

Supporting Information

One-pot mild and efficient synthesis of [1,3]thiazino[3,2-*a*]indol-4-ones and their anti-proliferative activity

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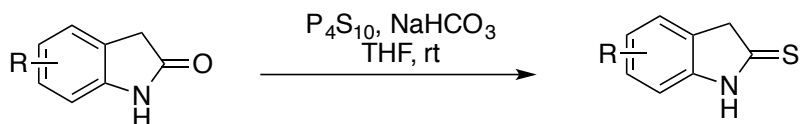
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Canada

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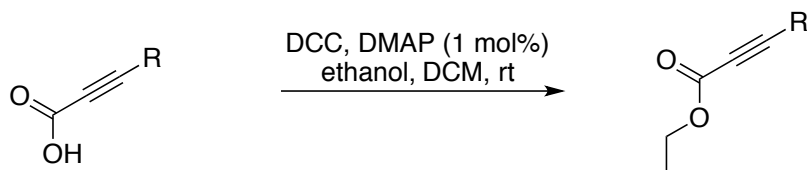
General Remarks: Melting points were determined in open capillary tubes on an automated melting point apparatus and are uncorrected. Reactions were monitored using thin layer chromatography (TLC) on 0.2 mm silica gel F254 plates. The chemical structures of final products were determined by their NMR spectra (^1H and ^{13}C NMR) using 300 MHz spectrometer. ^{13}C NMR spectra are fully decoupled. High-resolution mass spectra (HRMS) were carried out using a quadrupole time-of-flight (qTOF) mass spectrometer. Chemicals obtained from the commercial suppliers were used without further purification.

General Procedure for the Synthesis of Indoline-2-thiones **8**¹



To a solution of appropriate indolin-2-ones (22.53 mmol) in 60 mL anhydrous THF, NaHCO_3 (47.32 mmol) was added and the reaction was left to stir at room temperature for 10 minutes. Reagent P_4S_{10} (13.52 mmol) was then added portion wise and the resulting mixture was stirred at room temperature for 1 – 4 hr. On completion of the reaction, as indicated by TLC, the mixture was concentrated in *vacuo* to one fourth of its volume. Ice-cold water (30 mL) was then added in small portions to the oily residue with vigorous stirring, which resulted into precipitate formation. The mixture was left to stand in the ice-cold water for 15 minutes before vacuum filtration. The precipitates collected were washed with water followed by hexanes and air dried to yield various indoline-2-thions **8** in 80-90% yields.

General Procedure for the Synthesis of propiolate esters **18**²



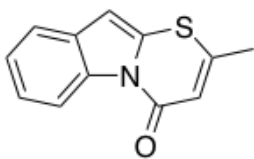
To a mixture of DCC (0.51 mmol) and DMAP (1 mol%) in 1 mL of DCM was added drop wise an ice-cold mixture of appropriated propiolic acid (0.51 mmol) and ethanol (0.56 mmol) dissolved in 1 ml of DCM. The reaction was then stirred at room temperature for 3 h. Upon completion of the reaction, based on TLC, the reaction mixture was diluted with water and extracted with ethyl acetate. The organic layer was then washed with brine (2 mL) and dried over Na_2SO_4 . Further, the dried organic layer was concentrated in *vacuo* and the resulting residue was purified using column chromatography using 10% ethyl acetate in hexanes go yield the propiolate esters **18** in 86-90% yields.

¹ M. Jha, G. M. Shelke, T. S. Cameron and A. Kumar, *J. Org. Chem.*, 2015, **80**, 5272-5278.

² P. V. Ramachandran, M. T. Rudd and M. V. Reddy, *Tetrahedron Lett.*, 2005, **46**, 2547-2549.

**^1H NMR and ^{13}C NMR Spectra
for compounds 10, 17, and 19-34**

2-methyl-4H-[1,3]thiazino[3,2-a]indol-4-one (10)

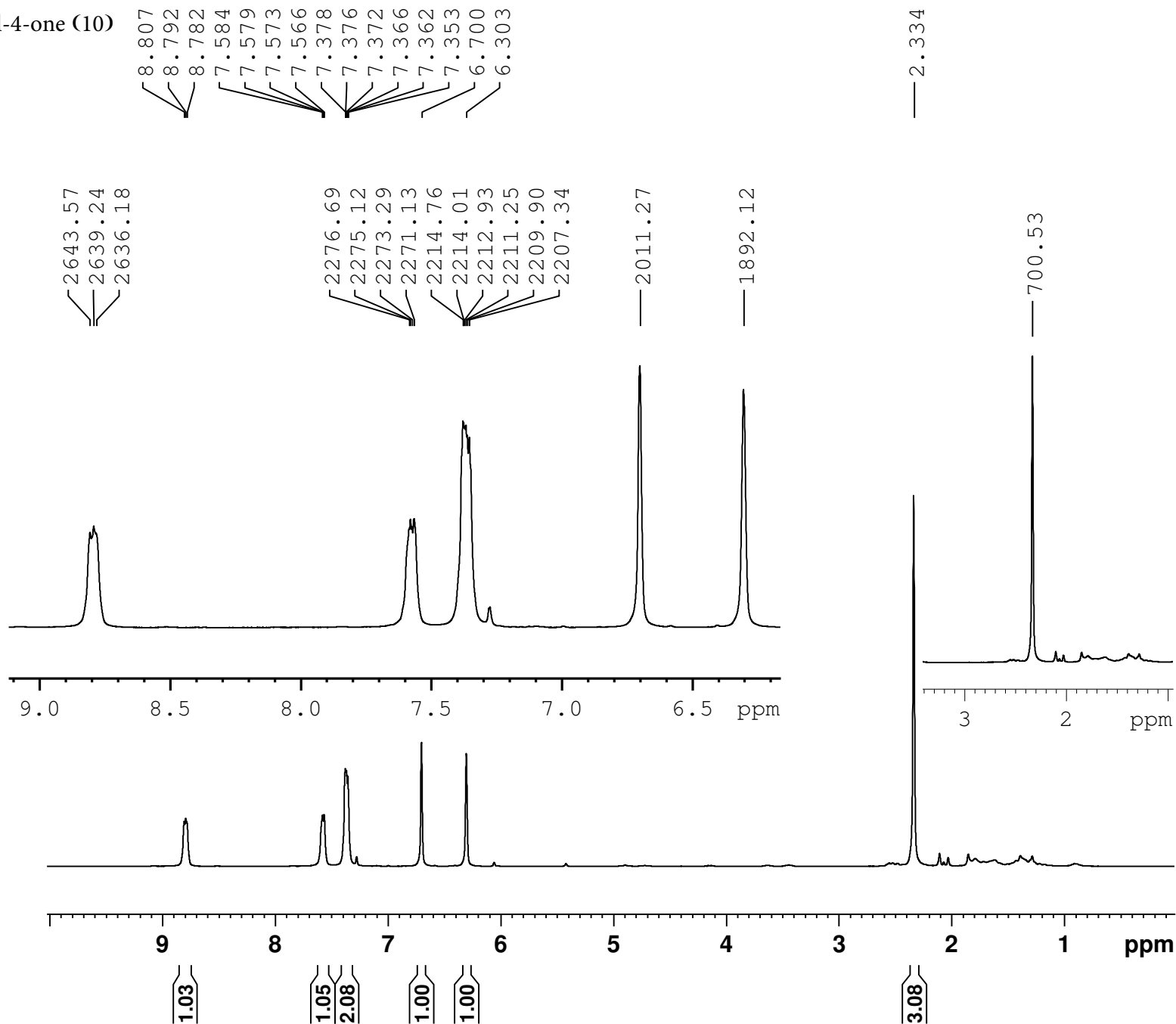


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 PROCNO 1

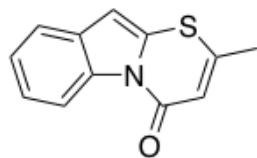
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 SOLVENT CDCl3
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 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 13.6231
 DW 81.920 usec
 DE 6.50 usec
 TE 293.8 K
 D1 1.00000000 sec
 TD0 1

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 NUC1 1H
 P1 12.00 usec
 PLW1 10.00000000 W

F2 - Processing parameters
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 SF 300.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



2-methyl-4H-[1,3]thiazino[3,2-a]indol-4-one (10)



Current Data Parameters
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 PROCNO 1

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 FIDRES 0.372529 Hz
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 RG 199.526
 DW 20.480 usec
 DE 6.50 usec
 TE 293.9 K
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 L5 57
 P32 90.00 usec
 TD0 1

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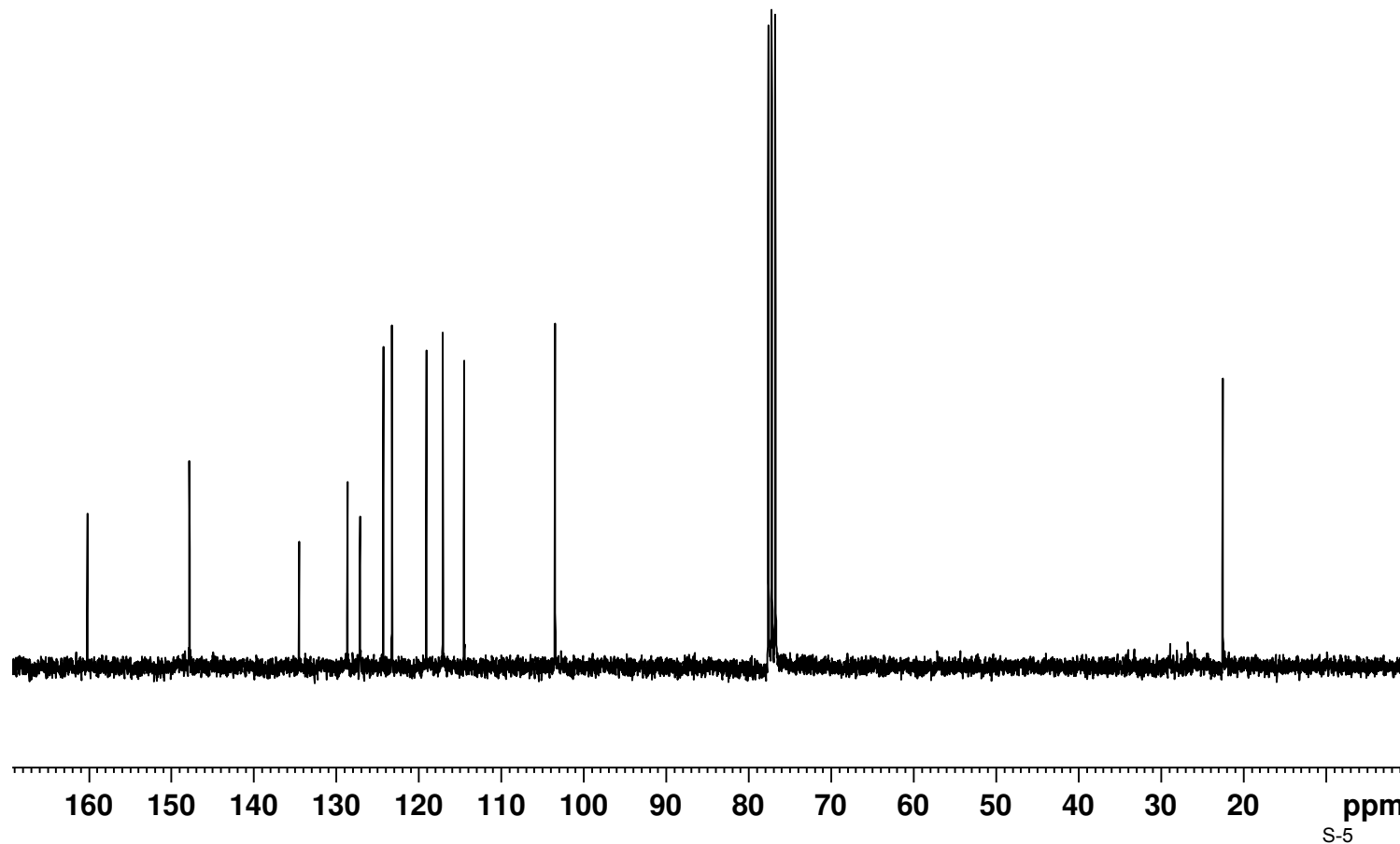
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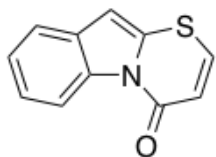
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F2 - Processing parameters

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4H-[1,3]thiazino[3,2-a]indol-4-one (17)



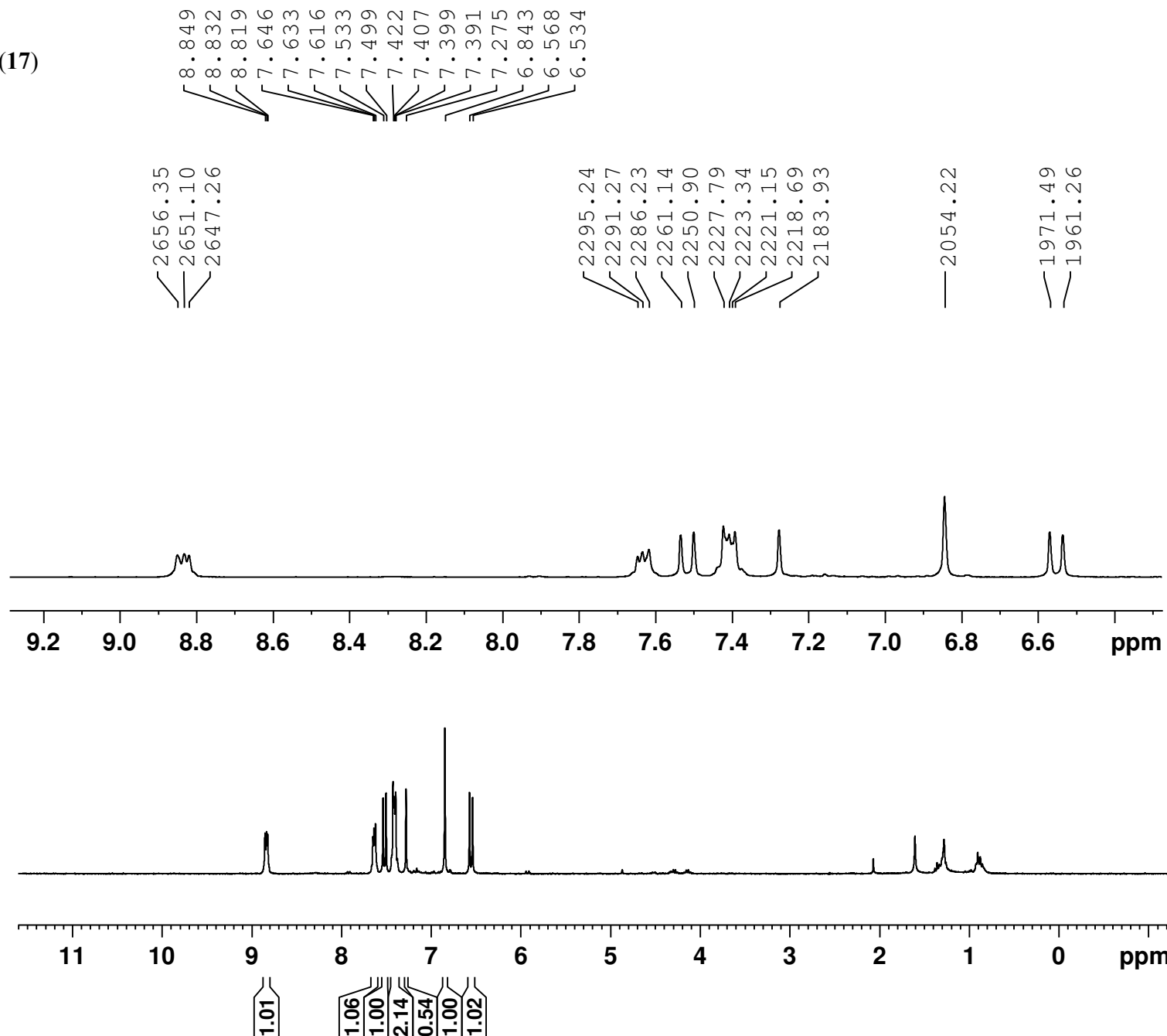
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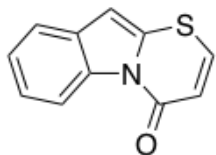
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SOLVENT CDCl3
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DS 2
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FIDRES 0.093132 Hz
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RG 83.5918
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DE 6.50 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1

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P1 12.00 usec
PLW1 10.00000000 W

F2 - Processing parameters
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4H-[1,3]thiazino[3,2-a]indol-4-one (17)



