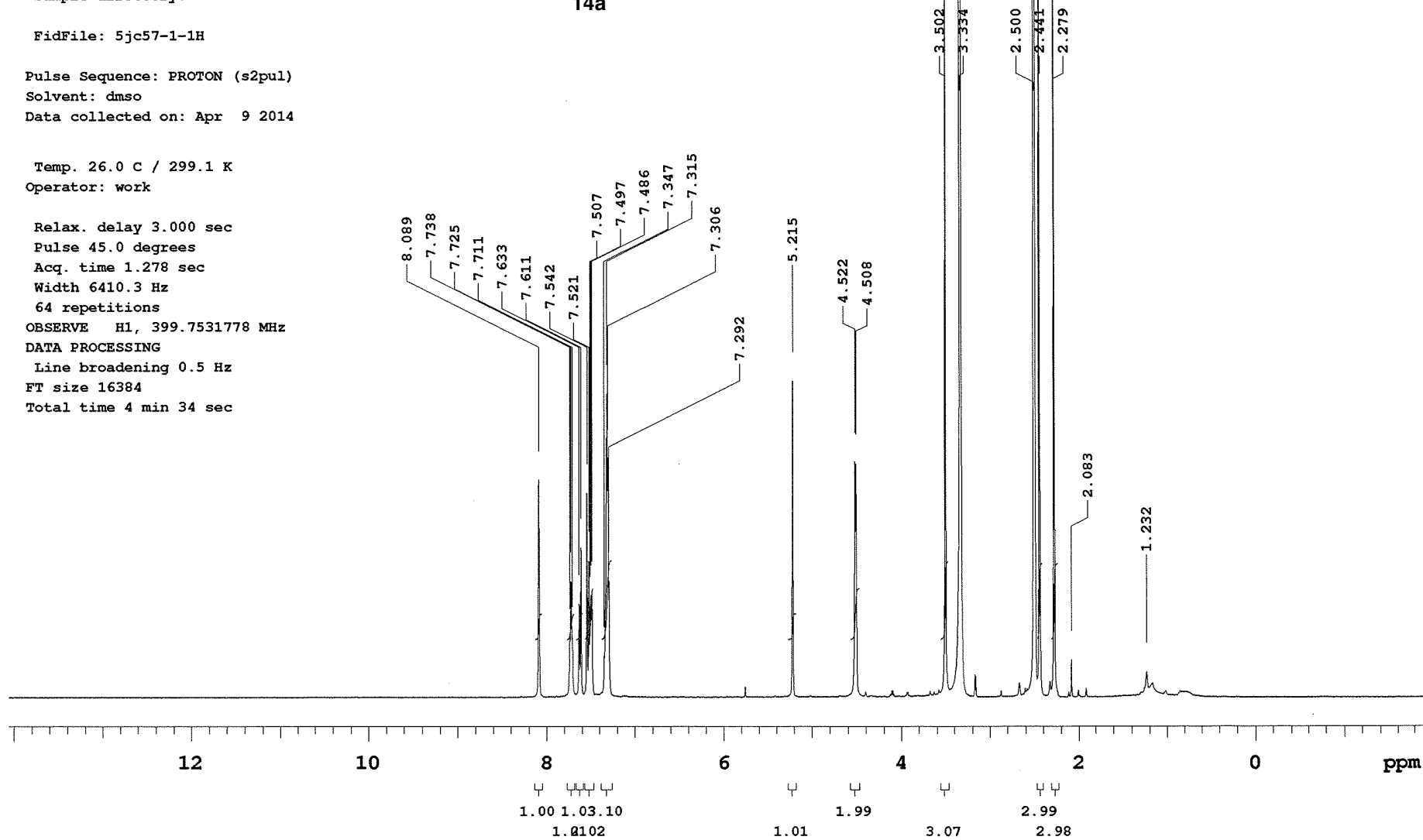
Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



14a



5jc57-1

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc57-1-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Apr 9 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

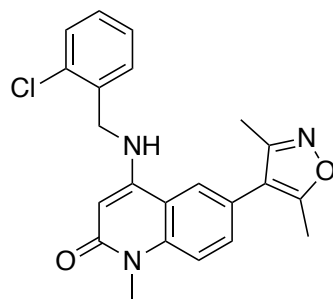
OBSERVE H1, 399.7531778 MHz

DATA PROCESSING

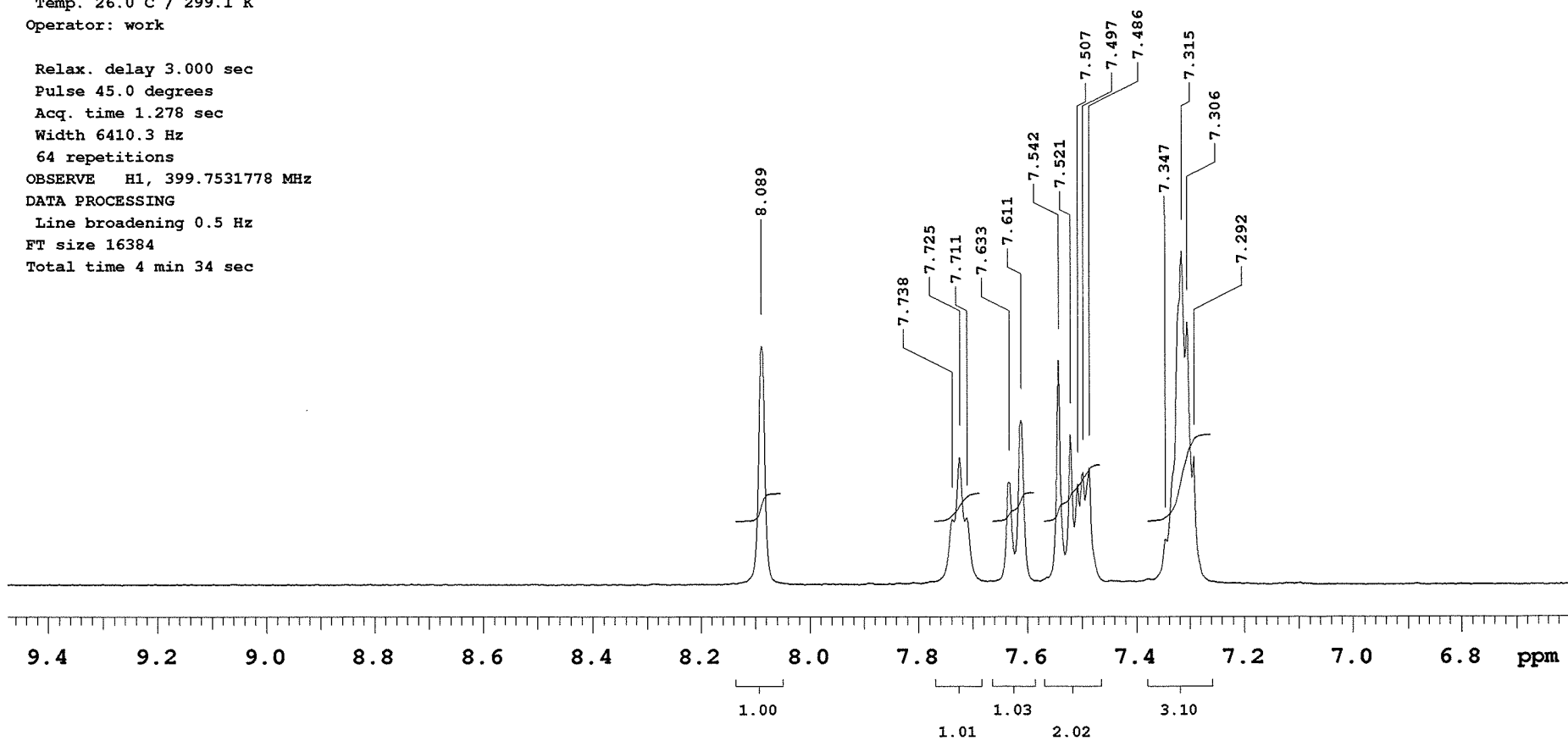
Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



14a



5jc57-2

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc57-2-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Apr 22 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

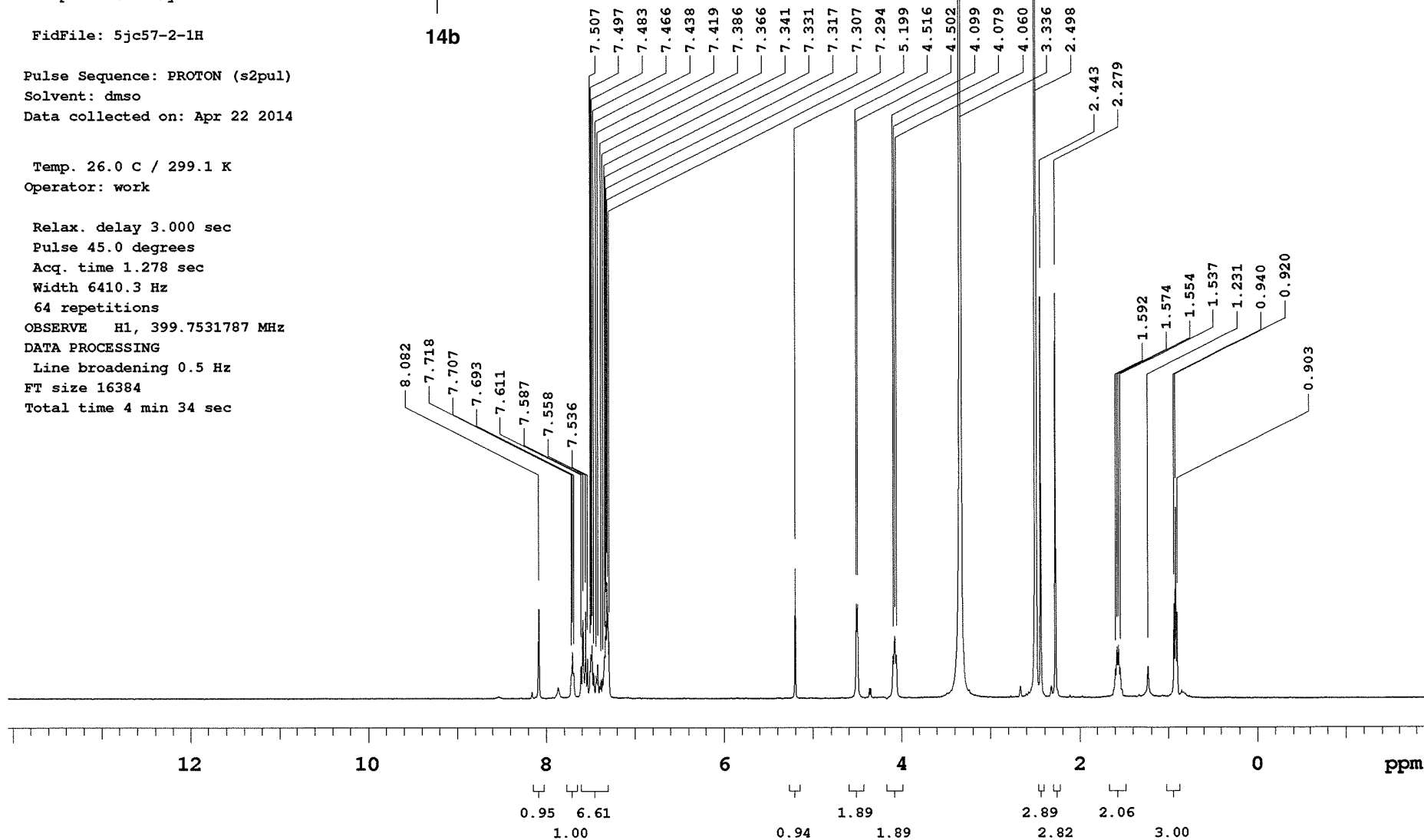
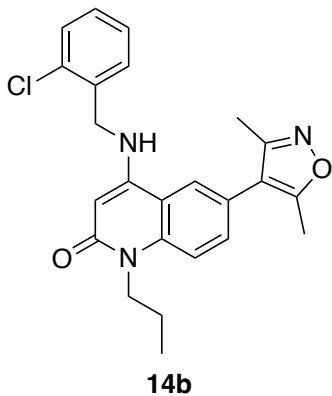
OBSERVE H1, 399.7531787 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



5jc57-2

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc57-2-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Apr 22 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

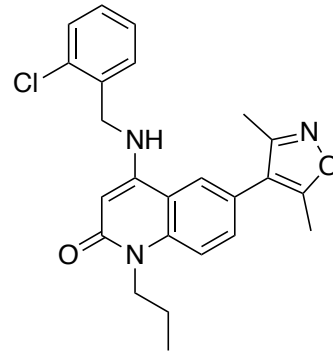
OBSERVE H1, 399.7531787 MHz

DATA PROCESSING

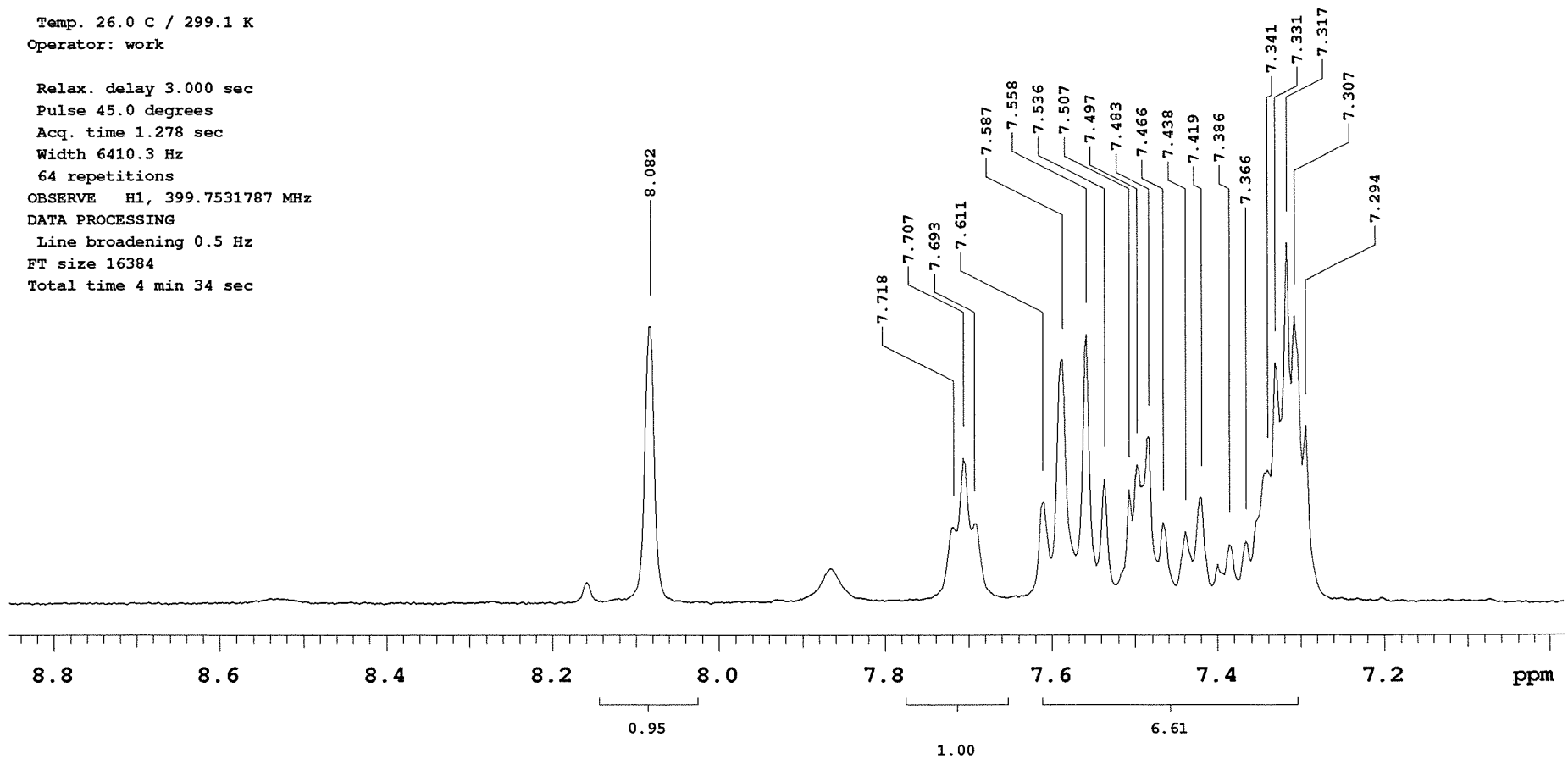
Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



14b



5jc59-1

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc59-1-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Apr 22 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

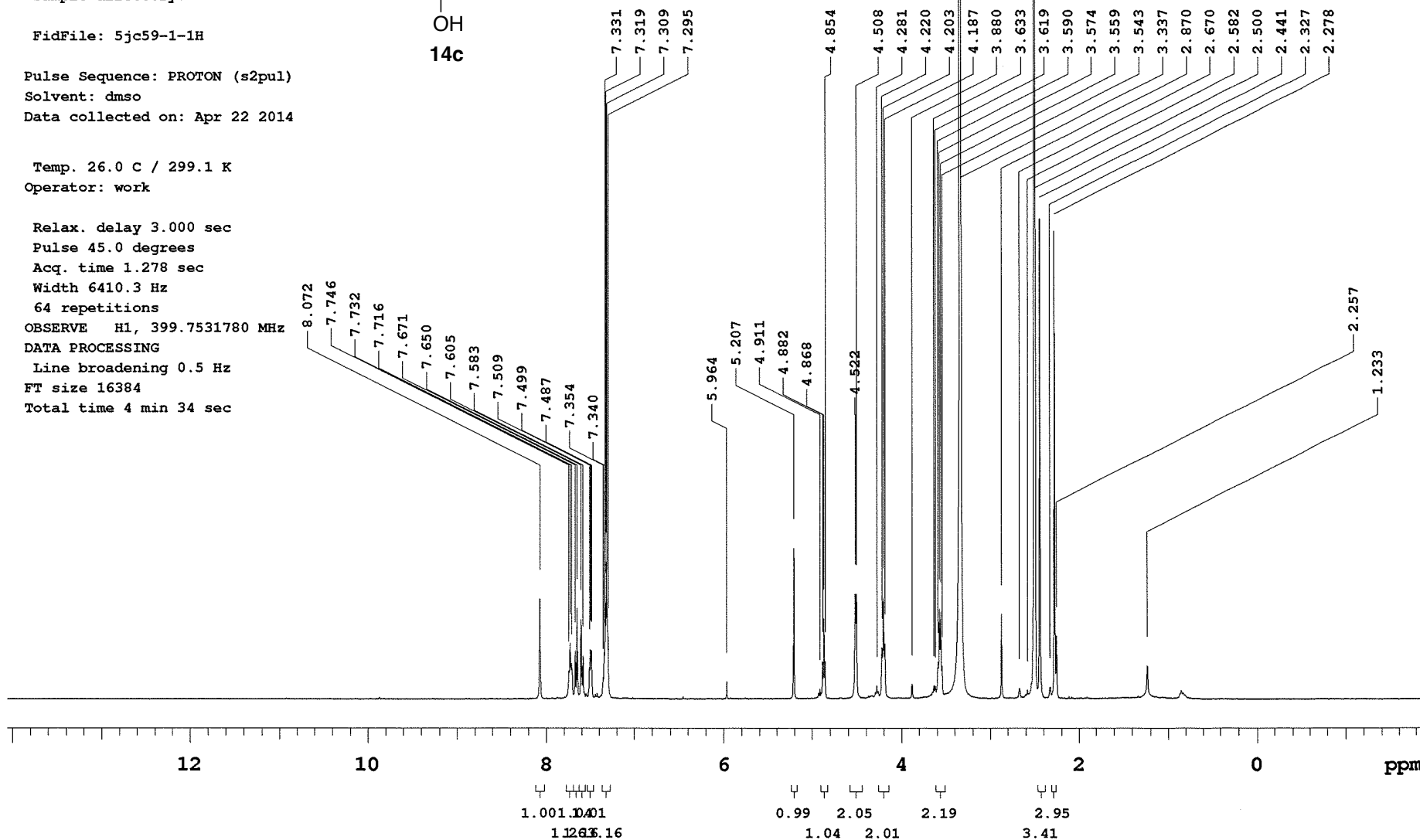
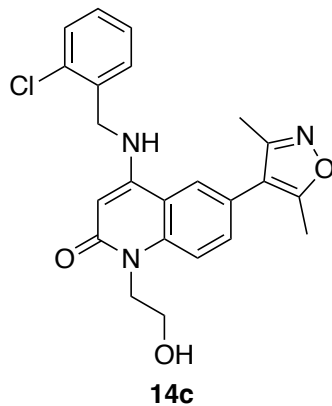
OBSERVE H1, 399.7531780 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



