

Supporting Information for

Rapid assembly of pyrrole-ligated 1,3,4-oxadiazoles and excellent antibacterial activity by iodophenol substituents

Hyein Kim,^{†1} Lina Gu,^{†1,2} Huisu Yeo,¹ Umji Choi,³ Chang-Ro Lee,^{*3} Haiyang Yu,⁴ and Sangho Koo^{*1,2}

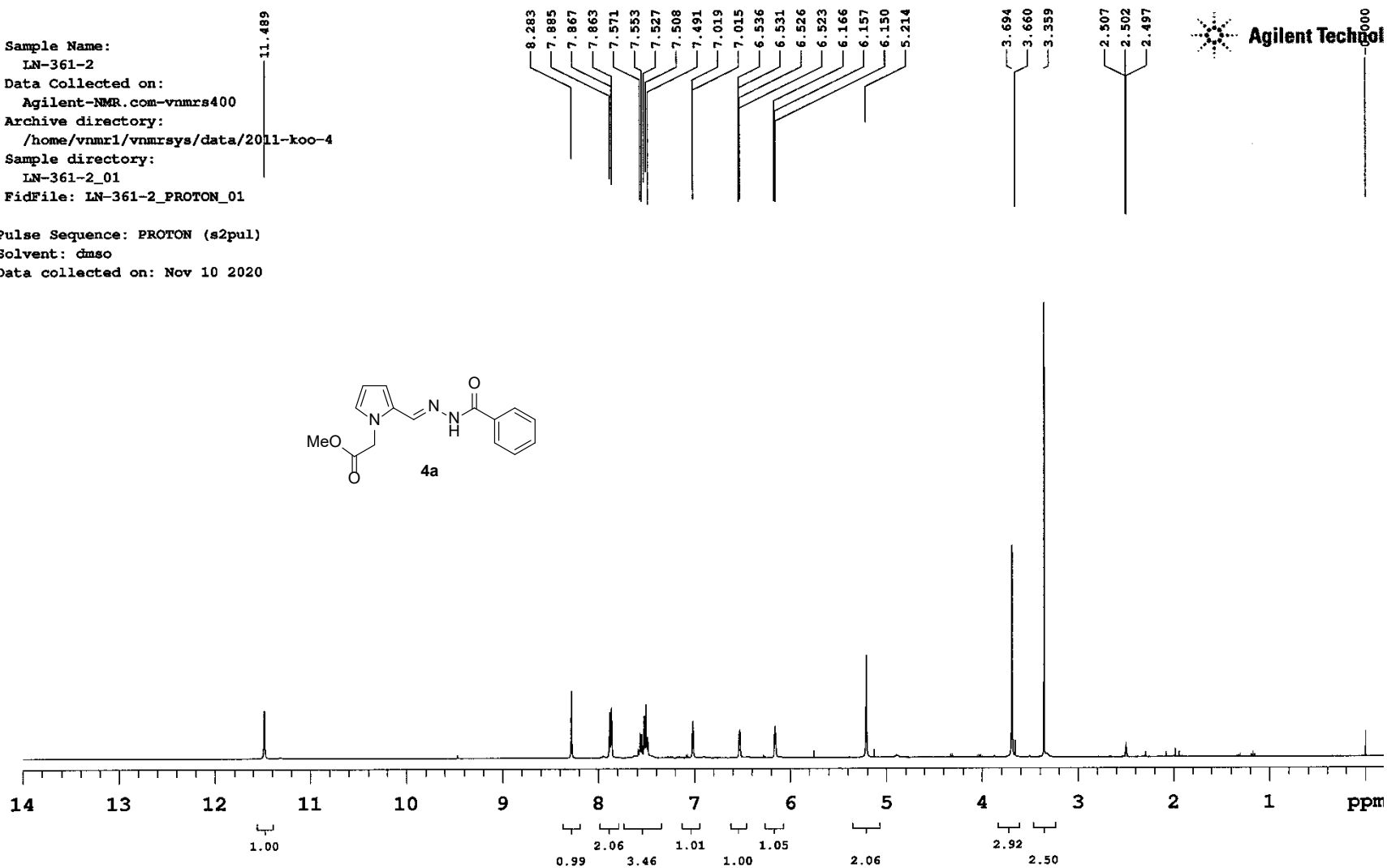
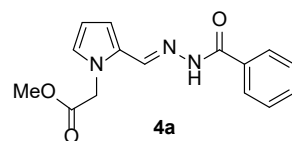
¹ Department of Chemistry, Myongji University, Myongji-Ro 116, Cheoin-Gu, Yongin, Gyeonggi-Do 17058, Korea; ² School of Pharmacy, East China University of Science and Technology, Meilong Road 130, Shanghai, 200237, China; ³ Department of Biological Sciences and Bioinformatics, Myongji University, Myongji-Ro 116, Cheoin-Gu, Yongin, Gyeonggi-Do 17058, Korea; ⁴ Tianjin State Key Laboratory of Modern Chinese Medicine, Tianjin University of Traditional Chinese Medicine, Tianjin 300193, China

[†]These authors contributed equally; Corresponding authors: *crlee@mju.ac.kr; *sangkoo@mju.ac.kr

(1) ¹ H/ ¹³ C-NMR Spectra	-----	S-2
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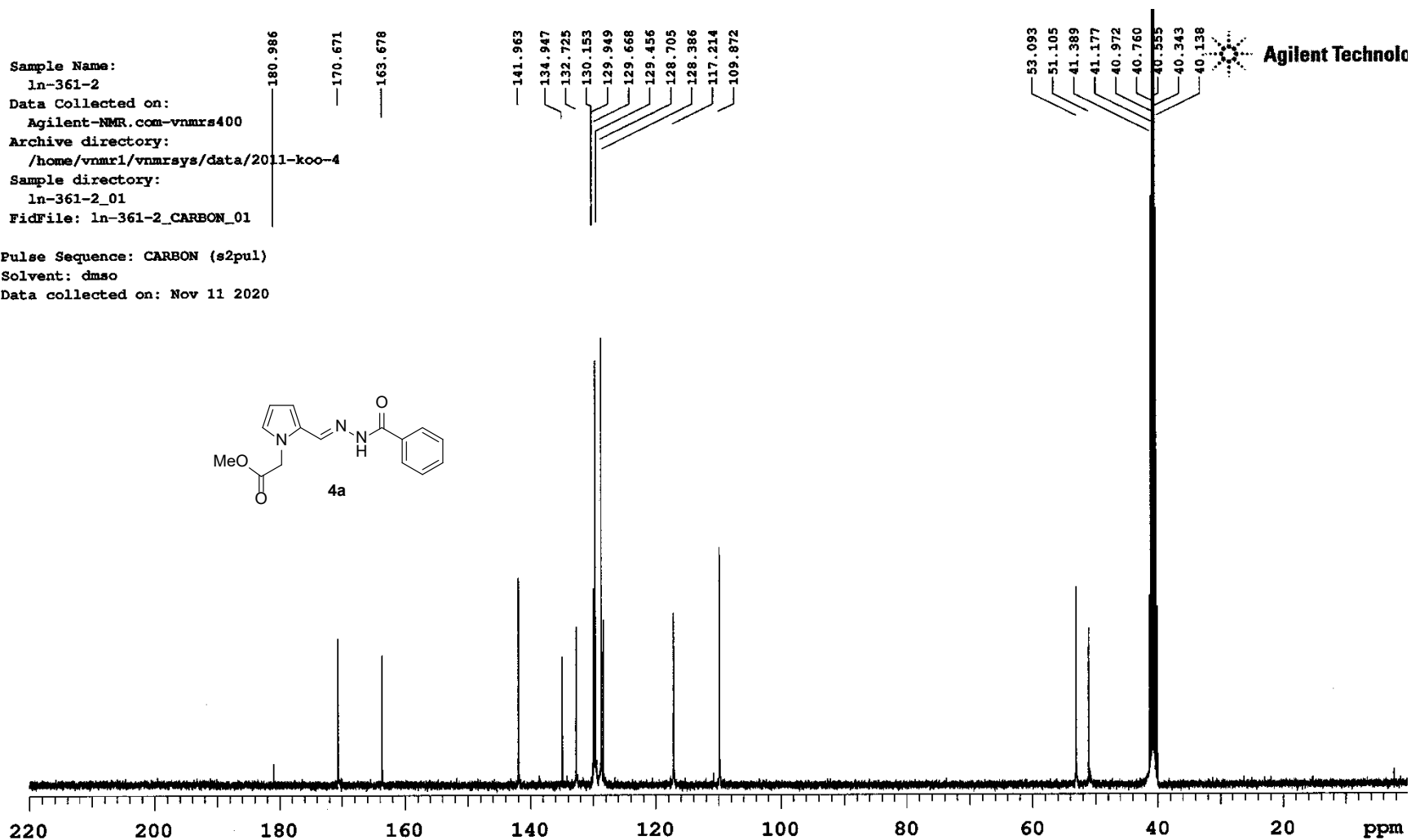
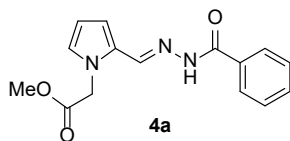
Sample Name:
 LN-361-2
 Data Collected on:
 Agilent-NMR.com-vnmrs400
 Archive directory:
 /home/vnmr1/vnmrsys/data/2011-koo-4
 Sample directory:
 LN-361-2_01
 FidFile: LN-361-2_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: dmsd
 Data collected on: Nov 10 2020



Sample Name: ln-361-2
 Data Collected on: Agilent-NMR.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2011-koo-4
 Sample directory: ln-361-2_01
 FidFile: ln-361-2_CARBON_01

Pulse Sequence: CARBON (s2pul)
 Solvent: dmso
 Data collected on: Nov 11 2020



Sample Name:

LN-381-P

Data Collected on:

Agilent-NMR.com-vnmrs400

Archive directory:

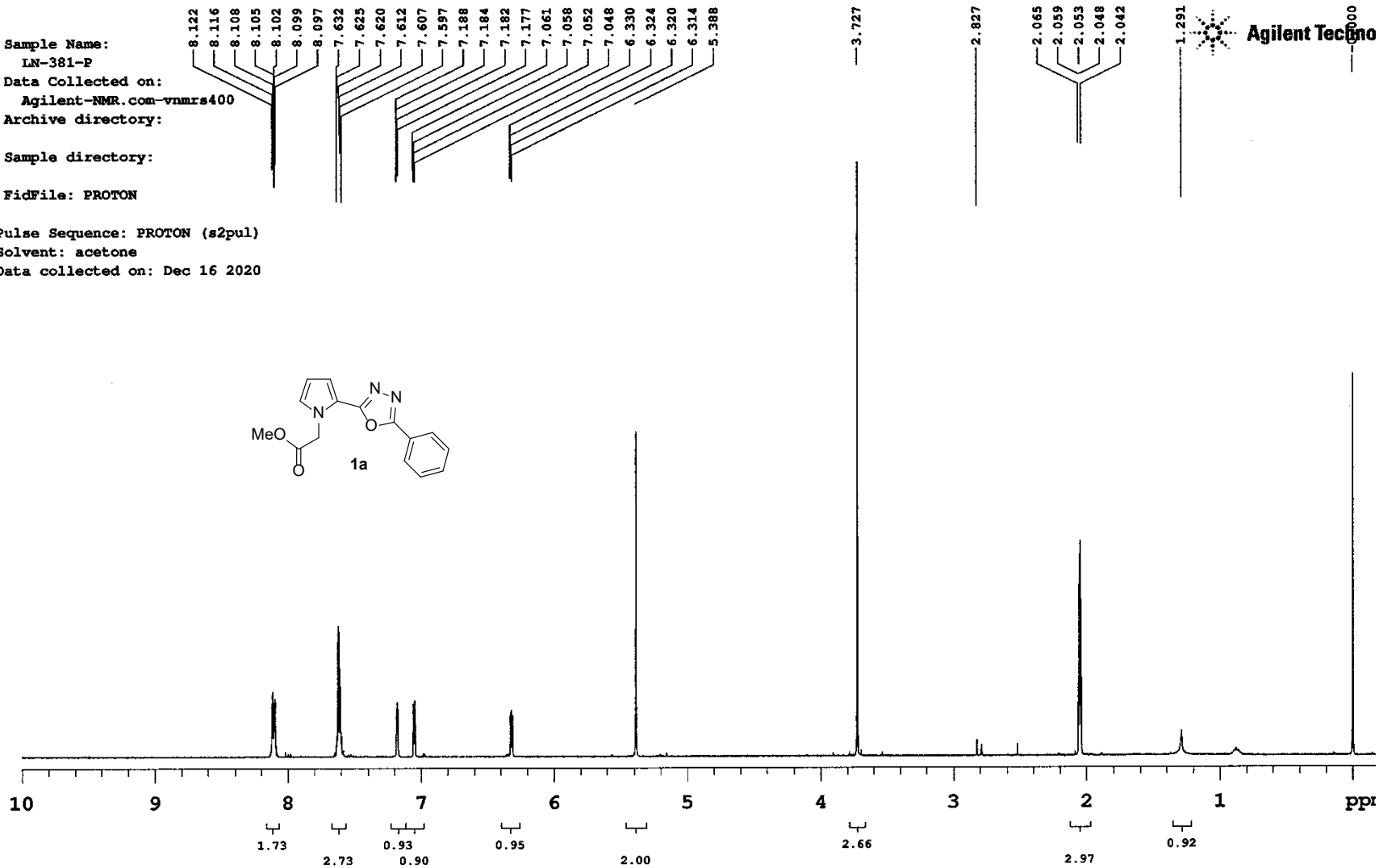
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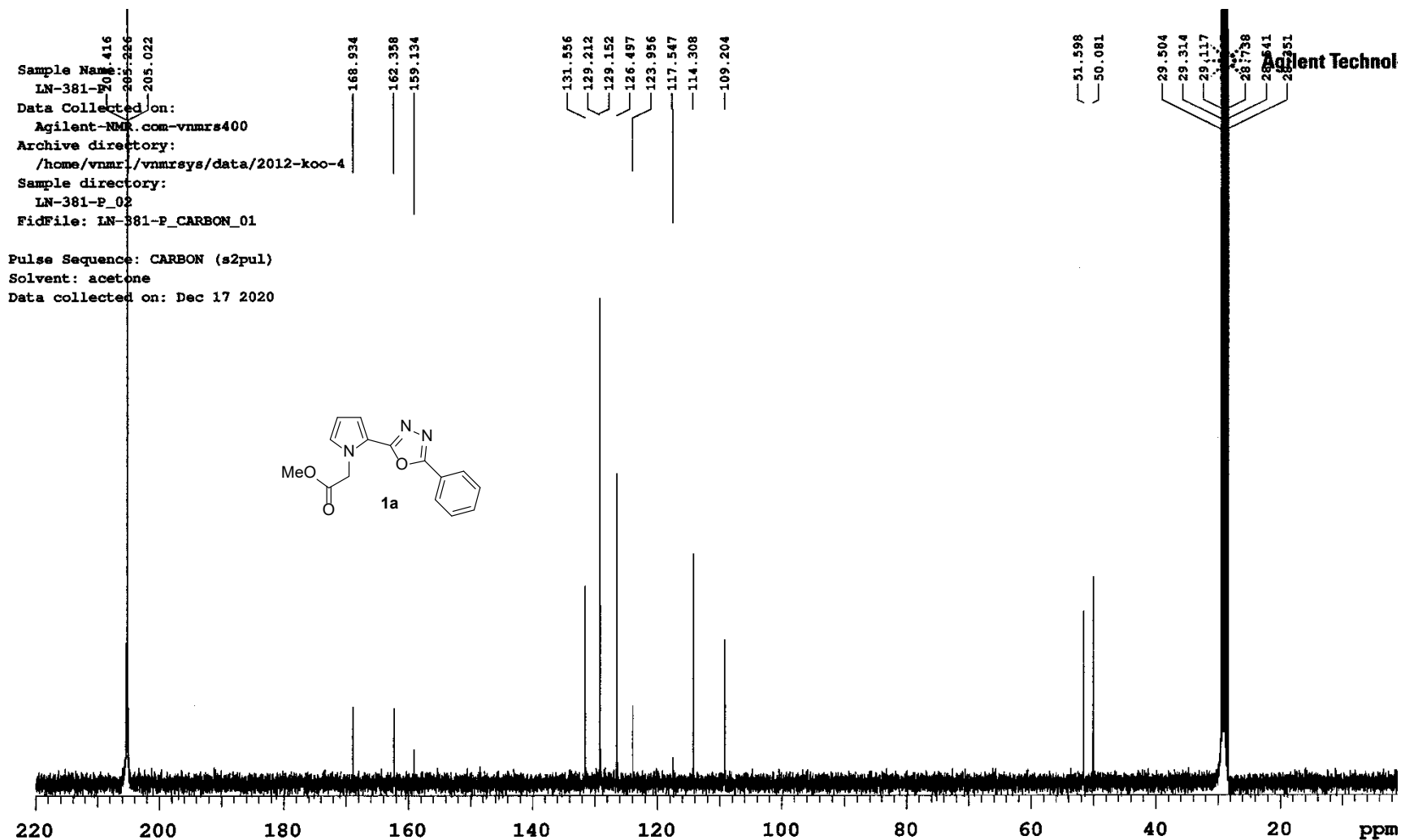
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: acetone

Data collected on: Dec 16 2020

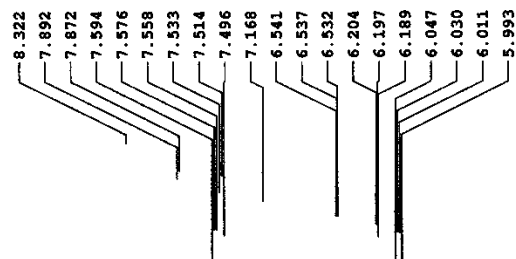




Sample Name:
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Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2012-koo-4
Sample directory:
LN-265-1_01
FidFile: LN-265-1_PROTON_01

Pulse Sequence: PROTON (s2pul)
Solvent: dmsd
Data collected on: Dec 4 2020

11.513



3.673

3.356

2.508

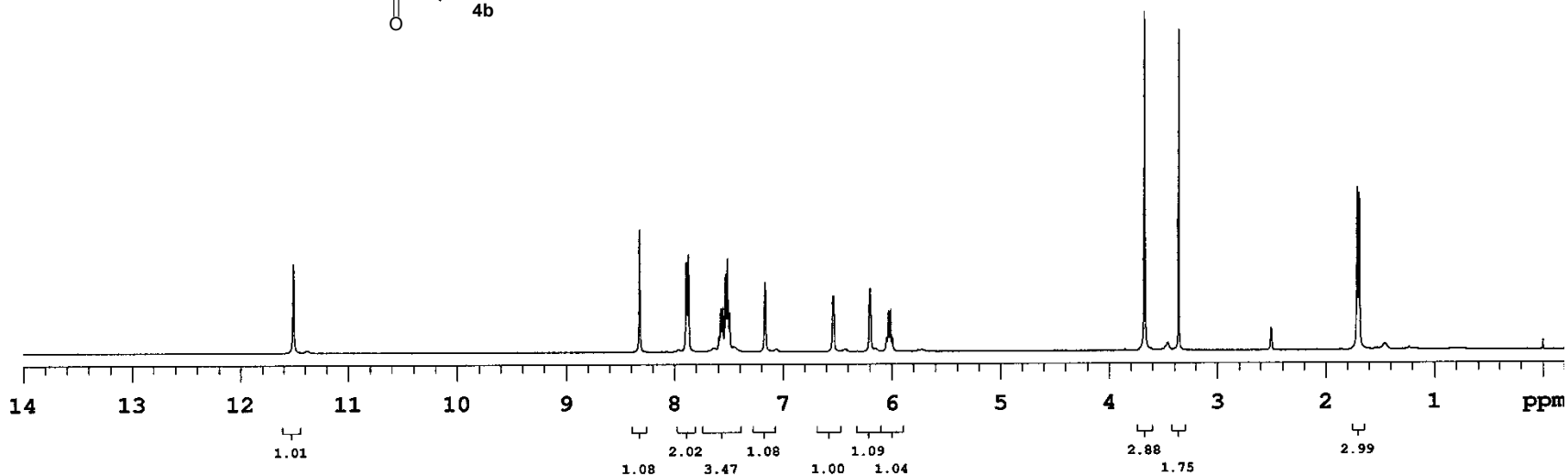
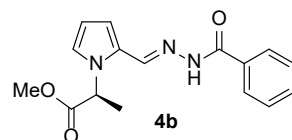
2.503

2.499

1.710

1.691

Agilent Technol



Sample Name:

LN-265-1

Data Collected on:

Agilent-NMR.com-vnmrs400

Archive directory:

/home/vnmr1/vnmrsys/data/2012-koo-4

Sample directory:

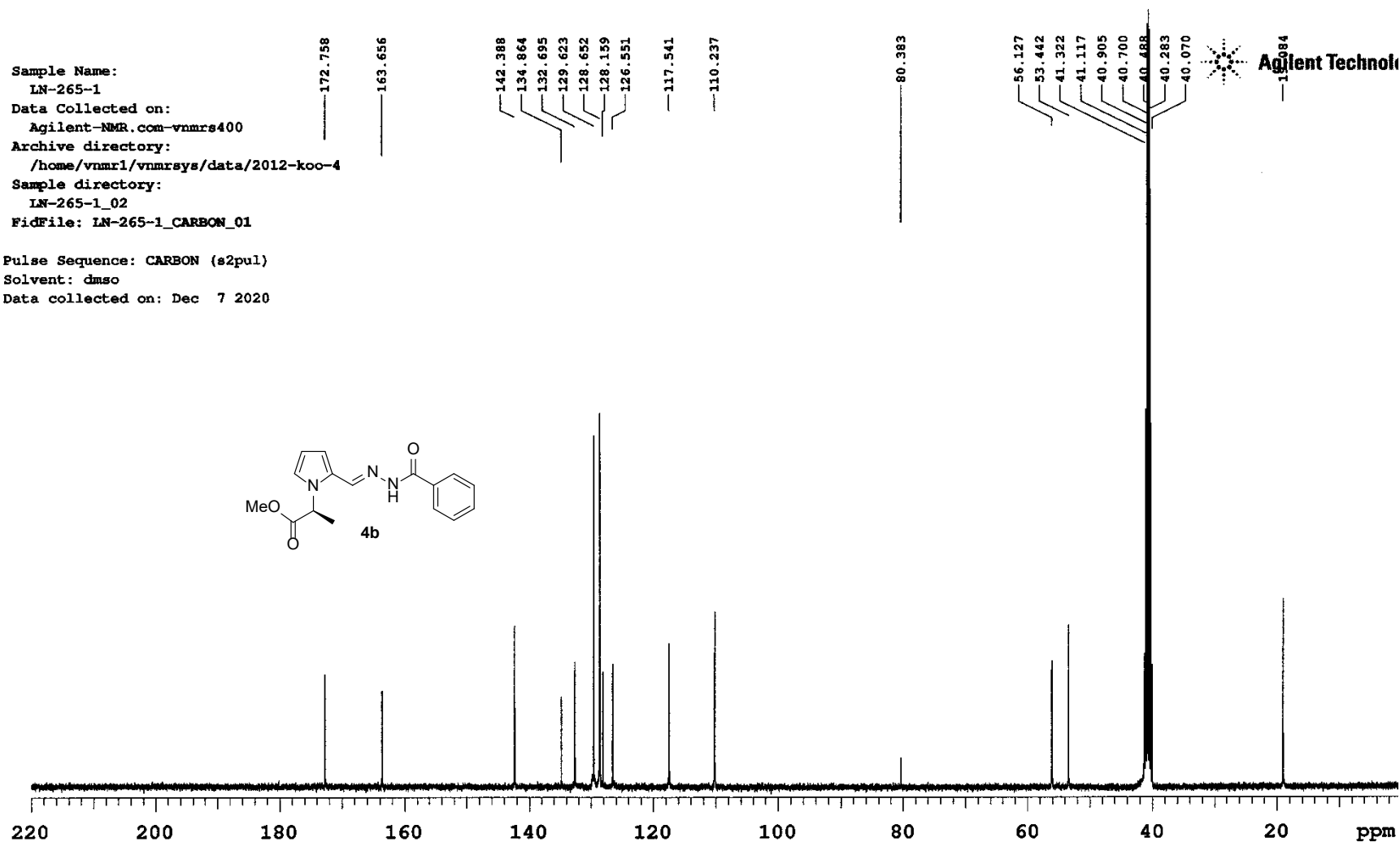
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FidFile: LN-265-1_CARBON_01

Pulse Sequence: CARBON (s2pul)

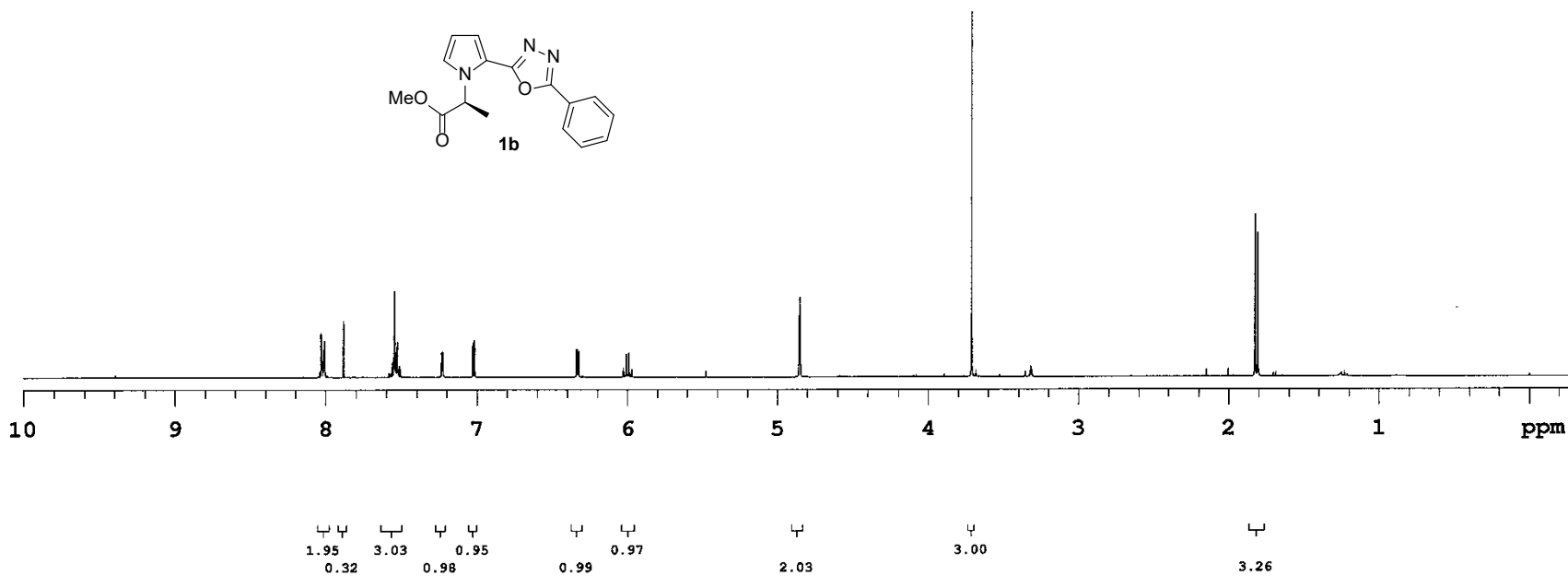
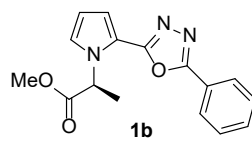
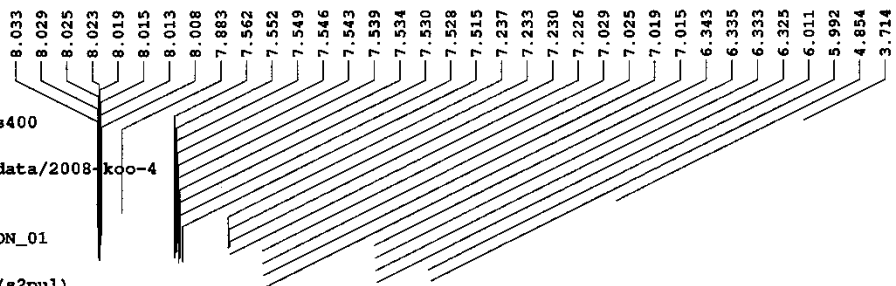
Solvent: dmsd

Data collected on: Dec 7 2020



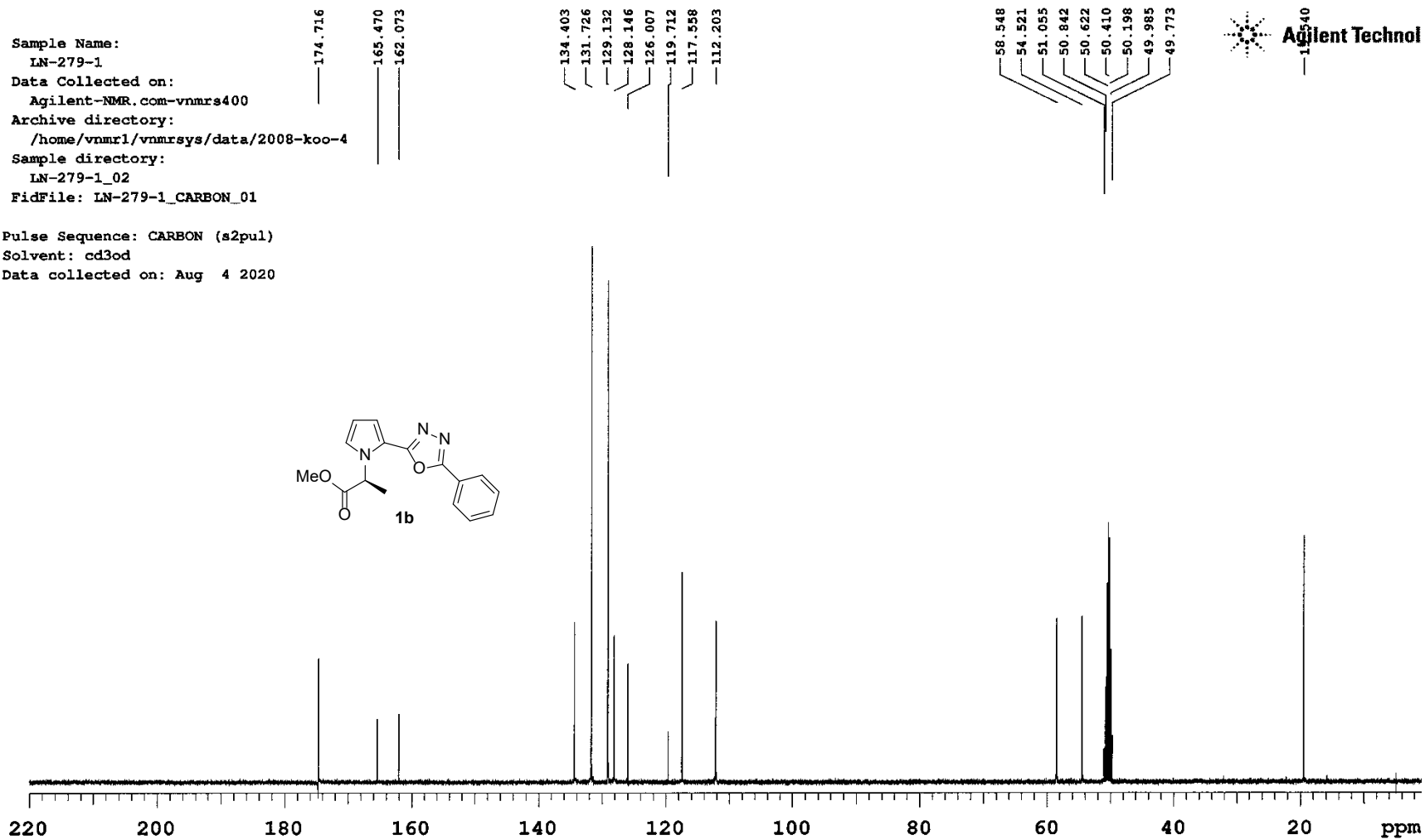
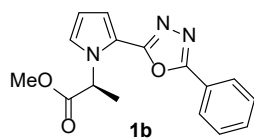
Sample Name:
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 Data Collected on:
 Agilent-NMR.com-vnmrs400
 Archive directory:
 /home/vnmr1/vnmrsys/data/2008-koo-4
 Sample directory:
 LN-279-P_01
 FidFile: LN-279-P_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cd3od
 Data collected on: Aug 6 2020



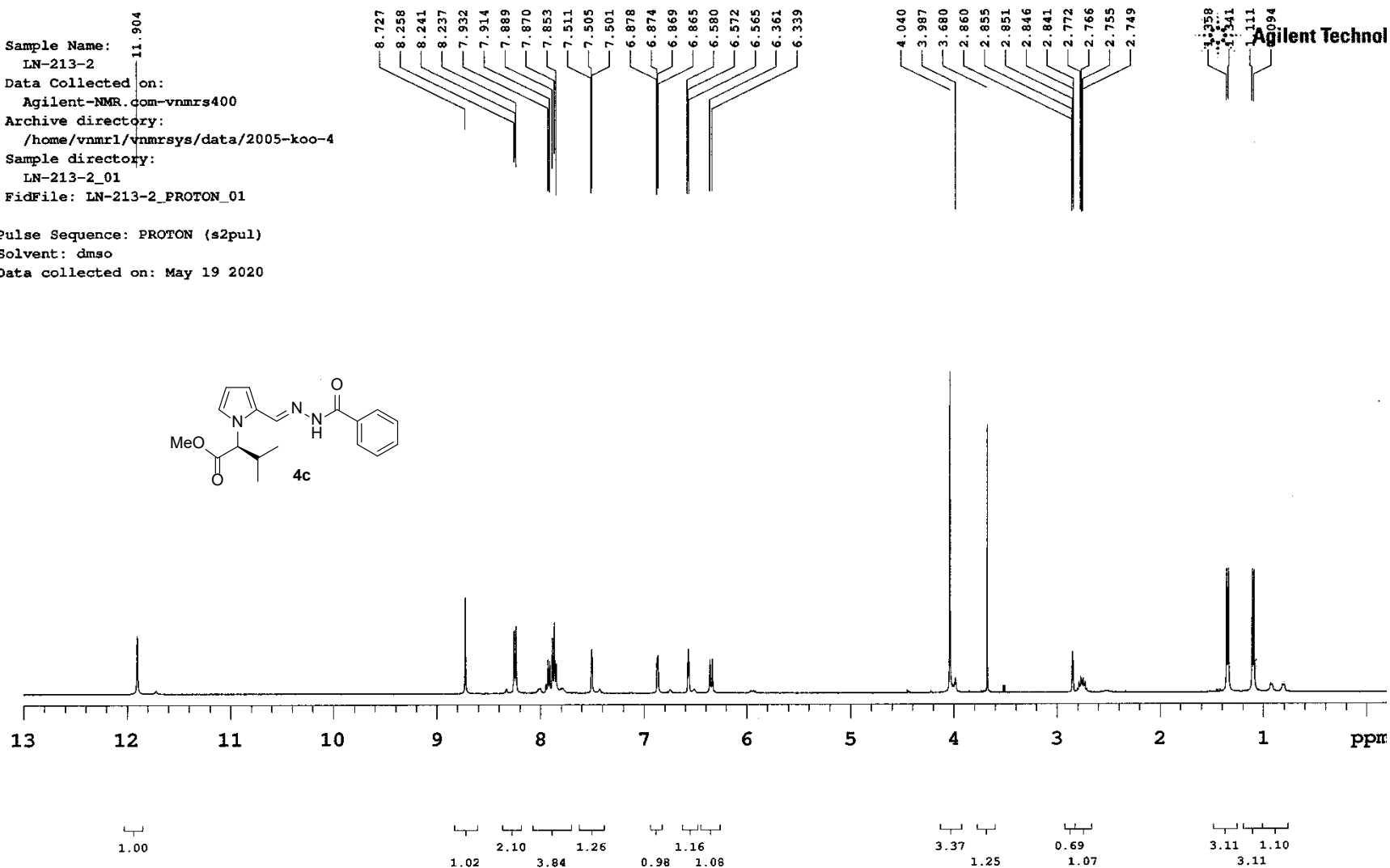
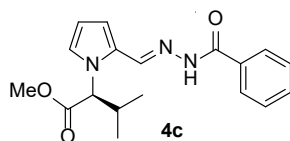
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LN-279-1
Data Collected on:
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Archive directory:
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Sample directory:
LN-279-1_02
FidFile: LN-279-1_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Aug 4 2020



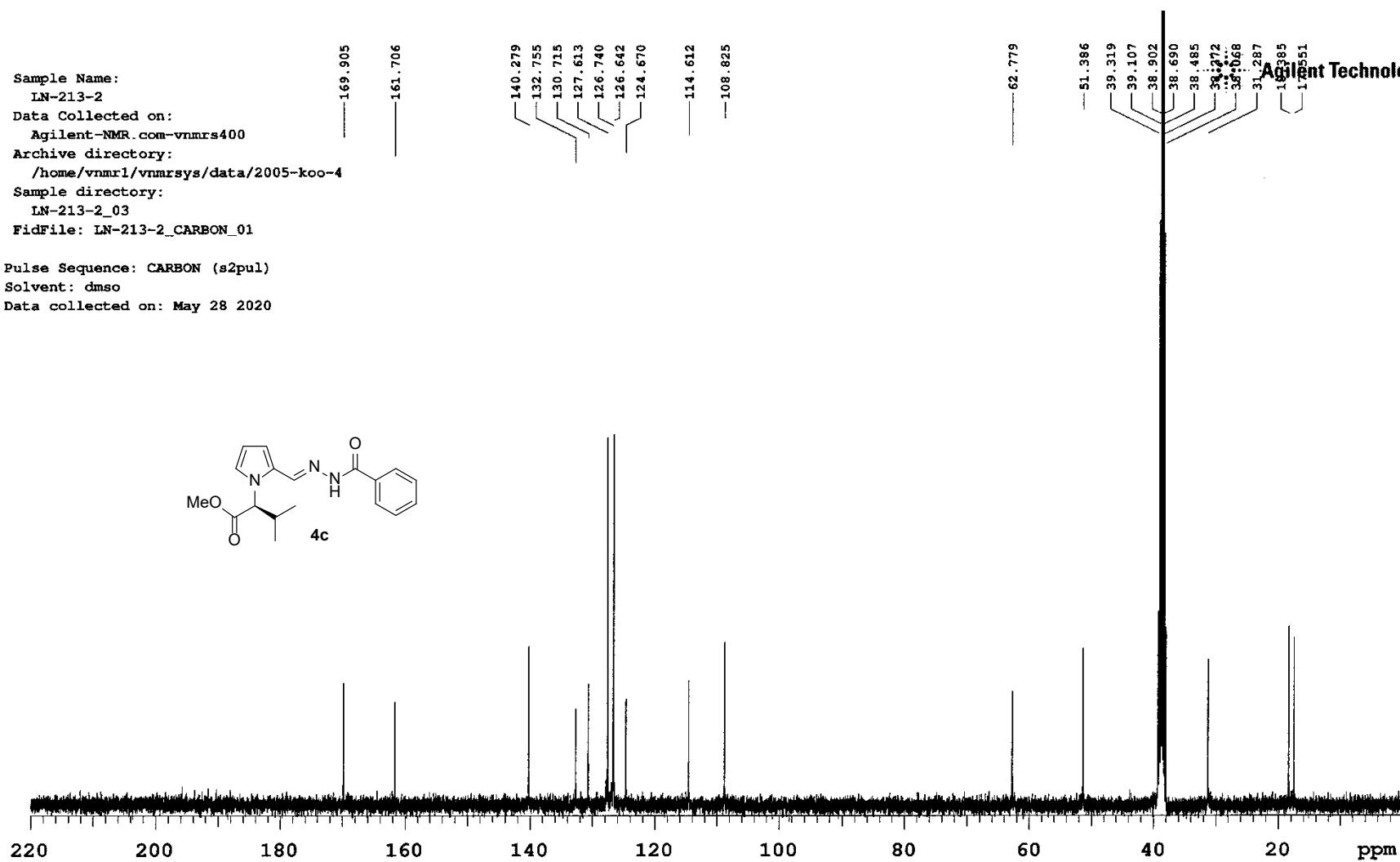
Sample Name: LN-213-2
 Data Collected on: Agilent-NMR.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2005-koo-4
 Sample directory: LN-213-2_01
 FidFile: LN-213-2_PROTON_01

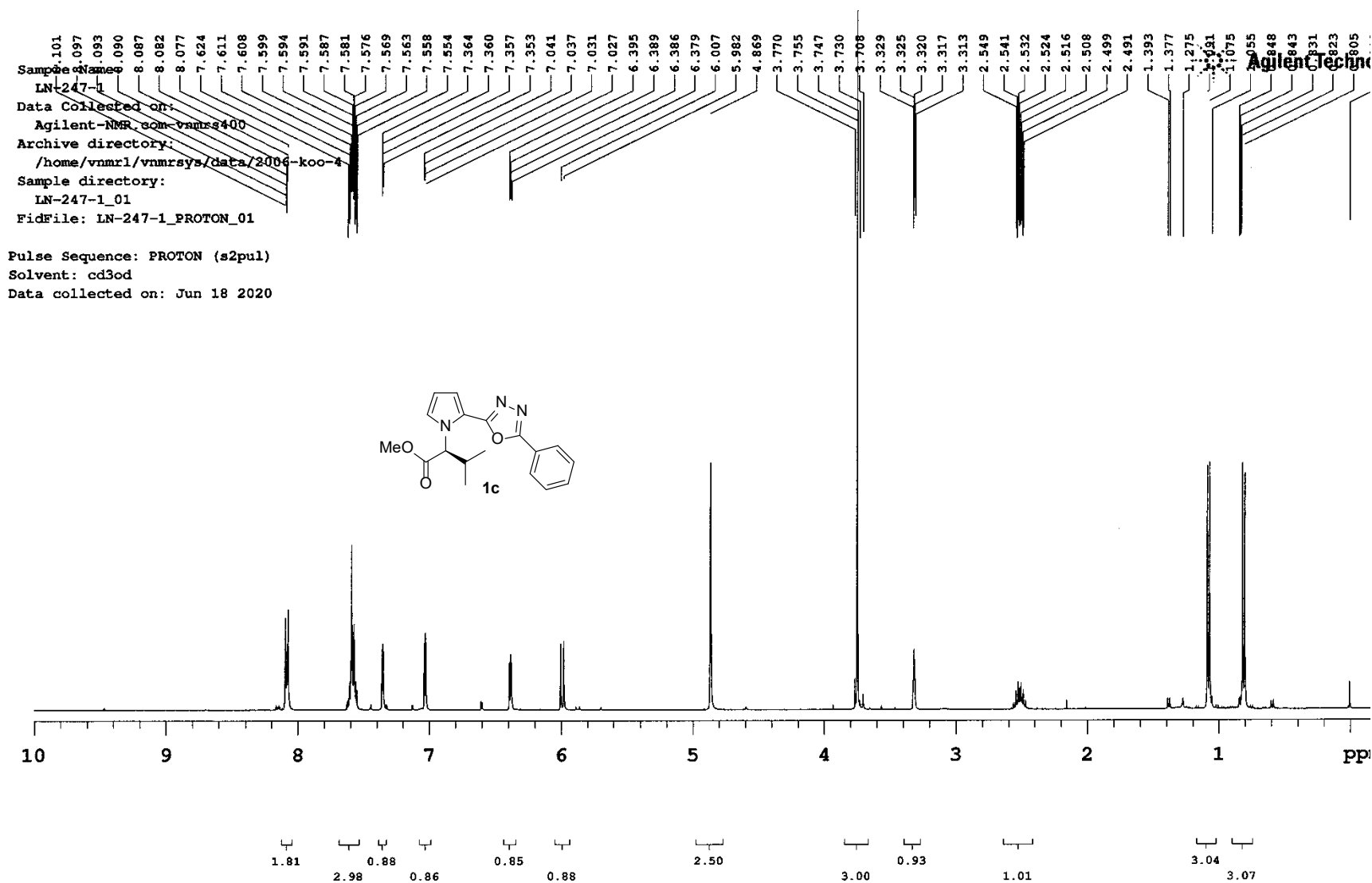
Pulse Sequence: PROTON (s2pul)
 Solvent: dmso
 Data collected on: May 19 2020



Sample Name:
LN-213-2
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2005-koo-4
Sample directory:
LN-213-2_03
FidFile: LN-213-2_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: dmsd
Data collected on: May 28 2020





Sample Name:

LN-367-2

Data Collected on:

Agilent-NMR.com-vnmrs400

Archive directory:

/home/vnmr1/vnmrsys/data/2011-koo-4

Sample directory:

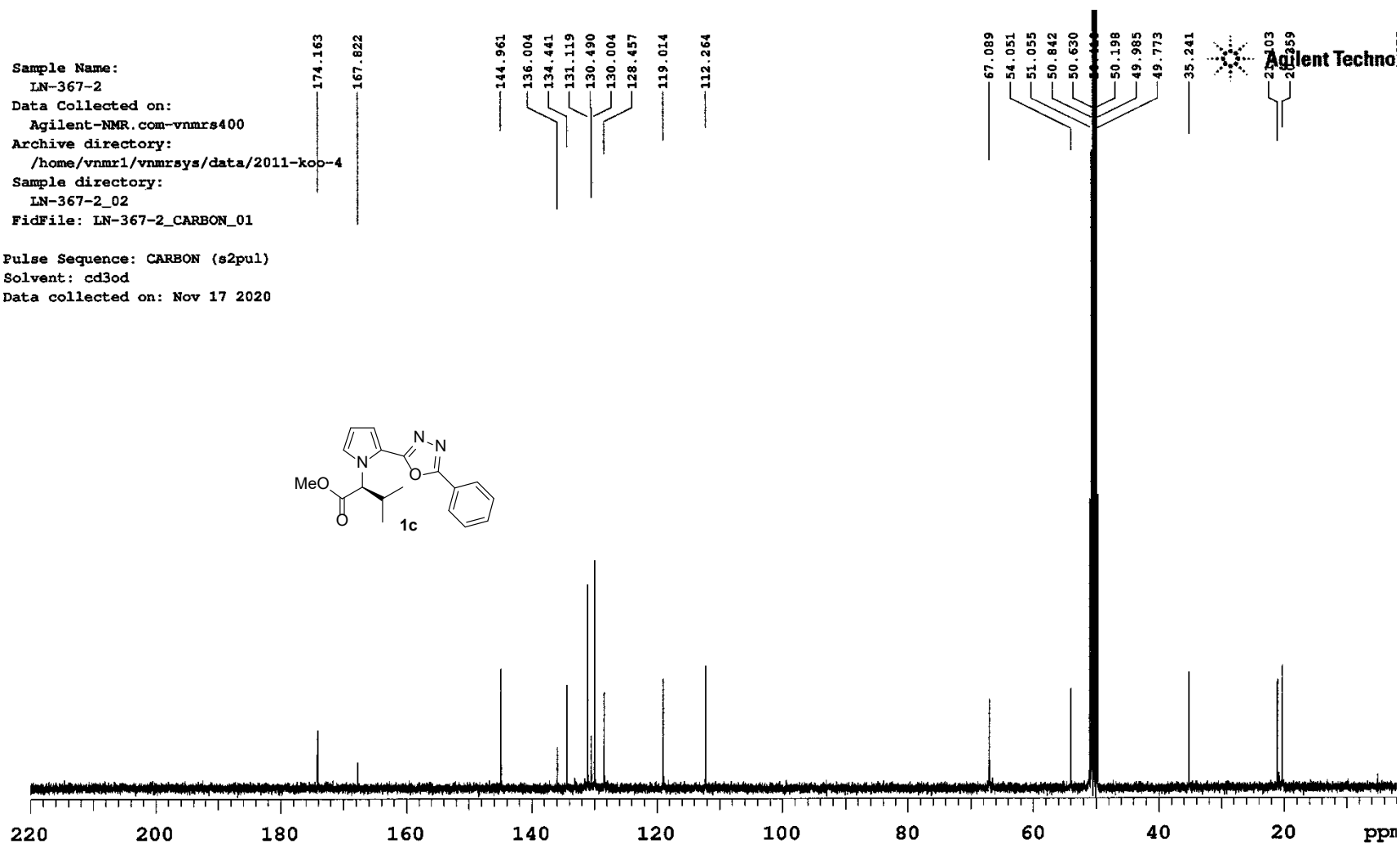
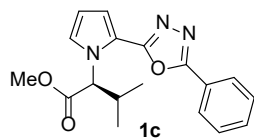
LN-367-2_02

FidFile: LN-367-2_CARBON_01

Pulse Sequence: CARBON (s2pul)

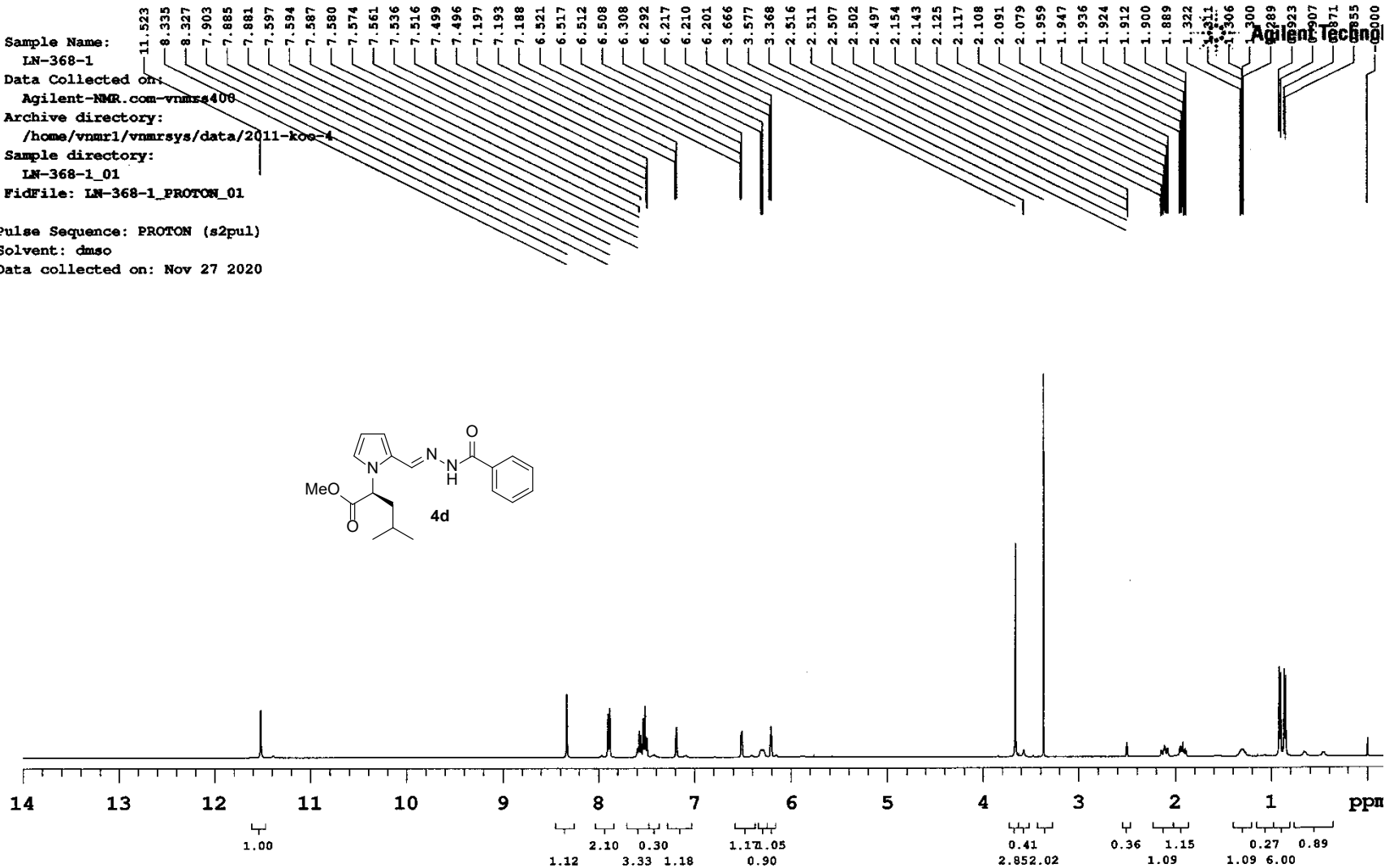
Solvent: cd3od

Data collected on: Nov 17 2020



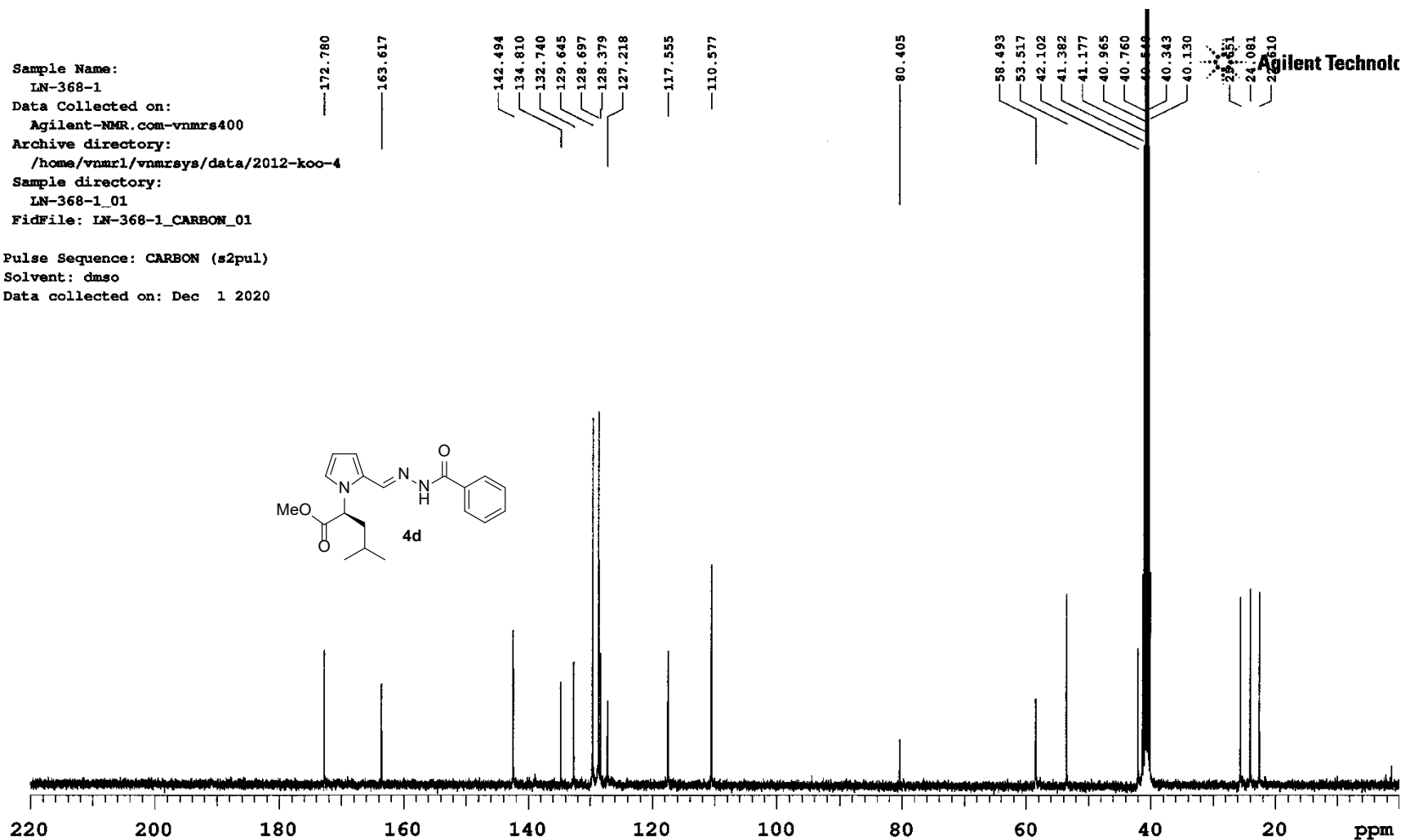
Sample Name: LN-368-1
 Data Collected on: Agilent-NMR.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2011-koe-4
 Sample directory: LN-368-1_01
 FidFile: LN-368-1_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: dmsc
 Data collected on: Nov 27 2020