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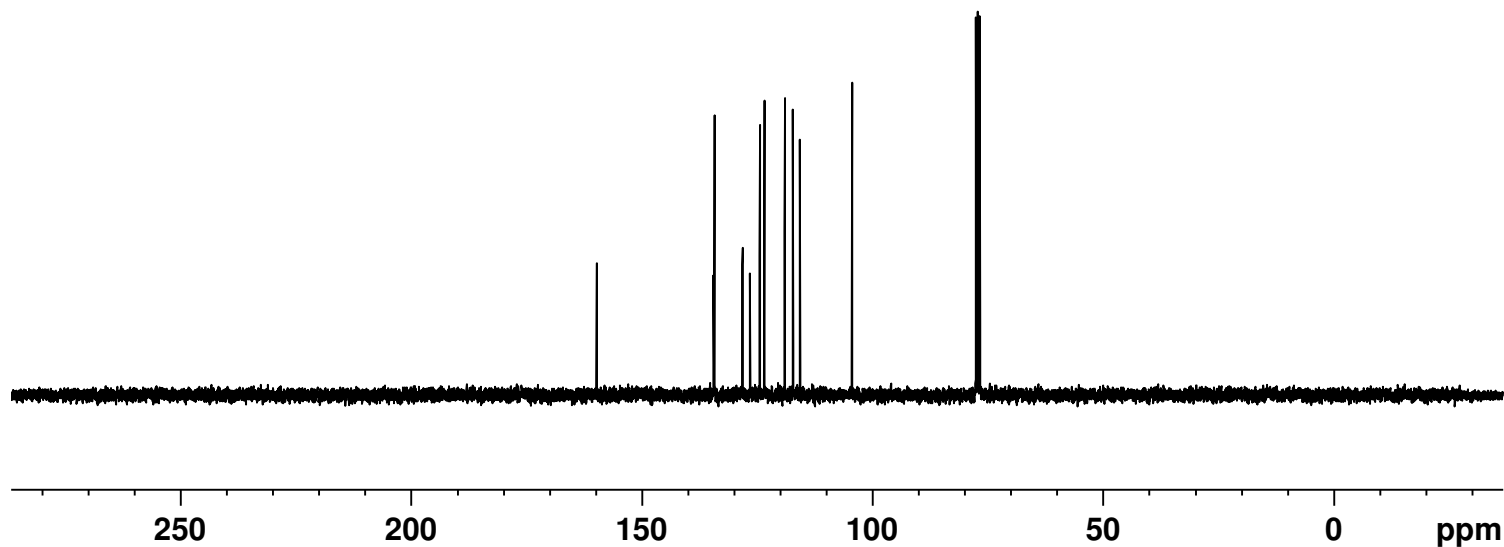
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SOLVENT CDC13
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FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 199.526
DW 20.480 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001200 sec
D40 0.02898005 sec
L4 40
L5 57
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TD0 1

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NUC1 13C
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PLW1 10.00000000 W

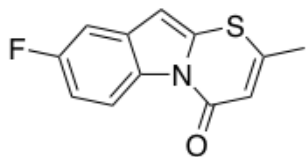
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PLW12 0.21333000 W
PLW13 0.17280000 W

F2 - Processing parameters
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SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

159.76
134.45
134.23
128.19
126.56
124.44
123.41
119.02
117.24
115.73
104.43



8-fluoro-2-methyl-4H-[1,3]thiazino[3,2-a]indol-4-one (20)

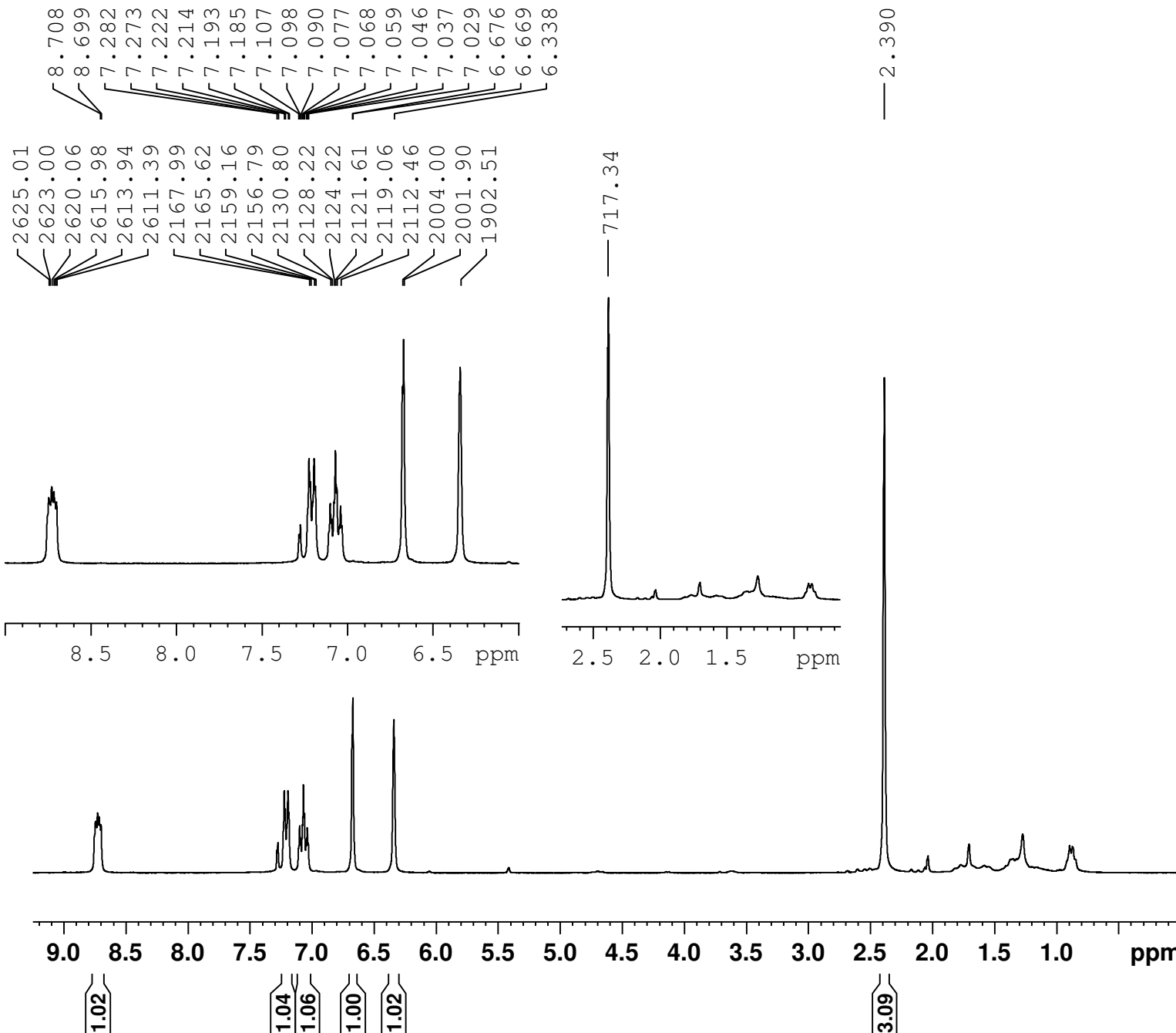


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PROCNO 1

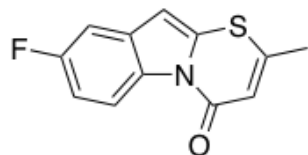
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 31.623
DW 81.920 usec
DE 6.50 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
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NUC1 1H
P1 12.00 usec
PLW1 10.00000000 W

F2 - Processing parameters
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SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



8-fluoro-2-methyl-4H-[1,3]thiazino[3,2-a]indol-4-one (20)



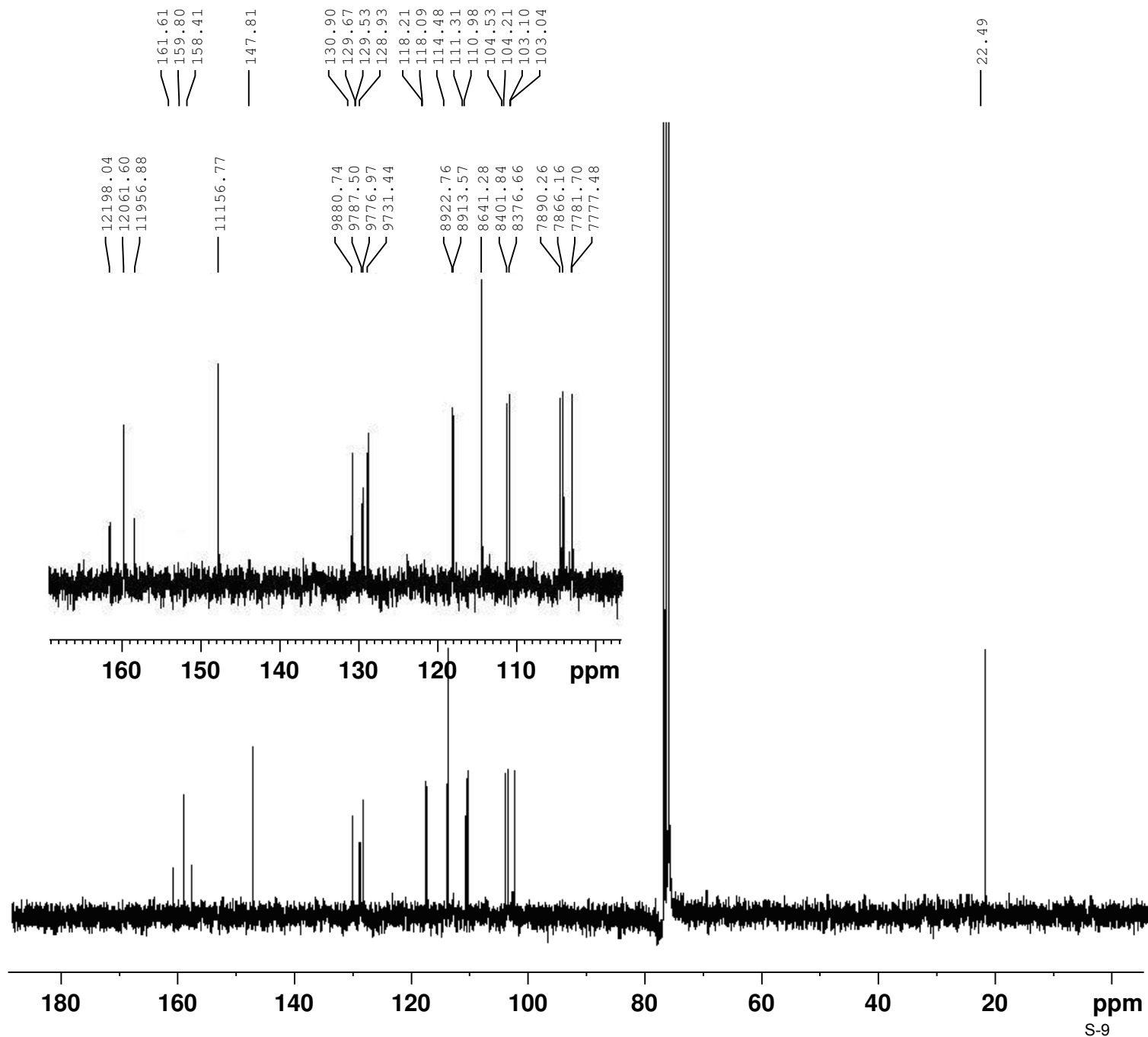
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PROCNO 1

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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1794
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 199.526
DW 20.480 usec
DE 6.50 usec
TE 293.9 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001200 sec
D40 0.02898005 sec
L4 40
L5 57
P32 90.00 usec
TD0 1

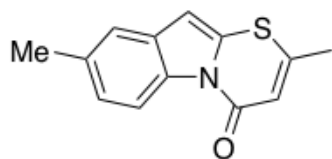
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NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
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PLW12 0.21333000 W
PLW13 0.17280000 W

F2 - Processing parameters
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SF 75.4803210 MHz
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LB 1.00 Hz
GB 0
PC 1.40



2,8-dimethyl-4H-[1,3]thiazino[3,2-a]indol-4-one (21)



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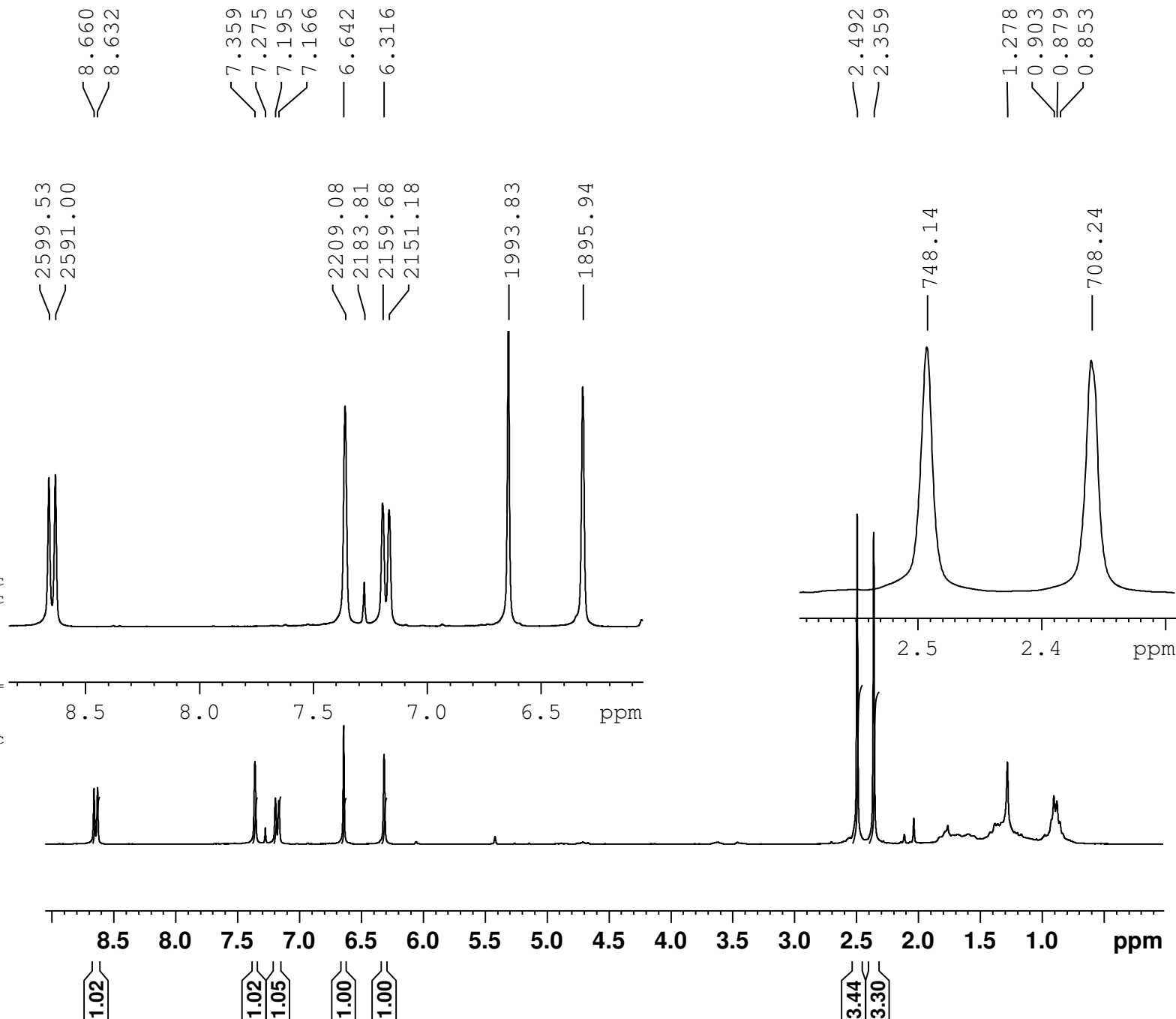
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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
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 RG 13.1704
 DW 81.920 usec
 DE 6.50 usec
 TE 293.1 K
 D1 1.00000000 sec
 TD0 1

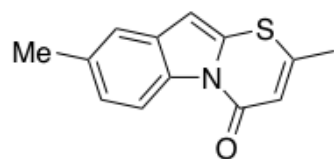
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 PLW1 10.00000000 W

F2 - Processing parameters

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 SF 300.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



2,8-dimethyl-4H-[1,3]thiazino[3,2-a]indol-4-one (21)



