

Supplementary Material

Unequivocal synthesis of substituted thiazolo[3,2-*a*]benzimidazoles

Gordon W. Rewcastle*

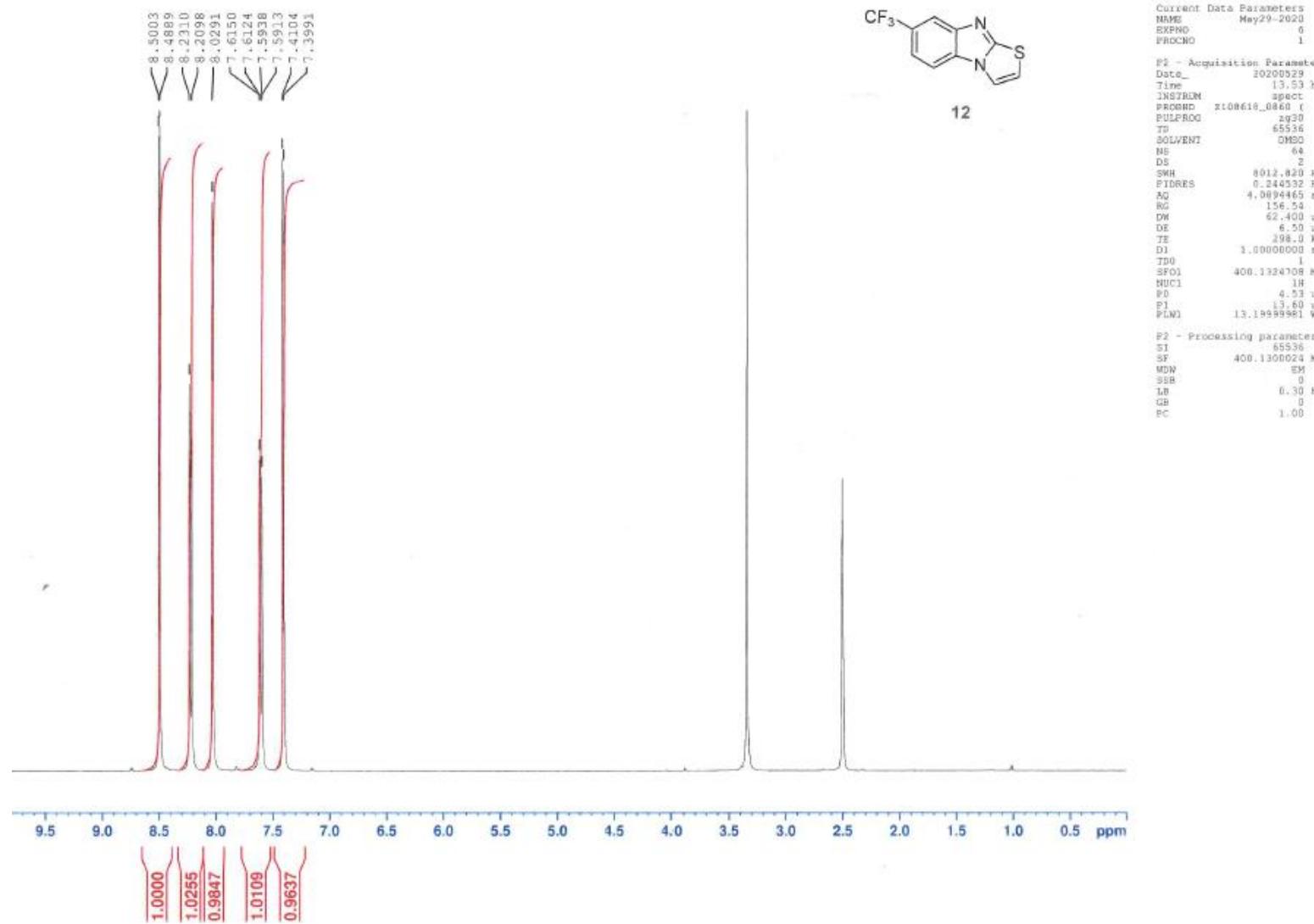
Auckland Cancer Society Research Centre, School of Medical Sciences, Faculty of Medical and Health Sciences, and Maurice Wilkins Centre for Molecular Biodiscovery, The University of Auckland, Private Bag 92019, Auckland 1142, New Zealand

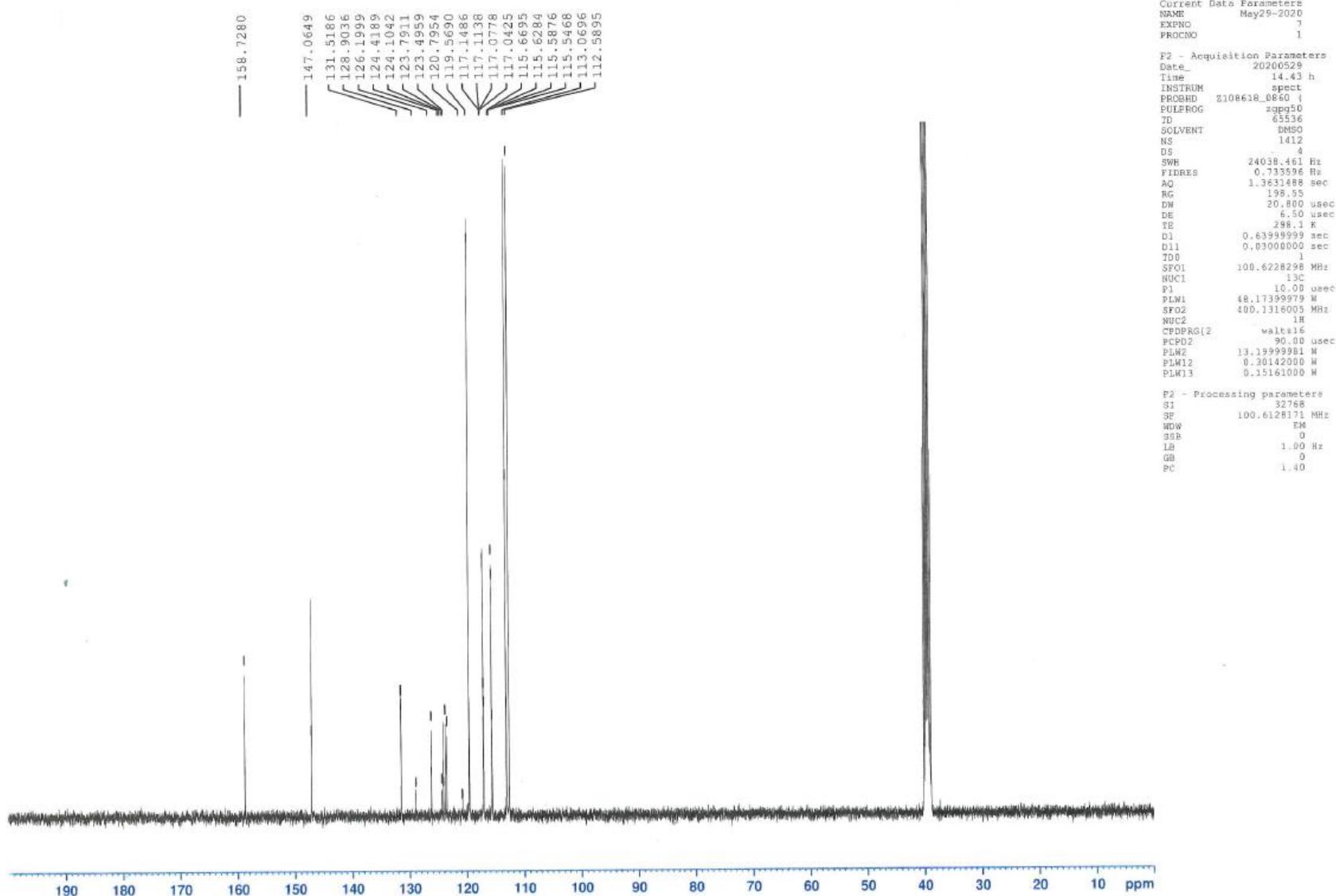
Email: g.rewcastle@auckland.ac.nz

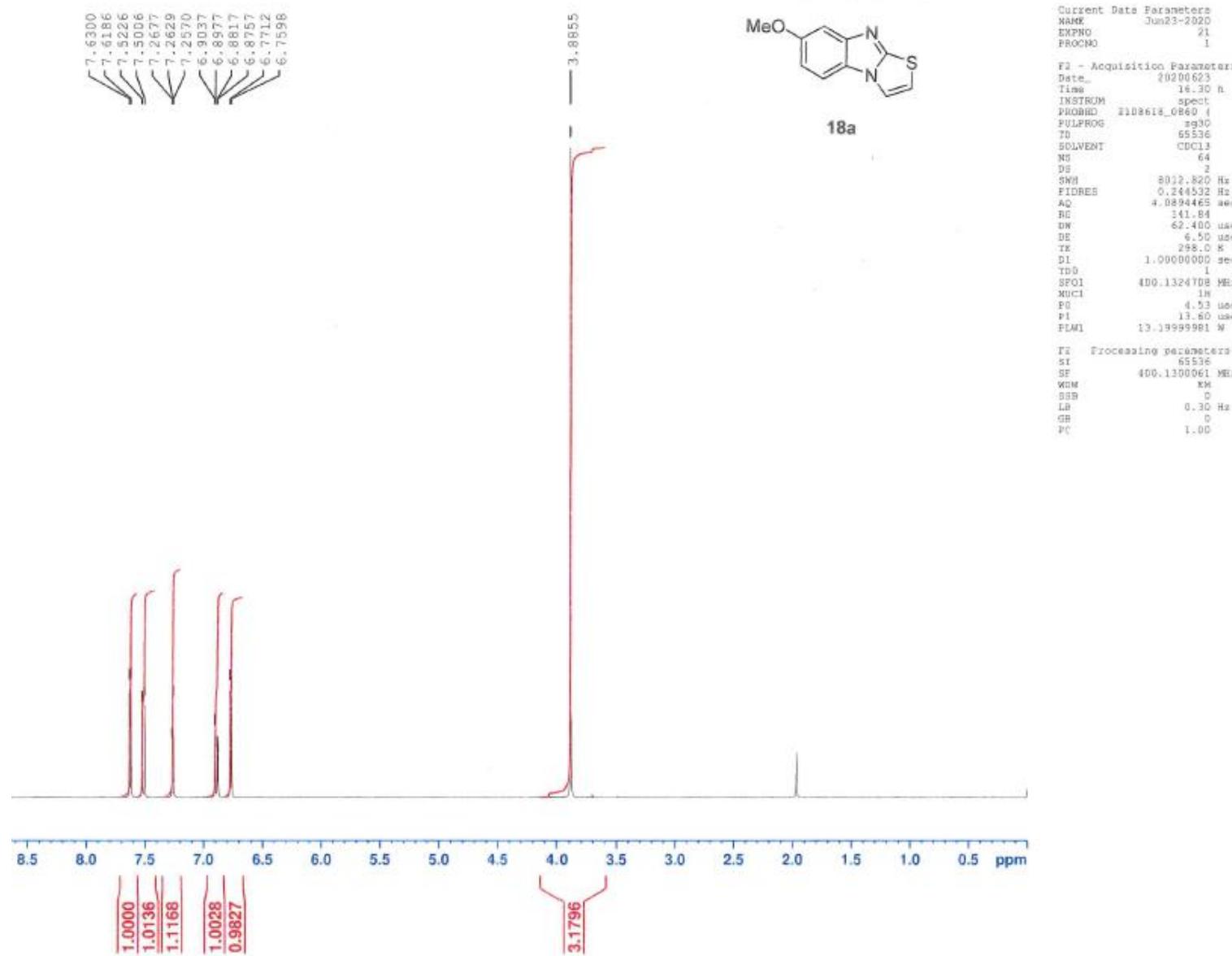
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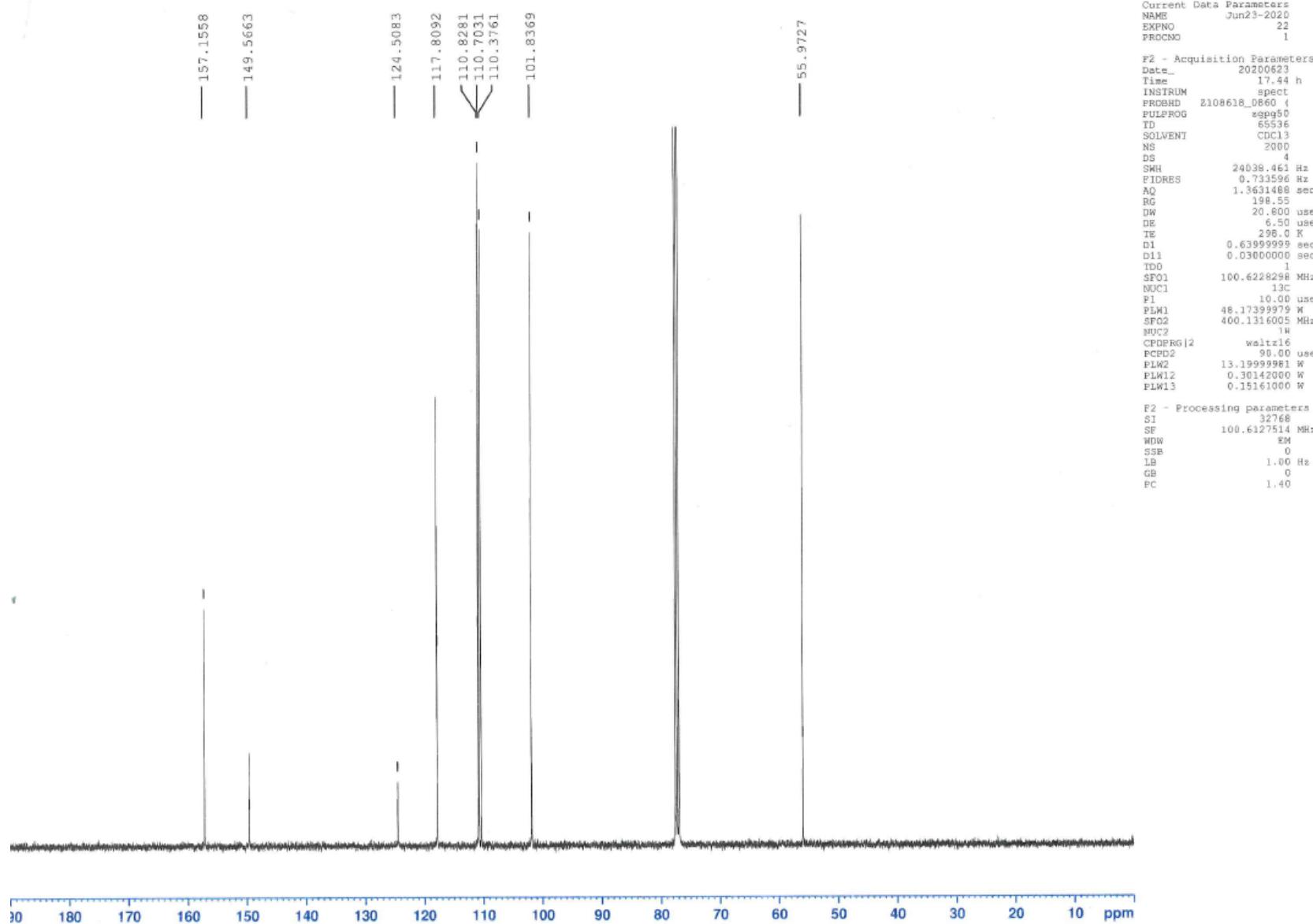
NMR Spectra

