

Synthesis and insecticidal evaluation of chiral neonicotinoids analogs: The Laurelt wilt case

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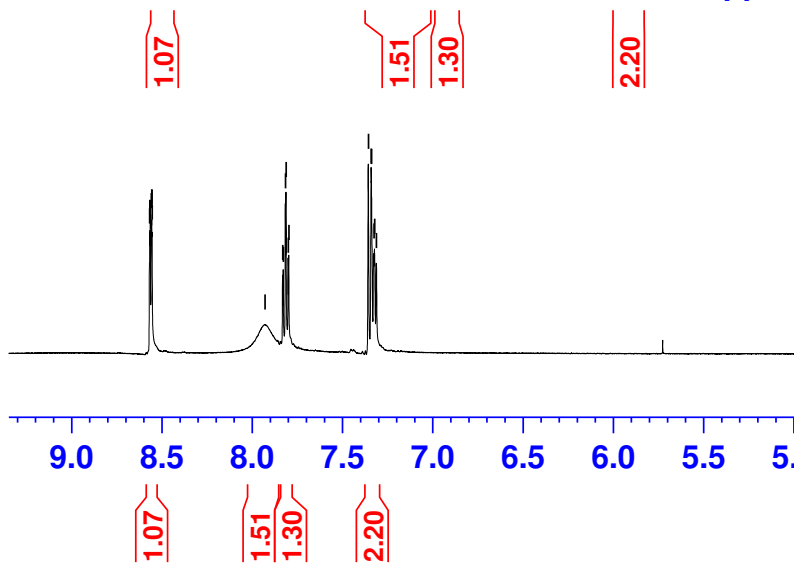
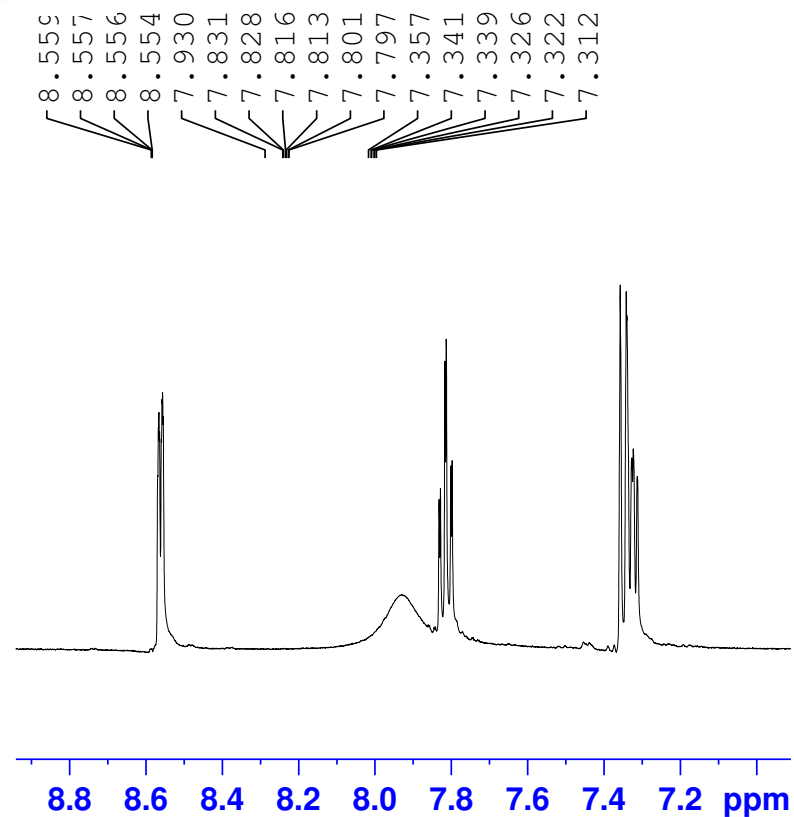
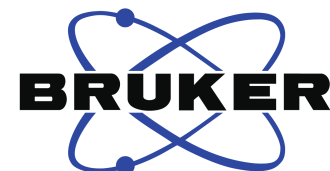
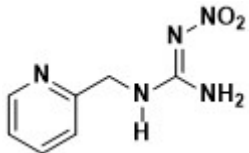
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This document contains all the ¹H and ¹³C NMR spectra for all compounds.



Current Data Parameters
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 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180703
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 TD 65536
 SOLVENT DMSO
 NS 5
 DS 1
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 139.09
 DW 50.000 usec
 DE 6.50 usec
 TE 323.1 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1830886 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 18.10400009 W

F2 - Processing parameters
 SI 65536
 SF 500.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

—159.42
—156.81

—129.71
—127.72

—114.52

—79.58
—77.30

—55.58
—50.41

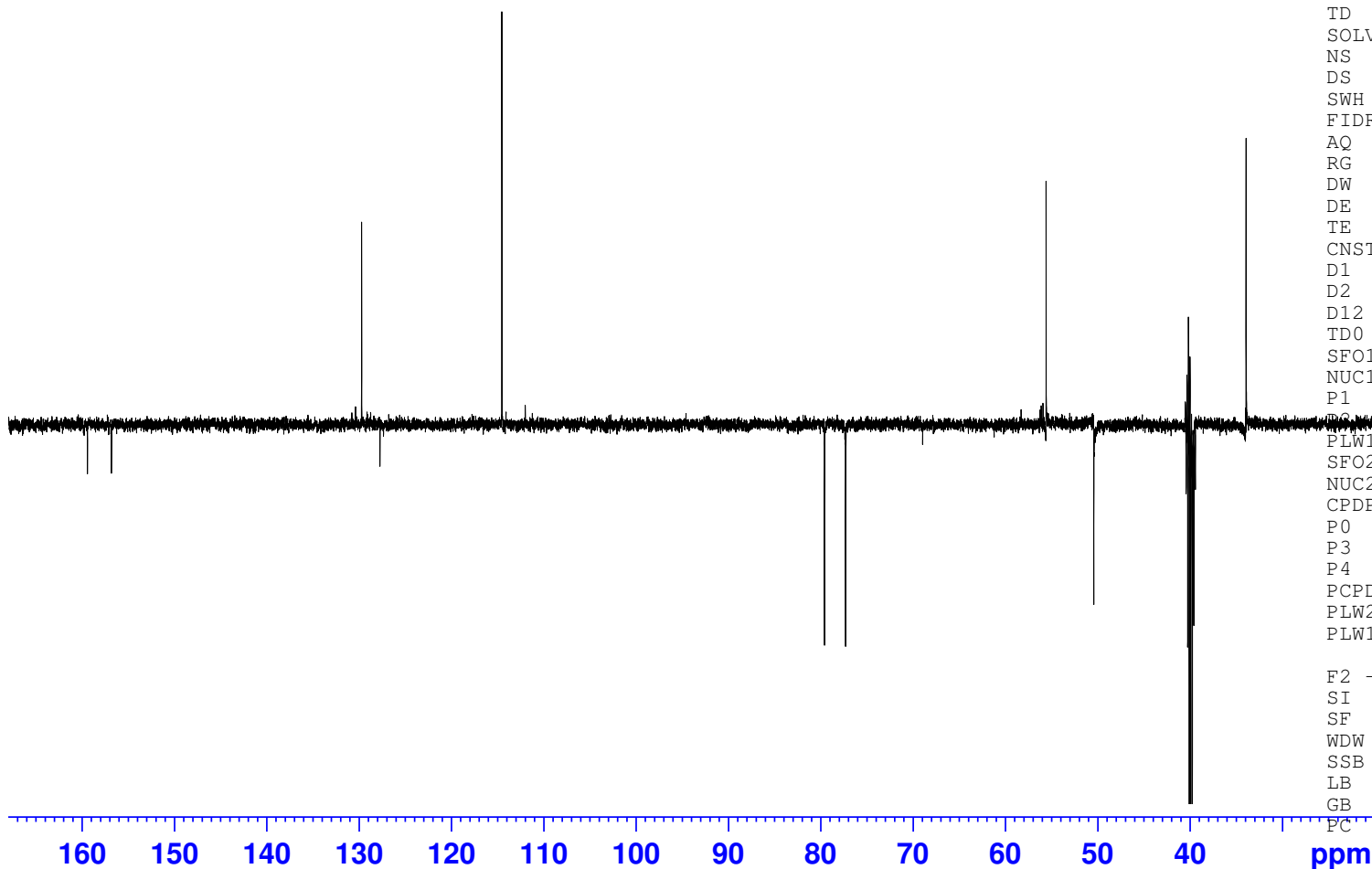
—33.91



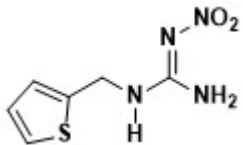
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PULPROG deptq135
TD 65536
SOLVENT DMSO
NS 200
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
PCPD 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
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P3 10.47 usec
P4 20.94 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
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F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



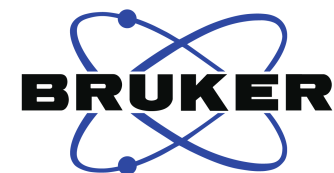
^{13}C (DEPTQ135) NMR (125 MHz, DMSO- d_6) of **47**



— 9.077

8.129
7.877
7.510
7.500
7.469
7.458
7.449
7.144
7.040
7.033
7.030
7.023
6.991
6.984

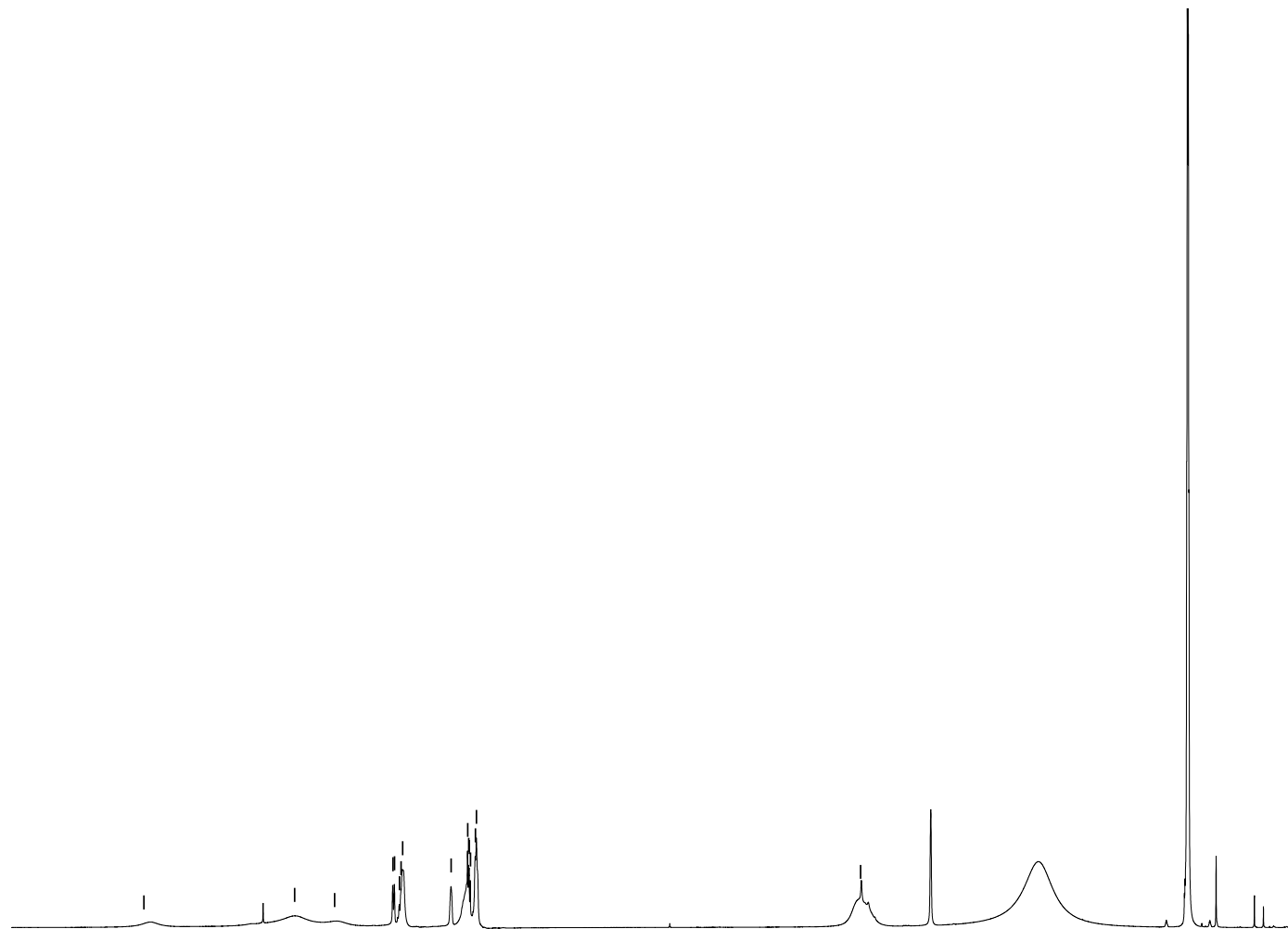
— 4.568



Current Data Parameters
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PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 88.37
DW 50.000 usec
DE 12.72 usec
TE 287.5 K
D1 5.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm

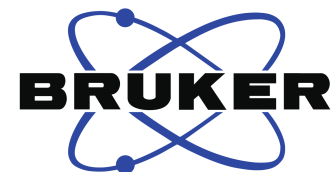
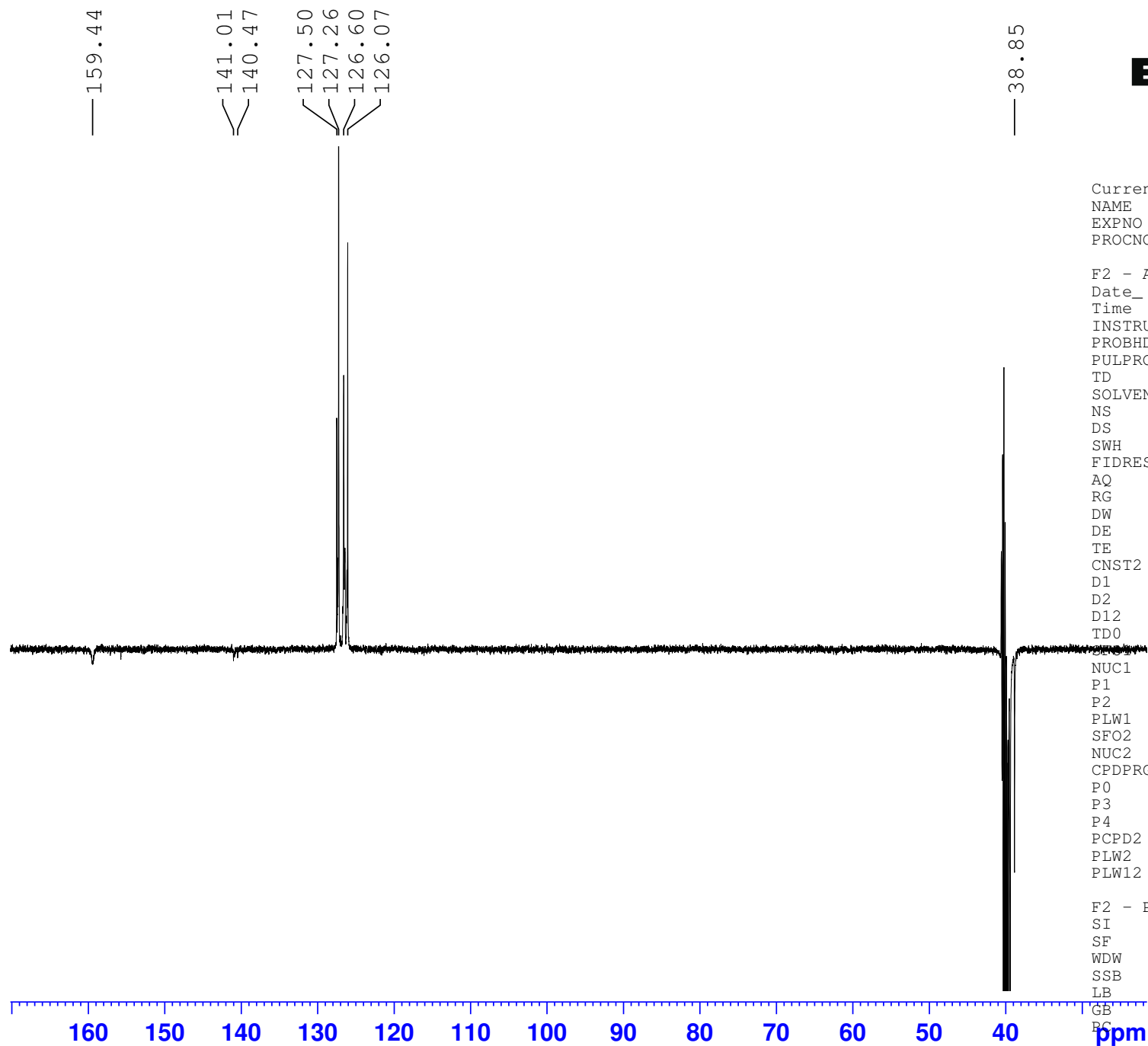
0.41

1.90

1.28

2.19

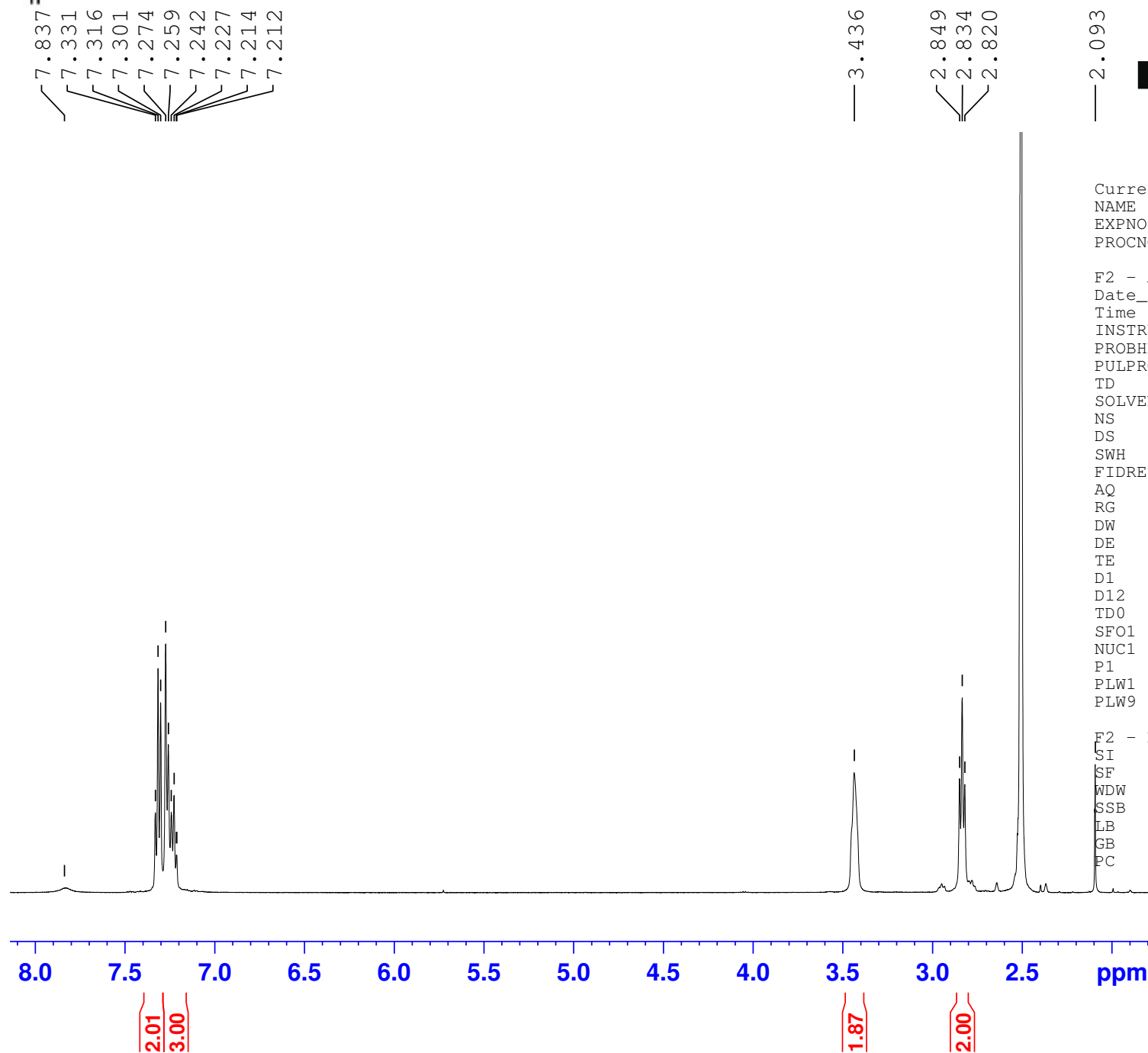
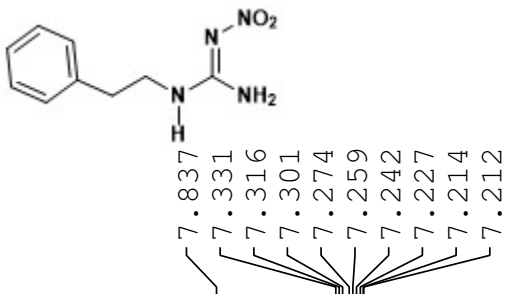
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 PROCNO 1

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 PULPROG deptq135
 TD 65536
 SOLVENT DMSO
 NS 16874
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 288.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 P2 20.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.00 usec
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28288001 W

F2 - Processing parameters
 SI 32768
 SF 125.7703610 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 BC 1.40



BRUKER

Current Data Parameters

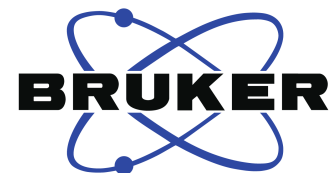
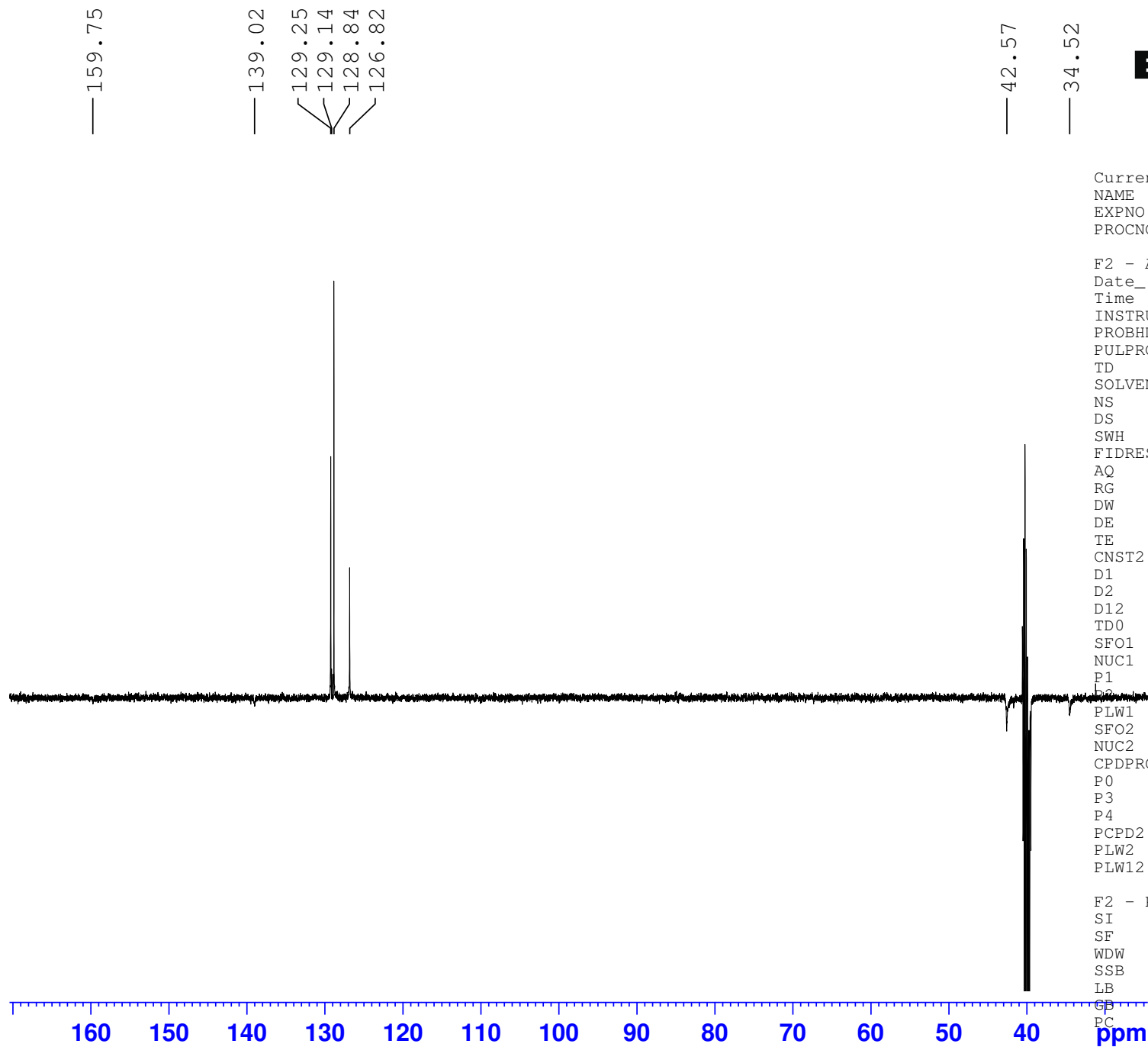
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EXPNO	3
PROCNO	1

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PULPROG	zgpgpr
TD	32768
SOLVENT	DMSO
NS	8
DS	4
SWH	8012.820 Hz
FIDRES	0.489064 Hz
AQ	2.0447233 sec
RG	123.82
DW	62.400 usec
DE	6.50 usec
TE	323.2 K
D1	2.00000000 sec
D12	0.00002000 sec
TD0	1
SFO1	500.1816031 MHz
NUC1	1H
P1	10.00 usec
PLW1	18.10400009 W
PLW9	0.00007242 W

F2 - Processing parameters

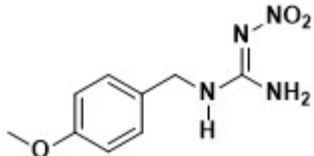
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SF	500.1800000 MHz
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SSB	0
LB	0.30 Hz
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Current Data Parameters
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 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180704
 Time 12.07 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG deptq135
 TD 65536
 SOLVENT DMSO
 NS 2422
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 291.4 K
 CNST2 145.0000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.00 usec
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28288001 W

F2 - Processing parameters
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 SF 125.7703610 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

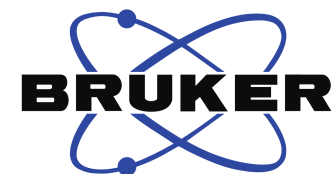


— 7.86;

7.266
7.249
6.935
6.918

— 4.339

— 3.754



Current Data Parameters

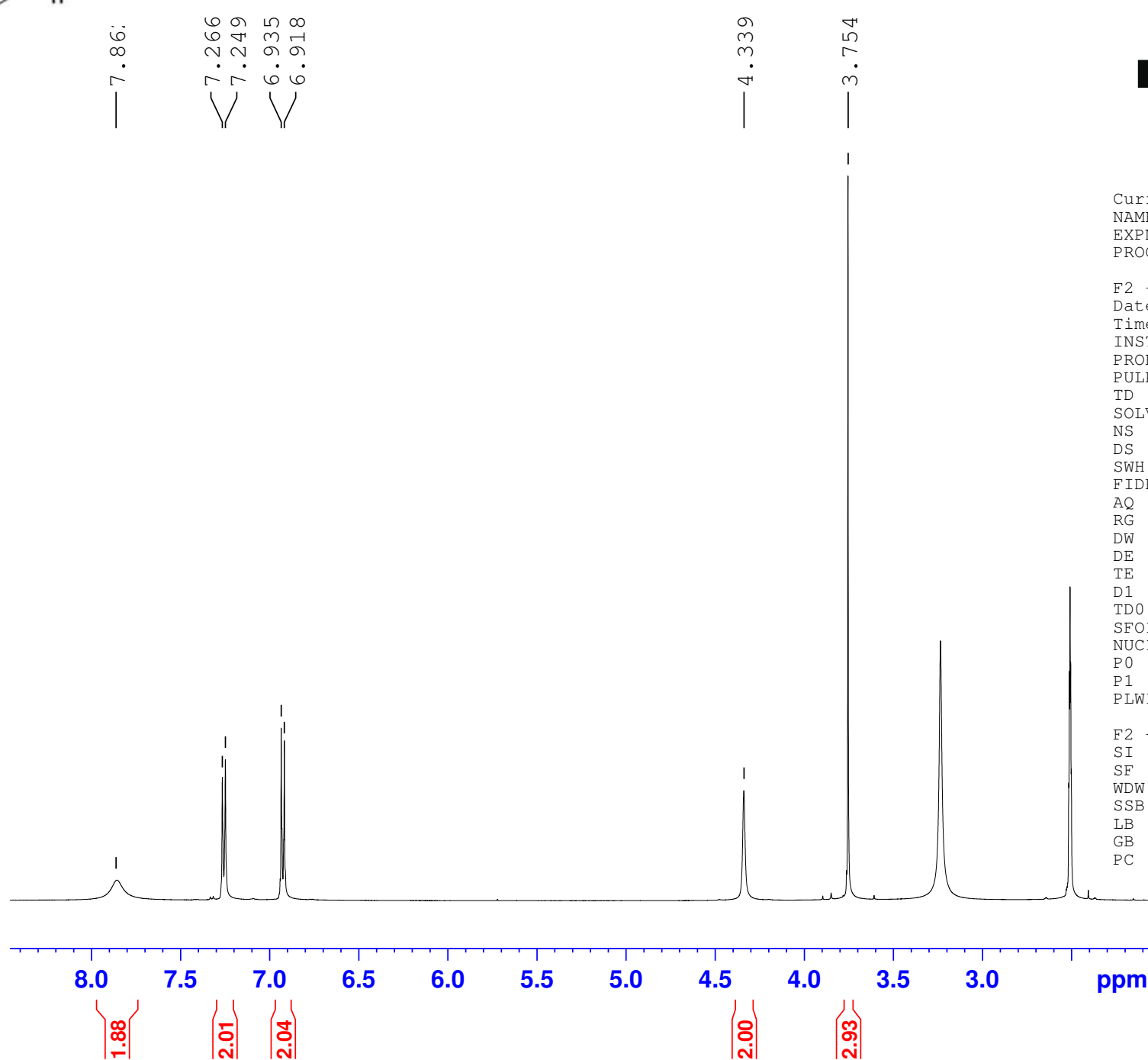
NAME 5
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

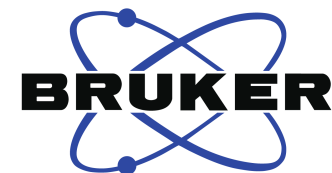
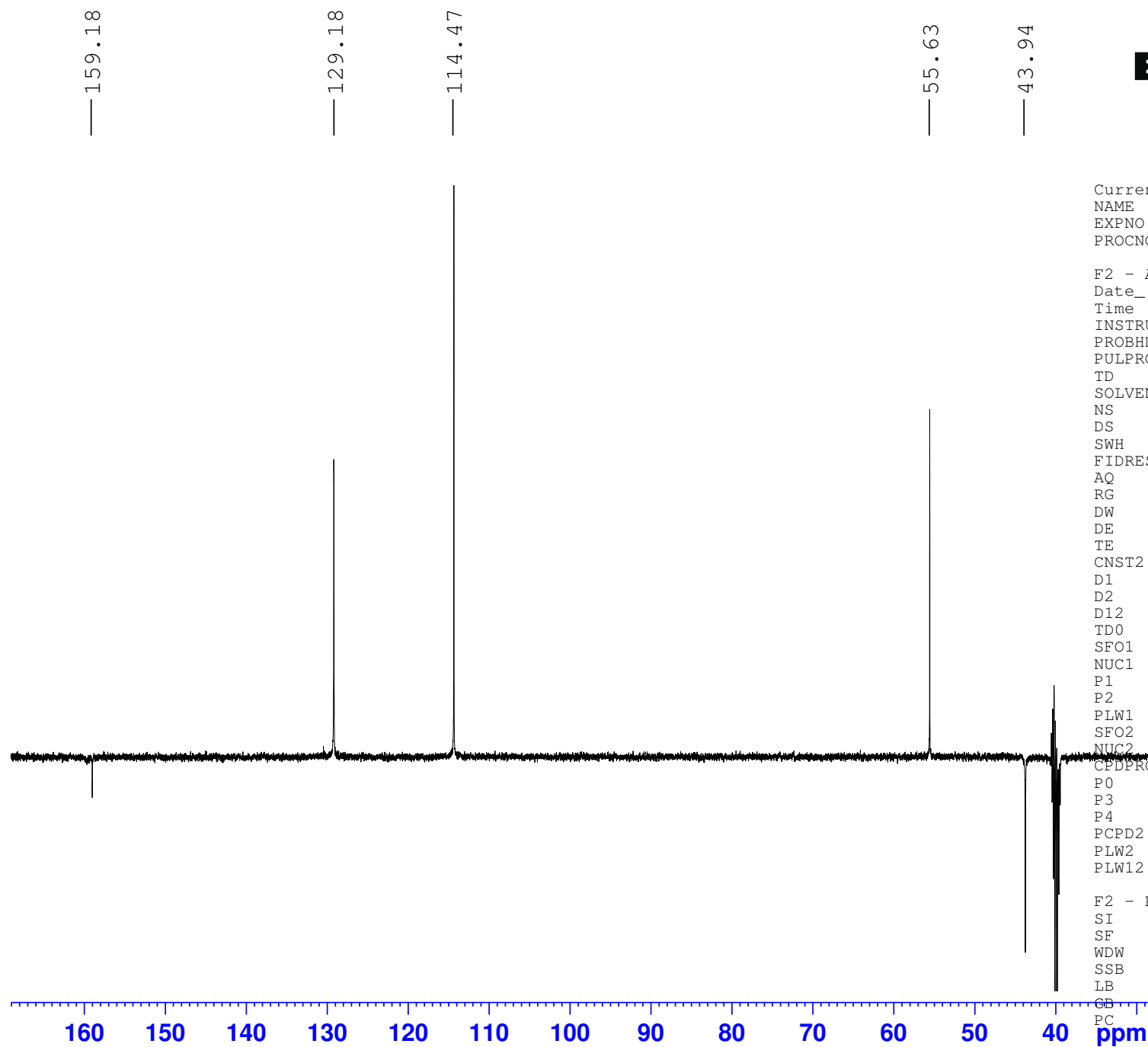
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PROBHD Z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 95.16
DW 50.000 usec
DE 6.50 usec
TE 323.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters

SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



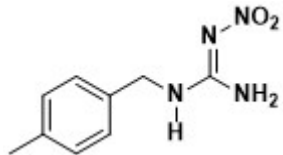
¹H NMR (500 MHz, DMSO-d₆, 50°C) of **5**



Current Data Parameters
NAME 5
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181204
Time 15.51 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT DMSO
NS 441
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 293.6 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.00 usec
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28288001 W

F2 - Processing parameters
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SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

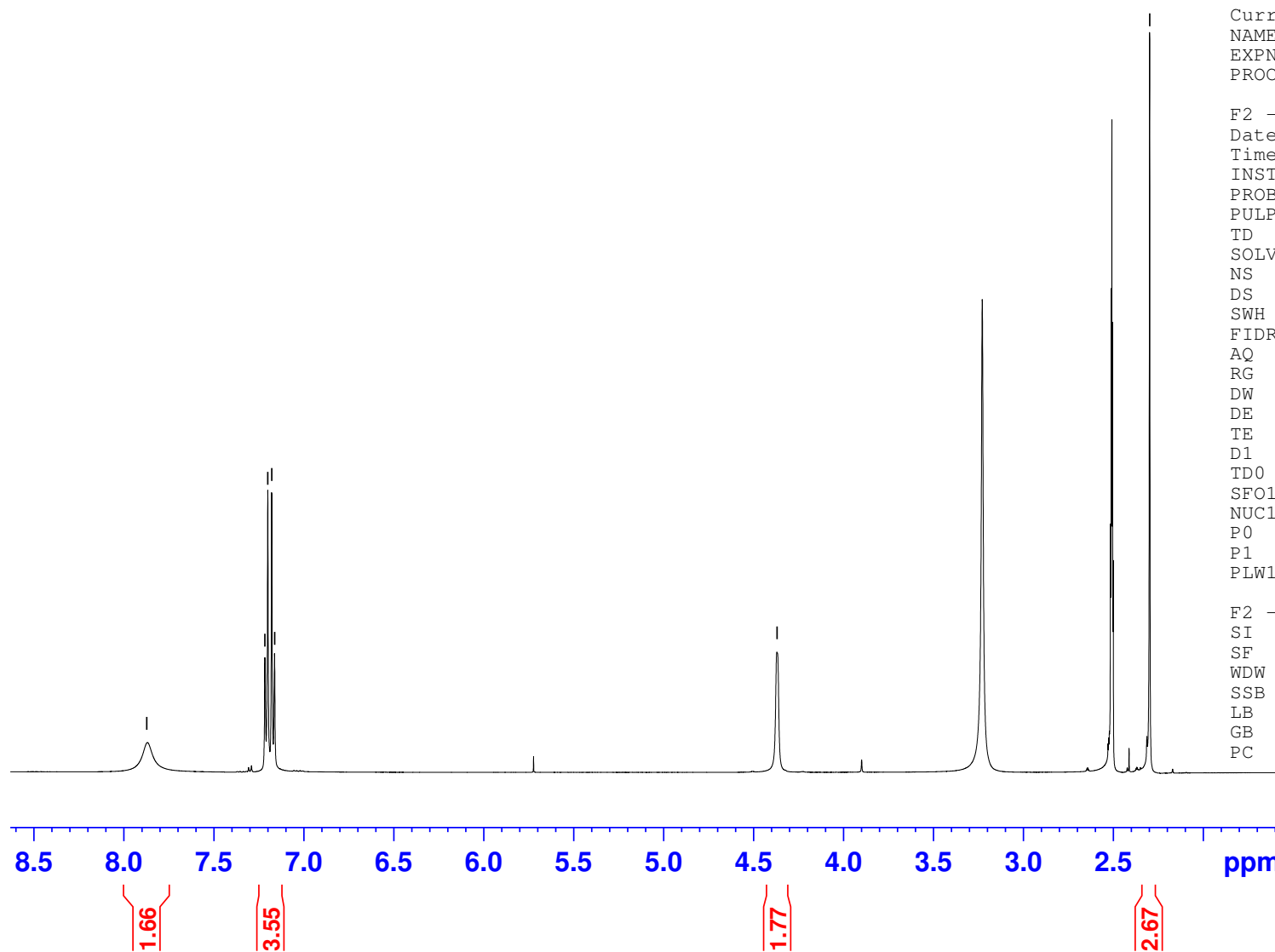


— 7.873

7.216
7.200
7.178
7.162

— 4.370

— 2.298

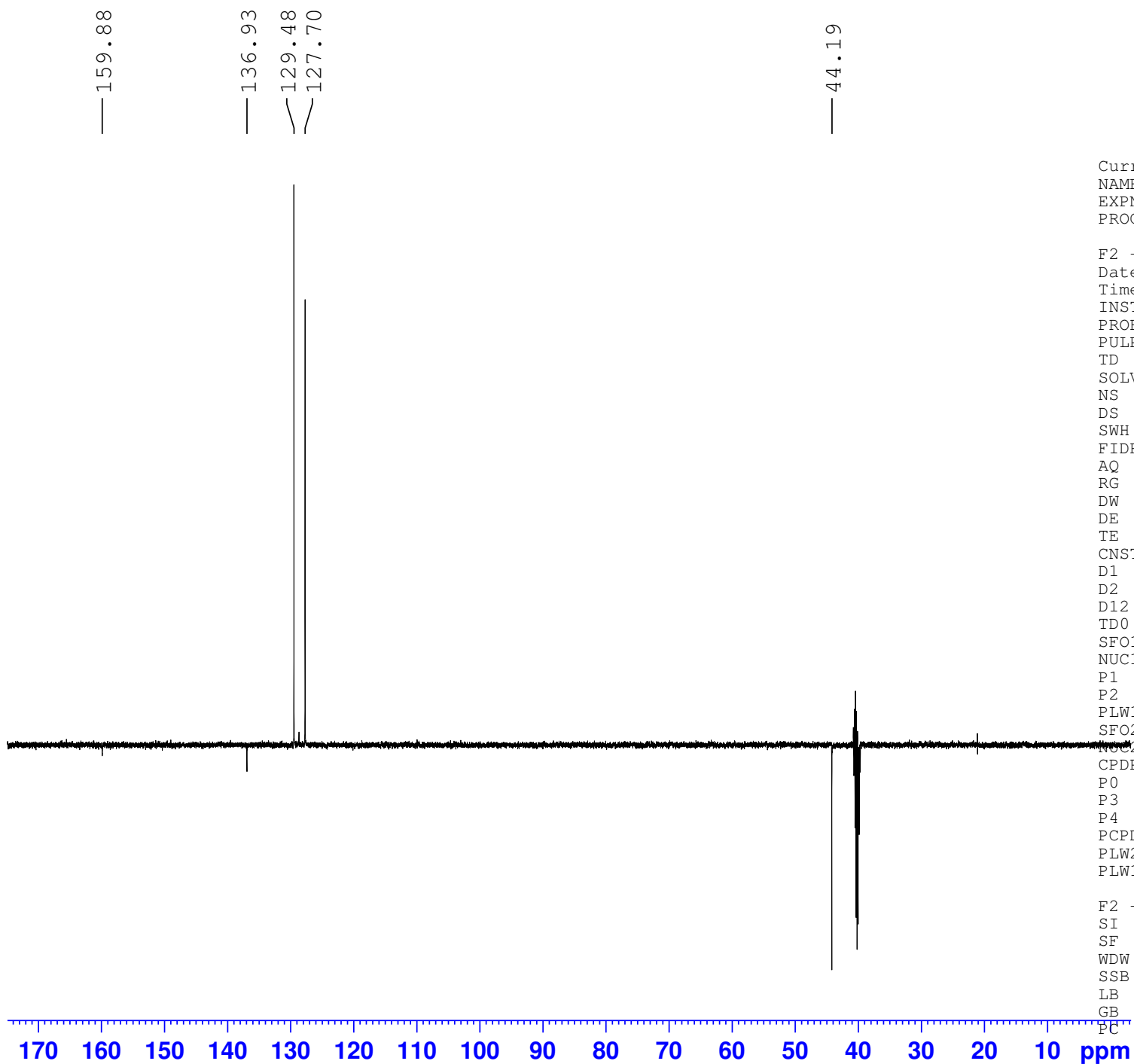
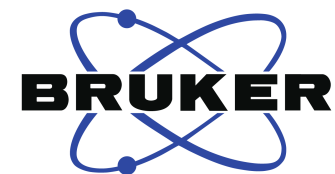


Current Data Parameters
NAME 6
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
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PROBHD Z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 108.3
DW 50.000 usec
DE 6.50 usec
TE 323.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

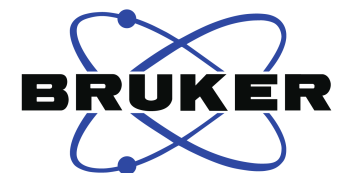
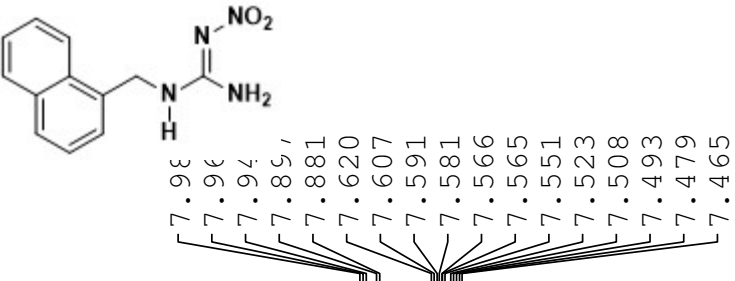
¹H NMR (500 MHz, DMSO-d₆, 50°C) of **6**



Current Data Parameters
NAME 6
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181204
Time 10.28 h
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PROBHD Z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT DMSO
NS 366
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 323.2 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.00 usec
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28288001 W

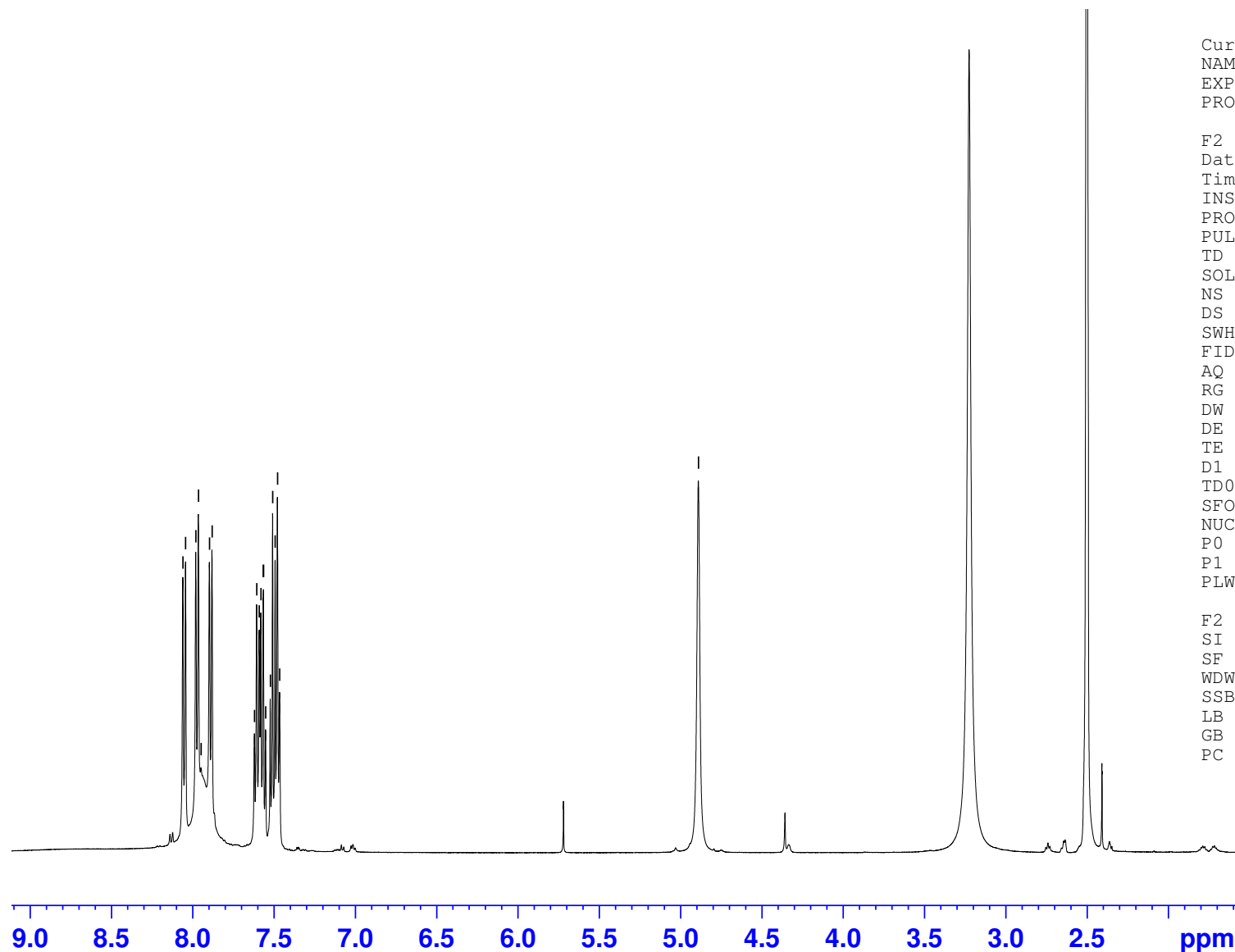
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SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
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 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181204
 Time 13.21 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 139.09
 DW 50.000 usec
 DE 6.50 usec
 TE 323.2 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1830886 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 18.10400009 W

F2 - Processing parameters
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 PC 1.00