5jc59-1

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

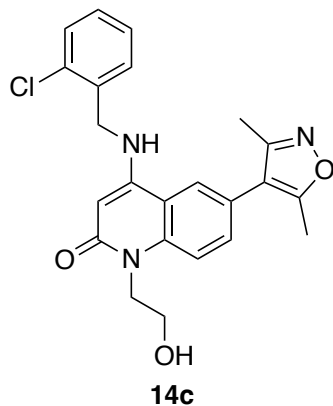
Sample directory:

FidFile: 5jc59-1-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Apr 22 2014



Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

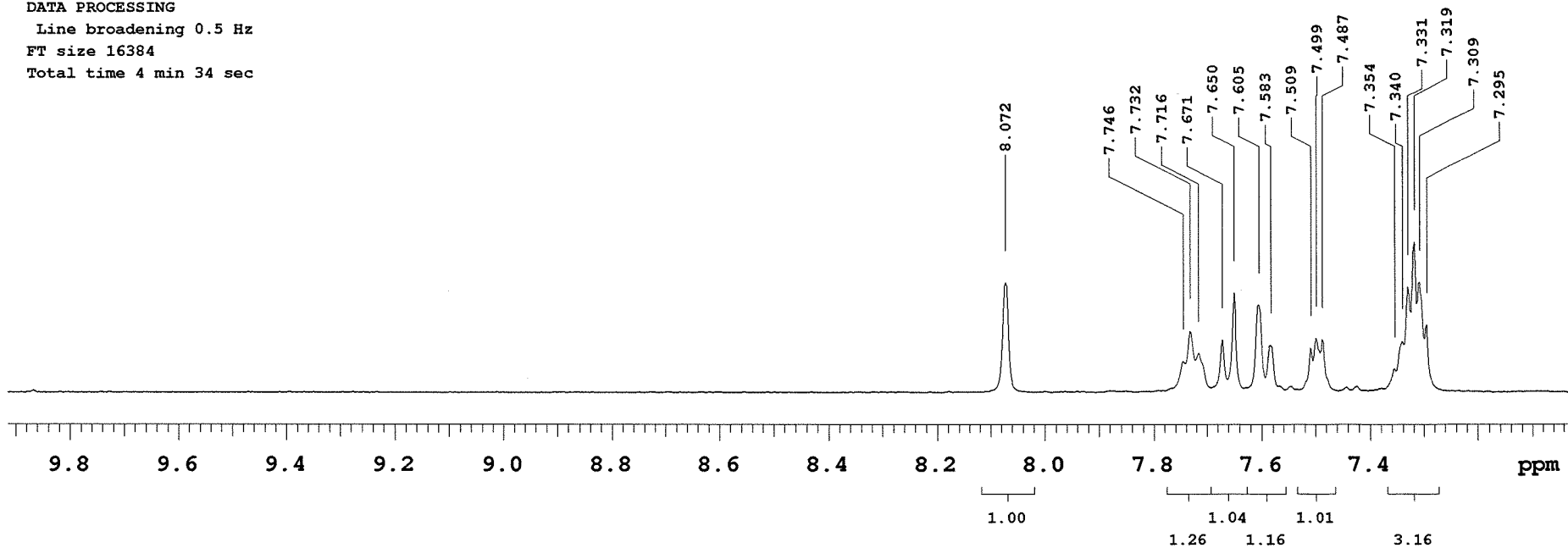
OBSERVE H1, 399.7531780 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



5jc70

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 5jc70-1H-pure

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Jun 11 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

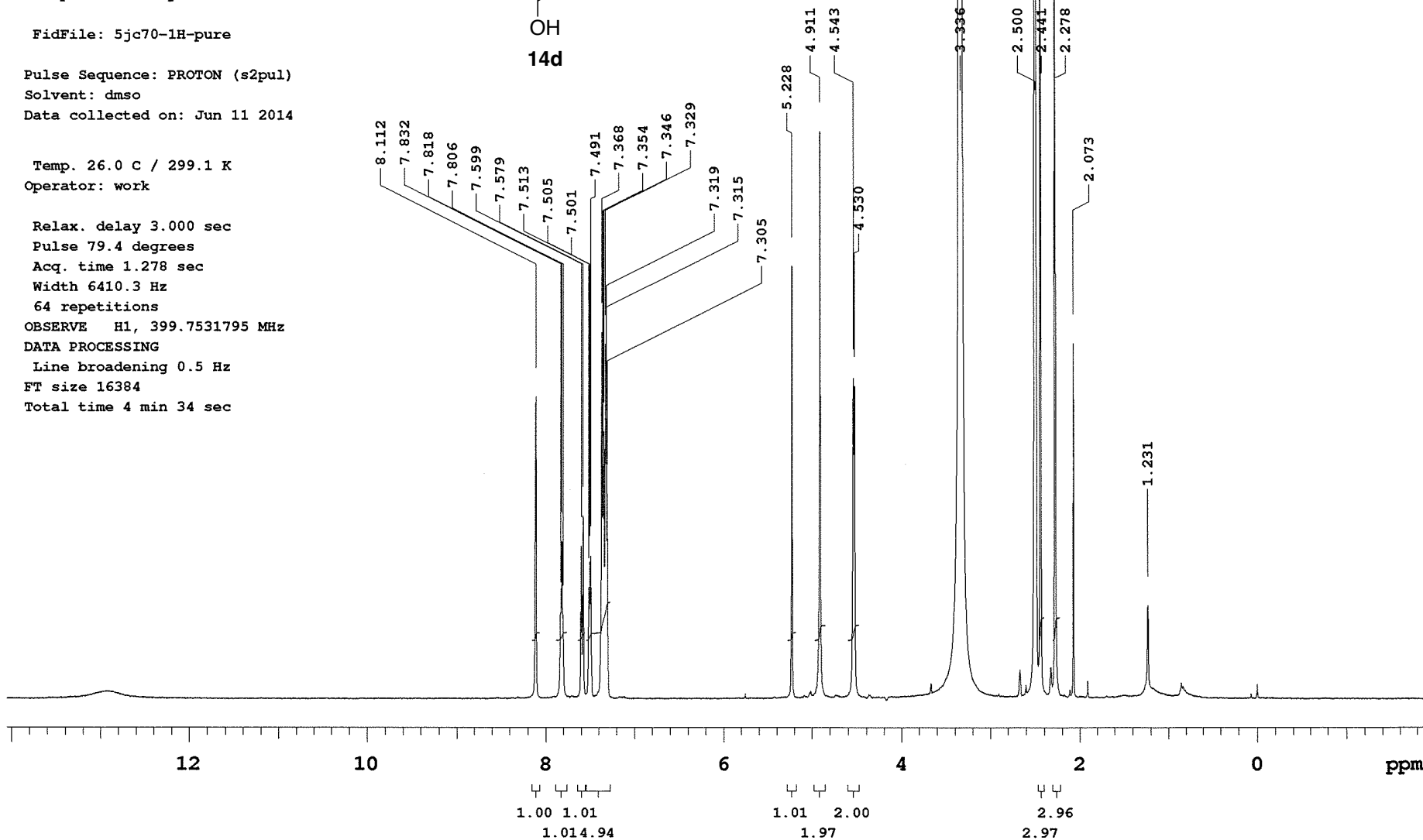
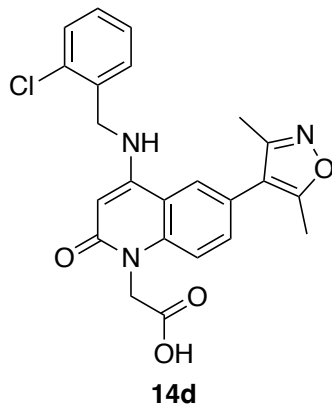
OBSERVE H1, 399.7531795 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec



7jc06

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 7jc06-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Sep 4 2015

Temp. 22.0 C / 295.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

32 repetitions

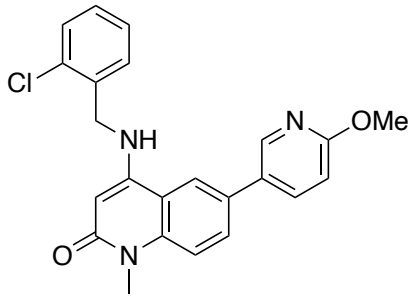
OBSERVE H1, 399.7531798 MHz

DATA PROCESSING

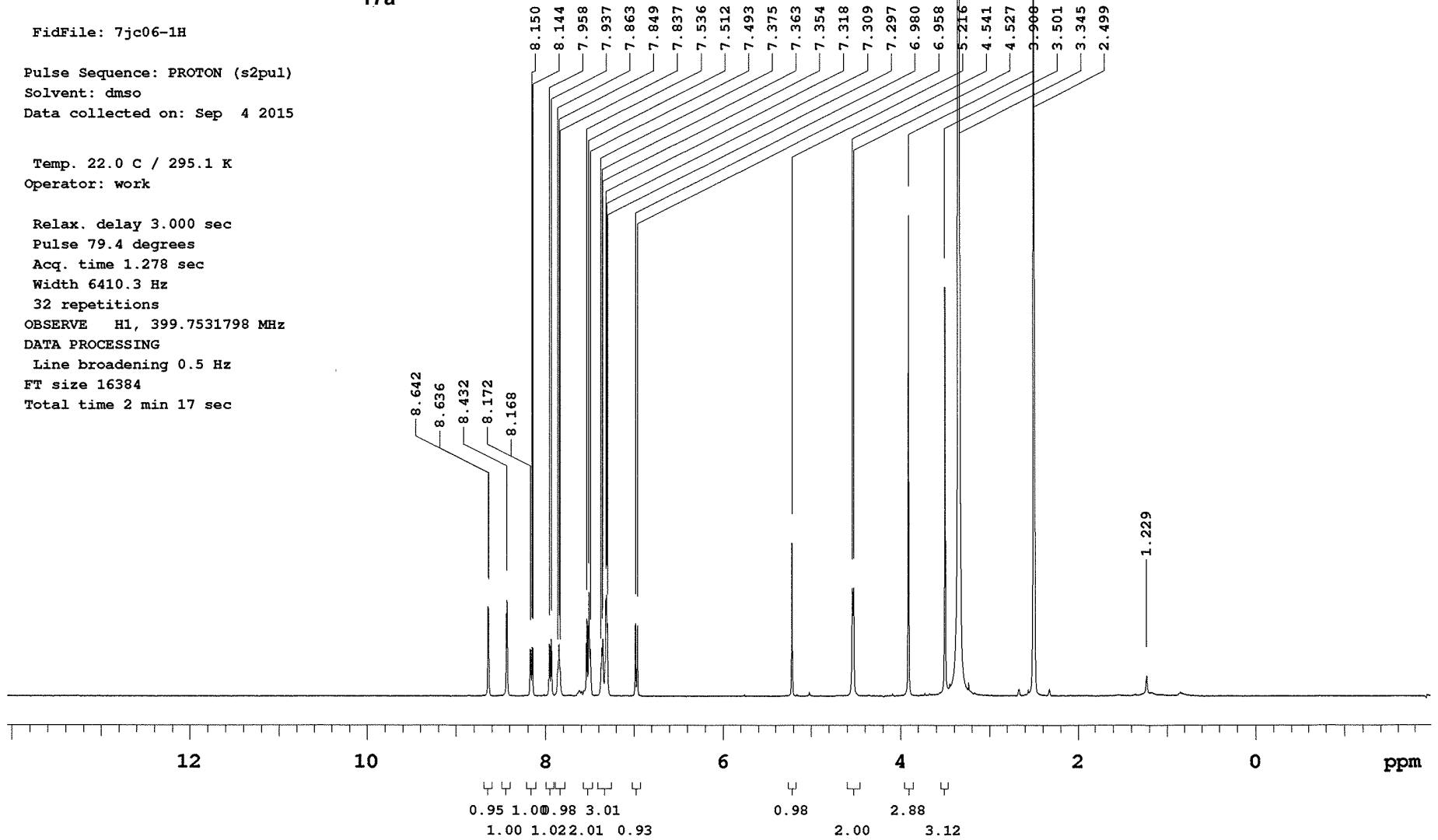
Line broadening 0.5 Hz

FT size 16384

Total time 2 min 17 sec



17a



7jc06

Sample Name:

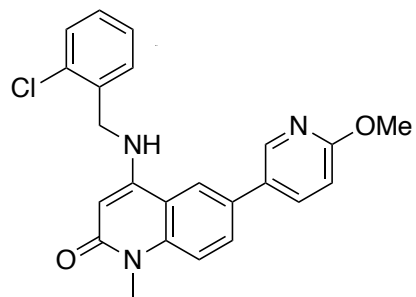
Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 7jc06-1H



17a

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Sep 4 2015

Temp. 22.0 C / 295.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

32 repetitions

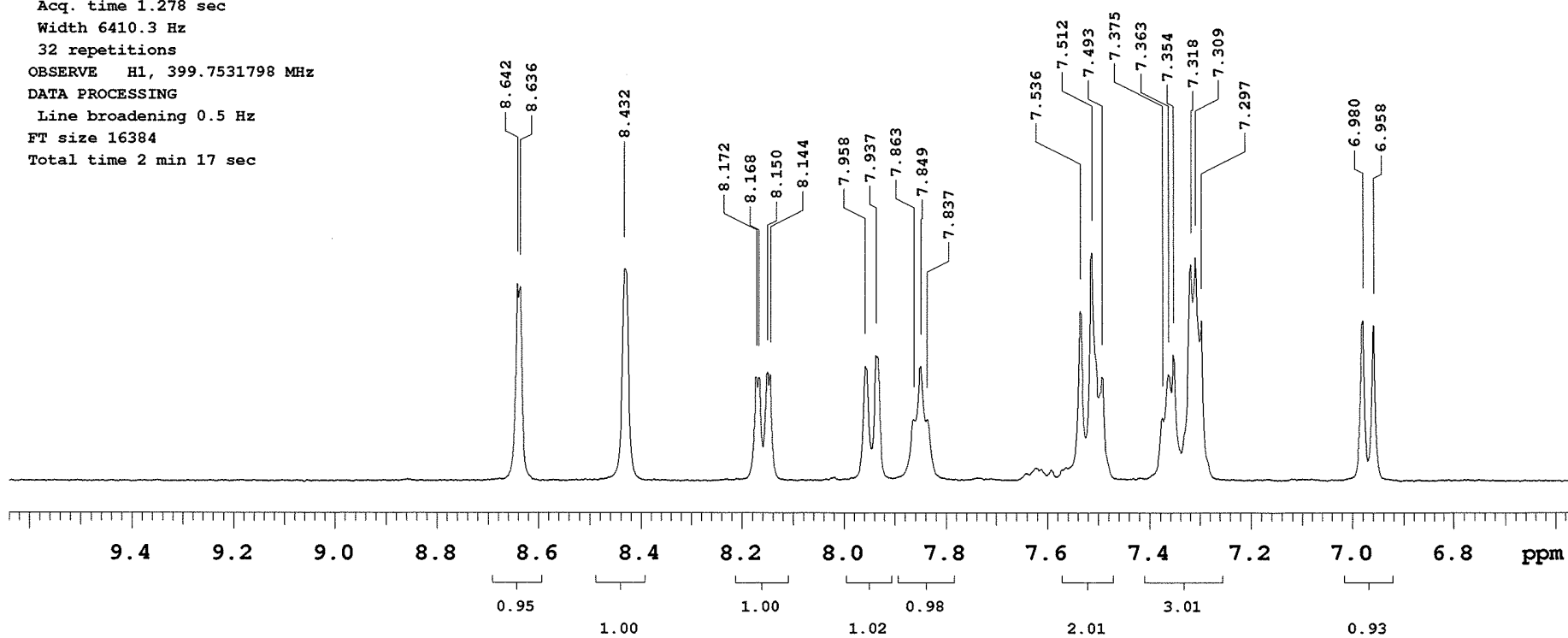
OBSERVE H1, 399.7531798 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 2 min 17 sec



7jc18

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 7jc18-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Oct 8 2015

