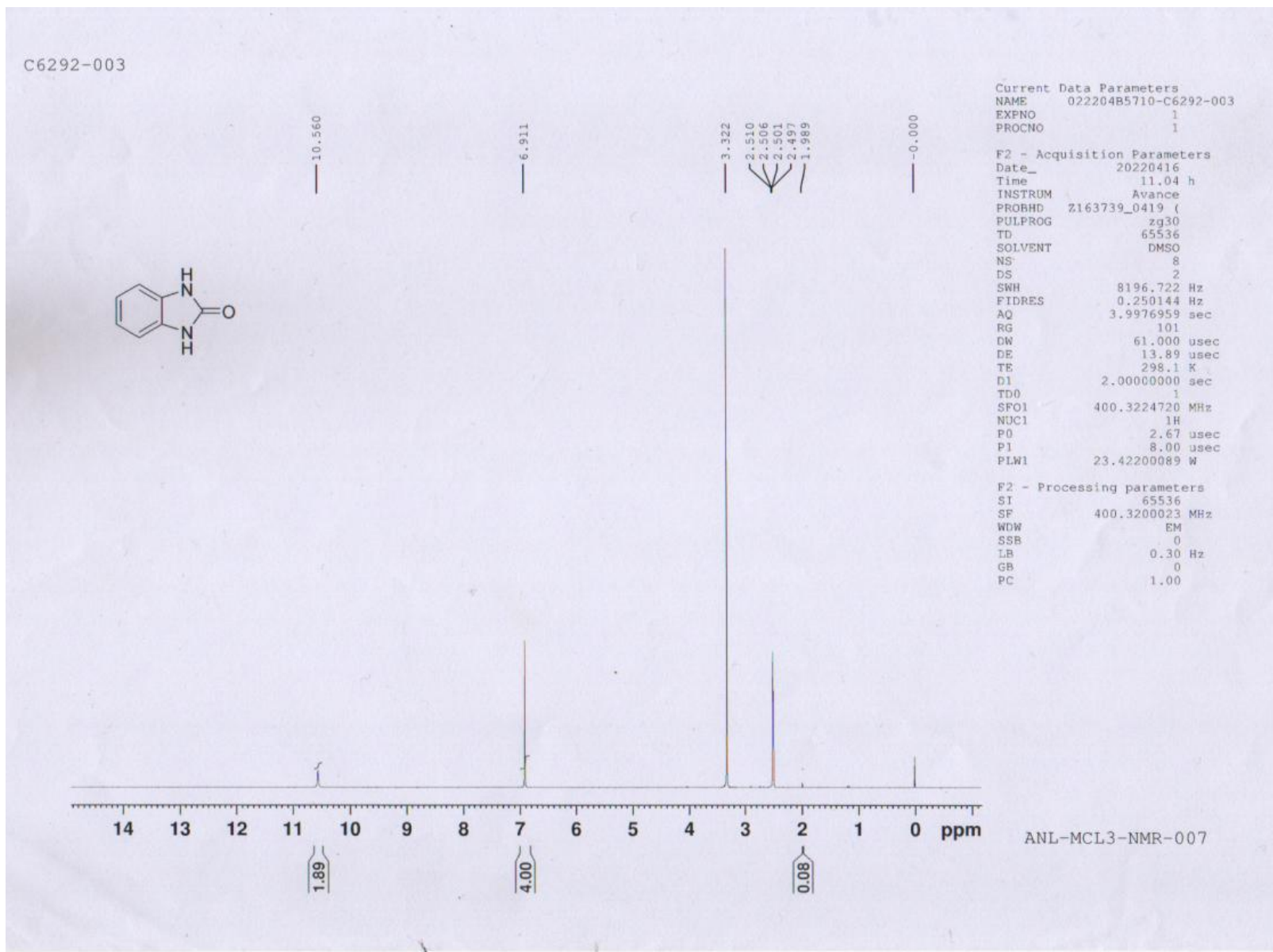
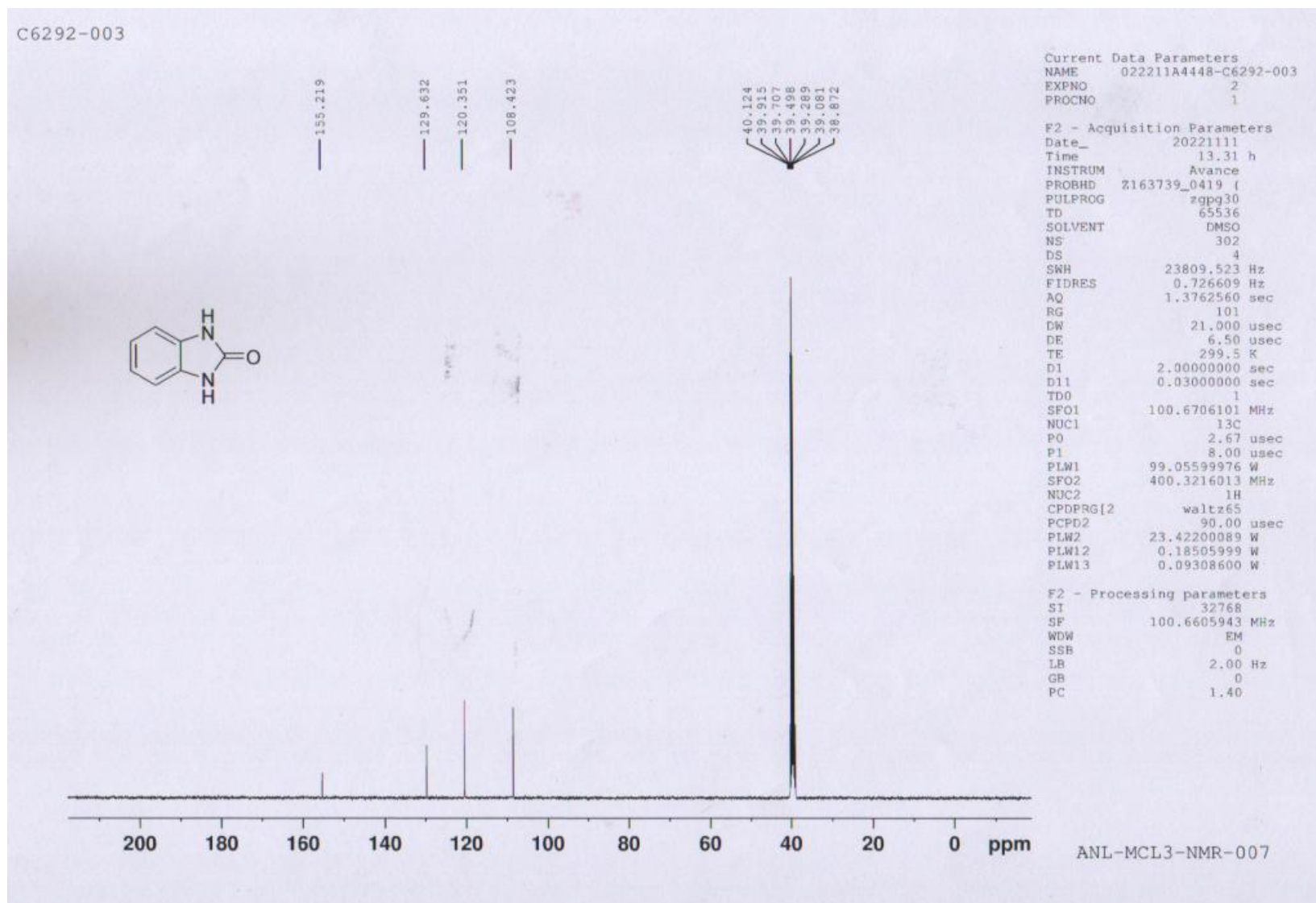


Spectrum:

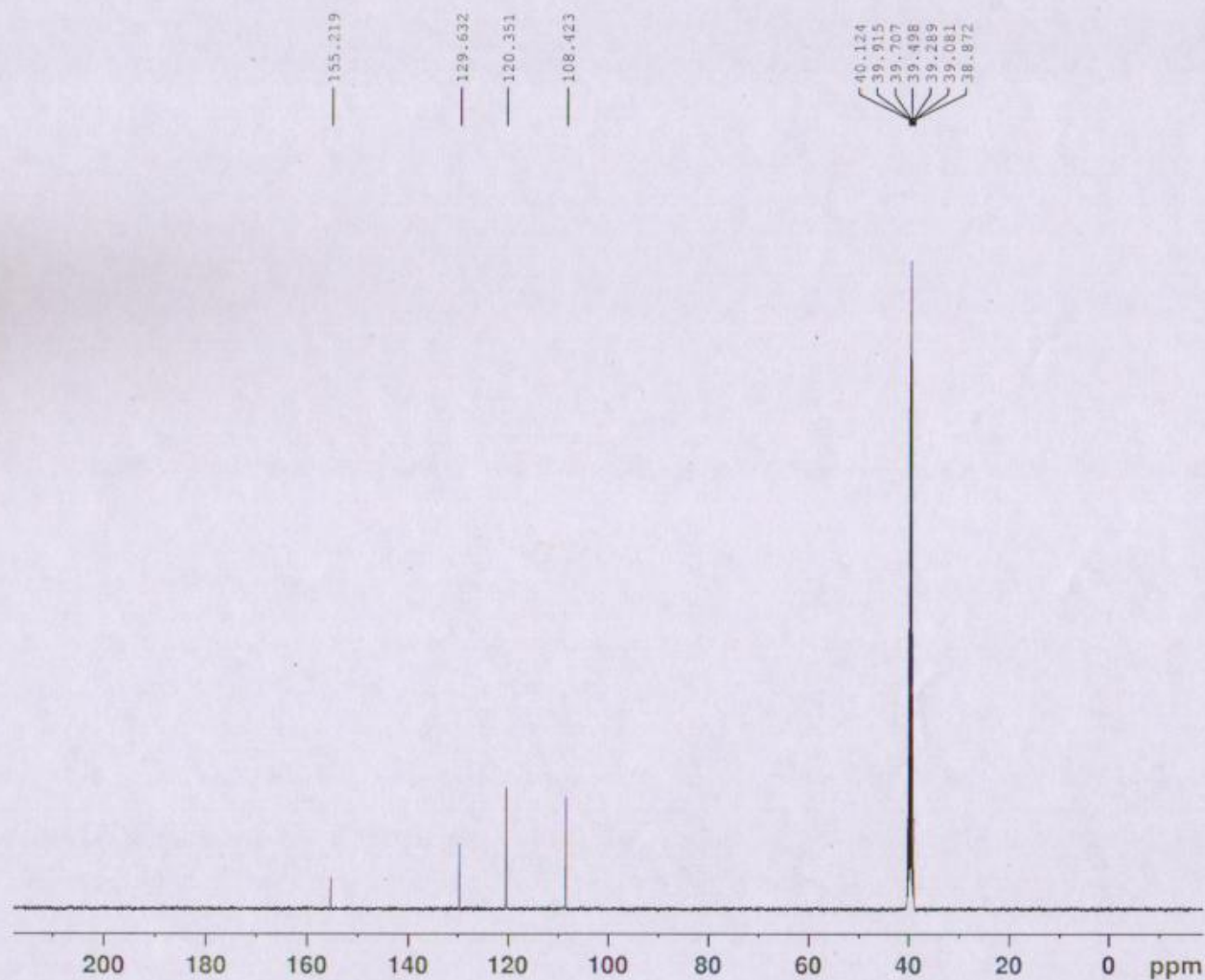
¹H NMR of benzimidazolone



¹³C NMR of benzimidazolone



C6292-003



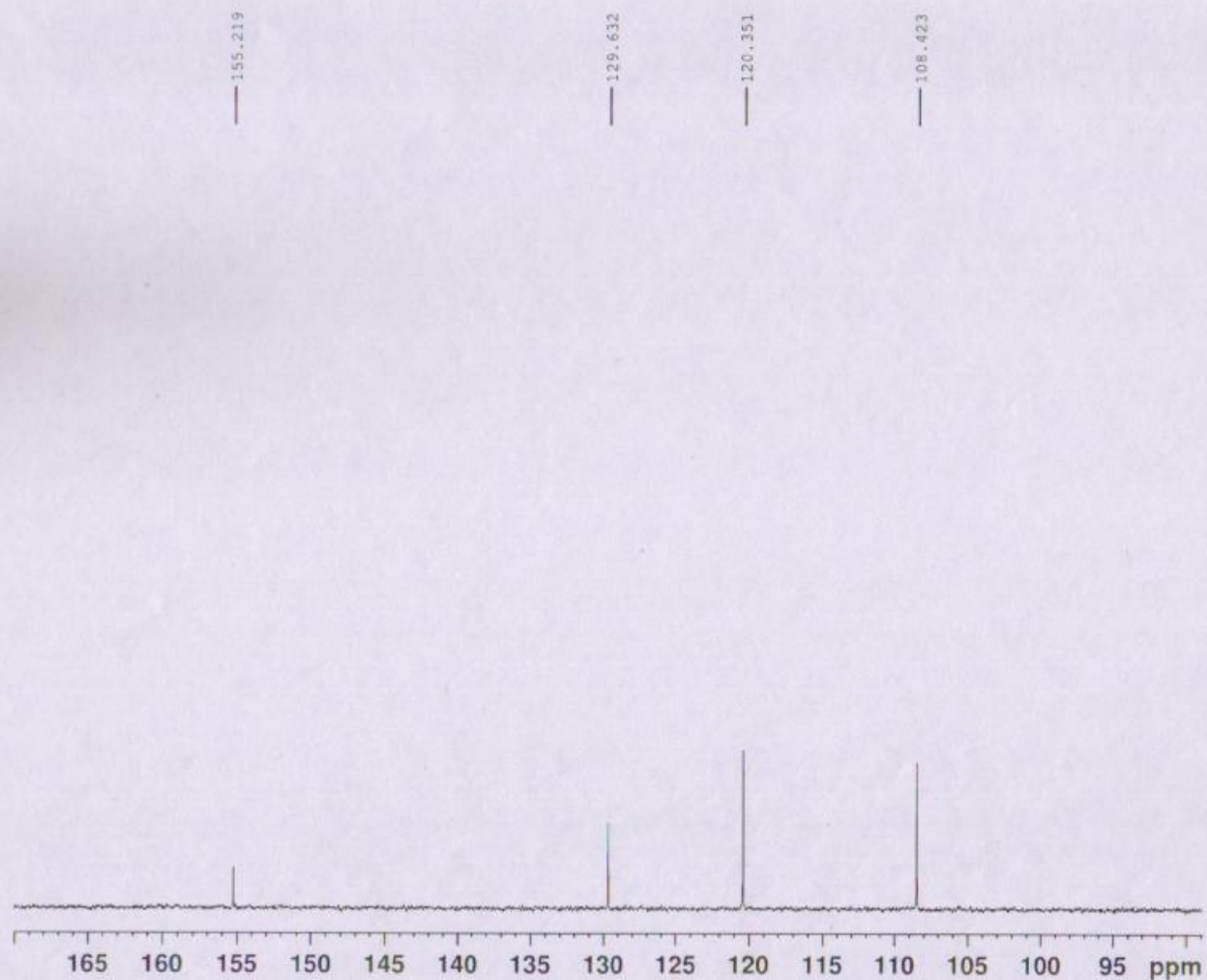
Current Data Parameters
NAME 022211A4448-C6292-003
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221111
Time 13.31 h
INSTRUM Avance
PROBHD Z163739_0419 1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 302
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 299.5 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6706101 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 99.05599976 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 23.42200089 W
PLW12 0.18505999 W
PLW13 0.09308600 W

F2 - Processing parameters
SI 32768
SF 100.6605943 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

ANL-MCL3-NMR-007

C6292-003



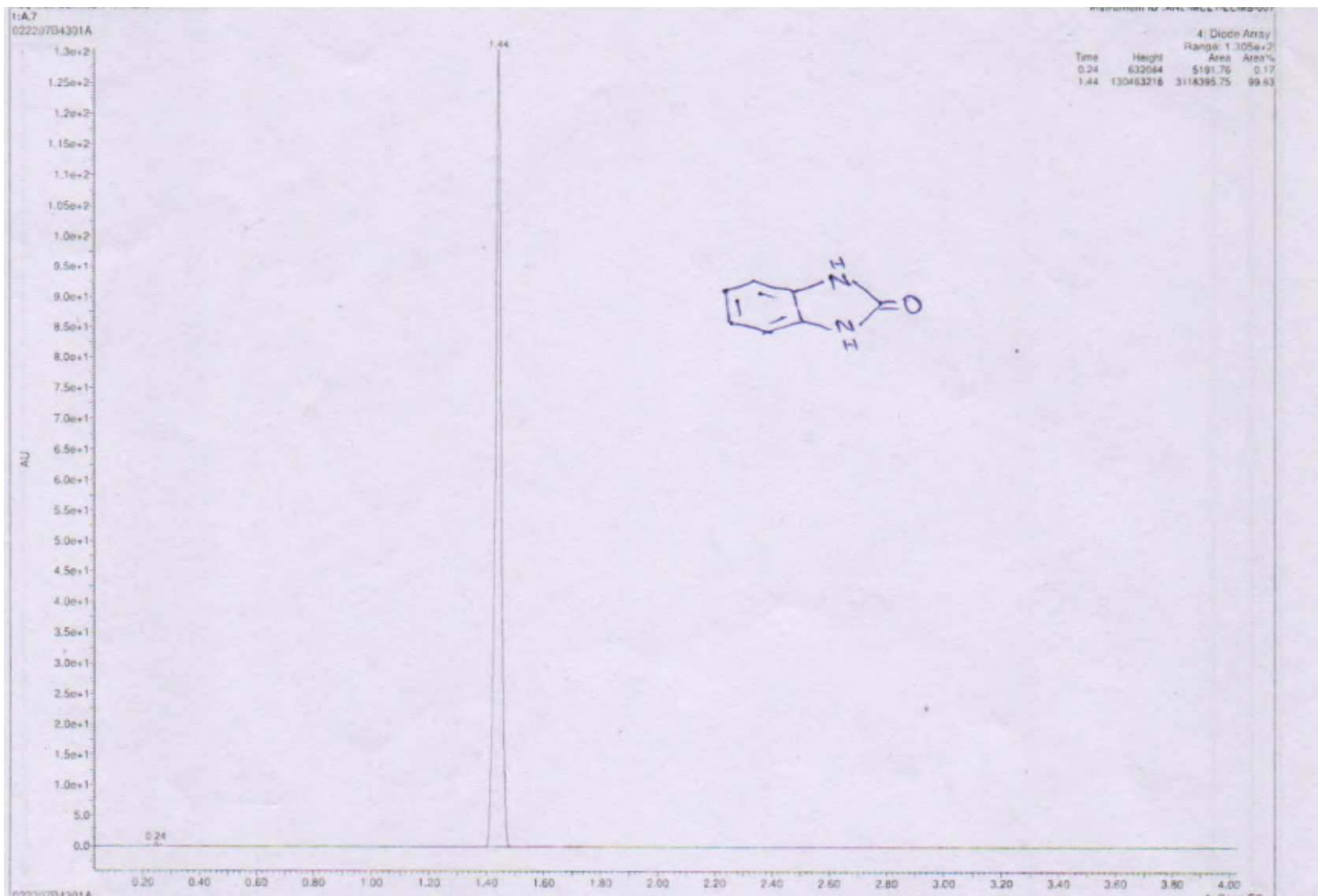
Current Data Parameters
NAME 022211A4448-C6292-003
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221111
Time 13.31 h
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 302
DS 4
SWH 23809.521 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 299.5 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6706101 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 99.05599976 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 23.42200089 W
PLW12 0.18505999 W
PLW13 0.09308600 W

F2 - Processing parameters
SI 32768
SF 100.6605943 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

ANL-MCL3-NMR-007

LCMS of benzimidazolone

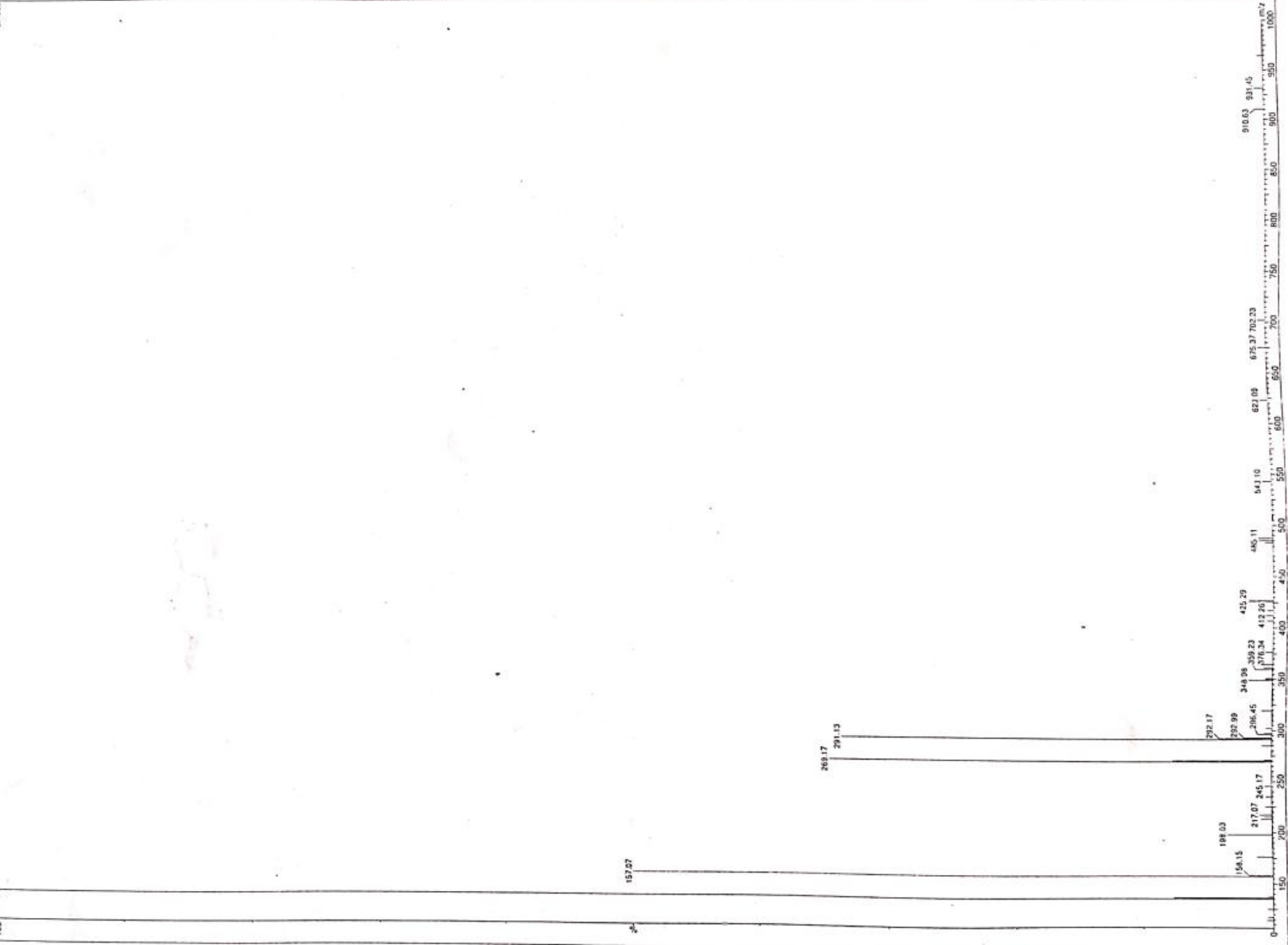


SAMPLE ID: C6390-003
Acq Method: FID-F-A4.MN
C2220704301A.S7 (1.457)

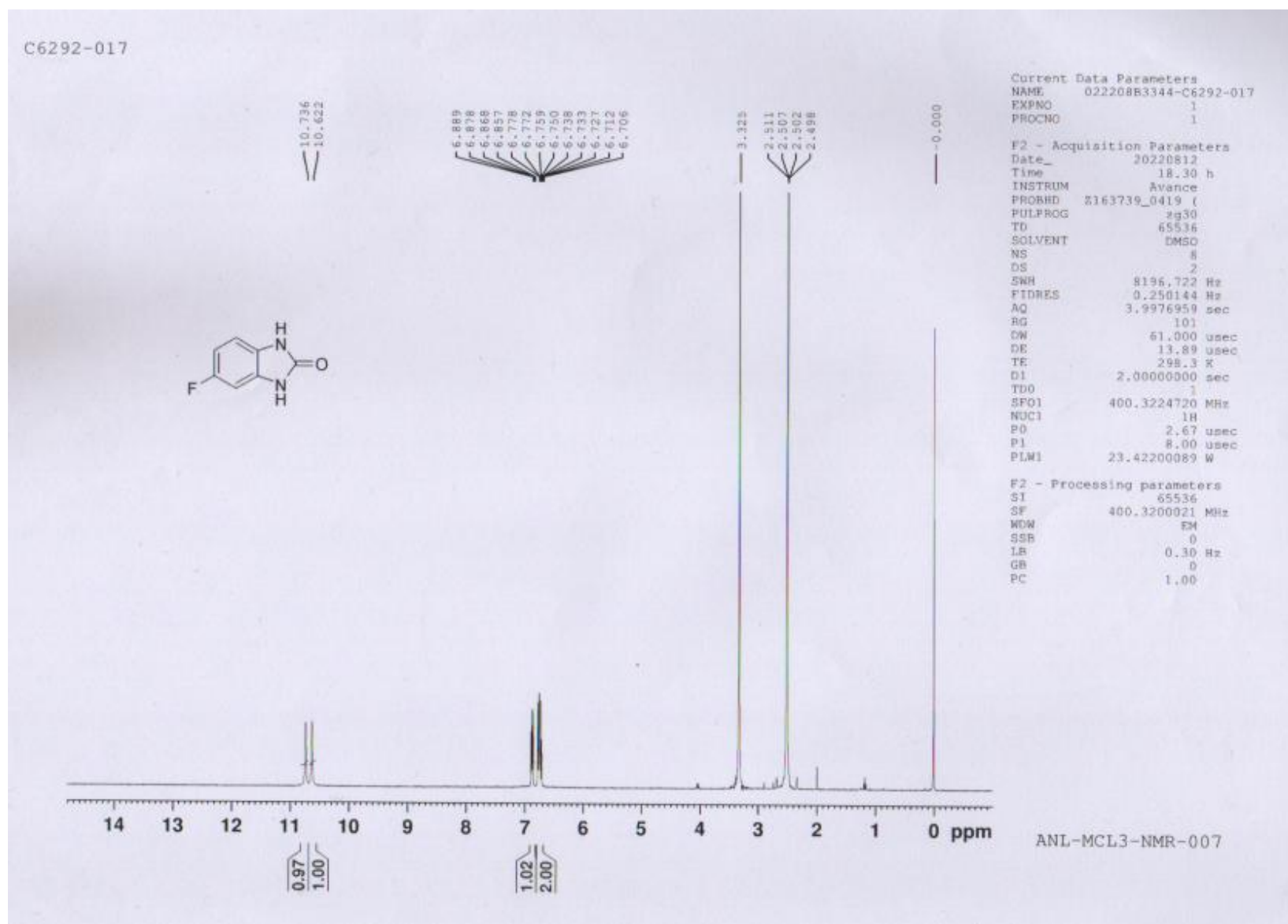
100 125.11

Date of Analysis: 15-Jul-2022 10:21:48
Instrument ID: ANI-HCL1-LCMS-007
1: Scan EC:
3.8826

100 125.11

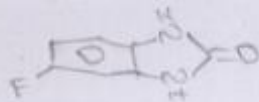


¹H NMR of 5-Fluoro-1,3-dihydro-2H-benzo[d]imidazol-2-one (2a)



C6292-017

10.736
10.622

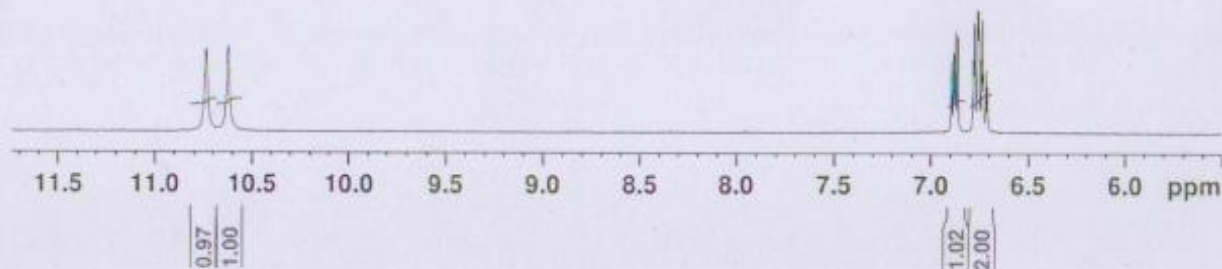


6.889
6.878
6.868
6.857
6.778
6.772
6.759
6.750
6.738
6.732
6.727
6.712
6.706

Current Data Parameters
NAME 022208B1344-C6292-017
EXPNO 1
PROCNO 1

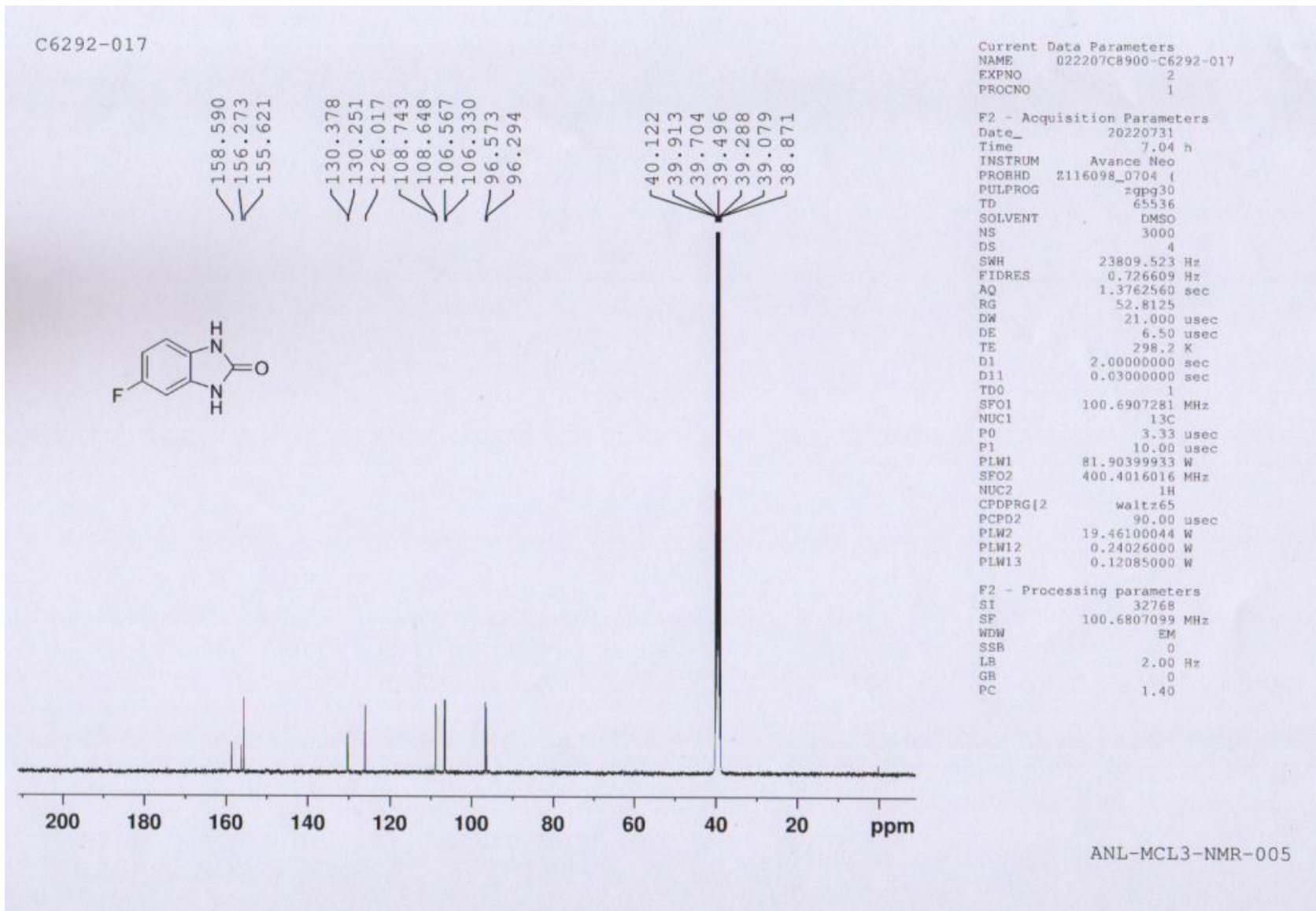
F2 - Acquisition Parameters
Date_ 20220812
Time 18.30 h
INSTRUM Avance
PROBHD Z163739_0419 f
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976559 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.3 K
D1 2.00000000 sec
TDO 1
SFO1 400.3224720 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 23.42200089 W

F2 - Processing parameters
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SF 400.3200071 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

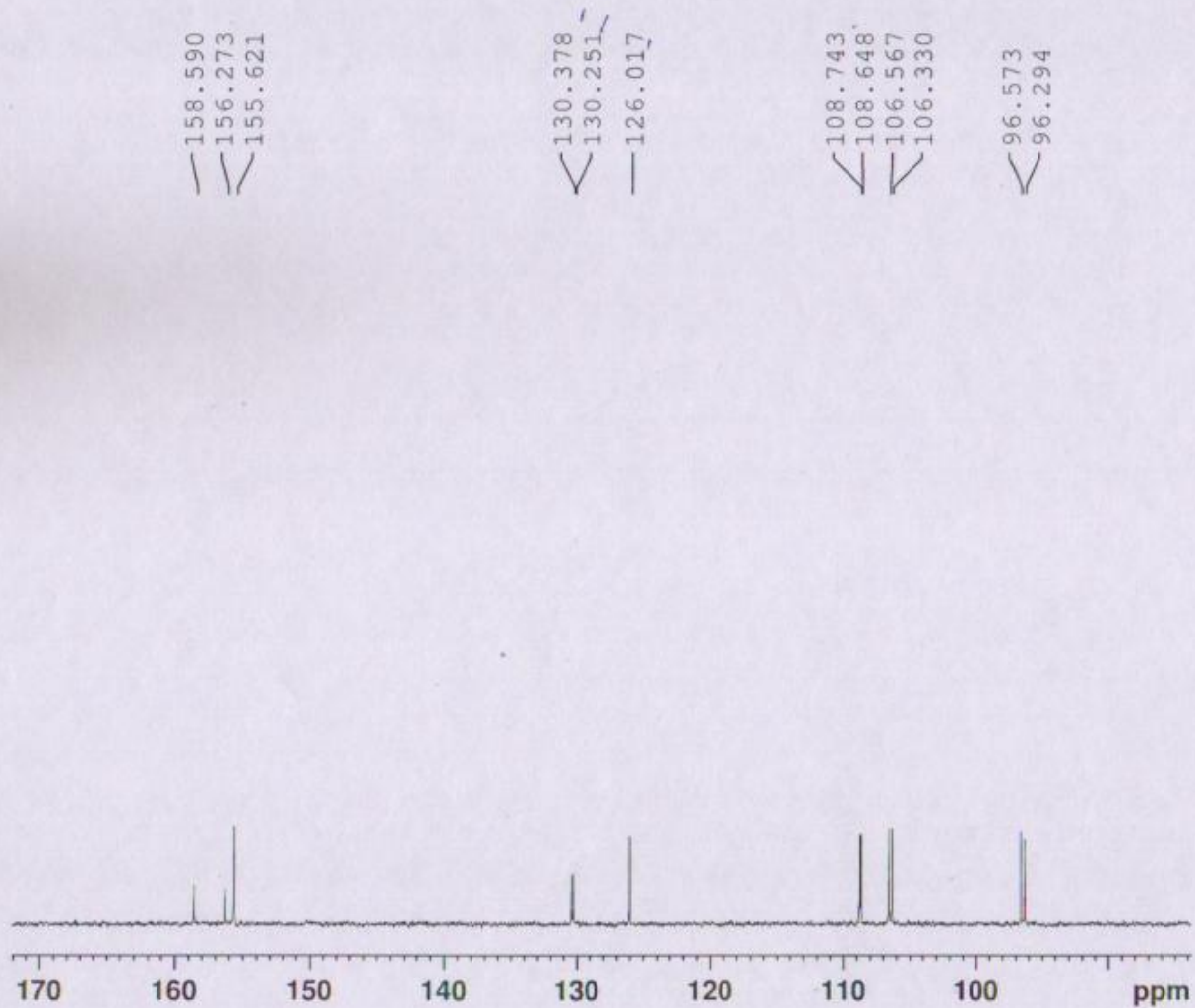


ANL-MCL3-NMR-007

¹³C NMR of 5-Fluoro-1,3-dihydro-2H-benzo[d]imidazol-2-one (2a)



C6292-017



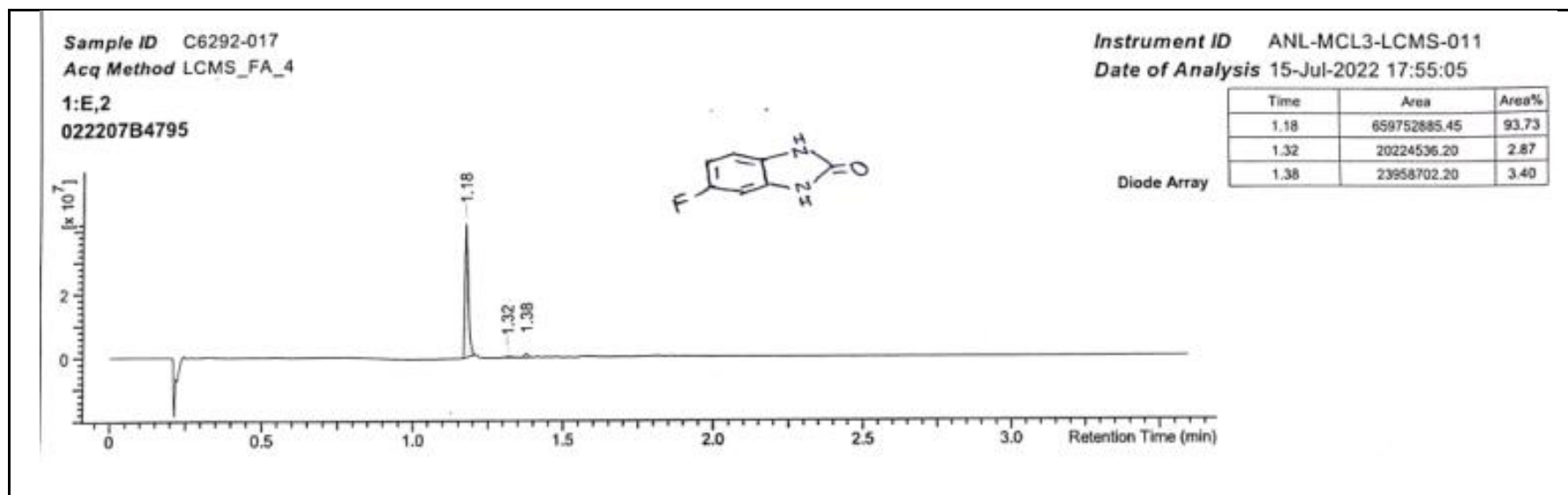
Current Data Parameters
NAME 022207C8900-C6292-017
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220731
Time 7.04 h
INSTRUM Avance Neo
PROBHD Z116098_0704 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3000
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 52.8125
DN 21.000 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6907281 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 81.90399933 W
SFO2 400.4016016 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 19.46100044 W
PLW12 0.24026000 W
PLW13 0.12085000 W

F2 - Processing parameters
SI 32768
SF 100.6807099 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

ANL-MCL3-NMR-005

LCMS of 5-Fluoro-1,3-dihydro-2H-benzo[d]imidazol-2-one (2a)



Sample ID C6292-017

Discovery Chemistry – Analytical Services

Instrument ID ANL-MCL3-LCMS-011

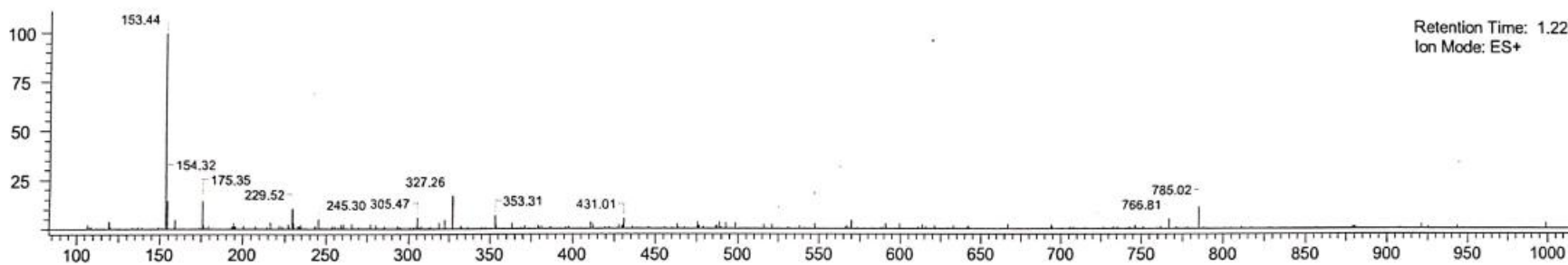
Acq Method LCMS_FA_4

Date of Analysis 15-Jul-2022 17:55:05

1:E,2

022207B4795

Retention Time: 1.226
Ion Mode: ES+

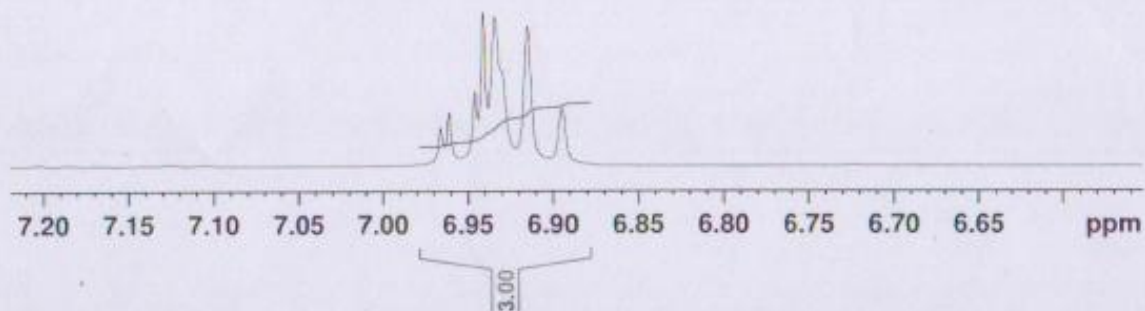


¹H NMR of 5-Chloro-1,3-dihydro-2H-benzo[d]imidazol-2-one (2b)



C6292-032

6.966
6.961
6.946
6.941
6.934
6.915
6.894



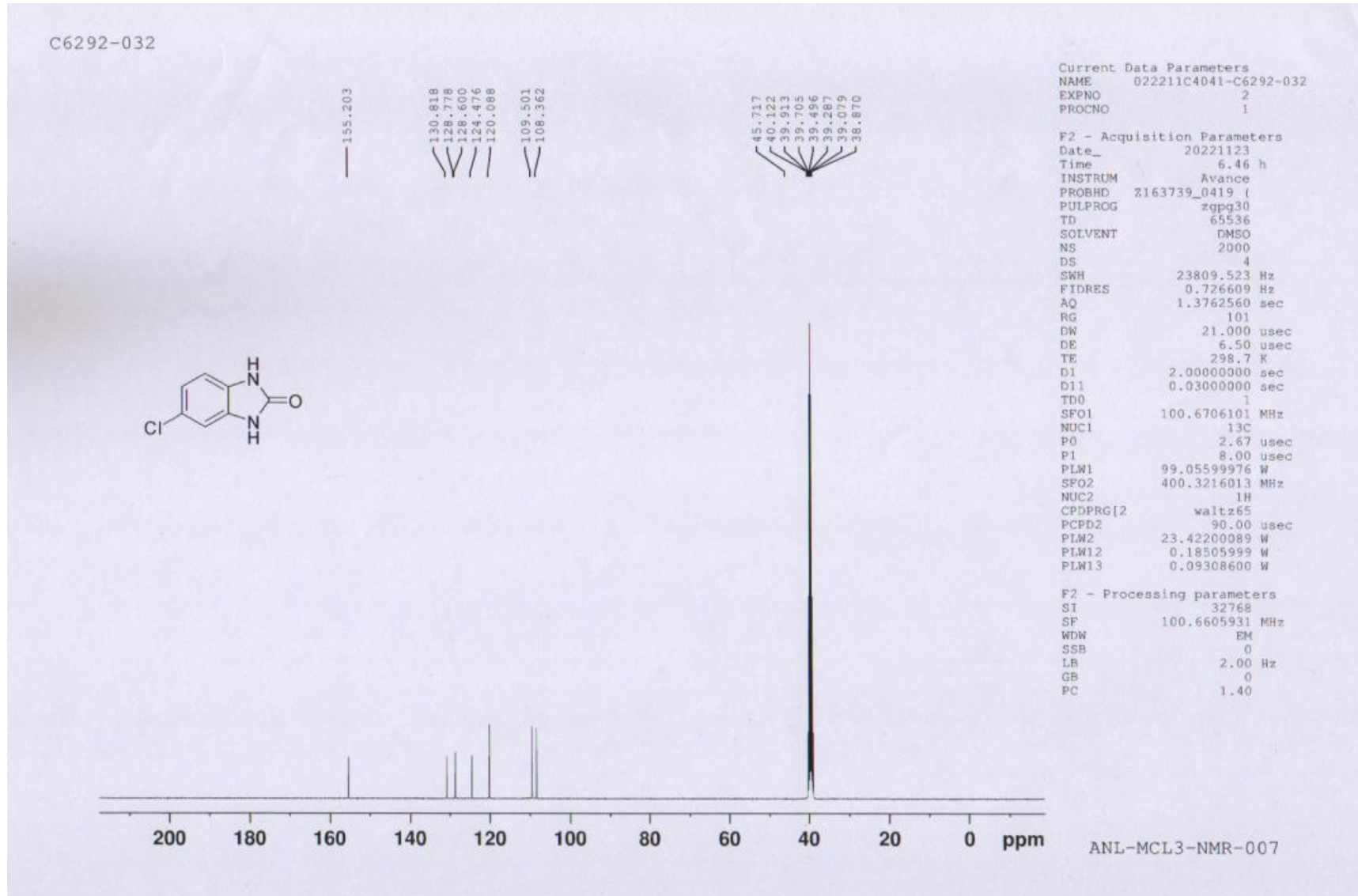
Current Data Parameters
NAME 02220862454-C6292-032
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220811
Time 21.19 h
INSTRUM Avance Neo
PROBHD E116098_0704 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 7142.857 Hz
FIDRES 0.217983 Hz
AQ 4.5875201 sec
RG 101
EW 70.000 usec
DE 7.04 usec
TE 298.1 K
D1 2.00000000 sec
TDO 1
SFO1 400.4024725 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PL1 19.46100044 W

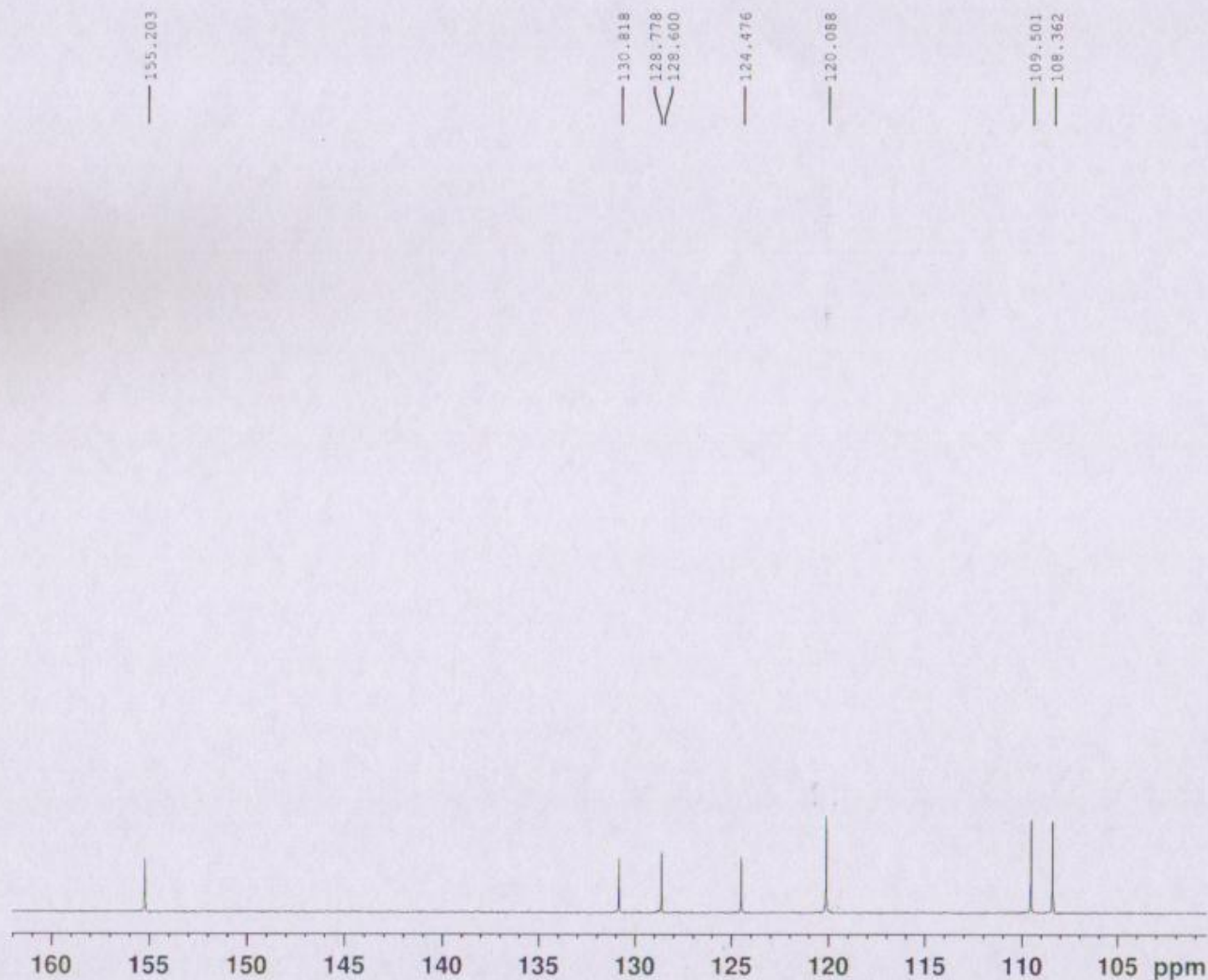
F2 - Processing parameters
SI 65536
SF 400.4000022 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ANL-MCL3-NMR-005

13C NMR of 5-Chloro-1,3-dihydro-2H-benzo[d]imidazol-2-one (2b)



C6292-032



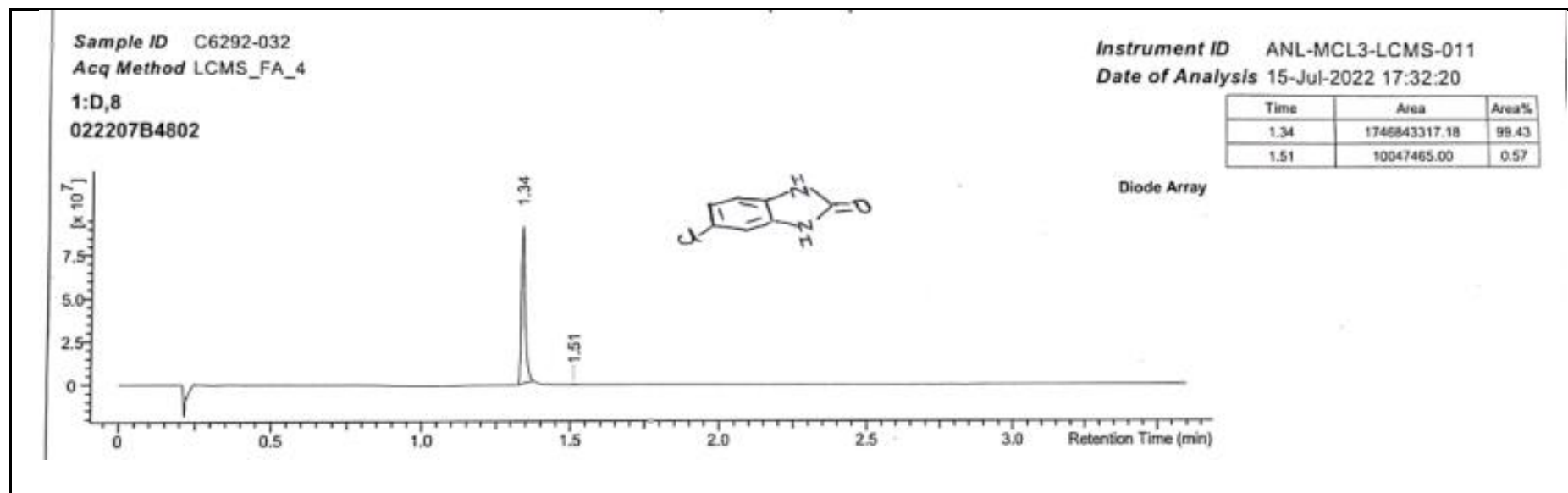
Current Data Parameters
NAME 022211C4041-C6292-032
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221123
Time 6.46 h
INSTRUM Avance
PROBHD Z163739_0419 ()
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6706101 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 99.05599976 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG2 waltz65
PCPD2 90.00 usec
PLW2 23.42200089 W
PLW12 0.18505999 W
PLW13 0.09308600 W

F2 - Processing parameters
SI 32768
SF 100.6605931 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

ANL-MCL3-NMR-007

LCMS of 5-Chloro-1,3-dihydro-2H-benzo[d]imidazol-2-one (2b)

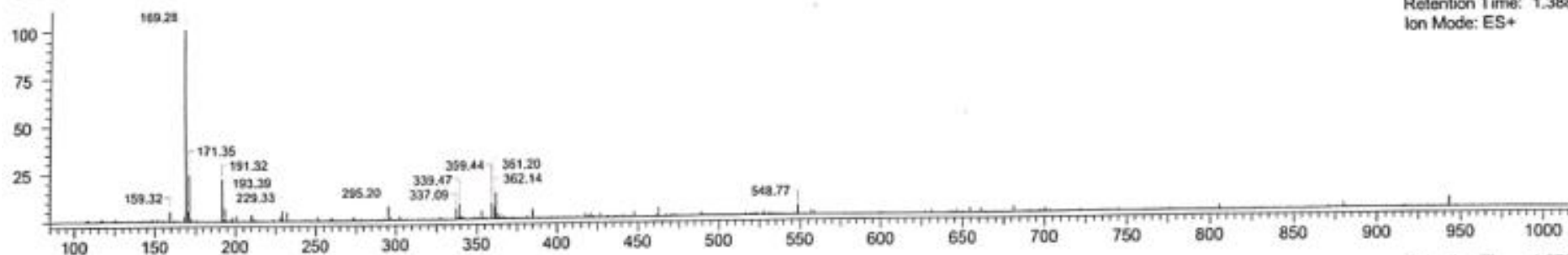


Sample ID C6292-032
Acq Method LCMS_FA_4
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022207B4802

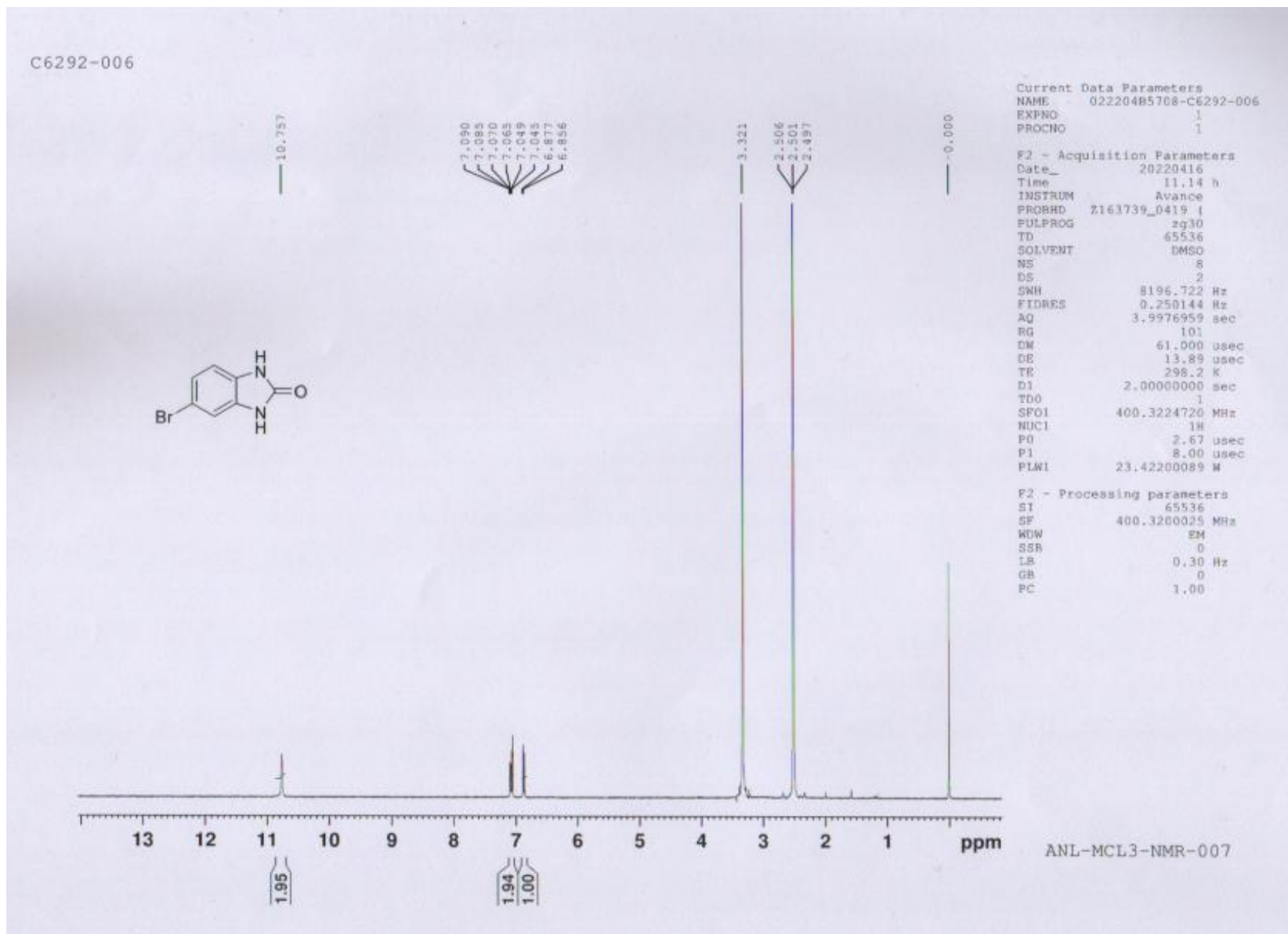
Discovery Chemistry – Analytical Services

Instrument ID ANL-MCL3-LCMS-011
Date of Analysis 15-Jul-2022 17:32:20

Retention Time: 1.388
Ion Mode: ES+



¹H NMR of 5-Bromo-1,3-dihydro-2H-benzo[d]imidazol-2-one (2c)



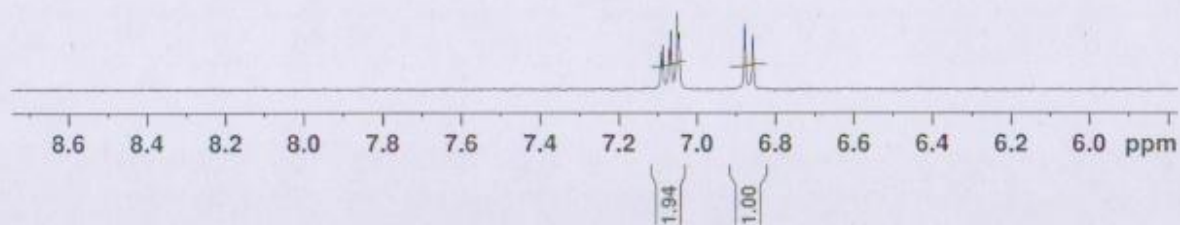
C6292-006

7.090
7.085
7.070
7.065
7.049
7.045
6.877
6.856

Current Data Parameters
NAME 022204B5708-C6292-006
EXPNO 1
PROCNO 1

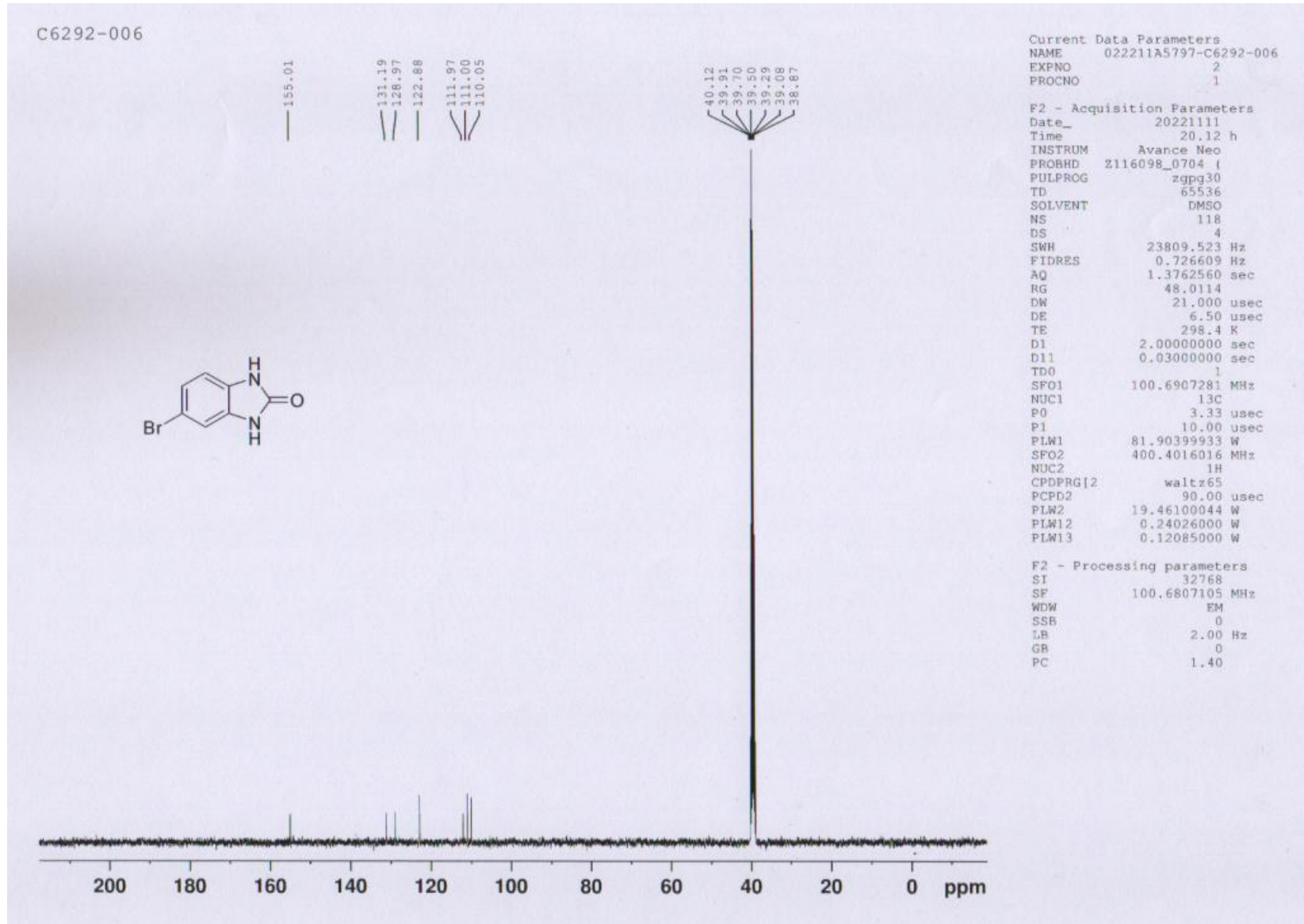
F2 - Acquisition Parameters
Date_ 20220416
Time 11.14 h
INSTRUM Avance
PROBHD 2163739_0419 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SKH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DK 61.000 usec
DE 13.89 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
SFO1 400.3224720 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 23.42200089 W

F2 - Processing parameters
SI 65536
SF 400.3200025 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

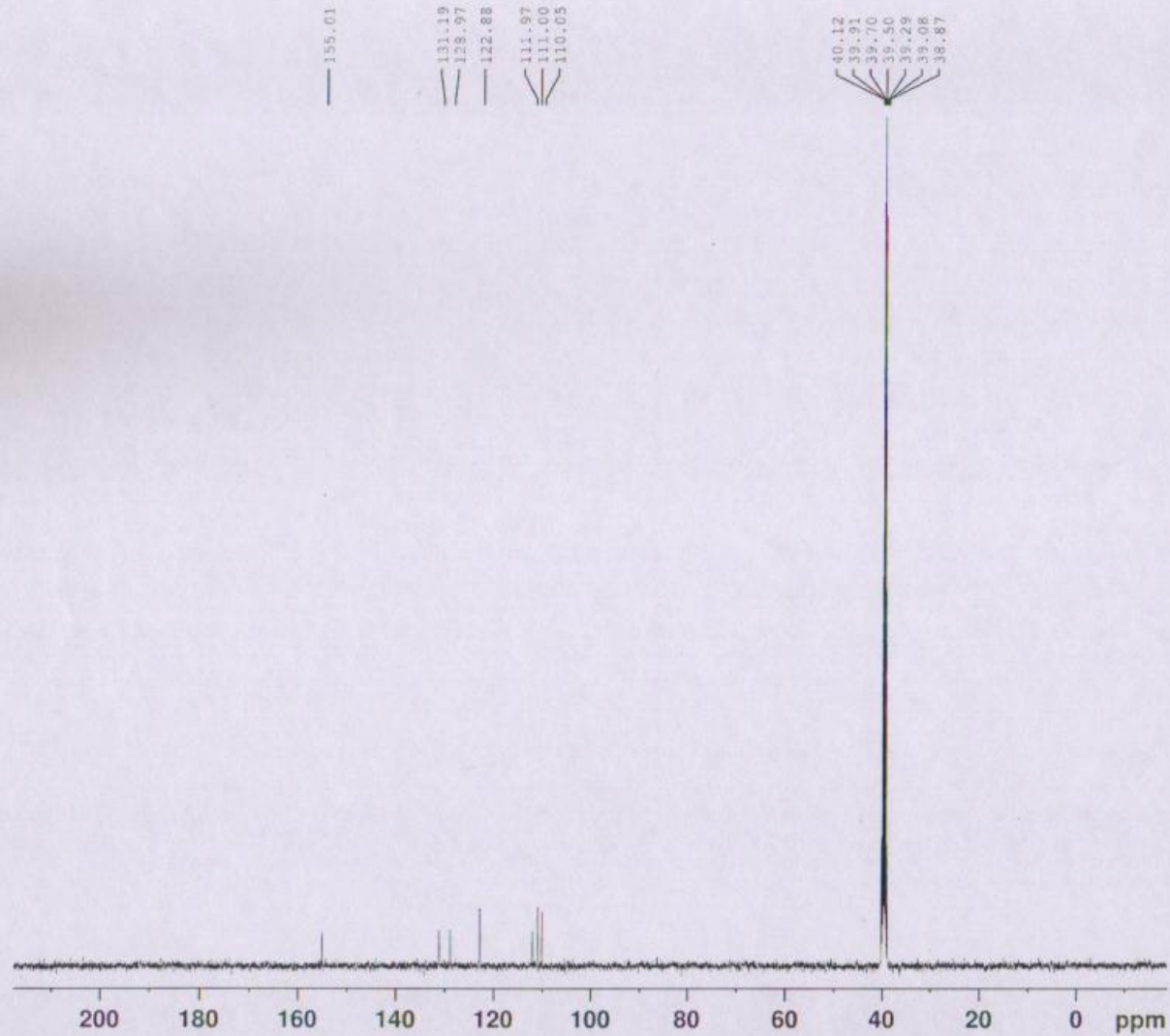


ANL-MCL3-NMR-007

¹³C NMR of 5-Bromo-1,3-dihydro-2H-benzo[d]imidazol-2-one (2c)