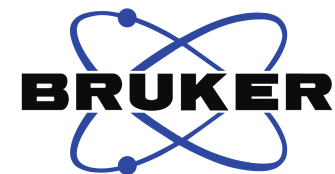


¹H NMR (500 MHz, DMSO-d₆, 50°C) of 7

—159.96

133.88
131.18
129.05
128.42
126.87
126.41
125.91
123.73

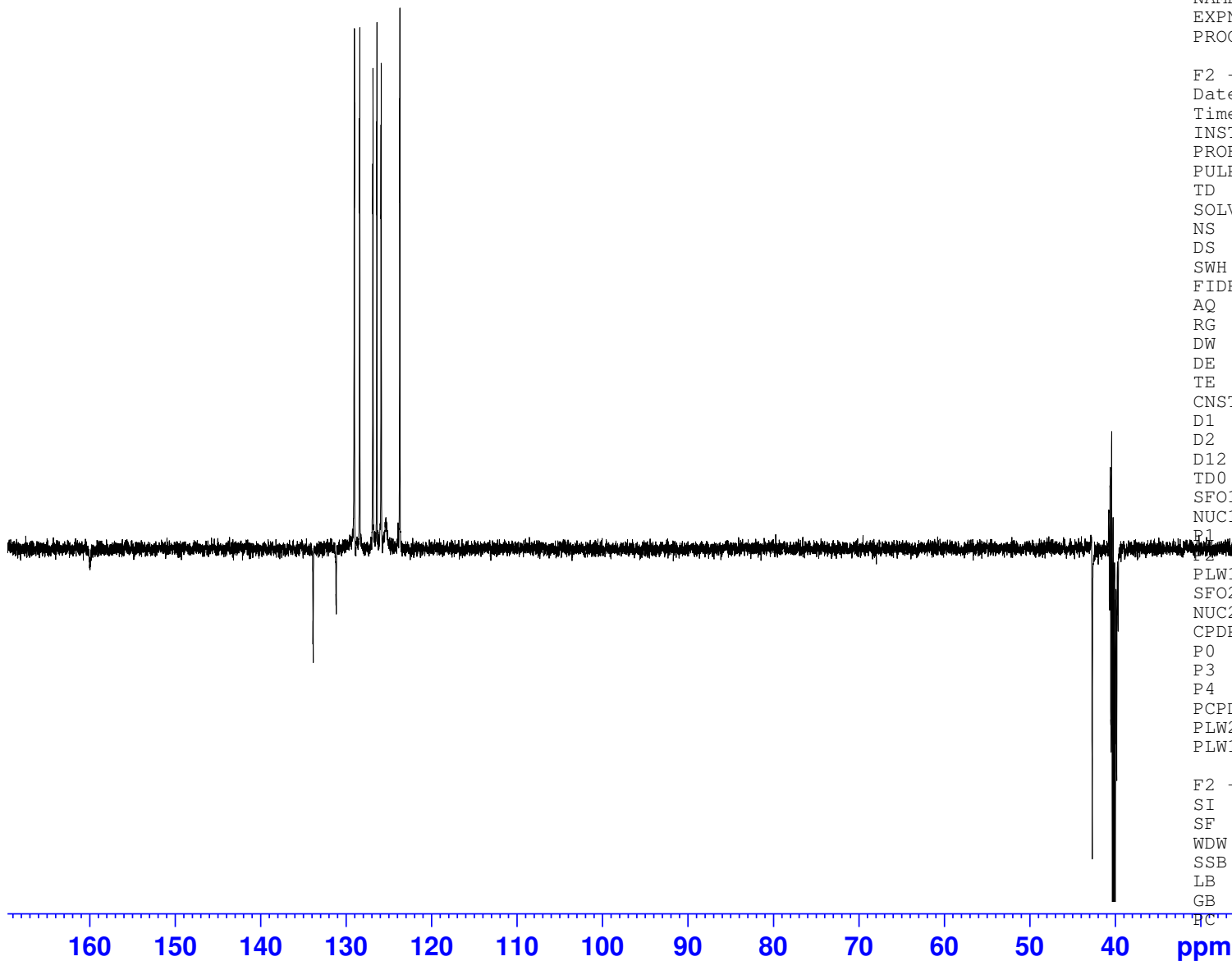
—42.70

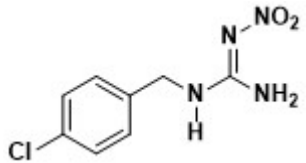


Current Data Parameters
NAME 7
EXPNO 2
PROCNO 1

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PULPROG deptq135
TD 65536
SOLVENT DMSO
NS 1536
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 323.1 K
CNST2 145.000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.00 usec
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28288001 W

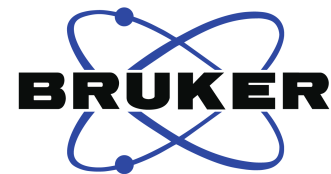
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SI 32768
SF 125.7703610 MHz
WDW EM
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LB 1.00 Hz
GB 0
Hc 1.40





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7.434
7.420
7.404
7.340
7.323

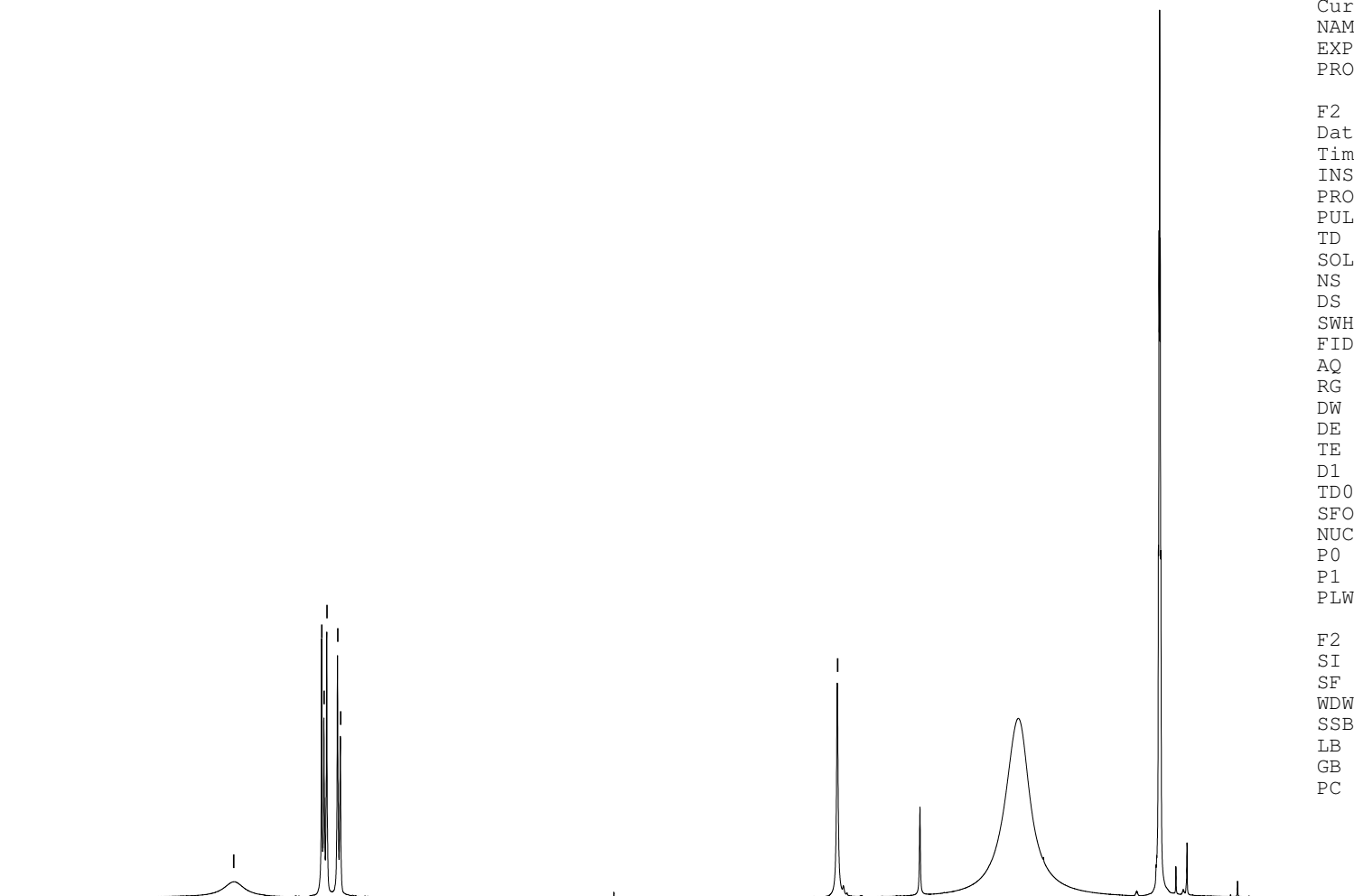
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Current Data Parameters
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EXPNO 1
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 95.16
DW 50.000 usec
DE 6.50 usec
TE 323.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm

1.47
2.44
1.66

1.61

¹H NMR (500 MHz, DMSO-d₆, 50°C) of **8**

—159.92

132.33
129.53
128.84

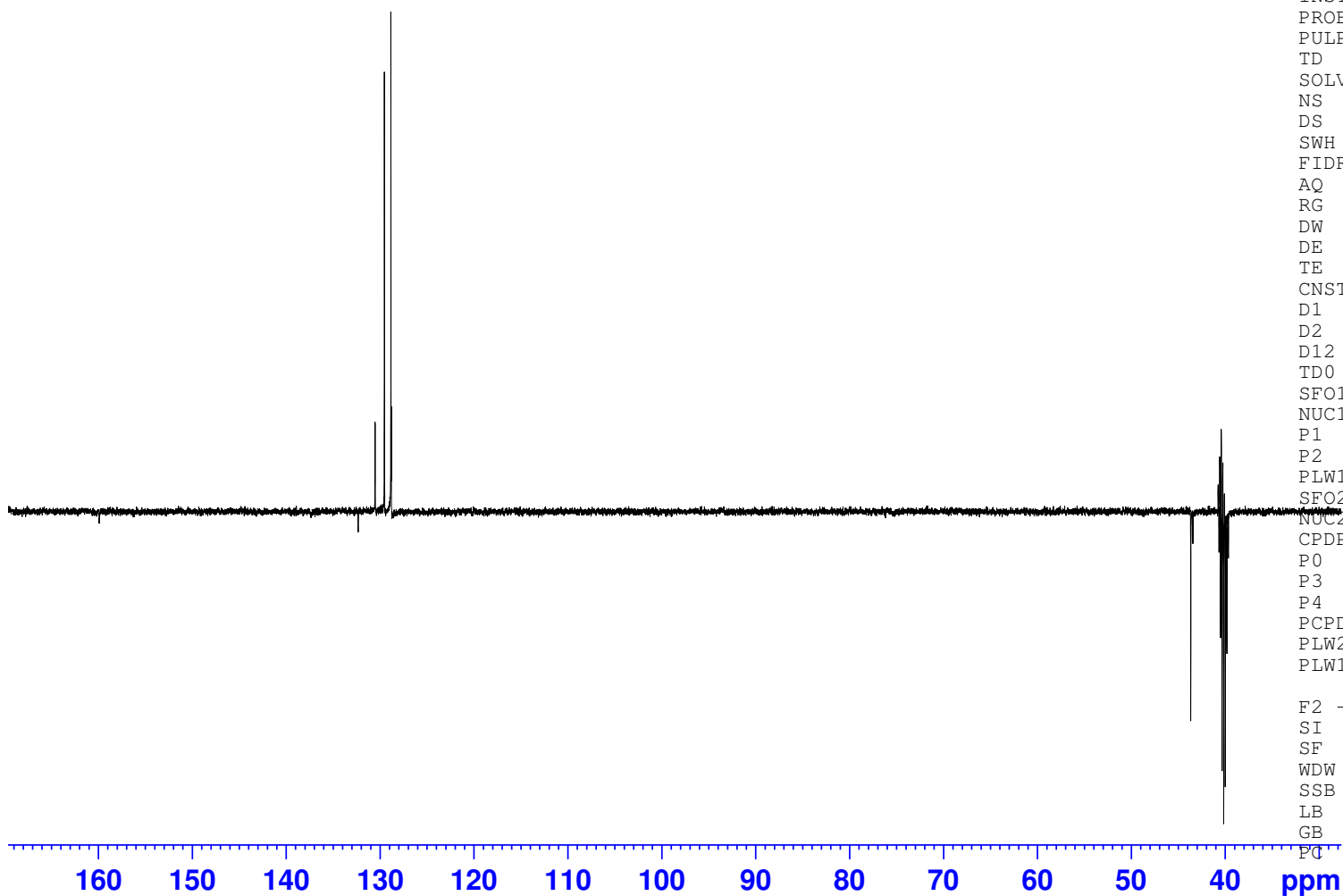
—43.65



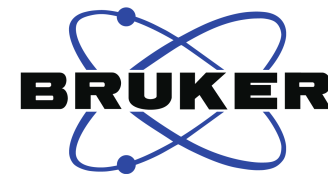
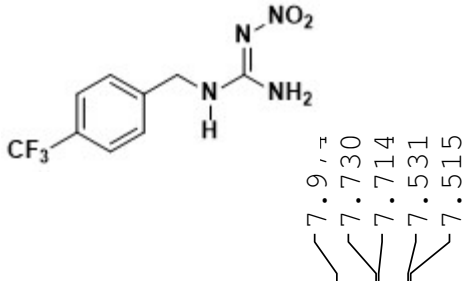
Current Data Parameters
NAME 8
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
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Time 9.54 h
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PROBHD z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT DMSO
NS 578
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 323.1 K
CNST2 145.000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SF01 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SF02 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.00 usec
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28288001 W

F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



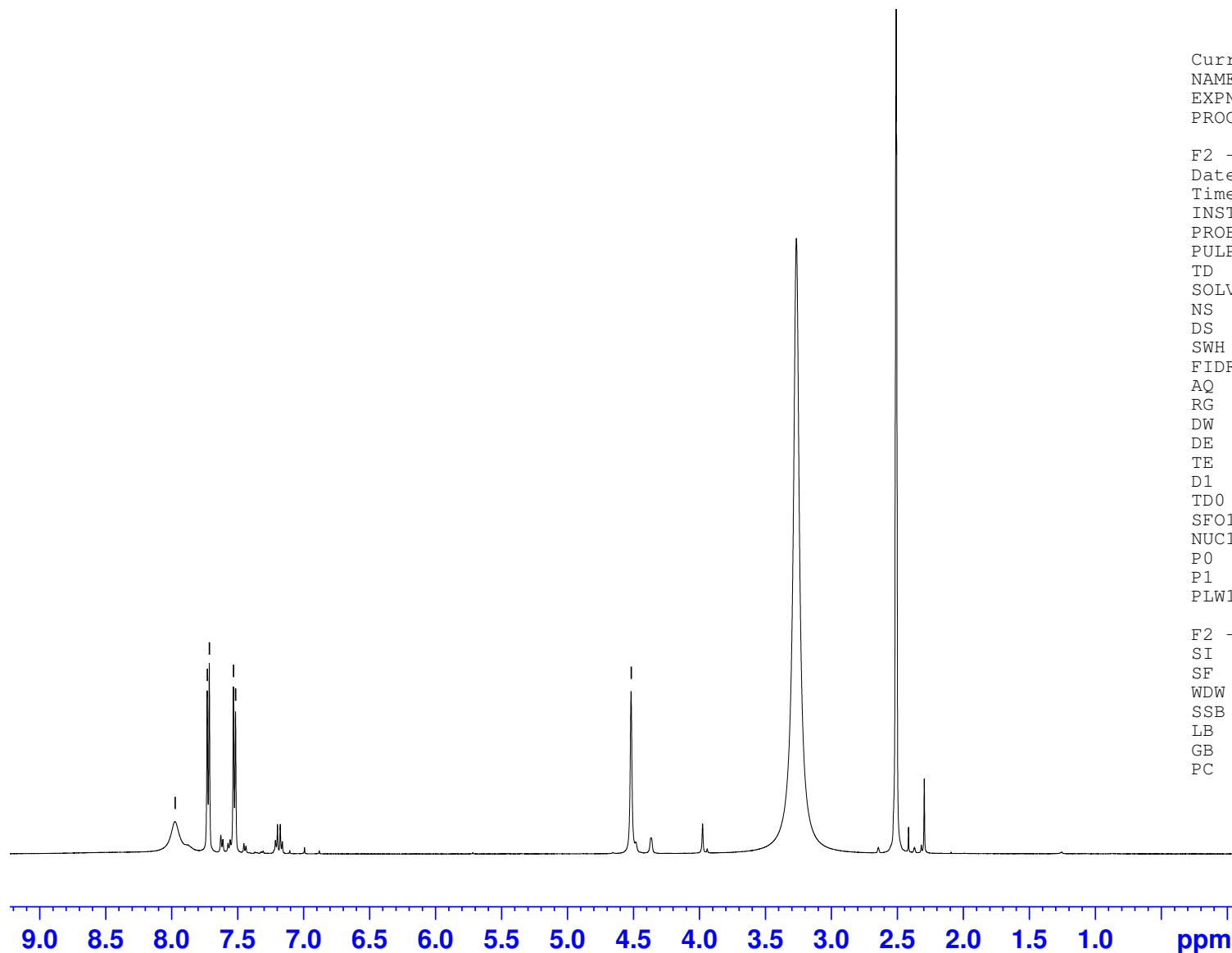
¹³C (DEPTQ135) NMR (125 MHz, DMSO-d₆, 50°C) of **8**



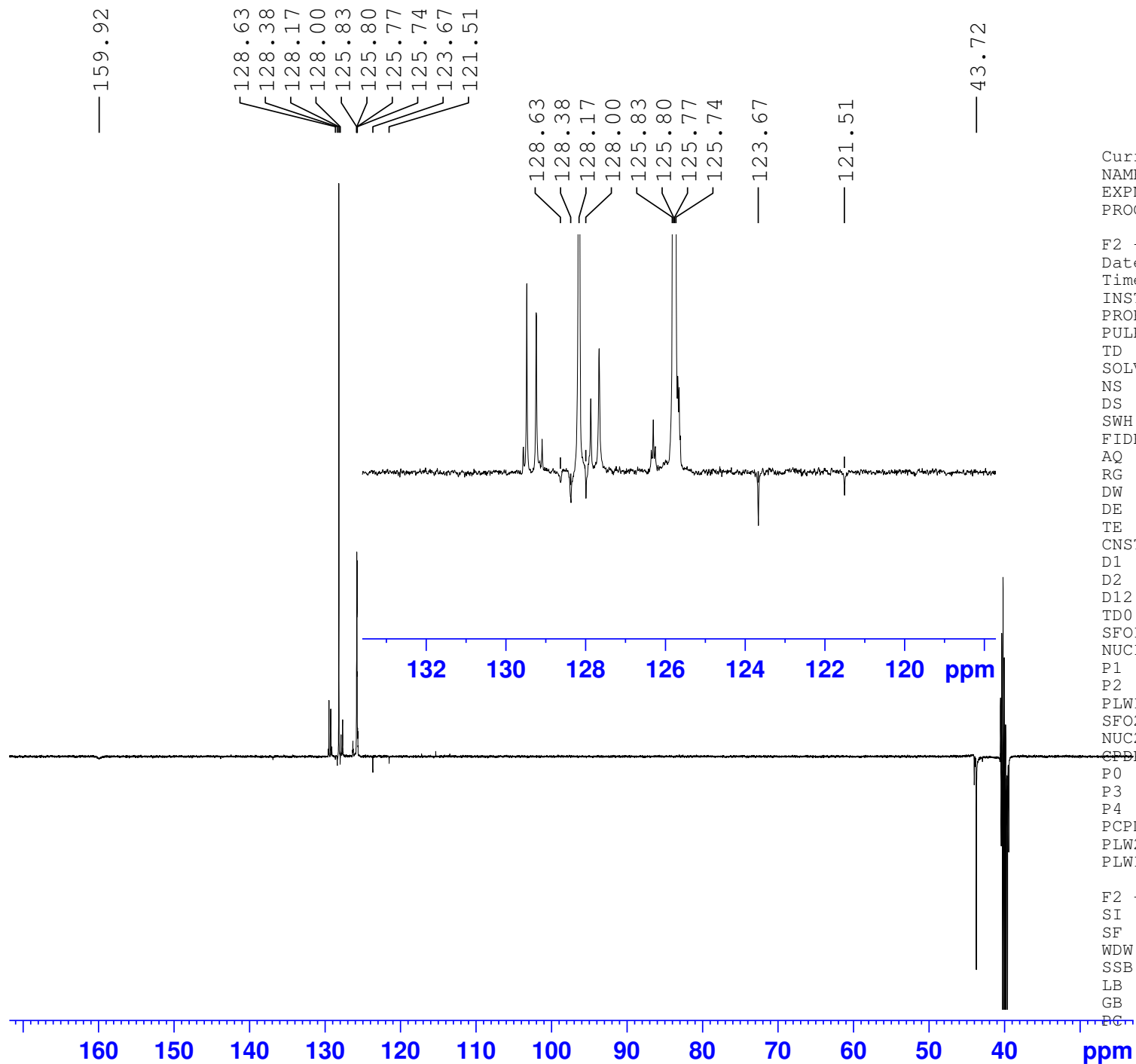
Current Data Parameters
 NAME 9
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180816
 Time 20.01 h
 INSTRUM spect
 PROBHD z119470_0187 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 88.37
 DW 50.000 usec
 DE 6.50 usec
 TE 323.4 K
 D1 1.00000000 sec
 TD0 1
 SF01 500.1830886 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 18.10400009 W

F2 - Processing parameters
 SI 65536
 SF 500.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



¹H NMR (500 MHz, DMSO-d₆, 50°C) of 9

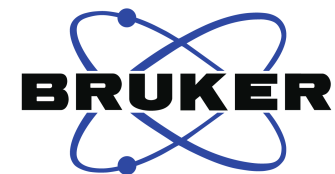


Current Data Parameters
 NAME 9
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180817
 Time 9.09 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG deptq135
 TD 65536
 SOLVENT DMSO
 NS 14945
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 297.1 K
 CNST2 145.000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 P2 20.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.00 usec
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28288001 W

F2 - Processing parameters
 SI 32768
 SF 125.7703610 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

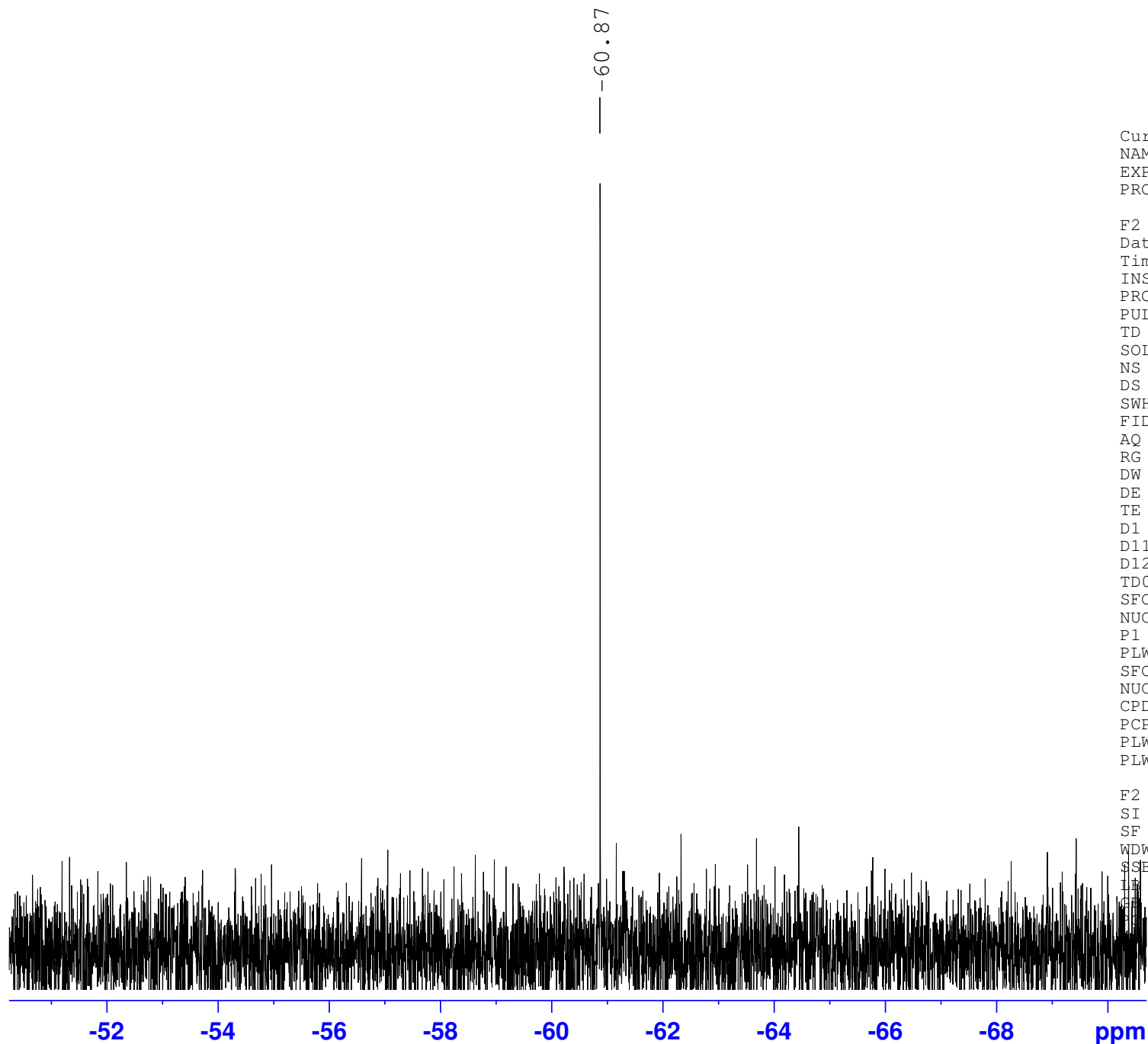
¹³C (DEPTQ135) NMR (125 MHz, DMSO-d₆) of 9



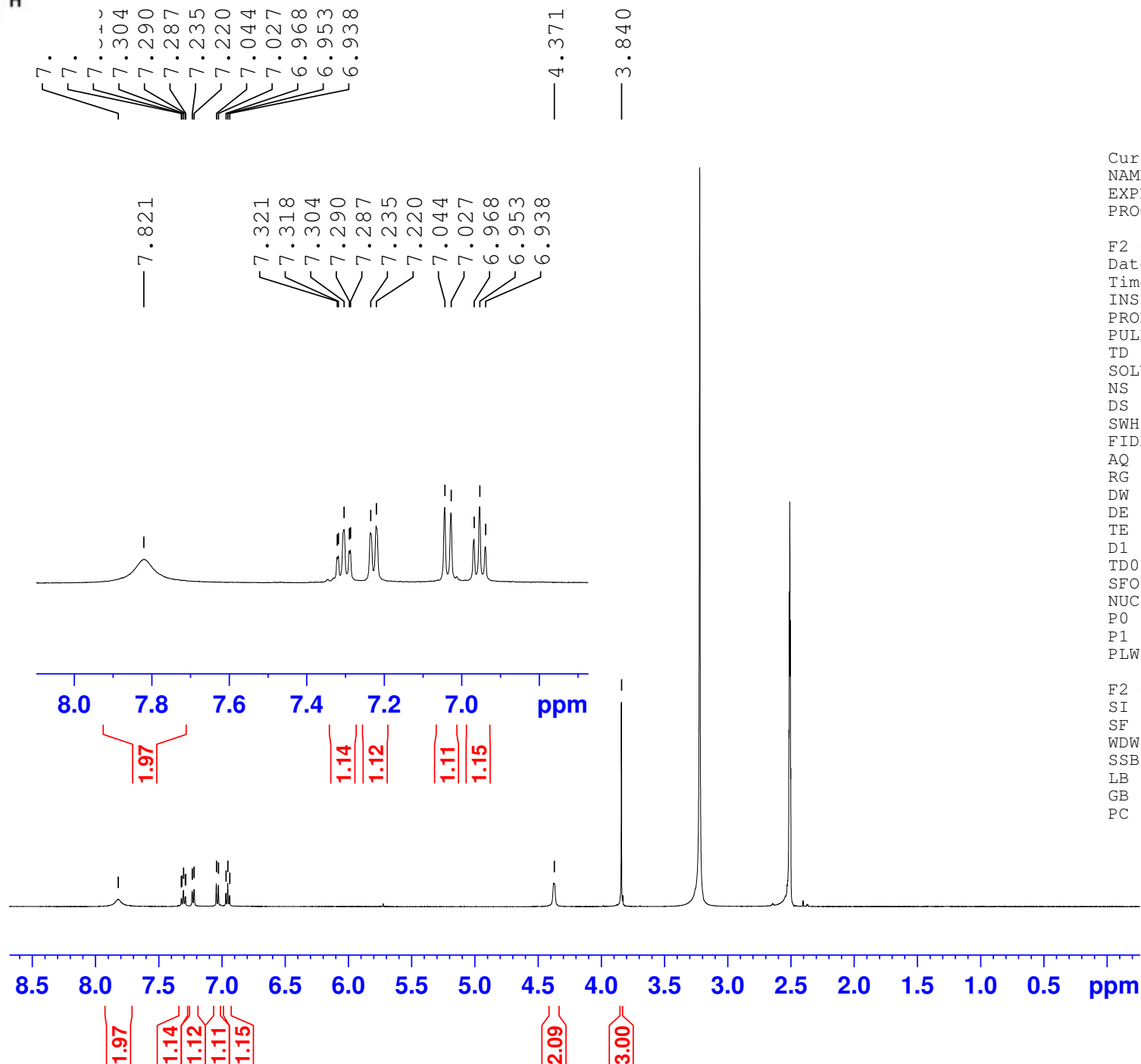
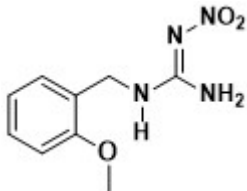
Current Data Parameters
NAME 9
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190801
Time 14.44 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zgfhigqn.2
TD 131072
SOLVENT DMSO
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 1.733953 Hz
AQ 0.5767168 sec
RG 11.27
DW 4.400 usec
DE 6.50 usec
TE 293.4 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
SFO1 470.5923603 MHz
NUC1 19F
P1 16.00 usec
PLW1 36.93899918 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.31009001 W

F2 - Processing parameters
SI 65536
SF 470.6394242 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
CB 1.00



¹⁹F NMR (470 MHz, DMSO-d₆) of 9

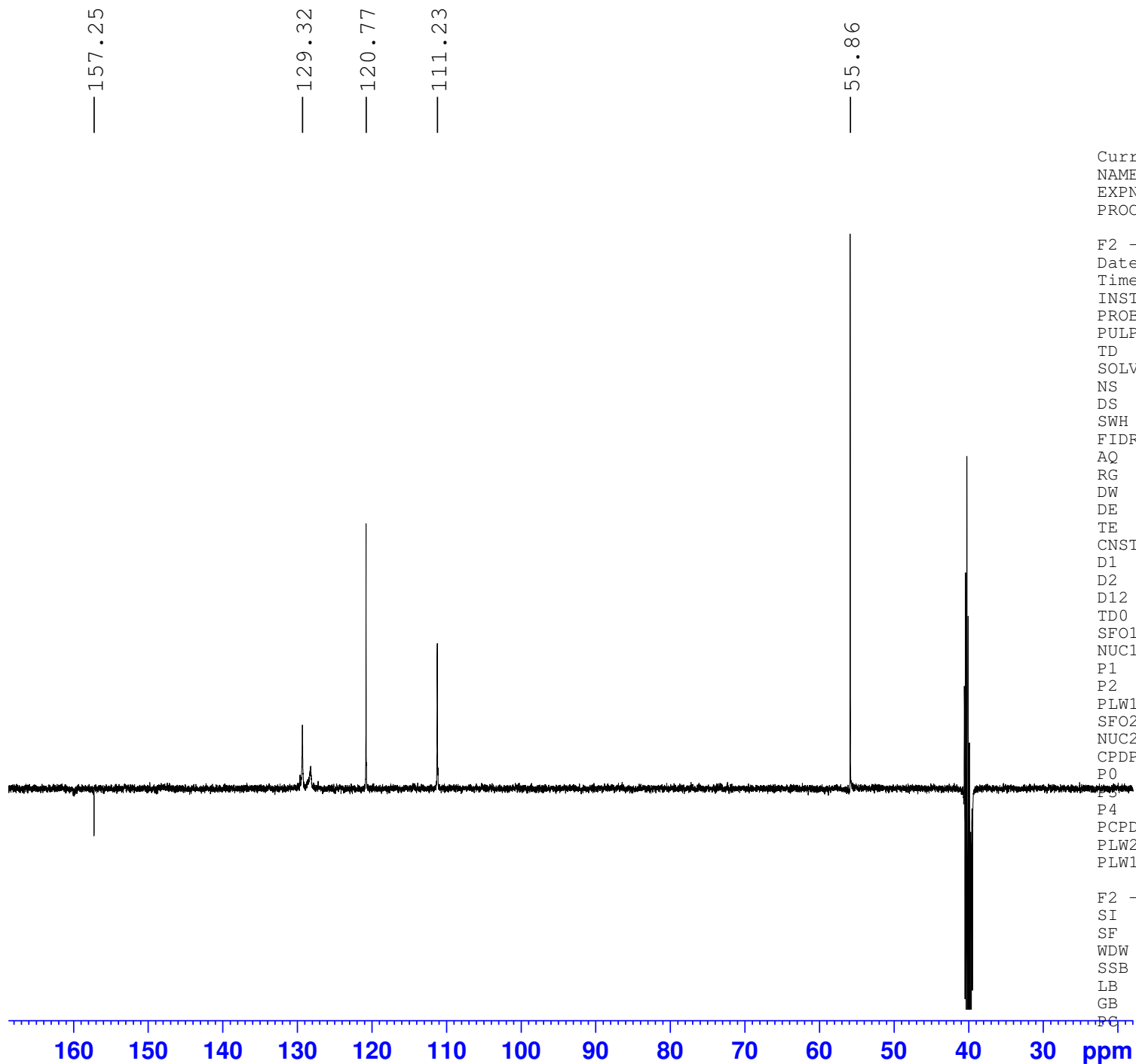
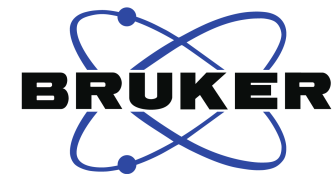


Current Data Parameters
NAME 10
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180817
Time 11.06 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 5
DS 1
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 139.09
DW 50.000 usec
DE 6.50 usec
TE 323.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

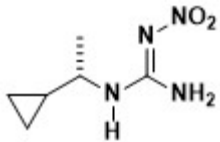
¹H NMR (500 MHz, DMSO-d₆, 50°C) of **10**



Current Data Parameters
NAME 10
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180817
Time 15.58 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT DMSO
NS 5120
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 290.9 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.00 usec
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28288001 W

F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



6.66
3.10
3.09
3.082
1.386
1.373
1.050
1.045
1.041
1.035
1.029
1.025
1.019
1.013
1.008
1.003
0.993
0.698
0.690
0.681
0.671
0.668
0.664
0.654
0.640
0.394
0.384
0.374
0.366
0.357
0.351
0.342
0.334
0.325
0.319
0.317
0.315
0.310

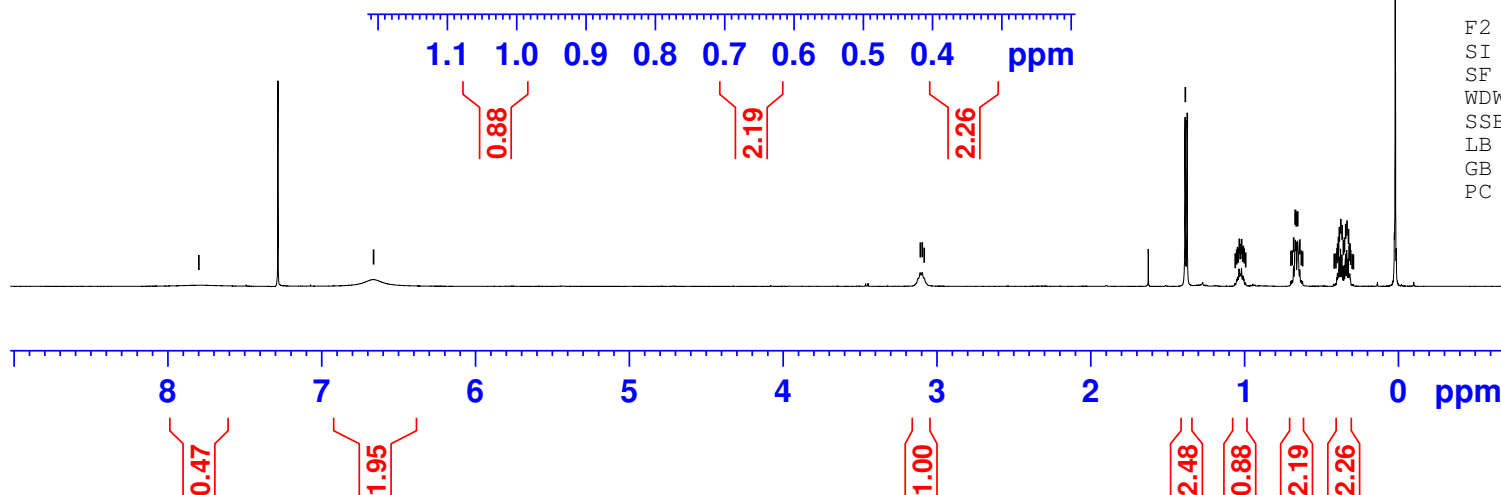


1.035
1.029
1.025
1.019
0.681
0.671
0.668
0.664
0.654
0.640
0.394
0.384
0.374
0.366
0.357
0.351
0.342
0.334
0.325
0.315

Current Data Parameters
NAME S-11
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180601
Time 10.34 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zgcppr
TD 32768
SOLVENT CDC13
NS 16
DS 4
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 2.0447233 sec
RG 139.09
DW 62.400 usec
DE 6.50 usec
TE 291.0 K
D1 2.00000000 sec
D12 0.00002000 sec
TD0 1
SFO1 500.1808034 MHz
NUC1 1H
P1 10.00 usec
PLW1 18.10400009 W
PLW9 0.00007242 W

F2 - Processing parameters
SI 32768
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H NMR (500 MHz, CDCl₃) of S-11

—158.62

—52.33

—20.21
—16.90

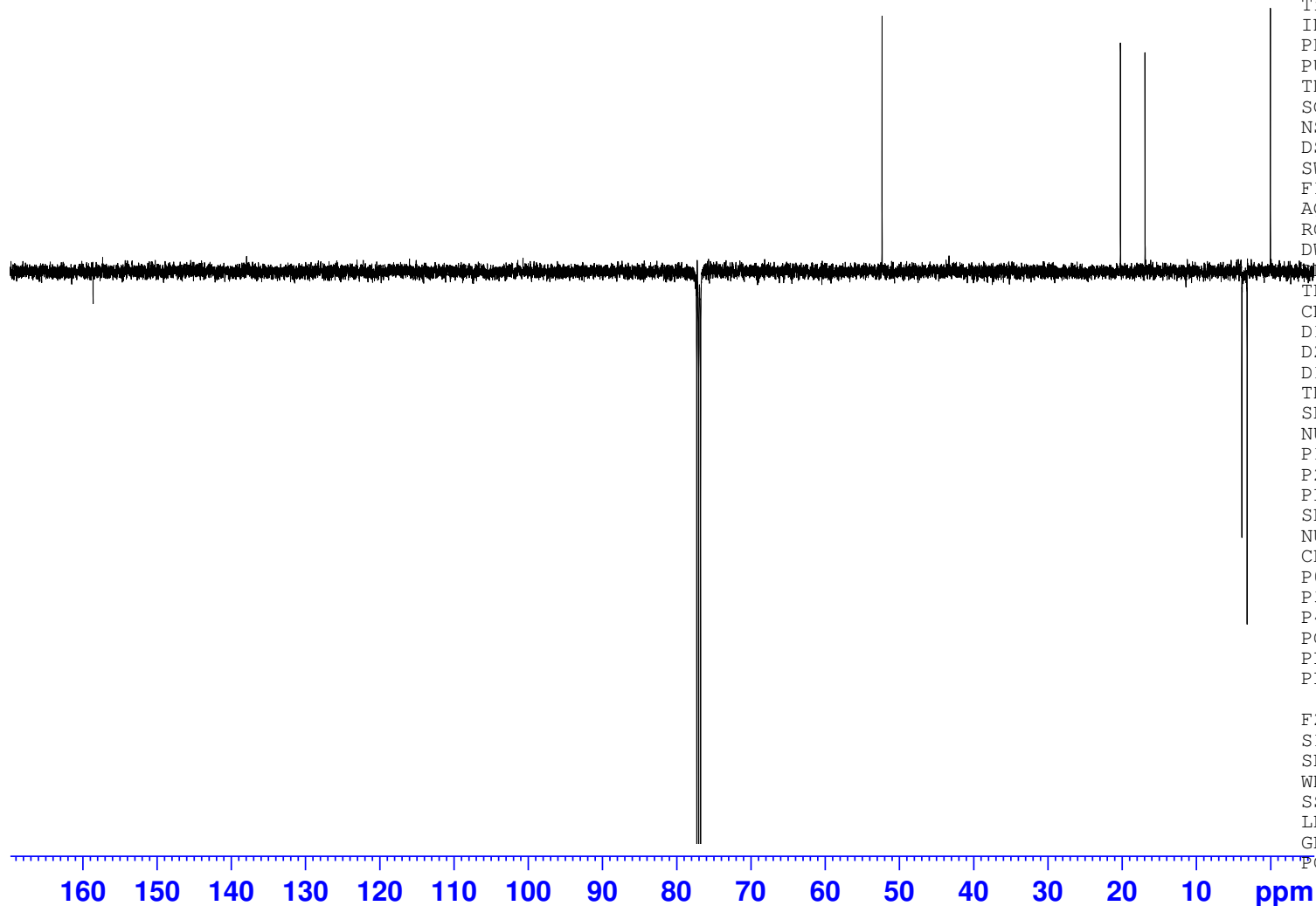
3.85
3.15
0.01



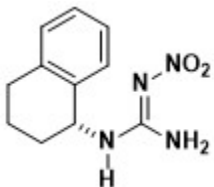
Current Data Parameters
NAME S-11
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180601
Time 13.59 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT CDC13
NS 3832
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 291.7 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.00 usec
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28288001 W

F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



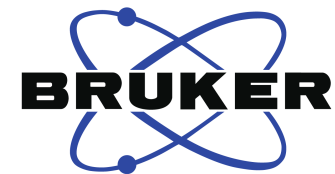
¹³C (DEPTQ135) NMR (125 MHz, CDCl₃) of S-11



7.267
7.255
7.252
7.186
7.135
7.122

— 4.998

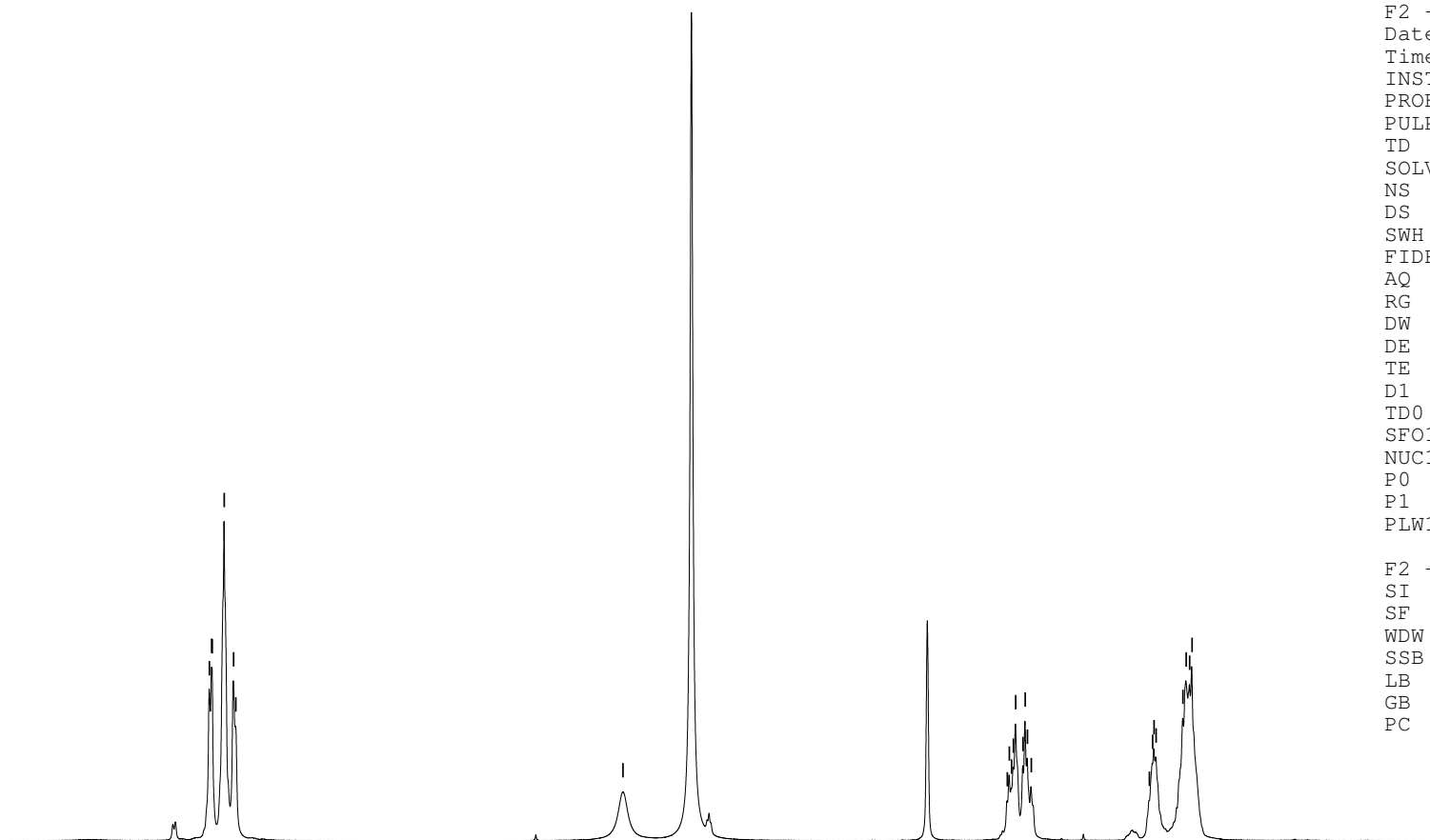
2.890
2.879
2.866
2.857
2.844
2.804
2.792
2.780
2.759
2.111
2.093
2.085
2.074
1.926
1.909
1.890
1.877



Current Data Parameters
NAME S-12
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200410
Time 13.04 h
INSTRUM spect
PROBHD z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.276799 sec
RG 95.16
DW 50.000 usec
DE 6.50 usec
TE 323.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.49 usec
P1 10.47 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm

4.68

1.00

2.11

1.22
3.24

¹H NMR (500 MHz, CD₃OD, 50°C) of **S-12**

—159.05

—137.35
128.89
128.01
127.30
125.93

—49.51

—29.62
—28.58

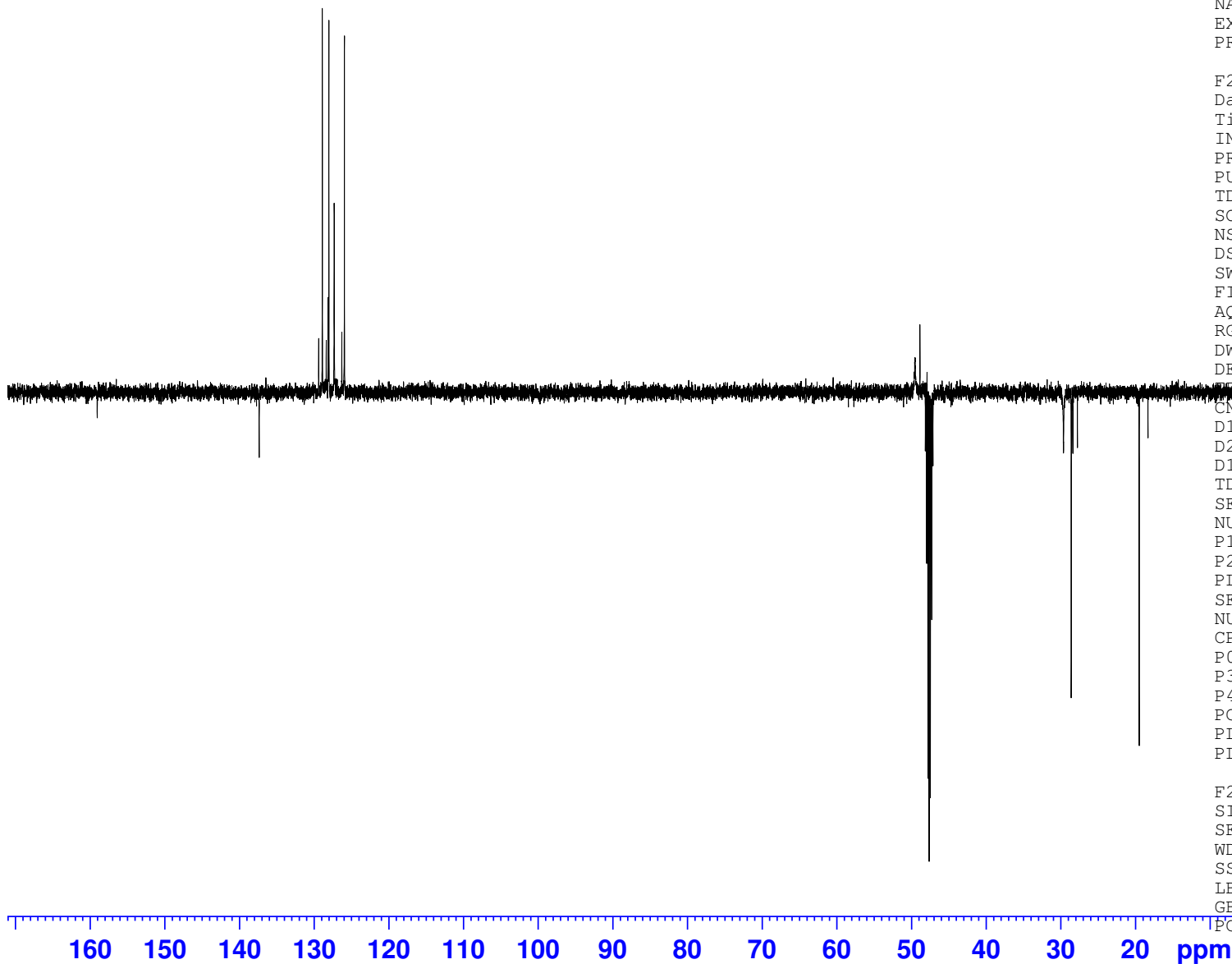
—19.48



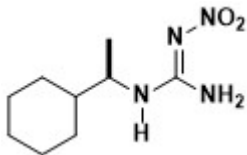
Current Data Parameters
NAME S-12
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200410
Time 13.16 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT MeOD
NS 203
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 323.1 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.70 usec
P3 10.47 usec
P4 20.94 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.31009001 W