Sample Name:
 LN-368-1
 Data Collected on:
 Agilent-NMR.com-vnmrs400
 Archive directory:
 /home/vnmr1/vnmrsys/data/2012-koo-4
 Sample directory:
 LN-368-1_01
 FidFile: LN-368-1_CARBON_01

Pulse Sequence: CARBON (s2pul)
 Solvent: dmsd
 Data collected on: Dec 1 2020



Sample Name:

LN-383-1

Data Collected on:

Agilent-NMR.com-vnmr400

Archive directory:

/home/vnmr1/vnmr400/data/2012-10-16

Sample directory:

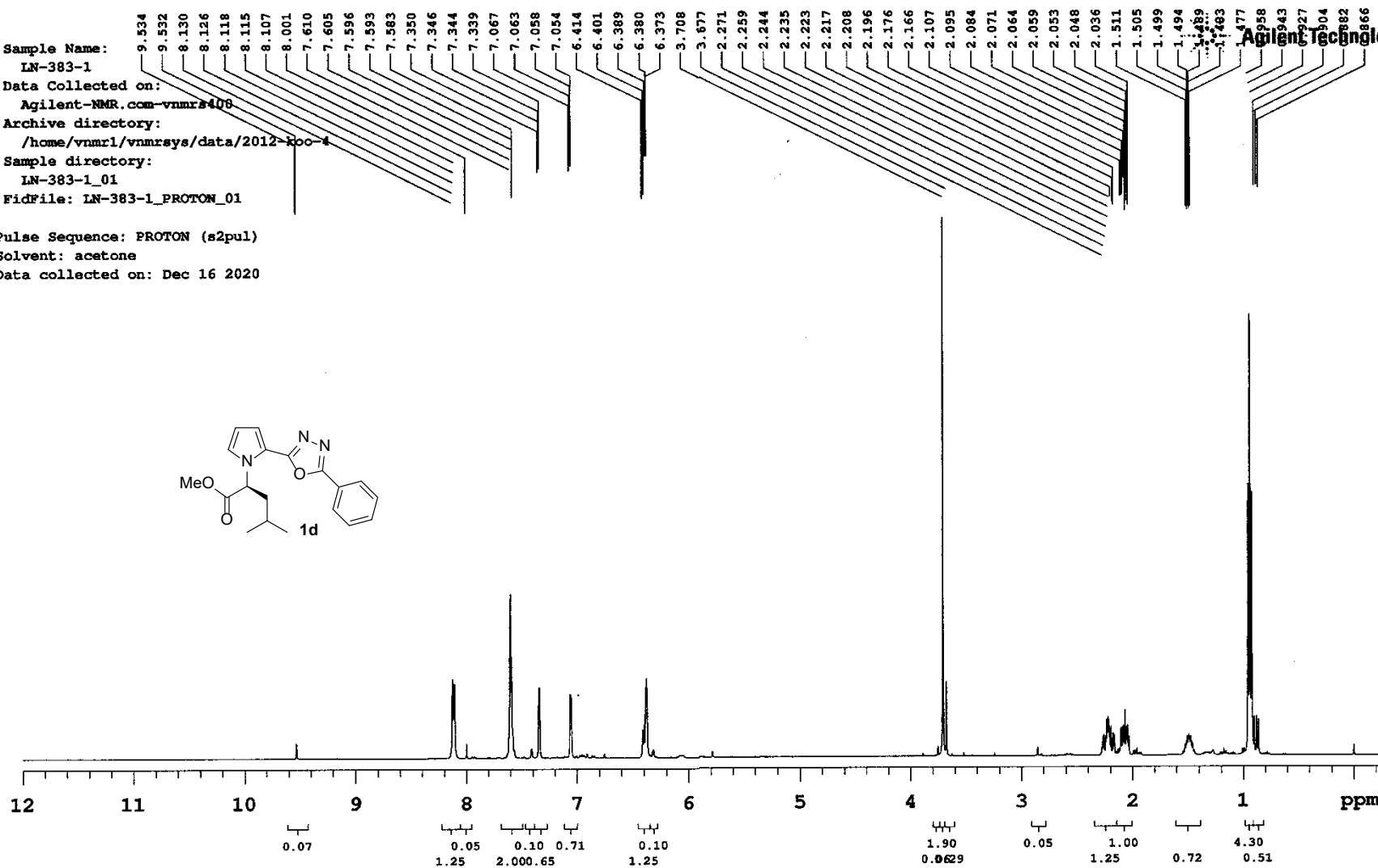
LN-383-1_01

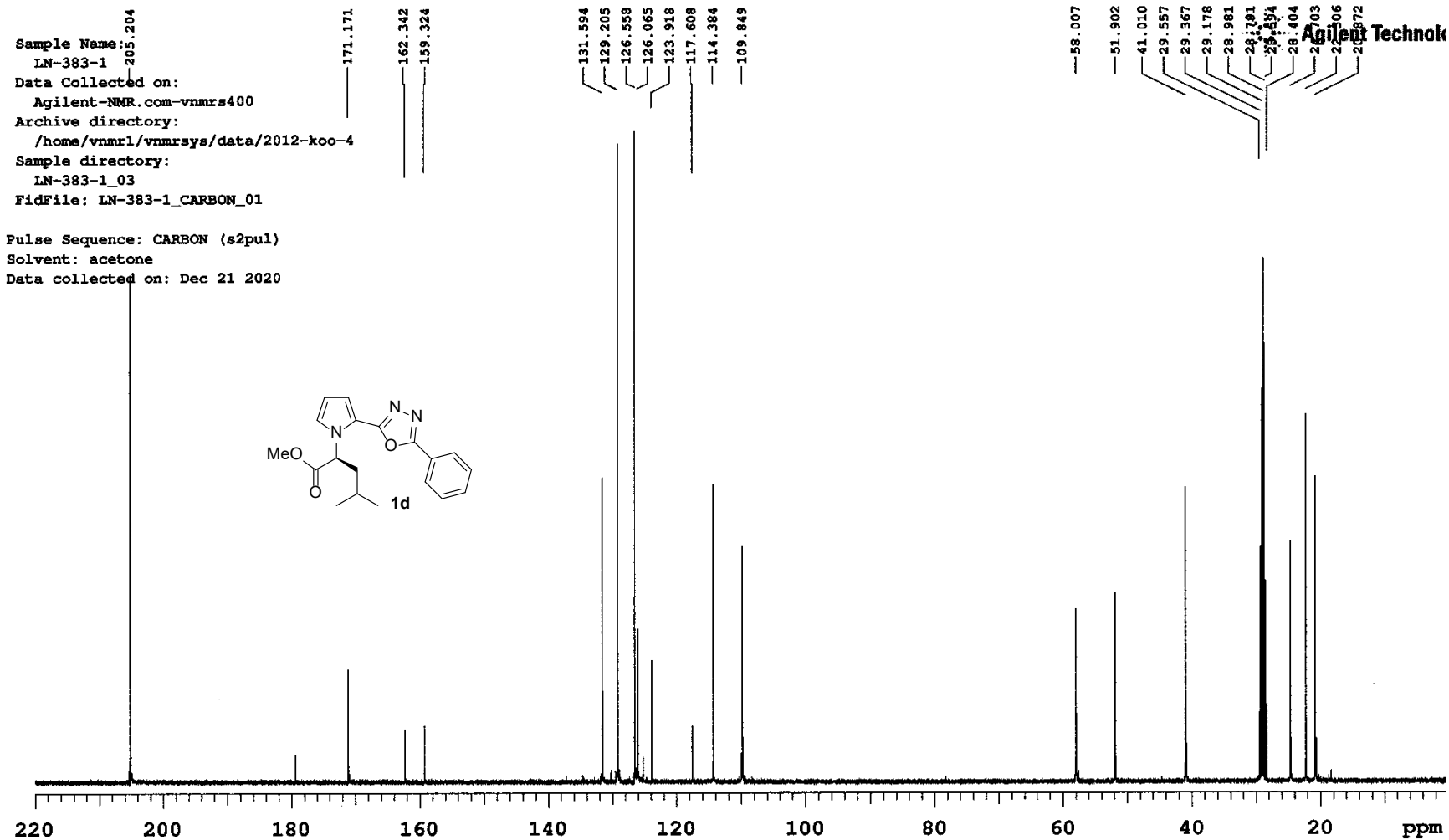
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Pulse Sequence: PROTON (s2pul)

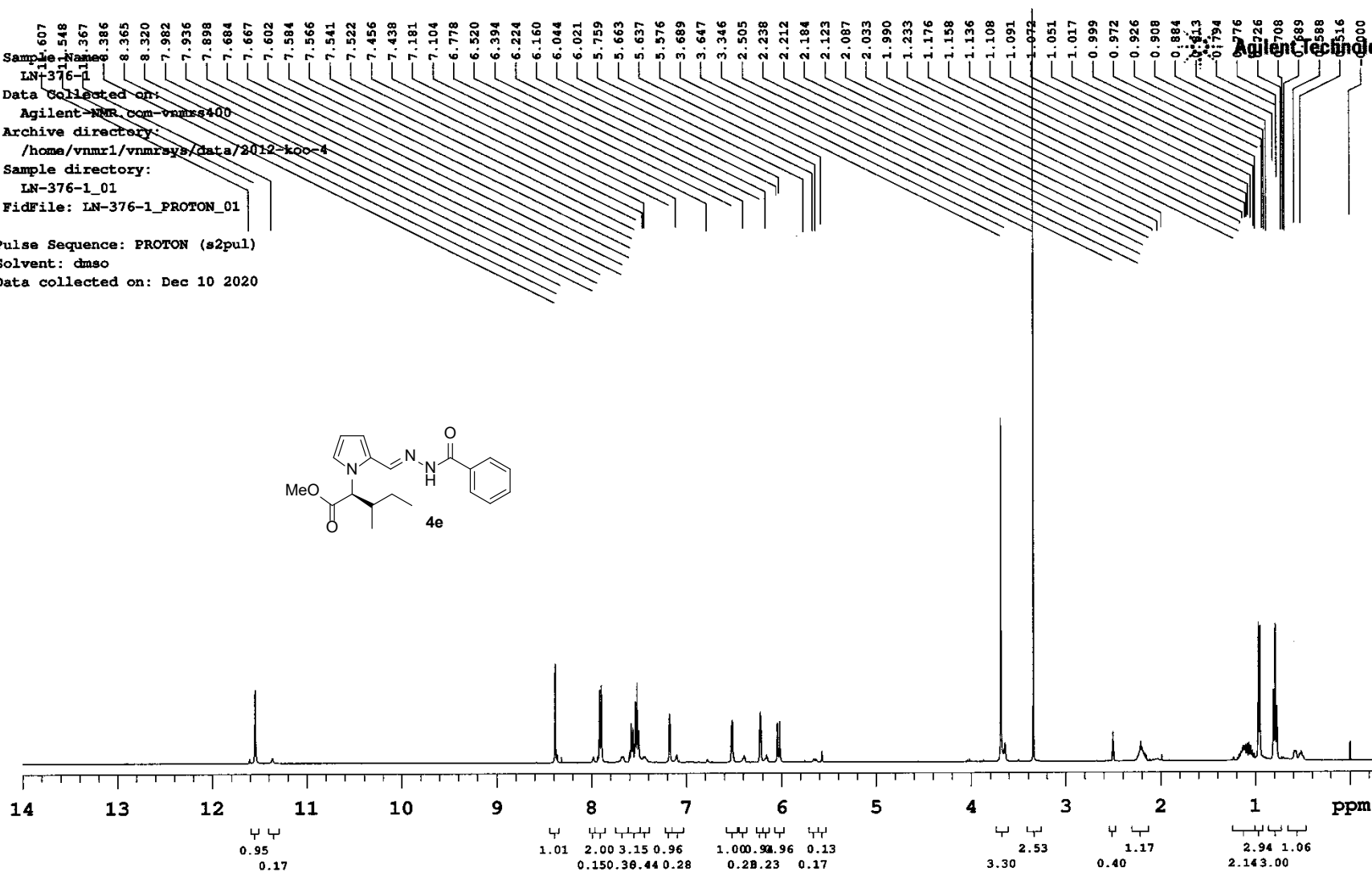
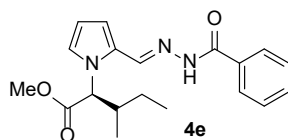
Solvent: acetone

Data collected on: Dec 16 2020



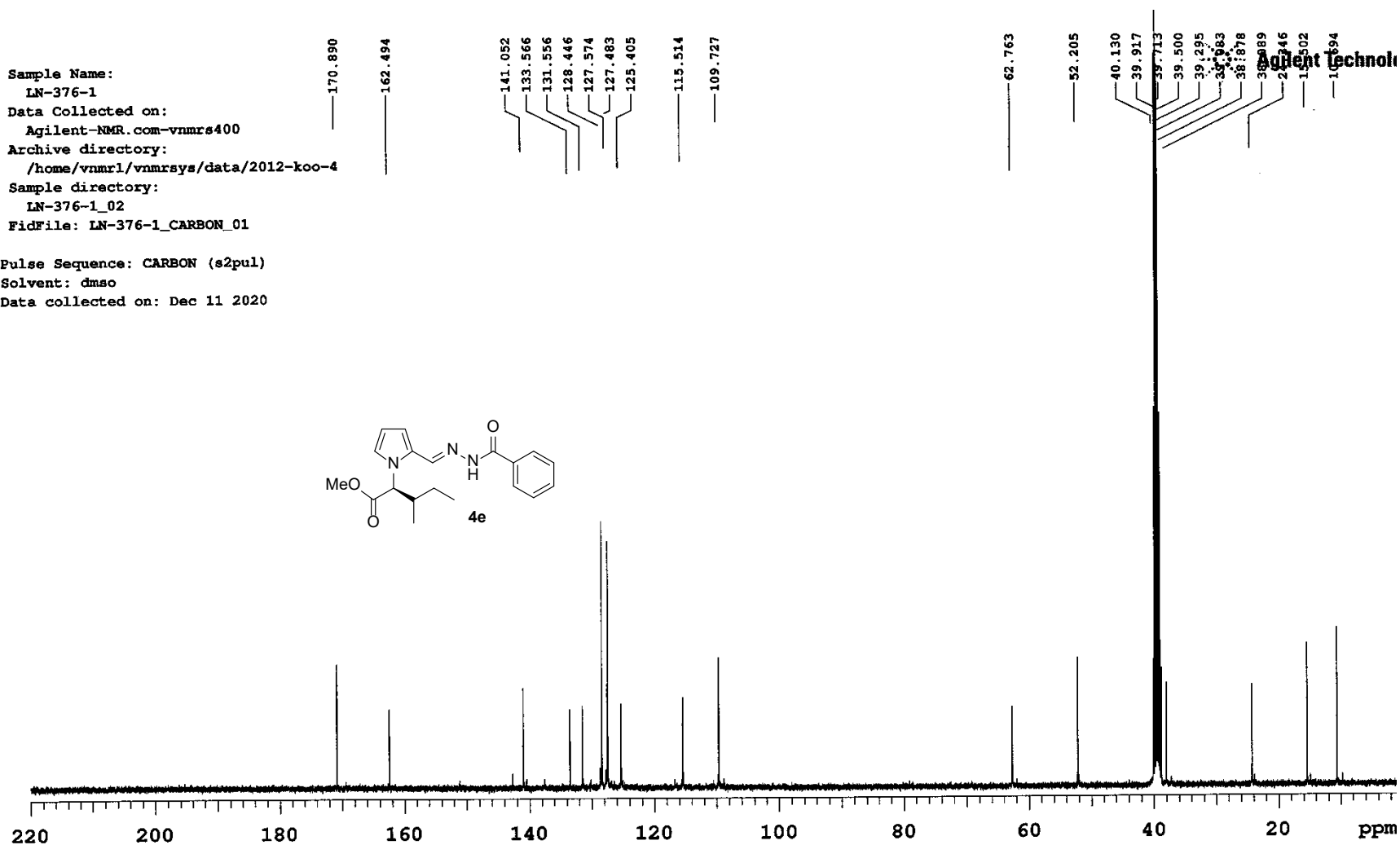


Sample Name: LN-376-1
 Data Collected on: Agilent-MMR-DM-VNMR400
 Archive directory: /home/vnmr1/vnmrsys/data/2012-koo-4
 Sample directory: LN-376-1_01
 FidFile: LN-376-1_PROTON_01
 Pulse Sequence: PROTON (s2pul)
 Solvent: dmsd
 Data collected on: Dec 10 2020



Sample Name:
LN-376-1
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2012-koo-4
Sample directory:
LN-376-1_02
FidFile: LN-376-1_CARBON_01

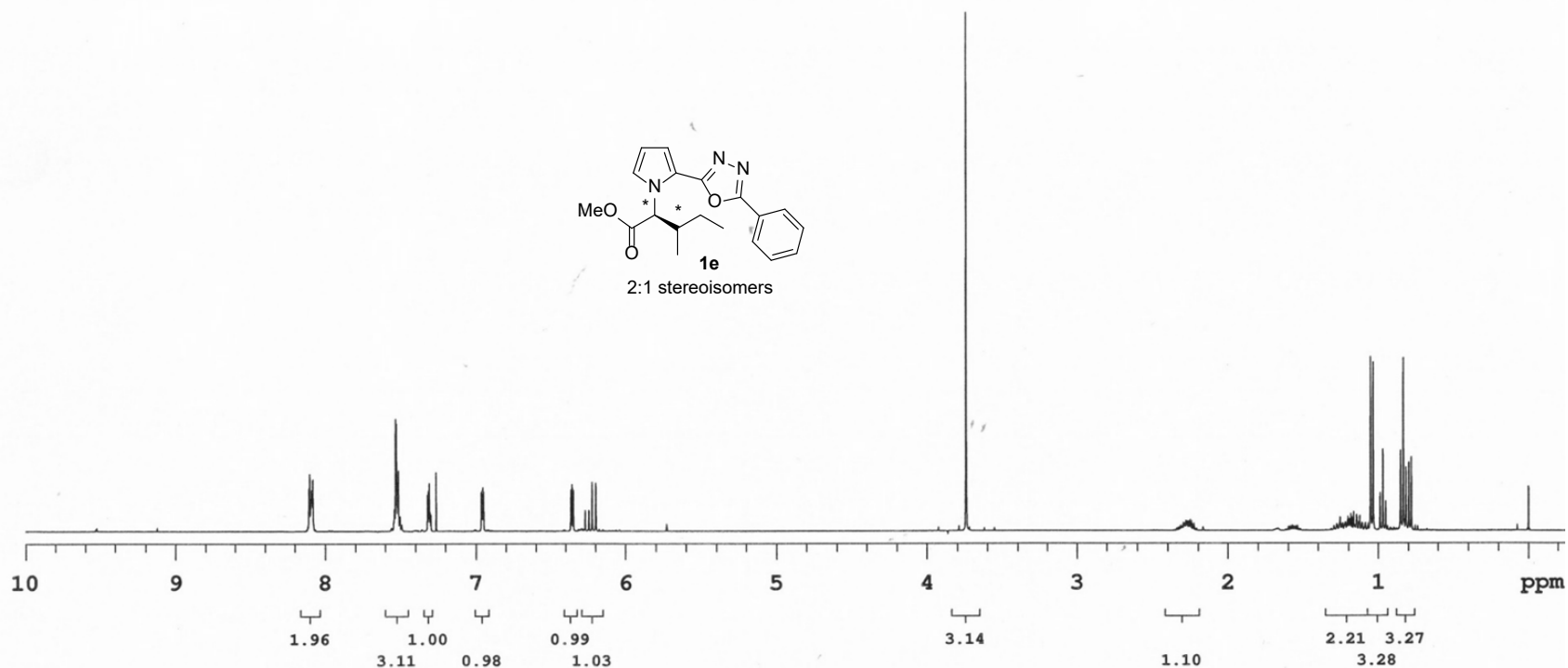
Pulse Sequence: CARBON (s2pul)
Solvent: dmsd
Data collected on: Dec 11 2020



108
 104
 096
 091
 8.084
 7.545
 7.540
 7.533
 7.528
 7.514
 7.506
 7.502
 7.320
 7.313
 7.309
 7.304
 7.297
 7.263
 6.966
 6.961
 6.956
 6.951
 6.366
 6.359
 6.356
 6.349
 6.270
 6.246
 6.223
 6.199
 3.744
 2.301
 2.292
 2.285
 2.276
 2.269
 2.261
 2.253
 2.245
 1.256
 1.238
 1.222
 1.209
 1.204
 1.194
 1.184
 1.176
 1.166
 1.147
 1.143
 1.130
 1.125
 1.109
 1.052
 1.036
 0.989
 0.970
 0.952
 0.953
 0.834
 0.826
 0.816
 0.796
 0.779
 0.000

Sample Name: YHS-396-aa
 Data Collected on: Agilent-NMR.chem.com-vnmrsg400
 Archive directory: /home/vnmr1/vnmrsys/data/2303-koo-1
 Sample directory: YHS-396-aa_01
 FidFile: YHS-396-aa_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Mar 29 2023



Sample Name:

YHS-396-aa-13C

Data Collected on:

Agilent-NMR.chem.com-vnmrs400

Archive directory:

/home/vnmr1/vnmrsys/data/2303-koo-1

Sample directory:

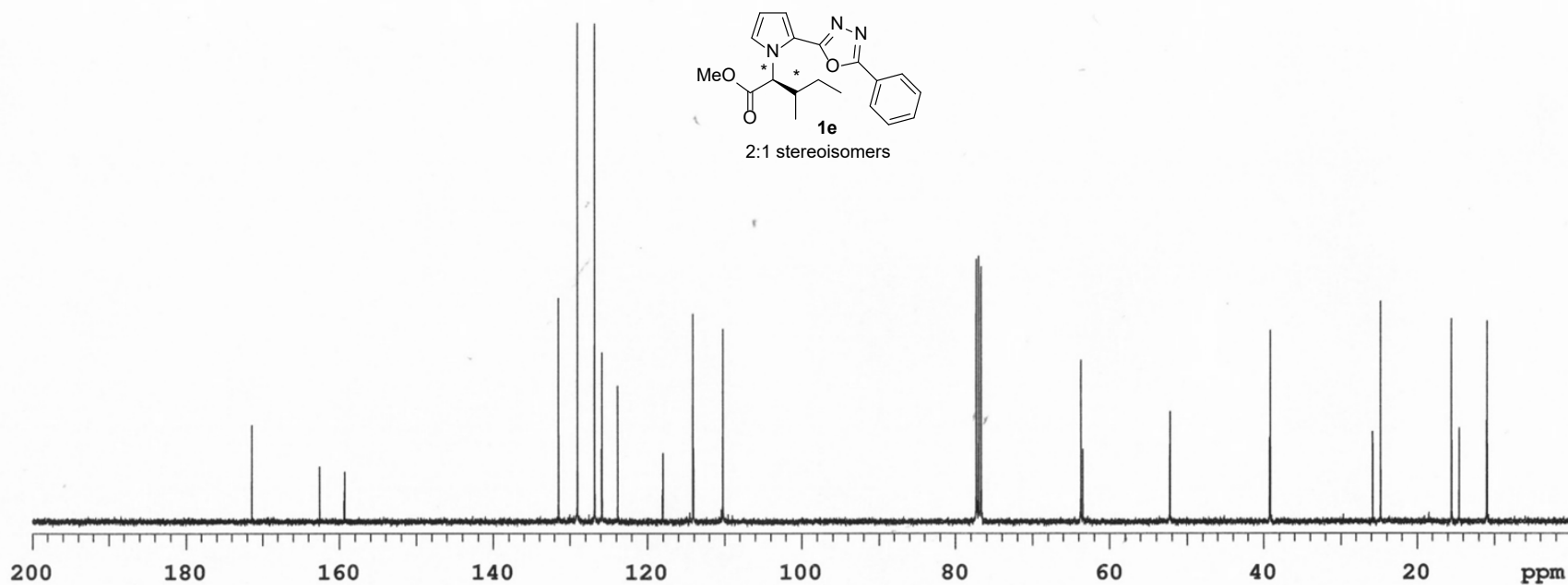
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FidFile: YHS-396-aa-13C CARBON_01

Pulse Sequence: CARBON (s2pul)

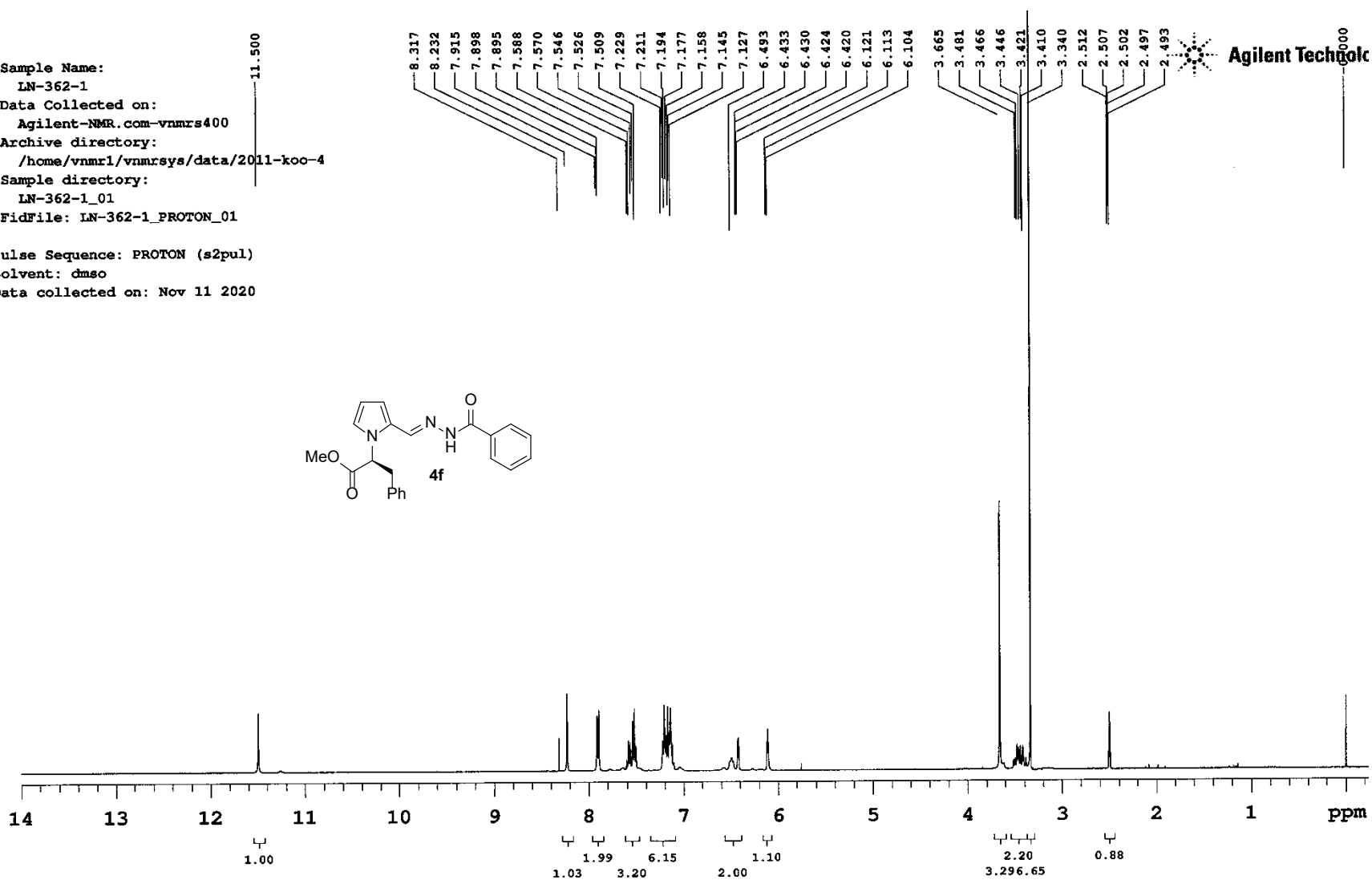
Solvent: cdcl3

Data collected on: Mar 29 2023



Sample Name:
 LN-362-1
 Data Collected on:
 Agilent-NMR.com-vnmrs400
 Archive directory:
 /home/vnmr1/vnmrsys/data/2011-koc-4
 Sample directory:
 LN-362-1_01
 FidFile: LN-362-1_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: dmsd
 Data collected on: Nov 11 2020

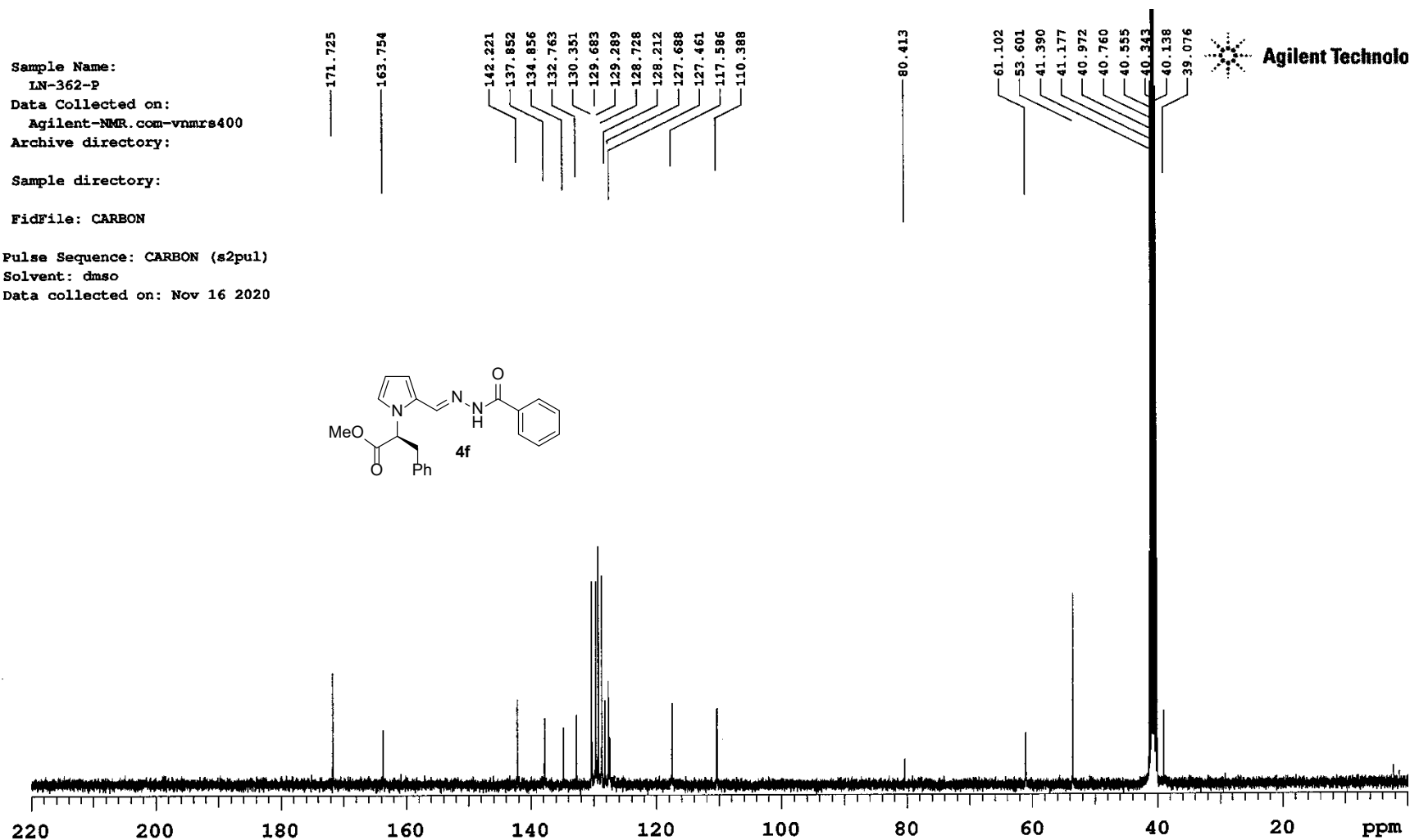
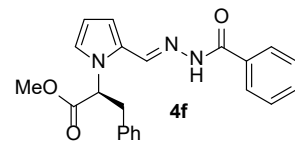


Sample Name:
LN-362-P
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:

Sample directory:

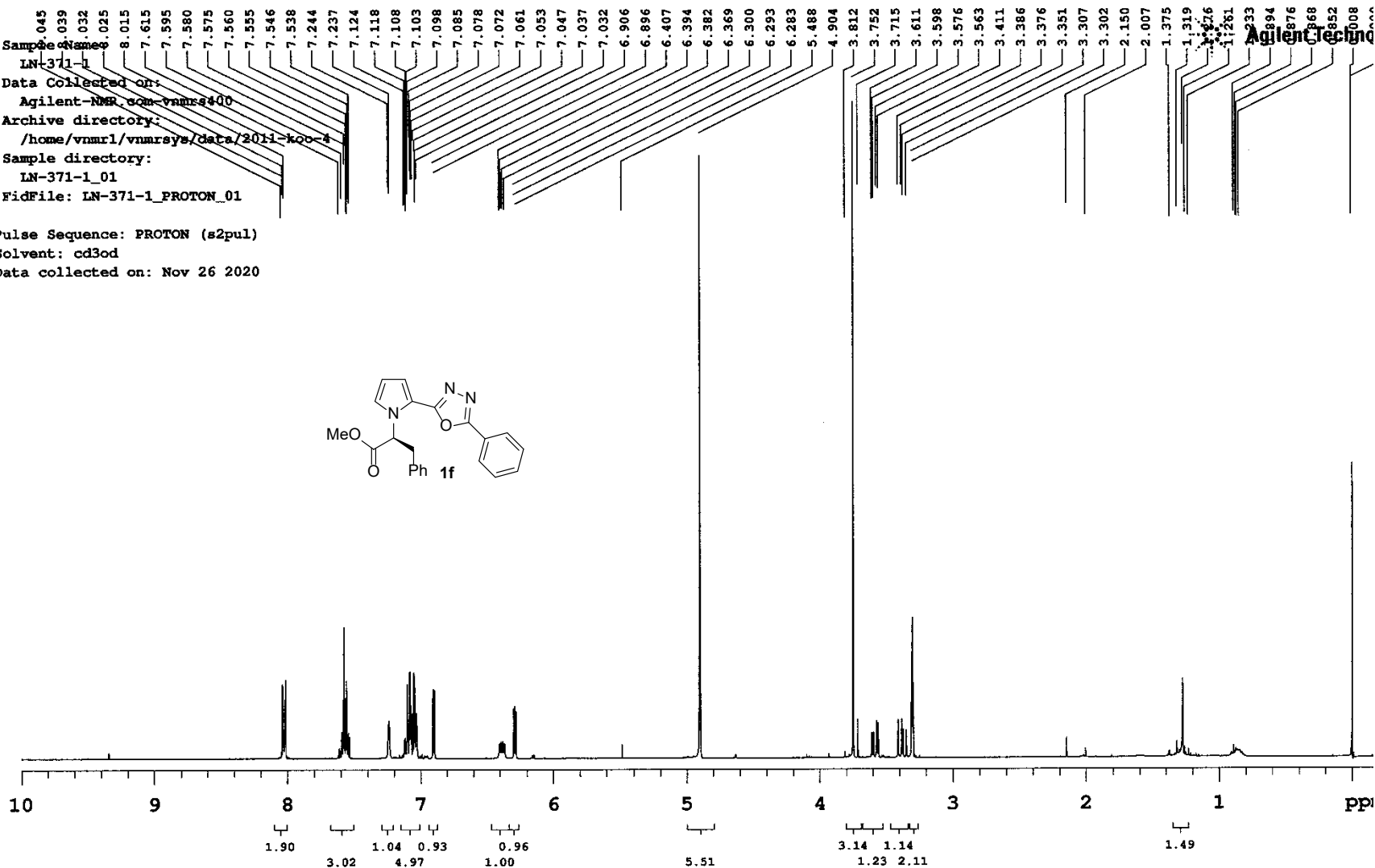
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: dmsd
Data collected on: Nov 16 2020



Sample Name: LN-371-1
 Data Collected on: Agilent-NMR.com-vnmr4400
 Archive directory: /home/vnmr1/vnmrsys/data/2011-koo-4
 Sample directory: LN-371-1_01
 FidFile: LN-371-1_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cd3od
 Data collected on: Nov 26 2020



Sample Name:

LN-371-1

Data Collected on:

Agilent-NMR.com-vnmrs400

Archive directory:

/home/vnmr1/vnmrsys/data/2011-koo-4

Sample directory:

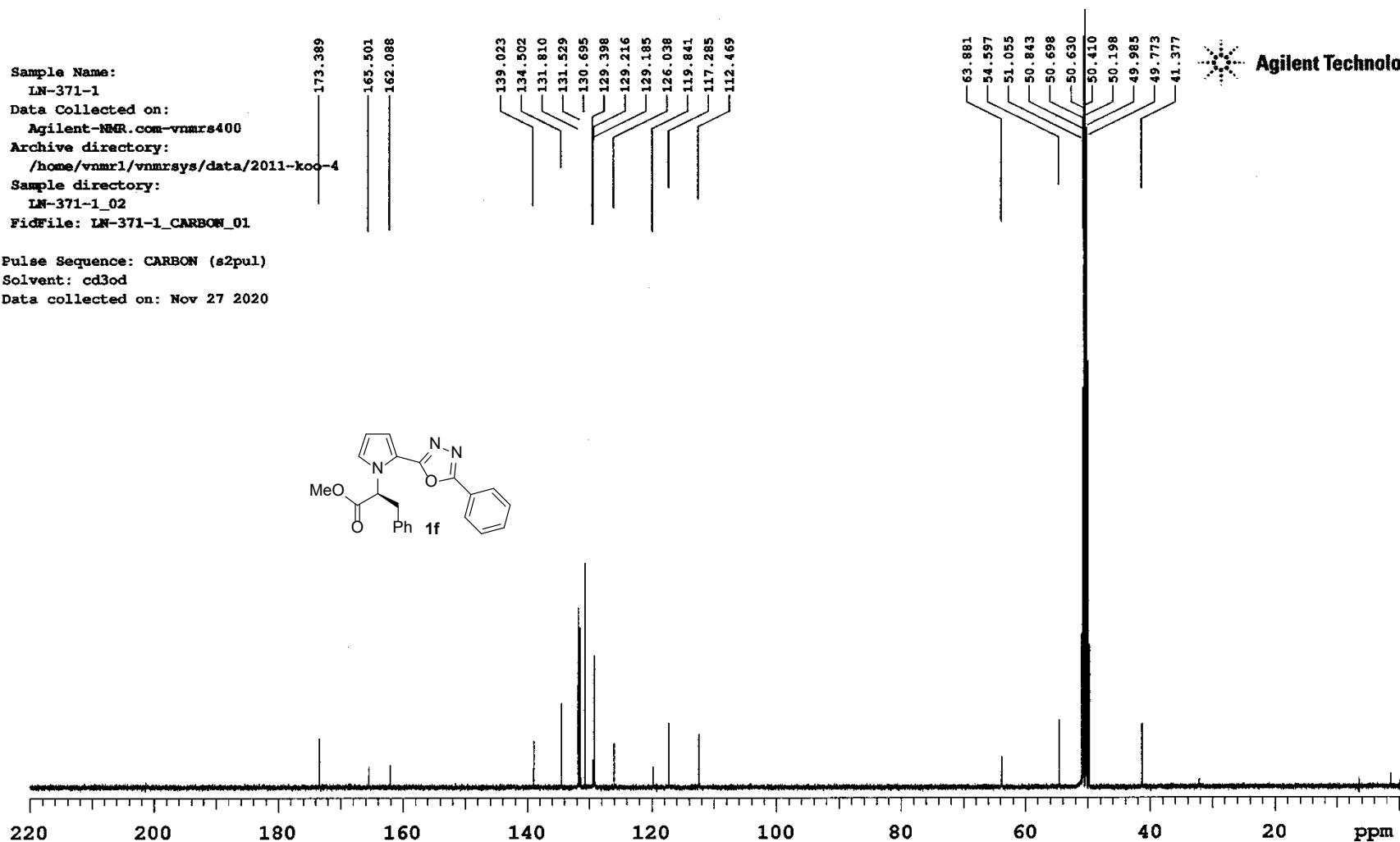
LN-371-1_02

FidFile: LN-371-1_CARBON_01

Pulse Sequence: CARBON (s2pul)

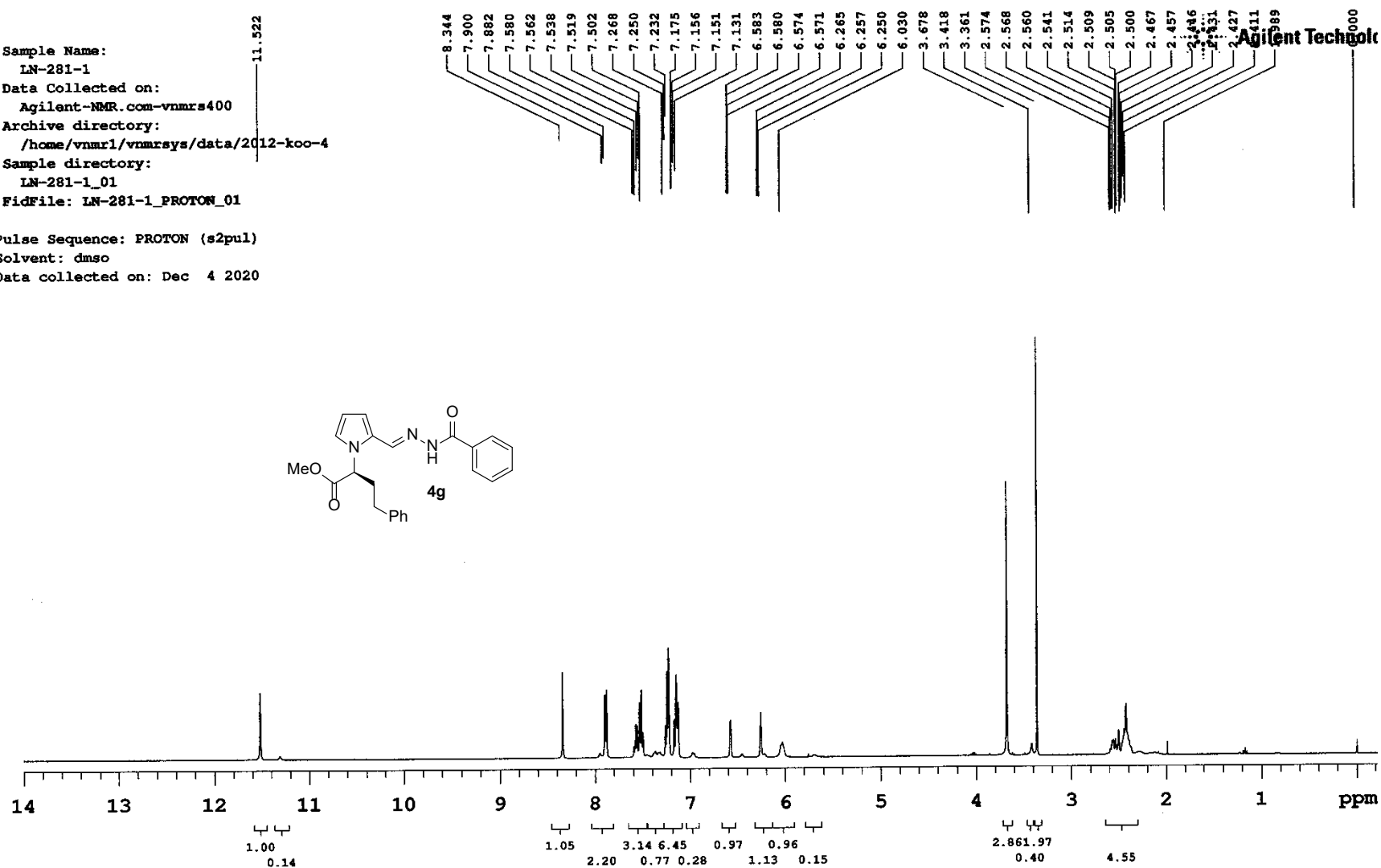
Solvent: cd3od

Data collected on: Nov 27 2020



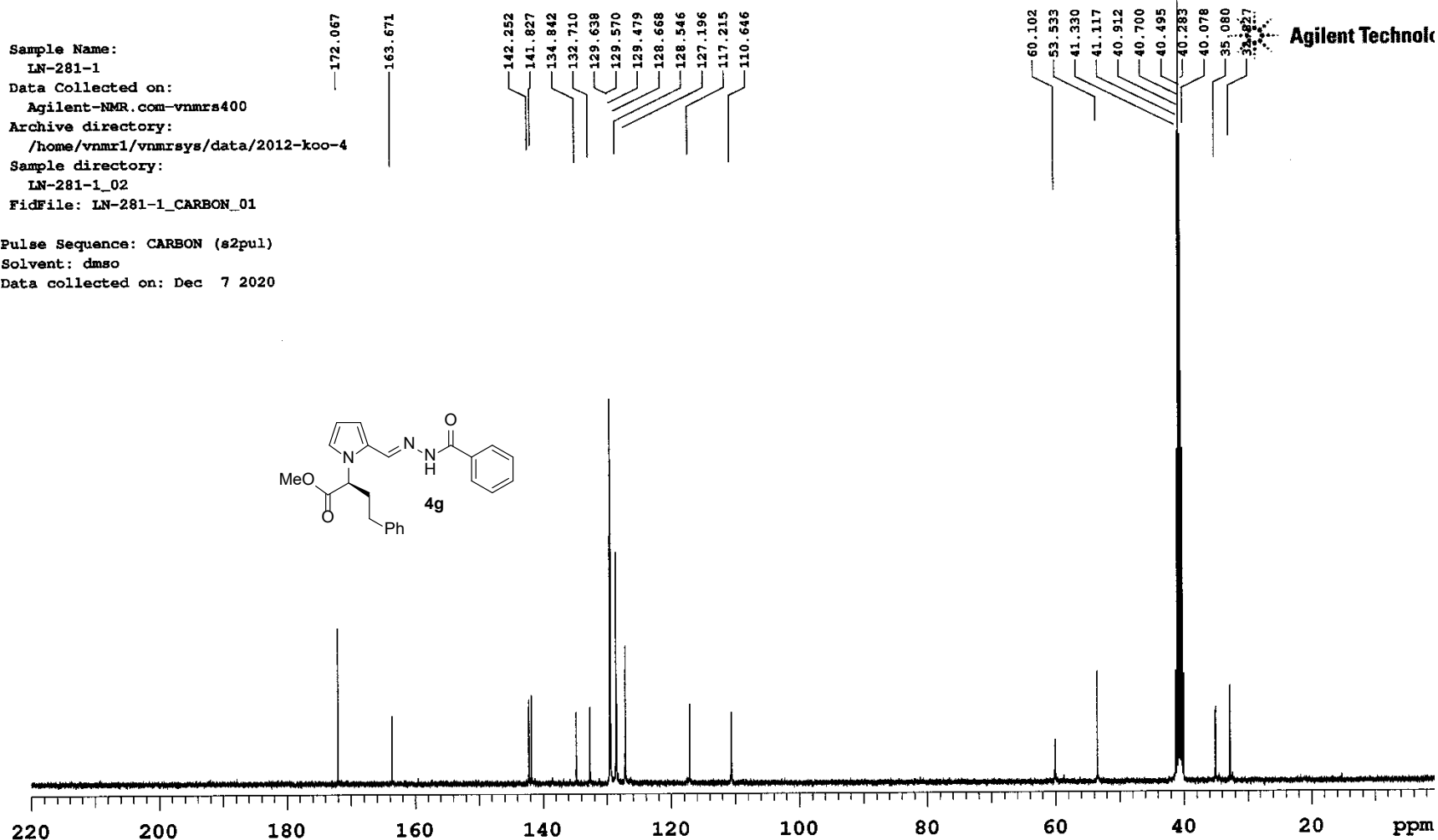
Sample Name:
 LN-281-1
 Data Collected on:
 Agilent-NMR.com-vnmrs400
 Archive directory:
 /home/vnmr1/vnmrsys/data/2012-koo-4
 Sample directory:
 LN-281-1_01
 FidFile: LN-281-1_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: dmsd
 Data collected on: Dec 4 2020

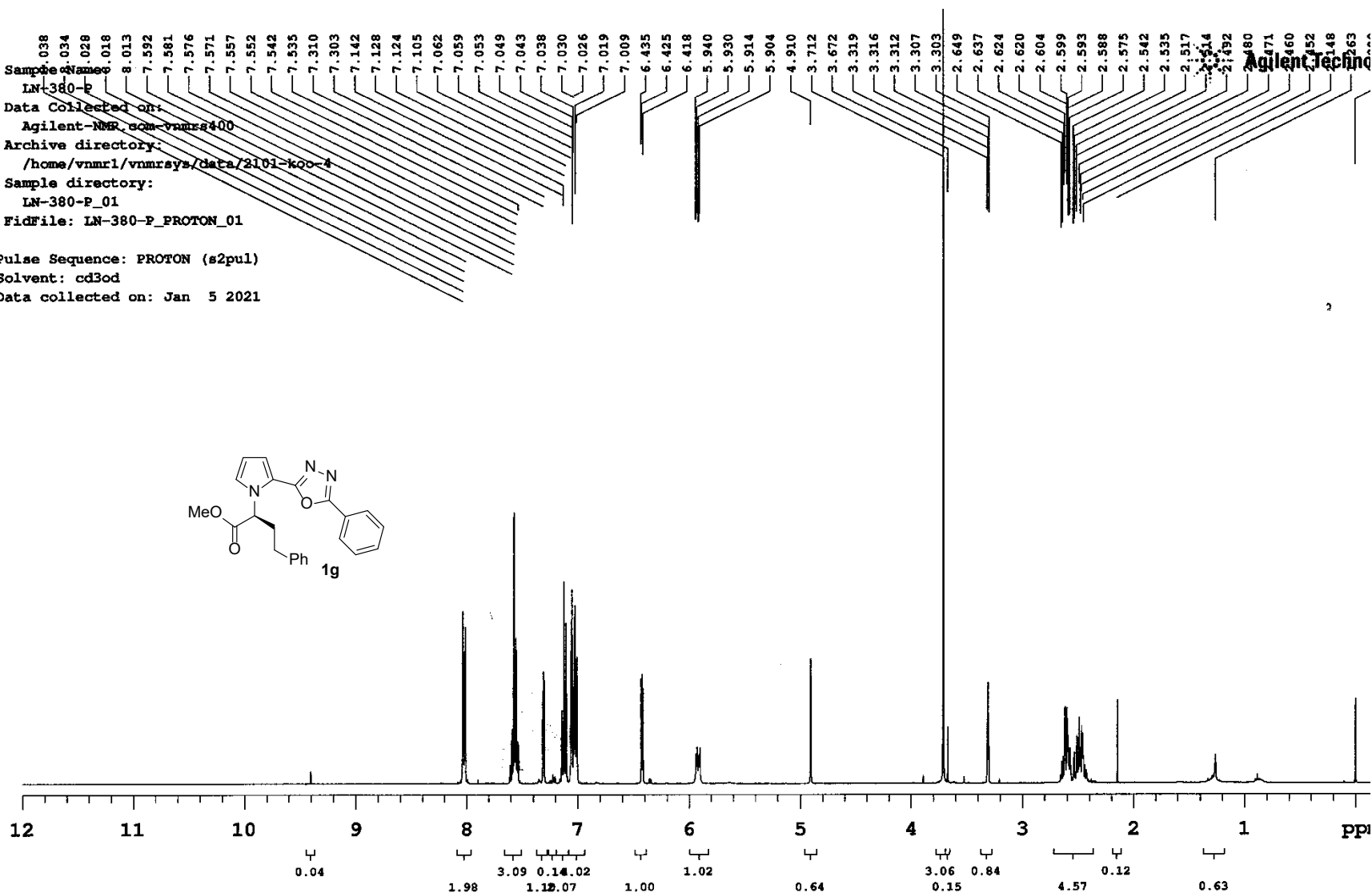


Sample Name:
LN-281-1
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
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Sample directory:
LN-281-1_02
FidFile: LN-281-1_CARBON_01