C6292-006

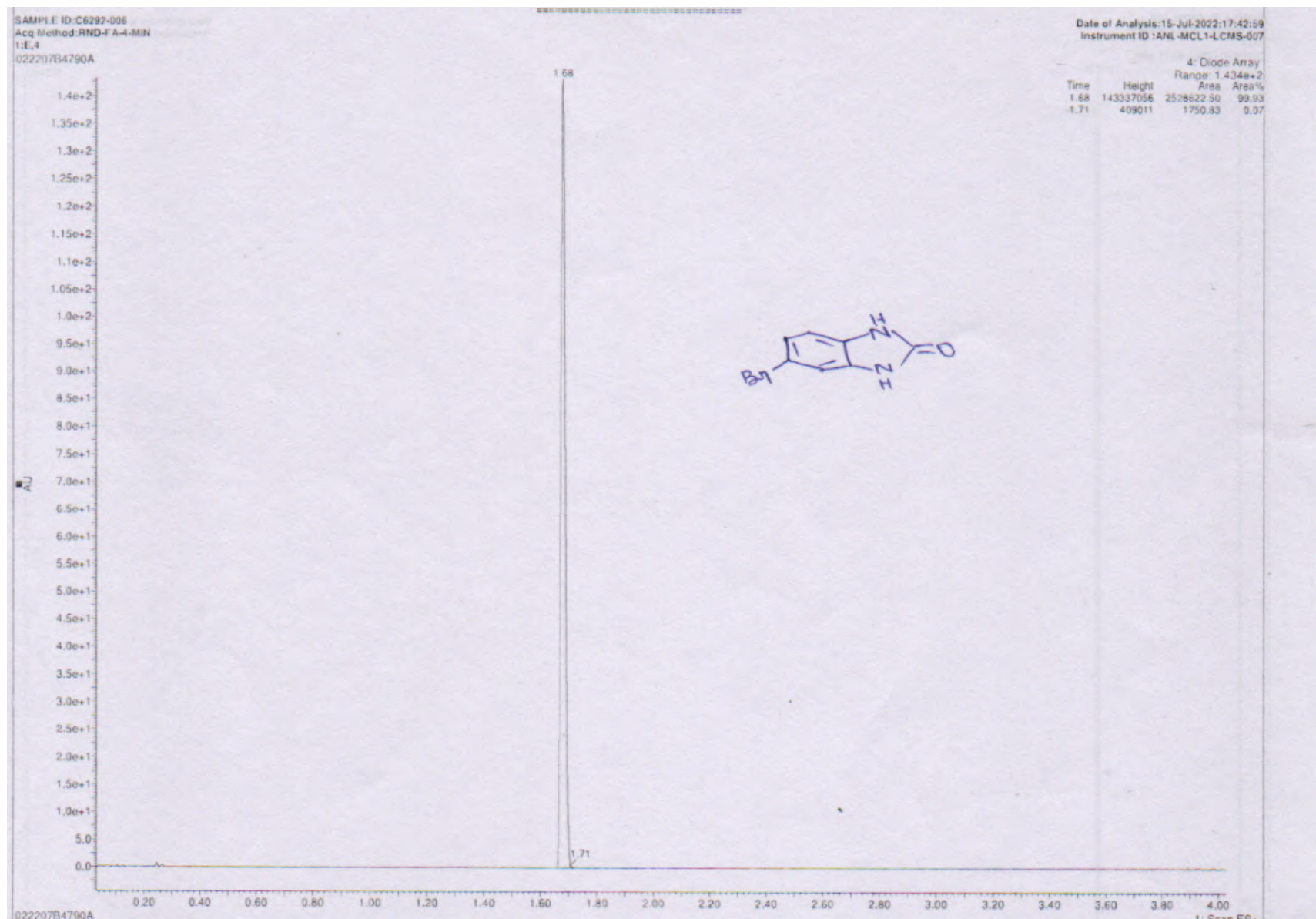


Current Data Parameters
NAME 022211A5797-C6292-006
EXPNO 2
PROCNO 1

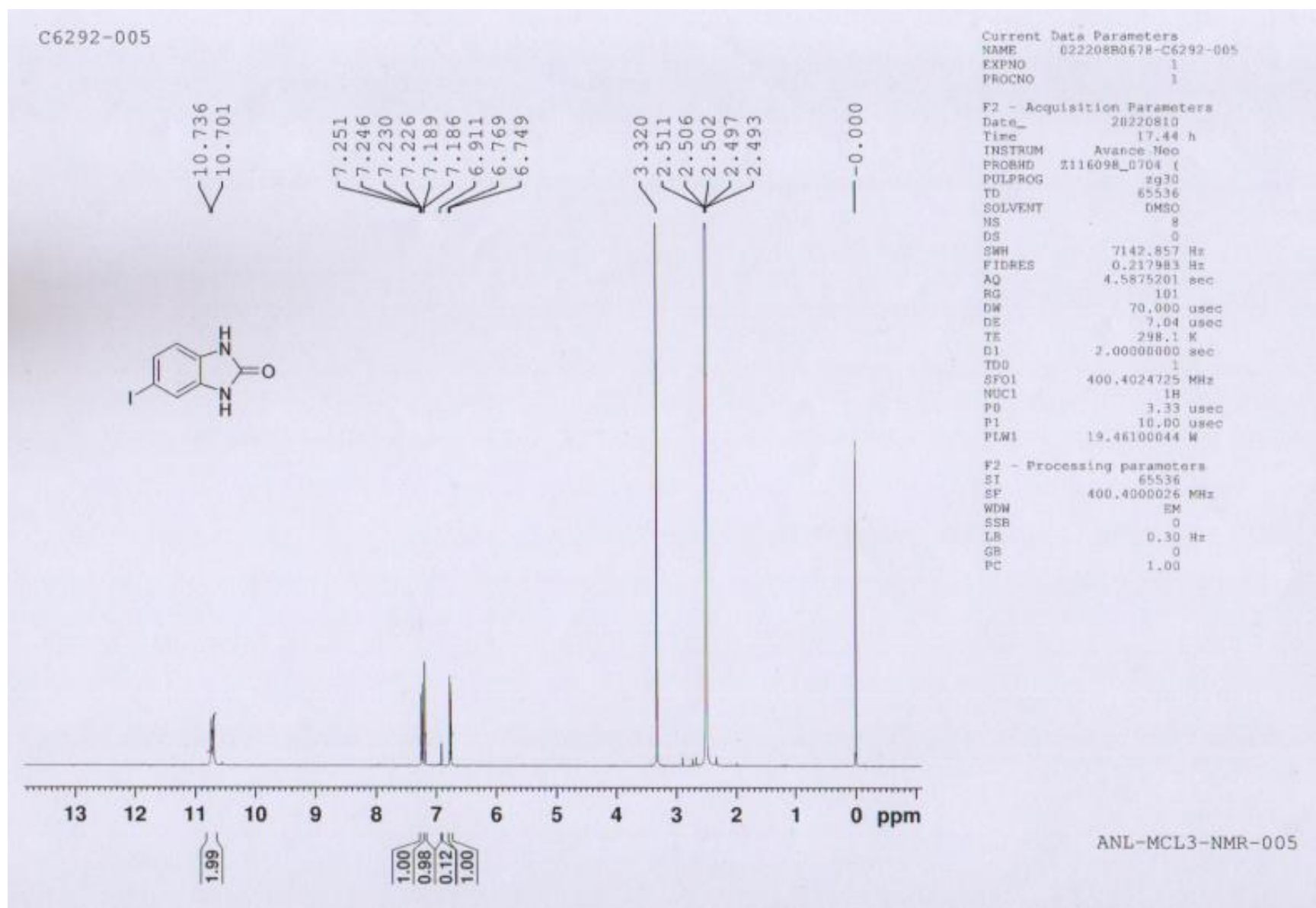
F2 - Acquisition Parameters
Date_ 20221111
Time 20.12 h
INSTRUM Avance Neo
PROBHD Z116098_0704 ()
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 118
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 48.0114
DW 21.000 usec
DE 6.50 usec
TE 298.4 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6907281 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 81.90399933 W
SFO2 400.4016016 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 19.46100044 W
PLW12 0.24026000 W
PLW13 0.12085000 W

F2 - Processing parameters
SI 32768
SF 100.6207105 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

LCMS of 5-Bromo-1,3-dihydro-2H-benzo[d]imidazol-2-one (2c)



¹H NMR of 5-Iodo-1,3-dihydro-2H-benzo[d]imidazol-2-one (2d)



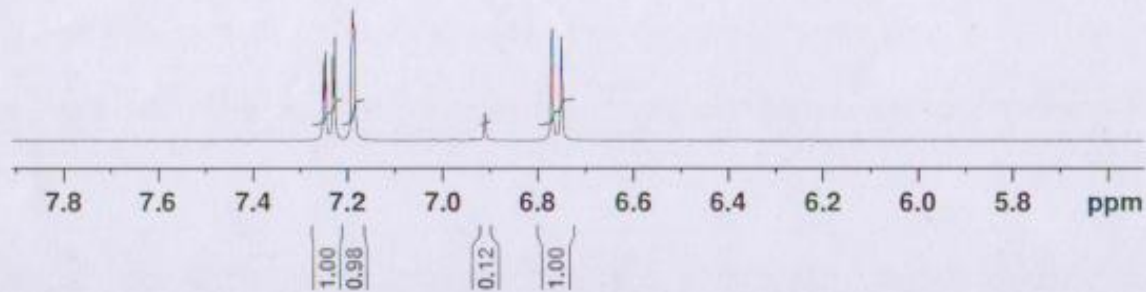
C6292-005

7.251
7.246
7.230
7.226
7.189
7.186
— 6.911
6.769
6.749

Current Data Parameters
NAME 02220880678-C6292-005
EXPNO 1
PROCNO 1

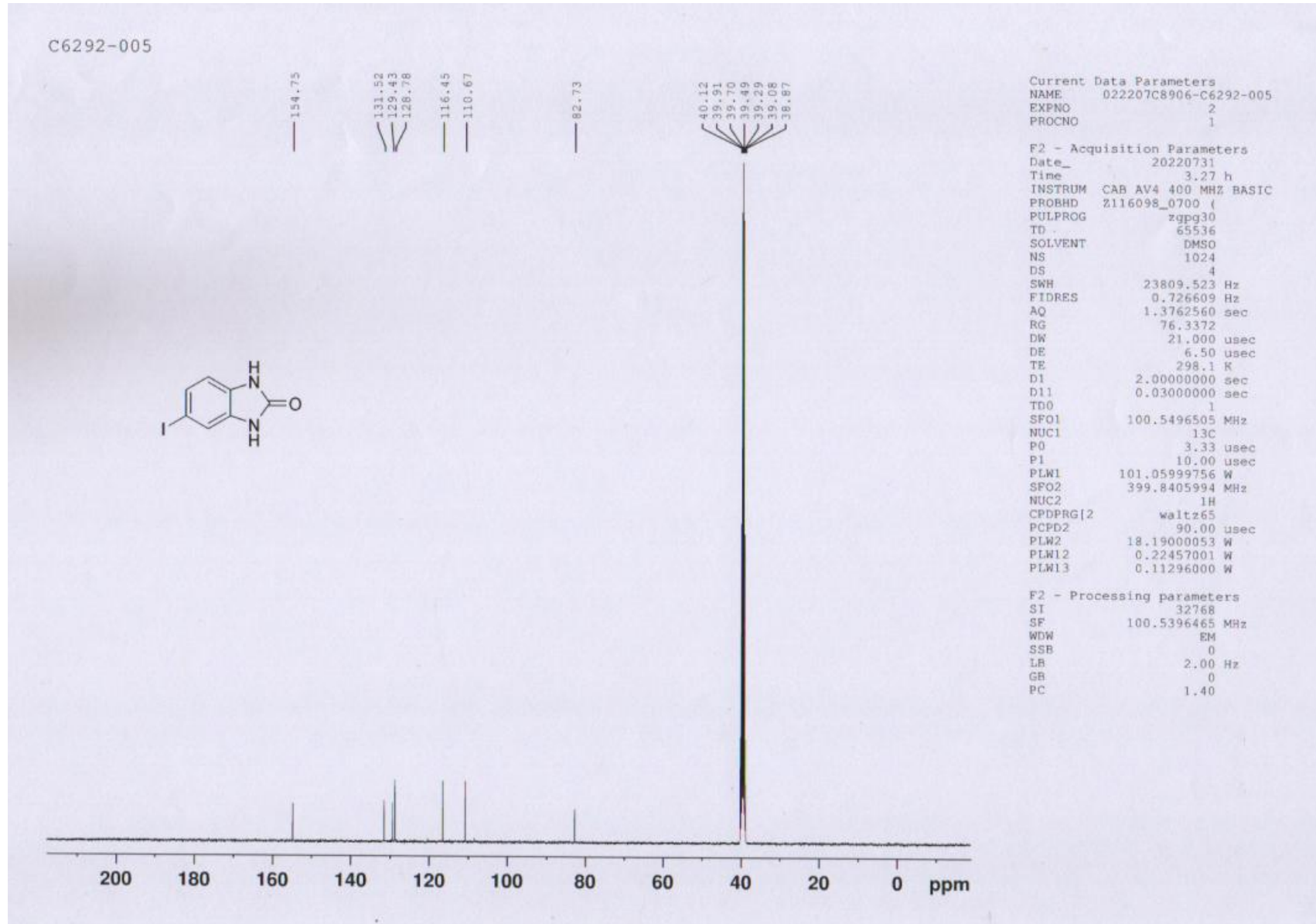
F2 - Acquisition Parameters
Date_ 20220810
Time 17.44 h
INSTRUM Avance Neo
PROBHD z116098_0704 (z)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 7142.857 Hz
FIDRES 0.217983 Hz
AQ 4.5875201 sec
RG 101
DM 70.000 usec
DE 7.04 usec
TE 298.1 K
D1 2.00000000 sec
TDO 1
SFO1 400.4024725 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLWI 19.46100044 W

F2 - Processing parameters
SI 65536
SF 400.4000026 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ANL-MCL3-NMR-005

¹³C NMR of 5-Iodo-1,3-dihydro-2H-benzo[d]imidazol-2-one (2d)



C6292-005

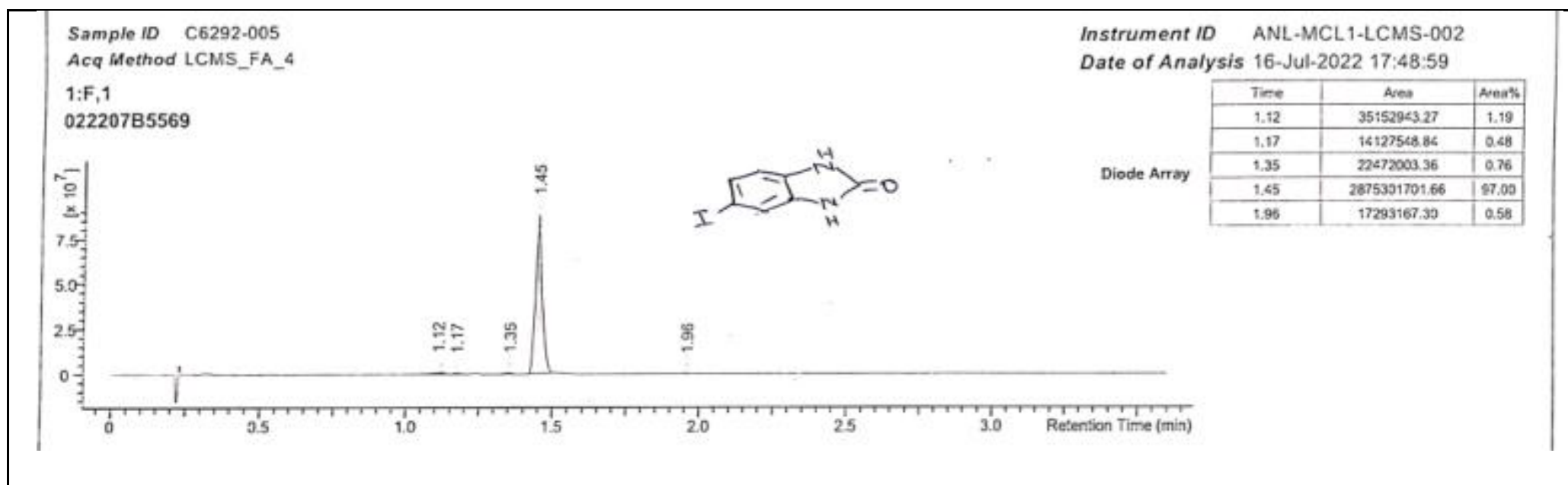


Current Data Parameters
NAME 022207C8906-C6292-005
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220731
Time 3.27 h
INSTRUM CAB AV4 400 MHZ BASIC
PROBHD Z116098_0700 ()
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 76.3372
DW 21.000 usec
DE 6.50 usec
TE 298.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.5496505 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 101.05999756 W
SFO2 399.8405994 MHz
NUC2 1H
CPDPRG2 waltz65
PCPD2 90.00 usec
PLW2 18.19000053 W
PLW12 0.22457001 W
PLW13 0.11296000 W

F2 - Processing parameters
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SF 100.5396465 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

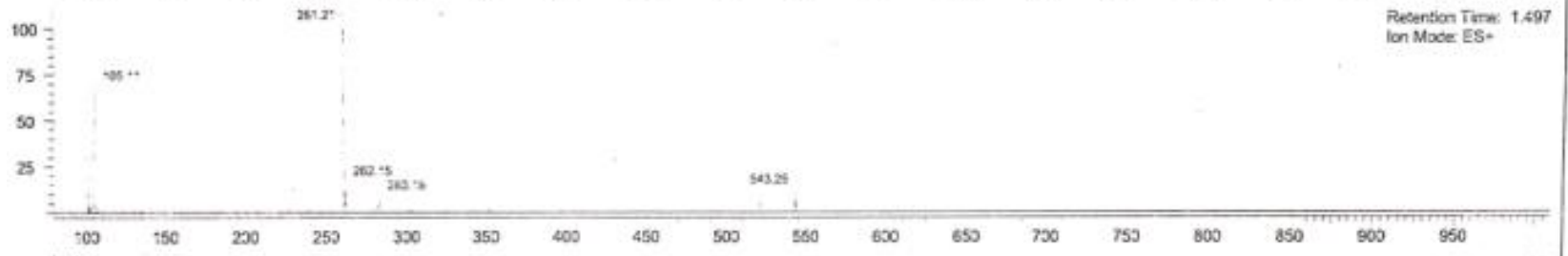
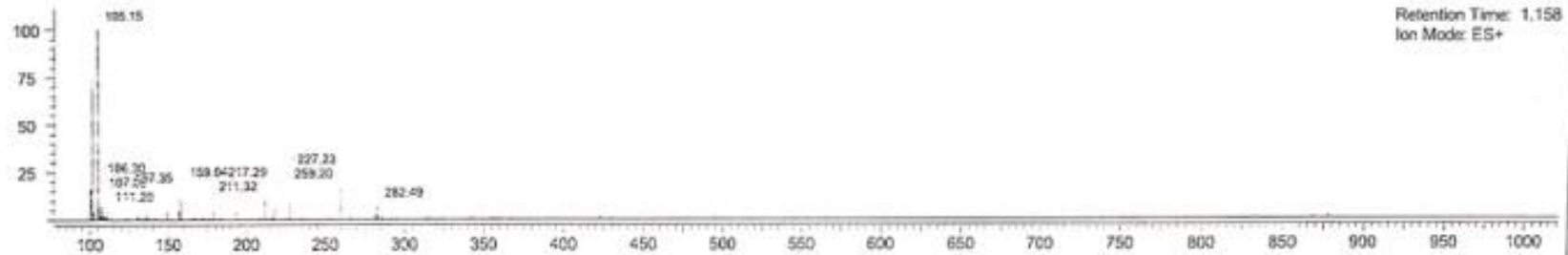
LCMS of 5-Iodo-1,3-dihydro-2H-benzo[d]imidazol-2-one (2d)



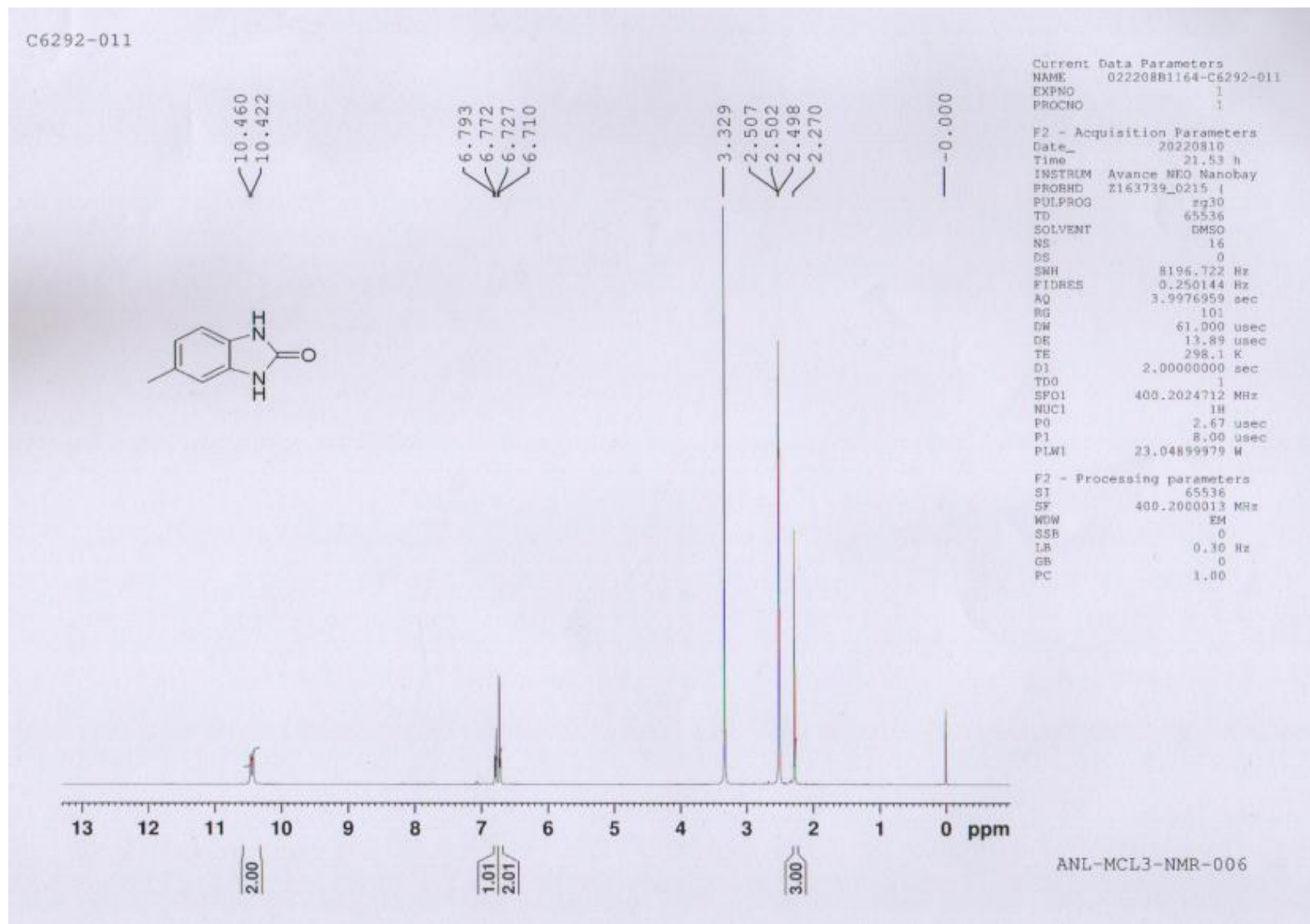
Sample ID C6292-005
Acq Method LCMS_FA_4
1:F,1
022207B5569

Discovery Chemistry – Analytical Services

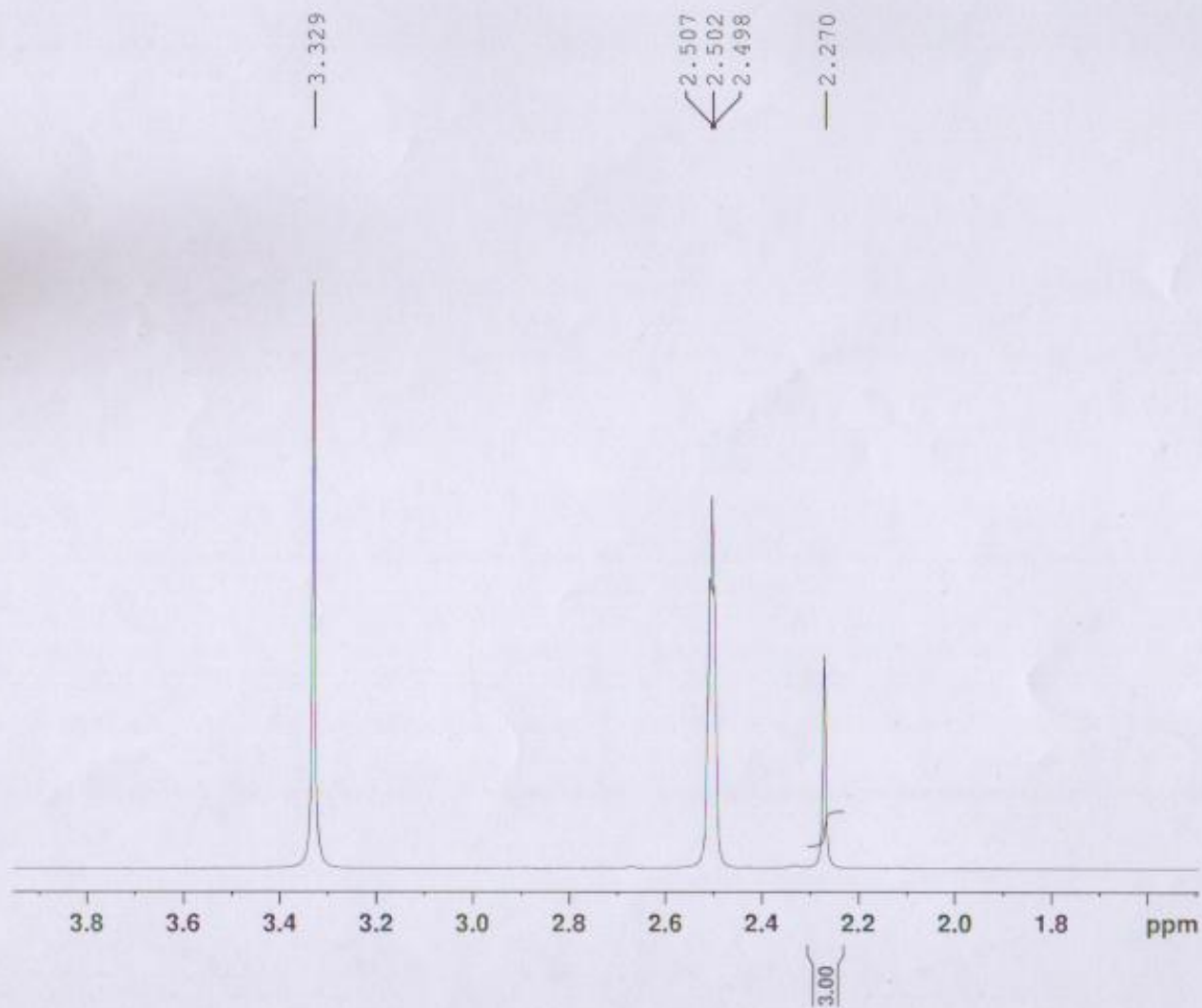
Instrument ID ANL-MCL1-LCMS-002
Date of Analysis 16-Jul-2022 17:48:59



¹H NMR of 5-Methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (2e)



C6292-011



Current Data Parameters
NAME 022208B1164-C6292-011
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220810
Time 21.53 h
INSTRUM Avance NEO Nanobay
PROBHD Z163739_0215 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.1 K
D1 2.00000000 sec
TDO 1
SFO1 400.2024712 MHz
NUC1 1H
P0 2.57 usec
P1 8.00 usec
PLM1 23.04899979 W

F2 - Processing parameters
SI 65536
SF 400.2000013 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ANL-MCL3-NMR-006

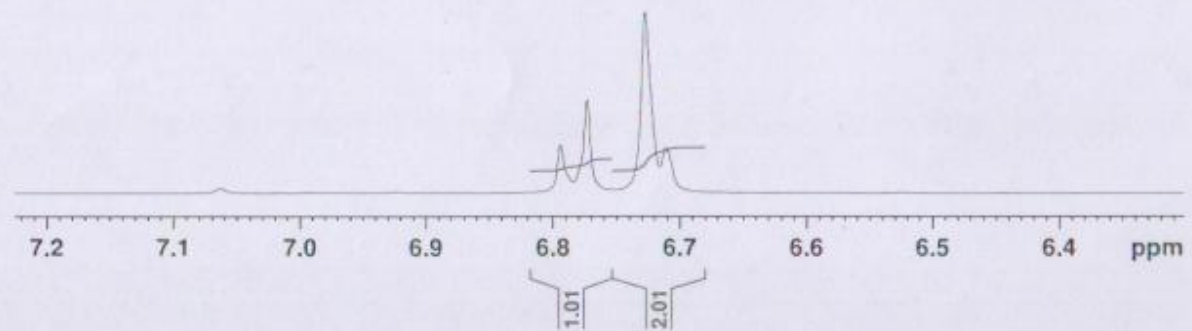
C6292-011

— 6.793
— 6.772
— 6.727
— 6.710

Current Data Parameters
NAME 022206B1164-C6292-011
EXPNO 1
PROCNO 1

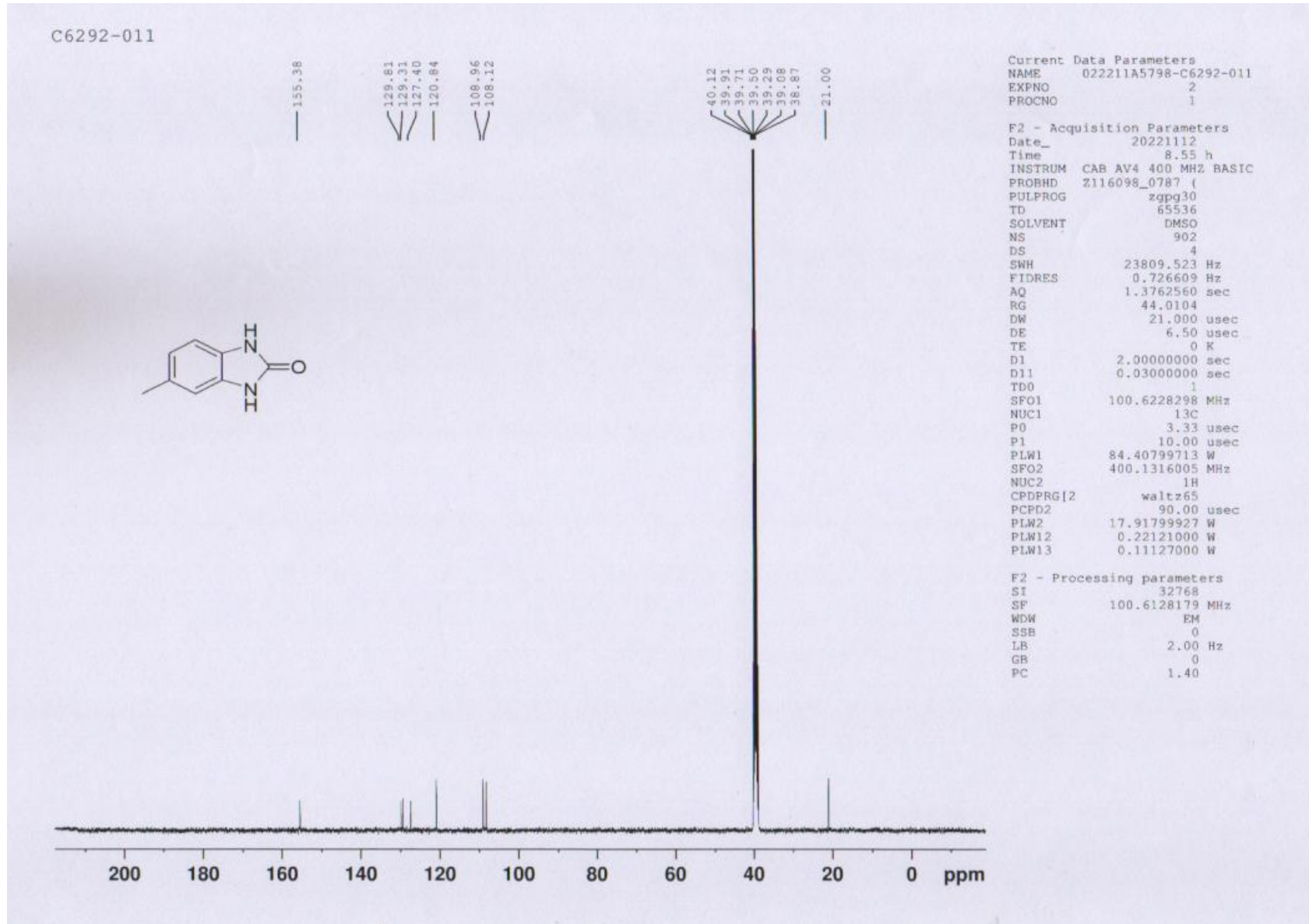
F2 - Acquisition Parameters
Date_ 20220810
Time 21.53 h
INSTRUM Avance NEO Nanobay
PROBHD Z163739_0215 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.1 K
D1 2.00000000 sec
TDO 1
SFO1 400.2024712 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 23.04899979 W

F2 - Processing parameters
SI 65536
SF 400.2000013 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

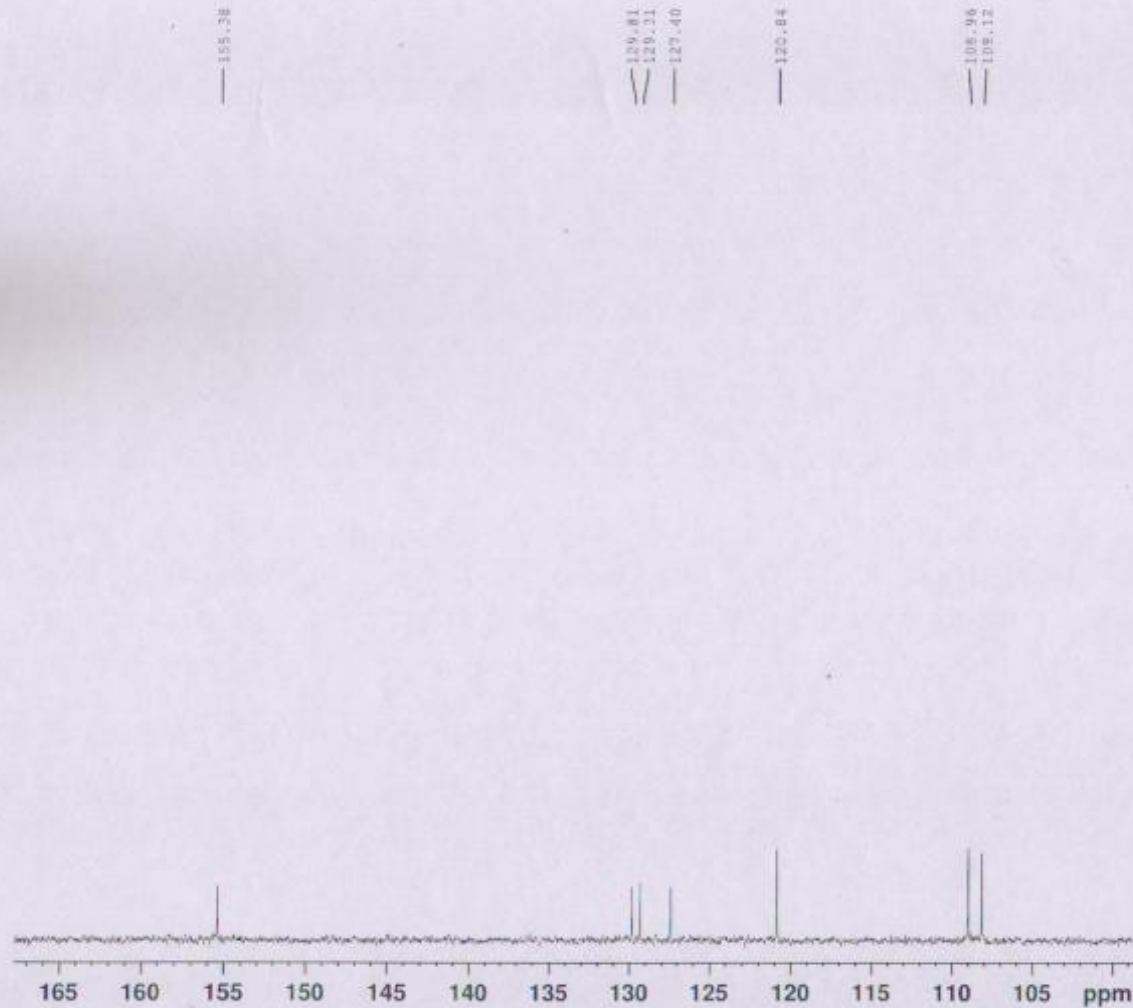


ANL-MCL3-NMR-006

¹³C NMR of 5-Methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (2e)



C6292-011

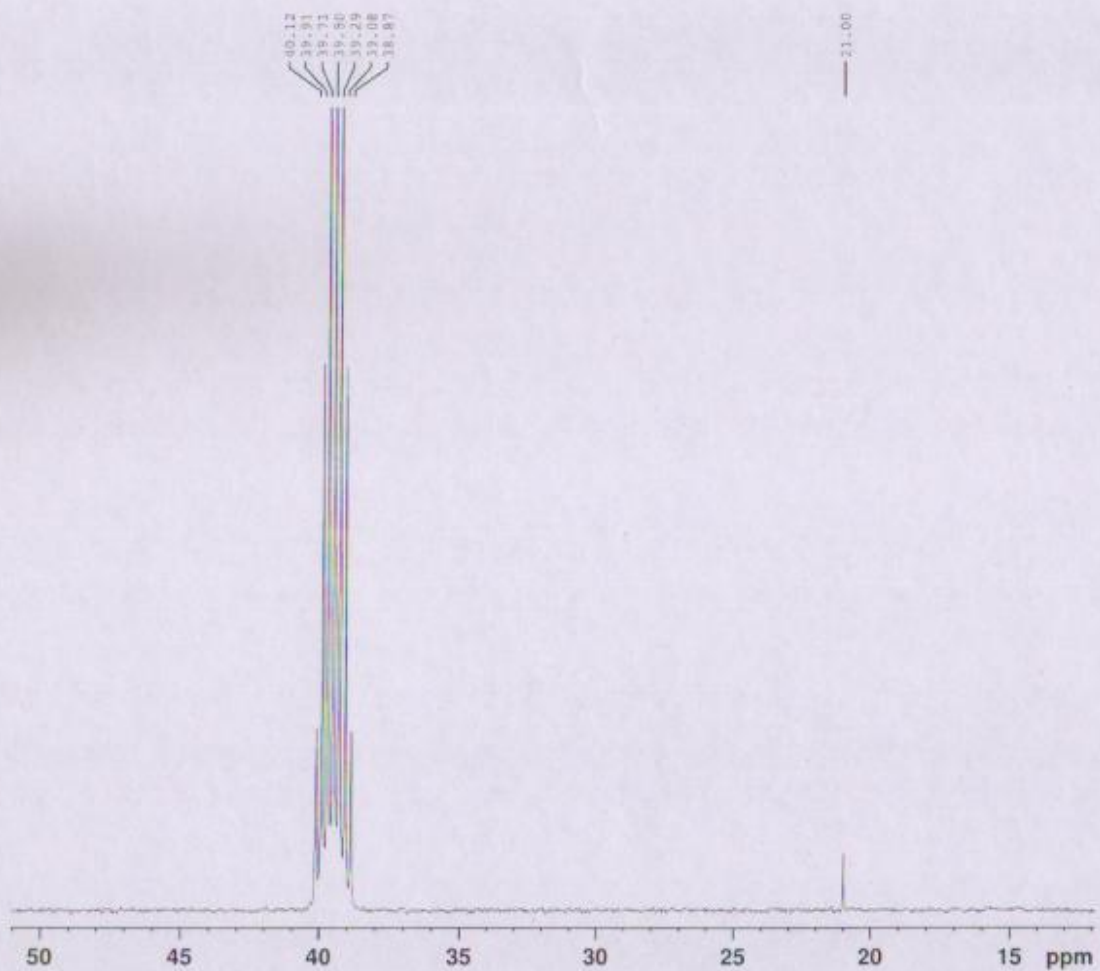


Current Data Parameters
NAME 012211A5798-C6292-011
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221112
Time 8.55 h
INSTRUM CAS AV4 400 MHz BASIC
PROBHD Z116098_0787 (1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 902
DS 4
SWH 21809.521 Hz
FIDRES 0.724609 Hz
AQ 1.3762560 sec
RG 44.0104
DW 21.000 usec
DE 6.50 usec
TE 300 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 84.40799713 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG12 waltz65
PCPD2 90.00 usec
PLW2 17.91799927 W
PLW12 0.22121000 W
PLW13 0.11127000 W

F2 - Processing parameters
SI 32768
SF 100.6128179 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

C6292-011



Current Data Parameters
NAME 012211A5798-c6292-011
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221112
Time 8.55 h
INSTRUM CAB AV4 400 MHz BASIC
PROBHD Z116098_0787 f
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 902
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 44.0104
DW 21.000 usec
DE 6.50 usec
TE C K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 84.40799713 W
SFO2 400.1316005 MHz
NUC2 1H
CFDPRG(2) waltz65
PCPD2 90.00 usec
PLW2 17.91799927 W
PLW12 0.22121000 W
PLW13 0.11127000 W

F2 - Processing parameters
SI 32768
SF 100.6128179 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

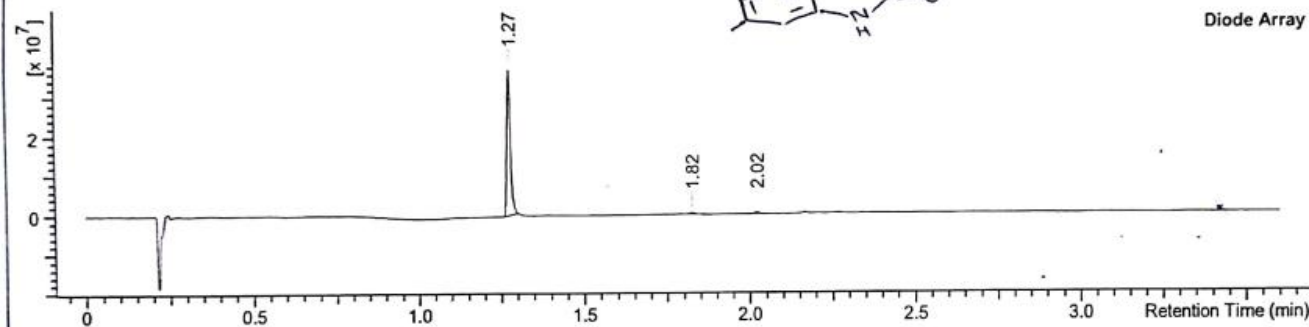
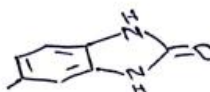
LCMS of 5-Methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (2e)

Sample ID C6292-011
Acq Method LCMS_FA_4
1:E,1
022207B4793

Instrument ID ANL-MCL3-LCMS-011
Date of Analysis 15-Jul-2022 17:43:43

Time	Area	Area%
1.27	600686468.86	94.37
1.82	23197185.74	3.64
2.02	12645678.90	1.99

Diode Array



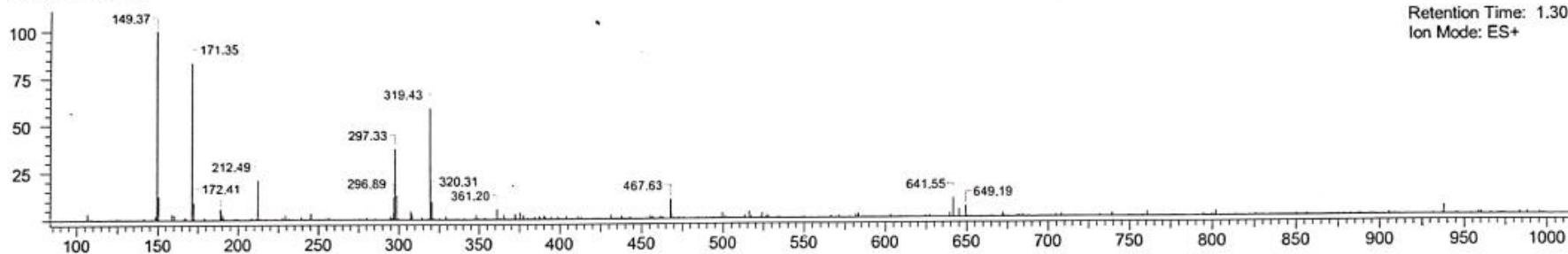
Sample ID C6292-011
Acq Method LCMS_FA_4

Discovery Chemistry – Analytical Services

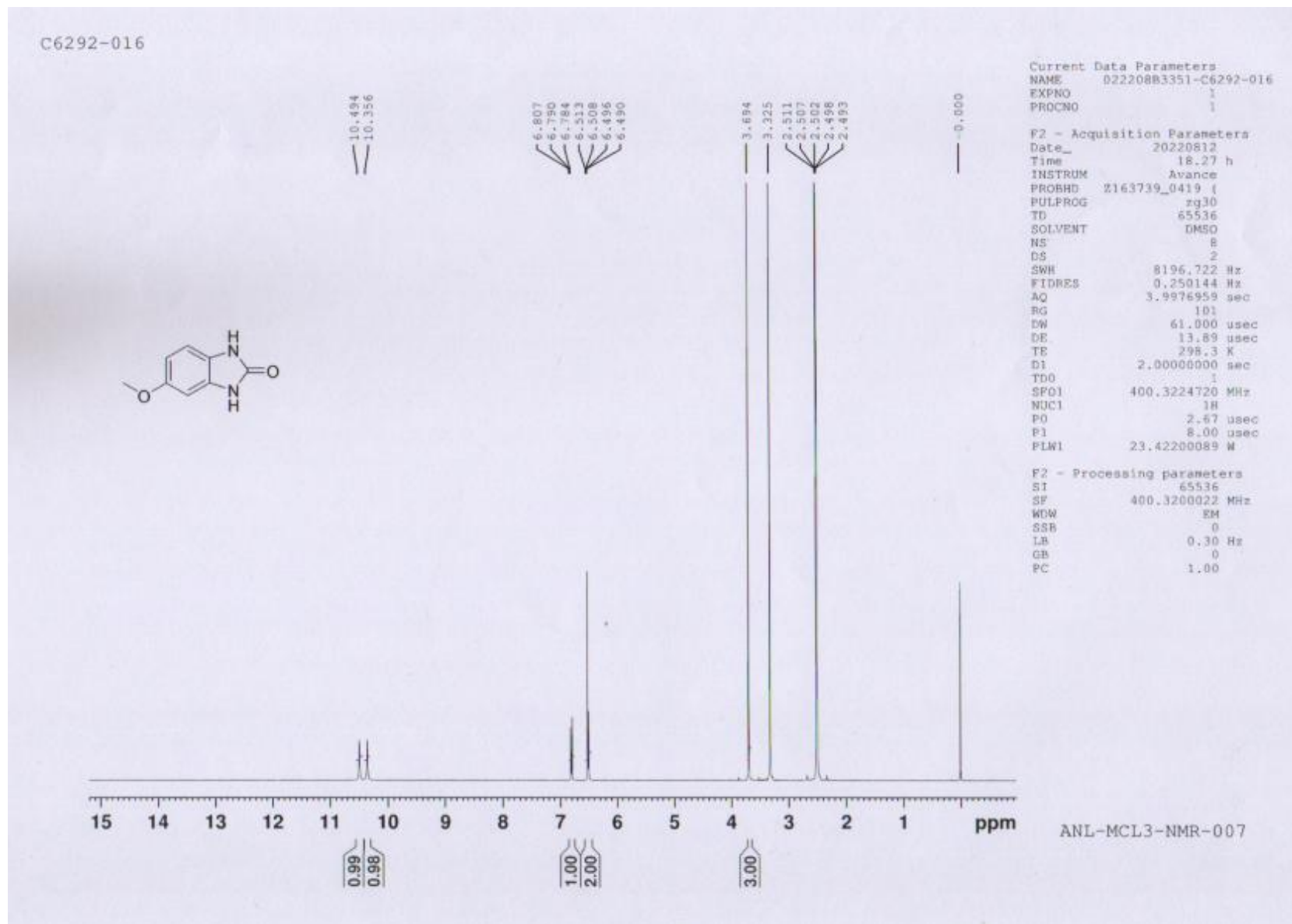
Instrument ID ANL-MCL3-LCMS-011
Date of Analysis 15-Jul-2022 17:43:43

1:E,1
022207B4793

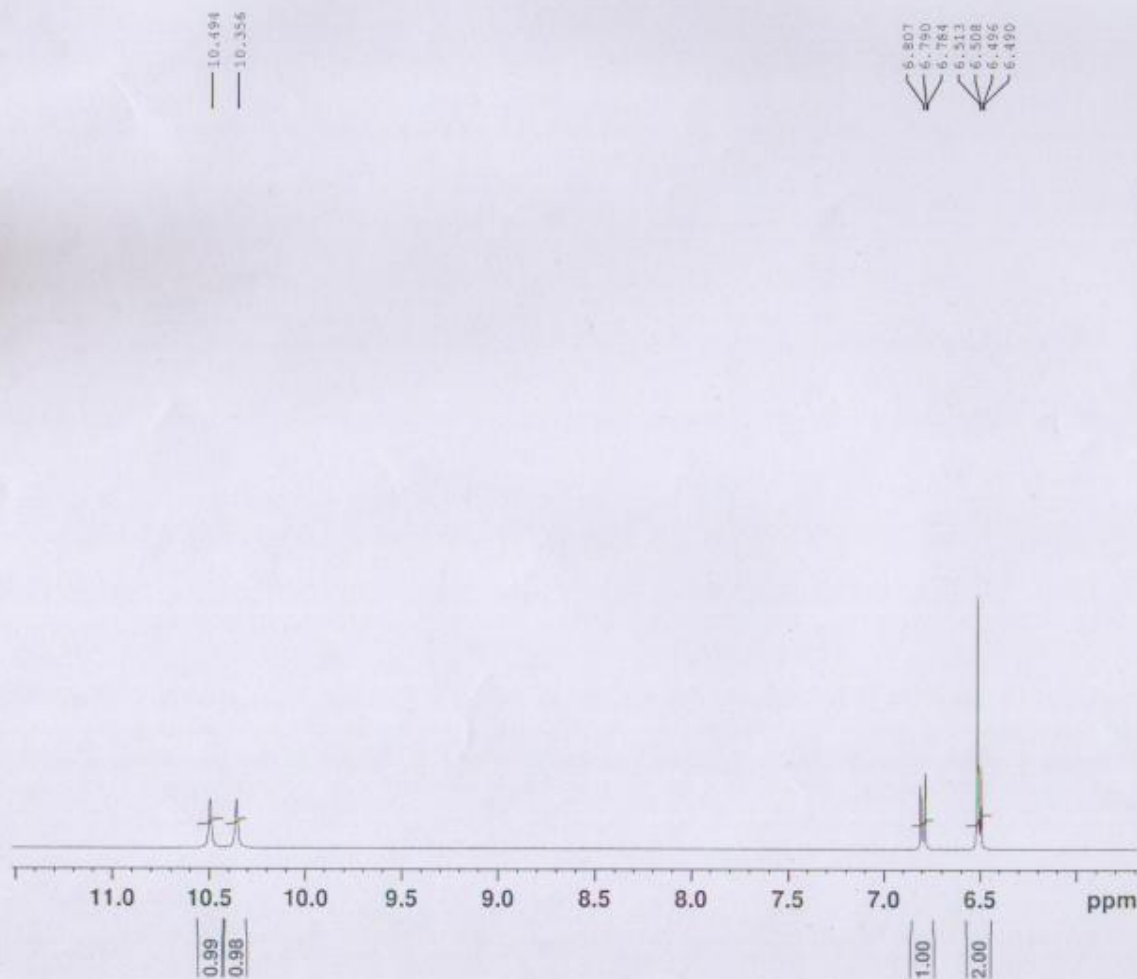
Retention Time: 1.307
Ion Mode: ES+



¹H NMR of 5-Methoxy-1,3-dihydro-2H-benzo[d]imidazol-2-one (2f)



C6292-016



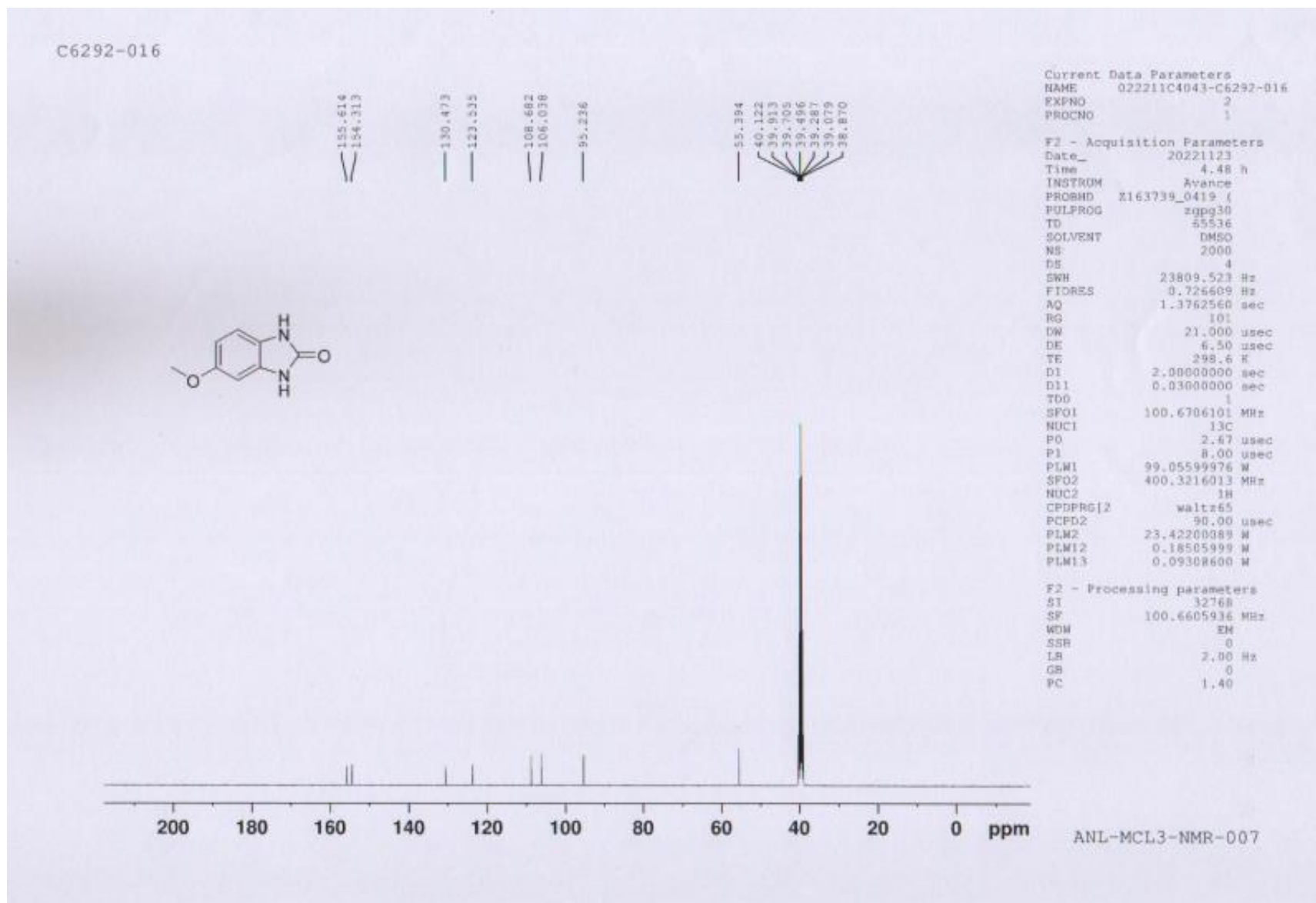
Current Data Parameters
NAME 022208B3351-C6292-016
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220812
Time 18.27 h
INSTRUM Avance
PROBHD Z163739_0419 1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
CW 61.000 usec
DE 13.89 usec
TE 298.3 K
D1 2.0000000 sec
TDO 1
SFO1 400.3224720 MHz
NUC1 1H
PO 2.67 usec
P1 8.00 usec
PLW1 23.42200089 W

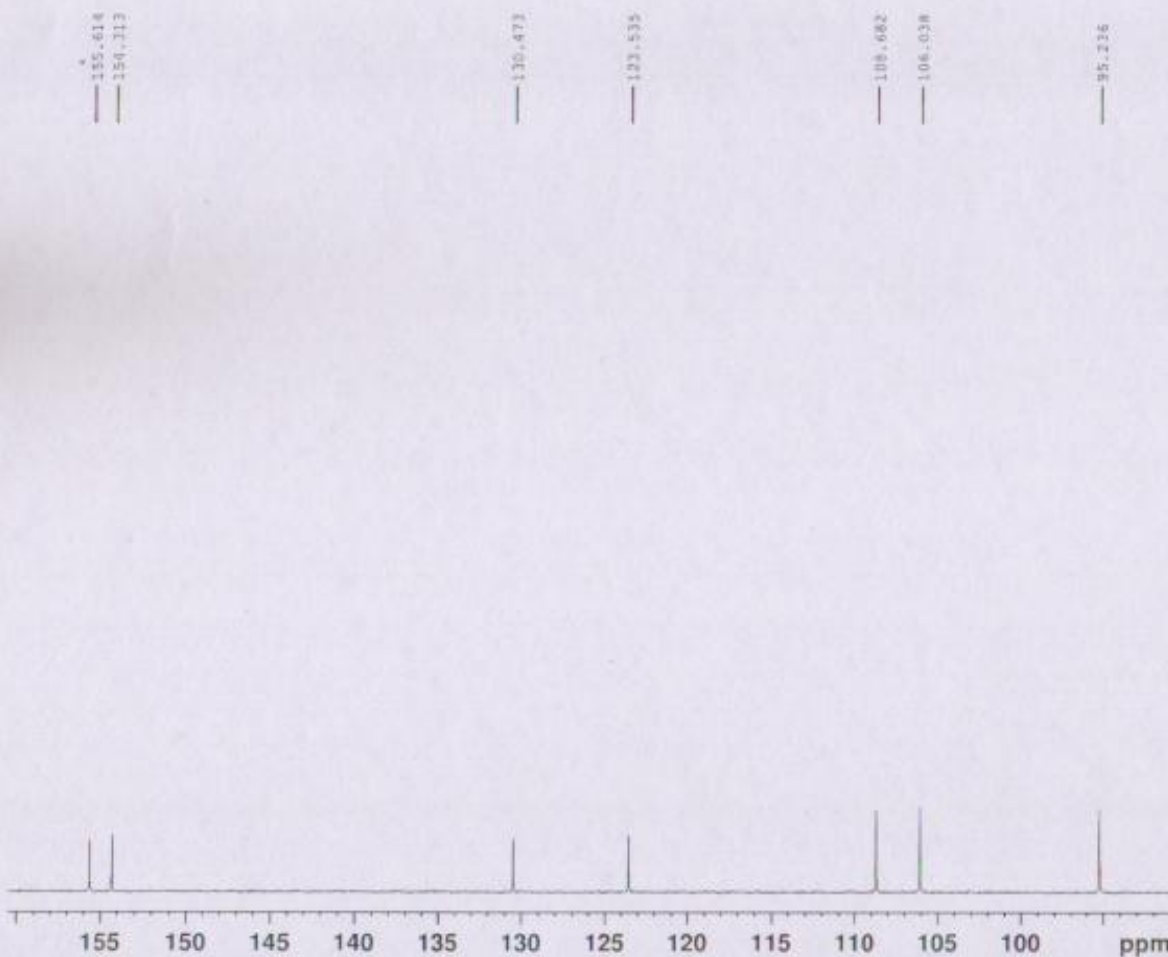
F2 - Processing parameters
SI 65536
SF 400.3200022 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ANL-MCL3-NMR-007

13C NMR of 5-Methoxy-1,3-dihydro-2H-benzo[d]imidazol-2-one (2f)



C6292-016



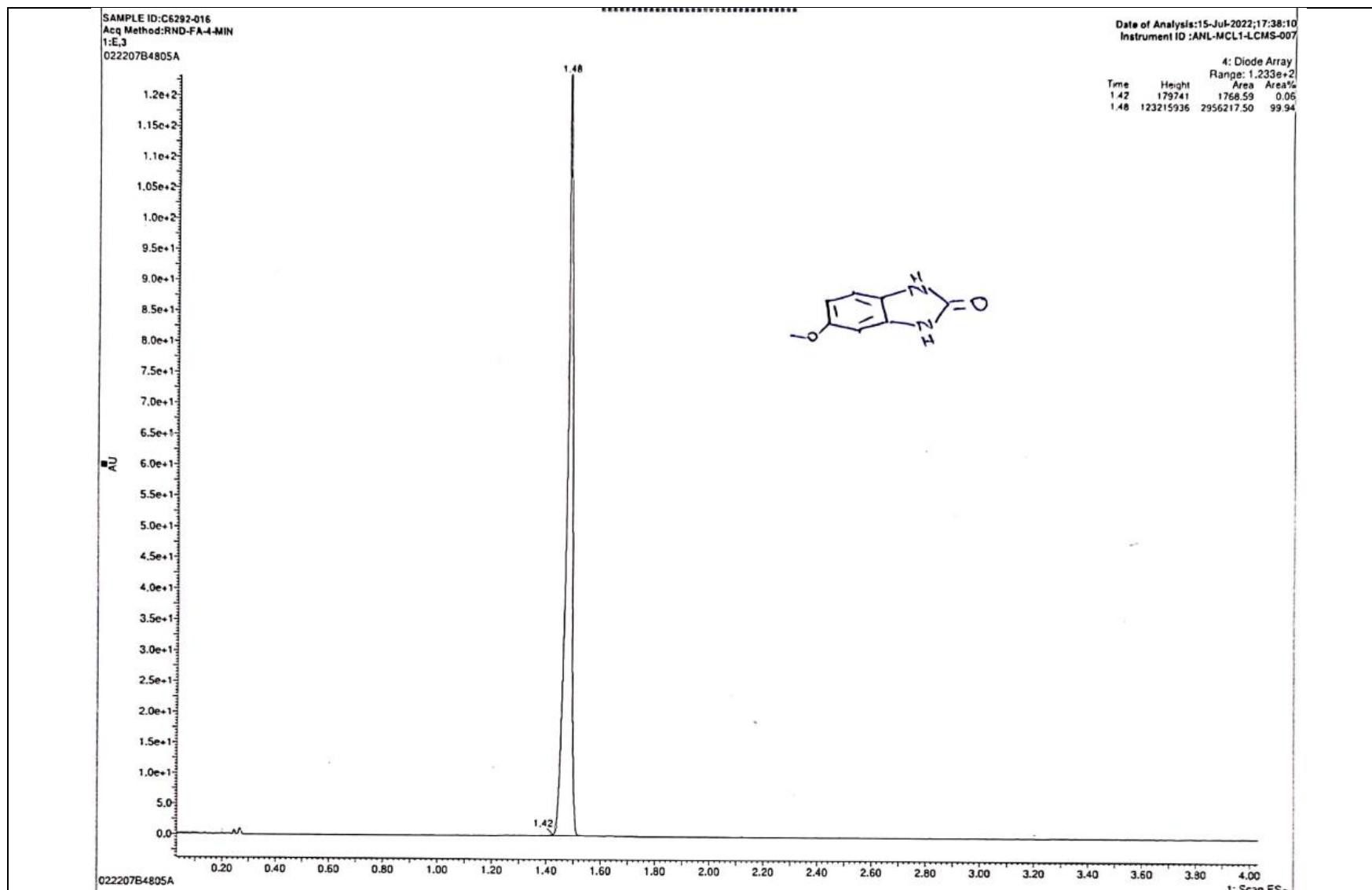
Current Data Parameters
NAME 022211C4043-C6292-016
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221123
Time 4.48 h
INSTRUM Avance
PROBHD Z163739_0419 1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DM 21.000 usec
DE 6.50 usec
TE 298.6 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6706101 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 99.05599976 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG12 waltz65
PCPD2 90.00 usec
PLW2 23.42200089 W
PLW12 0.10505999 W
PLW13 0.09308660 W

F2 - Processing parameters
SI 32768
SF 100.6605936 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

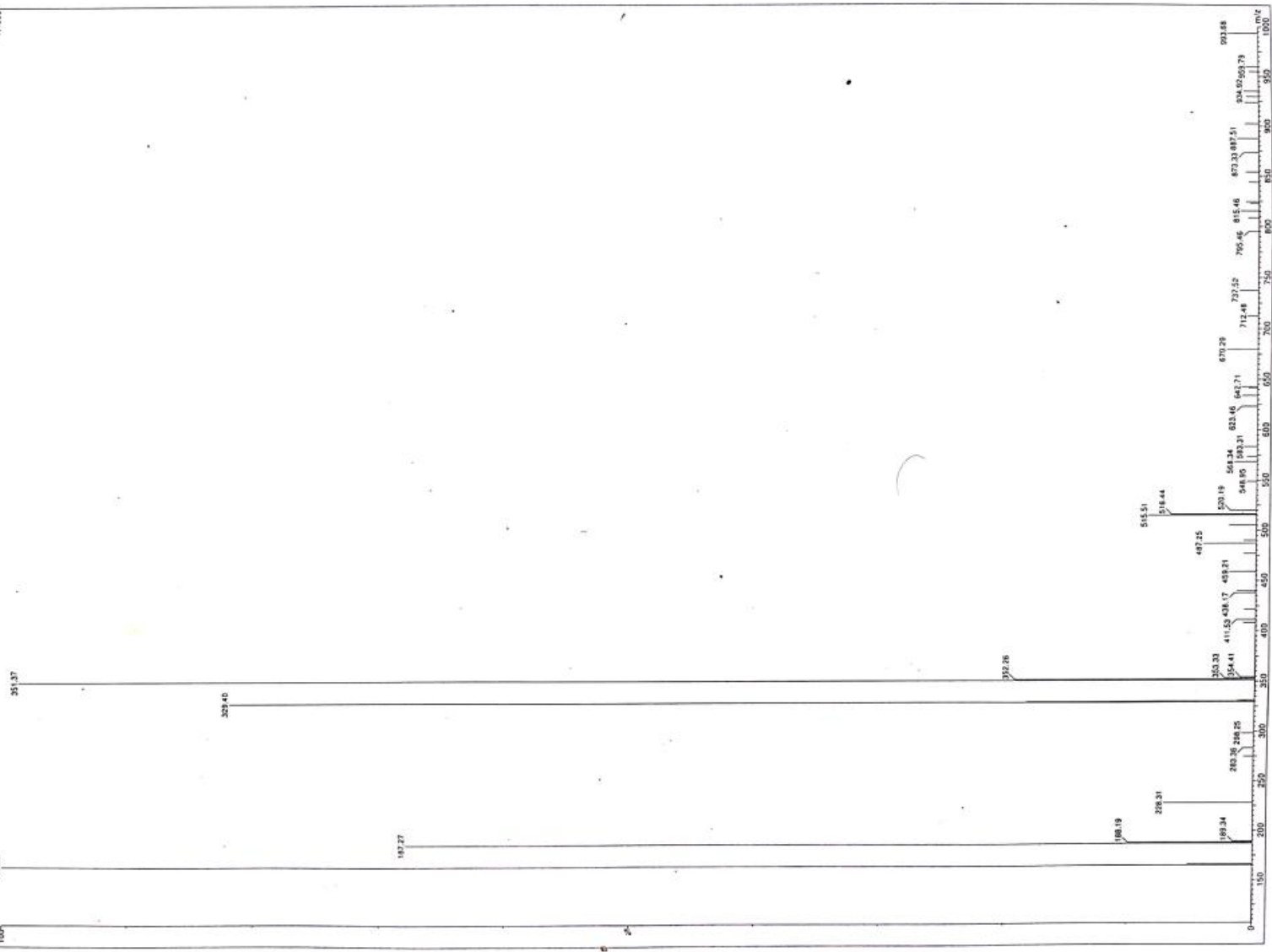
ANL-MCL3-NMR-007

LCMS of 5-Methoxy-1,3-dihydro-2H-benzo[d]imidazol-2-one (2f)

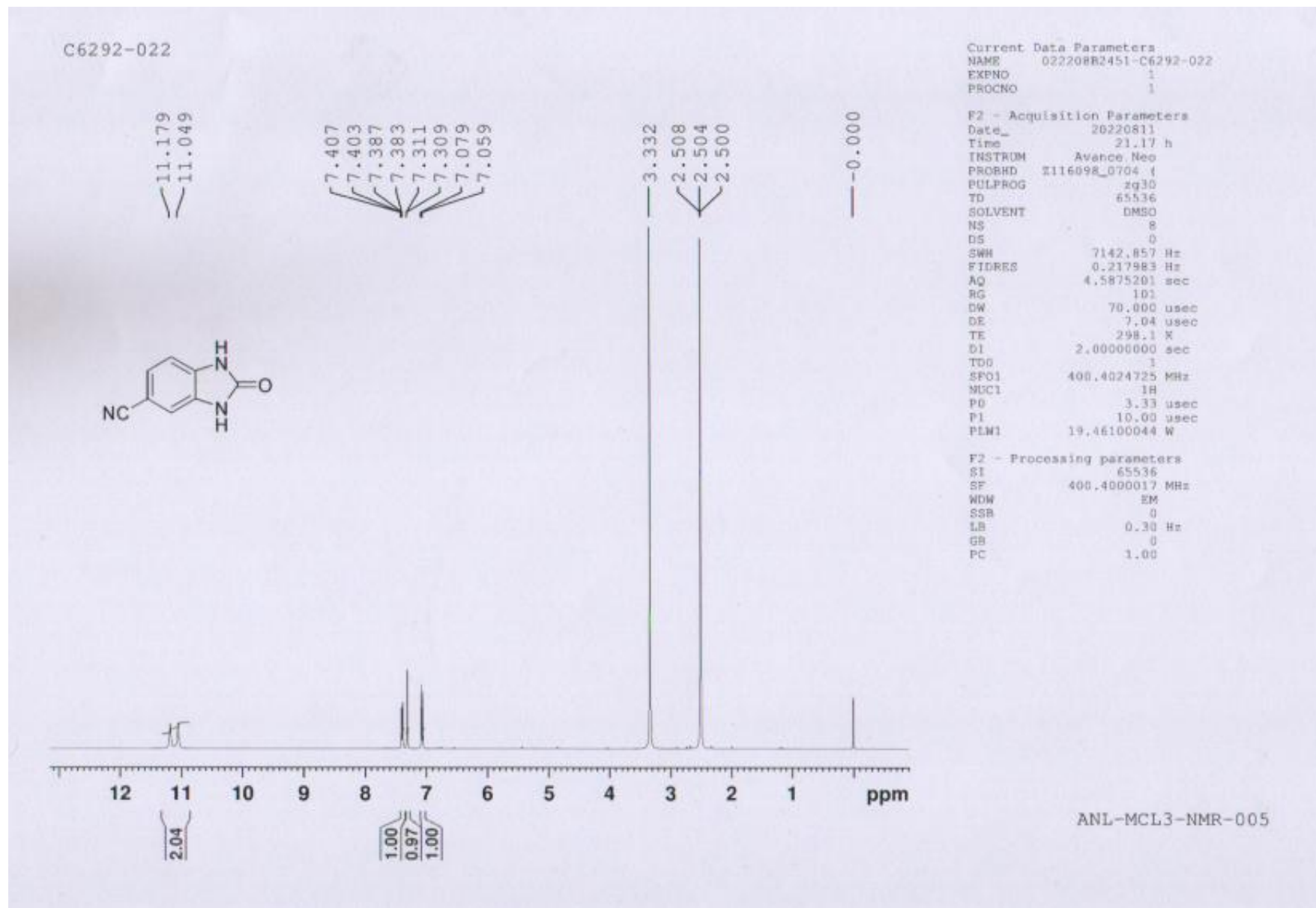


SAMPLE ID: 62327-016
Acq Method: JMW-P1-A1-1N
10/22/2016 05:58:11 (GMT)
163.26

Date of Analysis: 16-10-2016 05:58:11
Instrument ID: JMW-P1-A1-1N



¹H NMR of 2-Oxo-2,3-dihydro-1H-benzo[d]imidazole-5-carbonitrile (2g)