F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



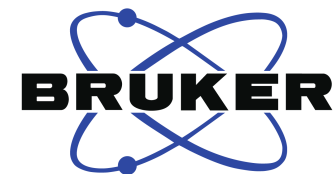
¹³C (DEPTQ135) NMR (125 MHz, CD₃OD, 50°C) of **S-12**



— 8.471

— 6.647

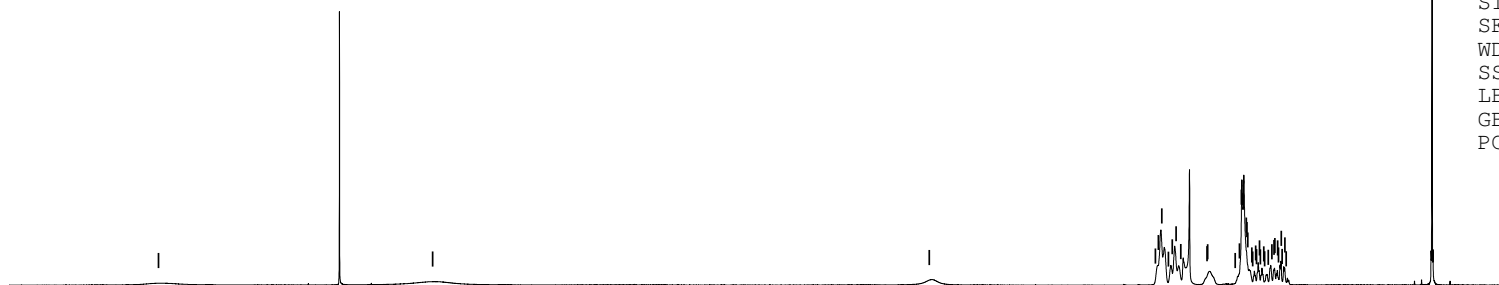
3.346
1.841
1.821
1.799
1.755
1.730
1.703
1.673
1.499
1.494
1.311
1.283
1.270
1.237
1.233
1.227
1.200
1.194
1.175
1.169
1.150
1.143



Current Data Parameters
NAME R-13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170810
Time 10.48 h
INSTRUM spect
PROBHD zg30
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 139.09
DW 50.000 usec
DE 6.50 usec
TE 292.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

0.80

1.83

1.00

6.27

1.15

9.52

¹H NMR (500 MHz, CDCl₃) of **R-13**

—158.63

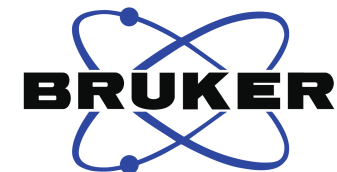
—42.97

—28.99

—26.12

—25.95

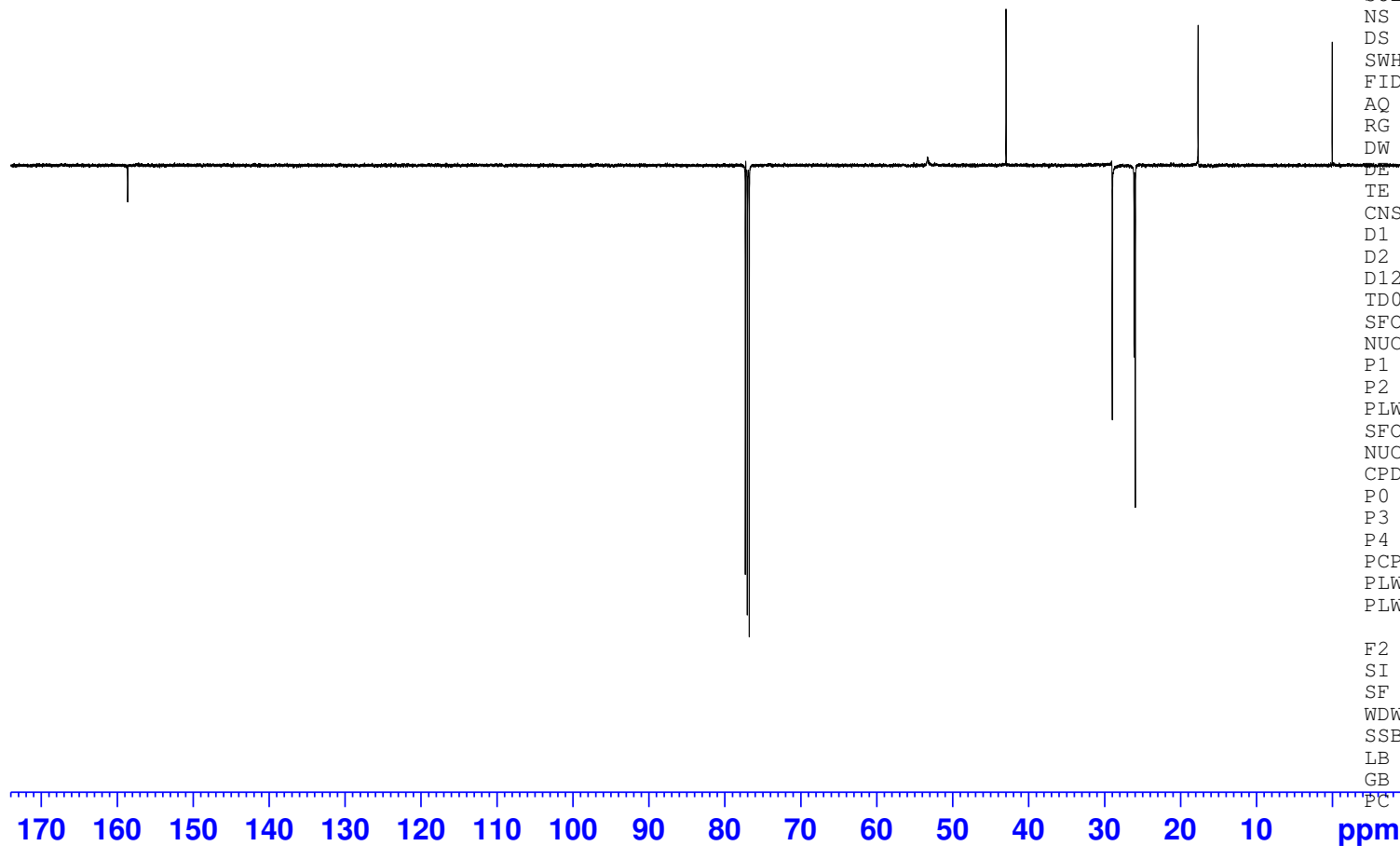
—17.68



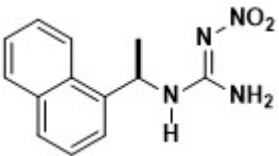
Current Data Parameters
NAME R-13
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170813
Time 1.58 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT CDCl3
NS 10240
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 291.3 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.00 usec
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28680280 W

F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

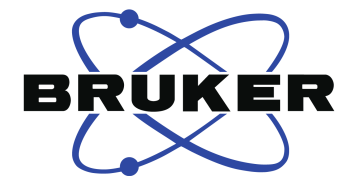


^{13}C (DEPTQ135) NMR (125 MHz, CDCl_3) of **R-13**



7.61
7.61
7.61
7.61
7.642
7.631
7.628
7.614
7.611
7.608
7.601
7.594
7.592
7.581
7.579
7.553
7.537
7.522
7.284
5.437

2.065
1.803
1.789
1.621
1.259

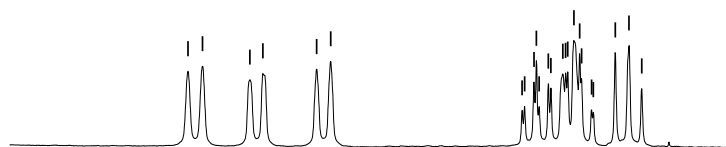


Current Data Parameters
NAME R-14
EXPNO 1
PROCNO 1

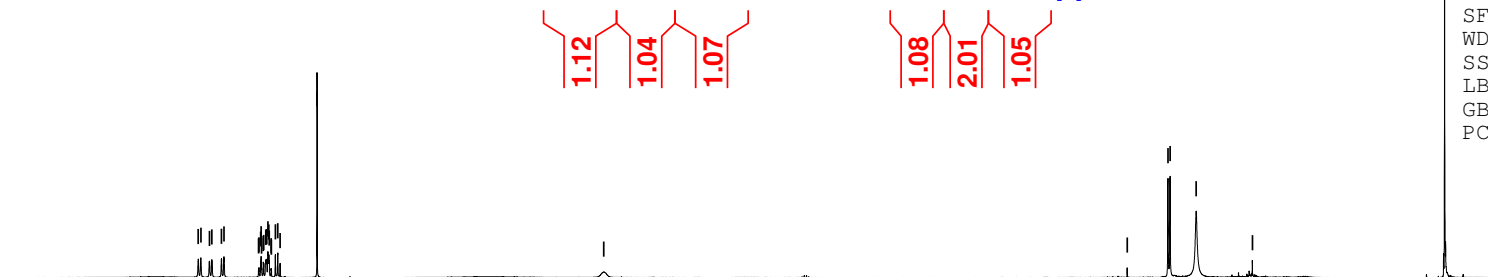
F2 - Acquisition Parameters
Date_ 20170519
Time 14.55 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 139.09
DW 50.000 usec
DE 6.50 usec
TE 292.6 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.050
8.033
7.978
7.963
7.900
7.884
7.658
7.648
7.645
7.642
7.631
7.628
7.614
7.611
7.608
7.601
7.594
7.592
7.553
7.537
7.522

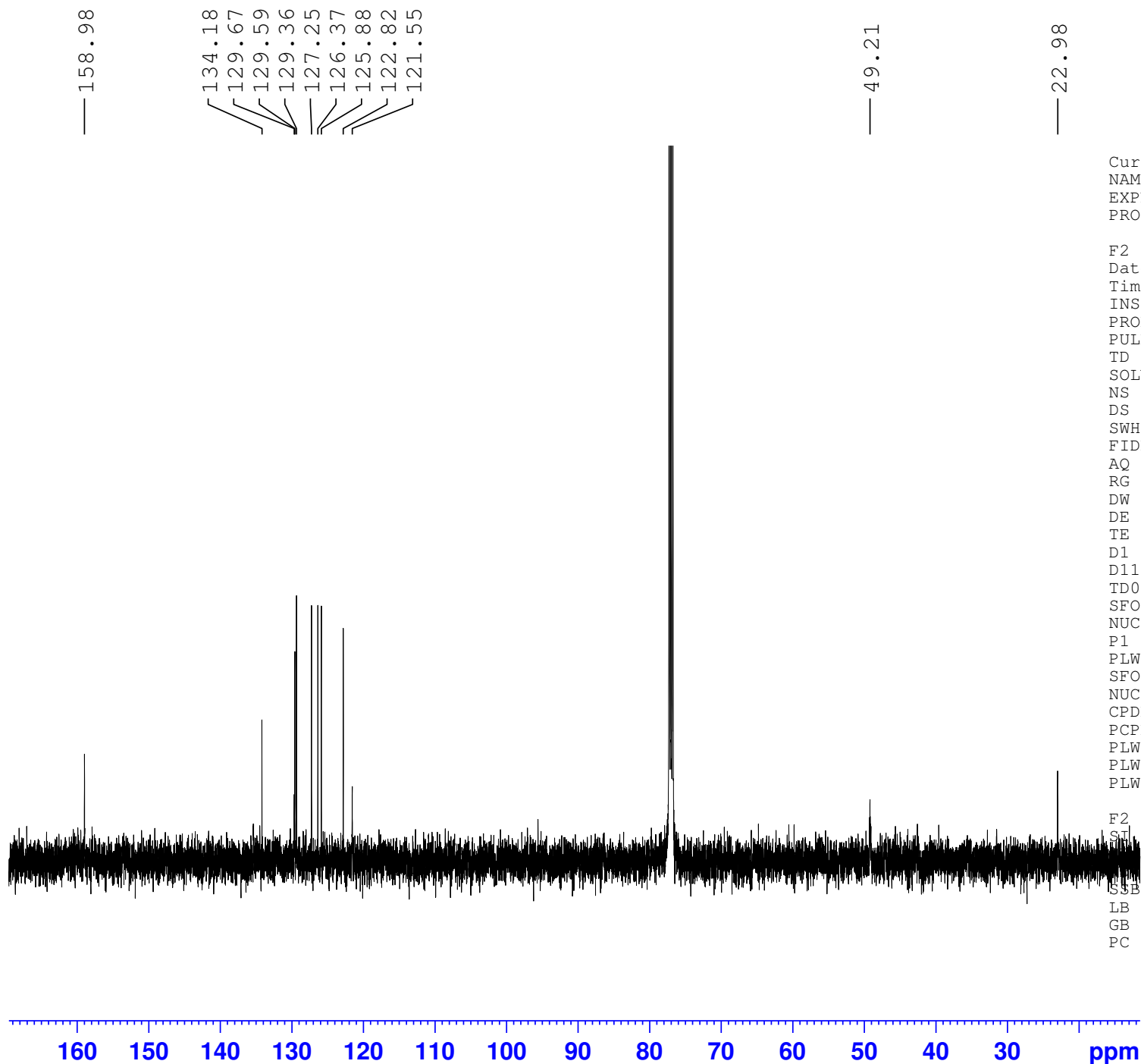


8.2 8.1 8.0 7.9 7.8 7.7 7.6 ppm



9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

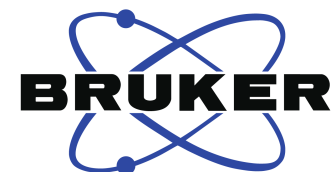
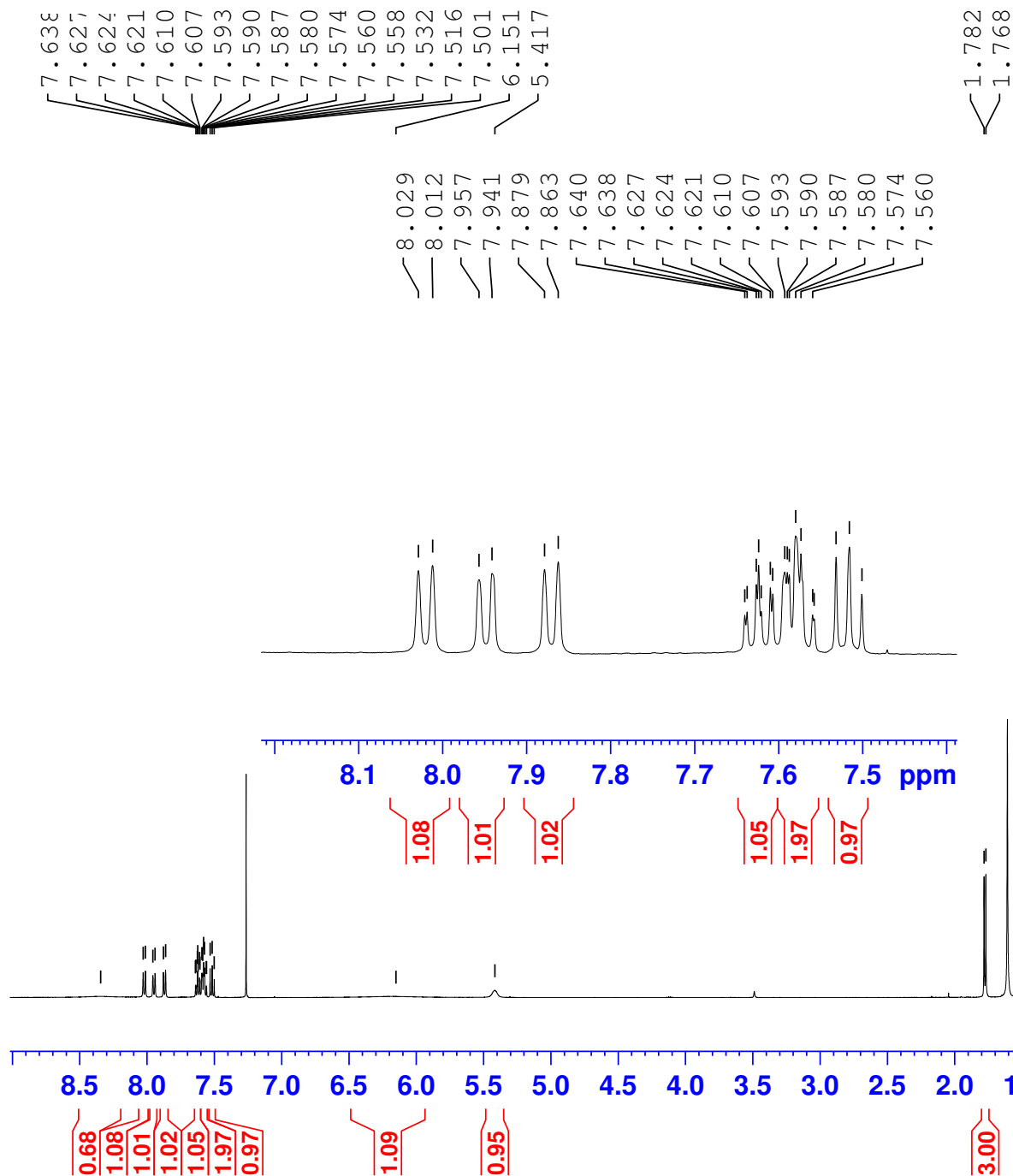
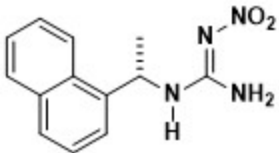
¹H NMR (500 MHz, CDCl₃) of *R*-14



Current Data Parameters
 NAME 13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170519
 Time 17.39 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 293.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28680280 W
 PLW13 0.14374560 W

F2 - Processing parameters
 SI 32768
 SF 125.7703631 MHz
 EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

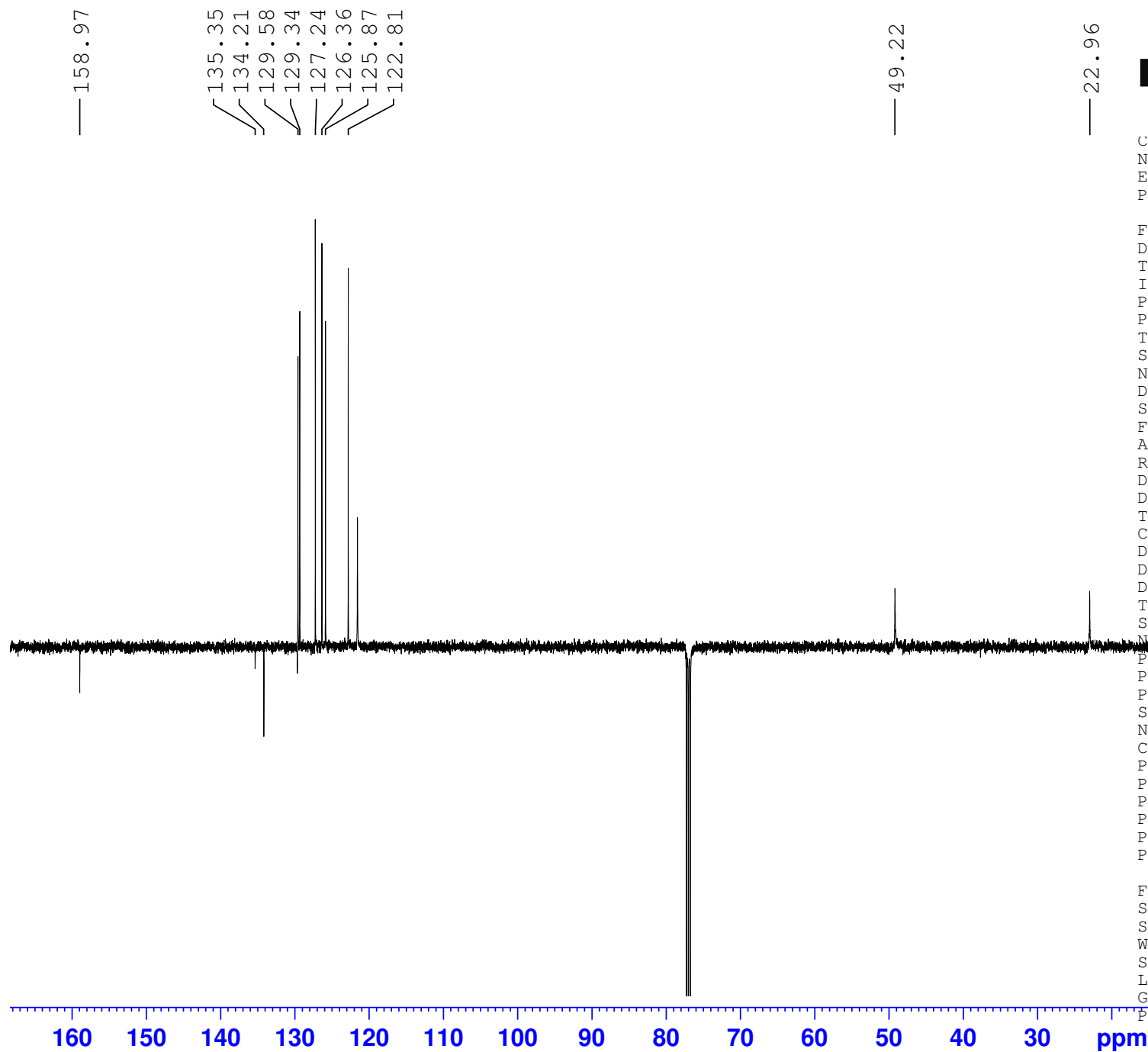


Current Data Parameters
NAME S-15
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170531
Time 17.19 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 139.09
DW 50.000 usec
DE 6.50 usec
TE 291.4 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

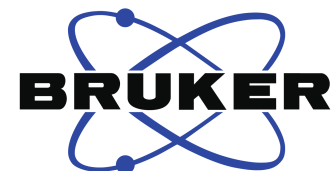
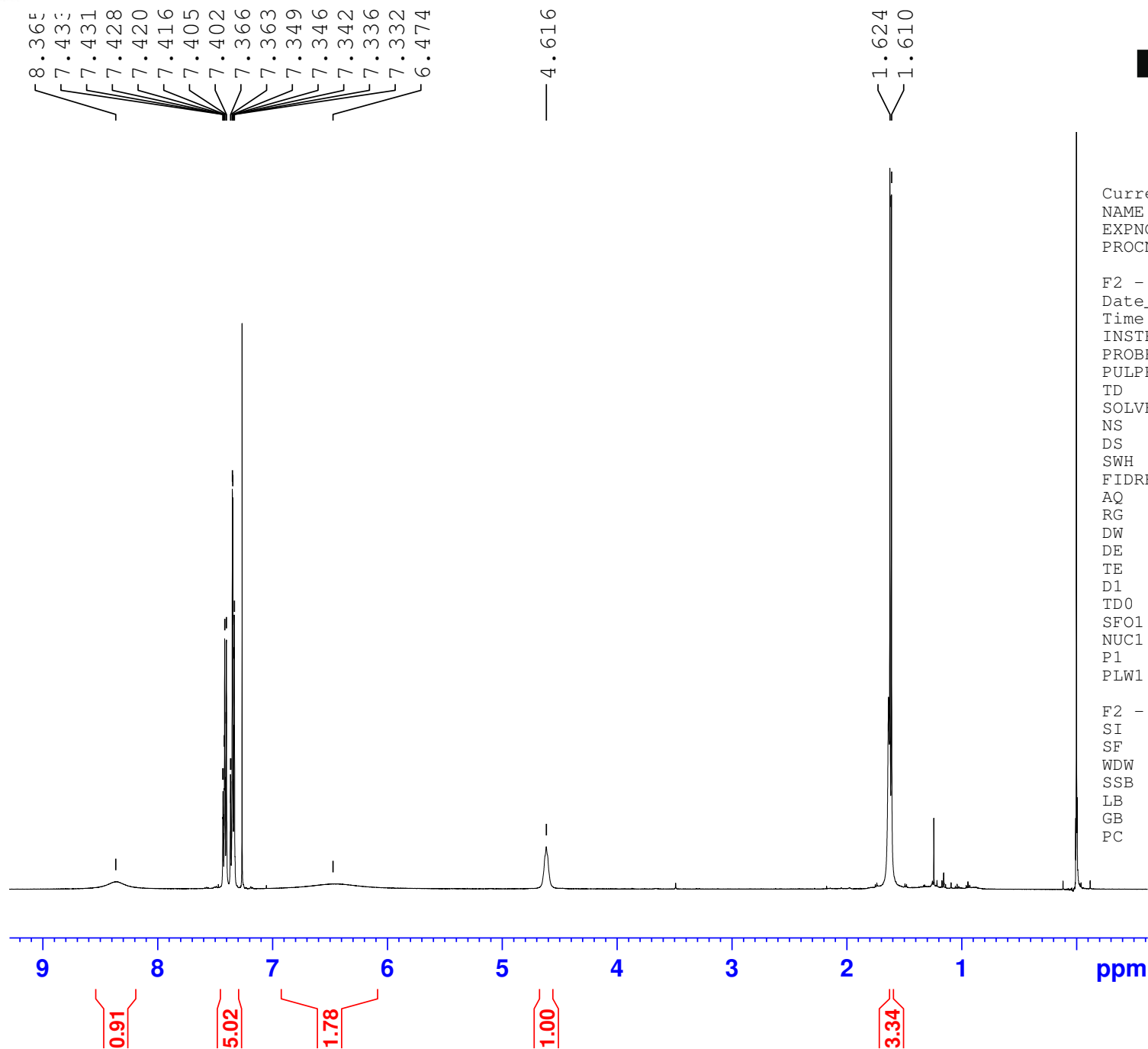
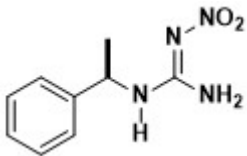
¹H NMR (500 MHz, CDCl₃) of S-15



Current Data Parameters
 NAME S-15
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170601
 Time 2.18 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG deptq135
 TD 65536
 SOLVENT CDCl3
 NS 10240
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 291.5 K
 CNST2 145.0000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 P2 20.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.00 usec
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28680280 W

F2 - Processing parameters
 SI 32768
 SF 125.7703639 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 FC 1.40

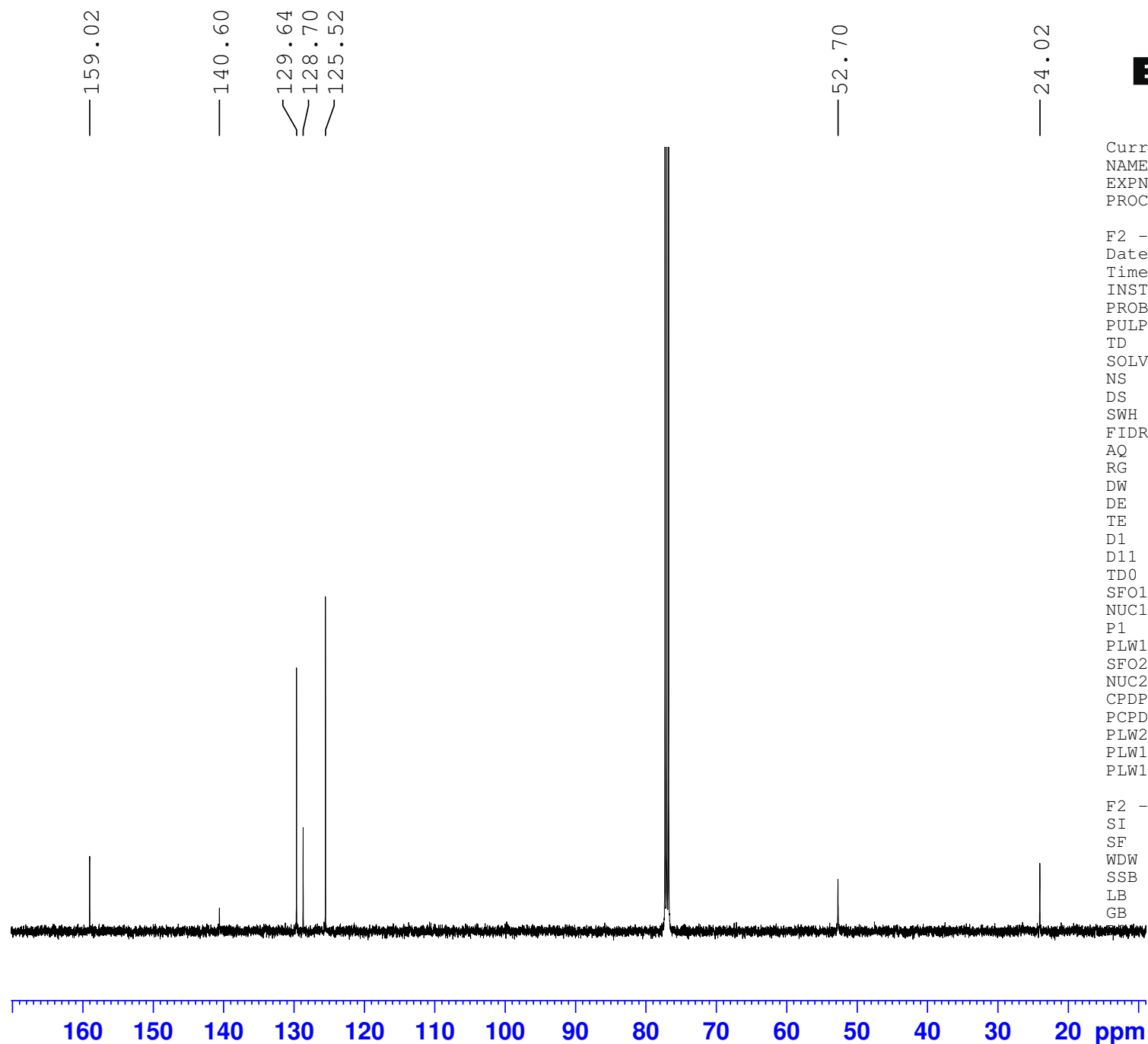


Current Data Parameters
 NAME 1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170519
 Time 14.42 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 139.09
 DW 50.000 usec
 DE 6.50 usec
 TE 292.6 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1830886 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 18.10400009 W

F2 - Processing parameters
 SI 65536
 SF 500.1800096 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

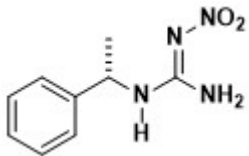
¹H NMR (500 MHz, CDCl₃) of **R-16**



Current Data Parameters
 NAME 2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170519
 Time 18.36 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 293.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28680280 W
 PLW13 0.14374560 W

F2 - Processing parameters
 SI 32768
 SF 125.7703632 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 1.40



8.40
7.427
7.412
7.401
7.398
7.362
7.359
7.348
7.345
7.335
7.331
6.536

— 4.622

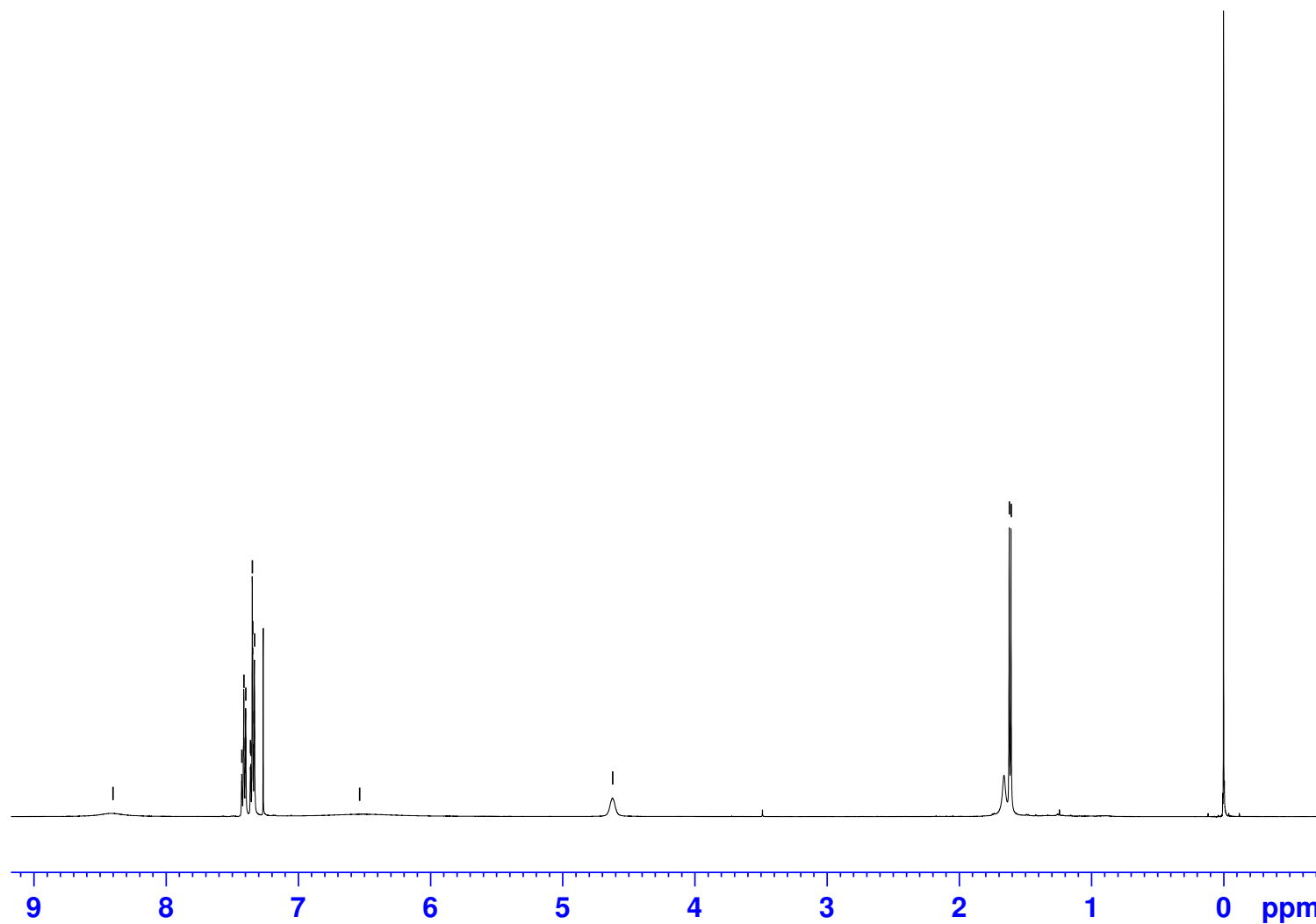
1.621
1.608



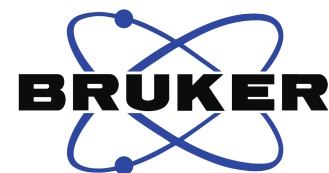
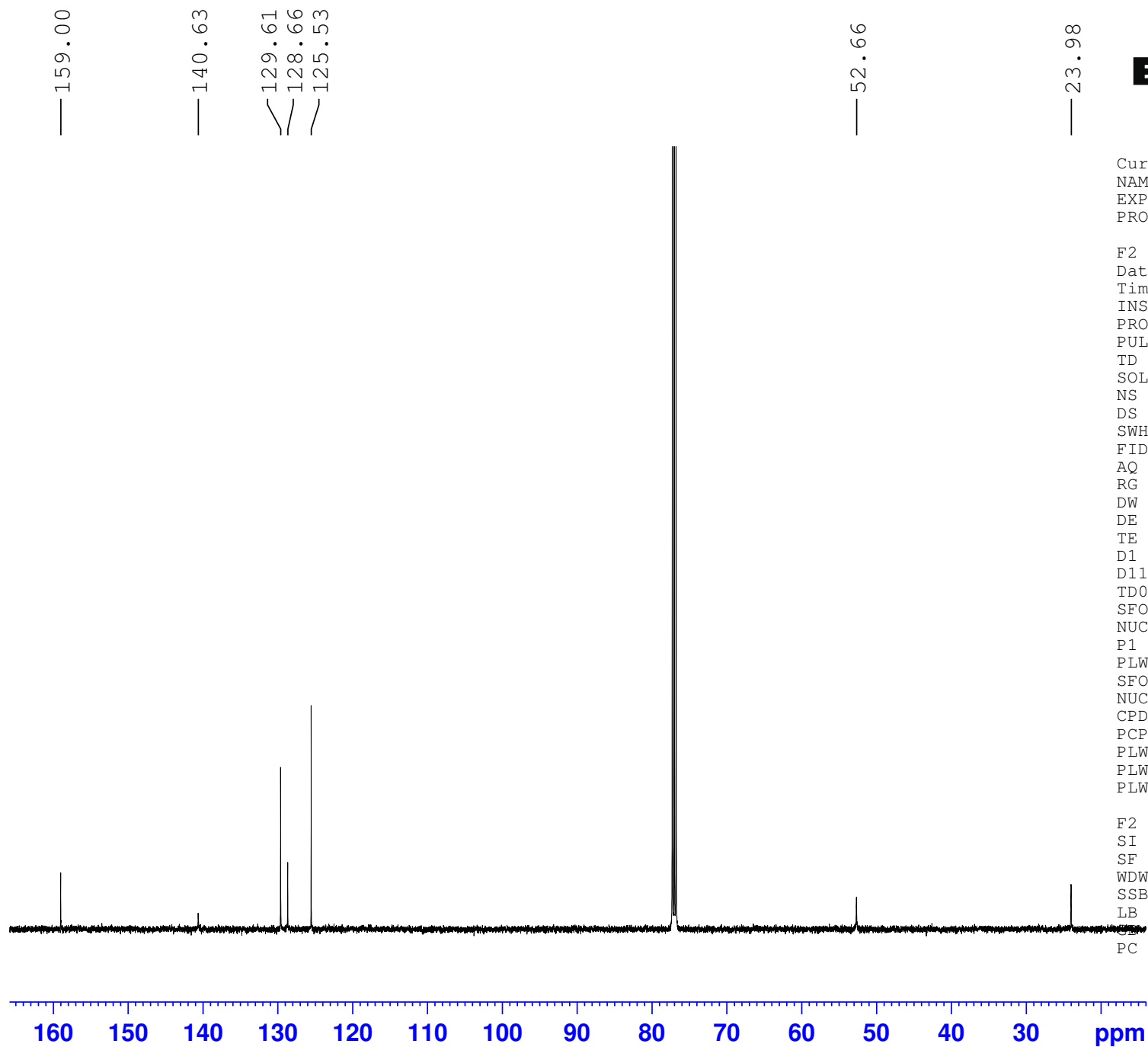
Current Data Parameters
NAME 1H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170519
Time 15.34 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 139.09
DW 50.000 usec
DE 6.50 usec
TE 292.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



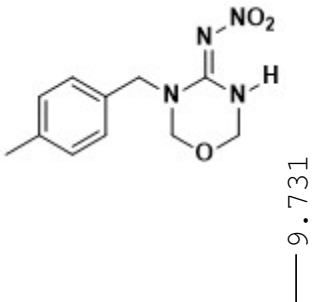
¹H NMR (500 MHz, CDCl₃) of **S-17**



Current Data Parameters
 NAME 13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170519
 Time 16.41 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 293.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28680280 W
 PLW13 0.14374560 W

F2 - Processing parameters
 SI 32768
 SF 125.7703633 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

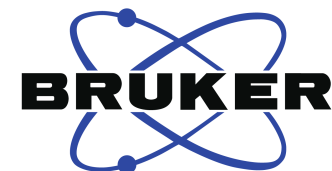


7.216
7.200
7.184
7.168

4.971
4.929
4.565

— 3.216

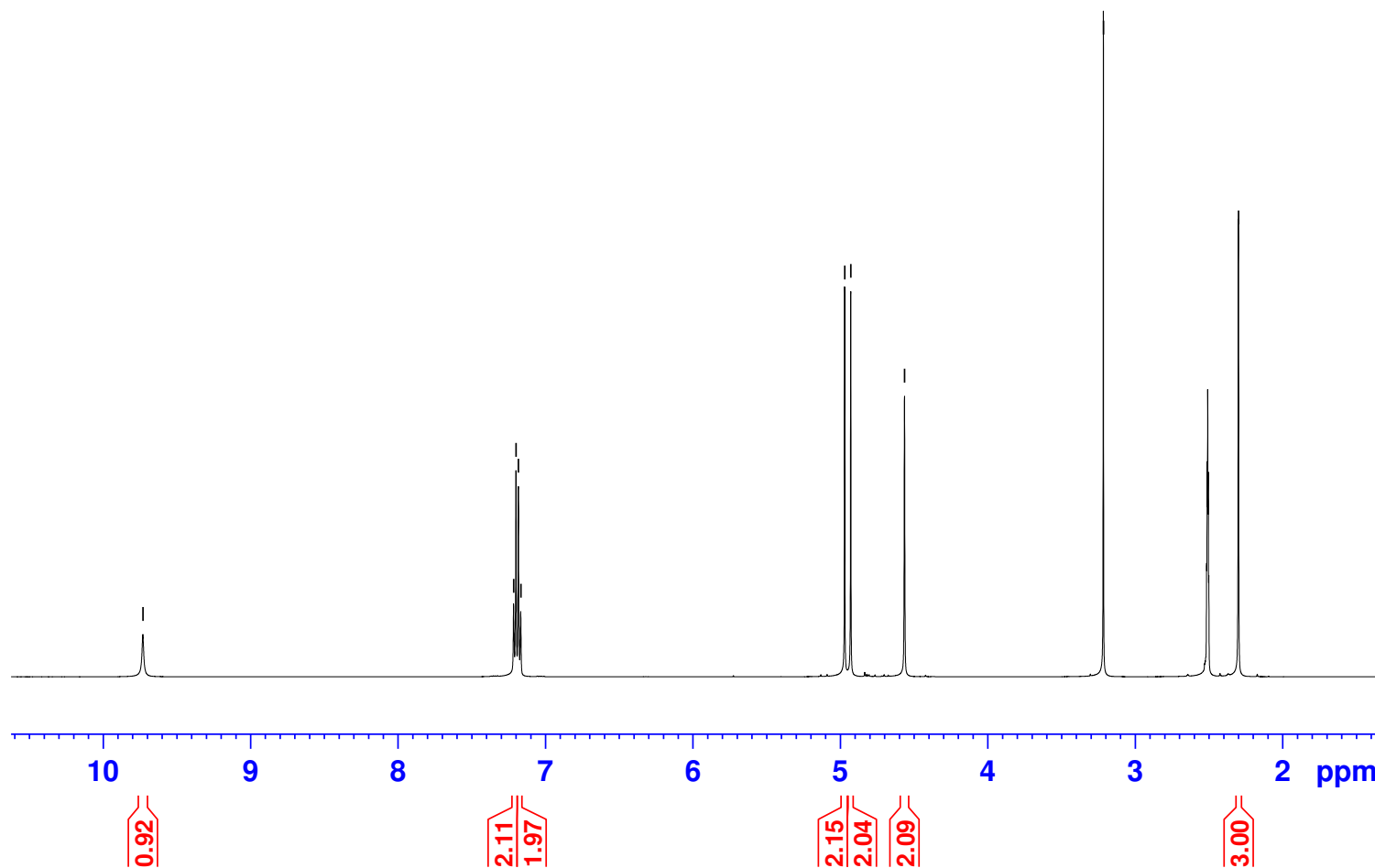
— 2.300



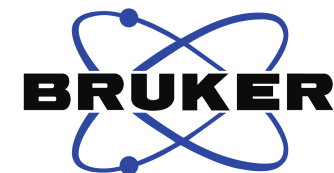
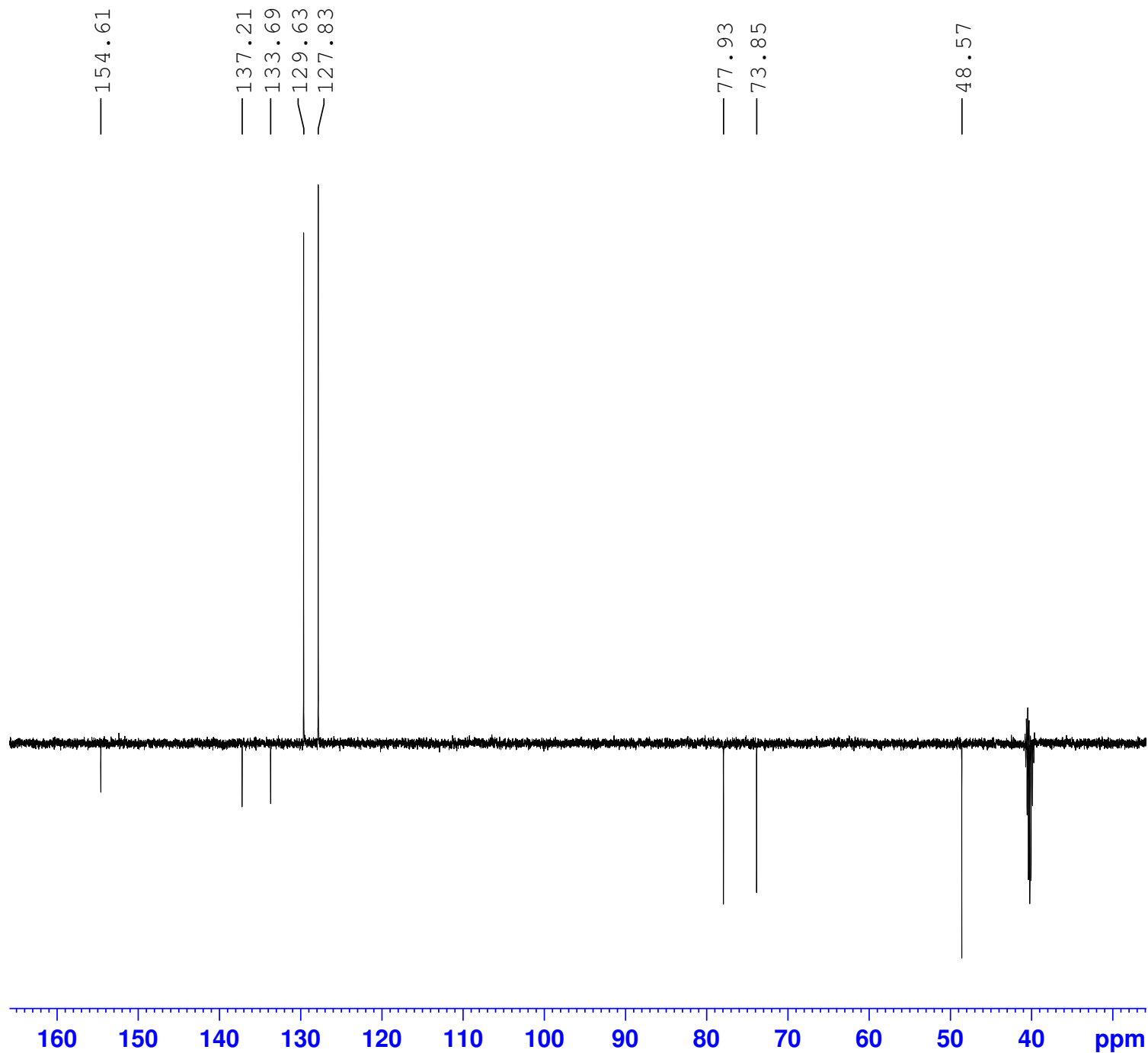
Current Data Parameters
NAME 18
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181204
Time 11.33 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 108.3
DW 50.000 usec
DE 6.50 usec
TE 323.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H NMR (500 MHz, DMSO-d₆, 50°C) of **18**