Temp. 22.0 C / 295.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

32 repetitions

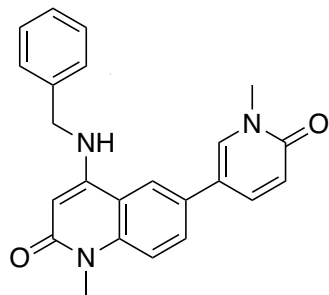
OBSERVE H1, 399.7531793 MHz

DATA PROCESSING

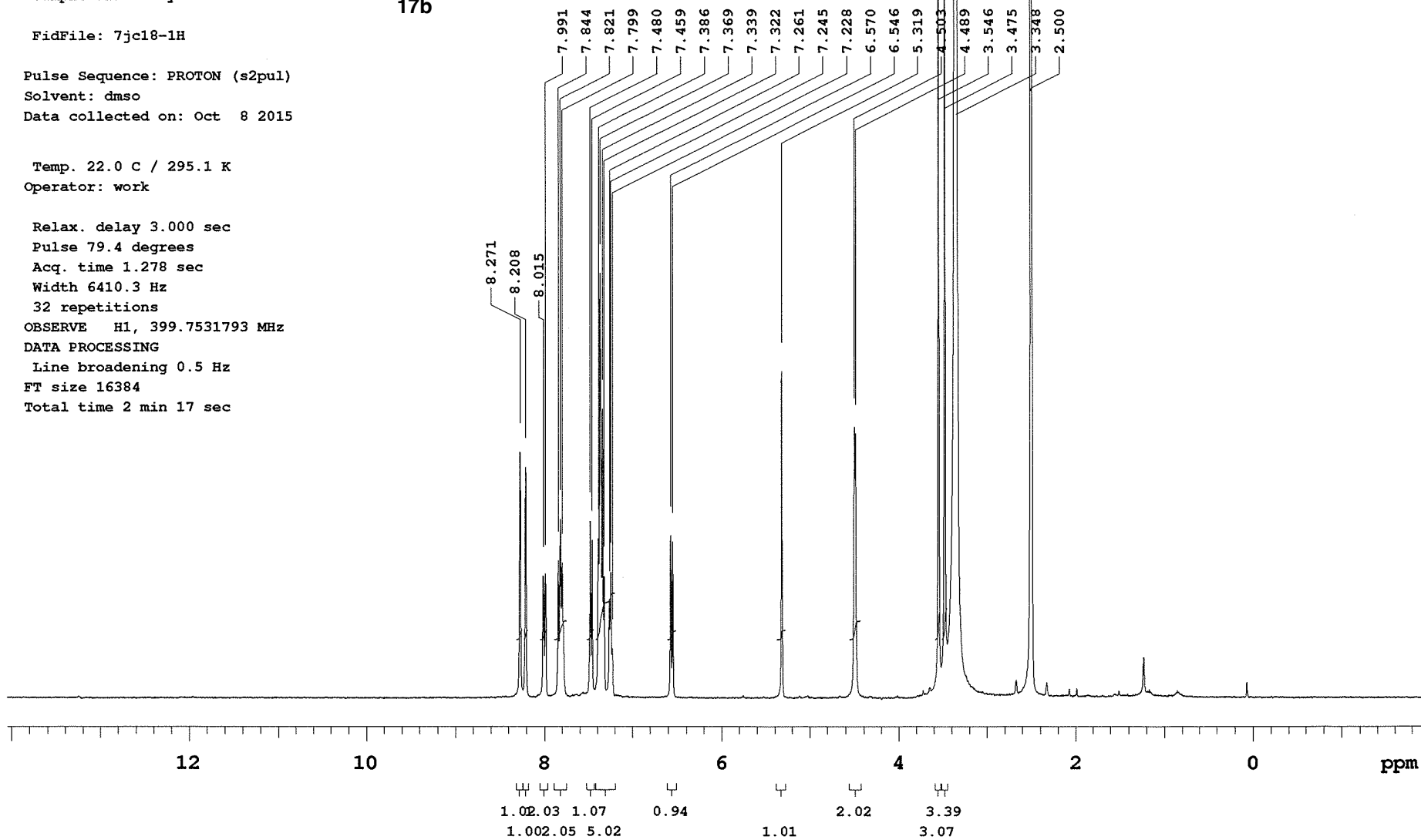
Line broadening 0.5 Hz

FT size 16384

Total time 2 min 17 sec



17b



7jc18

Sample Name:

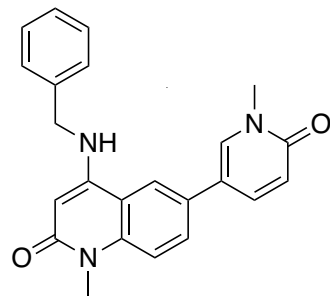
Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 7jc18-1H



17b

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Oct 8 2015

Temp. 22.0 C / 295.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

32 repetitions

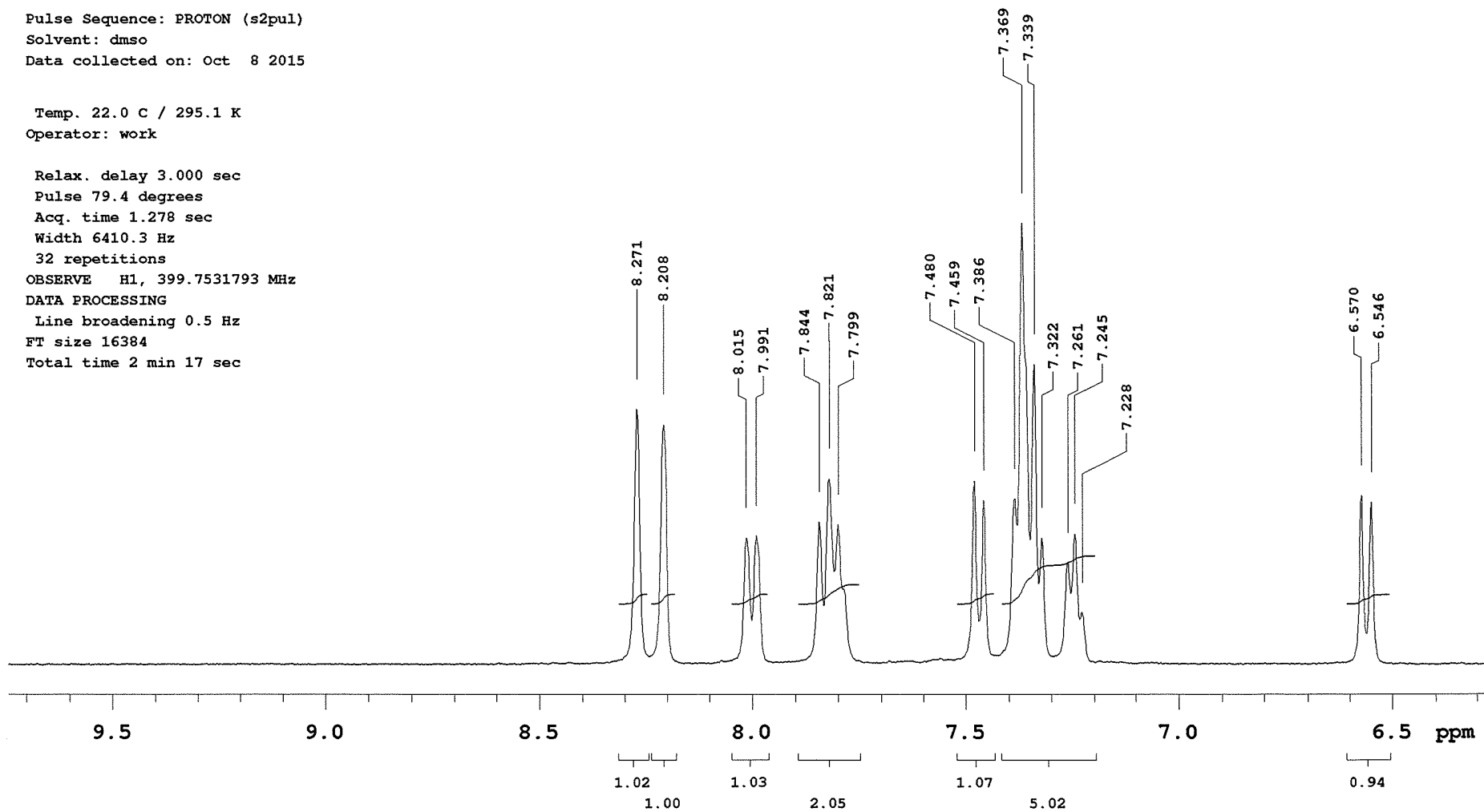
OBSERVE H1, 399.7531793 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 2 min 17 sec



7jc20-1

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 7jc20-1-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Oct 13 2015

Temp. 22.0 C / 295.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

32 repetitions

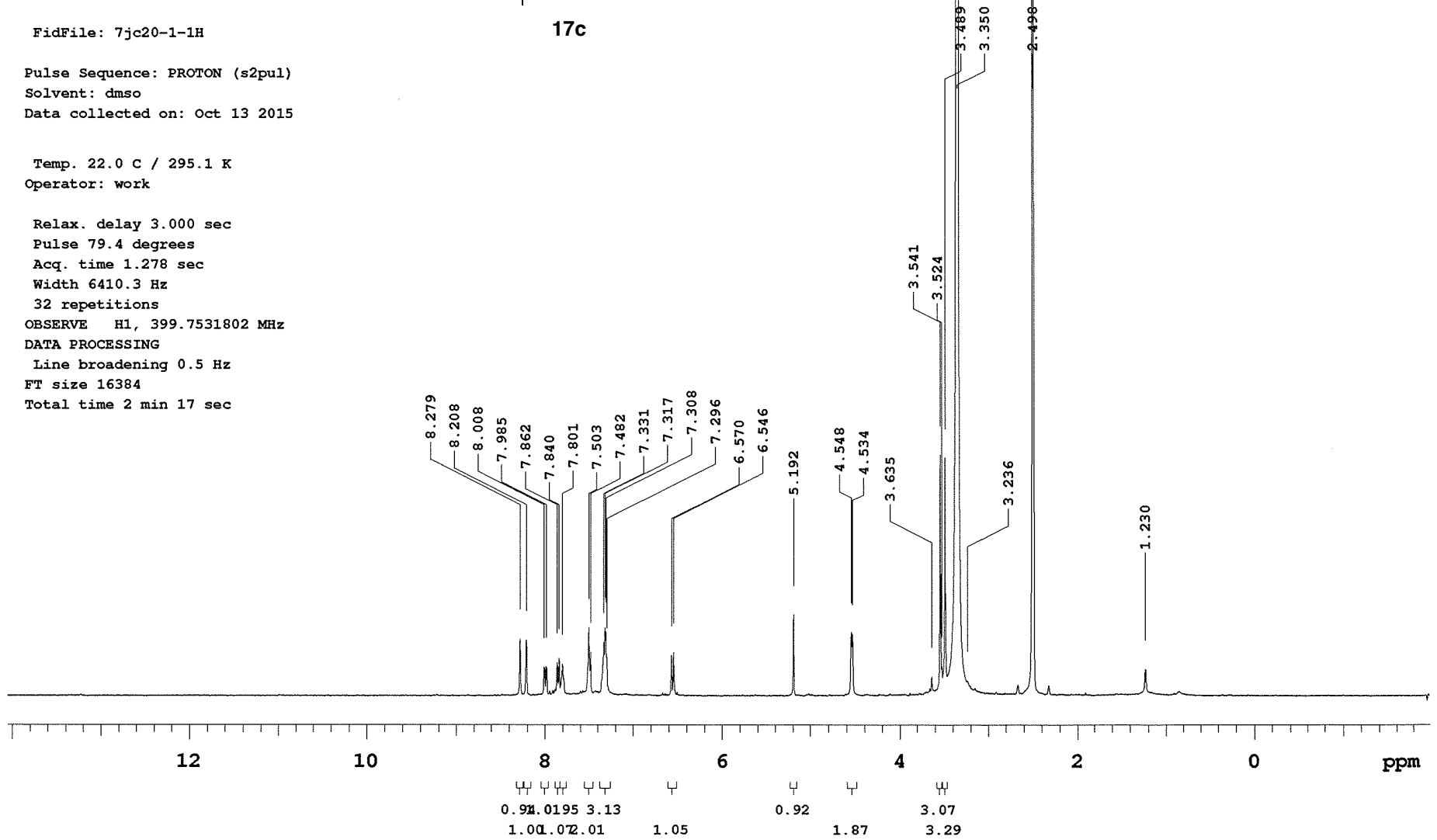
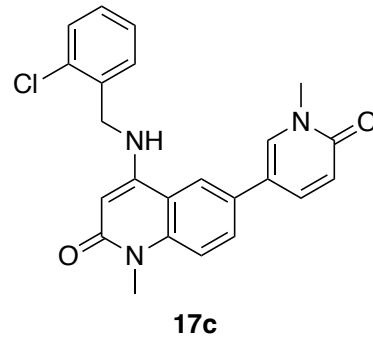
OBSERVE H1, 399.7531802 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 2 min 17 sec



7jc20-1

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 7jc20-1-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Oct 13 2015

Temp. 22.0 C / 295.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

32 repetitions

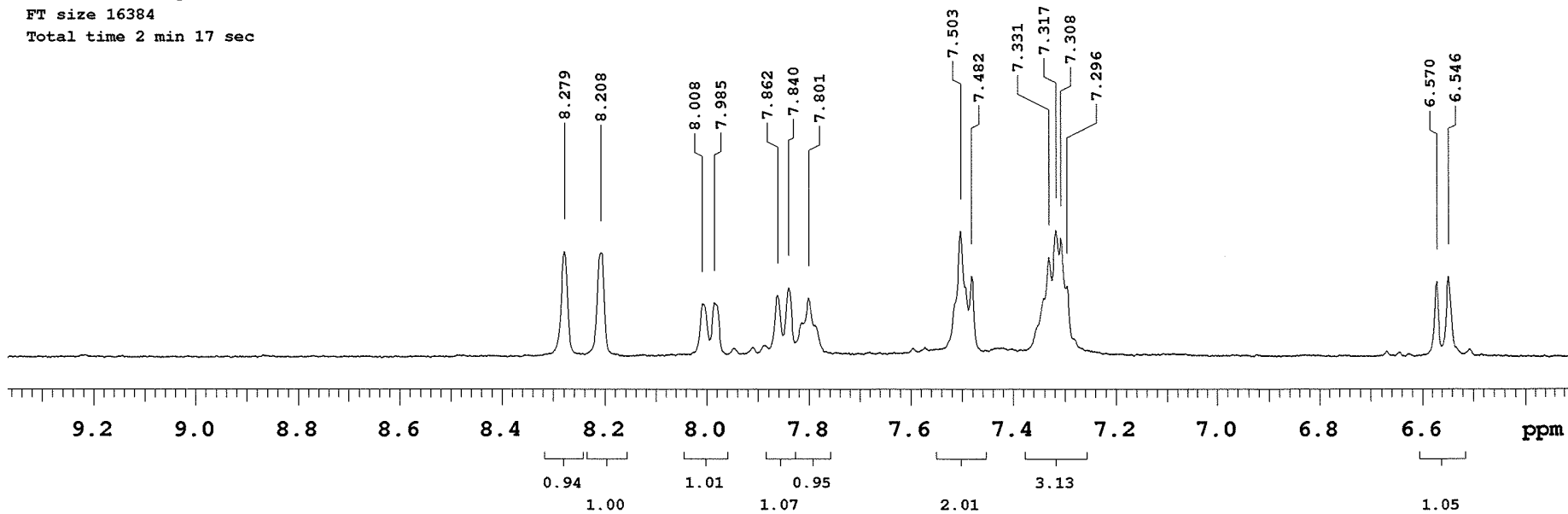
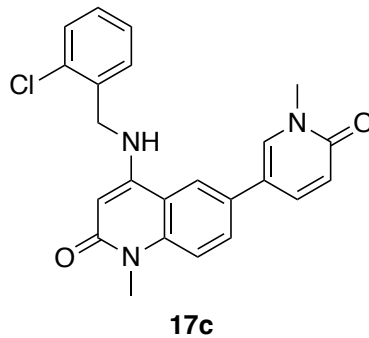
OBSERVE H1, 399.7531802 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 16384

Total time 2 min 17 sec



7jc19-3

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 7jc19-3-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Nov 2 2015

Temp. 22.0 C / 295.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

32 repetitions

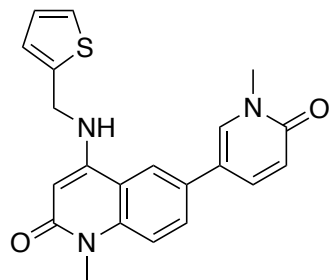
OBSERVE H1, 399.7531794 MHz

DATA PROCESSING

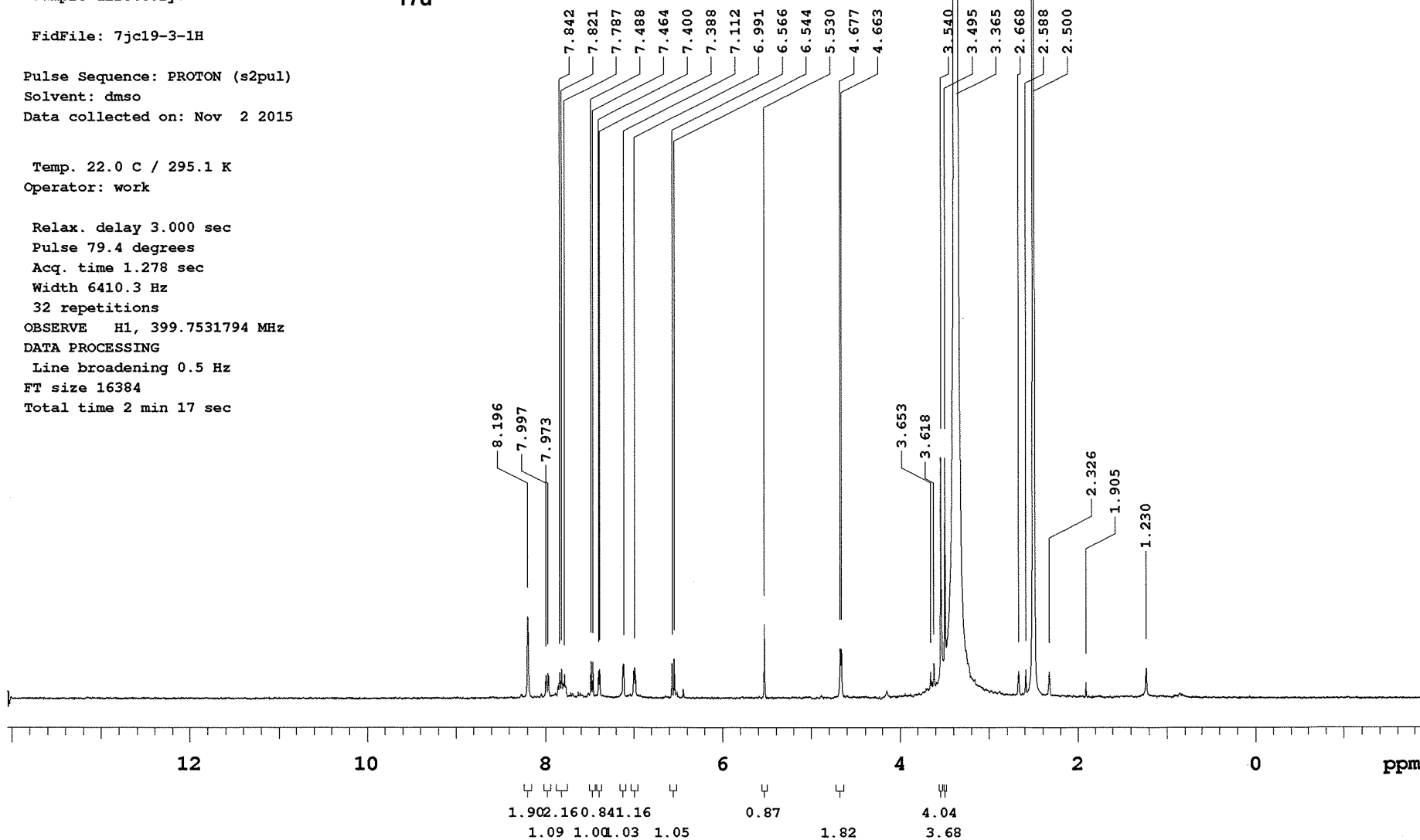
Line broadening 0.5 Hz

FT size 16384

Total time 2 min 17 sec



17d



7jc19-3

Sample Name:

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: 7jc19-3-1H

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Nov 2 2015

Temp. 22.0 C / 295.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

32 repetitions

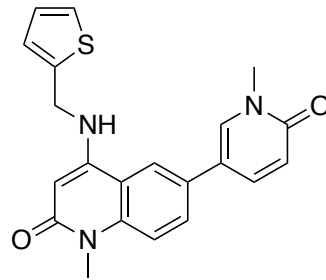
OBSERVE H1, 399.7531794 MHz

DATA PROCESSING

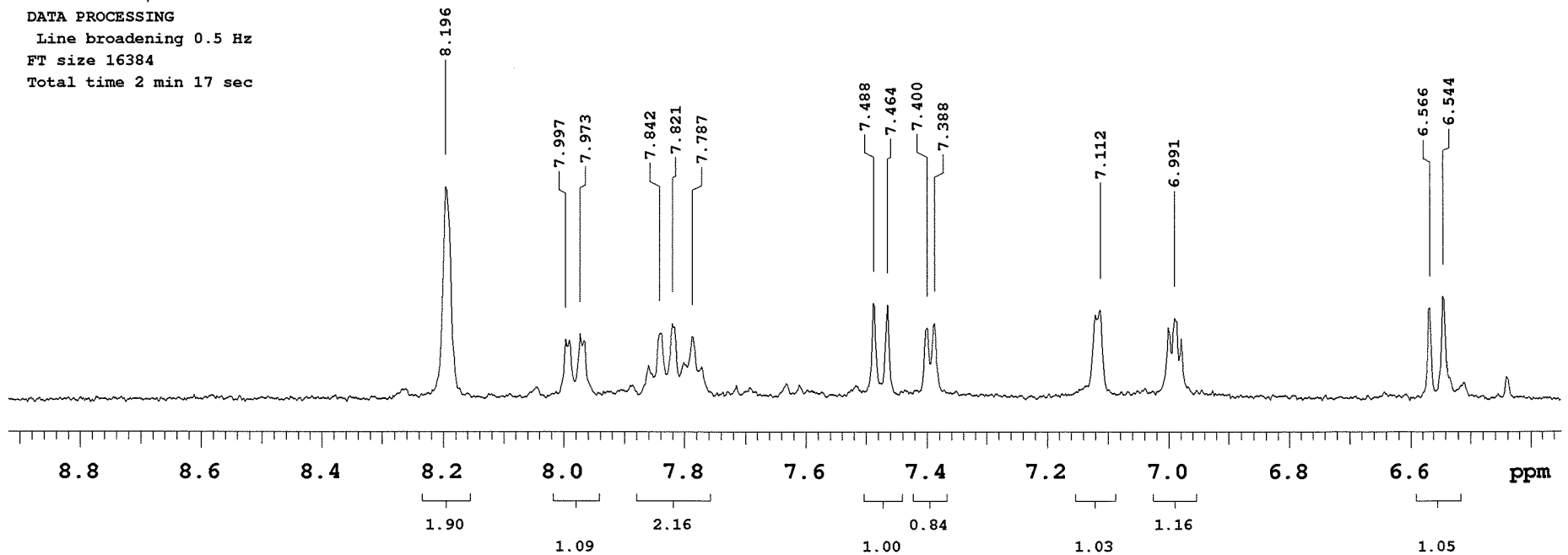
Line broadening 0.5 Hz

FT size 16384

Total time 2 min 17 sec



17d



MR\_45

Sample Name:  
MR\_45

Data Collected on:  
400mr-vnmrs400

Archive directory:

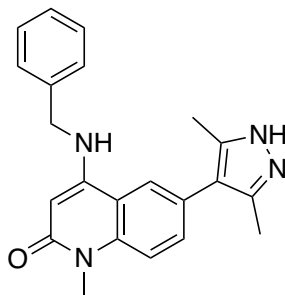
Sample directory:

FidFile: MR\_45

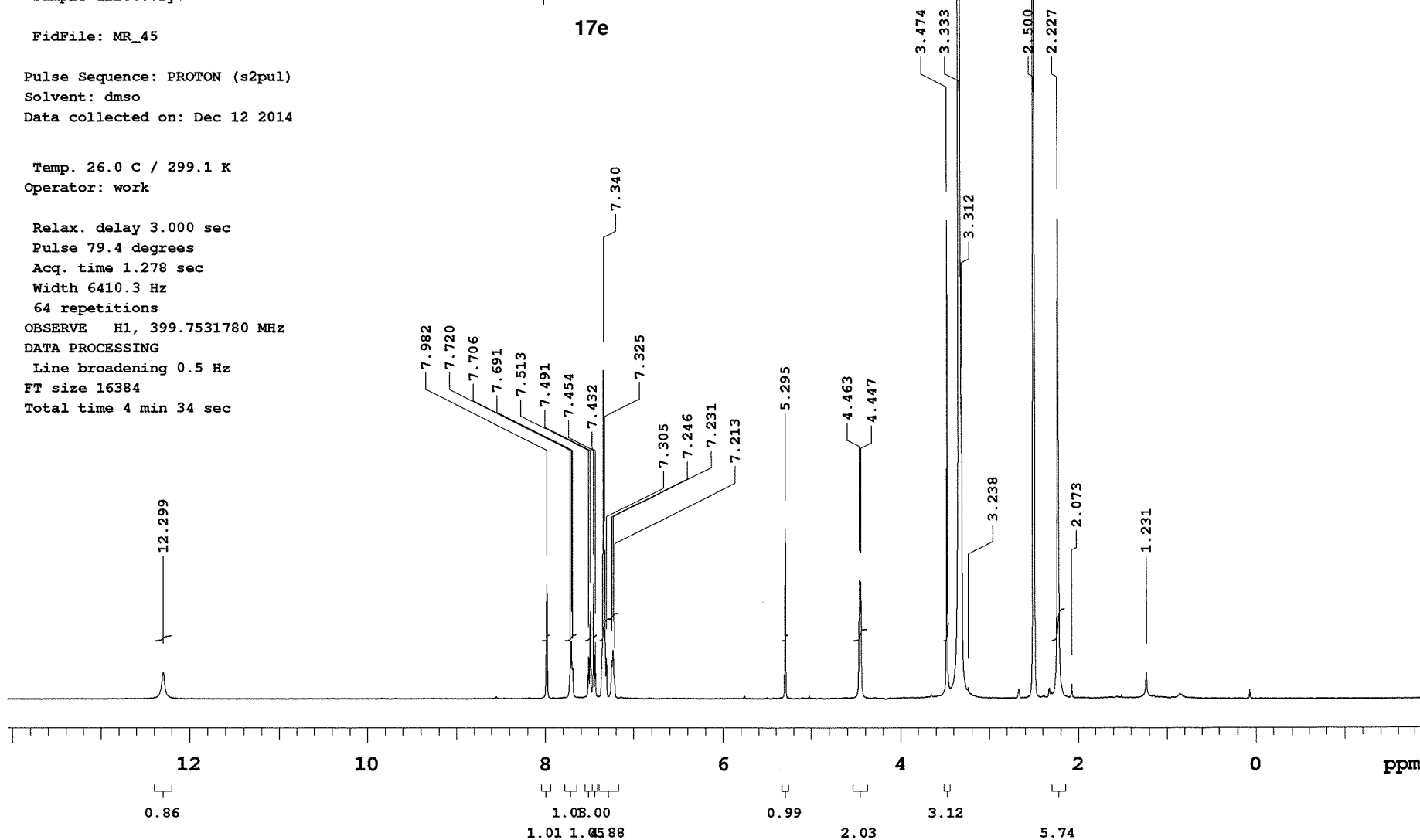
Pulse Sequence: PROTON (s2pul)  
Solvent: dms  
Data collected on: Dec 12 2014

Temp. 26.0 C / 299.1 K  
Operator: work

Relax. delay 3.000 sec  
Pulse 79.4 degrees  
Acq. time 1.278 sec  
Width 6410.3 Hz  
64 repetitions  
OBSERVE H1, 399.7531780 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 16384  
Total time 4 min 34 sec



17e



MR\_45

Sample Name:

MR\_45

Data Collected on:

400mr-vnmrs400

Archive directory:

Sample directory:

FidFile: MR\_45

Pulse Sequence: PROTON (s2pul)