C6292-022

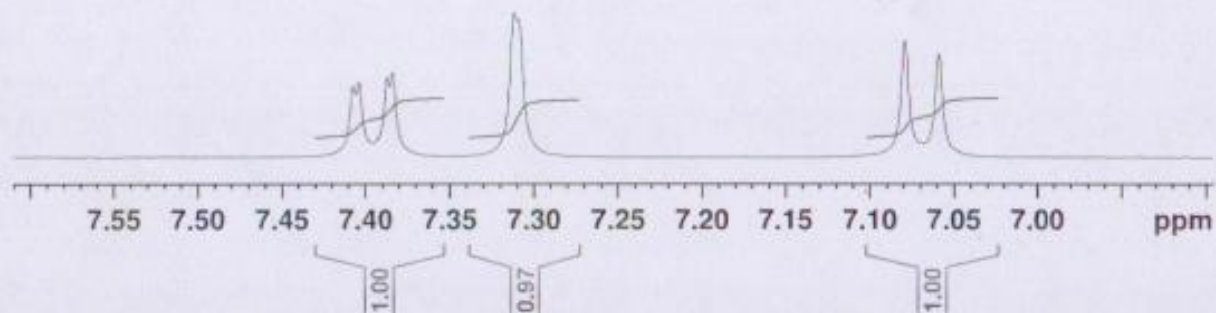
7.407
7.403
7.387
7.383
7.311
7.309

7.079
7.059

Current Data Parameters
NAME 022208B2451-C6292-022
EXPNO 1
PROCNO 1

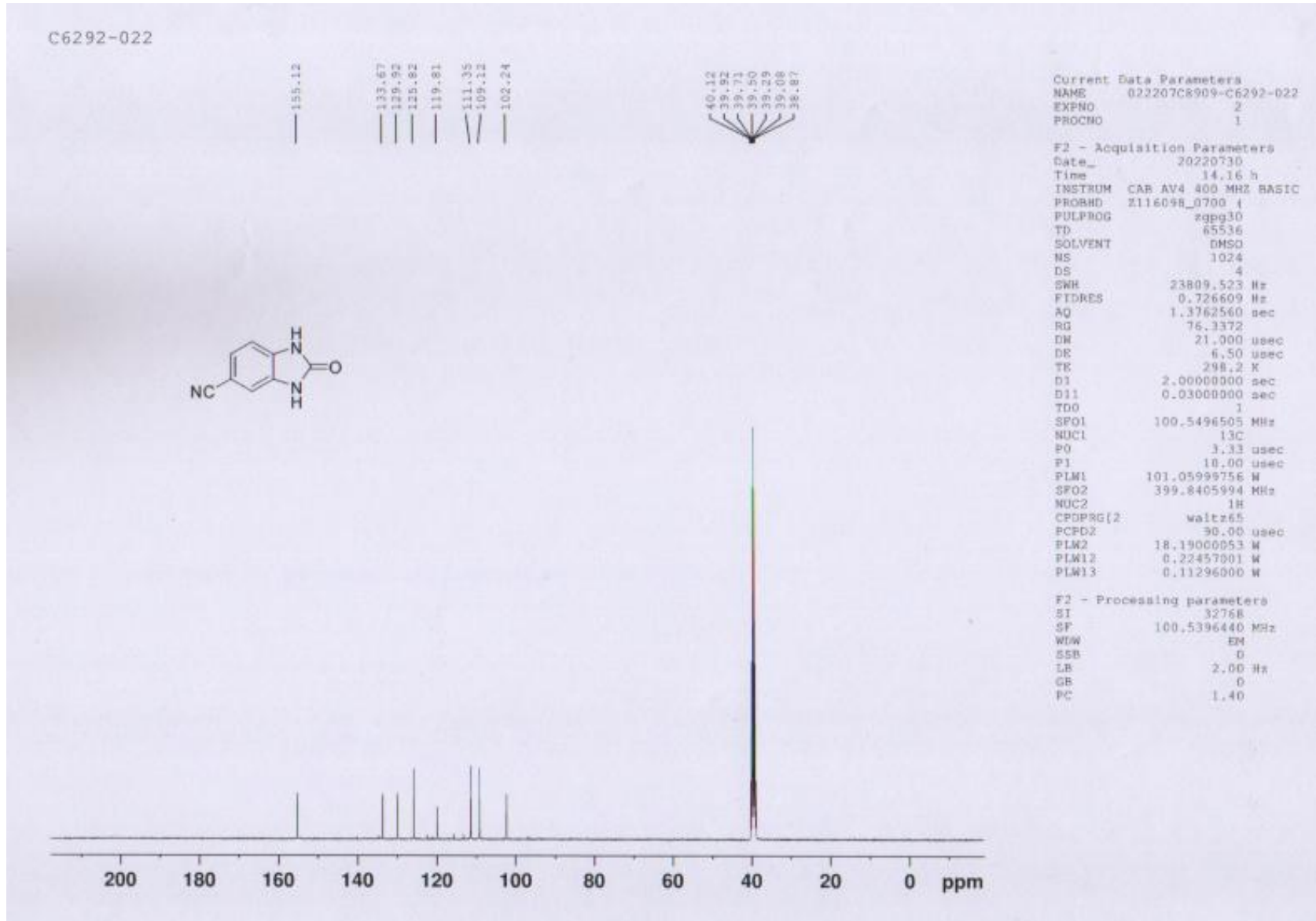
F2 - Acquisition Parameters
Date_ 20220811
Time 21.17 h
INSTRUM Avance Neo
PROBHD B116095_0704 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 7142.857 Hz
FIDRES 0.217983 Hz
AQ 4.5875201 sec
RG 101
DW 70.000 usec
DE 7.04 usec
TE 298.1 K
D1 2.00000000 sec
TDO 1
SFO1 400.4024725 MHz
NUC1 1H
PC 3.33 usec
F1 10.00 usec
PLW1 19.46100044 W

F2 - Processing parameters
SI 65536
SF 400.4000017 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ANL-MCL3-NMR-005

¹³C NMR of 2-Oxo-2,3-dihydro-1H-benzo[d]imidazole-5-carbonitrile (2g)



C6292-022

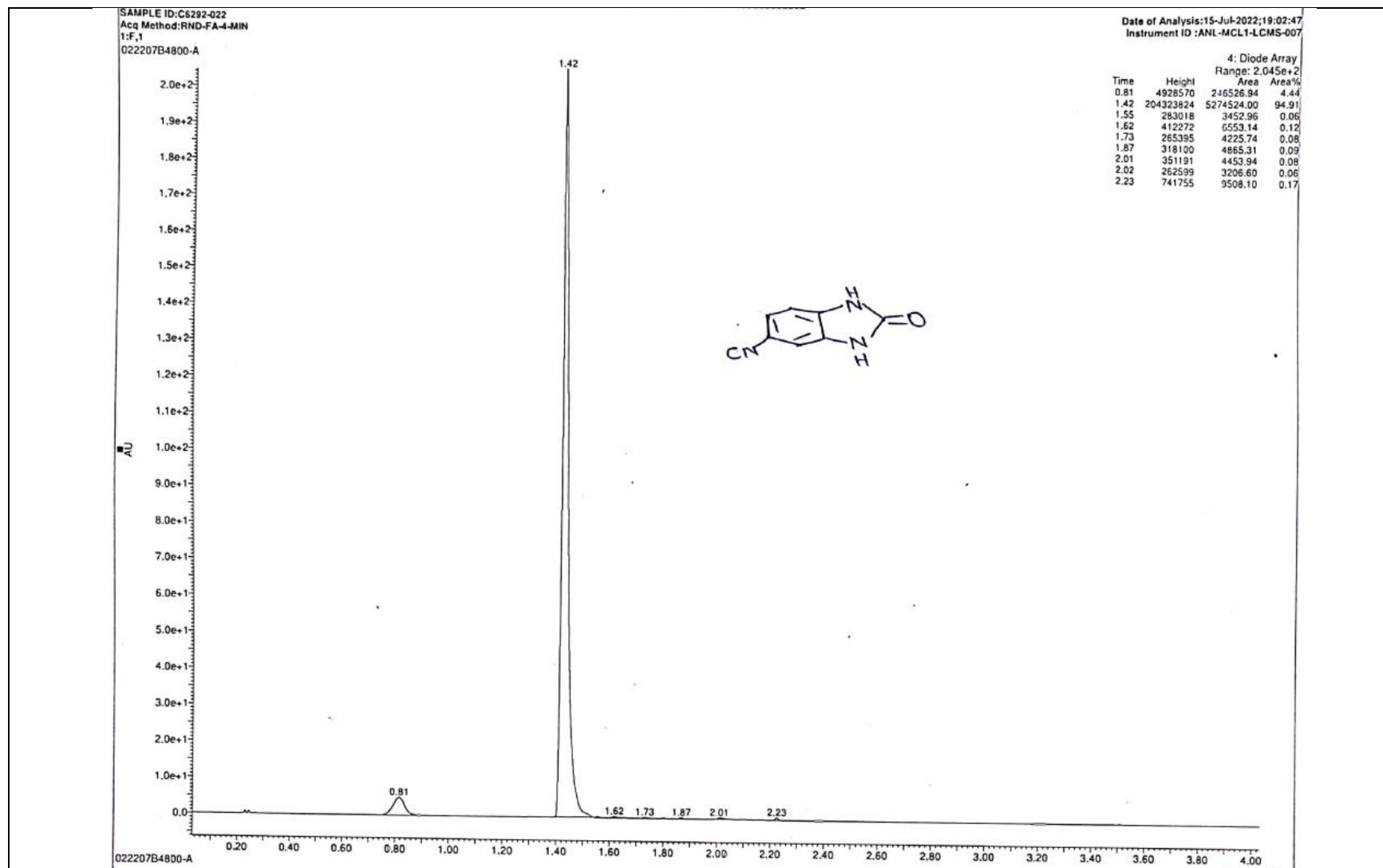


Current Data Parameters
NAME 822207C8909-C6292-022
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220730
Time 14.16 h
INSTRUM CAS AV4 400 MHZ BASIC
PROBHD Z116098_0700 4
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 76.3372
DW 21.000 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.5496505 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 101.05999756 W
SFO2 399.8405994 MHz
NUC2 1H
CPDPRG2 waltz65
PCPD2 90.00 usec
PLW2 18.19000053 W
PLW12 0.22457001 W
PLW13 0.11296000 W

F2 - Processing parameters
SI 32768
SF 100.5396440 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

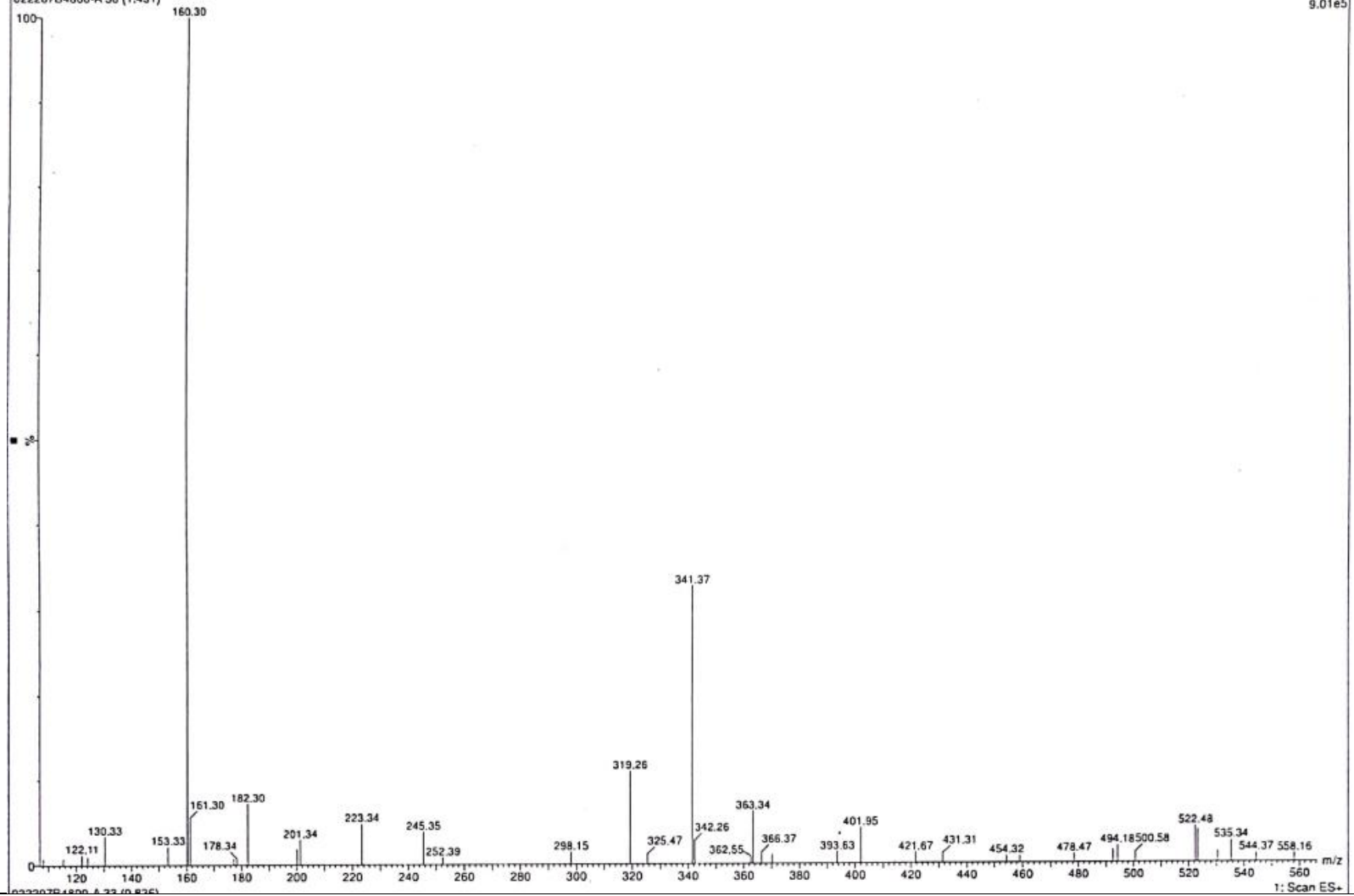
LCMS of 2-Oxo-2,3-dihydro-1H-benzo[d]imidazole-5-carbonitrile (2g)



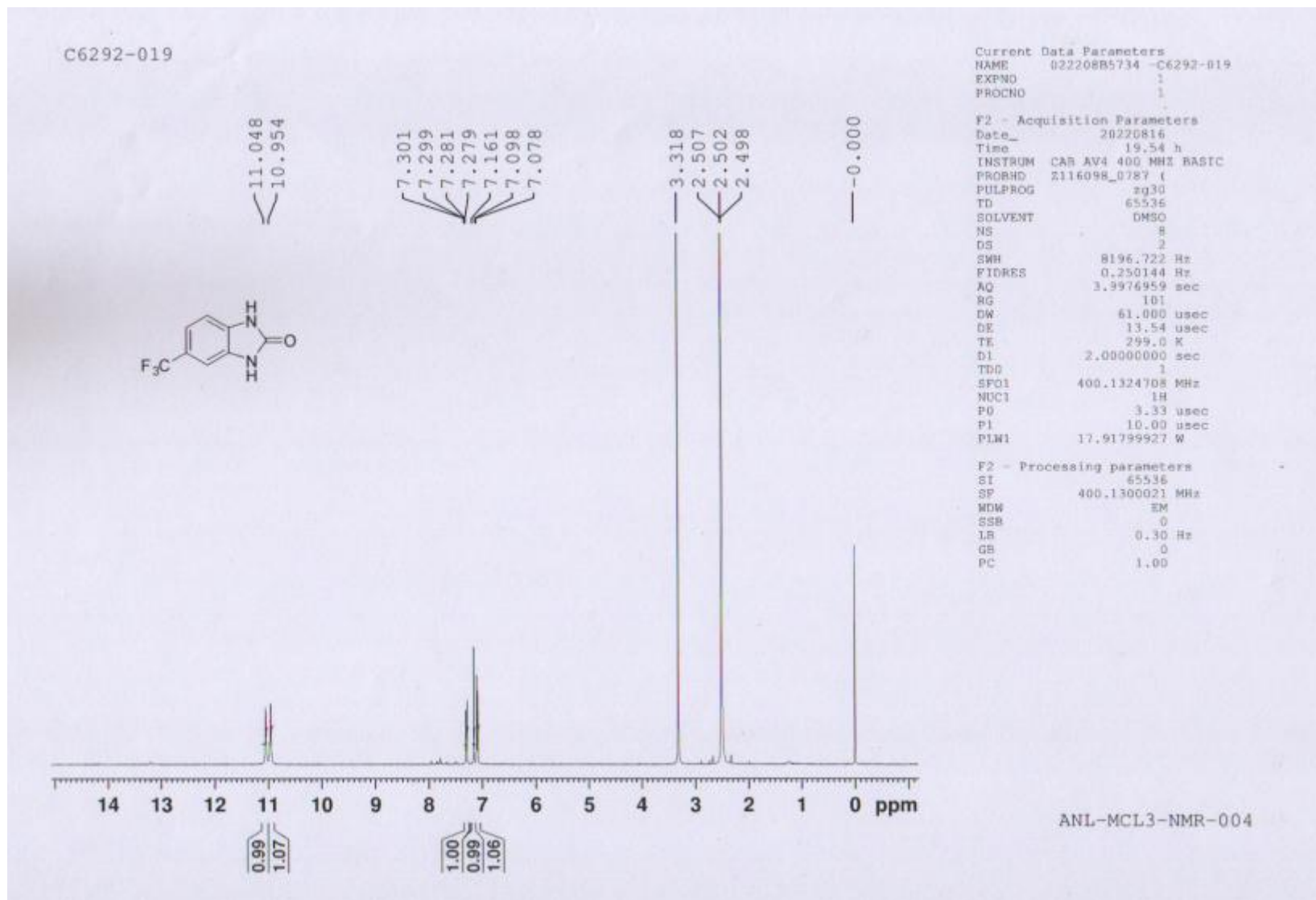
SAMPLE ID :C6292-022
Acq Method :RND-FA-4-MIN
1:F,1
022207B4800-A 56 (1.431)

Date of Analysis:15-Jul-2022:19:02:47
Instrument ID :ANL-MCL1-LCMS-007

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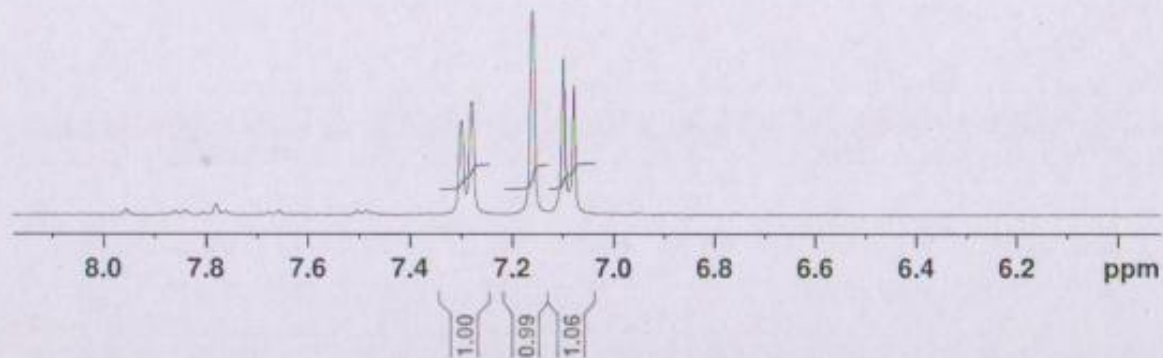


¹H NMR of 5-(Trifluoromethyl)-1,3-dihydro-2H-benzo[d]imidazol-2-one (2h)



C6292-019

7.301
7.299
7.281
7.279
7.161
7.098
7.078



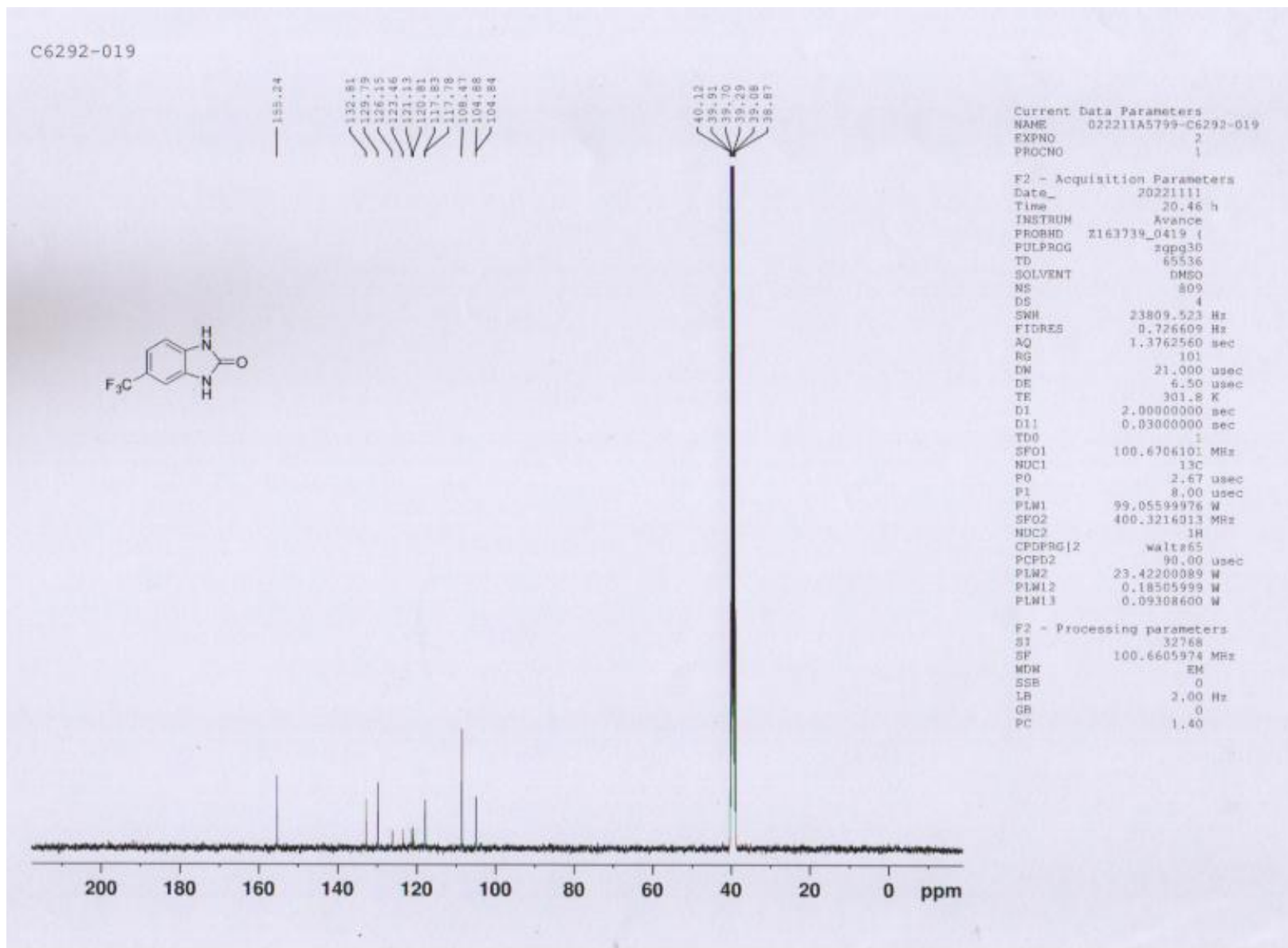
Current Data Parameters
NAME 022208B5734 -C6292-019
EXFNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220816
Time 19.54 h
INSTRUM CAB AV4 400 MHz BASIC
PROBHD Z116098_0787 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.54 usec
TE 299.0 K
D1 2.00000000 sec
TDD 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 17.91799927 W

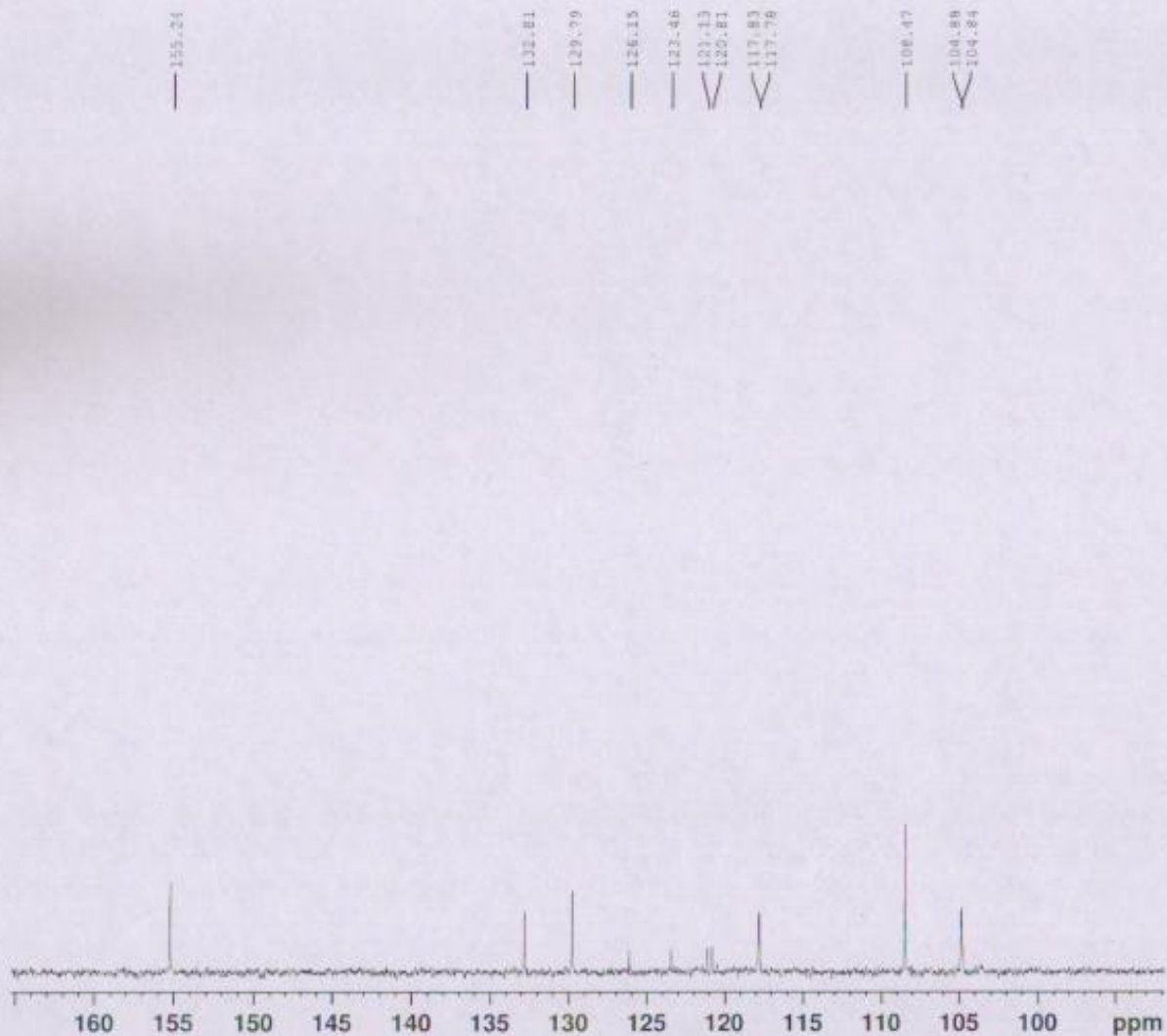
F2 - Processing parameters
SI 65536
SF 400.1300021 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ANL-MCL3-NMR-004

13C NMR of 5-(Trifluoromethyl)-1,3-dihydro-2H-benzo[d]imidazol-2-one (2h)



C6292-019

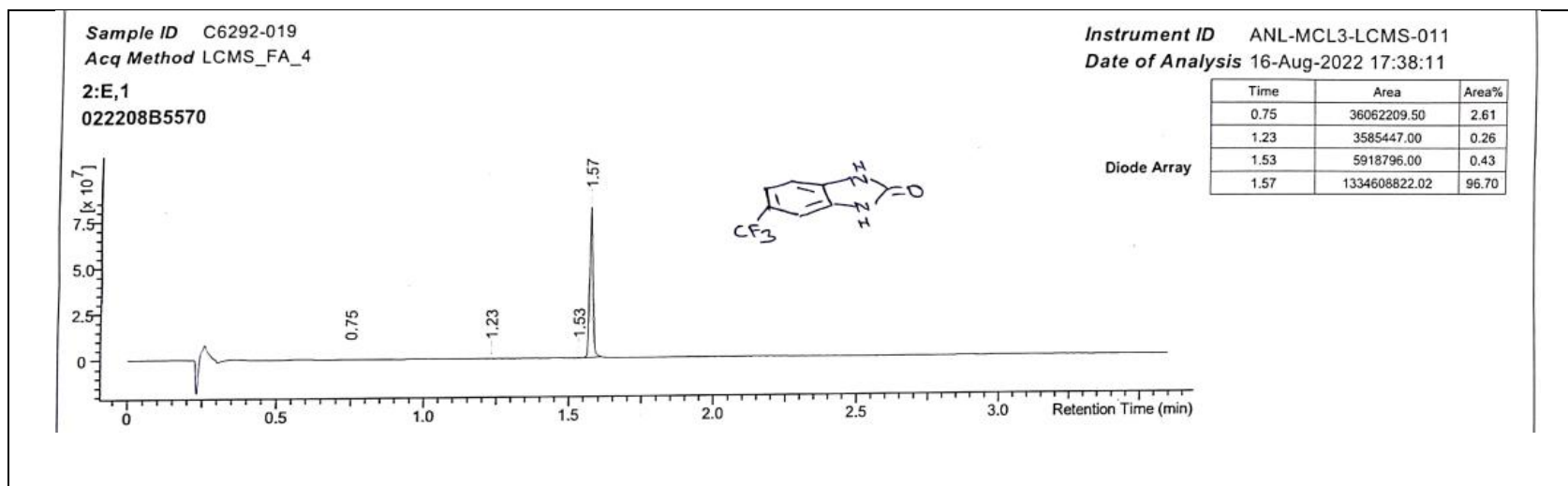


Current Data Parameters
NAME 022211A1799-C6292-019
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221111
Time 20.46 h
INSTRUM Avance
PROBHD z163735_0415 (1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 809
DS 4
SWH 23809.523 Hz
FIDRES 0.724609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 301.8 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6706101 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 99.05599976 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG12 waltz65
PCPD2 90.00 usec
PLW2 23.42200089 W
PLW12 0.18505999 W
PLW13 0.09308600 W

F2 - Processing parameters
SI 32768
SF 100.6605974 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

LCMS of 5-(Trifluoromethyl)-1,3-dihydro-2H-benzo[d]imidazol-2-one (2h)



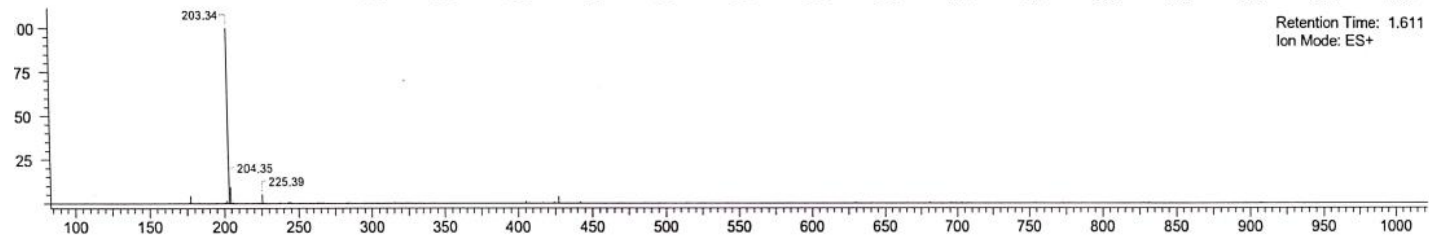
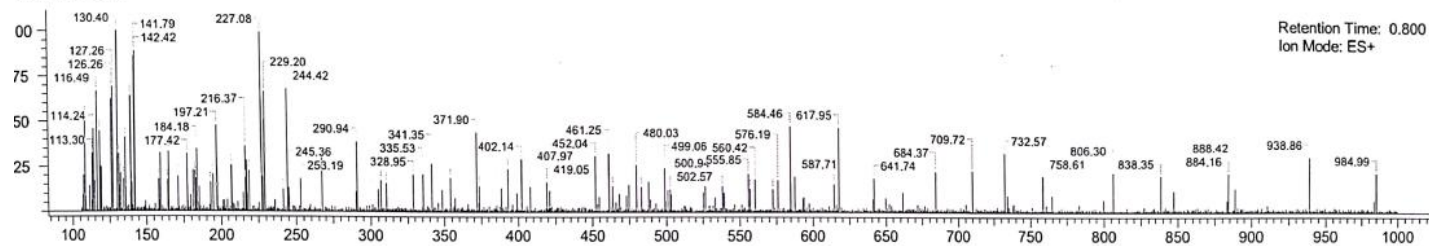
1cq Method LCMS_FA_4

1:E,1

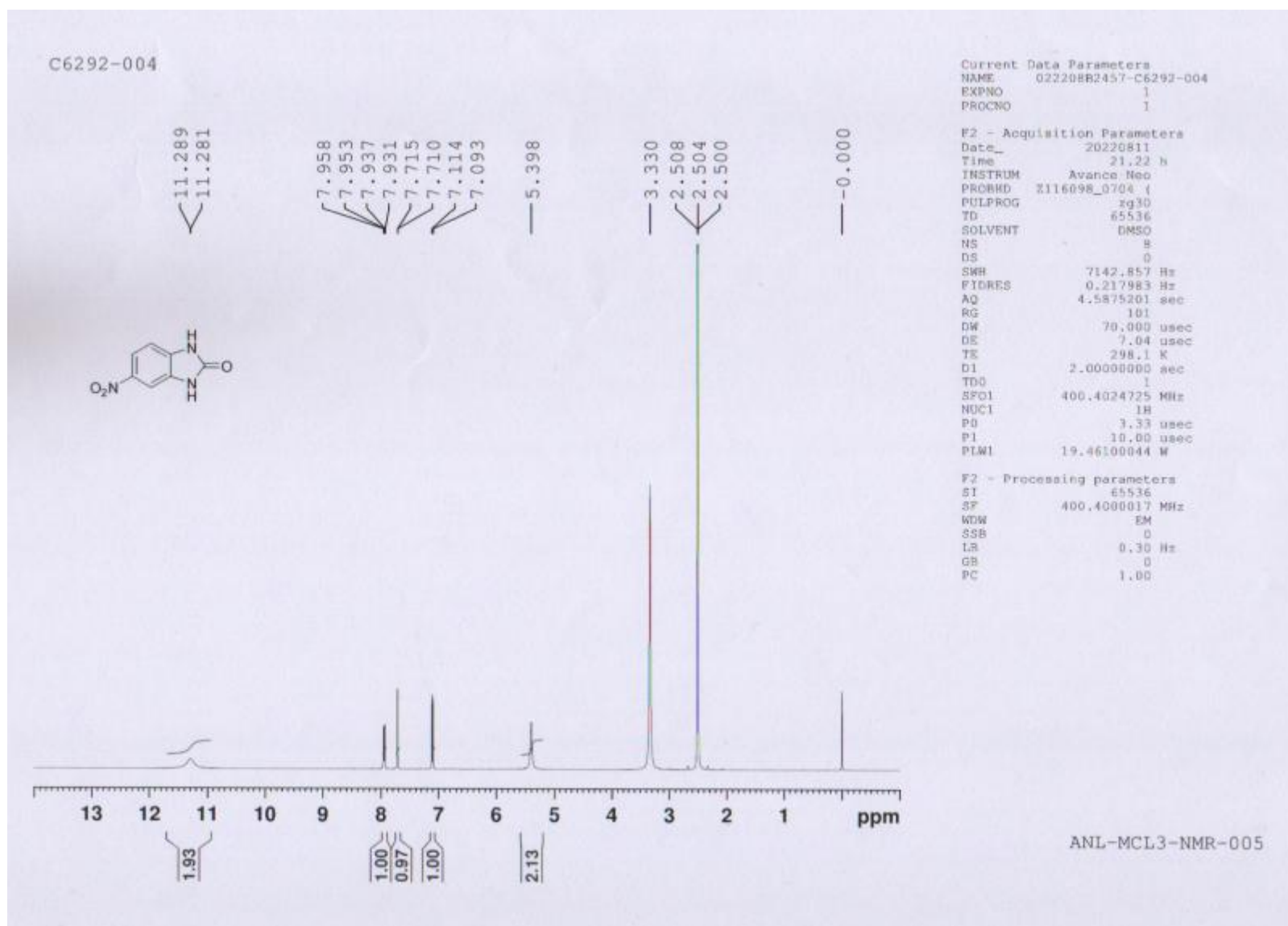
J22208B5570

Instrument ID ANL-MCL3-LCMS-011

Date of Analysis 16-Aug-2022 17:38:11



¹H NMR of 5-Nitro-1,3-dihydro-2H-benzo[d]imidazol-2-one (2i)



C6292-004

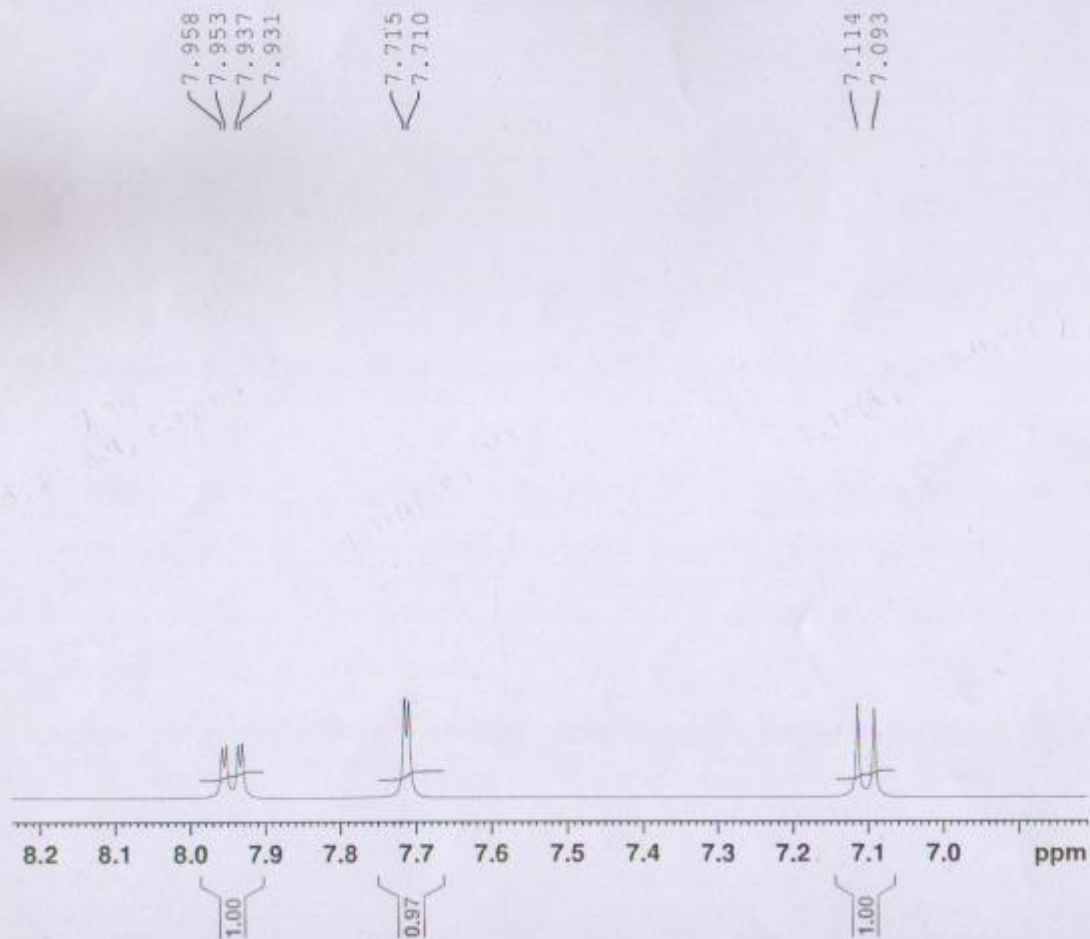
Current Data Parameters
NAME 02220882457-C6292-004
EXPMO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20220811
Time 21.22 h
INSTRUM Avance Neo
PROBHD 2116098_0704 (4
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 7142.857 Hz
FIDRES 0.217983 Hz
AQ 4.5875201 sec
RG 101
DW 70.000 usec
DE 7.04 usec
TE 298.1 K
D1 2.00000000 sec
TDO 1
SFO1 400.4024725 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 19.46100044 W

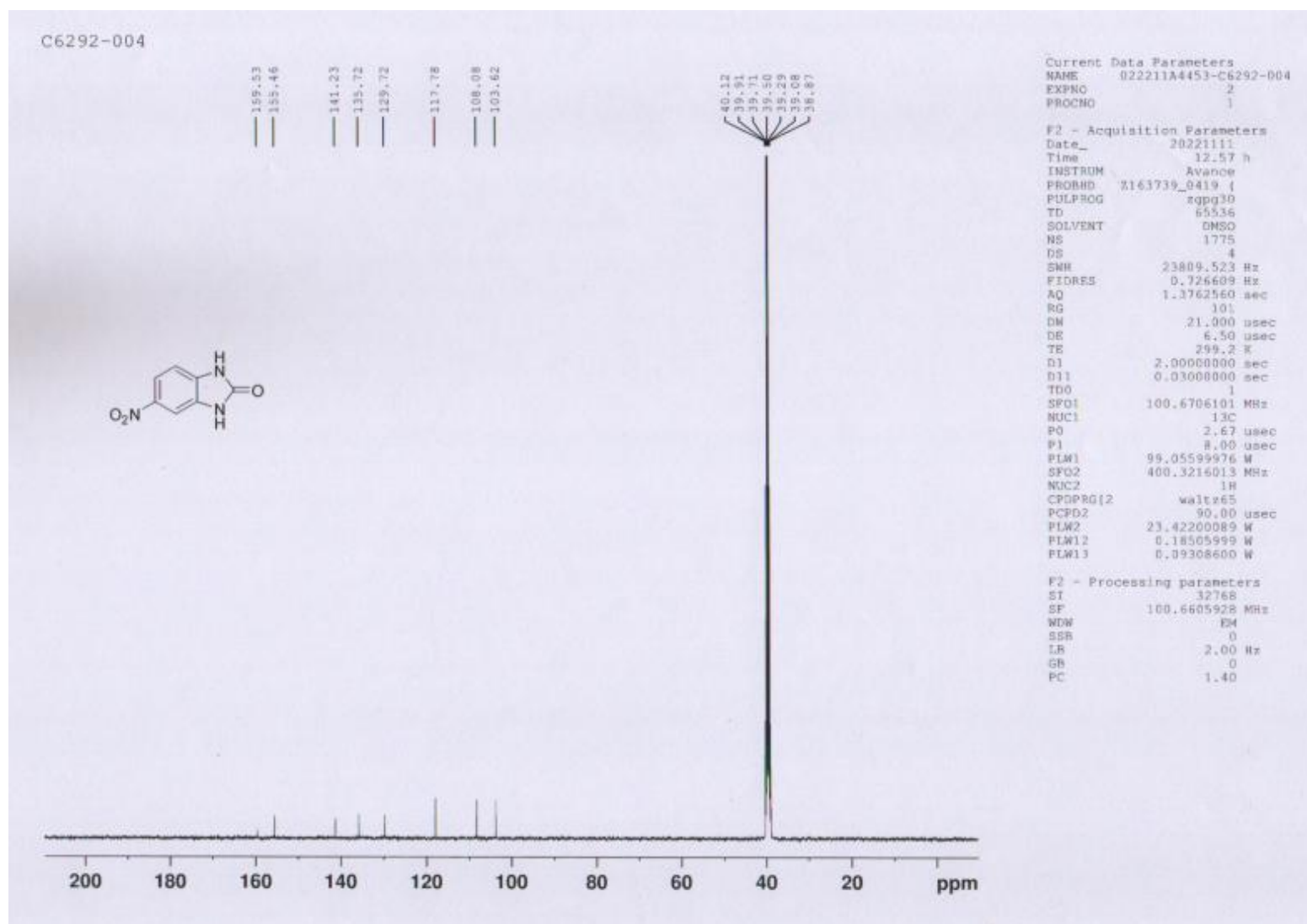
F2 - Processing parameters

SI 65536
SF 400.4000017 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ANL-MCL3-NMR-005

13C NMR of 5-Nitro-1,3-dihydro-2H-benzo[d]imidazol-2-one (2i)



C6292-004

159.53

155.46

141.23

135.72

129.72

117.78

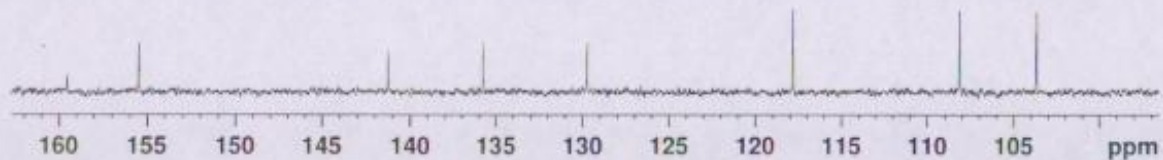
108.08

103.62

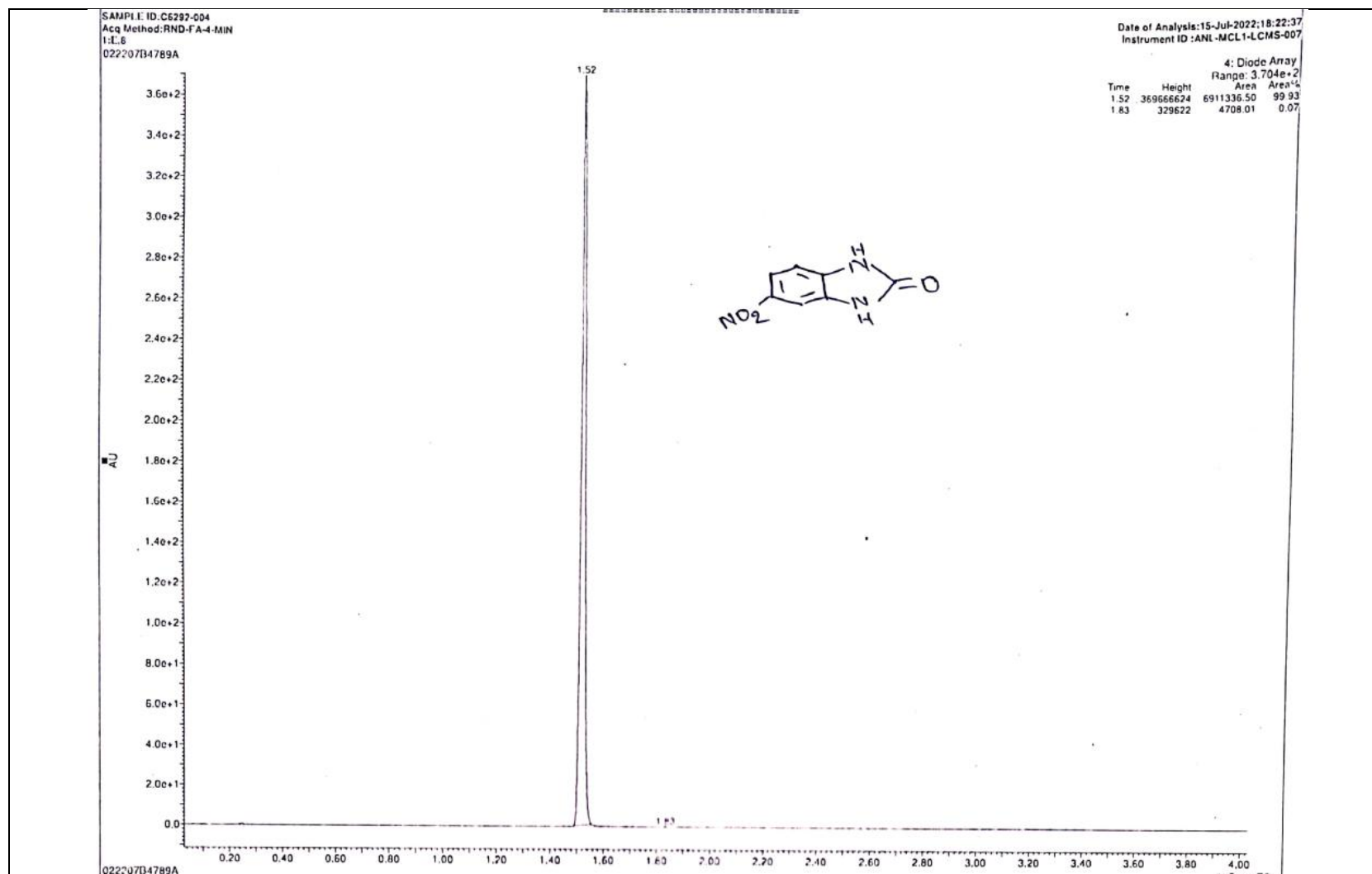
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NAME 022211A4453-C6292-004
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221111
Time 12:57 h
INSTRUM Avance
PROBHD Z163739_0419 1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1775
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 299.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6706101 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 99.05599976 W
SFO2 400.3216013 MHz
NUC2 1H
PCPD2 90.00 usec
PLW2 23.42200089 W
PLW12 0.18505999 W
PLW13 0.09308600 W

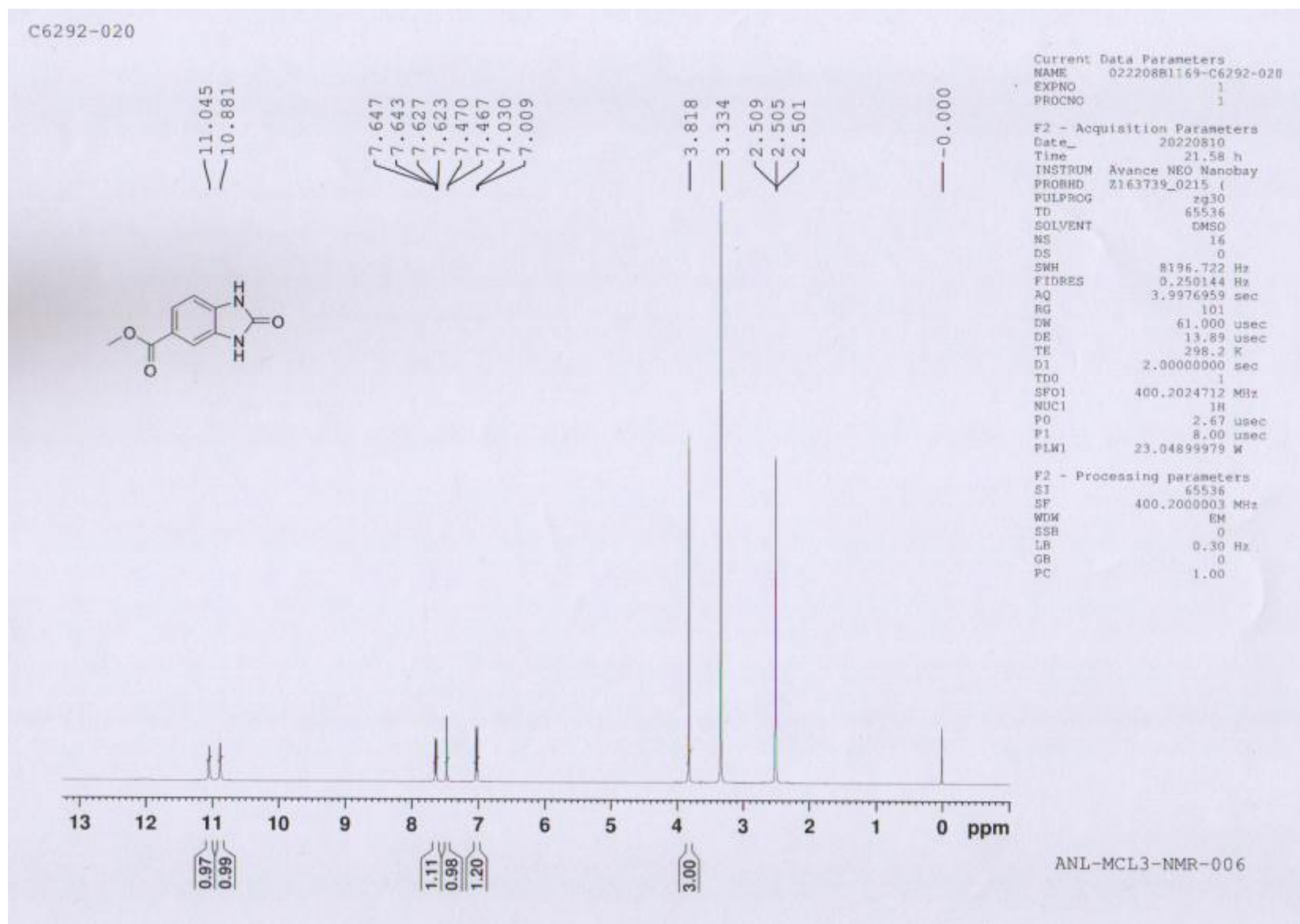
F2 - Processing parameters
SI 32768
SF 100.6605928 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



LCMS of 5-Nitro-1,3-dihydro-2H-benzo[d]imidazol-2-one (2i)



¹H NMR of Methyl 2-oxo-2,3-dihydro-1H-benzo[d]imidazole-5-carboxylate (2j)



C6292-020

7.647
7.643
7.627
7.623

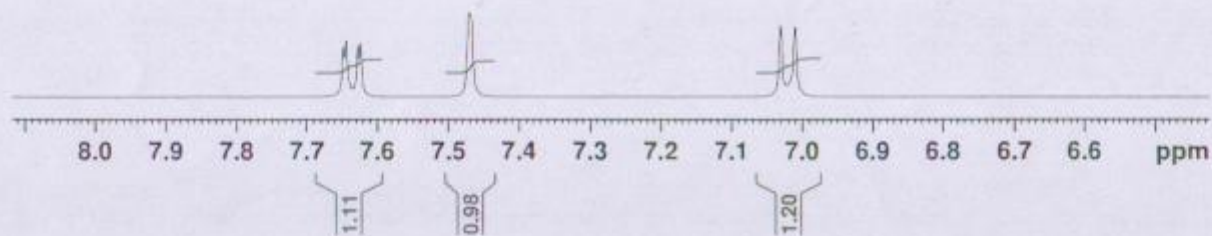
7.470
7.467

7.030
7.009

Current Data Parameters
NAME 022208B1169-C6292-020
EXPNO 1
PROCNO 1

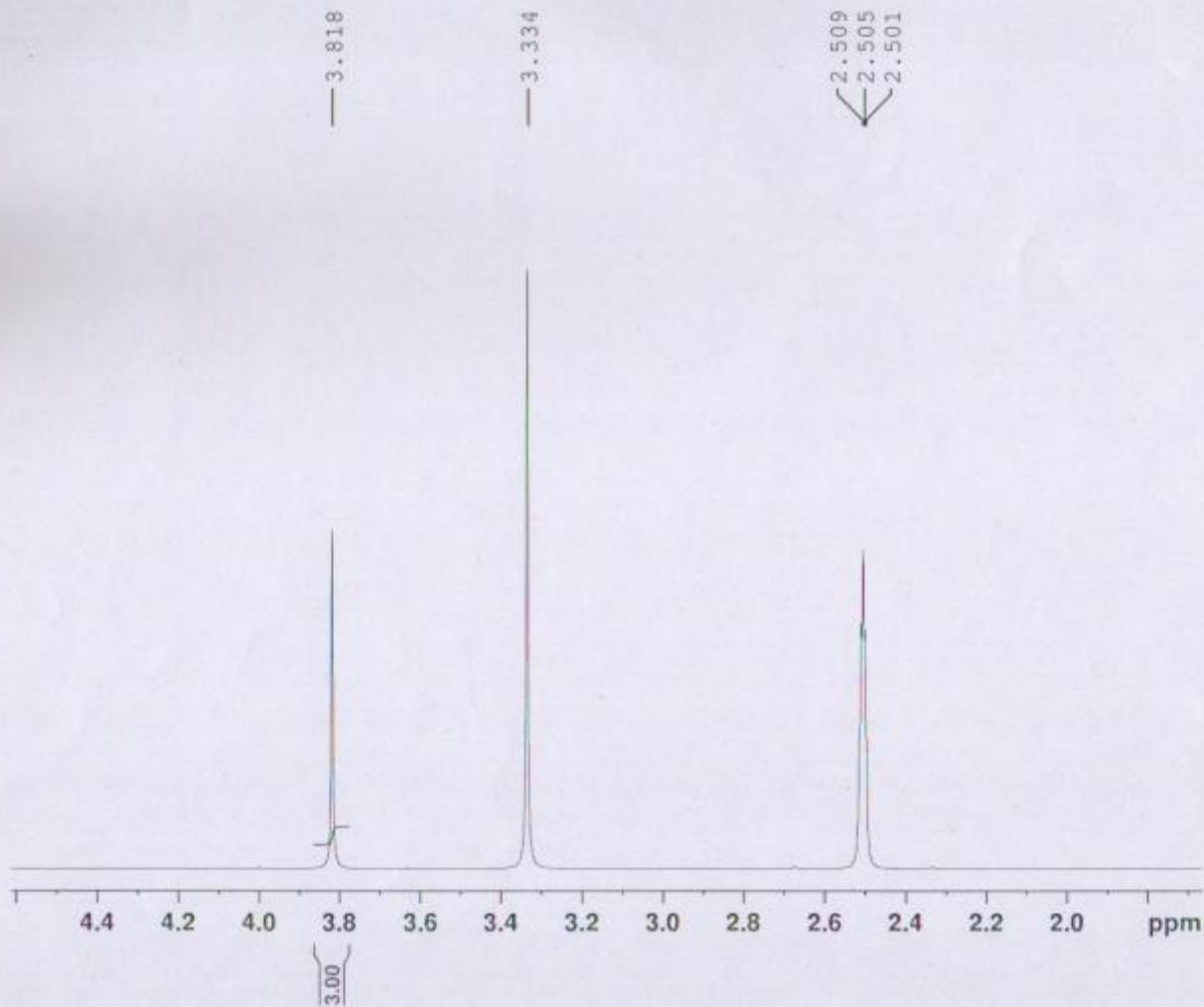
F2 - Acquisition Parameters
Date_ 20220810
Time 21.58 h
INSTRUM Avance NEO Nanobay
PROBHD Z163739_0215 (rg30
PULPROG zg30
ID 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
SFO1 400.2024712 MHz
NUC1 1H
PO 2.67 usec
PI 8.00 usec
PLW1 23.04899979 W

F2 - Processing parameters
SI 65536
SF 400.2000003 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ANL-MCL3-NMR-006

C6292-020



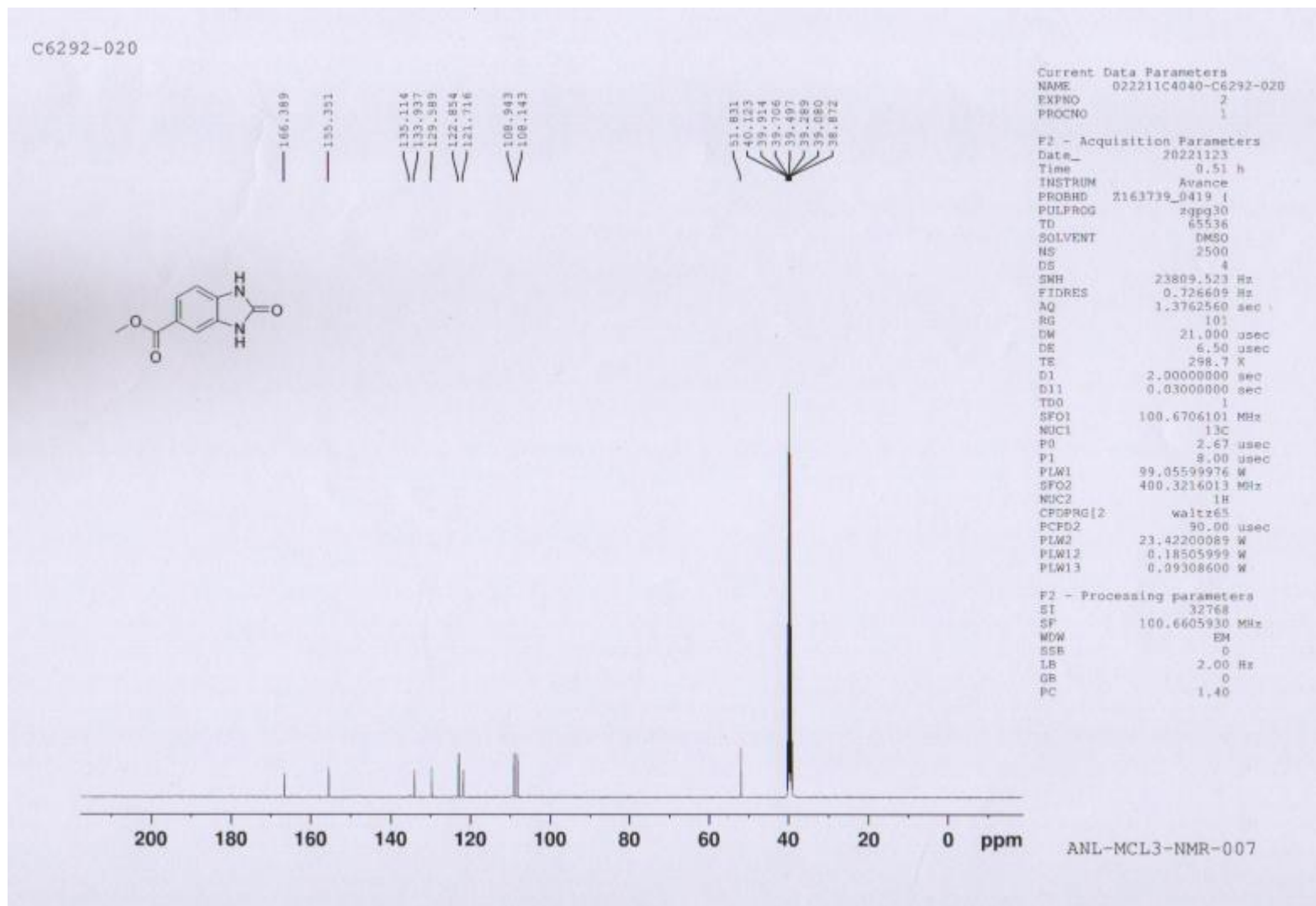
Current Data Parameters
NAME 022208B1169-C6292-020
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220810
Time 21.58 h
INSTRUM Avance NEO Nanobay
PROBHD Z163739_0215 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.2 K
D1 2.00000000 sec
TDD 1
SFO1 400.2024712 MHz
NUC1 1H
PO 2.67 usec
P1 8.00 usec
PLW1 23.04899979 W

F2 - Processing parameters
SI 65536
SF 400.2000003 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ANL-MCL3-NMR-006

13C NMR of Methyl 2-oxo-2,3-dihydro-1H-benzo[d]imidazole-5-carboxylate (2j)



C6292-020



Current Data Parameters
NAME 022211C4040-C6292-020
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221123
Time 0.51 h
INSTRUM Avance
PROBHD Z163735_0419 (4
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2500
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DM 21.000 usec
CE 6.50 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1
SFO1 100.6706101 MHz
NUC1 13C
P0 2.67 usec
P1 5.00 usec
PLW1 99.05599976 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG2 waltz165
PCPD2 90.00 usec
PLW2 23.42200089 W
PLW12 0.18505999 W
PLW13 0.09308600 W

F2 - Processing parameters
SI 32768
SF 100.6405930 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

ANL-MCL3-NMR-007

C6292-020



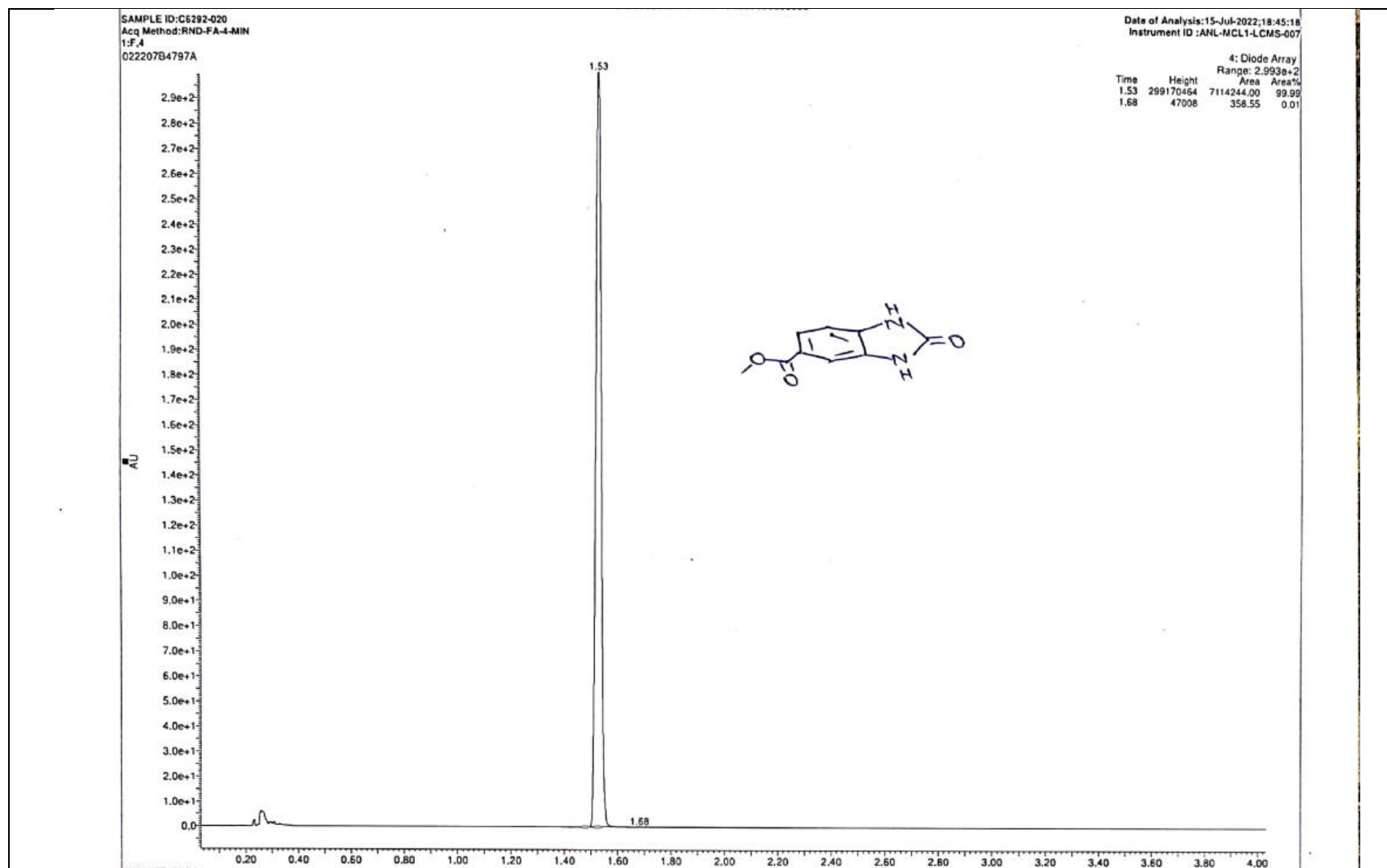
Current Data Parameters
NAME 022211C4040-C6292-020
EXPTNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221123
Time 0.51 h
INSTRUM Avance
PROBHD Z163739_0419 (
PULPROG epgg30
TD 65536
SOLVENT DMSO
NS 2500
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 298.7 K
D1 2.0000000 sec
D11 0.0300000 sec
TDD 1
SFO1 100.6706101 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLM1 99.05599976 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG2 waltz65
PCPD2 90.00 usec
PLM2 23.42200089 W
PLM12 0.18505999 W
PLM13 0.09308600 W

F2 - Processing parameters
SI 32768
SF 100.6605930 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

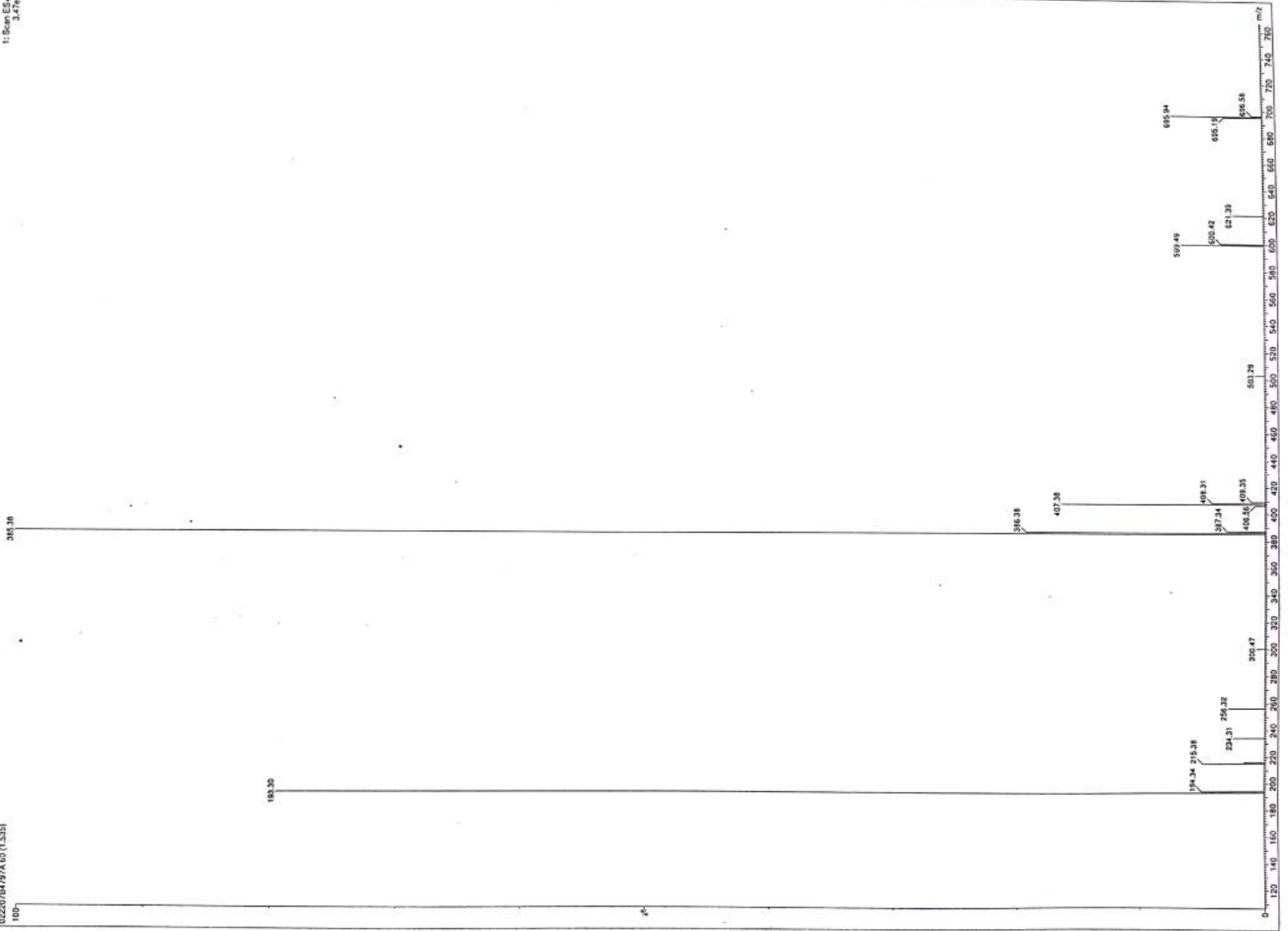
ANL-MCL3-NMR-007

LCMS of Methyl 2-oxo-2,3-dihydro-1*H*-benzo[*d*]imidazole-5-carboxylate (2j)