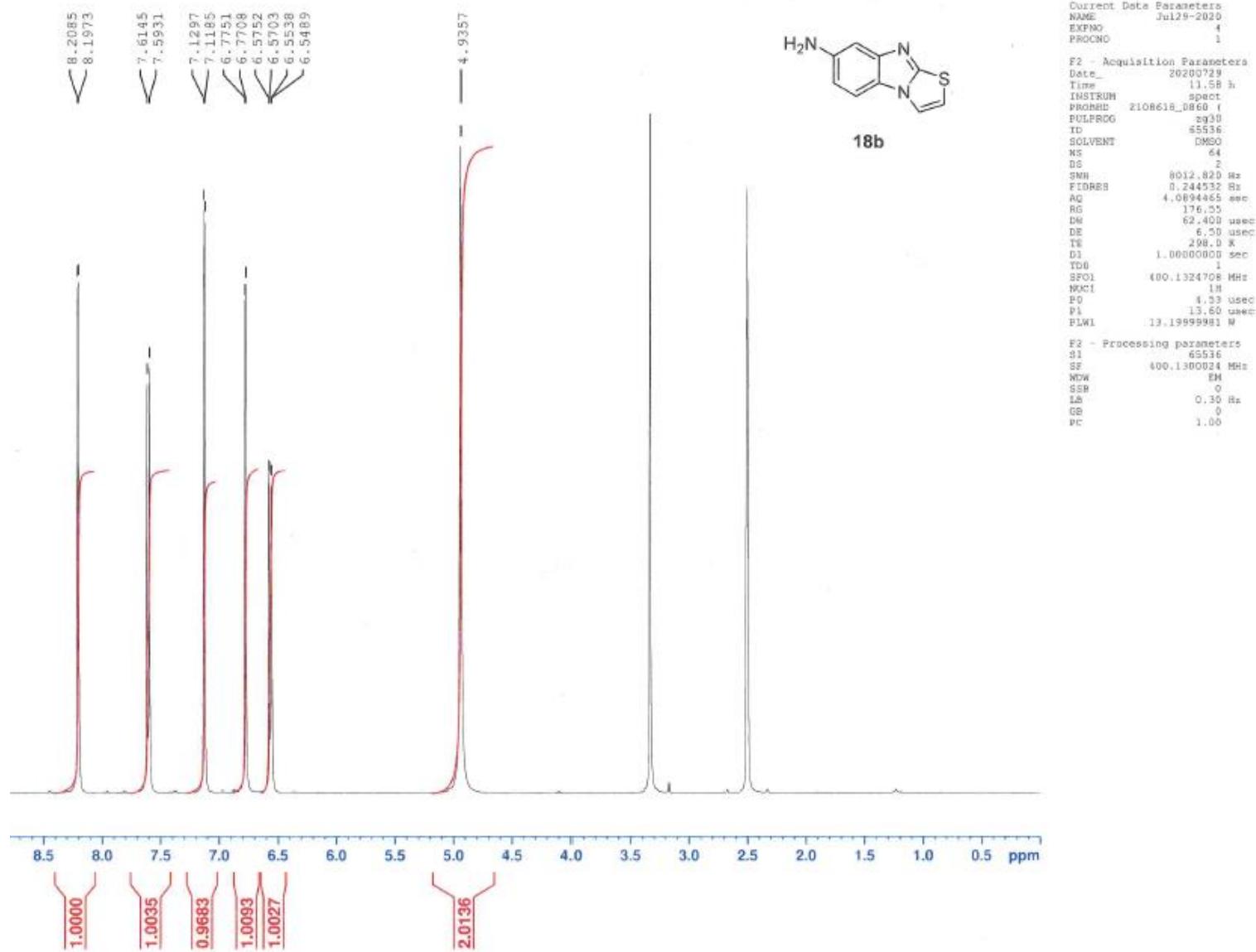
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Compound 18a	S4
Compound 18b	S6
Compound 18c	S8
Compound 18d	S10
Compound 18e	S12
Compound 21b	S14
Compound 21c	S16
Compound 21d	S18
Compound 21e	S20
Compound 21f	S22
Compound 25	S24
Compound 26	S26