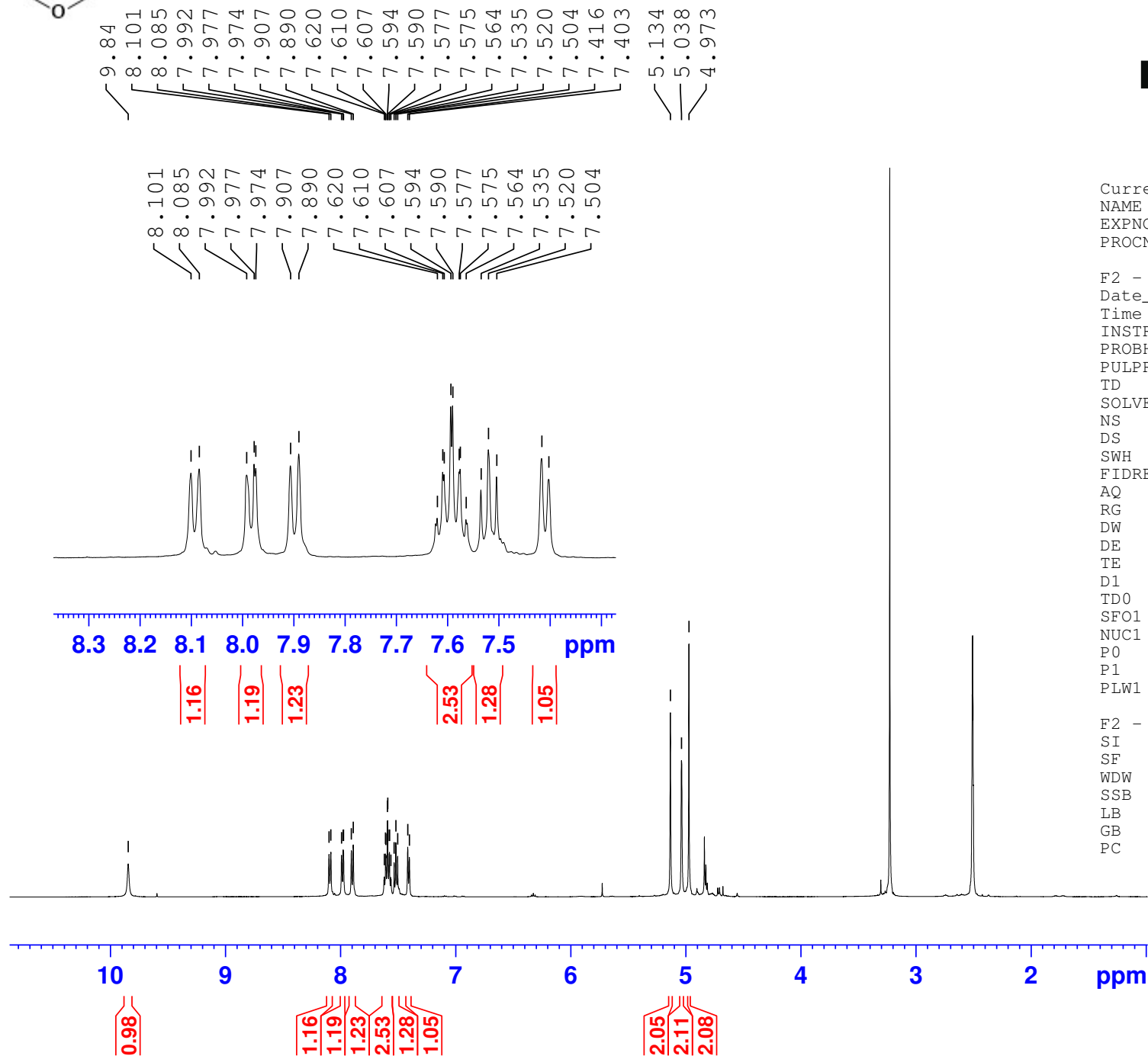
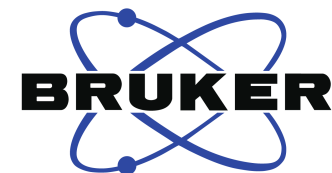
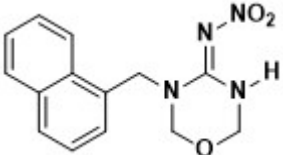


Current Data Parameters
NAME 18
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181204
Time 11.38 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT DMSO
NS 78
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 323.2 K
CNST2 145.000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.00 usec
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28288001 W

F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{13}C (DEPTQ135) NMR (125 MHz, DMSO- d_6 , 50°C) of **18**

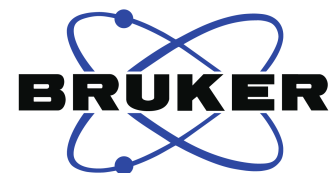
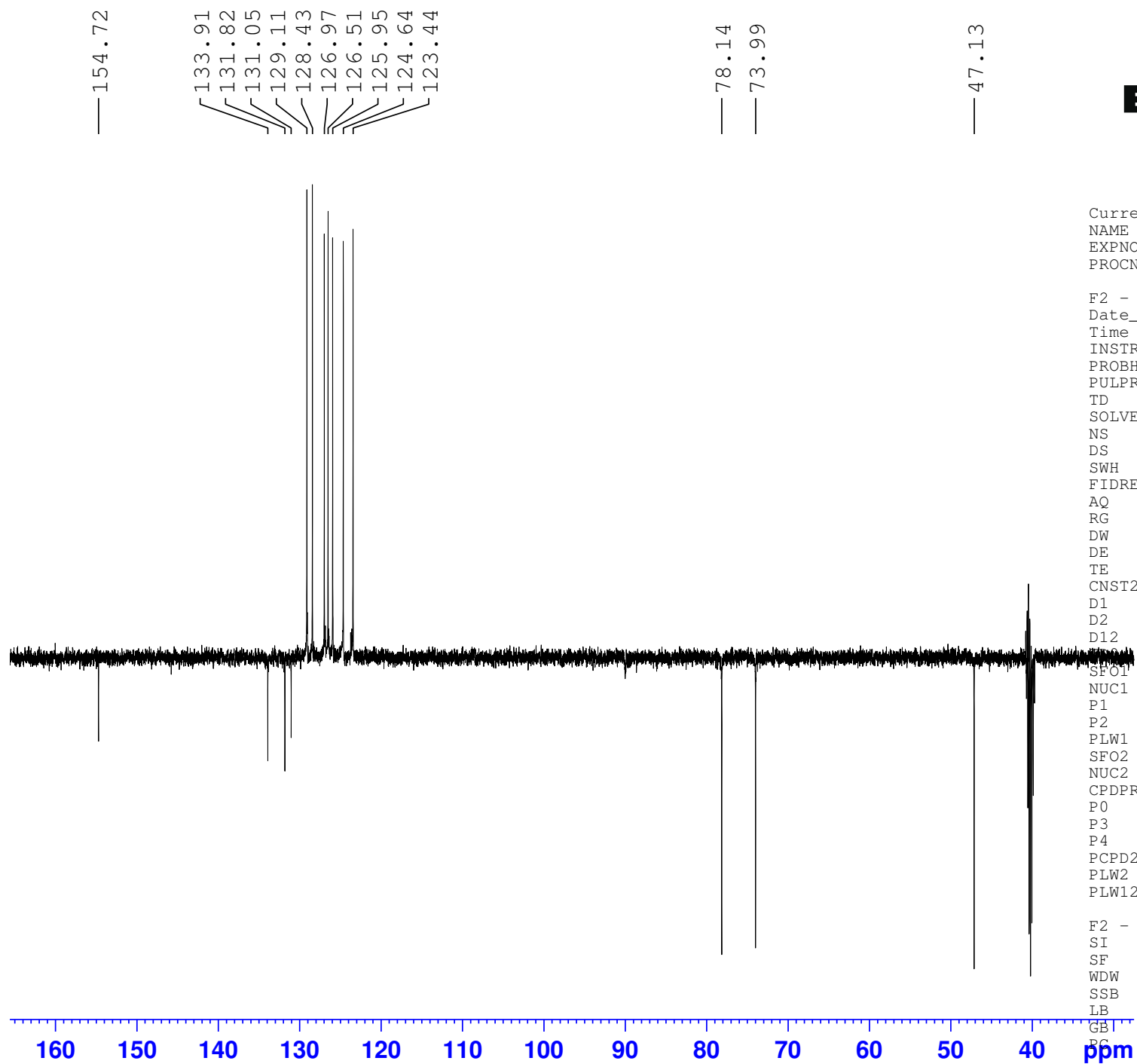


Current Data Parameters
NAME 19
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181204
Time 9.03 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 95.16
DW 50.000 usec
DE 6.50 usec
TE 323.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

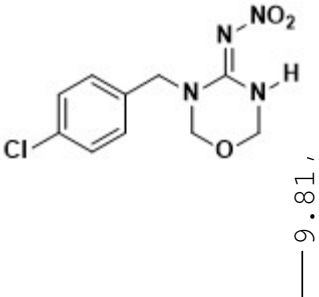
¹H NMR (500 MHz, DMSO-d₆, 50°C) of **19**



Current Data Parameters
NAME 19
EXPNO 2
PROCNO 1

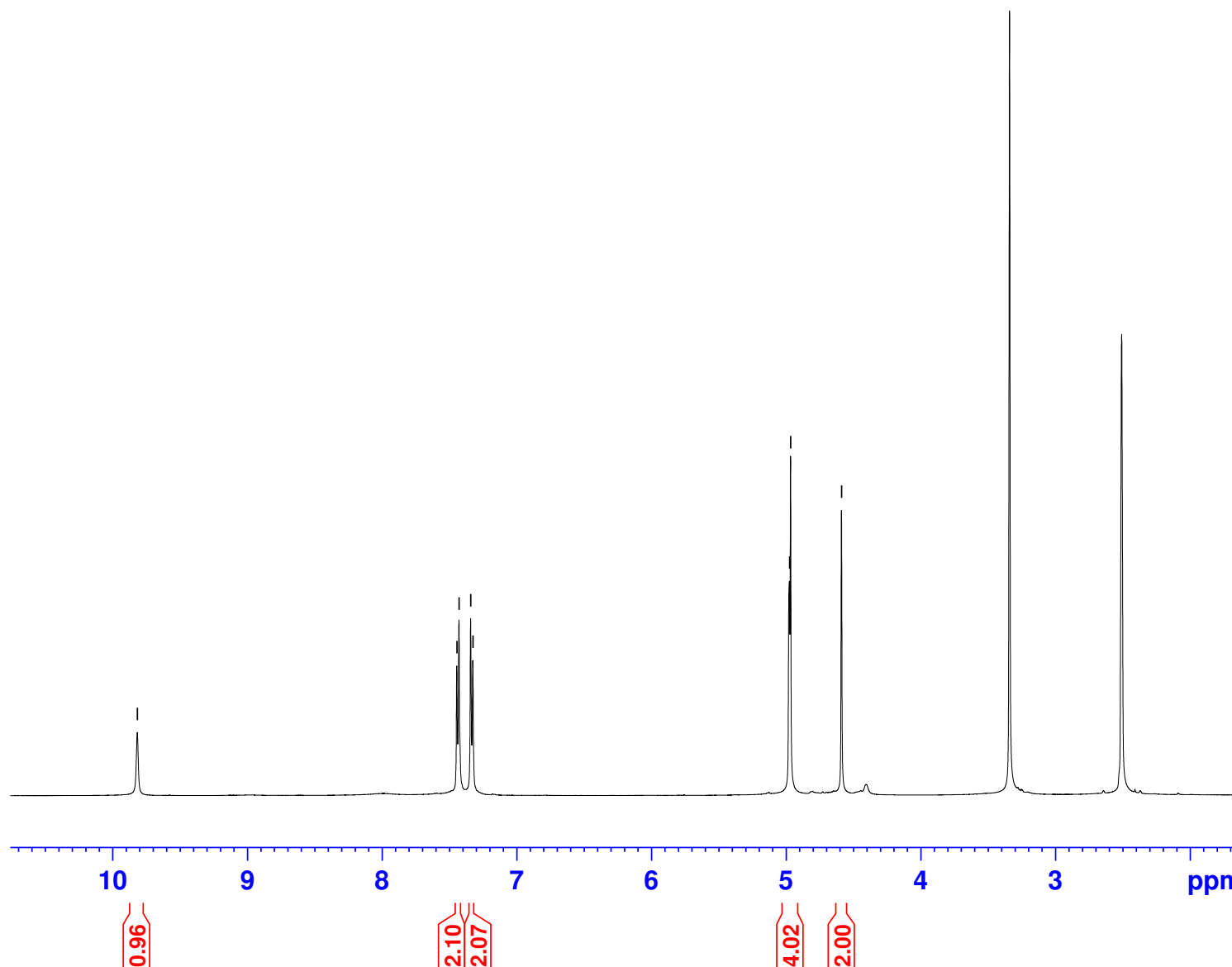
F2 - Acquisition Parameters
Date_ 20181204
Time 9.13 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT DMSO
NS 172
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 323.2 K
CNST2 145.000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.00 usec
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28288001 W

F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.445
7.429
7.342
7.326

4.975
4.966
4.588

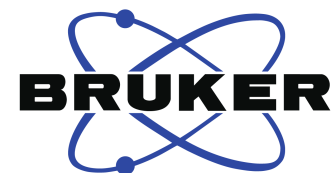
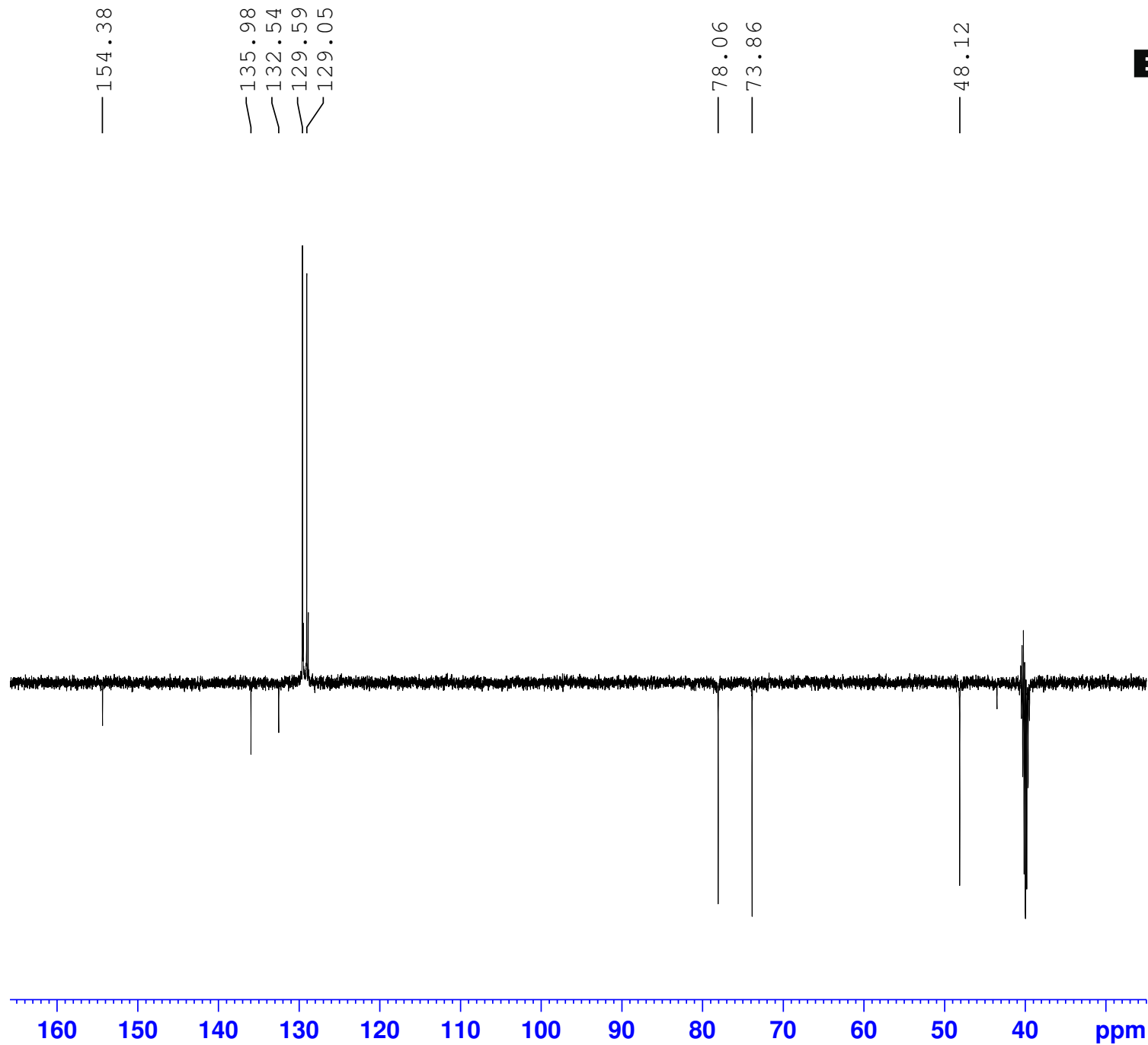


Current Data Parameters
NAME 20
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181204
Time 15.14 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 1
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 139.09
DW 50.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

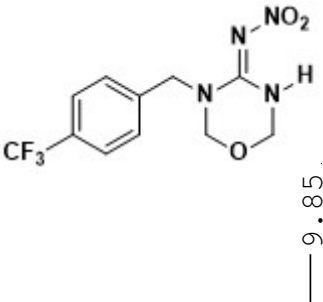
¹H NMR (500 MHz, DMSO-d₆) of **20**



Current Data Parameters
 NAME 20
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181204
 Time 15.21 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG deptq135
 TD 65536
 SOLVENT DMSO
 NS 122
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 296.0 K
 CNST2 145.000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 P2 20.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.00 usec
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28288001 W

F2 - Processing parameters
 SI 32768
 SF 125.7703610 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



7.756
7.740
7.517
7.501

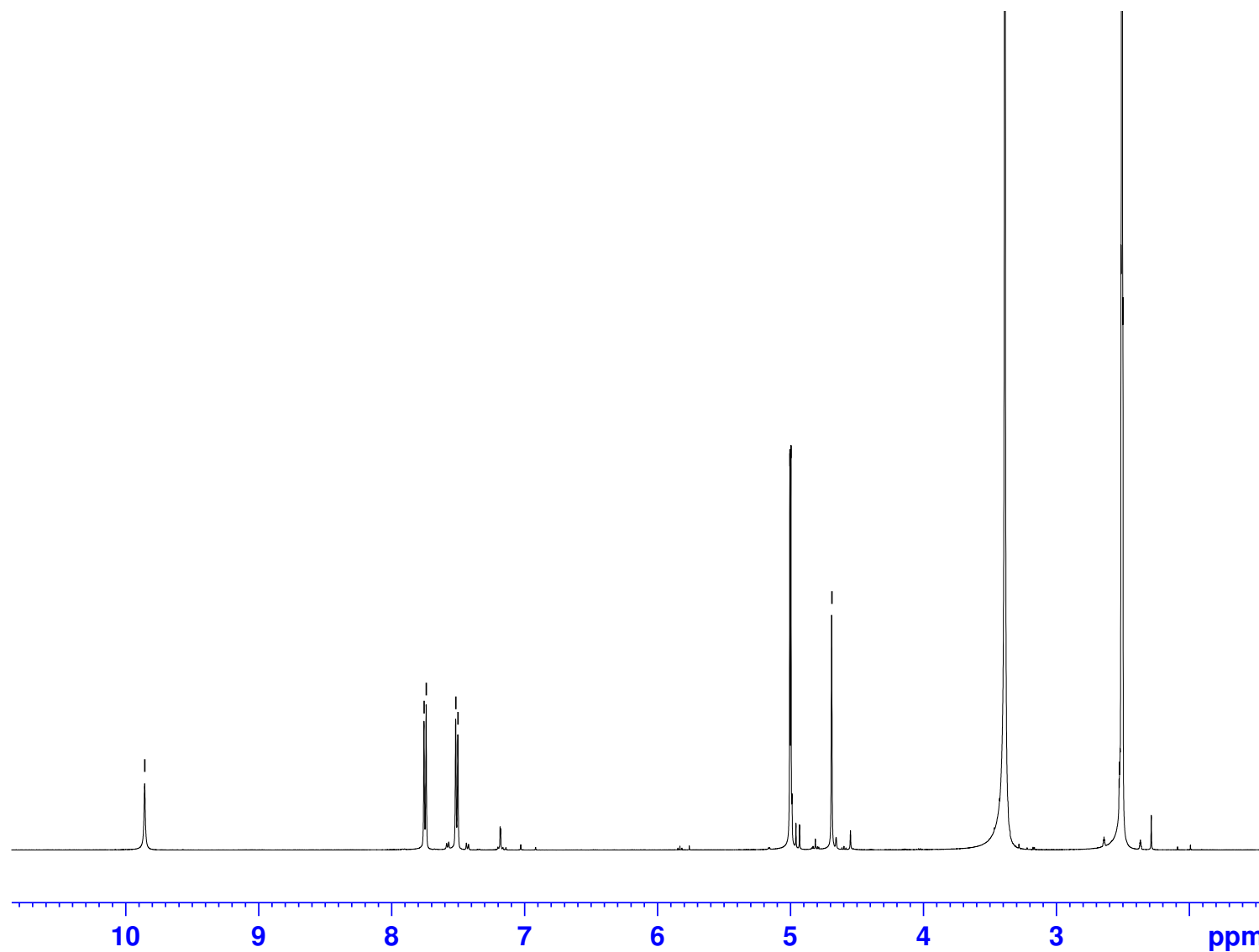
5.004
4.996
4.689



Current Data Parameters
NAME 21
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180907
Time 12.51 h
INSTRUM spect
PROBHD z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 88.37
DW 50.000 usec
DE 6.50 usec
TE 291.9 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

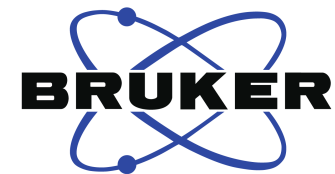
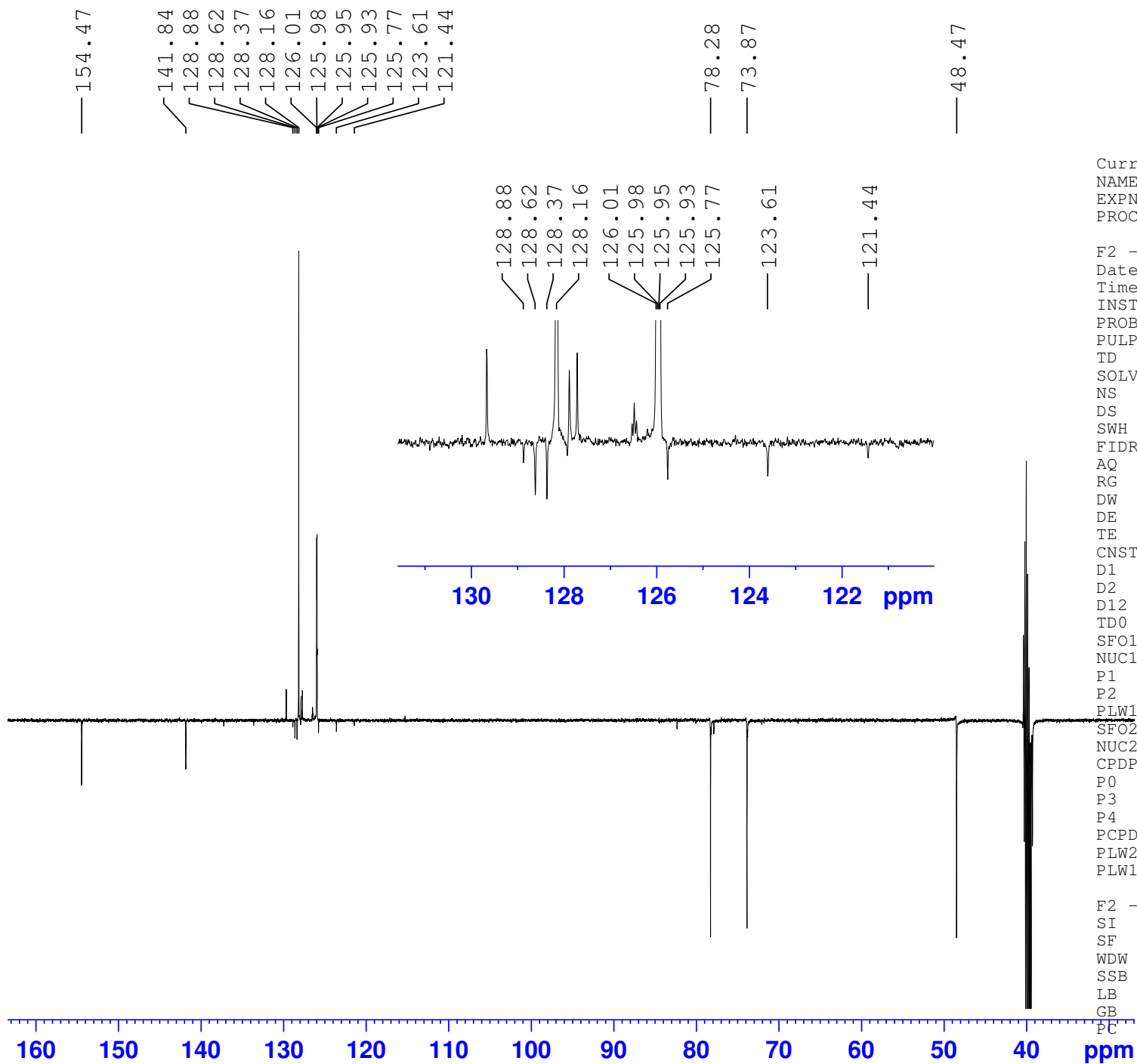


0.99

2.09 2.09

1.99 1.90 2.00

¹H NMR (500 MHz, DMSO-d₆) of **21**



Current Data Parameters

NAME 21
EXPNO 4
PROCNO 1

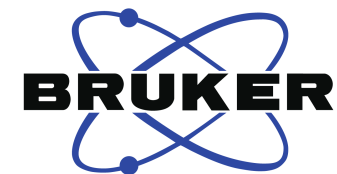
F2 - Acquisition Parameters

Date_ 20180926
Time 10.05 h
INSTRUM spect
PROBHD z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT DMSO
NS 17064
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 295.4 K
CNST2 145.000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SF01 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SF02 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.00 usec
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28288001 W

F2 - Processing parameters

SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

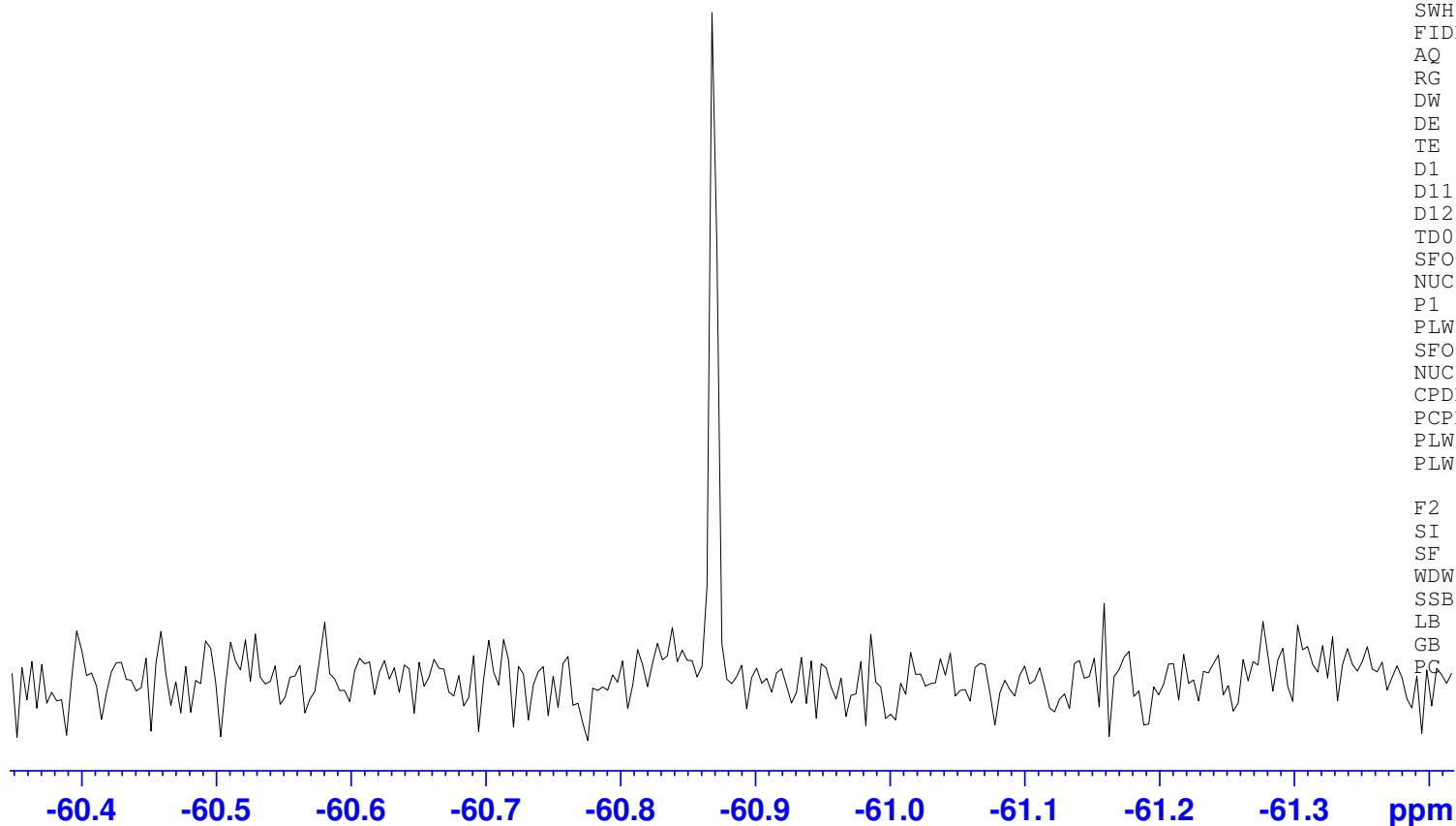
— -60.87

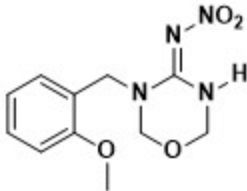


Current Data Parameters
NAME ARH-8
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190801
Time 14.44 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zgfhigqn.2
TD 131072
SOLVENT DMSO
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 1.733953 Hz
AQ 0.5767168 sec
RG 11.27
DW 4.400 usec
DE 6.50 usec
TE 293.4 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
SFO1 470.5923603 MHz
NUC1 19F
P1 16.00 usec
PLW1 36.93899918 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.31009001 W

F2 - Processing parameters
SI 65536
SF 470.6394242 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



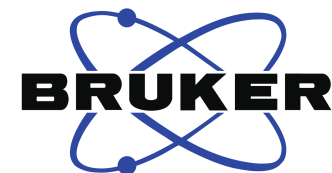
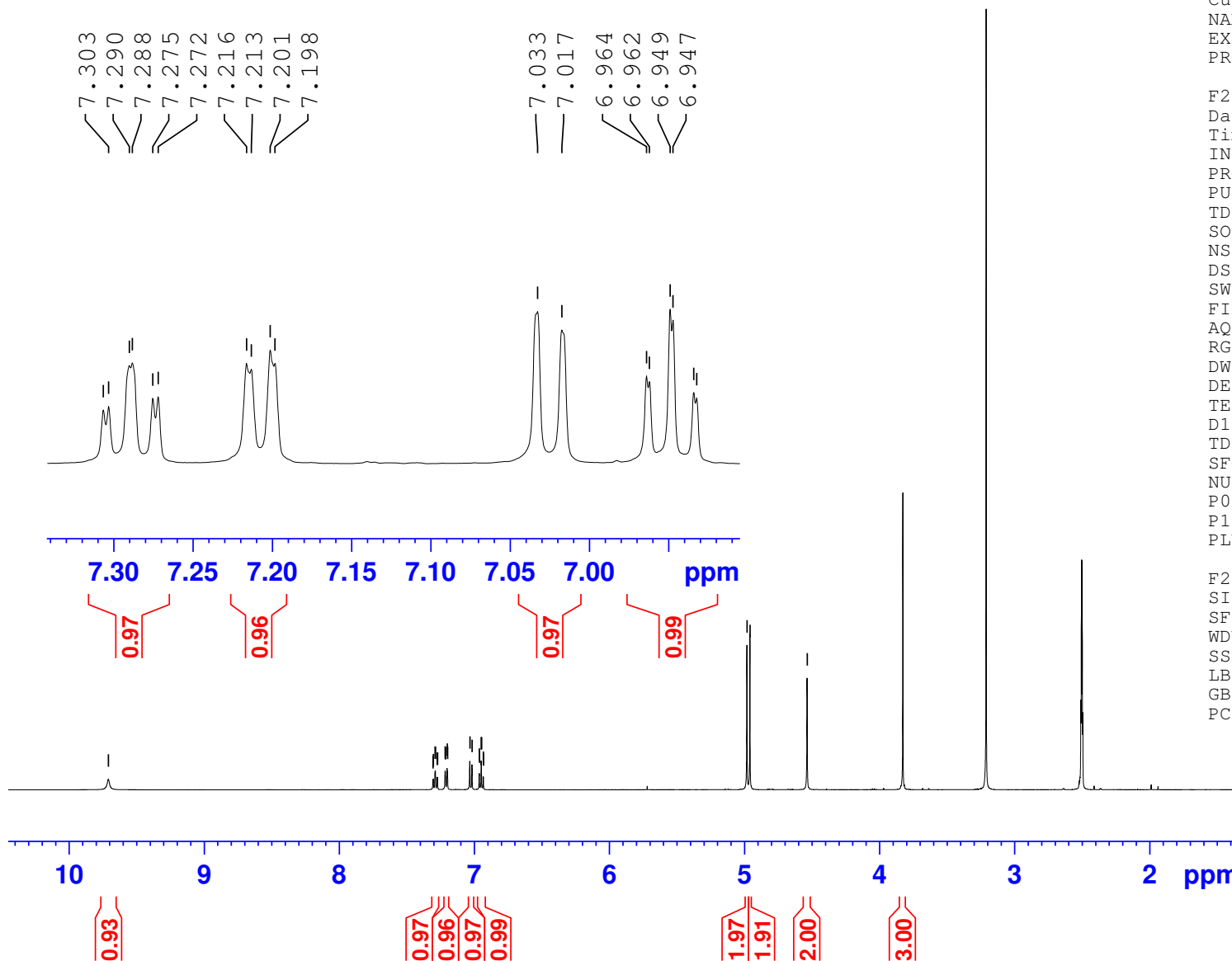


— 9.709

7.307
7.303
7.290
7.288
7.275
7.272
7.216
7.213
7.201
7.198
7.033
7.017
6.964
6.962
6.949
6.947
6.934
6.932
4.982
4.959
— 4.536

7.303
7.290
7.288
7.275
7.272
7.216
7.213
7.201
7.198

7.033
7.017
6.964
6.962
6.949
6.947

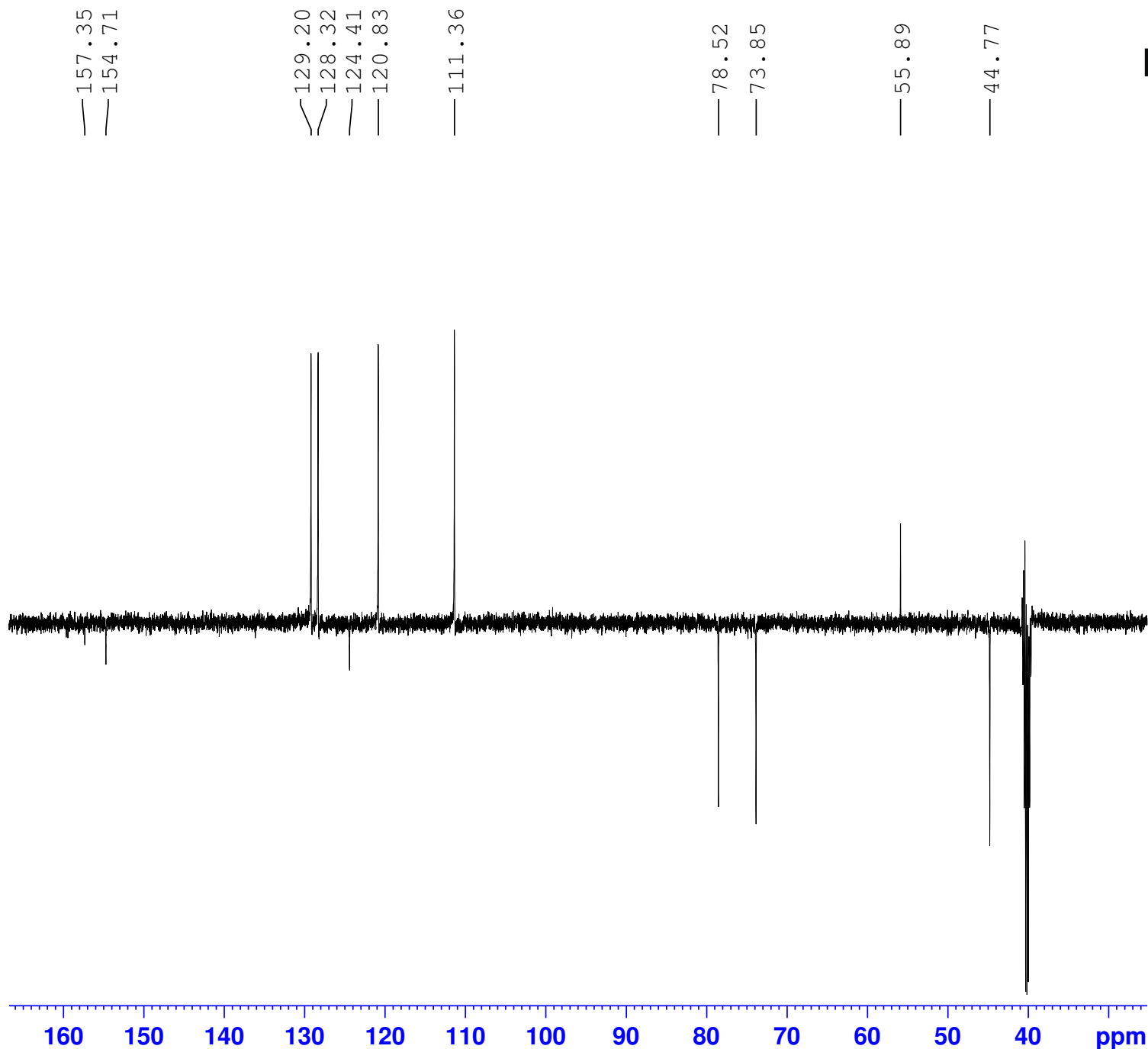


Current Data Parameters
NAME 22
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181204
Time 12.30 h
INSTRUM spect
PROBHD z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 139.09
DW 50.000 usec
DE 6.50 usec
TE 323.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR (500 MHz, DMSO-d₆, 50°C) of **22**

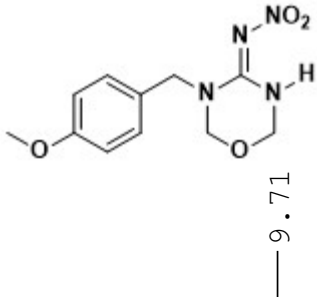


Current Data Parameters
 NAME 22
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181204
 Time 13.04 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG deptq135
 TD 65536
 SOLVENT DMSO
 NS 633
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 323.1 K
 CNST2 145.0000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 P2 20.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.00 usec
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28288001 W

F2 - Processing parameters
 SI 32768
 SF 125.7703610 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

^{13}C (DEPTQ135) NMR (125 MHz, DMSO- d_6 , 50°C) of **22**



7.272
7.255
6.938
6.921

4.961
4.957
4.925
4.536

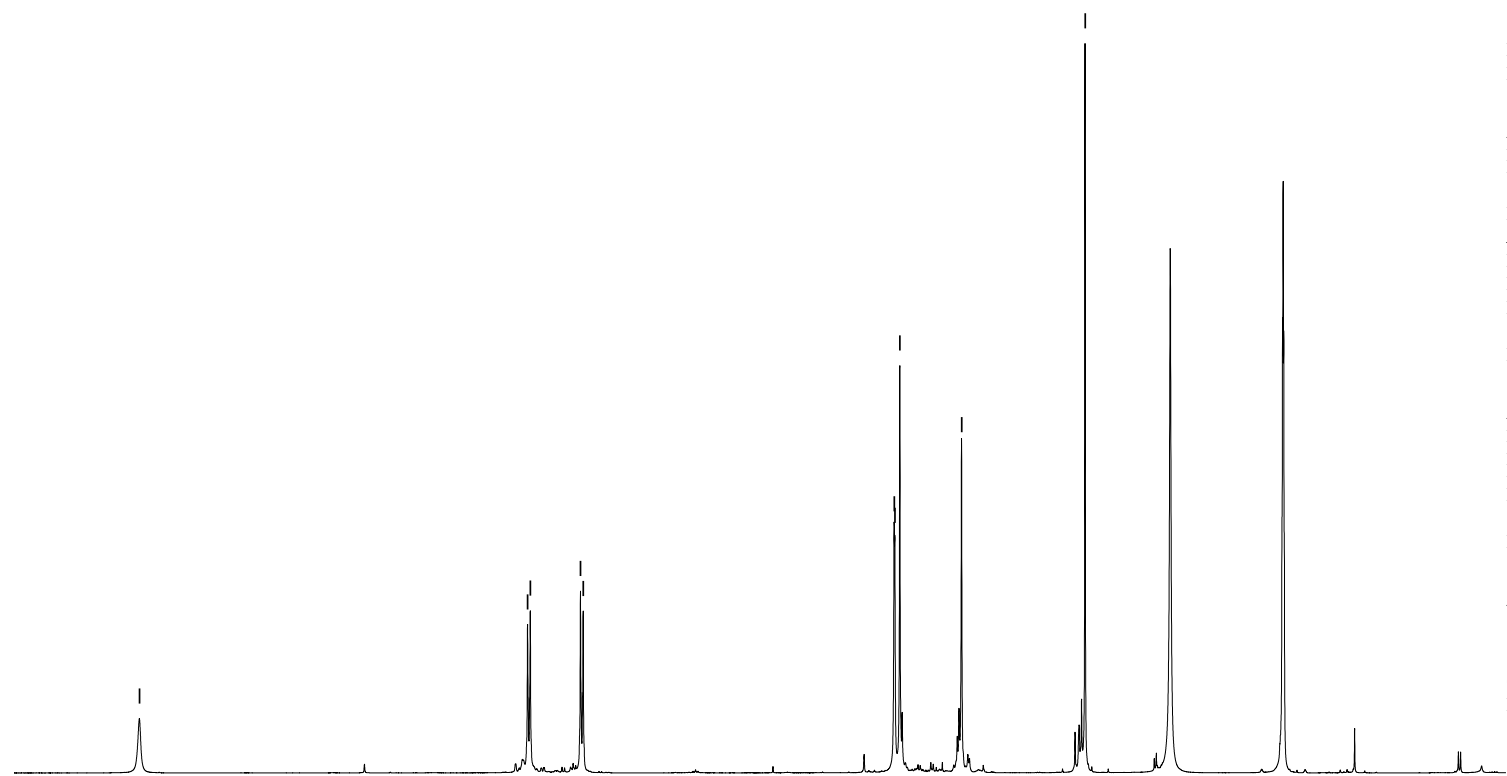
— 3.757



Current Data Parameters
NAME 23
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181204
Time 11.43 h
INSTRUM spect
PROBHD z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 139.09
DW 50.000 usec
DE 6.50 usec
TE 323.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



10 9 8 7 6 5 4 3 2 ppm

1.10

2.04

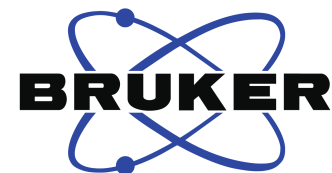
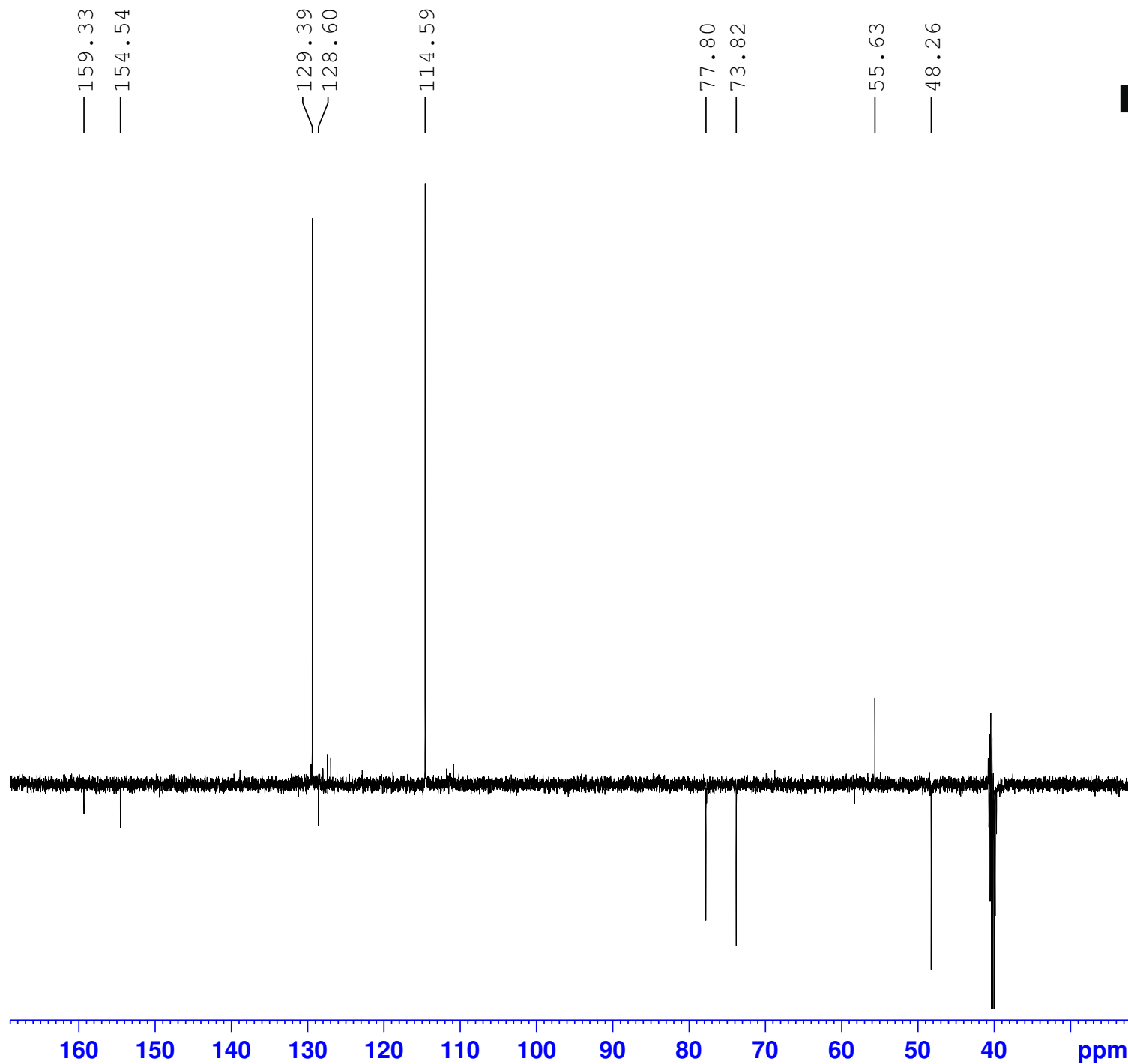
2.00

4.79

2.28

3.07

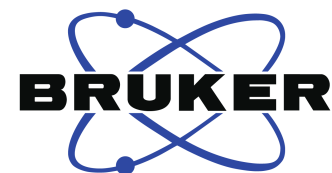
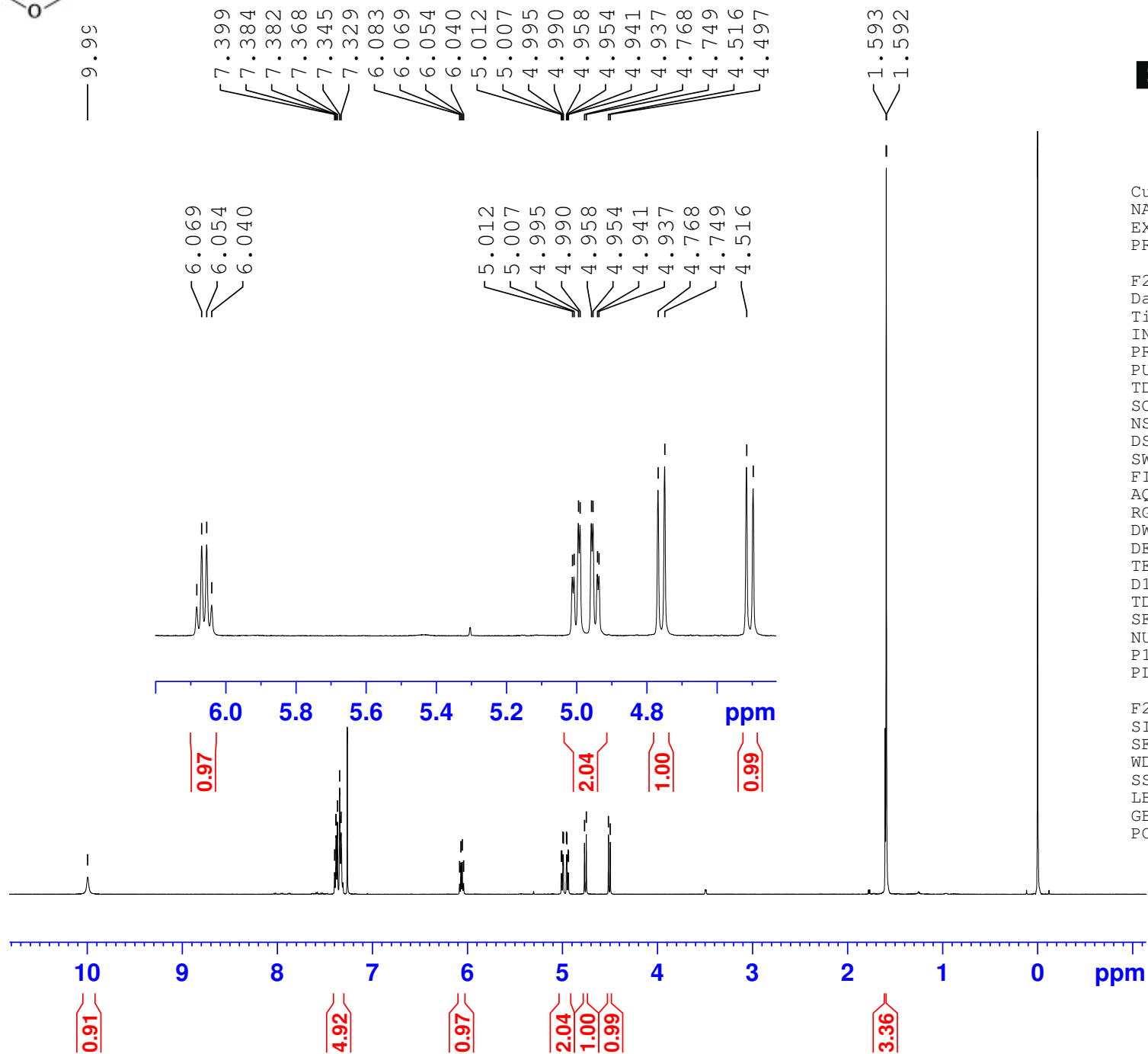
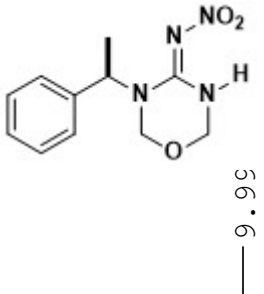
¹H NMR (500 MHz, DMSO-d₆, 50°C) of **23**