— 160.03

— 147.52

133.91

132.69

128.85

126.97

124.67

118.83

116.62

114.48

— 103.13

22.44
21.61

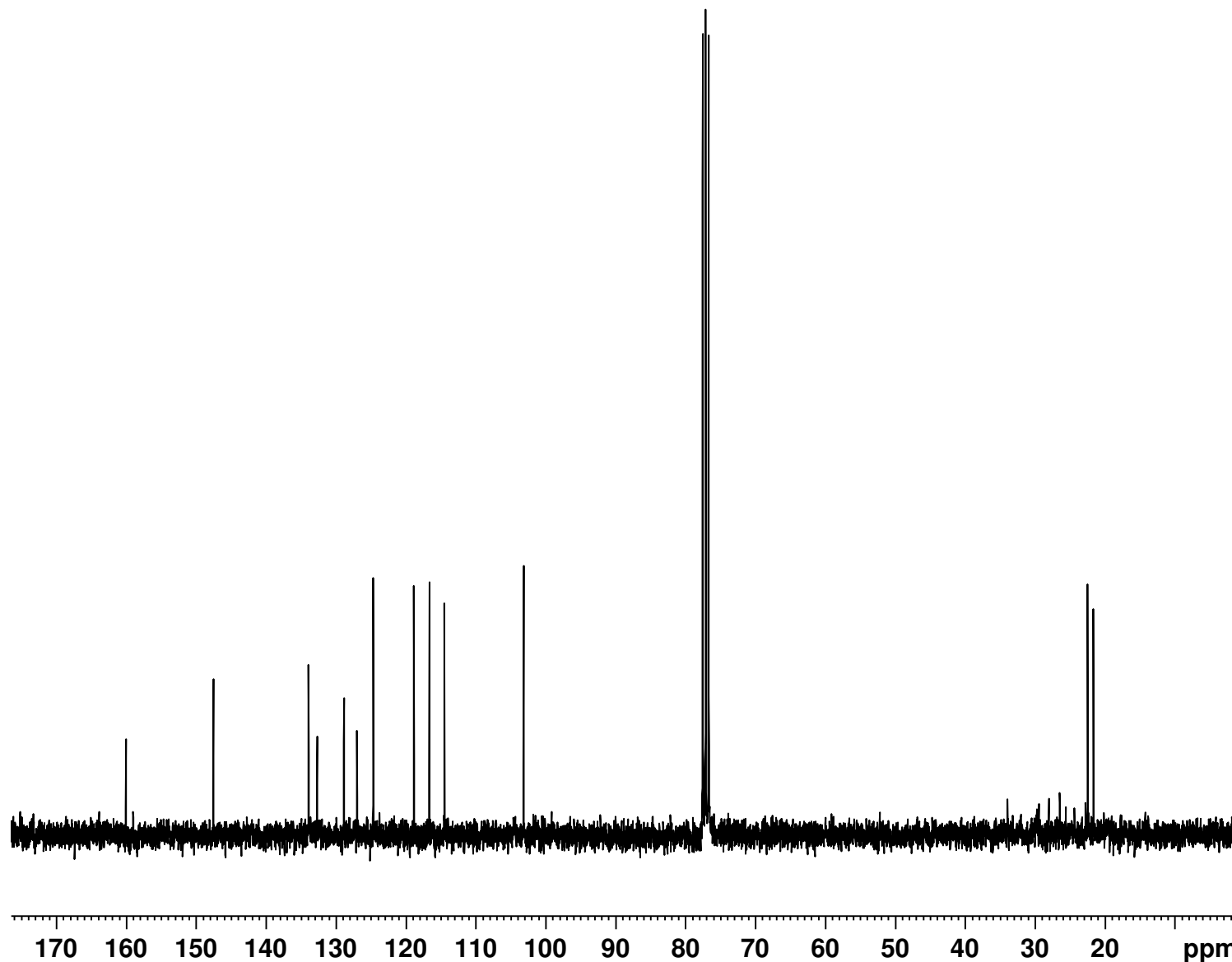
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EXPNO 2
PROCNO 1

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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 284
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 199.526
DW 20.480 usec
DE 6.50 usec
TE 293.2 K
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D11 0.03000000 sec
D31 0.00001200 sec
D40 0.02898005 sec
L4 40
L5 57
P32 90.00 usec
TD0 1

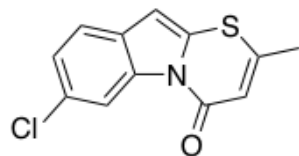
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NUC2 1H
CPDPRG[2] waltz65
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PLW12 0.21333000 W
PLW13 0.17280000 W

F2 - Processing parameters
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SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7-chloro-2-methyl-4H-[1,3]thiazino[3,2-a]indol-4-one (22)



Current Data Parameters

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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

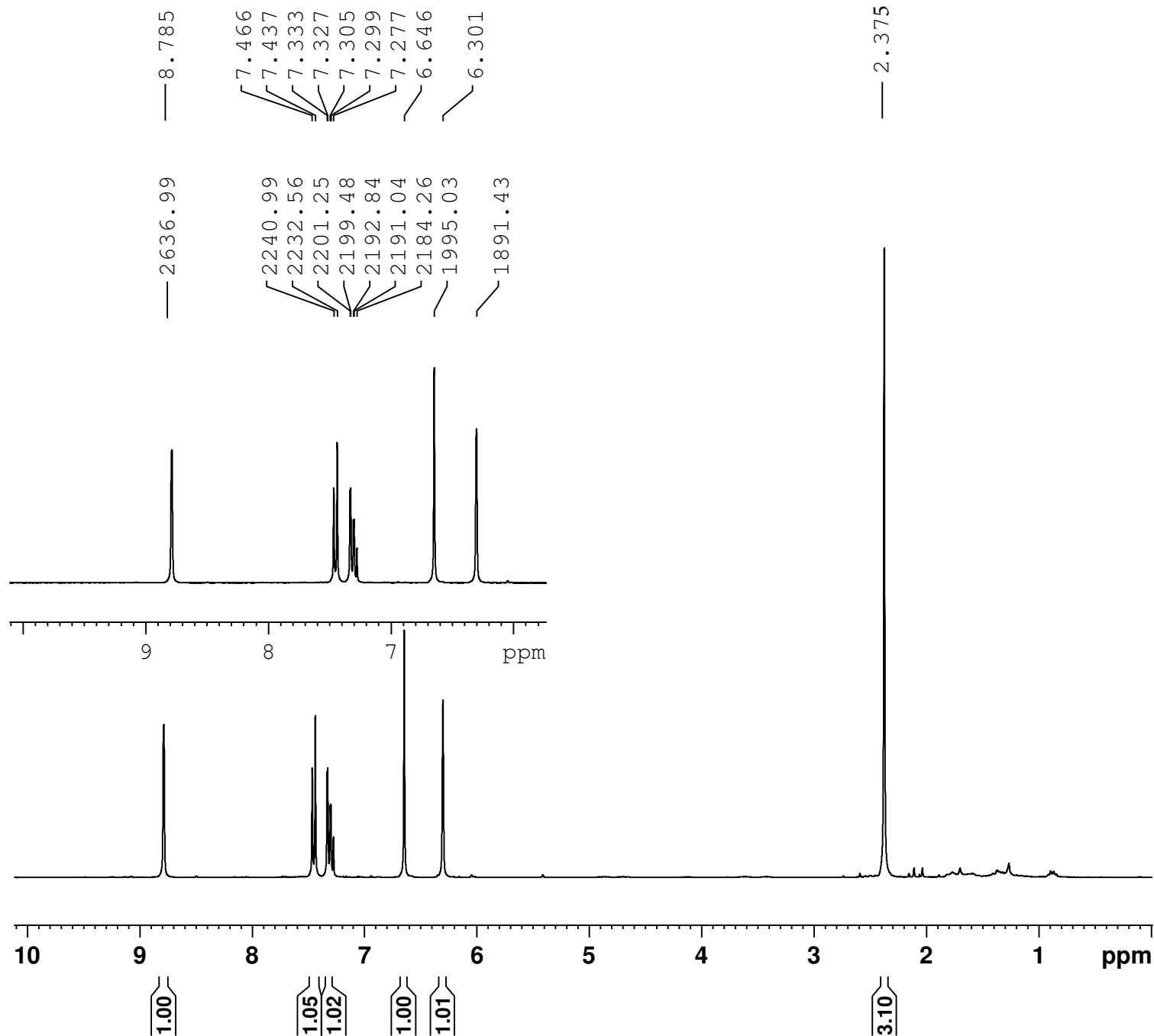
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SOLVENT CDC13
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DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
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RG 31.623
DW 81.920 usec
DE 6.50 usec
TE 292.2 K
D1 1.00000000 sec
TD0 1

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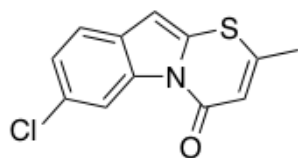
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F2 - Processing parameters

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WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



7-chloro-2-methyl-4H-[1,3]thiazino[3,2-a]indol-4-one (22)



— 159.82
— 148.24
— 134.49
— 129.00
— 127.77
— 127.00
— 124.83
— 119.63
— 117.04
— 114.32
— 103.05

— 22.53

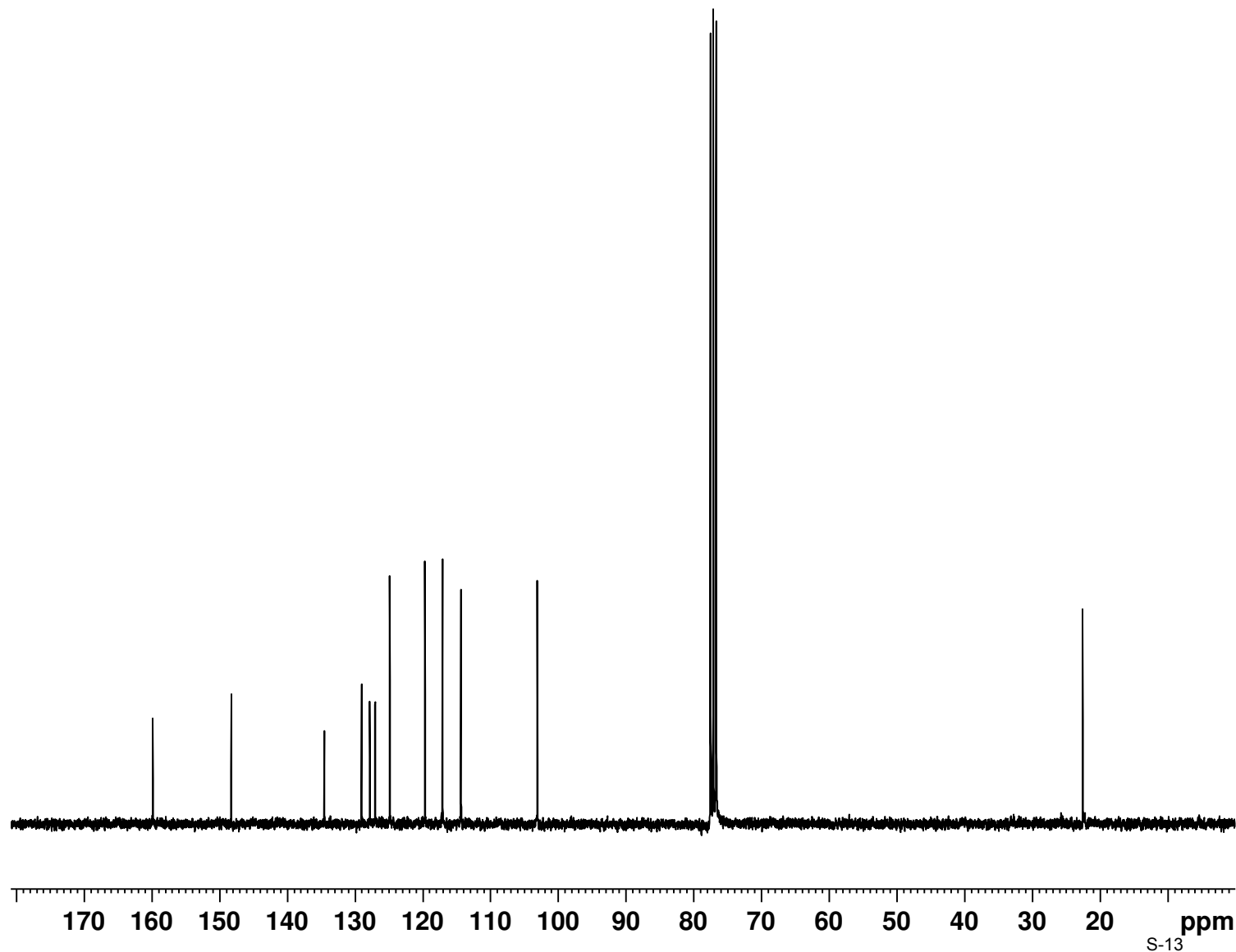
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PROCNO 1

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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1639
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 292.8 K
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D31 0.00001200 sec
D40 0.02898005 sec
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L5 57
P32 90.00 usec
TD0 1

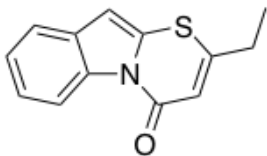
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NUC2 1H
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PCPD2 90.00 usec
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PLW12 0.21333000 W
PLW13 0.17280000 W

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



2-ethyl-4H-[1,3]thiazino[3,2-a]indol-4-one (23)

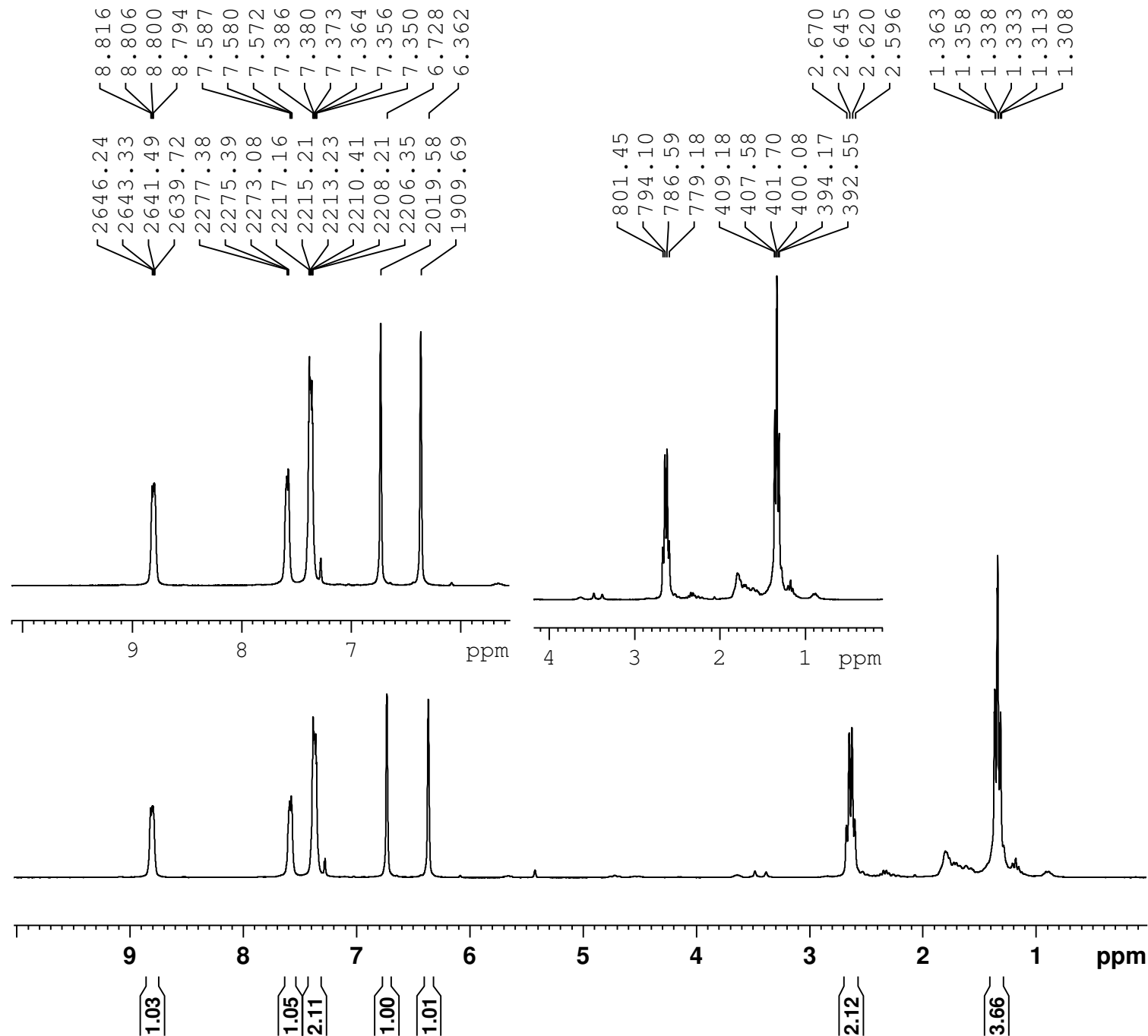


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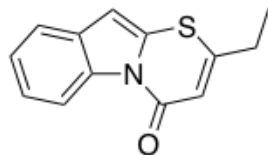
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 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 14.2884
 DW 81.920 usec
 DE 6.50 usec
 TE 293.5 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
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 NUC1 1H
 P1 12.00 usec
 PLW1 10.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1800000 MHz
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 PC 1.00