Solvent: dms0

Data collected on: Dec 12 2014

Temp. 26.0 C / 299.1 K

Operator: work

Relax. delay 3.000 sec

Pulse 79.4 degrees

Acq. time 1.278 sec

Width 6410.3 Hz

64 repetitions

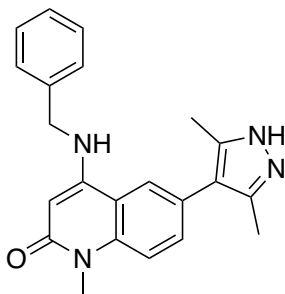
OBSERVE H1, 399.7531780 MHz

DATA PROCESSING

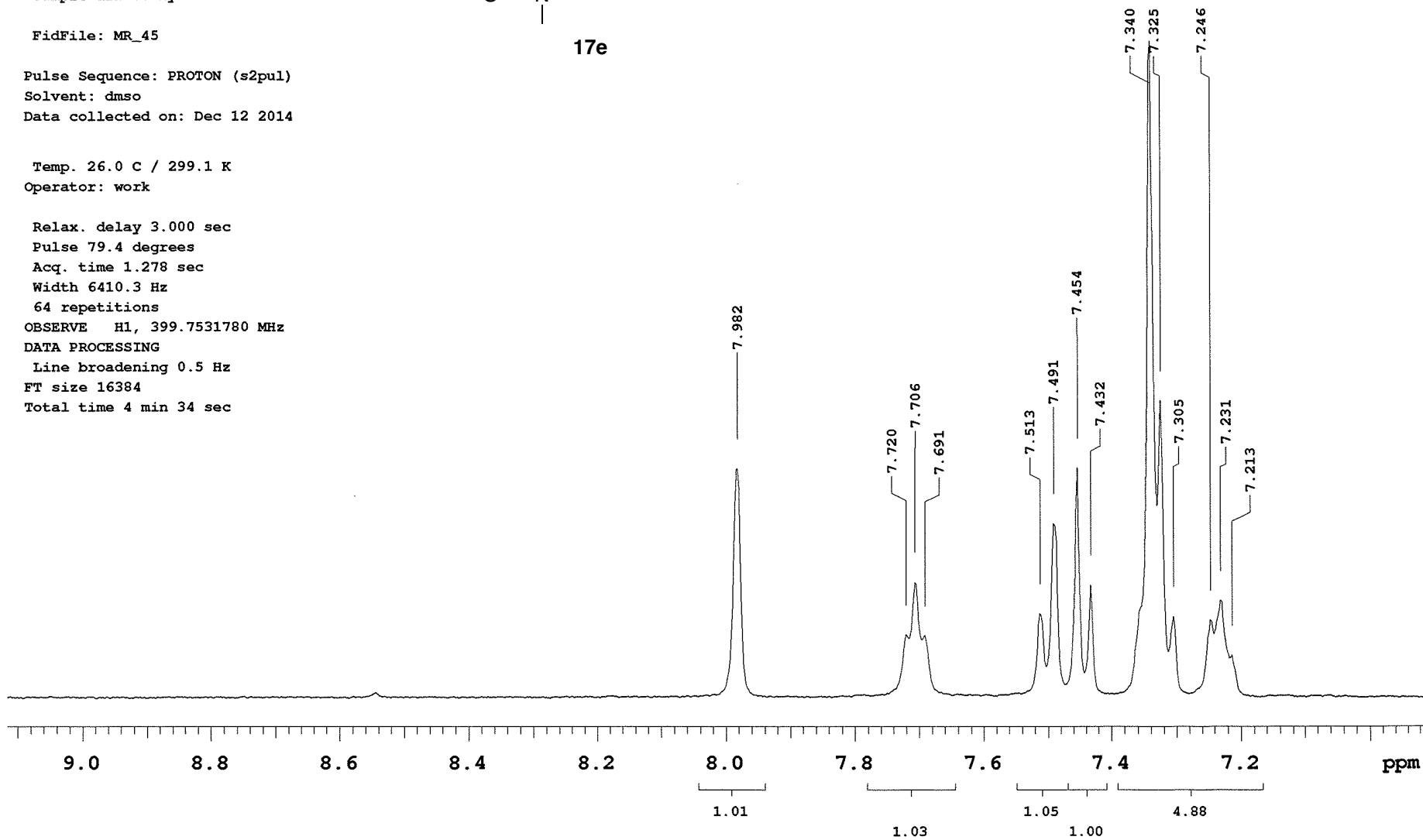
Line broadening 0.5 Hz

FT size 16384

Total time 4 min 34 sec

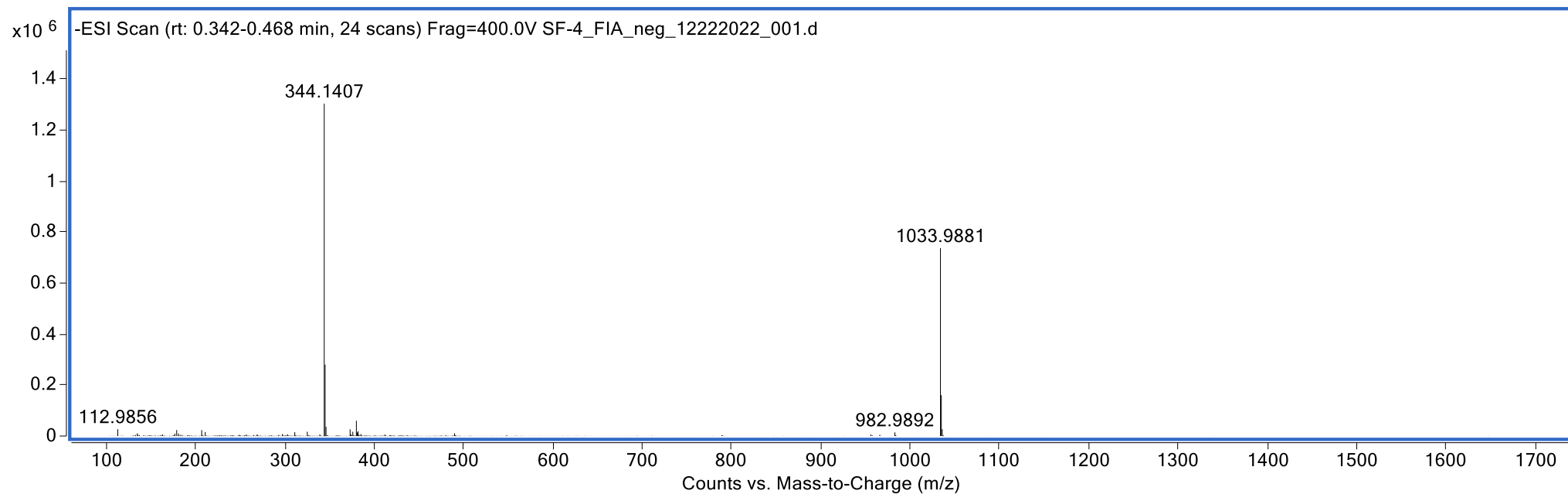


17e

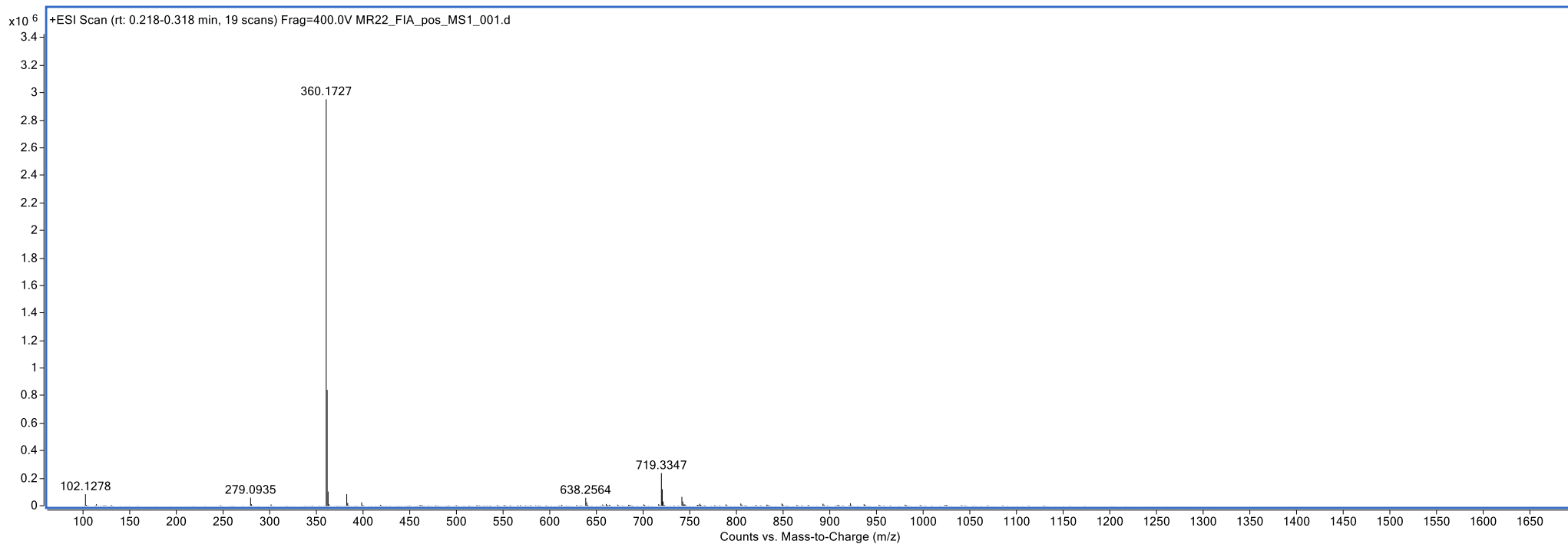


# HRMS Spectra

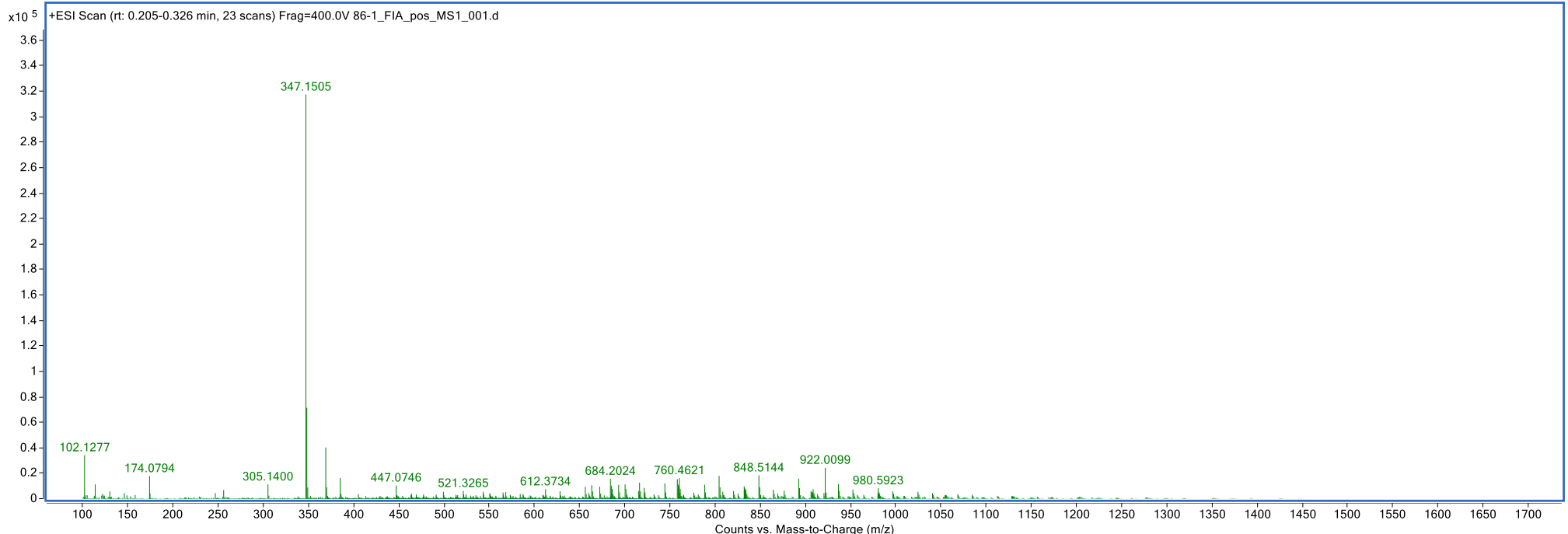
## Compound 6 (5jc21, CG13250)