Current Data Parameters
 NAME 23
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181204
 Time 11.49 h
 INSTRUM spect
 PROBHD z119470_0187 (
 PULPROG deptq135
 TD 65536
 SOLVENT DMSO
 NS 104
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 323.2 K
 CNST2 145.000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 P2 20.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.00 usec
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28288001 W

F2 - Processing parameters
 SI 32768
 SF 125.7703610 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

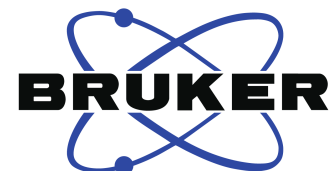
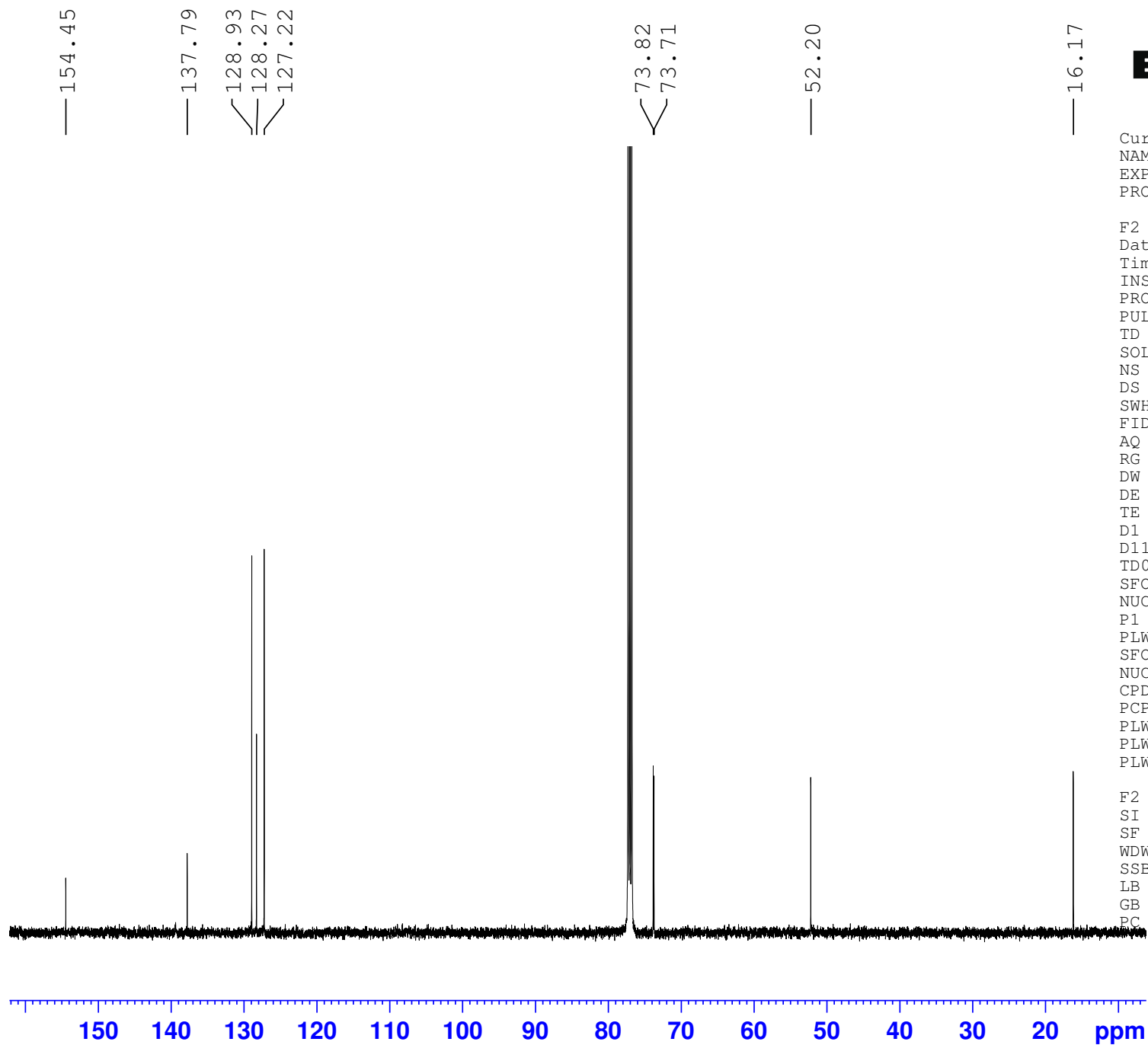


Current Data Parameters
 NAME 1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170826
 Time 8.08 h
 INSTRUM spect
 PROBHD z119470_0187 (
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 192.72
 DW 50.000 usec
 DE 6.50 usec
 TE 291.9 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1830886 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 18.10400009 W

F2 - Processing parameters
 SI 65536
 SF 500.1800100 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

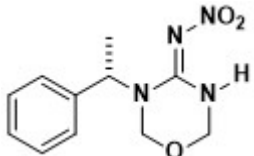
¹H NMR (500 MHz, CDCl₃) of **R-24**



Current Data Parameters
 NAME 13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170826
 Time 8.05 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 5120
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 292.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28680280 W
 PLW13 0.14374560 W

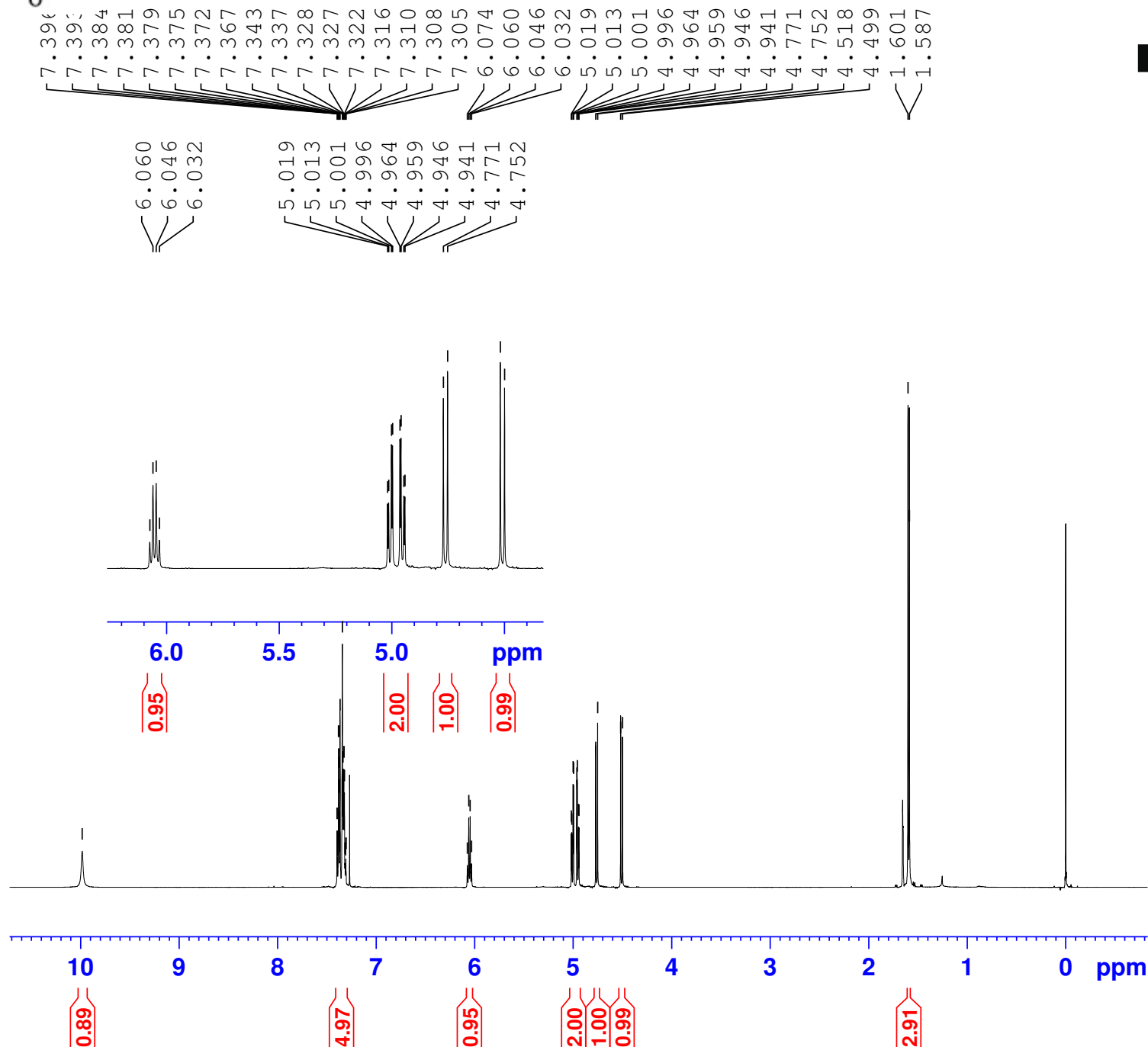
F2 - Processing parameters
 SI 32768
 SF 125.7703636 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



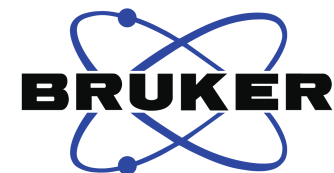
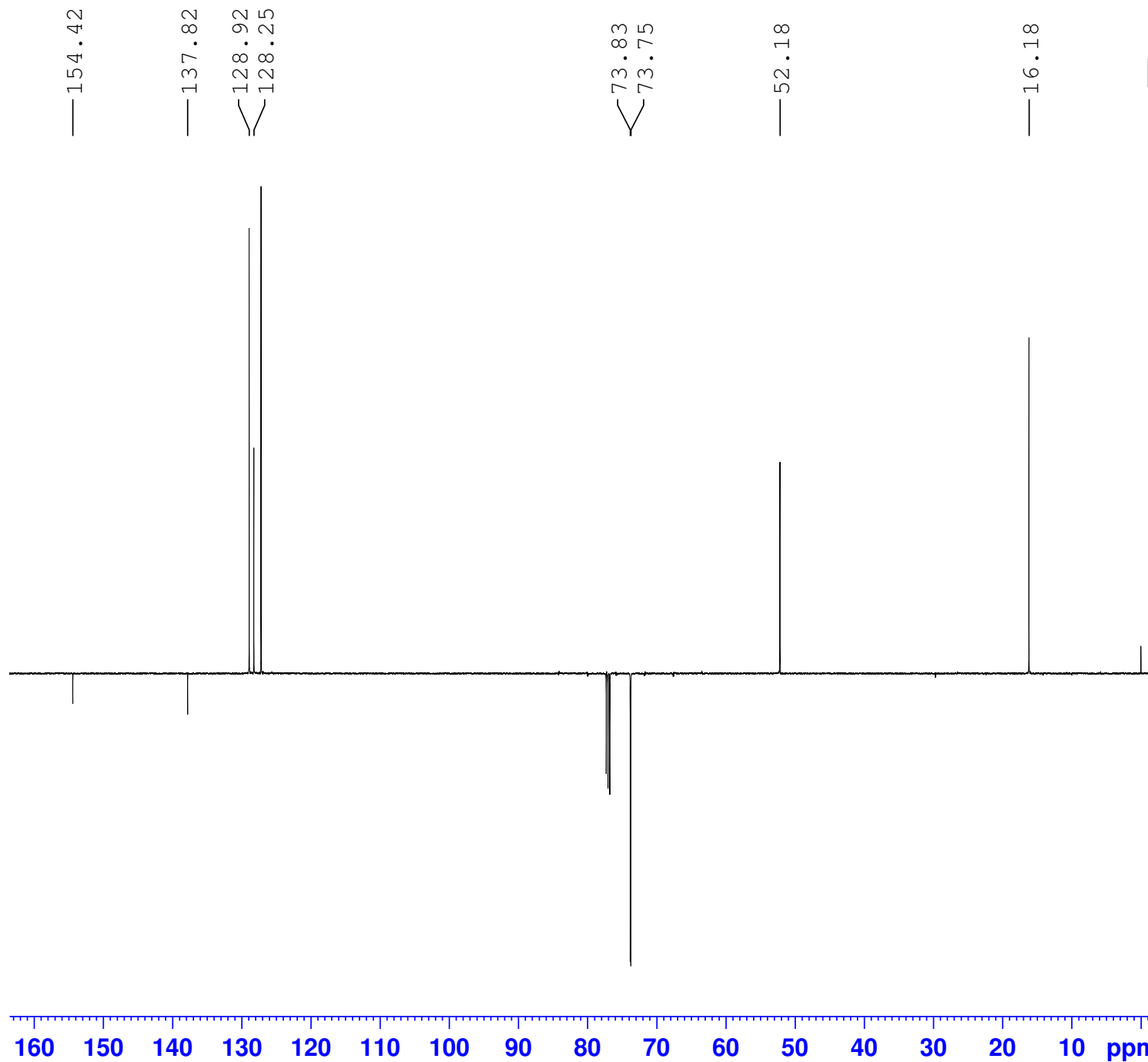
Current Data Parameters
 NAME S-25
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170622
 Time 10.51 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 95.16
 DW 50.000 usec
 DE 6.50 usec
 TE 291.3 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1830886 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 18.10400009 W

F2 - Processing parameters
 SI 65536
 SF 500.180074 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



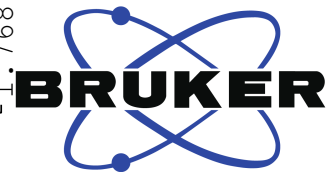
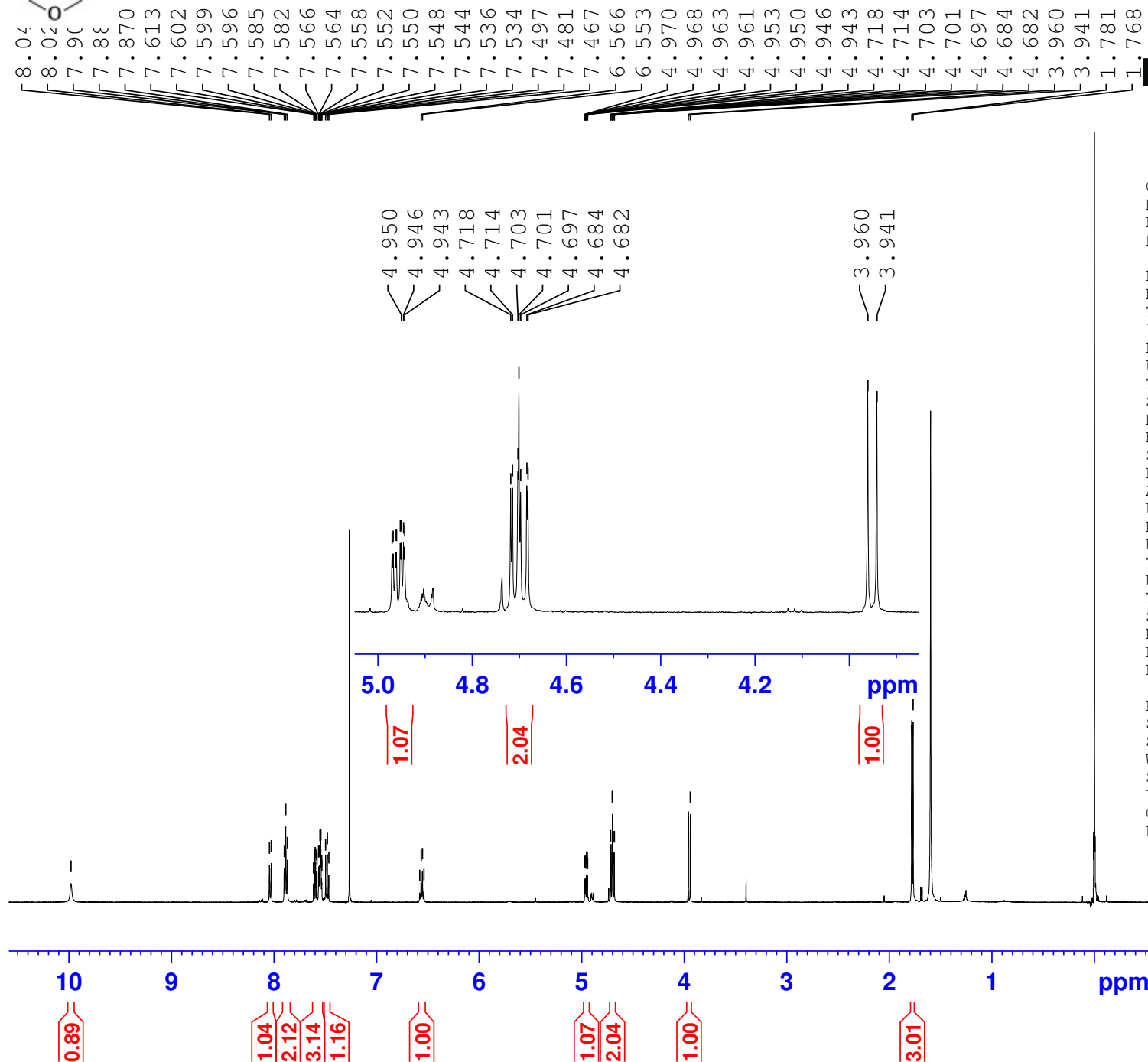
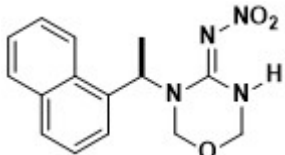
¹H NMR (500 MHz, CDCl₃) of S-25



Current Data Parameters
NAME S-25
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170622
Time 14.35 h
INSTRUM spect
PROBHD z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT CDCl3
NS 4097
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 291.7 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.00 usec
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28680280 W

F2 - Processing parameters
SI 32768
SF 125.7703641 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

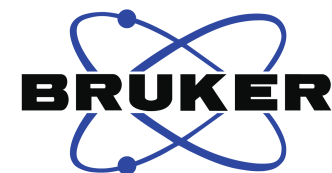
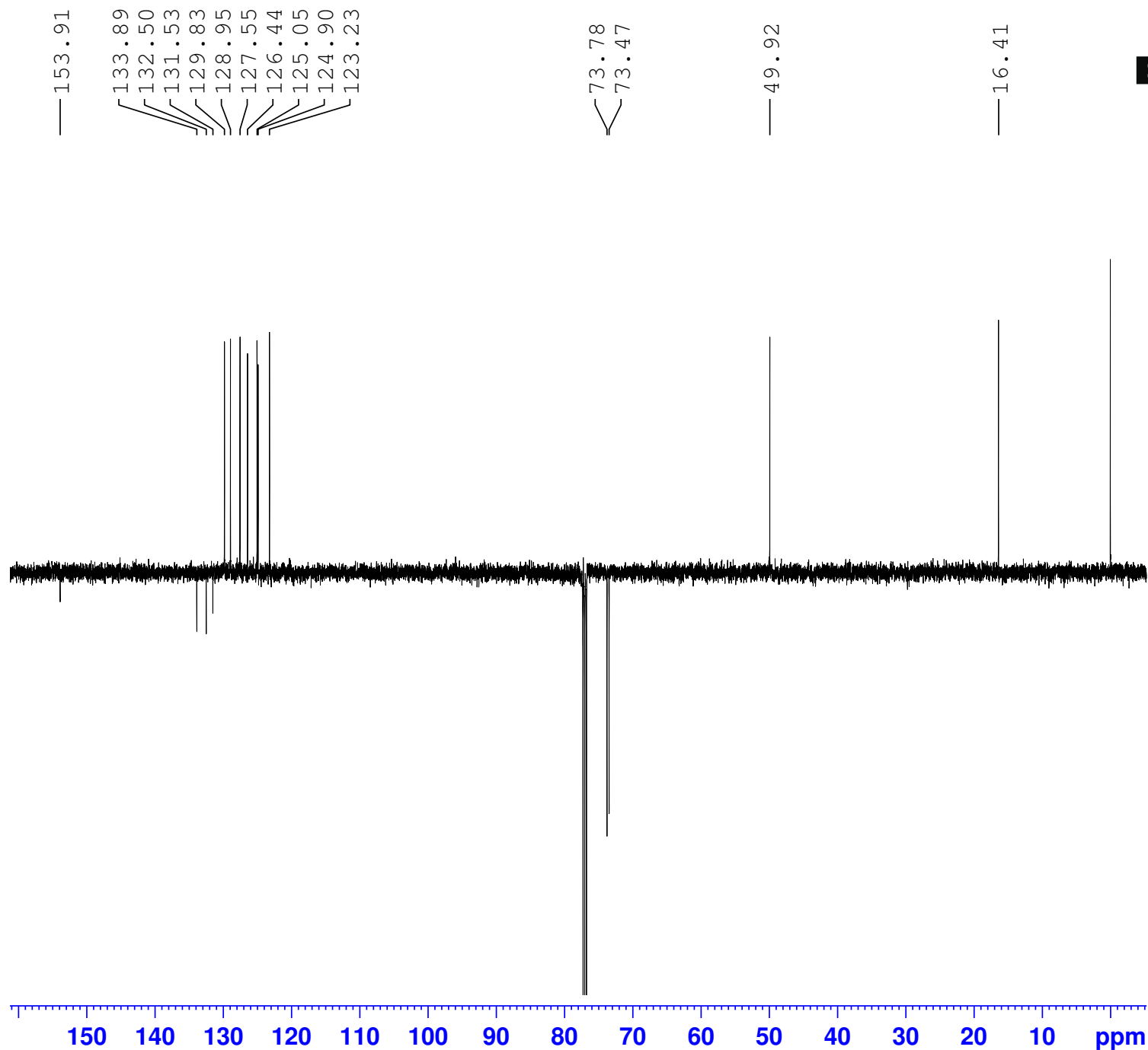


Current Data Parameters
 NAME R-26
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170825
 Time 13.02 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 139.09
 DW 50.000 usec
 DE 6.50 usec
 TE 291.2 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1830886 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 18.10400009 W

F2 - Processing parameters
 SI 65536
 SF 500.1800098 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H NMR (500 MHz, CDCl₃) of **R-26**

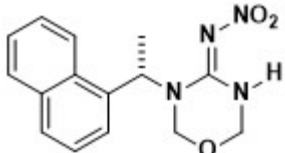


Current Data Parameters
 NAME R-26
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170825
 Time 14.23 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG deptq135
 TD 65536
 SOLVENT CDCl3
 NS 1479
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 291.6 K
 CNST2 145.000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 P2 20.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.00 usec
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28680280 W

F2 - Processing parameters
 SI 32768
 SF 125.7703610 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 52 1.40

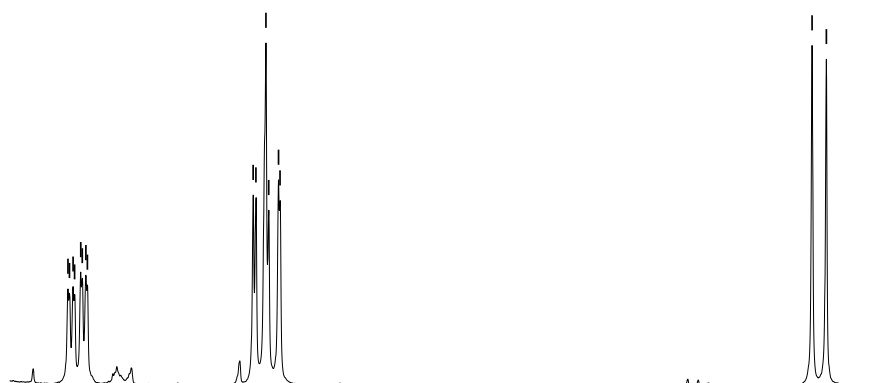
^{13}C (DEPTQ135) NMR (125 MHz, CDCl_3) of **R-26**



9.98
8.04
8.03
7.90
7.886
7.870
7.615
7.613
7.602
7.599
7.596
7.585
7.582
7.566
7.564
7.558
7.550
7.547
7.544
7.536
7.534
7.497
7.481
7.466
6.568
6.554
4.969
4.967
4.962
4.960
4.952
4.950
4.945
4.943
4.718
4.714
4.701
4.697
4.684
4.682
3.961
3.942
1.782
1.768

4.960
4.952
4.950
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4.701
4.697
4.684
4.682

3.961
3.942

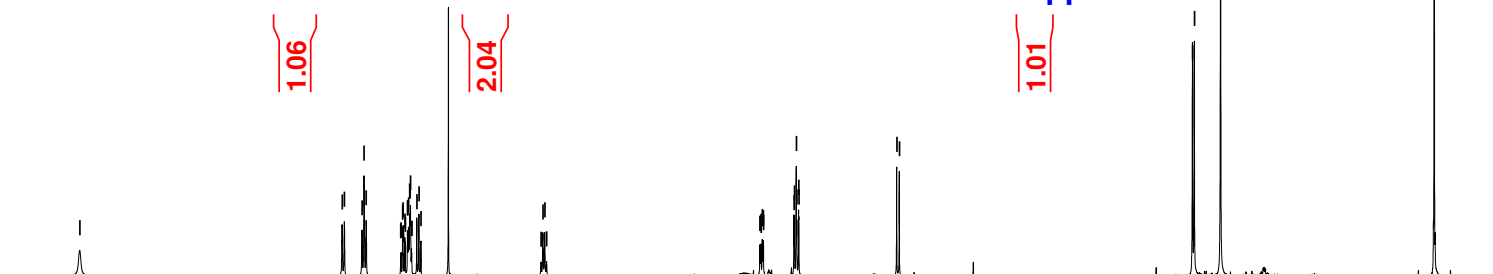


5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 ppm

1.06

2.04

1.01



10 9 8 7 6 5 4 3 2 1 ppm

0.86

1.00

1.95

0.98

2.01

1.01

1.00

1.06

2.04

1.01

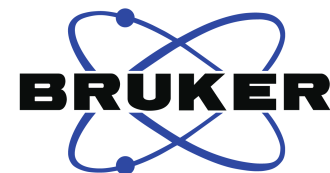
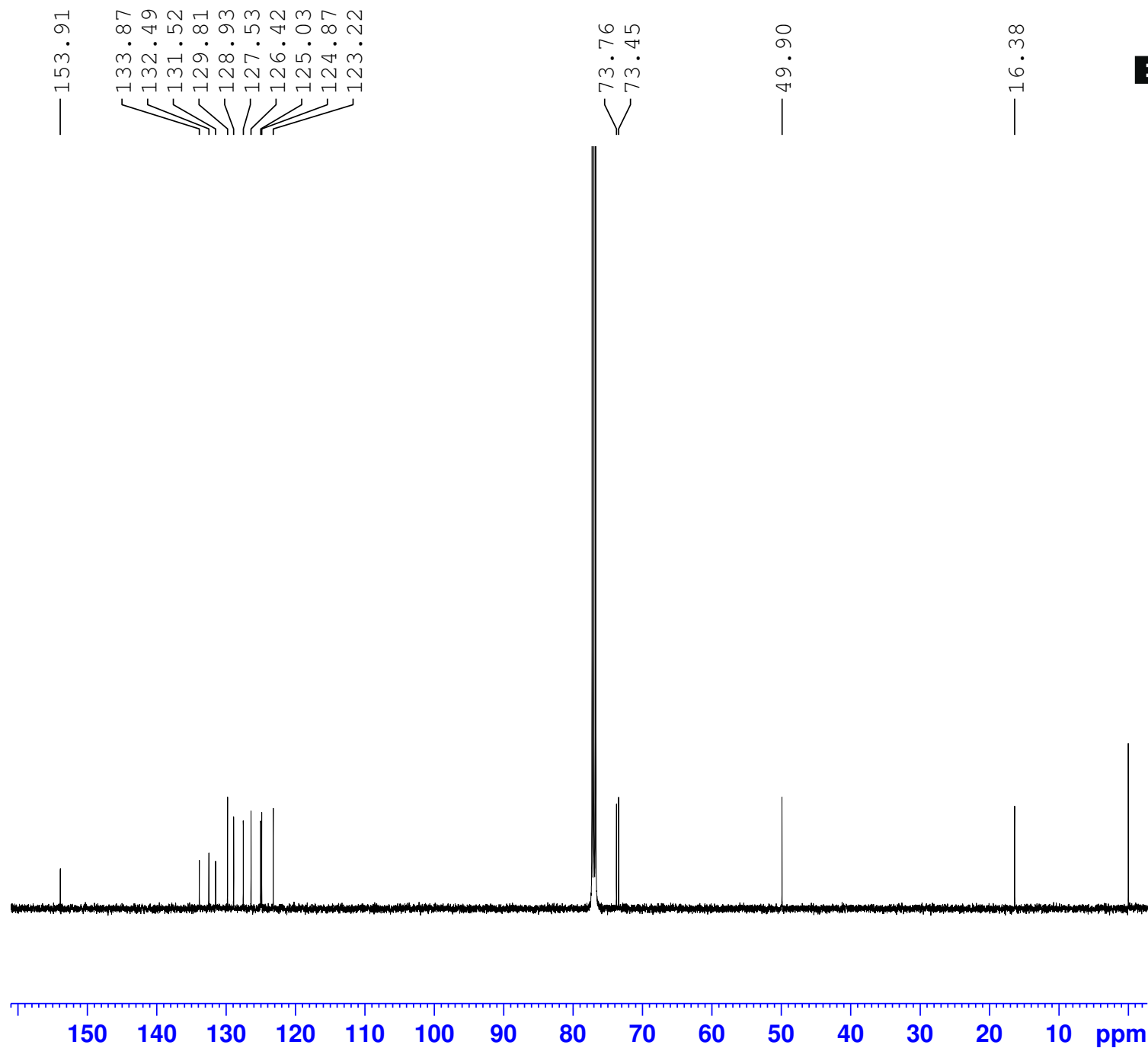
3.00



Current Data Parameters
NAME 1H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170826
Time 20.01 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 192.72
DW 50.000 usec
DE 6.50 usec
TE 292.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P1 10.00 usec
PLW1 18.10400009 W

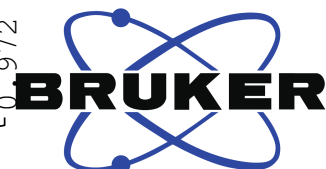
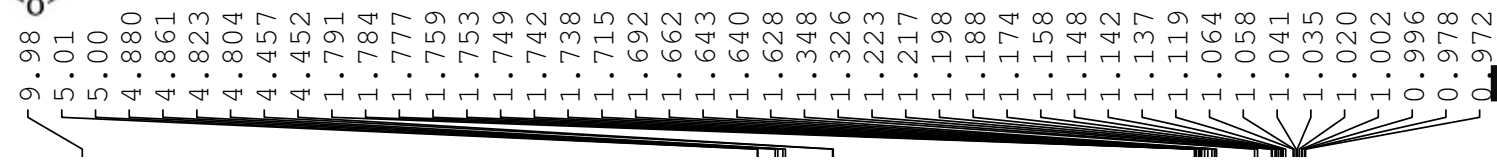
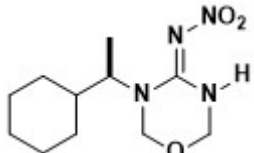
F2 - Processing parameters
SI 65536
SF 500.1800101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170826
Time 19.59 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5120
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 292.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28680280 W
PLW13 0.14374560 W

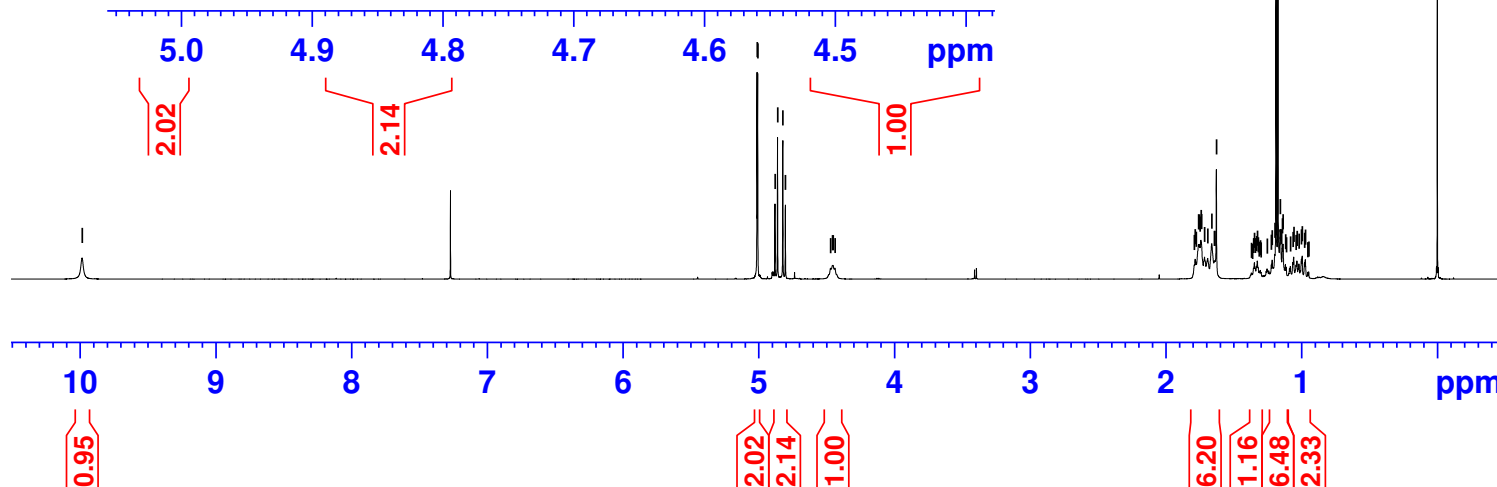
F2 - Processing parameters
SI 32768
SF 125.7703632 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
 NAME 1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181101
 Time 11.56 h
 INSTRUM spect
 PROBHD z119470_0187 (
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 5
 DS 1
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.276799 sec
 RG 95.16
 DW 50.000 usec
 DE 6.50 usec
 TE 292.1 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1830886 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 18.10400009 W

F2 - Processing parameters
 SI 65536
 SF 500.1800069 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



¹H NMR (500 MHz, CDCl₃) of **R-28**

—154.91

<73.73
<73.33

—55.52

—40.84

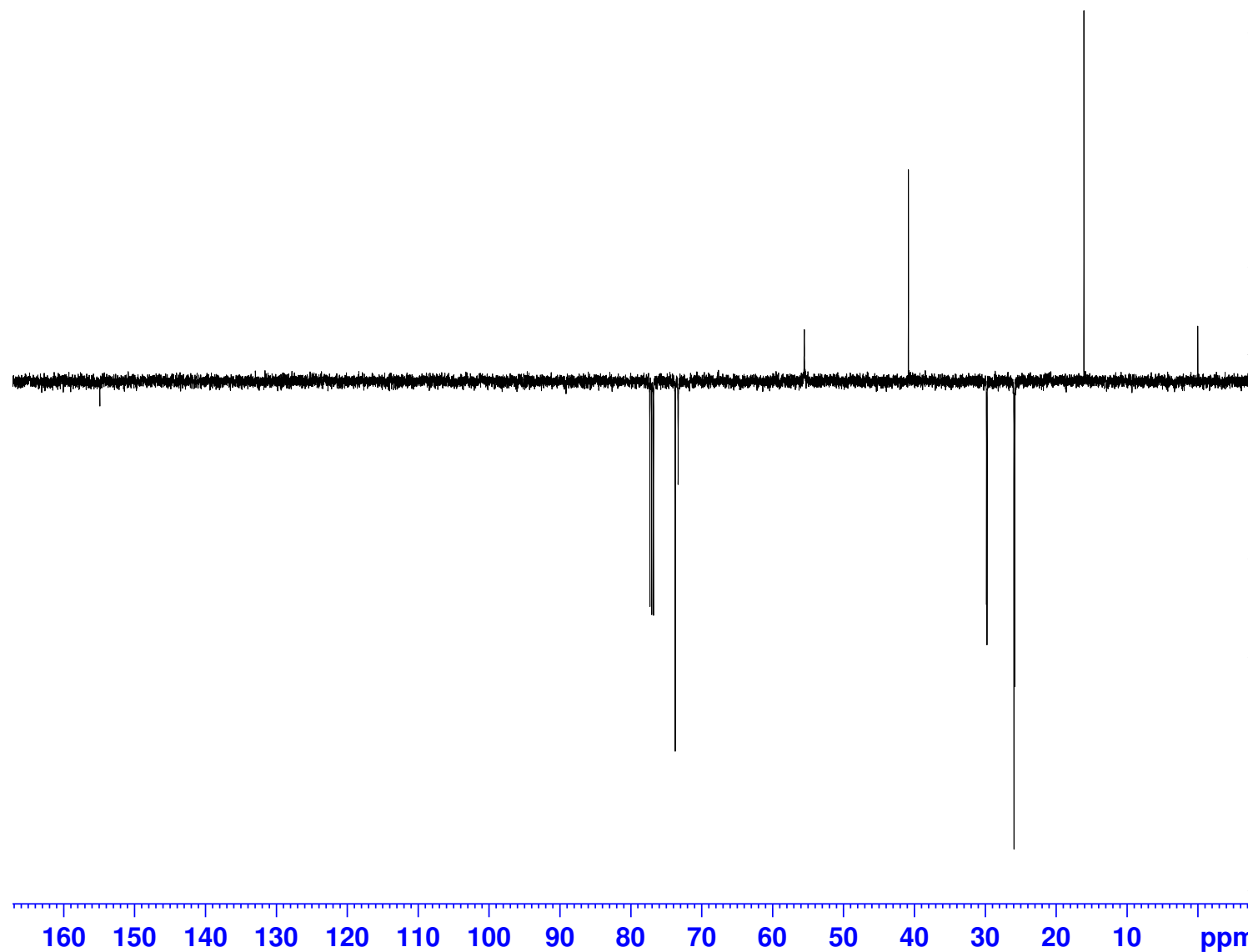
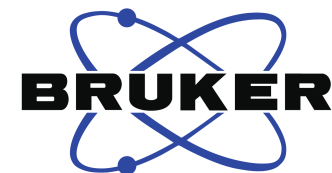
<29.82

<29.75

<25.94

<25.82

—16.08

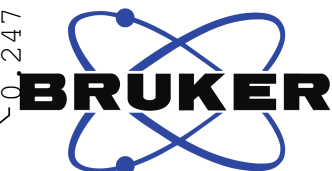
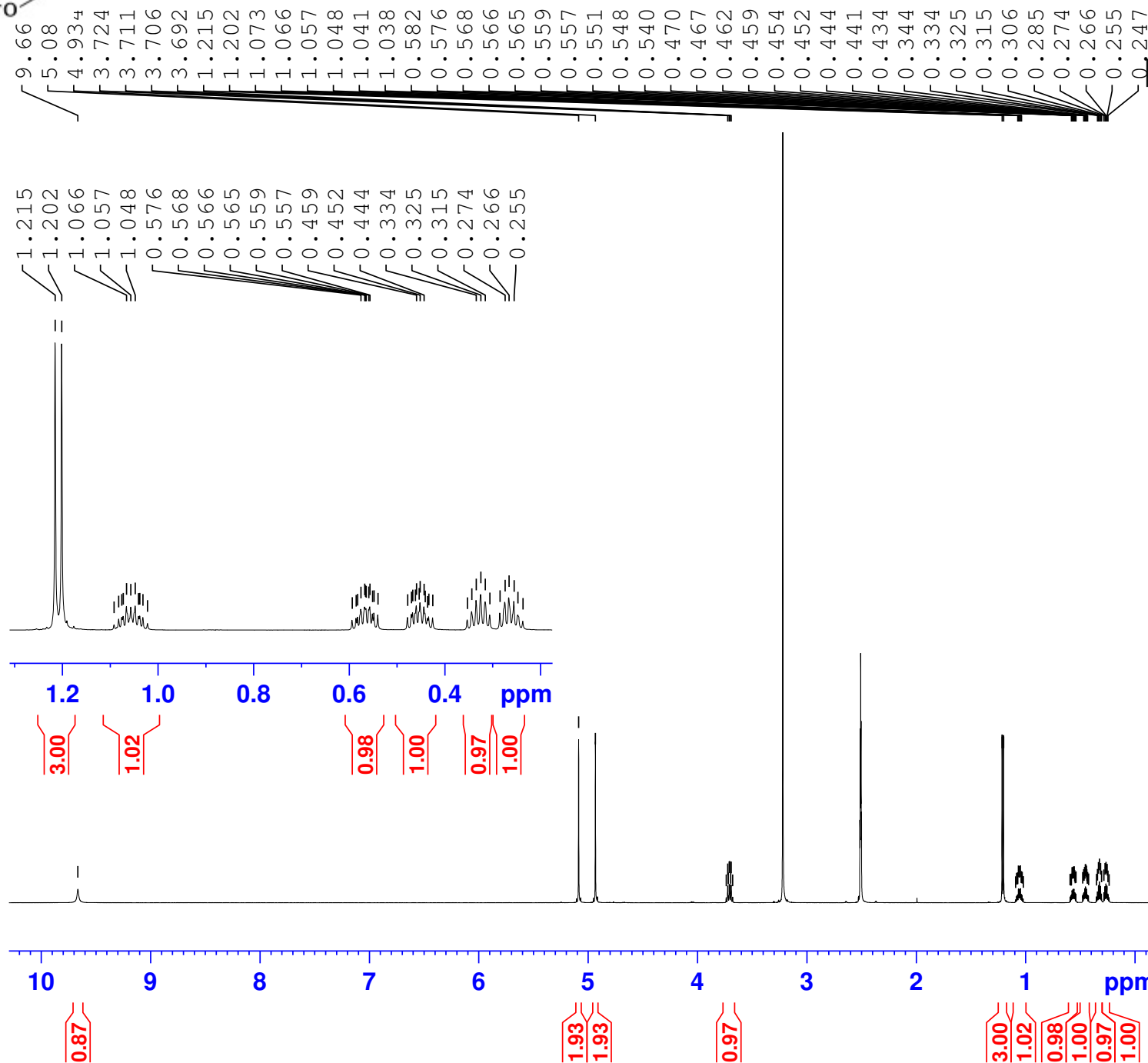
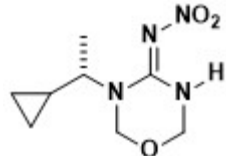


Current Data Parameters
NAME 13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181101
Time 12.07 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT CDCl3
NS 146
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
RW 16.800 usec
DE 6.50 usec
TE 292.5 K
CNST2 145.000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.00 usec
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28288001 W

F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 5640

^{13}C (DEPTQ135) NMR (125 MHz, CDCl_3) of **R-28**

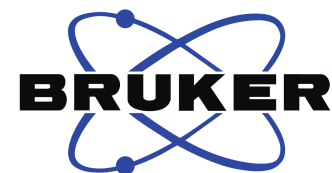
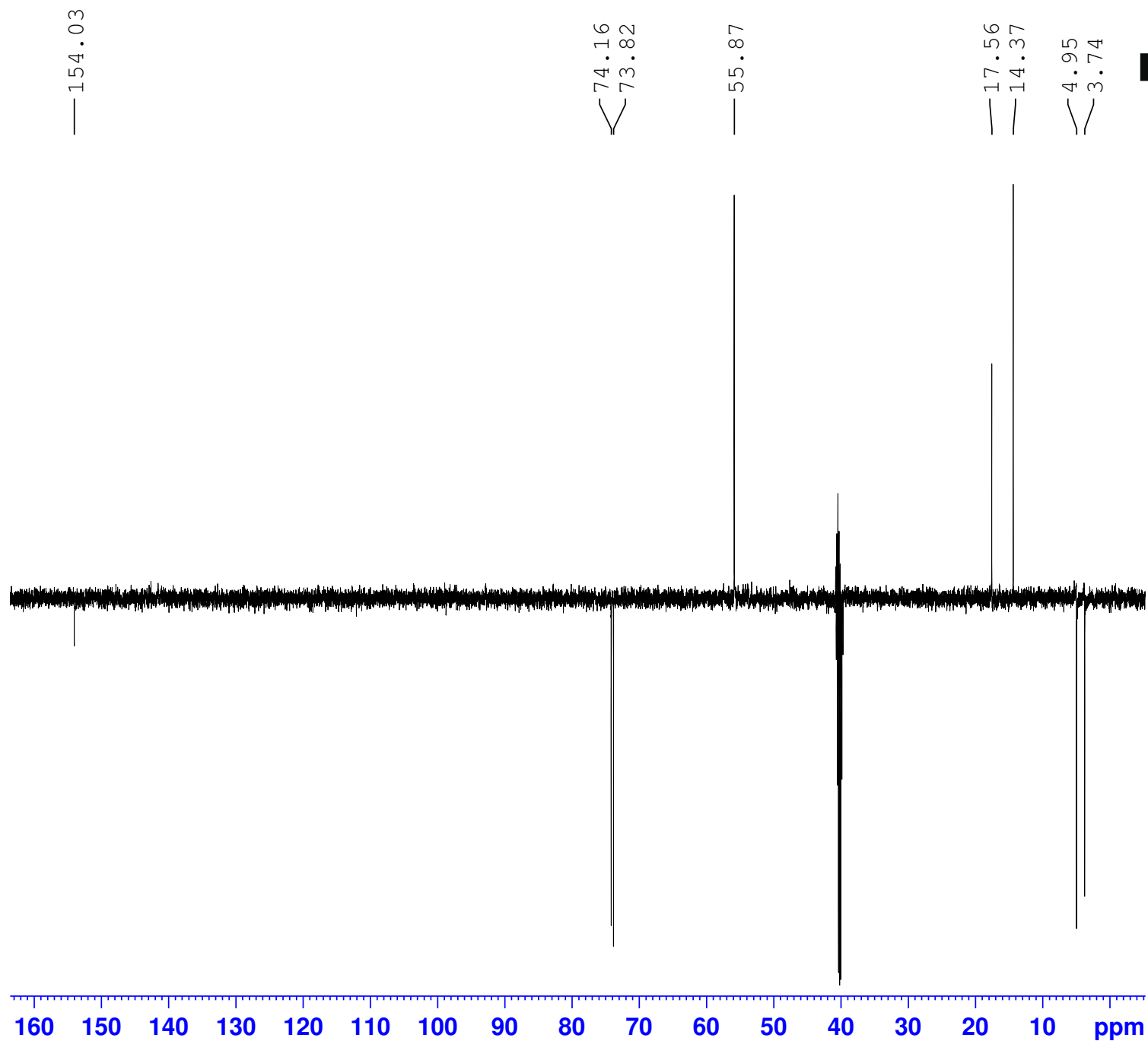


Current Data Parameters
NAME S-29
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180920
Time 11.21 h
INSTRUM spect
PROBHD z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 5
DS 1
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.276799 sec
RG 108.3
DW 50.000 usec
DE 6.50 usec
TE 323.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