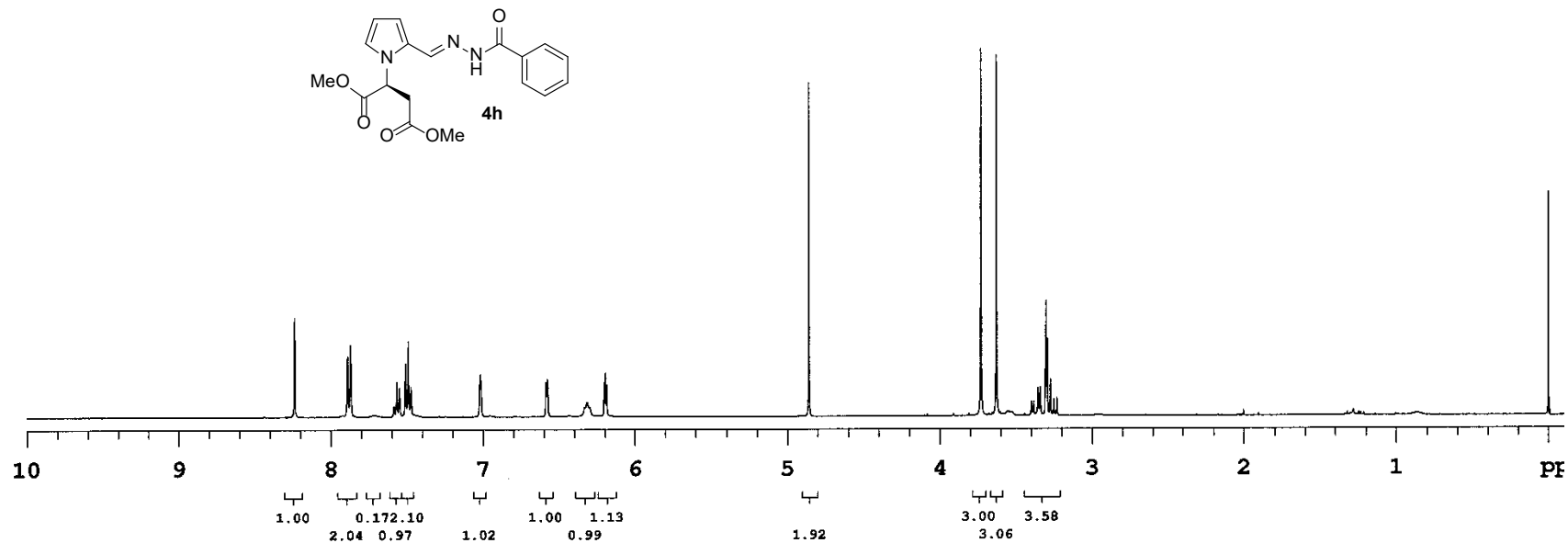
Pulse Sequence: CARBON (s2pul)
Solvent: dmsd
Data collected on: Dec 7 2020



Sample Name: LN-380-P
 Data Collected on: Agilent-NMR, vnmr400
 Archive directory: /home/vnmr1/vnmr400/data/2101-koo-4
 Sample directory: LN-380-P_01
 Fidfile: LN-380-P_PROTON_01
 Pulse Sequence: PROTON (s2pul)
 Solvent: cd3od
 Data collected on: Jan 5 2021

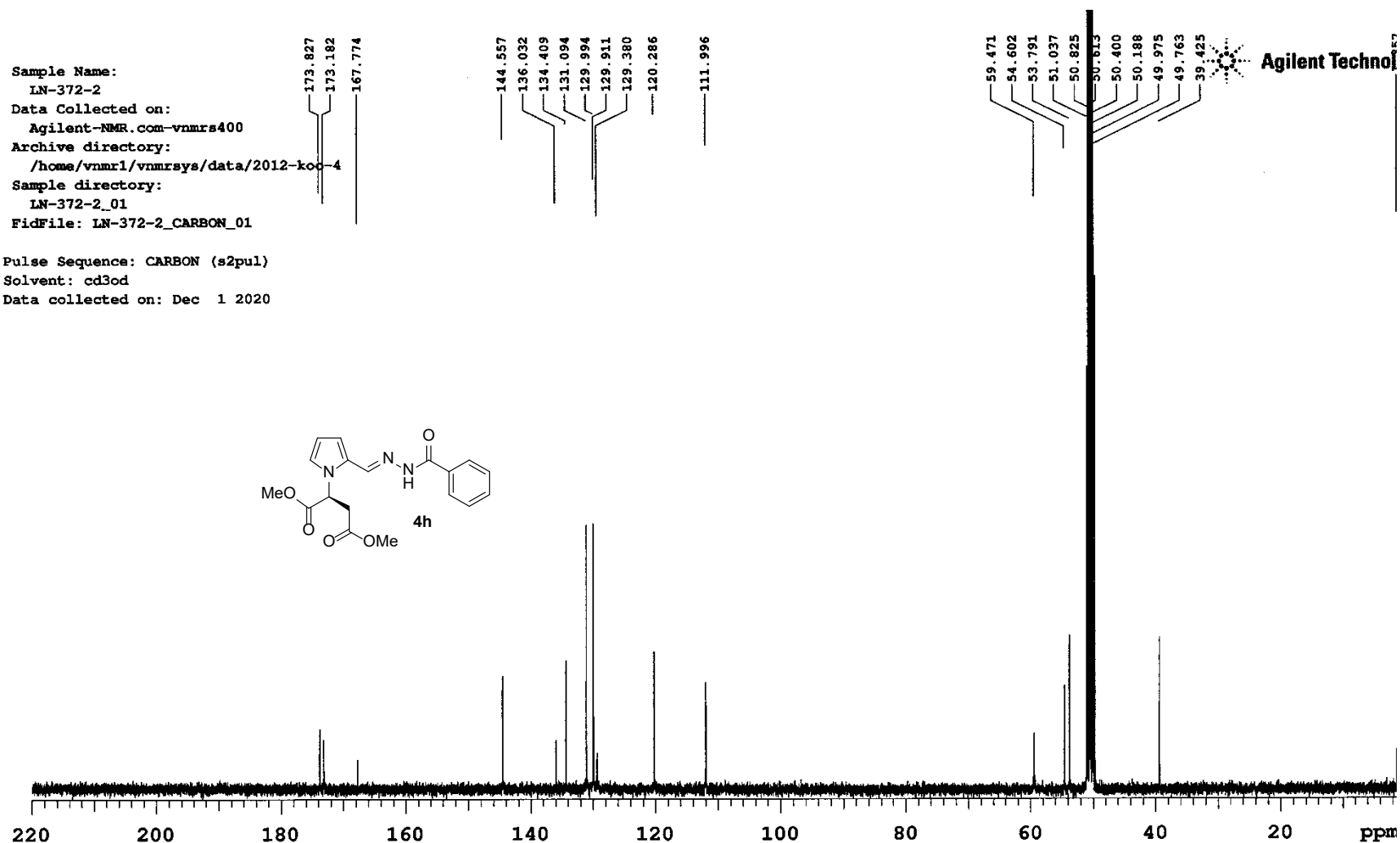


Sample Name: LN-372-2
 Data Collected on: Agilent-NMR-gcm-vnmrse400
 Archive directory: /home/vnmr1/vnmrsys/data/2011-kob-4
 Sample directory: LN-372-2_01
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 Pulse Sequence: PROTON (s2pul)
 Solvent: cd3od
 Data collected on: Nov 30 2020

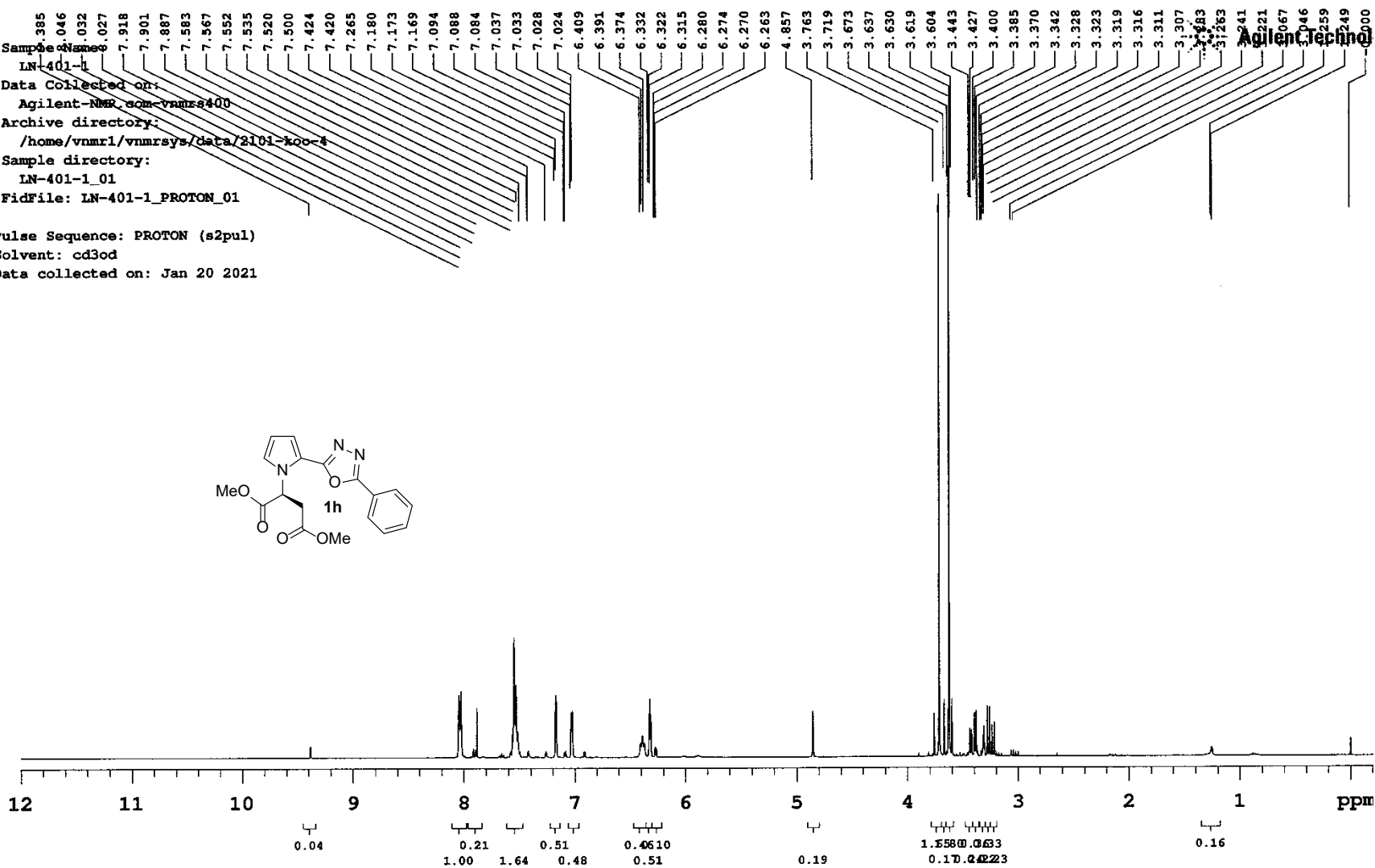
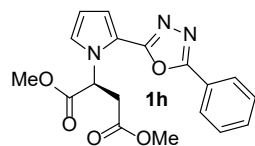


Sample Name:
LN-372-2
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
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Sample directory:
LN-372-2_01
FidFile: LN-372-2_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Dec 1 2020



Sample Name: LN-401-1
 Data Collected on: Agilent-NMR.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2101-koo-4
 Sample directory: LN-401-1_01
 FidFile: LN-401-1_PROTON_01
 Pulse Sequence: PROTON (s2pul)
 Solvent: cd3od
 Data collected on: Jan 20 2021



Sample Name:

LN-401-1

Data Collected on:

Agilent-NMR.com-vnmrs400

Archive directory:

/home/vnmr1/vnmrsys/data/2101-koo-4

Sample directory:

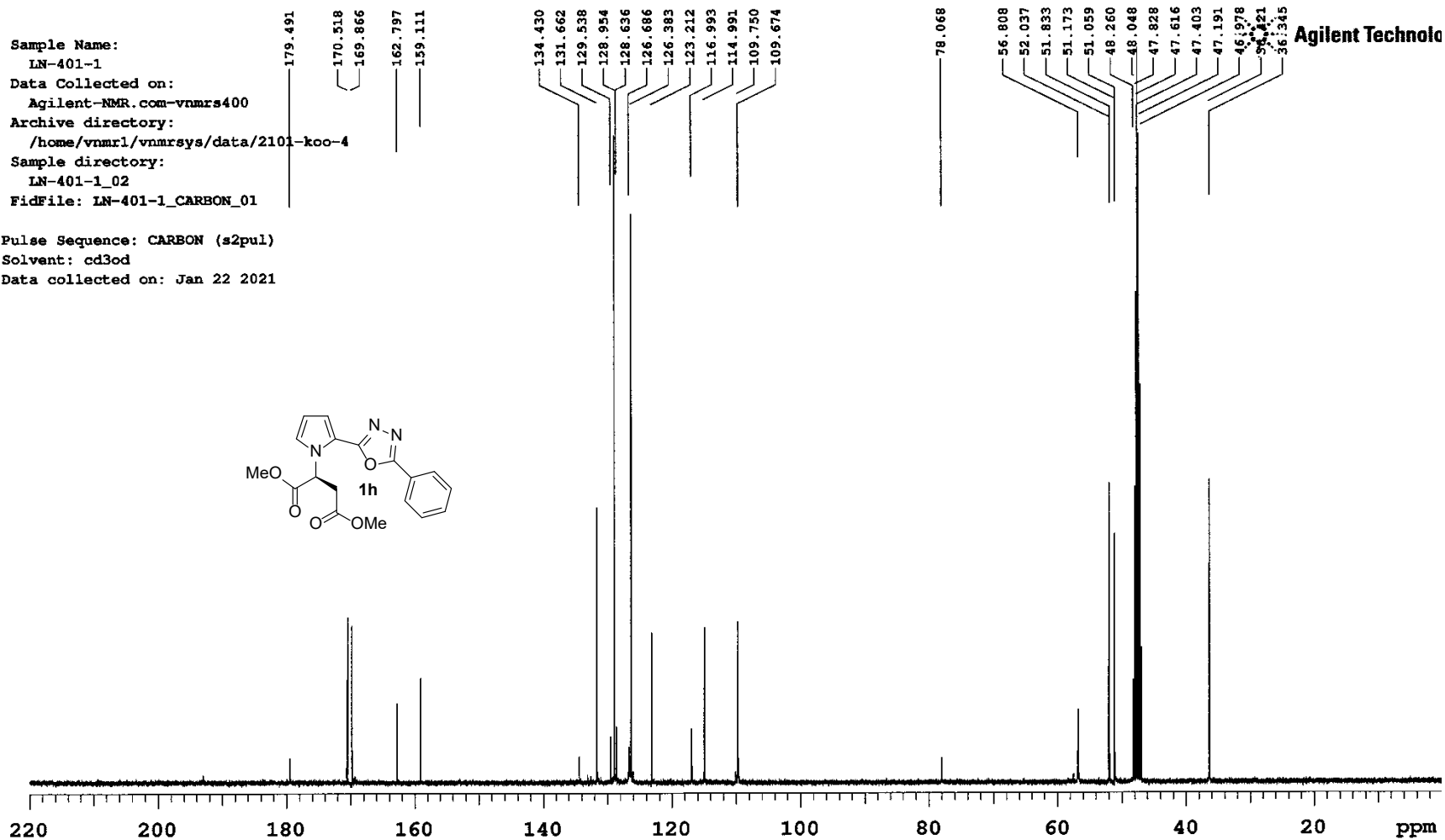
LN-401-1_02

FidFile: LN-401-1_CARBON_01

Pulse Sequence: CARBON (s2pul)

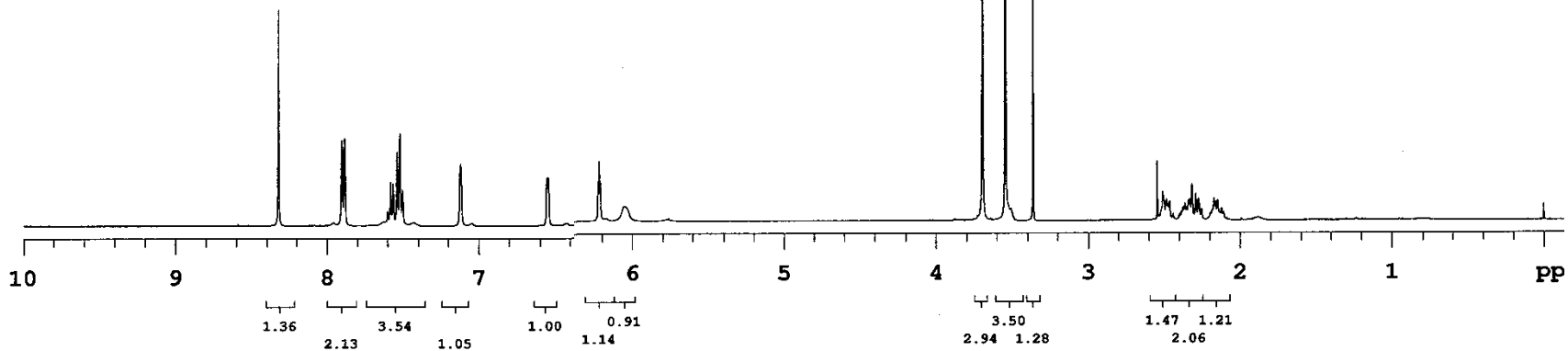
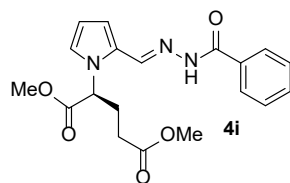
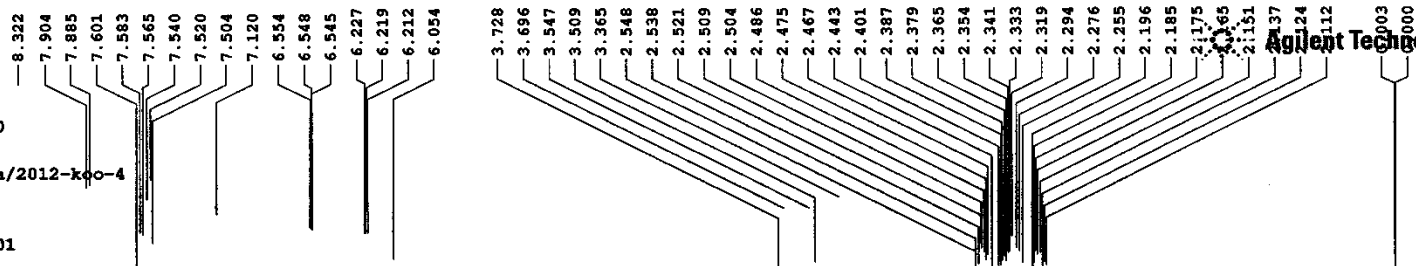
Solvent: cd3od

Data collected on: Jan 22 2021



Sample Name:
 LN-374-1
 Data Collected on:
 Agilent-NMR.com-vnmrs400
 Archive directory:
 /home/vnmr1/vnmrsys/data/2012-ko-4
 Sample directory:
 LN-374-1_01
 FidFile: LN-374-1_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: dmsd
 Data collected on: Dec 4 2020



Sample Name:

LN-374-1

Data Collected on:

Agilent-NMR.com-vnmrs400

Archive directory:

/home/vnmr1/vnmrsys/data/2012-koo-4

Sample directory:

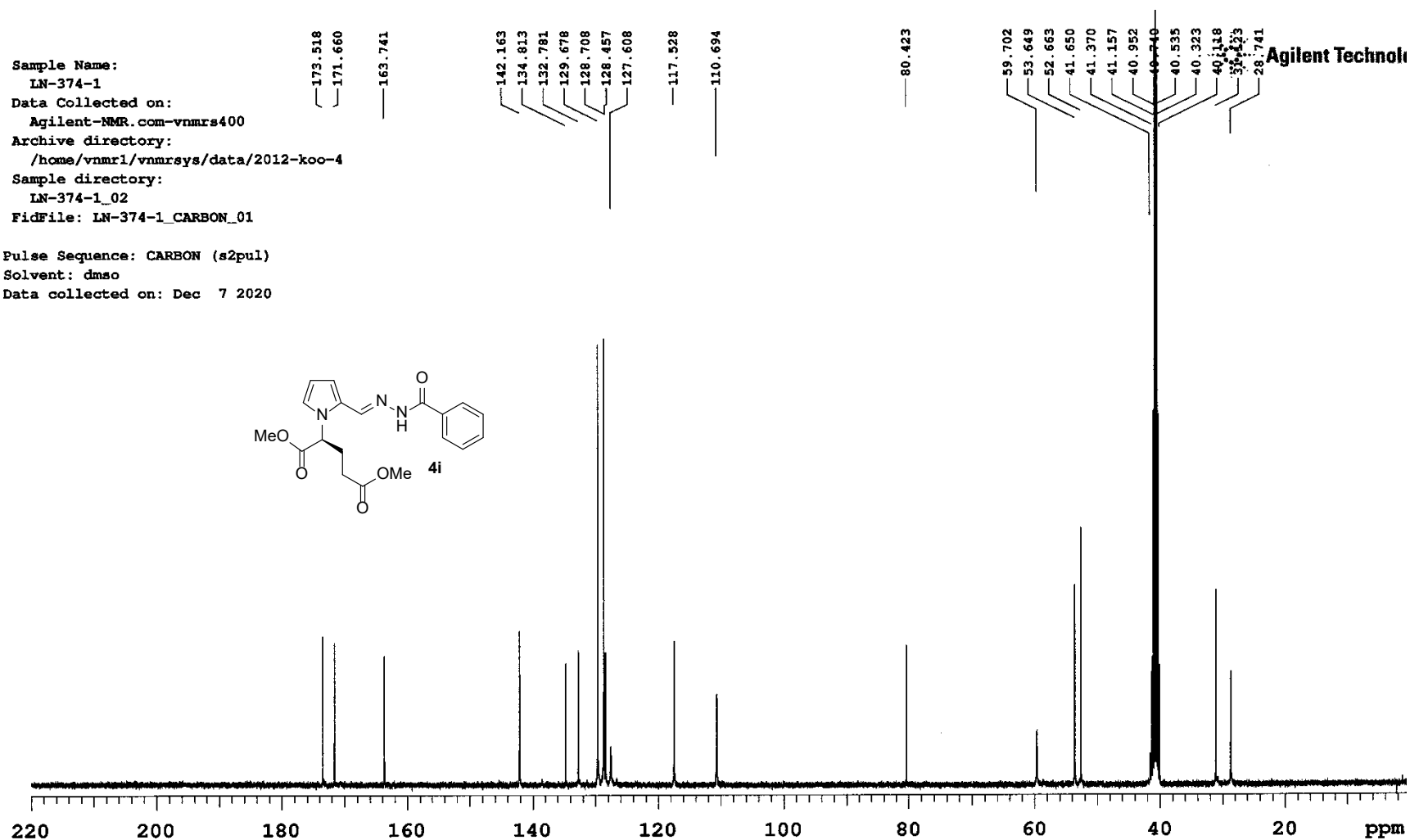
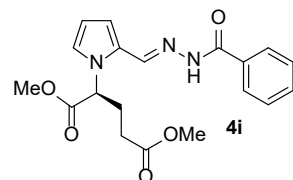
LN-374-1_02

FidFile: LN-374-1 CARBON_01

Pulse Sequence: CARBON (s2pul)

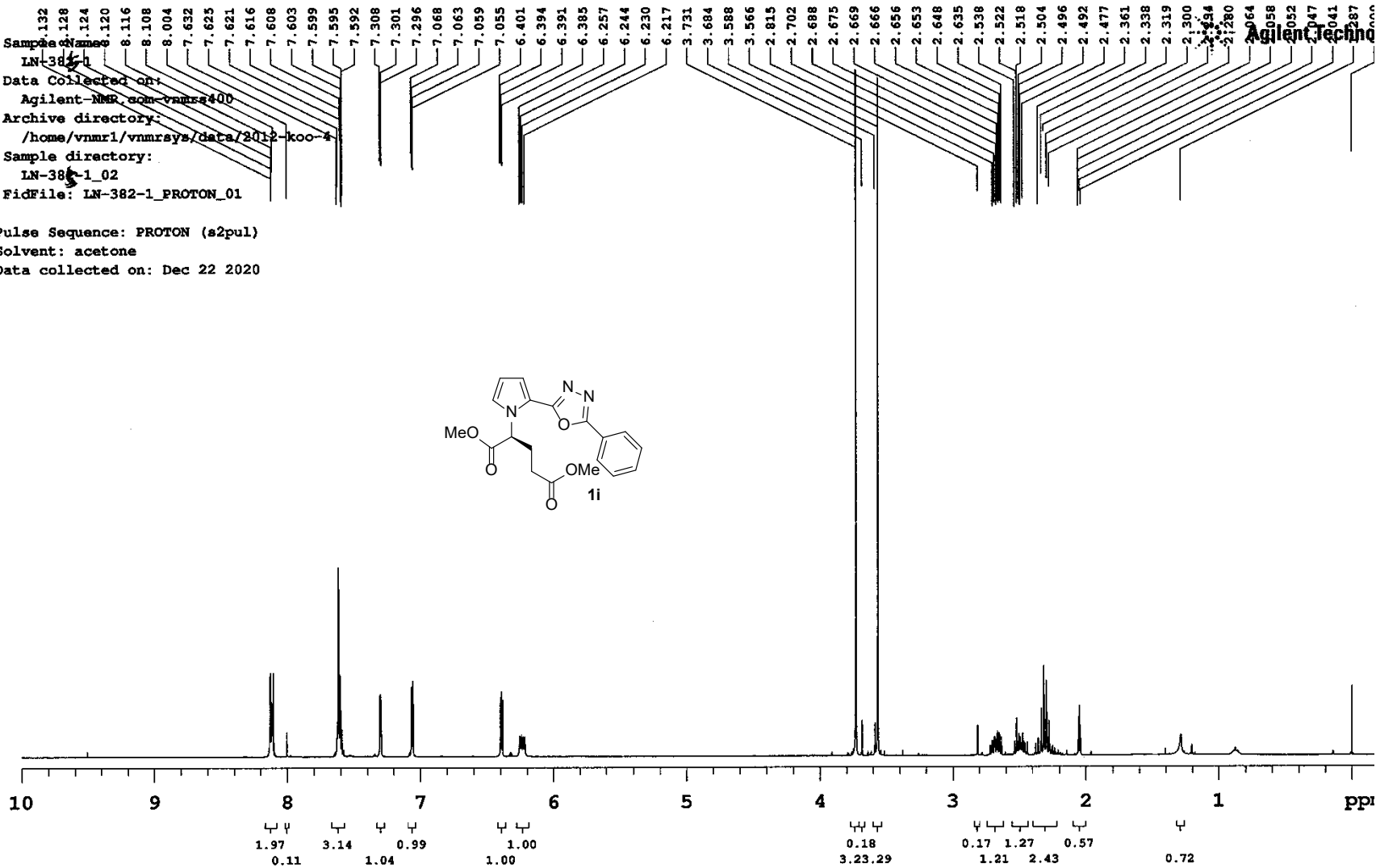
Solvent: dmsd

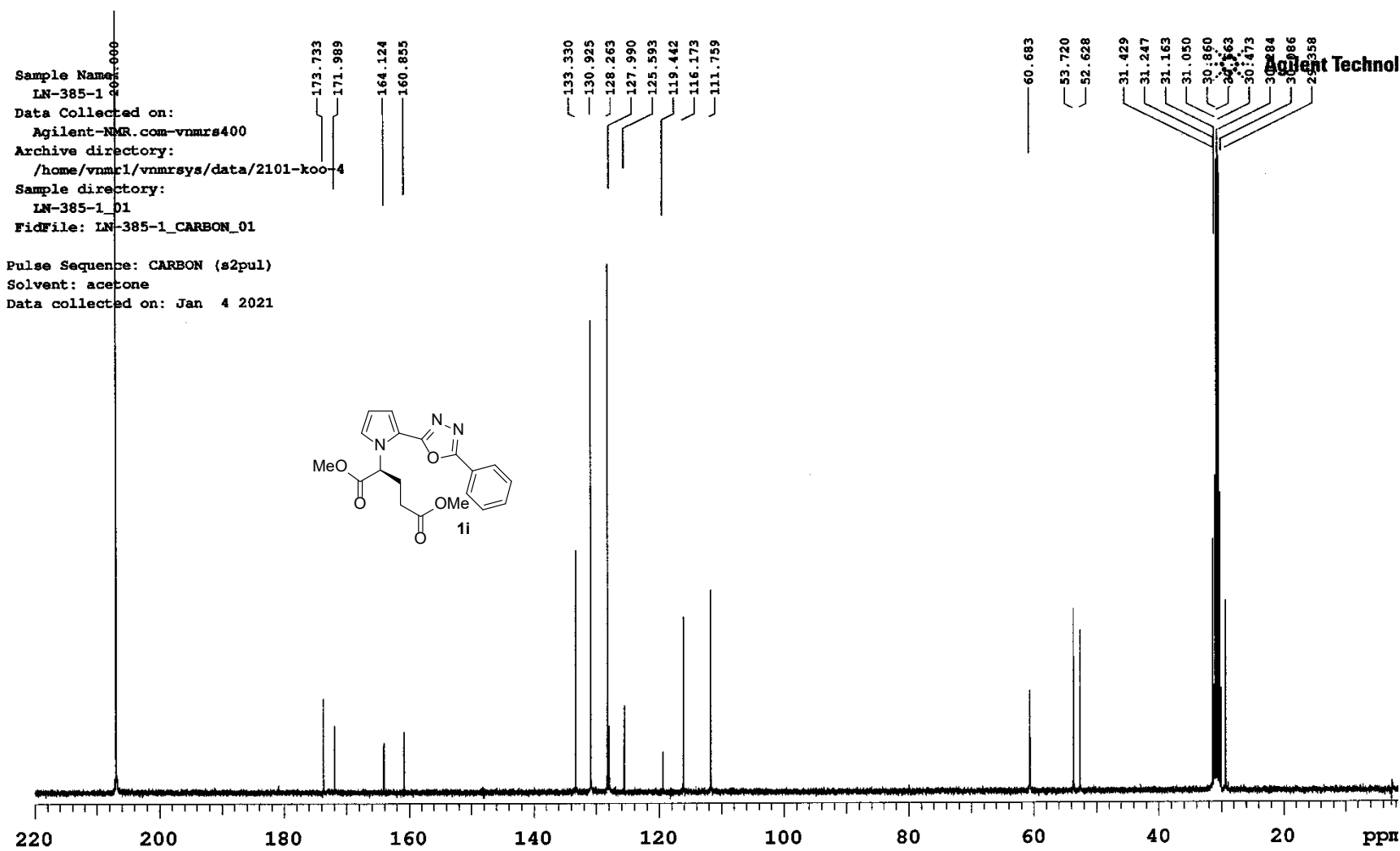
Data collected on: Dec 7 2020

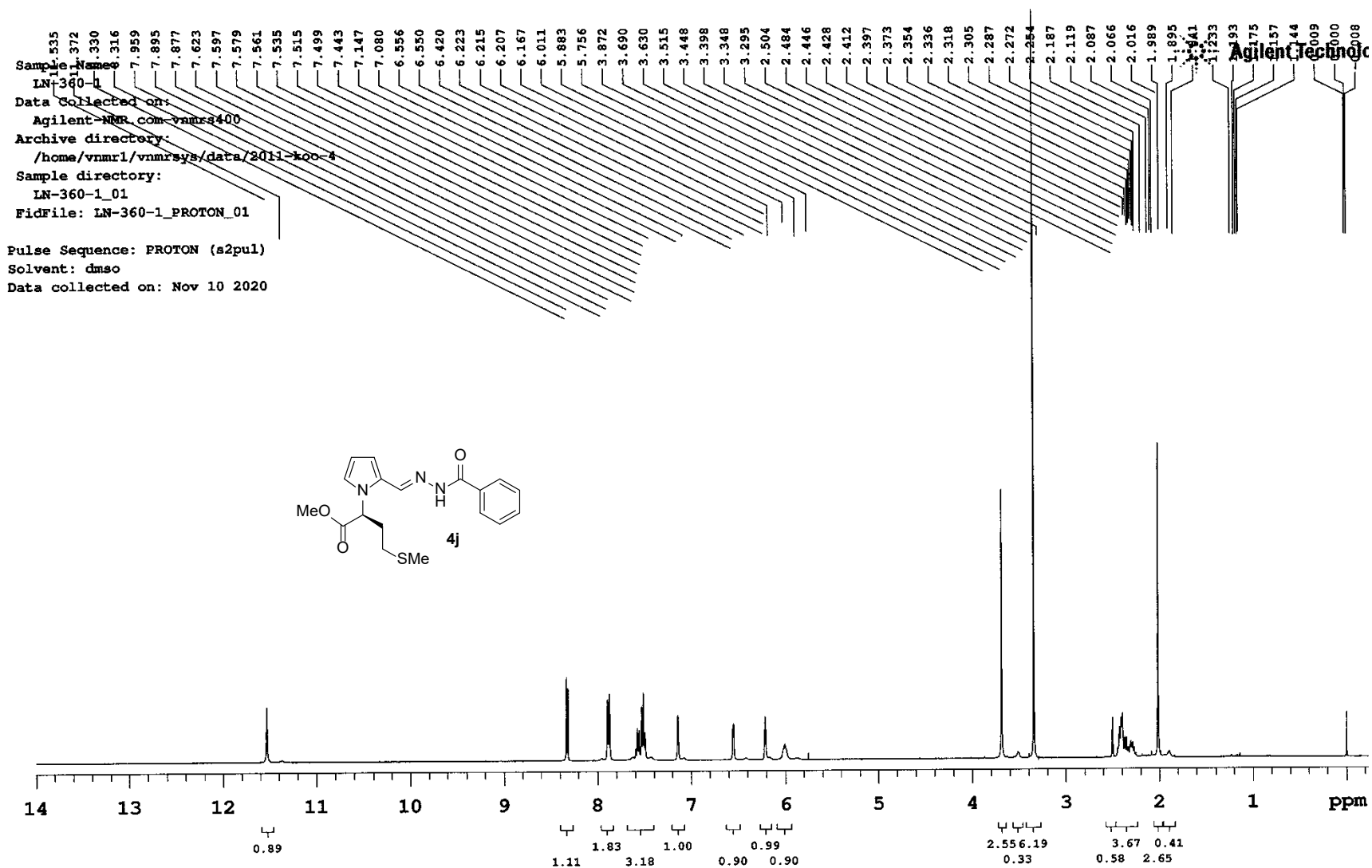


Sample Name: LN-382-1
 Data Collected on: Agilent NMR spectrometer
 Archive directory: /home/vnmr1/vnmrsys/data/2012-koo-4
 Sample directory: LN-382-1_02
 FidFile: LN-382-1_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: acetone
 Data collected on: Dec 22 2020

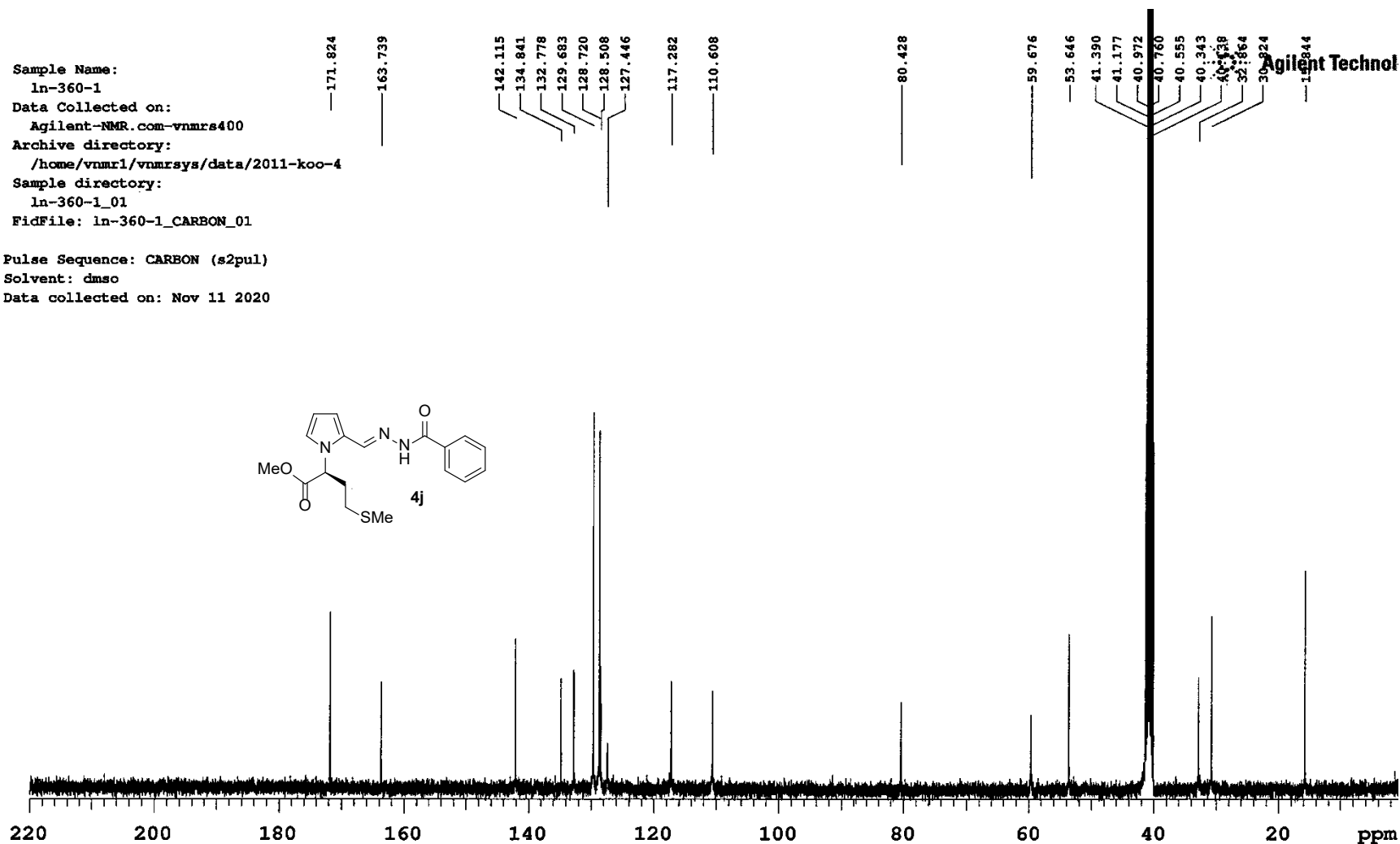


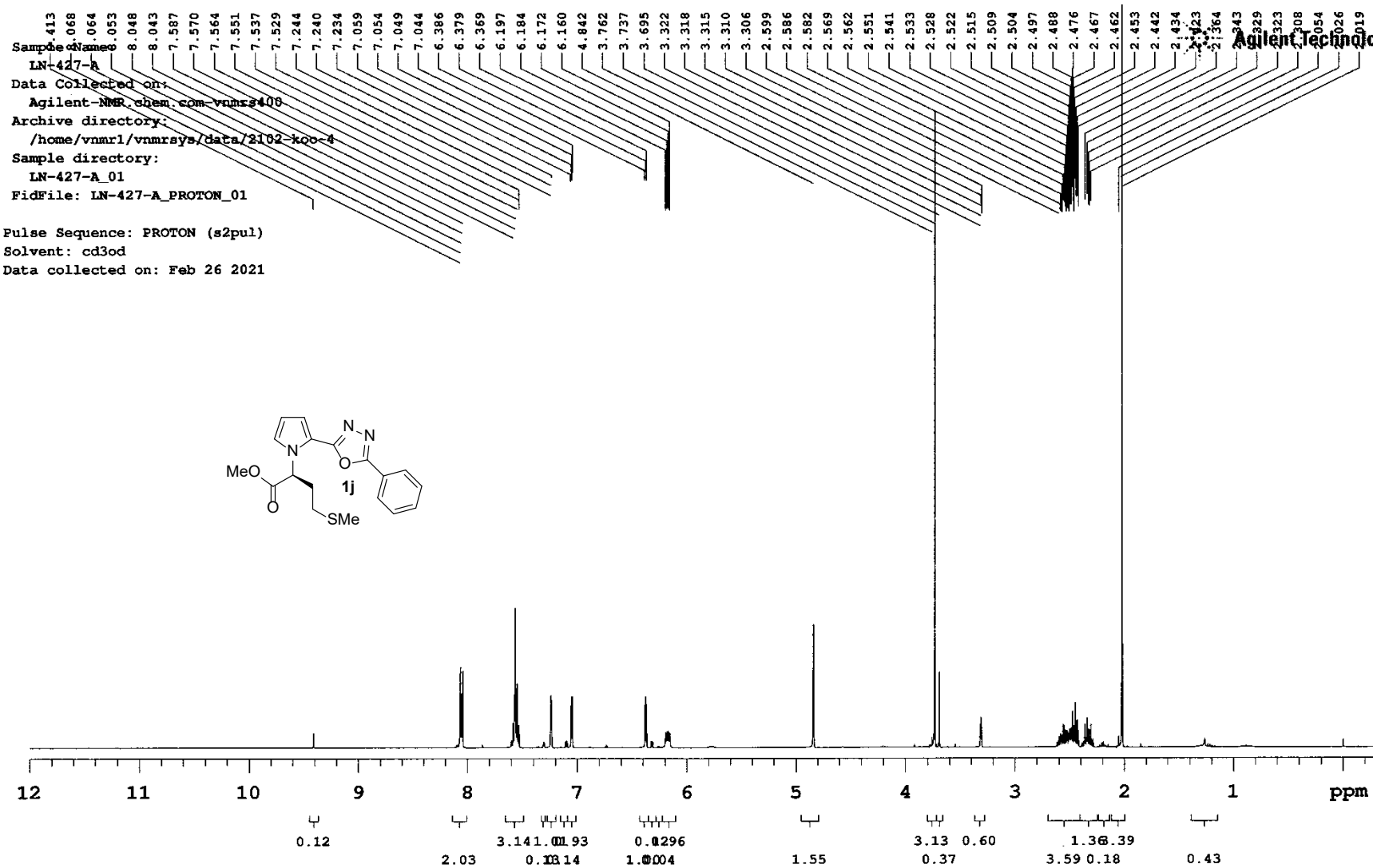




Sample Name:
ln-360-1
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2011-koo-4
Sample directory:
ln-360-i_01
FidFile: ln-360-1_CARBON_01

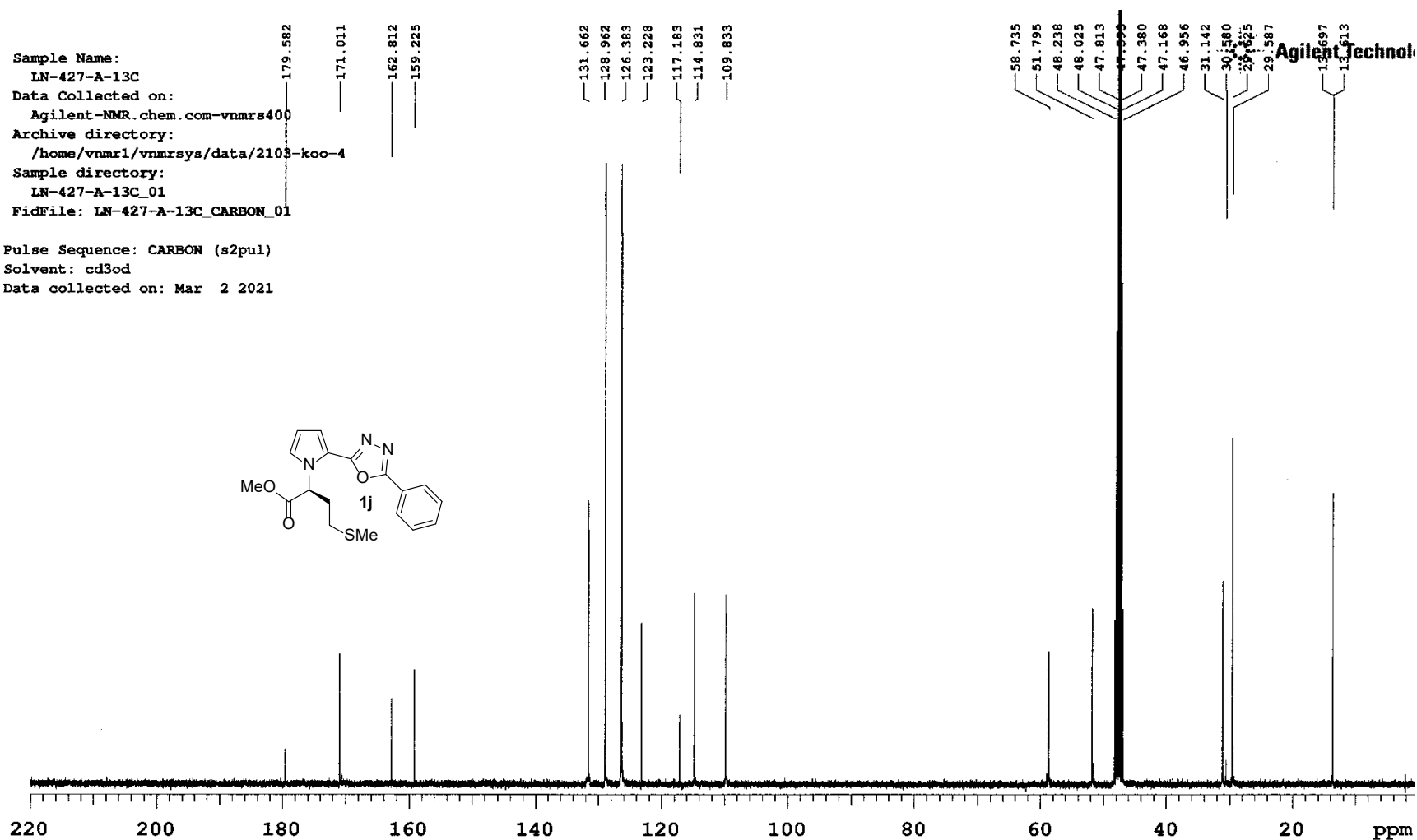
Pulse Sequence: CARBON (s2pul)
Solvent: dmsc
Data collected on: Nov 11 2020



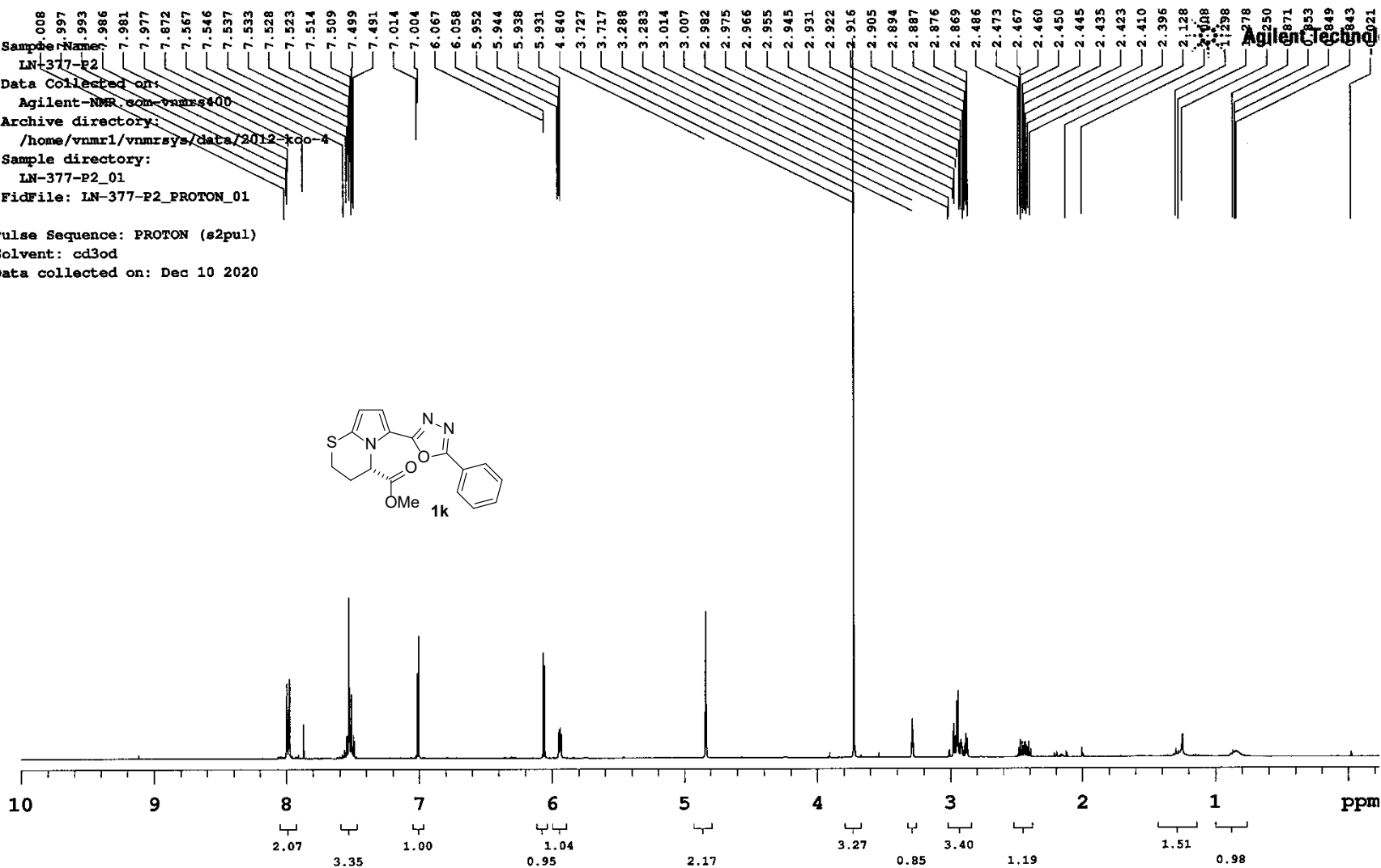
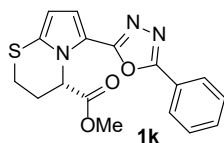


Sample Name:
 LN-427-A-13C
 Data Collected on:
 Agilent-NMR.chem.com-vnmrs400
 Archive directory:
 /home/vnmr1/vnmrsys/data/2103-koo-4
 Sample directory:
 LN-427-A-13C_01
 FidFile: LN-427-A-13C CARBON_01