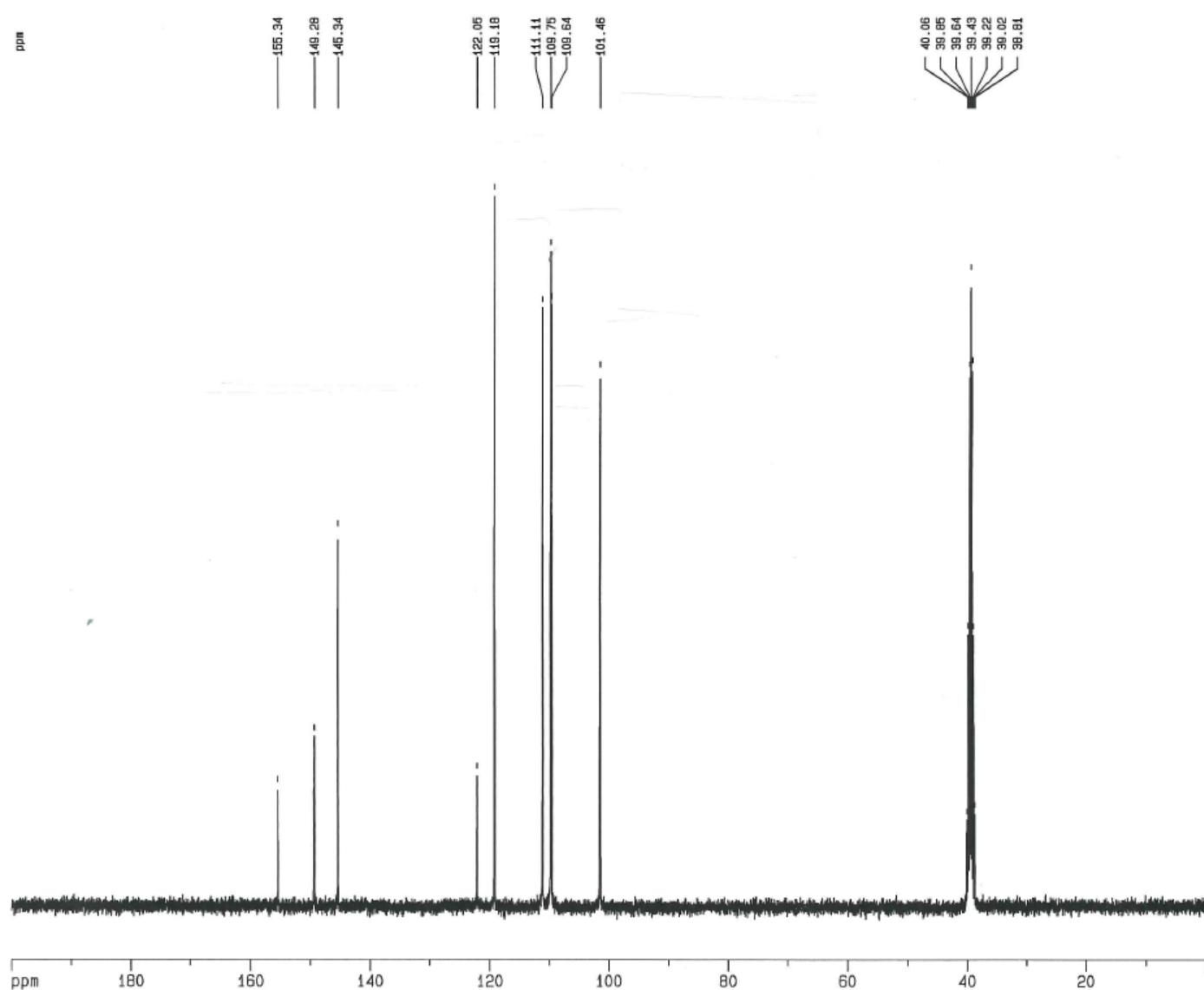








ppm

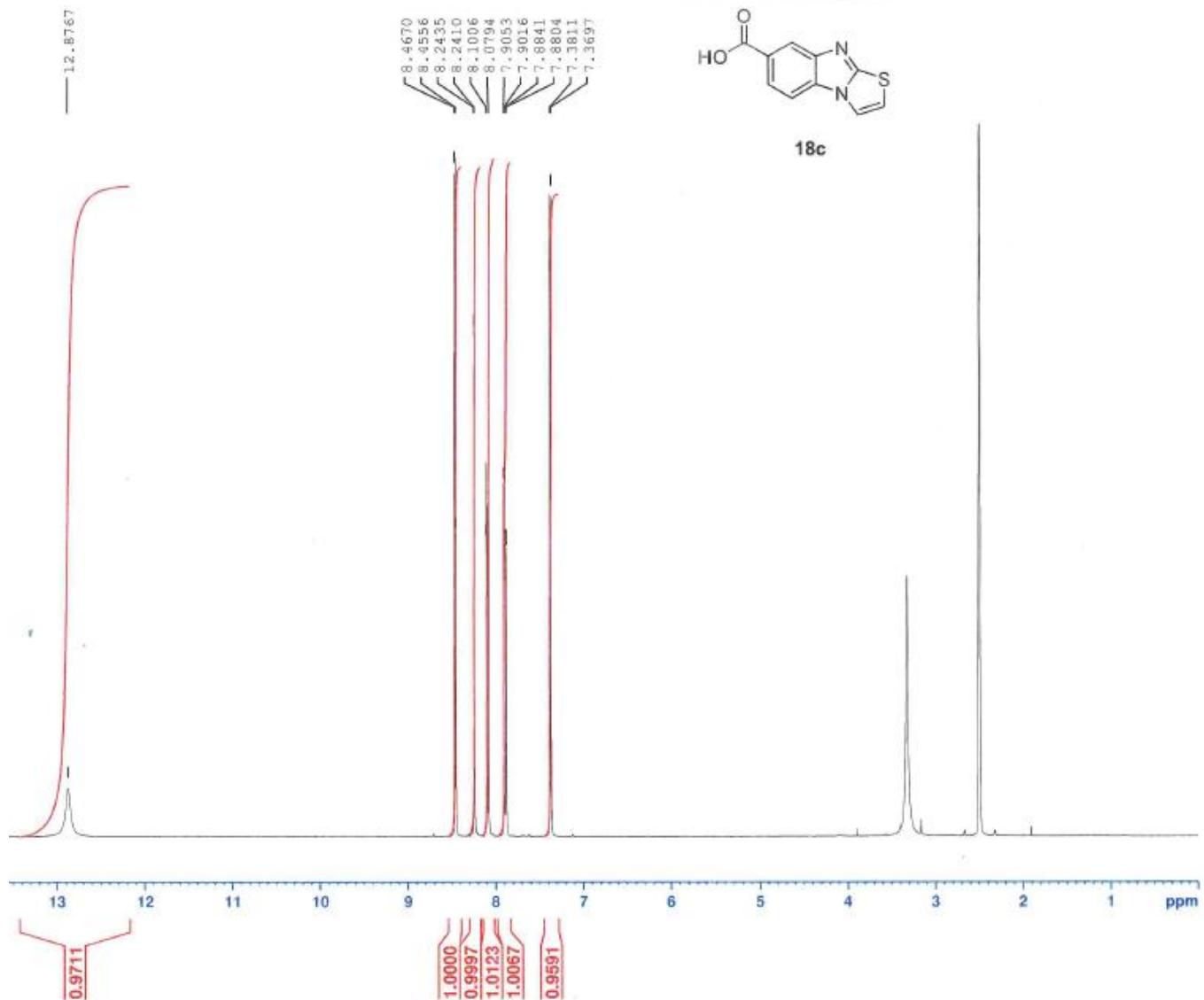


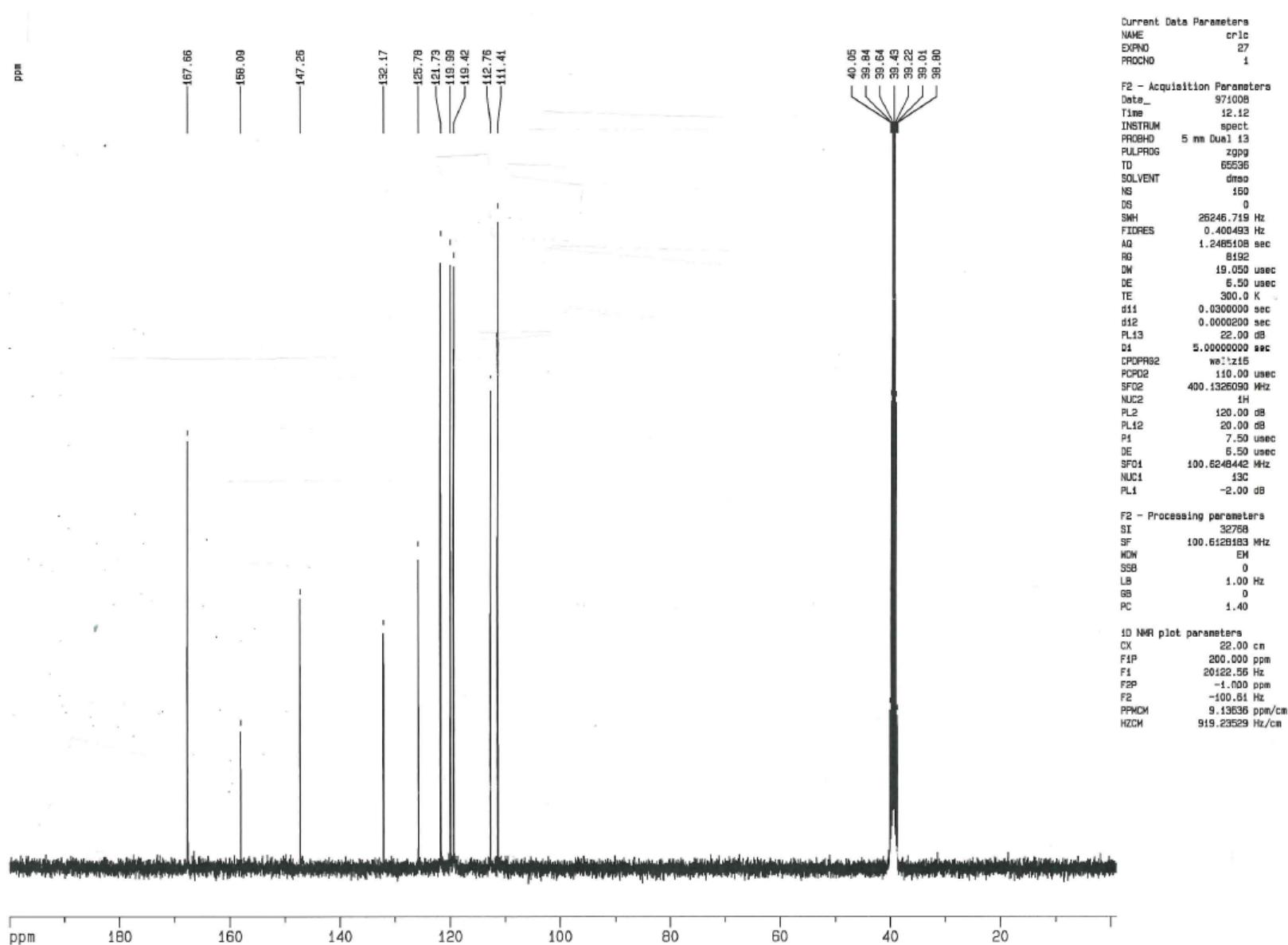
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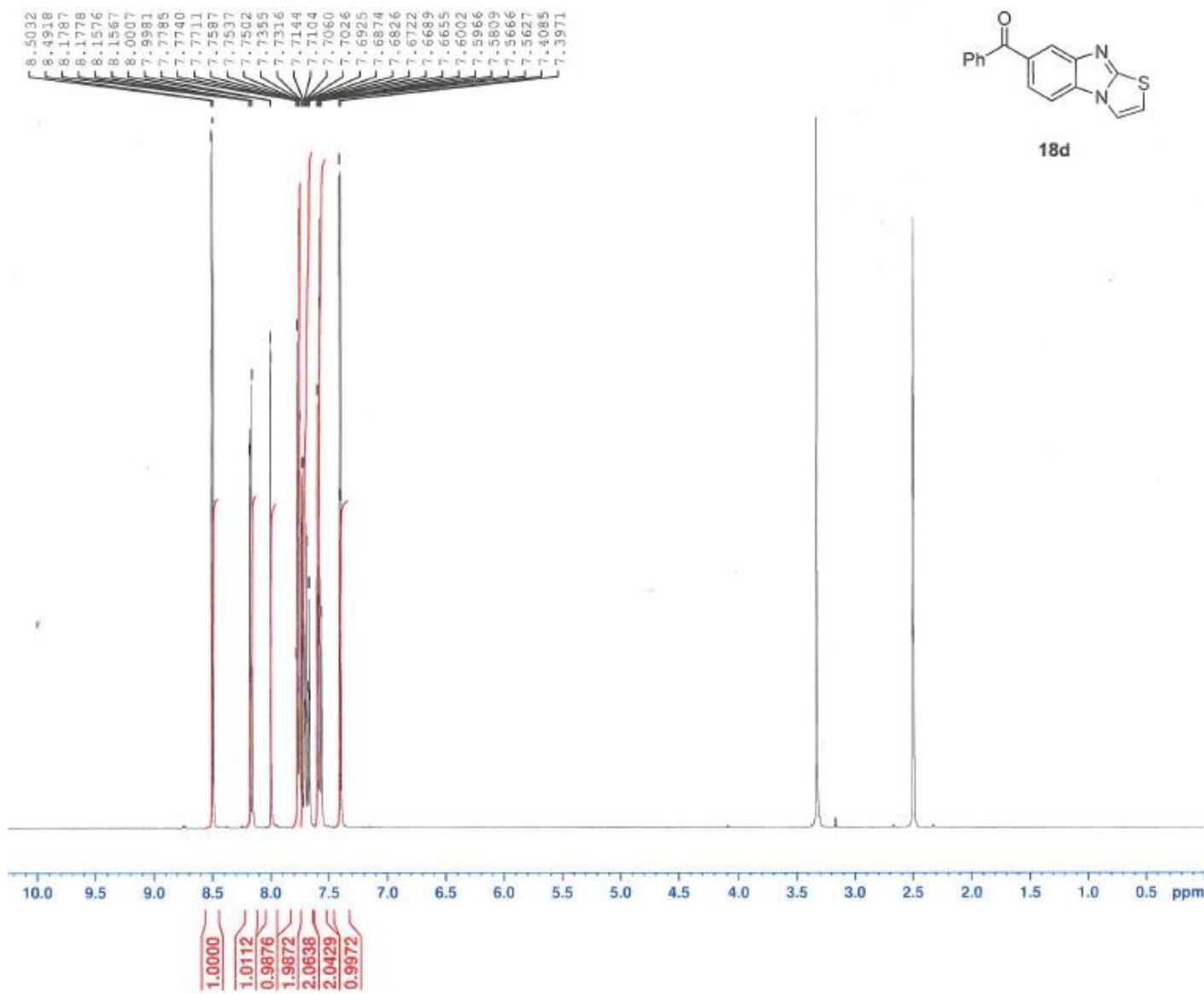
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 Time 9.39
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 SOLVENT dmo
 NS 128
 DS 0
 SWH 26245.719 Hz
 FIDRES 0.400493 Hz
 AQ 1.2485108 sec
 RG 8192
 DW 19.050 usec
 DE 6.50 usec
 TE 300.0 K
 d11 0.0300000 sec
 d12 0.0000200 sec
 PL13 22.00 dB
 D1 5.00000000 sec
 CPDPG2 Waltz16
 PCPD2 110.00 usec
 SF02 400.1326090 MHz
 NUC2 1H
 PL2 120.00 dB
 PL12 20.00 dB
 P1 7.50 usec
 DE 6.50 usec
 SF01 100.5246442 MHz
 NUC1 13C
 PL1 -2.00 dB

F2 - Processing parameters
 SI 32768
 SF 100.5126839 MHz
 NDN EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 22.00 cm
 F1P 200.000 ppm
 F1 20122.55 Hz
 F2P -1.000 ppm
 F2 -100.51 Hz
 PPMH 9.13635 ppm/cm
 HZCM 919.23535 Hz/cm



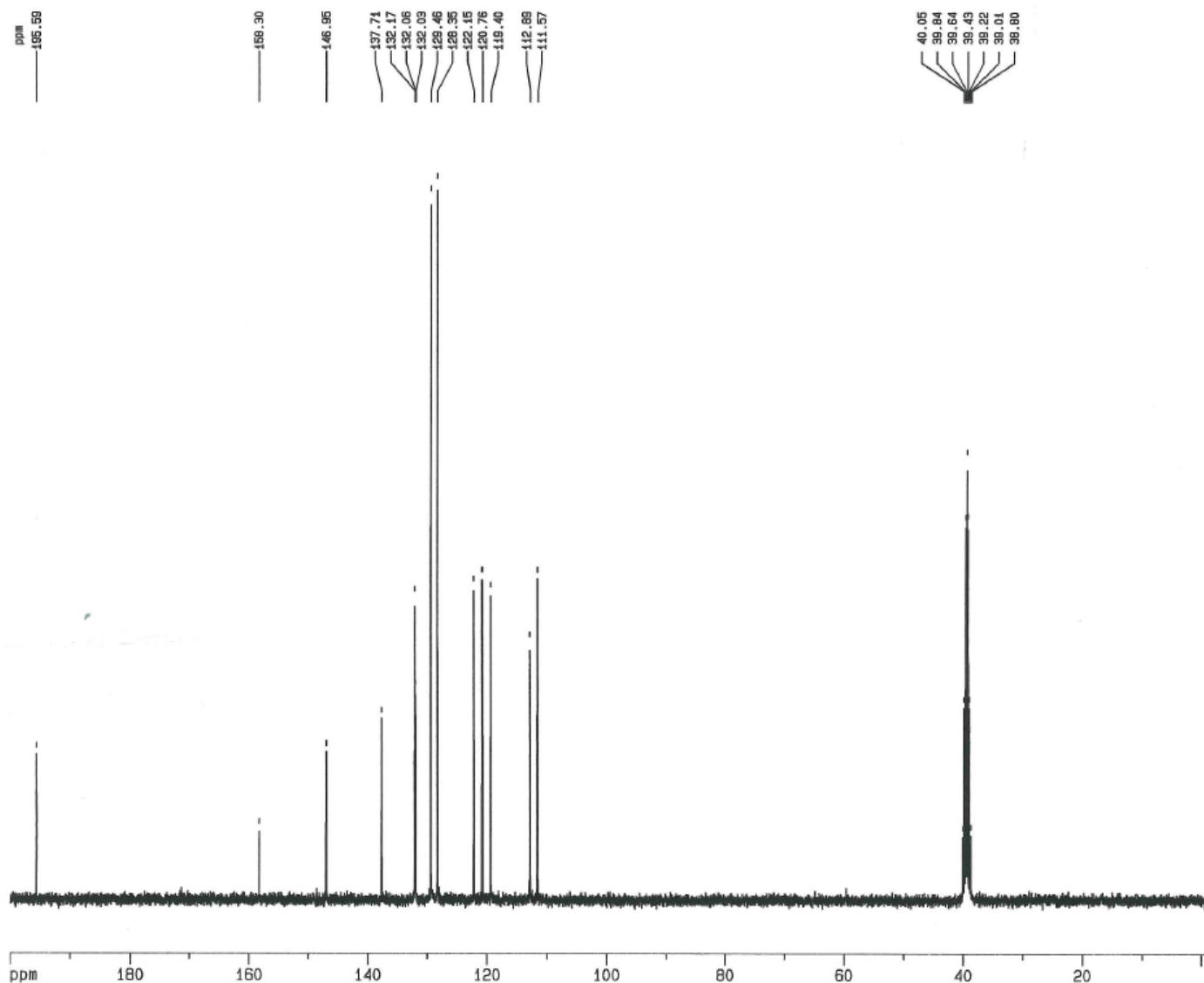




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 EXPNO 3
 PROCNO 1

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 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 64
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
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 RG 174.55
 DW 62.400 usec
 DE 6.50 usec
 TE 299.0 K
 D1 1.00000000 sec
 TDS 3
 SRQ1 400.1324708 MHz
 NDC1 1R
 P0 4.53 usec
 P1 13.60 usec
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 PC 1.00