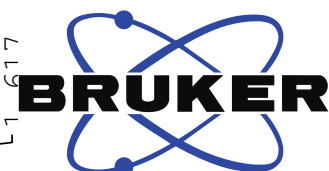
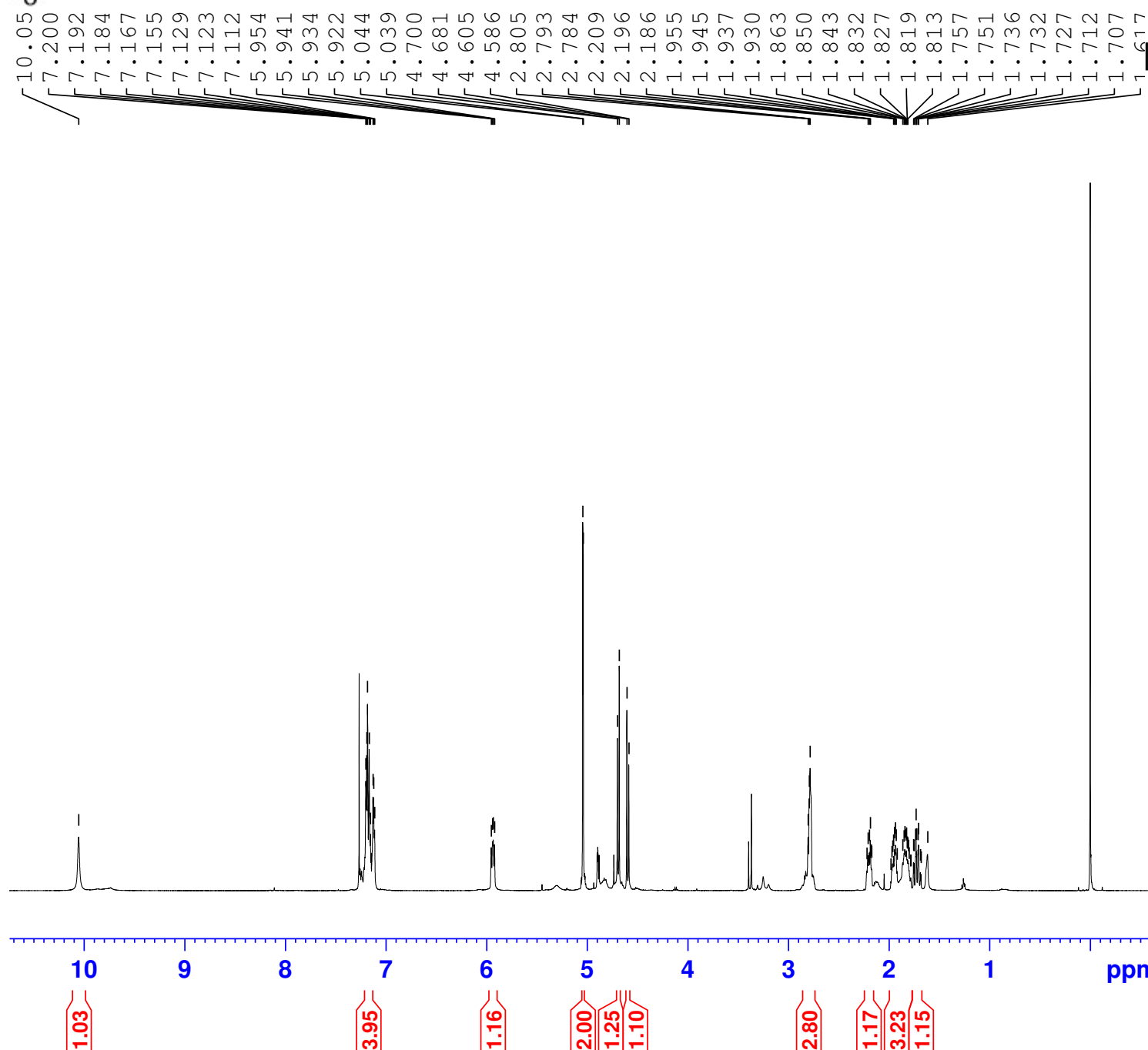
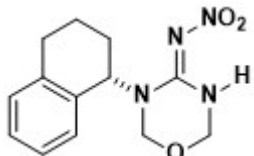
¹H NMR (500 MHz, DMSO-d₆, 50°C) of S-29



Current Data Parameters
 NAME S-29
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180920
 Time 11.32 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG deptq135
 TD 65536
 SOLVENT DMSO
 NS 185
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 323.2 K
 CNST2 145.000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 P2 20.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.00 usec
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28288001 W

F2 - Processing parameters
 SI 32768
 SF 125.7703610 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

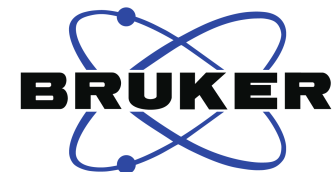
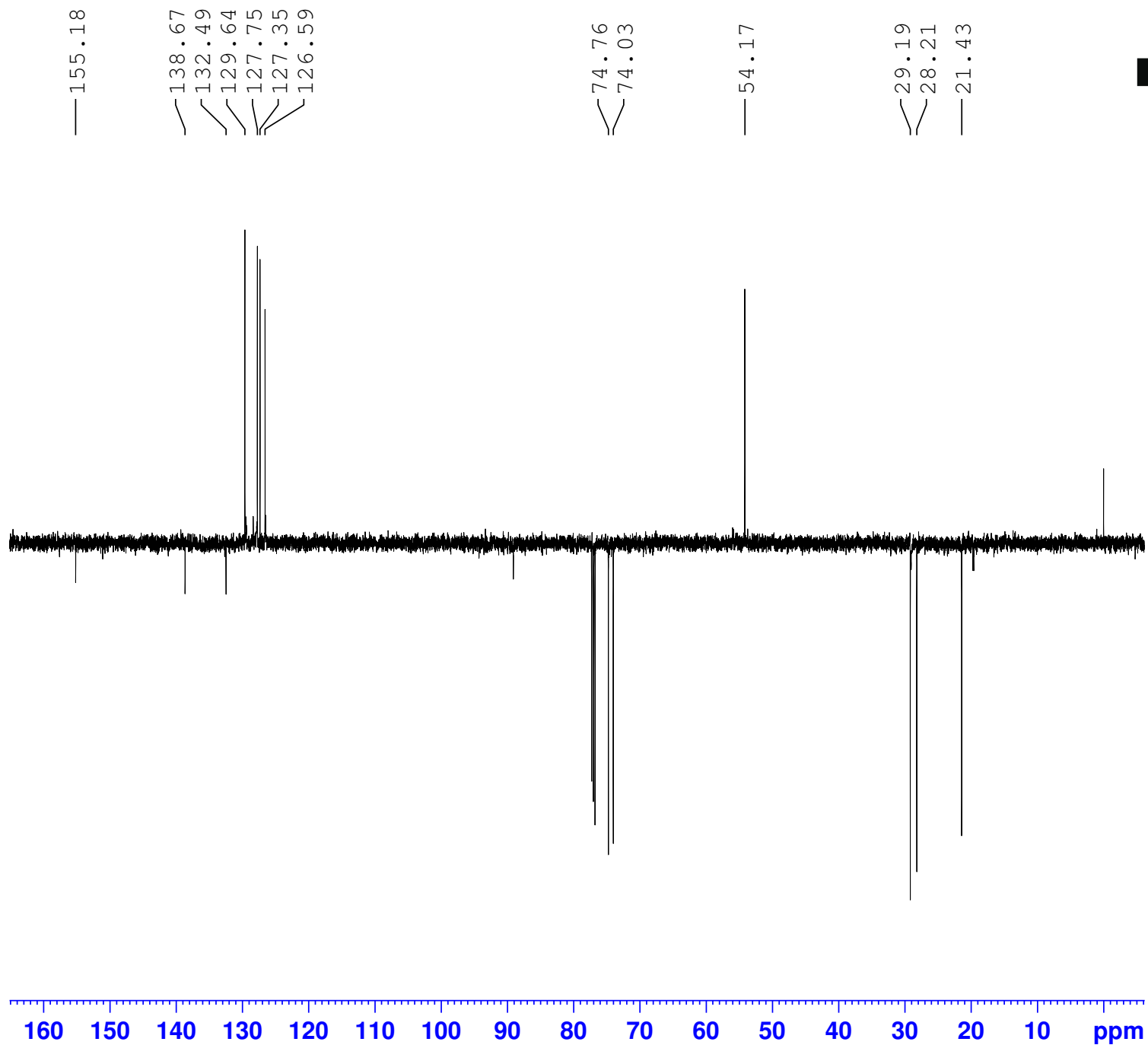


Current Data Parameters
NAME S-30
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180829
Time 17.18 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 10
DS 1
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 108.3
DW 50.000 usec
DE 6.50 usec
TE 291.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR (500 MHz, CDCl₃) of S-30

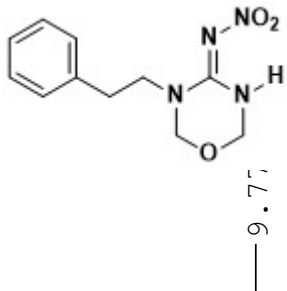


Current Data Parameters
 NAME S-30
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180829
 Time 17.29 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG deptq135
 TD 65536
 SOLVENT CDCl3
 NS 157
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 291.7 K
 CNST2 145.0000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 P2 20.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.00 usec
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28288001 W

F2 - Processing parameters
 SI 32768
 SF 125.7703642 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 60.40

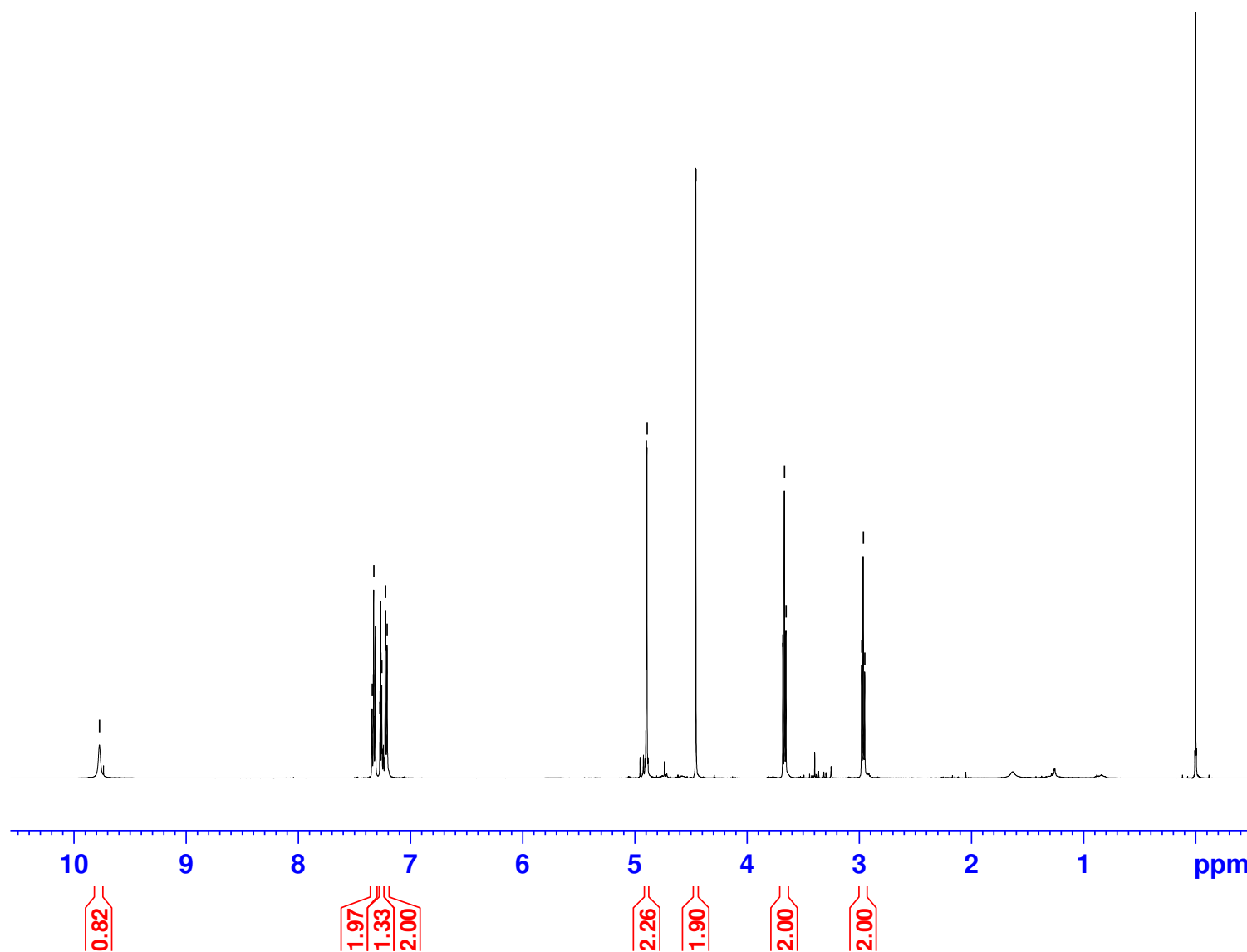
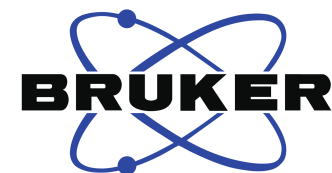
^{13}C (DEPTQ135) NMR (125 MHz, CDCl_3) of S-30



7.342
7.331
7.328
7.316
7.313
7.273
7.270
7.266
7.256
7.225
7.222
7.209

4.897
4.892
4.456

3.680
3.666
3.653
2.977
2.964
2.950

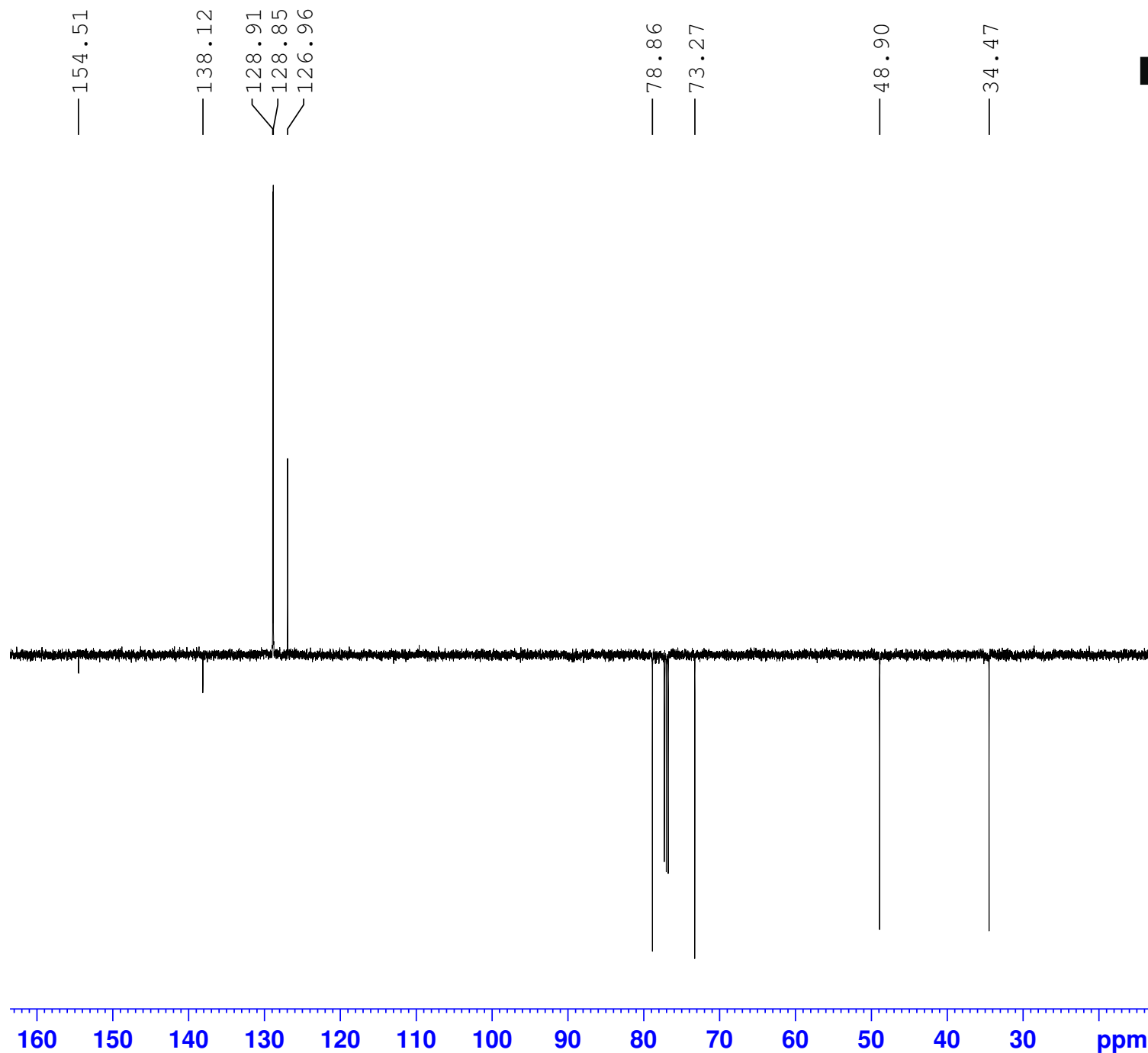


Current Data Parameters
NAME R-31
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180829
Time 17.35 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 139.09
DW 50.000 usec
DE 6.50 usec
TE 291.8 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

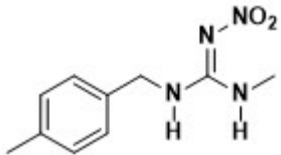
¹H NMR (500 MHz, CDCl₃) of **R-31**



Current Data Parameters
NAME R-31
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180829
Time 17.50 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT CDCl3
NS 256
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 292.3 K
CNST2 145.000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.00 usec
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28288001 W

F2 - Processing parameters
SI 32768
SF 125.7703641 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



— 9.174

— 7.791

7.197

7.181

7.161

7.146

— 4.380

— 2.842

— 2.282



Current Data Parameters
NAME 33
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181012
Time 18.21 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 1
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 77.78
DW 50.000 usec
DE 6.50 usec
TE 292.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



10 9 8 7 6 5 4 3 2 ppm

0.57

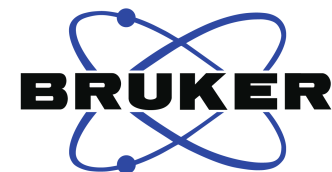
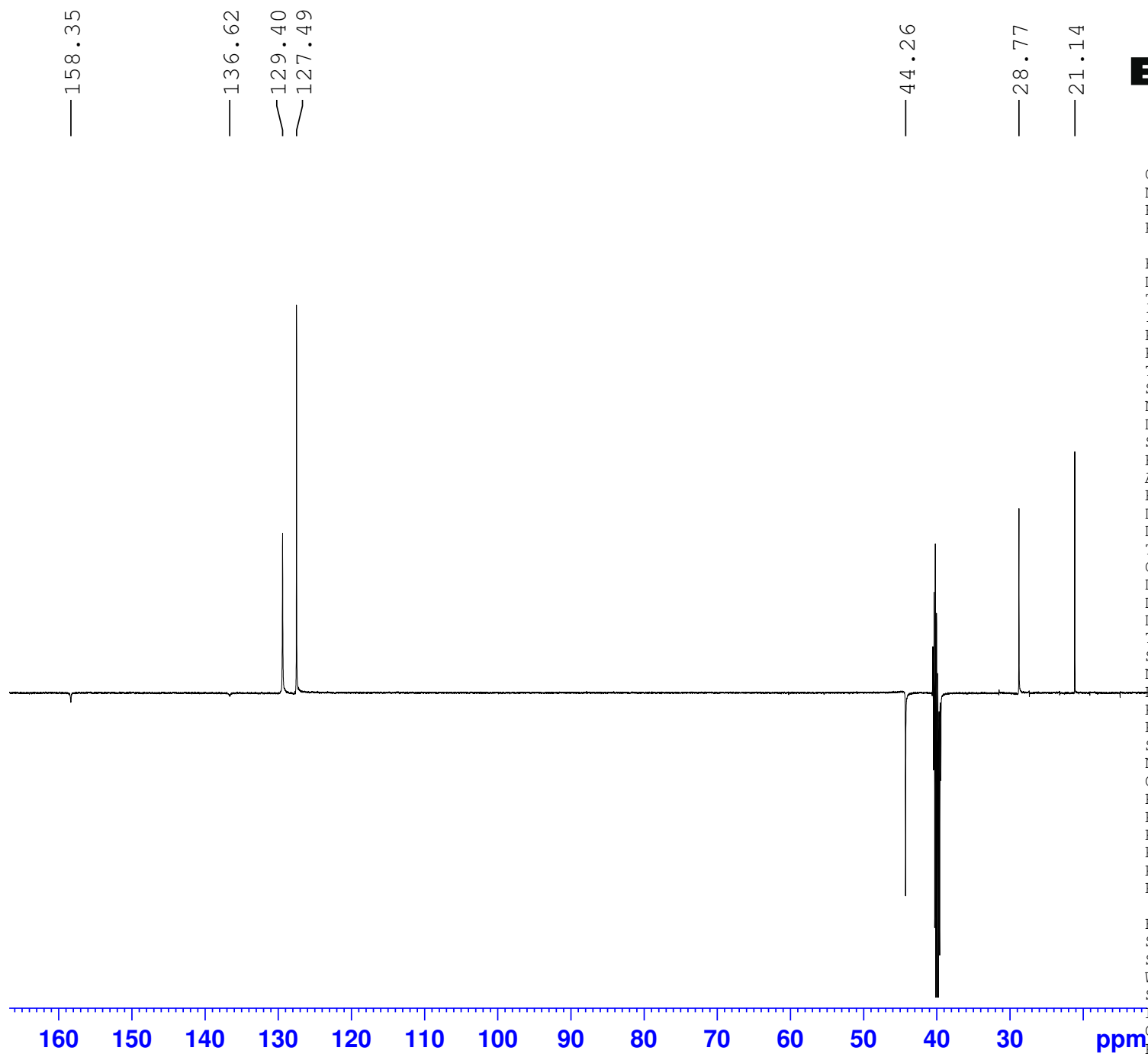
0.58

4.01

2.02

3.02

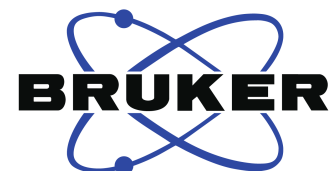
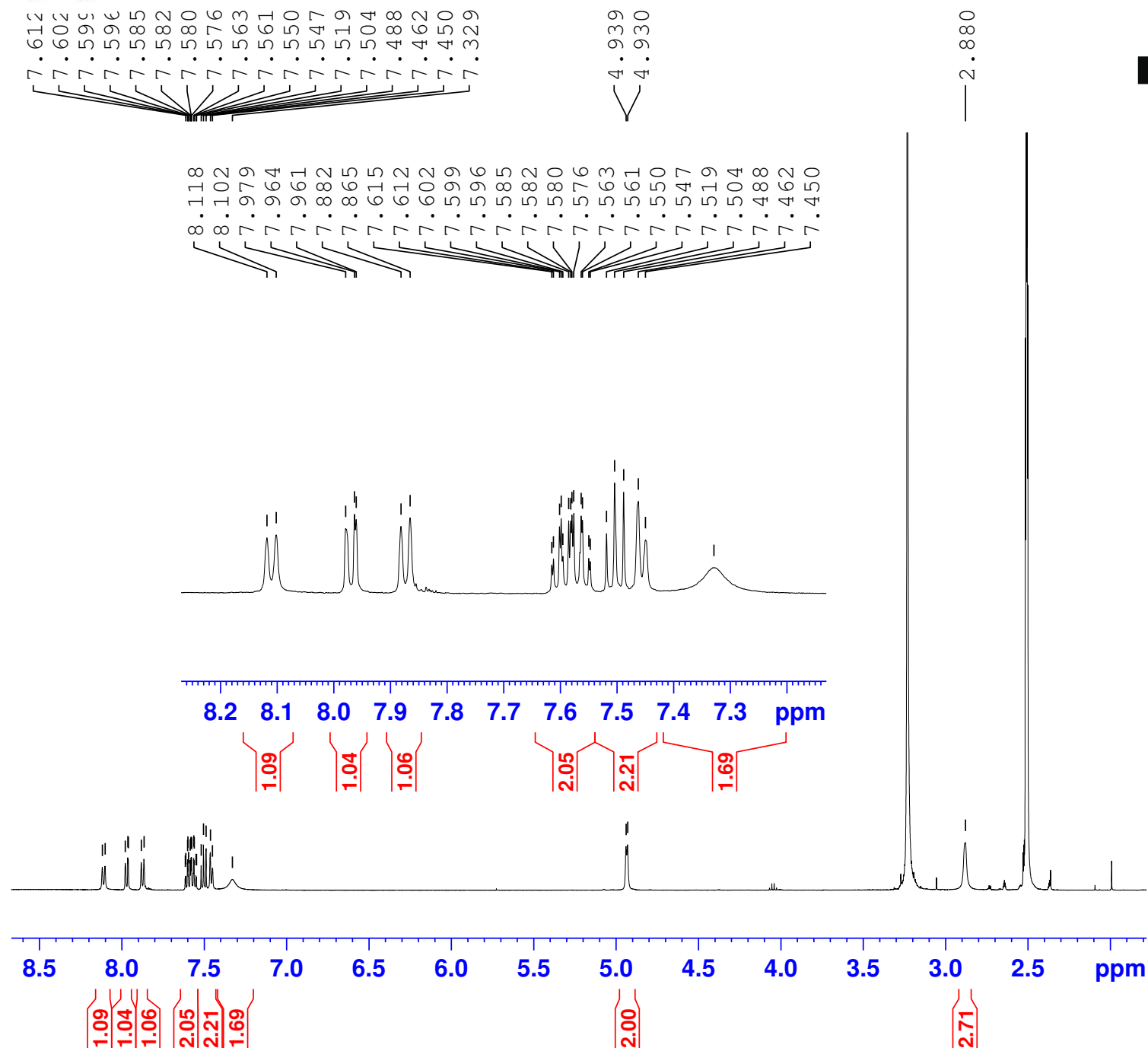
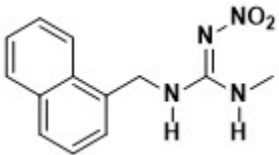
3.00



Current Data Parameters
 NAME 33
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181013
 Time 12.17 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG deptq135
 TD 65536
 SOLVENT DMSO
 NS 20480
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 292.1 K
 CNST2 145.0000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 P2 20.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.00 usec
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28288001 W

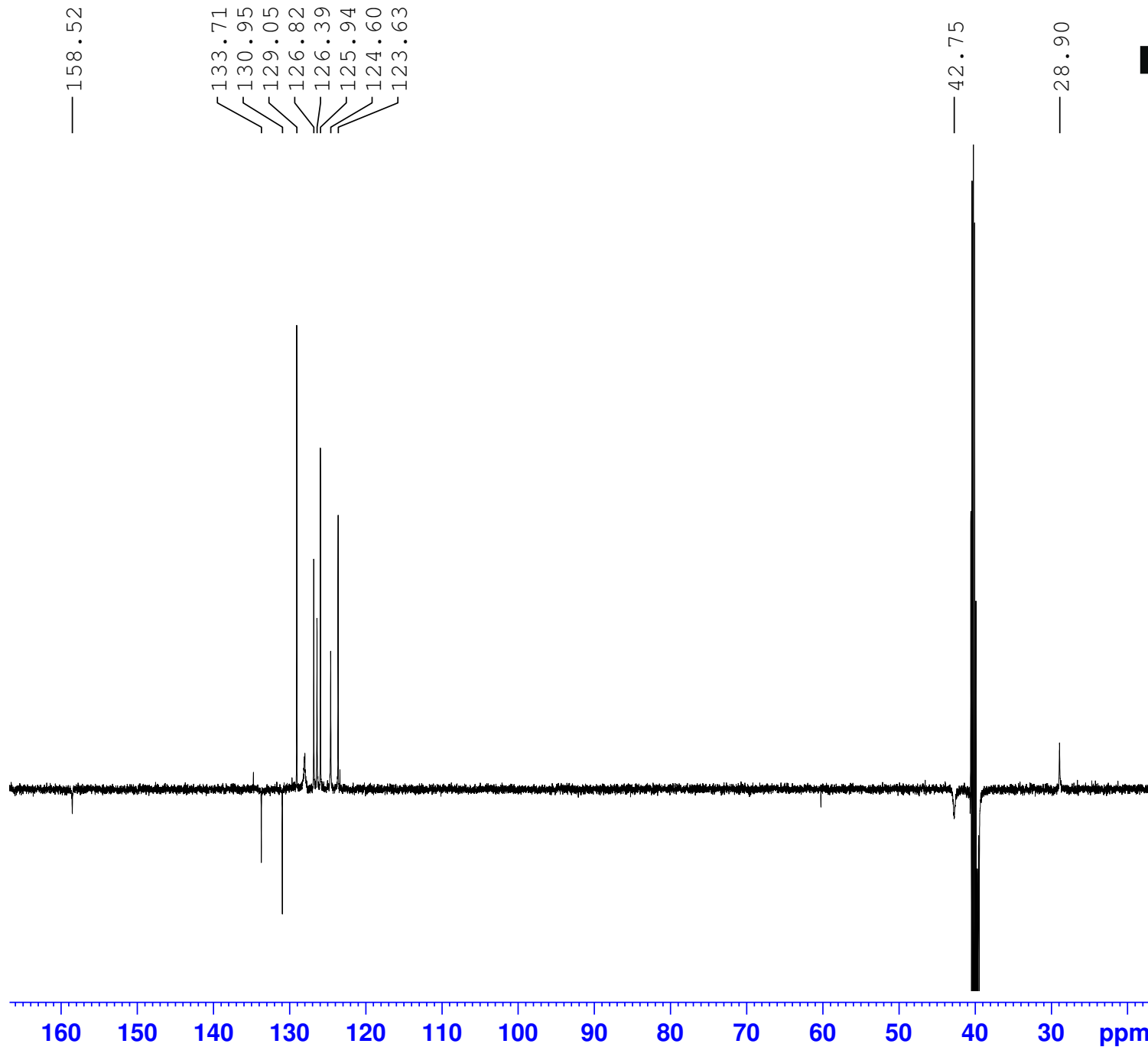
F2 - Processing parameters
 SI 32768
 SF 125.7703610 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME 34
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180904
 Time 17.08 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 139.09
 DW 50.000 usec
 DE 6.50 usec
 TE 323.3 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1830886 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 18.10400009 W

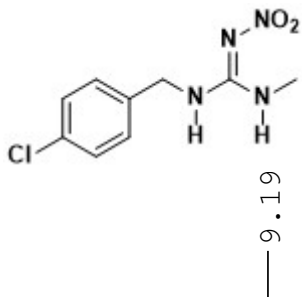
F2 - Processing parameters
 SI 65536
 SF 500.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME 34
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180905
Time 9.23 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT DMSO
NS 18519
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 297.9 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.00 usec
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28288001 W

F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



— 7.856
 — 7.417
 — 7.400
 — 7.330
 — 7.313

— 4.411

— 2.853



Current Data Parameters
 NAME 35
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180831
 Time 12.22 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 77.78
 DW 50.000 usec
 DE 6.50 usec
 TE 292.8 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1830886 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 18.10400009 W

F2 - Processing parameters
 SI 65536
 SF 500.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm

0.63

0.66

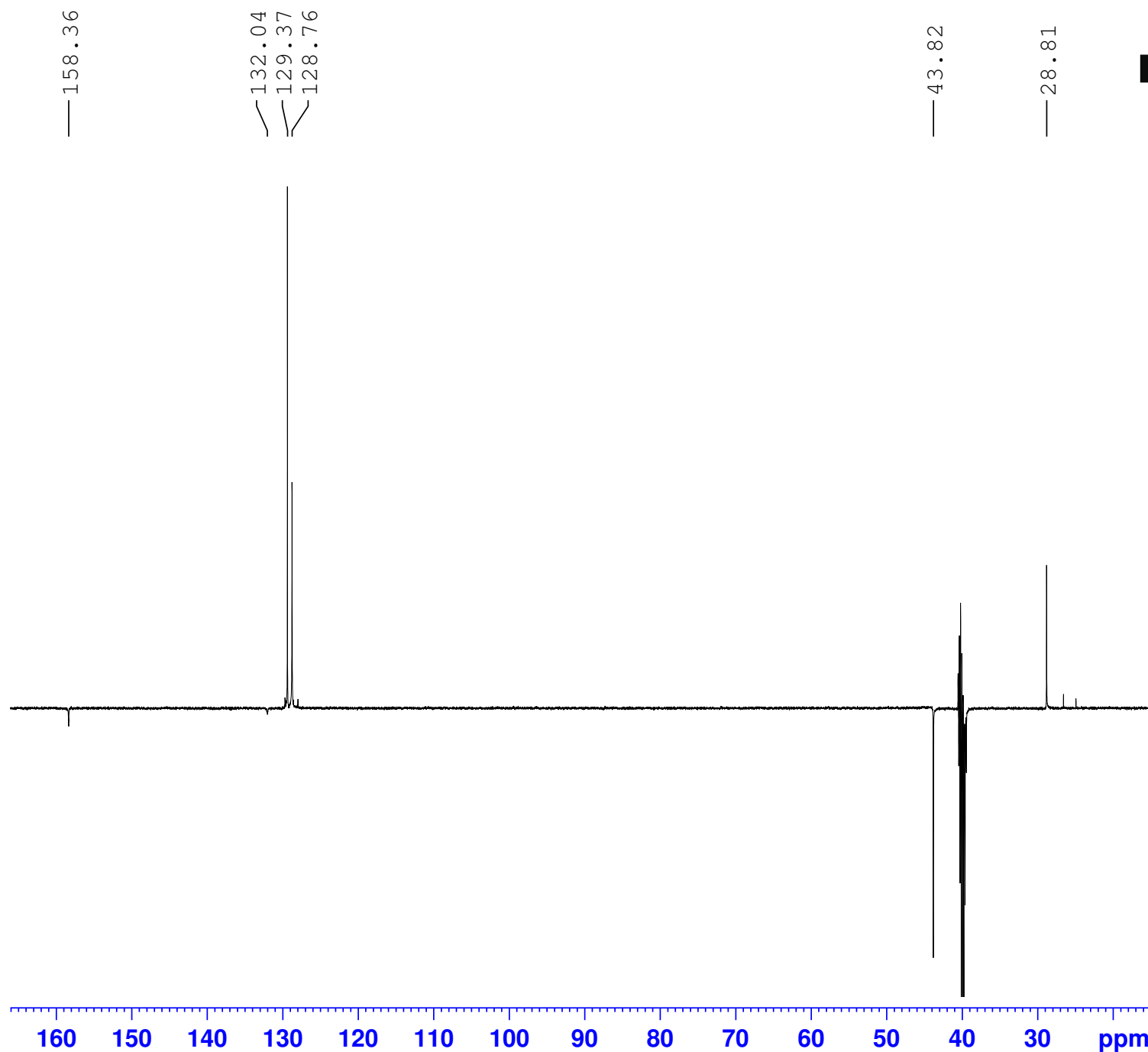
2.07

2.06

2.00

2.99

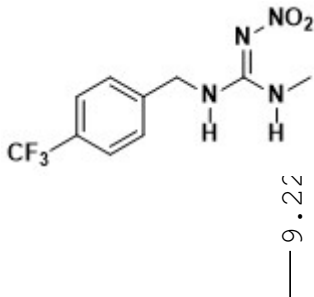
¹H NMR (500 MHz, DMSO-d₆) of **35**



Current Data Parameters
 NAME 35
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180831
 Time 18.49 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG deptq135
 TD 65536
 SOLVENT DMSO
 NS 6952
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 294.1 K
 CNST2 145.0000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 P2 20.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.00 usec
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28680280 W

F2 - Processing parameters
 SI 32768
 SF 125.7703610 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



7.890
7.726
7.710
7.517
7.501

— 4.513

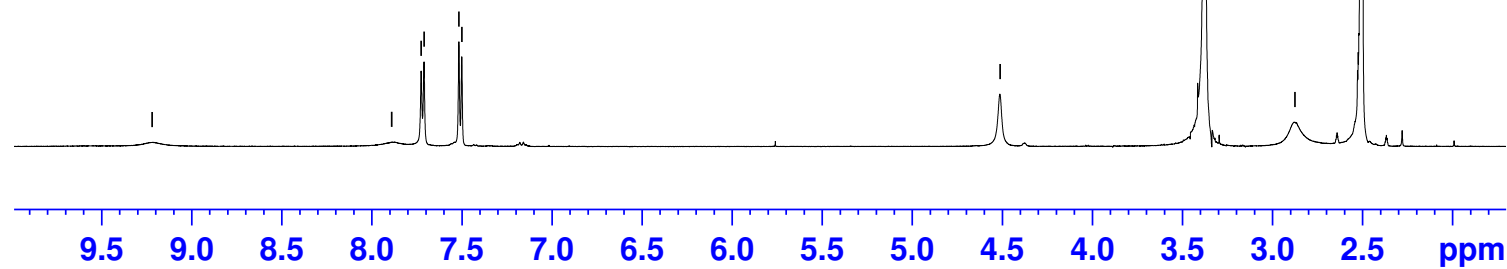
— 2.875



Current Data Parameters
NAME 36
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180928
Time 12.49 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 5
DS 1
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 108.3
DW 50.000 usec
DE 6.50 usec
TE 293.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



0.61

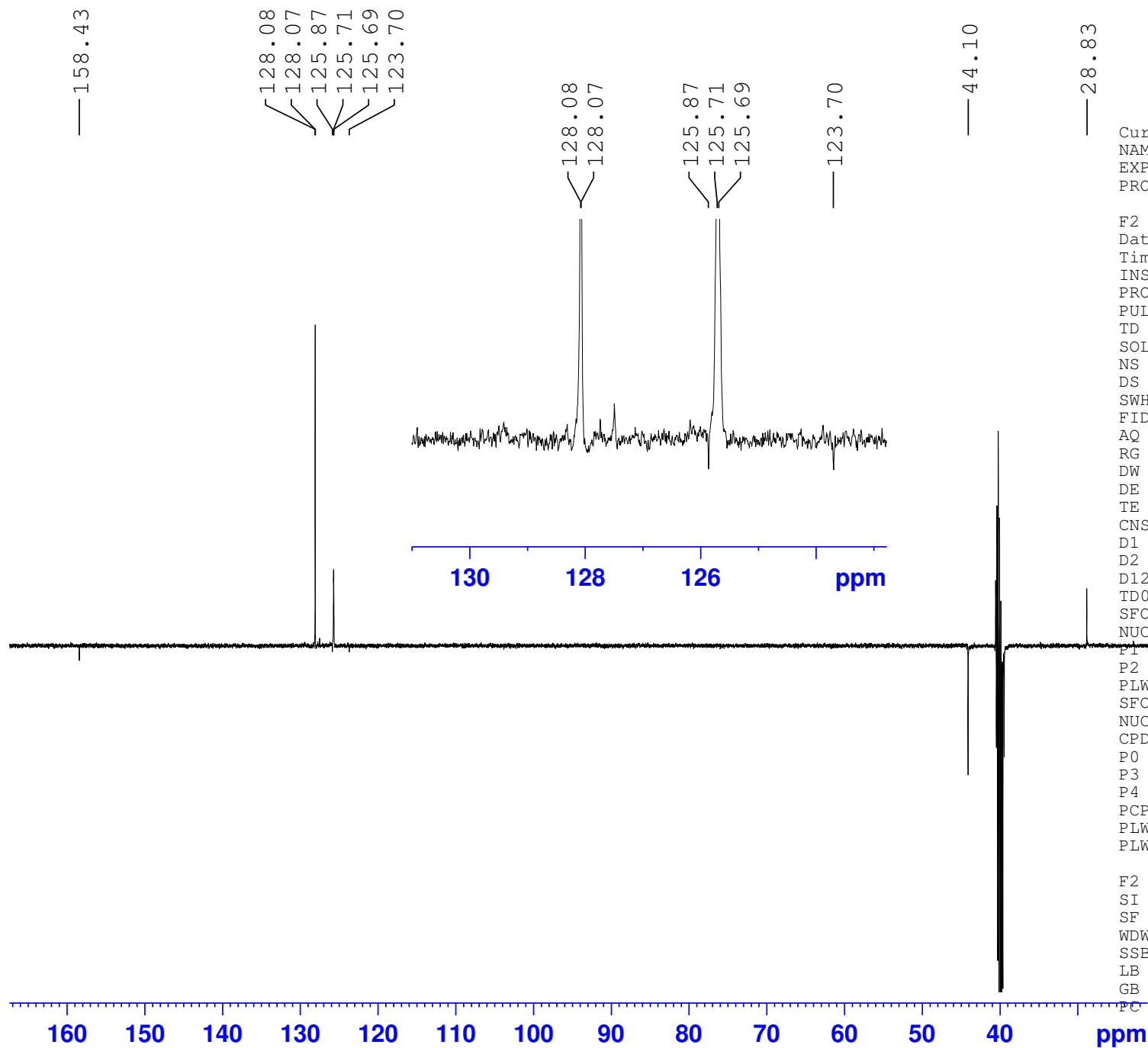
0.62

2.00

2.02

1.93

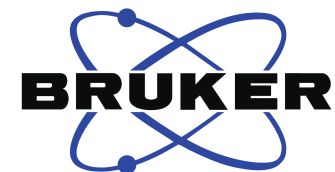
2.71



Current Data Parameters
NAME 36
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180928
Time 17.03 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT DMSO
NS 4764
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 293.4 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.00 usec
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28288001 W

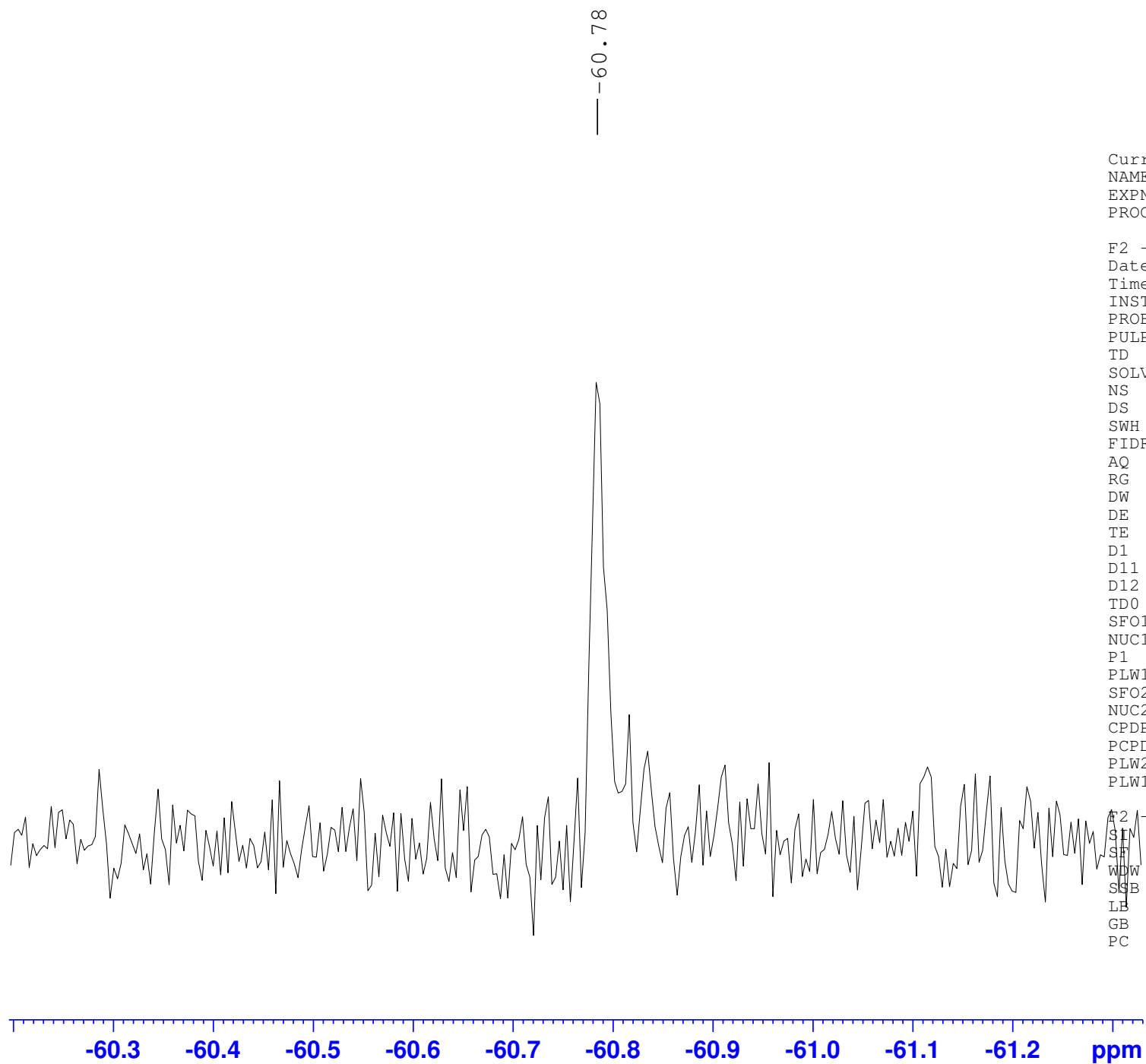
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



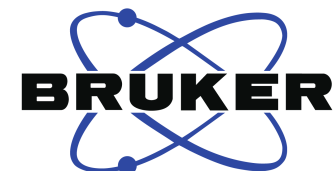
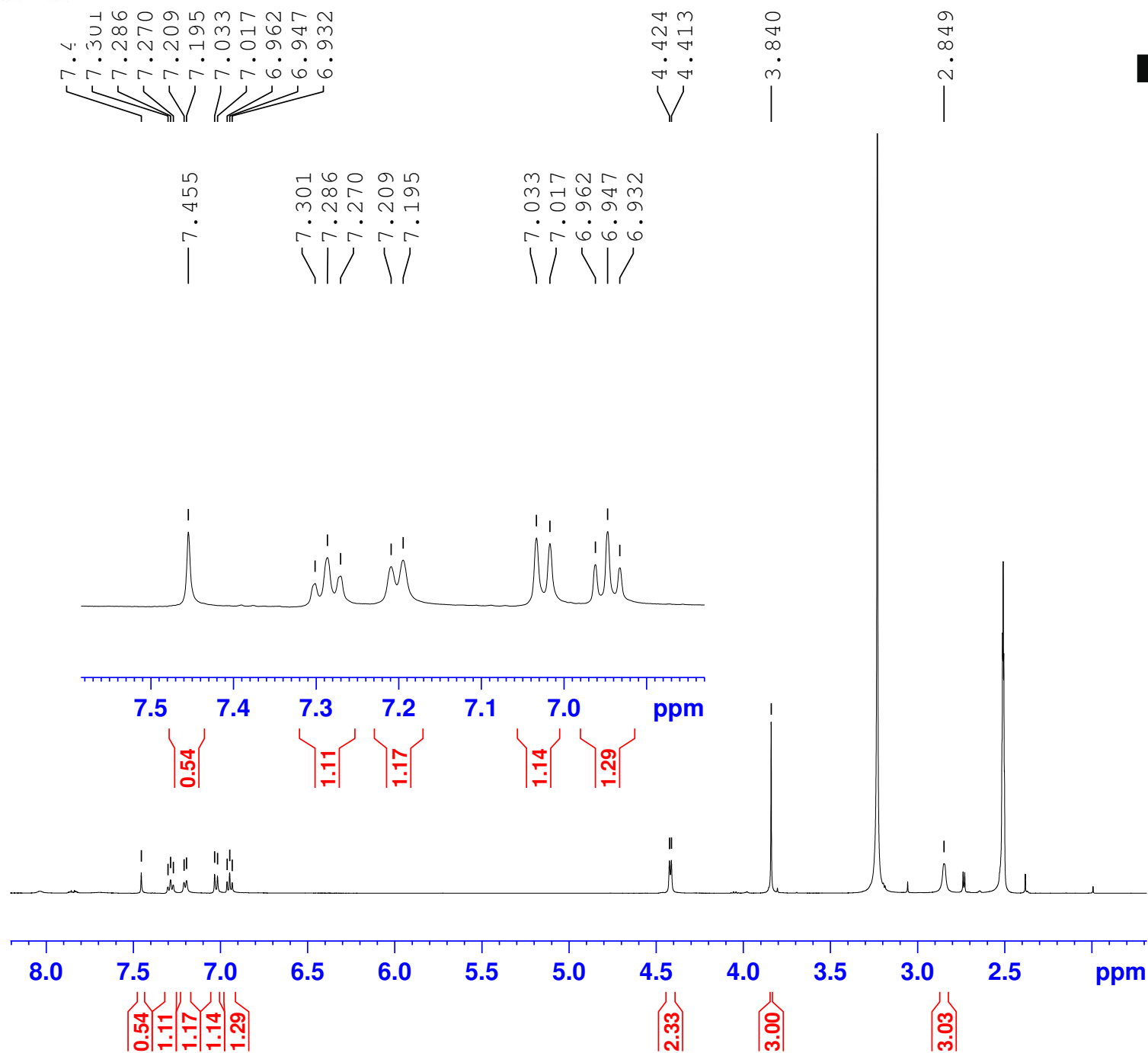
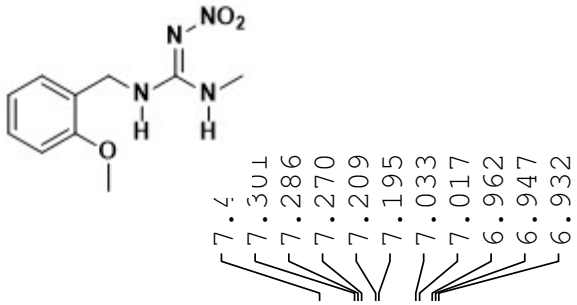
Current Data Parameters
NAME ARH-14
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190801
Time 14.40 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zgfhigqn.2
TD 131072
SOLVENT DMSO
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 1.733953 Hz
AQ 0.5767168 sec
RG 11.27
DW 4.400 usec
DE 6.50 usec
TE 293.4 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
SFO1 470.5923603 MHz
NUC1 19F
P1 16.00 usec
PLW1 36.93899918 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.31009001 W

F2 - Processing parameters
SI 65536
SF 470.6394242 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