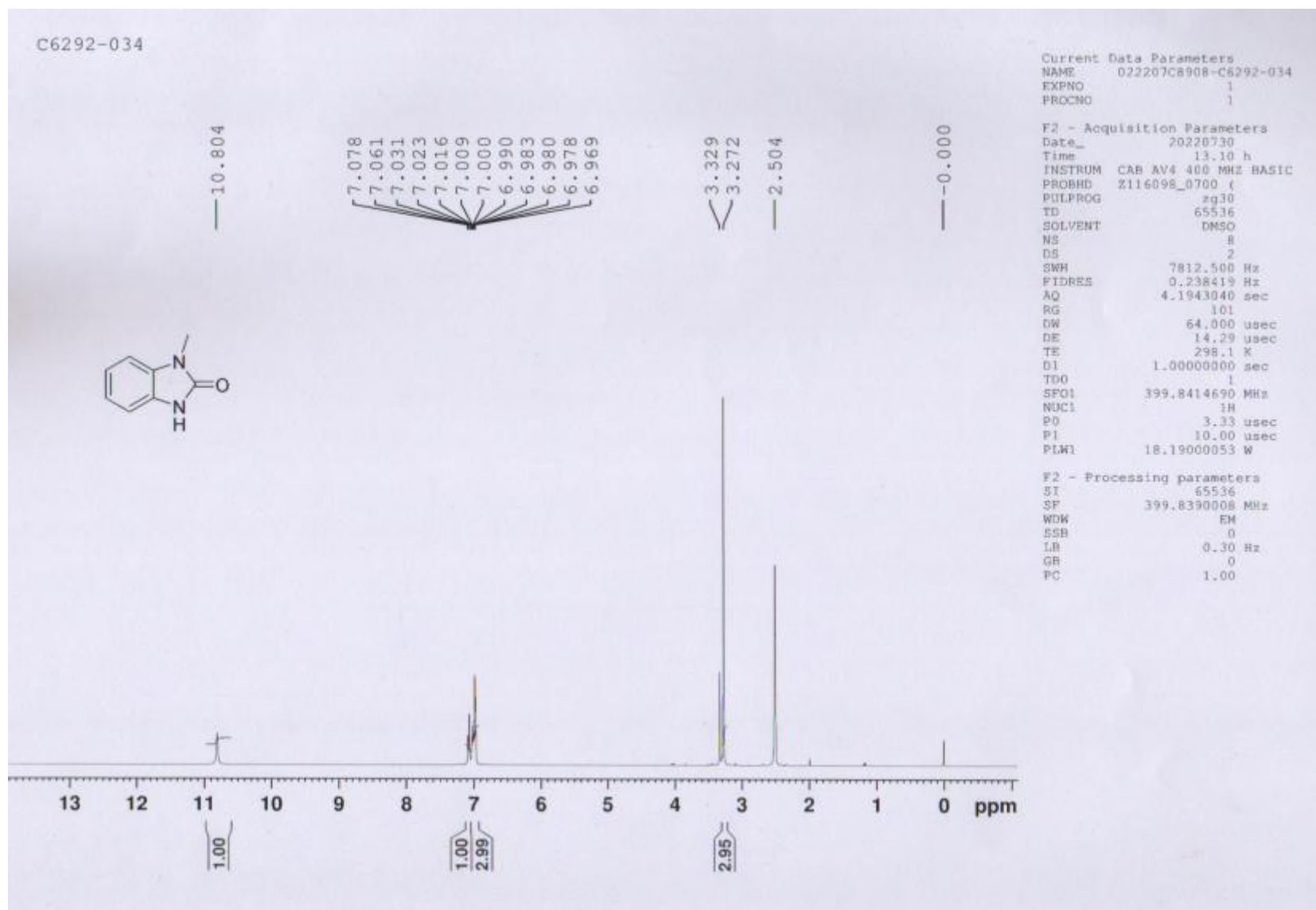


SAMPLE ID: CENY-009
FID: FID-7444M
022078197A.G0 (1.53)

Date of Analysis: Jul-2022 18:45:18
Instrument ID: JNL-MCL-LCMS-007
11 Scan ES+
3.47ug



¹H NMR of 1-Methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (2k)



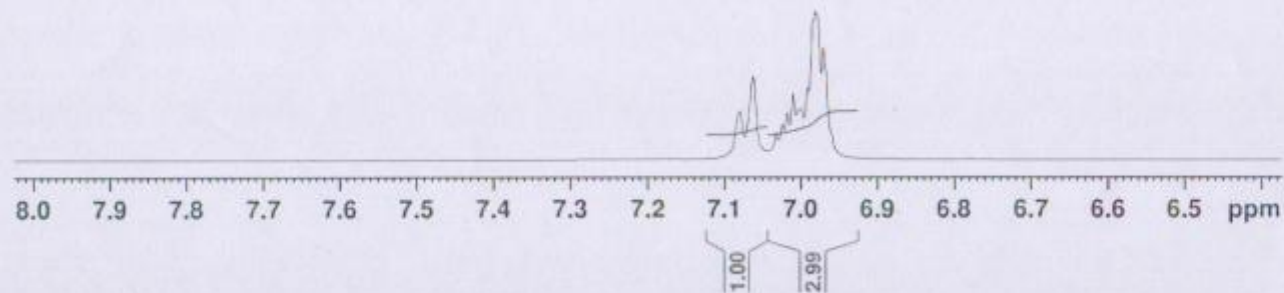
C6292-034

7.078
7.061
7.031
7.023
7.016
7.009
7.000
6.990
6.983
6.980
6.978
6.969

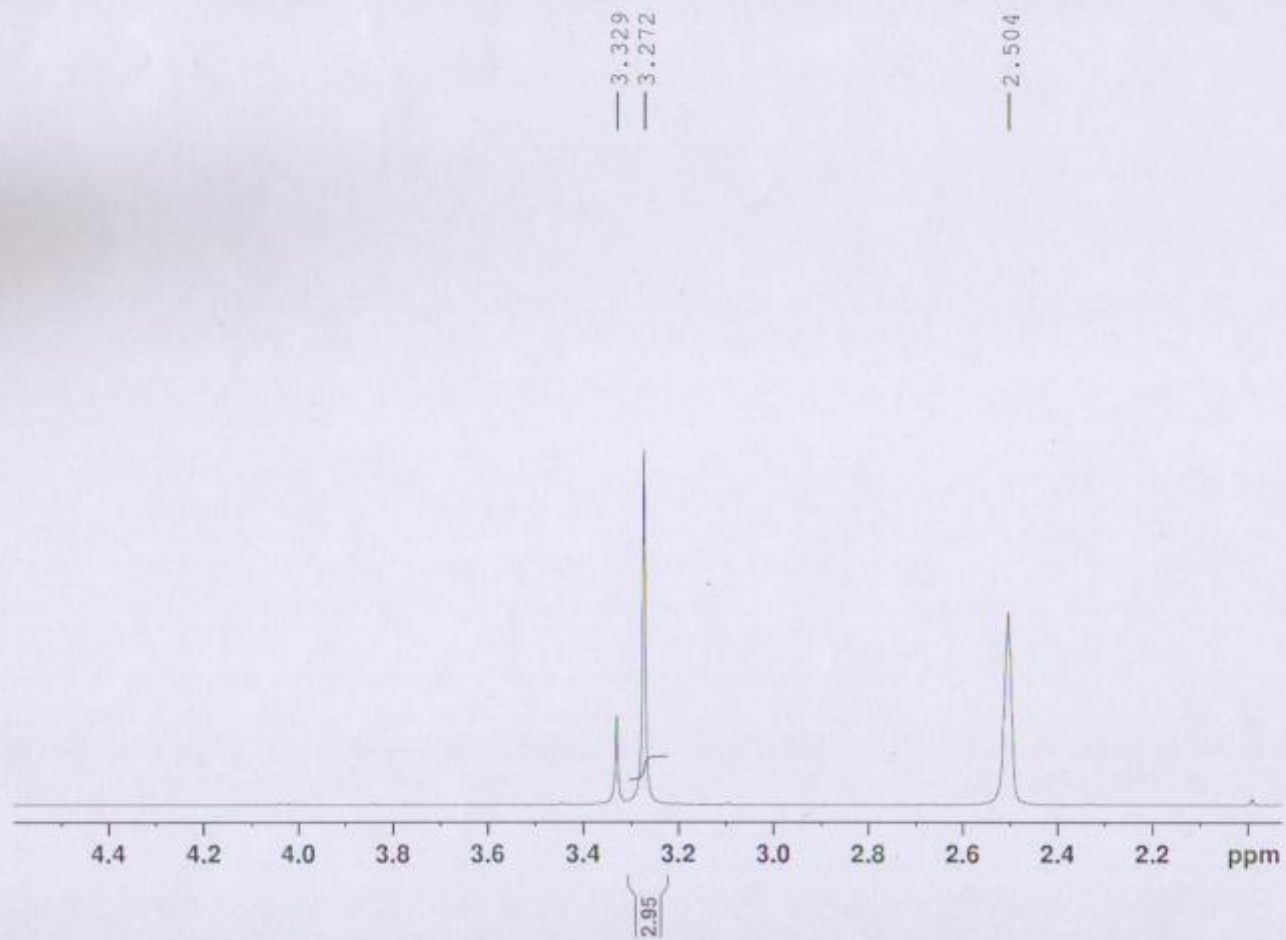
Current Data Parameters
NAME 022207C8908-C6292-034
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220730
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PROBHD Z116098_0700 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 4.1943040 sec
RG 101
DW 64.000 usec
DE 14.29 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 399.8414590 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.19000053 W

F2 - Processing parameters
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WDW EM
SSB 0
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PC 1.00



C6292-034

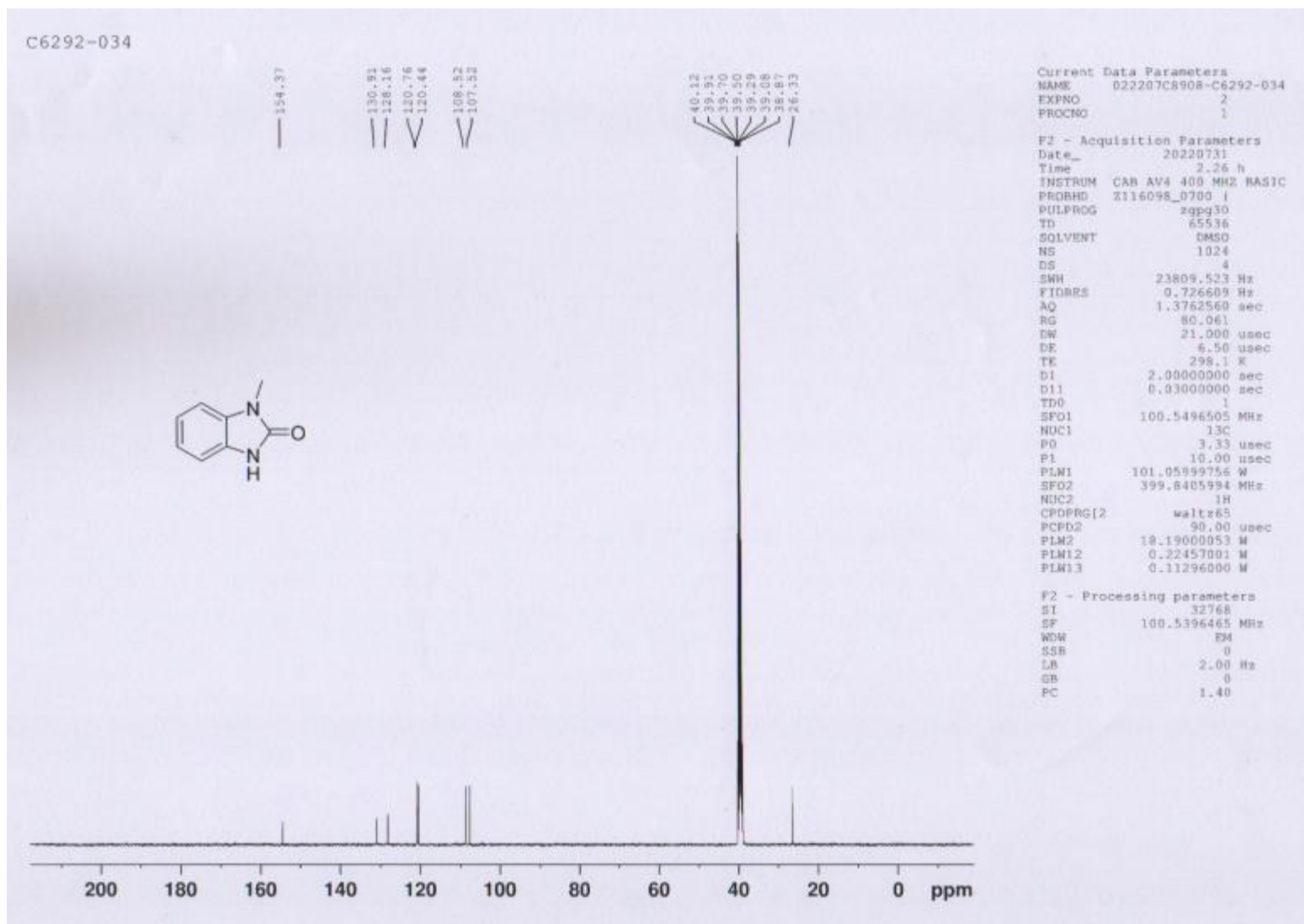


Current Data Parameters
NAME 022207C8908-C6292-034
EXPNO 1
PROCNO 1

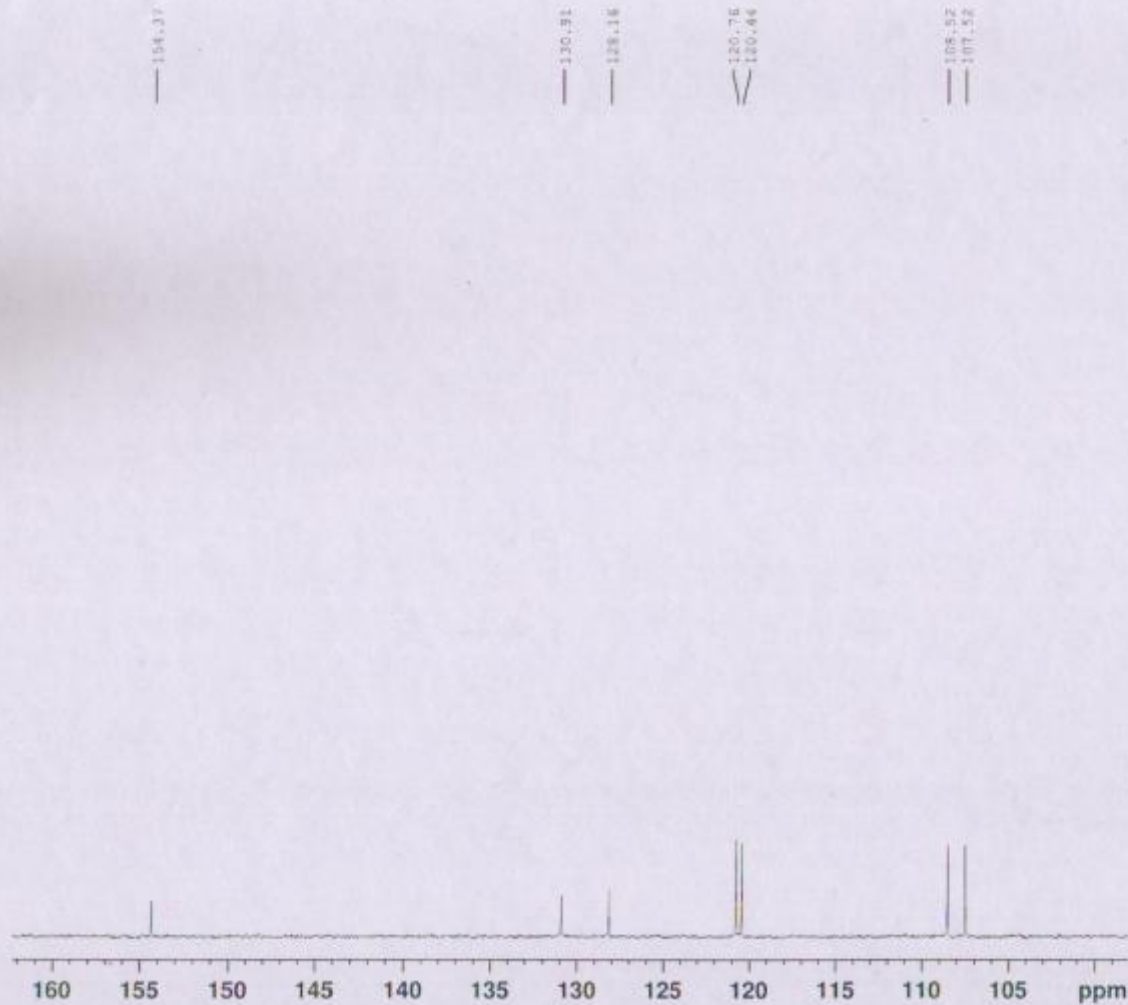
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PROBHD Z116098_0700 4
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 4.1943040 sec
RG 101
DW 64.000 usec
DE 14.29 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1
SFO1 399.8414690 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.19000053 W

F2 - Processing parameters
SI 65536
SF 399.8390008 MHz
WDW EM
SSB 0
LB 0.30 Hz
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PC 1.00

¹³C NMR of 1-Methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (2k)



C6292-034

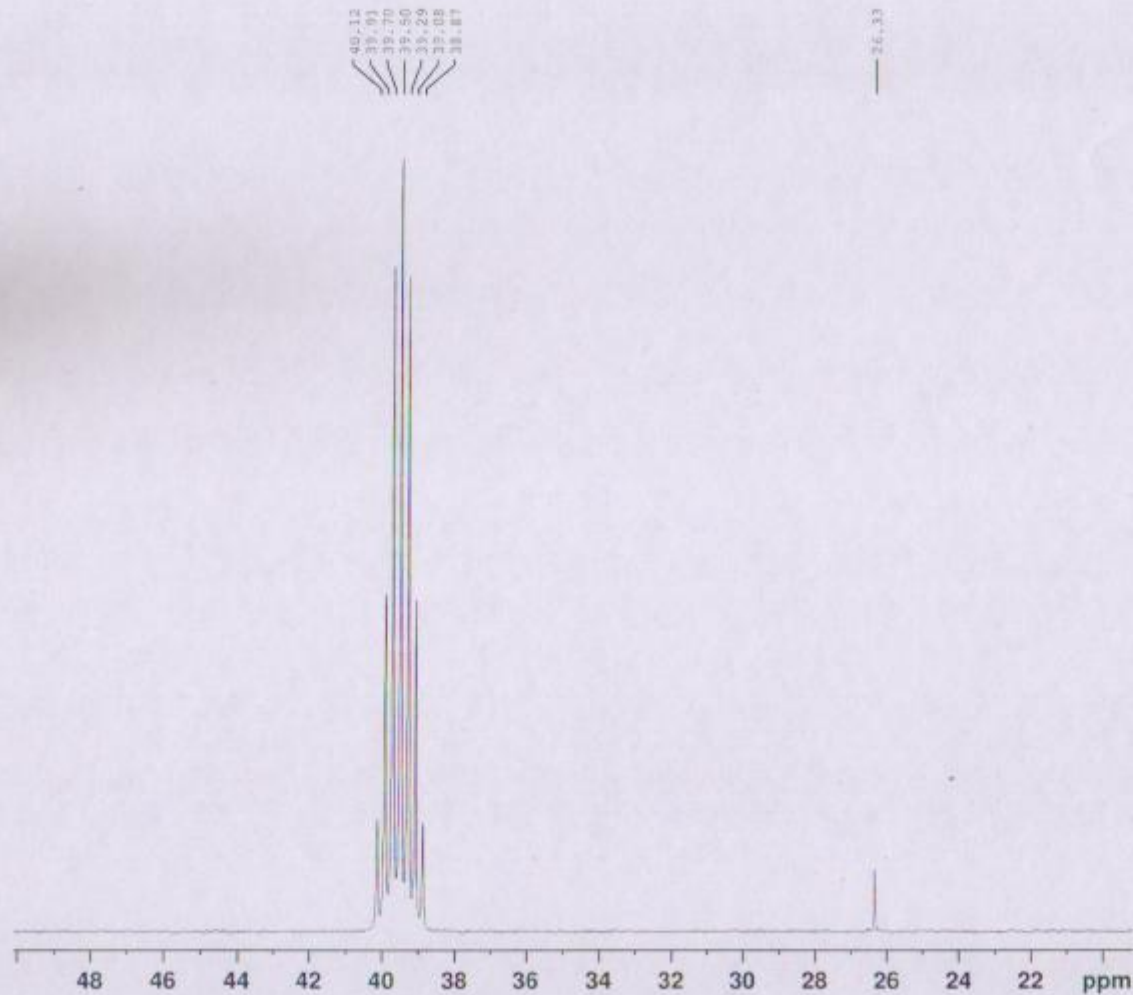


Current Data Parameters
NAME 022207C8908-C6292-034
EXENO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220731
Time 2.26 h
INSTRUM CAS AV4 400 MHz BASIC
PROBHD Z116098_0700 1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 23809.523 Hz
FIDRES 0.725609 Hz
AQ 1.3762560 sec
RG 80.061
DN 21.000 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TDD 1
SFO1 100.5496505 MHz
NUC1 13C
PC 3.33 usec
P1 10.00 usec
PLW1 101.05999756 W
SFO2 399.8405994 MHz
NUC2 1H
CPDPRG2 waltz165
PCPD2 90.00 usec
PLW2 18.19000053 W
PLW12 0.22457001 W
PLW13 0.11296000 W

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SF 100.5396465 MHz
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SSB 0
LB 2.00 Hz
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PC 1.40

C6292-034

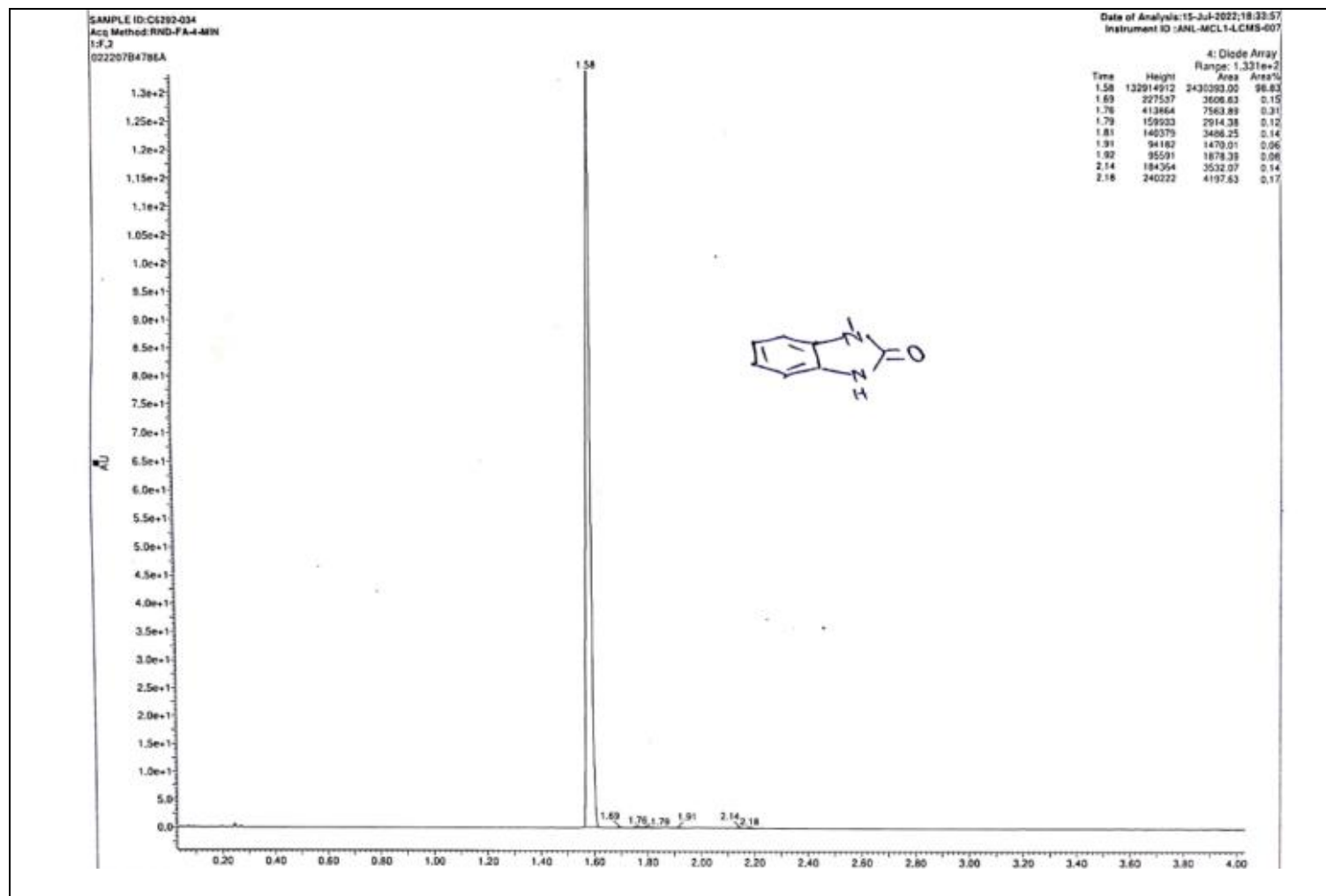


Current Data Parameters
NAME 022207C8908-C6292-034
EXPNO 2
PROCNO 1

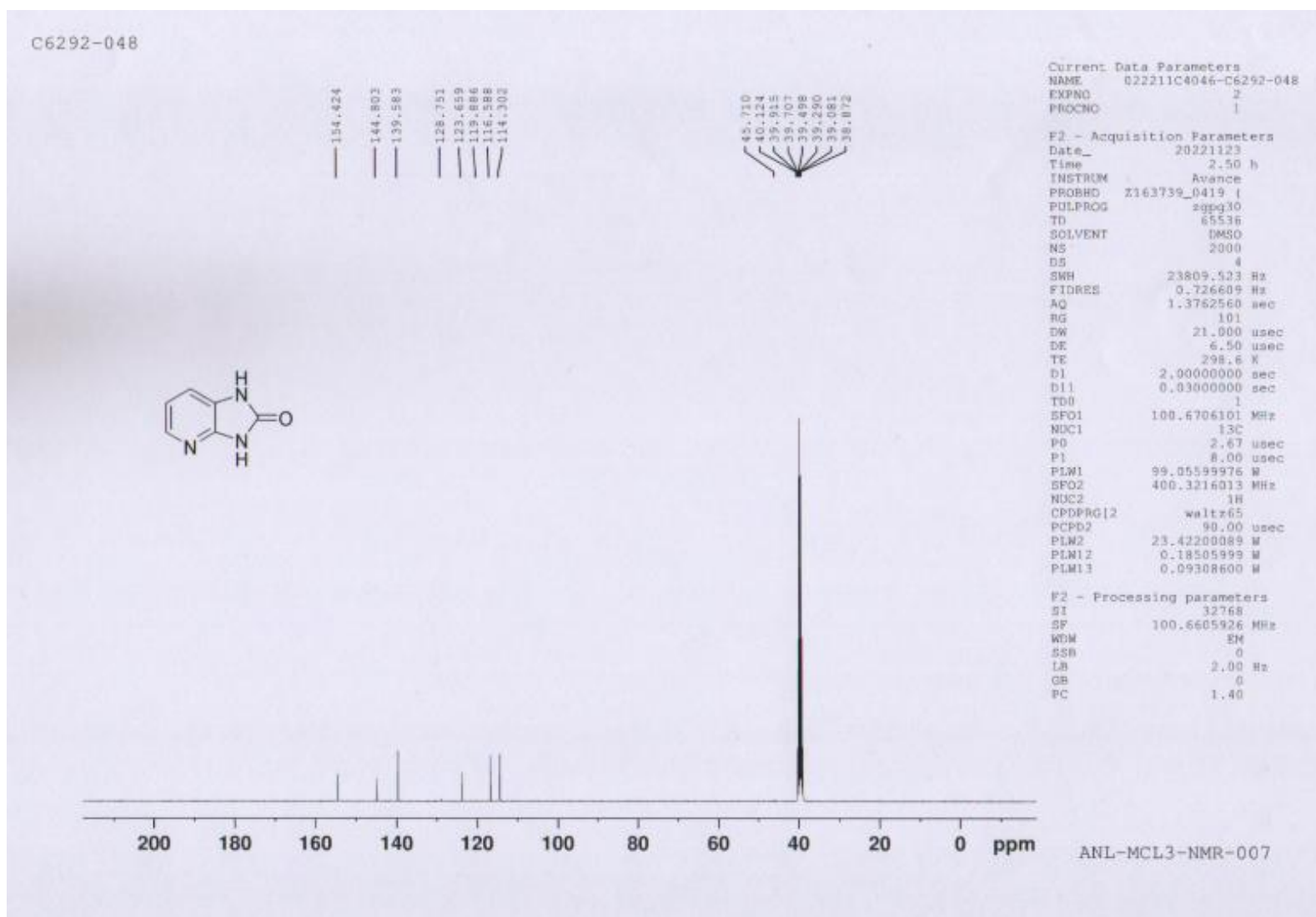
F2 - Acquisition Parameters
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Time 2.26 h
INSTRUM CAS AV4 400 MHZ BASIC
PROBHD Z116098_0700 1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 23869.523 Hz
FIDRES 0.726605 Hz
AQ 1.3762560 sec
RG 80.061
CW 21.000 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.5496505 MHz
NUC1 13C
PO 3.33 usec
PI 10.00 usec
PLW1 101.03999756 W
SFO2 399.8405994 MHz
NUC2 1H
CPDPRG2 waltz65
PCPD2 90.00 usec
PLW2 18.19000053 W
PLW12 0.22457001 W
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F2 - Processing parameters
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SF 100.5396465 MHz
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SSB 0
LB 2.00 Hz
GB 0
PC 1.40

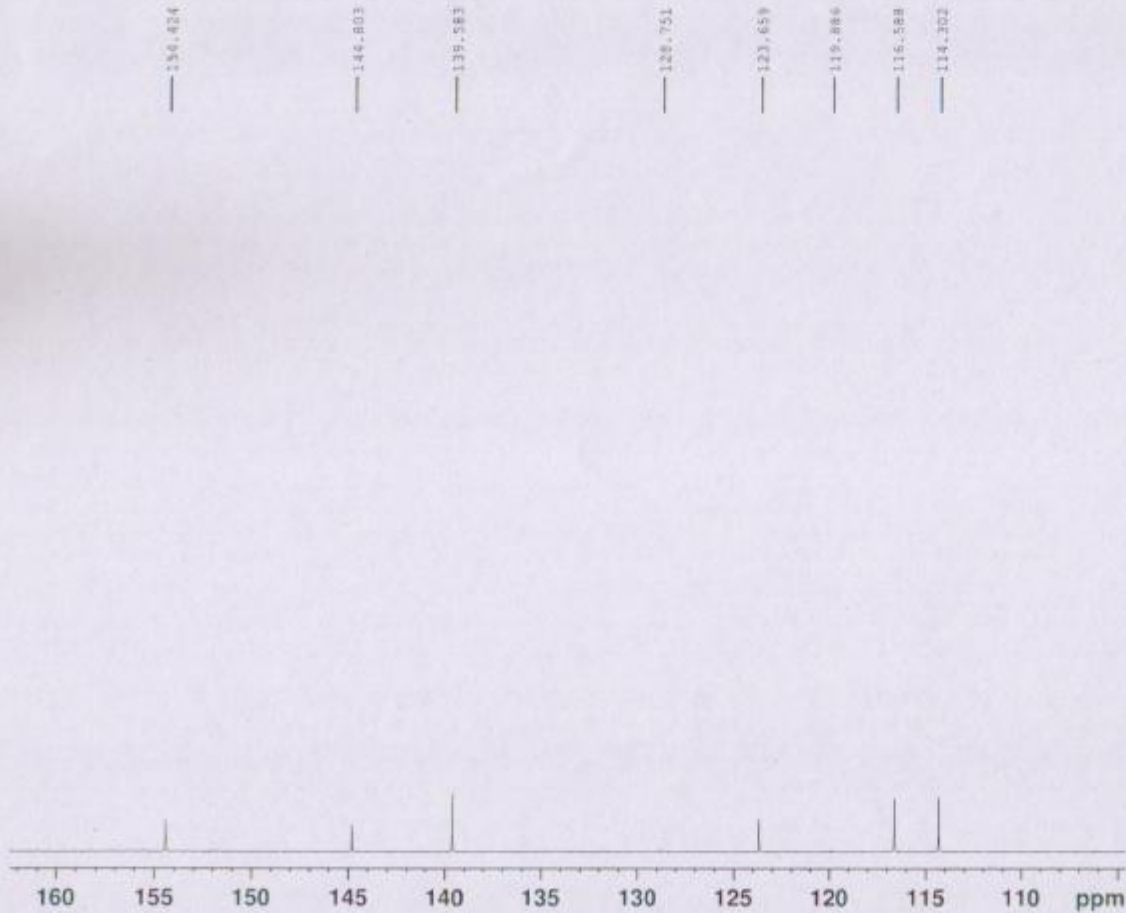
LCMS of 1-Methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (2k)



¹³C NMR of 1,3-Dihydro-2*H*-imidazo[4,5-*b*]pyridin-2-one (2l)



C6292-048



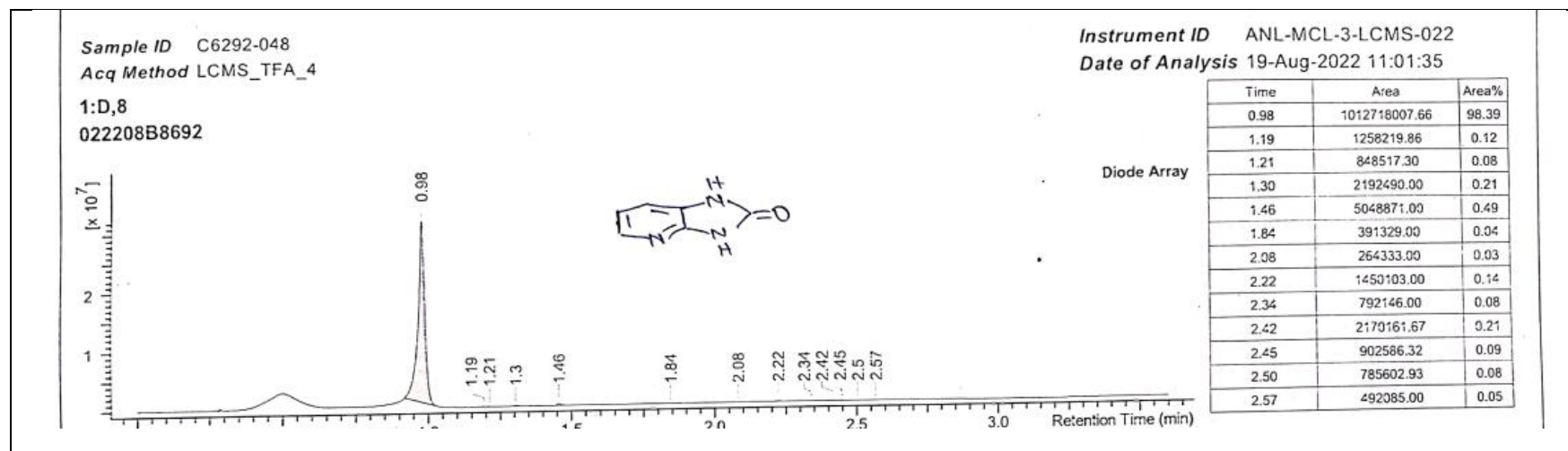
Current Data Parameters
NAME 022211C4046-C6292-048
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221123
Time 2.50 h
INSTRUM Avance
PROBHD Z163739_0419 1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6706101 MHz
NUC1 13C
PO 2.67 usec
P1 8.00 usec
PLW1 99.05599976 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG2 waltz65
PCPD2 90.00 usec
PLW2 23.42200089 W
PLW12 0.18505999 W
PLW13 0.09308600 W

F2 - Processing parameters
SI 32768
SF 100.6605926 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

ANL-MCL3-NMR-007

LCMS of 1,3-Dihydro-2H-imidazo[4,5-b]pyridin-2-one (2I)

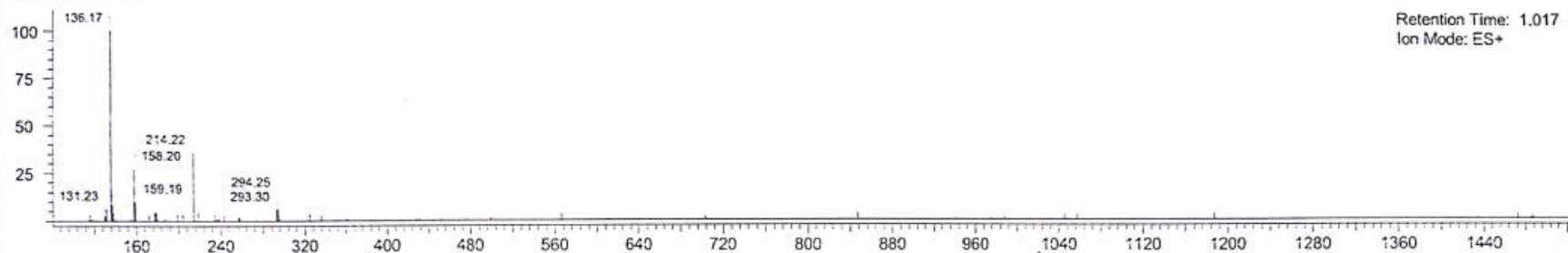


Sample ID C6292-048
Acq Method LCMS_TFA_4

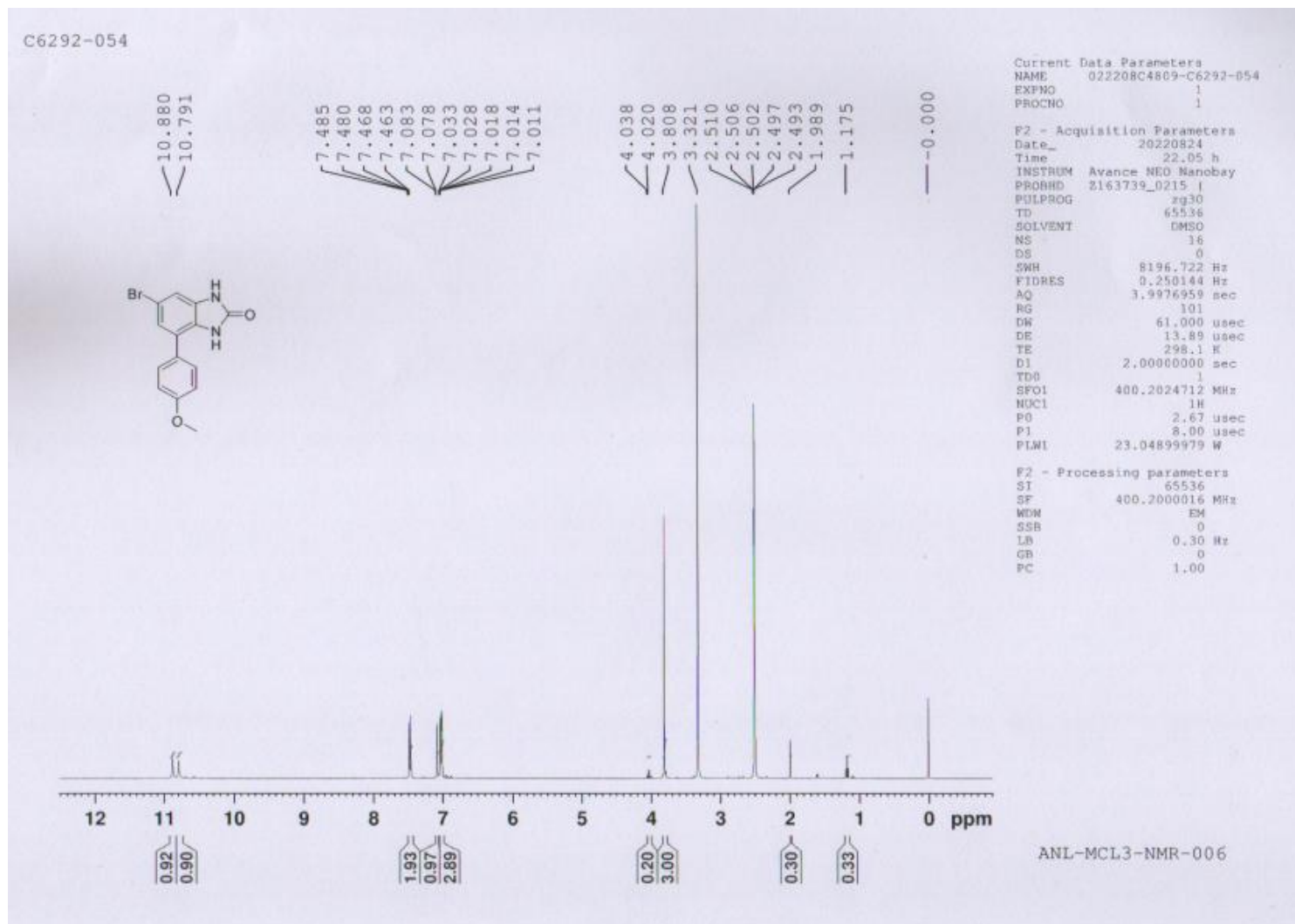
Discovery Chemistry Analytical Services

Instrument ID ANL-MCL-3-LCMS-022
Date of Analysis 19-Aug-2022 11:01:35

1:D,8
022208B8692



¹H NMR of 6-Bromo-4-(4-methoxyphenyl)-1,3-dihydro-2H-benzo[d]imidazol-2-one (2m)



C6292-054

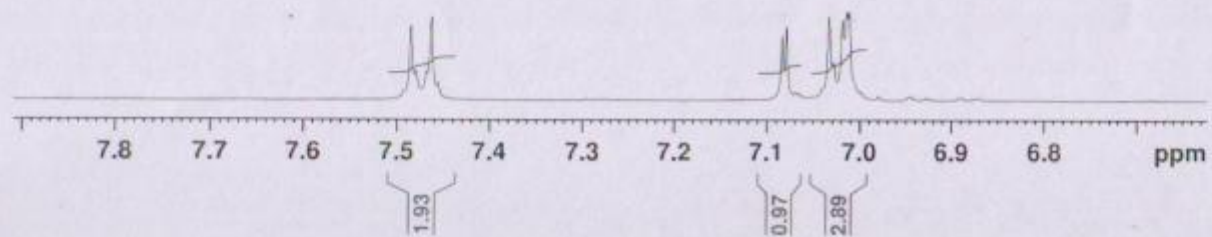
7.485
7.480
7.468
7.463

7.083
7.078
7.033
7.028
7.018
7.014
7.011

Current Data Parameters
NAME 022208C4809-C6292-054
EXPNO 1
PROCNO 1

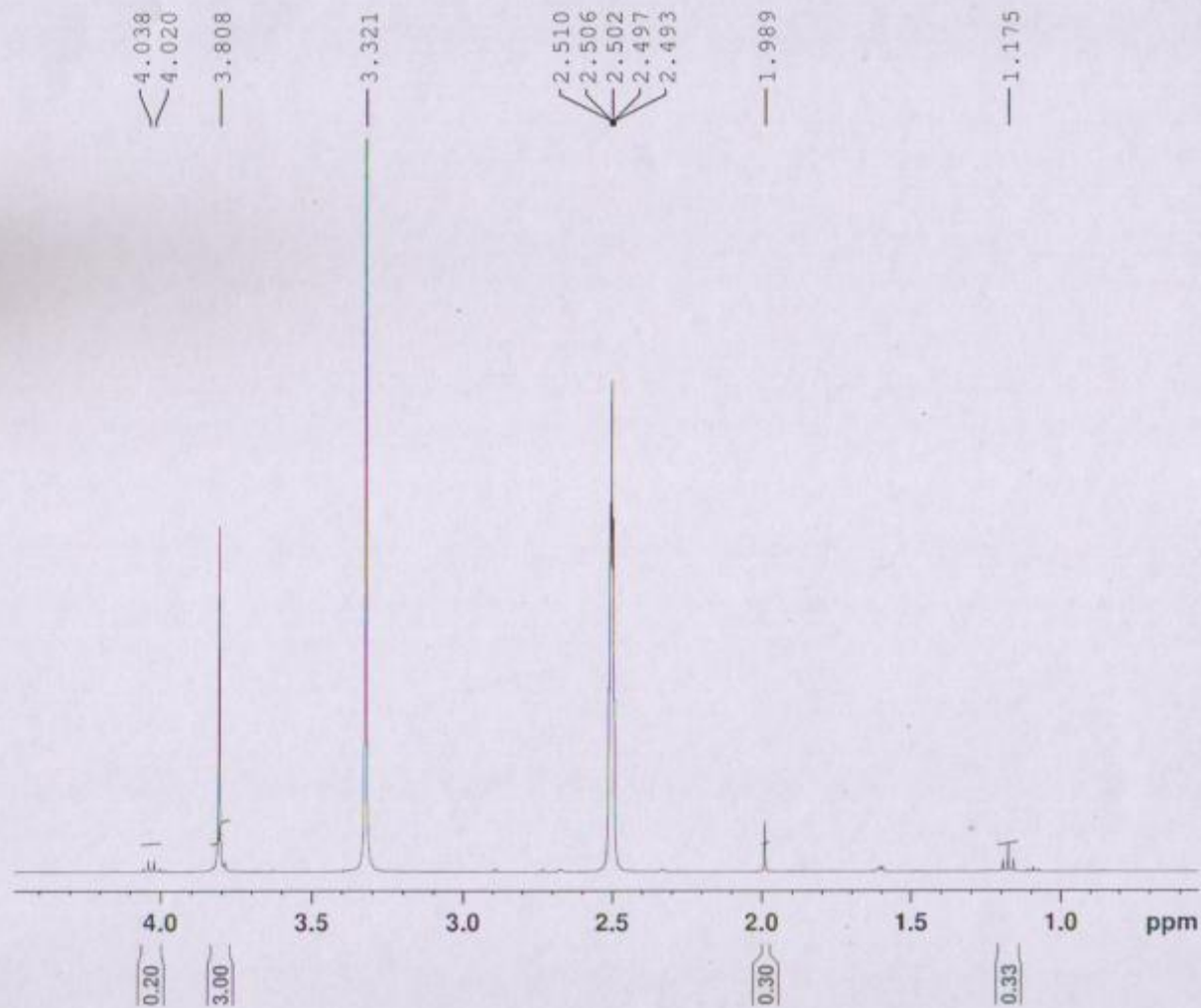
F2 - Acquisition Parameters
Date_ 20220824
Time 22.05 h
INSTRUM Avance NEO Nanobay
PROBHD Z163739_0215 (1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DN 61.000 usec
DE 13.89 usec
TE 298.1 K
D1 2.0000000 sec
TDO 1
SFO1 400.2024712 MHz
NUC1 1H
PQ 2.67 usec
PI 8.00 usec
PLW1 23.04899979 W

F2 - Processing parameters
SI 65536
SF 400.200016 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ANL-MCL3-NMR-006

C6292-054



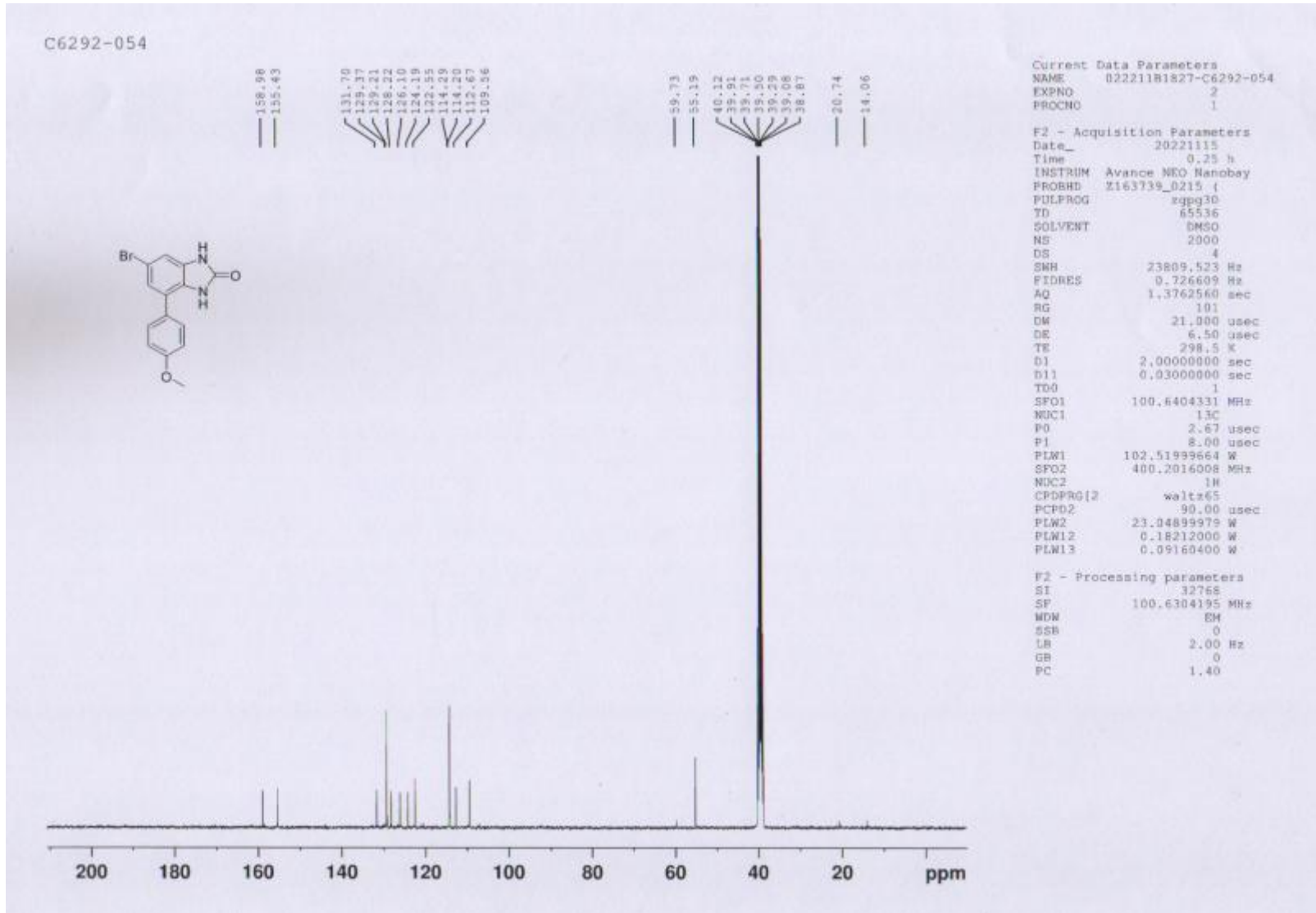
Current Data Parameters
NAME 022208C4809-C6292-054
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220824
Time 22.05 h
INSTRUM Avance NEO Nanobay
PROBHD Z163739_0215 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.1 K
D1 2.00000000 sec
TDO 1
SFO1 400.2024712 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 23.04899979 W

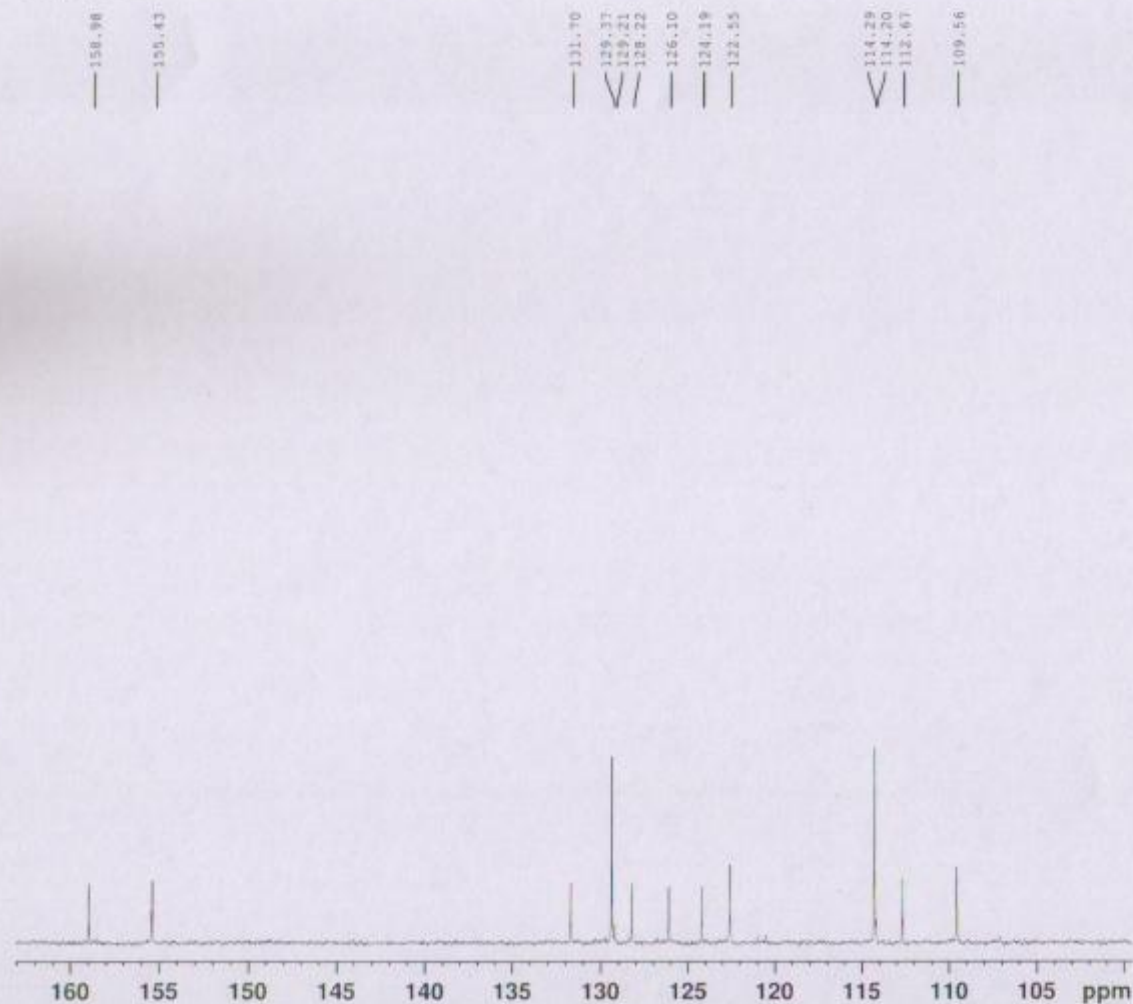
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SF 400.2000016 MHz
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SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ANL-MCL3-NMR-006

13C NMR of 6-Bromo-4-(4-methoxyphenyl)-1,3-dihydro-2H-benzo[d]imidazol-2-one (2m)



C6292-054

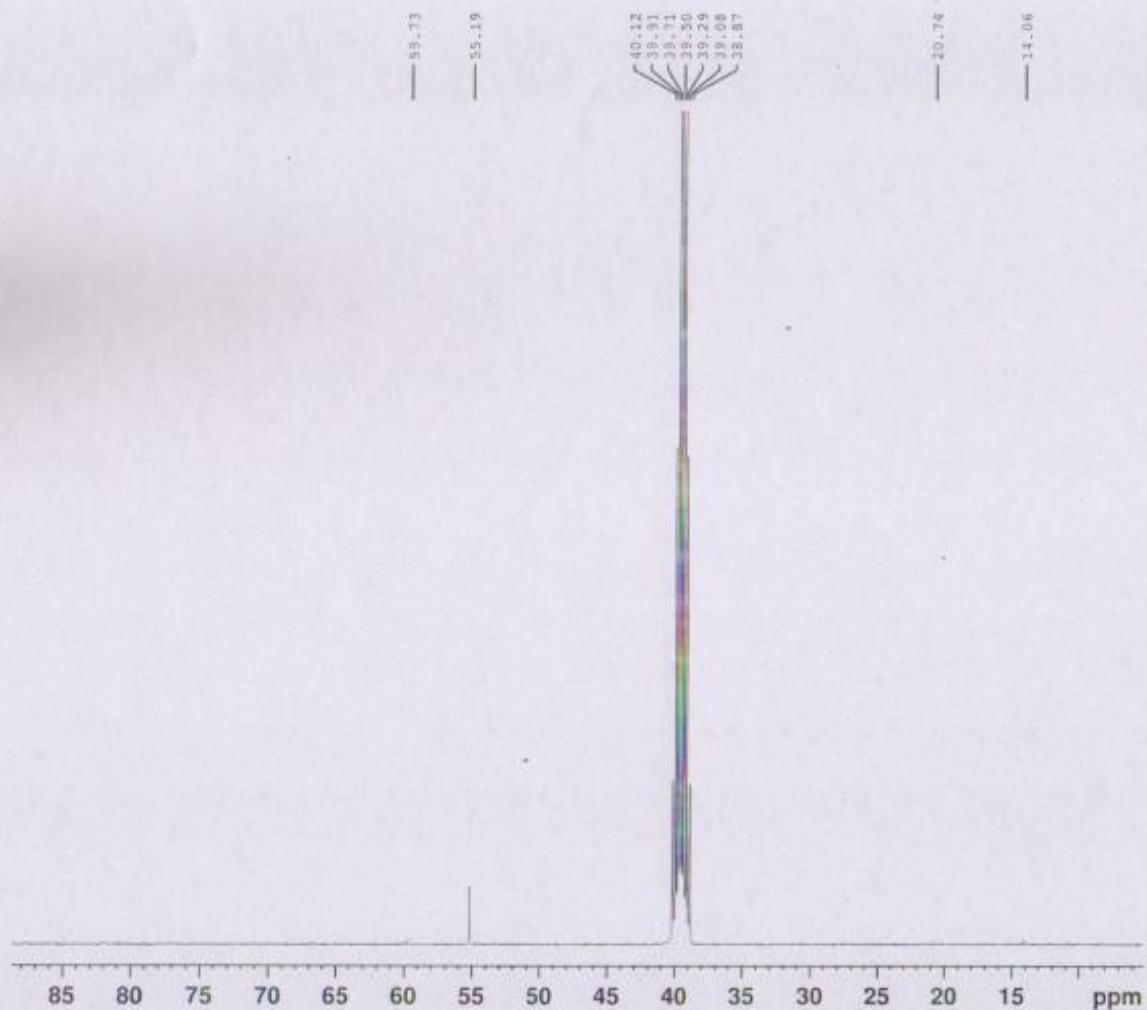


Current Data Parameters
NAME 02221181827-C6292-054
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221115
Time 0.25 h
INSTRUM Avance NEO Nanobay
PROBHD X161718_0215 1
PULPROG zgpg30
TD 63336
SOLVENT DMSO
NS 2000
DS 4
SWH 23809.521 Hz
FIDRES 0.726699 Hz
AQ 1.3762560 sec
RG 101
DN 21.000 usec
DE 6.50 usec
TE 298.5 K
D1 2.0000000 sec
D11 0.0300000 sec
TDD 1
SFO1 100.6404331 MHz
NUC1 13C
PO 2.67 usec
P1 8.00 usec
PLW1 102.51999664 W
SFO2 400.2016008 MHz
NUC2 1H
CPDPRG12 waltz65
PCPD2 90.00 usec
PLW2 23.04895979 W
PLW12 8.18212000 W
PLW13 0.09160400 W

F2 - Processing parameters
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SF 100.6304195 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

C6292-054

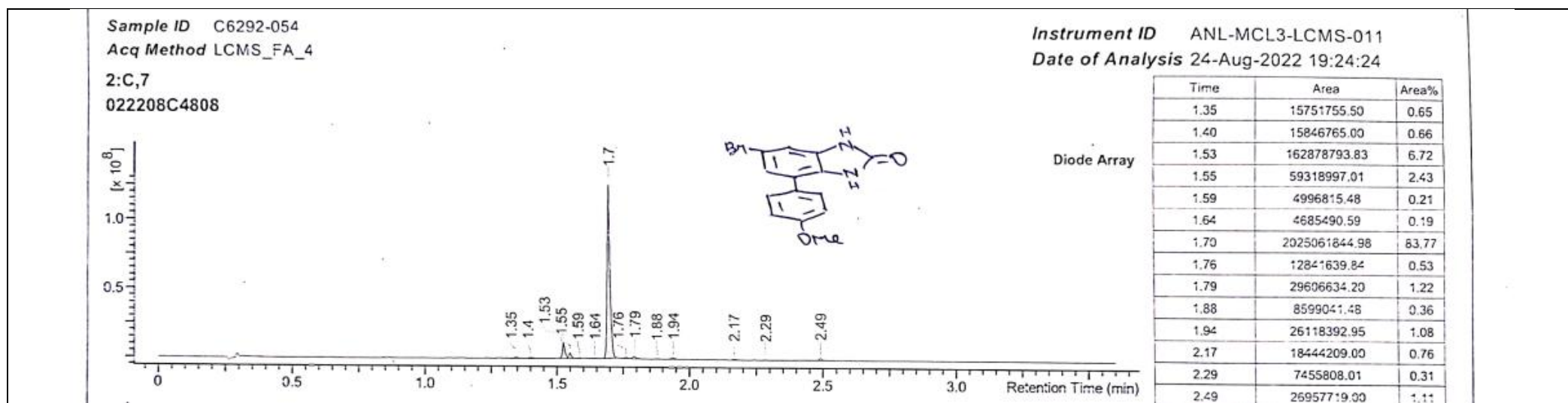


Current Data Parameters
NAME 02221181827-C6292-054
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221115
Time 0.25 h
INSTRUM Avance NEO Nanobay
PROBHD 2163739_0215 1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DM 21.000 usec
SE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
S11 0.03000000 sec
TD0 1
SFO1 100.6404331 MHz
NUC1 13C
PD 2.67 usec
P1 8.00 usec
PLW1 102.51999664 W
SFO2 400.2016008 MHz
NUC2 1H
CPDPRG12 waltz65
PCPD2 90.00 usec
PLW2 23.04899979 W
PLW12 0.18212000 W
PLW13 0.09160400 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 2.00 Hz
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PC 1.40

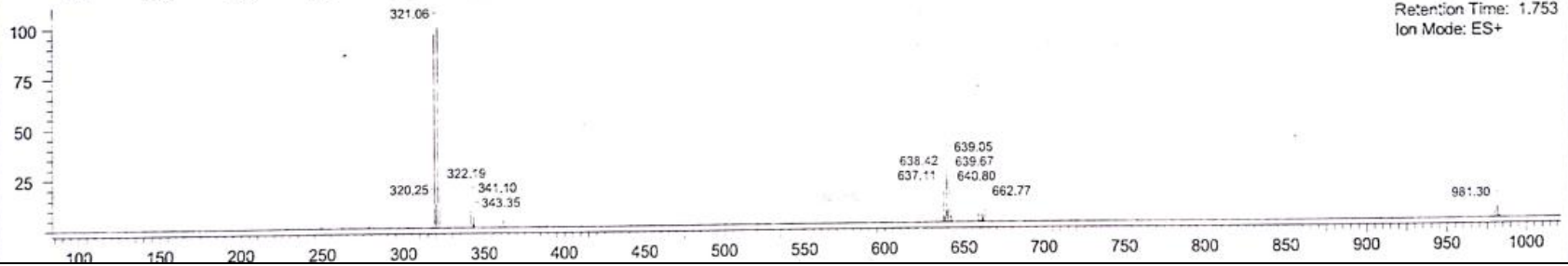
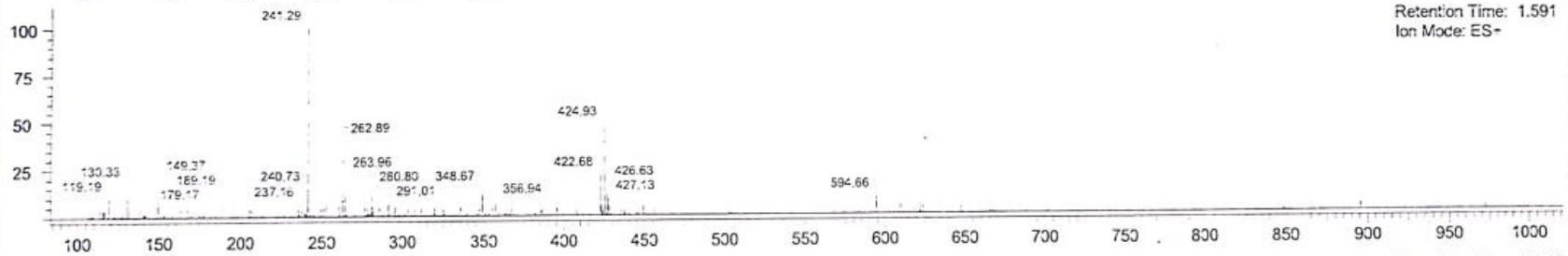
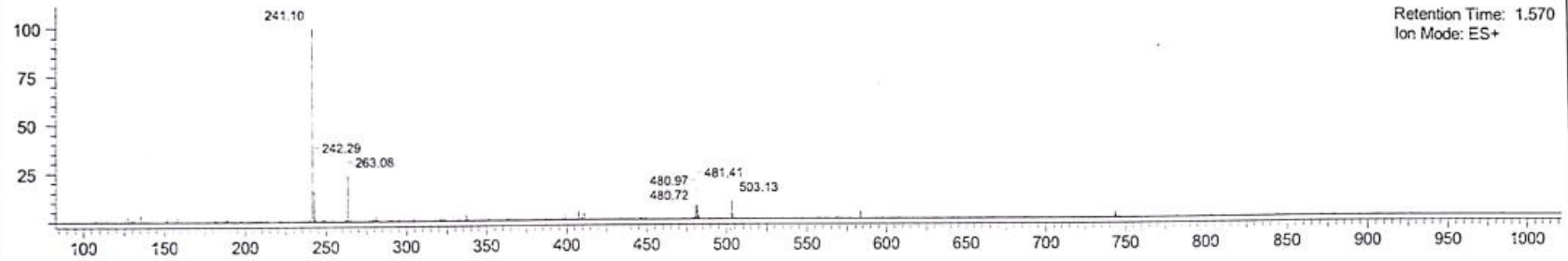
LCMS of 6-Bromo-4-(4-methoxyphenyl)-1,3-dihydro-2H-benzo[d]imidazol-2-one (2m)



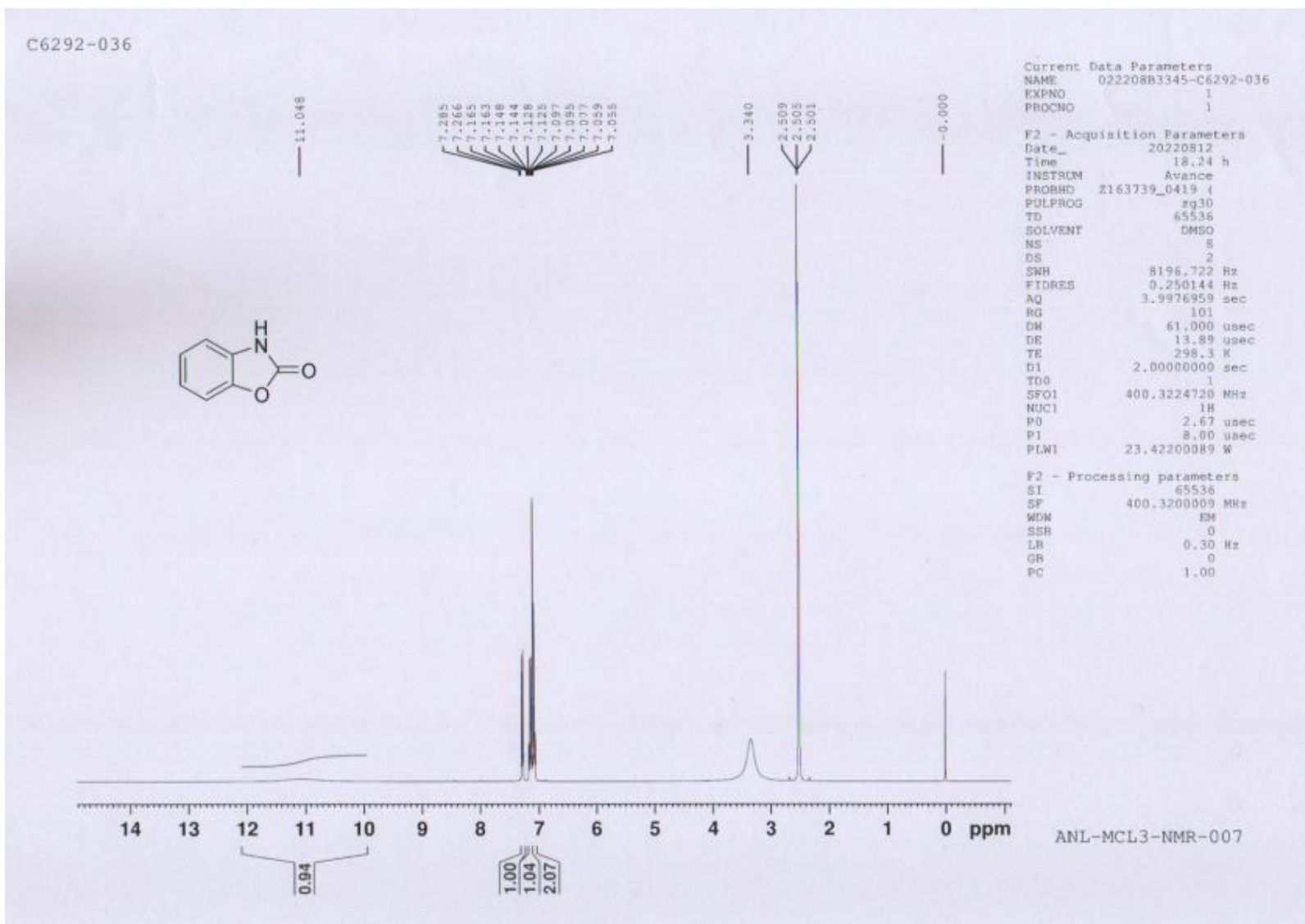
Sample ID C6292-054
Acq Method LCMS_FA_4
2:C,7
022208C4808