2-ethyl-4H-[1,3]thiazino[3,2-a]indol-4-one (23)



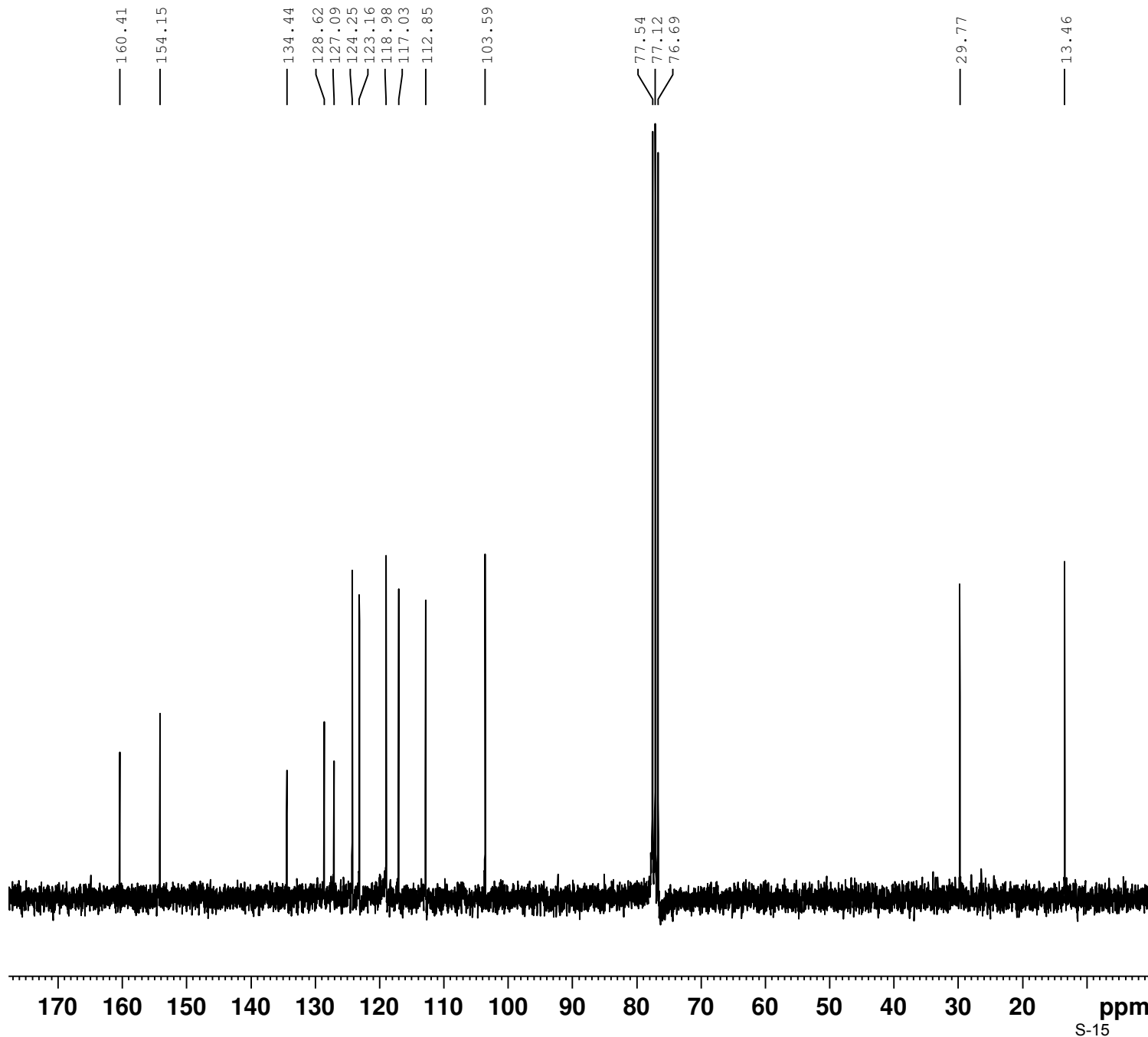
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 PROCNO 1

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 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 888
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 199.526
 DW 20.480 usec
 DE 6.50 usec
 TE 293.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00001200 sec
 D40 0.02898005 sec
 L4 40
 L5 57
 P32 90.00 usec
 TD0 1

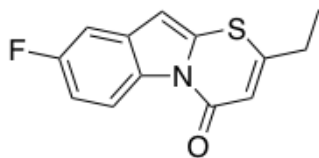
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===== CHANNEL f2 =====
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 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.21333000 W
 PLW13 0.17280000 W

F2 - Processing parameters
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2-ethyl-8-fluoro-4H-[1,3]thiazino[3,2-a]indol-4-one (24)

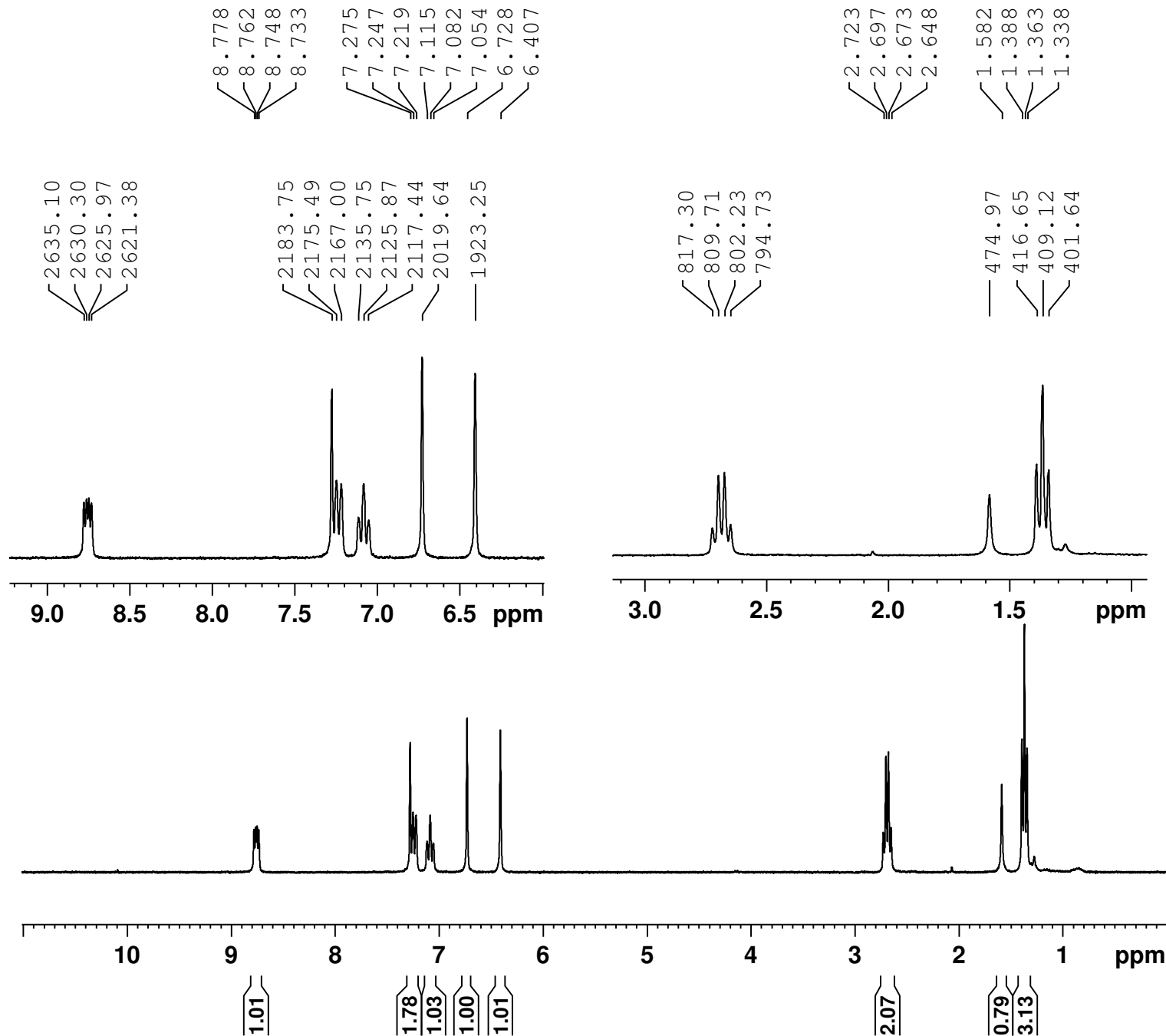


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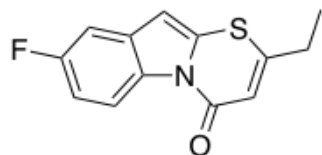
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 123.399
DW 81.920 usec
DE 6.50 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1818537 MHz
NUC1 1H
P1 12.00 usec
PLW1 10.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2-ethyl-8-fluoro-4H-[1,3]thiazino[3,2-a]indol-4-one (24)



Current Data Parameters
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 EXPNO 8
 PROCNO 1

F2 - Acquisition Parameters

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 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 10240
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 199.526
 DW 20.480 us
 DE 6.50 us
 TE 293.6
 D1 2.00000000 s
 D11 0.03000000 sec
 D31 0.00001200 sec
 D40 0.02898005 sec
 L4 40
 L5 57
 P32 90.00 usec
 TD0 1

===== CHANNEL f1 =====

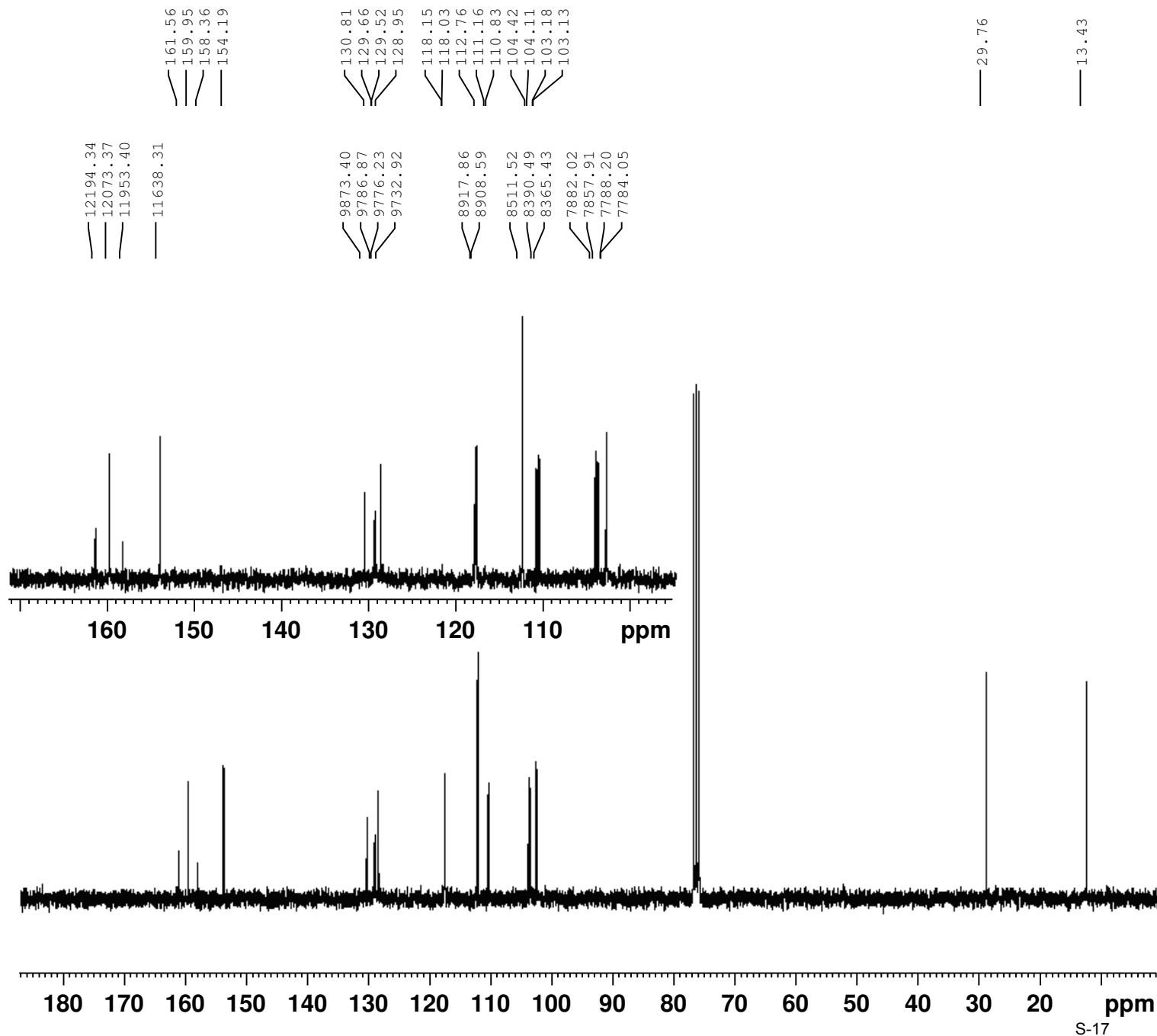
SFO1 75.4897560
 NUC1
 P1 12.00 us
 PLW1 10.000000

===== CHANNEL f2 =====

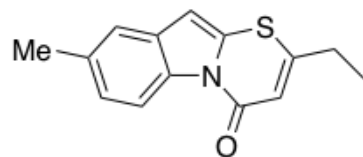
SFO2 300.1812007
 NUC2
 CPDPRG[2]
 PCPD2 90.00
 PLW2 12.000000
 PLW12 0.21333
 PLW13 0.17280

F2 - Processing parameters

SI 327
 SF 75.4803210 M
 WDW
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



2-ethyl-8-methyl-4H-[1,3]thiazino[3,2-a]indol-4-one (25)



8.670
8.641

7.381
7.278
7.173
6.692
6.382

2.708
2.684
2.658
2.633
2.500

1.384
1.358
1.333

Current Data Parameters

NAME SR-02-209
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters

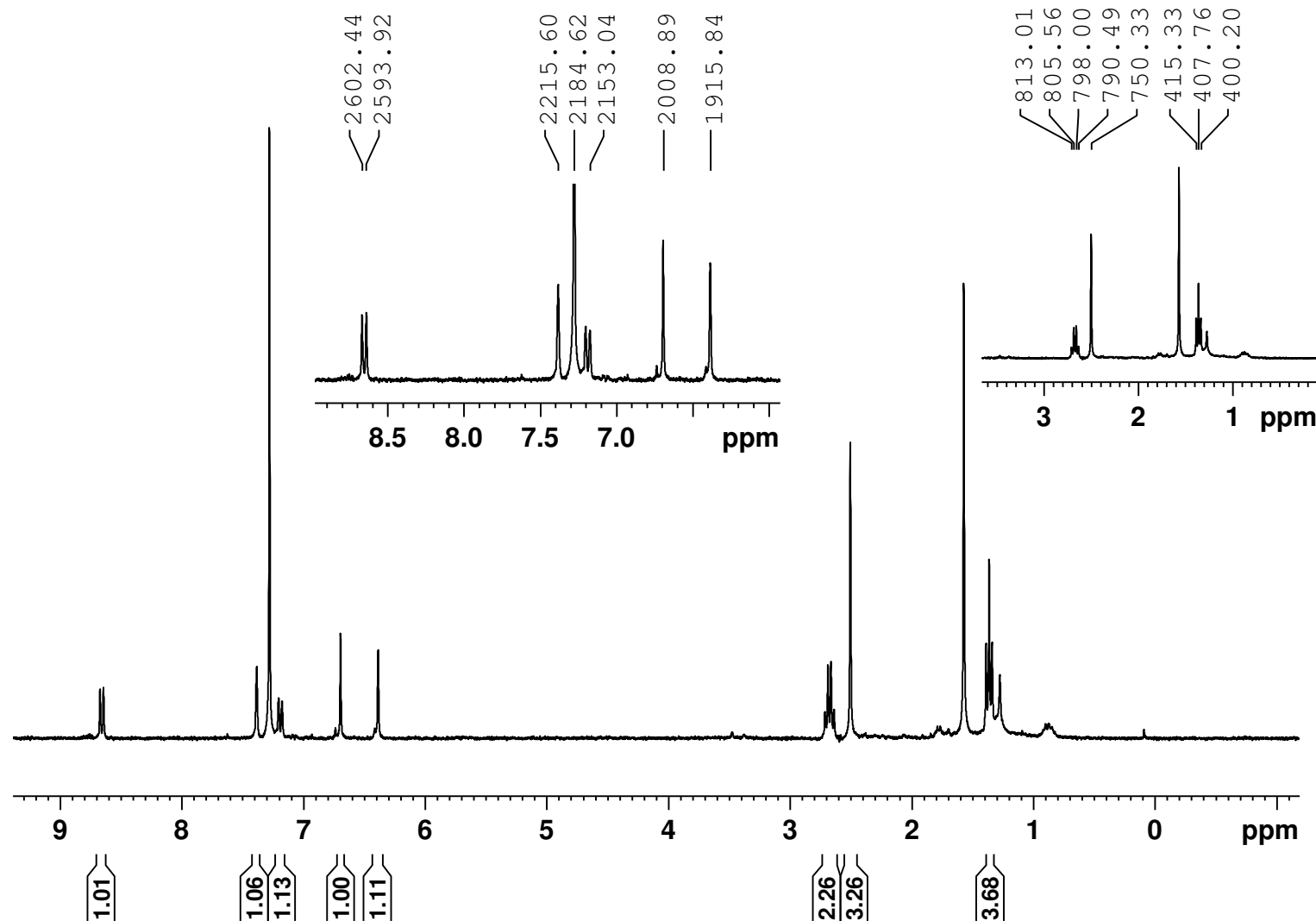
Date_ 20190322
Time 17.19
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 264.027
DW 81.920 usec
DE 6.50 usec
TE 293.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====