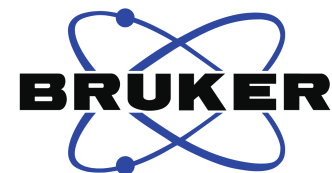
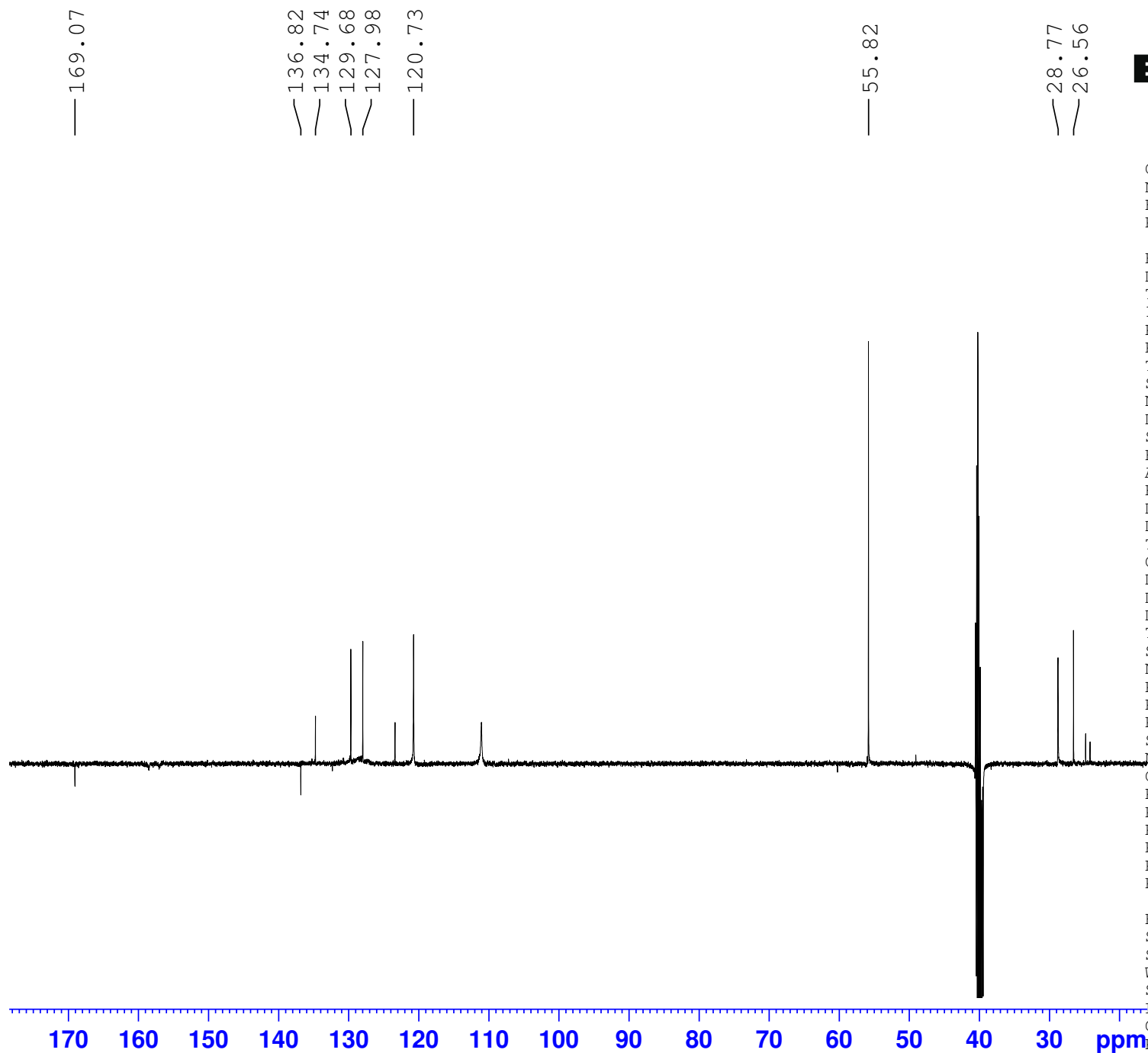
^{19}F NMR (470 MHz, DMSO-d_6) of **36**



Current Data Parameters
 NAME 37
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180829
 Time 18.09 h
 INSTRUM spect
 PROBHD z119470_0187 ()
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 139.09
 DW 50.000 usec
 DE 6.50 usec
 TE 323.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1830886 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 18.10400009 W

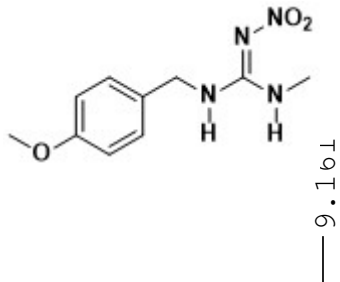
F2 - Processing parameters
 SI 65536
 SF 500.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 37
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180831
 Time 10.08 h
 INSTRUM spect
 PROBHD z119470_0187 (
 PULPROG deptq135
 TD 65536
 SOLVENT DMSO
 NS 16926
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 293.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 P2 20.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.00 usec
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28288001 W

F2 - Processing parameters
 SI 32768
 SF 125.7703610 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



— 7.768
 < 7.251
 < 7.235
 < 6.919
 < 6.902

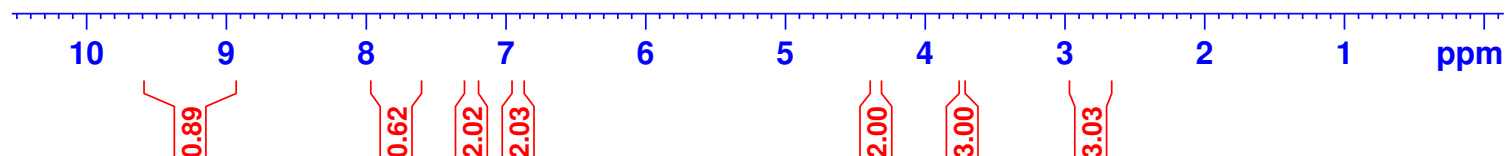
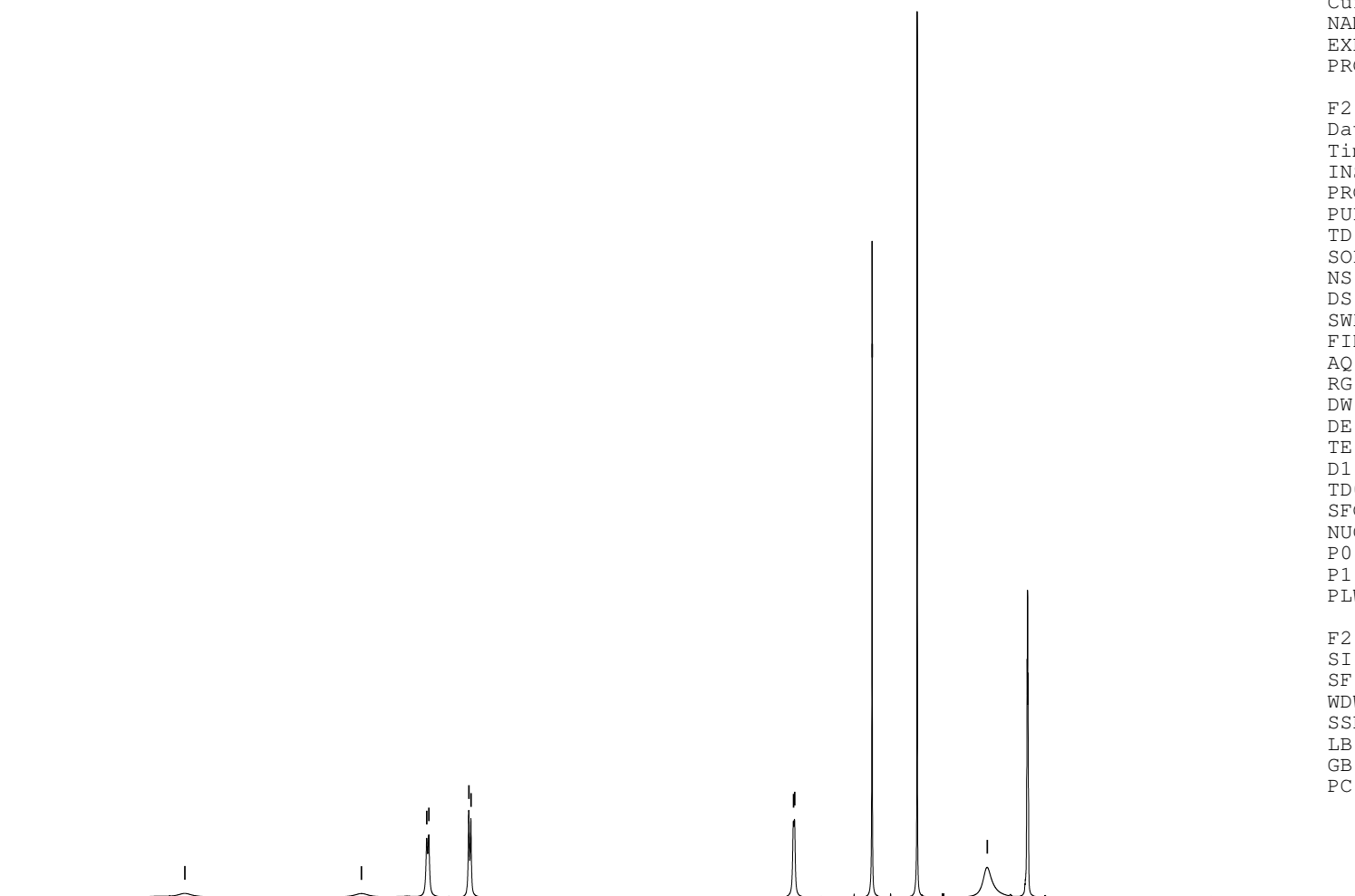
< 4.356
 < 4.347
 — 3.735
 — 2.826



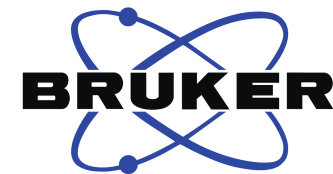
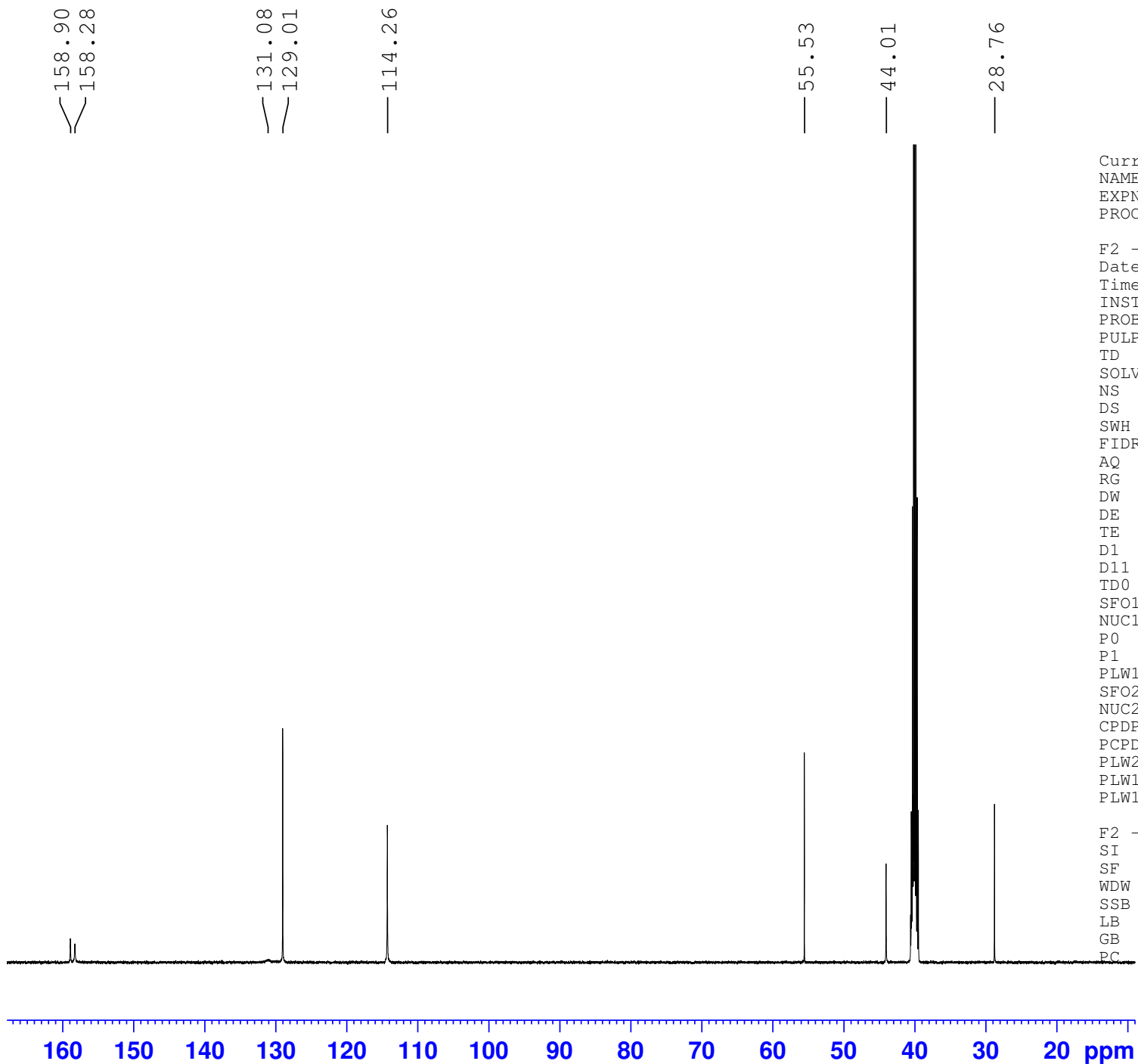
Current Data Parameters
 NAME 38
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181205
 Time 10.53 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 70.58
 DW 50.000 usec
 DE 6.50 usec
 TE 291.1 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1830886 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 18.10400009 W

F2 - Processing parameters
 SI 65536
 SF 500.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



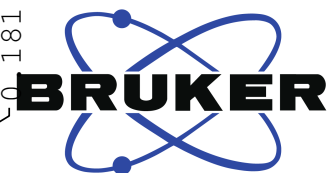
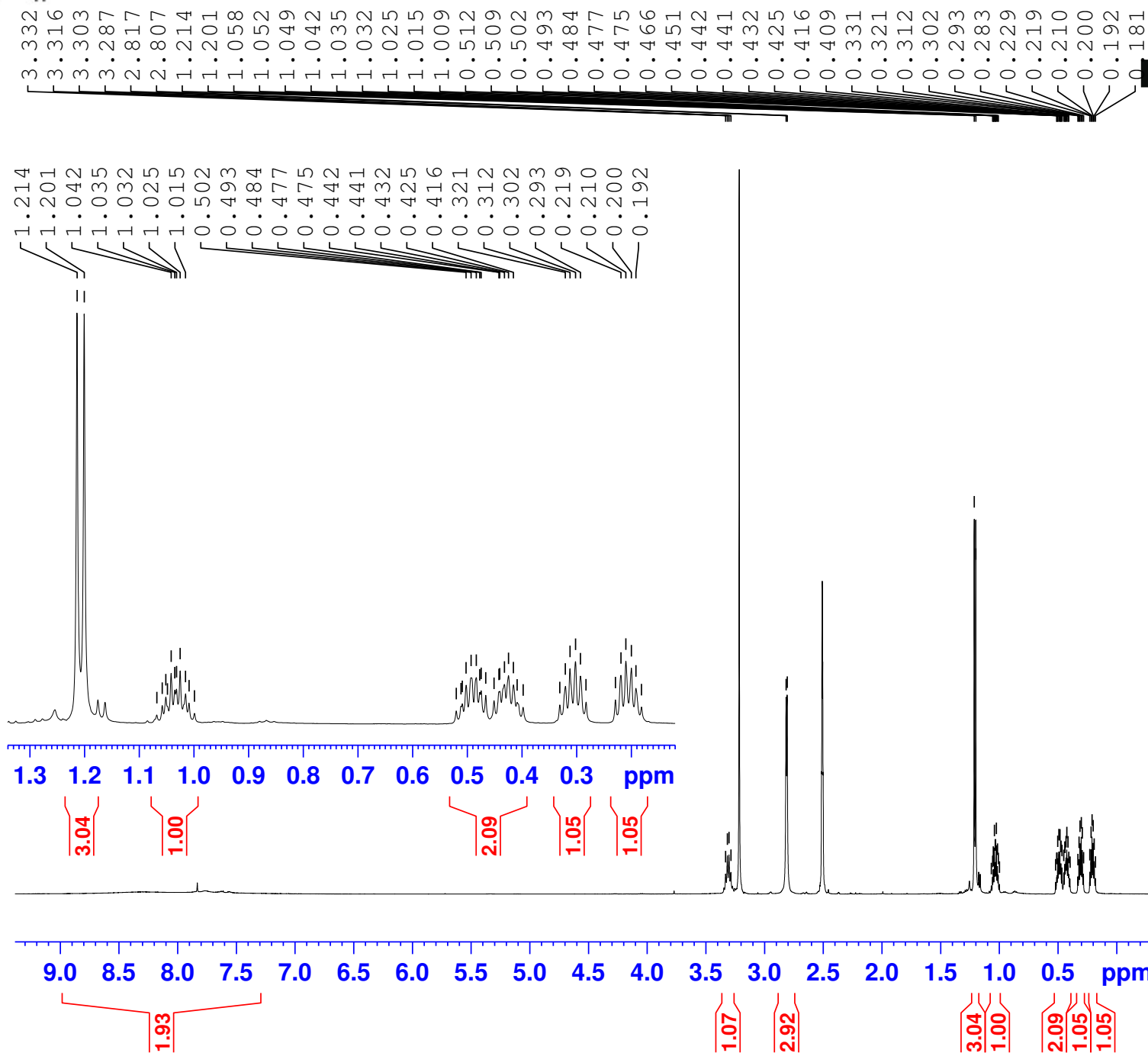
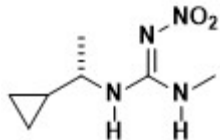
¹H NMR (500 MHz, DMSO-d₆, 50°C of **38**)



Current Data Parameters
NAME 38
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181205
Time 12.54 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1973
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 291.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28288001 W
PLW13 0.14228000 W

F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

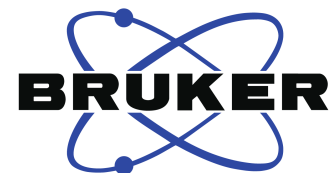
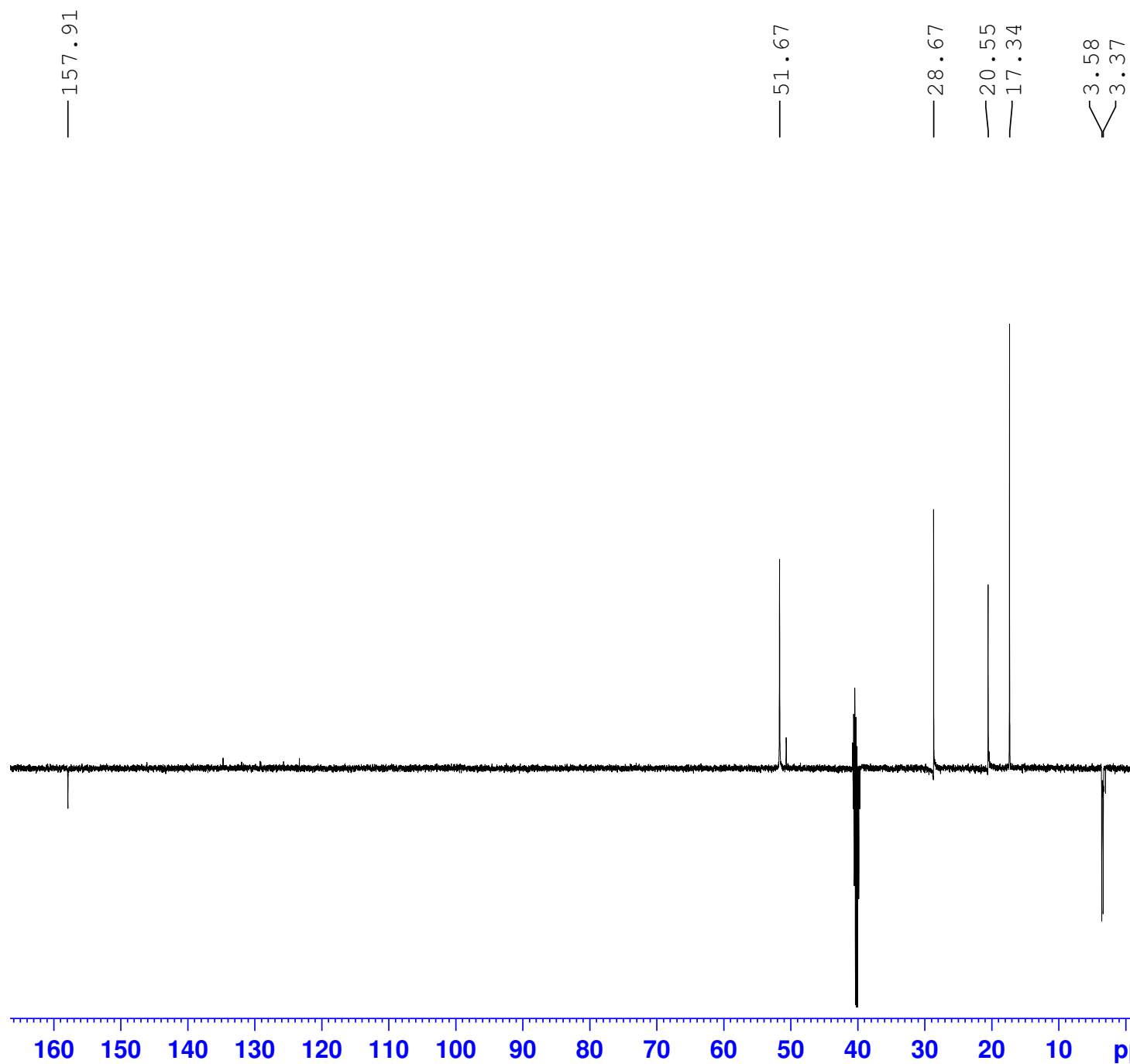


Current Data Parameters
 NAME S-39
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180905
 Time 17.57 h
 INSTRUM spect
 PROBHD Z119470_0187 (zg30)
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 5
 DS 1
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.276799 sec
 RG 77.78
 DW 50.000 usec
 DE 6.50 usec
 TE 323.2 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1830886 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 18.10400009 W

F2 - Processing parameters
 SI 65536
 SF 500.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H NMR (500 MHz, DMSO-d₆, 50°C) of S-39

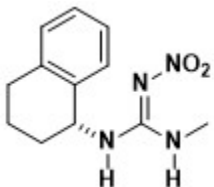


Current Data Parameters
 NAME S-39
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180906
 Time 11.34 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG deptq135
 TD 65536
 SOLVENT DMSO
 NS 1087
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 323.3 K
 CNST2 145.0000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 P2 20.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.00 usec
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28288001 W

F2 - Processing parameters
 SI 32768
 SF 125.7703610 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 140

¹³C (DEPTQ135) NMR (125 MHz, DMSO-d₆, 50°C) of **S-39**

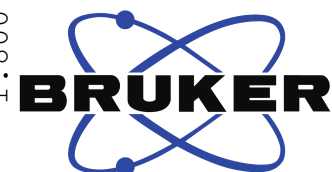


— 8.806

7.220
7.191
7.140
7.128

— 5.051

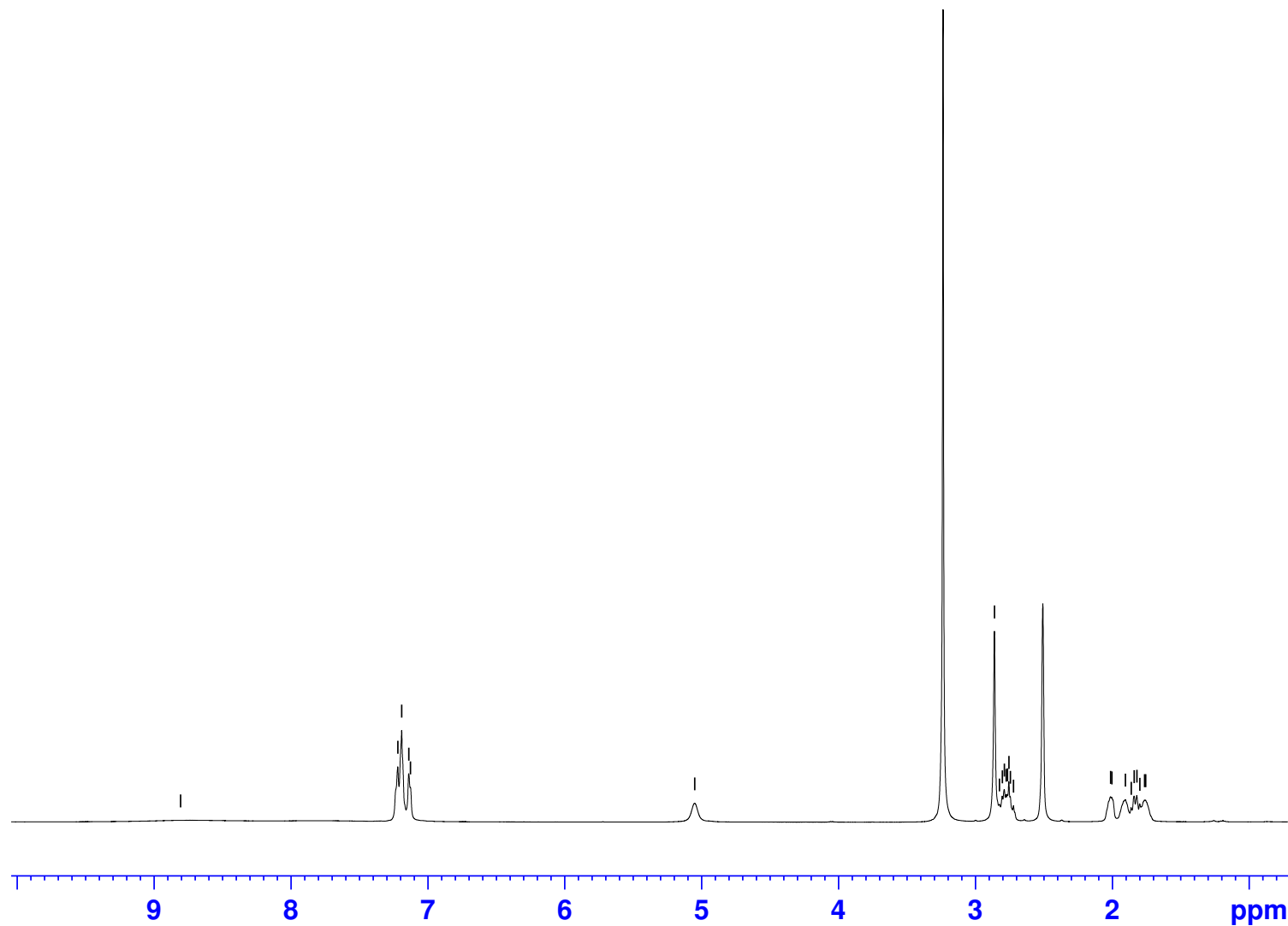
2.861
2.825
2.804
2.789
2.776
2.766
2.755
2.745
2.722
2.012
2.004
1.905
1.862
1.841
1.821
1.800



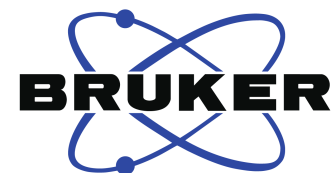
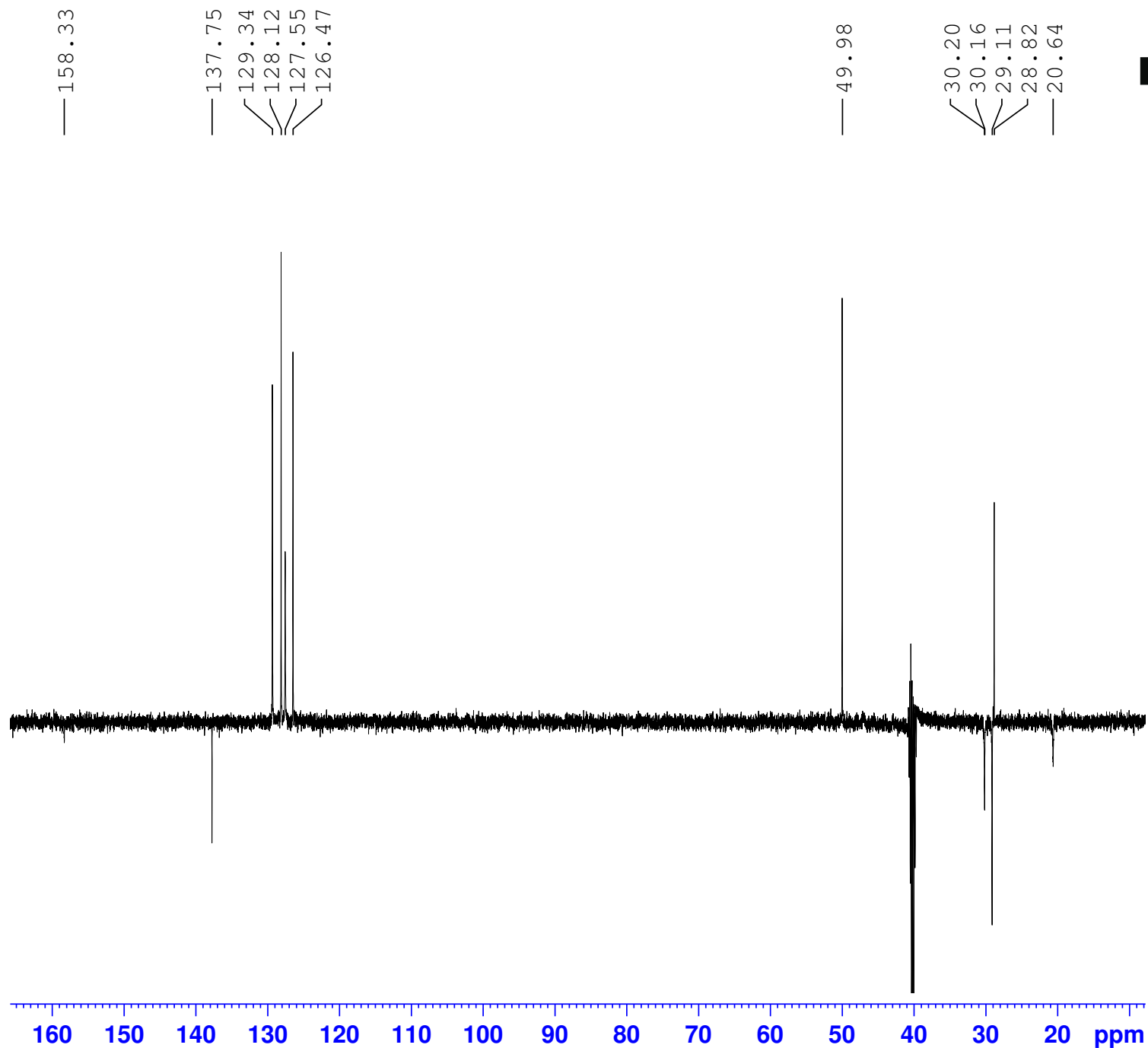
Current Data Parameters
NAME S-40
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180920
Time 10.42 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 77.78
DW 50.000 usec
DE 6.50 usec
TE 323.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H NMR (500 MHz, DMSO-d₆, 50°C) of **S-40**

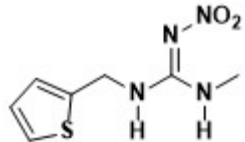


Current Data Parameters
 NAME S-40
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180920
 Time 10.59 h
 INSTRUM spect
 PROBHD z119470_0187 (
 PULPROG deptq135
 TD 65536
 SOLVENT DMSO
 NS 256
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 323.2 K
 CNST2 145.0000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 P2 20.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.00 usec
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28288001 W

F2 - Processing parameters
 SI 32768
 SF 125.7703610 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 791.40

¹³C (DEPTQ135) NMR (125 MHz, DMSO-d₆, 50°C) of **S-40**

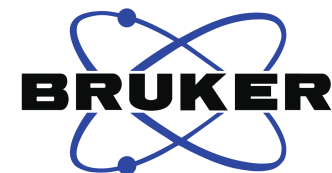


— 9.180

7.920
7.914
7.909
7.903
7.423
7.415
7.031
6.982
6.973
6.966

— 4.573

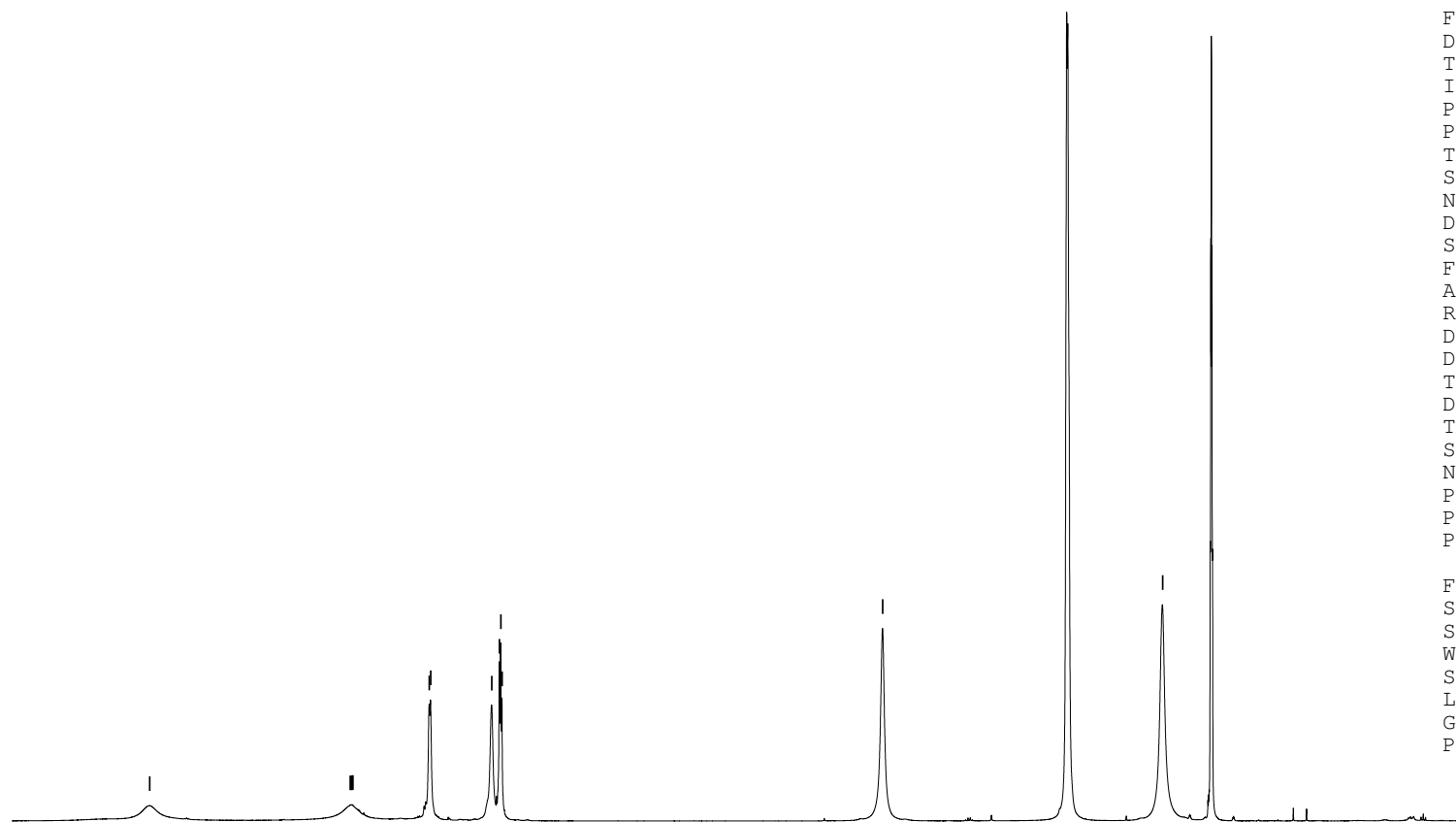
— 2.815



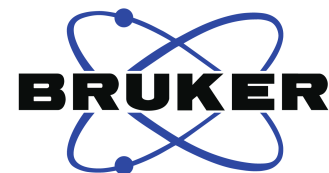
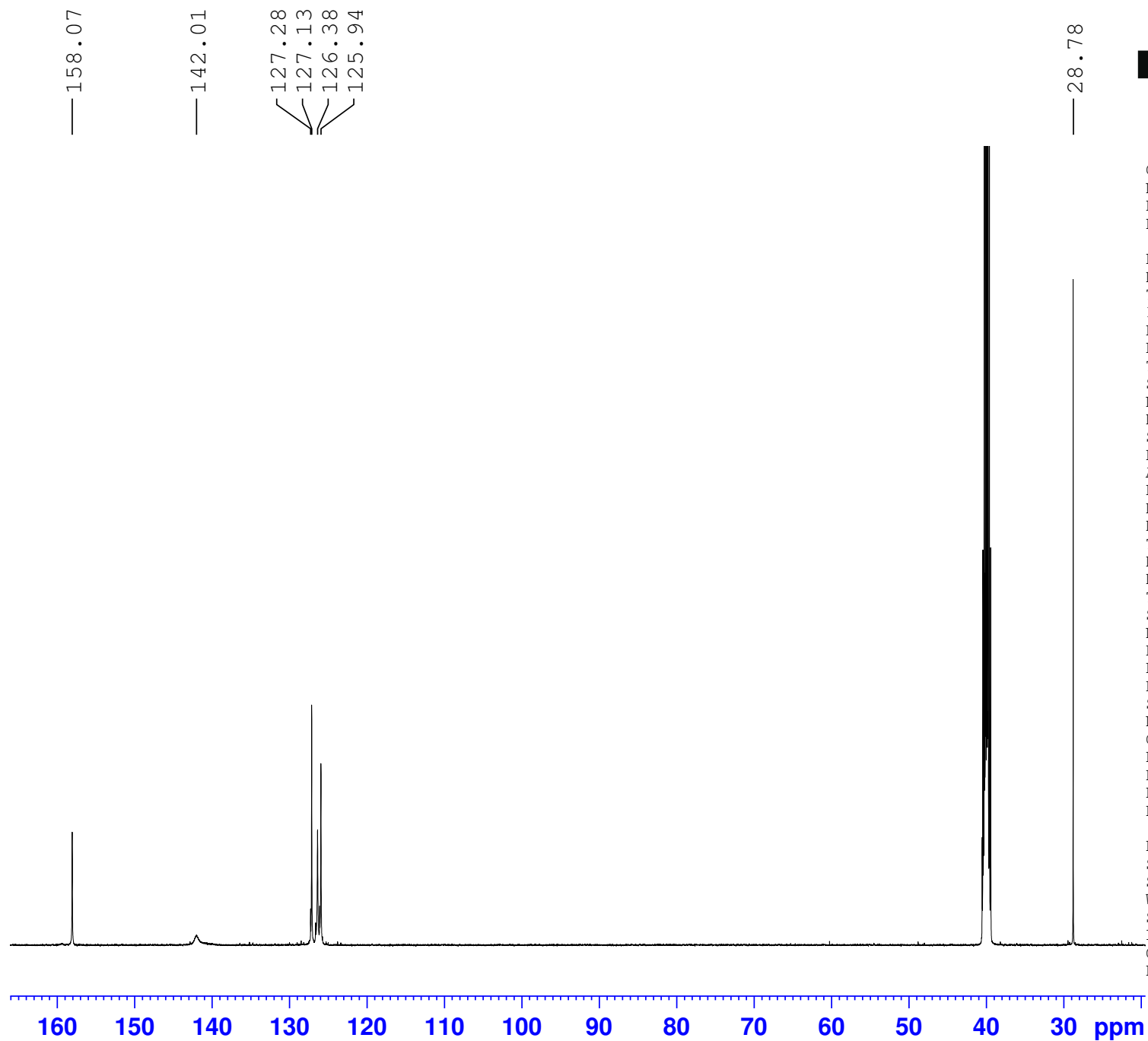
Current Data Parameters
NAME 41
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181008
Time 18.53 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 5
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 62.71
DW 50.000 usec
DE 6.50 usec
TE 291.7 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.180000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



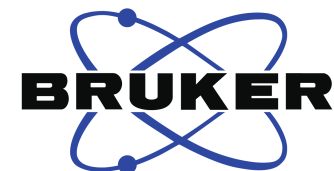
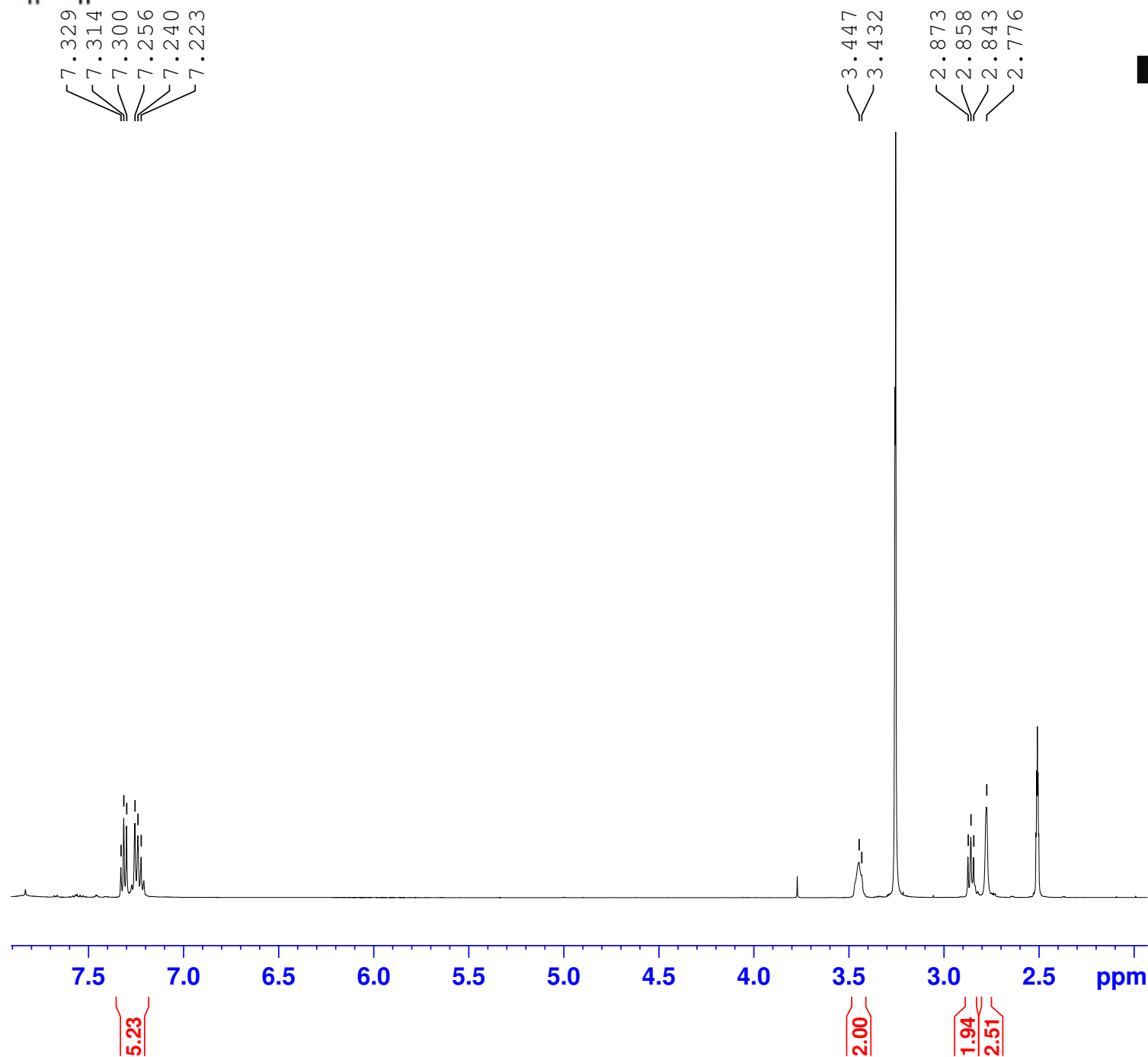
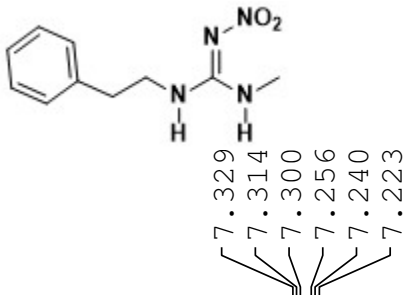
¹H NMR (500 MHz, DMSO-d₆) of 41



Current Data Parameters
 NAME 41
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181016
 Time 21.44 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 30720
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 292.7 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28288001 W
 PLW13 0.14228000 W

F2 - Processing parameters
 SI 32768
 SF 125.7703610 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

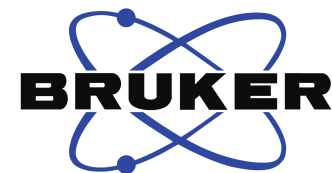
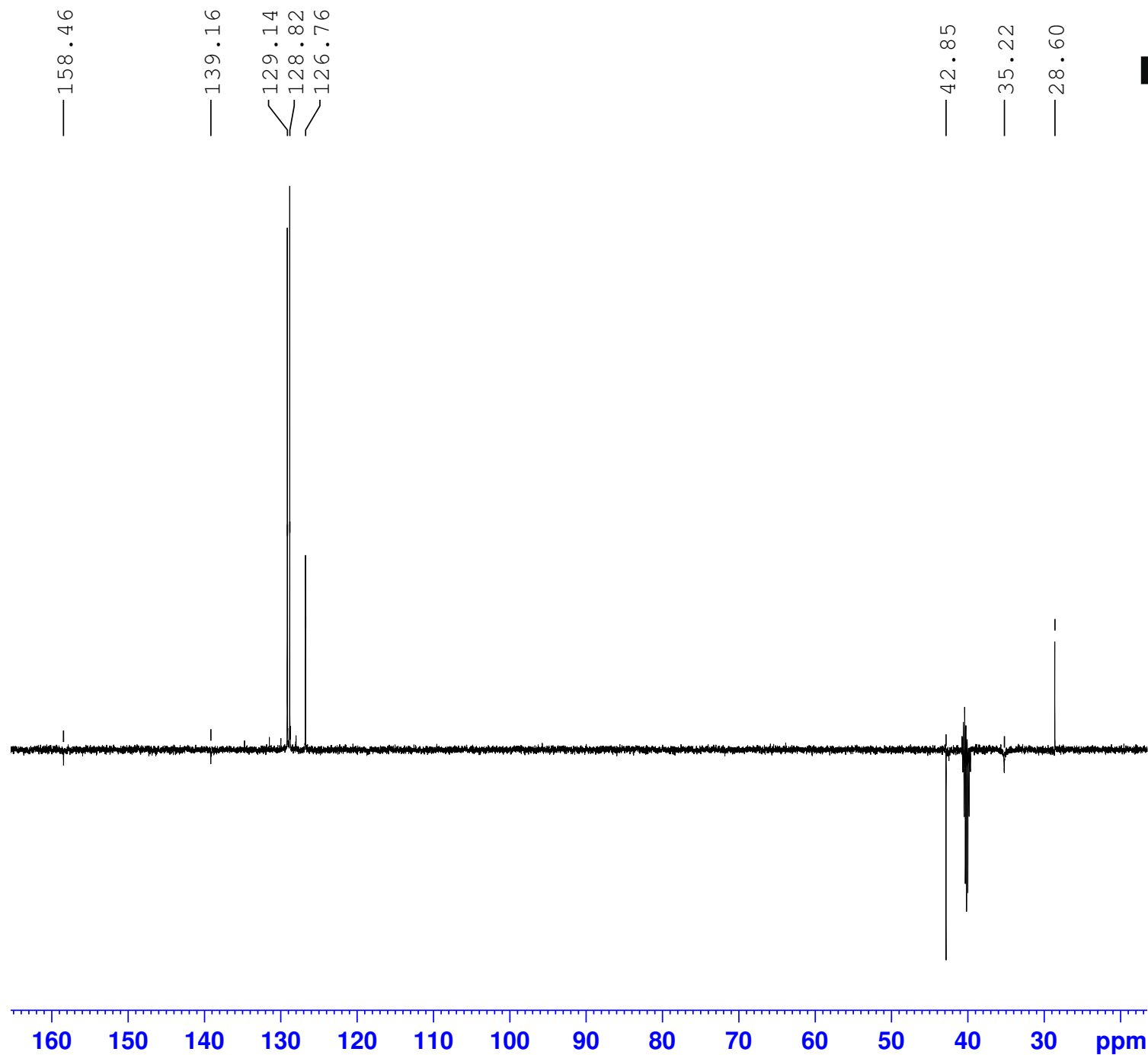


Current Data Parameters
 NAME 42
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180920
 Time 11.05 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 5
 DS 1
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 77.78
 DW 50.000 usec
 DE 6.50 usec
 TE 323.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1830886 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 18.10400009 W

F2 - Processing parameters
 SI 65536
 SF 500.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