Pulse Sequence: CARBON (s2pul)
 Solvent: cd3od
 Data collected on: Mar 2 2021

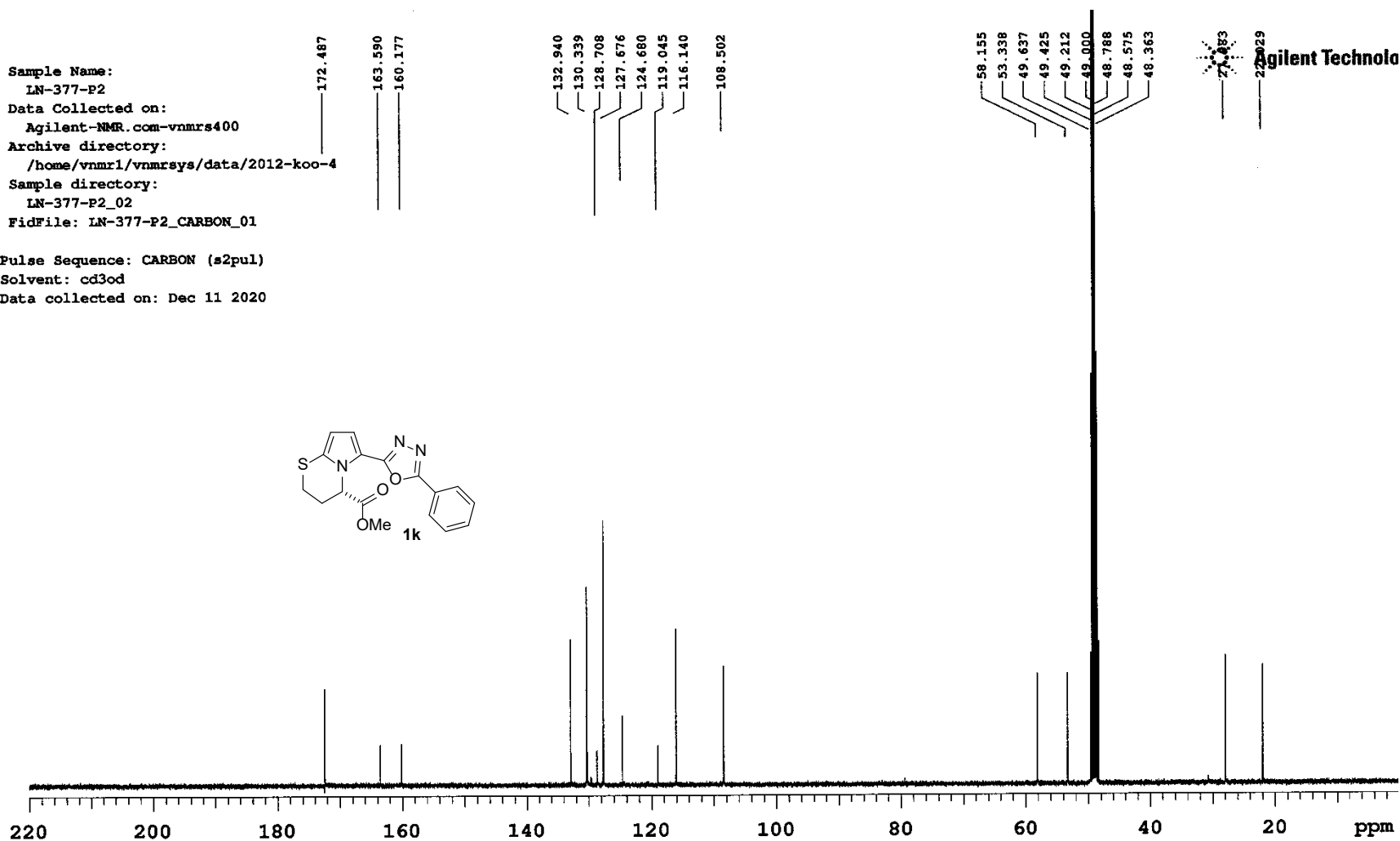


Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Dec 10 2020



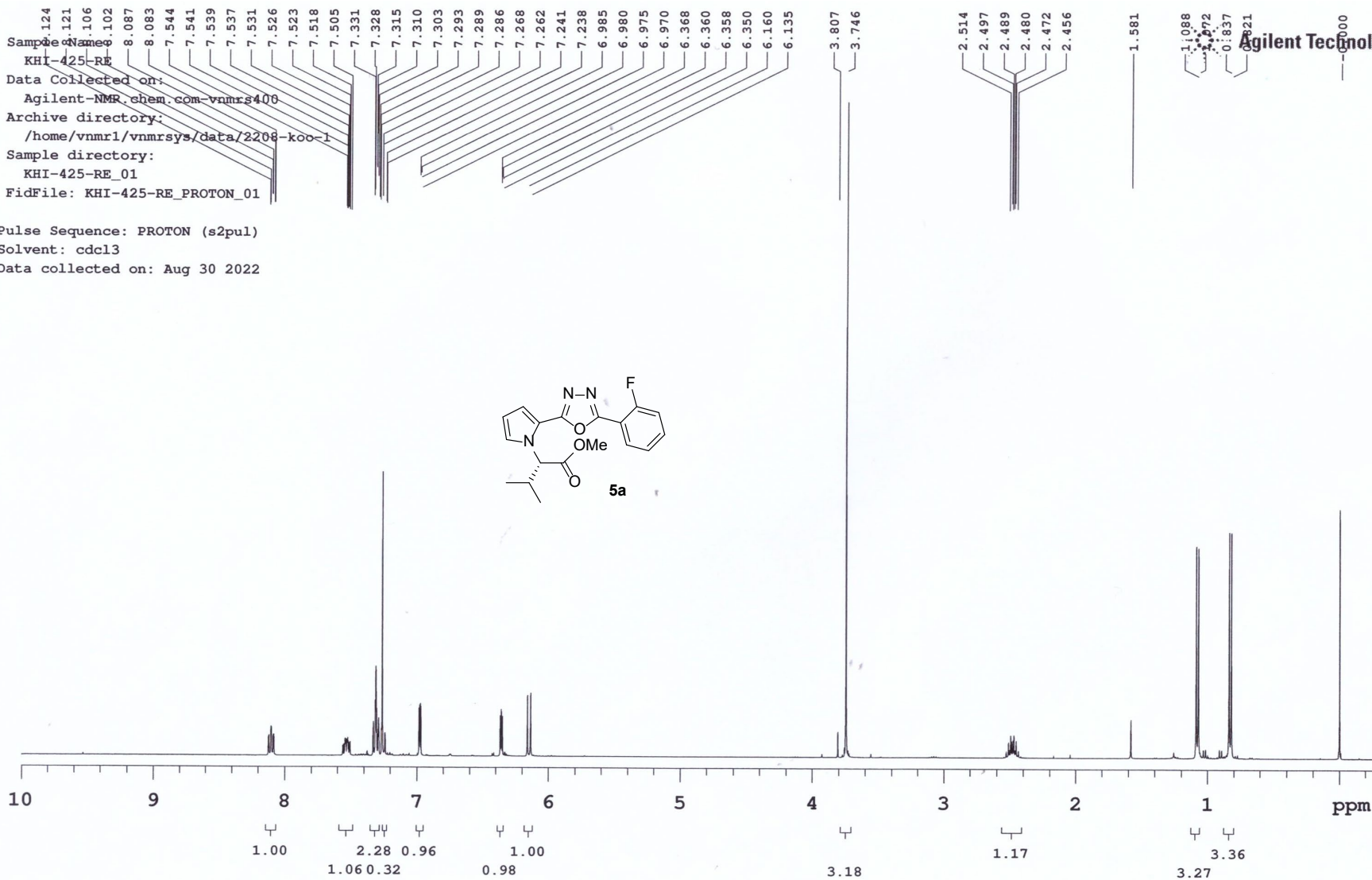
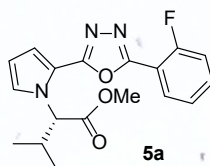
Sample Name:
 LN-377-P2
 Data Collected on:
 Agilent-NMR.com-vnmrs400
 Archive directory:
 /home/vnmr1/vnmrsys/data/2012-koo-4
 Sample directory:
 LN-377-P2_02
 FidFile: LN-377-P2_CARBON_01

Pulse Sequence: CARBON (s2pul)
 Solvent: cd3od
 Data collected on: Dec 11 2020



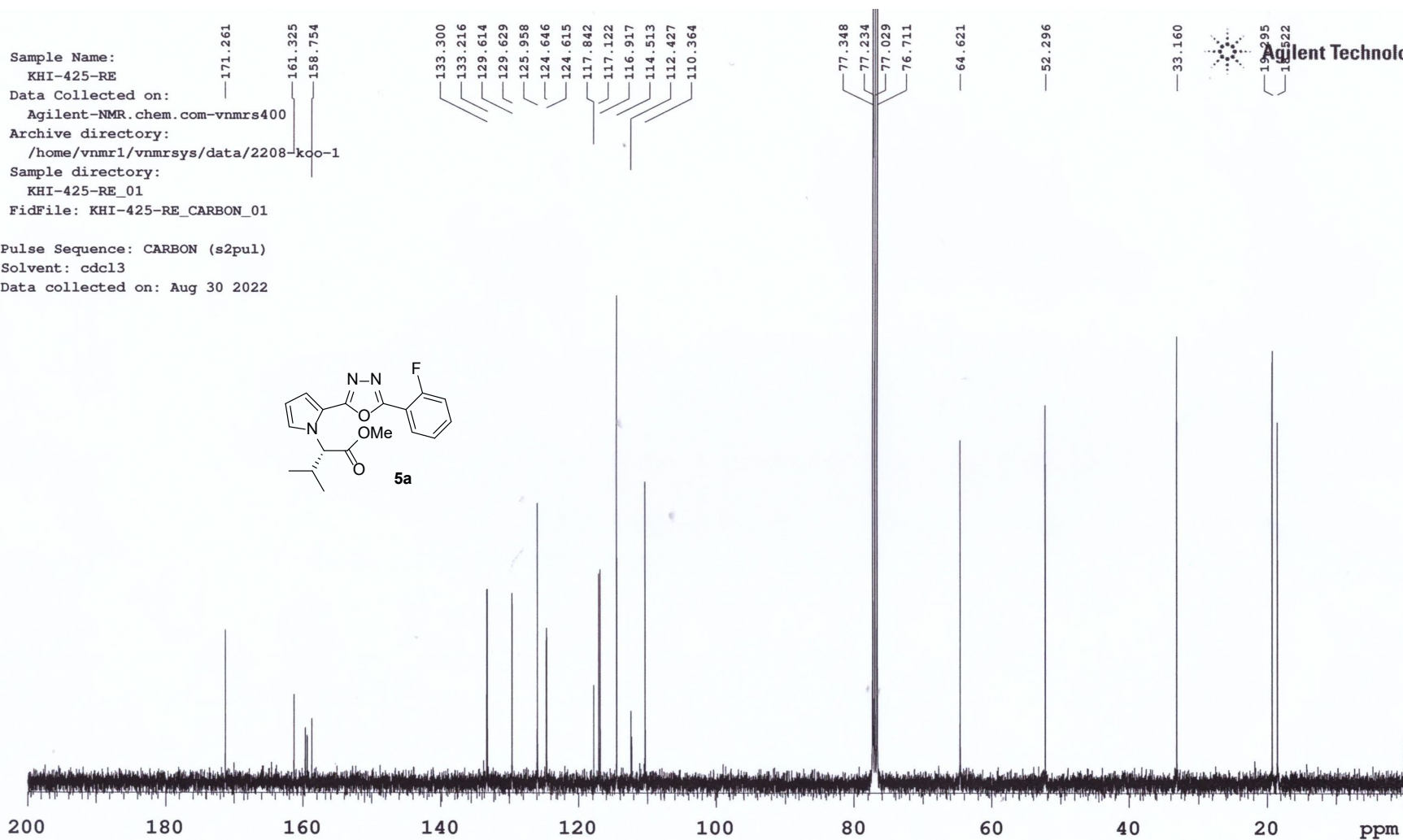
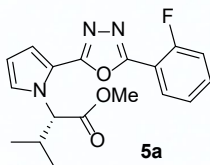
Sample Name: KHI-425-RE
 Data Collected on: Agilent-NMR.chem.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2208-koo-1
 Sample directory: KHI-425-RE_01
 FidFile: KHI-425-RE_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Aug 30 2022



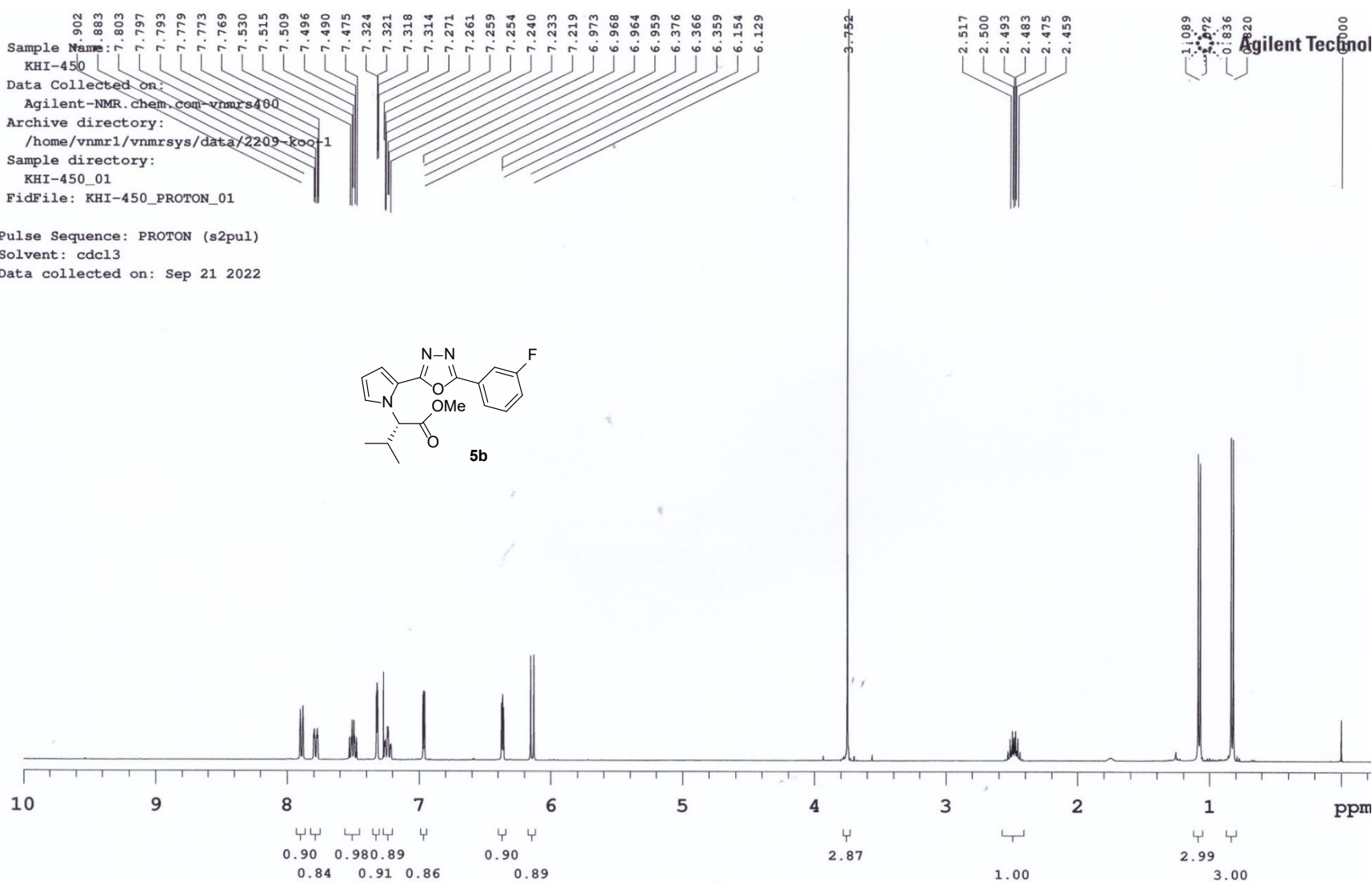
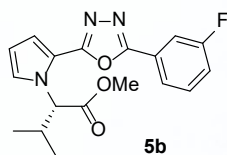
Sample Name:
KHI-425-RE
Data Collected on:
Agilent-NMR.chem.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2208-koo-1
Sample directory:
KHI-425-RE_01
FidFile: KHI-425-RE_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 30 2022



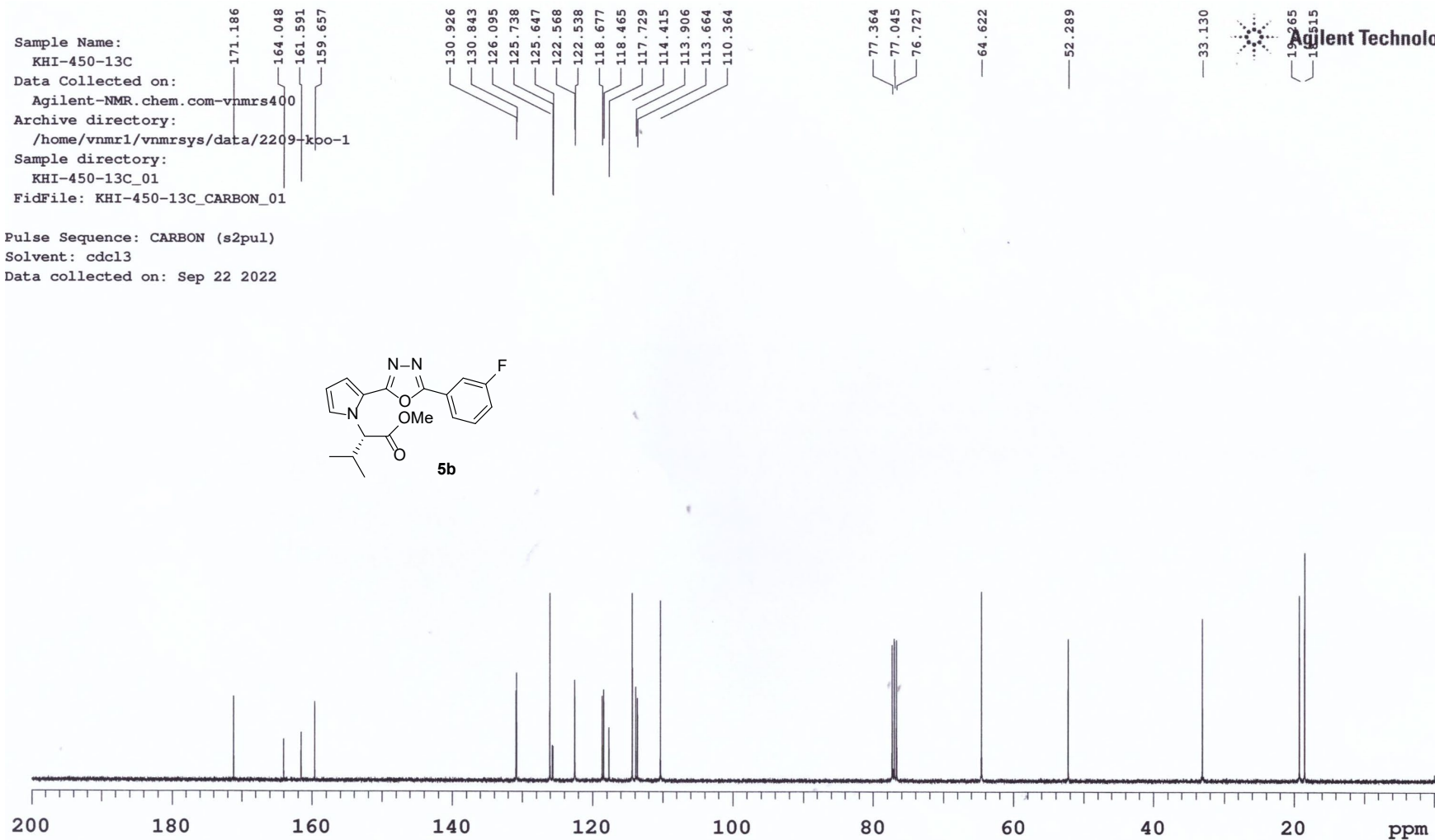
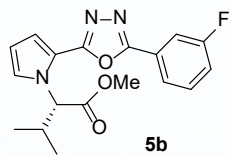
Sample Name: KHI-450
 Data Collected on: Agilent-NMR.chem.com-vnmrs460
 Archive directory: /home/vnmr1/vnmrsys/data/2209-koo-1
 Sample directory: KHI-450_01
 FidFile: KHI-450_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Sep 21 2022



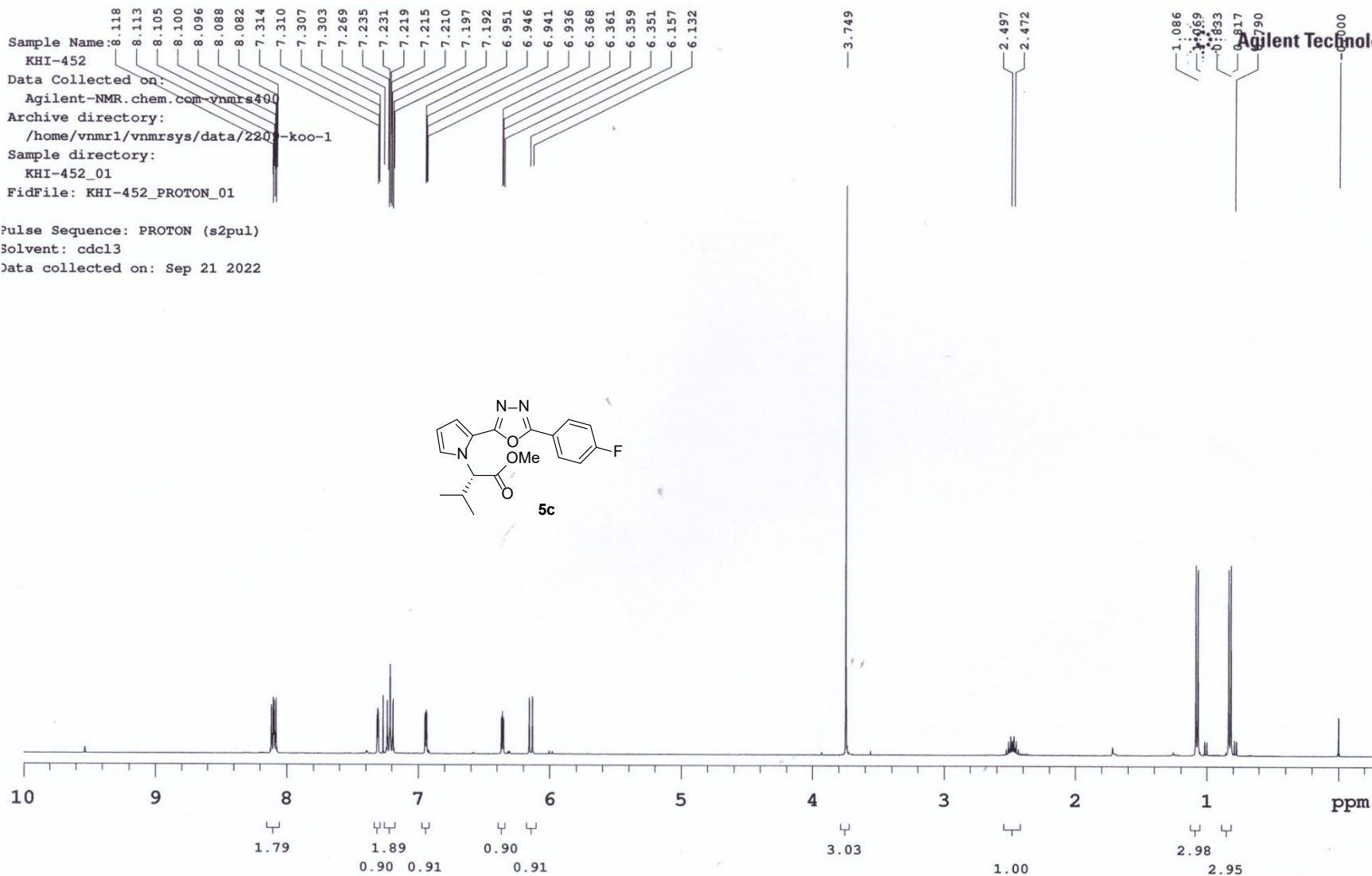
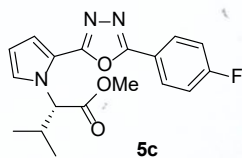
Sample Name:
KHI-450-13C
Data Collected on:
Agilent-NMR.chem.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2209-koo-1
Sample directory:
KHI-450-13C_01
FidFile: KHI-450-13C_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 22 2022



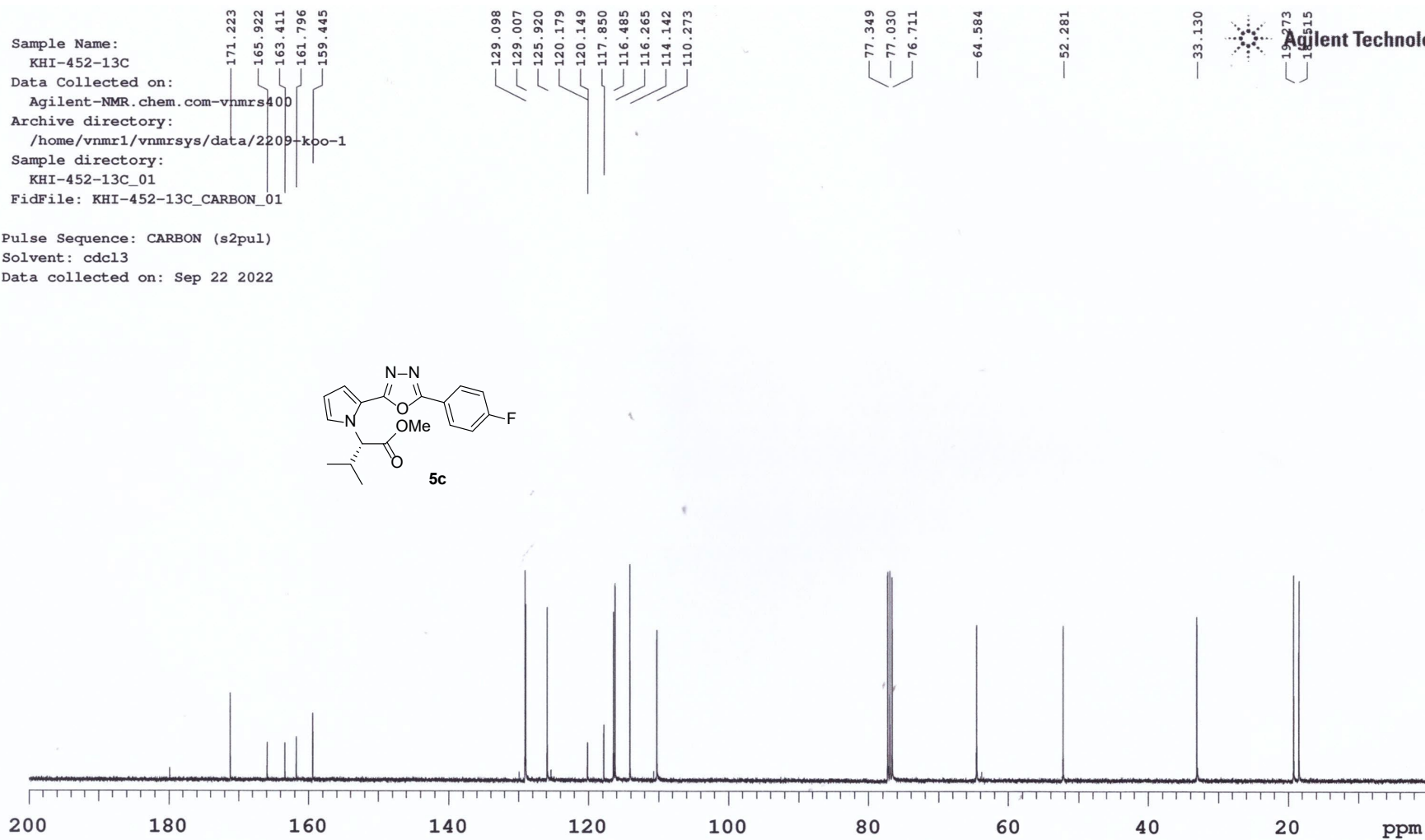
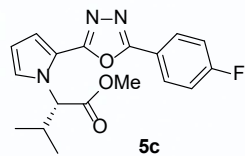
Sample Name: KHI-452
 Data Collected on: Agilent-NMR.chem.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2207-koo-1
 Sample directory: KHI-452_01
 FidFile: KHI-452_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Sep 21 2022



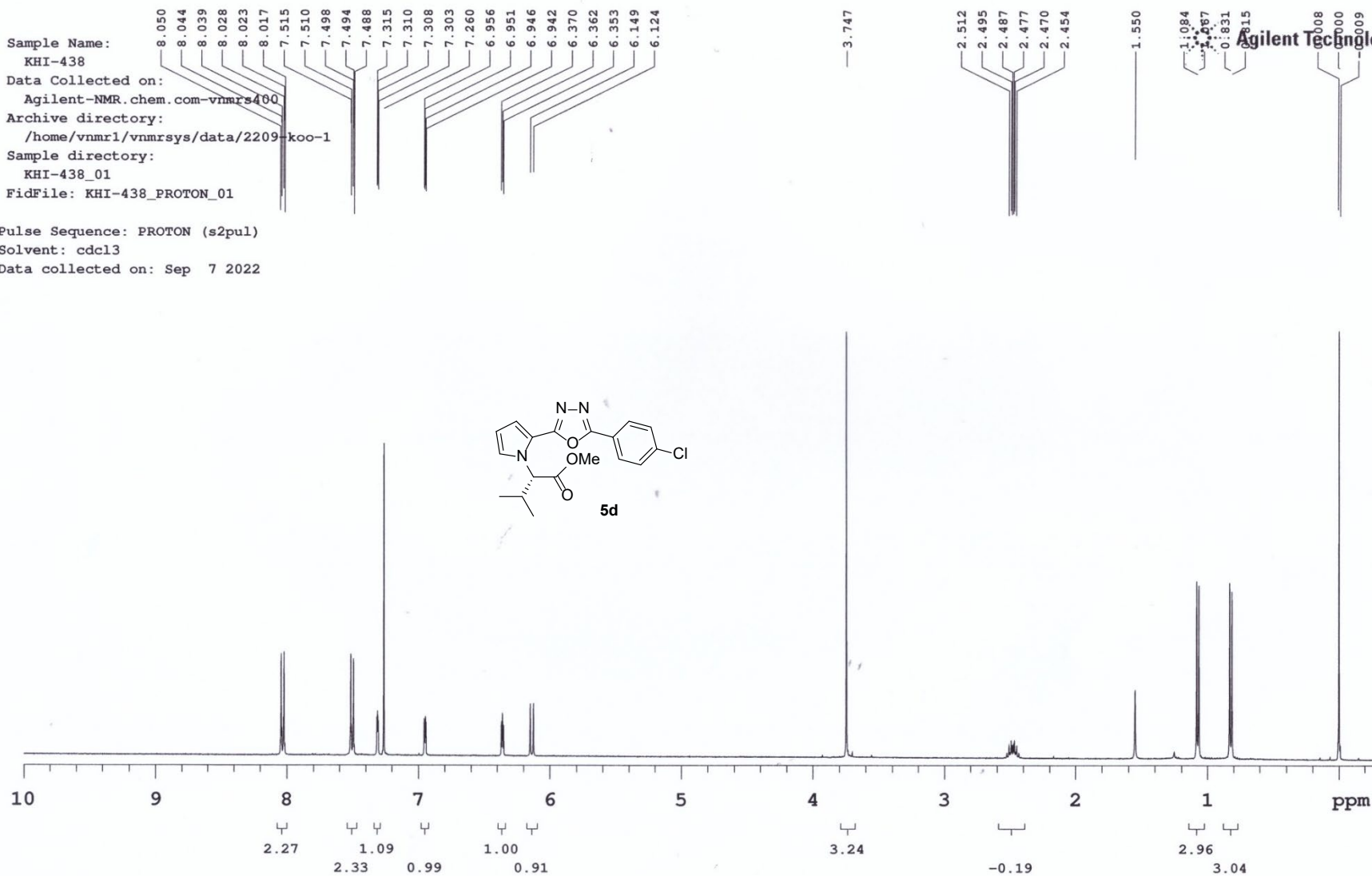
Sample Name:
KHI-452-13C
Data Collected on:
Agilent-NMR.chem.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2209-kpo-1
Sample directory:
KHI-452-13C_01
FidFile: KHI-452-13C_CARBO_N_01

Pulse Sequence: CARBO_N (s2pul)
Solvent: cdcl₃
Data collected on: Sep 22 2022



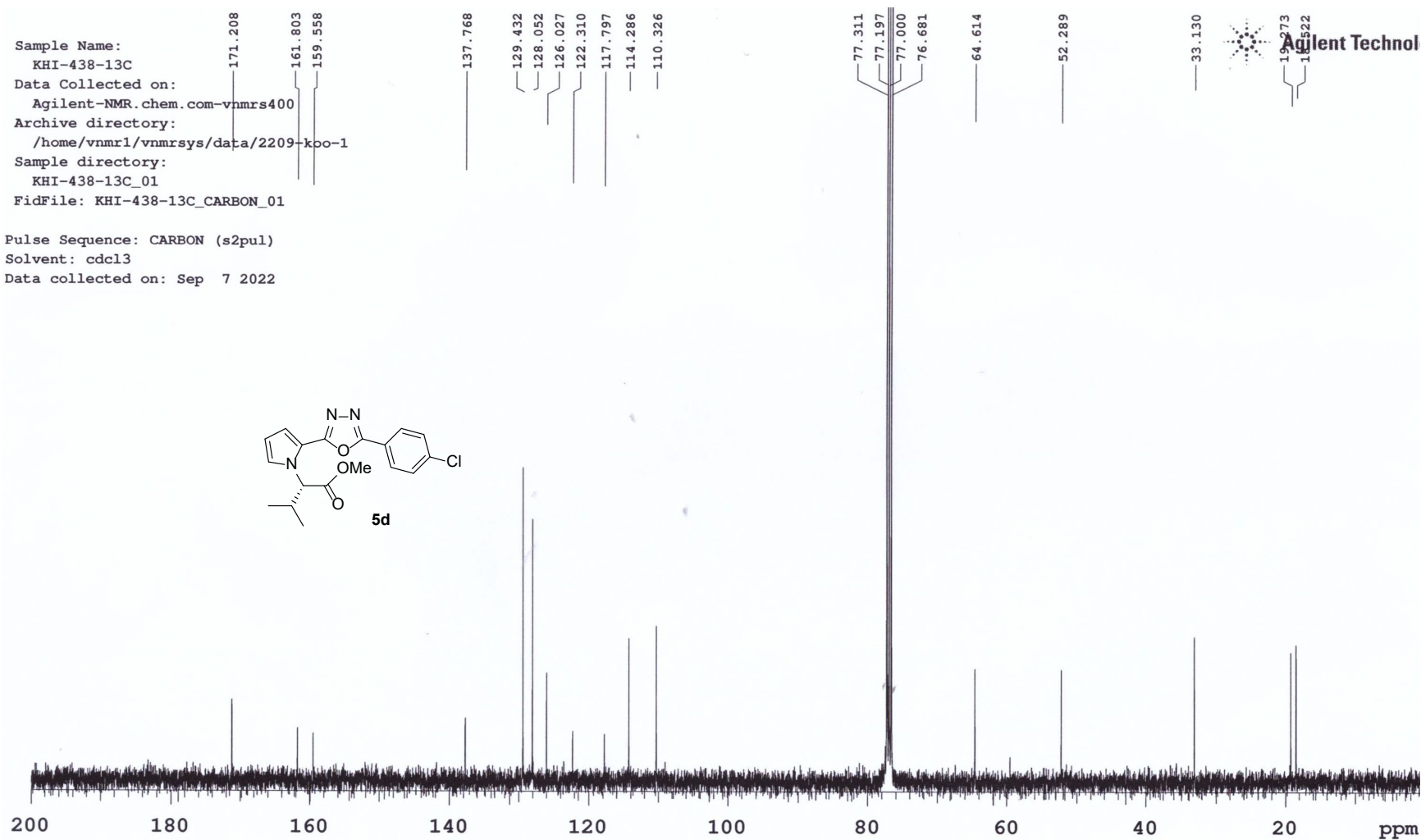
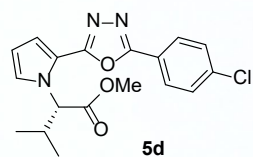
Sample Name:
KHI-438
Data Collected on:
Agilent-NMR.chem.com-vnmr400
Archive directory:
/home/vnmr1/vnmrsys/data/2209-koo-1
Sample directory:
KHI-438_01
FidFile: KHI-438_PROTON_01

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 7 2022



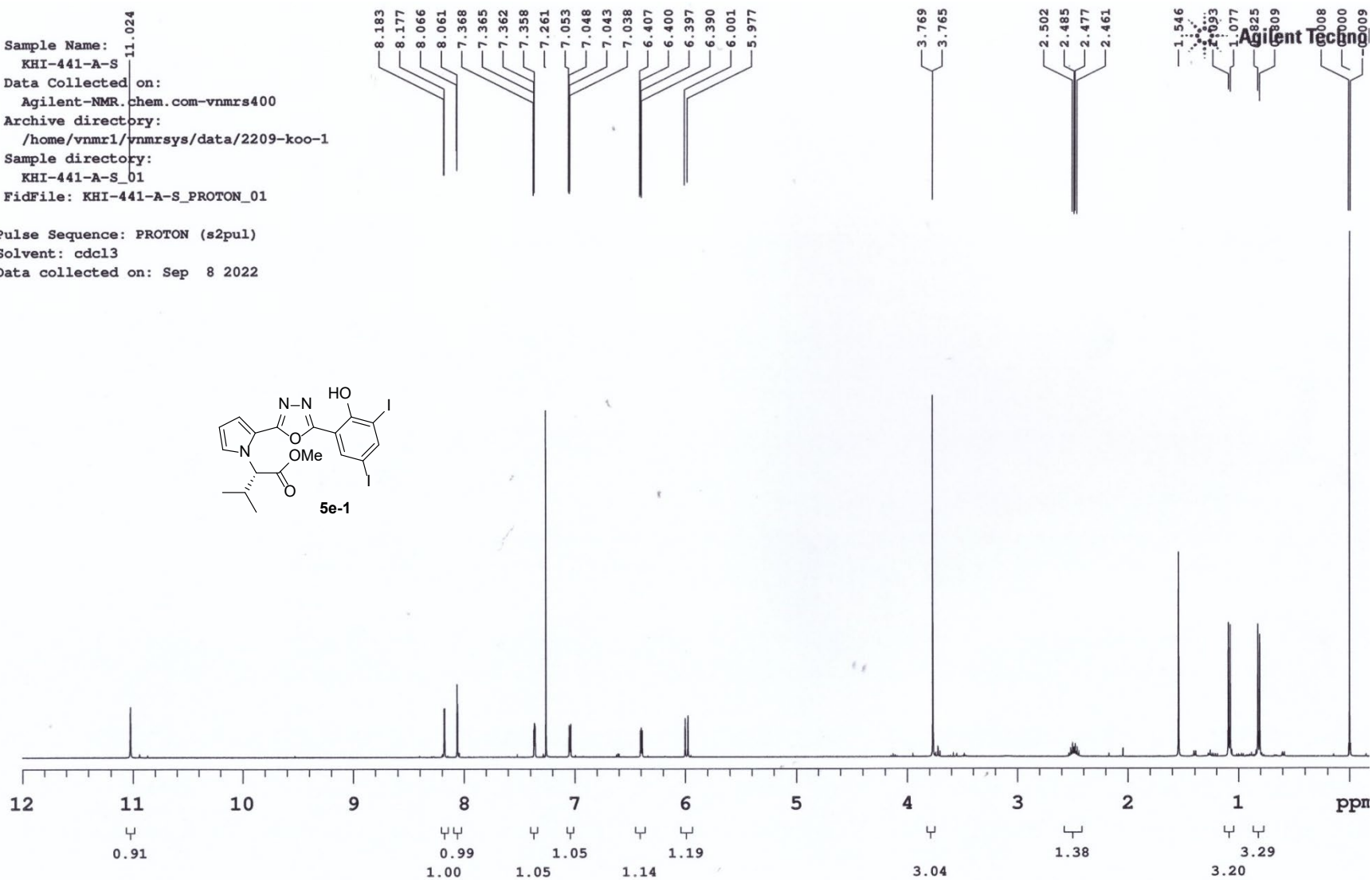
Sample Name:
 KHI-438-13C
 Data Collected on:
 Agilent-NMR.chem.com-vnmrs400
 Archive directory:
 /home/vnmr1/vnmrsys/data/2209-kpo-1
 Sample directory:
 KHI-438-13C_01
 FidFile: KHI-438-13C_CARBO_01

Pulse Sequence: CARBON (s2pul)
 Solvent: cdcl3
 Data collected on: Sep 7 2022



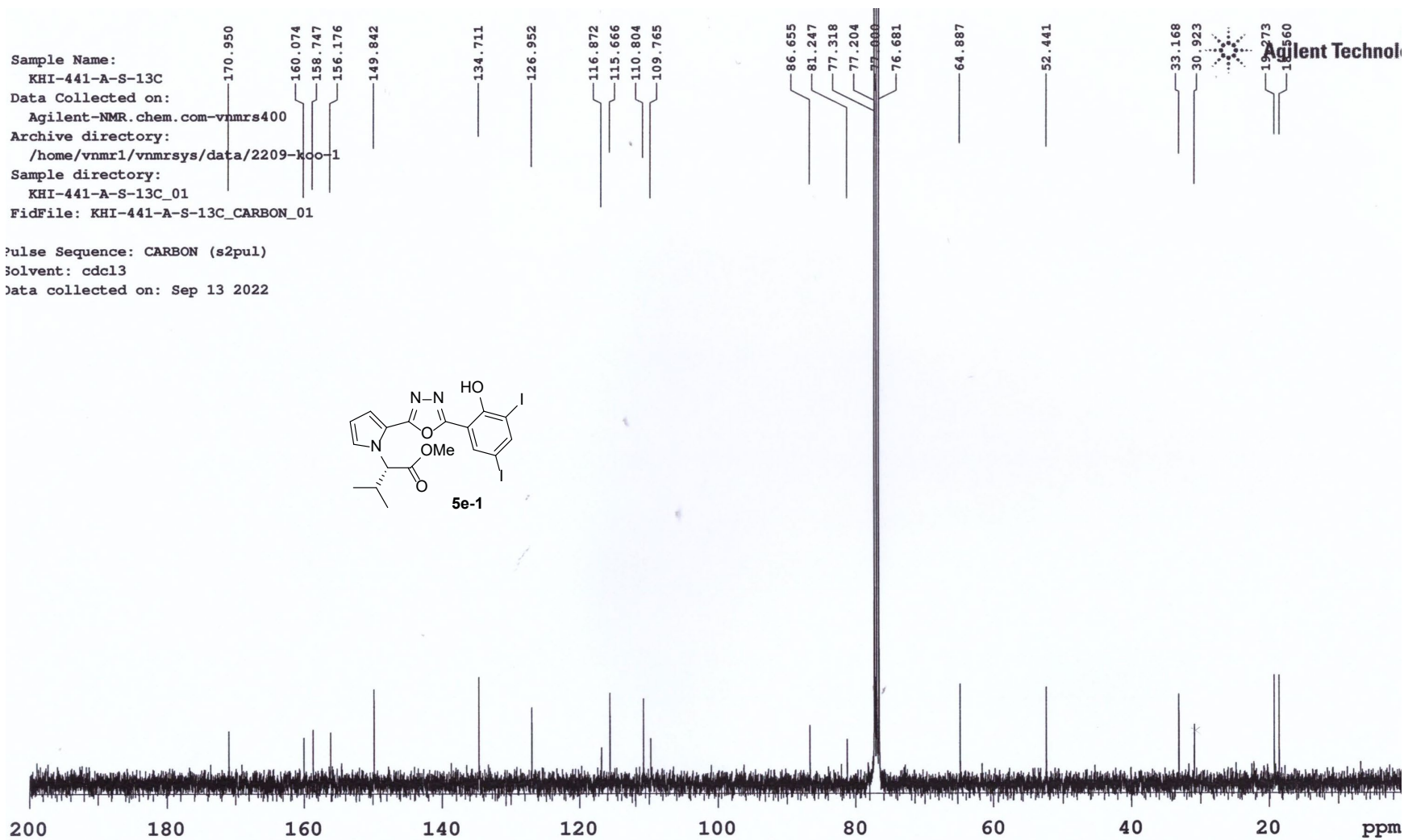
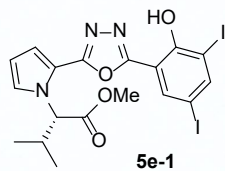
Sample Name: KHI-441-A-S
 Data Collected on: Agilent-NMR.chem.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2209-koo-1
 Sample directory: KHI-441-A-S_01
 FidFile: KHI-441-A-S_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Sep 8 2022



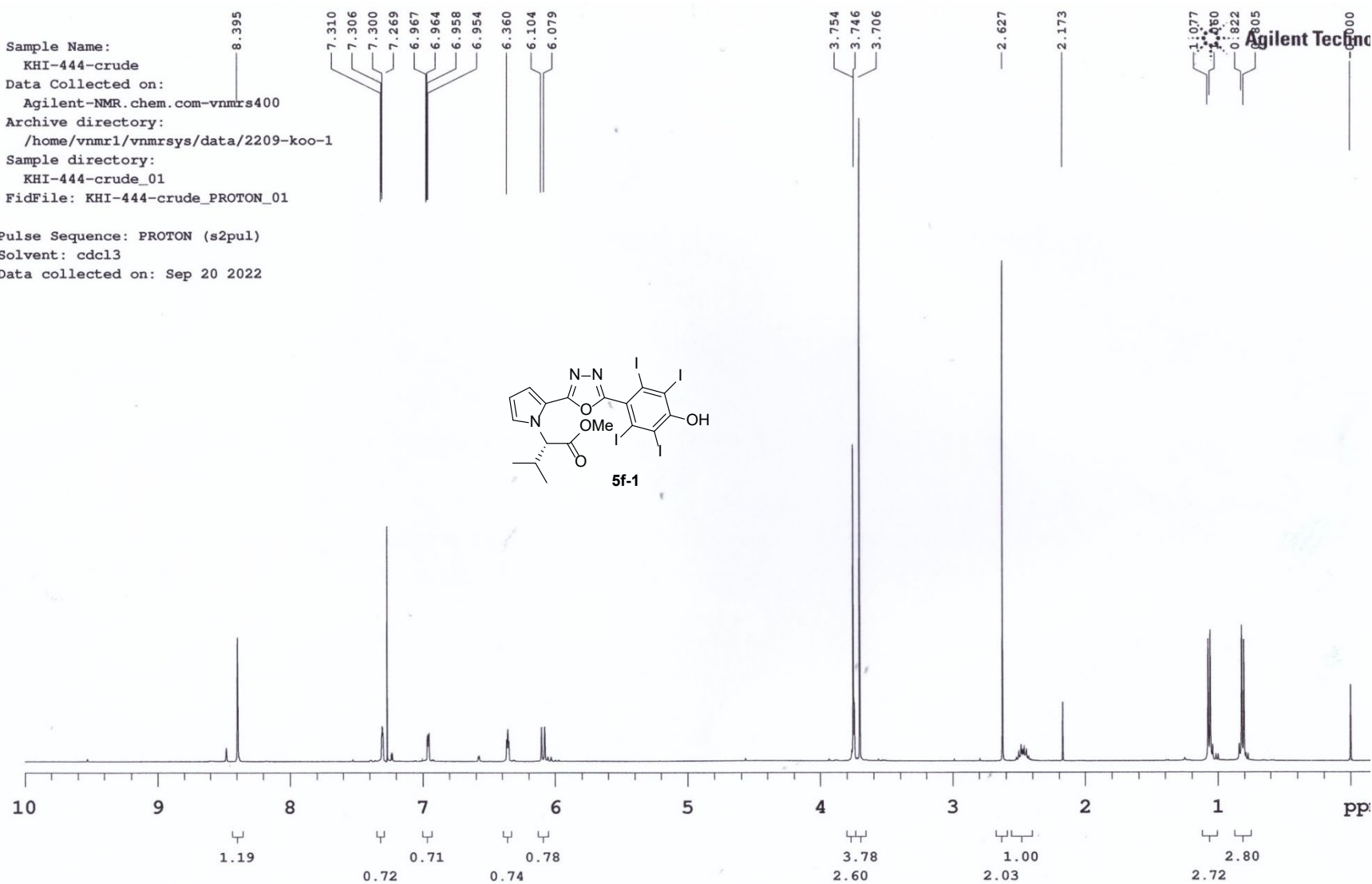
Sample Name:
KHI-441-A-S-13C
Data Collected on:
Agilent-NMR.chem.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2209-kco-1
Sample directory:
KHI-441-A-S-13C_01
FidFile: KHI-441-A-S-13C CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 13 2022



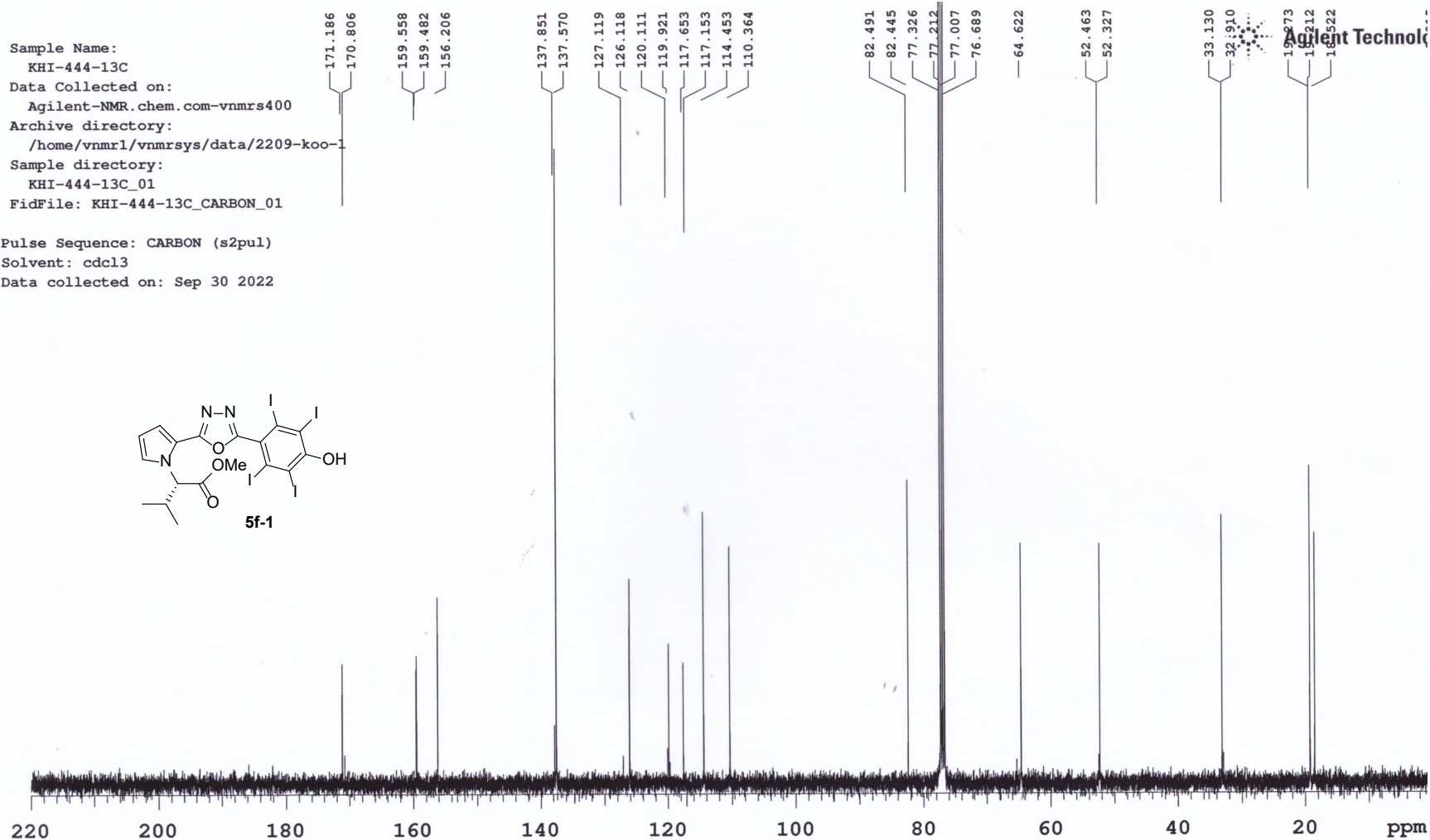
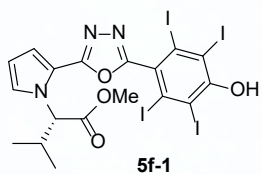
Sample Name:
KHI-444-crude
Data Collected on:
Agilent-NMR.chem.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2209-koo-1
Sample directory:
KHI-444-crude_01
FidFile: KHI-444-crude_PROTON_01