Discovery Chemistry – Analytical Services

Instrument ID ANL-MCL3-LCMS-011
Date of Analysis 24-Aug-2022 19:24:24

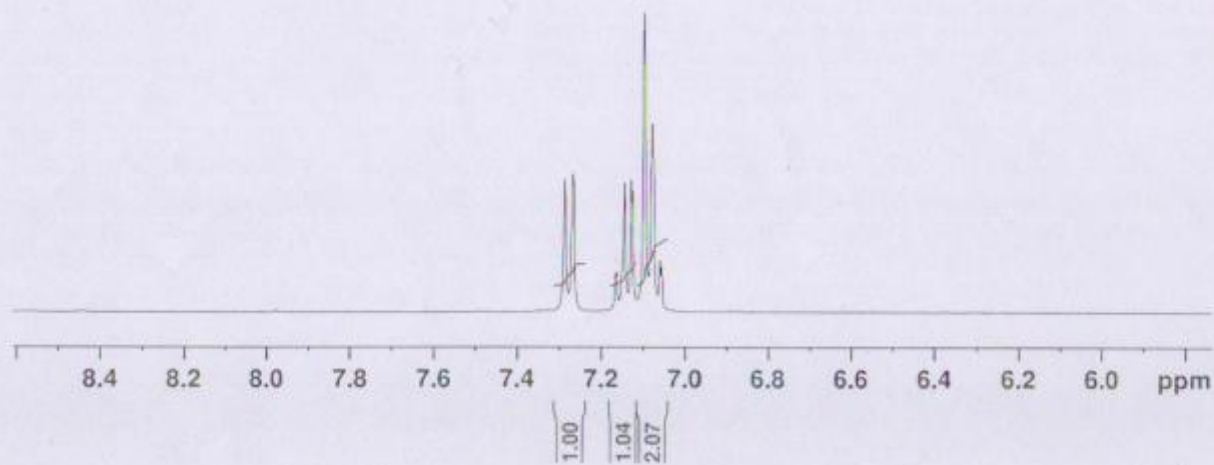


¹H NMR of 2-benzoxazolone (2p)



C6292-036

7.285
7.266
7.165
7.163
7.148
7.148
7.128
7.125
7.097
7.095
7.077
7.059
7.055



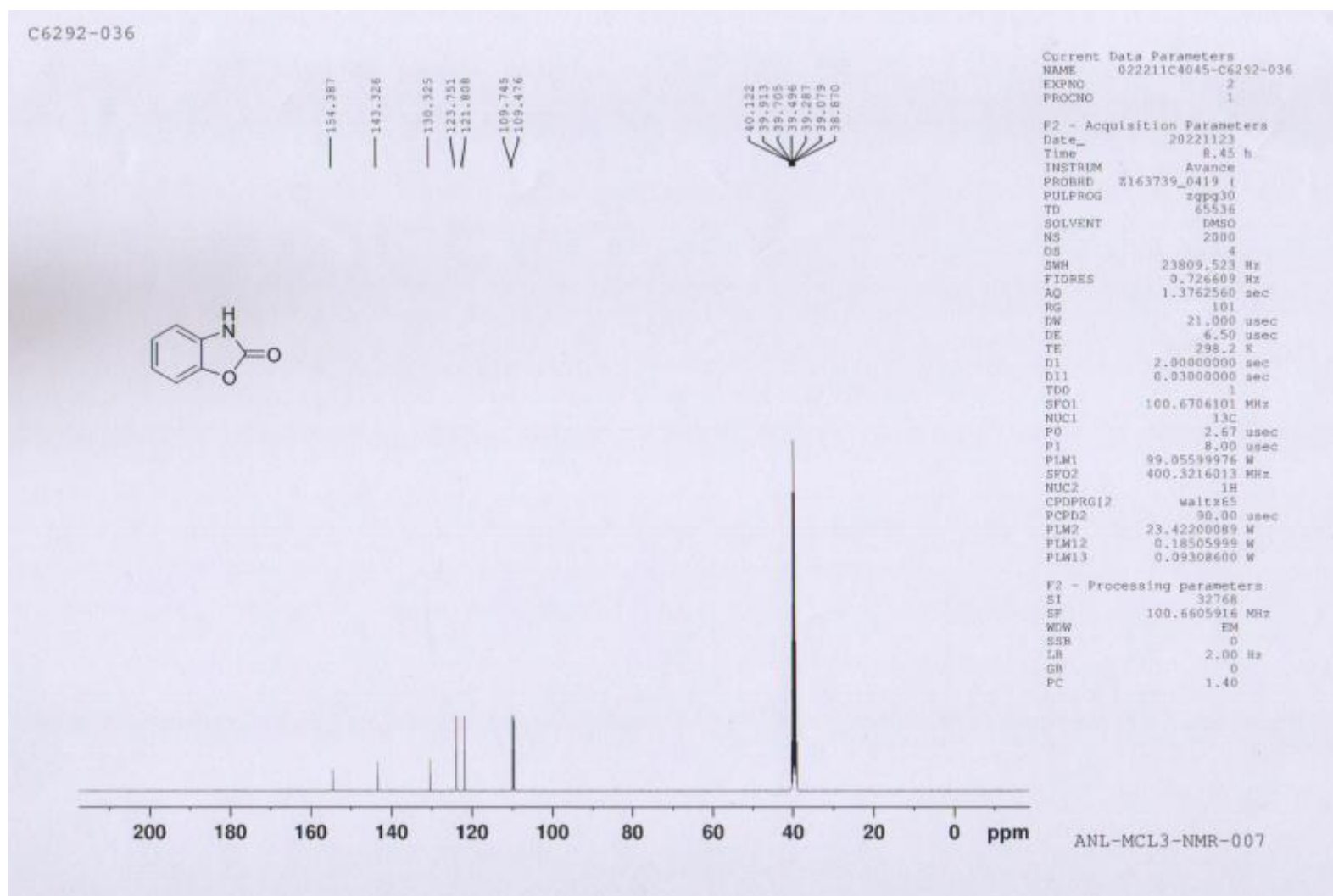
Current Data Parameters
NAME 022208B3345-C6292-036
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220812
Time 18.24 h
INSTRUM Avance
PROBHD Z163739_0419 1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SMH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DM 61.000 usec
DE 13.89 usec
TE 298.3 K
D1 2.00000000 sec
TDO 1
SFO1 400.3224720 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 23.42200089 W

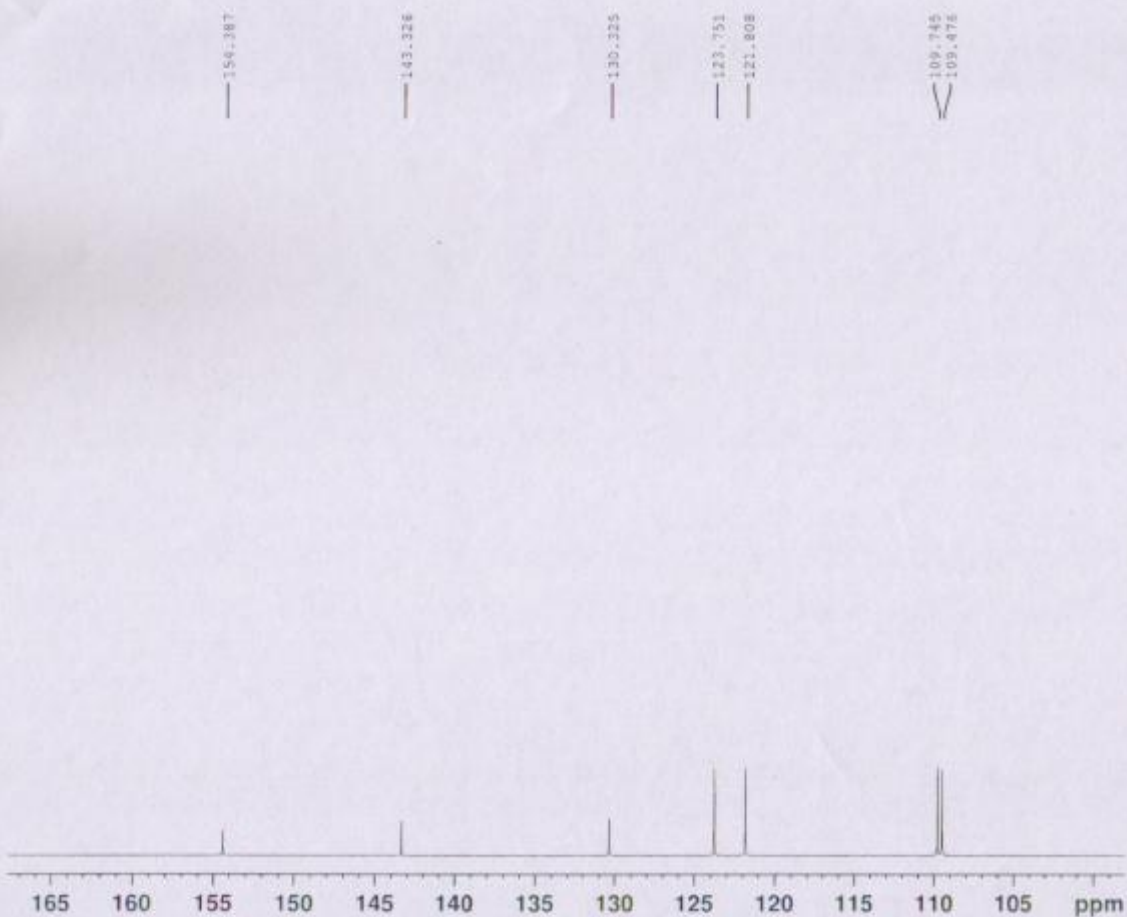
F2 - Processing parameters
SI 65536
SF 400.3200009 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ANL-MCL3-NMR-007

¹³C NMR of 2-benzoxazolone (2p)



C6292-036



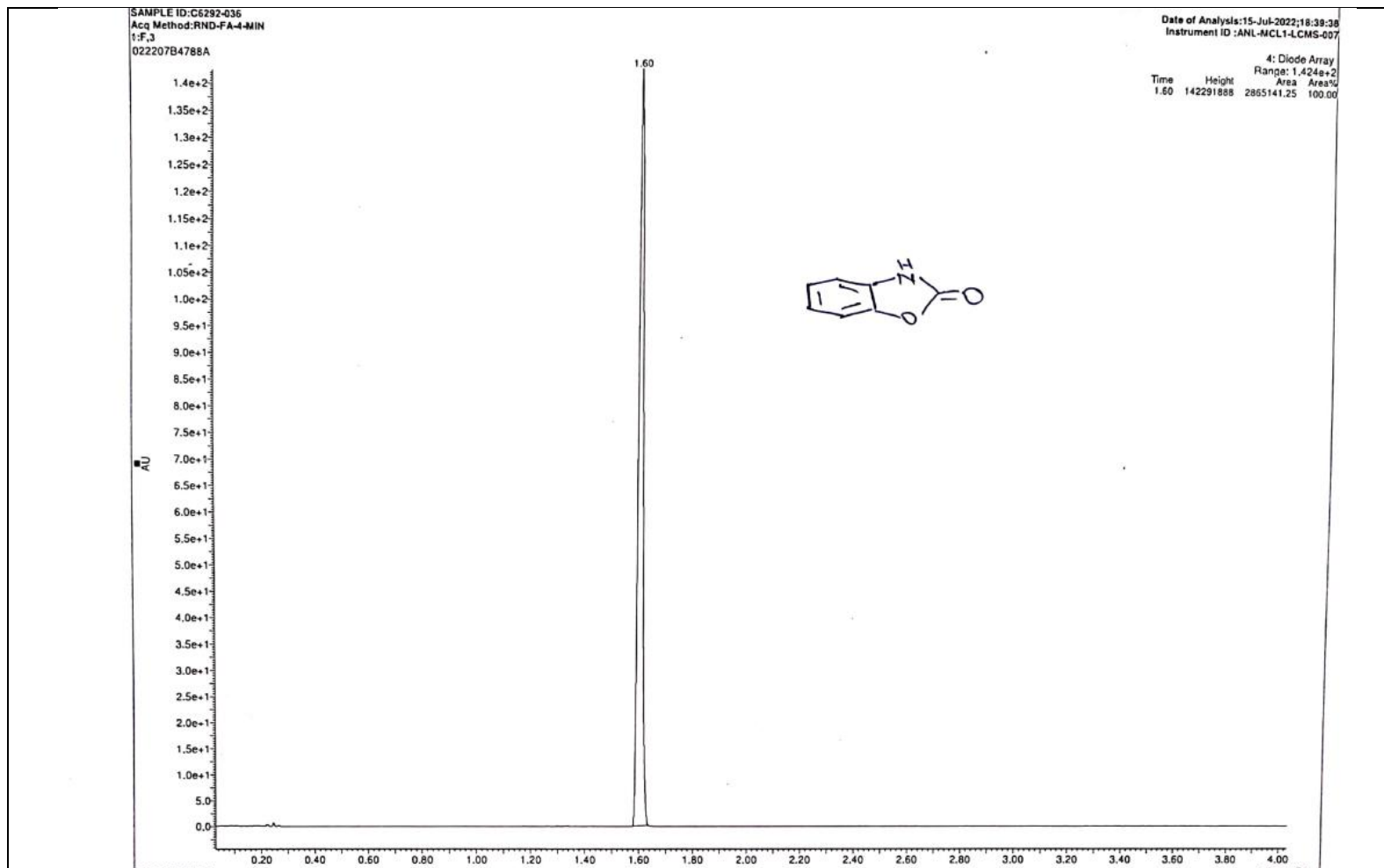
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NAME 022211C4045-C6292-036
EXPNO 2
PROCNO 1

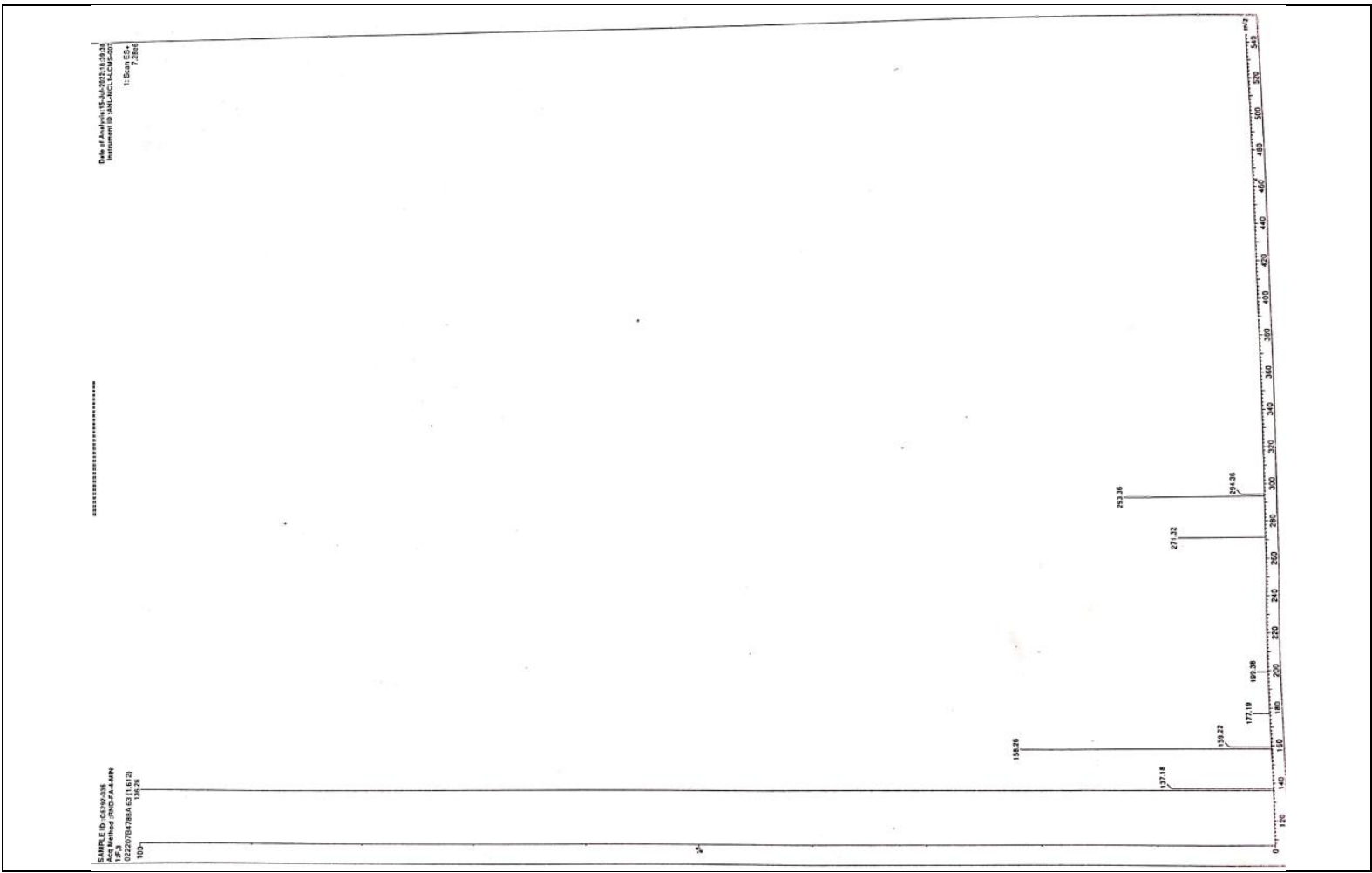
F2 - Acquisition Parameters
Date_ 20221123
Time 8.45 h
INSTRUM Avance
PROBHD Z163739_0419 (4
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 23809.521 Hz
FIDRES 0.726609 Hz
AQ 1.1762560 sec
RG 101
DM 21.000 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6706101 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 99.05599976 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG2 waltz65
PCPD2 90.00 usec
PLW2 23.42200089 W
PLW12 0.18505999 W
PLW13 0.09308600 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

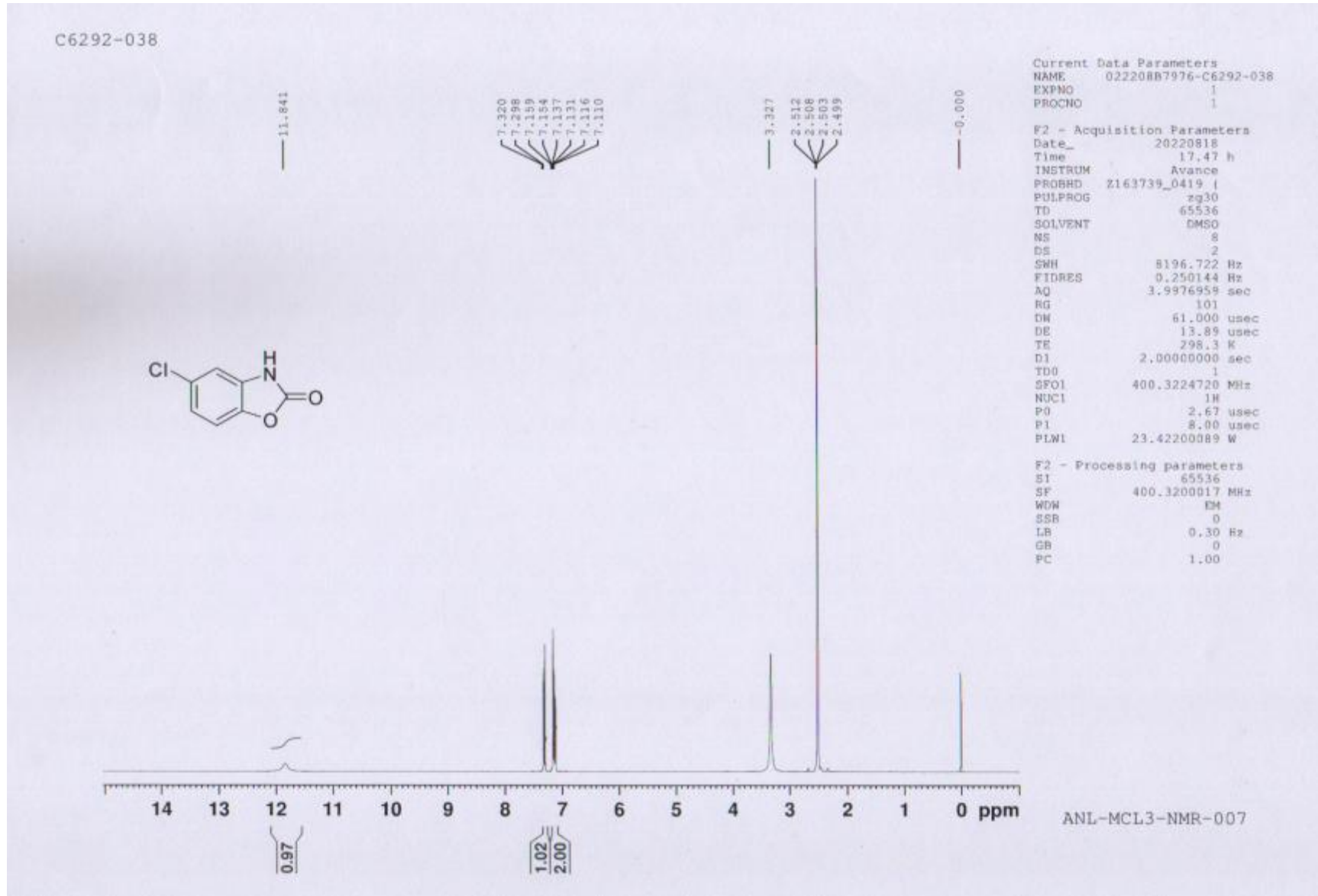
ANL-MCL3-NMR-007

LCMS of 2-benzoxazolone (2p)





¹H NMR of 5-Chlorobenzo[d]oxazol-2(3H)-one (2q)



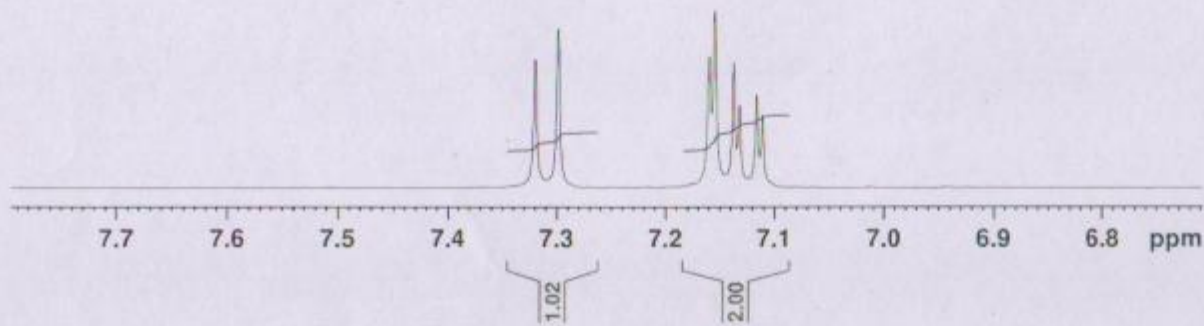
C6292-038

7.320
7.298
7.158
7.154
7.150
7.146
7.142
7.140

Current Data Parameters
NAME 022208B7976-C6292-038
EXPNO 1
PROCNO 1

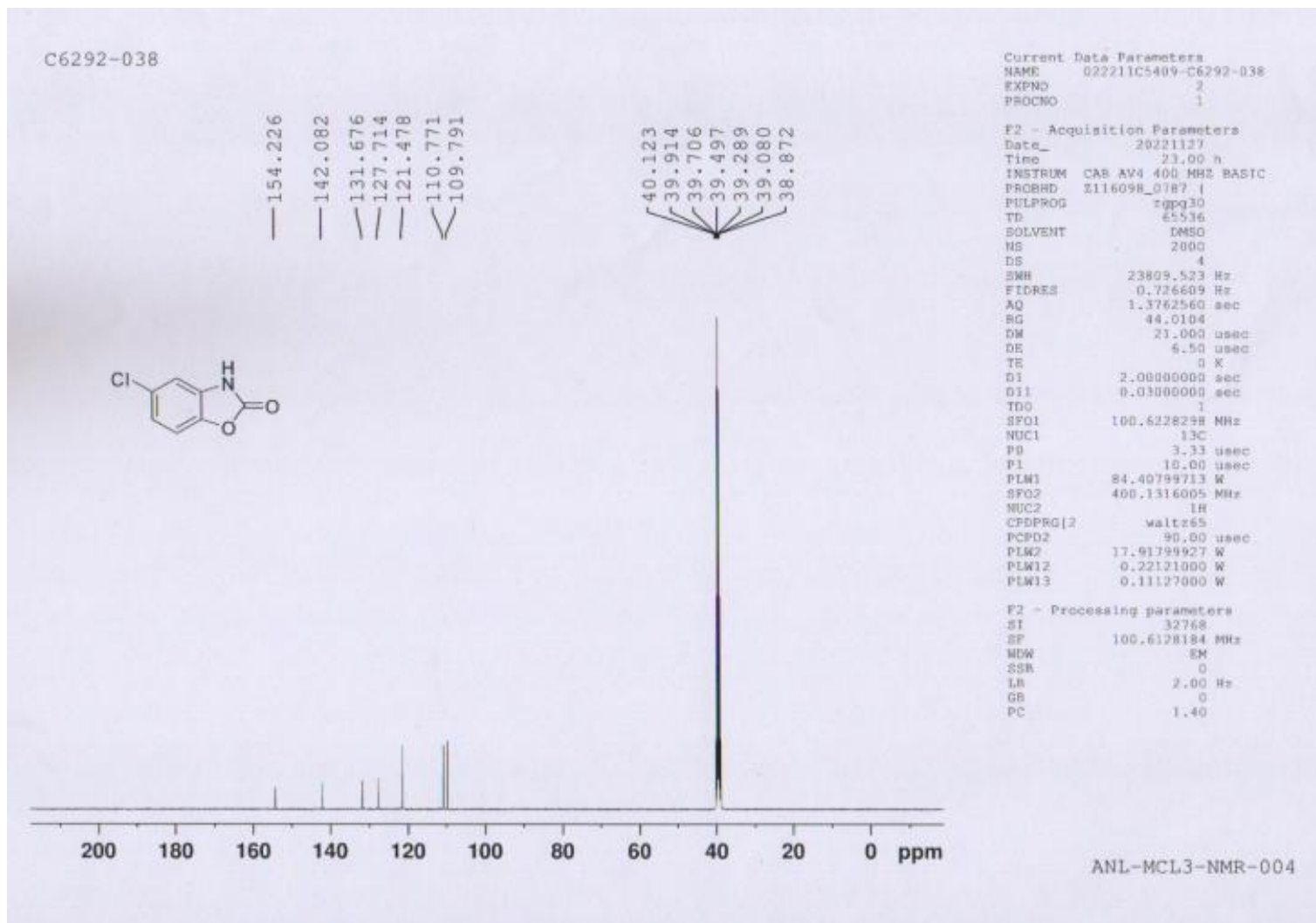
F2 - Acquisition Parameters
Date_ 20220818
Time 17.47 h
INSTRUM Avance
PROBRD W161739_0419 f
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9974959 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.3 K
D1 2.0000000 sec
TDO 1
SFO1 400.3224720 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 23.42200089 W

F2 - Processing parameters
SI 65536
SF 400.3200017 MHz
WDM EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

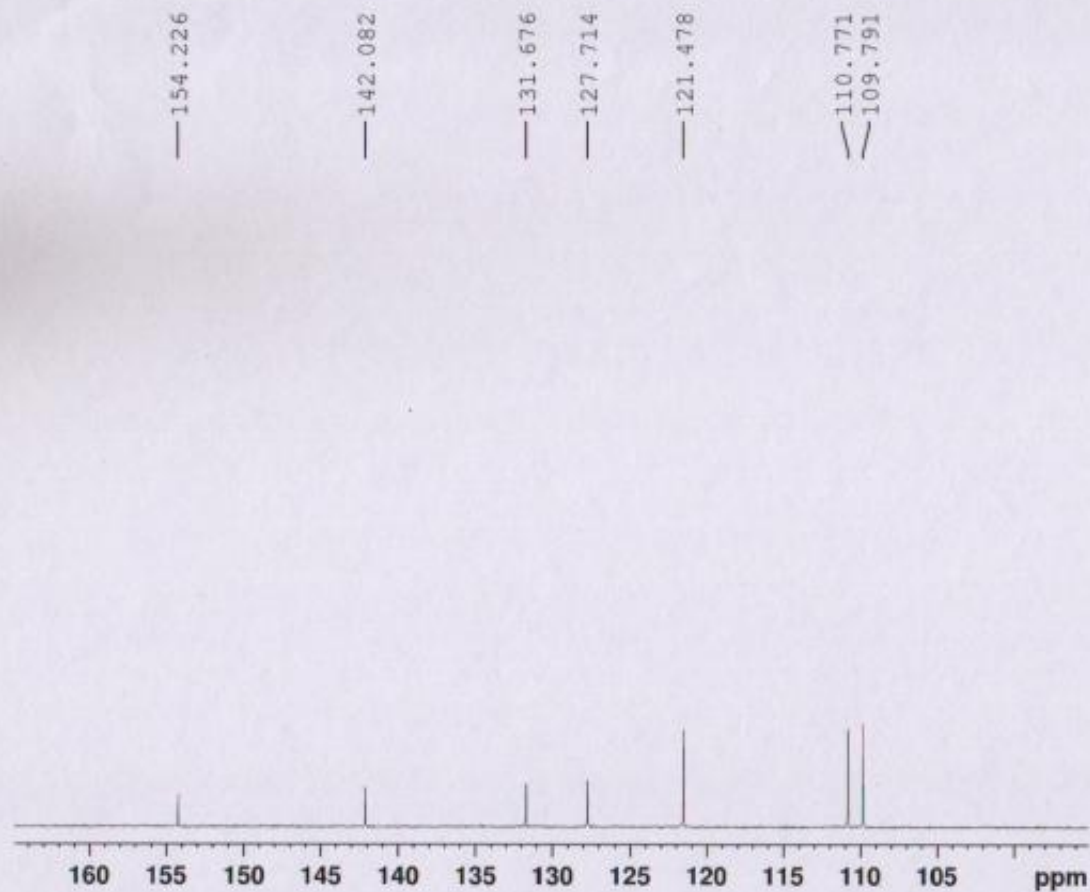


ANL-MCL3-NMR-007

¹³C NMR of 5-Chlorobenzo[d]oxazol-2(3H)-one (2q)



C6292-038



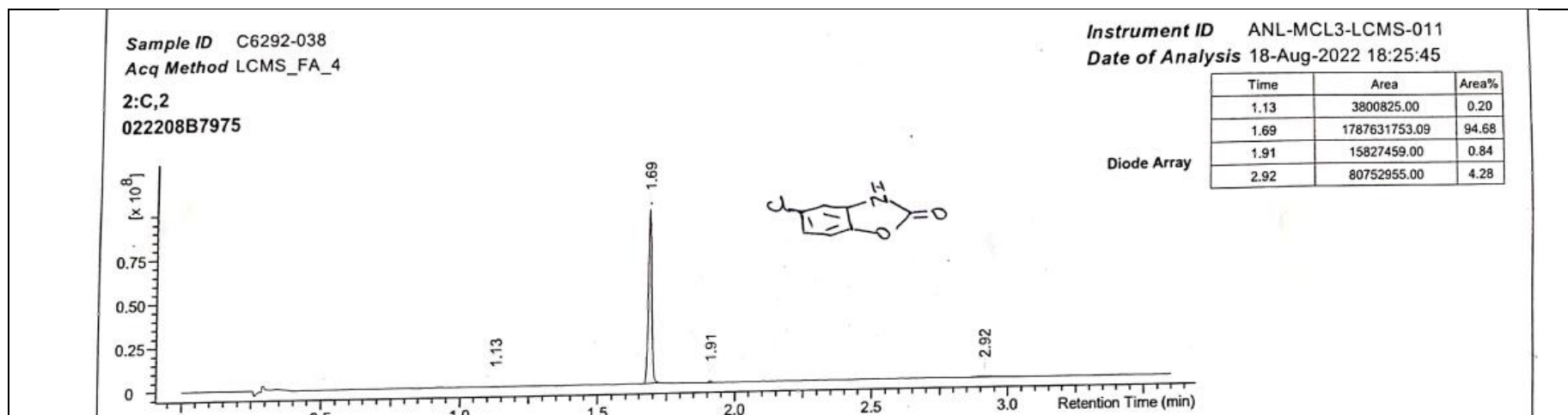
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NAME 022211C5409-C6292-038
EXPNO 2
PROCNO 1

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Time 23.00 h
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PROBHD E116096_0787 i
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 44.0104
DM 21.000 usec
DE 6.50 usec
TE 0 K
D1 2.0000000 sec
D11 0.0100000 sec
TDC 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 84.40799713 W
SFO2 400.1316005 MHz
NUC2 1H
PCPDPC12 waltz65
PCPD2 90.00 usec
PLW2 17.91799927 W
PLW12 0.22121000 W
PLW13 0.11127000 W

F2 - Processing parameters
S1 32768
SF 100.6128184 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

ANL-MCL3-NMR-004

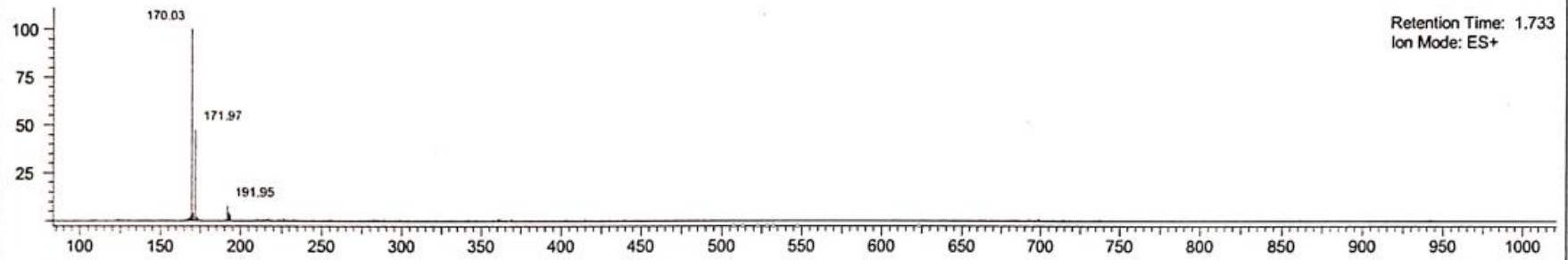
LCMS of 5-Chlorobenzo[d]oxazol-2(3H)-one (2q)



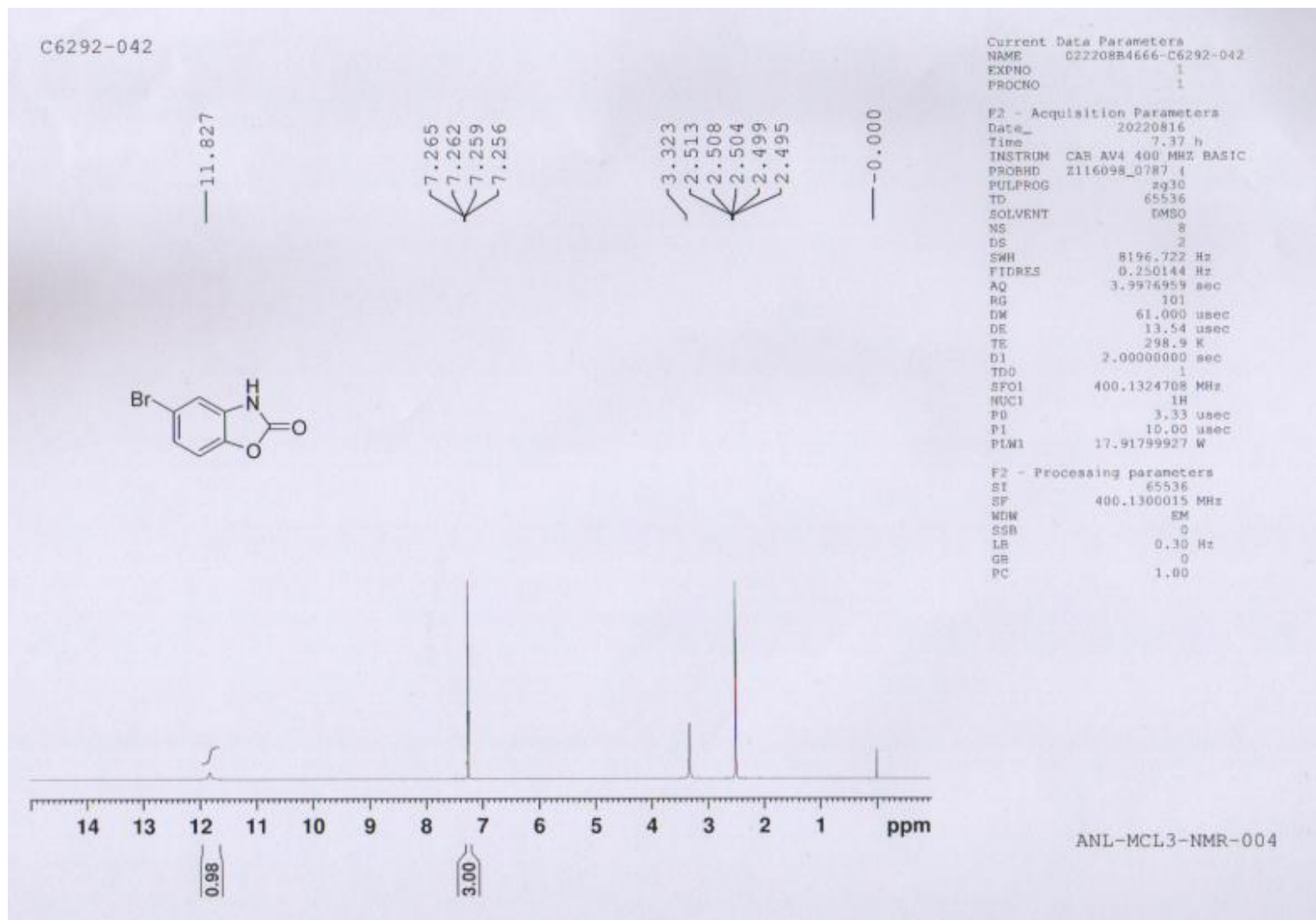
Sample ID C6292-038
Acq Method LCMS_FA_4
2:C,2
022208B7975

Discovery Chemistry – Analytical Services

Instrument ID ANL-MCL3-LCMS-011
Date of Analysis 18-Aug-2022 18:25:45

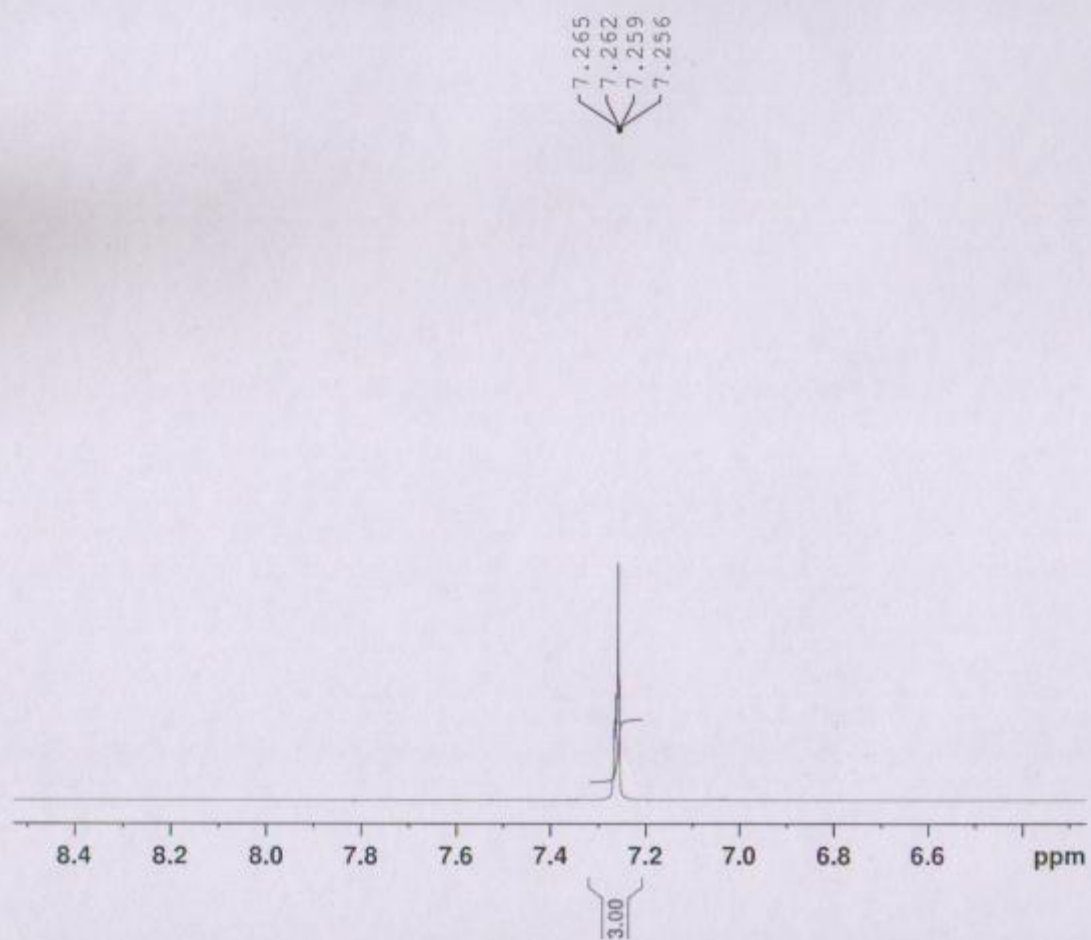


¹H NMR of 5-Bromobenzo[d]oxazol-2(3H)-one (2r)



ANL-MCL3-NMR-004

C6292-042



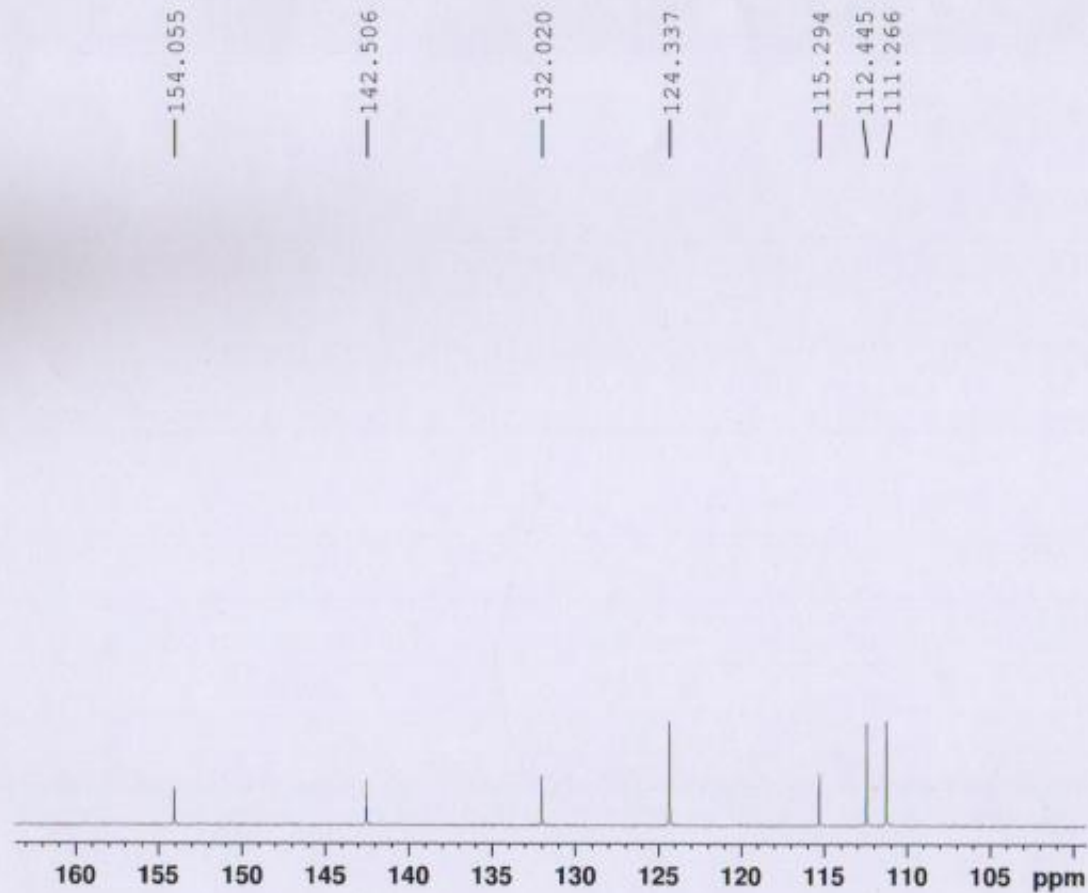
Current Data Parameters
NAME 022208B4666-C6292-042
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220816
Time 7.37 h
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PROBHD S116098_0787 (1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.54 usec
TE 298.9 K
D1 2.00000000 sec
TDC 1
SFO1 400.1324708 MHz
NUC1 1H
PQ 3.33 usec
PI 10.00 usec
PLW1 17.91799927 W

F2 - Processing parameters
SI 65536
SF 400.1300015 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ANL-MCL3-NMR-004

C6292-042



Current Data Parameters
NAME 022211C5405-C6292-042
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221128
Time 0.58 h
INSTRUM CAB AV4 400-MHZ BASIC
PROBHD X116098_0787 4
PULPROG zgpg30
TD 45536
SOLVENT DMSO
NS 2000
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 40.625
DW 21.000 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 84.40799713 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG12 waltz155
PCPD2 90.00 usec
PLW2 17.91799927 W
PLW12 0.22121000 W
PLW13 0.11127000 W

F2 - Processing parameters
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SSB 0
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GB 0
PC 1.40

ANL-MCL3-NMR-004

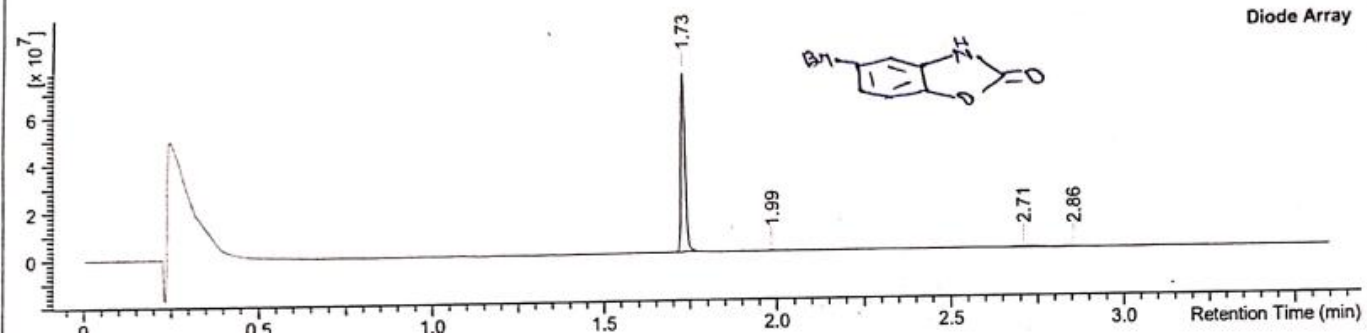
LCMS of 5-Bromobenzo[d]oxazol-2(3H)-one (2r)

Sample ID C6292-042
Acq Method LCMS_FA_4
1:A,6
022208B4665

Instrument ID ANL-MCL3-LCMS-011
Date of Analysis 16-Aug-2022 08:33:07

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2.71	51307921.13	3.62
2.86	24568117.08	1.73

Diode Array



Sample ID C629Z-04Z

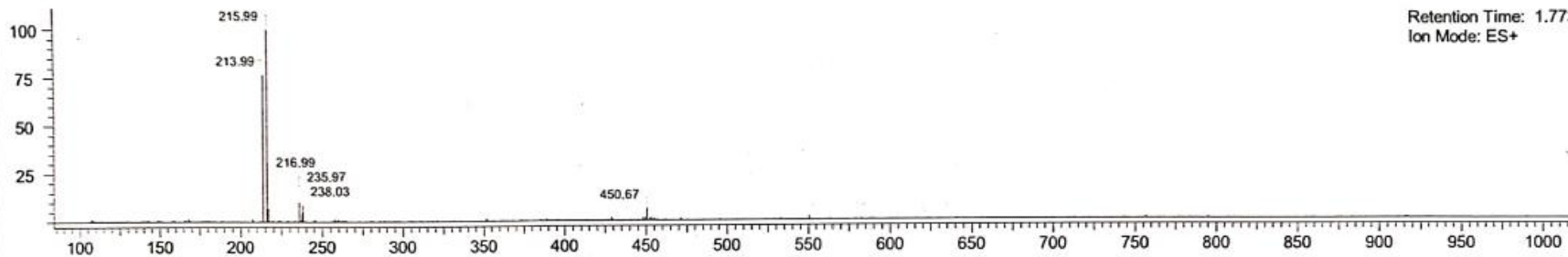
Acq Method LCMS_FA_4

1:A,6

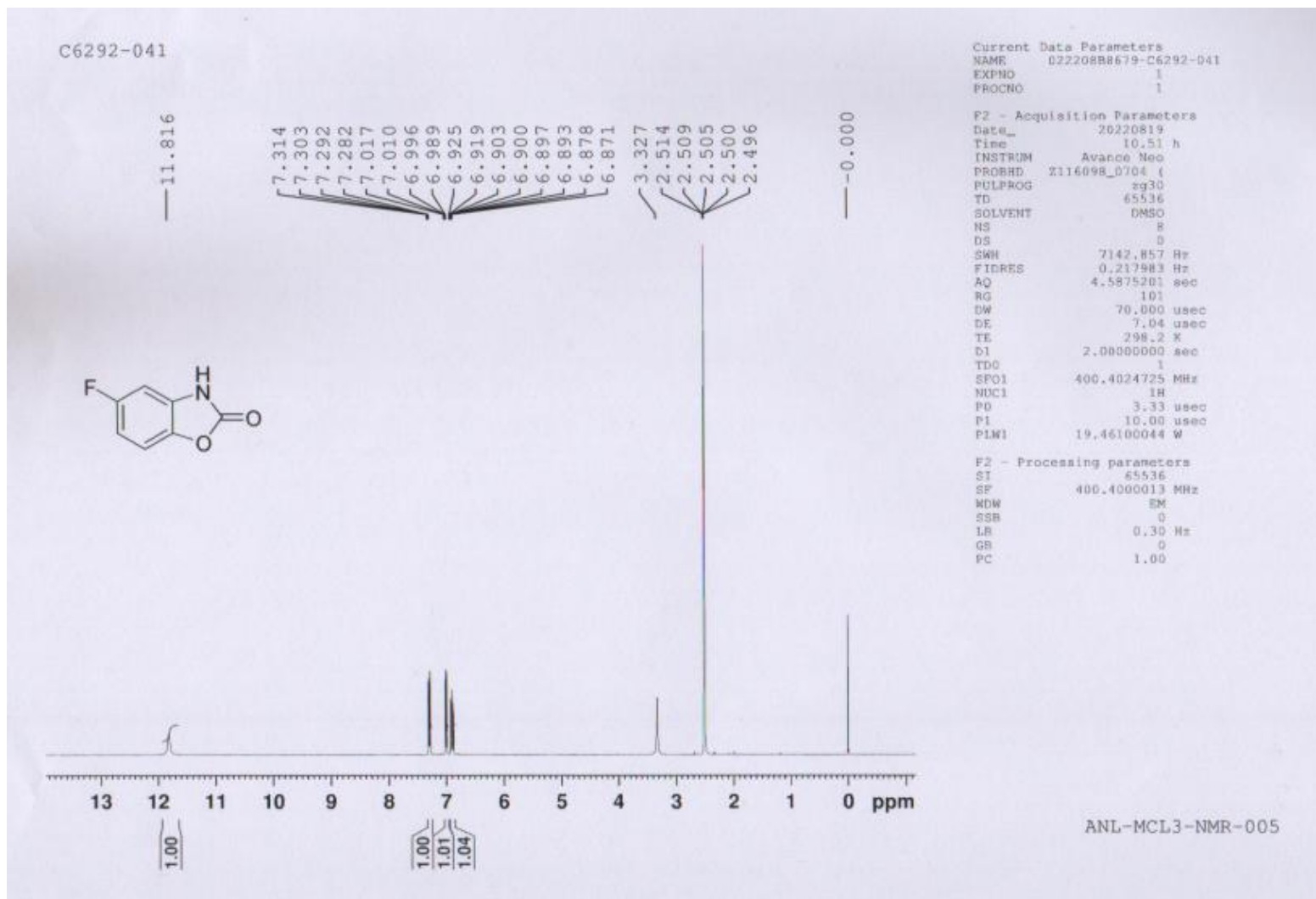
022208B4665

Instrument ID ANL-MCL3-LCMS-011

Date of Analysis 16-Aug-2022 08:33:07



¹H NMR of 5-Fluorobenzo[d]oxazol-2(3H)-one (2s)



C6292-041

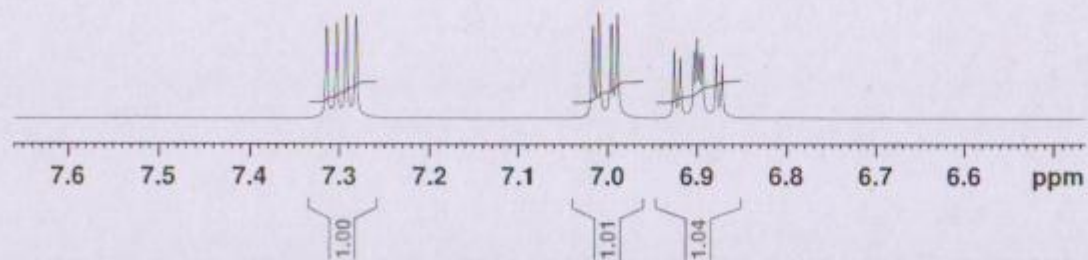
7.314
7.303
7.292
7.282

7.017
7.010
6.996
6.989
6.925
6.919
6.903
6.900
6.897
6.893
6.878
6.871

Current Data Parameters
NAME 022208B8679-C6292-041
EXPNO 1
PROCNO 1

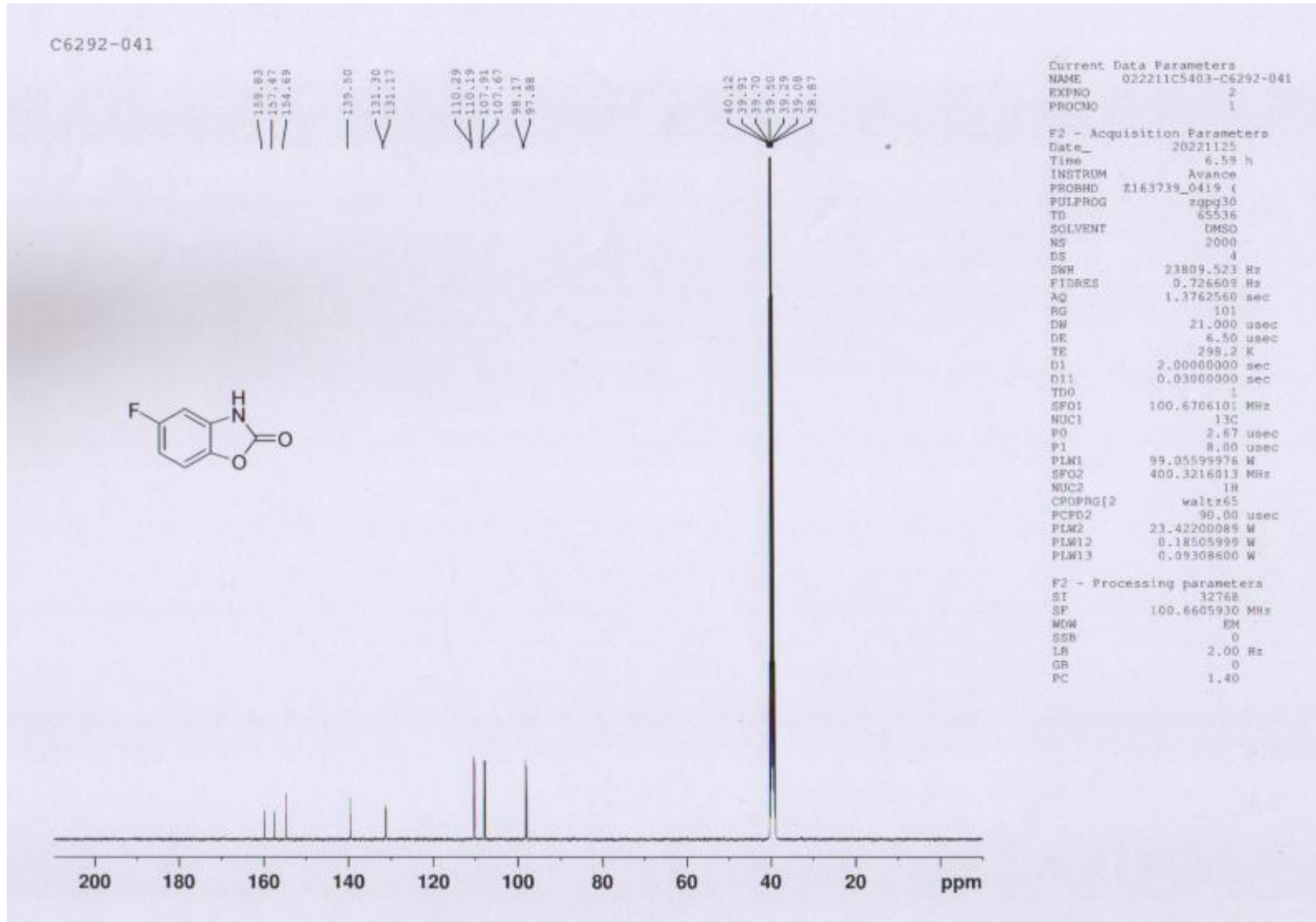
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PROBHD Z116096_0704 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 7142.857 Hz
FIDRES 0.217983 Hz
AQ 4.5875201 sec
RG 101
DW 70.000 usec
DE 7.04 usec
TE 298.2 K
D1 2.00000000 sec
TDO 1
SFO1 400.4024725 MHz
NUC1 1H
PO 3.33 usec
P1 10.00 usec
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F2 - Processing parameters
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LB 0.30 Hz
GB 0
PC 1.00

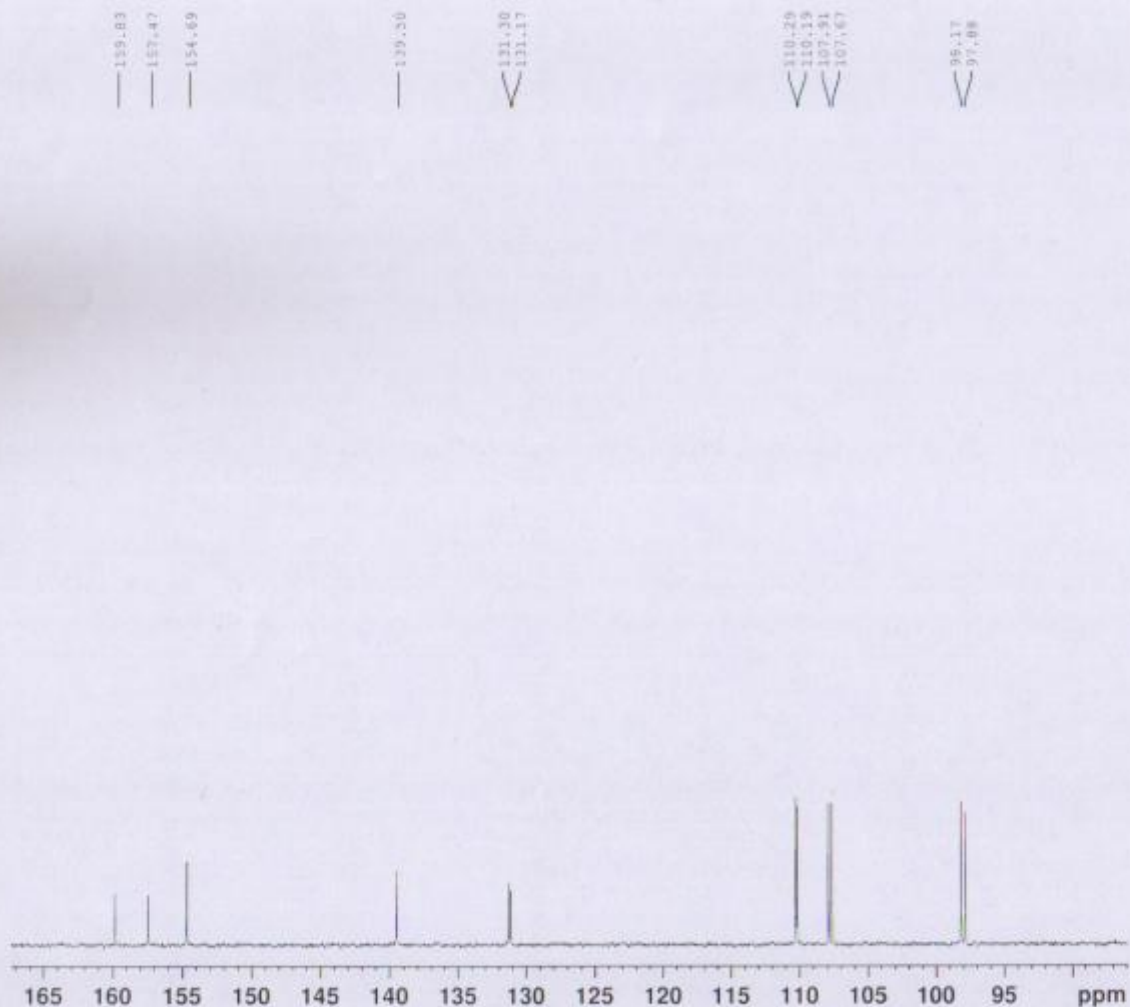


ANL-MCL3-NMR-005

¹³C NMR of 5-Fluorobenzo[d]oxazol-2(3H)-one (2s)



C6292-041

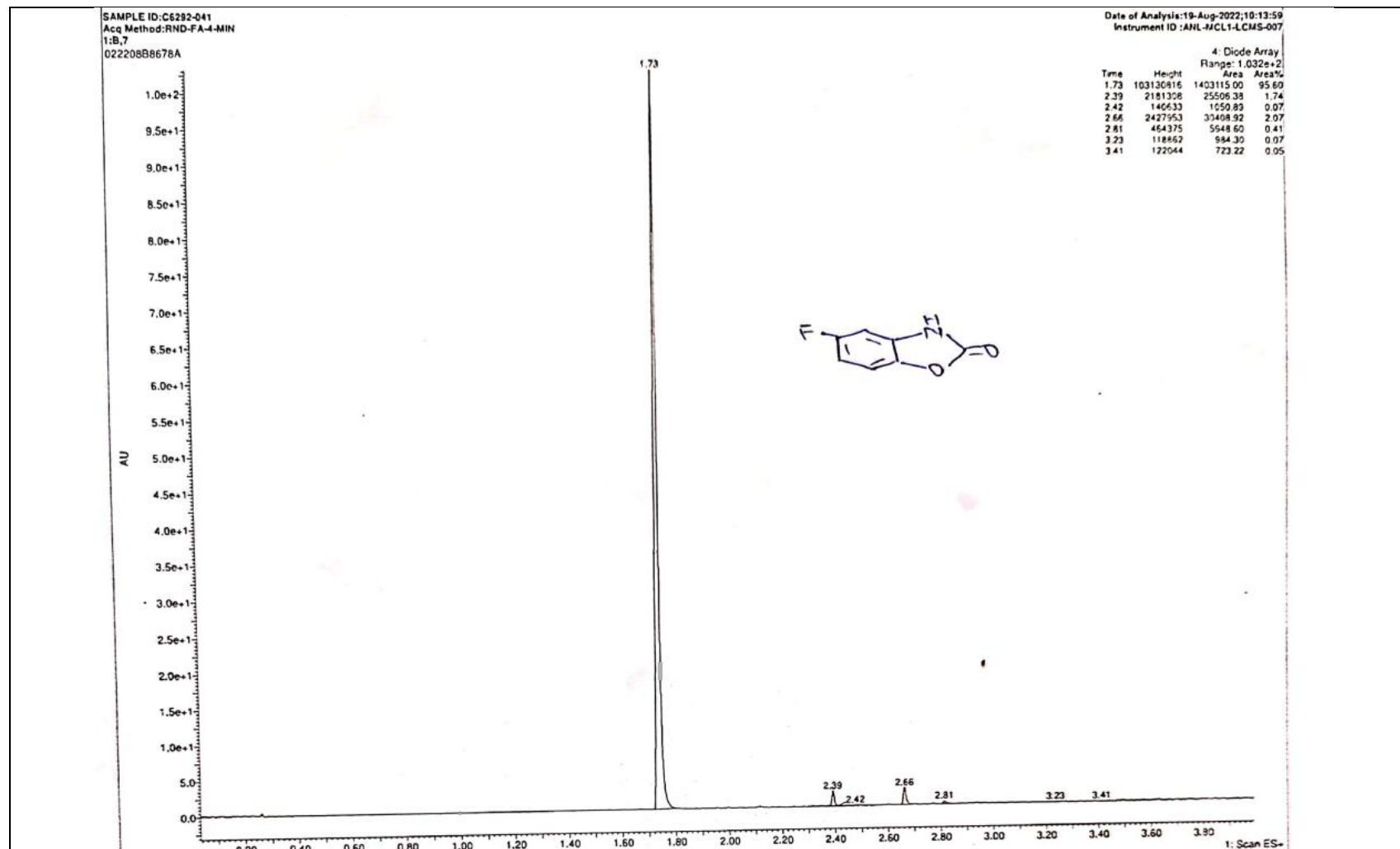


Current Data Parameters
NAME 022211C5403-C6292-041
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221125
Time 6.59 h
INSTRUM Avance
PROBHD E163739_0419 1
PULPROG zgpg30
ID 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6706101 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 99.05599976 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG2 waltz165
PCPD02 90.00 usec
PLW2 23.42200089 W
PLW12 0.18505999 W
PLW13 0.09308600 W

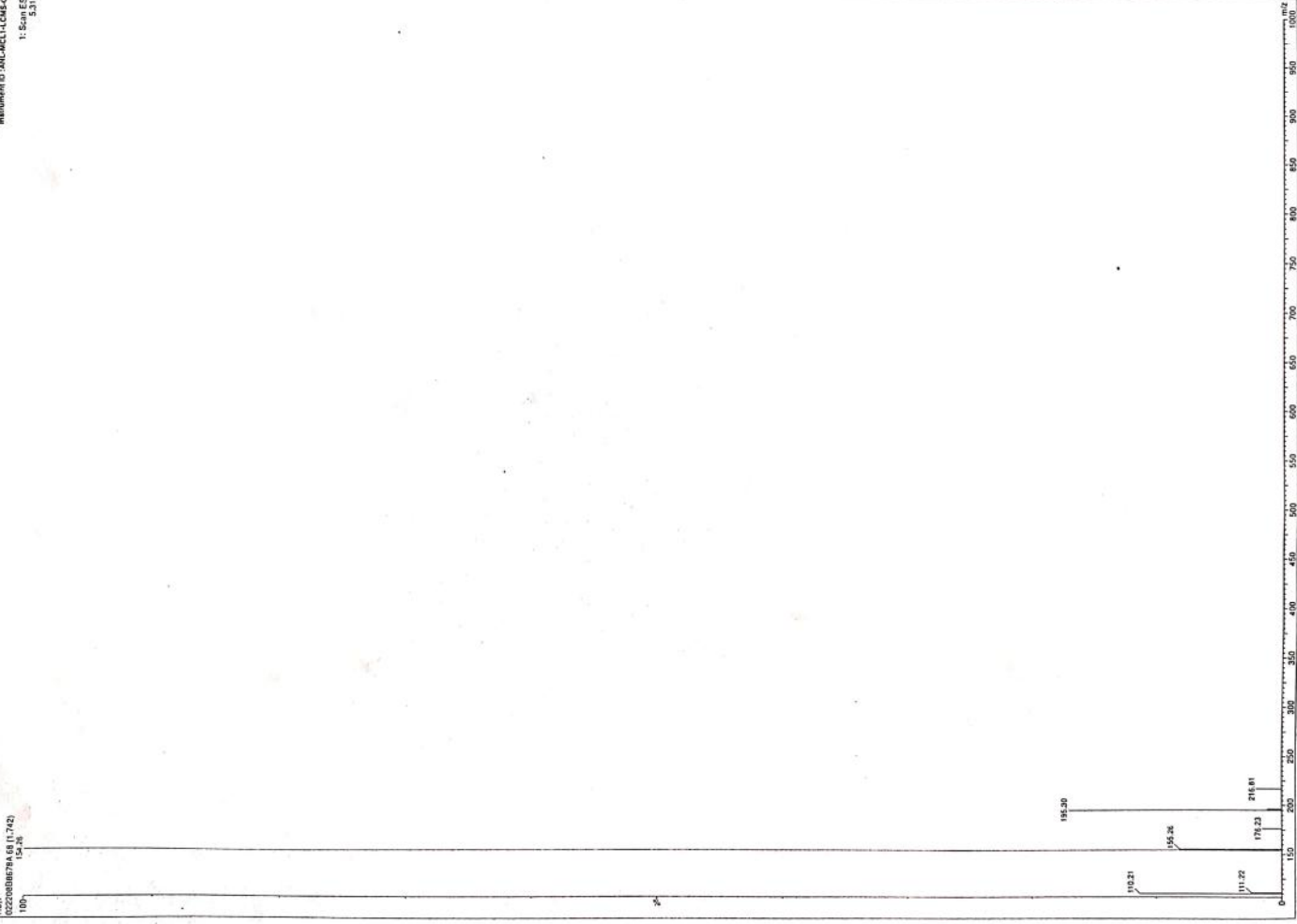
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SI 32768
SF 100.6605930 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

LCMS of 5-Fluorobenzo[d]oxazol-2(3H)-one (2s)