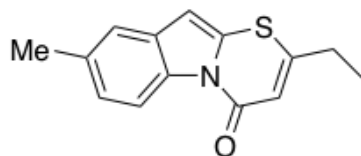
SFO1 300.1818537 MHz
NUC1 1H
P1 12.00 usec
PLW1 10.00000000 W

F2 - Processing parameters

SI 65536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2-ethyl-8-methyl-4H-[1,3]thiazino[3,2-a]indol-4-one (25)



160.30
153.94
133.90
132.68
128.88
126.99
124.63
118.78
116.63
112.86
103.30

29.76
21.61
13.48

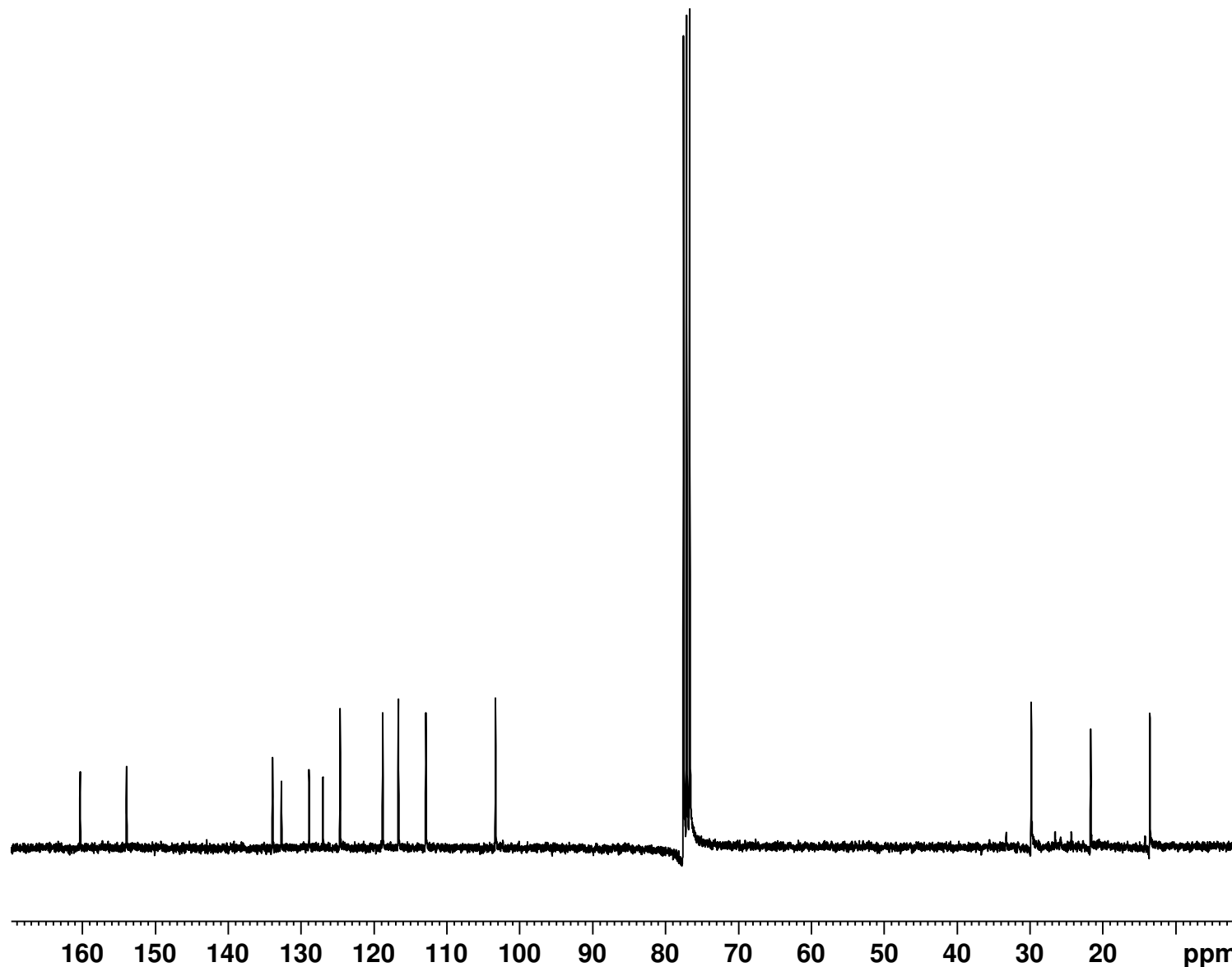
Current Data Parameters
NAME SR-02-209
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180515
Time 9.21
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 7799
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 199.526
DW 20.480 usec
DE 6.50 usec
TE 293.6 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001200 sec
D40 0.02898005 sec
L4 40
L5 57
P32 90.00 usec
TD0 1

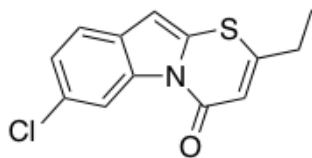
===== CHANNEL f1 =====
SFO1 75.4897560 MHz
NUC1 13C
P1 12.00 usec
PLW1 10.00000000 W

===== CHANNEL f2 =====
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.21333000 W
PLW13 0.17280000 W

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7-chloro-2-ethyl-4H-[1,3]thiazino[3,2-a]indol-4-one (26)



Current Data Parameters
 NAME SR-02-198
 EXPNO 21
 PROCNO 1

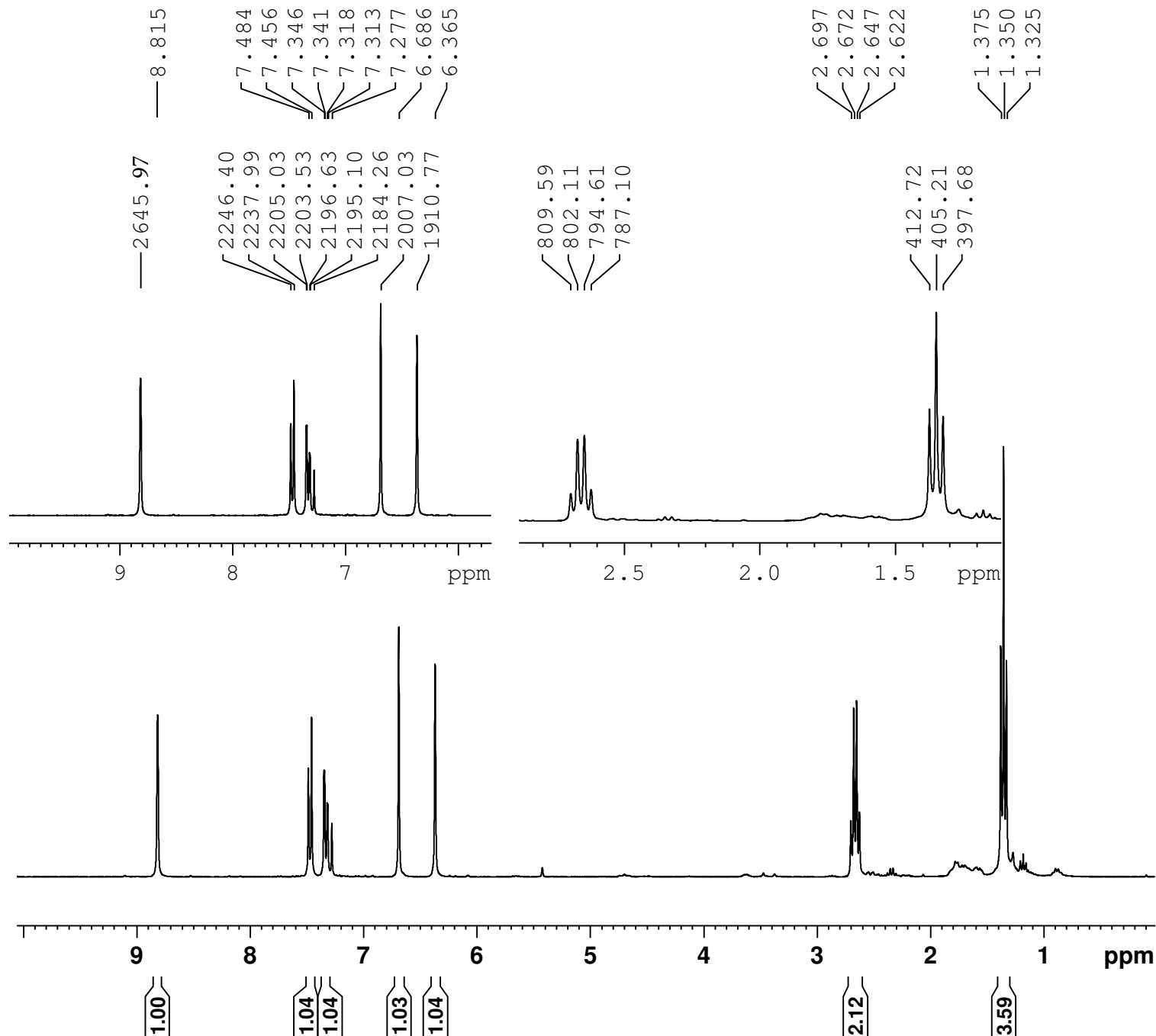
F2 - Acquisition Parameters

Date_ 20180423
 Time 11.23
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 31.623
 DW 81.920 usec
 DE 6.50 usec
 TE 292.2 K
 D1 1.00000000 sec
 TD0 1

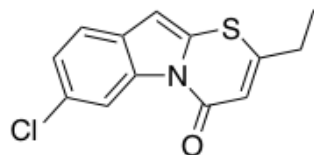
===== CHANNEL f1 =====
 SFO1 300.1818537 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 10.00000000 W

F2 - Processing parameters

SI 65536
 SF 300.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



7-chloro-2-ethyl-4H-[1,3]thiazino[3,2-a]indol-4-one (26)



— 160.12
— 154.63
— 134.52
— 128.98
— 127.80
— 127.05
— 124.86
— 119.59
— 117.06
— 112.72
— 103.25

— 29.84
— 13.45

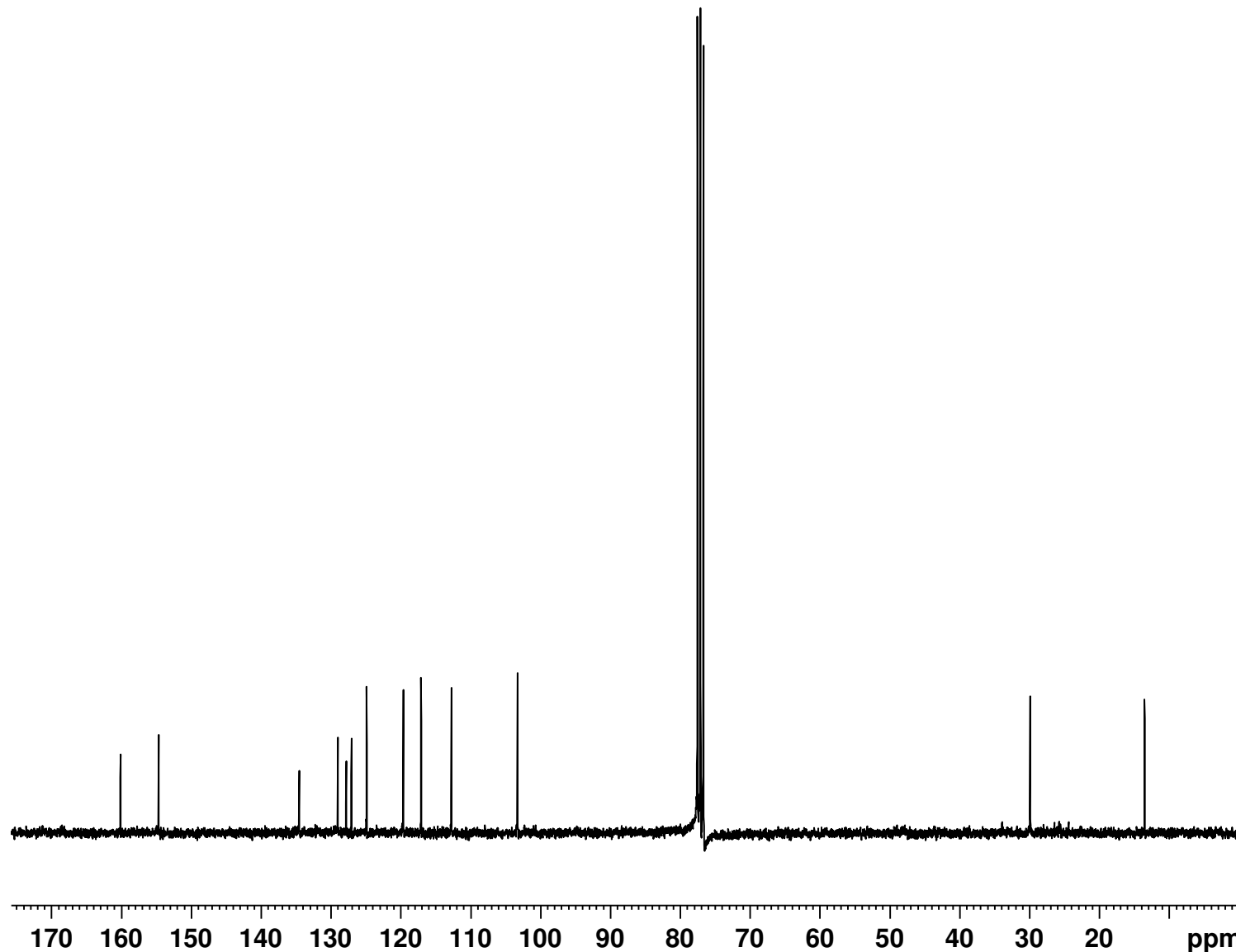
Current Data Parameters
NAME SR-02-198
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180423
Time_ 11.30
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1846
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 199.526
DW 20.480 usec
DE 6.50 usec
TE 292.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001200 sec
D40 0.02898005 sec
L4 40
L5 57
P32 90.00 usec
TD0 1

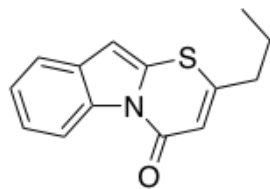
===== CHANNEL f1 =====
SFO1 75.4821747 MHz
NUC1 13C
P1 12.00 usec
PLW1 10.00000000 W

===== CHANNEL f2 =====
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.21333000 W
PLW13 0.17280000 W

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



2-propyl-4H-[1,3]thiazino[3,2-a]indol-4-one (27)