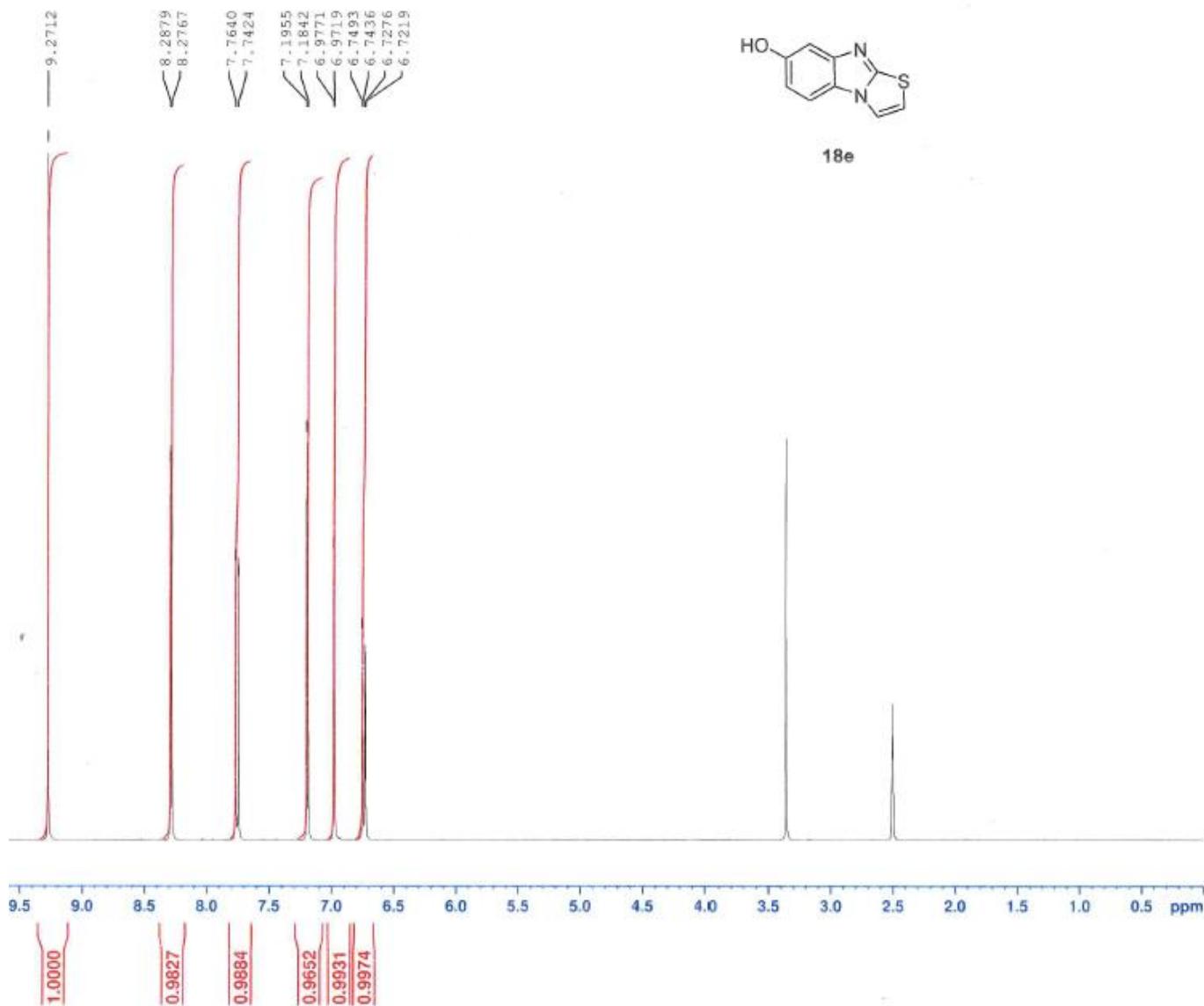


Current Data Parameters
NAME crie.fr
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PROCNO 1

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PULPROG zgpg
TD 65536
SOLVENT dmso
NB 72
DS 0
SWH 26246.719 Hz
FIDRES 0.400493 Hz
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RG 6502
DM 19.050 usec
DE 6.50 usec
TE 300.0 K
d11 0.0300000 sec
d12 0.0000200 sec
PL13 22.00 dB
D1 5.0000000 sec
CPDPRE2 waltz16
PCPD2 10.00 usec
SF02 400.1326090 MHz
NUC2 1H
PL2 120.00 dB
PL12 20.00 dB
P1 7.50 usec
DE 6.50 usec
SF01 100.6248442 MHz
NUC1 13C
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F2 - Processing parameters
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SSB 0
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GB 0
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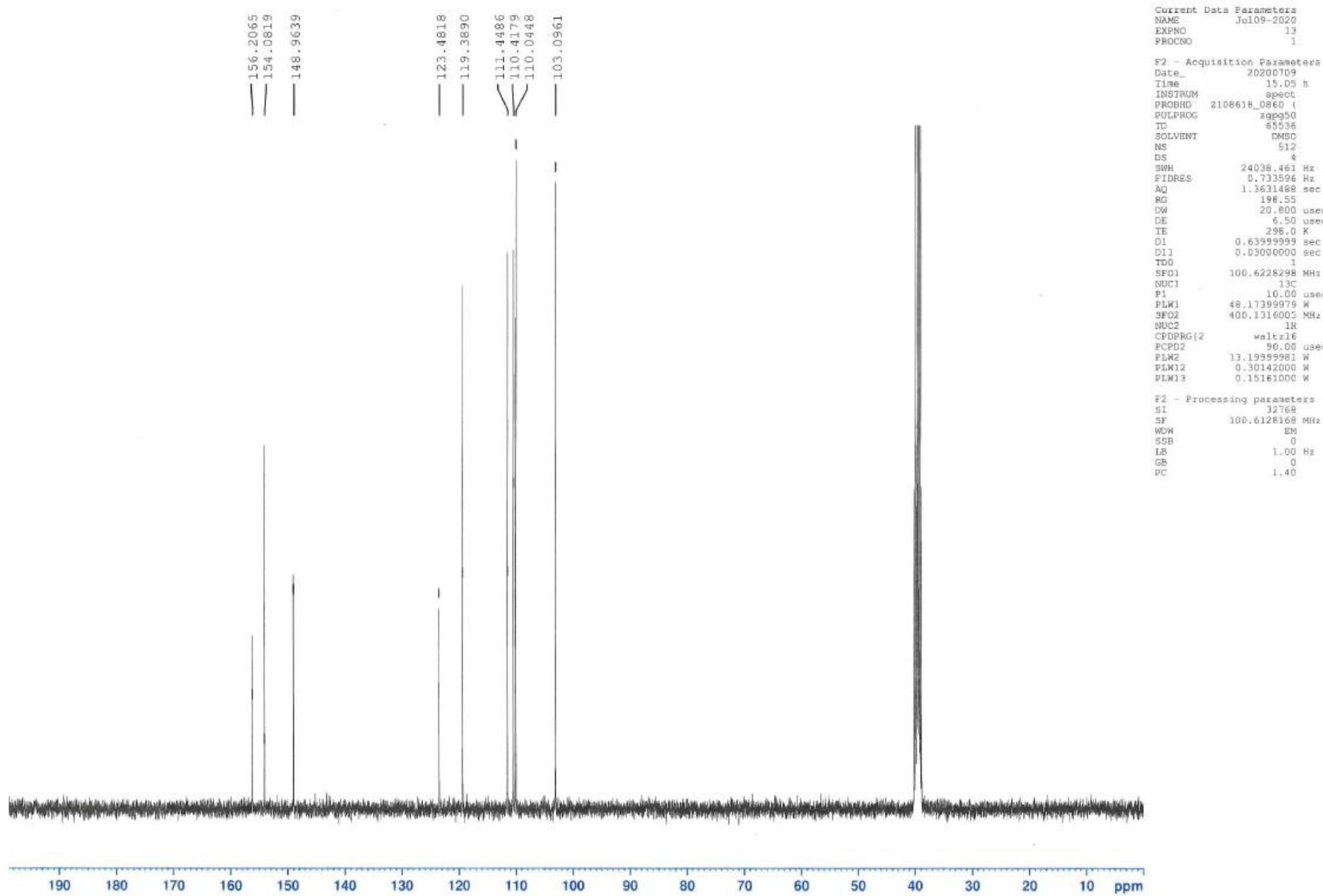
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F1 20122.56 Hz
F2P -1.000 ppm
F2 -100.51 Hz
PPMCH 9.13636 ppm/cm
HZCH 919.23535 Hz/cm