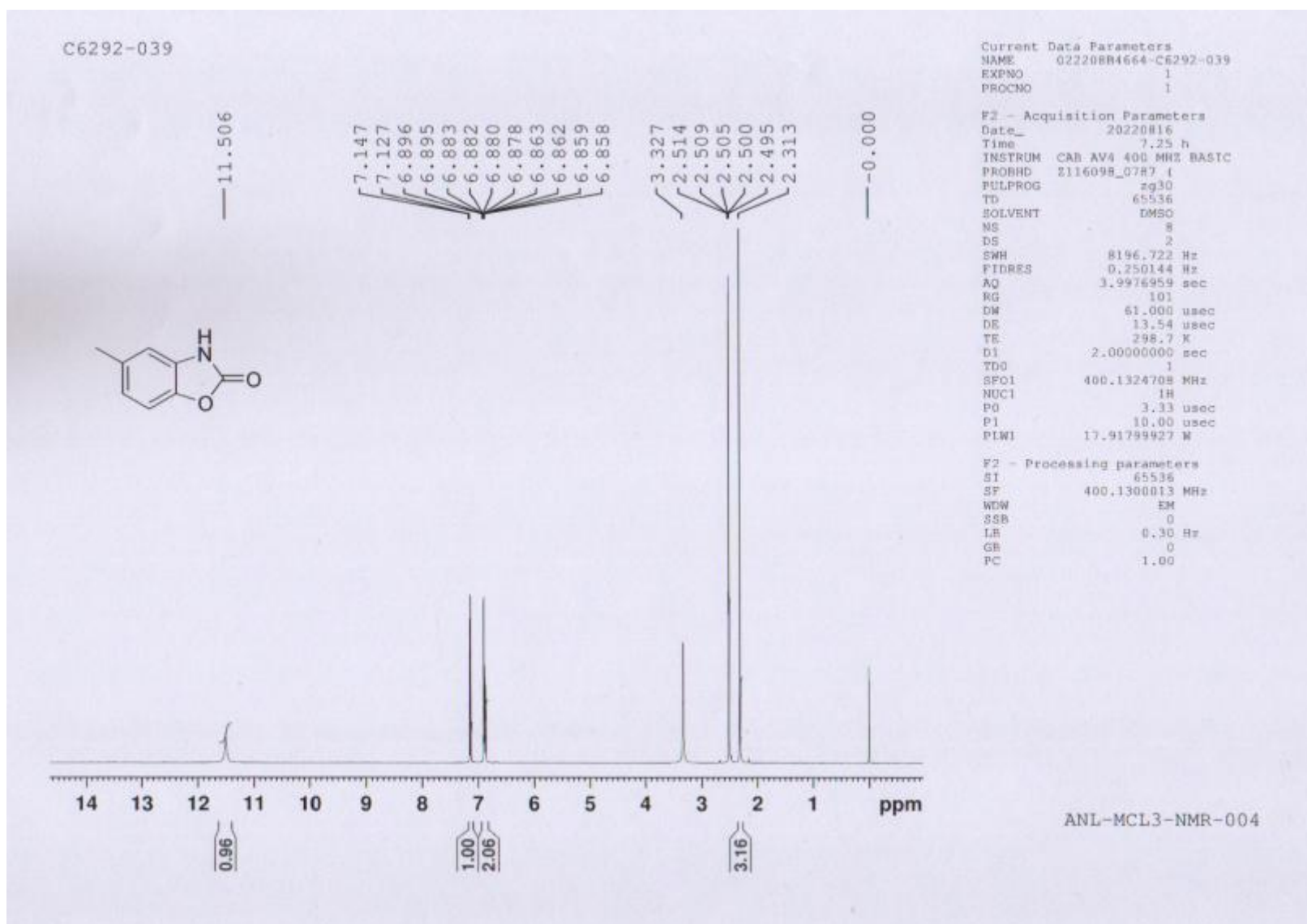


SAMPLE ID: C025041
Acq Method: FID-FA-AJVN
022008678A.SI (1.742)
100%

Date of Analysis: 19-Aug-2022 10:13:39
Instrument ID: JNL-MCL1-L08-007
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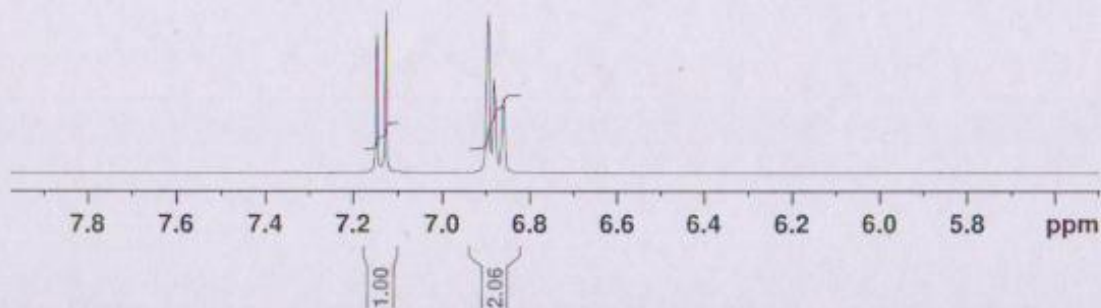


¹H NMR of 5-Methylbenzo[d]oxazol-2(3H)-one (2t)



C6292-039

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7.127
6.896
6.895
6.883
6.882
6.880
6.878
6.863
6.862
6.859
6.858



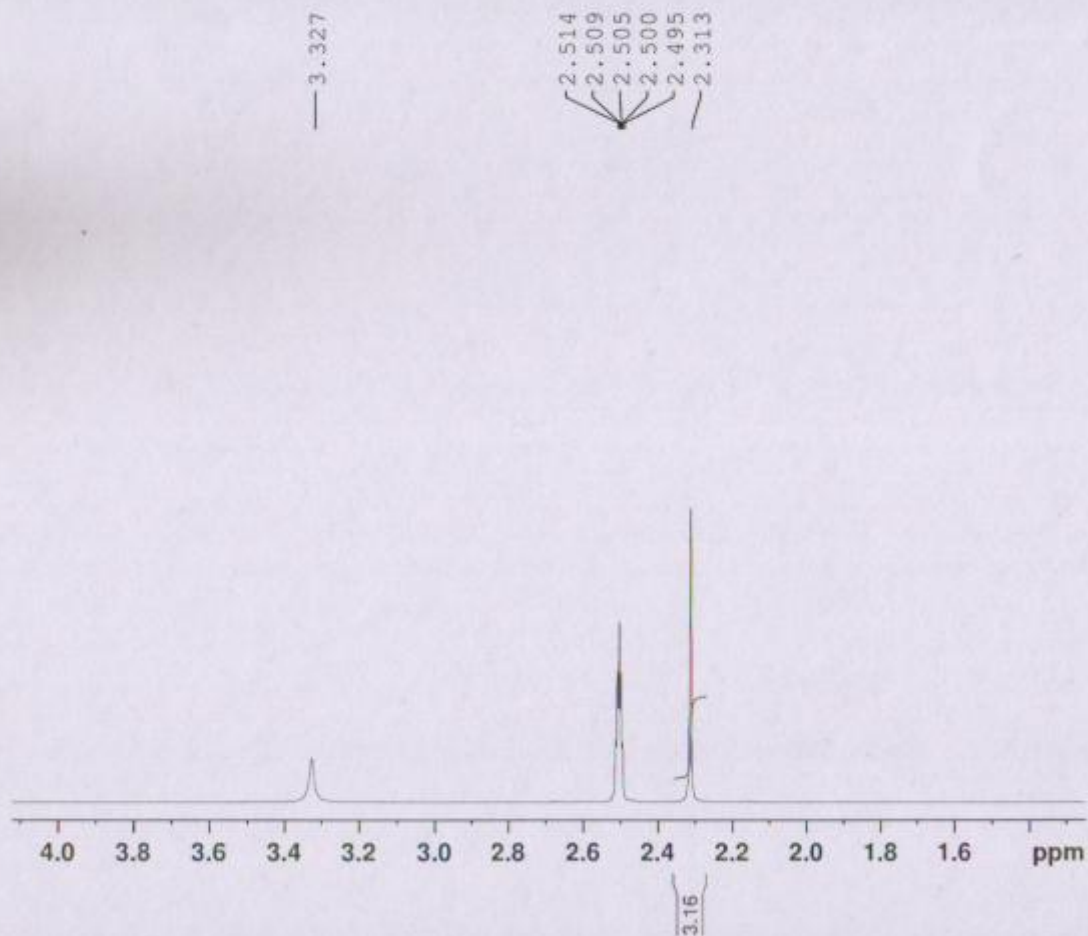
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220816
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PROBHD Z116098_0787 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.54 usec
TE 298.7 K
D1 2.00000000 sec
TDO 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 17.91799927 W

F2 - Processing parameters
SI 65536
SF 400.1300013 MHz
WDW EM
SSB 0
LB 0.30 Hz
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PC 1.00

ANL-MCL3-NMR-004

C6292-039



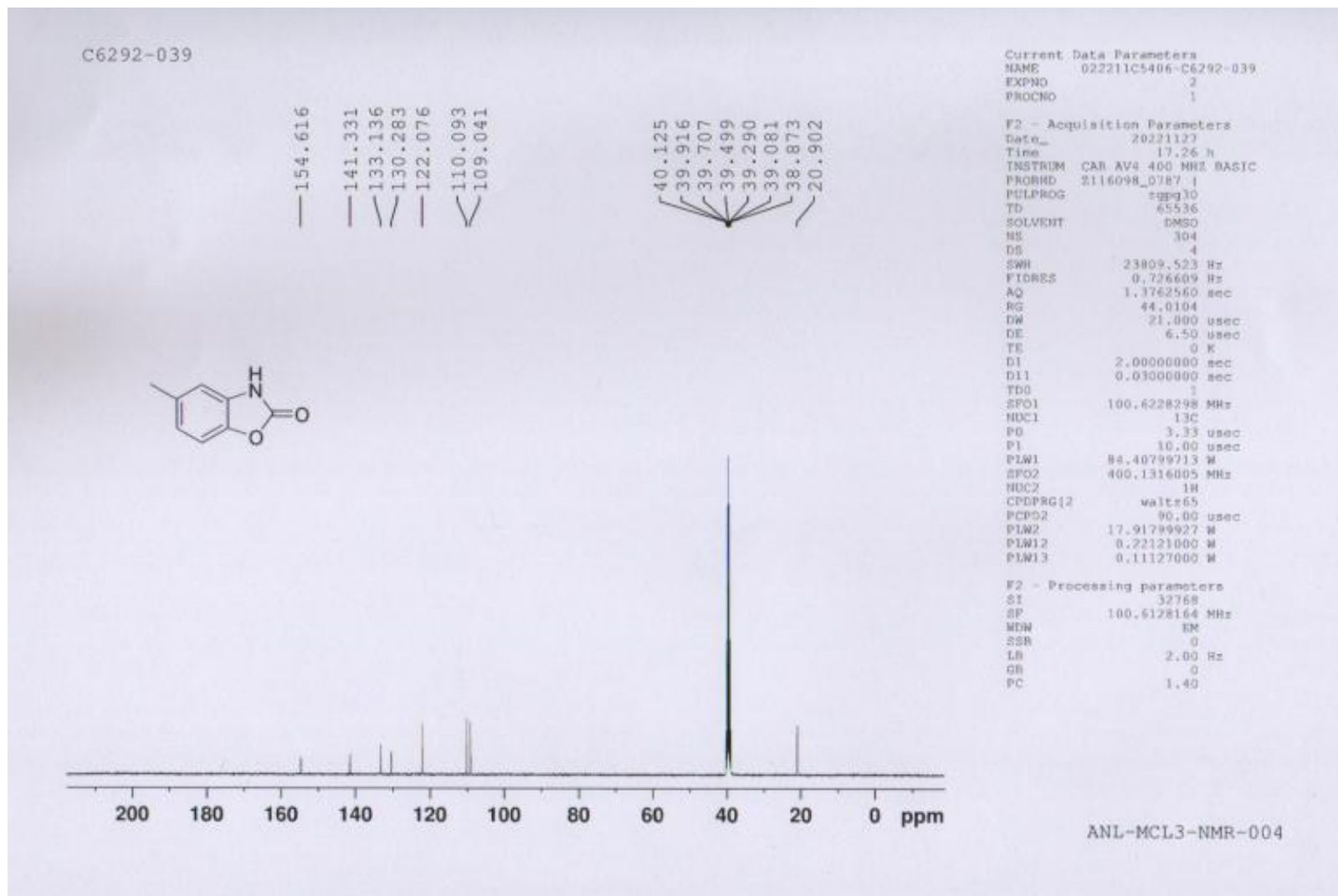
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NAME 022208B4664-C6292-039
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220816
Time 7.25 h
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PROBHD Z116098_0787 4
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DN 61.000 usec
DE 13.54 usec
TE 298.7 K
D1 2.00000000 sec
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PI 10.00 usec
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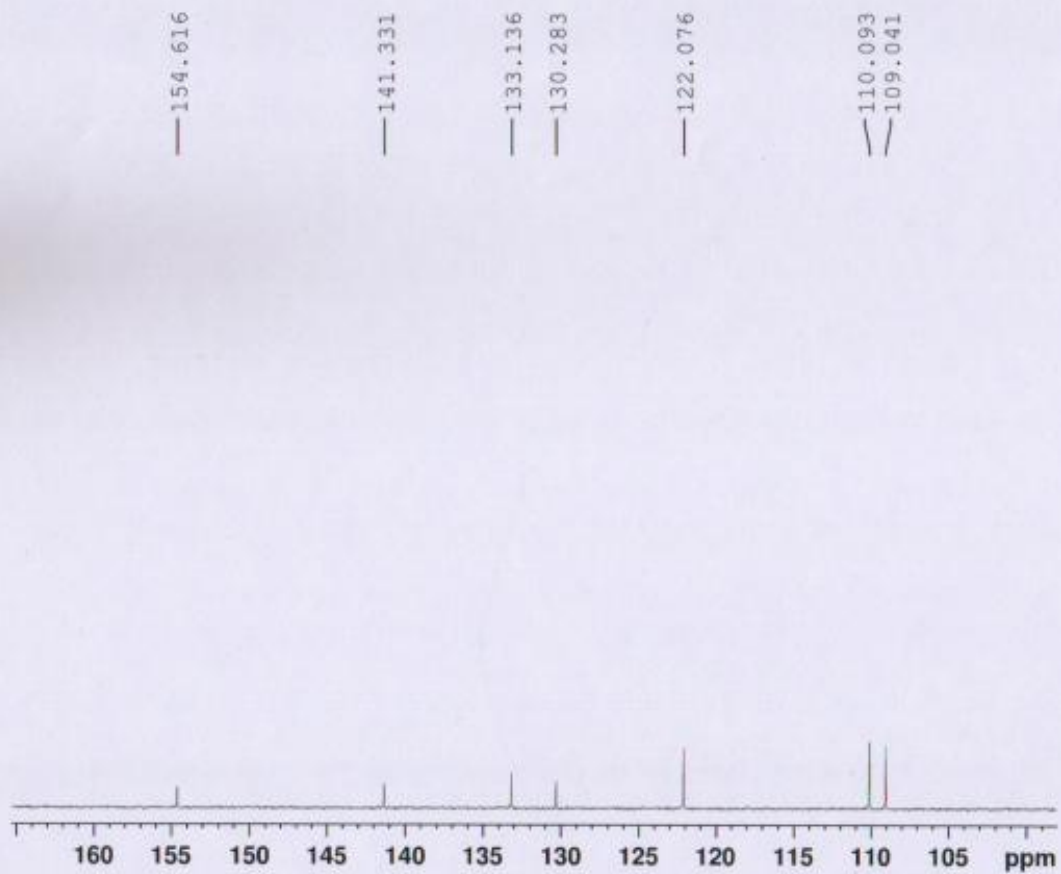
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SSB 0
LB 0.30 Hz
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PC 1.00

ANL-MCL3-NMR-004

¹³C NMR of 5-Methylbenzo[d]oxazol-2(3H)-one (2t)



C6292-039



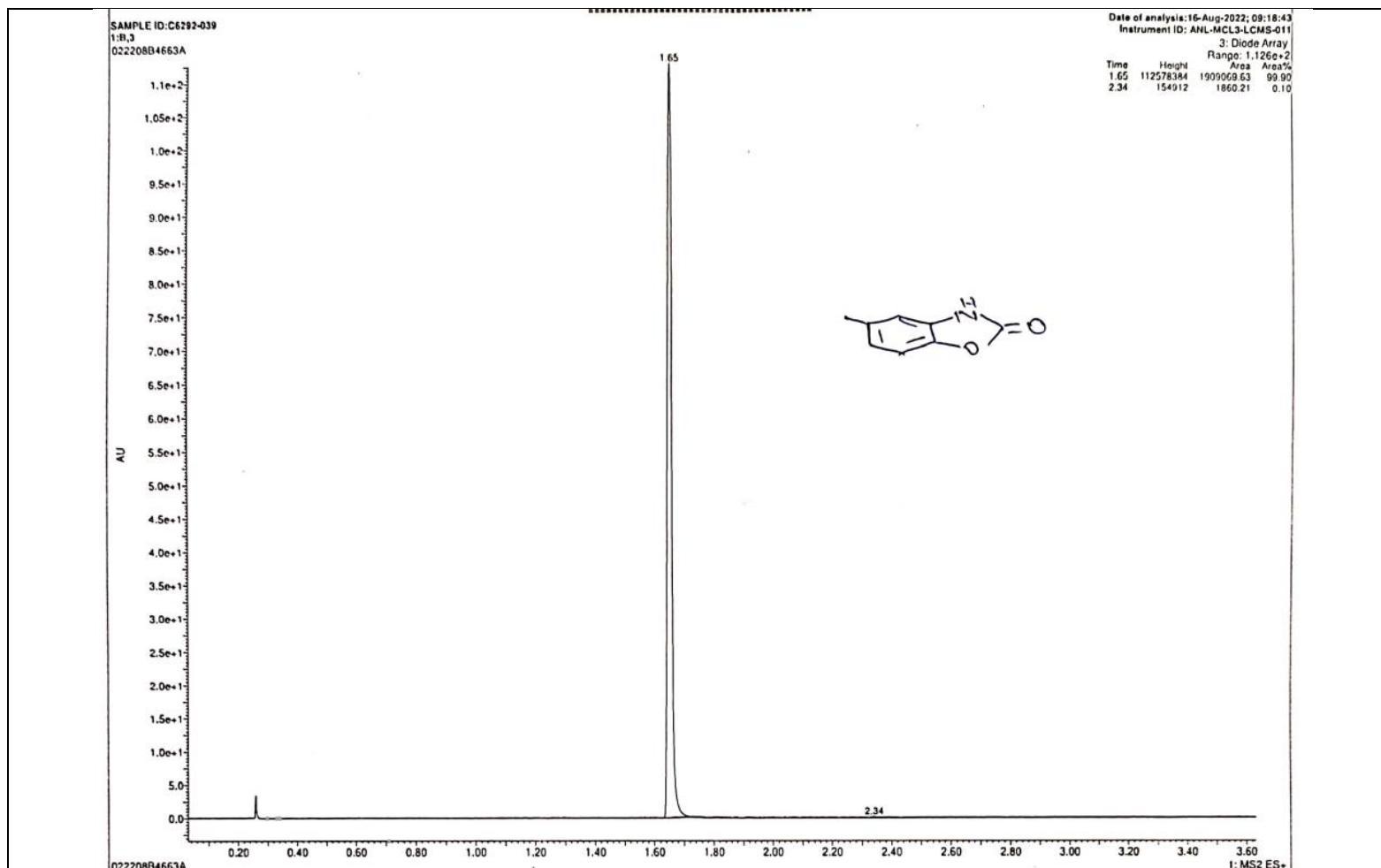
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NAME 022211C5406-C6292-039
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221127
Time 17.26 h
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PROBHD 2116098_0787 f
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 304
DS 4
SMH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 44.0104
DM 21.000 usec
DE 6.50 usec
TE 0 K
D1 2.0000000 sec
D11 0.0300000 sec
TDS 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 84.40799713 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz65
PCPD2 90.00 usec
PLW2 17.91799927 W
PLW12 0.22121000 W
PLW13 0.11127000 W

F2 - Processing parameters
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SF 100.6128164 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

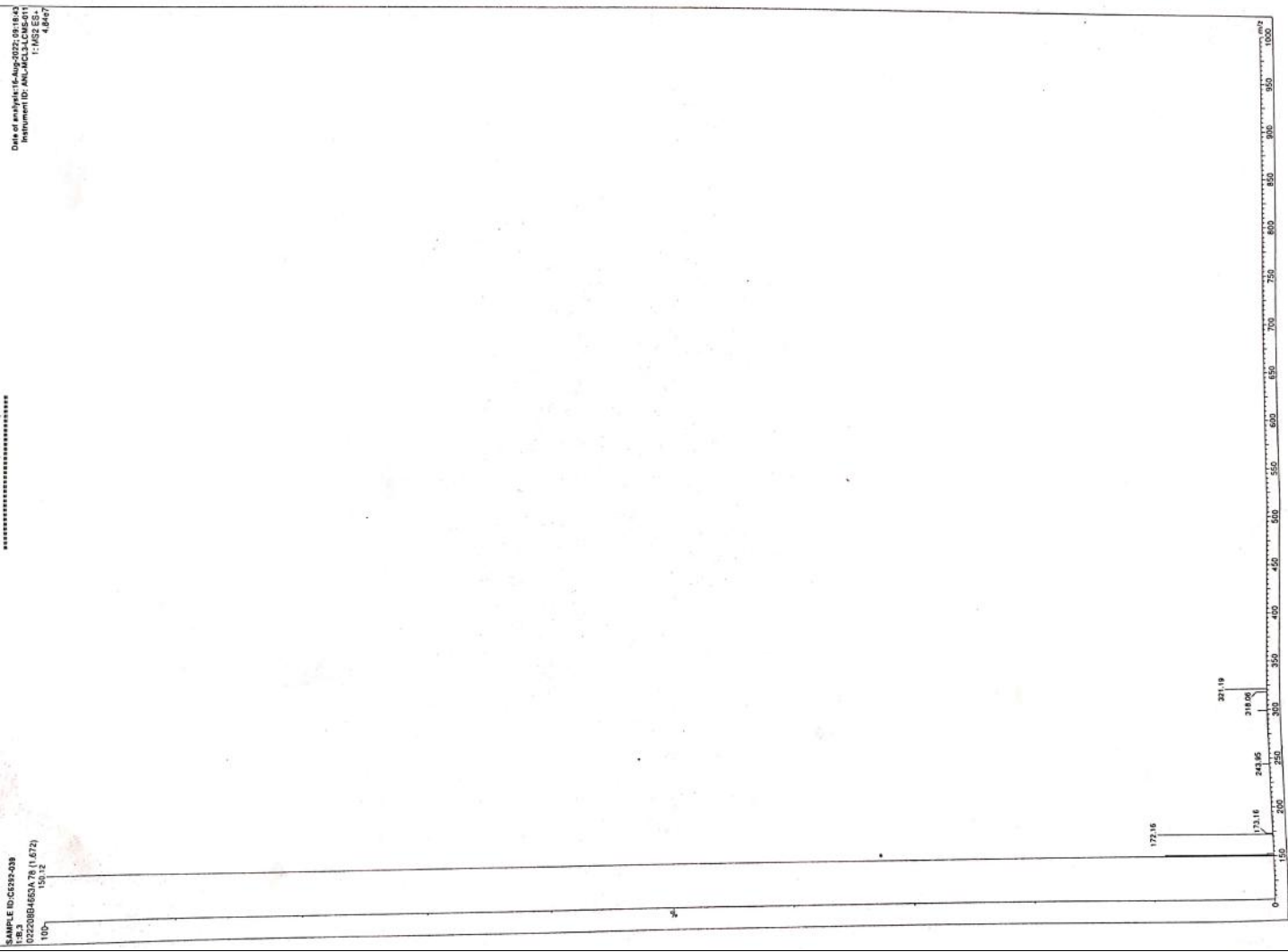
ANL-MCL3-NMR-004

LCMS of 5-Methylbenzo[d]oxazol-2(3H)-one (2t)

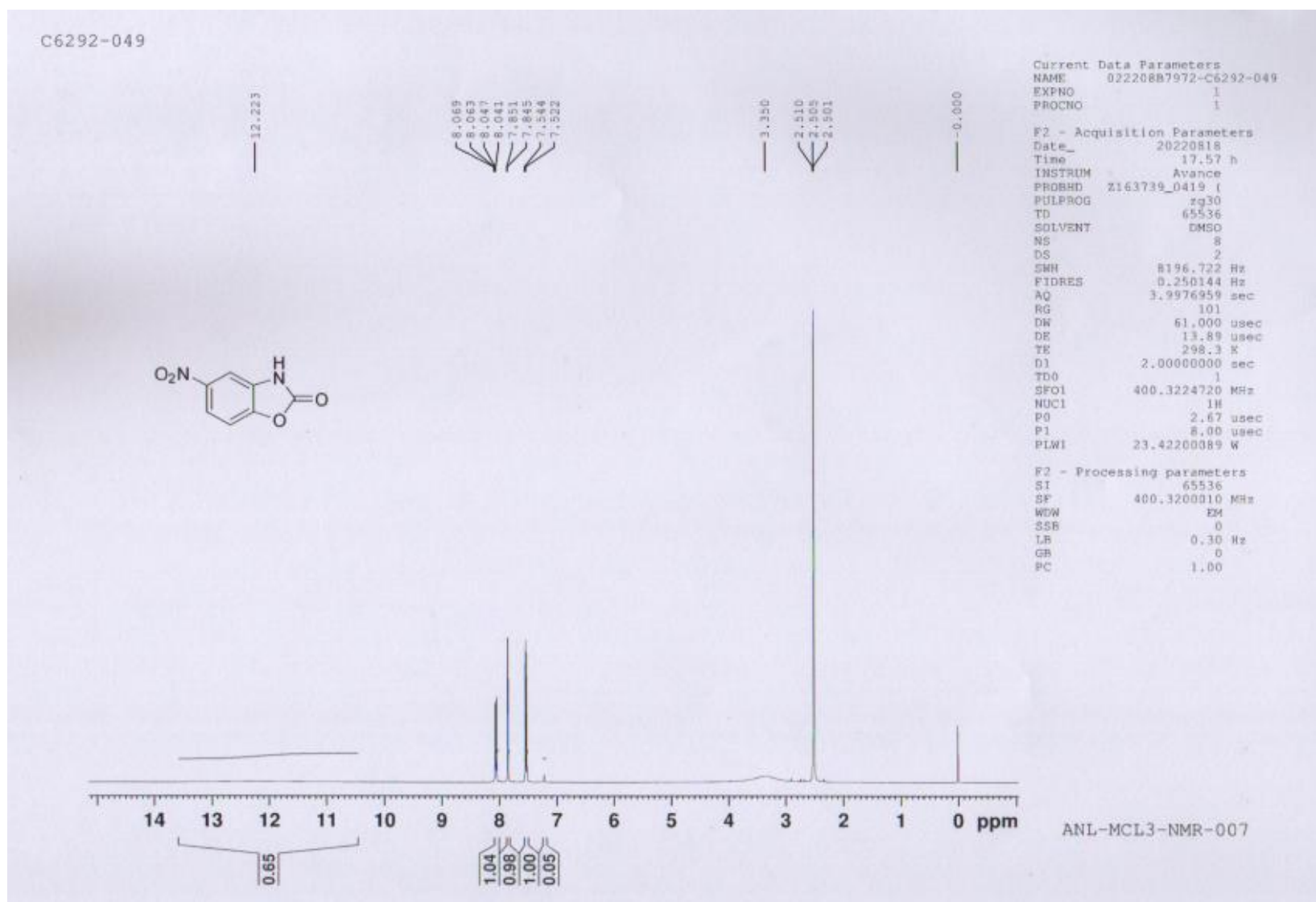


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U.S. 2
022208465A.P (1.67)
13012

Data analysis: July 2007, 08:54
Instrument: JMS-6000
1: MS2 ES+
4.847



¹H NMR of 5-Nitrobenzo[d]oxazol-2(3H)-one (2u)

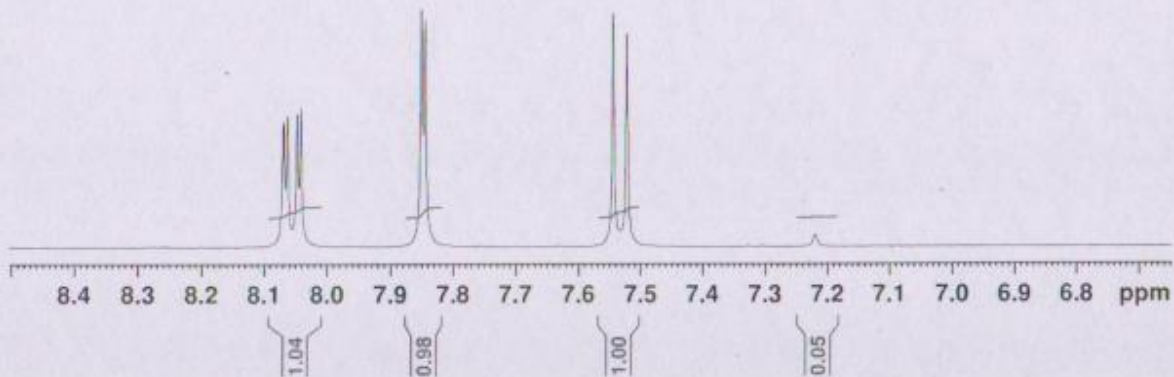


C6292-049

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8.063
8.047
8.041

7.851
7.845

7.544
7.522



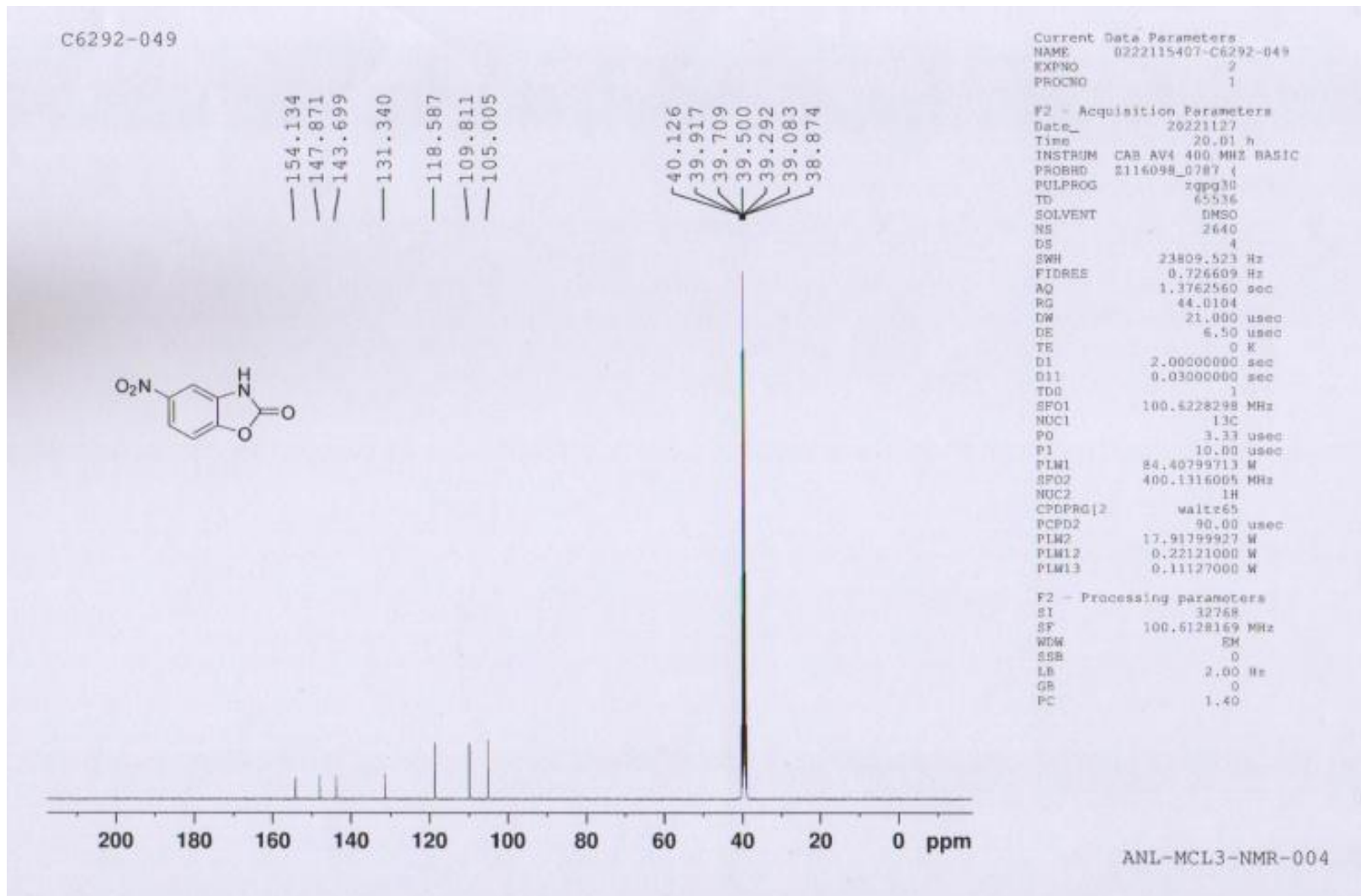
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NAME 02220887972-C6292-049
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time 17.57 h
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PROBHD Z163739_0419 (4
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.3 K
D1 2.00000000 sec
TD0 1
SFO1 400.3224720 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 23.42200089 W

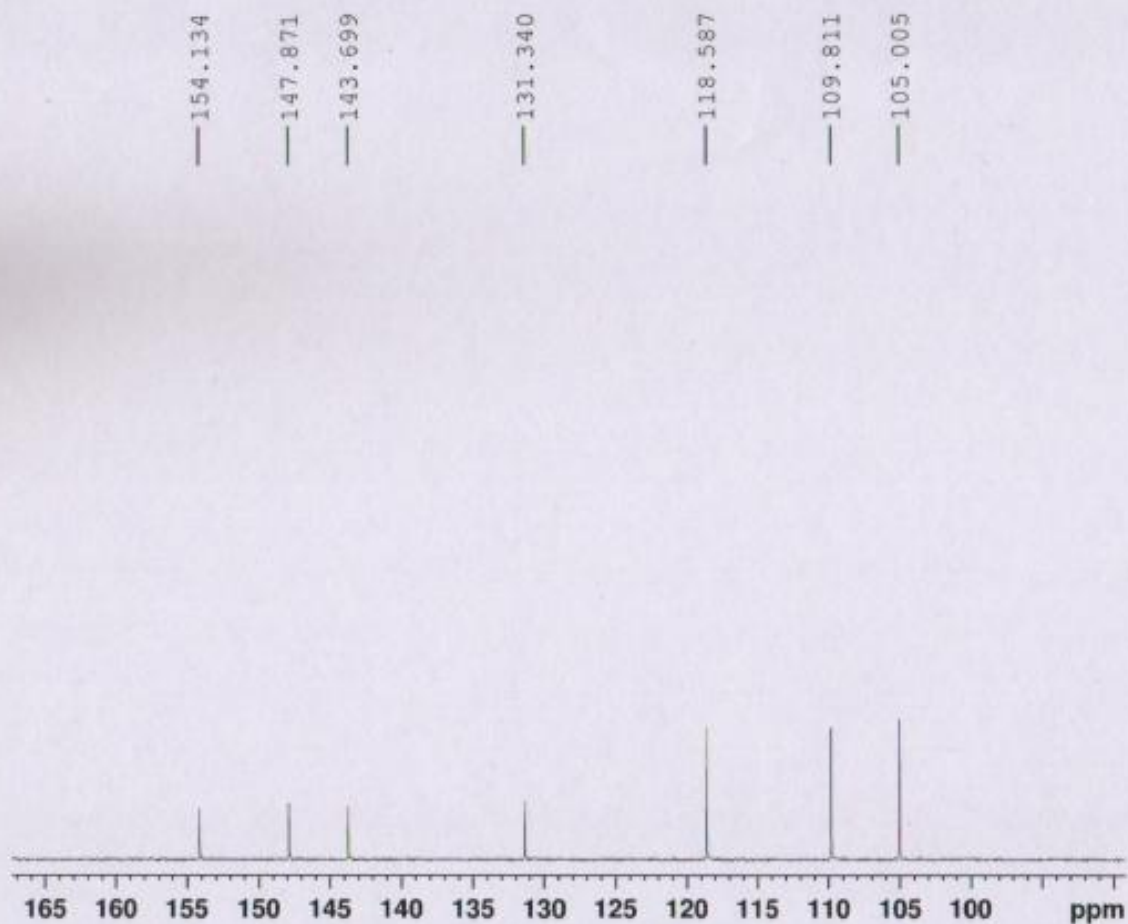
F2 - Processing parameters
SI 65536
SF 400.3200010 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ANL-MCL3-NMR-007

¹³C NMR of 5-Nitrobenzo[d]oxazol-2(3H)-one (2u)



C6292-049



Current Data Parameters
NAME 0222115407-C6292-049
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221127
Time 20.01 h
INSTRUM CAB AV4 400 MHz BASIC
PROBHD 2116098_0787 ()
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2640
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 44.0104
DW 21.000 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 84.40799713 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG(2) waltz65
PCPD2 90.00 usec
PLW2 17.91799927 W
PLW12 0.22121000 W
PLW13 0.11127000 W

F2 - Processing parameters
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SF 100.6128169 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

ANL-MCL3-NMR-004

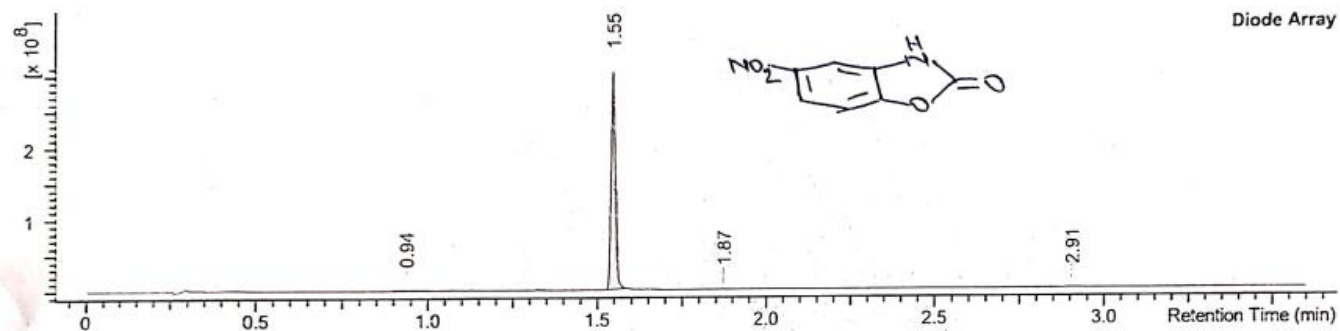
LCMS of 5-Nitrobenzo[d]oxazol-2(3H)-one (2u)

Sample ID C6292-049
Acq Method LCMS_FA_4
2:B,6
022208B7971

Instrument ID ANL-MCL3-LCMS-011
Date of Analysis 18-Aug-2022 17:40:13

Time	Area	Area%
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1.87	7648244.00	0.13
2.91	58820665.50	1.01

Diode Array



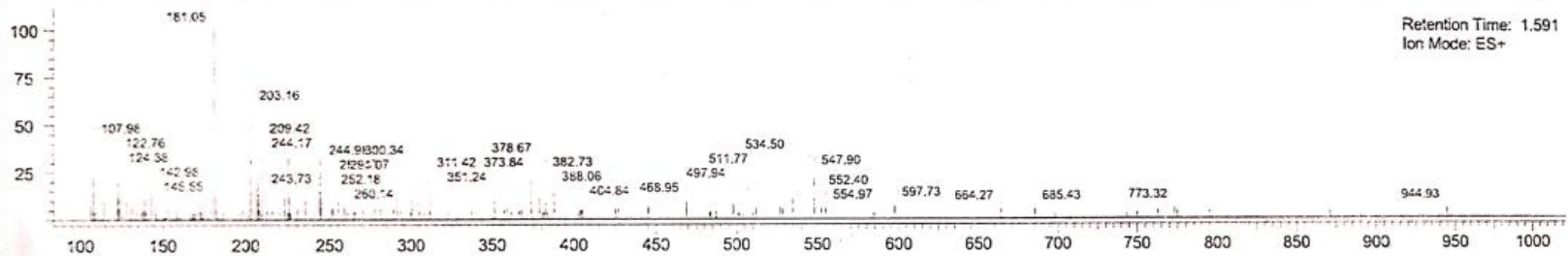
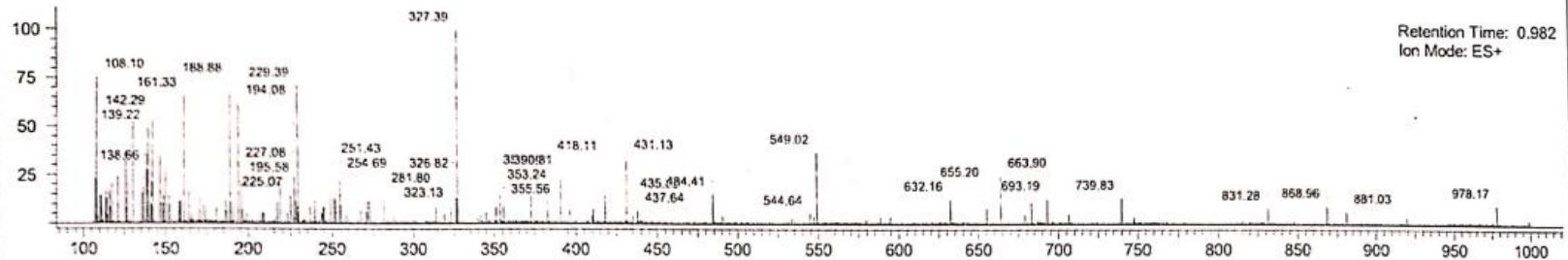
Acq Method LCMS_FA_4

2:B,6

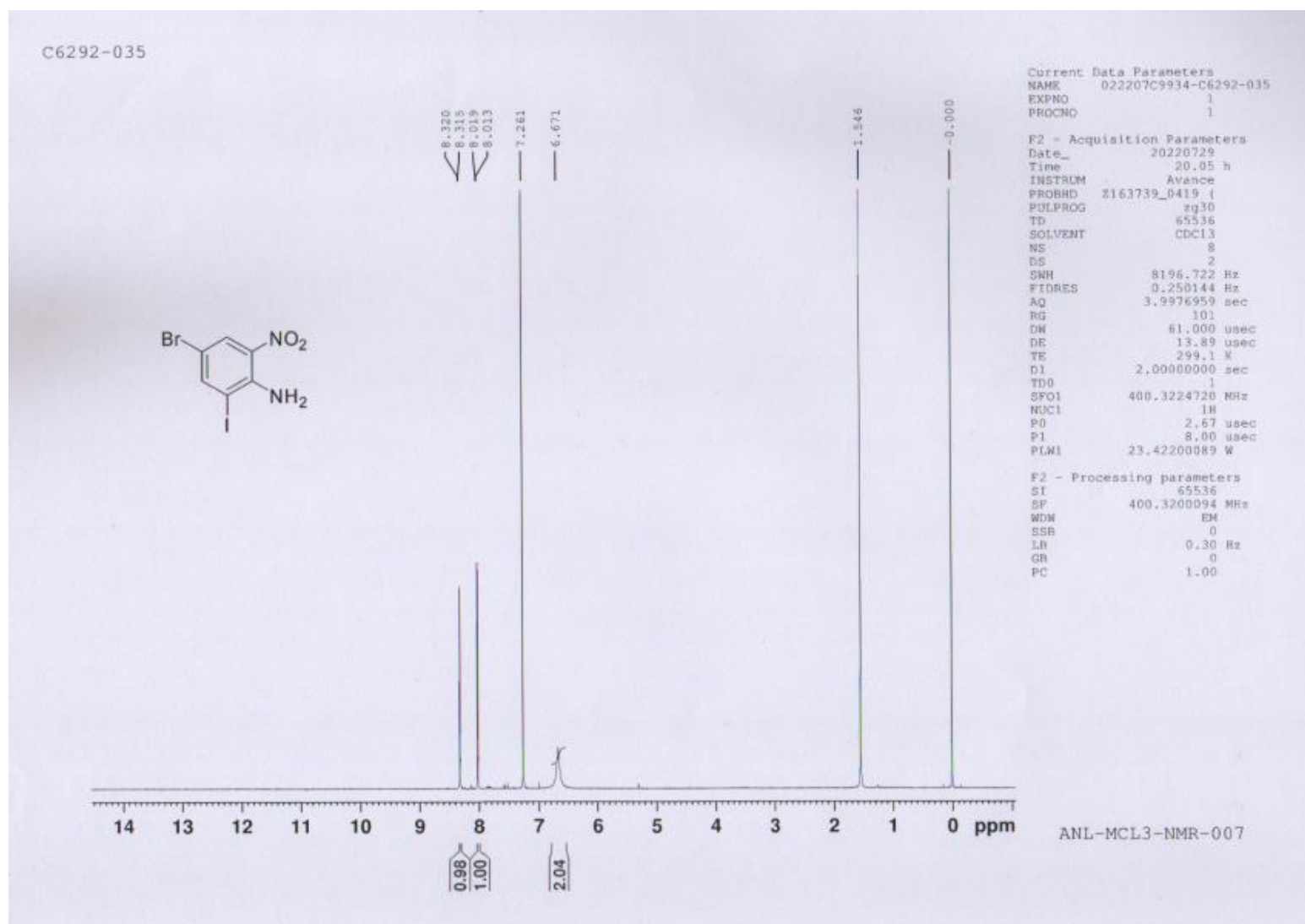
022208B7971

Instrument ID ANL-MCL3-LCMS-011

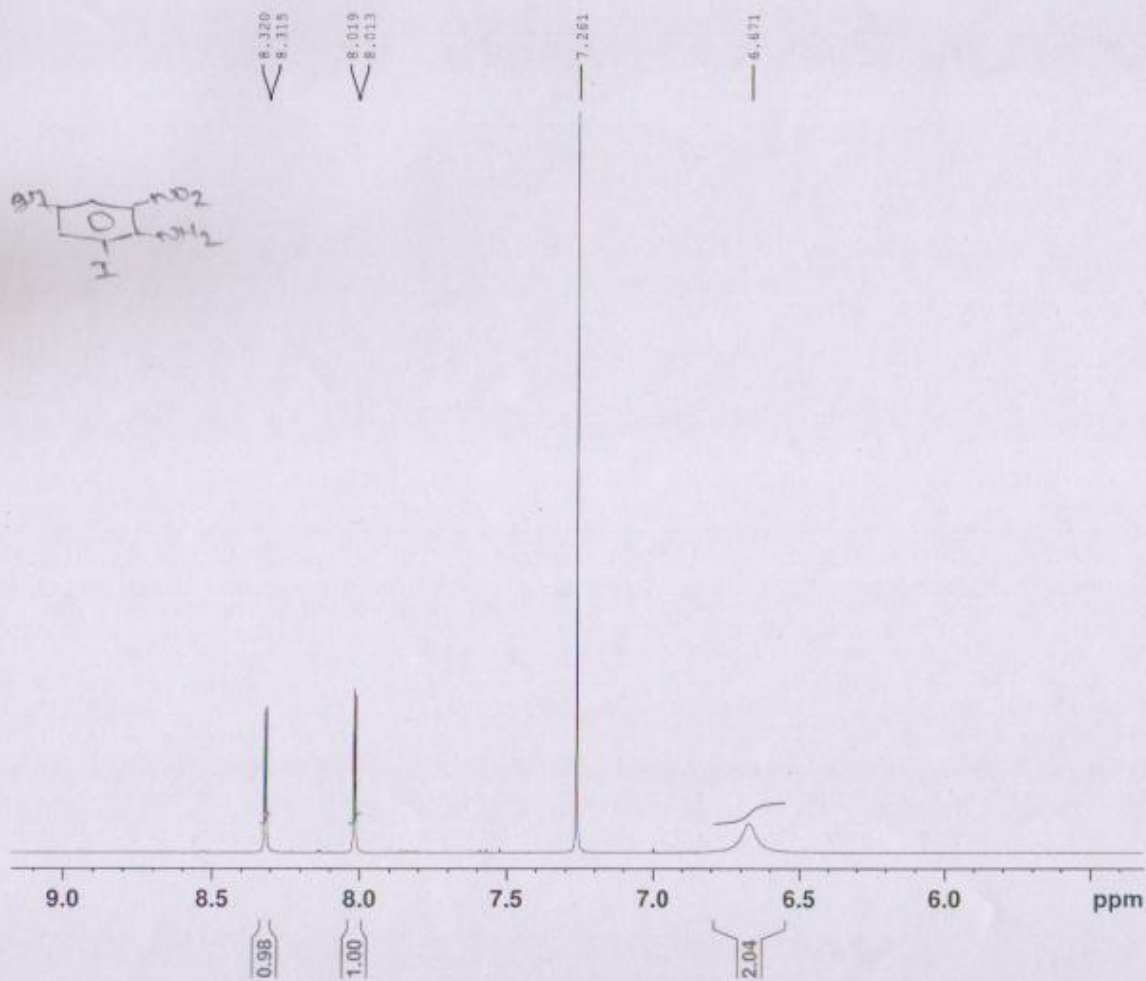
Date of Analysis 18-Aug-2022 17:40:13



¹H NMR of 4-Bromo-2-iodo-6-nitroaniline (2)



C6292-035



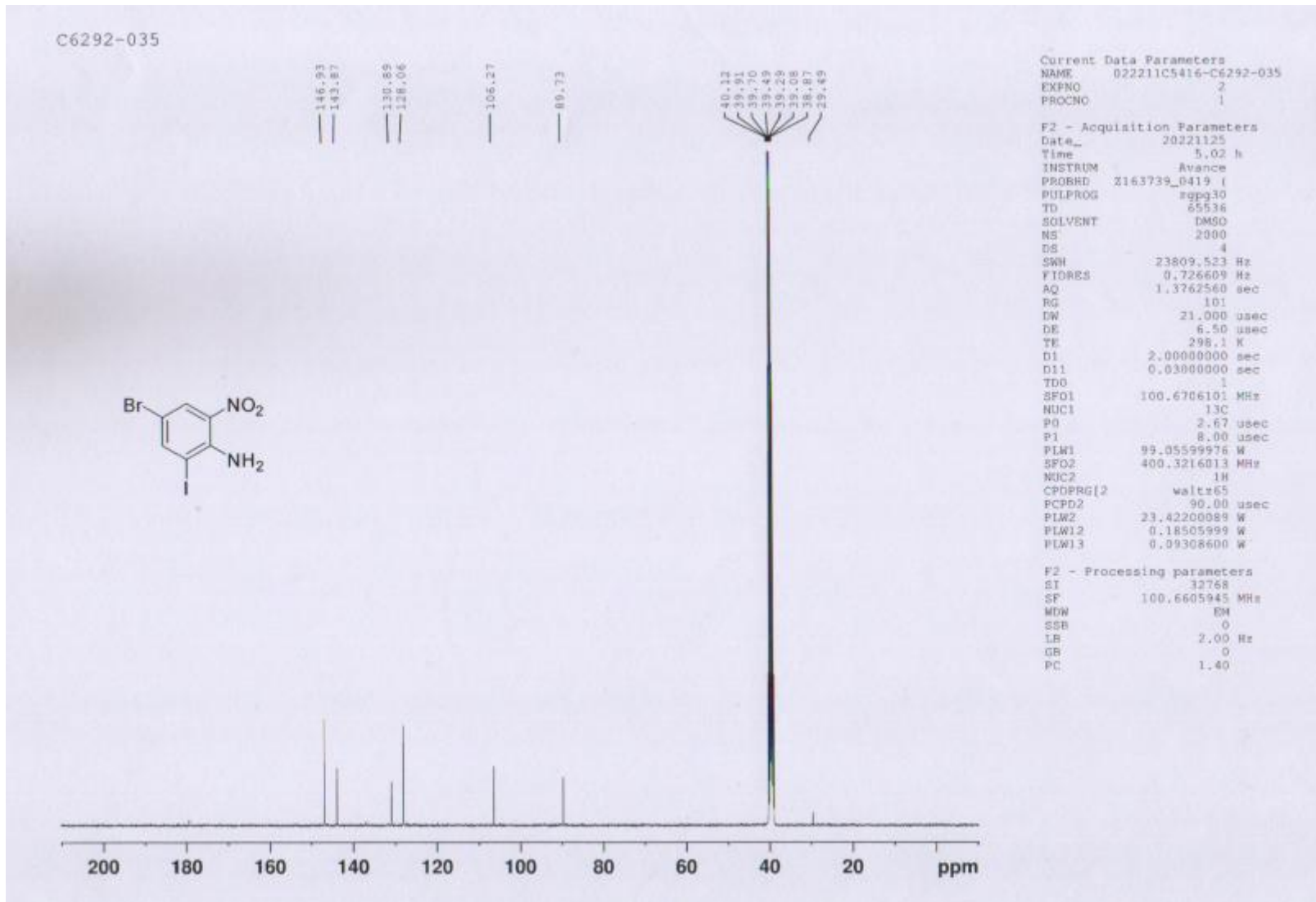
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time 20.05 h
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SMH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DN 61.000 usec
DE 13.89 usec
TE 299.1 K
D1 2.0000000 sec
TDD 1
SFO1 400.3224720 MHz
NUC1 1H
PD 2.67 usec
P1 8.00 usec
PLWI 23.42200089 W

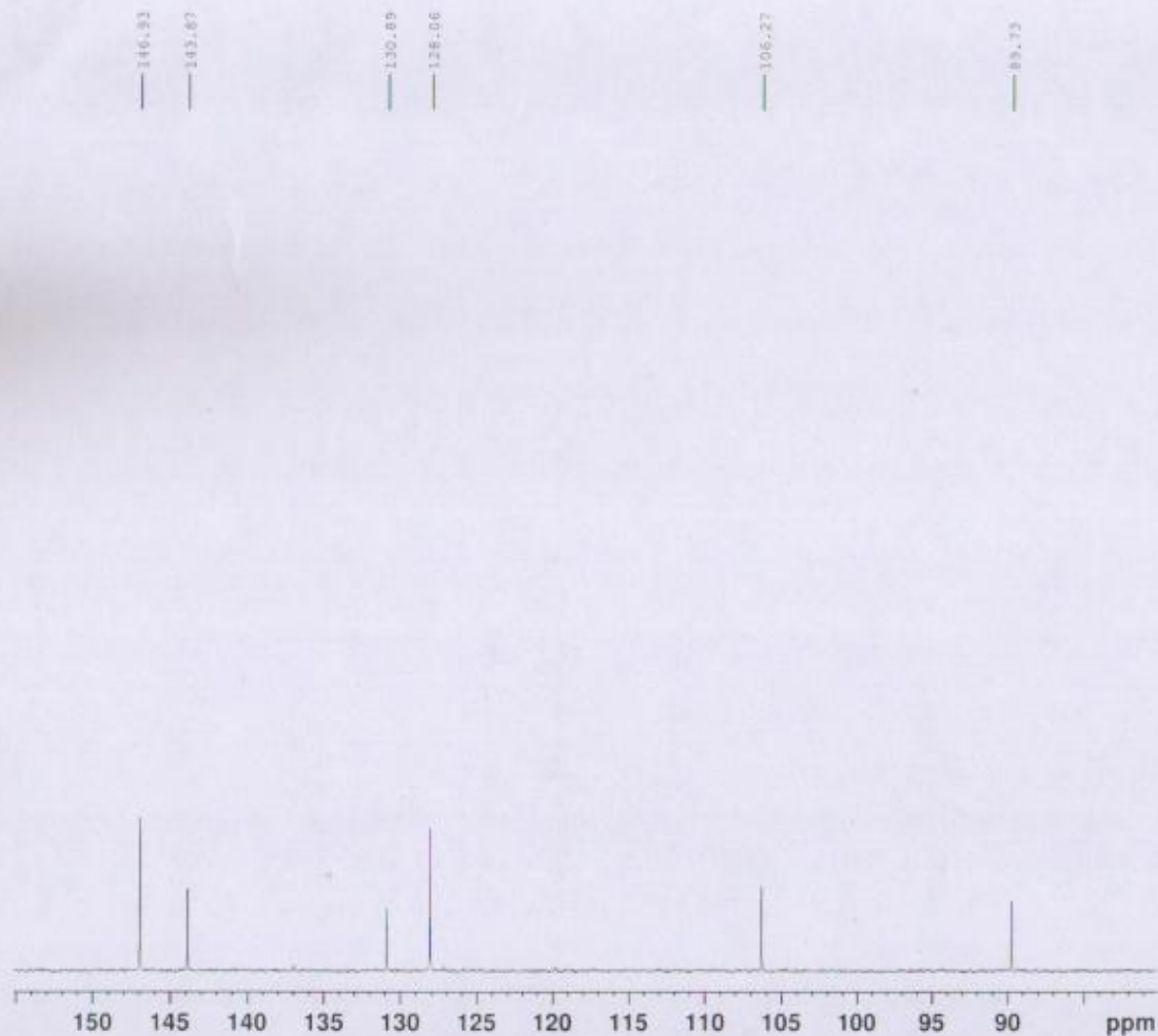
F2 - Processing parameters
SI 65536
SF 400.3200094 MHz
WDW EM
SSB 0
LA 0.30 Hz
GB 0
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ANL-MCL3-NMR-007

¹³C NMR of 4-Bromo-2-iodo-6-nitroaniline (2)



C6292-035

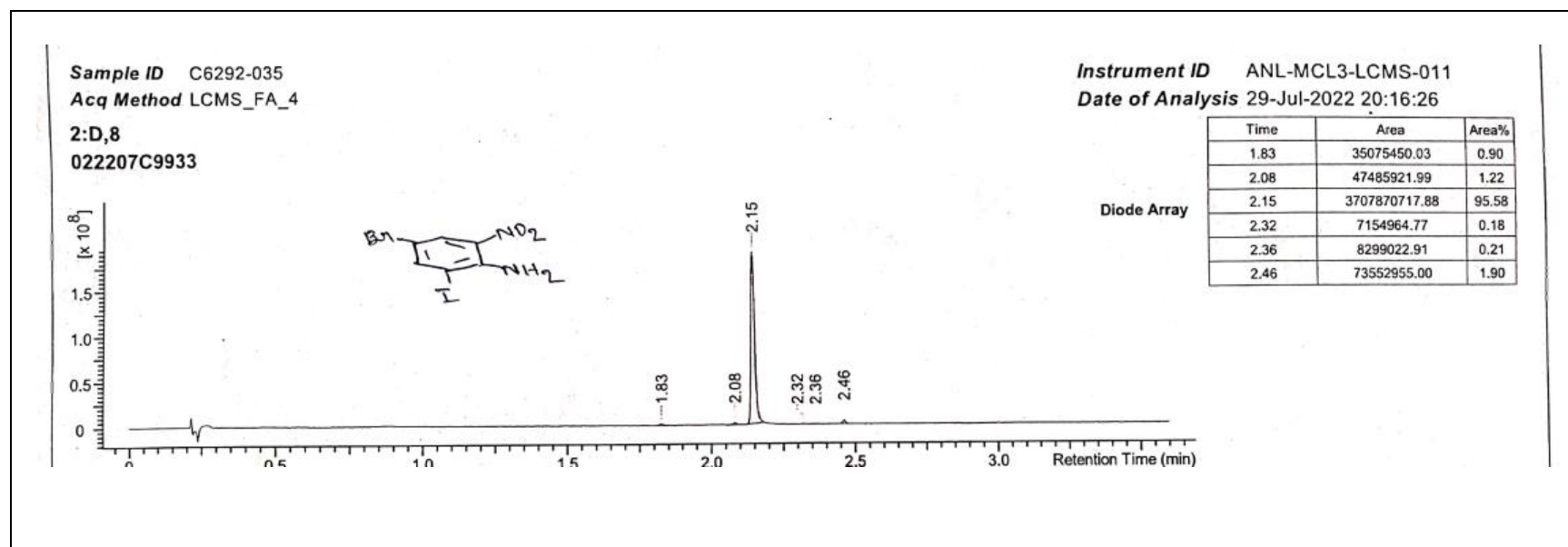


Current Data Parameters
NAME 022211C5416-C6292-035
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221125
Time 5.02 h
INSTRUM Avance
PROBHD 2163739_0419 (4
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 298.1 K
D1 2.0000000 sec
D11 0.9300000 sec
TD0 1
SFO1 100.6706101 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 89.05599876 W
SFO2 400.3216813 MHz
NUC2 1H
CPOPRG12 waltz65
PCPD2 90.00 usec
PLW2 23.42200089 W
PLW12 0.18505999 W
PLW13 0.09308600 W

F2 - Processing parameters
SI 32768
SF 100.6605945 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

LCMS of 4-Bromo-2-iodo-6-nitroaniline (2)



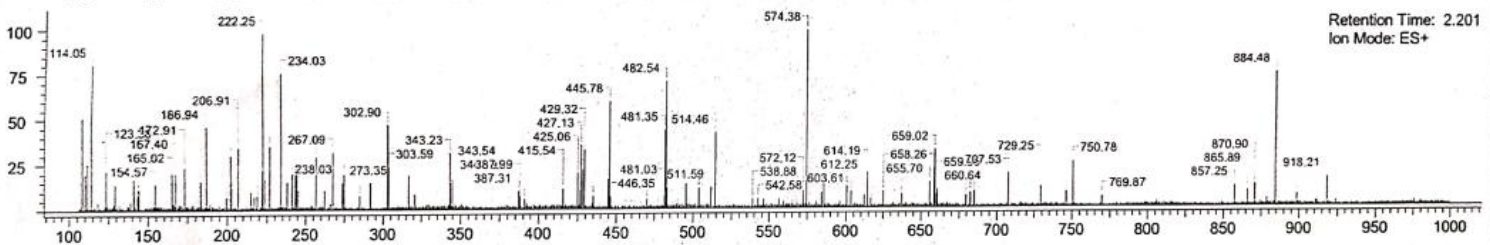
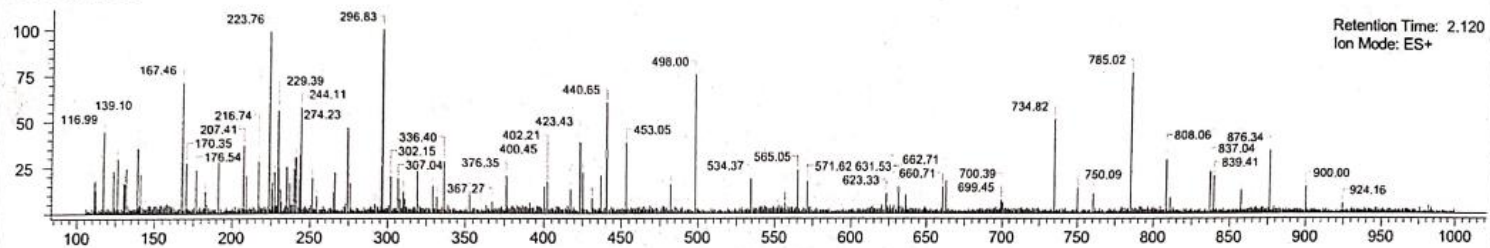
Acq Method LCMS_FA_4

2:D,8

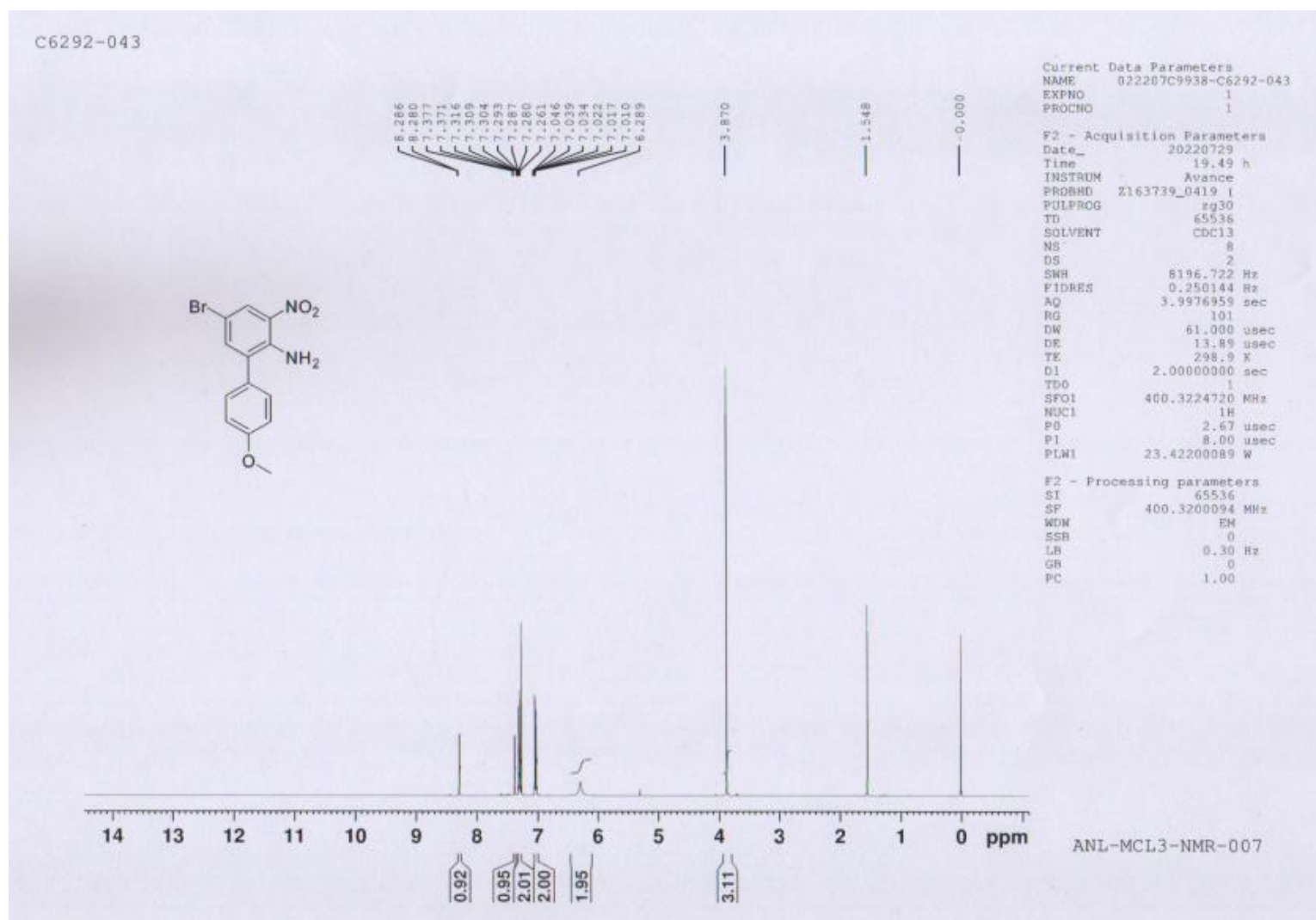
022207C9933

Instrument ID ANL-MCL3-LCMS-011

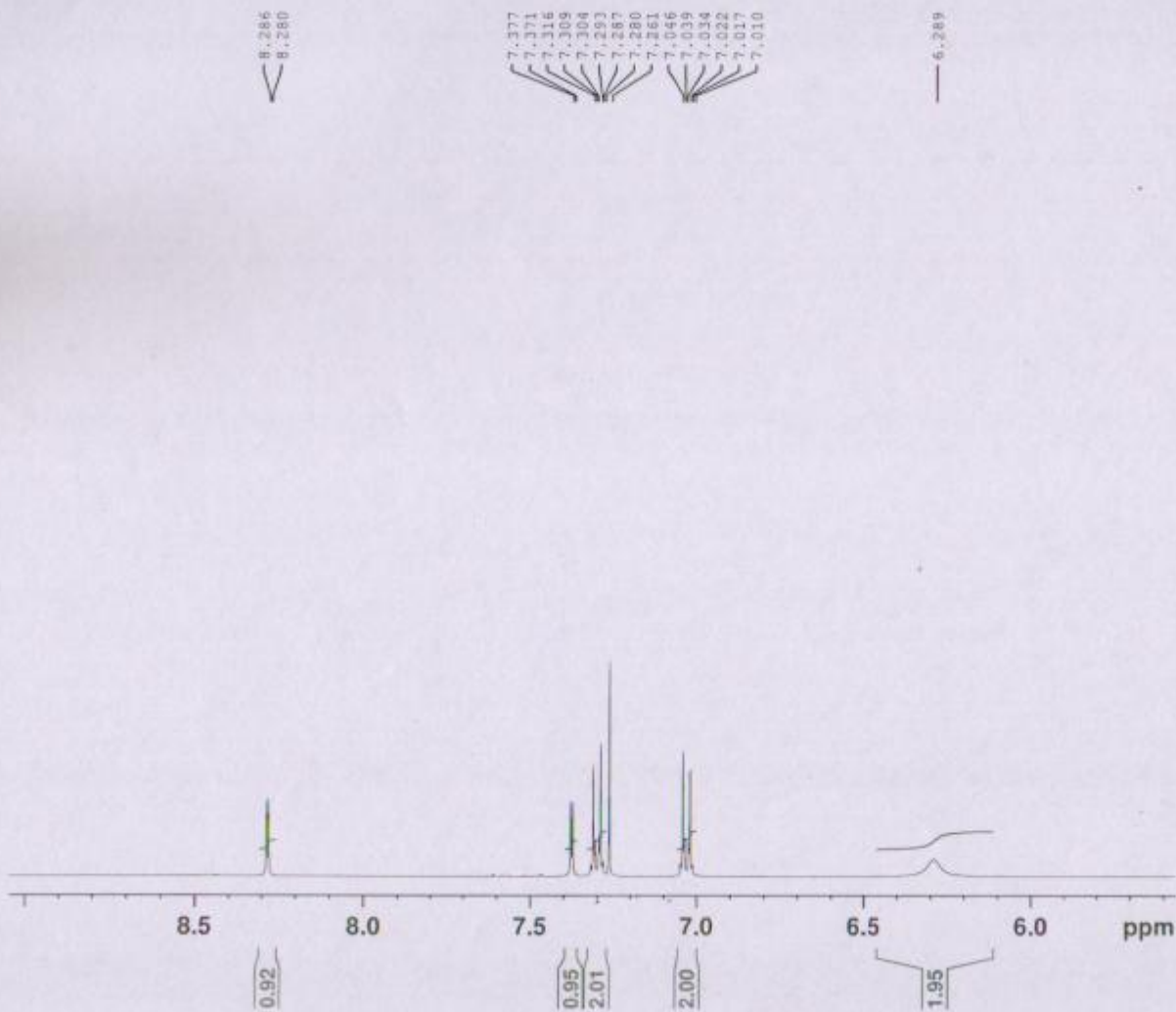
Date of Analysis 29-Jul-2022 20:16:26



¹H NMR of 5-Bromo-4'-methoxy-3-nitro-[1,1'-biphenyl]-2-amine (4)