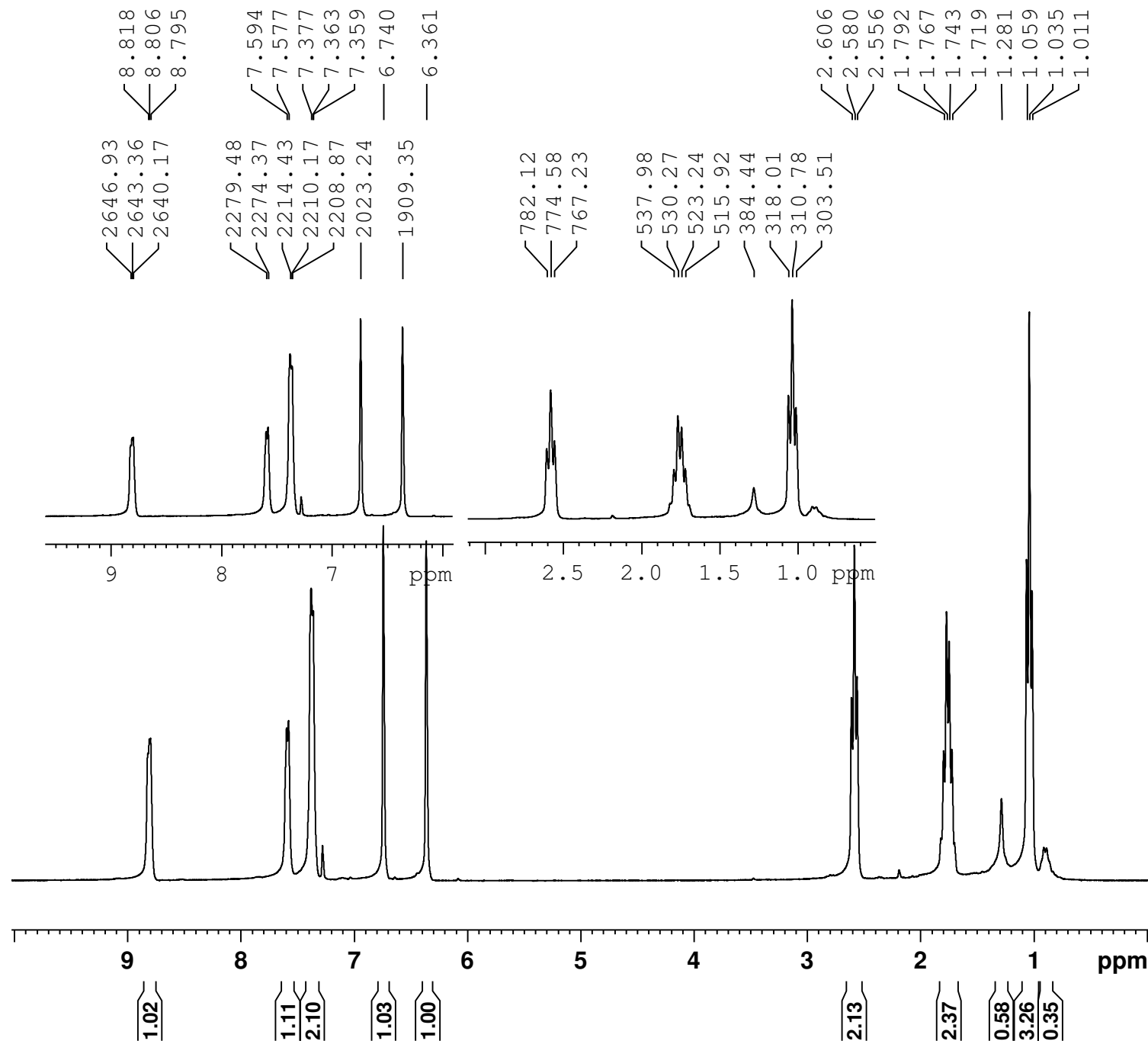


Current Data Parameters
 NAME SR-02-204
 EXPNO 2
 PROCNO 1

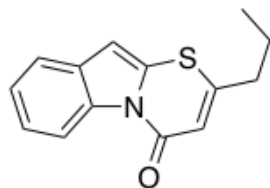
F2 - Acquisition Parameters
 Date_ 20180511
 Time 12.05
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 13.4589
 DW 81.920 usec
 DE 6.50 usec
 TE 293.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1818537 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 10.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



2-propyl-4H-[1,3]thiazino[3,2-a]indol-4-one (27)



— 160.35 — 152.64 — 134.44 — 128.61 — 127.15 — 124.25 — 123.17 — 118.98 — 117.04 — 113.63 — 103.58 — 38.43 — 22.43 — 13.41

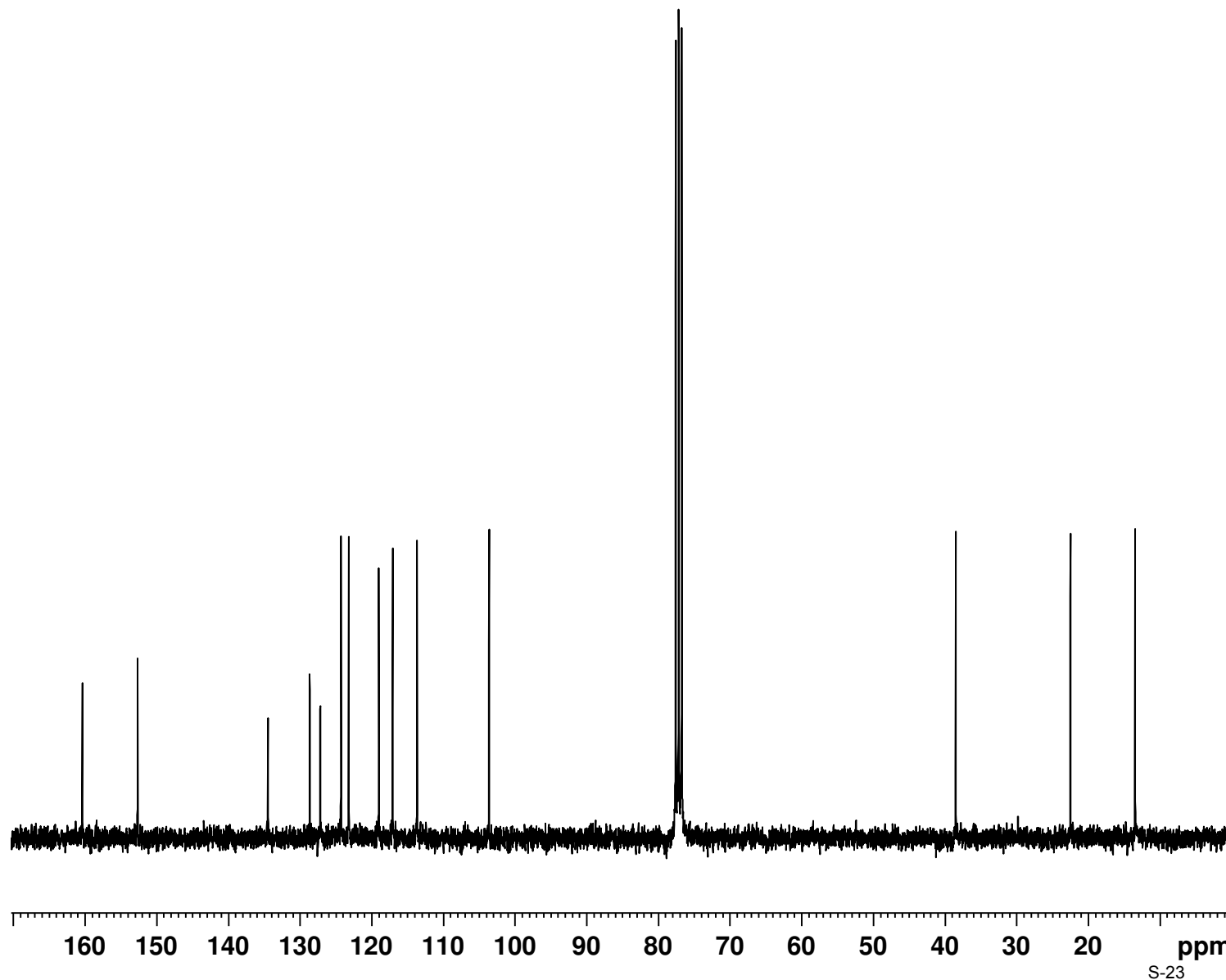
Current Data Parameters
NAME SR-02-204
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180511
Time 12.12
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 644
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 199.526
DW 20.480 usec
DE 6.50 usec
TE 293.3 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001200 sec
D40 0.02898005 sec
L4 40
L5 57
P32 90.00 usec
TD0 1

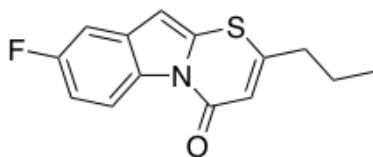
===== CHANNEL f1 =====
SFO1 75.4897560 MHz
NUC1 13C
P1 12.00 usec
PLW1 10.00000000 W

===== CHANNEL f2 =====
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.21333000 W
PLW13 0.17280000 W

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



8-fluoro-2-propyl-4H-[1,3]thiazino[3,2-a]indol-4-one (28)

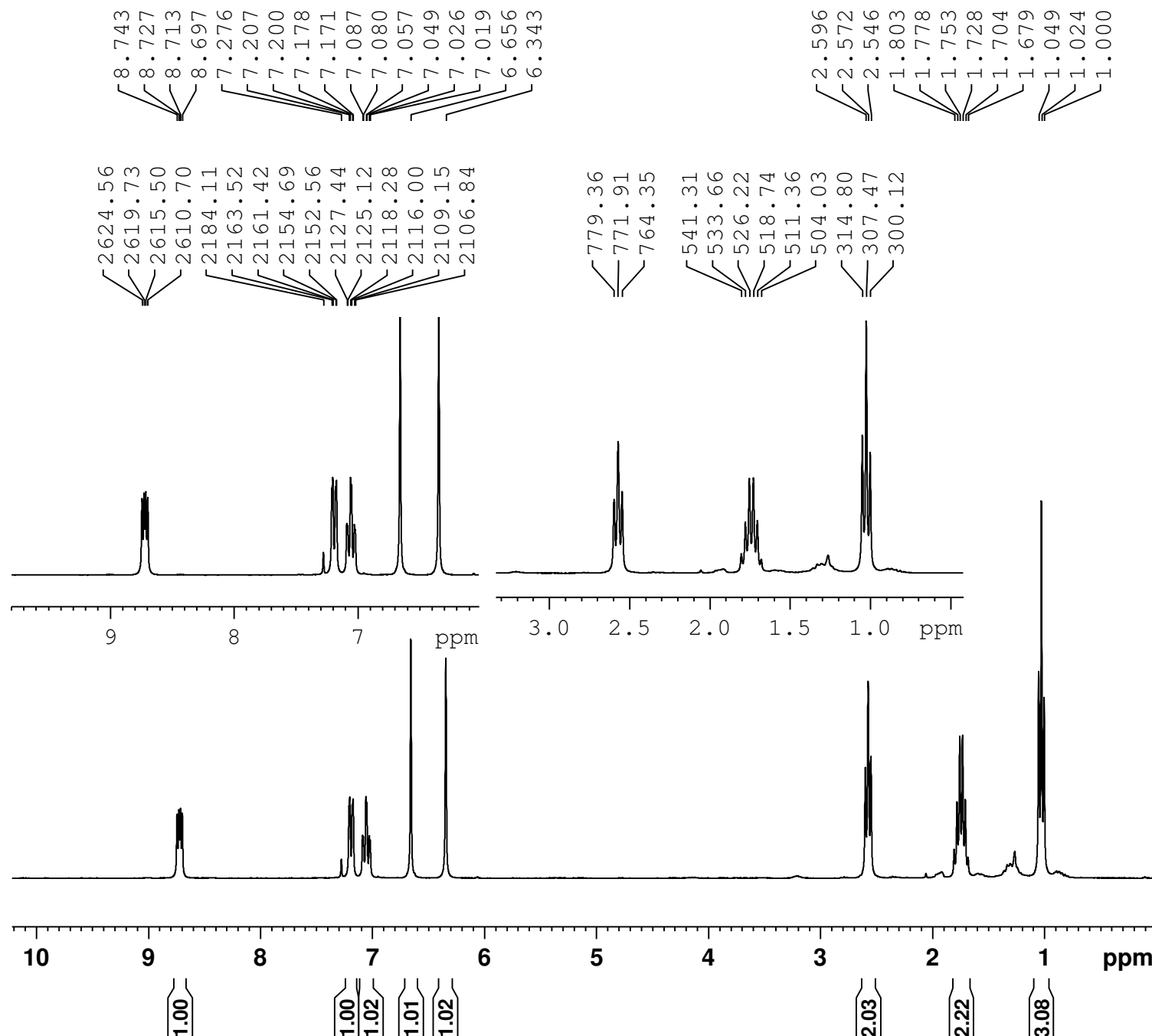


Current Data Parameters
 NAME SR-02-196
 EXPNO 2
 PROCNO 1

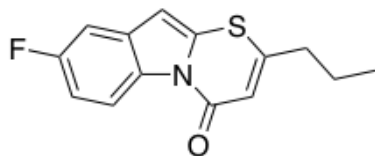
F2 - Acquisition Parameters
 Date_ 20180425
 Time 10.39
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 12.2513
 DW 81.920 usec
 DE 6.50 usec
 TE 293.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1818537 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 10.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



8-fluoro-2-propyl-4H-[1,3]thiazino[3,2-a]indol-4-one (28)



Current Data Parameters
 NAME SR-02-196
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

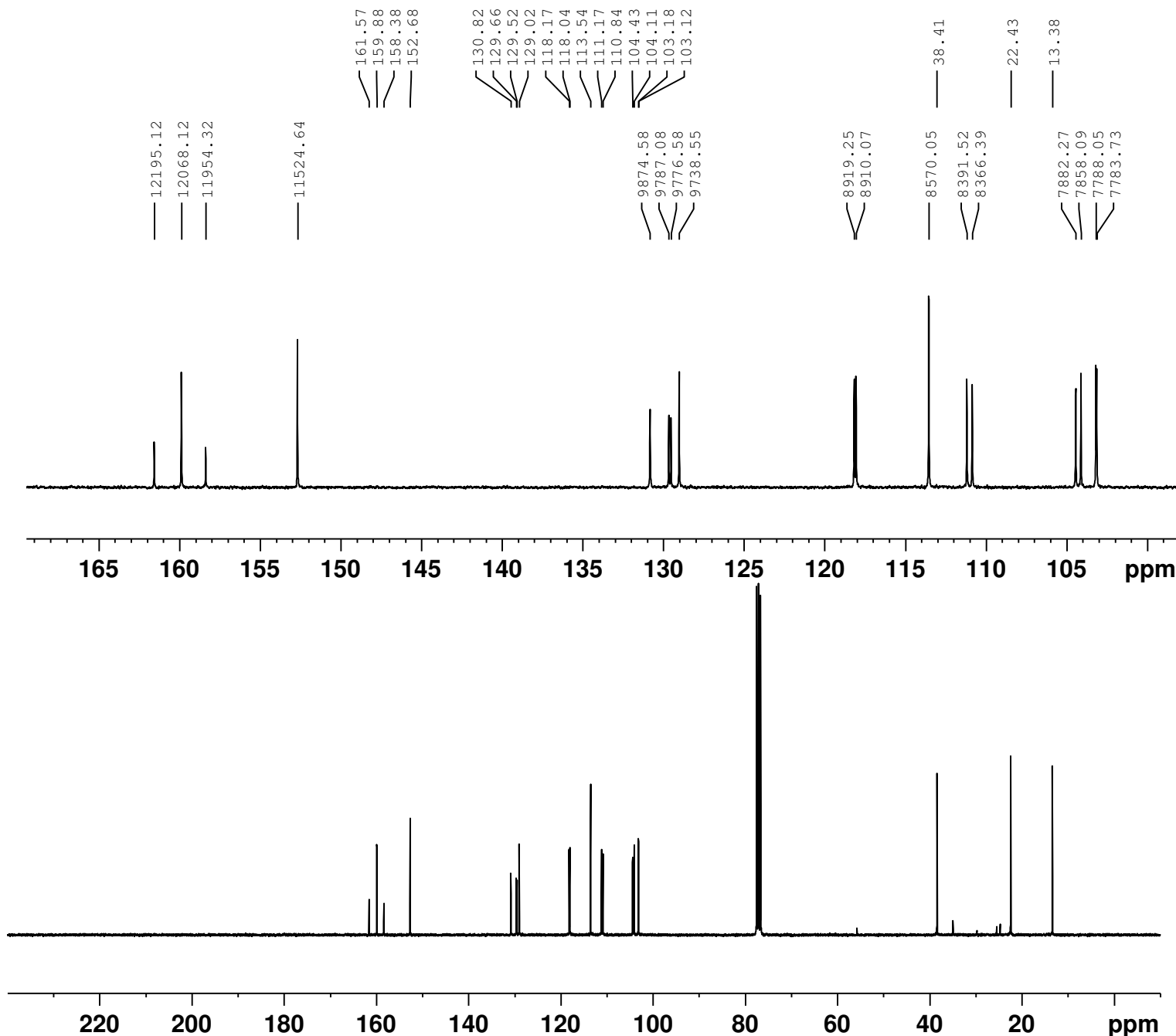
Date_ 20180425
 Time 11.03
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 10240
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 293.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00001200 sec
 D40 0.02898005 sec
 L4 40
 L5 57
 P32 90.00 usec
 TD0 1