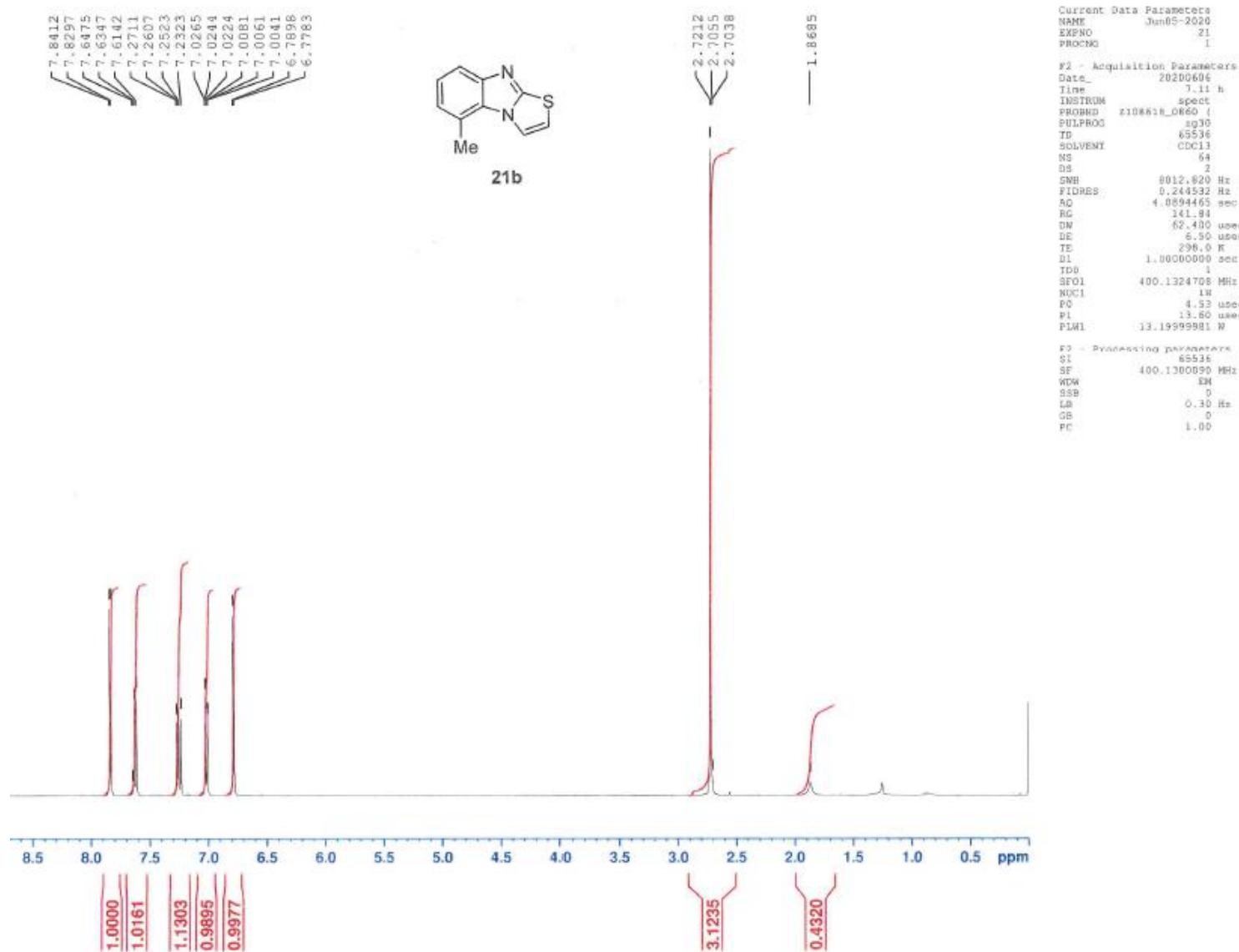


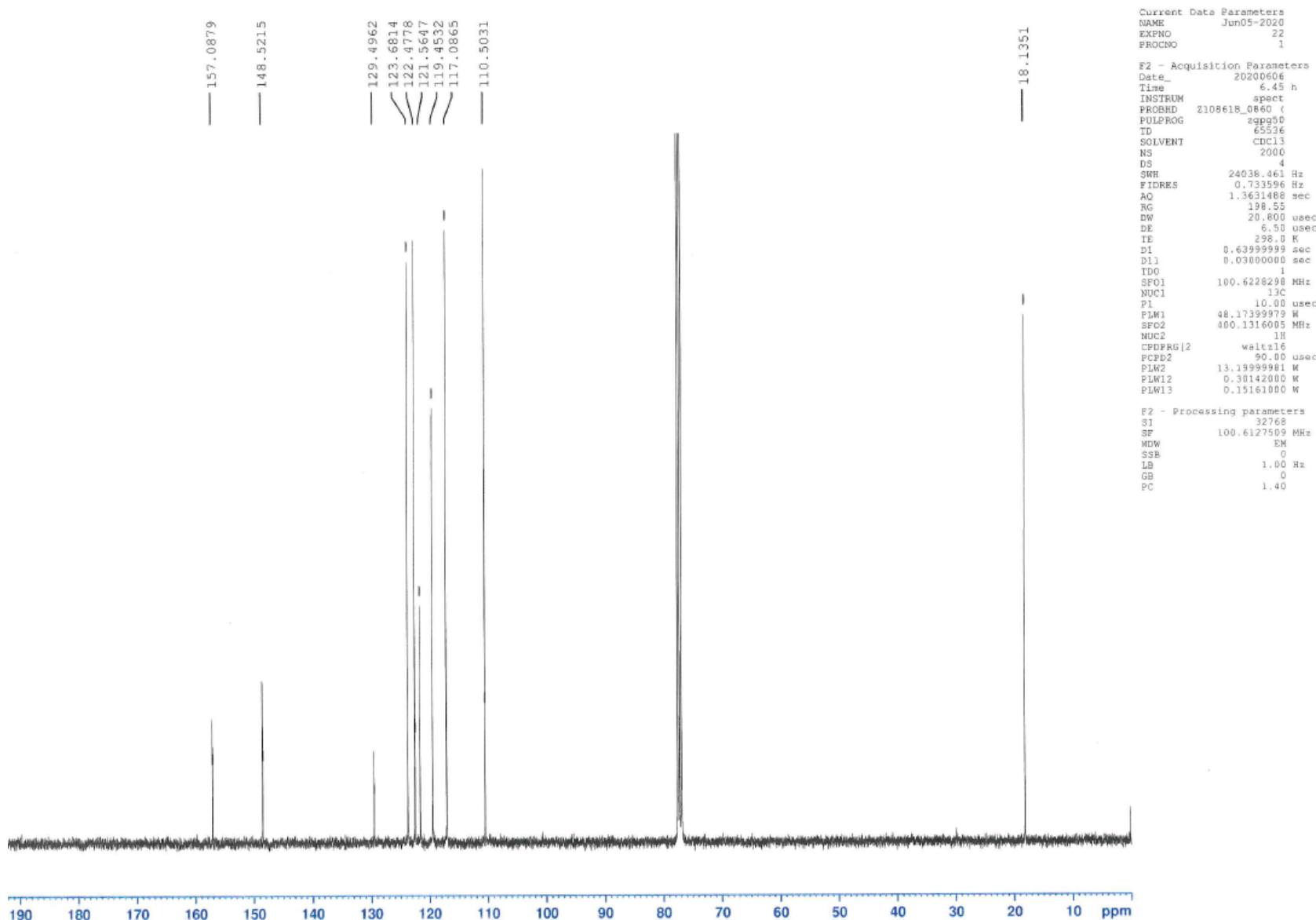
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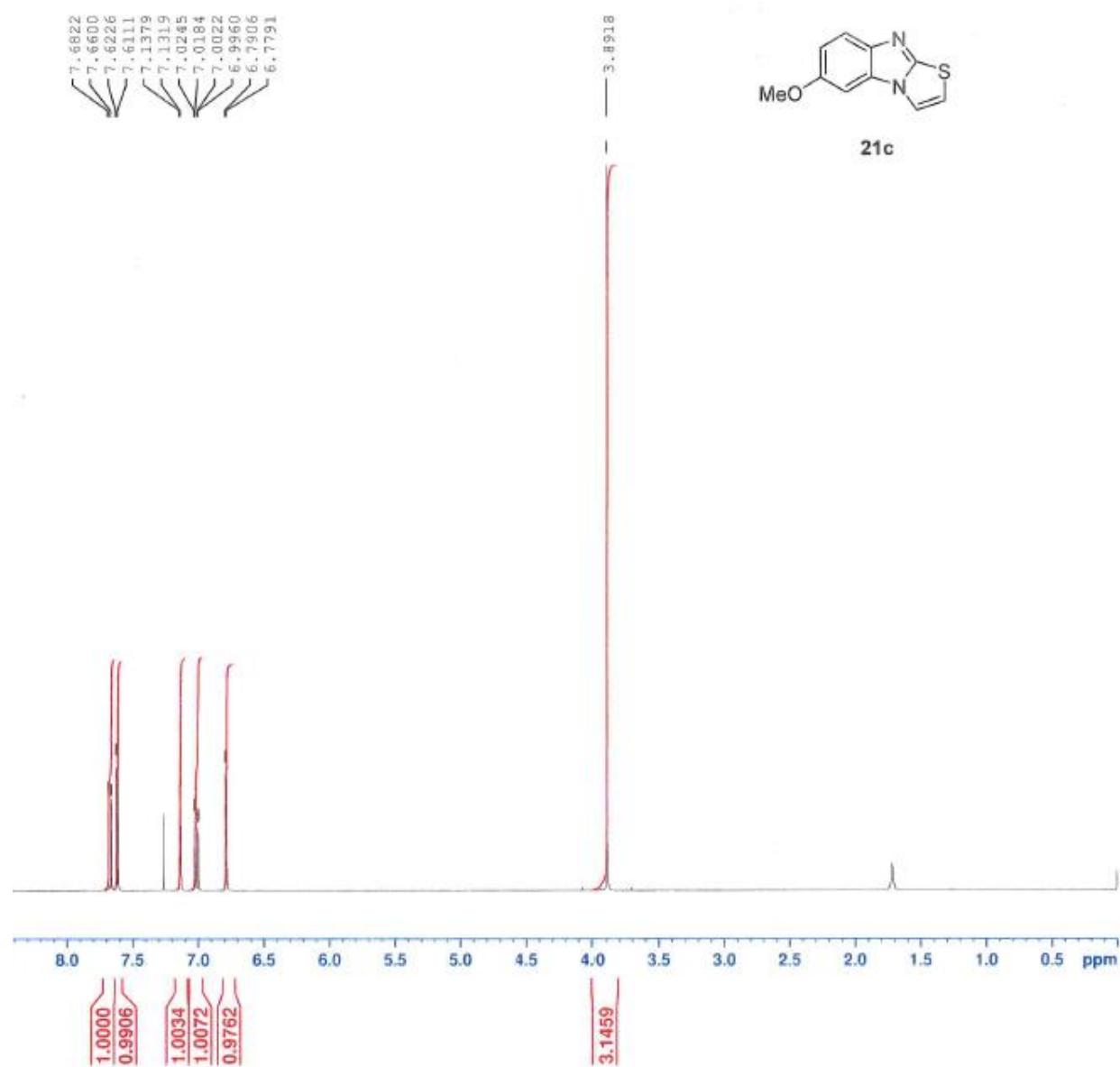
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 PULPROG zap30
 TD 65536
 SOLVENT DMSO
 NS 64
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 141.84
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDR 1
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 NUC1 1H
 PC 4.53 usec
 PL 13.60 usec
 P1M1 13.1999991 N

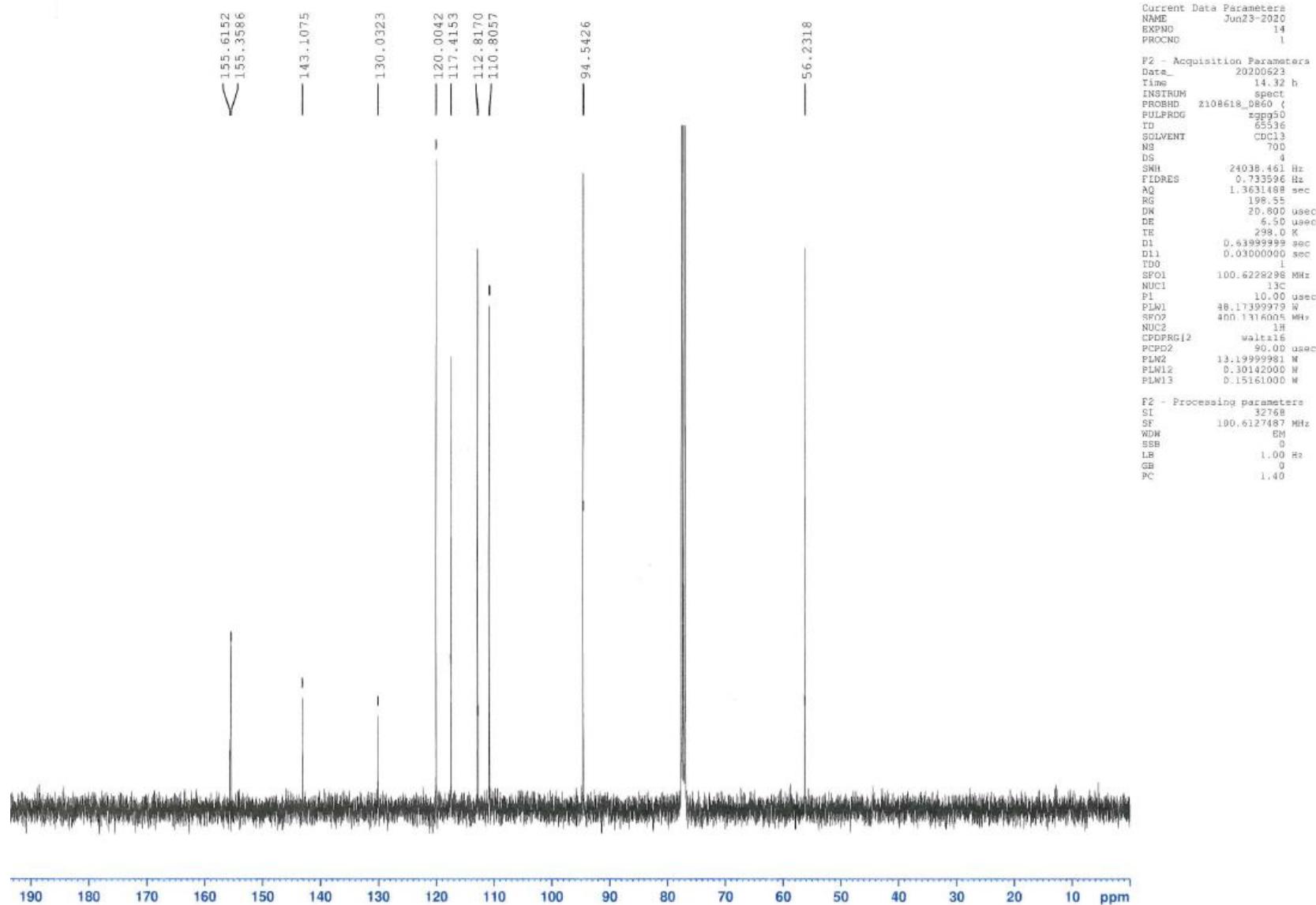
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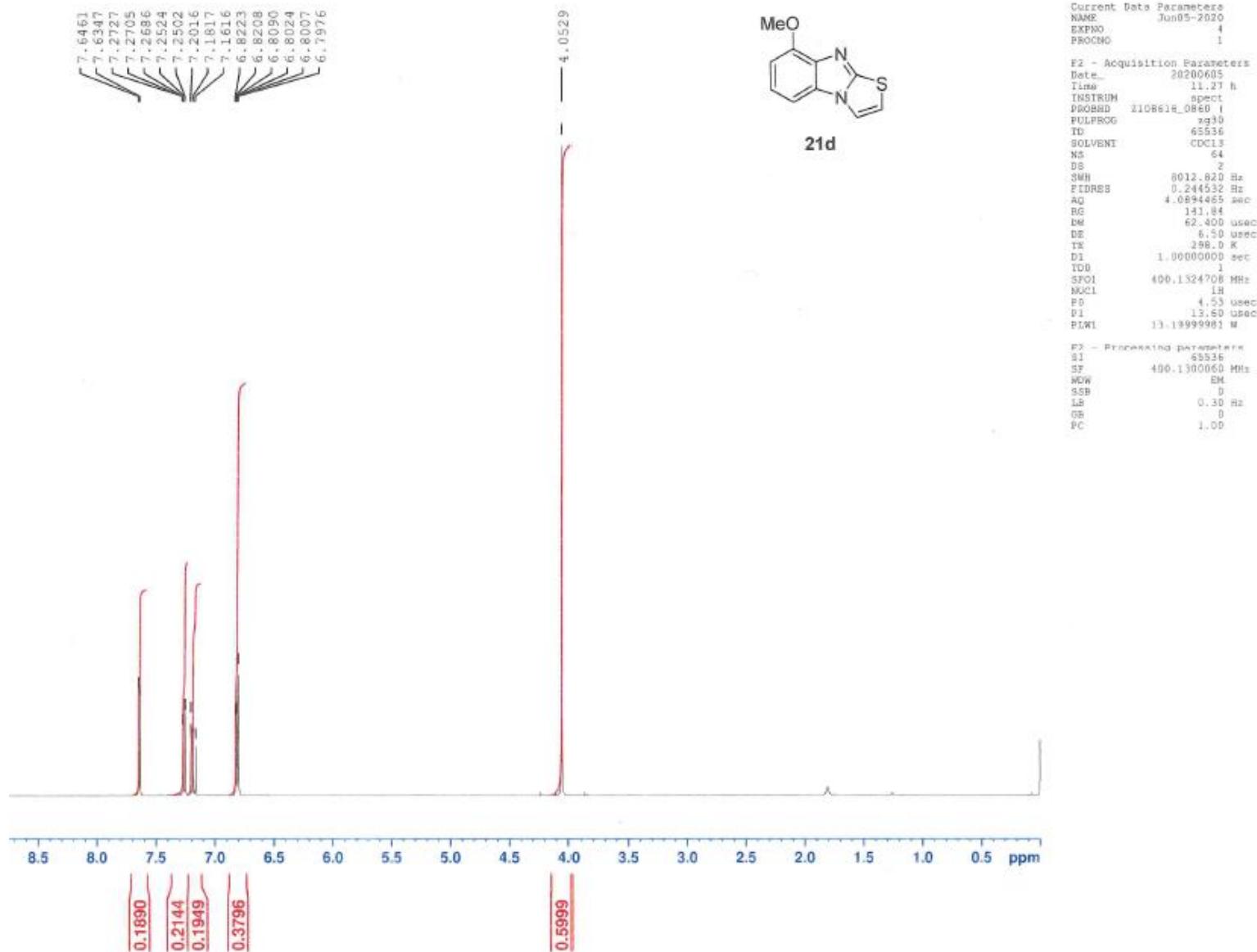