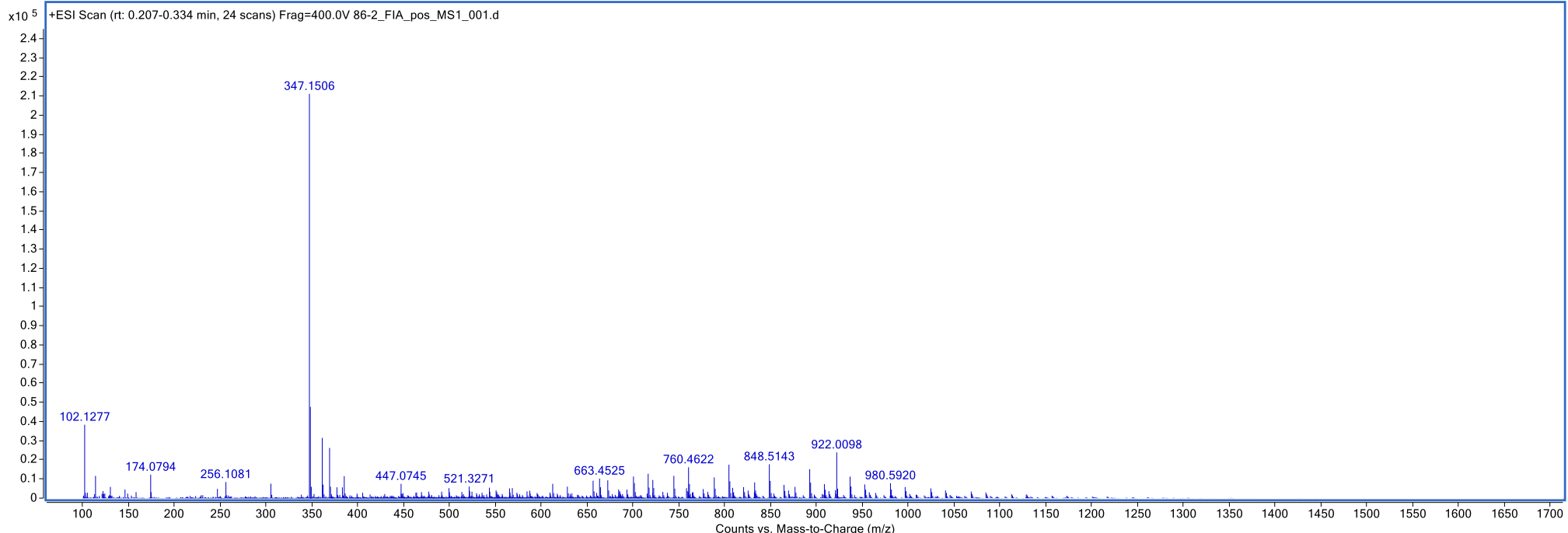
## Compound 13a



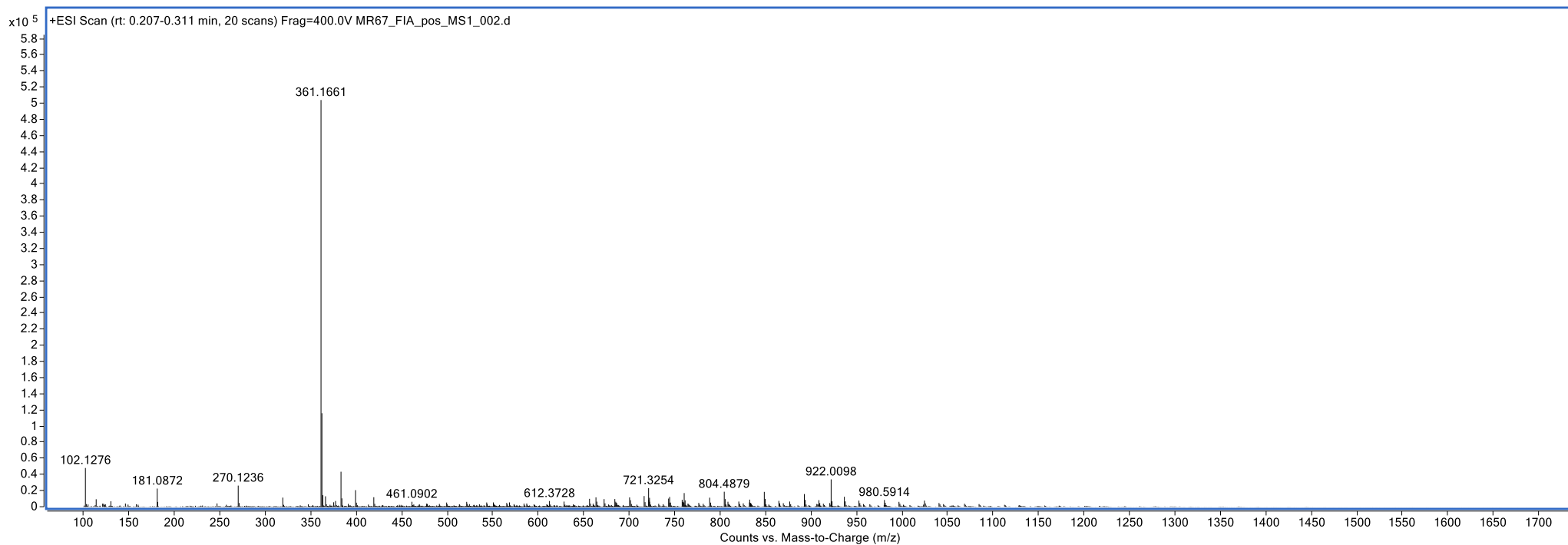
**Compound 12a**



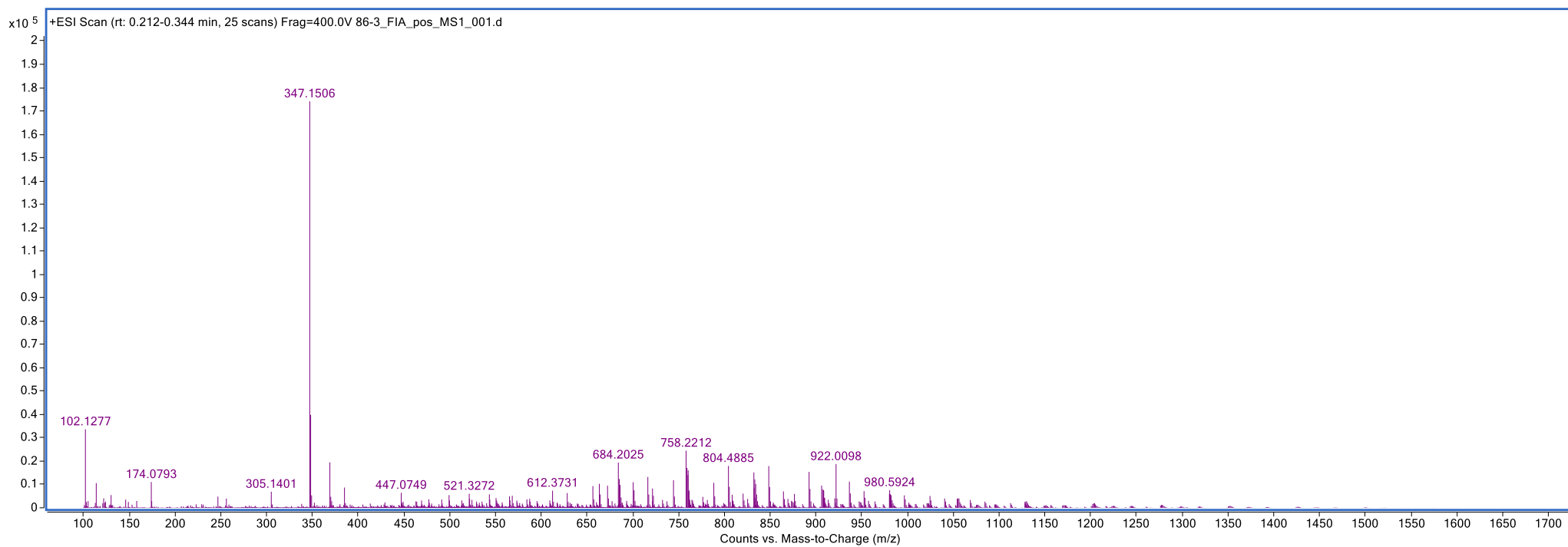
**Compound 12b**



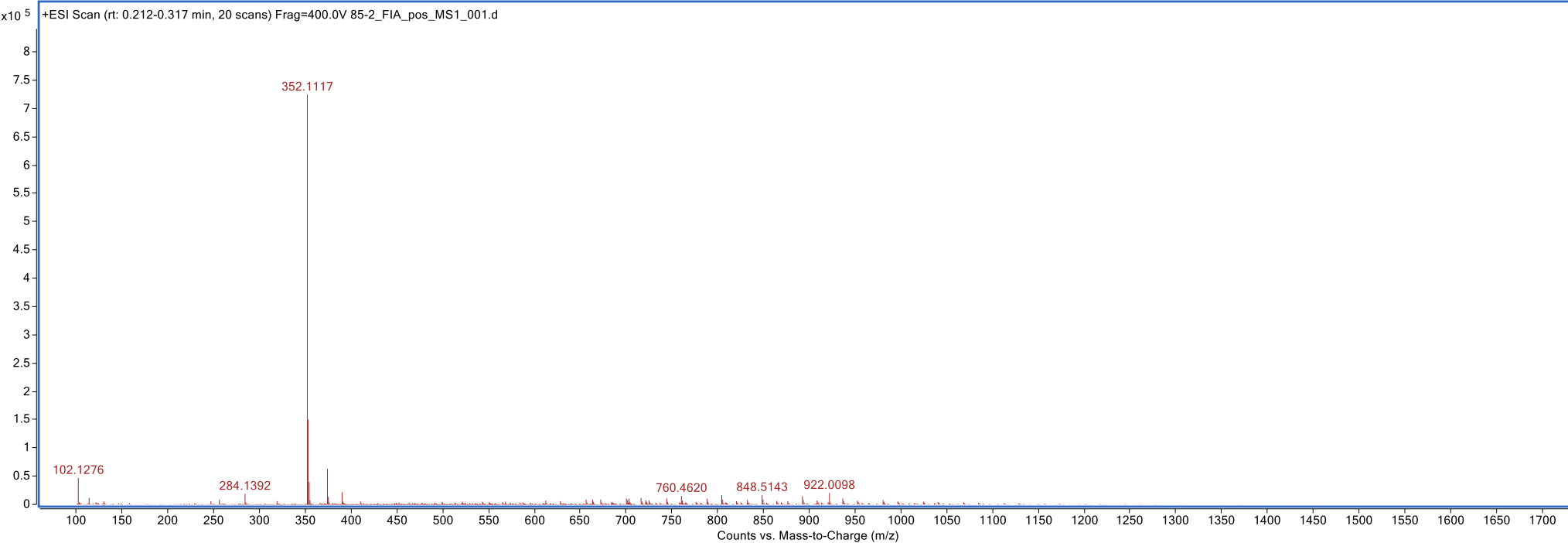
## Compound 13b



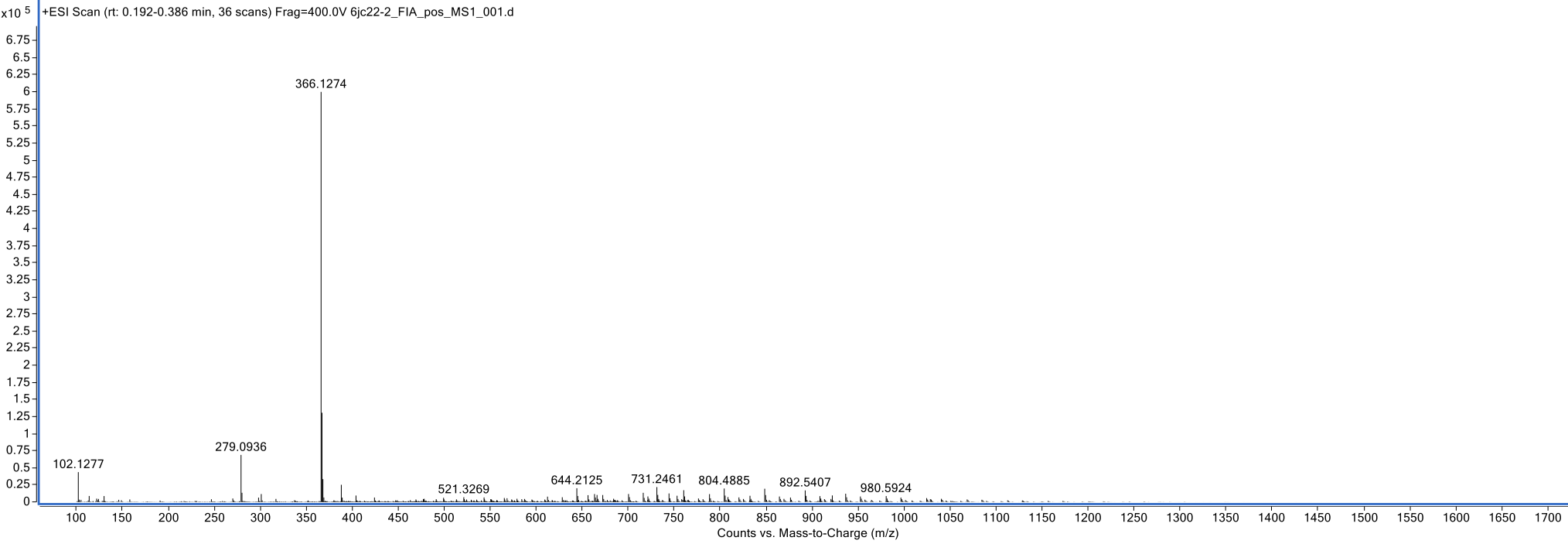
## Compound 12c



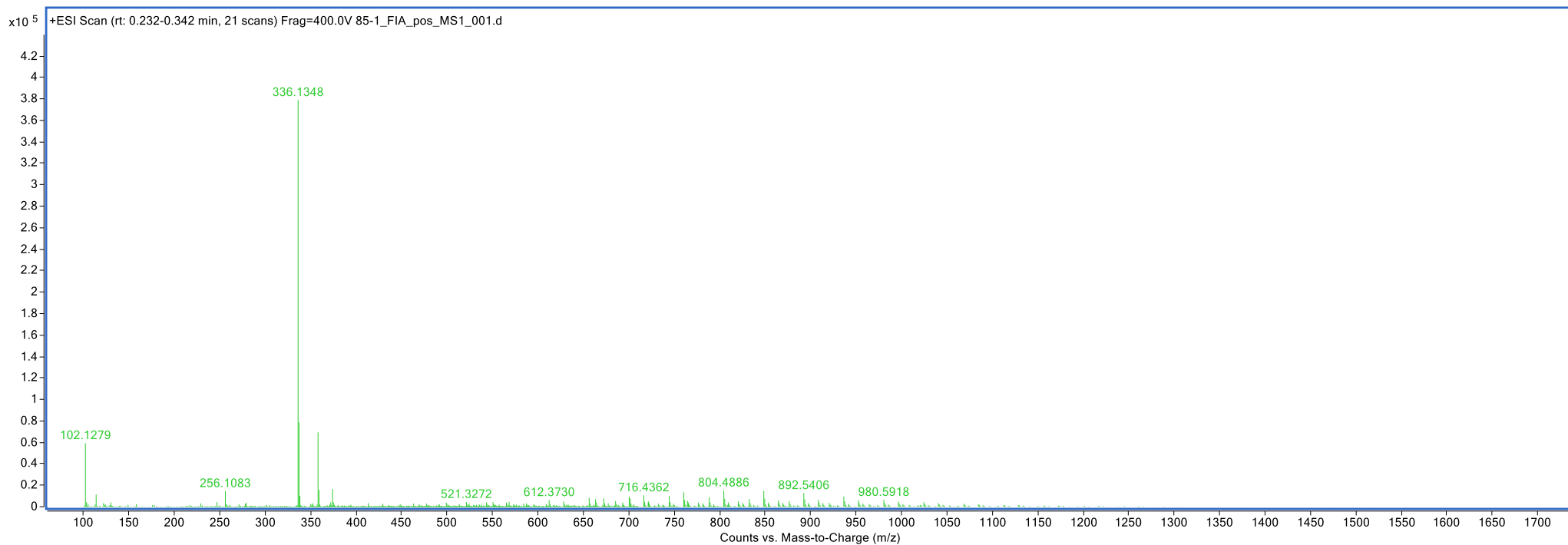
**Compound 12h**



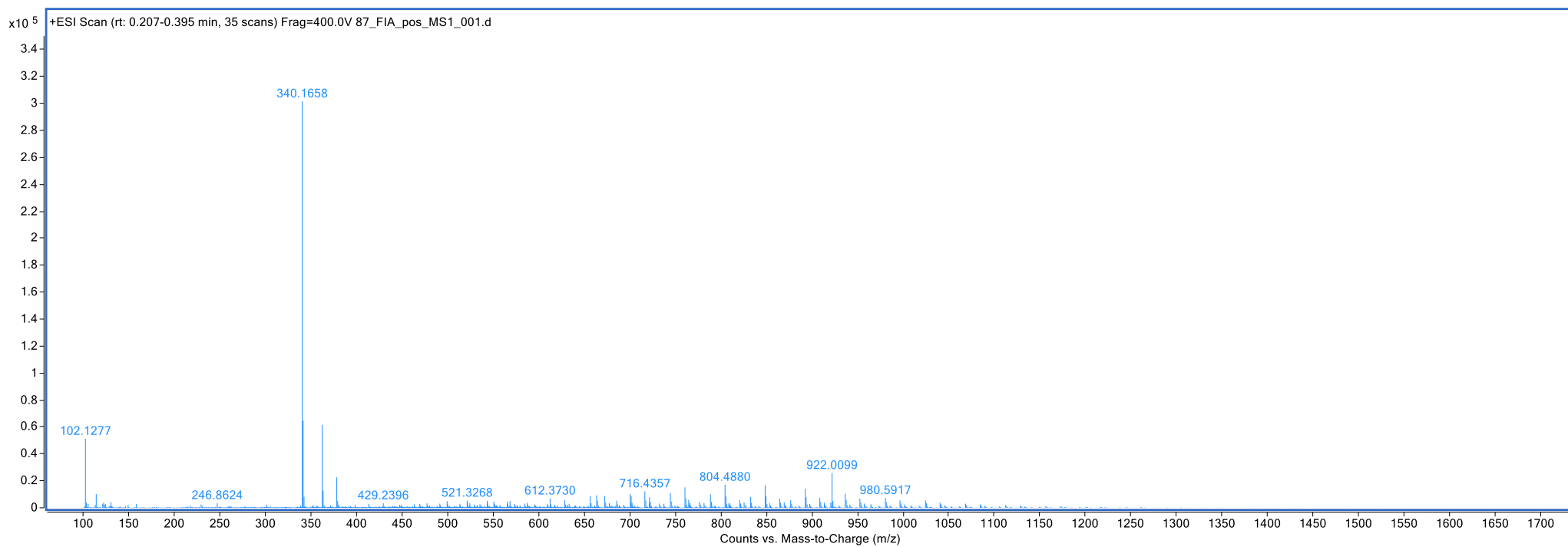
**Compound 13c**



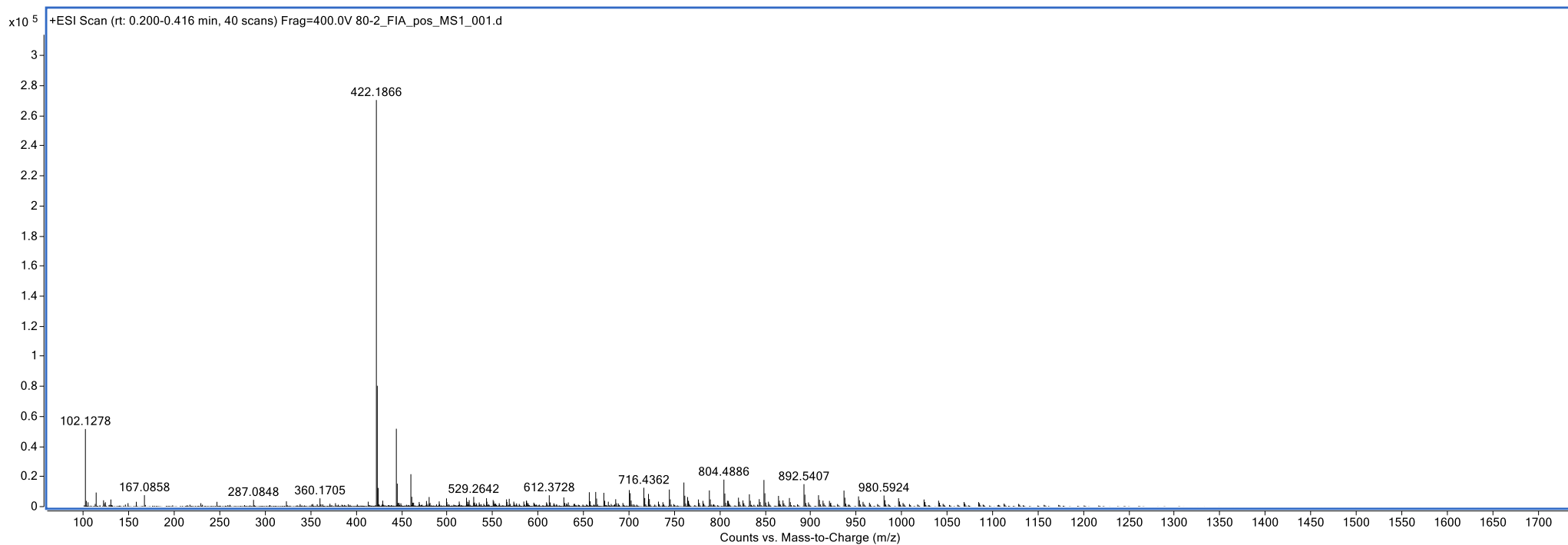
## Compound 12i



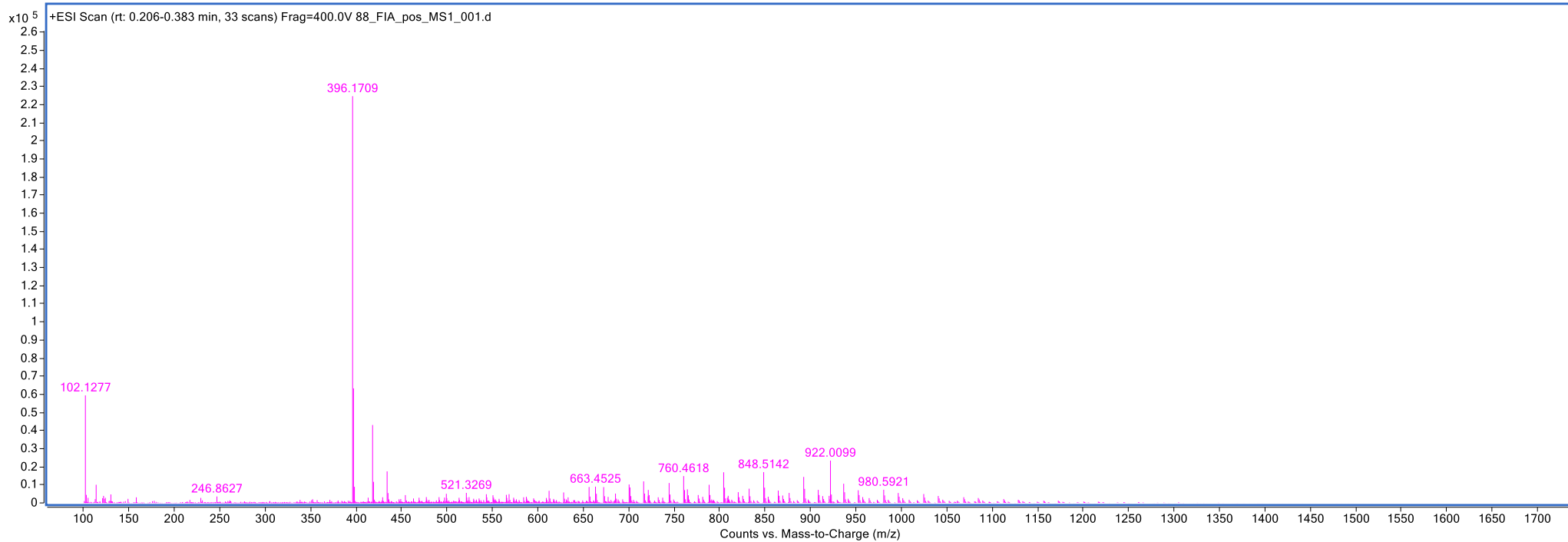