===== CHANNEL f1 =====
 SFO1 75.4897560 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 10.00000000 W

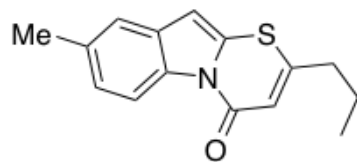
===== CHANNEL f2 =====
 SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.21333000 W
 PLW13 0.17280000 W

F2 - Processing parameters

SI 32768
 SF 75.4803210 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



8-methyl-2-propyl-4H-[1,3]thiazino[3,2-a]indol-4-one (29)



Current Data Parameters
 NAME SR-02-210
 EXPNO 2
 PROCNO 1

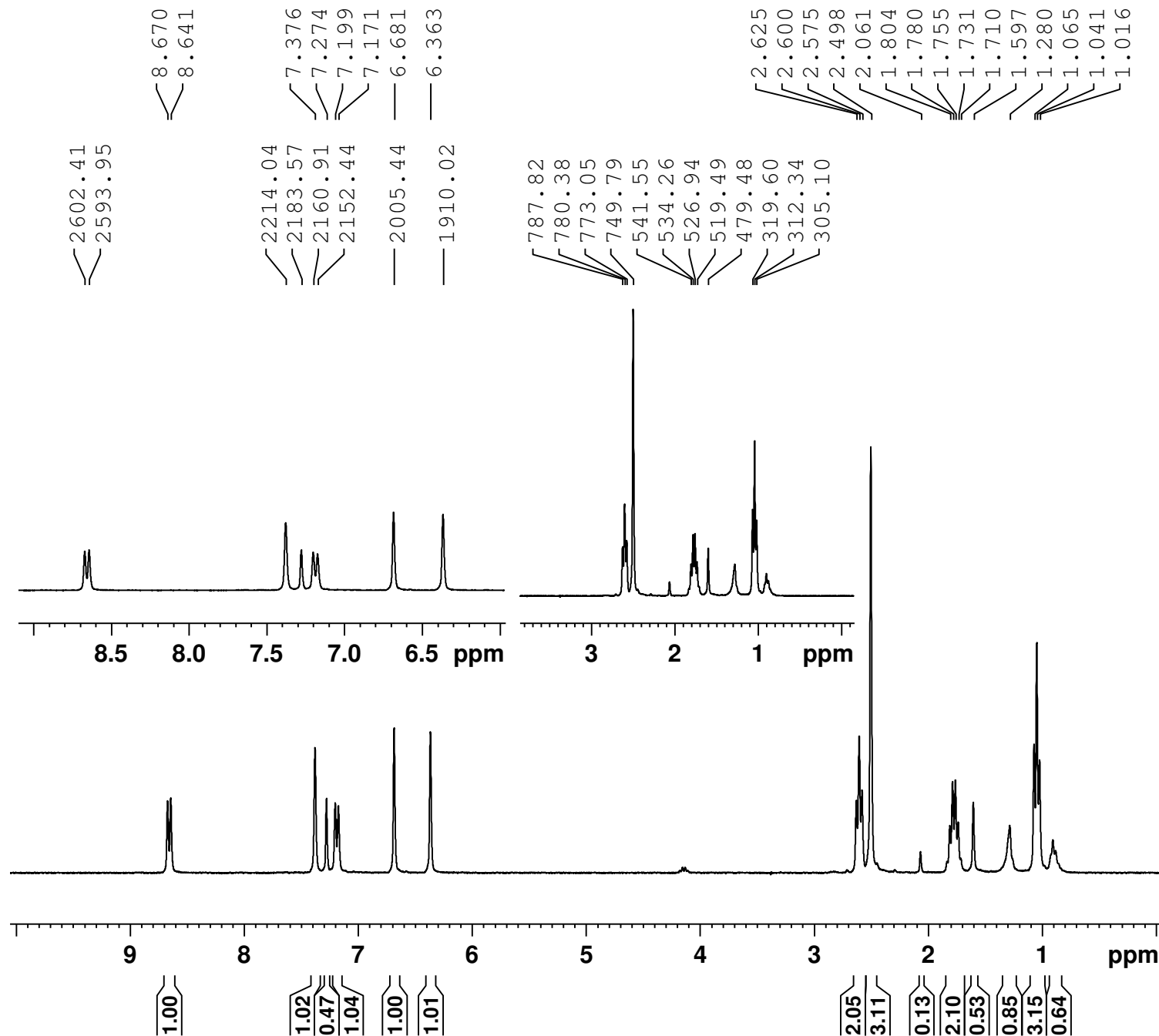
F2 - Acquisition Parameters

Date_ 20181217
 Time 12.04
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 62.5134
 DW 81.920 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.00000000 sec
 TD0 1

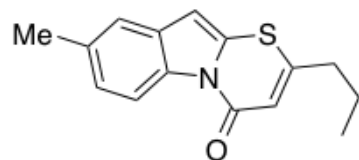
===== CHANNEL f1 =====
 SFO1 300.1818537 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 10.00000000 W

F2 - Processing parameters

SI 65536
 SF 300.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



8-methyl-2-propyl-4H-[1,3]thiazino[3,2-a]indol-4-one (29)



160.21
152.37
133.90
132.70
128.88
127.05
124.64
118.77
116.63
113.67
103.28

38.44
22.44
21.58
13.38

Current Data Parameters
NAME SR-02-210
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20181217
Time 17.42
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10240
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001000 sec
D40 0.02898005 sec
L4 40
L5 57
P32 90.00 usec
TD0 1

===== CHANNEL f1 =====

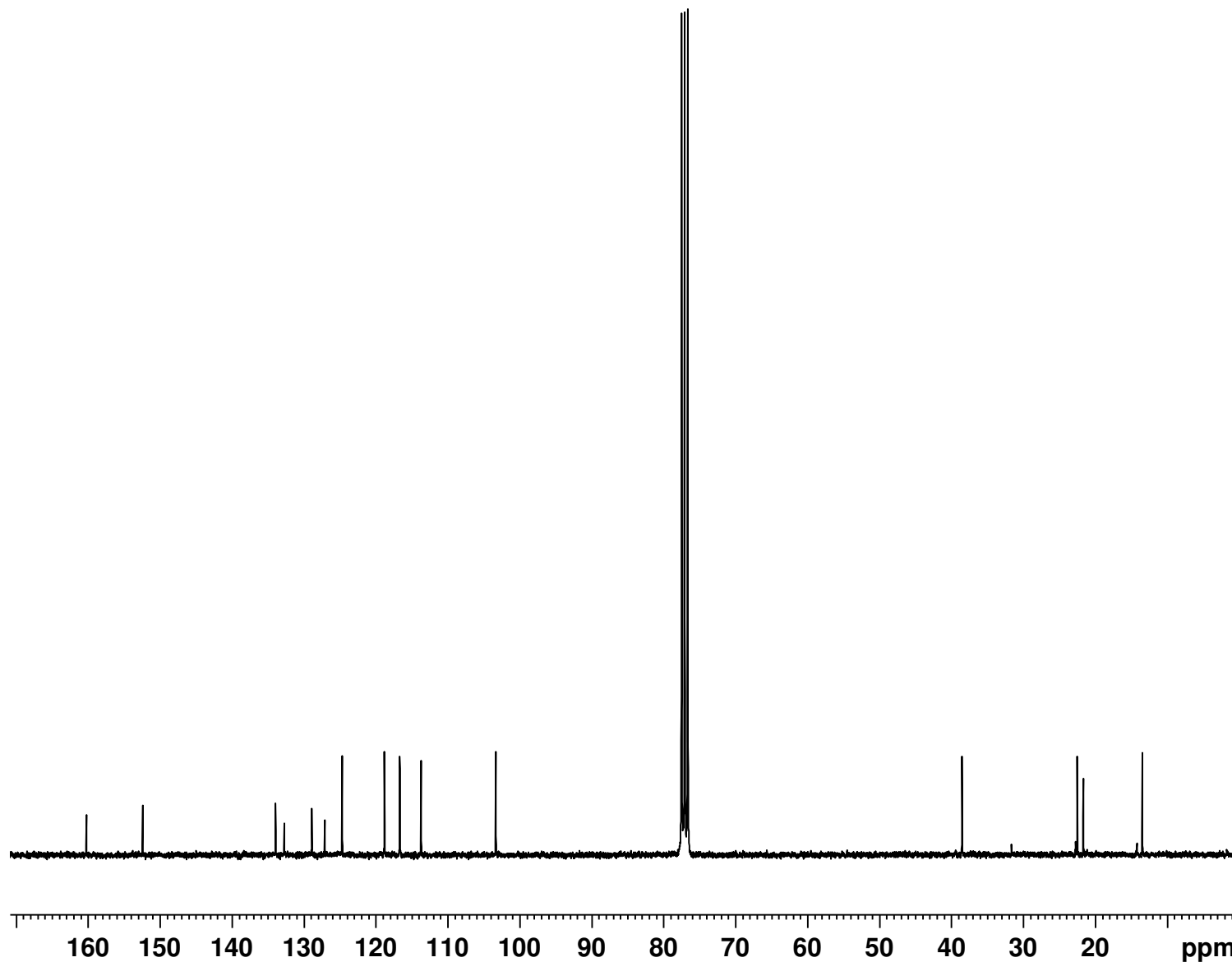
SFO1 75.4897560 MHz
NUC1 13C
P1 10.00 usec
PLW1 32.50899887 W

===== CHANNEL f2 =====

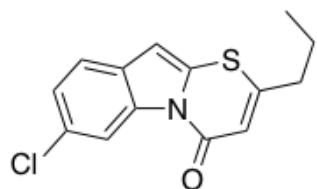
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.21333000 W
PLW13 0.17280000 W

F2 - Processing parameters

SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7-chloro-2-propyl-4H-[1,3]thiazino[3,2-a]indol-4-one (30)



Current Data Parameters
 NAME SR-02-199
 EXPNO 1
 PROCNO 1

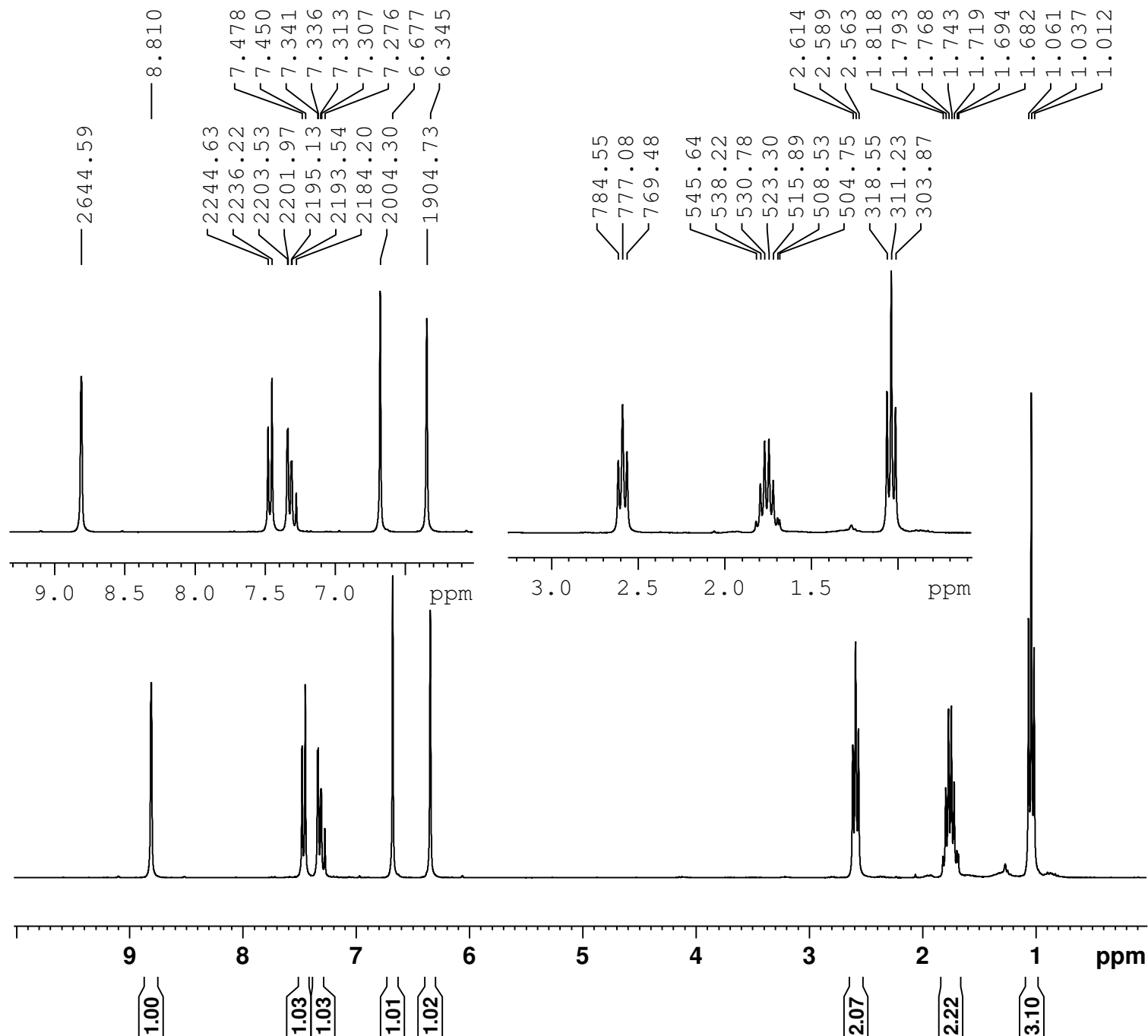
F2 - Acquisition Parameters

Date_ 20180420
 Time 12.57
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 31.623
 DW 81.920 usec
 DE 6.50 usec
 TE 292.7 K
 D1 1.00000000 sec
 TD0 1

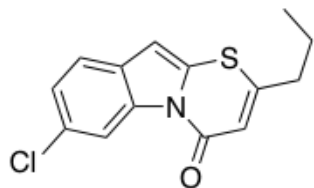
===== CHANNEL f1 =====
 SFO1 300.1818537 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 10.00000000 W

F2 - Processing parameters

SI 65536
 SF 300.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



7-chloro-2-propyl-4H-[1,3]thiazino[3,2-a]indol-4-one (30)



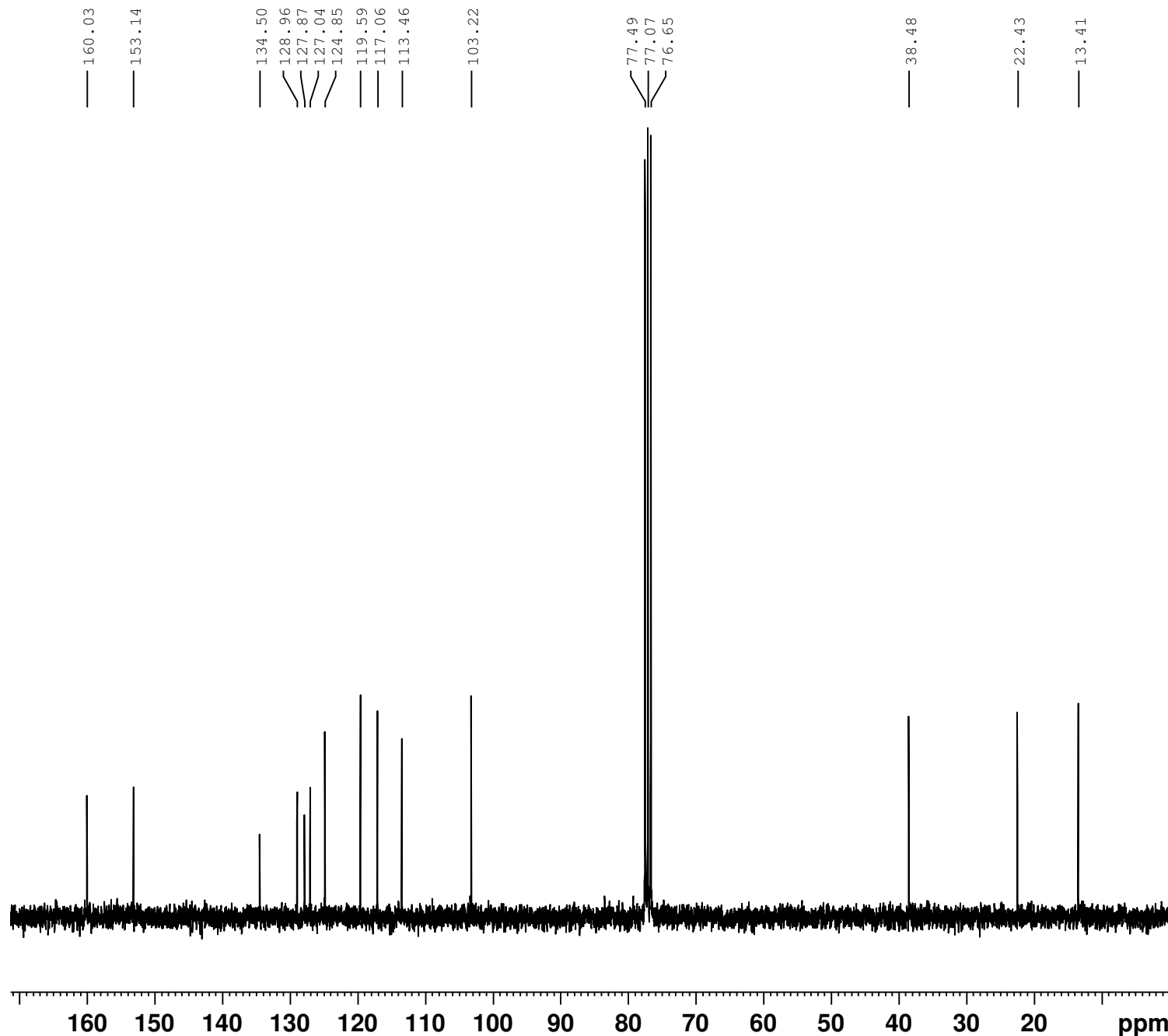
Current Data Parameters
 NAME SR-02-199
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180420
 Time 13.10
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 327
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 199.526
 DW 20.480 usec
 DE 6.50 usec
 TE 292.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00001200 sec
 D40 0.02898005 sec
 L4 40
 L5 57
 P32 90.00 usec
 TD0 1