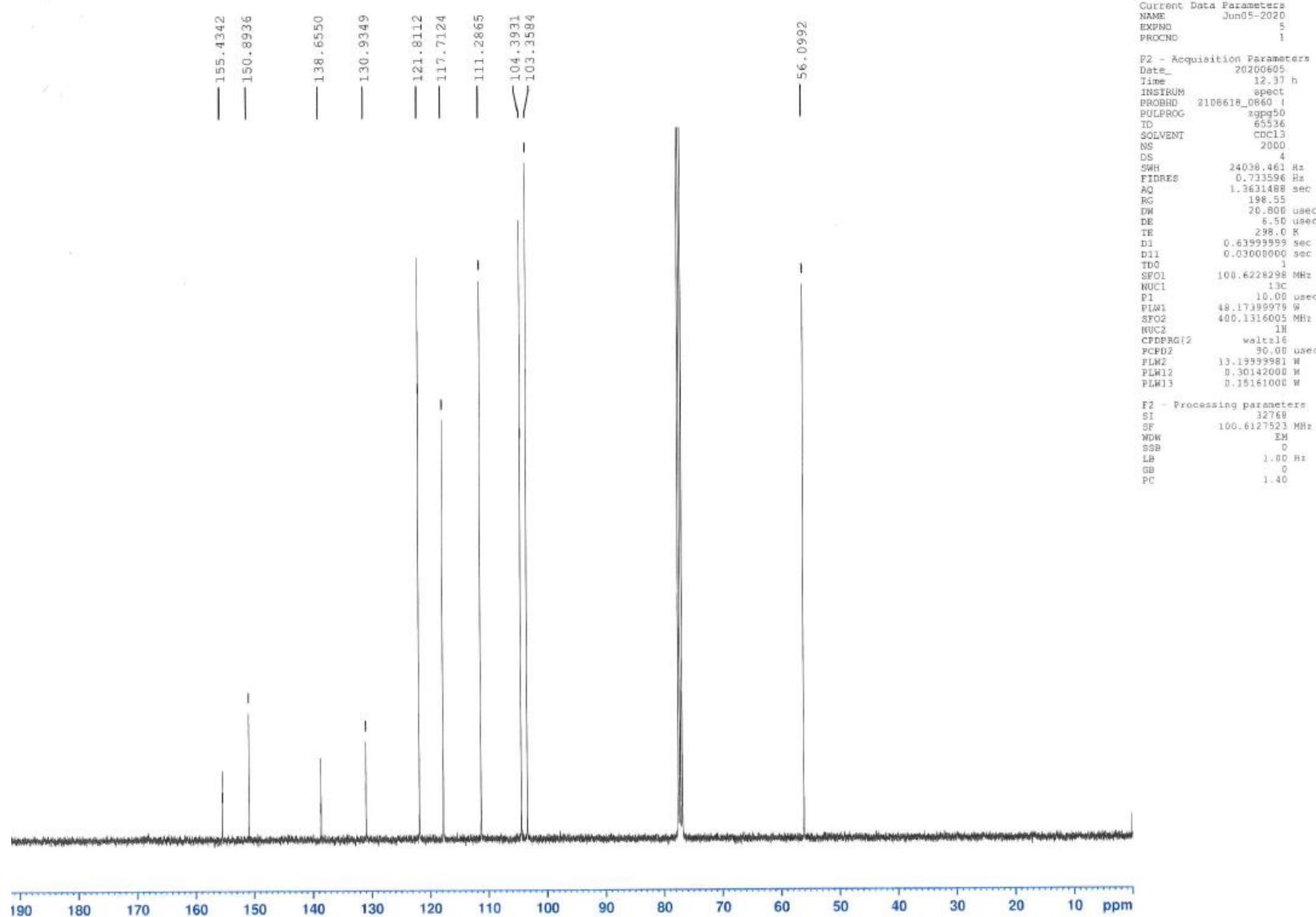


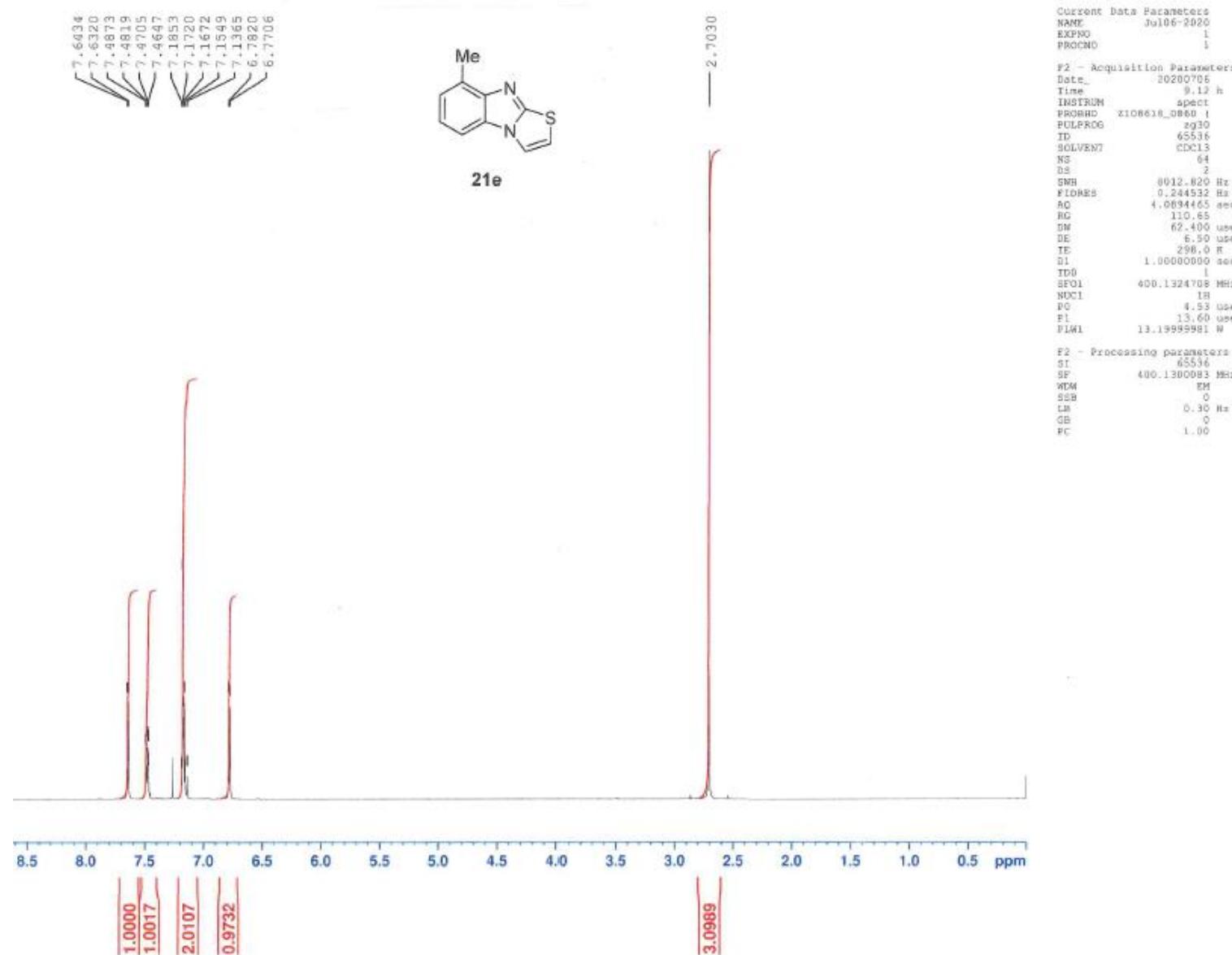


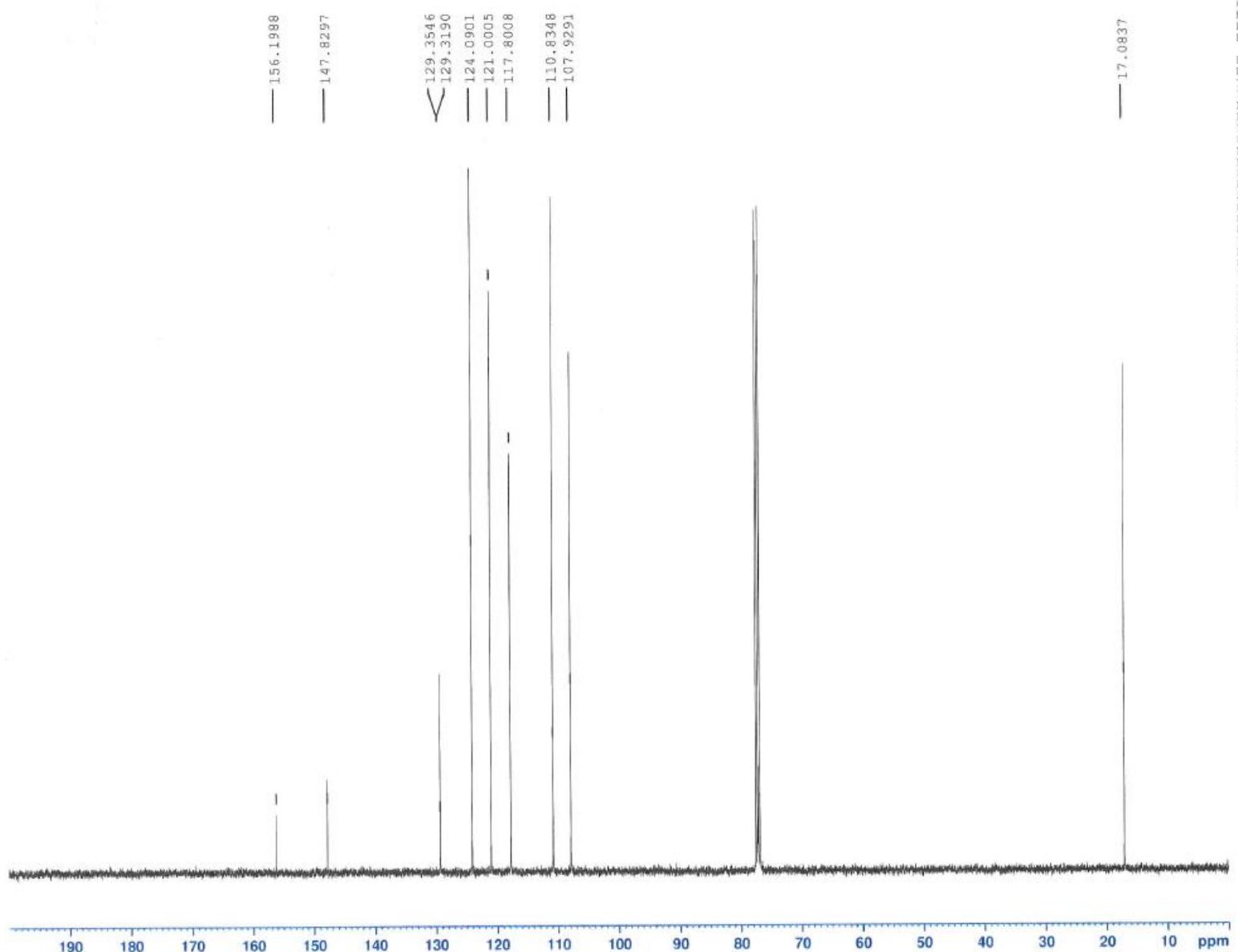


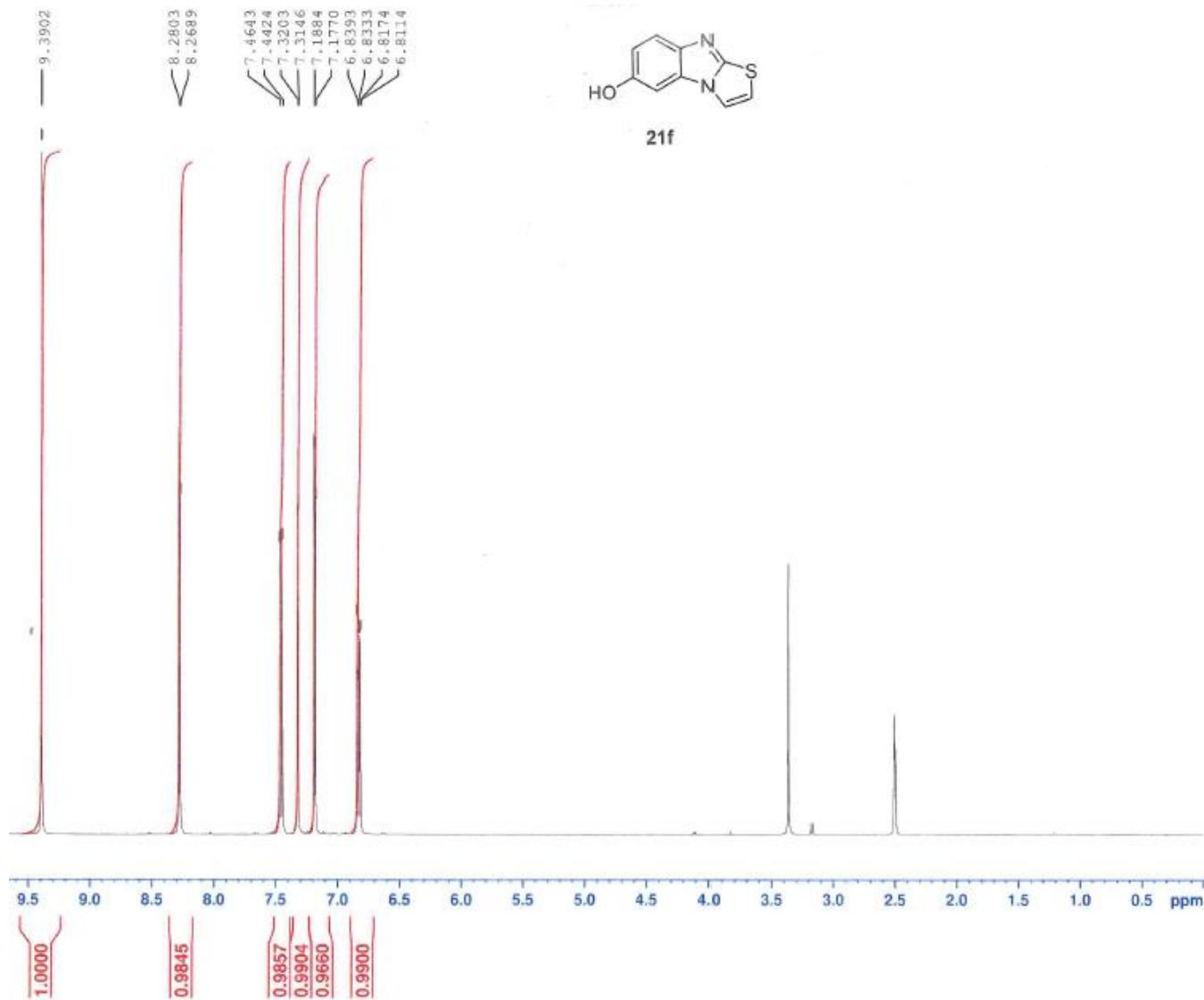








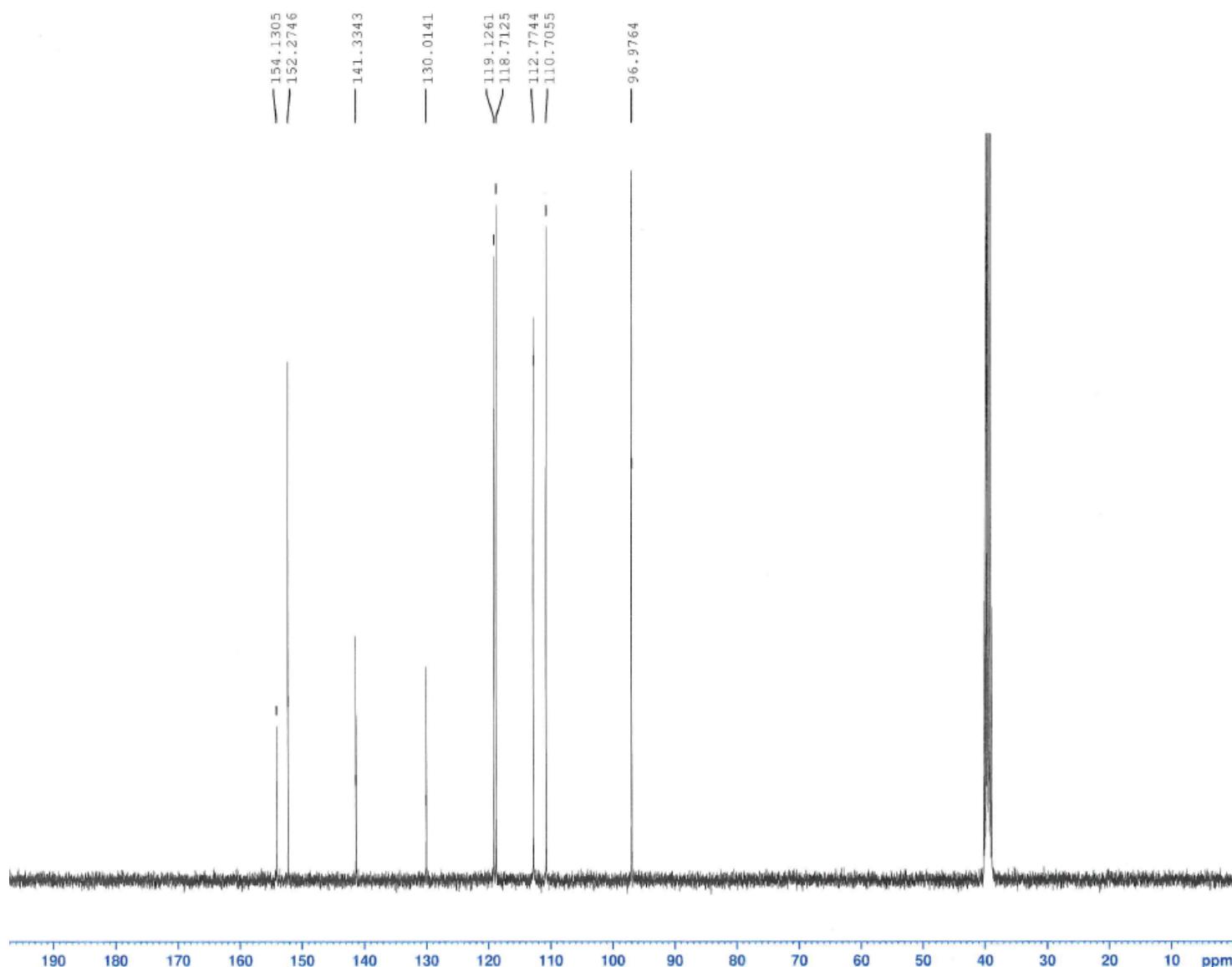




Current Data Parameters
NAME Jul09-2020
EXPNO 1
PROCNO 1

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Time_ 13.46 h
INSTRUM spect