C6292-043



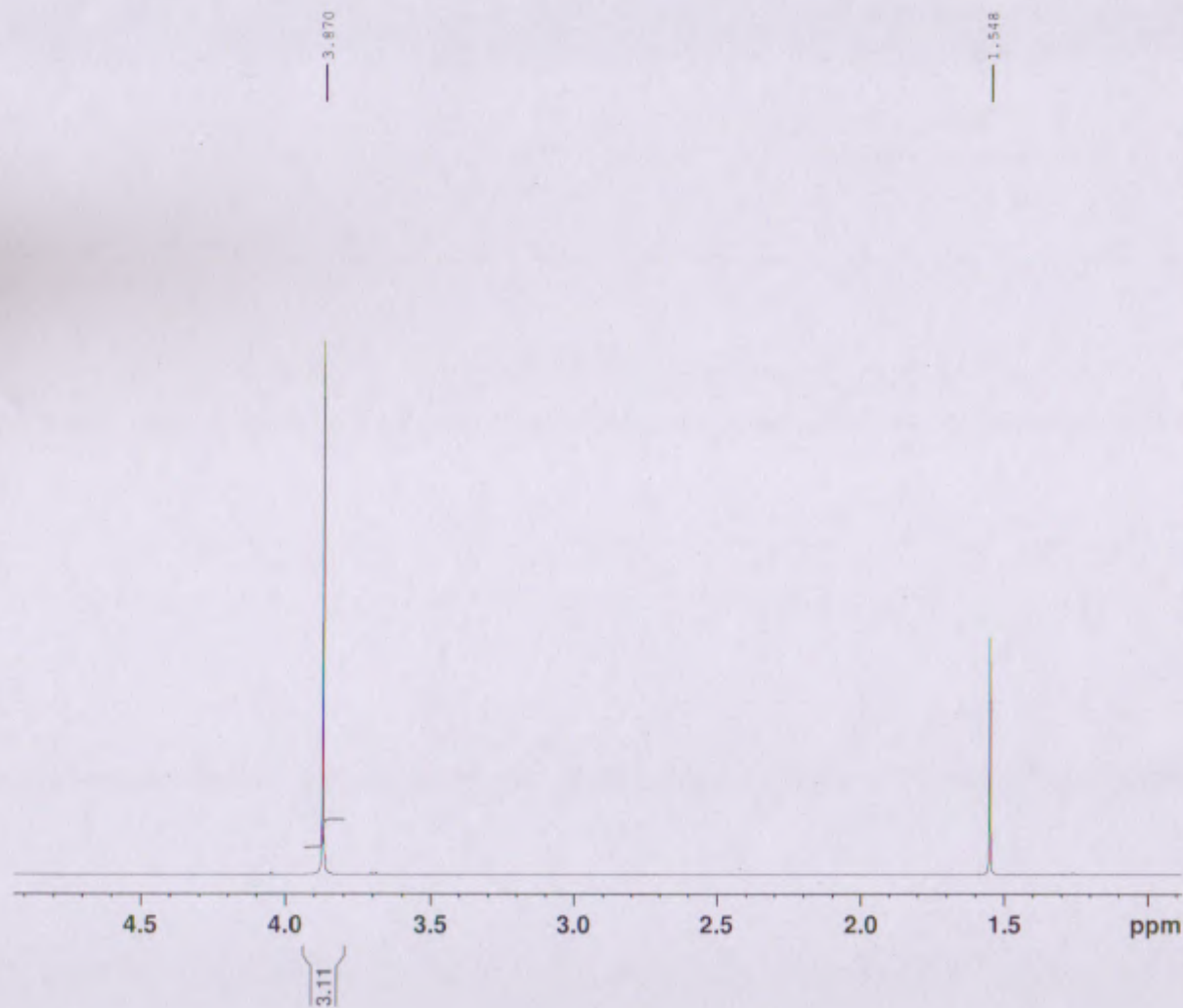
Current Data Parameters
NAME 022207C9938-C6292-043
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time 19.49 h
INSTRUM Avance
PROBHD Z163739_0419 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.9 K
D1 2.00000000 sec
TD0 1
SFO1 400.3224720 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 23.42200089 W

F2 - Processing parameters
SI 65536
SF 400.3200094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ANL-MCL3-NMR-007

C6292-043



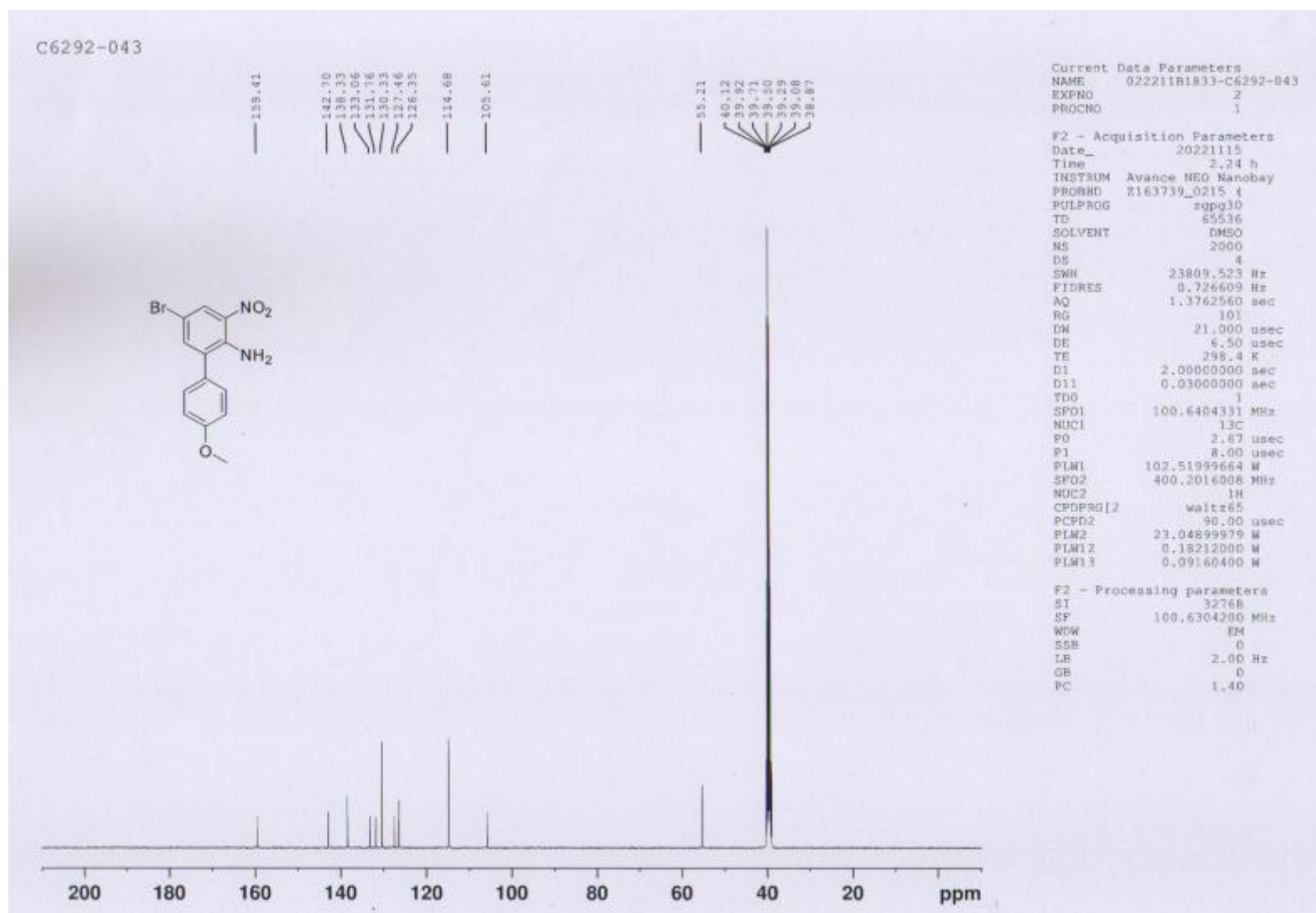
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EXPNO 1
PROCNO 1

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SOLVENT CDC13
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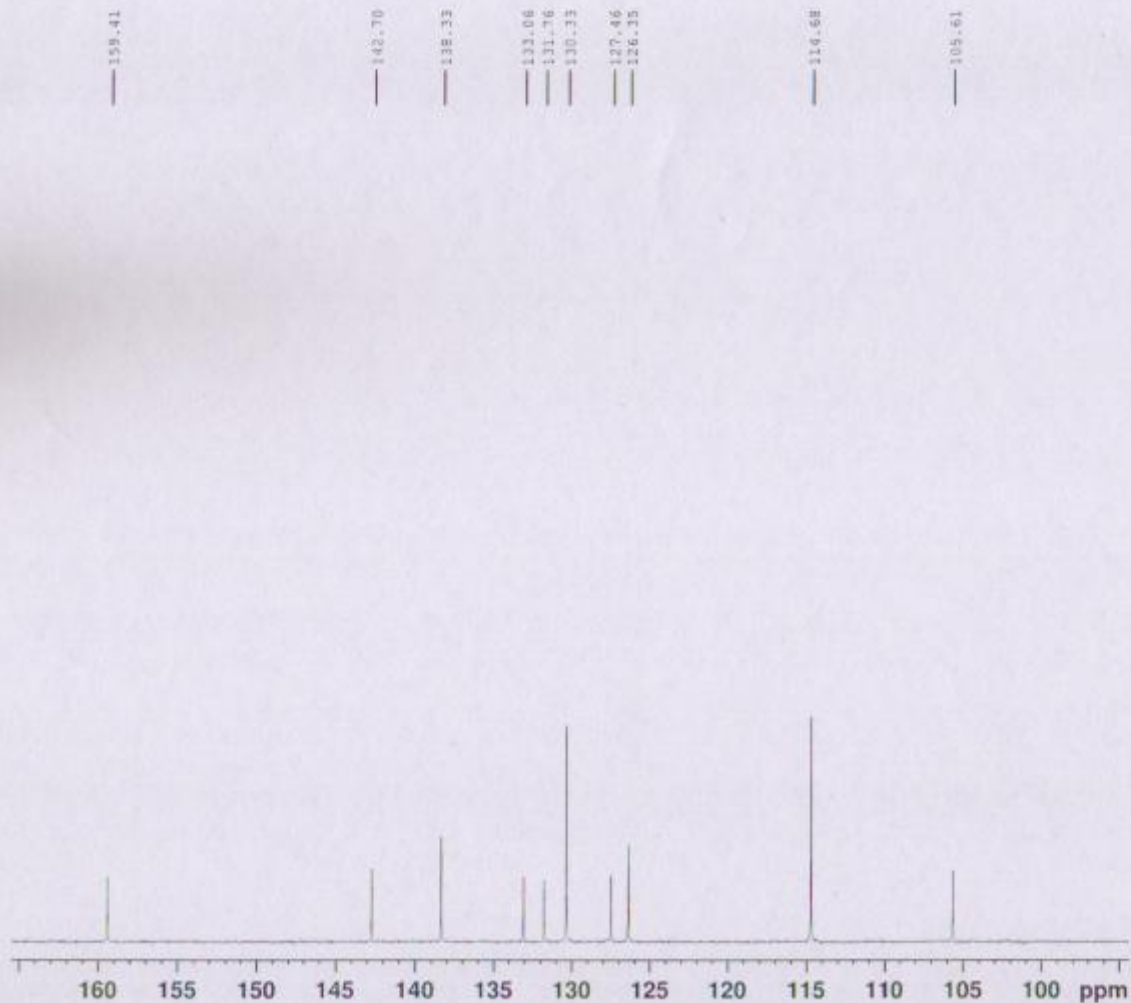
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ANL-MCL3-NMR-007

13C NMR of 5-Bromo-4'-methoxy-3-nitro-[1,1'-biphenyl]-2-amine (4)



C6292-043

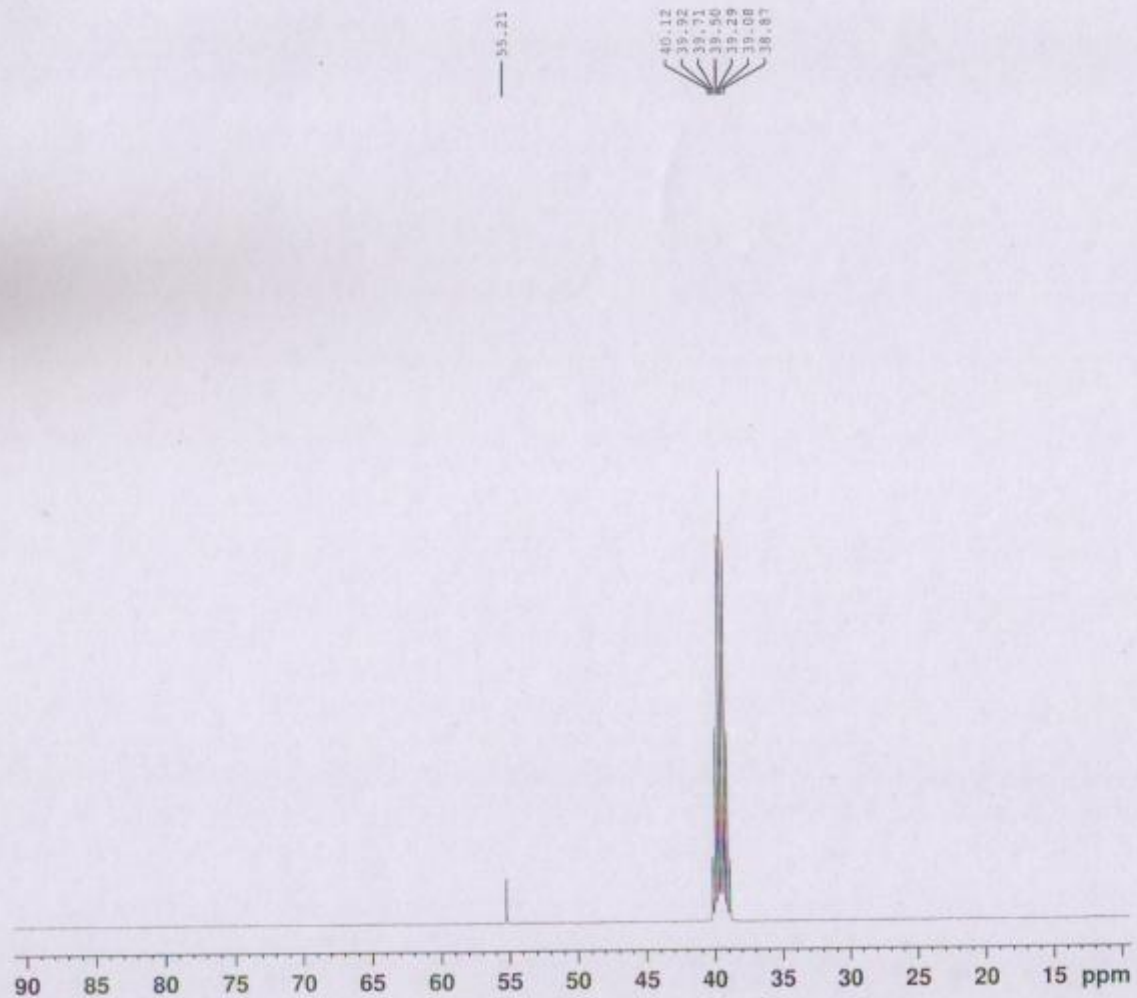


Current Data Parameters
NAME 022211P1833-C6292-043
EXPNO 2
PROCNO 1

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FIDRES 0.726609 Hz
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D11 0.0300000 sec
TDO 1
SFO1 100.6404331 MHz
NUC1 13C
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PLW1 102.51999664 W
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NUC2 1H
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C6292-043

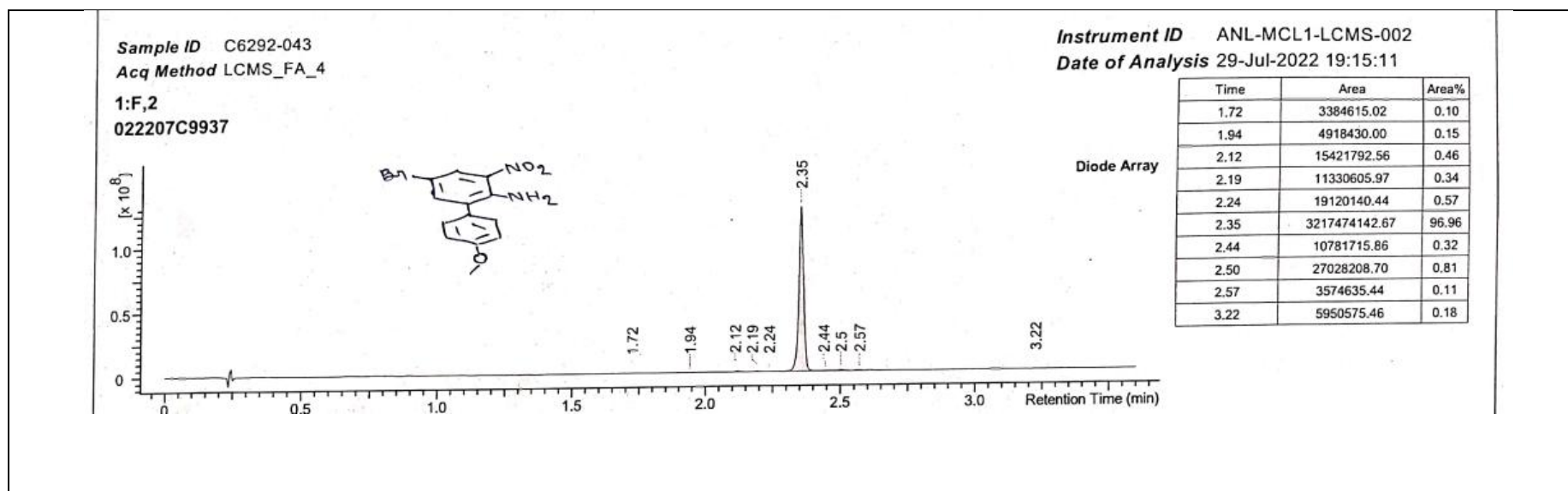


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EXPNO 2
PROCNO 1

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LCMS of 5-Bromo-4'-methoxy-3-nitro-[1,1'-biphenyl]-2-amine (4)

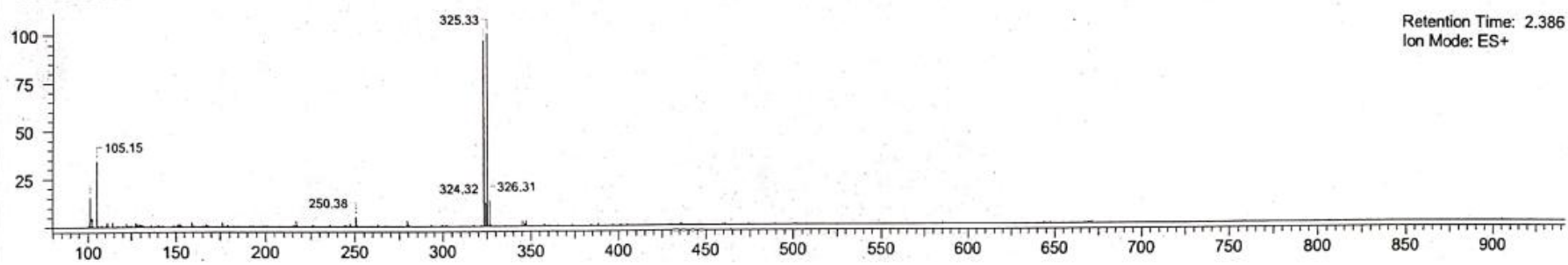


Sample ID C6292-043
Acq Method LCMS_FA_4

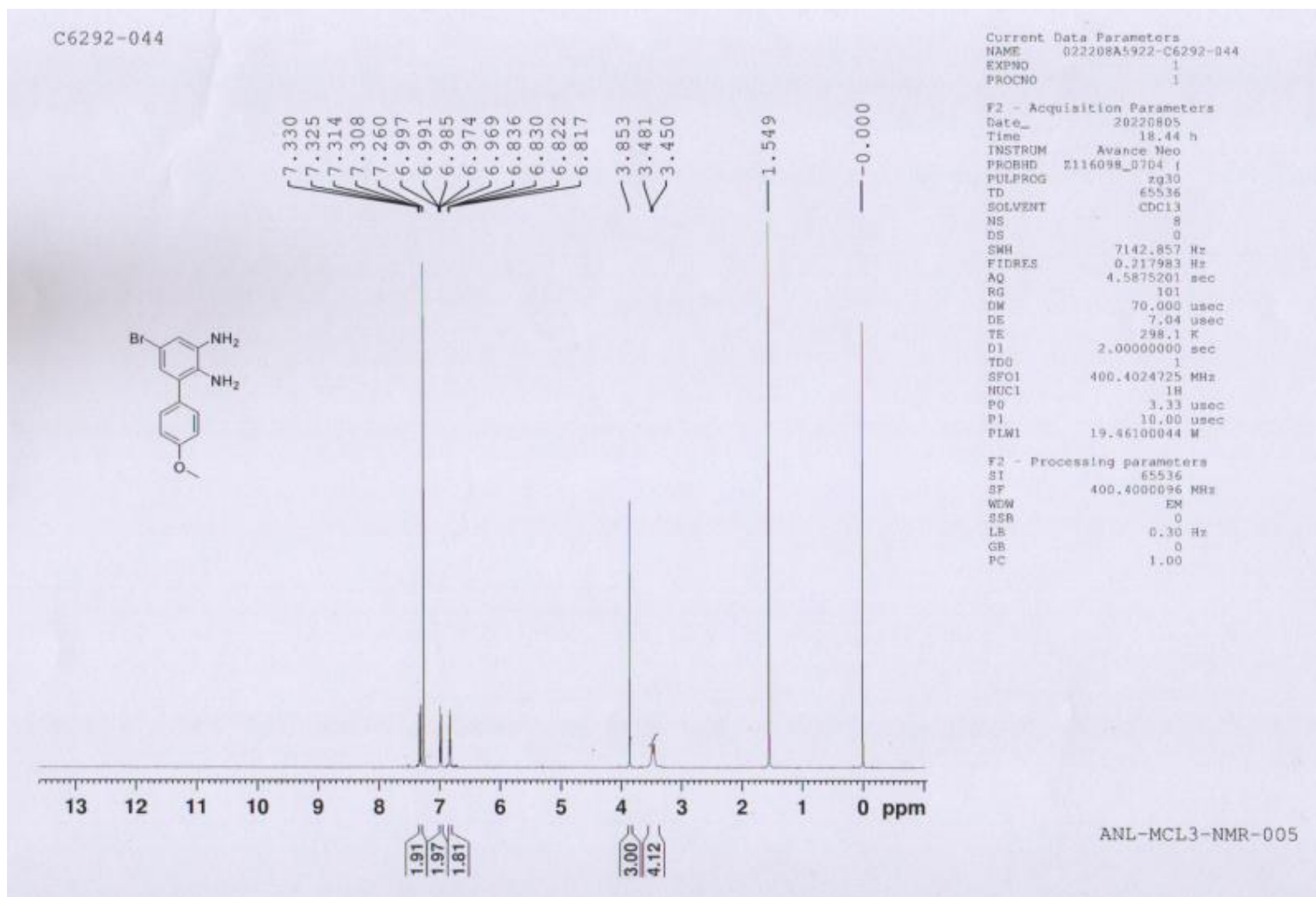
Discovery Chemistry Analytical Services

Instrument ID ANL-MCL1-LCMS-002
Date of Analysis 29-Jul-2022 19:15:11

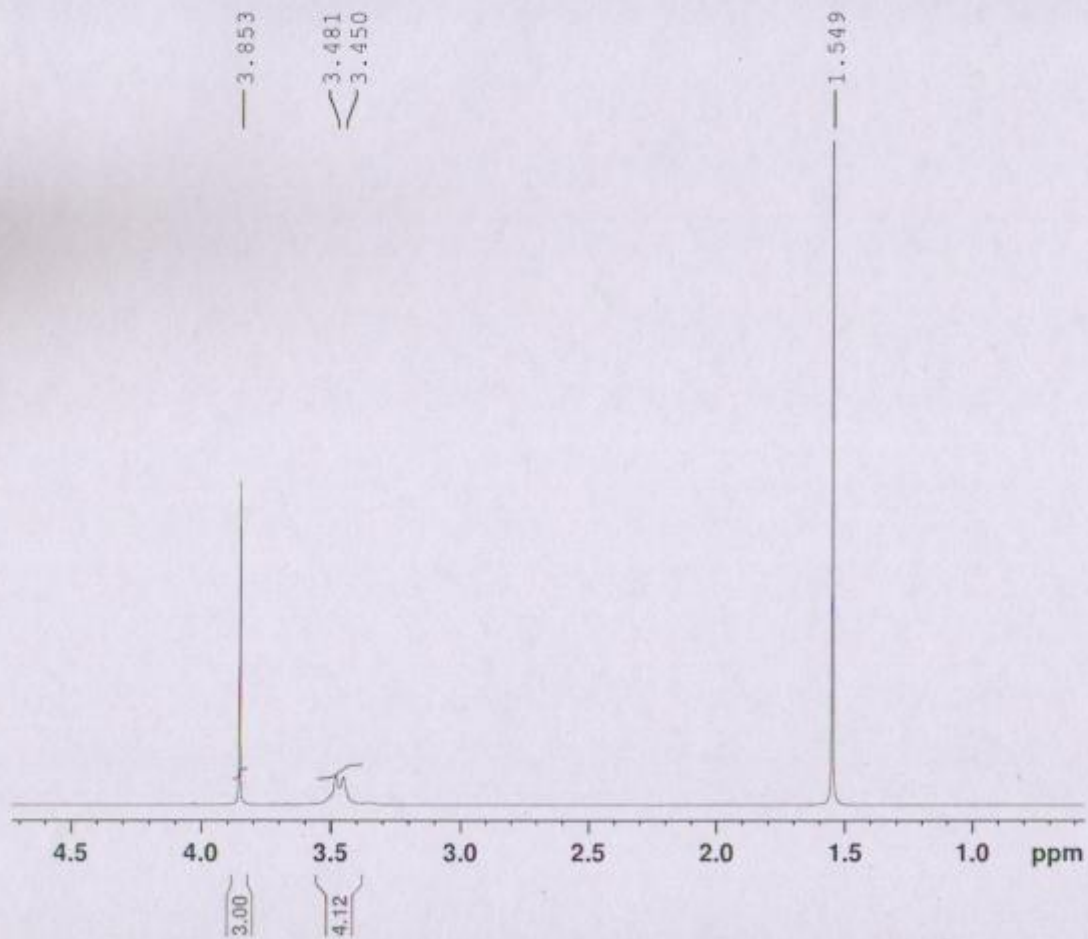
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022207C9937



¹H NMR of 5-Bromo-4'-methoxy-[1,1'-biphenyl]-2,3-diamine (5)



C6292-044



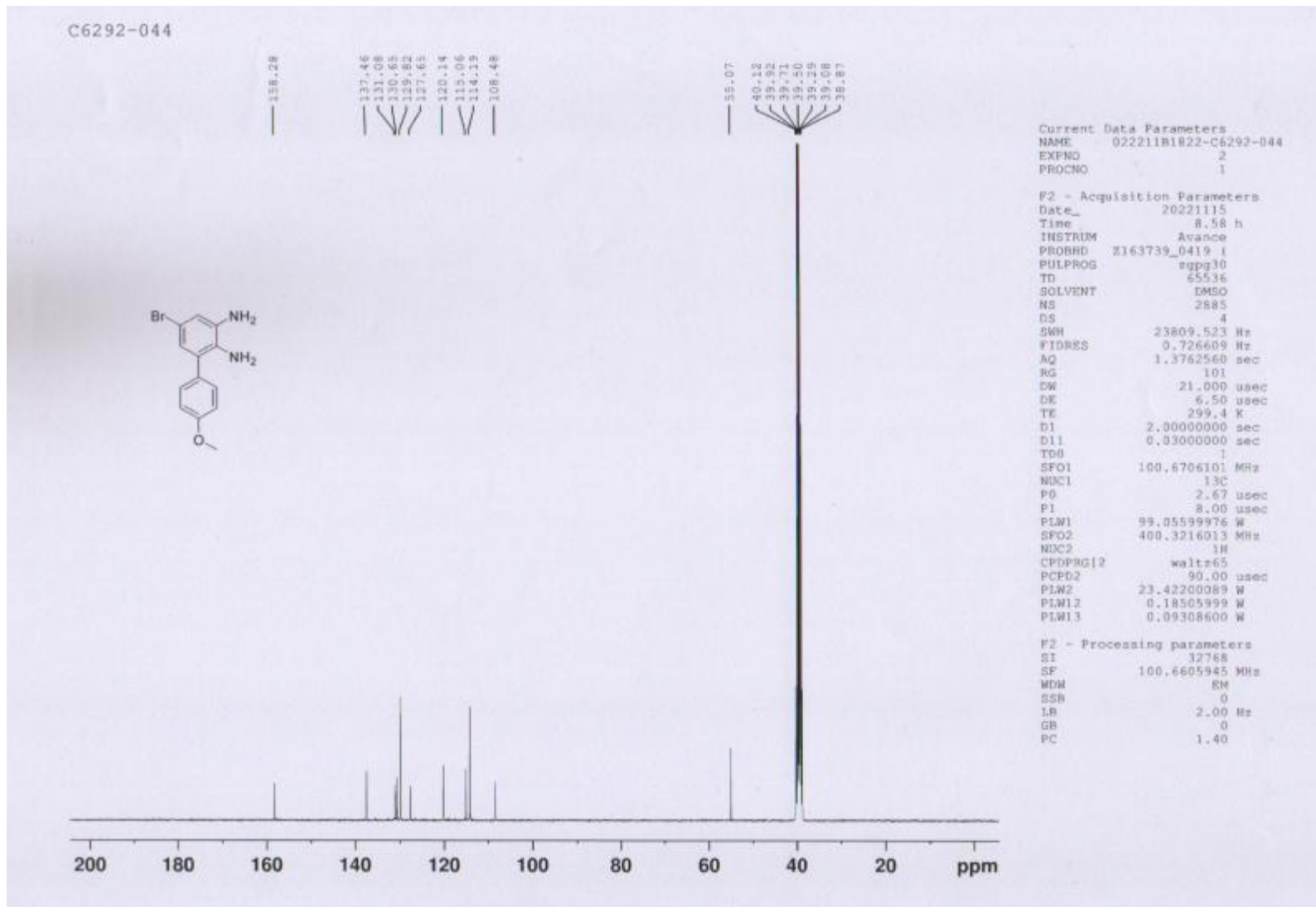
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PROCNO 1

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SOLVENT CDCl3
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AQ 4.5875201 sec
RG 101
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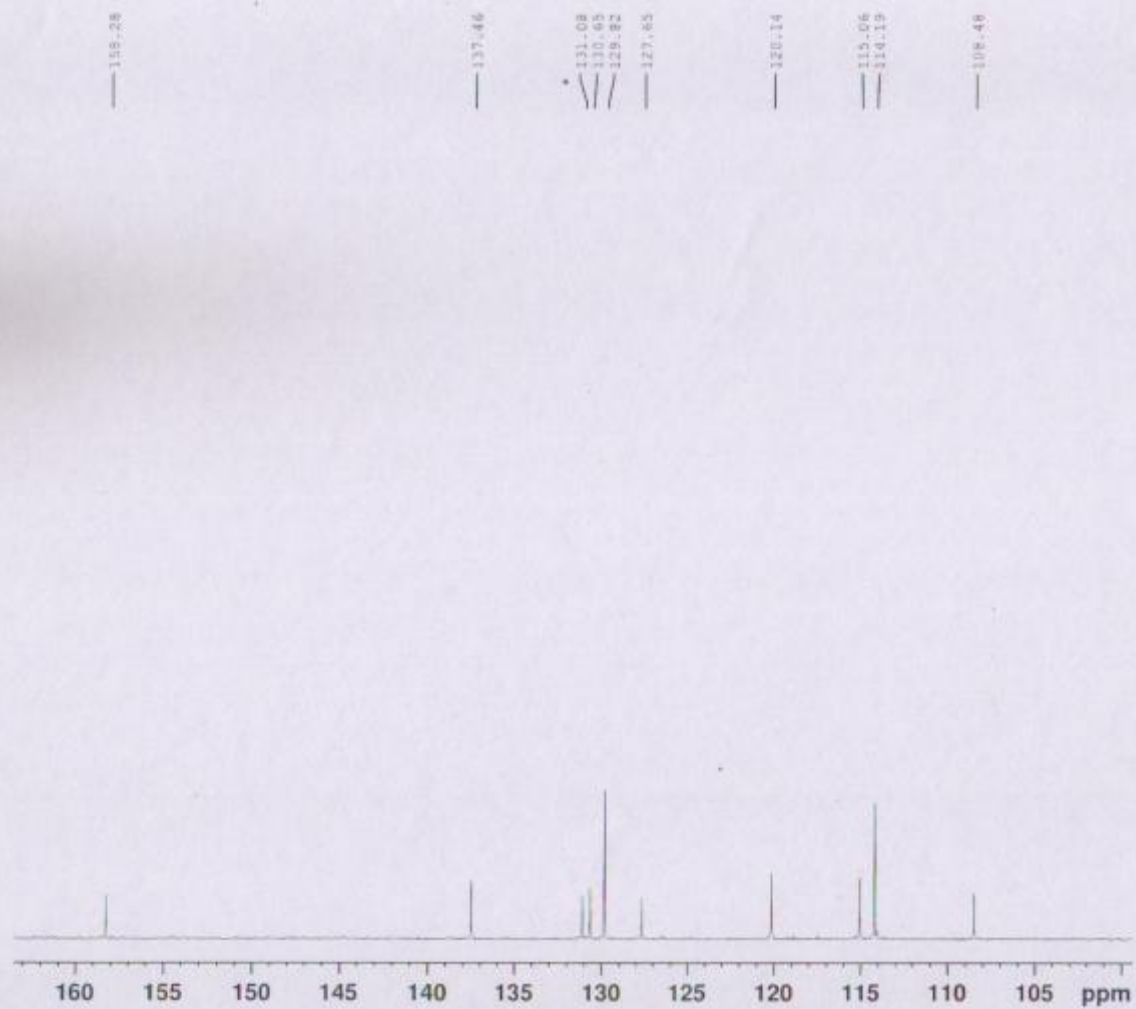
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ANL-MCL3-NMR-005

13C NMR of 5-Bromo-4'-methoxy-[1,1'-biphenyl]-2,3-diamine (5)



C6292-044

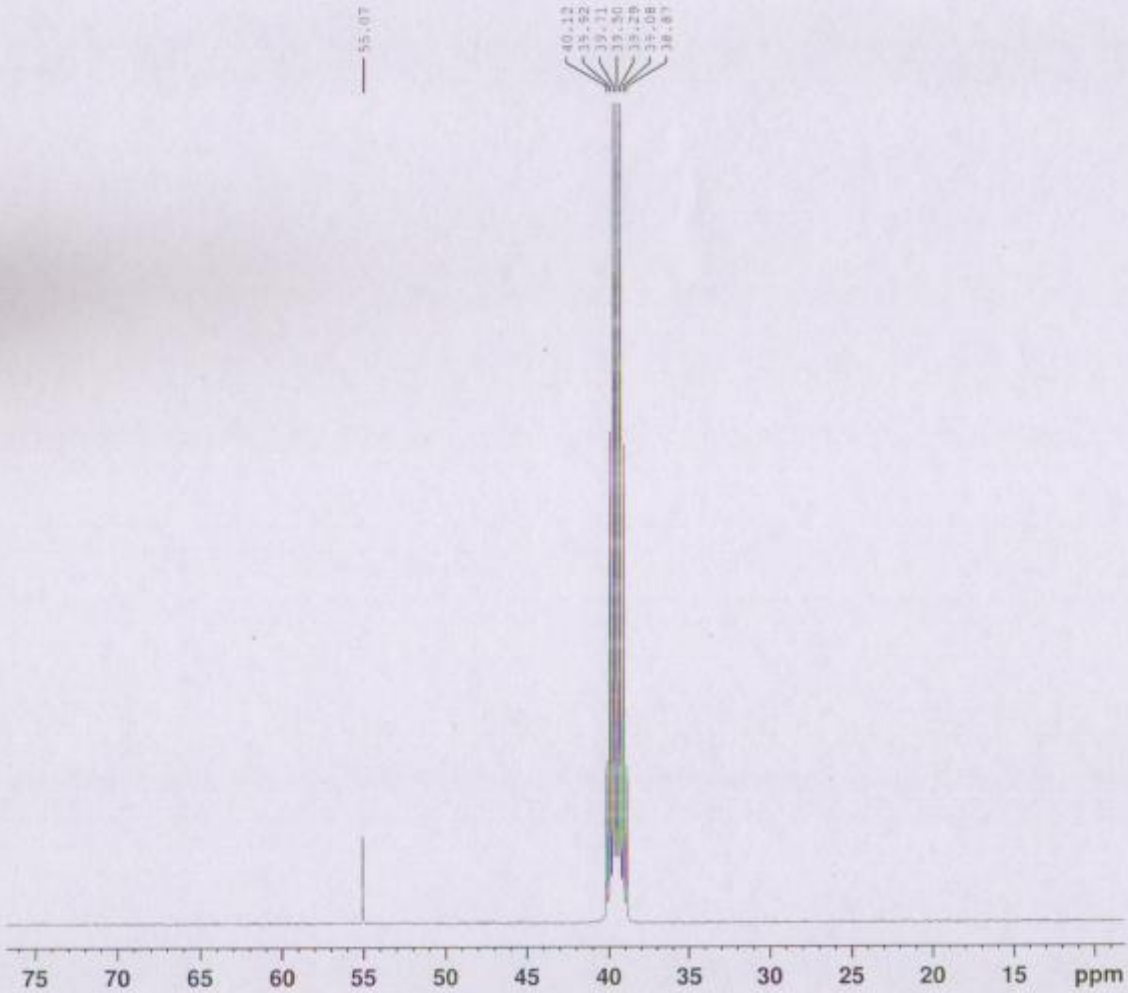


Current Data Parameters
NAME 02221181822-C6292-044
EXPNO 2
PROCNO 1

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SOLVENT DMSO
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FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DM 21.000 usec
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D1 2.0000000 sec
D11 0.0300000 sec
TDO 1
SFO1 100.6706101 MHz
NUC1 13C
PQ 2.67 usec
PI 5.00 usec
PLW1 99.05599976 M
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG12 waltz65
PCPD2 90.00 usec
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PLW12 0.18505999 M
PLW13 0.09308600 M

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C6292-044

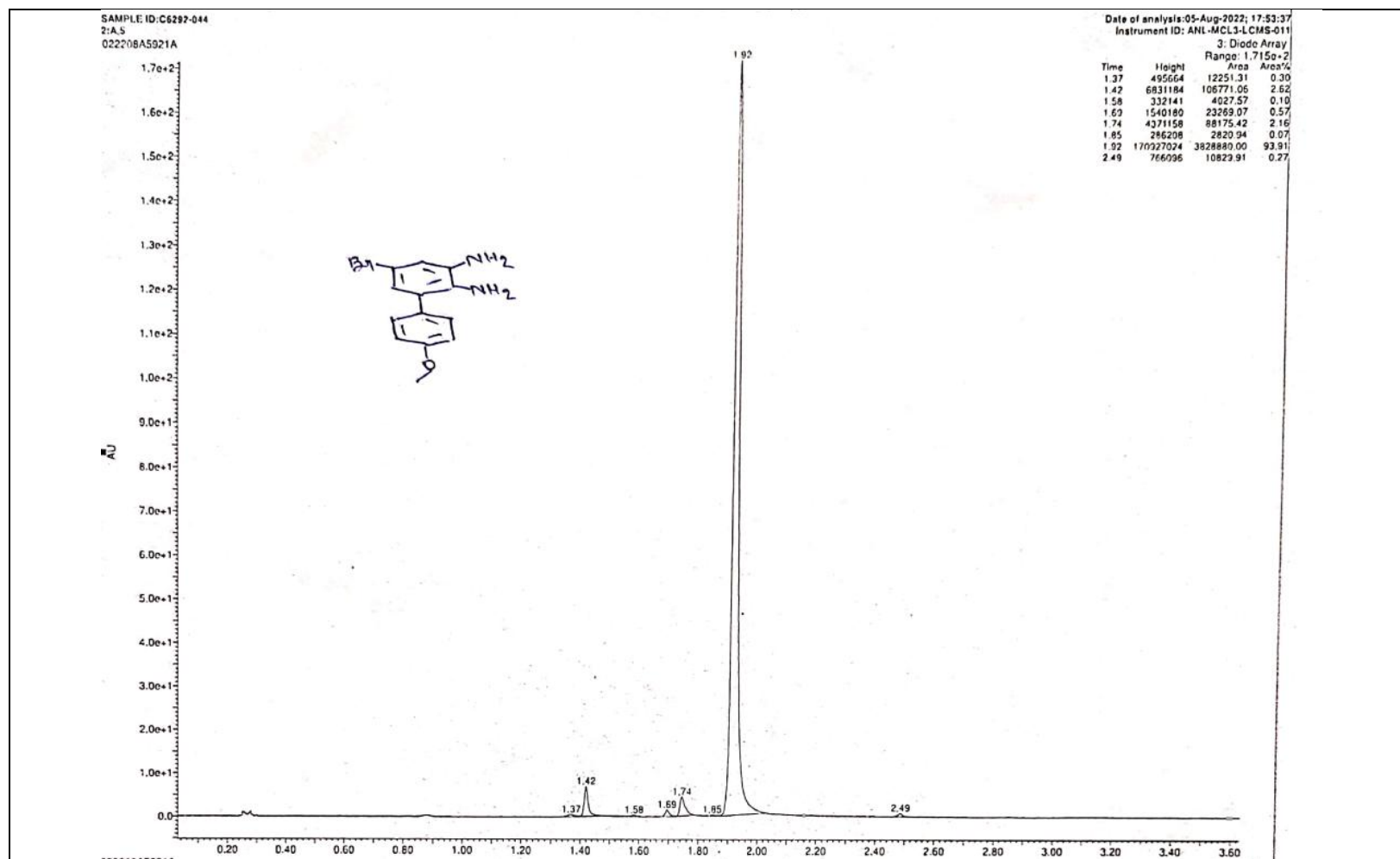


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PROCNO 1

F2 - Acquisition Parameters
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DE 6.50 usec
TE 299.4 K
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O11 0.03000000 sec
TDO 1
SFO1 100.6706101 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 99.05599976 W
SFO2 400.3216013 MHz
NUC2 1H
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PCPD2 90.00 usec
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PLW12 0.18505999 W
PLW13 0.09308600 W

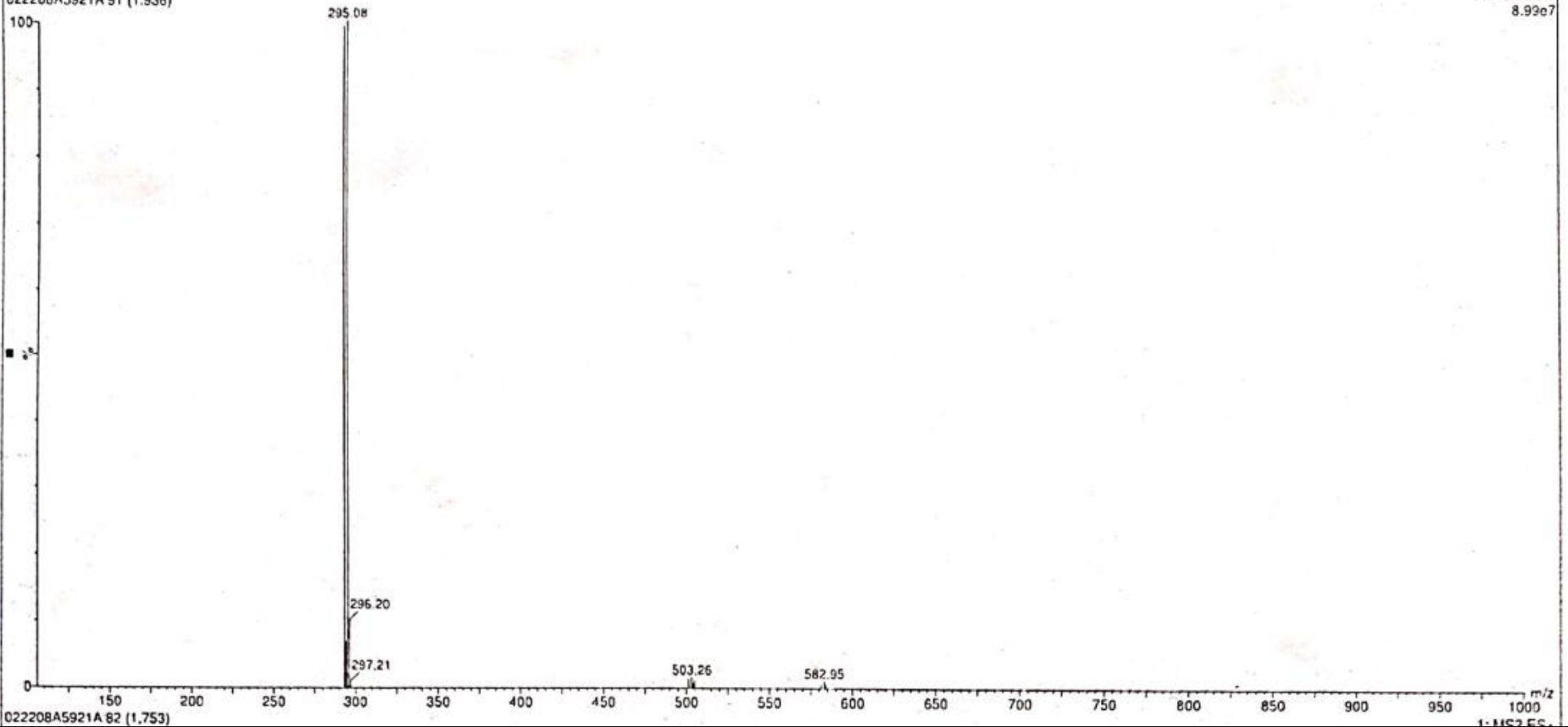
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LCMS of 5-Bromo-4'-methoxy-[1,1'-biphenyl]-2,3-diamine (5)



SAMPLE ID: C6292-044
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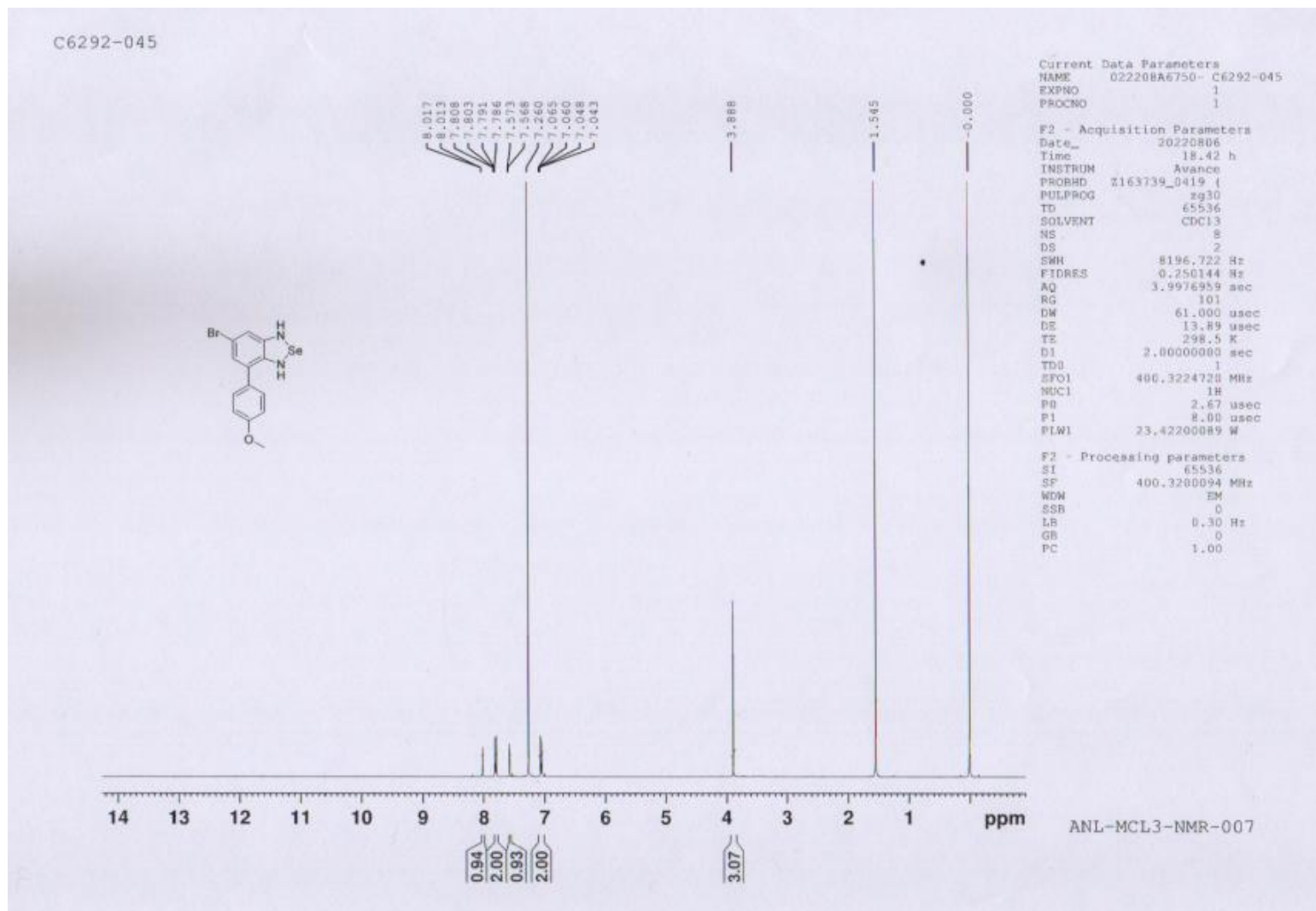
Date of analysis: 05-Aug-2022; 17:53:37
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8.99e7



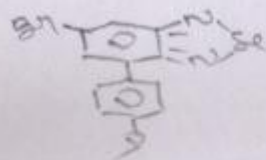
022208A5921A 82 (1.753)

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¹H NMR of 6-Bromo-4-(4-methoxyphenyl)benzo[c][1,2,5]selenadiazole (6)



C6292-045



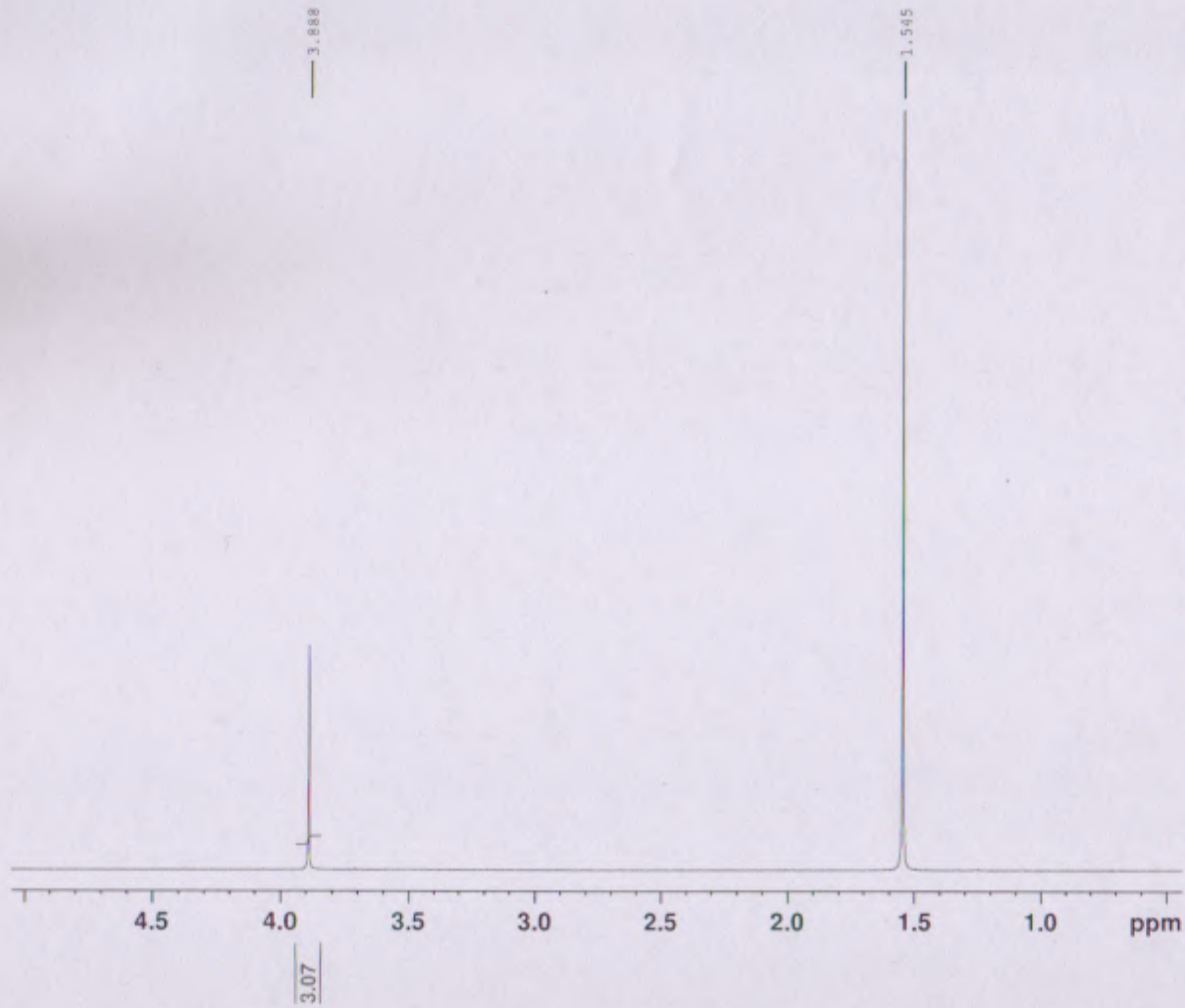
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FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
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DE 13.89 usec
TE 298.5 K
D1 2.00000000 sec
TDO 1
SFO1 400.3224720 MHz
NUC1 1H
PO 2.67 usec
P1 8.00 usec
PL1 23.42200089 W

F2 - Processing parameters
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ANL-MCL3-NMR-007

C6292-045



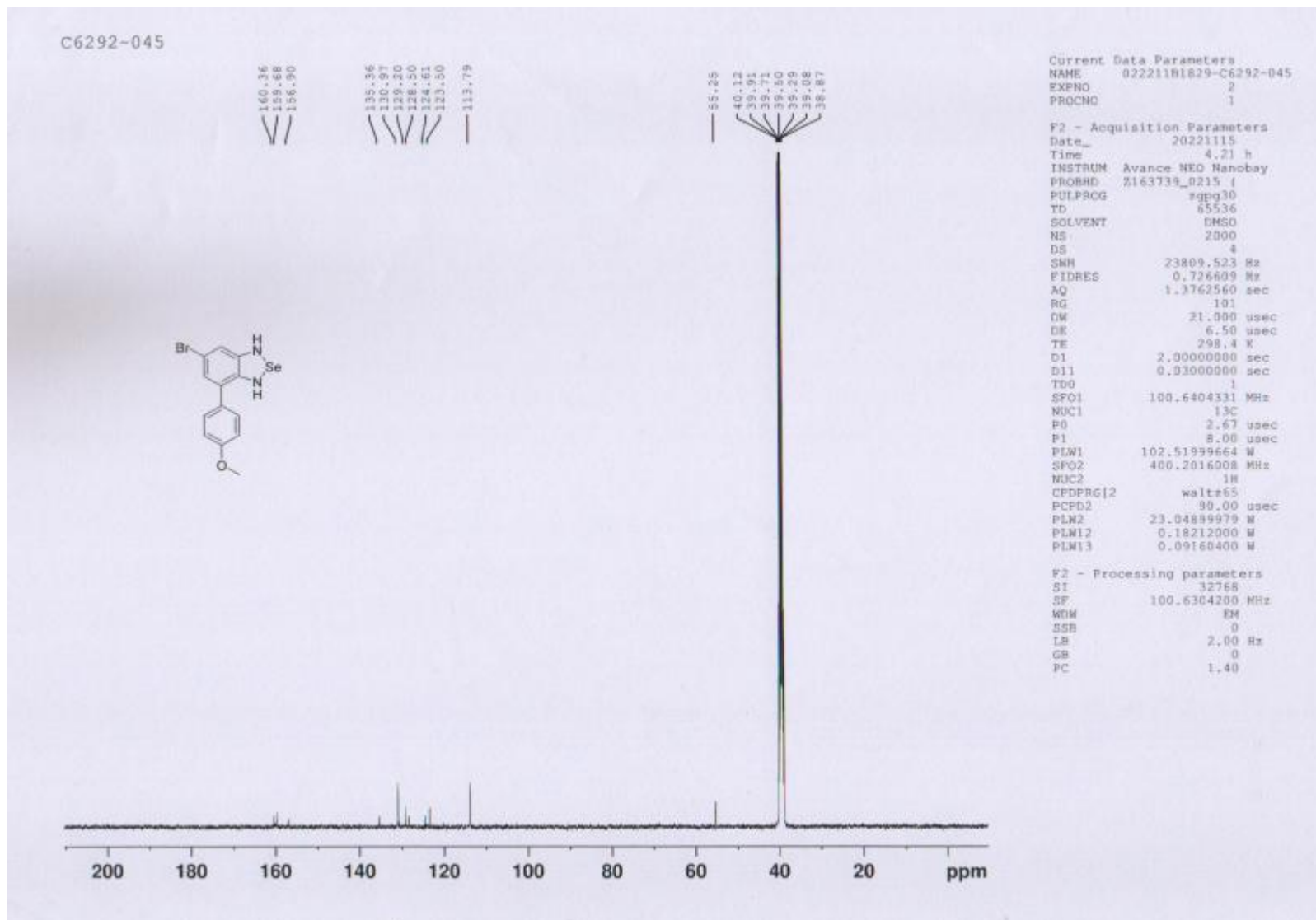
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EXPNO 1
PROCNO 1

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DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.5 K
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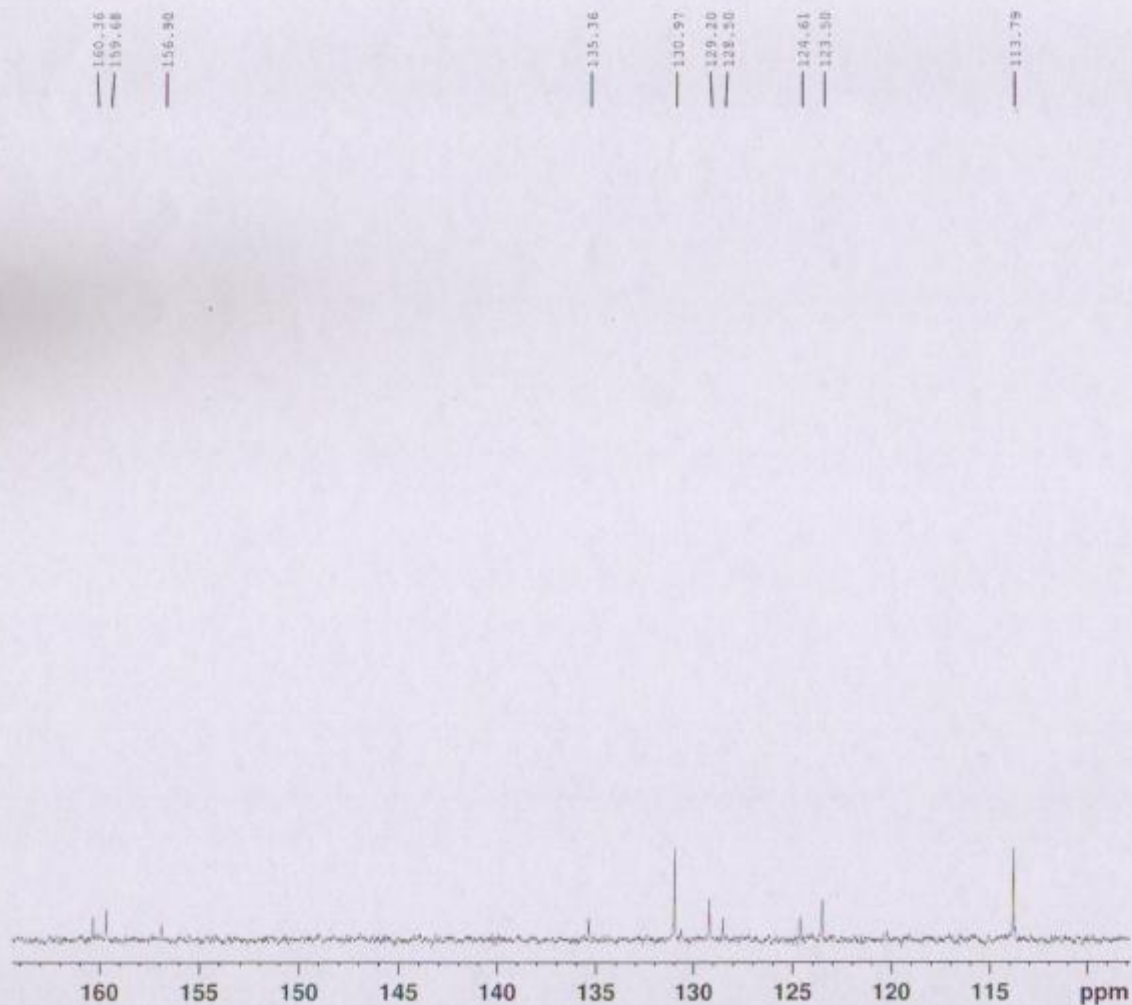
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LB 0.30 Hz
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PC 1.00

ANL-MCL3-NMR-007

13C NMR of 6-Bromo-4-(4-methoxyphenyl)benzo[c][1,2,5]selenadiazole (6)



C6292-045



Current Data Parameters
NAME 022211B1829-C6292-045
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221115
Time 4.21 h
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 73809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 298.4 K
D1 2.0000000 sec
D11 0.6300000 sec
TDO 1
SFO1 100.6404331 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLM1 102.51999664 W
SFO2 400.2016008 MHz
NUC2 1H
CPDPRG12 waltz65
PCPD2 90.00 usec
PLM2 23.04899979 W
PLM12 0.18212000 W
PLM13 0.09160400 W

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C6292-045

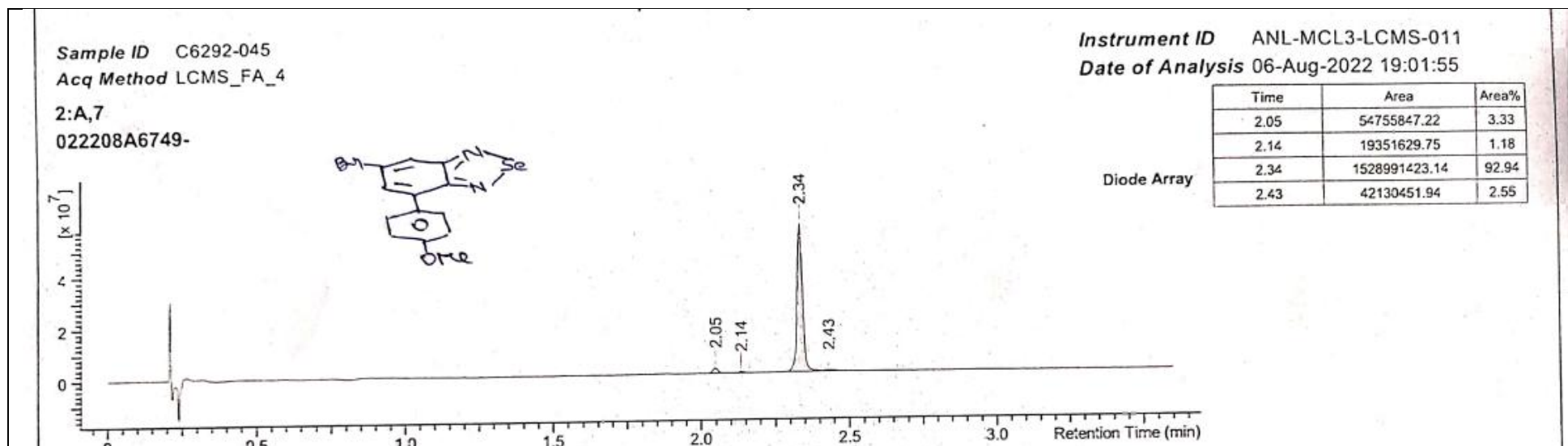


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EXPNO 2
PROCNO 1

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TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
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RG 181
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TE 298.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
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NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLM1 102.51999664 W
SFO2 400.2016008 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 23.04899979 W
PLW12 0.18212000 W
PLW13 0.09160400 W

F2 - Processing parameters
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LCMS of 6-Bromo-4-(4-methoxyphenyl)benzo[c][1,2,5]selenadiazole (6)



Sample ID C6292-045

Discovery Chemistry - Analytical Services

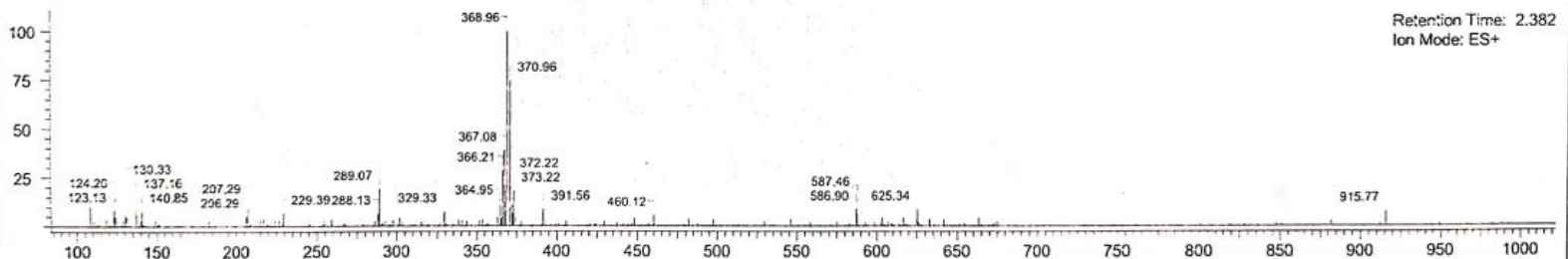
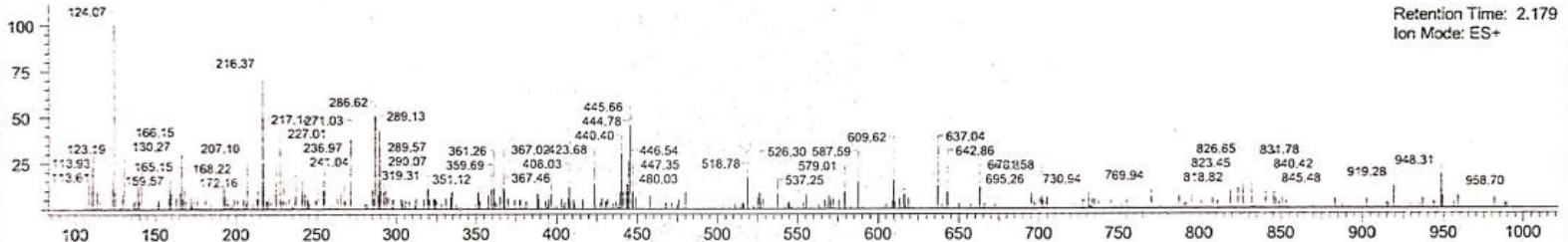
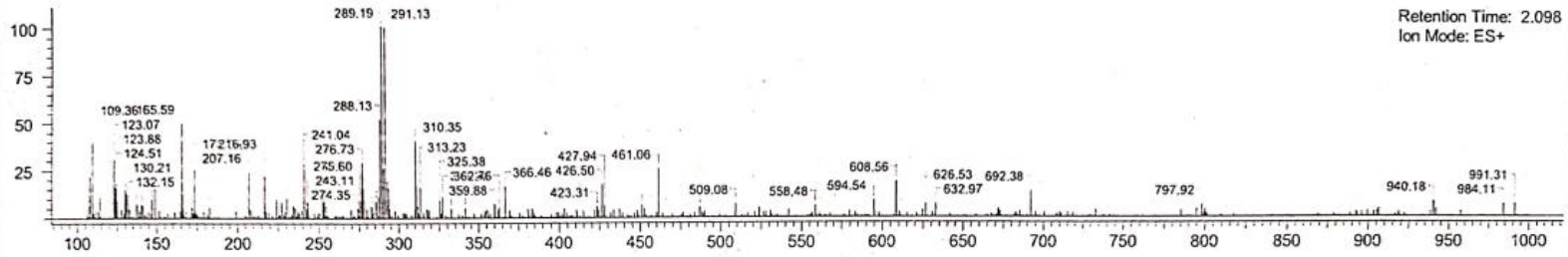
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Acq Method LCMS_FA_4