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 20 2022



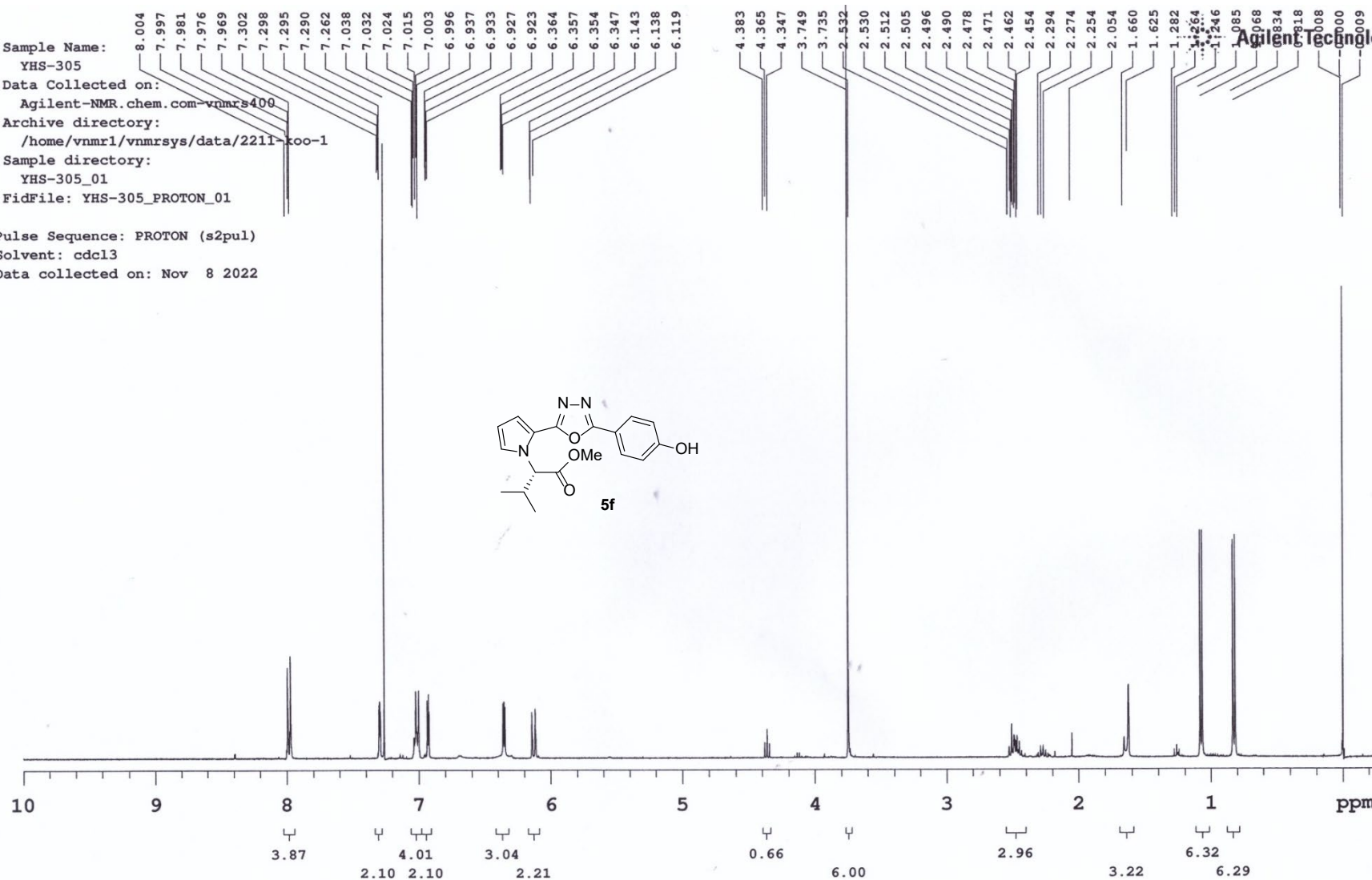
Sample Name:
KHI-444-13C
Data Collected on:
Agilent-NMR.chem.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2209-koo-1
Sample directory:
KHI-444-13C_01
FidFile: KHI-444-13C_CARBO_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 30 2022



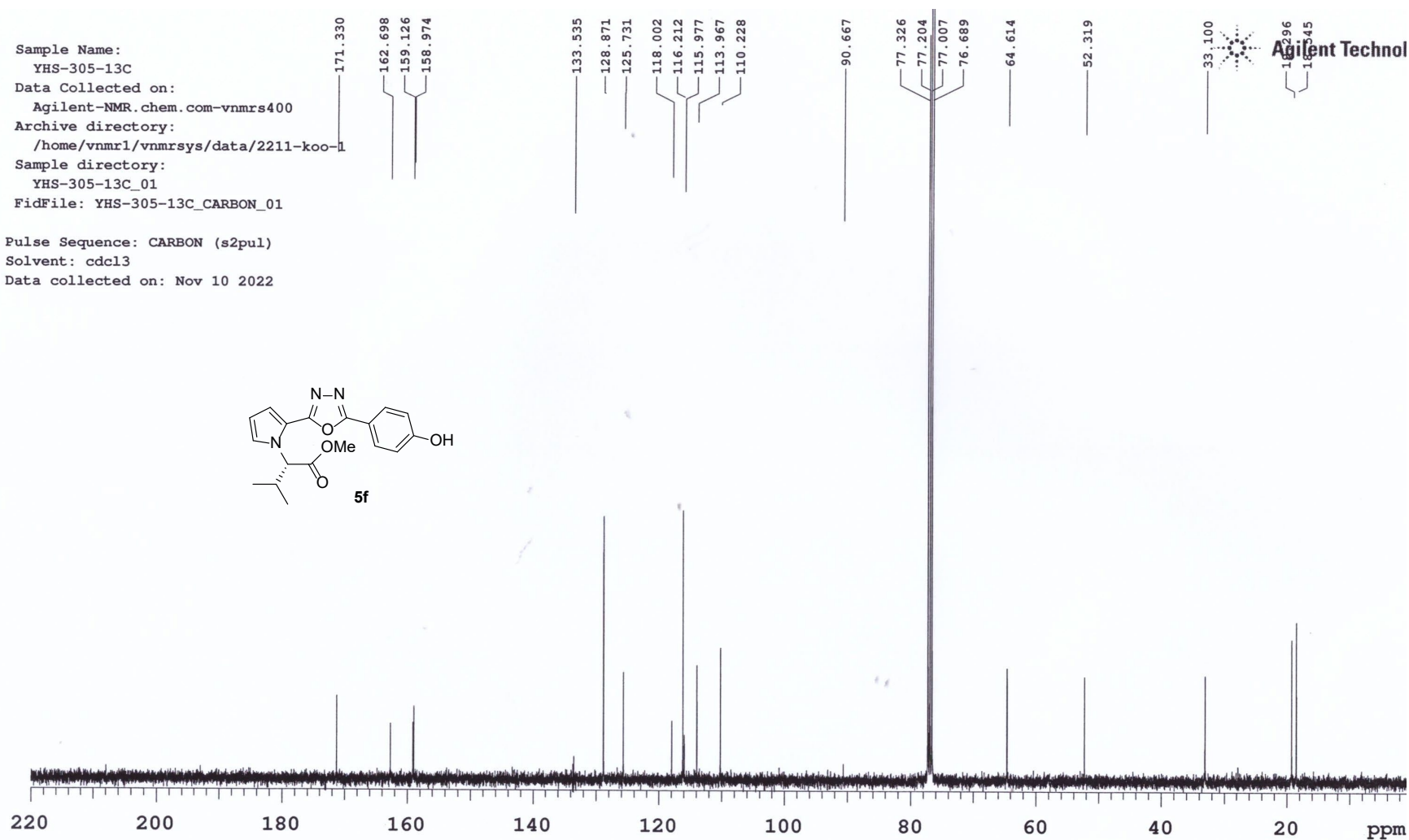
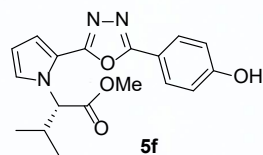
Sample Name: YHS-305
 Data Collected on: Agilent-NMR.chem.com-vnmr400
 Archive directory: /home/vnmr1/vnmrsys/data/2211-koo-1
 Sample directory: YHS-305_01
 FidFile: YHS-305_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Nov 8 2022



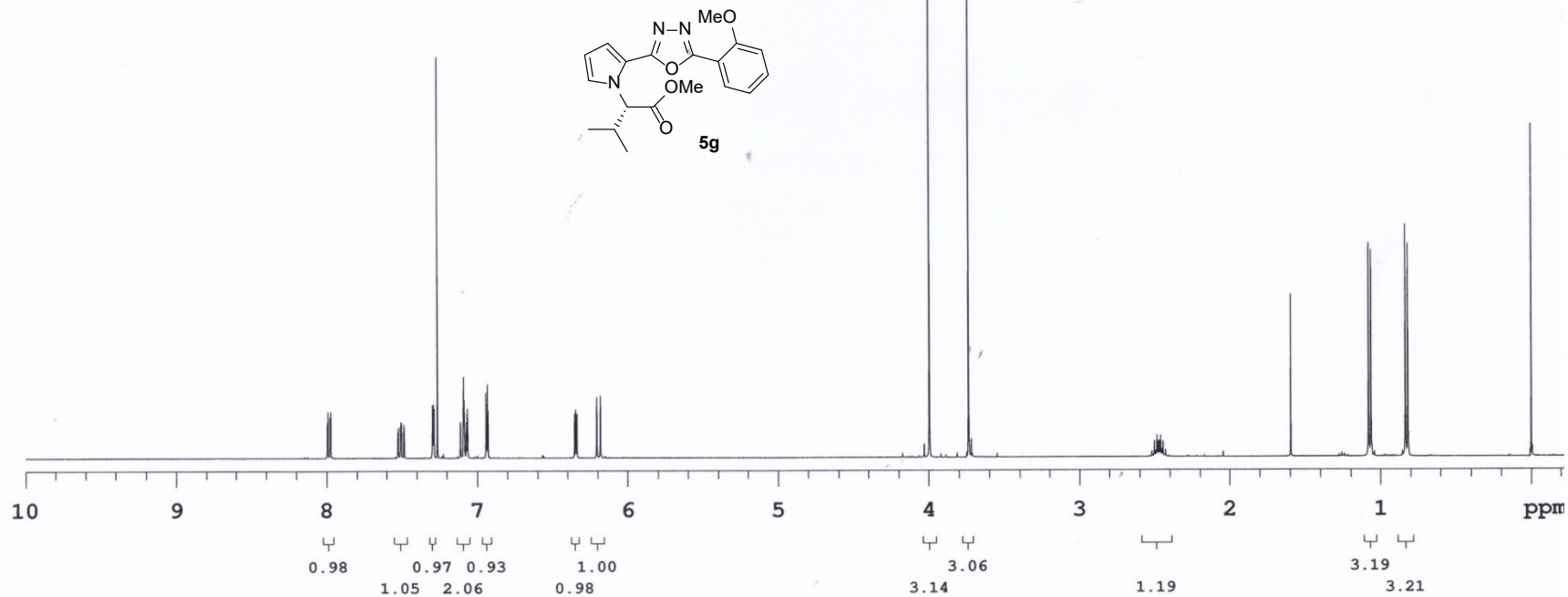
Sample Name:
YHS-305-13C
Data Collected on:
Agilent-NMR.chem.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2211-koo-1
Sample directory:
YHS-305-13C_01
FidFile: YHS-305-13C_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 10 2022



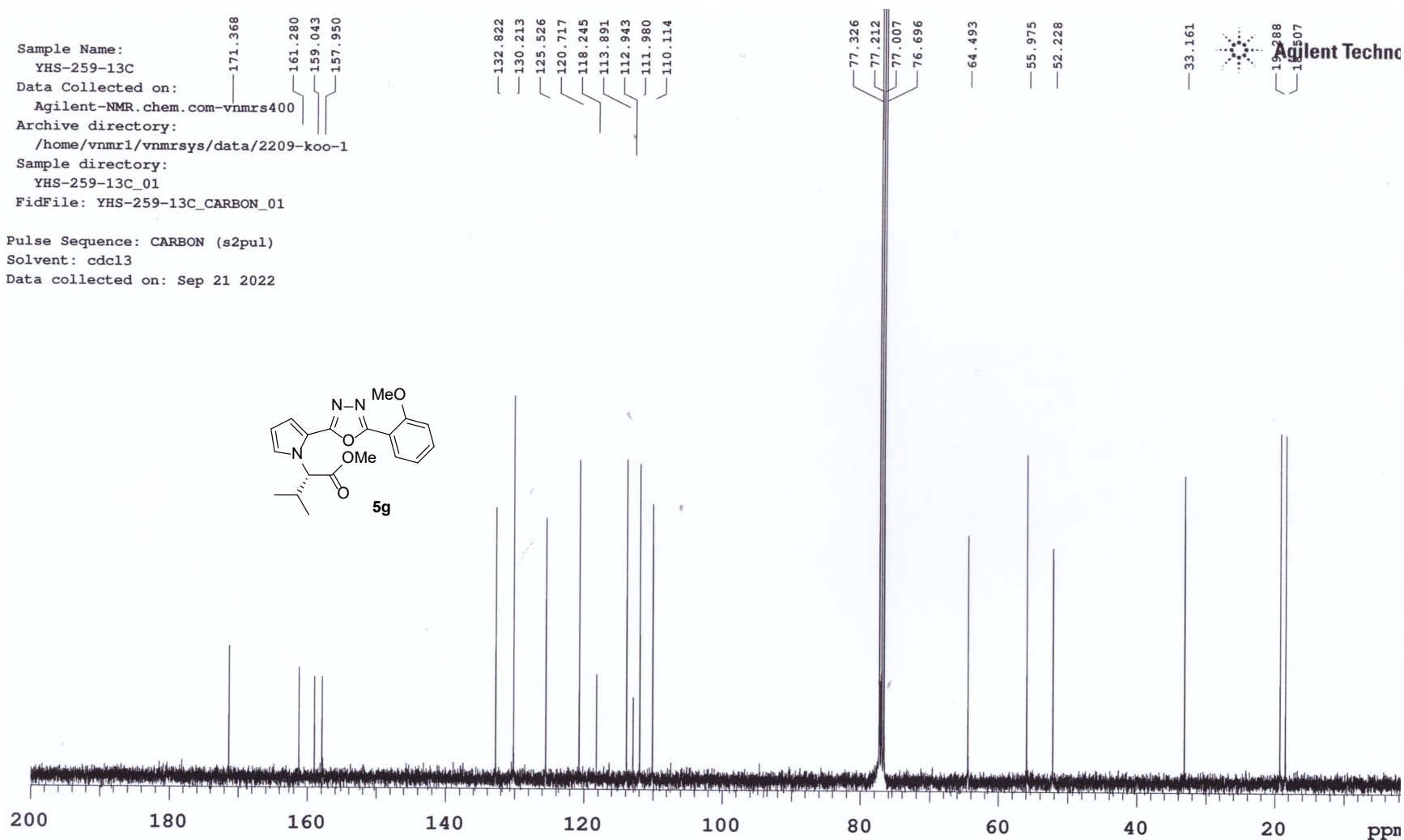
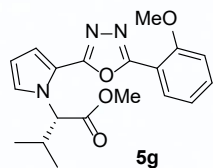
Sample Name: YHS-259
 Data Collected on: Agilent-NMR.chem.com-vnmr400
 Archive directory: /home/vnmr1/vnmrsys/data/2209-koo-1
 Sample directory: YHS-259_02
 FidFile: YHS-259_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Sep 21 2022



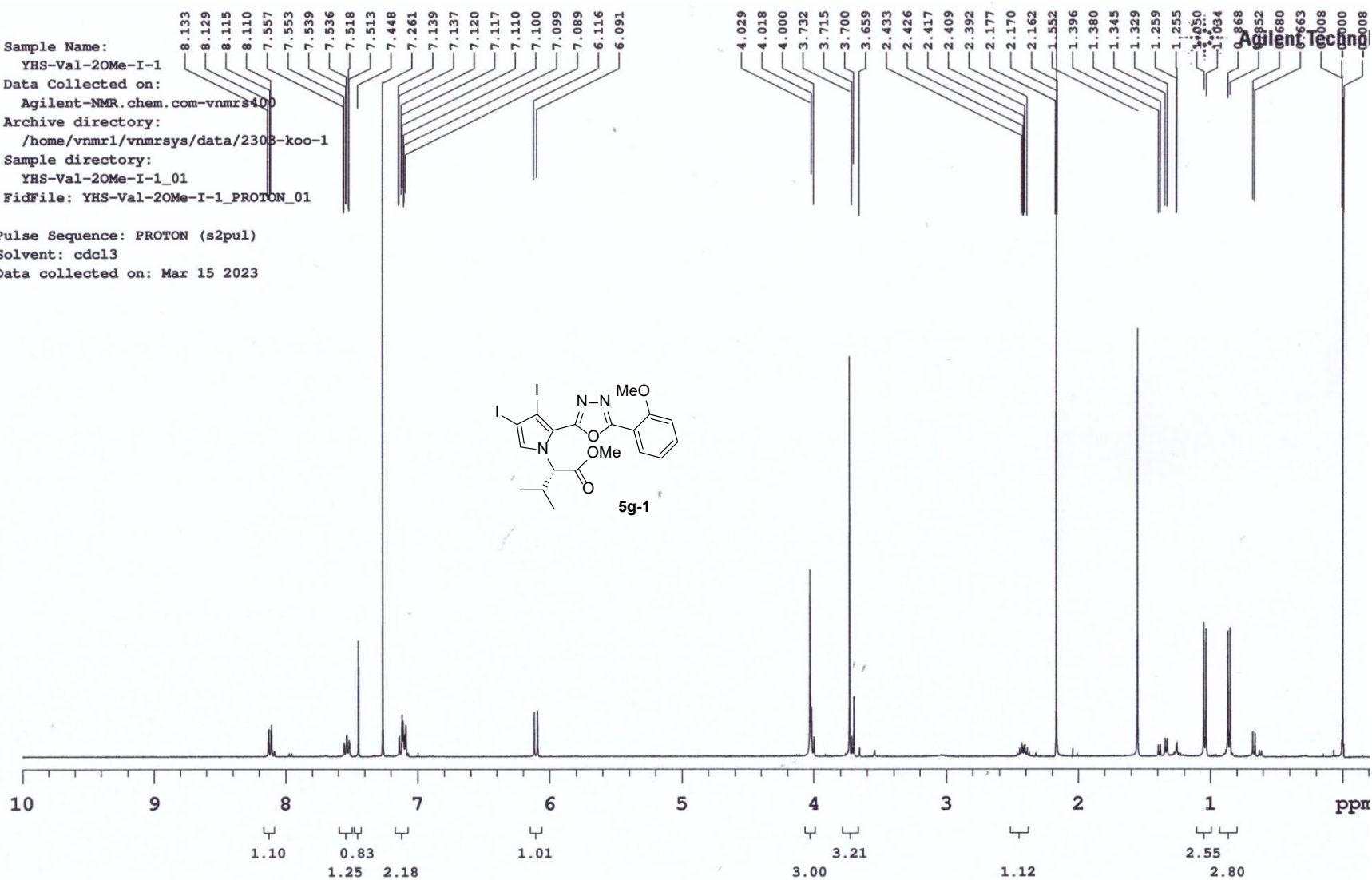
Sample Name:
YHS-259-13C
Data Collected on:
Agilent-NMR.chem.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2209-koo-1
Sample directory:
YHS-259-13C_01
FidFile: YHS-259-13C_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 21 2022



Sample Name:
 YHS-Val-2OMe-I-1
 Data Collected on:
 Agilent-NMR.chem.com-vnmrs400
 Archive directory:
 /home/vnmr1/vnmrsys/data/2308-koo-1
 Sample directory:
 YHS-Val-2OMe-I-1_01
 FidFile: YHS-Val-2OMe-I-1_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Mar 15 2023



Sample Name:

YHS-val-20Me-I-2-13C

Data Collected on:

Agilent-NMR.chem.com-vnmrs400

Archive directory:

/home/vnmr1/vnmrsys/data/2303-koo-1

Sample directory:

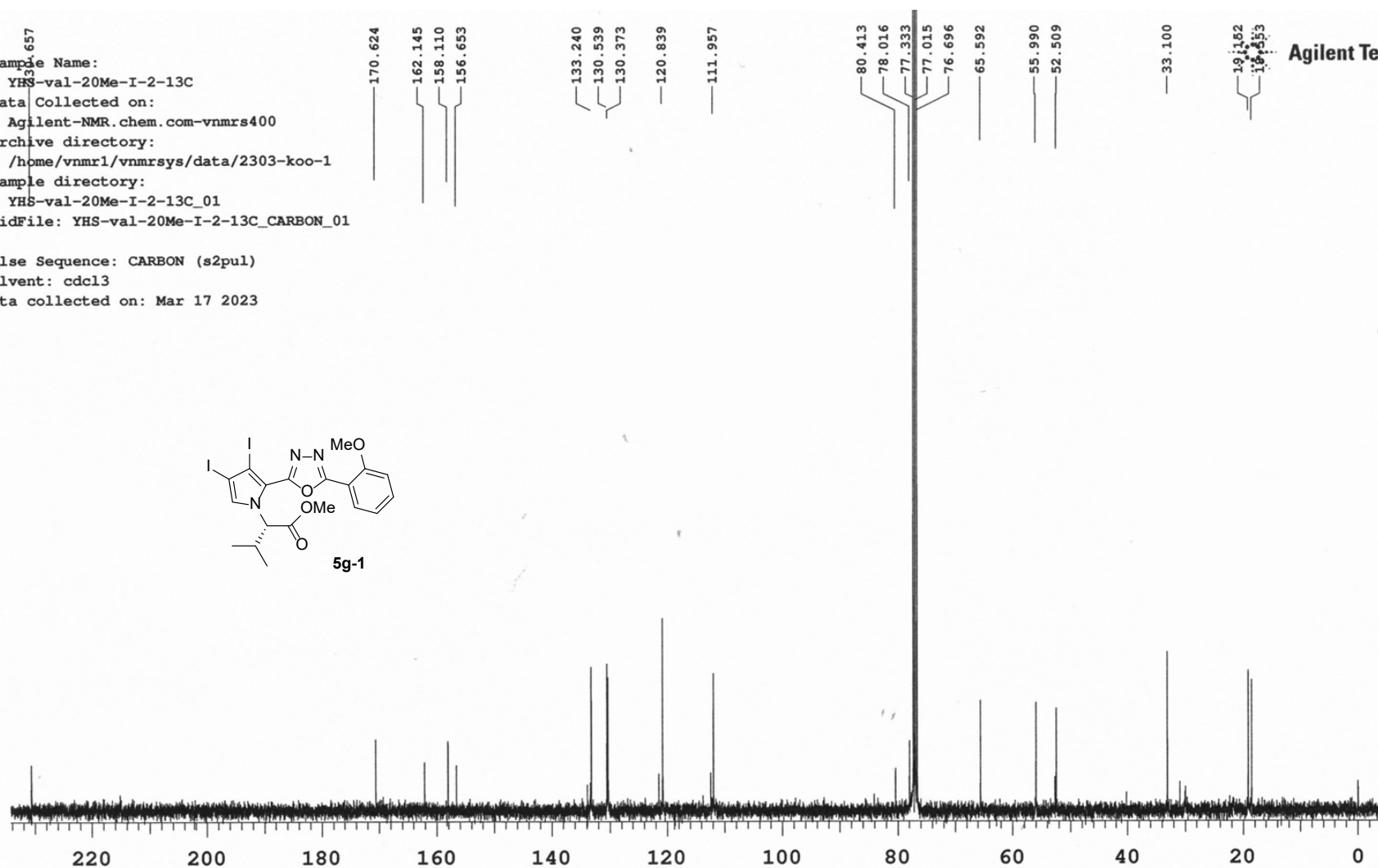
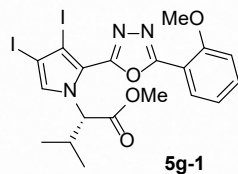
YHS-val-20Me-I-2-13C_01

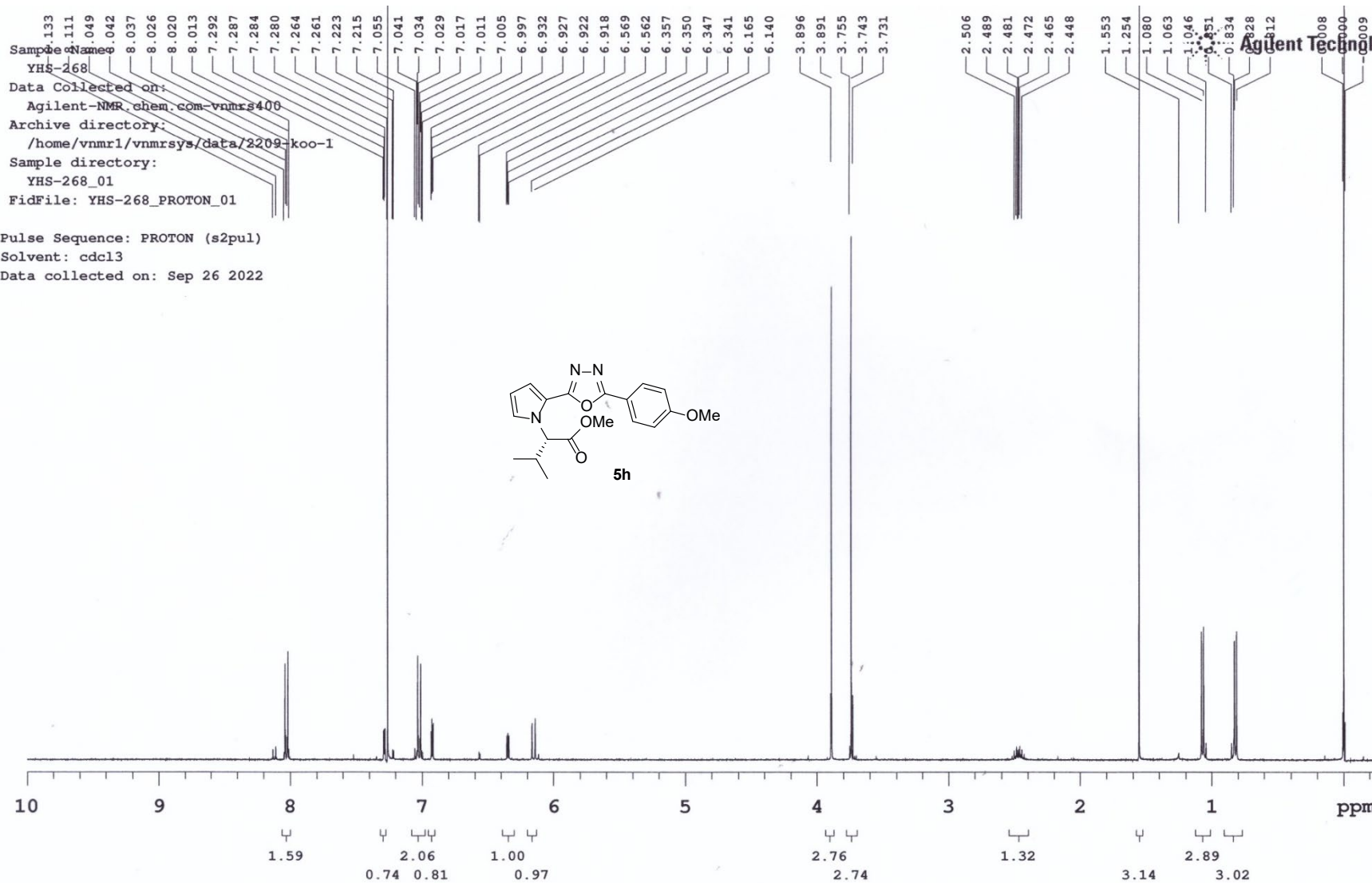
FidFile: YHS-val-20Me-I-2-13C_CARBON_01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

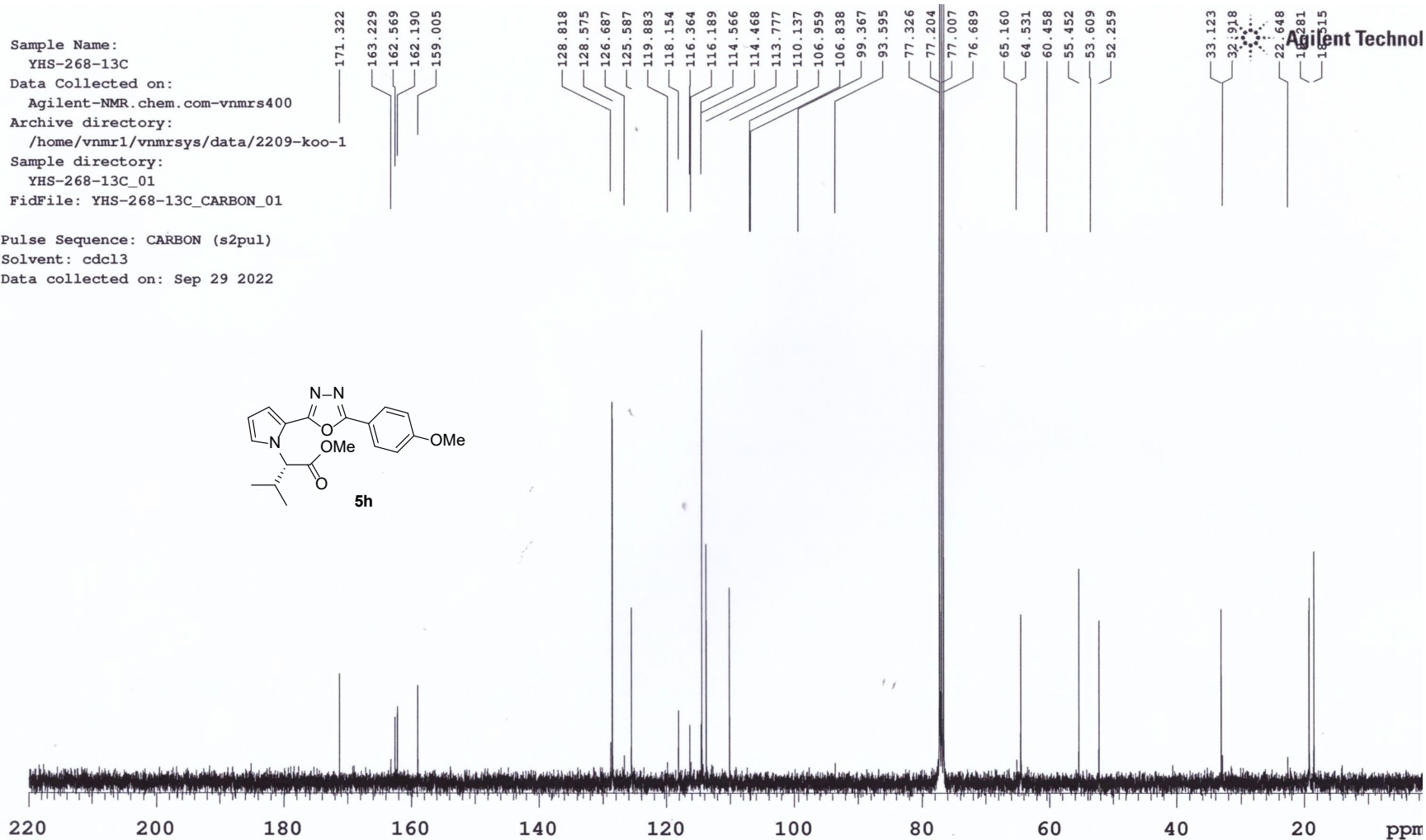
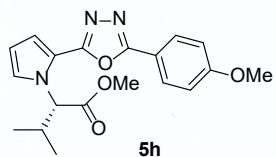
Data collected on: Mar 17 2023





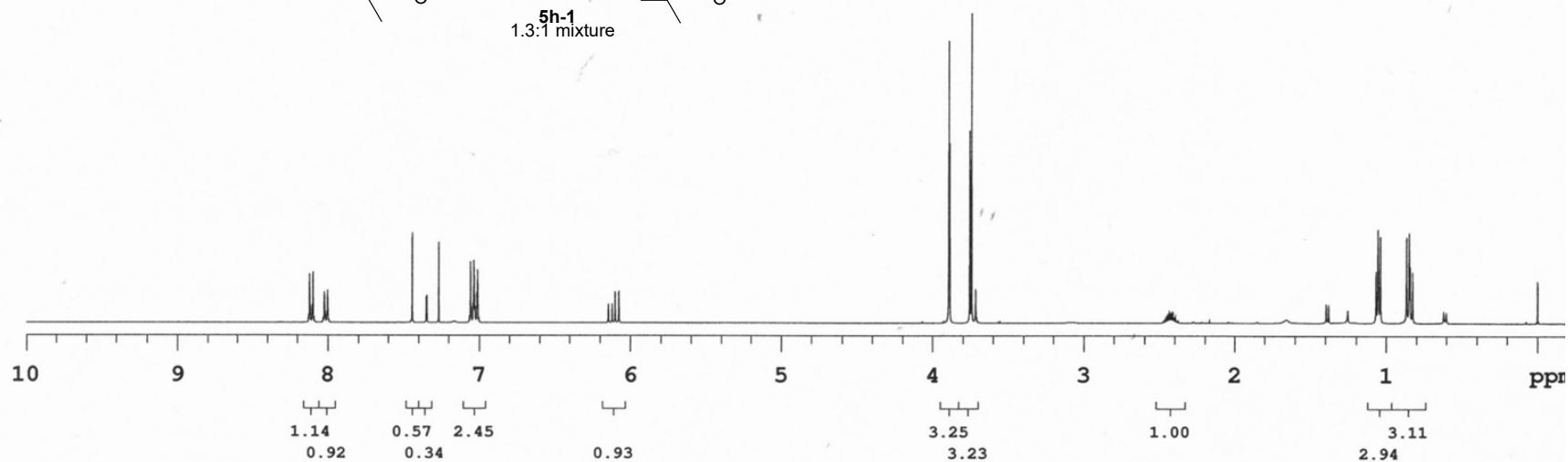
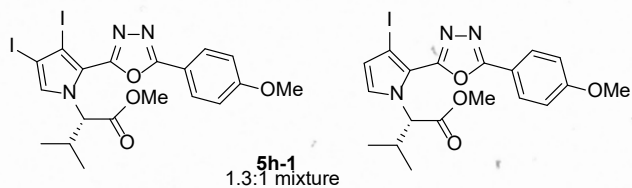
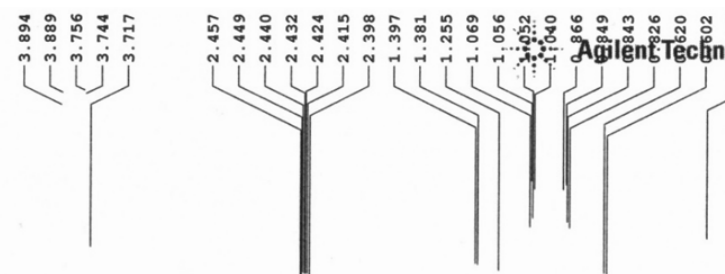
Sample Name:
YHS-268-13C
Data Collected on:
Agilent-NMR.chem.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2209-koo-1
Sample directory:
YHS-268-13C_01
FidFile: YHS-268-13C_CARBO_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 29 2022



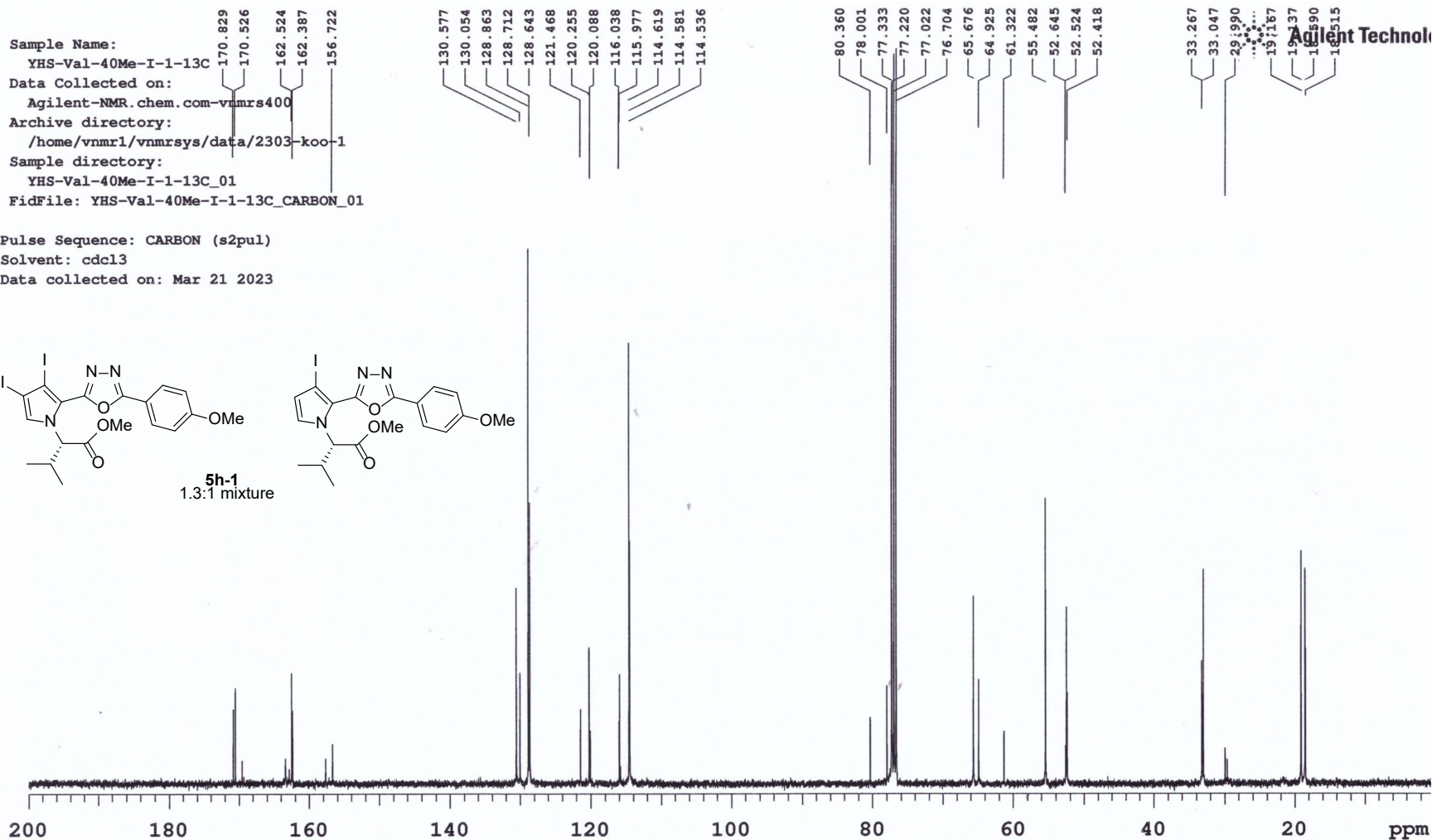
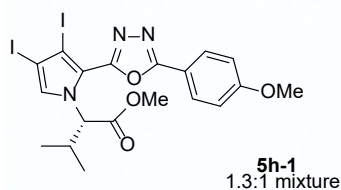
Sample Name: YHS-Val-40Me-I-1
 Data Collected on: Agilent-NMR.chem.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2303-koo-1
 Sample directory: YHS-Val-40Me-I-1_01
 FidFile: YHS-Val-40Me-I-1_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Mar 20 2023



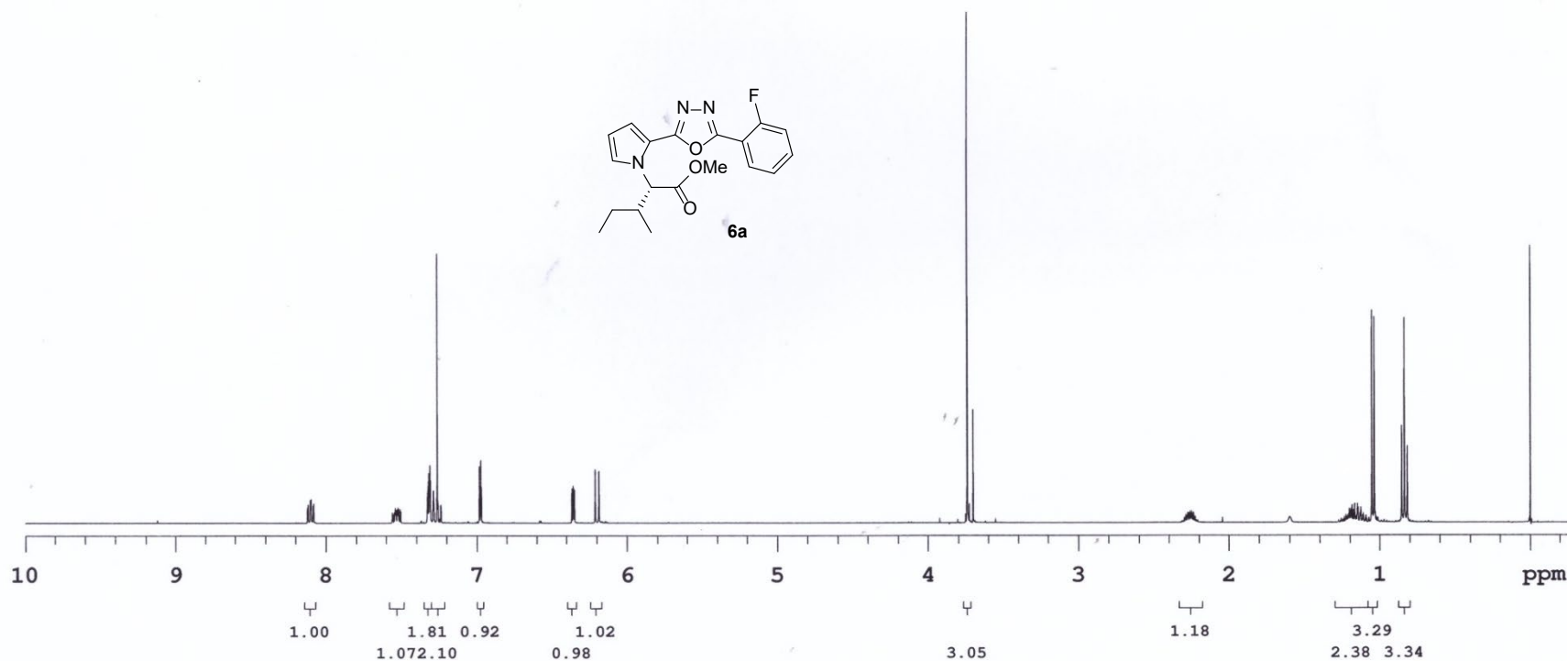
Sample Name:
 YHS-Val-4OMe-I-1-13C
 Data Collected on:
 Agilent-NMR.chem.com-vnmrs400
 Archive directory:
 /home/vnmr1/vnmrsys/data/2303-koo-1
 Sample directory:
 YHS-Val-4OMe-I-1-13C_01
 FidFile: YHS-Val-4OMe-I-1-13C_CARBON_01

Pulse Sequence: CARBON (s2pul)
 Solvent: cdcl3
 Data collected on: Mar 21 2023



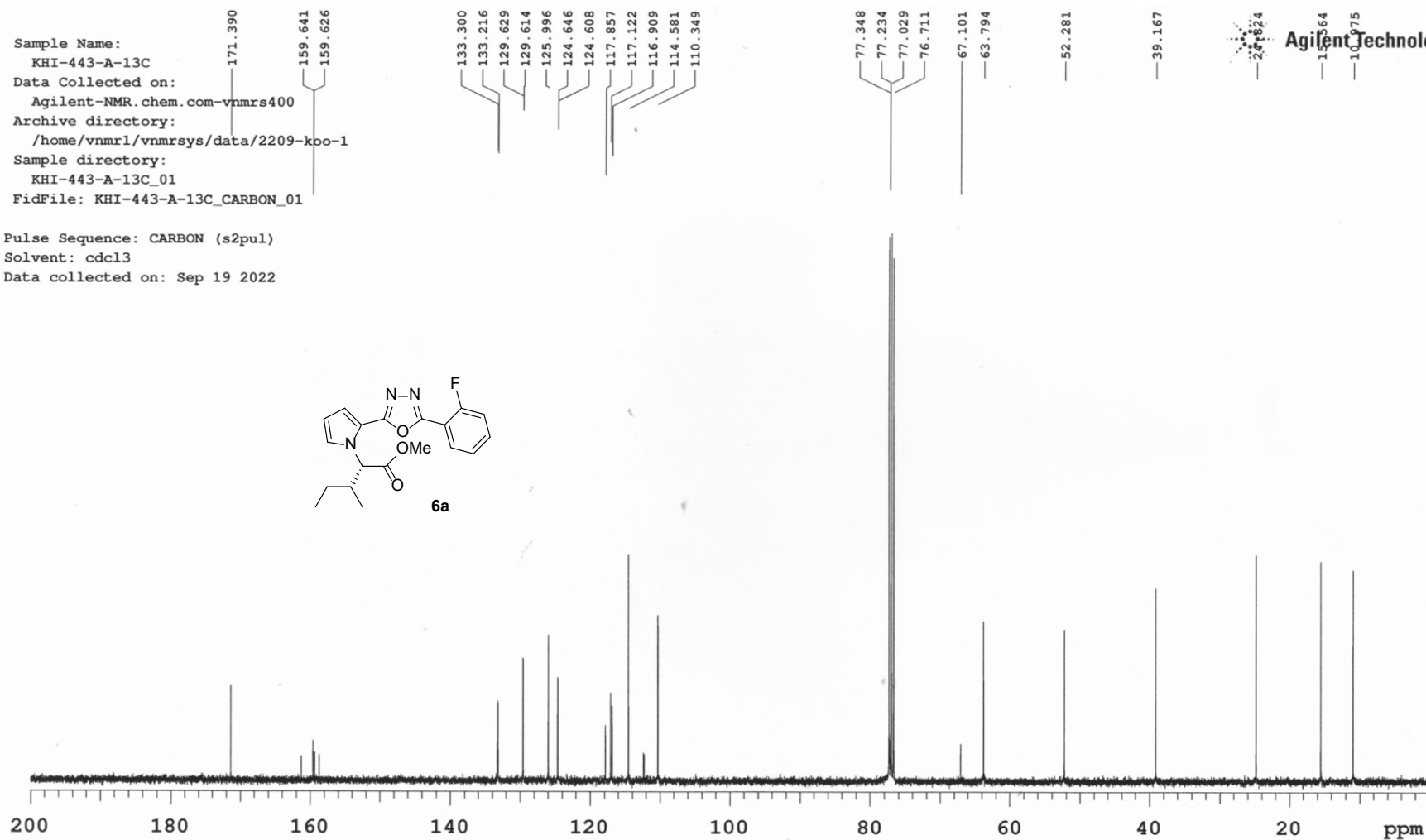
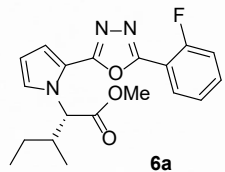
Sample Name: KHI-443-A
 Data Collected on: Agilent-NMR.chem.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2209-koo-1
 Sample directory: KHI-443-A_01
 FidFile: KHI-443-A_PROTON_01

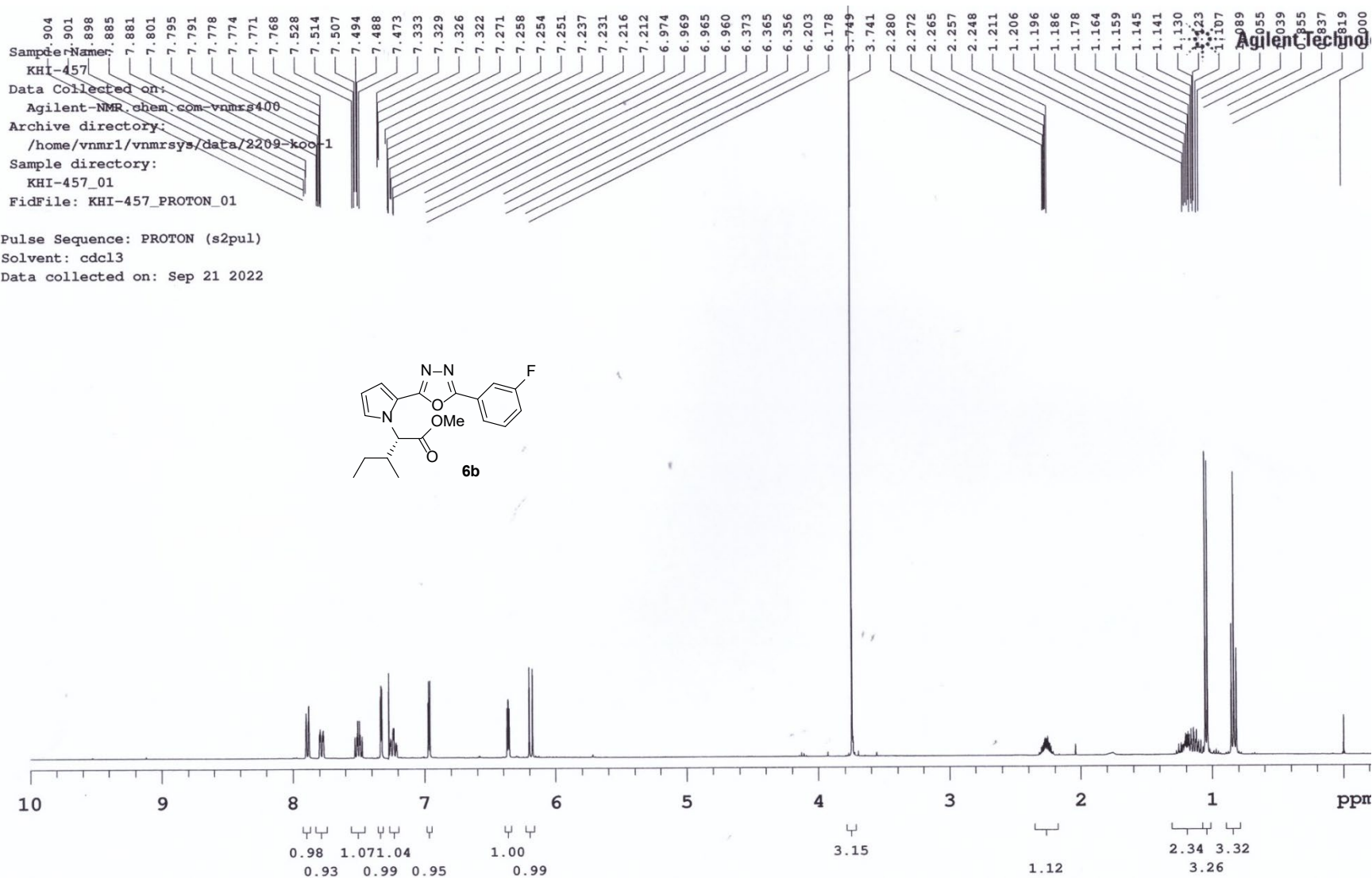
Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Sep 16 2022



Sample Name:
KHI-443-A-13C
Data Collected on:
Agilent-NMR.chem.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2209-kpo-1
Sample directory:
KHI-443-A-13C_01
FidFile: KHI-443-A-13C_CARBO_01

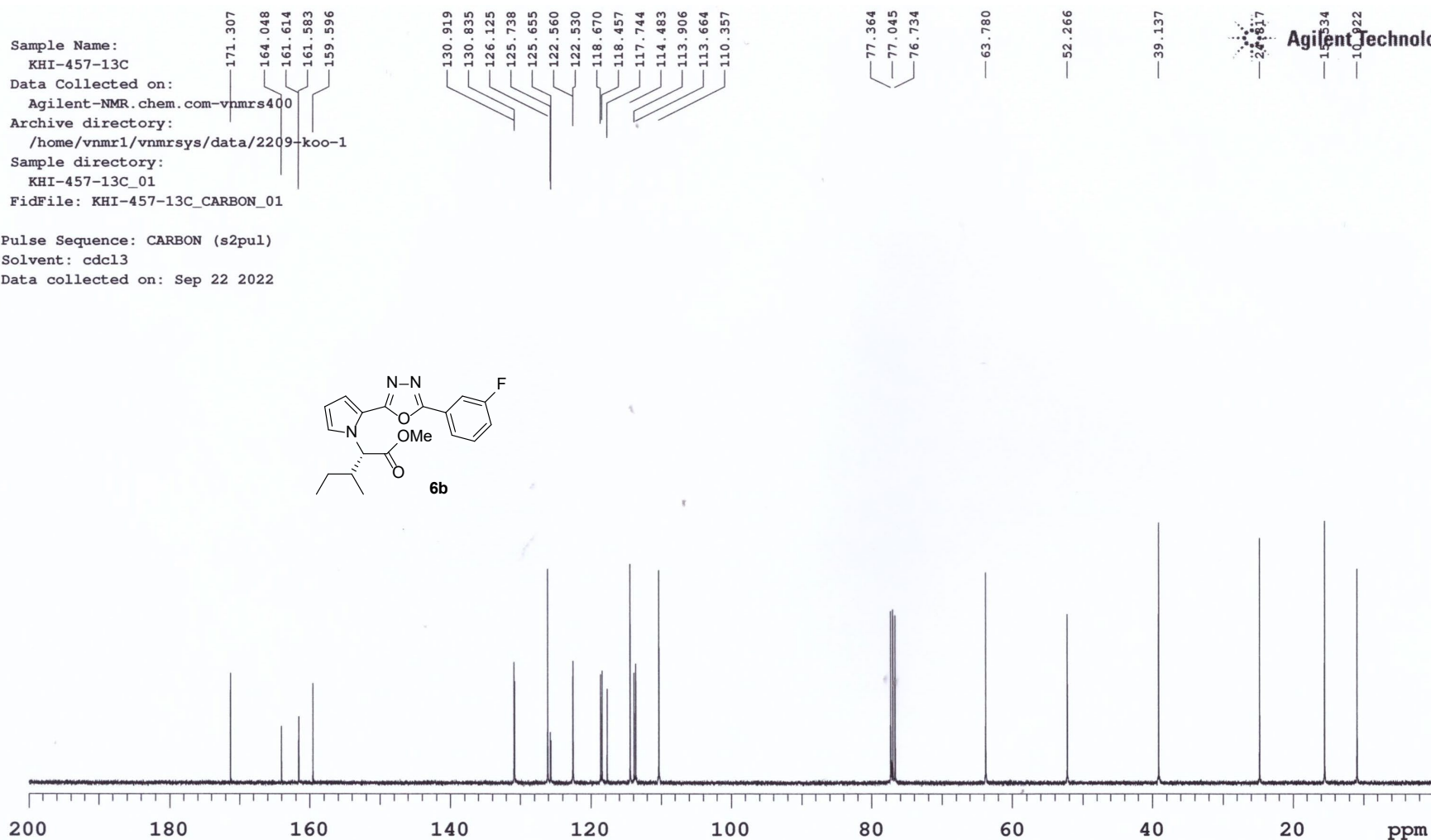
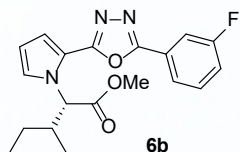
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 19 2022