PROBHD 2108618_0860 (PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWR 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 141.80
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1
SFO1 400.1324798 MHz
MUC1 1H
PO 4.53 usec
P1 13.60 usec
PLW1 13.19999981 M

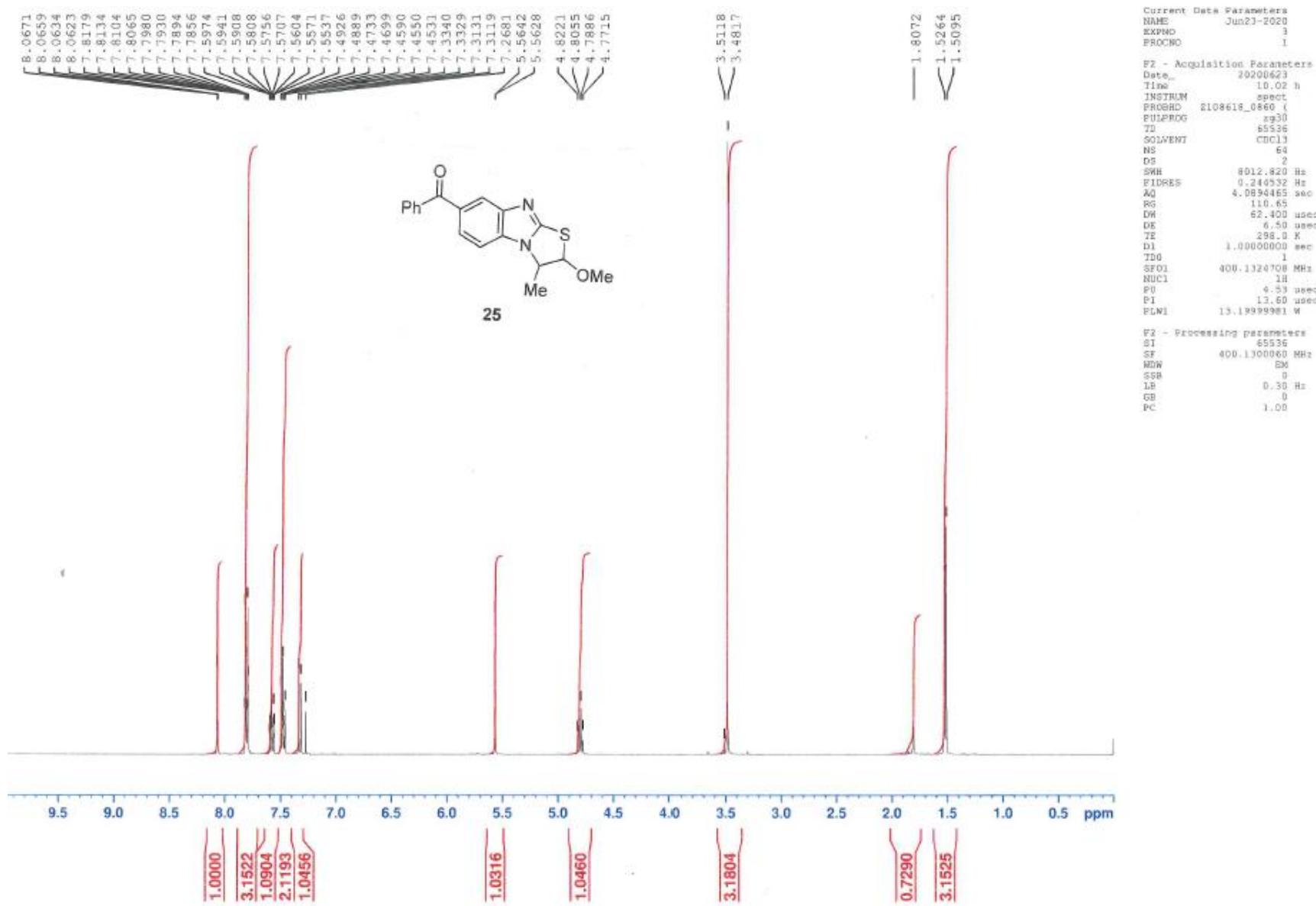
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SSB 0
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GB 0
PC 1.00