## Compound 12j



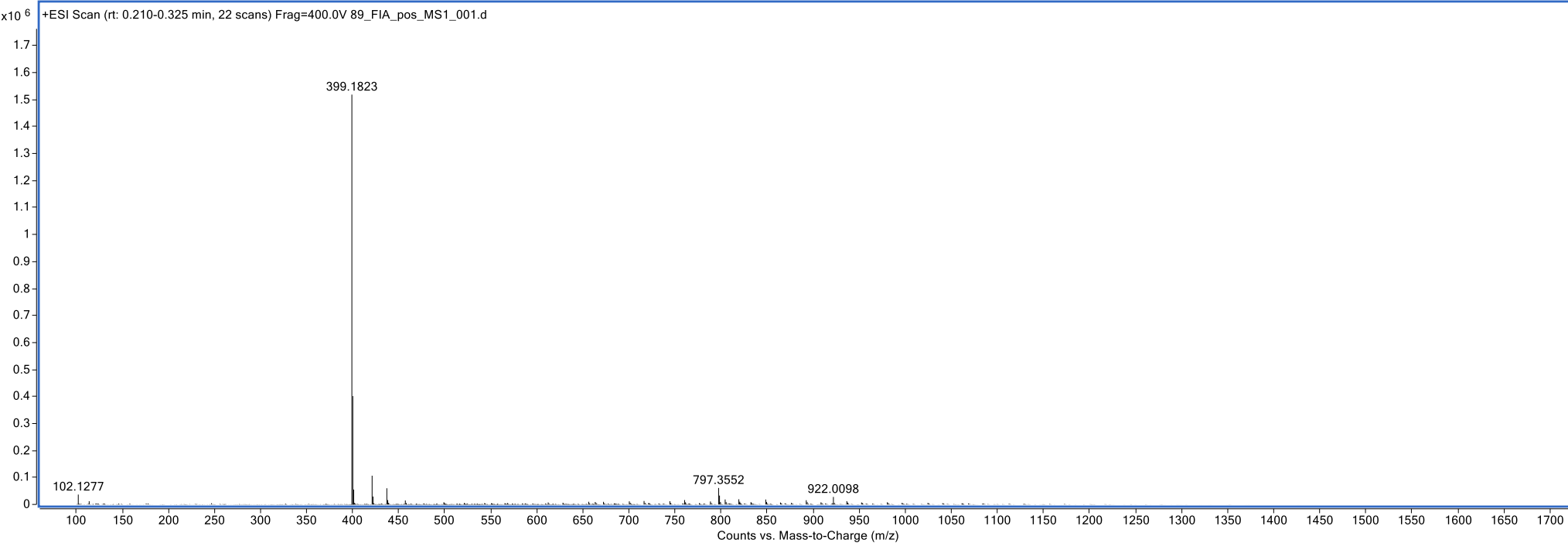
## Compound 12k



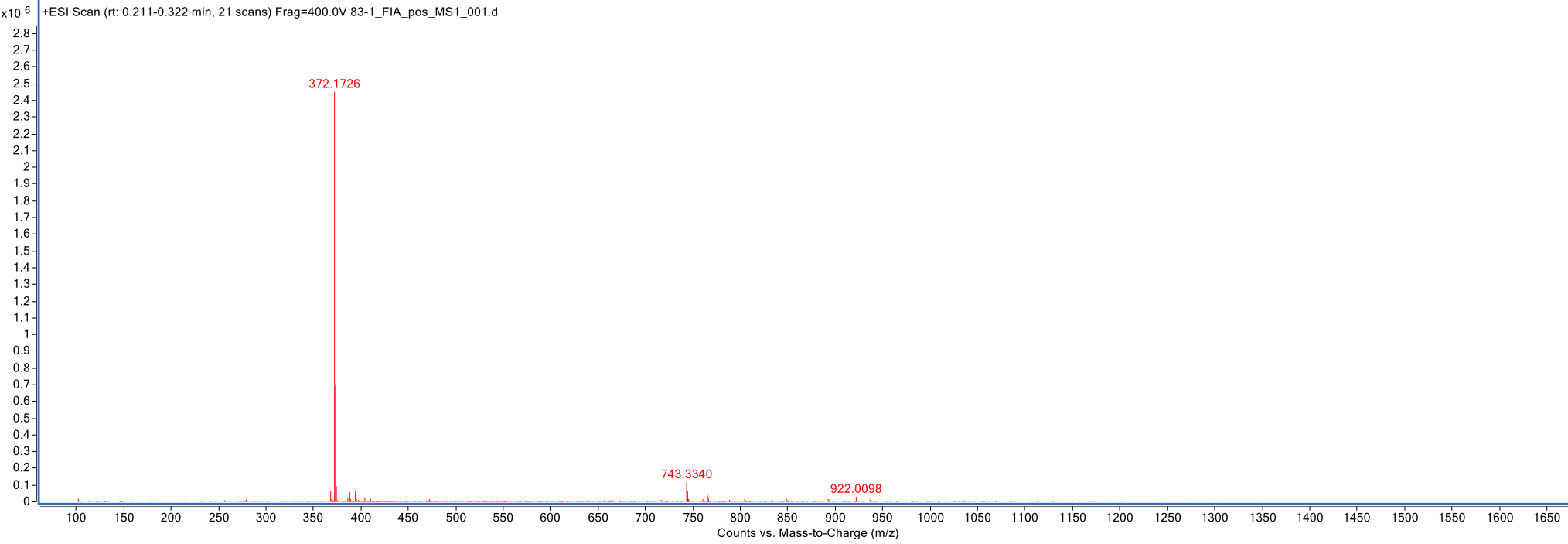
## Compound 12l



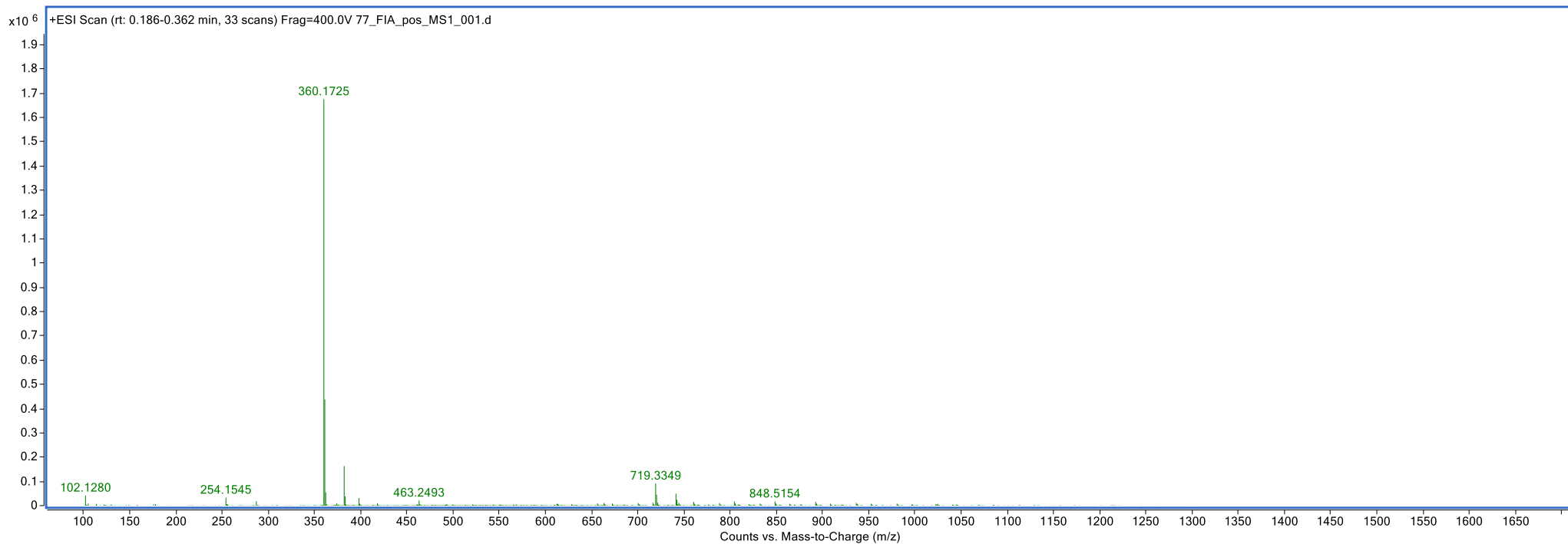
**Compound 12m**



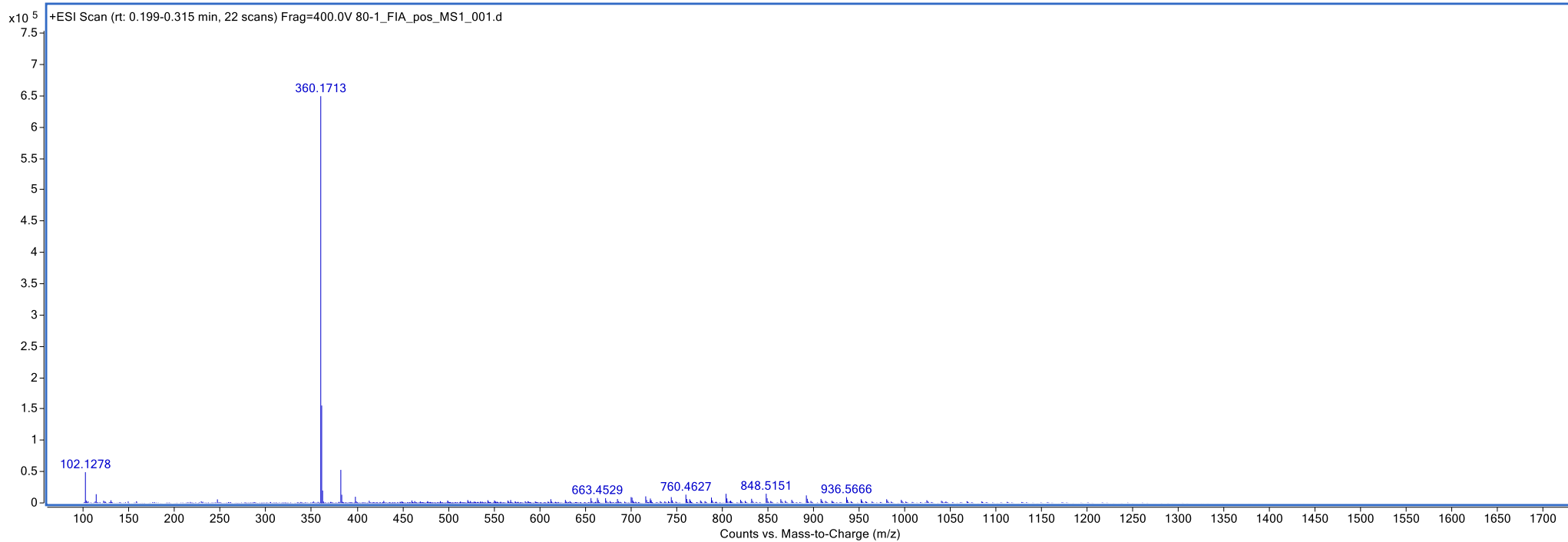
**Compound 12p**



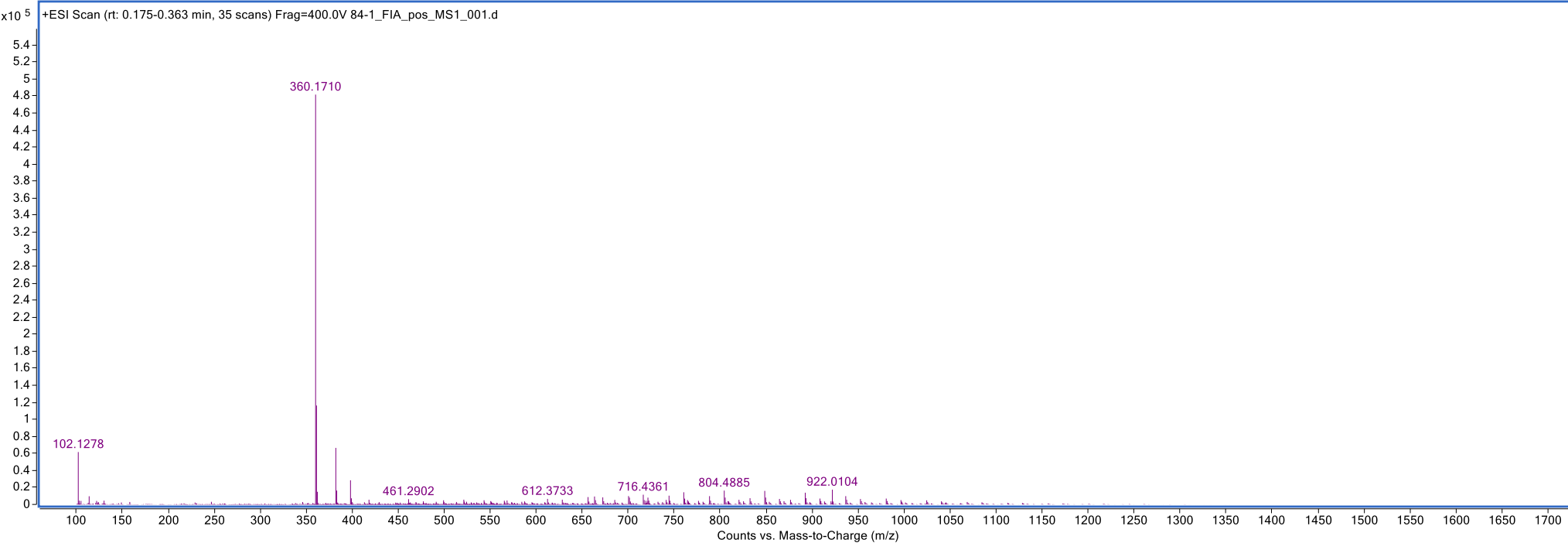
## Compound 12q



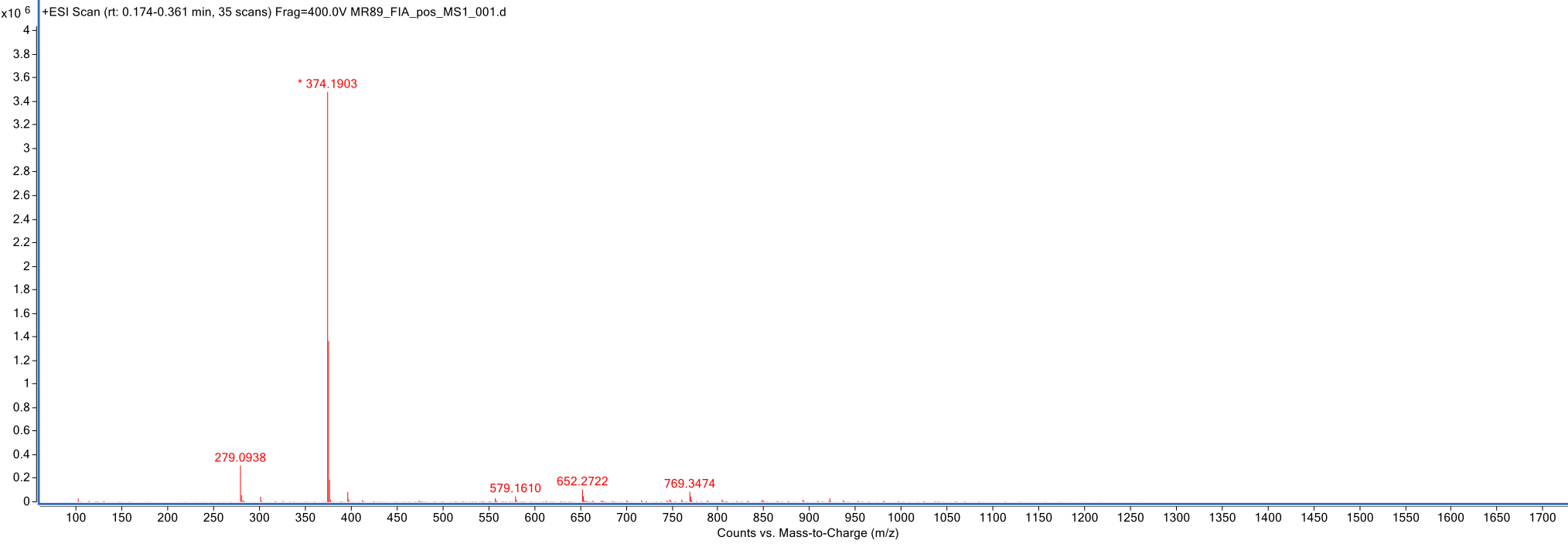
## Compound 12r



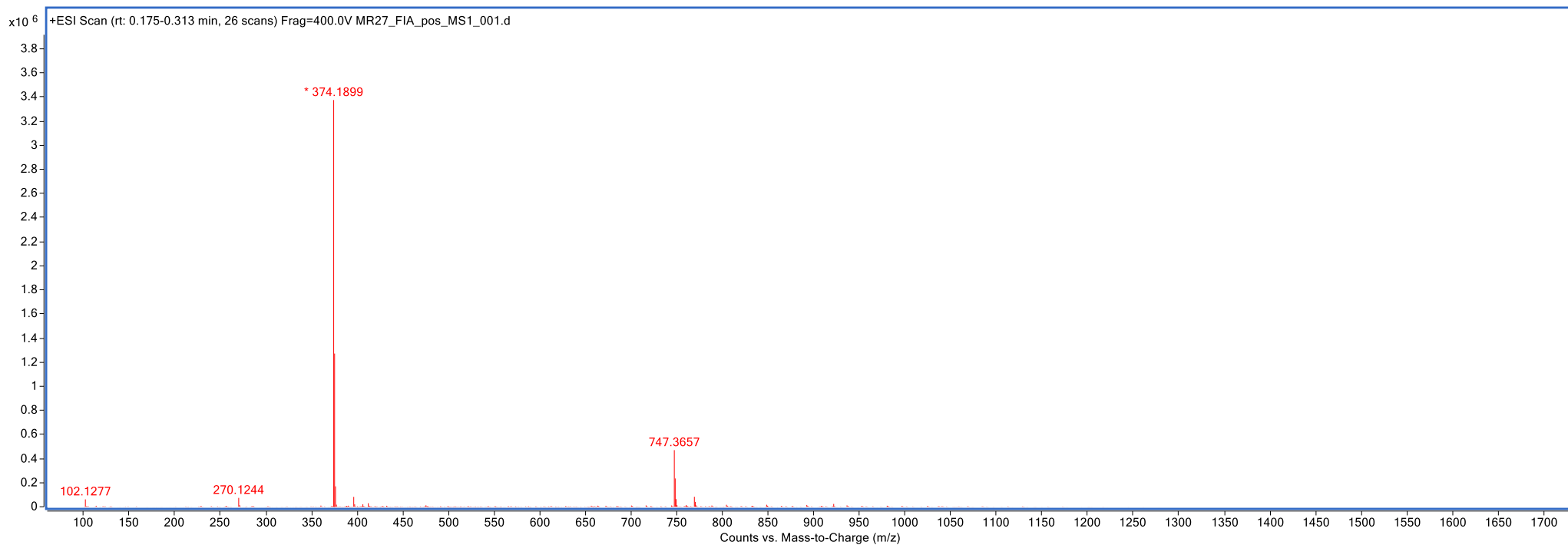
**Compound 12s**



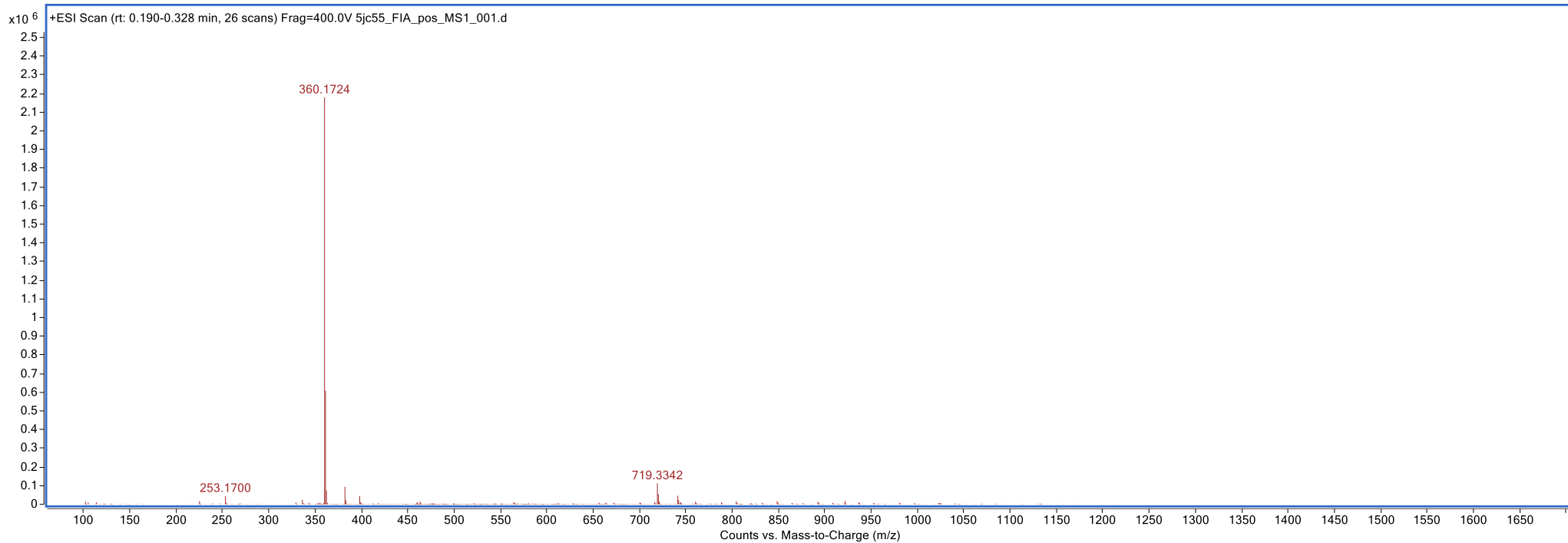
**Compound 13d**



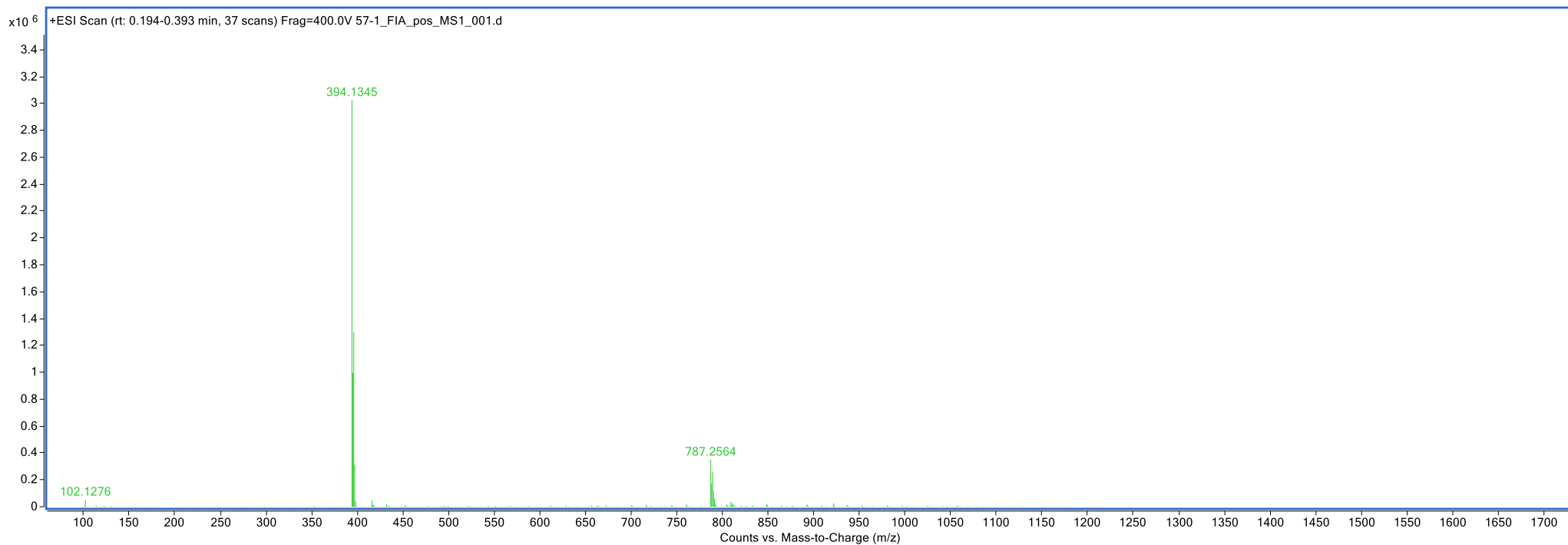