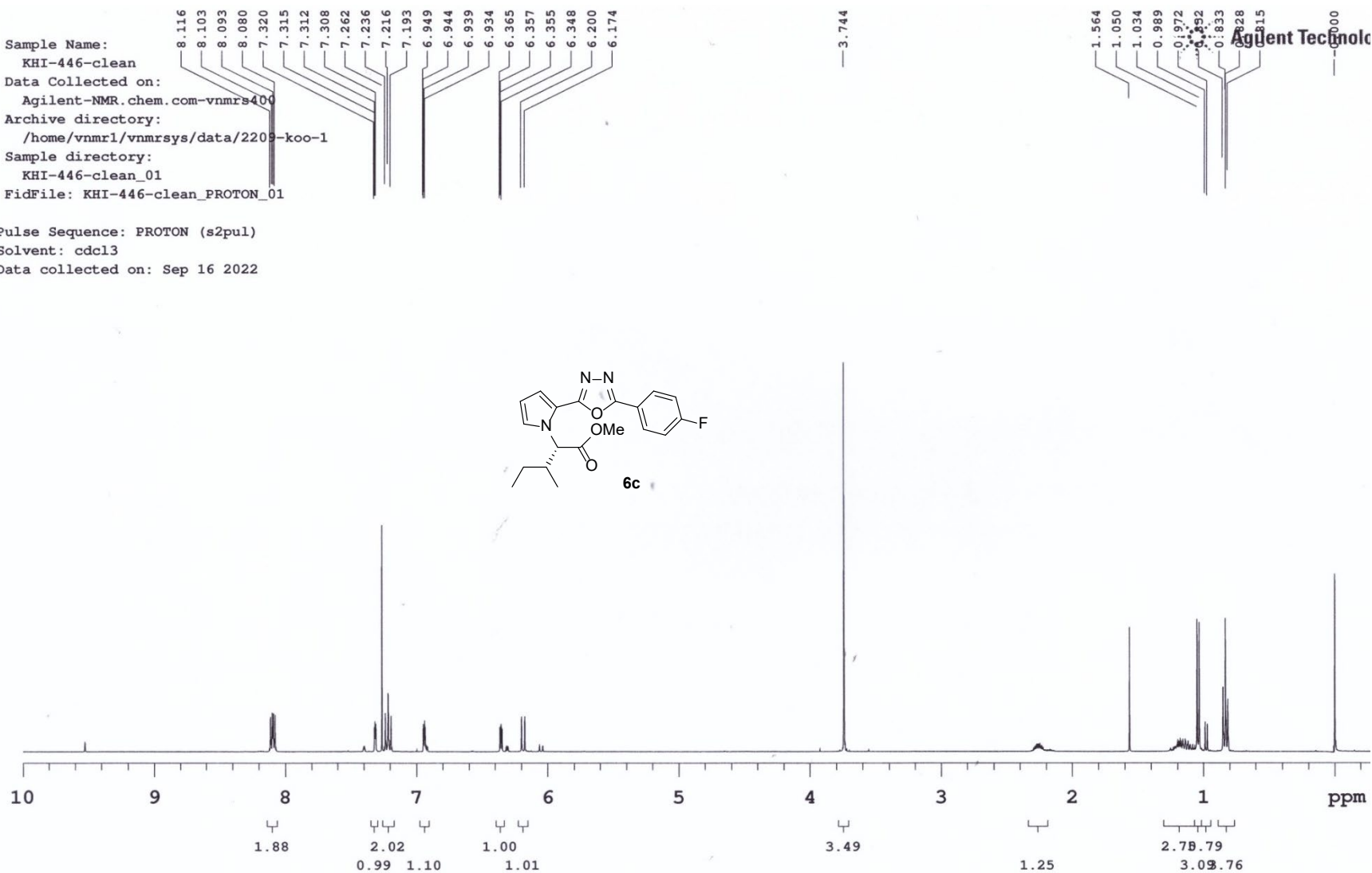
Sample Name:
KHI-457-13C
Data Collected on:
Agilent-NMR.chem.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2209-koo-1
Sample directory:
KHI-457-13C_01
FidFile: KHI-457-13C_CARBO_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 22 2022



Sample Name:
KHI-446-clean
Data Collected on:
Agilent-NMR.chem.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2209-koo-1
Sample directory:
KHI-446-clean_01
FidFile: KHI-446-clean_PROTON_01

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 16 2022



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Agilent-NMR.chem.com-vnmrs400

Archive directory:

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Sample directory:

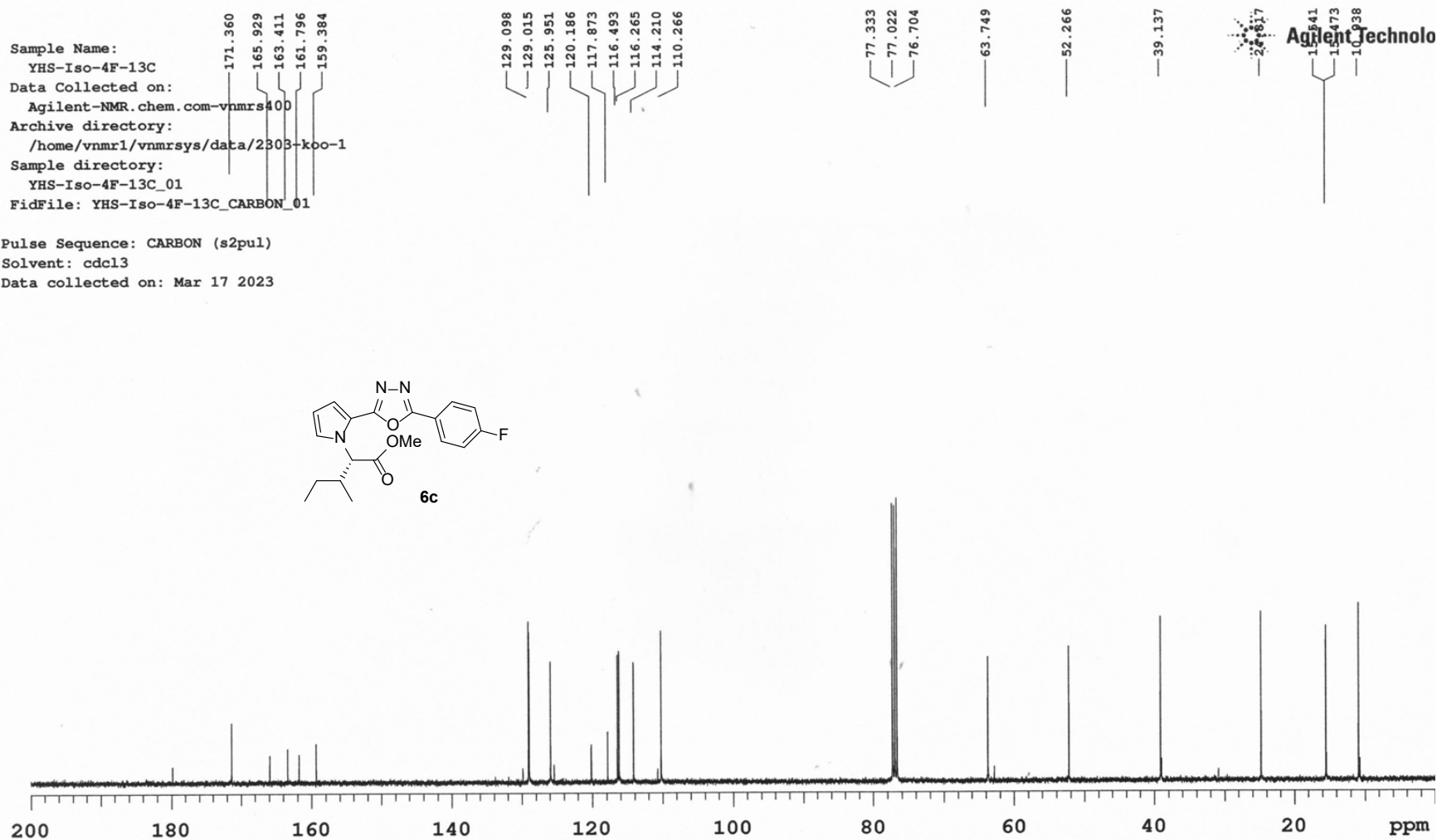
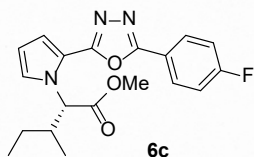
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Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Mar 17 2023



KHI-448-A

Data Collected on:

Agilent-NMR.chem.com-vnmrs400

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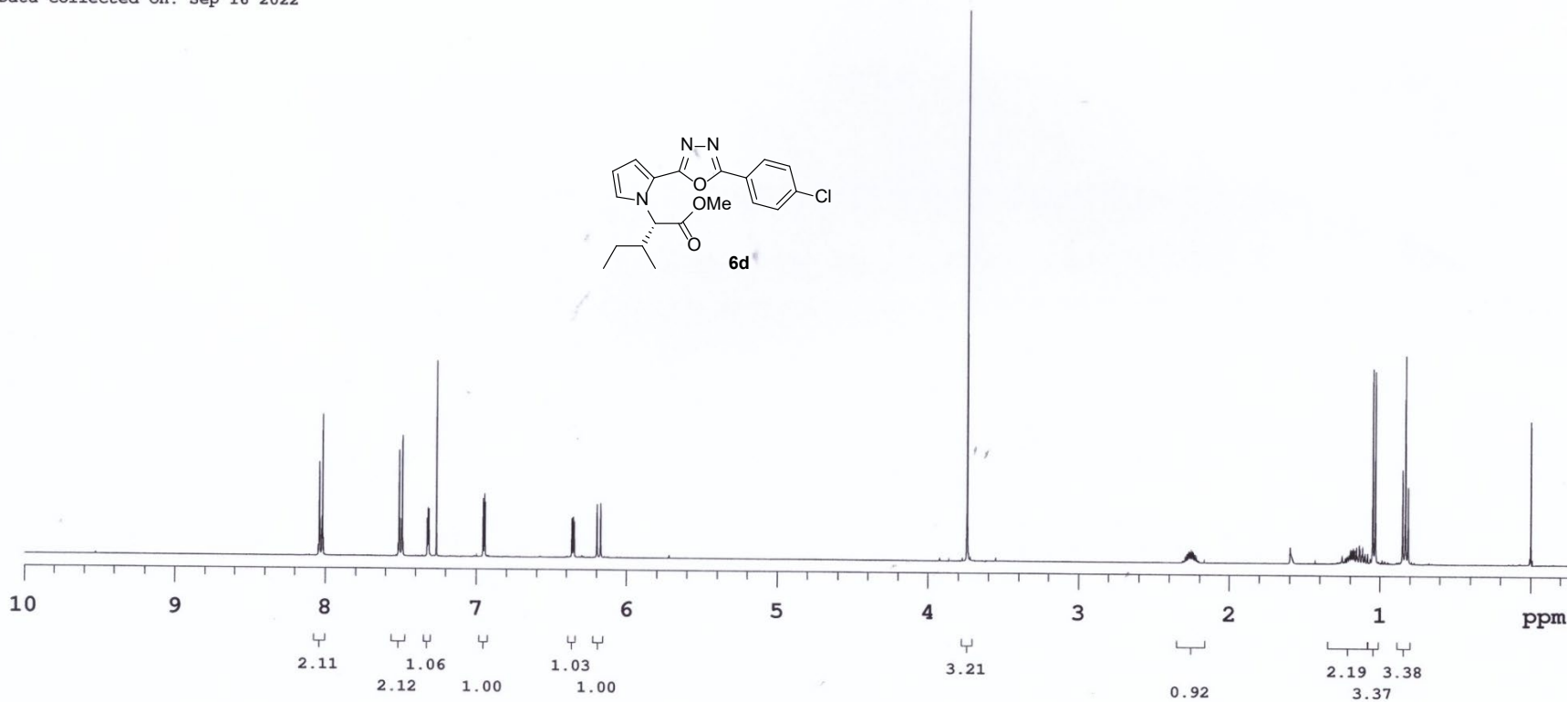
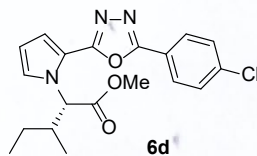
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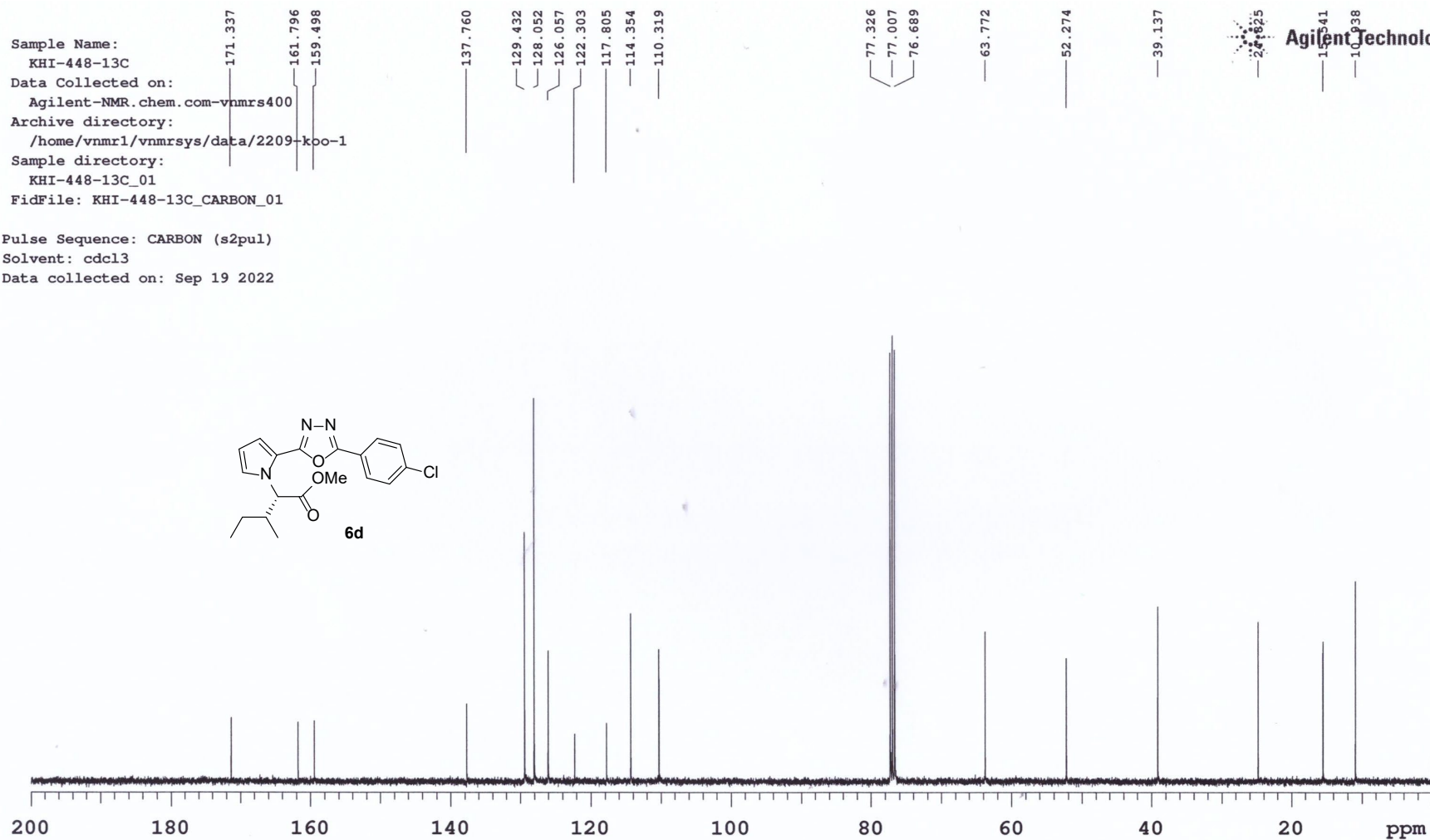
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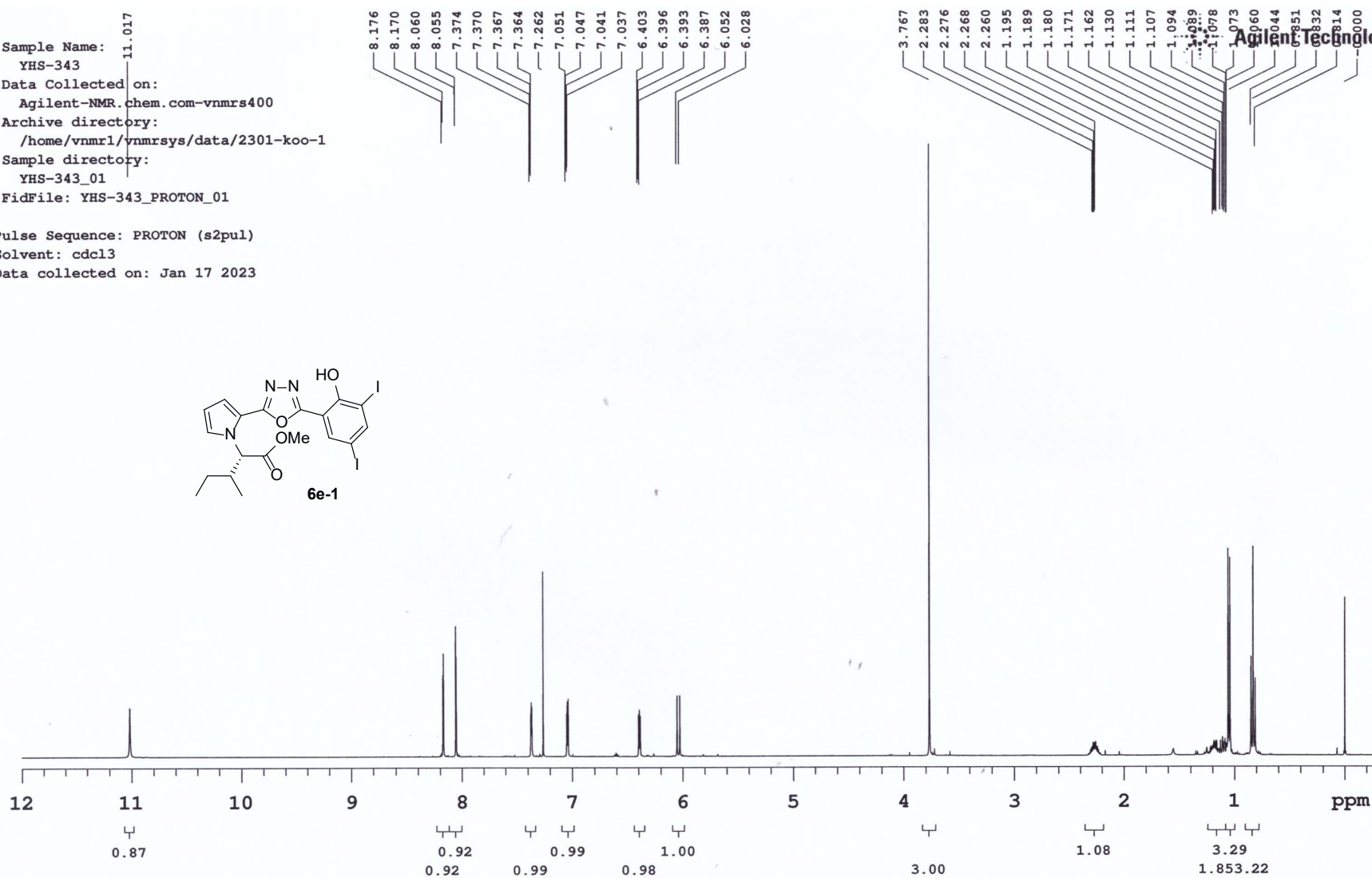
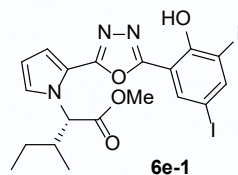
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Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 19 2022



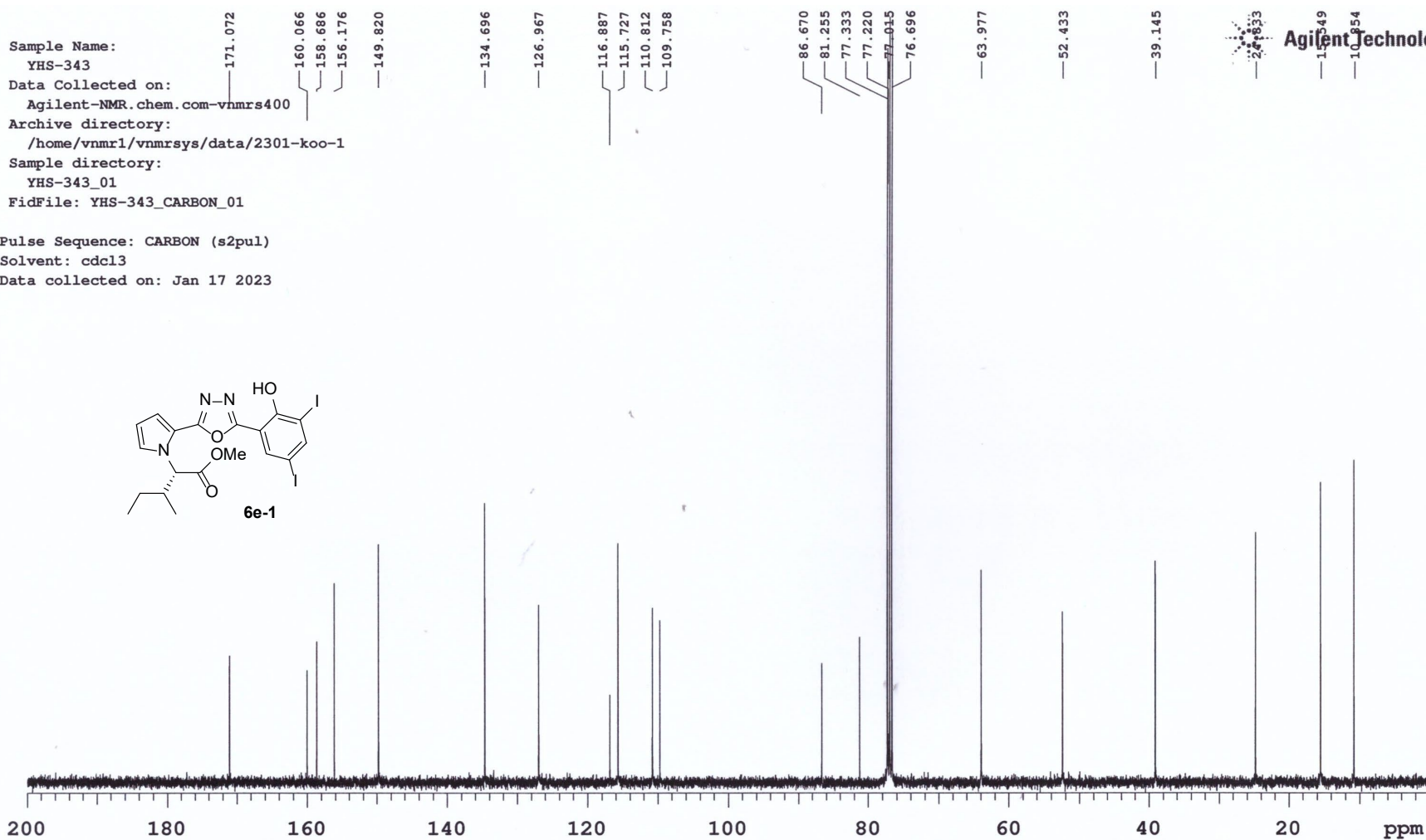
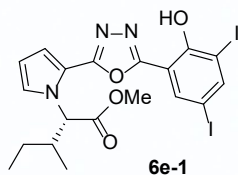
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Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Jan 17 2023



Sample Name:
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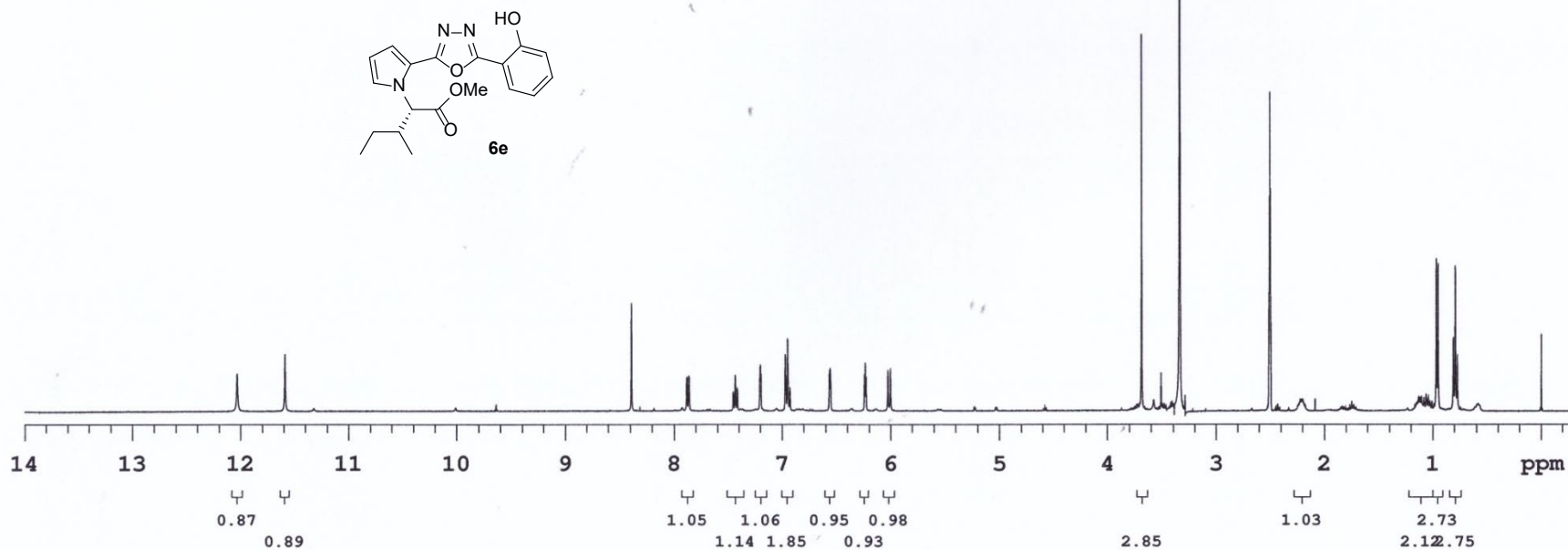
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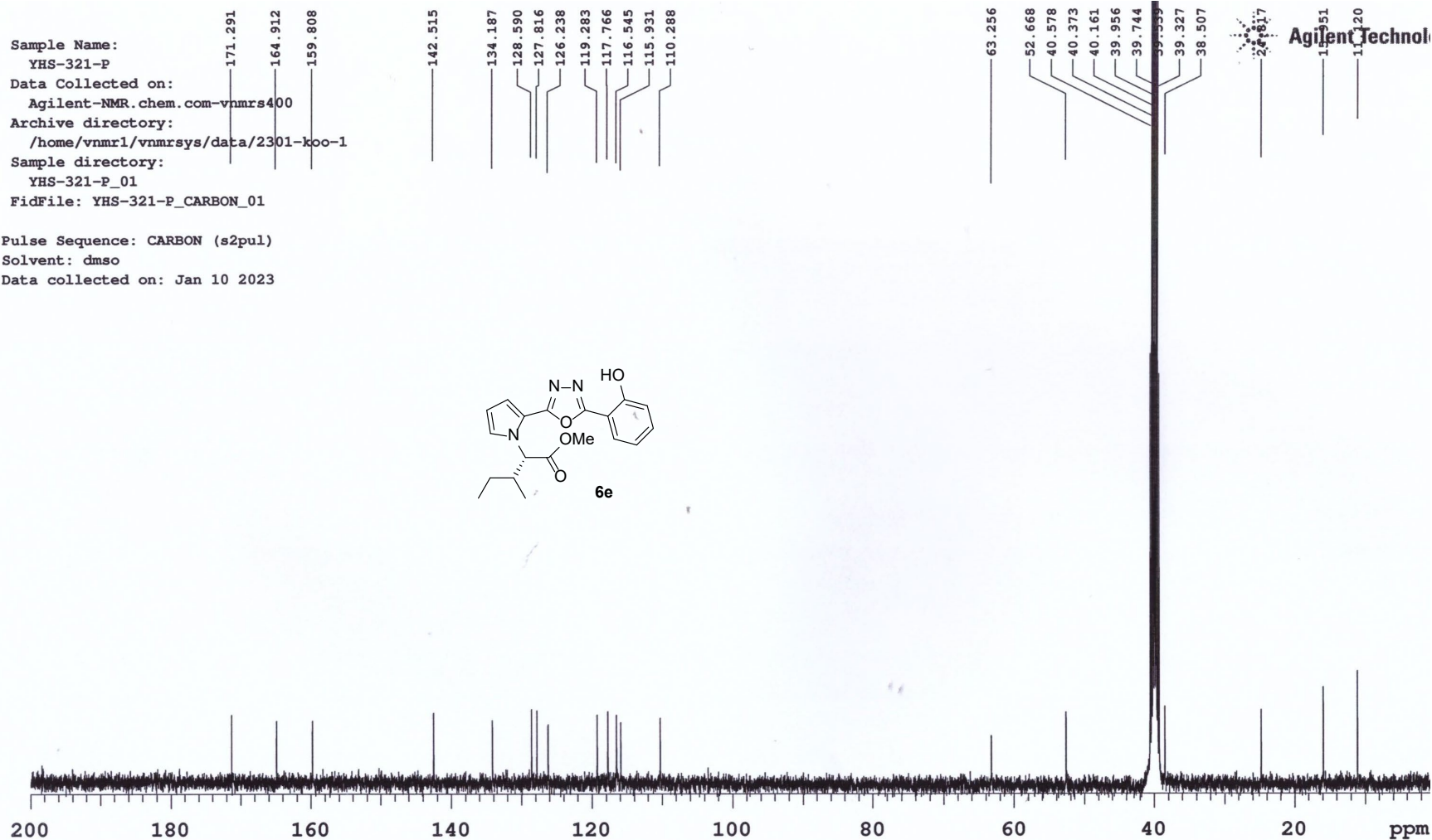
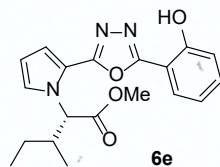
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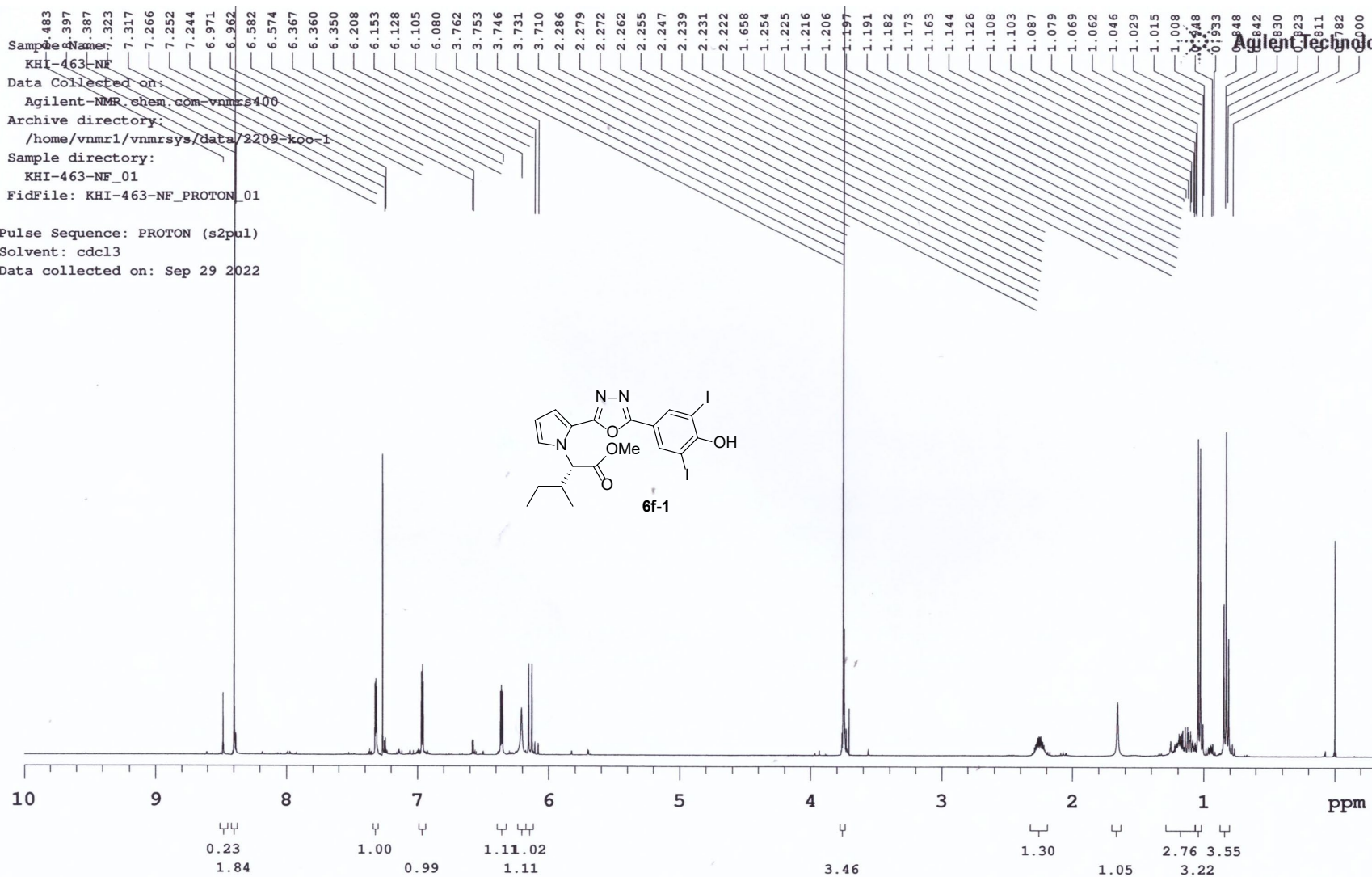
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 Solvent: dmsd
 Data collected on: Jan 10 2023



Sample Name: YHS-321-P
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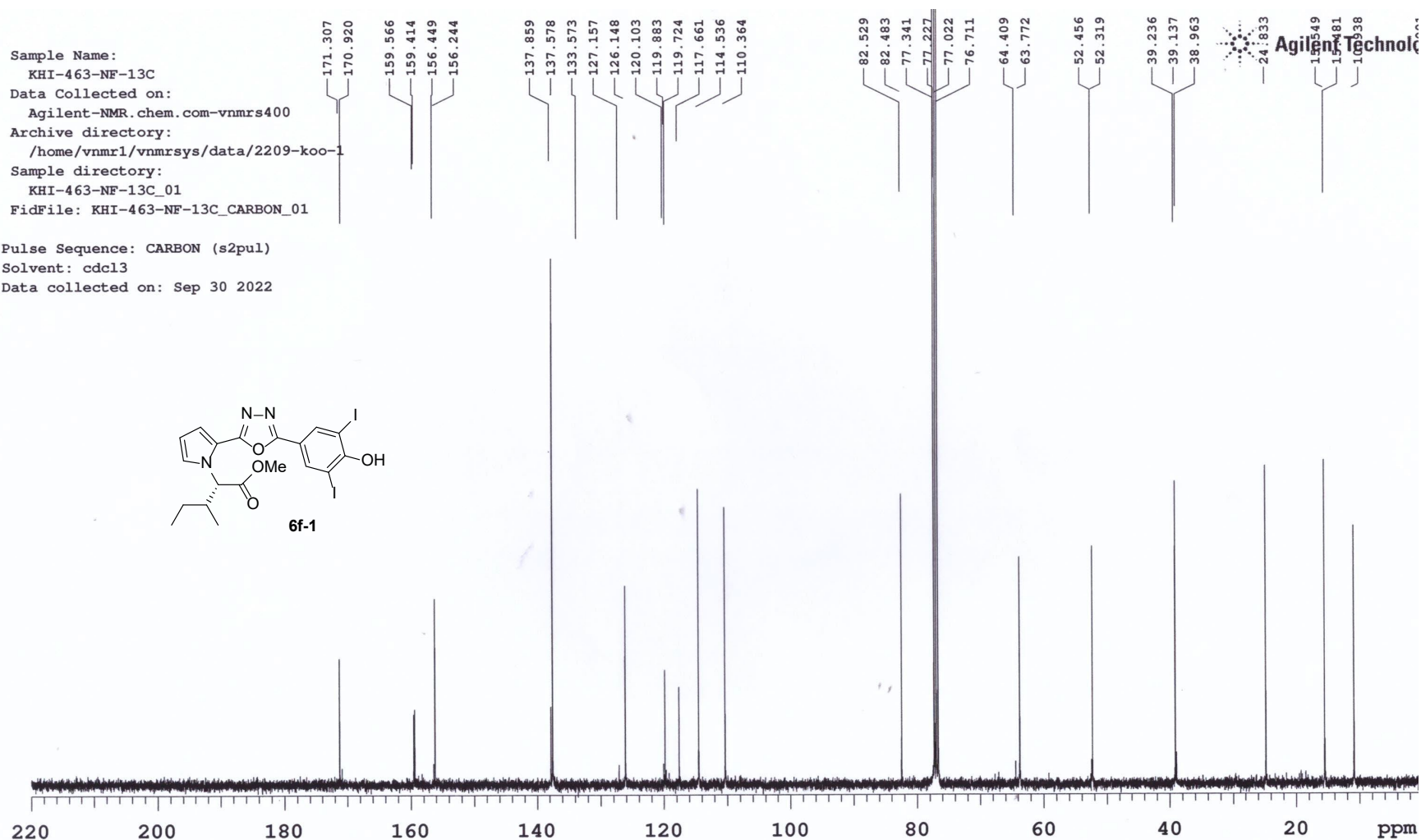
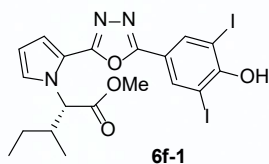
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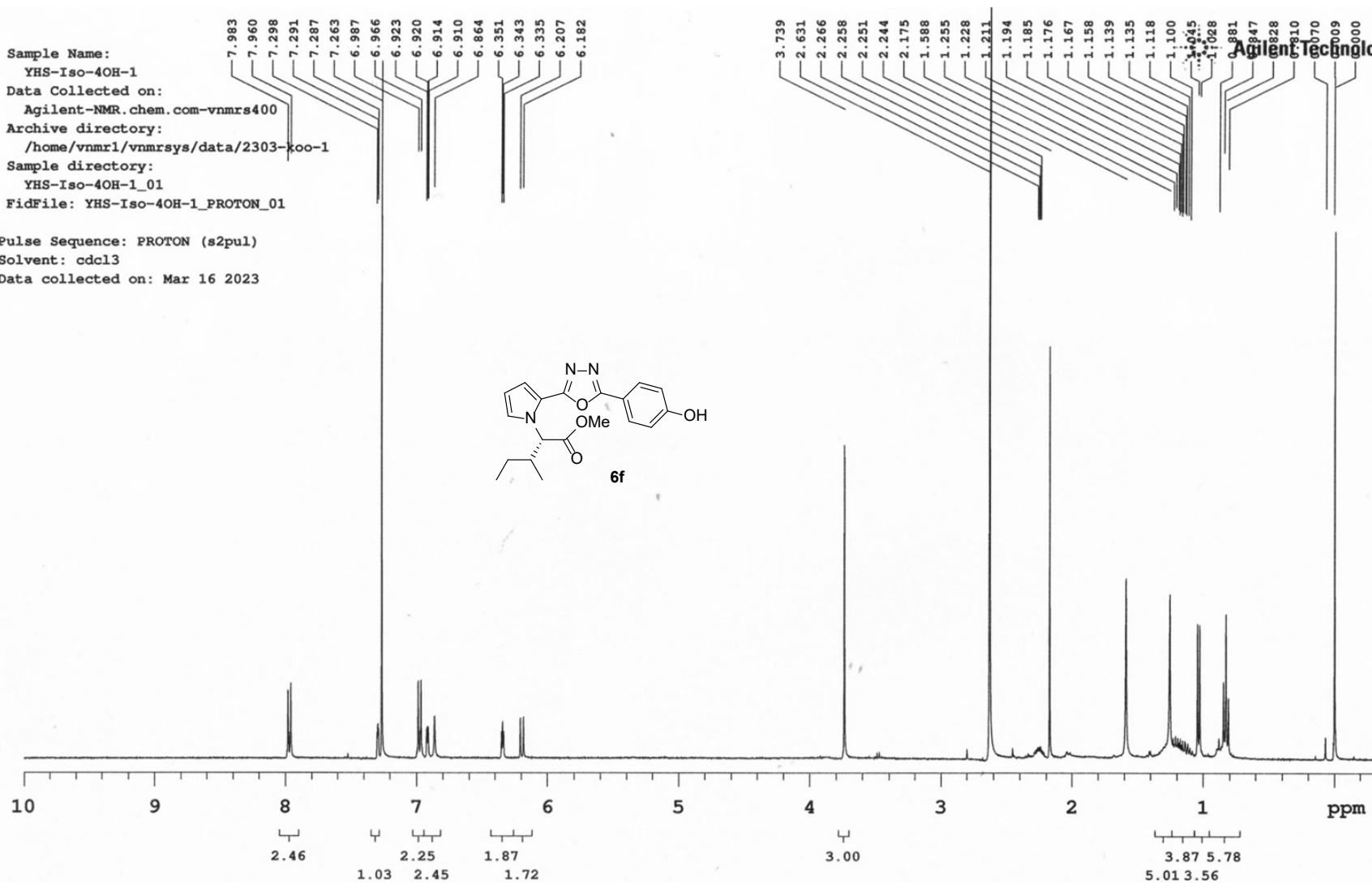
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Pulse Sequence: CARBON (s2pul)
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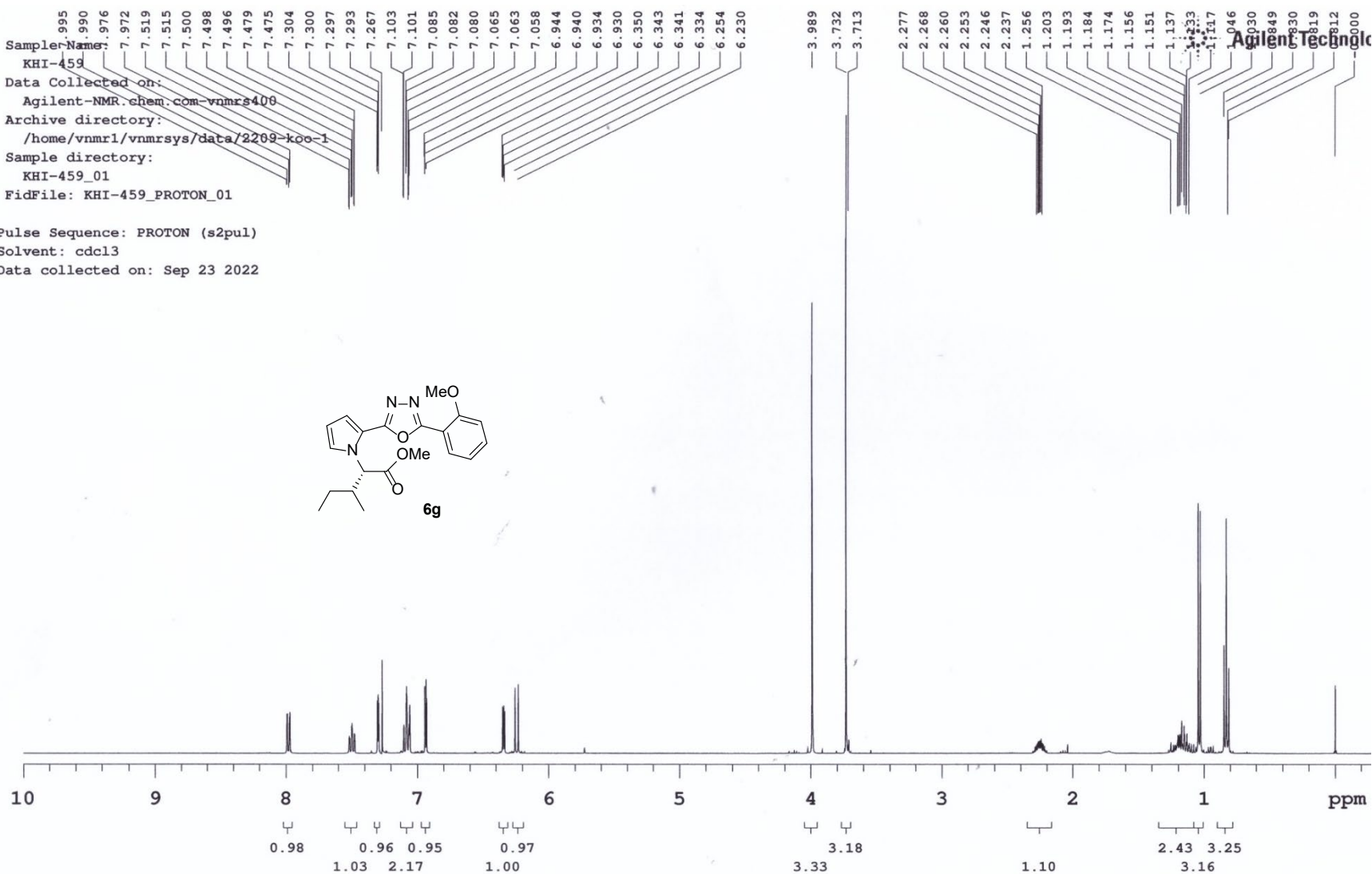
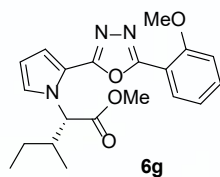
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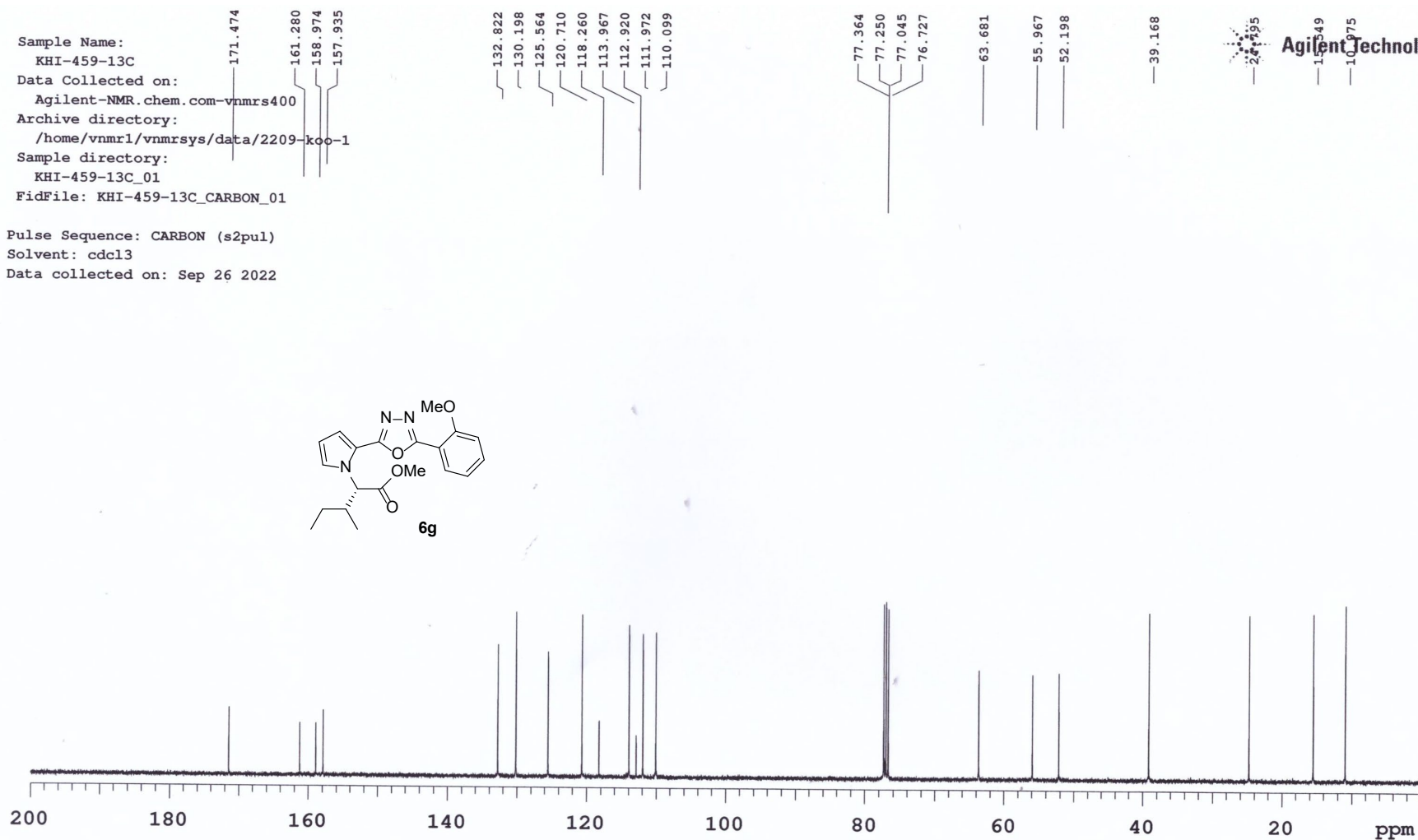
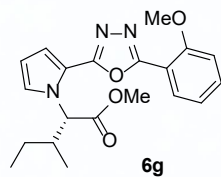
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Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Sep 23 2022



Sample Name:
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FidFile: KHI-459-13C_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 26 2022



Sample Name:

KHI-461

Data Collected on:

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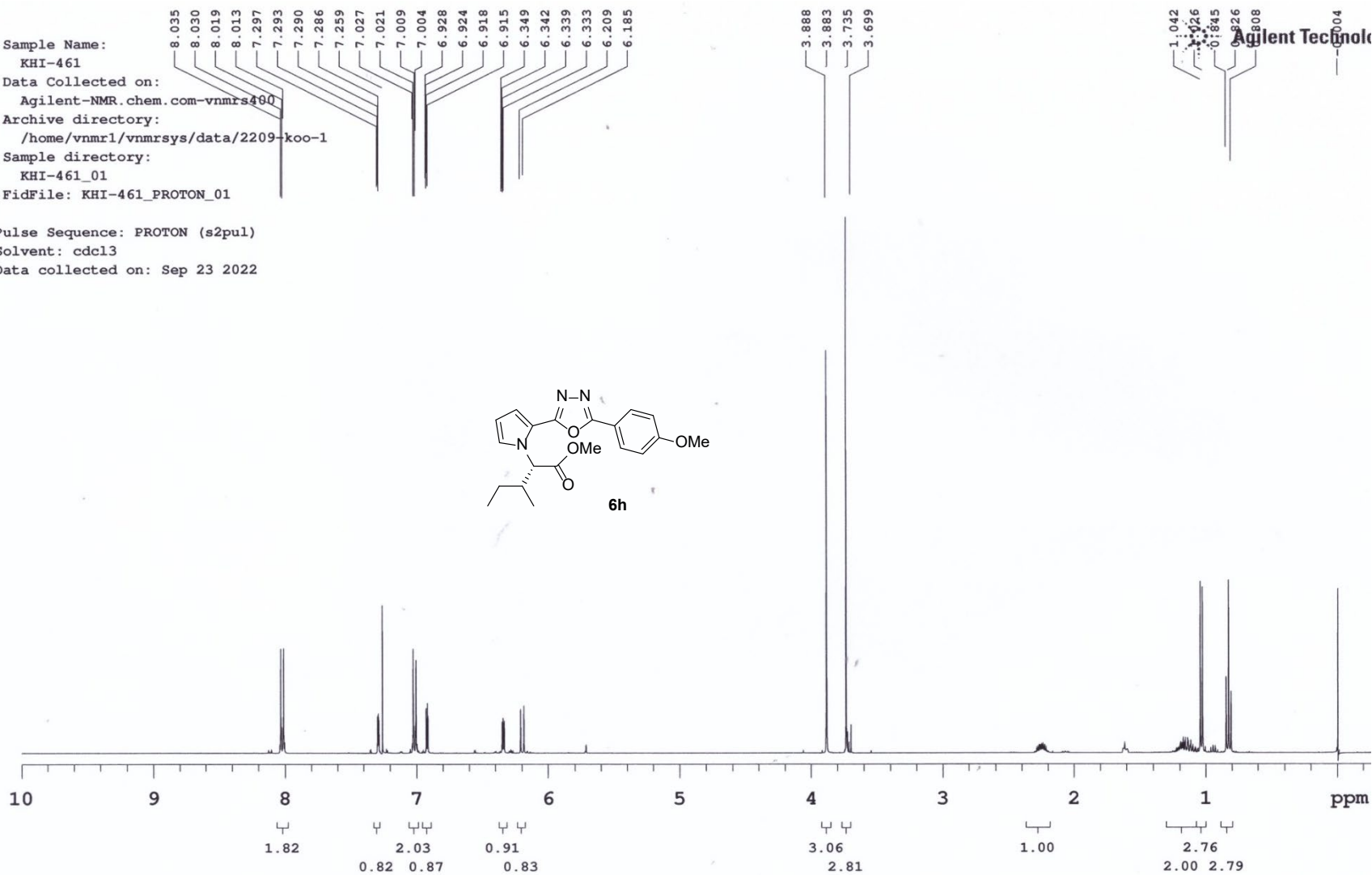
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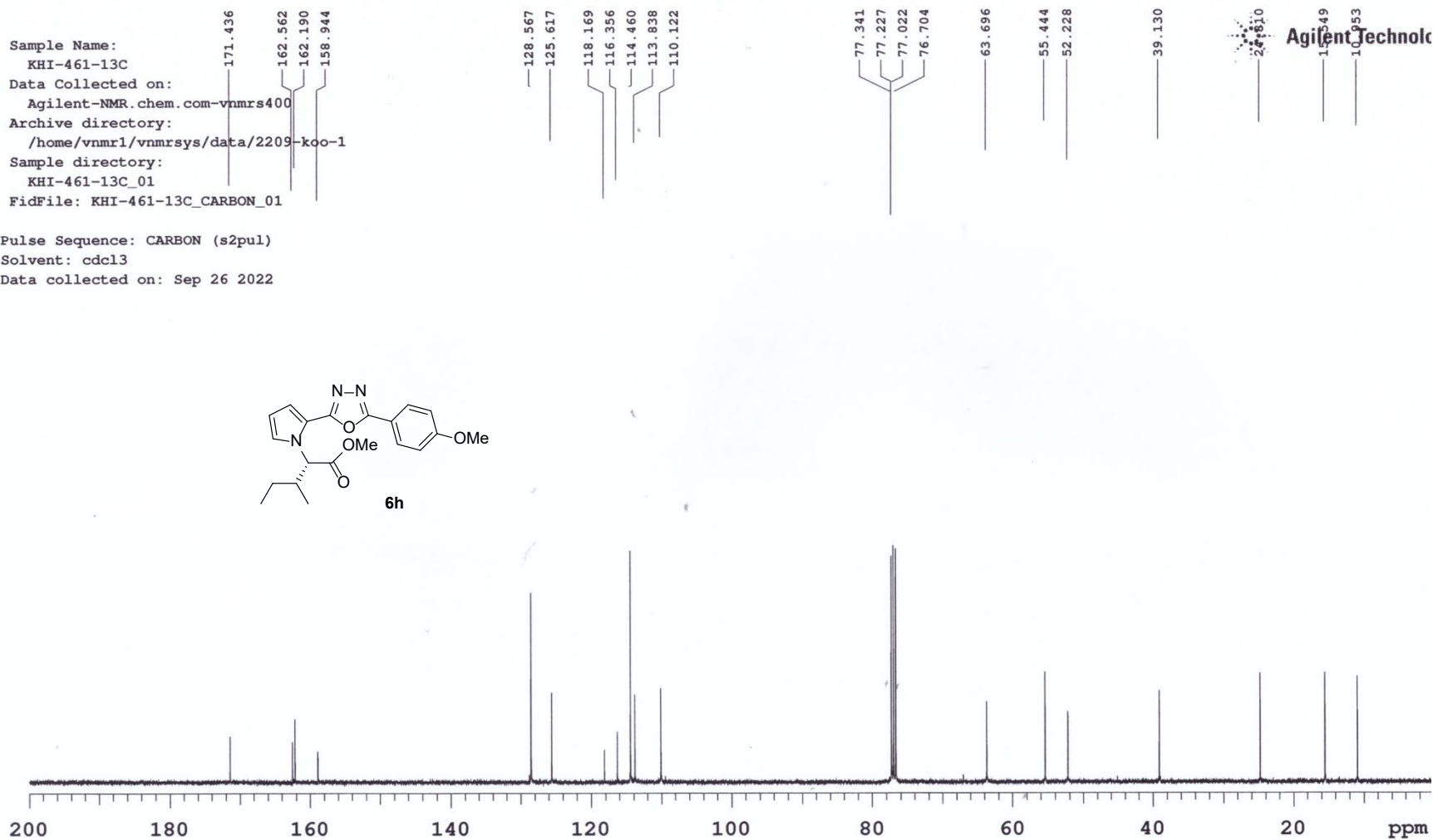
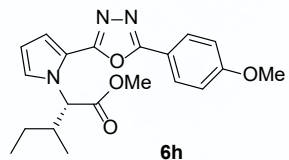
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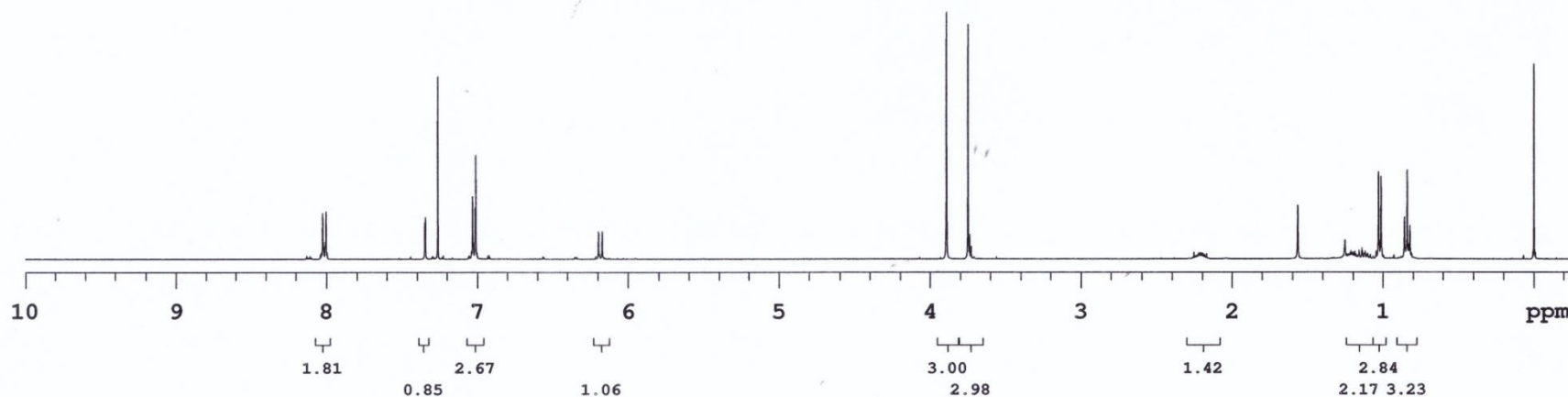
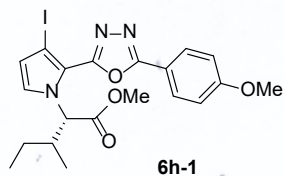
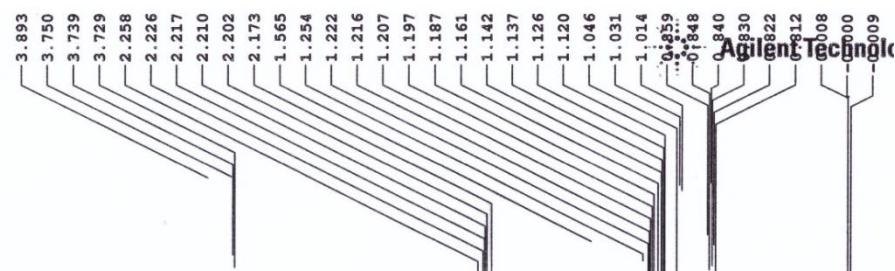
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Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 26 2022



Sample Name:
 YHS-Iso-4OMe-I-re
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 Archive directory:
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 Sample directory:
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 FidFile: YHS-Iso-4OMe-I-re_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Mar 17 2023



Sample Name:
 YHS-Iso-40Me-13C
 Data Collected on:
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 Sample directory:
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Pulse Sequence: CARBON (s2pul)
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 Data collected on: Mar 17 2023

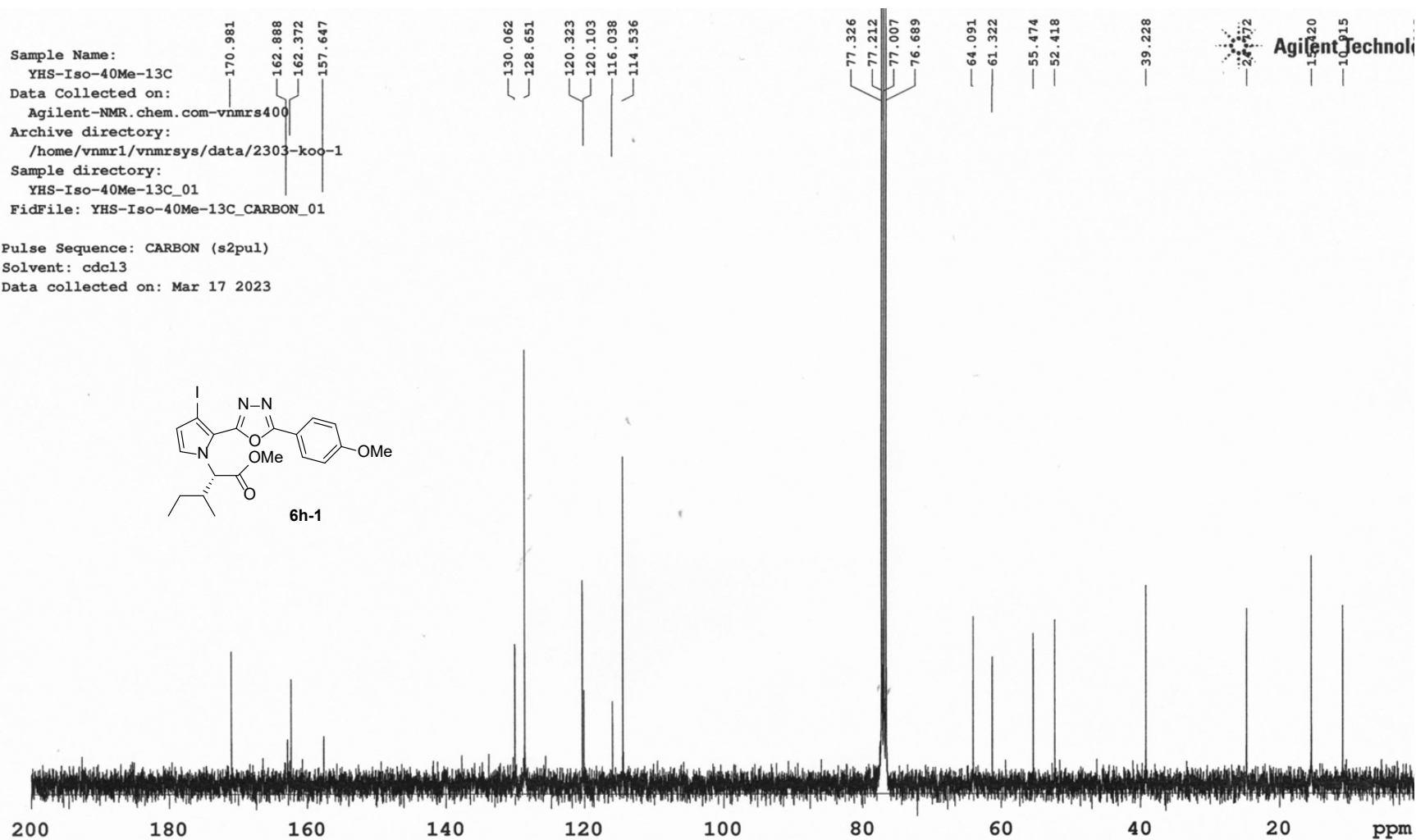
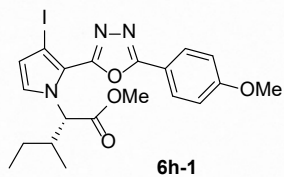


Table S1. Determination of MIC for **1** for *E. coli* and *S. aureus* by OD₆₀₀ (20 h). Each value was obtained as an average of at least triple measurements.

OD ₆₀₀	Average	100% DMSO	2048 µg/mL	1024 µg/mL	512 µg/mL	256 µg/mL	128 µg/mL	64 µg/mL	32 µg/mL	16 µg/mL	8 µg/mL	4 µg/mL	Triple Distilled Water
	Standard Deviation												
1a	<i>E. coli</i>	0.3478 0.030547	0.289233 0.850022	0.8507 0.714032	0.151167 0.472498	0.3022 0.163467	0.426367 0.045185	0.331567 0.03466	0.323967 0.024543	0.309567 0.017898	0.307567 0.025528	0.279 0.007448	0.654767 0.032528
	<i>S. aureus</i>	0.2505 0.000424	-0.0939 0.03182	0.27025 0.215597	0.1779 0.02291	0.2686 0.011172	0.3424 0.033517	0.2688 0.019375	0.2575 0.006788	0.2414 0.018668	0.23315 0.026941	0.226 0.004667	0.5288 0.028567
1b	<i>E. coli</i>	0.33185 0.03783	-0.5113 0.087665	-0.47107 0.099417	-0.24387 0.075585	0.2371 0.057446	0.323167 0.055494	0.311667 0.053523	0.3073 0.034963	0.2944 0.031323	0.298667 0.043386	0.2851 0.046392	0.644167 0.021711
	<i>S. aureus</i>	0.21535 0.03684	-0.665 0.032244	-0.7692 0.024324	-0.58615 0.008839	0.104 0.000141	0.19055 0.010536	0.18395 0.003748	0.1696 0.006223	0.17765 0.000778	0.17695 0.003323	0.18175 0.004455	0.4575 0.005233
1c	<i>E. coli</i>	0.33135 0.035567	-0.4664 0.050321	-0.62733 0.02021	-0.51347 0.090596	-0.1628 0.036104	0.101767 0.043366	0.231333 0.043653	0.288167 0.03173	0.319667 0.036844	0.3146 0.054097	0.296833 0.050751	0.646467 0.026931
	<i>S. aureus</i>	0.22985 0.028214	-0.4684 0.069438	-0.6106 0.212698	-0.68205 0.2856	-0.3628 0.078065	-0.06505 0.003465	0.10315 0.005445	0.17225 0.006293	0.19655 0.015061	0.19245 0.012799	0.18055 0.005162	0.47835 0.008415
1d	<i>E. coli</i>	0.3297 0.035214	-0.35697 0.055124	-0.18807 0.079664	0.0547 0.062815	0.136567 0.025095	0.245367 0.046661	0.282333 0.036691	0.313767 0.027534	0.3293 0.029802	0.3124 0.042749	0.296633 0.051993	0.655067 0.027386
	<i>S. aureus</i>	0.2168 0.032951	-0.5331 0.21793	-0.48685 0.358008	-0.21885 0.238224	-0.03435 0.061589	0.0706 0.011879	0.1423 0	0.1725 0.000849	0.1717 0.003111	0.1677 0.007071	0.17205 7.07E-05	0.4882 0.037194
1e	<i>E. coli</i>	0.32355 0.036982	-0.24903 0.031268	-0.19493 0.04301	-0.04953 0.06383	0.048233 0.030179	0.1481 0.031921	0.2334 0.047883	0.269967 0.031503	0.305833 0.026131	0.3231 0.039861	0.313467 0.055979	0.638467 0.029372
	<i>S. aureus</i>	0.21815 0.015627	-0.2259 0.067458	-0.16365 0.081529	-0.13155 0.12042	-0.08995 0.114905	-0.0194 0.023759	0.0853 0.009192	0.14685 0.006718	0.17255 0.010394	0.1912 0.000283	0.1758 0.003818	0.47435 0.017183
1f	<i>E. coli</i>	0.33405 0.052962	-0.2903 0.09575	-0.256 0.036979	0.178533 0.083553	0.5189 0.039168	0.447633 0.026536	0.346633 0.041134	0.299733 0.026318	0.3095 0.031795	0.323633 0.055569	0.298933 0.049194	0.646933 0.028221
	<i>S. aureus</i>	0.2372 0.02588	-0.32965 0.135411	-0.3046 0.188939	0.035 0.238295	0.21185 0.158321	0.24615 0.056639	0.2057 0.000566	0.16555 0.010253	0.17325 0.004172	0.19085 0.002192	0.1656 0.005233	0.4664 0.050063
1g	<i>E. coli</i>	0.3458 0.055296	-0.32957 0.084745	-0.2146 0.024778	0.271 0.038061	0.461733 0.010671	0.415333 0.036195	0.347033 0.037208	0.316833 0.024892	0.3149 0.034566	0.316267 0.046847	0.298967 0.053796	0.652733 0.024363

	<i>S. aureus</i>	0.23595 0.022415	-0.3185 0.145381	-0.25655 0.155776	0.00045 0.223516	0.15445 0.119572	0.21035 0.071771	0.18 0.020648	0.17185 0.001626	0.1809 0.000283	0.2007 0.010748	0.18405 0.020435	0.45085 0.060033
1h	<i>E. coli</i>	0.3743 0.091924	-0.14843 0.144926	0.286733 0.07582	0.337267 0.027097	0.358567 0.04007	0.368367 0.042204	0.3572 0.04702	0.351733 0.027555	0.356733 0.064329	0.323433 0.039783	0.2907 0.073212	0.659467 0.006788
	<i>S. aureus</i>	0.26115 0.026234	-0.16995 0.050417	0.0988 0.082307	0.1624 0.055296	0.2799 0.014425	0.24735 0.015344	0.2239 0.016971	0.2181 0.037477	0.21875 0.023547	0.21805 0.005303	0.20855 0.003465	0.5153 0.086833
1i	<i>E. coli</i>	0.29705 0.045043	-0.07643 0.134622	0.302533 0.062365	0.2503 0.014714	0.287533 0.004665	0.285167 0.008344	0.284033 0.01954	0.2734 0.009896	0.28 0.01815	0.277267 0.020188	0.280767 0.026755	0.601667 0.007808
	<i>S. aureus</i>	0.25425 0.047023	-0.08225 0.236386	0.13875 0.169776	0.22455 0.032032	0.28055 0.029486	0.24695 0.008415	0.2318 0.002263	0.2303 0.015556	0.2213 0.017253	0.23295 0.019304	0.2204 0.006364	0.55235 0.057629
1j	<i>E. coli</i>	0.29785 0.04278	0.102133 0.052547	0.321467 0.018309	0.2305 0.020705	0.225867 0.009965	0.257767 0.006839	0.286467 0.020582	0.282867 0.016959	0.2803 0.018865	0.284767 0.019558	0.2814 0.039122	0.626967 0.019843
	<i>S. aureus</i>	0.2189 0.023476	-0.0115 0.08457	0.12025 0.098641	0.1411 0.014142	0.1658 0.038467	0.2065 0.00099	0.2115 0.001273	0.2006 0.008627	0.20105 0.001202	0.1877 0.002828	0.19245 0.008839	0.5254 0.009617
1k	<i>E. coli</i>	0.3603 0.102248	-1.5086 0.072676	-1.35513 0.043698	-0.6903 0.248257	-0.04887 0.061502	0.292933 0.104457	0.324833 0.030421	0.314667 0.019211	0.340767 0.042656	0.308833 0.033313	0.303367 0.026279	0.665167 0.028111
	<i>S. aureus</i>	0.2184 0.004243	-1.61145 0.167655	-1.4803 0.087116	-0.8555 0.24876	-0.1416 0.128835	0.1075 0.042709	0.19625 0.012092	0.1868 0.014142	0.19645 0.003889	0.1896 0.007212	0.20035 0.002616	0.5429 0.000707

Table S2. Determination of MIC for **5** and **6** for *E. coli*, *S. aureus*, and *A. baumannii* by OD₆₀₀ (20 h). Each value was obtained as an average of at least triple measurements (vancomycin and erythromycin as positive controls).

OD ₆₀₀	Average	5% DMSO	1024 µg/mL	512 µg/mL	256 µg/mL	128 µg/mL	64 µg/mL	32 µg/mL	16 µg/mL	8 µg/mL	4 µg/mL	2 µg/mL	Triple Distilled Water
	Standard Deviation												
5a <i>o</i> -F	<i>E. coli</i>	0.5663	-0.0935	-0.00173	0.181667	0.269833	0.5345	0.525867	0.559767	0.496167	0.6068	0.317	0.420467
		0.004779	0.031166	0.056804	0.043941	0.06155	0.022098	0.025765	0.020482	0.156749	0.137563	0.400098	0.236646
	<i>S. aureus</i>	0.4818	0.069367	-0.02667	0.052733	0.117067	0.301067	0.2923	0.3547	0.380767	0.4321	0.339567	0.289467
		0.039473	0.004285	0.056203	0.072894	0.031306	0.018322	0.035823	0.050483	0.046983	0.384518	0.138847	0.327076
	<i>A. baumannii</i>	0.2678	-0.19767	-0.19657	-0.00073	-0.03173	0.253667	0.1872	0.217867	0.226933	0.053	0.22915	-0.09783
		0.028071	0.193864	0.167014	0.115973	0.022621	0.143279	0.01693	0.022806	0.031214	0.073103	0.394707	0.070474
5b <i>m</i> -F	<i>E. coli</i>	0.585533	0.131	0.198133	0.317167	0.394467	0.4791	0.5444	0.571467	0.6097	0.4236	0.631833	0.5571
		0.032805	0.119208	0.189769	0.039728	0.018809	0.010886	0.009372	0.021289	0.029182	0.188151	0.027663	0.098856
	<i>S. aureus</i>	0.487633	0.102767	0.1662	0.246933	0.279233	0.279633	0.329767	0.332633	0.375433	0.3622	0.415733	0.359433
		0.029329	0.001986	0.085839	0.023332	0.024953	0.029252	0.016905	0.018159	0.01323	0.038219	0.09099	0.406902
	<i>A. baumannii</i>	0.134133	-0.01857	0.0047	0.113567	0.198433	0.227733	0.217367	0.2452	0.238567	0.211633	0.202567	0.481167
		0.169371	0.028894	0.066938	0.030551	0.008556	0.017352	0.028045	0.018368	0.031305	0.005845	0.07391	0.173203
5c <i>p</i> -F	<i>E. coli</i>	0.548433	0.151733	0.236633	0.3586	0.429	0.503267	0.540967	0.561633	0.561433	0.152067	0.567367	0.496467
		0.021914	0.026979	0.069258	0.069205	0.020637	0.018661	0.014262	0.025335	0.031601	0.409621	0.036247	0.141964
	<i>S. aureus</i>	0.441133	0.058333	0.1148	0.169867	0.254333	0.2757	0.334067	0.372167	0.380333	0.1813	0.289833	0.602933
		0.010098	0.03269	0.010253	0.029358	0.006962	0.011774	0.023027	0.046016	0.041734	0.271455	0.234179	0.076836
	<i>A. baumannii</i>	0.2341	-0.05587	-0.02777	0.0701	0.115767	0.179367	0.240467	0.260667	0.279733	0.0995	0.121733	0.623067
		0.024456	0.021574	0.044891	0.026683	0.025335	0.041527	0.024751	0.113443	0.11848	0.099321	0.127833	0.285097

OD ₆₀₀	Average	5% DMSO	1024 µg/mL	512 µg/mL	256 µg/mL	128 µg/mL	64 µg/mL	32 µg/mL	16 µg/mL	8 µg/mL	4 µg/mL	2 µg/mL	Triple Distilled Water
	Standard Deviation												
5d <i>p</i> -Cl	<i>E. coli</i>	0.579033	-0.14127	0.0054	0.3527	0.474933	0.5682	0.589033	0.598533	0.596467	0.5875	0.594733	0.648133
		0.053497	0.04099	0.118053	0.035666	0.055678	0.021054	0.007596	0.026585	0.008654	0.013396	0.04294	0.37161
	<i>S. aureus</i>	0.447033	-0.2376	-0.08727	-0.0187	0.254167	0.300367	0.380367	0.336767	0.3453	0.3313	0.080633	0.525
		0.004936	0.032193	0.043104	0.007732	0.051822	0.026651	0.021373	0.014327	0.013305	0.065115	0.413322	0.202245
	<i>A. baumannii</i>	0.246833	-0.16697	-0.12503	0.153567	0.236833	0.242933	0.371167	0.223533	0.2197	0.229133	0.174033	0.527267
		0.026606	0.031151	0.05423	0.071986	0.082996	0.026258	0.014022	0.012529	0.01149	0.015652	0.059859	0.164986
5e-1 <i>o</i> -OH	<i>E. coli</i>	0.584033	-0.00397	0.1366	0.406833	0.4453	0.535633	0.6021	0.555633	0.353433	0.4878	0.3224	0.337533
		0.036057	0.049138	0.015221	0.03456	0.025638	0.028504	0.02205	0.014318	0.368088	0.128463	0.126218	0.216063
	<i>S. aureus</i>	0.4603	-0.12153	-0.33813	-0.1466	-0.10913	-0.0546	-0.03017	-0.0187	-0.00907	0.031433	0.3362	0.4777
		0.028008	0.010365	0.117167	0.047326	0.011721	0.011049	0.003121	0.00423	0.094579	0.432203	0.039103	0.190024
	<i>A. baumannii</i>	0.257133	-0.1009	-0.18663	-0.11497	0.078667	0.021633	0.196133	0.193967	0.121967	0.0963	0.234567	0.141767
		0.019135	0.020148	0.108839	0.076689	0.068777	0.085558	0.1074	0.040734	0.128972	0.337207	0.156701	0.163562
5f-1 <i>p</i> -OH	<i>E. coli</i>	0.610767	-0.04497	0.304967	0.444	0.347633	0.4712	0.469867	0.571967	0.465867	0.376667	0.2635	0.494967
		0.032207	0.025902	0.055612	0.05995	0.121436	0.02763	0.145089	0.037334	0.227569	0.336678	0.384056	0.265685
	<i>S. aureus</i>	0.476367	-0.11507	-0.22337	-0.14757	-0.13423	0.039433	-0.0043	-0.28307	-0.22003	-0.34043	0.289467	0.242267
		0.011828	0.126333	0.225514	0.130583	0.10695	0.159668	0.028178	0.258498	0.206889	0.435493	0.126238	0.289827
	<i>A. baumannii</i>	0.207467	-0.09443	-0.25543	-0.13213	0.002233	-0.12997	-0.02577	0.001133	-0.01047	-0.25243	-0.00337	0.140033
		0.03379	0.115879	0.186161	0.053673	0.036527	0.30727	0.150633	0.393035	0.266581	0.443574	0.270916	0.268719

OD ₆₀₀	Average	5% DMSO	1024 µg/mL	512 µg/mL	256 µg/mL	128 µg/mL	64 µg/mL	32 µg/mL	16 µg/mL	8 µg/mL	4 µg/mL	2 µg/mL	Triple Distilled Water
	Standard Deviation												
5f o-OH	<i>E. coli</i>	0.5628	0.1427	0.2282	0.269467	0.3946	0.5437	0.607867	0.6051	0.617233	0.584533	0.576067	0.6816
		0.00374	0.018266	0.074549	0.041967	0.047099	0.029865	0.032888	0.039824	0.040086	0.033624	0.010333	0.029025
	<i>S. aureus</i>	0.4341	-0.1521	-0.1373	-0.14833	0.027633	0.136333	0.195033	0.0272	0.268333	0.239333	0.389833	0.5614
		0.010235	0.069882	0.085083	0.078398	0.059014	0.028494	0.027081	0.240389	0.075575	0.130233	0.021768	0.051241
	<i>A. baumannii</i>	0.203633	-0.0818	-0.09567	-0.1738	-0.0636	0.163067	0.207967	0.164	0.1454	0.102533	0.0891	0.6636
		0.018188	0.079953	0.086918	0.085729	0.056571	0.022547	0.048014	0.132417	0.143797	0.123057	0.250629	0.173474
5g o-OMe	<i>E. coli</i>	0.5669	0.1844	0.274633	0.378867	0.4271	0.511633	0.564233	0.582333	0.580233	0.5568	0.540567	0.1807
		0.019918	0.017485	0.0352	0.002577	0.019901	0.018367	0.008656	0.00369	0.015509	0.014681	0.027802	0.38267
	<i>S. aureus</i>	0.480267	0.038367	0.057167	0.147533	0.1874	0.2207	0.2516	0.2973	0.324133	0.257033	0.276667	0.207167
		0.009955	0.01766	0.044252	0.036703	0.03826	0.042948	0.018	0.02287	0.030935	0.192673	0.131945	0.386512
	<i>A. baumannii</i>	0.211433	-0.0343	-0.00167	0.051733	0.106567	0.1529	0.211833	0.220733	-0.2874	0.114633	0.1702	0.668733
		0.020501	0.021118	0.033471	0.018607	0.028527	0.02335	0.0195	0.020325	0.448755	0.12236	0.082064	0.043359
5g-1 o-OMe	<i>E. coli</i>	0.5811	0.089967	-0.06553	0.514867	0.461267	0.558367	0.622933	0.644933	0.574267	0.599167	0.5497	0.3087
		0.011607	0.305614	0.172808	0.329993	0.112704	0.037812	0.012552	0.019053	0.119493	0.060493	0.07266	0.504621
	<i>S. aureus</i>	0.151767	-0.4264	-0.19373	0.1073	0.214567	0.1032	0.052933	0.218667	0.2879	0.271567	0.035433	0.574567
		0.228957	0.252254	0.209641	0.063035	0.0491	0.245718	0.380542	0.175763	0.041644	0.068112	0.419599	0.032973
	<i>A. baumannii</i>	0.2284	-0.28307	-0.2196	-0.00743	0.119033	0.201433	0.294033	0.3238	0.0616	0.1952	0.1544	0.1093
		0.038088	0.172324	0.130771	0.124592	0.093969	0.094973	0.042036	0.523788	0.309035	0.174984	0.114535	0.335283

OD ₆₀₀	Average	5% DMSO	1024 µg/mL	512 µg/mL	256 µg/mL	128 µg/mL	64 µg/mL	32 µg/mL	16 µg/mL	8 µg/mL	4 µg/mL	2 µg/mL	Triple Distilled Water
	Standard Deviation												
5h <i>p</i> -OMe	<i>E. coli</i>	0.6065	0.2759	0.2894	0.388967	0.425267	0.463333	0.539967	0.5749	0.589633	0.599633	0.297133	0.665533
		0.043278	0.033042	0.089637	0.024927	0.008003	0.019803	0.014063	0.013524	0.028575	0.029255	0.480936	0.012708
	<i>S. aureus</i>	0.232567	0.0714	0.074533	0.105967	0.1629	0.1887	0.230767	0.265933	0.285	0.349367	0.323133	0.4444
		0.202334	0.058215	0.095632	0.044127	0.023381	0.012562	0.008674	0.005498	0.014389	0.015651	0.078875	0.134025
	<i>A. baumannii</i>	0.231867	0.022633	-0.00797	0.059267	0.1346	0.1992	0.2569	0.2641	0.258533	0.260933	0.225033	0.376767
		0.034406	0.05872	0.021548	0.056912	0.01599	0.014936	0.022995	0.017201	0.011692	0.003873	0.041971	0.430816
5h-1 <i>p</i> -OMe	<i>E. coli</i>	0.582233	-0.6511	-0.31983	0.321533	0.2436	0.3794	0.587367	0.596533	0.592	0.481	0.515933	0.680767
		0.015767	0.548606	0.41569	0.23707	0.390896	0.21503	0.04358	0.057936	0.012968	0.20526	0.089811	0.020469
	<i>S. aureus</i>	0.4426	-0.74527	-0.58953	0.0805	0.188533	0.2749	0.1625	0.1872	0.295733	0.3309	0.2201	0.5721
		0.019235	0.529512	0.517887	0.090981	0.099146	0.078272	0.125207	0.078118	0.062152	0.048683	0.322145	0.041743
	<i>A. baumannii</i>	0.135633	-0.24467	-0.56443	-0.21503	-0.01423	0.130133	0.122467	0.336233	0.181967	0.0584	0.290167	0.782967
		0.069146	0.244337	0.015529	0.30294	0.300765	0.090814	0.253604	0.152639	0.130578	0.338963	0.015167	0.018312
6a <i>o</i> -F	<i>E. coli</i>	0.563267	0.013467	0.055867	0.2771	0.405467	0.493067	0.5474	0.602033	0.590133	0.495167	0.497233	0.5904
		0.014833	0.059975	0.039829	0.071188	0.061659	0.028513	0.02019	0.023157	0.011302	0.082901	0.070453	0.060836
	<i>S. aureus</i>	0.3412	-0.1639	-0.07717	0.063533	0.145033	0.205	0.268267	0.316	0.322533	0.3593	0.402567	0.487833
		0.235327	0.034927	0.061558	0.06494	0.026627	0.037385	0.030399	0.042011	0.048313	0.047546	0.035848	0.218122
	<i>A. baumannii</i>	0.227233	-0.07443	-0.0908	-0.01367	0.101867	0.183	0.173467	0.266	0.228667	0.2411	-0.09203	0.661067
		0.050281	0.046175	0.024187	0.012133	0.023599	0.073893	0.041175	0.037129	0.016805	0.027742	0.061919	0.010594

OD ₆₀₀	Average	5% DMSO	1024 µg/mL	512 µg/mL	256 µg/mL	128 µg/mL	64 µg/mL	32 µg/mL	16 µg/mL	8 µg/mL	4 µg/mL	2 µg/mL	Triple Distilled Water
	Standard Deviation												
6b <i>m-F</i>	<i>E. coli</i>	0.580167	0.068733	0.103333	0.319667	0.410067	0.5444	0.560233	0.5988	0.5935	0.6024	0.4003	0.6172
		0.016053	0.049793	0.042423	0.014895	0.04715	0.01473	0.00889	0.021391	0.0218	0.004951	0.338978	0.089482
	<i>S. aureus</i>	0.3399	-0.17217	-0.02323	0.0732	0.153733	0.243367	0.2494	0.2927	0.2784	0.322467	0.309233	0.415967
		0.09231	0.066646	0.076326	0.050608	0.018056	0.0171	0.012946	0.011887	0.013586	0.049838	0.122567	0.12531
	<i>A. baumannii</i>	0.052033	-0.18307	-0.0763	0.012967	0.141433	0.348033	0.2747	0.349567	0.2578	0.272667	0.0699	0.645967
		0.133533	0.044449	0.057484	0.058517	0.037086	0.021735	0.05032	0.04814	0.01255	0.015233	0.276596	0.021989
6c <i>p-F</i>	<i>E. coli</i>	0.533967	0.144567	0.2717	0.413133	0.4972	0.564533	0.6045	0.614467	0.6126	0.590133	0.553333	0.647433
		0.059126	0.077264	0.030135	0.022098	0.016179	0.005781	0.041701	0.034766	0.029313	0.008946	0.030374	0.017528
	<i>S. aureus</i>	0.389267	0.082067	0.088433	0.180133	0.227167	0.276667	0.3111	0.328633	0.3426	0.3163	0.0376	0.683933
		0.196708	0.010492	0.038193	0.03482	0.03857	0.038653	0.025268	0.039157	0.035958	0.130464	0.314667	0.034948
	<i>A. baumannii</i>	0.212767	-0.05533	-0.04417	0.101167	0.129267	0.236533	0.2822	0.240533	0.267933	0.2421	0.242267	0.303567
		0.03289	0.034027	0.009846	0.018472	0.011427	0.035897	0.056385	0.04485	0.022347	0.037164	0.008719	0.2164
6d <i>p-Cl</i>	<i>E. coli</i>	0.5225	-0.05783	0.047933	0.3123	0.4468	0.538733	0.575433	0.599233	0.600867	0.6024	0.6279	0.669533
		0.073983	0.035173	0.034061	0.047372	0.049501	0.009252	0.008523	0.013413	0.01839	0.003559	0.02374	0.004352
	<i>S. aureus</i>	0.523767	-0.14937	-0.0628	0.1049	0.206933	0.279	0.311467	0.340467	0.353933	0.373833	0.3242	0.3406
		0.017647	0.053102	0.040789	0.029518	0.016909	0.018285	0.0052	0.019755	0.022413	0.042236	0.140104	0.337874
	<i>A. baumannii</i>	0.128867	-0.23597	-0.0958	0.087667	0.1727	0.251267	0.273167	0.2813	0.280467	0.285567	0.281733	0.652833
		0.254936	0.020526	0.034295	0.026702	0.027623	0.041322	0.026016	0.006437	0.016511	0.014398	0.023003	0.024892

OD ₆₀₀	Average	5% DMSO	1024 µg/mL	512 µg/mL	256 µg/mL	128 µg/mL	64 µg/mL	32 µg/mL	16 µg/mL	8 µg/mL	4 µg/mL	2 µg/mL	Triple Distilled Water
	Standard Deviation												
6e-1 o-OH	<i>E. coli</i>	0.482667	-0.03527	0.174567	0.5121	0.4774	0.488033	0.553267	0.66	0.6265	0.5765	0.589333	0.579333
		0.007044	0.026736	0.0824	0.088496	0.08139	0.10833	0.1059	0.032215	0.041559	0.058123	0.047768	0.106689
	<i>S. aureus</i>	0.409867	-0.06263	-0.1663	-0.32883	-0.1252	-0.05663	-0.06527	-0.02003	-0.7117	0.0345	-0.032	0.200967
		0.115135	0.031599	0.168687	0.25205	0.143971	0.016998	0.057151	0.007566	0.052551	0.13493	0.277024	0.388297
	<i>A. baumannii</i>	0.2263	-0.09757	0.0136	0.113933	-0.03577	-0.07657	0.0375	0.218233	-0.6665	0.2268	0.202433	0.403367
		0.014309	0.009657	0.079975	0.030953	0.228161	0.260033	0.162924	0.042339	0.023822	0.024996	0.063747	0.245056
6e o-OH	<i>E. coli</i>	0.550533	-0.71263	-0.6685	-0.2245	0.193367	0.423567	0.621433	0.663833	0.641033	0.620533	0.476133	0.6734
		0.079447	0.043027	0.087305	0.077585	0.05575	0.053036	0.025778	0.068848	0.029336	0.014524	0.092484	0.006509
	<i>S. aureus</i>	0.432267	-1.35967	-1.18427	-0.76853	-0.43957	0.055967	0.2072	0.211067	0.265833	0.3209	0.3583	0.538633
		0.031379	0.018284	0.139737	0.0292	0.139406	0.049015	0.014823	0.011113	0.013699	0.054685	0.042579	0.055584
	<i>A. baumannii</i>	0.193033	-1.30287	-1.08353	-0.5868	-0.2114	-0.0019	0.1532	0.221233	0.2962	0.323867	0.297067	0.824367
		0.04258	0.074684	0.035826	0.146309	0.056868	0.087508	0.125707	0.069535	0.03509	0.046317	0.036712	0.017131
6f-1 p-OH	<i>E. coli</i>	0.555333	0.038167	0.222533	0.456233	0.281633	0.546267	0.433933	0.5596	0.6226	0.4277	0.637433	0.692567
		0.024134	0.031092	0.25179	0.030192	0.196759	0.033515	0.196451	0.088235	0.020352	0.241129	0.008542	0.009547
	<i>S. aureus</i>	0.441433	-0.1143	-0.21467	-0.28177	-0.2246	-0.29967	-0.40083	-0.2534	-0.3732	-0.2752	-0.4245	0.065033
		0.043428	0.026457	0.133408	0.164958	0.34139	0.451706	0.395107	0.274966	0.24689	0.395395	0.311968	0.521248
	<i>A. baumannii</i>	0.210167	-0.08037	-0.06343	0.022367	-0.08597	0.095833	-0.33263	-0.40203	-0.16833	0.2602	0.1809	0.6579
		0.061093	0.038218	0.030068	0.03716	0.17361	0.079832	0.246976	0.12486	0.456569	0.017804	0.09659	0.068942

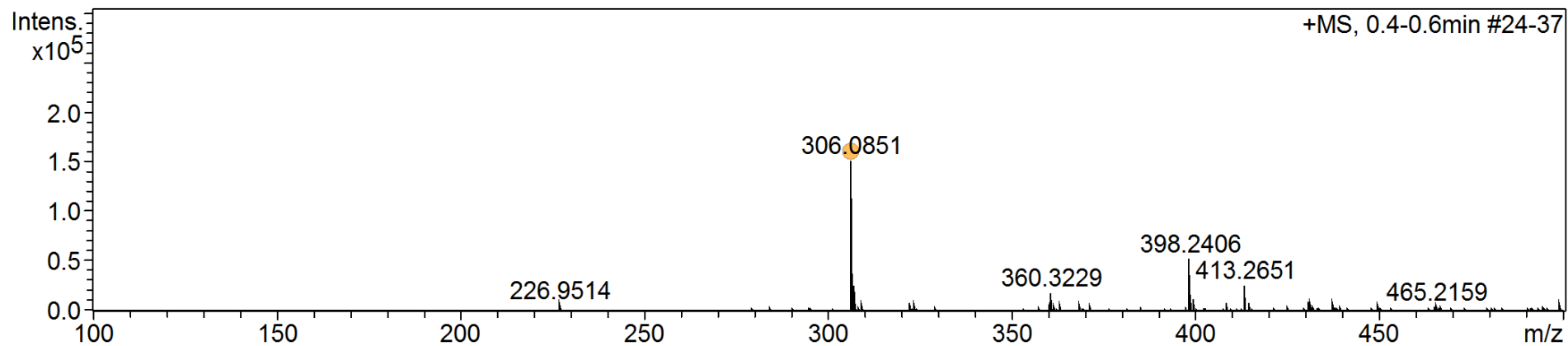
OD ₆₀₀	Average	5% DMSO	1024 µg/mL	512 µg/mL	256 µg/mL	128 µg/mL	64 µg/mL	32 µg/mL	16 µg/mL	8 µg/mL	4 µg/mL	2 µg/mL	Triple Distilled Water
	Standard Deviation												
6f <i>p</i> -OH	<i>E. coli</i>	0.580333	-0.55103	0.123533	0.5112	0.630767	0.516333	0.6104	0.622433	0.382067	0.644033	0.635333	0.6159
		0.005499	0.050954	0.051951	0.034334	0.032991	0.16293	0.022578	0.017579	0.42362	0.027766	0.054606	0.184714
	<i>S. aureus</i>	0.467367	-0.81597	-0.25553	0.083433	0.0425	0.0302	0.0004	-0.00203	-0.37443	0.2321	0.2364	0.5281
		0.024451	0.082553	0.071841	0.050228	0.042171	0.014697	0.00466	0.000416	0.50661	0.019489	0.157819	0.08503
	<i>A. baumannii</i>	0.2466	-0.77193	-0.2757	0.1809	0.2156	0.156367	0.004967	0.2751	0.1911	0.0836	0.066467	0.814933
		0.006974	0.079612	0.144879	0.037529	0.033036	0.054103	0.345068	0.229765	0.051765	0.139431	0.193652	0.098204
6g <i>o</i> -OMe	<i>E. coli</i>	0.514467	0.1212	0.256367	0.381667	0.5117	0.583033	0.617733	0.619233	0.625867	0.6043	0.509067	0.643467
		0.029871	0.041836	0.050119	0.025005	0.041626	0.031352	0.017664	0.013107	0.008832	0.00318	0.156222	0.062531
	<i>S. aureus</i>	0.351333	0.000967	0.086433	0.153367	0.221033	0.2471	0.282867	0.2767	0.274767	0.1091	0.4166	0.478733
		0.054321	0.08218	0.029258	0.037778	0.046923	0.04224	0.044203	0.016877	0.08942	0.238055	0.012454	0.201722
	<i>A. baumannii</i>	0.215233	-0.0594	-0.01203	0.060067	0.136333	0.193233	0.241033	0.240833	0.244267	0.2418	0.253933	0.3972
		0.007883	0.013868	0.01411	0.027256	0.025108	0.024043	0.012936	0.016836	0.027722	0.030545	0.010719	0.36455
6h <i>p</i> -OMe	<i>E. coli</i>	0.5625	0.141167	0.276133	0.368633	0.467233	0.541333	0.5983	0.623833	0.6327	0.394467	0.4689	0.509133
		0.036105	0.05724	0.00245	0.045647	0.033821	0.011793	0.01515	0.004051	0.003122	0.338243	0.282118	0.137559
	<i>S. aureus</i>	0.4173	-0.04433	0.016167	0.099667	0.1279	0.194733	0.22	0.2507	0.268333	0.317967	0.377733	0.564767
		0.153597	0.024286	0.031005	0.041051	0.038384	0.028184	0.010567	0.007572	0.017802	0.024059	0.029382	0.022851
	<i>A. baumannii</i>	0.194567	-0.06657	-0.05227	0.065067	0.161333	0.2098	0.2658	0.2876	0.302133	0.298467	0.279	0.753033
		0.083458	0.021736	0.041927	0.051276	0.036087	0.035985	0.035222	0.011166	0.030312	0.006313	0.02645	0.021247

OD ₆₀₀	Average	5% DMSO	1024 µg/mL	512 µg/mL	256 µg/mL	128 µg/mL	64 µg/mL	32 µg/mL	16 µg/mL	8 µg/mL	4 µg/mL	2 µg/mL	Triple Distilled Water
	Standard Deviation												
6h-1 <i>p</i> -OMe	<i>E. coli</i>	0.602033	0.0413	0.178267	0.402767	0.562833	0.622233	0.625767	0.613133	0.386733	0.594333	0.629533	0.677833
		0.0141	0.043315	0.058042	0.055404	0.055585	0.018501	0.01123	0.059871	0.40273	0.070062	0.010652	0.008664
	<i>S. aureus</i>	0.474433	0.0119	0.0536	0.186533	0.256567	0.283067	0.275167	0.2778	0.2863	0.318	0.003033	0.516733
		0.039822	0.040041	0.0414	0.03982	0.024243	0.01216	0.005953	0.017562	0.021674	0.027731	0.405709	0.106848
	<i>A. baumannii</i>	0.270233	-0.01317	-0.00273	0.151333	0.228867	0.280867	0.2116	0.013733	0.2785	0.22545	0.0679	0.875633
		0.046391	0.089113	0.101433	0.119789	0.10617	0.025088	0.131107	0.401343	0.107985	0.21022	0.15906	0.059901

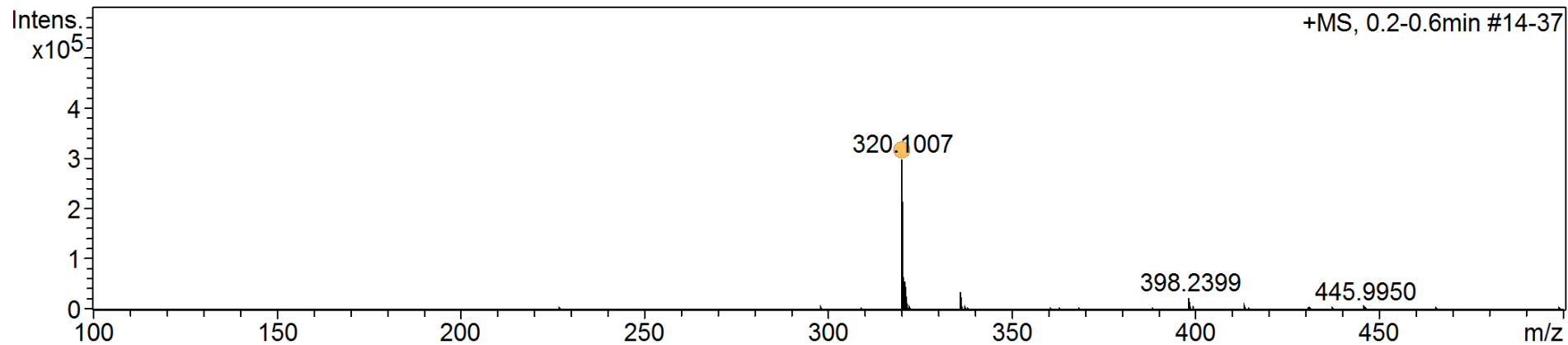
OD ₆₀₀	Average	5% DMSO	1024 µg/mL	512 µg/mL	256 µg/mL	128 µg/mL	64 µg/mL	32 µg/mL	16 µg/mL	8 µg/mL	4 µg/mL	2 µg/mL	Triple Distilled Water
	Standard Deviation												
Vancomycin	<i>E. coli</i>	0.8013	0.4901	0.708433	0.752867	0.746967	0.742067	0.7827	0.772167	0.781967	0.855167	0.871733	0.605967
		0.039069	0.030212	0.022352	0.008937	0.021712	0.021561	0.048403	0.057	0.023133	0.091893	0.10263	0.00325
	<i>S. aureus</i>	0.461433	0.0395	0.0391	0.039233	0.039333	0.0396	0.039667	0.041167	0.041367	0.042967	0.278133	0.487167
		0.01291	0.000854	0.000819	0.000643	0.000379	0.000436	0.000643	0.001193	0.001922	0.003197	0.135305	0.025012
	<i>A. baumannii</i>	0.6197	0.141267	0.232567	0.4701	0.574167	0.59	0.609667	0.599567	0.594367	0.600067	0.585467	0.643733
		0.010897	0.027308	0.039094	0.042326	0.075942	0.048362	0.048319	0.054458	0.053718	0.054685	0.013527	0.011796
Erythromycin	<i>E. coli</i>	0.778333	0.098533	0.315367	0.4438	0.543867	0.666633	0.700233	0.797567	0.790167	0.743067	0.782833	0.607333
		0.024451	0.086119	0.025522	0.025811	0.028514	0.011809	0.03331	0.047561	0.077885	0.043578	0.01501	0.018113
	<i>S. aureus</i>	0.4564	0.038133	0.037767	0.038367	0.0383	0.038633	0.039733	0.040433	0.042333	0.0501	0.147433	0.466767
		0.034787	0.000839	0.000451	0.00085	0.000721	0.000874	0.001815	0.00168	0.002894	0.006022	0.049306	0.012881
	<i>A. baumannii</i>	0.616867	0.038133	0.0384	0.038333	0.0973	0.148733	0.184367	0.226433	0.3081	0.407467	0.4603	0.6226
		0.024035	0.00095	0.000781	0.000929	0.006762	0.009729	0.007223	0.015602	0.007879	0.018736	0.010046	0.005151

High resolution mass spectra (ESI)

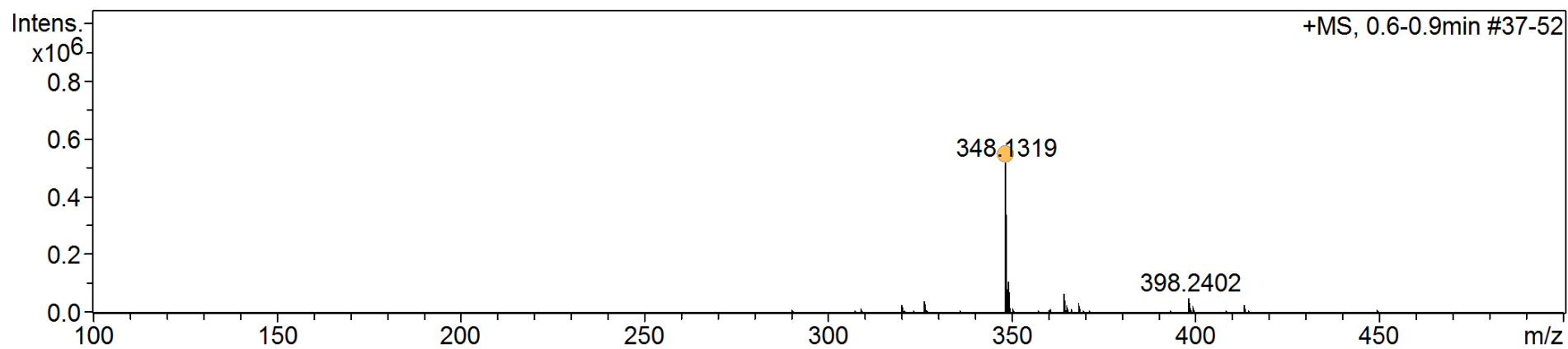
1a: calcd for $C_{15}H_{13}N_3O_3+Na$, 306.0849, found 306.0851.



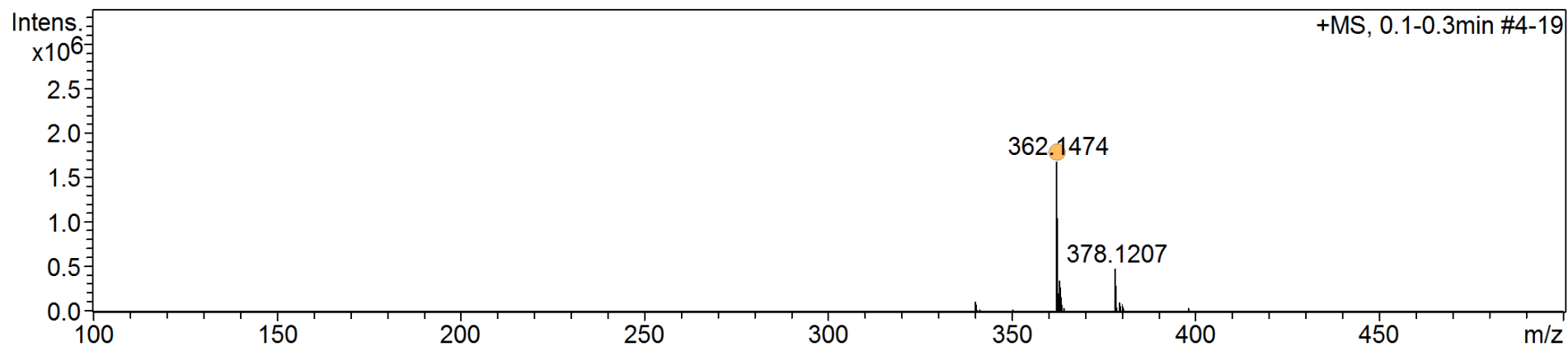
1b: calcd for $C_{16}H_{15}N_3O_3+Na$, 320.1006, found 320.1007.