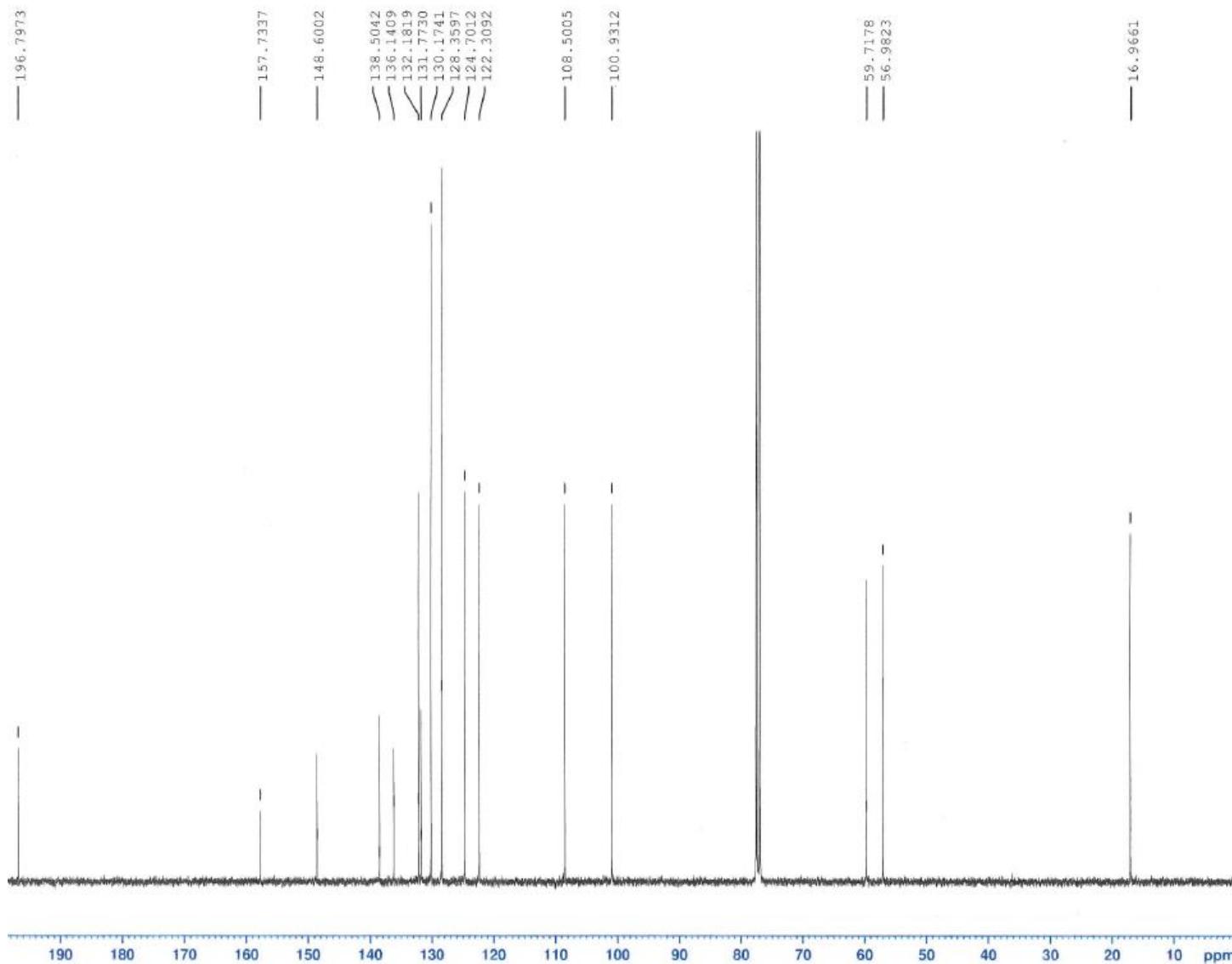


Current Data Parameters
NAME Jul09-2020
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
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Time 14.05 h
INSTRUM spect
PROBHD Z108618_0860_1
PULPROG zgpg50
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24036.461 Hz
FIDRES 0.73595 Hz
AQ 1.3631488 sec
RG 198.55
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 0.6399999 sec
D11 0.0300000 sec
TDQ 1
SP01 100.6228298 MHz
NUC1 ¹³C
P1 10.00 usec
PLW1 4E.17399979 W
SP02 400.1316005 MHz
NUC2 ¹H
CPDPFG[2] waltz16
PCPD2 90.00 usec
PLW2 13.19999981 W
PLW12 0.30142000 W
PLW13 0.15161000 W

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SSB D
LB 1.00 Hz
GB D
PC 1.40

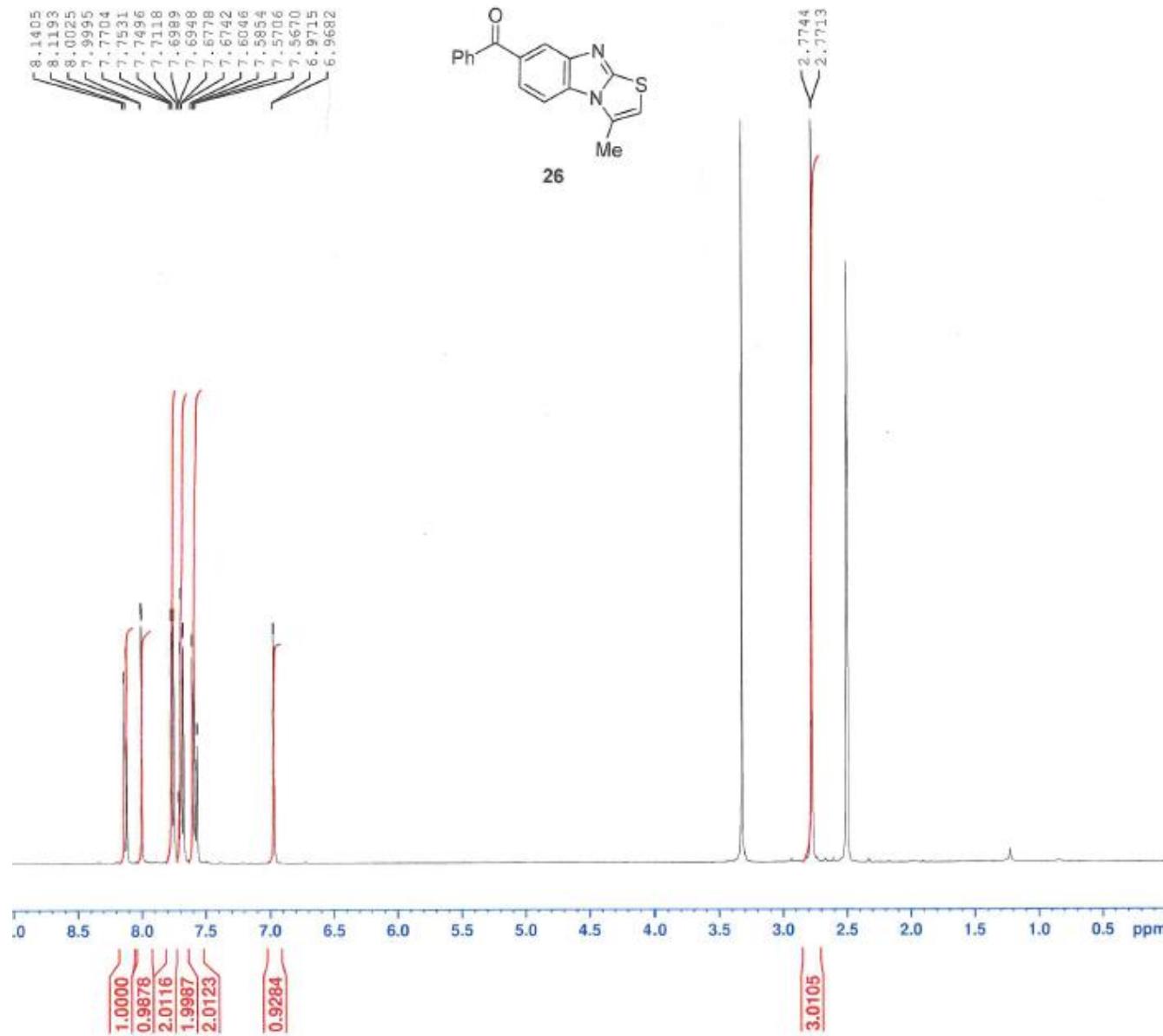




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 EXPNO 4
 PROCN0 1

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 Time_ 10.52 h
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 PULPROG zgpg50
 TD 65536
 SOLVENTI CDCl3
 NS 1161
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 1.3631488 sec
 RG 198.55
 DW 20.800 usec
 DE 6.50 usec
 JE 298.0 K
 D1 0.63999999 sec
 D11 0.03000000 sec
 TDD 1
 SF01 100.6228298 MHz
 NUC1 13C
 F1 10.00 usec
 PLW1 48.17399979 w
 SF02 400.1316005 MHz
 NUC2 1H
 CPDPFG[1]2 wait16
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 PLW2 13.19999981 w
 PLW12 0.30142000 w
 PLW13 0.15161000 w

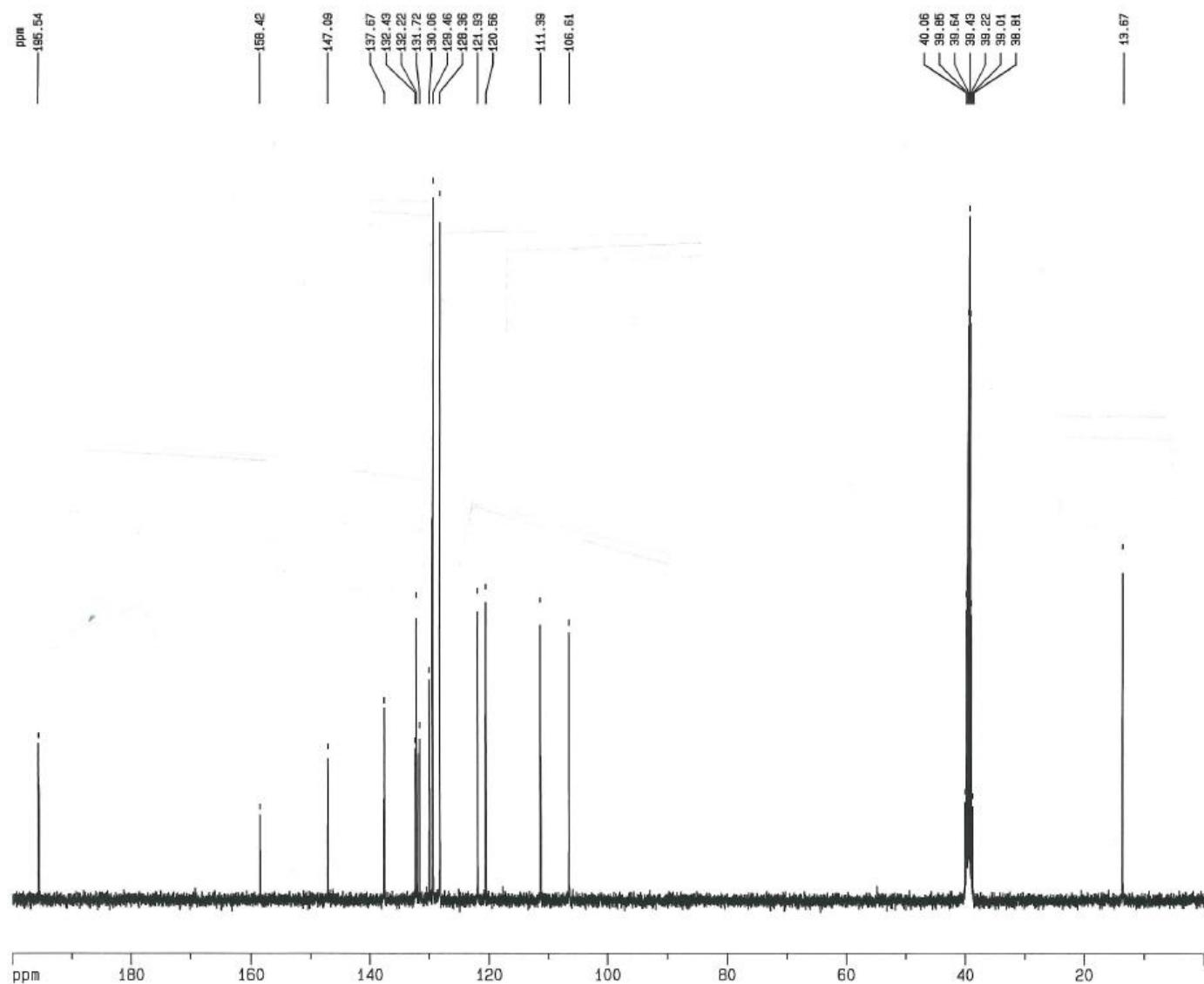
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 LB 1.00 Hz
 GB 0
 FC 1.00



Current Data Parameters
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 EXPNO 5
 PROCNO 1

P2 - Acquisition Parameters
 Date_ 20200729
 Time 12.07 h
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 PULPROG zg30
 T1 65536
 SOLVENT DMSO
 MS 64
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 198.55
 DW 62.400 usec
 DR 6.50 usec
 TR 298.0 K
 D1 1.0000000 sec
 TDO 1
 SF01 100.1324708 MHz
 NUC1 1H
 P0 4.53 usec
 P1 13.60 usec
 PLW1 13.19999981 K

P3 - Processing parameters
 DT 65536
 SF 400.1300024 MHz
 WM EM
 SSF 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME criex.fr
 EXPNO 5
 PROCN 1

F2 - Acquisition Parameters
 Date_ 971024
 Time 8.42
 INSTRUM spect
 PROBHD 5 mm Dual 13
 PULPROG zgpg
 TD 65536
 SOLVENT dmoa
 NS 128
 DS 0
 SWH 26246.719 Hz
 FIDRES 0.400493 Hz
 AQ 1.2485108 sec
 RG 8192
 DM 19.050 usec
 DE 6.50 usec
 TE 300.0 K
 d11 0.0300000 sec
 d12 0.0000200 sec
 PL13 22.00 dB
 D1 5.0000000 usec
 CPDPRG2 waltz15
 PCP02 110.00 usec
 SF02 400.13265090 MHz
 NUC2 1H
 PL2 120.00 dB
 PL12 20.00 dB
 P1 7.50 usec
 DE 6.50 usec
 SF01 100.6246442 MHz
 NUC1 13C
 PL1 -2.00 dB

F2 - Processing parameters
 SI 32768
 SF 100.6126255 MHz
 WM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 22.00 cm
 F1P 200.000 ppm
 F1 20122.56 Hz
 F2P -1.000 ppm
 F2 -100.61 Hz
 PPWCH 9.13636 ppm/cm
 HZCH 919.23535 Hz/cm