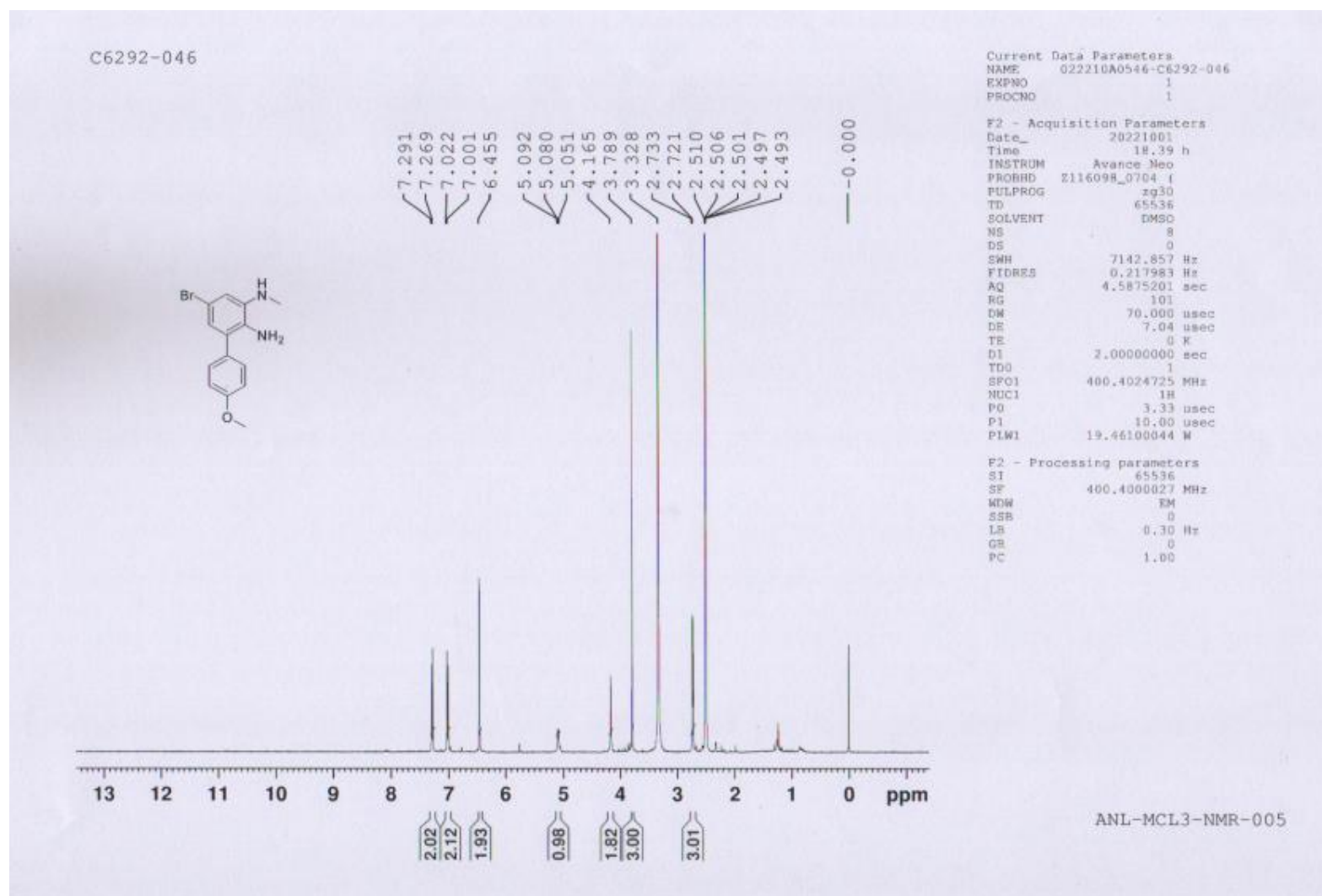
Date of Analysis 06-Aug-2022 19:01:55

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022208A6749-



¹H NMR of 5-Bromo-4'-methoxy-N³-methyl-[1,1'-biphenyl]-2,3-diamine (7)

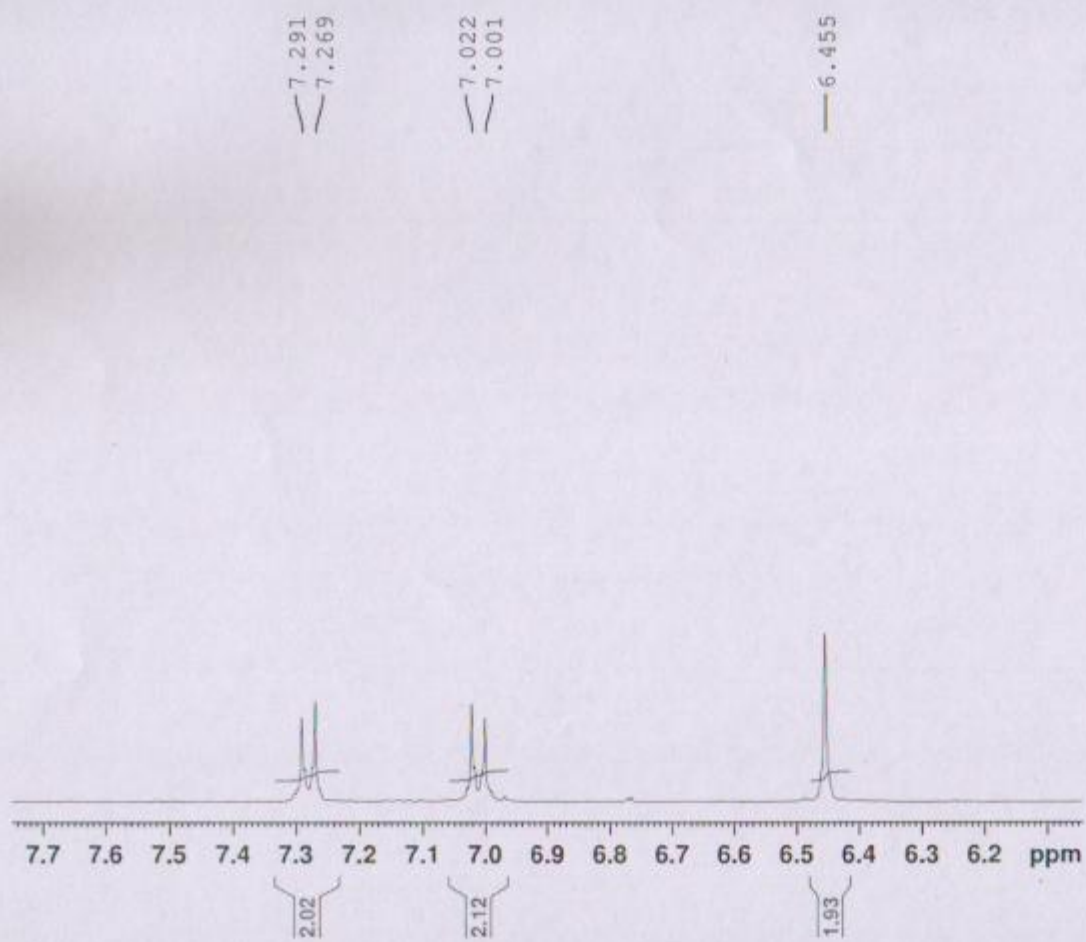


C6292-046

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PROCNO 1

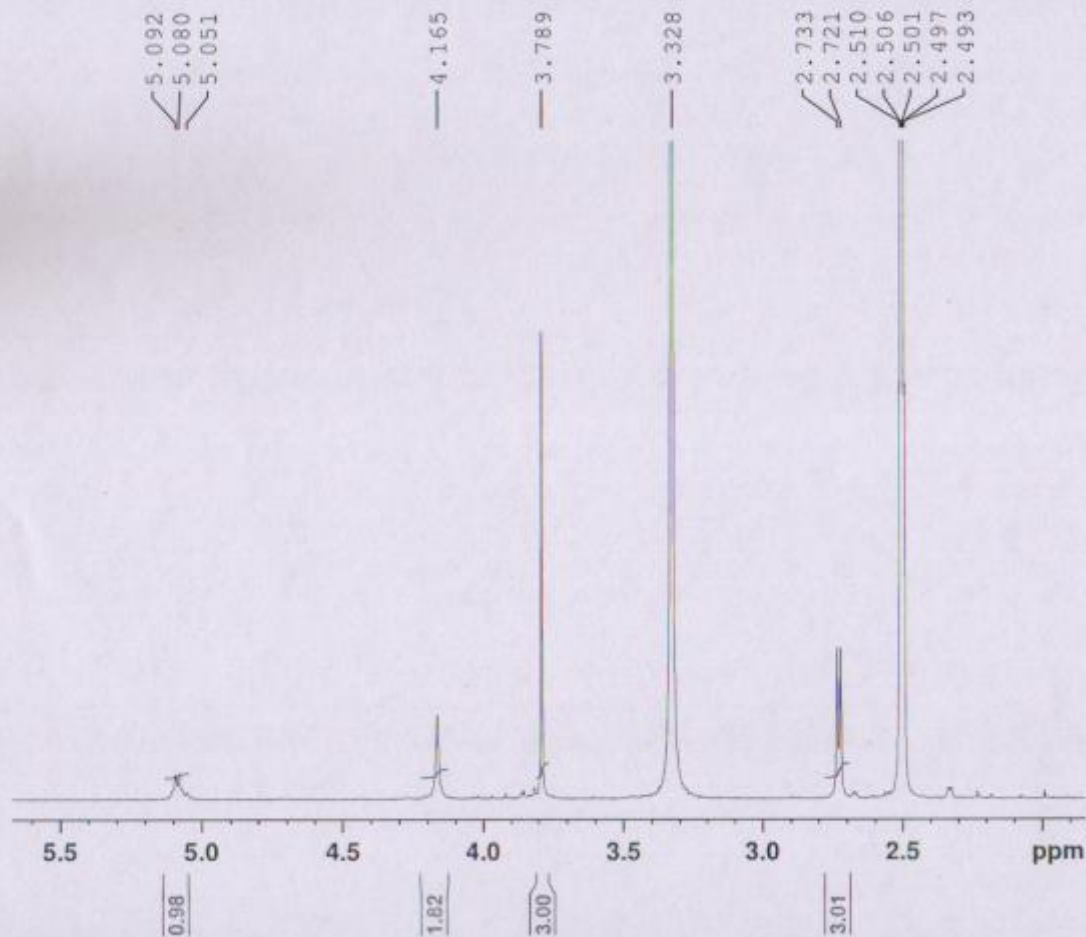
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NS 8
DS 0
SWH 7142.857 Hz
FIDRES 0.217983 Hz
AQ 4.5875201 sec
RG 101
DW 70.000 usec
DE 7.04 usec
TE 0 K
D1 2.00000000 sec
TDO 1
SFO1 400.4024725 MHz
NUC1 1H
PO 3.33 usec
P1 10.00 usec
PLW1 19.46100044 W

F2 - Processing parameters
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ANL-MCL3-NMR-005

C6292-046



Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 7142.857 Hz
FIDRES 0.217983 Hz
AQ 4.5875201 sec
RG 101
DW 70.000 usec
DE 7.04 usec
TE 0 K
D1 2.0000000 sec
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SFO1 400.4024725 MHz
NUC1 1H
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PLW1 19.46100044 W

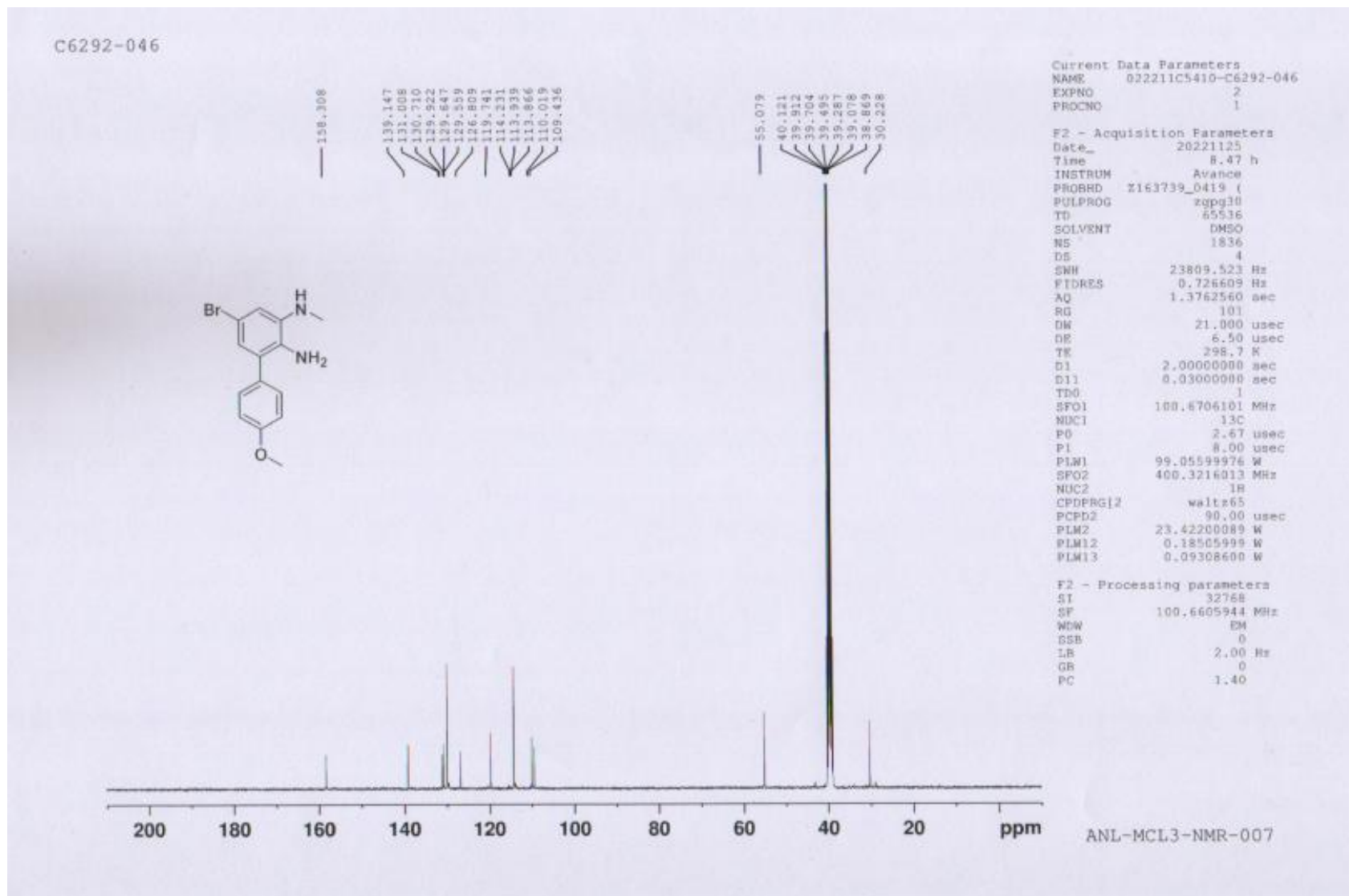
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ANL-MCL3-NMR-005

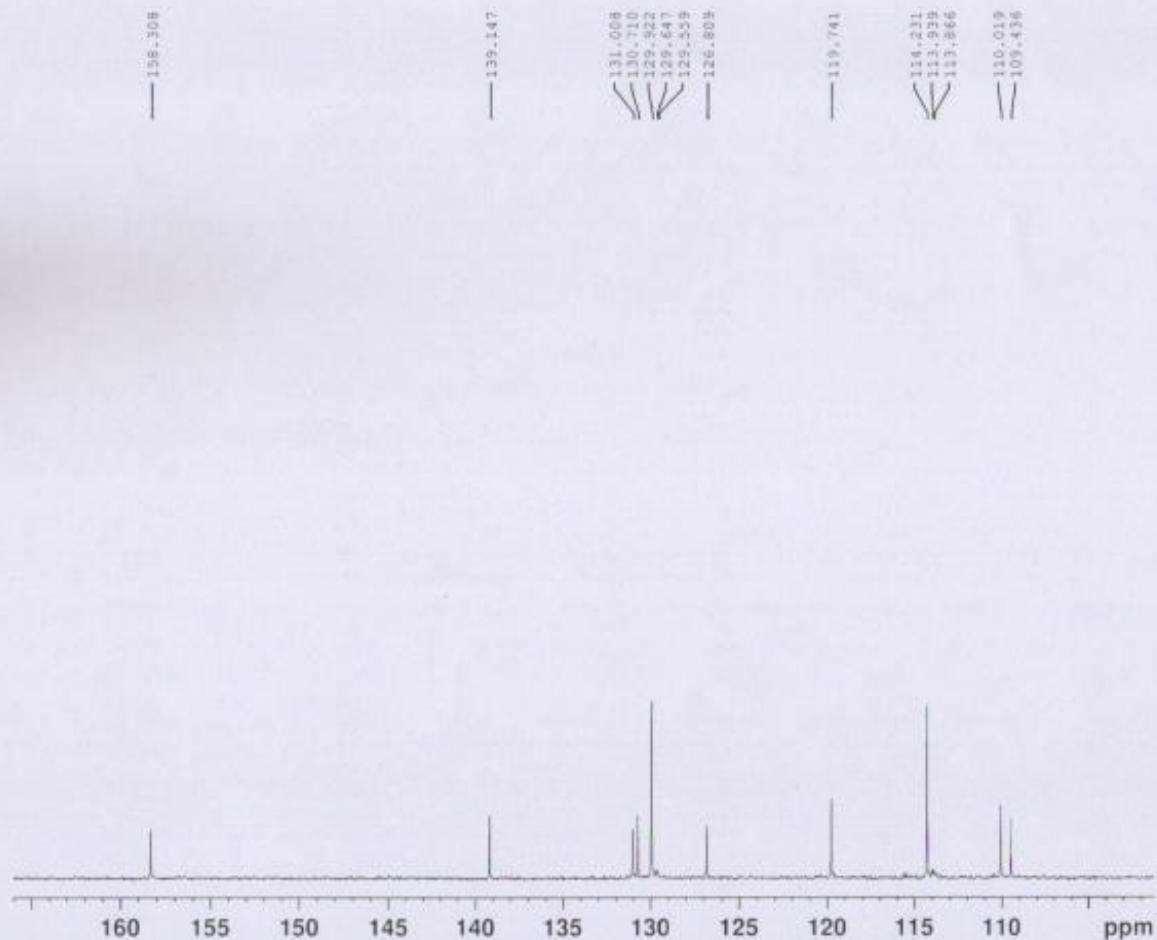
NOE of 5-Bromo-4'-methoxy-*N*³-methyl-[1,1'-biphenyl]-2,3-diamine (7)



¹³C NMR of 5-Bromo-4'-methoxy-N³-methyl-[1,1'-biphenyl]-2,3-diamine (7)



C6292-046



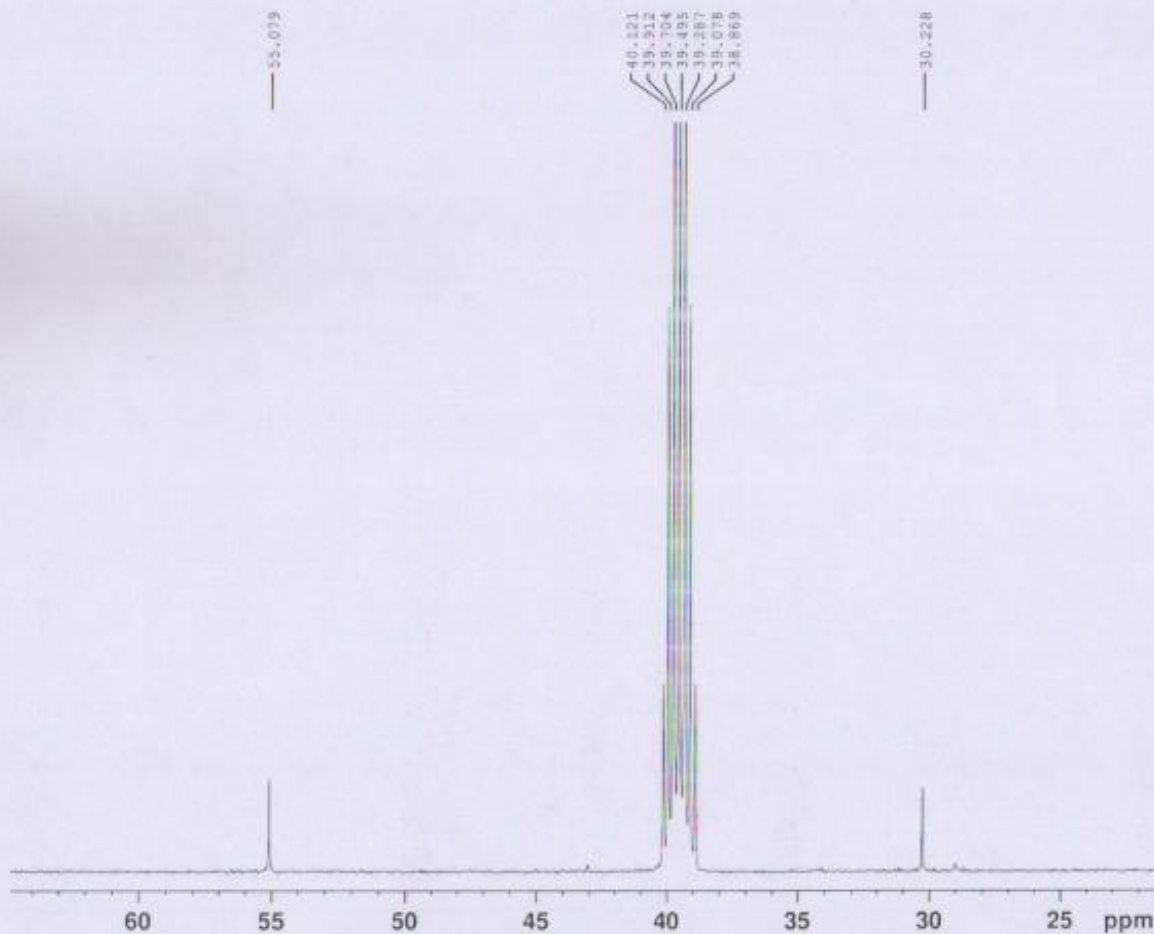
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SOLVENT DMSO
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SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 298.7 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6706101 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 99.05599976 W
SFO2 400.3216013 MHz
NUC2 1H
CPOPRG(2) waltz65
PCPD2 90.00 usec
PLW2 23.42200089 W
PLW12 0.18505999 W
PLW13 0.09308600 W

F2 - Processing parameters
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ANL-MCL3-NMR-007

C6292-046



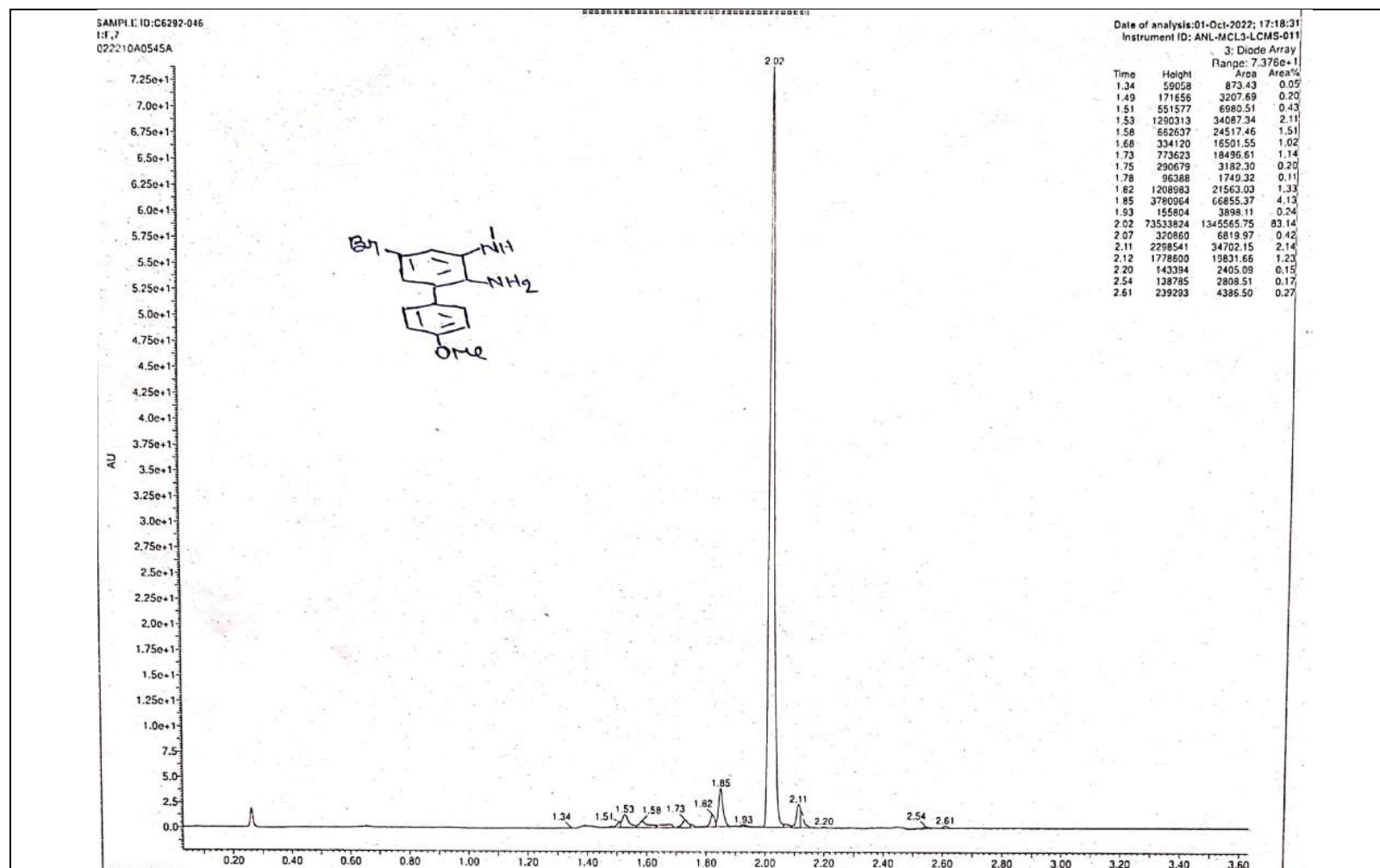
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FIDRES 0.726609 Hz
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P0 2.67 usec
P1 8.00 usec
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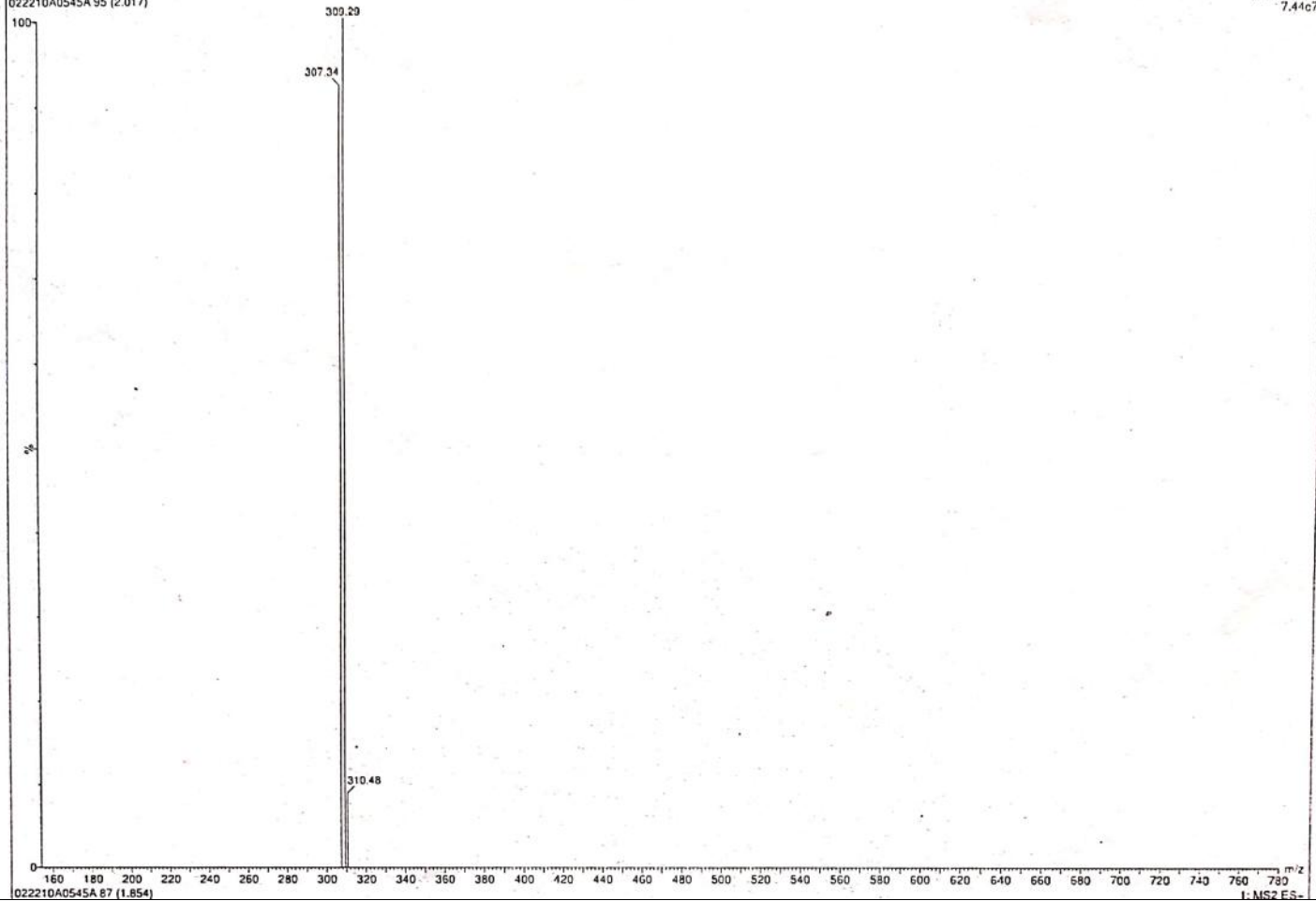
ANL-MCL3-NMR-007

LCMS of 5-Bromo-4'-methoxy-*N*³-methyl-[1,1'-biphenyl]-2,3-diamine (7)

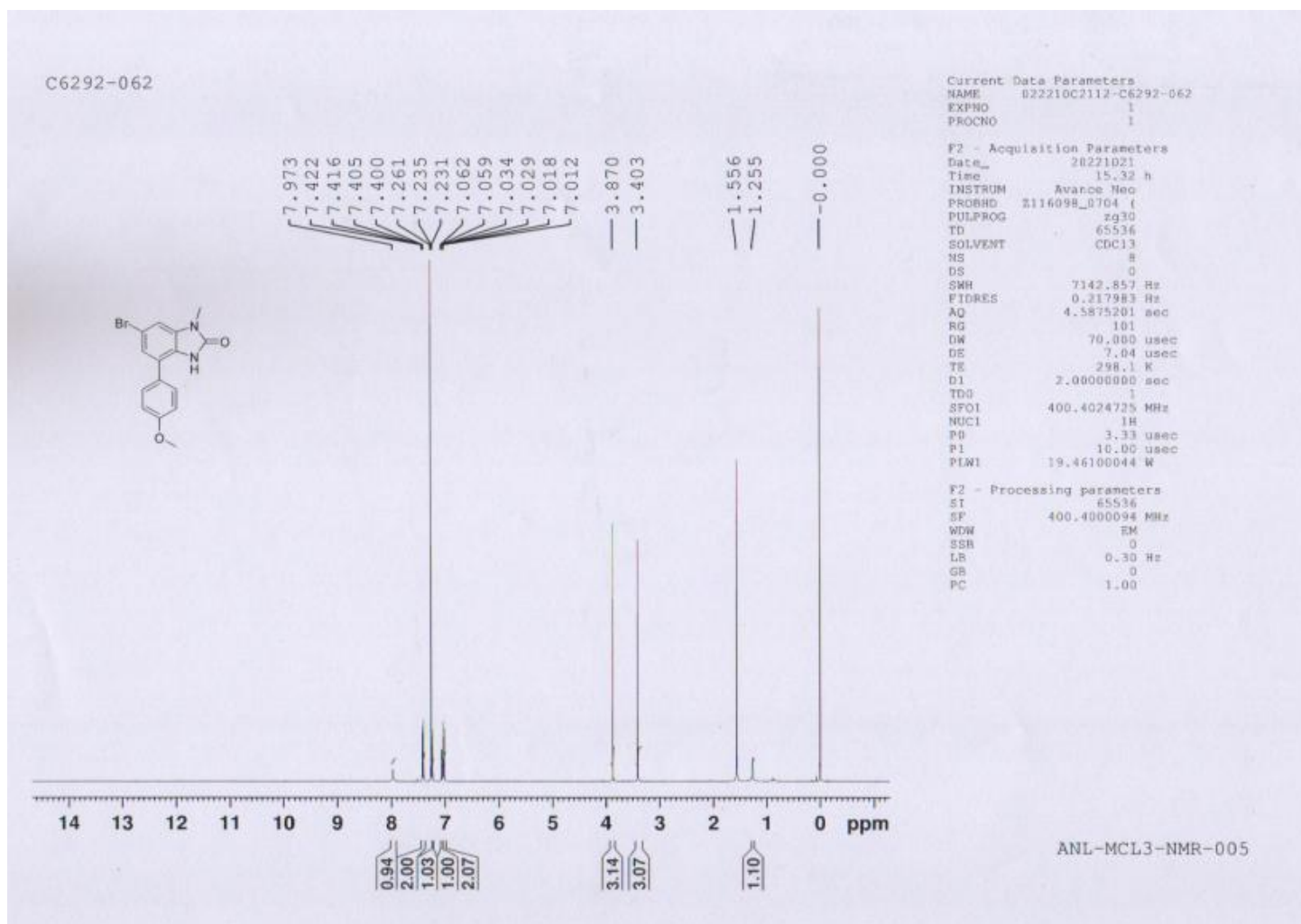


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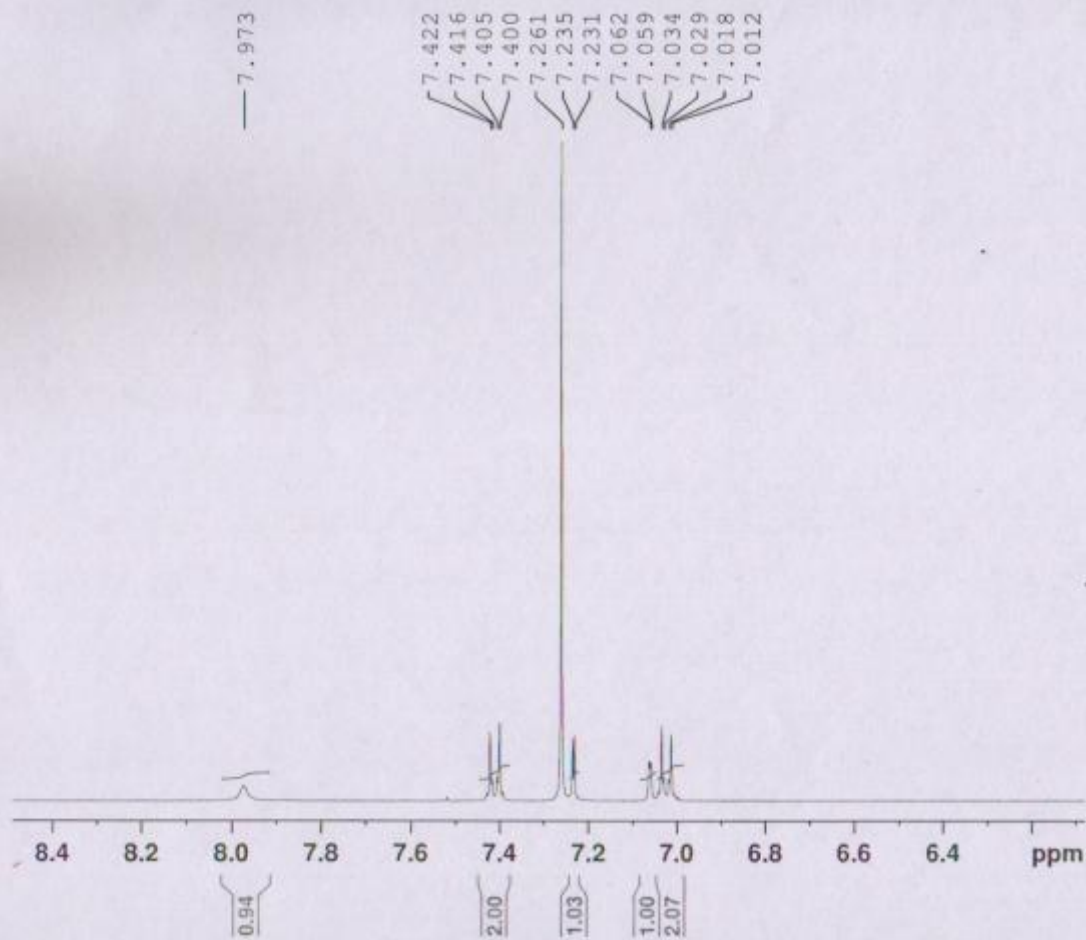
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¹H NMR of 6-Bromo-4-(4-methoxyphenyl)-1-methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (8)



C6292-062



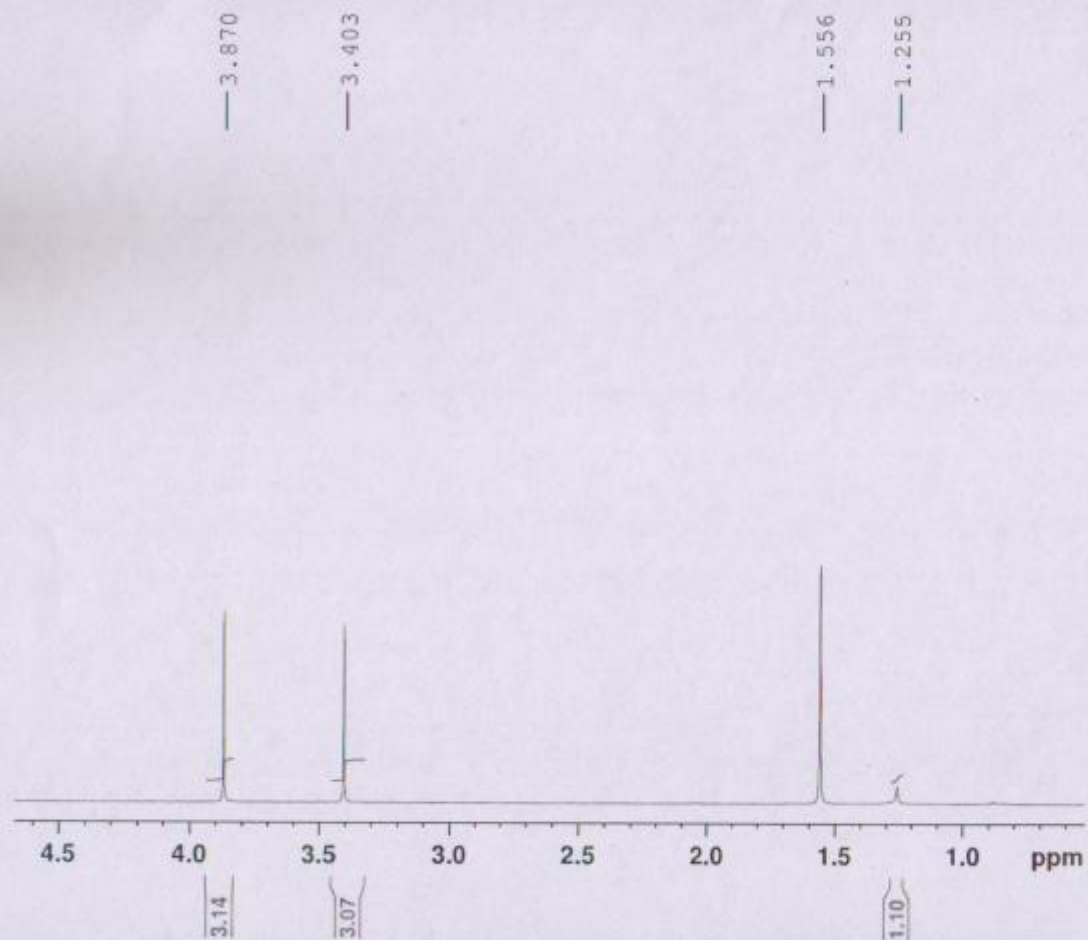
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EXPNO 1
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 7142.857 Hz
FIDRES 0.217983 Hz
AQ 4.5875201 sec
RG 101
DW 70.000 usec
DE 7.04 usec
TE 298.1 K
D1 2.00000000 sec
TDO 1
SFO1 400.4024725 MHz
NUC1 1H
PO 3.33 usec
PI 10.00 usec
PLW1 19.46100044 W

F2 - Processing parameters
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SSB 0
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GB 0
PC 1.00

ANL-MCL3-NMR-005

C6292-062



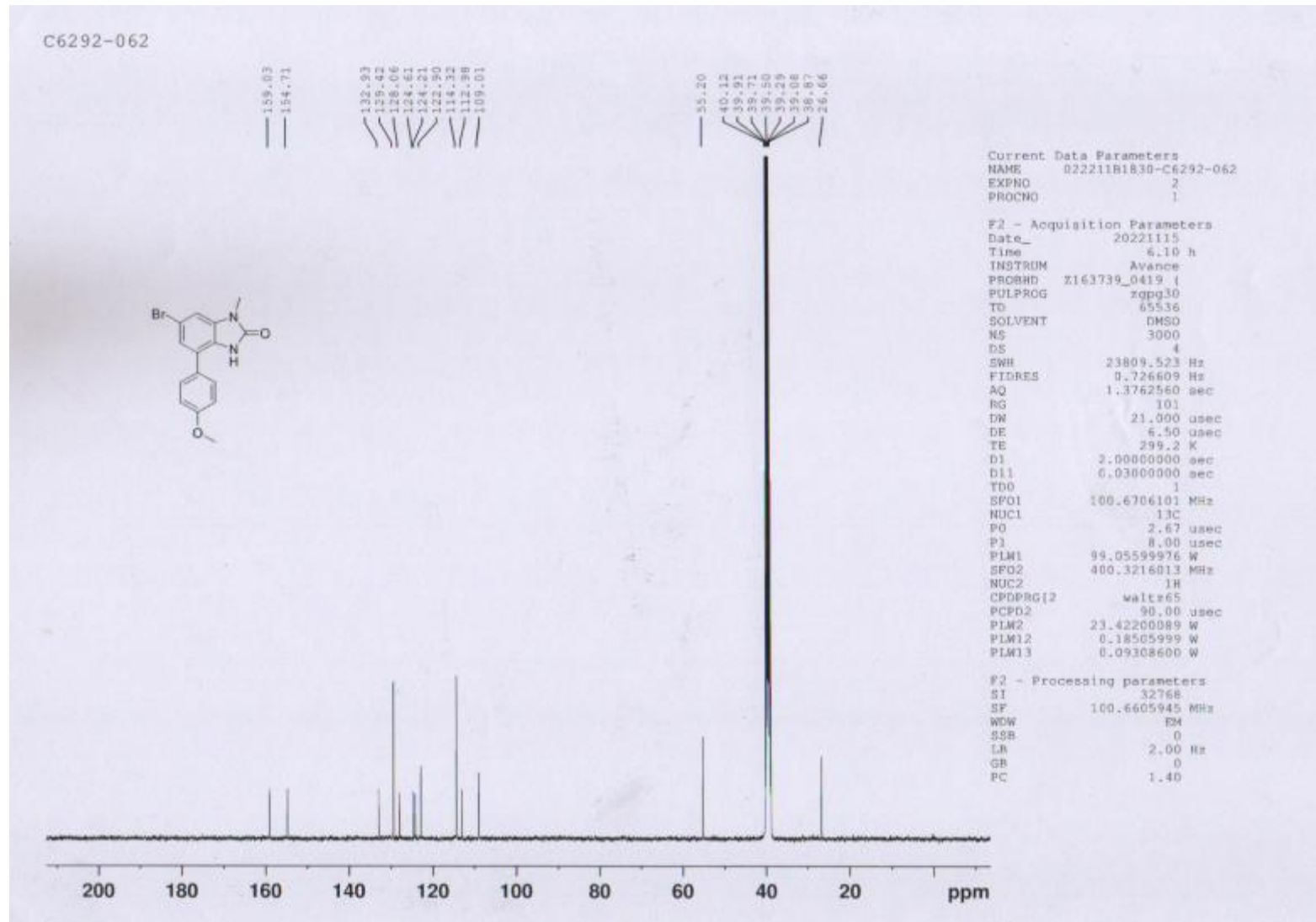
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EXPNO 1
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SOLVENT CDCl3
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DE 7.04 usec
TE 298.1 K
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P1 10.00 usec
PLW1 19.46100044 W

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PC 1.00

ANL-MCL3-NMR-005

¹³C NMR of 6-Bromo-4-(4-methoxyphenyl)-1-methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (8)



C6292-062

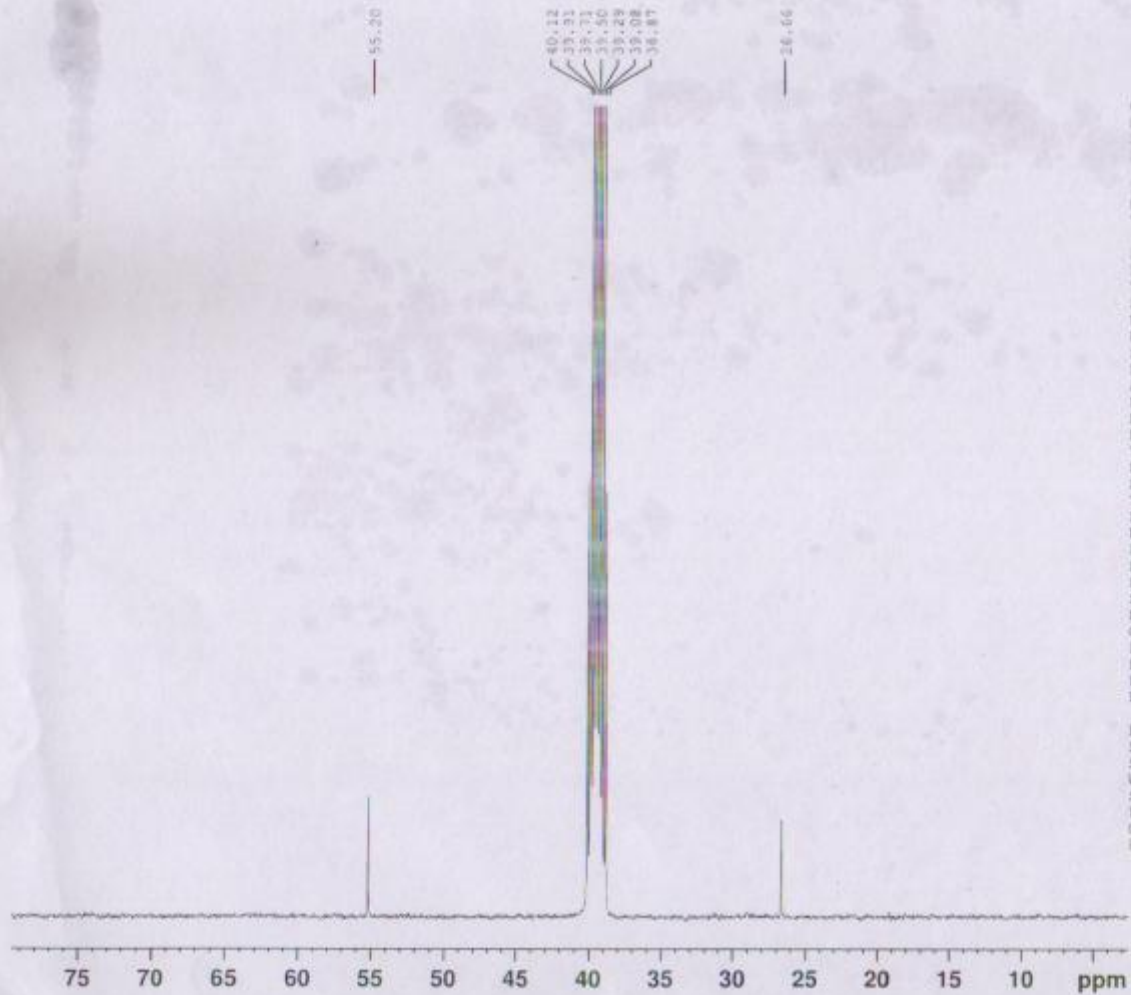


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EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3000
DS 4
SWH 23809.523 Hz
FIDRES 0.724609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 299.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6706101 MHz
NUC1 13C
PC 2.67 usec
P1 8.00 usec
PLW1 99.05599976 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG12 waltz165
PCPD2 90.00 usec
PLW2 23.42200089 W
PLW12 0.18505999 W
PLW13 0.09308600 W

F2 - Processing parameters
SI 32768
SF 100.6605945 MHz
WDW EM
SSB 0
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GB 0
PC 1.40

C6292-062



Current Data Parameters
NAME 022211b1830-C6292-062
EXPRD 2
PROCNO 1

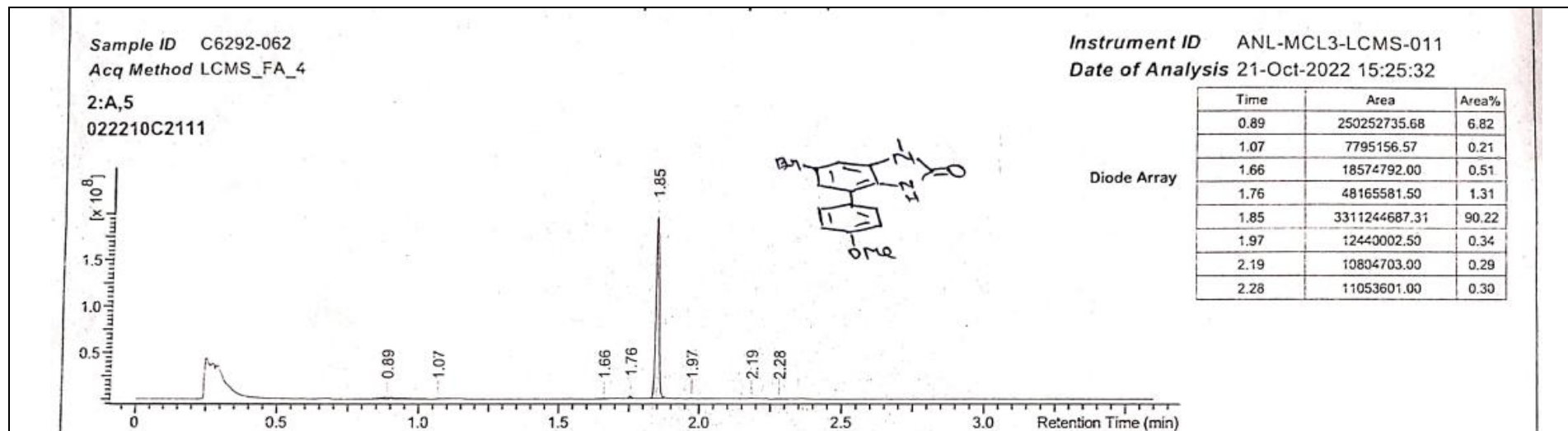
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Date_ 20221115
Time 6.10 h
INSTRM Avance
PROBHD 1143739_0419 1
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TD 65536
SOLVENT DMSO
NS 1000
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DM 21.000 usec
DE 6.50 usec
TE 299.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1
SFO1 100.6706101 MHz
NUC1 13C
PD 2.67 usec
P1 8.00 usec
PLW1 99.05599876 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG12 waltz65
PCPD2 90.00 usec
PLW2 23.42200089 W
PLW12 0.18505999 W
PLW13 0.09308600 W

F2 - Processing parameters

SI 32768
SF 100.6605945 MHz
WDW EM
SSM 0
LB 2.00 Hz
GB 0
PC 1.40

LCMS of 6-Bromo-4-(4-methoxyphenyl)-1-methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (8)



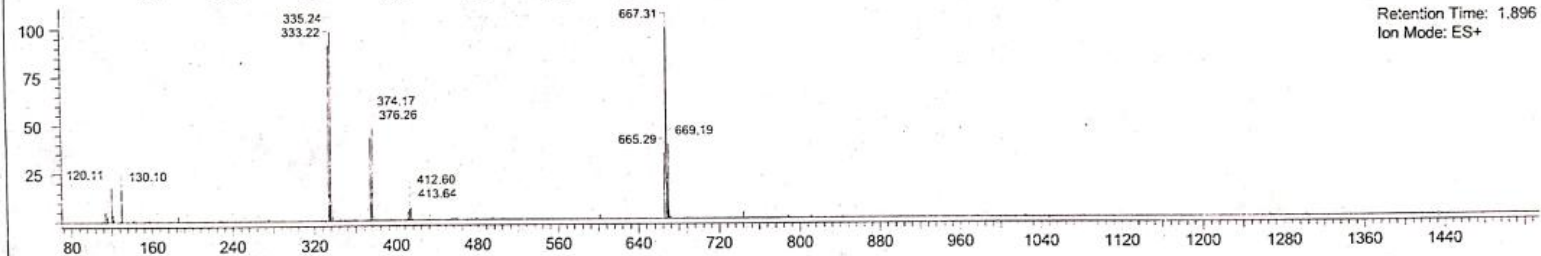
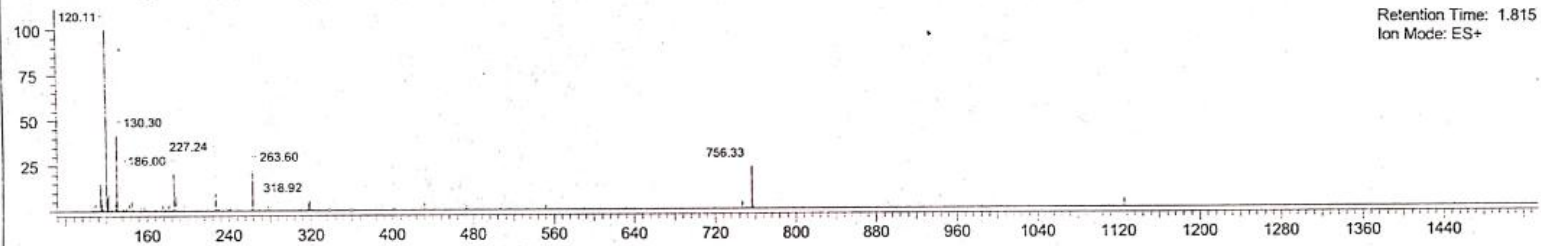
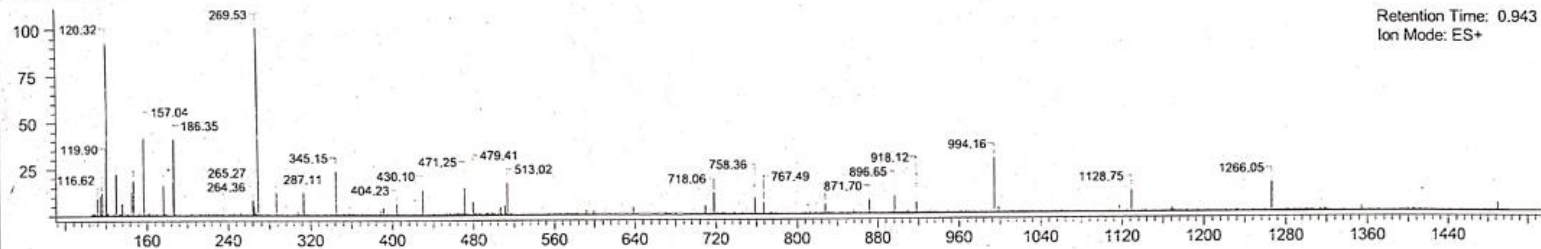
Acq Method LCMS_FA_4

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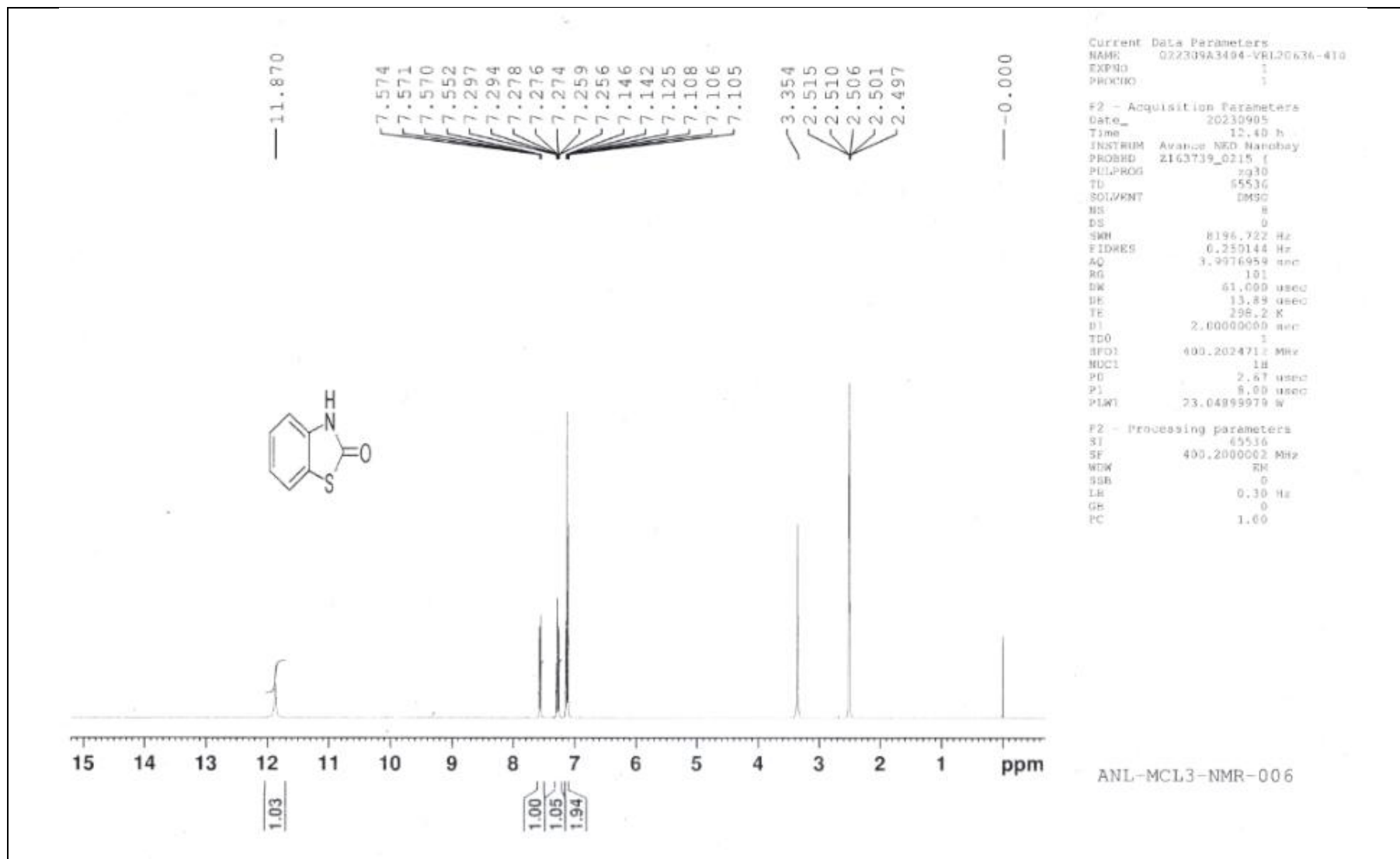
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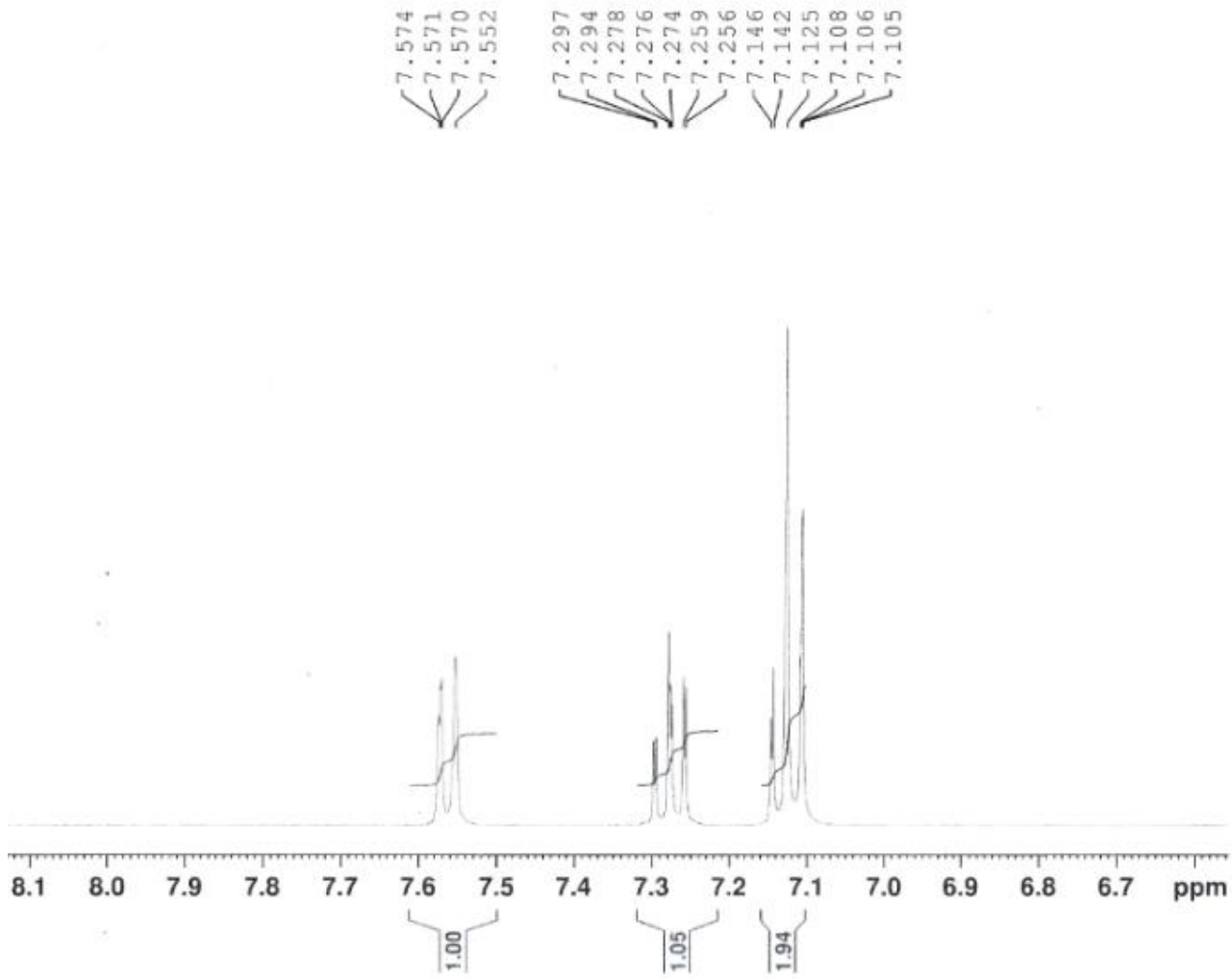
Instrument ID ANL-MCL3-LCMS-011

Date of Analysis 21-Oct-2022 15:25:32



¹H NMR of benzo[d]thiazol-2(3H)-one (2v)





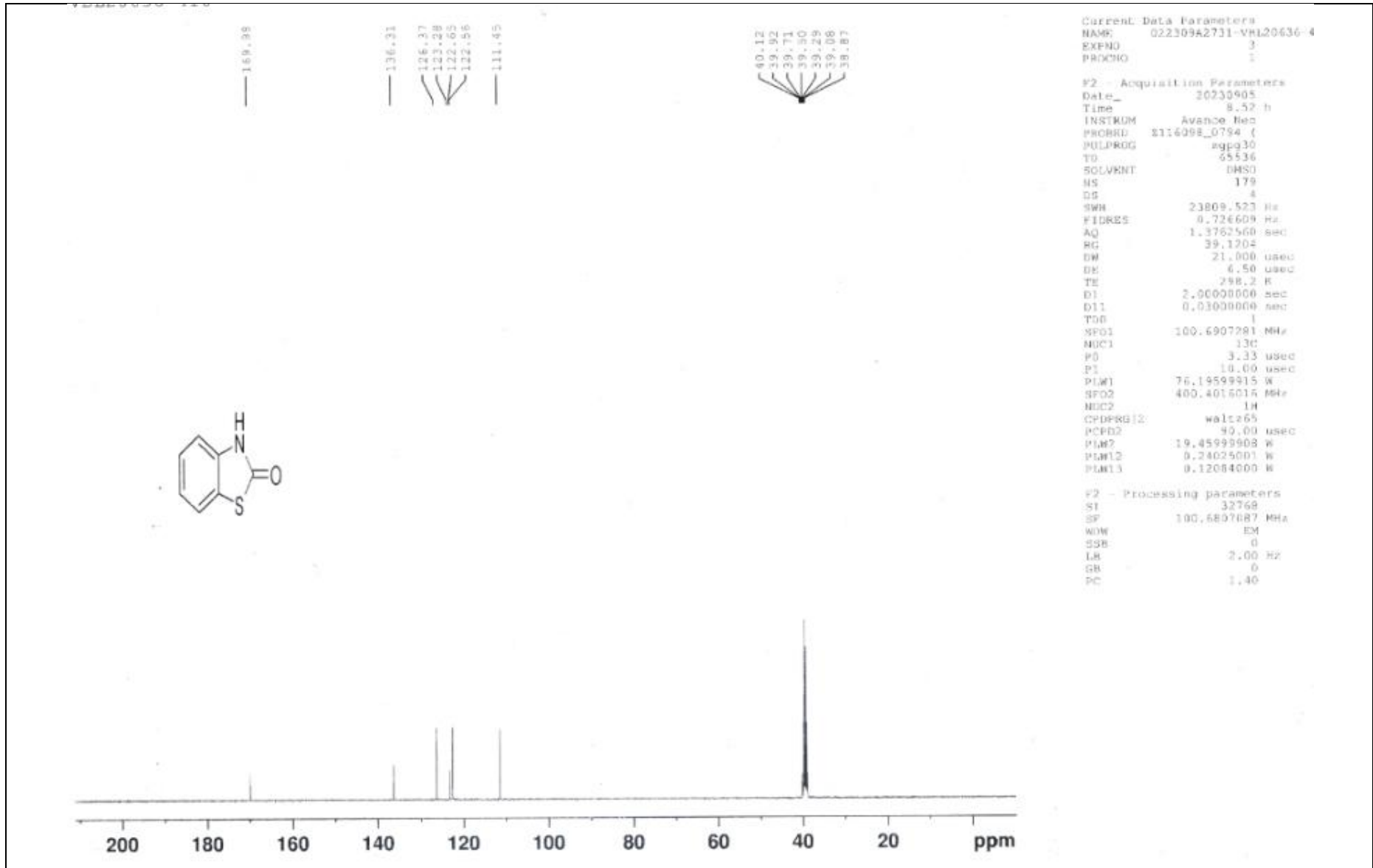
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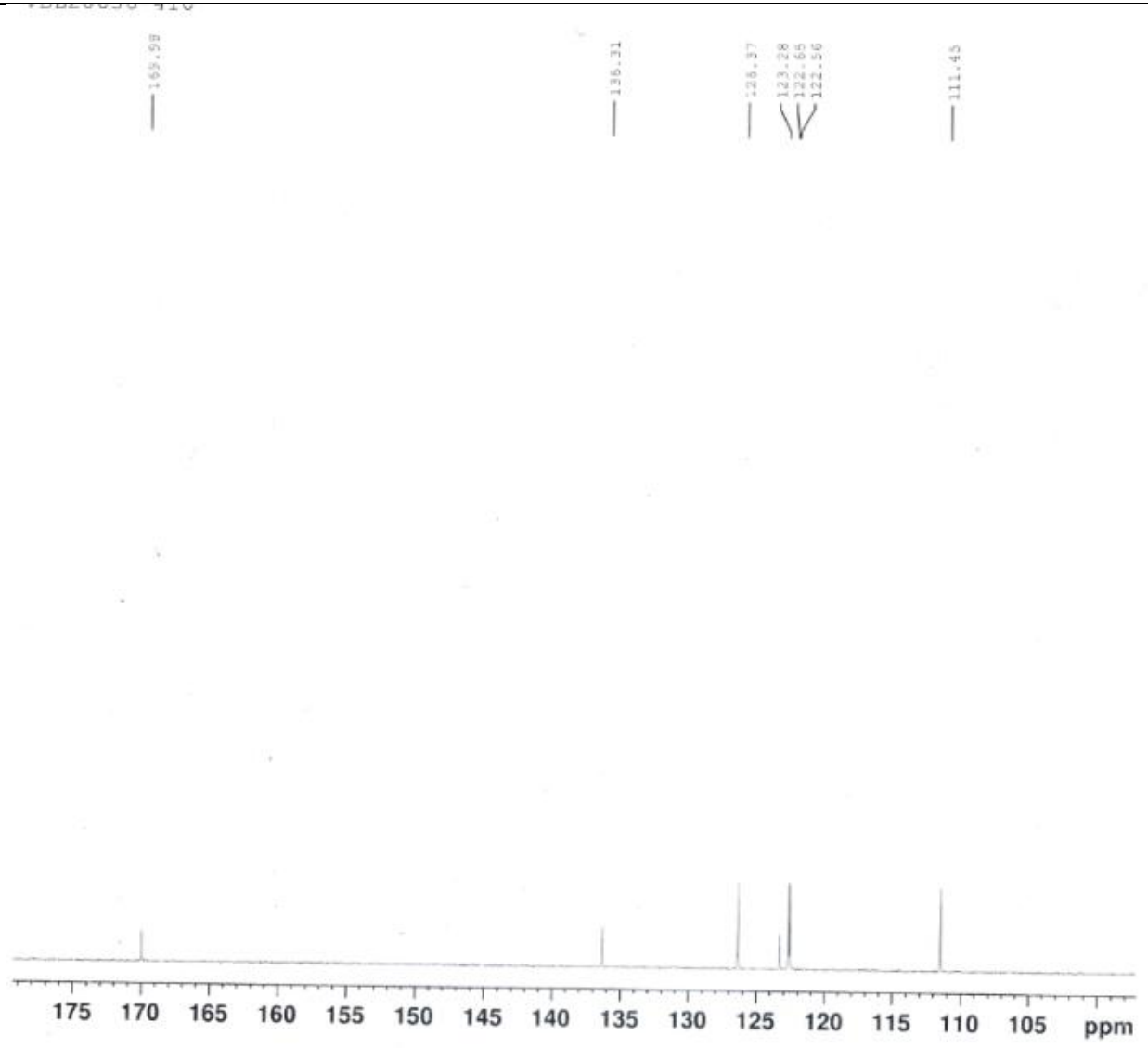
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 Time 12.40 h
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 PROBHD Z163739_0215 1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 8196.722 Hz
 FIDRES 0.250144 Hz
 AQ 3.9976959 sec
 RG 101
 CM 61.000 usec
 DE 13.89 usec
 TE 298.2 K
 DI 2.0000000 sec
 TDD 1
 SFO1 400.2024713 MHz
 NUC1 1H
 P0 2.67 usec
 P1 8.00 usec
 PLW1 25.04899979 W

F2 - Processing parameters
 SI 65536
 SF 400.2000002 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

ANL-MCL3-NMR-006

¹³C NMR of of benzo[d]thiazol-2(3H)-one (2v)





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Current Data Parameters
NAME      022309A2731-VBL20636-41
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20230905
Time      8.52 h
INSTRUM   Avance Neo
PROBHD    Z116098_0794 f
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         179
DS         4
SWH        23809.523 Hz
FIDRES     0.726609 Hz
AQ         1.3762560 sec
RG         39.1204
DN         21.000 usec
DE         6.50 usec
TE         298.2 K
D1         2.0000000 sec
D11        0.03000000 sec
TDO        1
SFO1       100.6207281 MHz
NUC1       13C
P0         3.33 usec
P1         10.00 usec
PLW1       76.19599915 W
SFO2       400.4016016 MHz
NUC2       1H
CPDPRG2    waltz65
PCPD2      90.00 usec
PLW2       19.45999908 W
PLW12      0.24025001 W
PLW13      0.12084000 W

F2 - Processing parameters
SI         32768
SF         100.6207087 MHz
WDW        EM
SSR         0
LB         2.00 Hz
GB         0
PC         1.40
  
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LCMS of of of benzo[d]thiazol-2(3H)-one (2v)