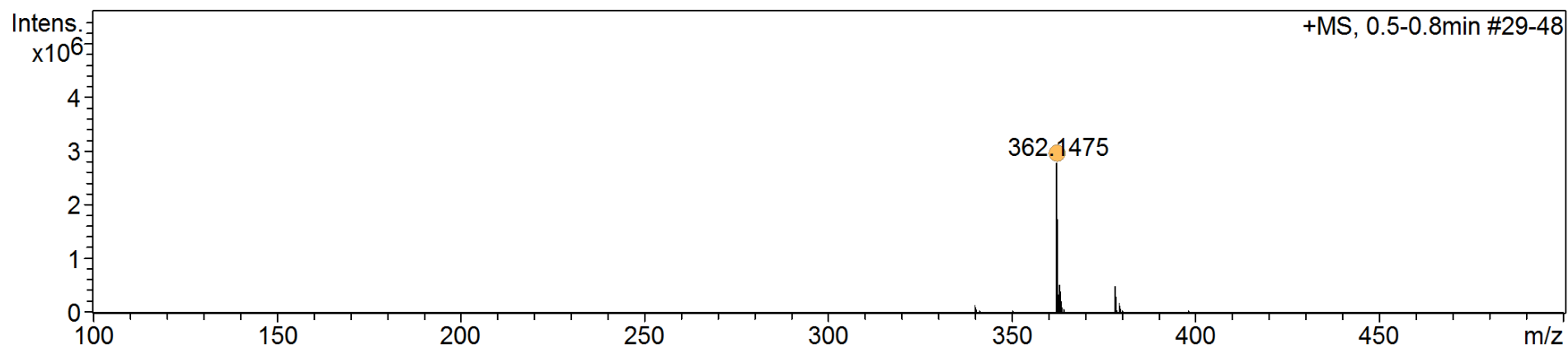
1c: calcd for $C_{18}H_{19}N_3O_3+Na$, 348.1319, found 348.1319.



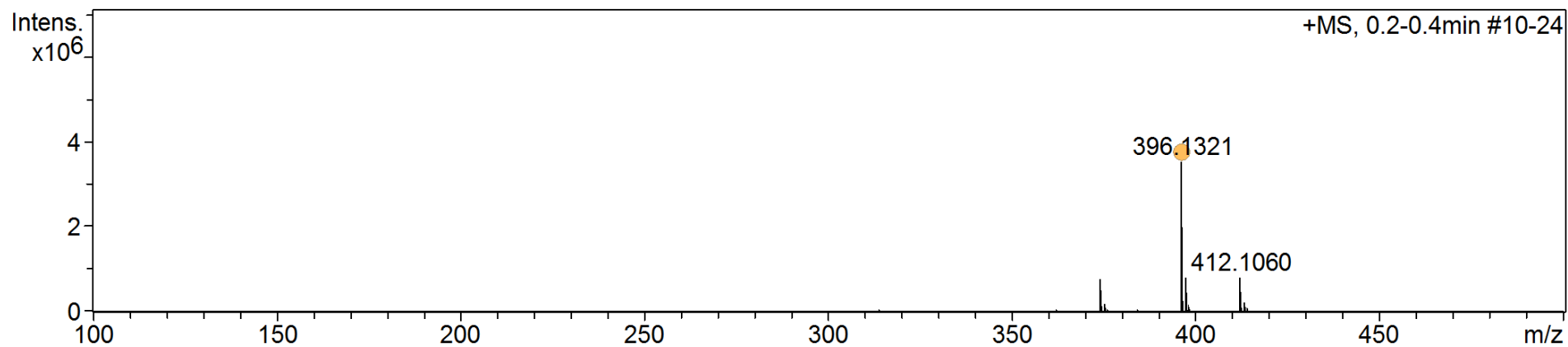
1d: calcd for $C_{19}H_{21}N_3O_3+Na$, 362.1475, found 362.1474.



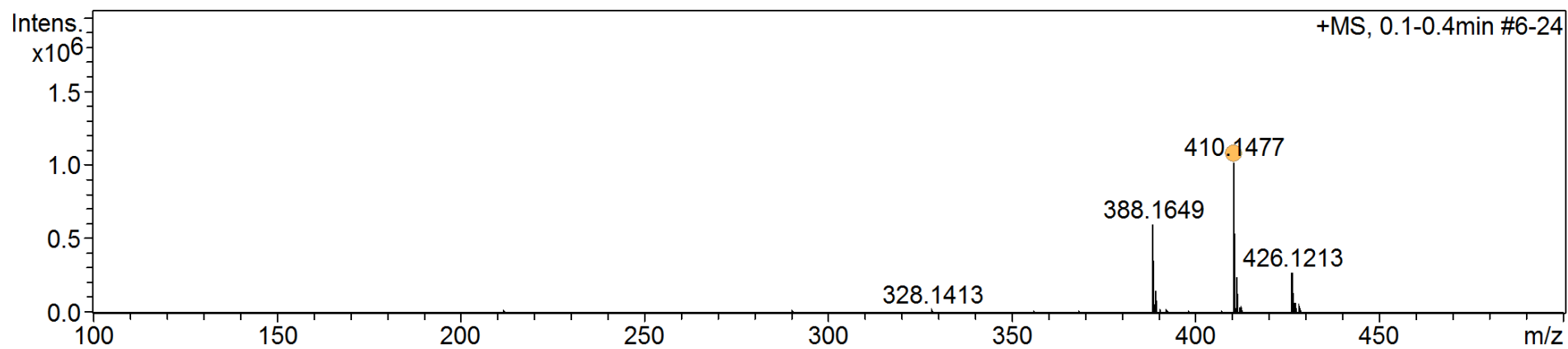
1e: calcd for $C_{19}H_{21}N_3O_3+Na$, 362.1475, found 362.1475.



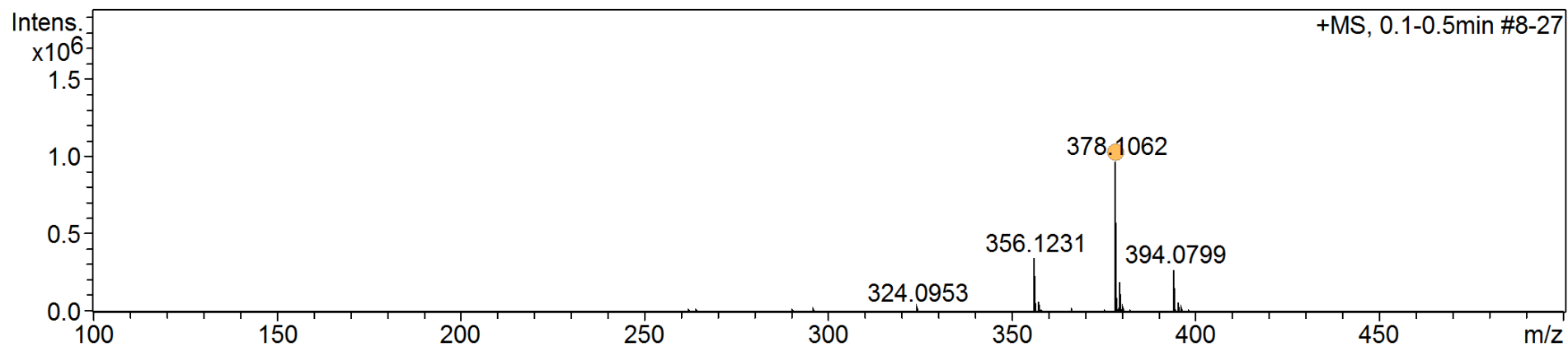
1f: calcd for $C_{22}H_{19}N_3O_3+Na$ 396.1319, found 396.1321.



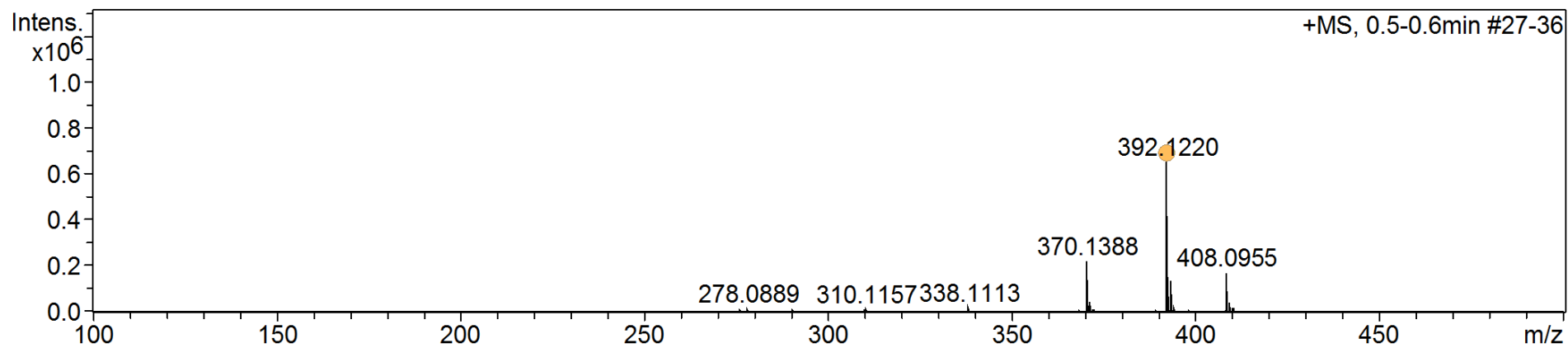
1g: calcd for $C_{23}H_{21}N_3O_3+Na$, 410.1475, found 410.1477.



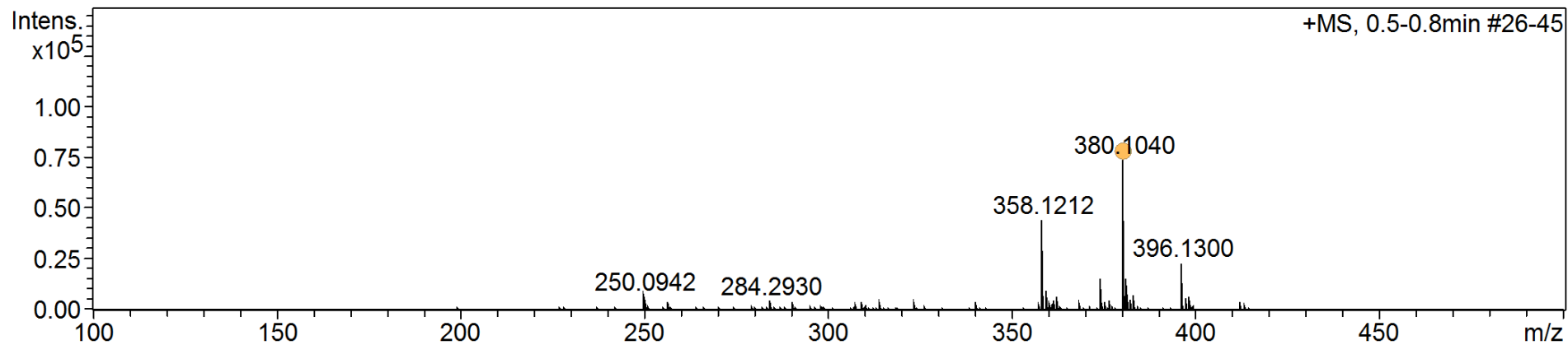
1h: calcd for $C_{18}H_{17}N_3O_5+Na$, 378.1060, found 378.1062.



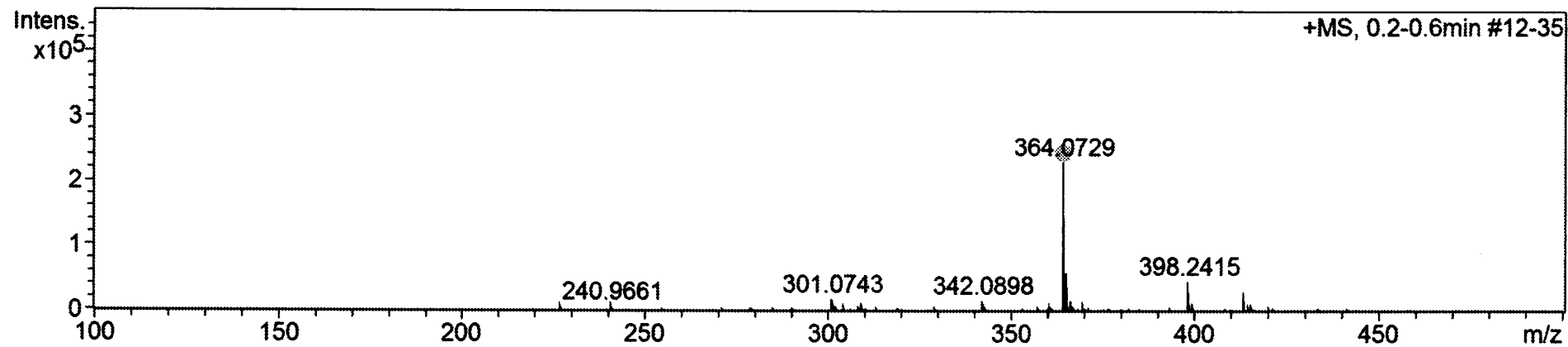
1i: calcd for $C_{19}H_{19}N_3O_5+Na$, 392.1217, found 392.1220.



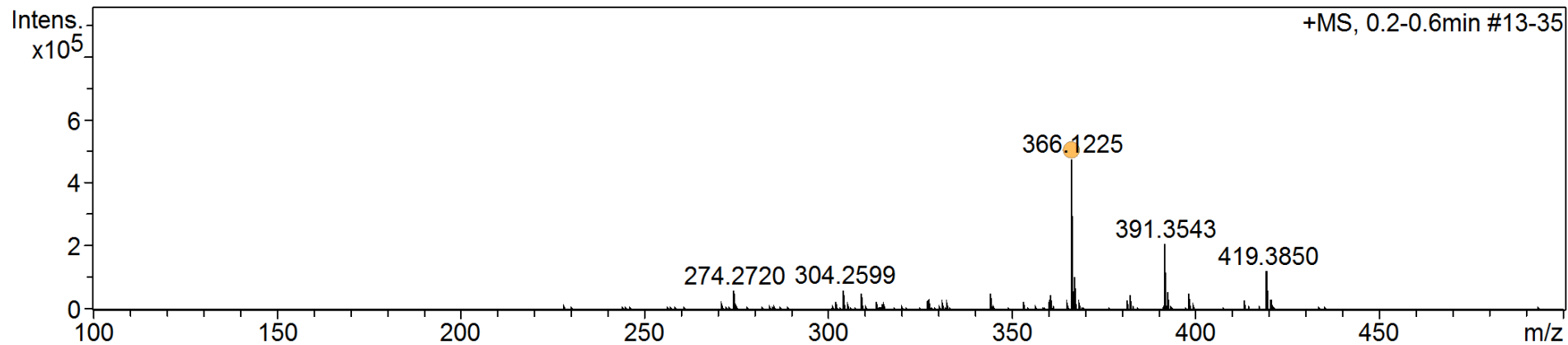
1j: calcd for $C_{18}H_{19}N_3O_3S+Na$, 380.1039, found 380.1040.



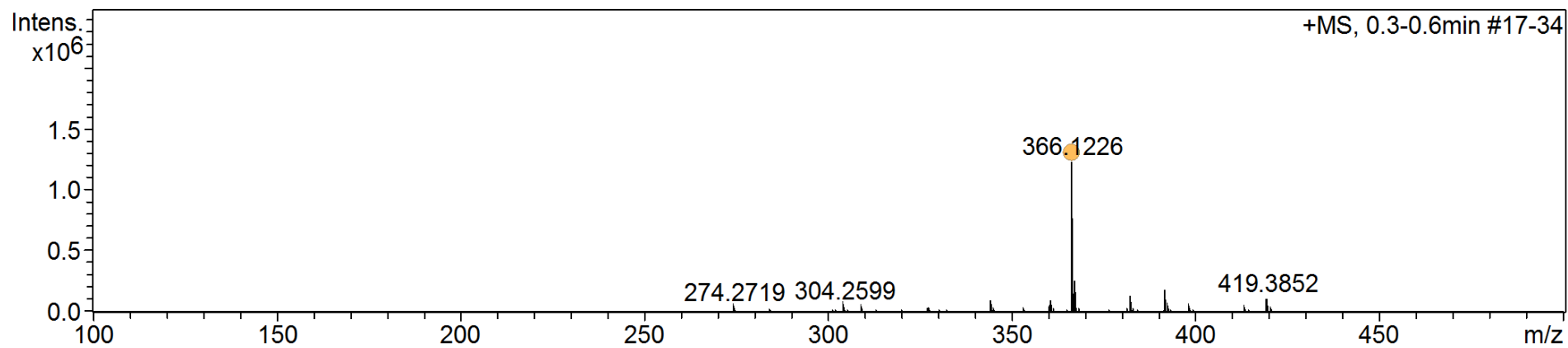
1k: calcd for $C_{17}H_{15}N_3O_3S+Na$, 364.0726, found 364.0729.



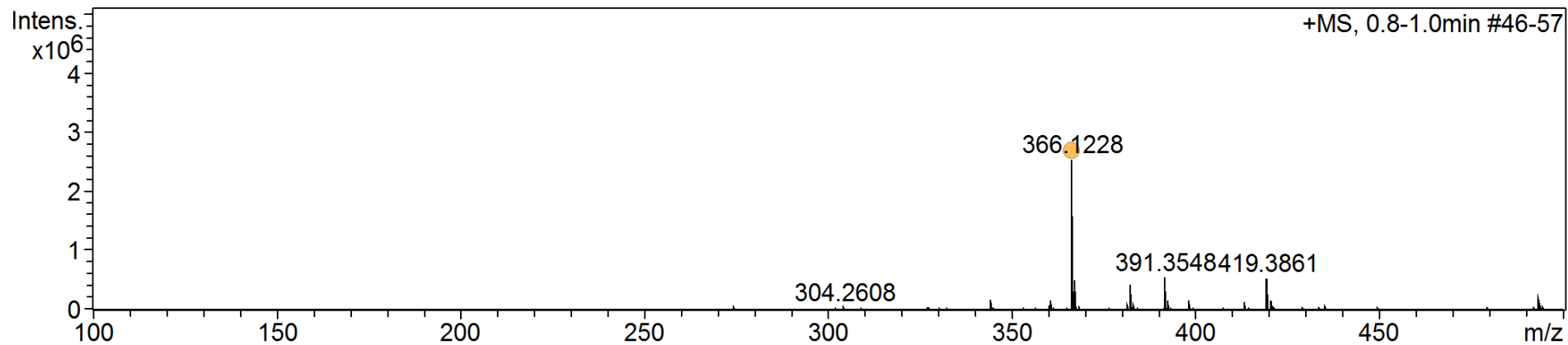
5a: calcd for $C_{18}H_{18}FN_3O_3+Na$ 366.1224, found 366.1225.



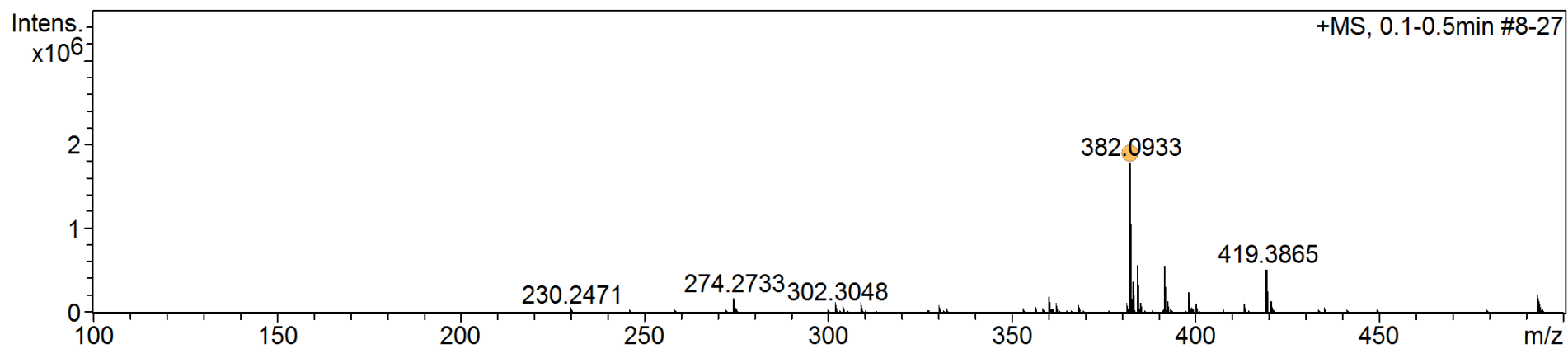
5b: calcd for $C_{18}H_{18}FN_3O_3+Na$ 366.1224, found 366.1226.



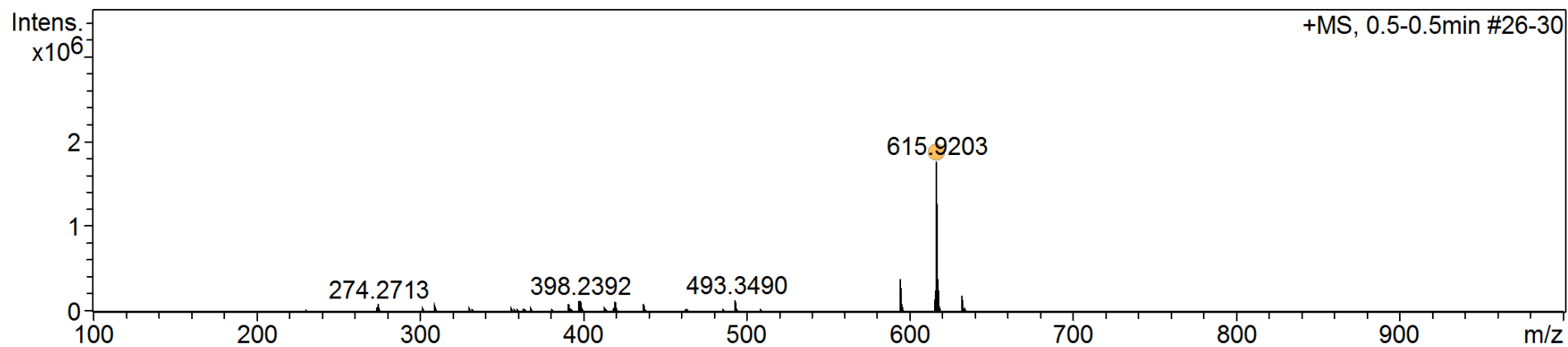
5c: calcd for $C_{18}H_{18}FN_3O_3+Na$ 366.1224, found 366.1228.



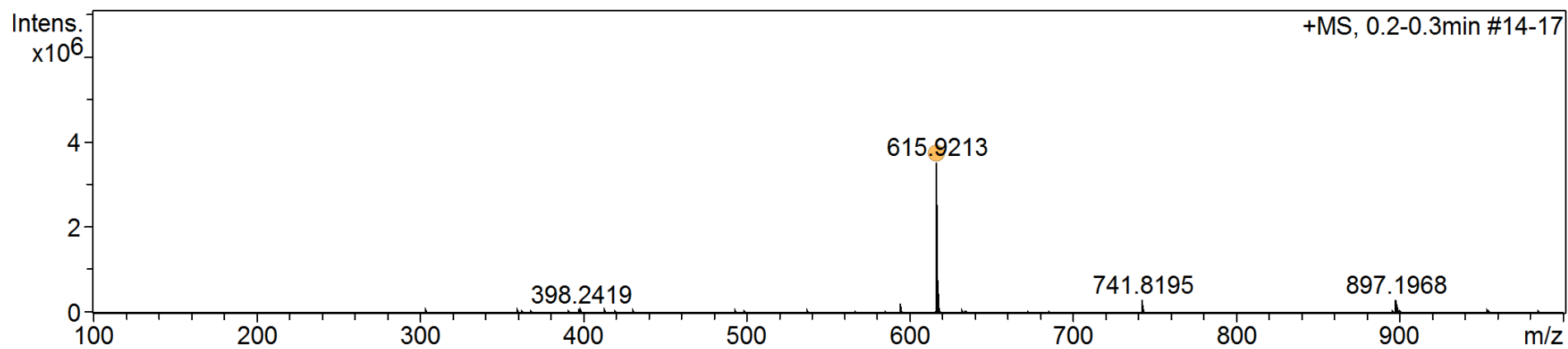
5d: calcd for $C_{18}H_{18}ClN_3O_3+Na$ 382.0929, found 382.0933.



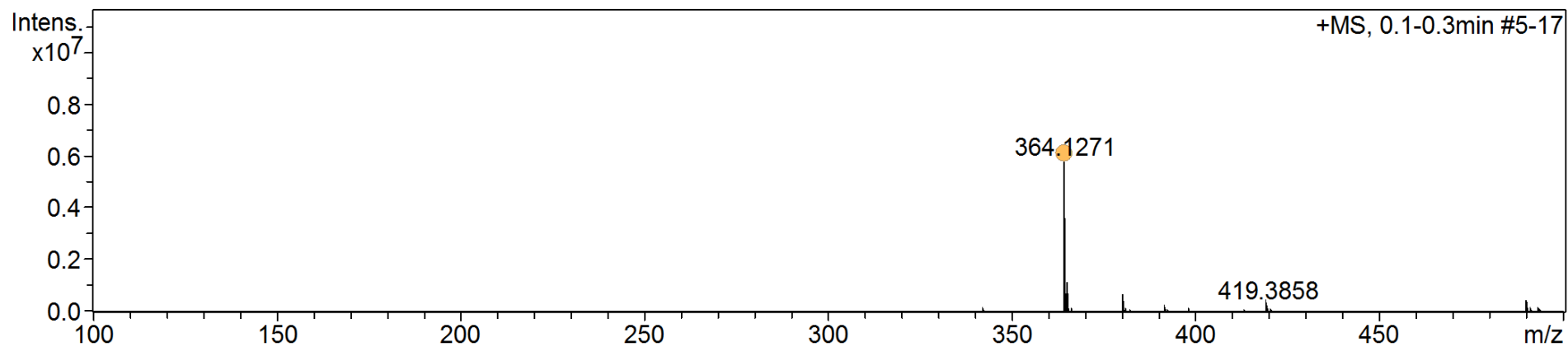
5e-1: calcd for $C_{18}H_{17}I_2N_3O_4+Na$ 615.9201, found 615.9203.



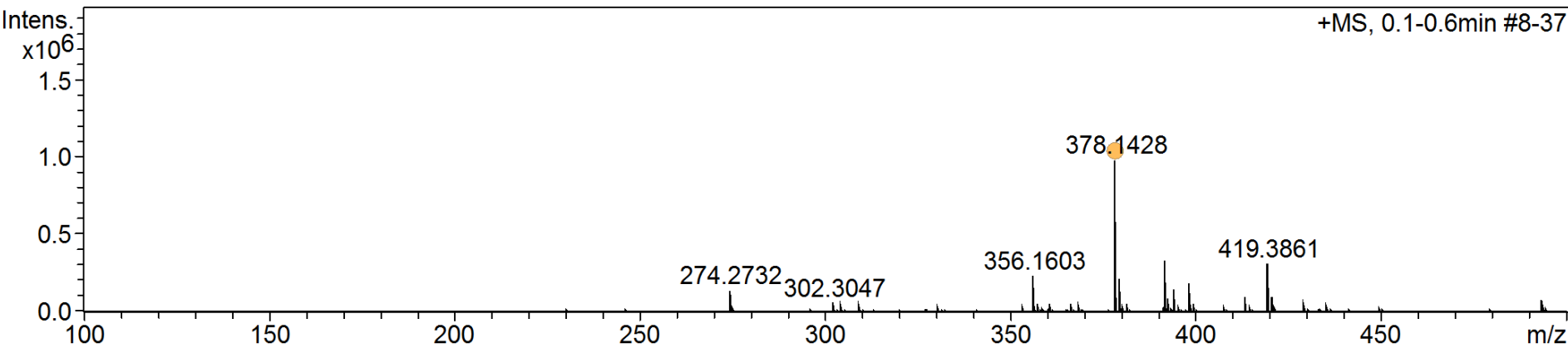
5f-1: calcd for $[\text{C}_{18}\text{H}_{15}\text{I}_4\text{N}_3\text{O}_4 - \text{I}_2 + \text{H}_2] + \text{Na}$ 615.9201, found 615.9213.



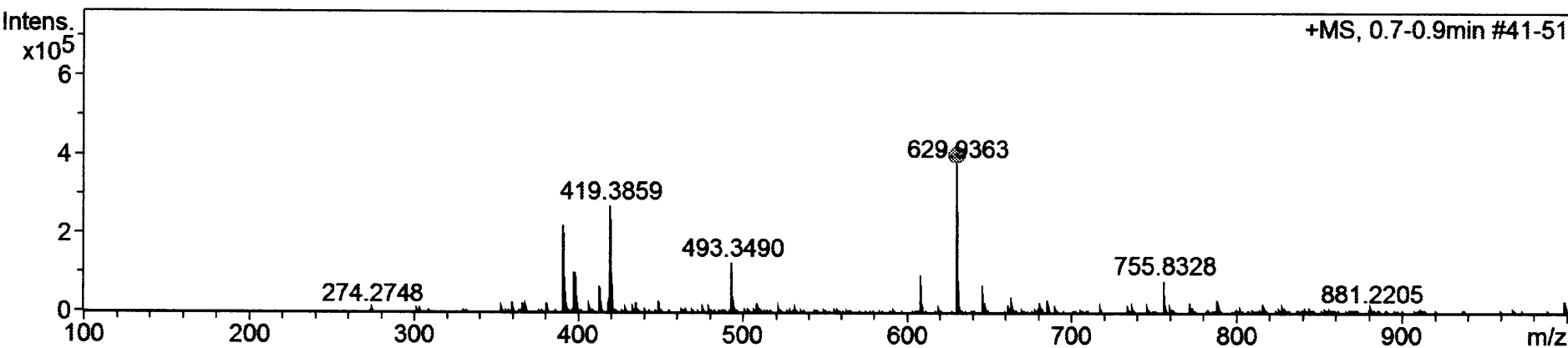
5f: calcd for $\text{C}_{18}\text{H}_{19}\text{N}_3\text{O}_4 + \text{Na}$ 364.1268, found 365.1271.



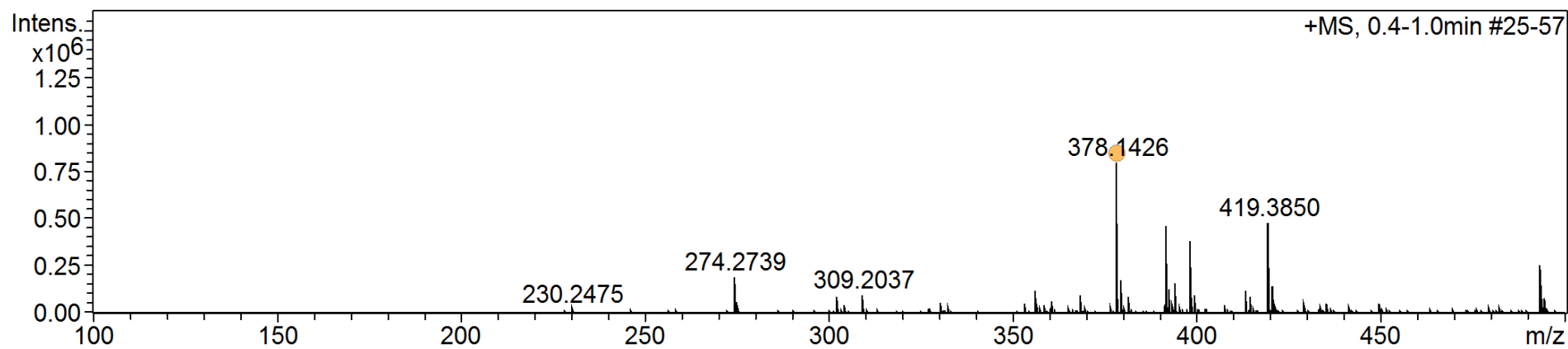
5g: calcd for C₁₉H₂₁N₃O₄+Na 378.1424, found 378.1428.



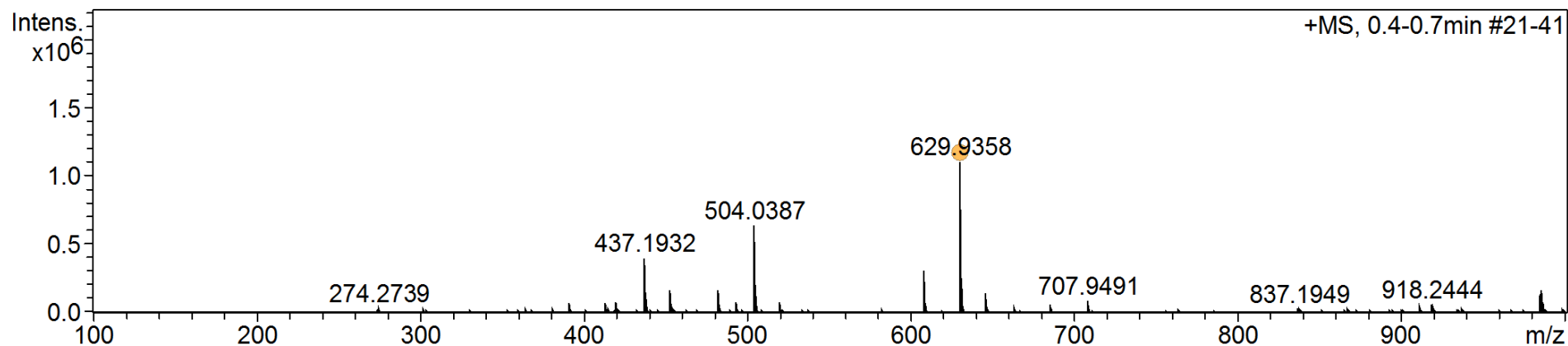
5g-1: calcd for C₁₉H₁₉I₂N₃O₄+Na 629.9357, found 629.9363.



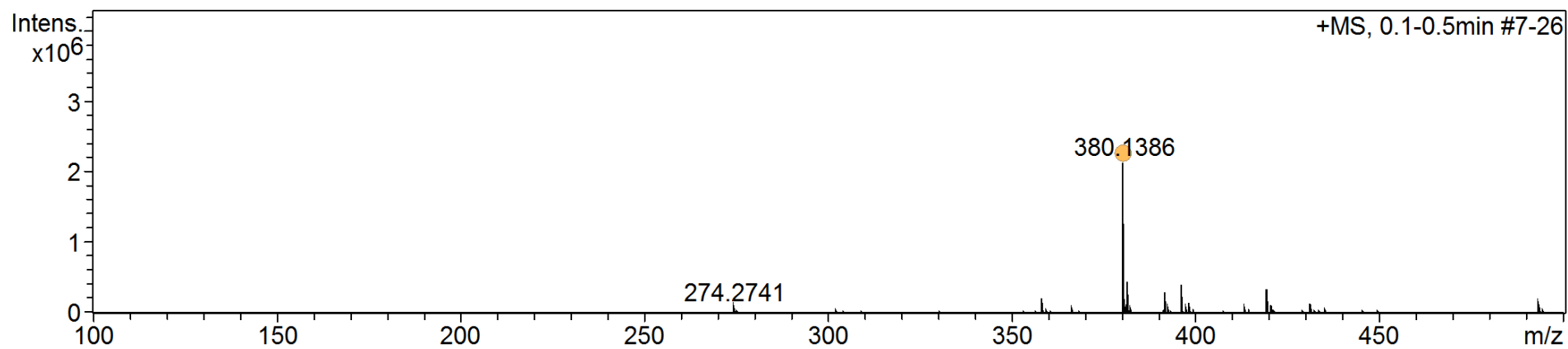
5h: calcd for $C_{19}H_{21}N_3O_4+Na$ 378.1424, found 378.1426.



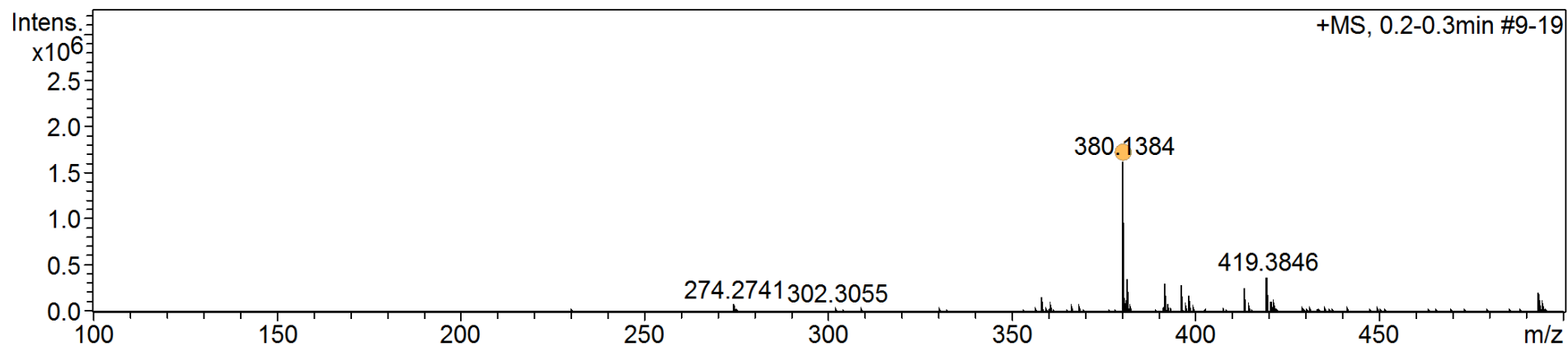
5h-1: calcd for $C_{19}H_{20}IN_3O_4+Na$ 504.0396, found 504.0387; calcd for $C_{19}H_{19}I_2N_3O_4+Na$ 629.9357, found 629.9358.



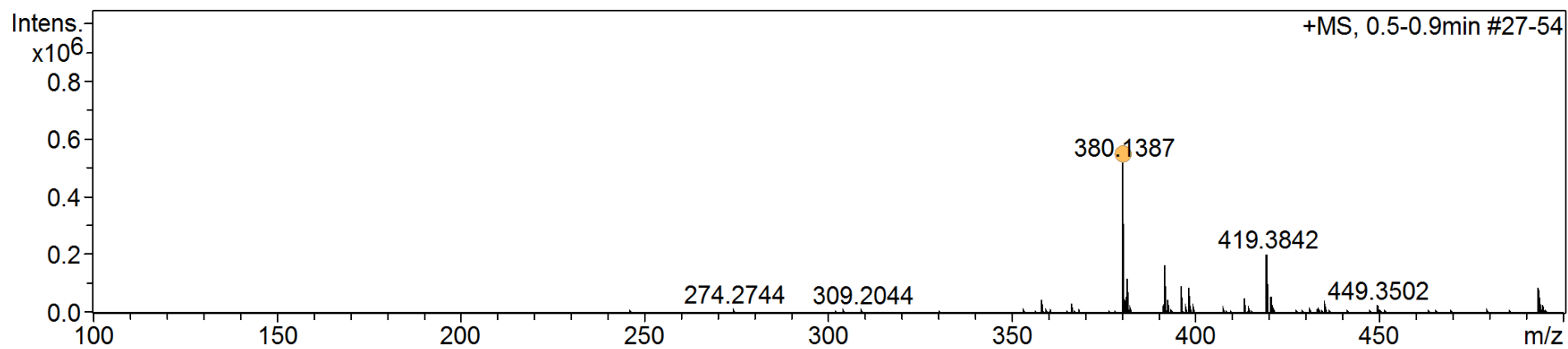
6a: calcd for $C_{19}H_{20}FN_3O_3+Na$ 380.1381, found 380.1386.



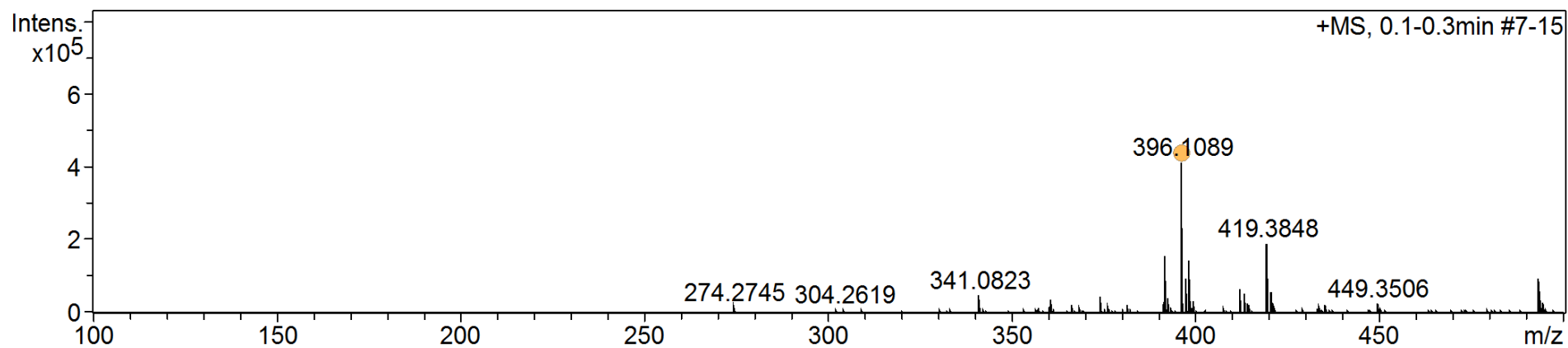
6b: calcd for $C_{19}H_{20}FN_3O_3+Na$ 380.1381, found 380.1384.



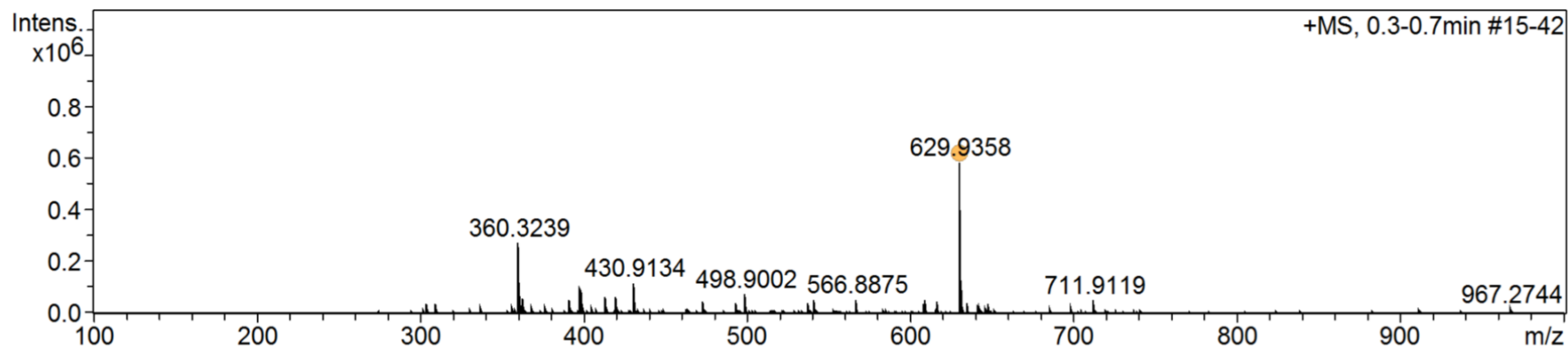
6c: calcd for $C_{19}H_{20}FN_3O_3+Na$ 380.1381, found 380.1387.



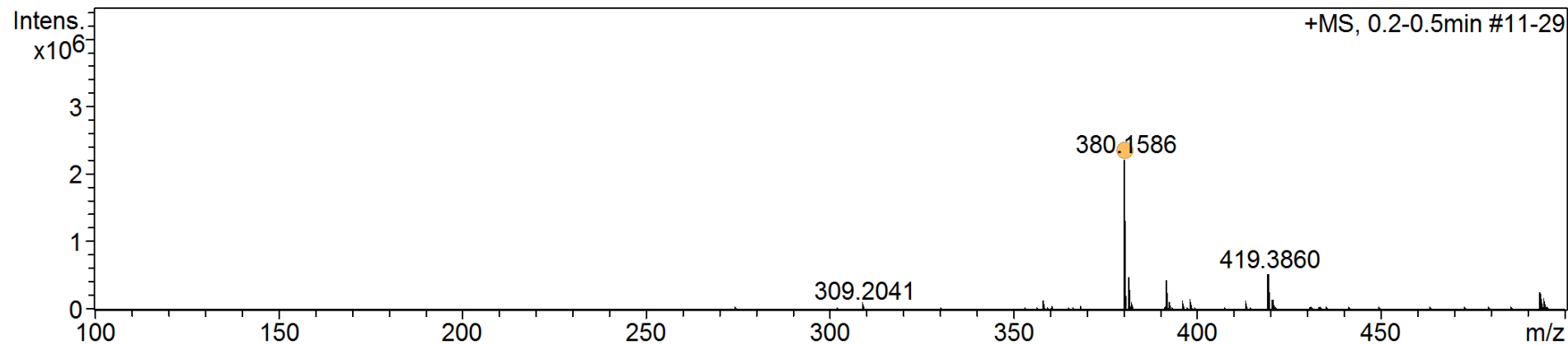
6d: calcd for $C_{19}H_{20}ClN_3O_3+Na$ 396.1085, found 396.1089.



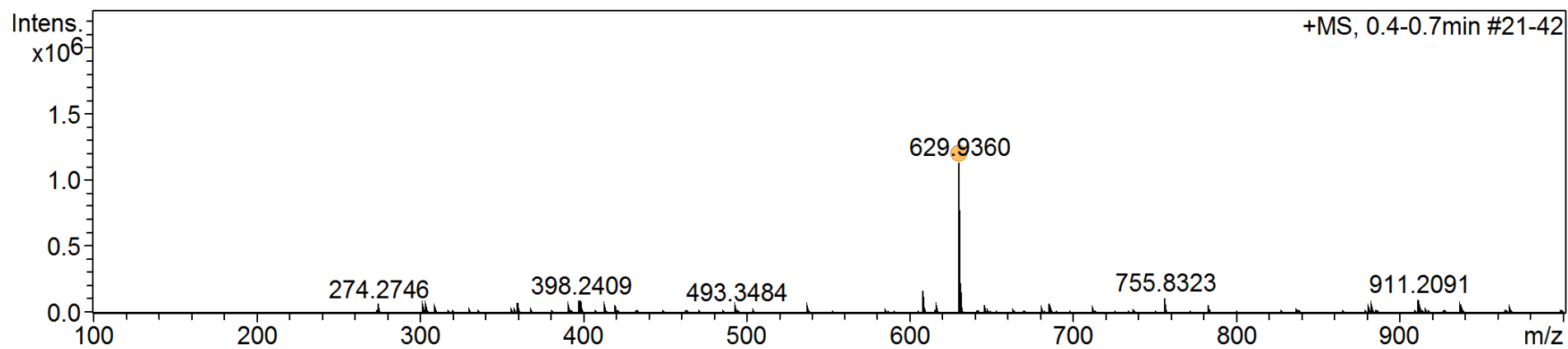
6e-1: calcd for $C_{19}H_{19}I_2N_3O_4+Na$ 629.9357, found 629.9358.



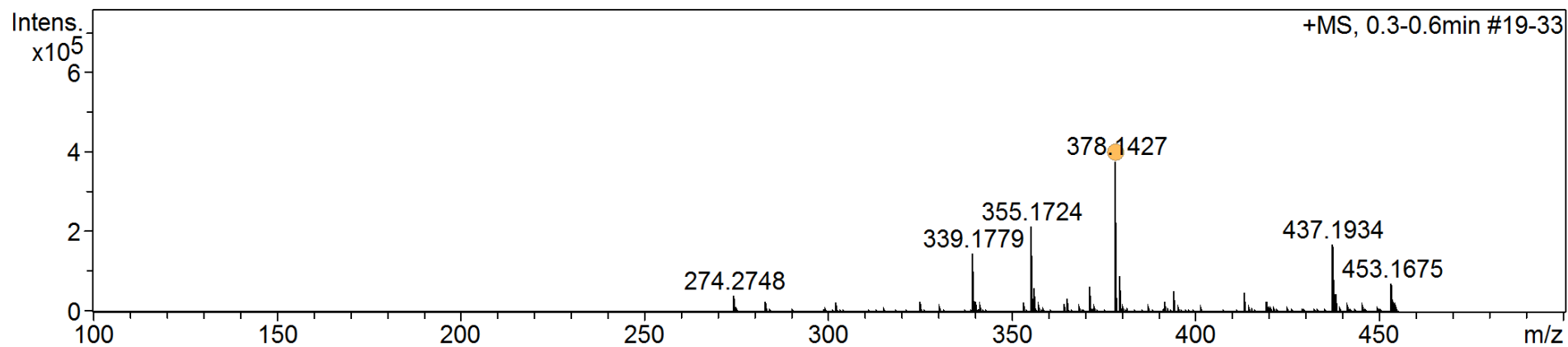
6e: calcd for $C_{19}H_{23}N_3O_4+Na$ 380.1581, found 380.1586.



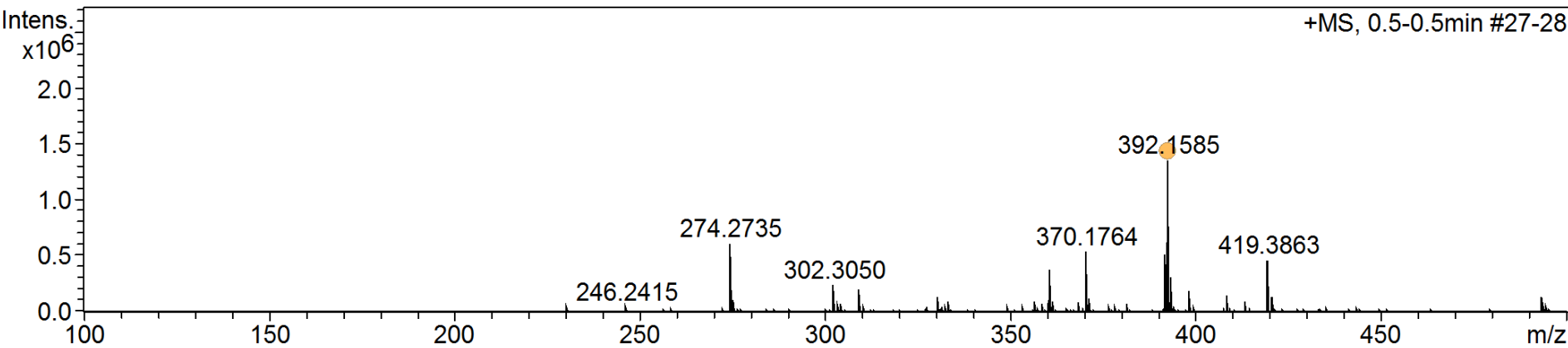
6f-1: calcd for $C_{19}H_{19}I_2N_3O_4+Na$ 629.9357, found 629.9360.



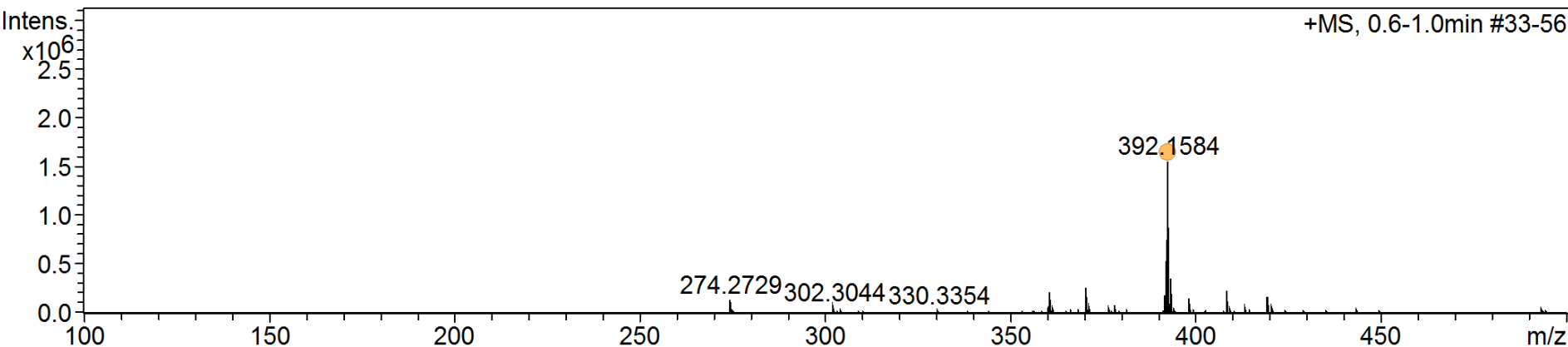
6f: calcd for $C_{19}H_{21}N_3O_4+Na$ 378.1424, found 378.1427.



6g: calcd for C₂₀H₂₃N₃O₄+Na 392.1581, found 392.1585.



6h: calcd for C₂₀H₂₃N₃O₄+Na 392.1581, found 392.1584.



6h-1: calcd for C₂₀H₂₂IN₃O₄+Na 518.0547, found 518.0548.