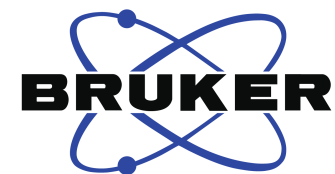
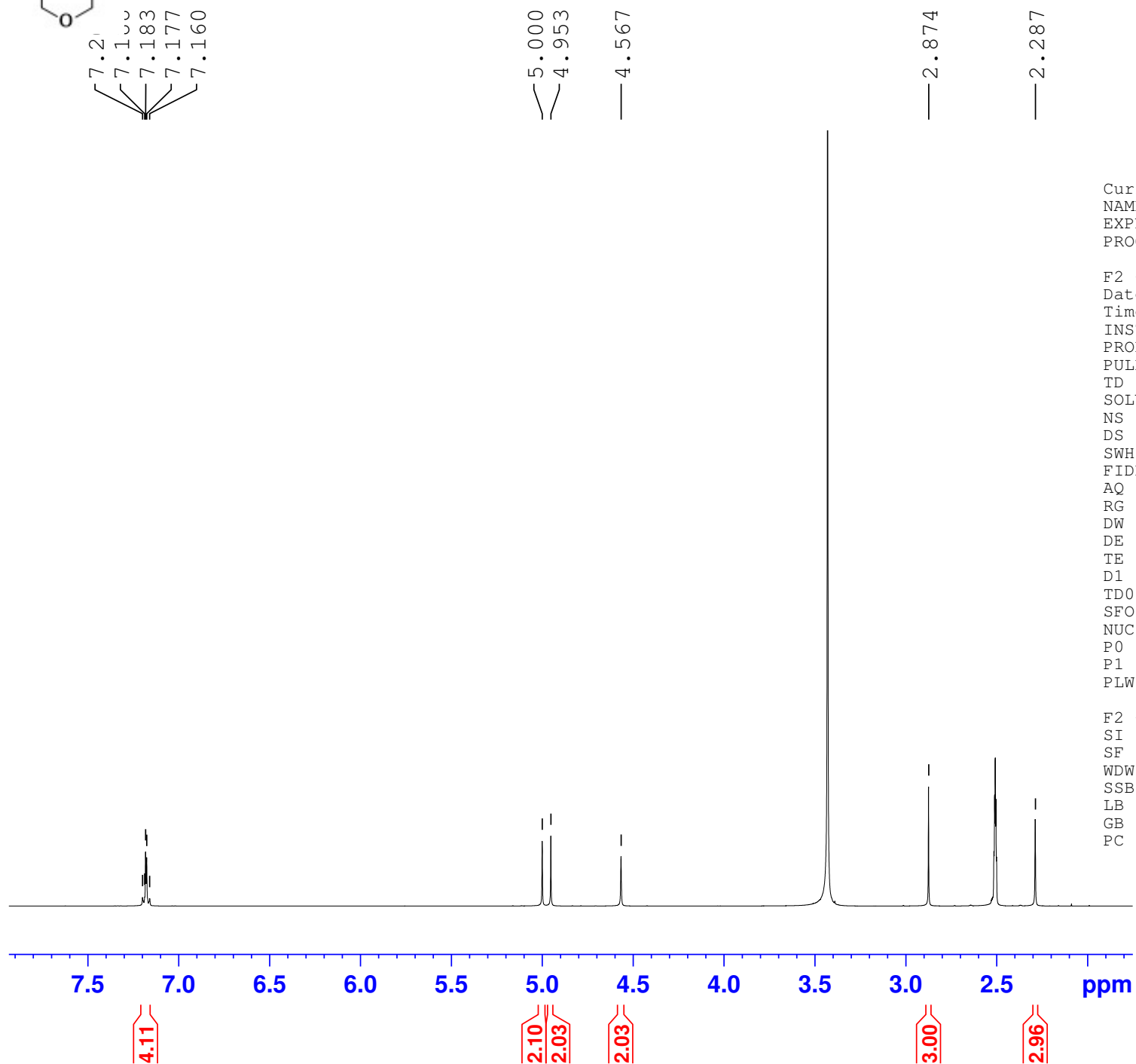
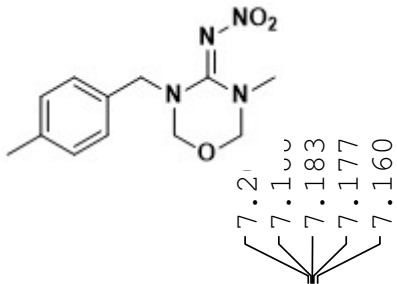
¹H NMR (500 MHz, DMSO-d₆) of 42



Current Data Parameters
 NAME 42
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180920
 Time 11.15 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG deptq135
 TD 65536
 SOLVENT DMSO
 NS 156
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 323.1 K
 CNST2 145.0000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 P2 20.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.00 usec
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28288001 W

F2 - Processing parameters
 SI 32768
 SF 125.7703610 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME 43
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181126
 Time 18.15 h
 INSTRUM spect
 PROBHD z119470_0187 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 62.71
 DW 50.000 usec
 DE 6.50 usec
 TE 291.0 K
 D1 1.00000000 sec
 TD0 1
 SF01 500.1830886 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 18.10400009 W

F2 - Processing parameters
 SI 65536
 SF 500.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H NMR (500 MHz, DMSO-d₆) of **43**

—156.88

—137.57

—132.92

—129.68

—128.13

—79.60

—77.42

—50.70

—33.93

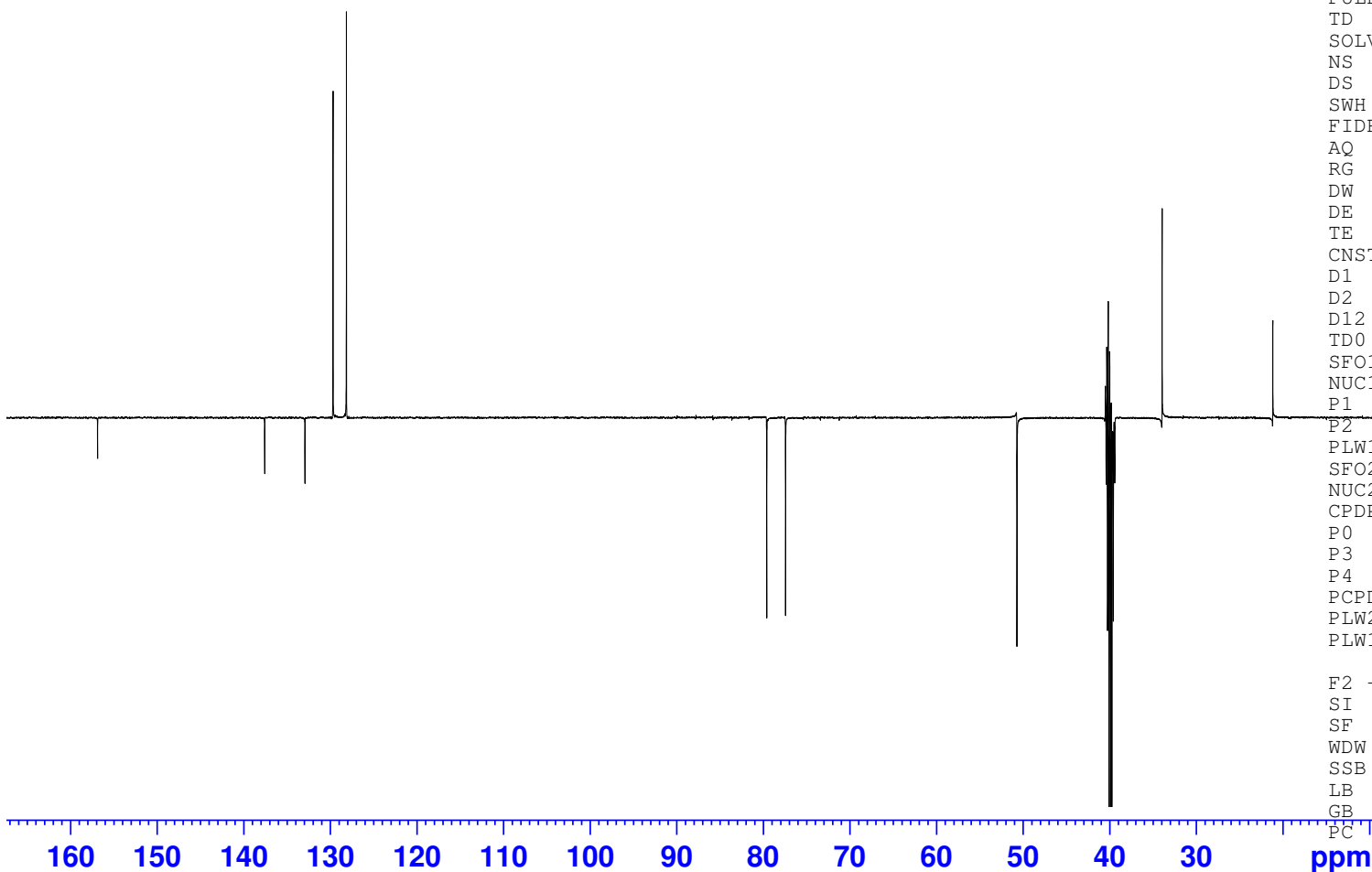
—21.15

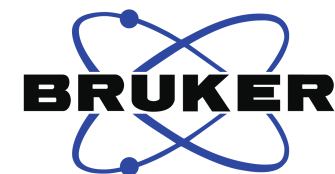
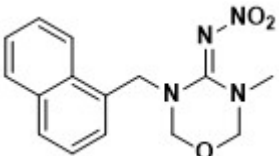


Current Data Parameters
NAME 43
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181128
Time 9.25 h
INSTRUM spect
PROBHD z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT DMSO
NS 16720
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 291.7 K
CNST2 145.000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.00 usec
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28288001 W

F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

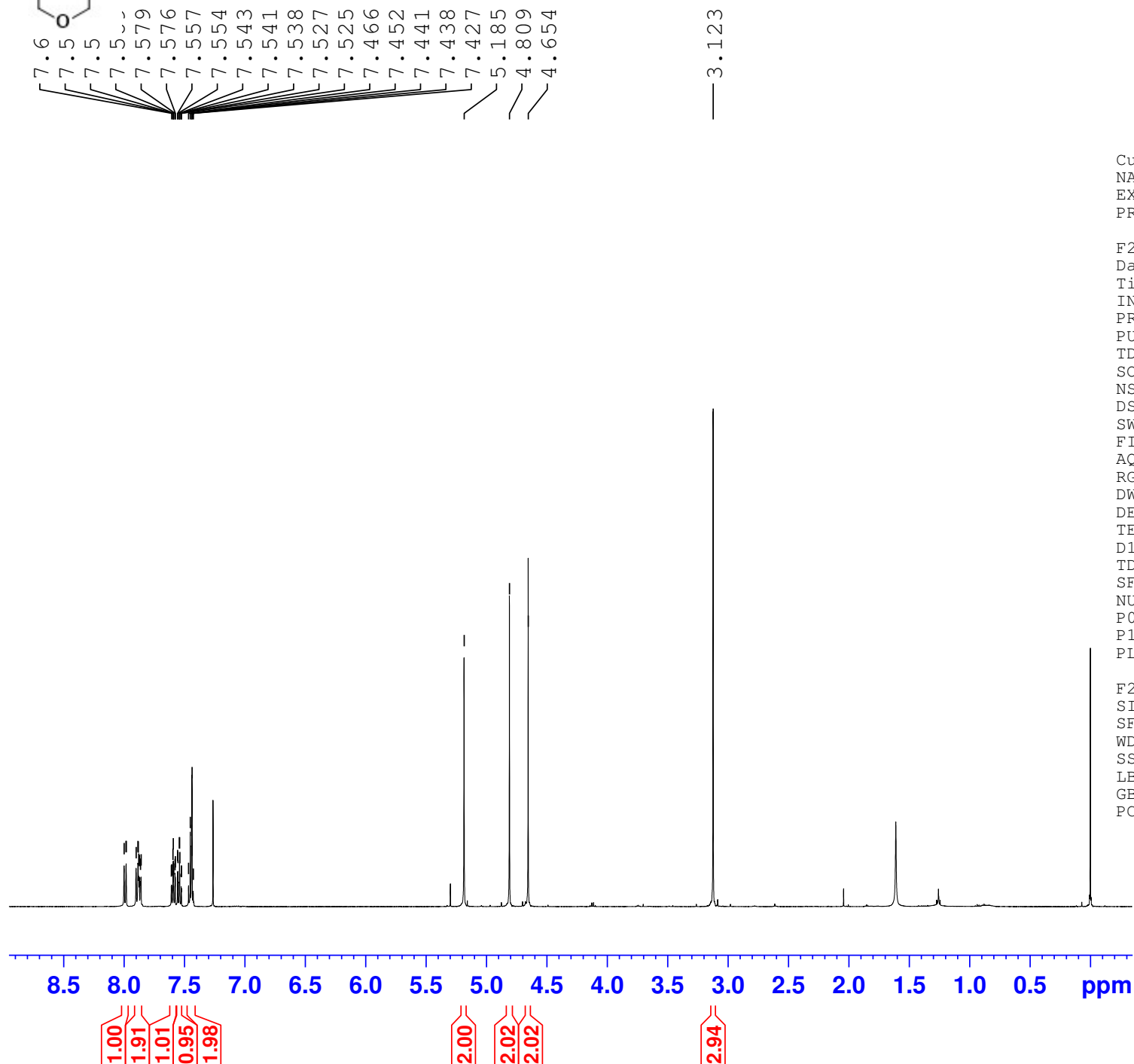




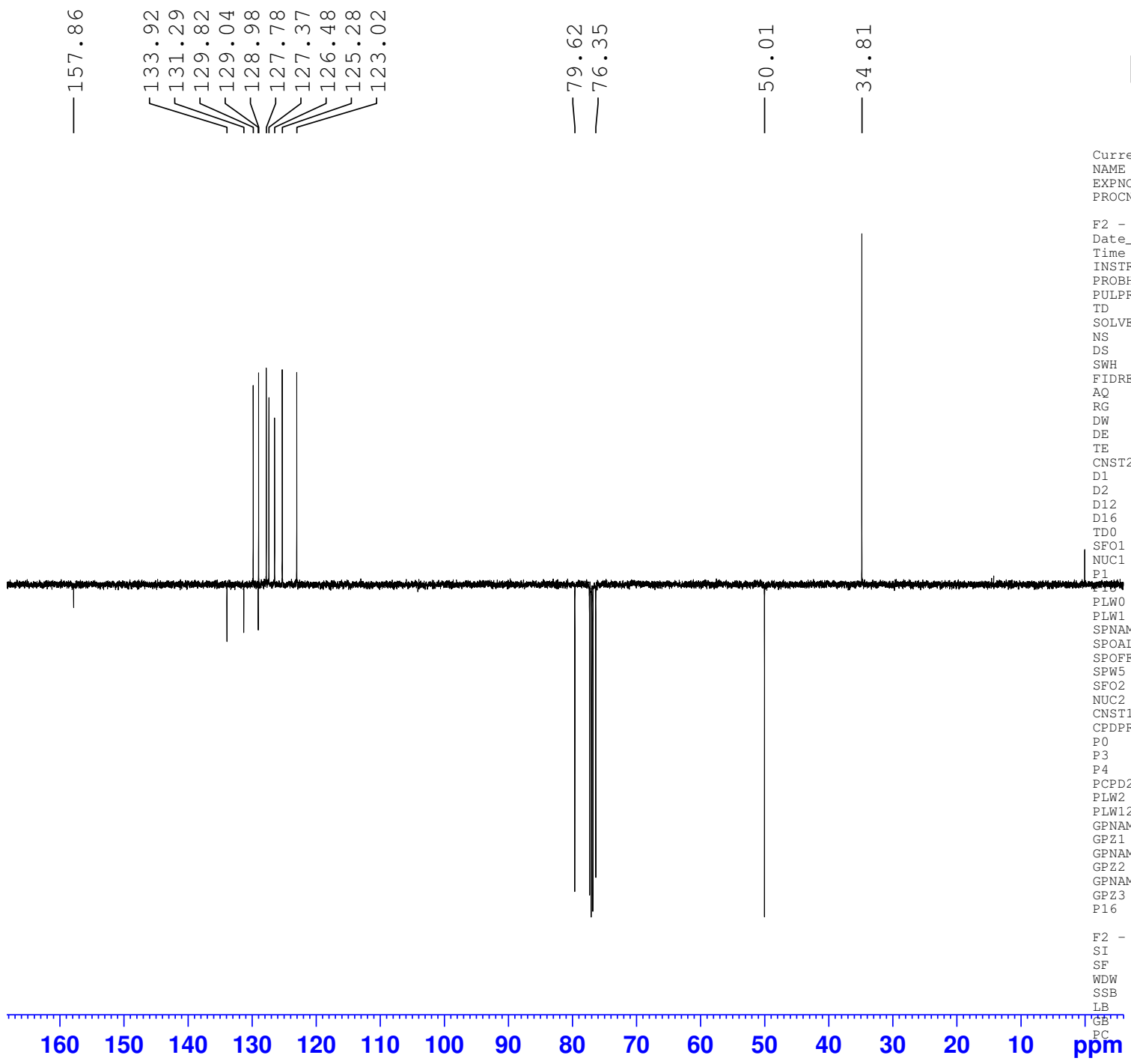
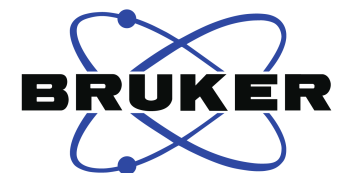
Current Data Parameters
NAME 44
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190613
Time 18.37 h
INSTRUM spect
PROBHD zg30
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 5
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 139.09
DW 50.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.49 usec
P1 10.47 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H NMR (500 MHz, CDCl₃) of **44**

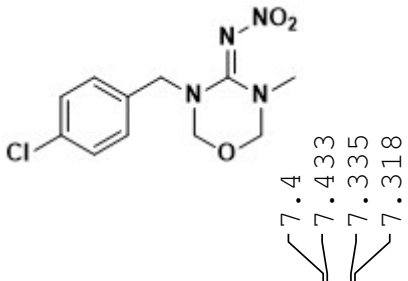


Current Data Parameters
 NAME 44
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190620
 Time 18.54 h
 INSTRUM spect
 PROBHD z119470_0187 (
 PULPROG deptqgppsp
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 291.1 K
 CNST2 145.0000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 D16 0.00020000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 P2 2000.00 usec
 PLW0 0 W
 PLW1 82.09700012 W
 SPNAM[5] Crp60comp.4
 SPOAL5 0.500
 SPOFFS5 0 Hz
 SPW5 12.54300022 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CNST12 1.5000000
 CPDPRG[2] waltz65
 P0 15.70 usec
 P3 10.47 usec
 P4 20.94 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.31009001 W
 GPNAM[1] SMSQ10.100
 GPZ1 31.00 %
 GPNAM[2] SMSQ10.100
 GPZ2 31.00 %
 GPNAM[3] SMSQ10.100
 GPZ3 31.00 %
 P16 1000.00 usec

F2 - Processing parameters
 SI 32768
 SF 125.7703610 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹³C (DEPTQ135) NMR (125 MHz, CDCl₃) of 44



5.020
5.000
4.618

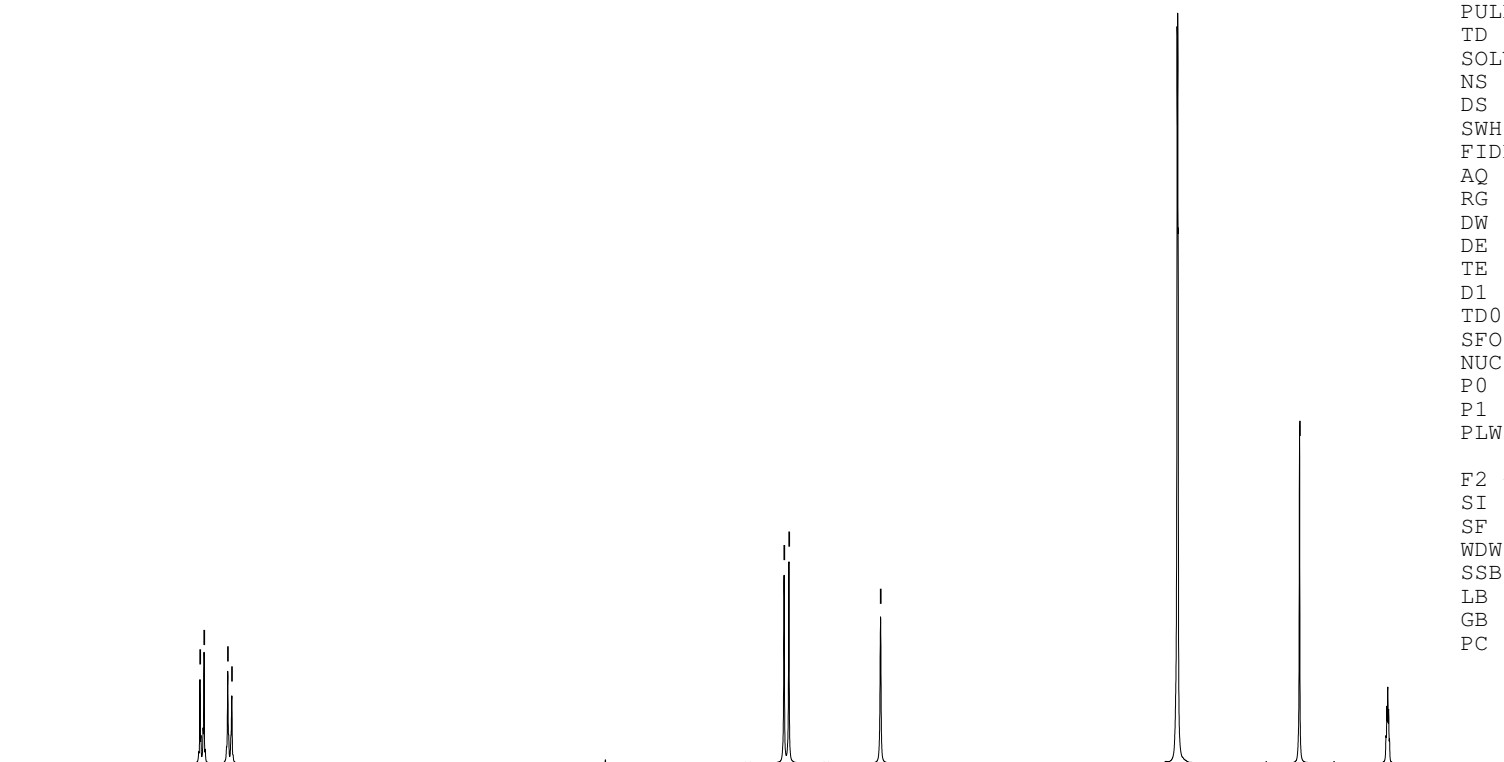
2.875



Current Data Parameters
NAME 45
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190115
Time 10.26 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 95.16
DW 50.000 usec
DE 6.50 usec
TE 291.4 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 18.10400009 W

F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm

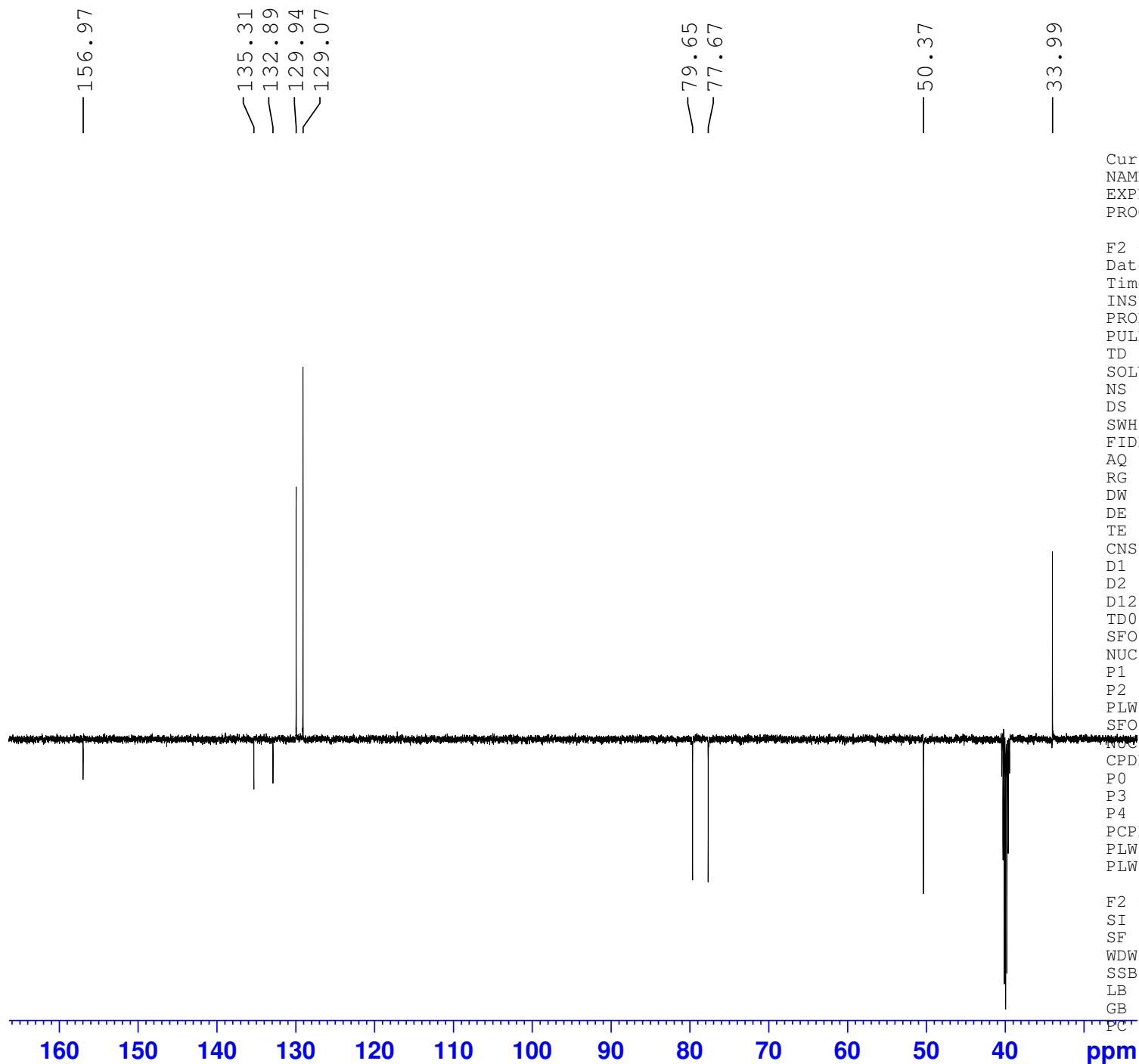
2.02
2.06

2.08
2.03

2.00

3.05

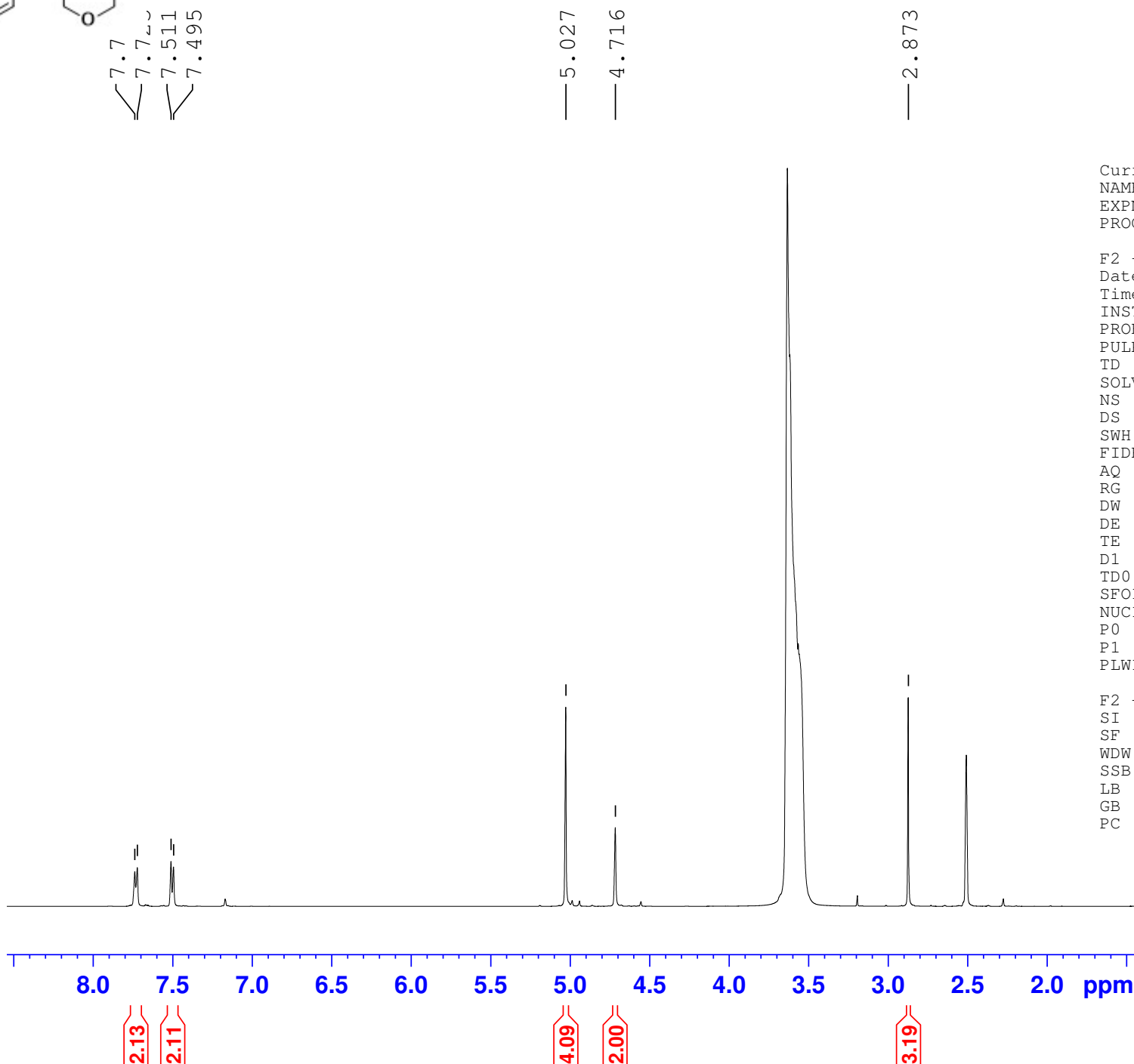
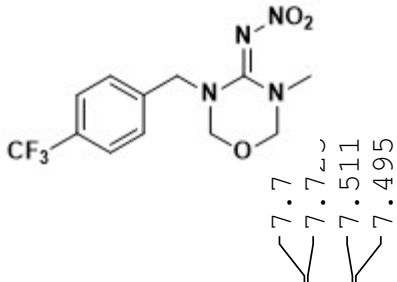
¹H NMR (500 MHz, DMSO-d₆) of 45



Current Data Parameters
 NAME 45
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190115
 Time 10.33 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG deptq135
 TD 65536
 SOLVENT DMSO
 NS 116
 DS 8
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 192.72
 DW 16.800 usec
 DE 6.50 usec
 TE 291.8 K
 CNST2 145.0000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 125.7829381 MHz
 NUC1 13C
 P1 10.00 usec
 P2 20.00 usec
 PLW1 82.09700012 W
 SFO2 500.1820007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.00 usec
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 18.10400009 W
 PLW12 0.28288001 W

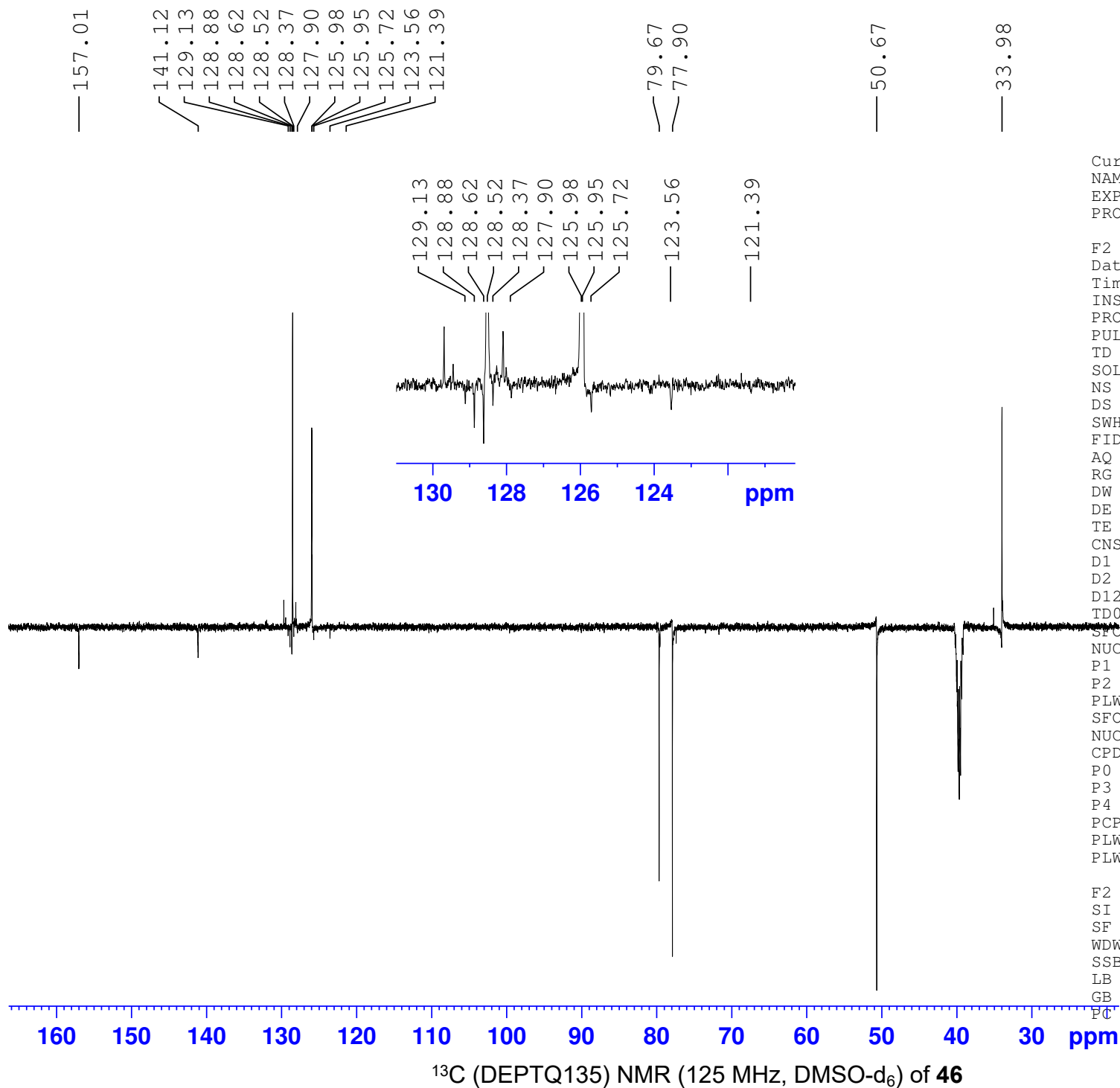
F2 - Processing parameters
 SI 32768
 SF 125.7703610 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME 46
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190115
 Time 9.35 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 19.48
 DW 50.000 usec
 DE 6.50 usec
 TE 291.1 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1830886 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 18.10400009 W

F2 - Processing parameters
 SI 65536
 SF 500.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

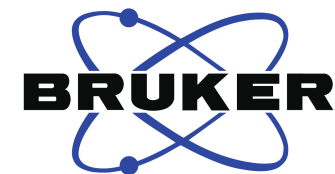


Current Data Parameters
NAME 46
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190115
Time 10.17 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT DMSO
NS 741
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 291.6 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.00 usec
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.28288001 W

F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

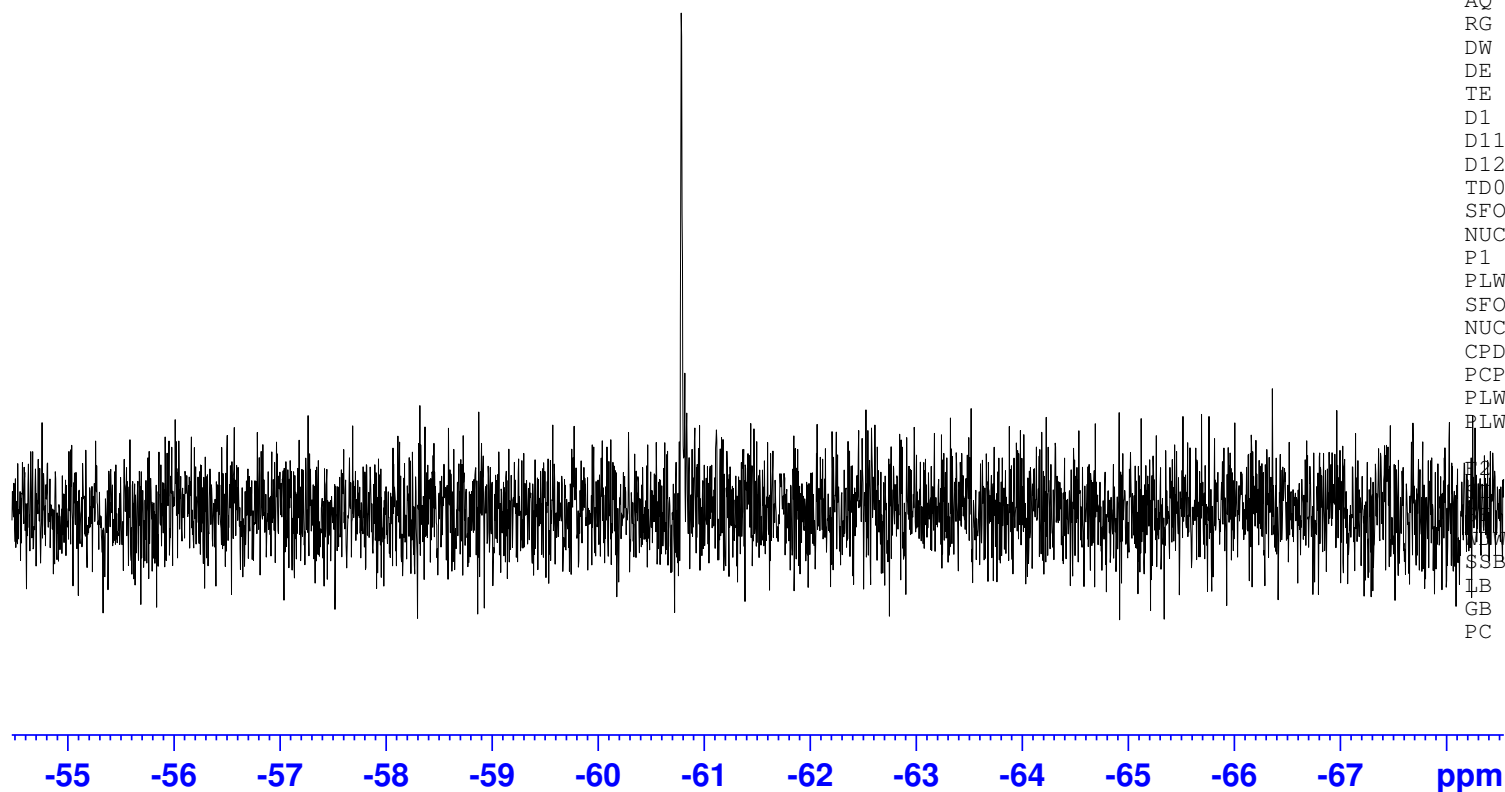
— -60.78



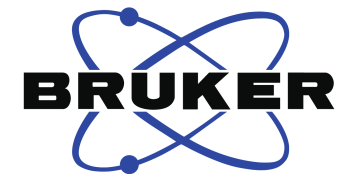
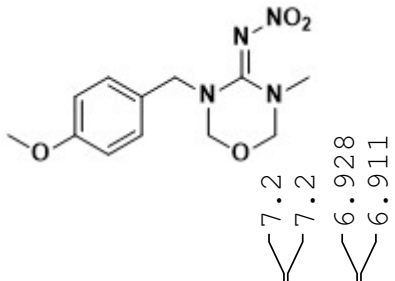
Current Data Parameters
NAME 46
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190801
Time 14.40 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG zgfhigqn.2
TD 131072
SOLVENT DMSO
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 1.733953 Hz
AQ 0.5767168 sec
RG 11.27
DW 4.400 usec
DE 6.50 usec
TE 293.4 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
SFO1 470.5923603 MHz
NUC1 19F
P1 16.00 usec
PLW1 36.93899918 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.31009001 W

F2 - Processing parameters
65536
470.6394242 MHz
EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



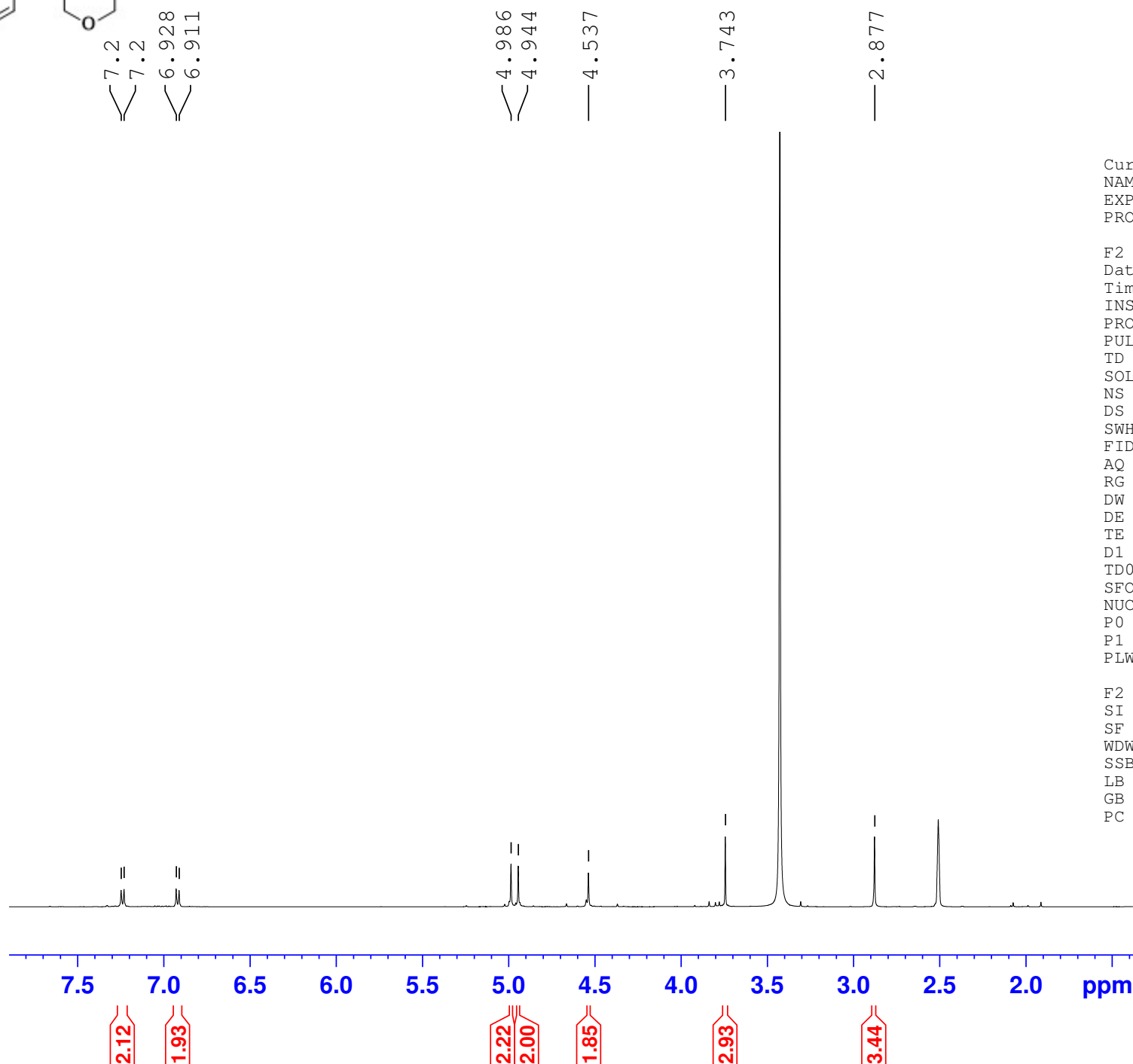
¹⁹F NMR (470 MHz, DMSO-d₆) of **46**



Current Data Parameters
 NAME 47
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190611
 Time 18.00 h
 INSTRUM spect
 PROBHD Z119470_0187 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 48.27
 DW 50.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1830886 MHz
 NUC1 1H
 P0 3.49 usec
 P1 10.47 usec
 PLW1 18.10400009 W

F2 - Processing parameters
 SI 65536
 SF 500.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



¹H NMR (500 MHz, DMSO-d₆) of **47**

—159.42
—156.81

—129.71
—127.72

—114.52

—79.58
—77.30

—55.58
—50.41

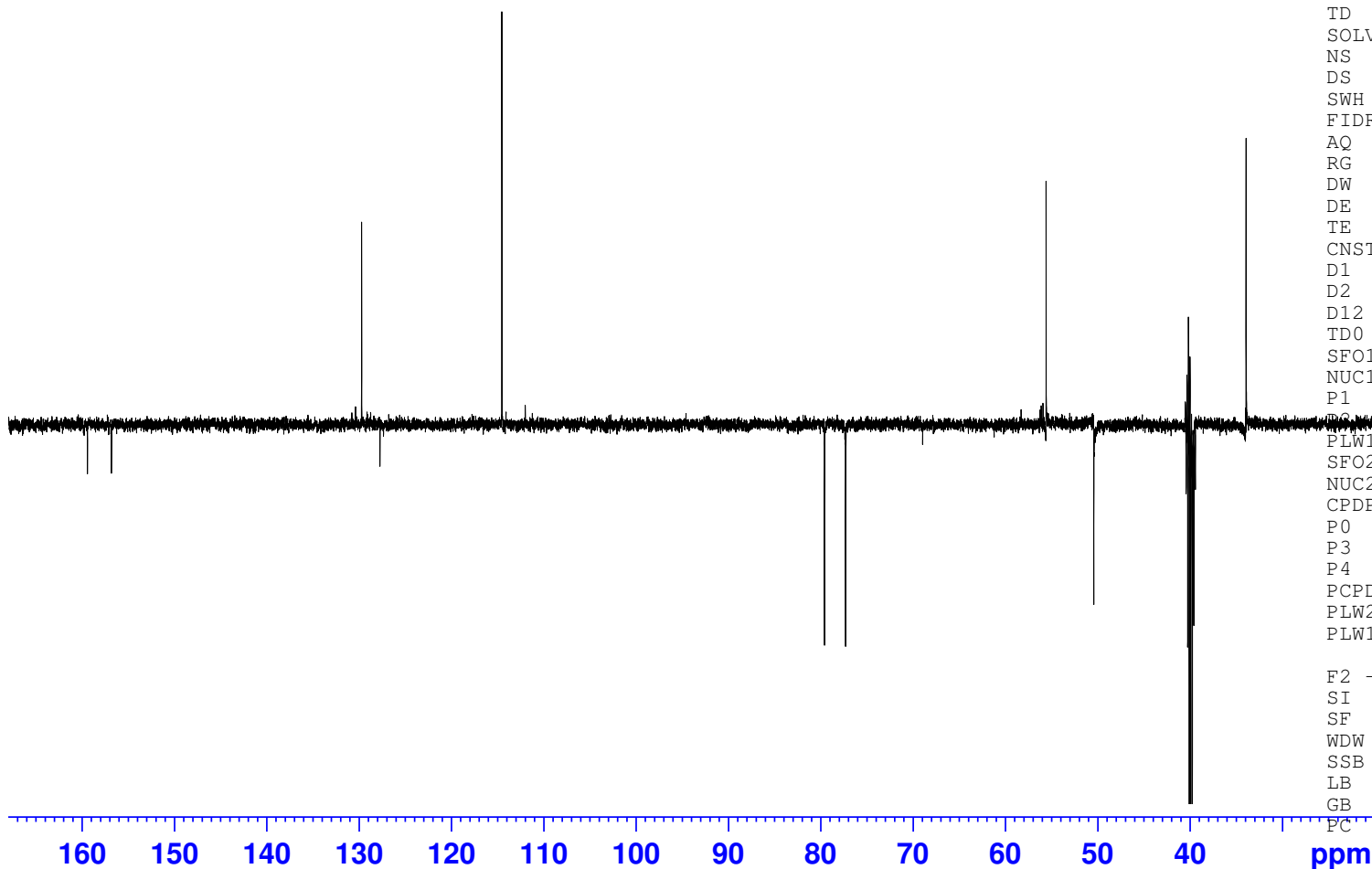
—33.91



Current Data Parameters
NAME 47
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190611
Time 18.18 h
INSTRUM spect
PROBHD Z119470_0187 (
PULPROG deptq135
TD 65536
SOLVENT DMSO
NS 200
DS 8
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.72
DW 16.800 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P1 10.00 usec
PCPD 20.00 usec
PLW1 82.09700012 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.70 usec
P3 10.47 usec
P4 20.94 usec
PCPD2 80.00 usec
PLW2 18.10400009 W
PLW12 0.31009001 W

F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



¹³C (DEPTQ135) NMR (125 MHz, DMSO-d₆) of **47**