## Compound 13e



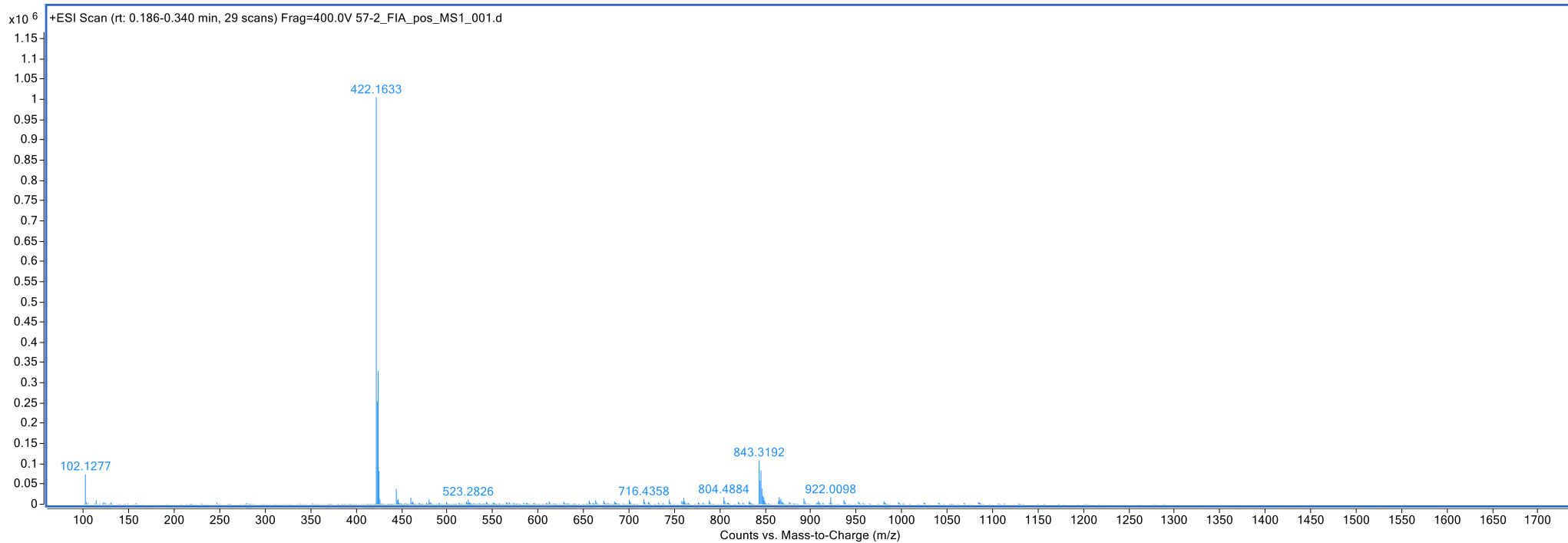
## Compound 12t



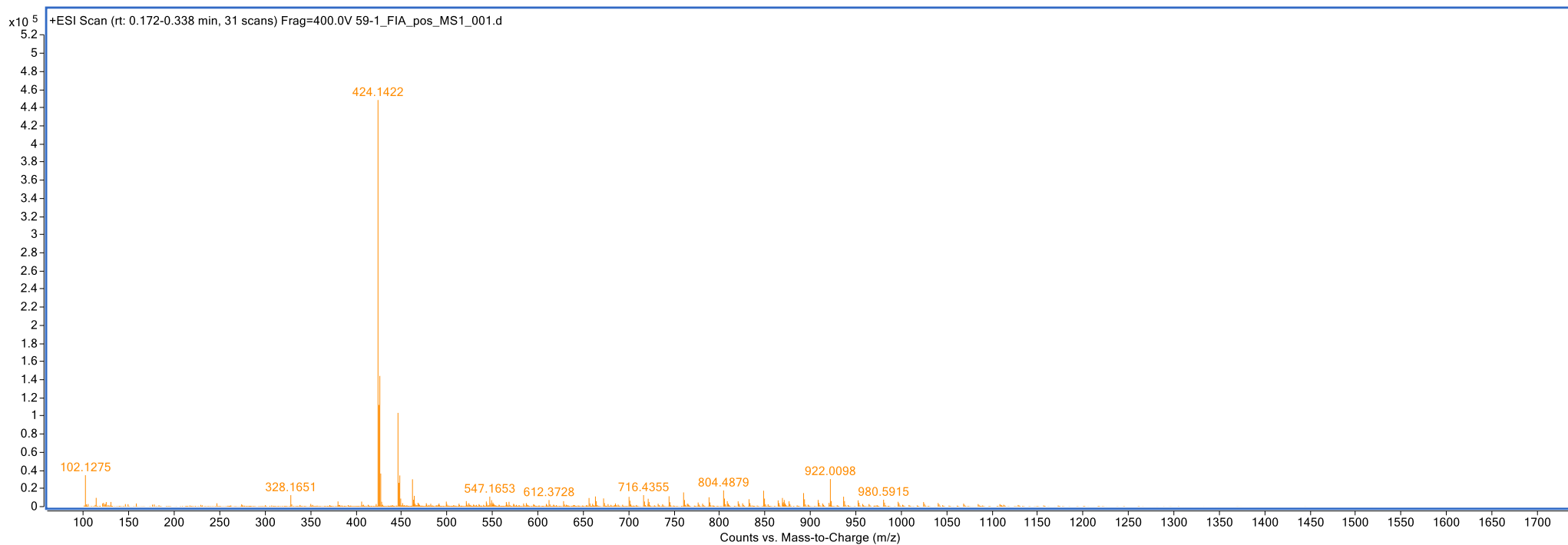
## Compound 14a



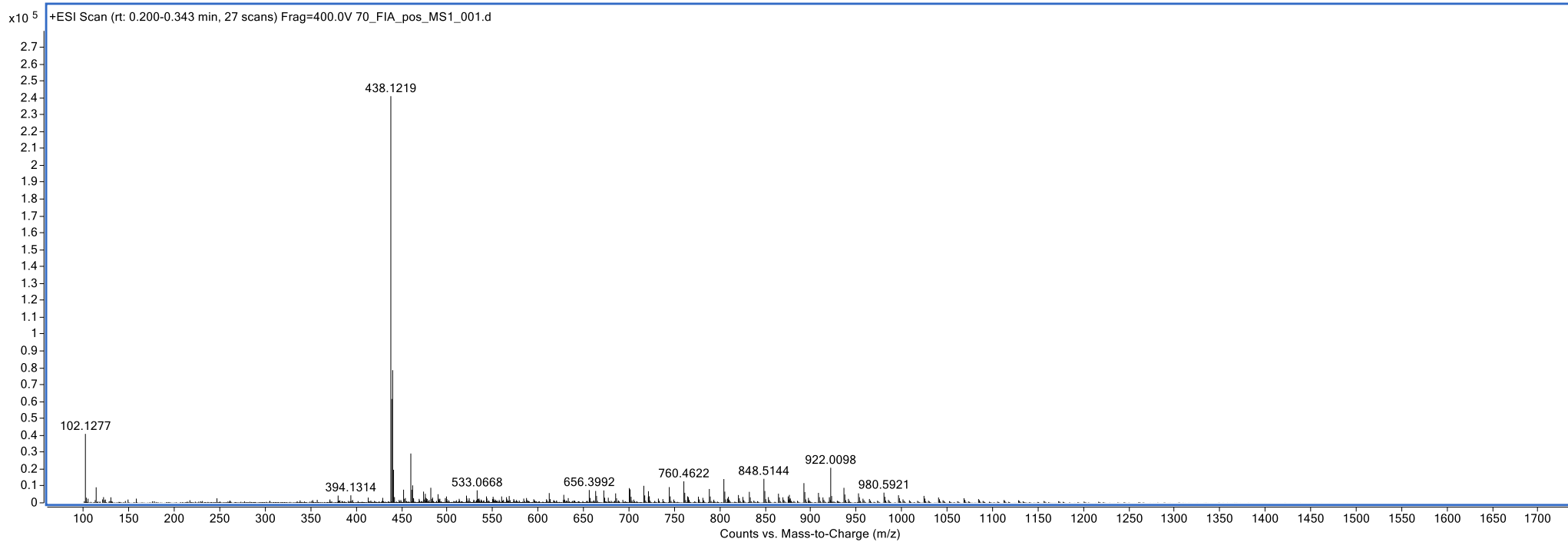
## Compound 14b



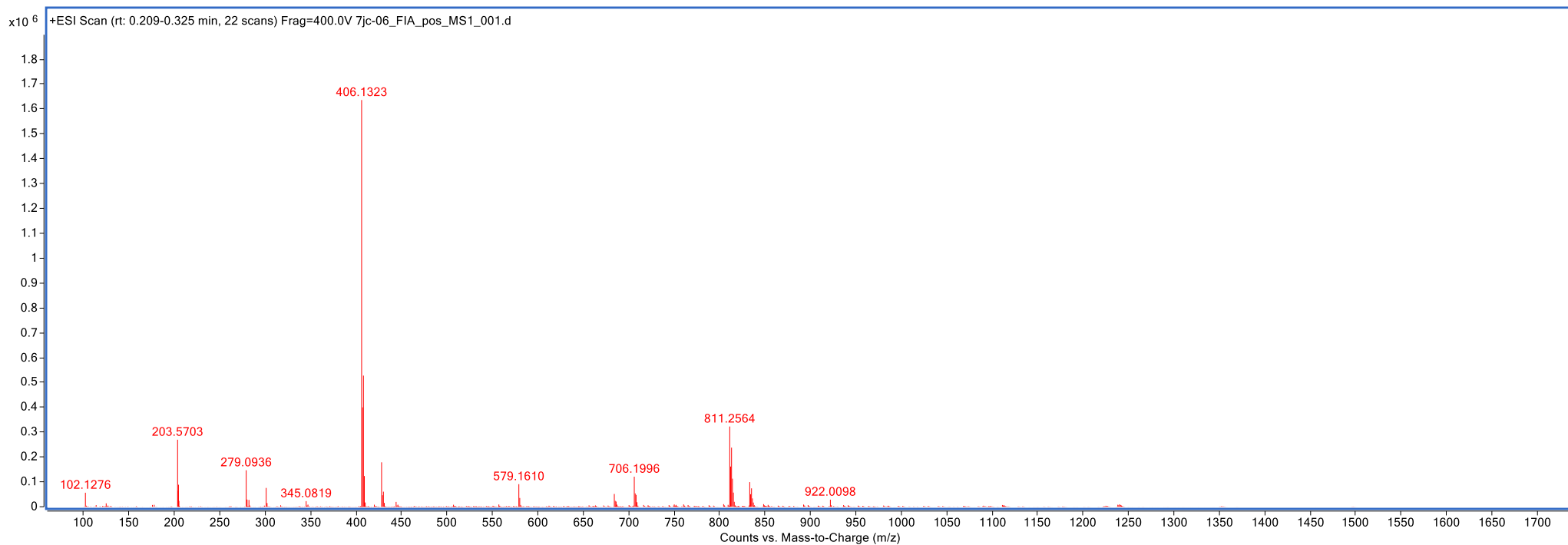
### Compound 14c



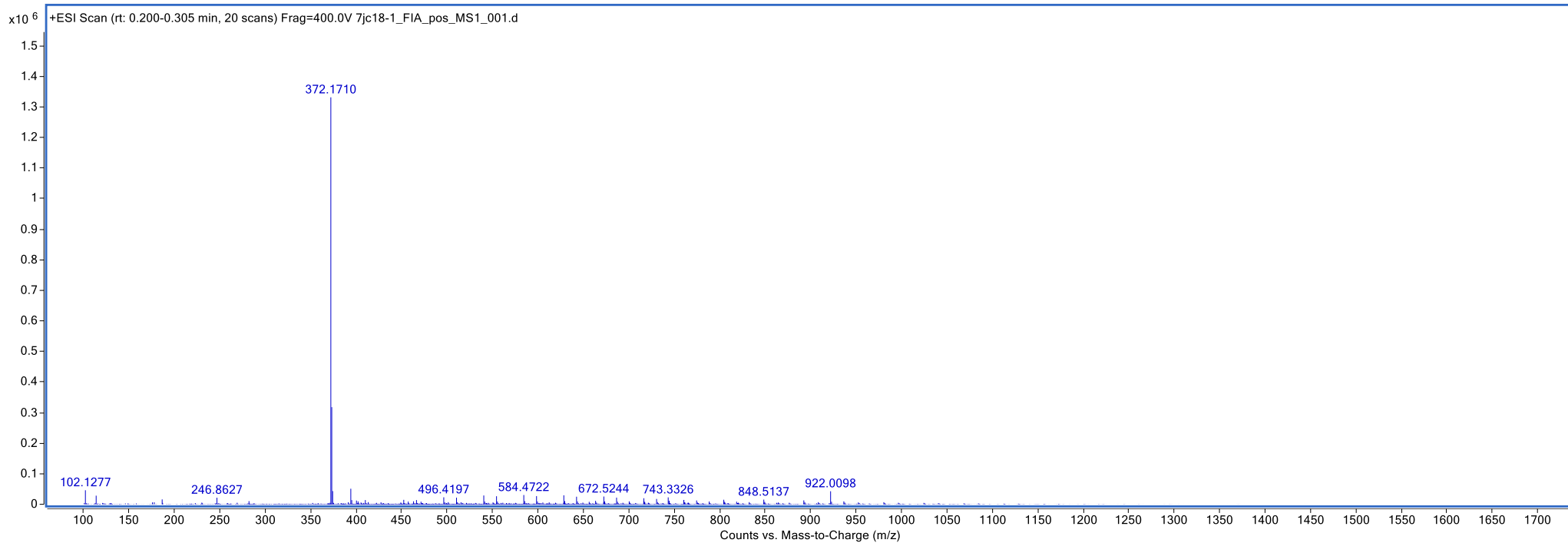
### Compound 14d



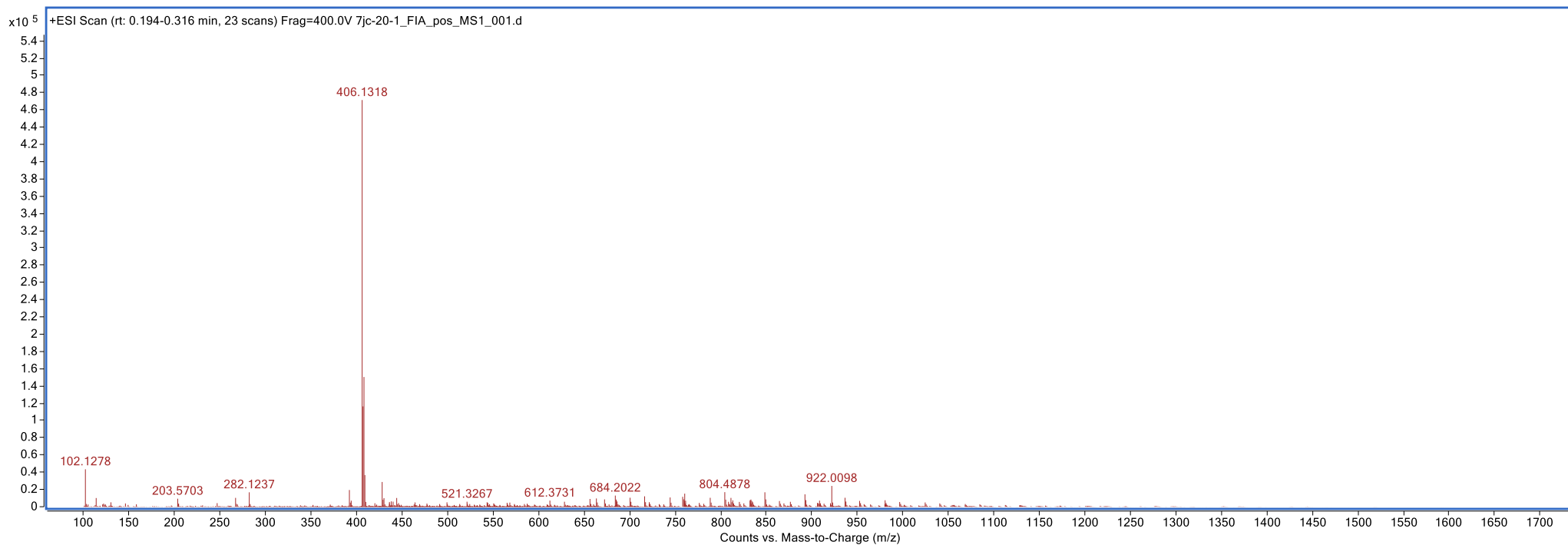
## Compound 17a



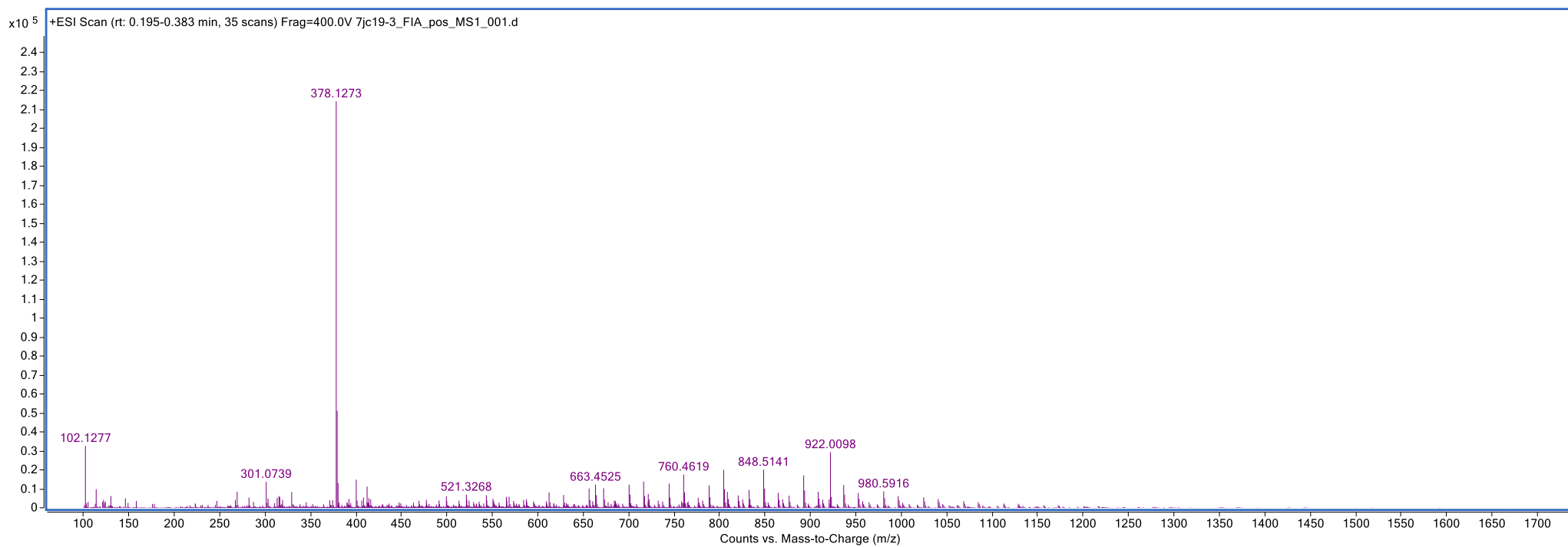
## Compound 17b



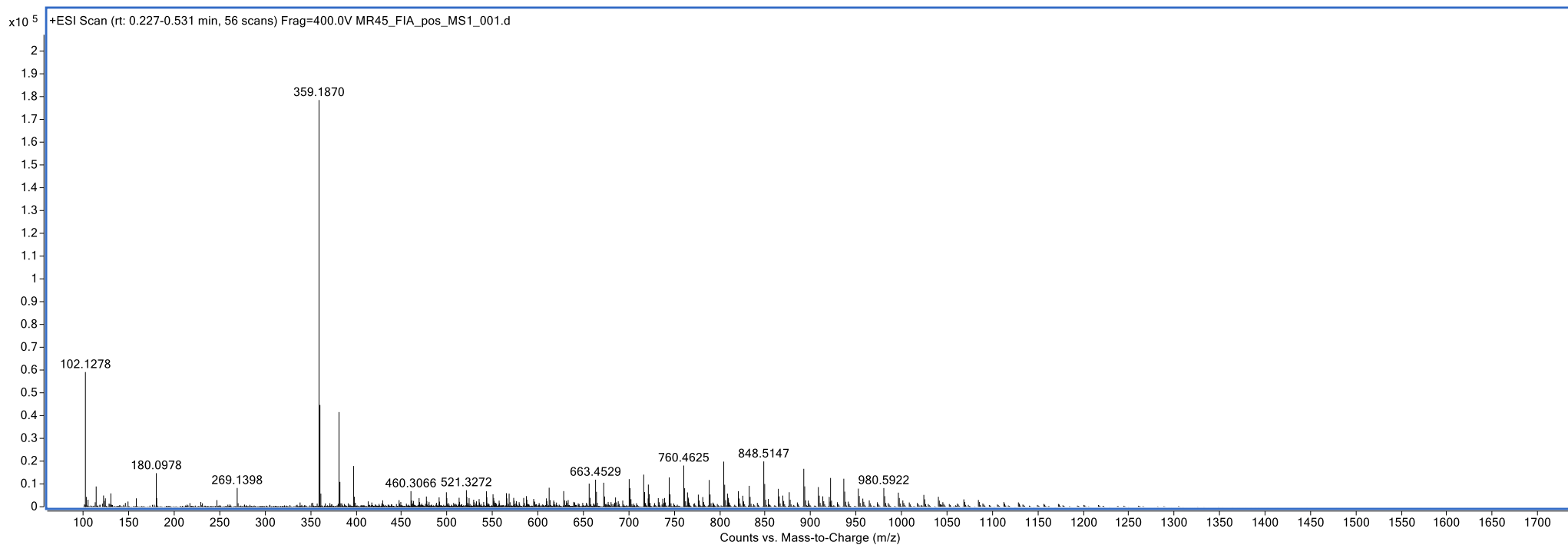
## Compound 17c



## Compound 17d



## Compound 17e



## Compound 17f