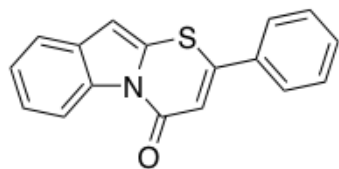
===== CHANNEL f1 =====
 SFO1 75.4897560 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 10.00000000 W

===== CHANNEL f2 =====
 SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.21333000 W
 PLW13 0.17280000 W

F2 - Processing parameters
 SI 32768
 SF 75.4803210 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



2-phenyl-4H-[1,3]thiazino[3,2-a]indol-4-one (31)

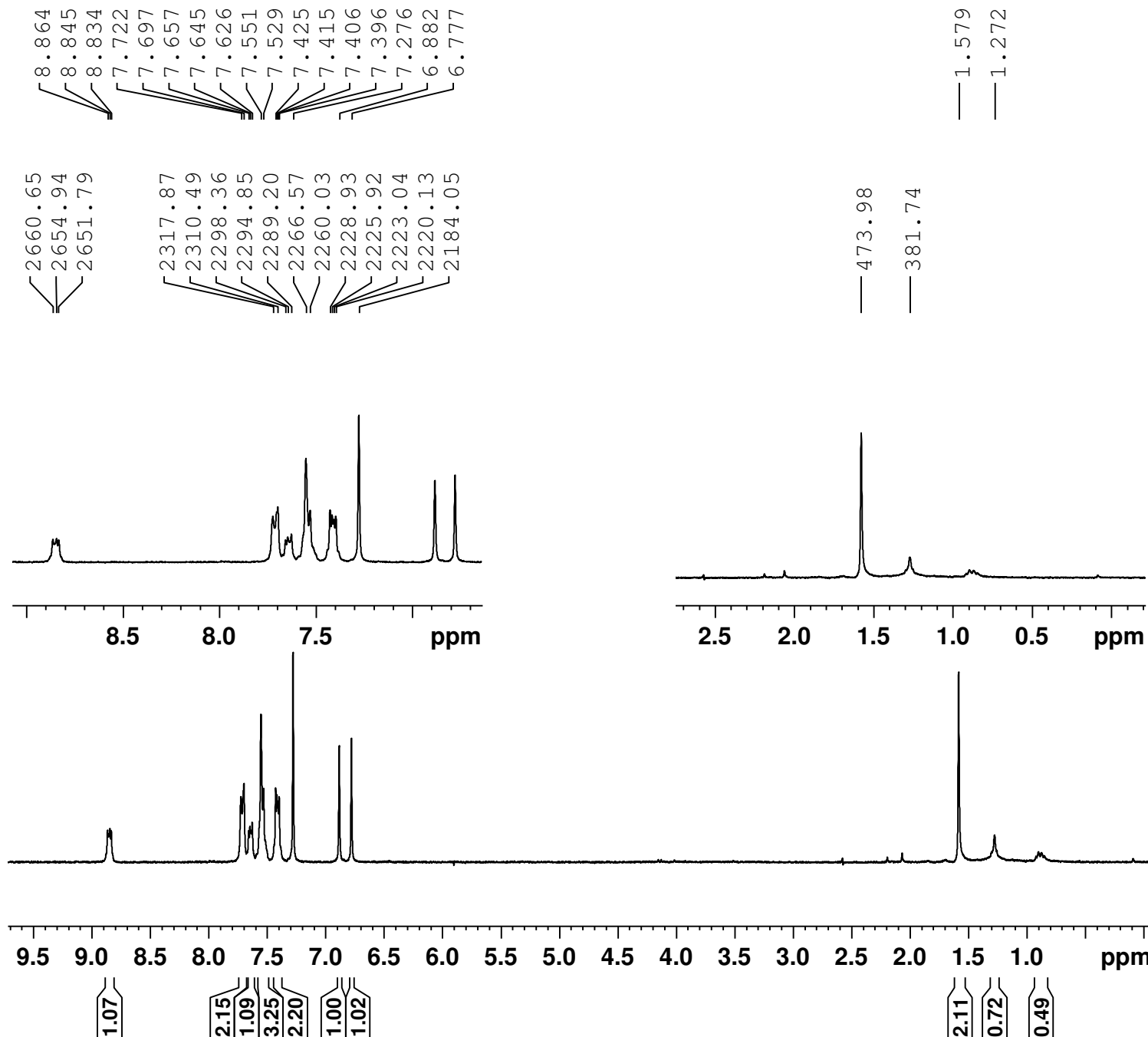


Current Data Parameters
 NAME SR-02-188
 EXPNO 1
 PROCNO 1

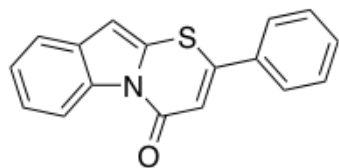
F2 - Acquisition Parameters
 Date_ 20180315
 Time 14.52
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 213.475
 DW 81.920 usec
 DE 6.50 usec
 TE 293.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1818537 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 10.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



2-phenyl-4H-[1,3]thiazino[3,2-a]indol-4-one (31)



— 160.56

— 149.60

— 135.13

— 134.41

— 131.32

— 129.37

— 128.73

— 126.97

— 126.79

— 124.44

— 123.44

— 119.11

— 117.08

— 112.83

— 104.21

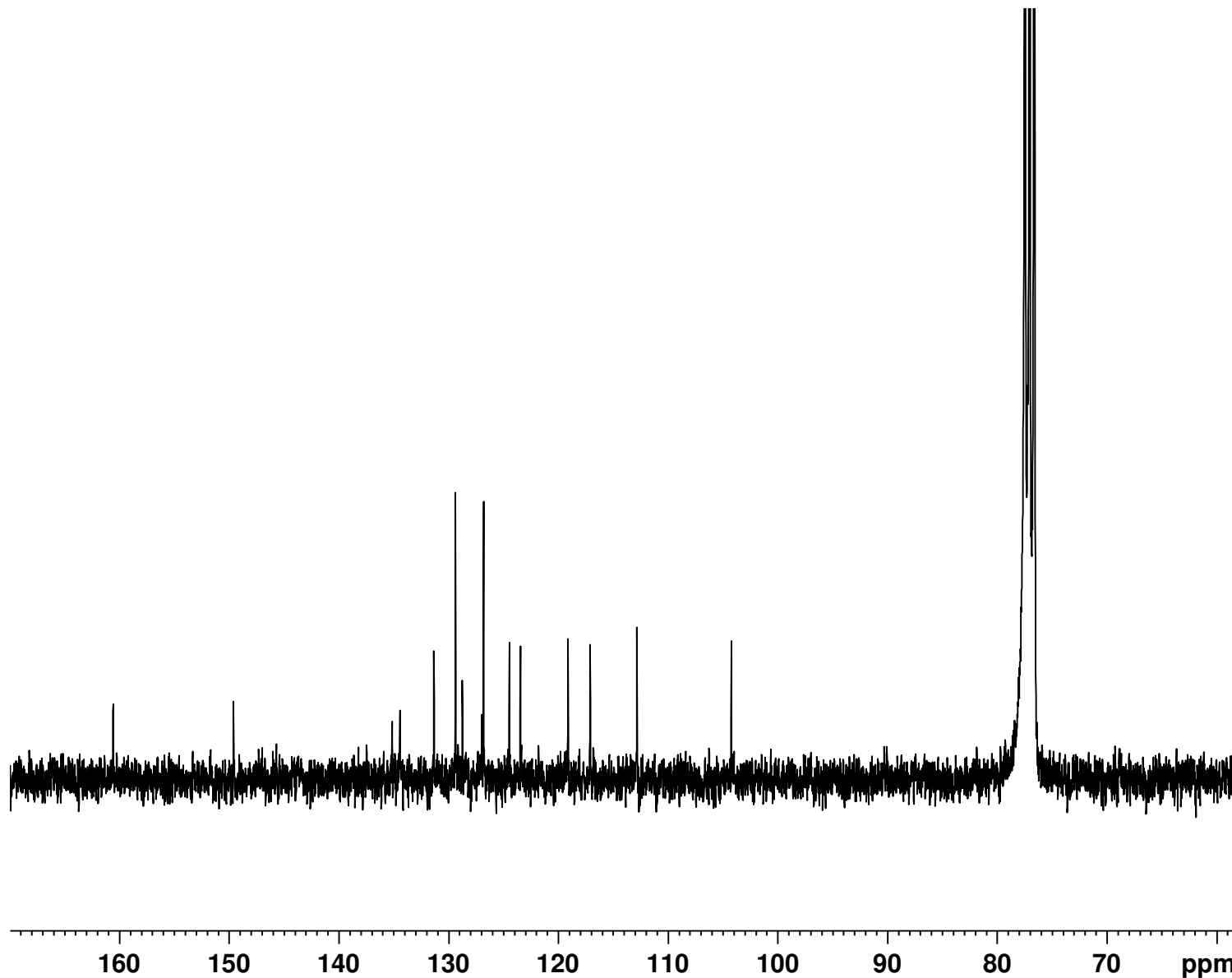
Current Data Parameters
NAME SR-02-188
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180319
Time 16.52
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10240
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 293.5 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001200 sec
D40 0.02898005 sec
L4 40
L5 57
P32 90.00 usec
TD0 1

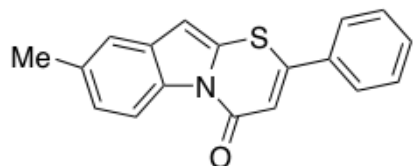
===== CHANNEL f1 =====
SFO1 75.4897560 MHz
NUC1 13C
P1 12.00 usec
PLW1 10.00000000 W

===== CHANNEL f2 =====
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.21333000 W
PLW13 0.17280000 W

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



8-methyl-2-phenyl-4H-[1,3]thiazino[3,2-a]indol-4-one (32)

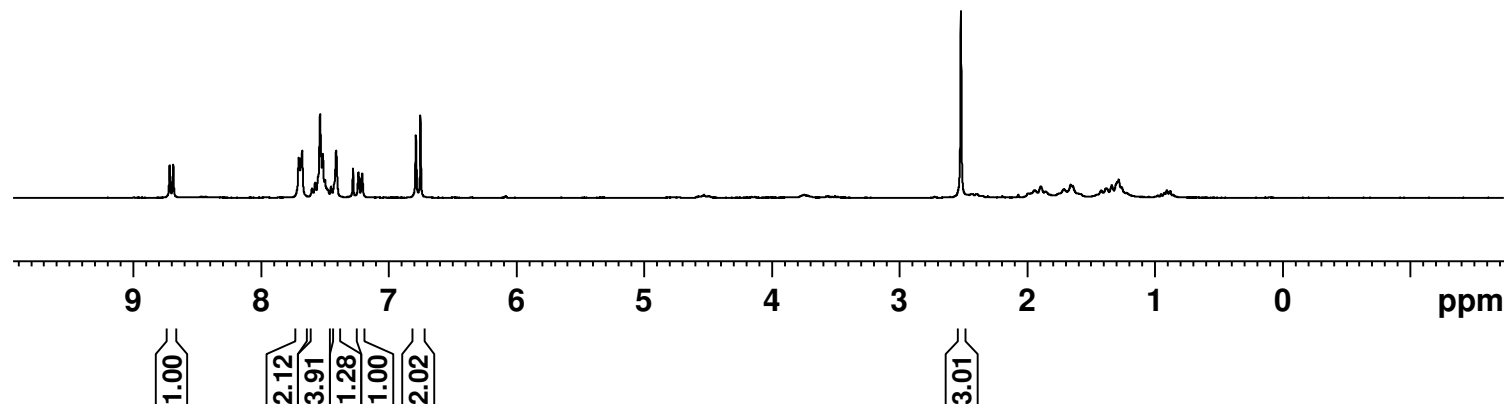
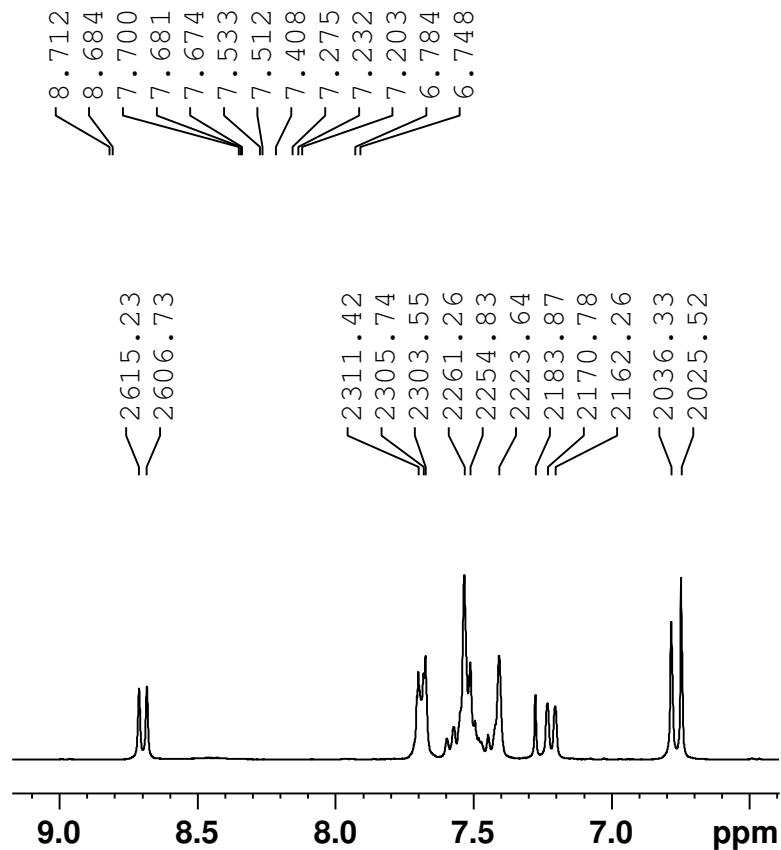


Current Data Parameters
 NAME SR-02-211
 EXPNO 1
 PROCNO 1

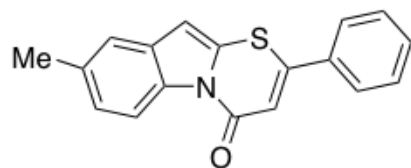
F2 - Acquisition Parameters
 Date_ 20180529
 Time 12.29
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 31.623
 DW 81.920 usec
 DE 6.50 usec
 TE 294.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1818536 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 10.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



8-methyl-2-phenyl-4H-[1,3]thiazino[3,2-a]indol-4-one (32)



160.40
149.38
135.17
134.13
132.66
132.61
131.24
129.33
128.99
126.76
124.90
118.91
116.66
112.78
103.89

21.64

Current Data Parameters

NAME SR-02-211
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20180529
Time 12.36
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 918
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 199.526
DW 20.480 usec
DE 6.50 usec
TE 294.5 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001200 sec
D40 0.02898005 sec
L4 40
L5 57
P32 90.00 usec
TD0 1

===== CHANNEL f1 =====

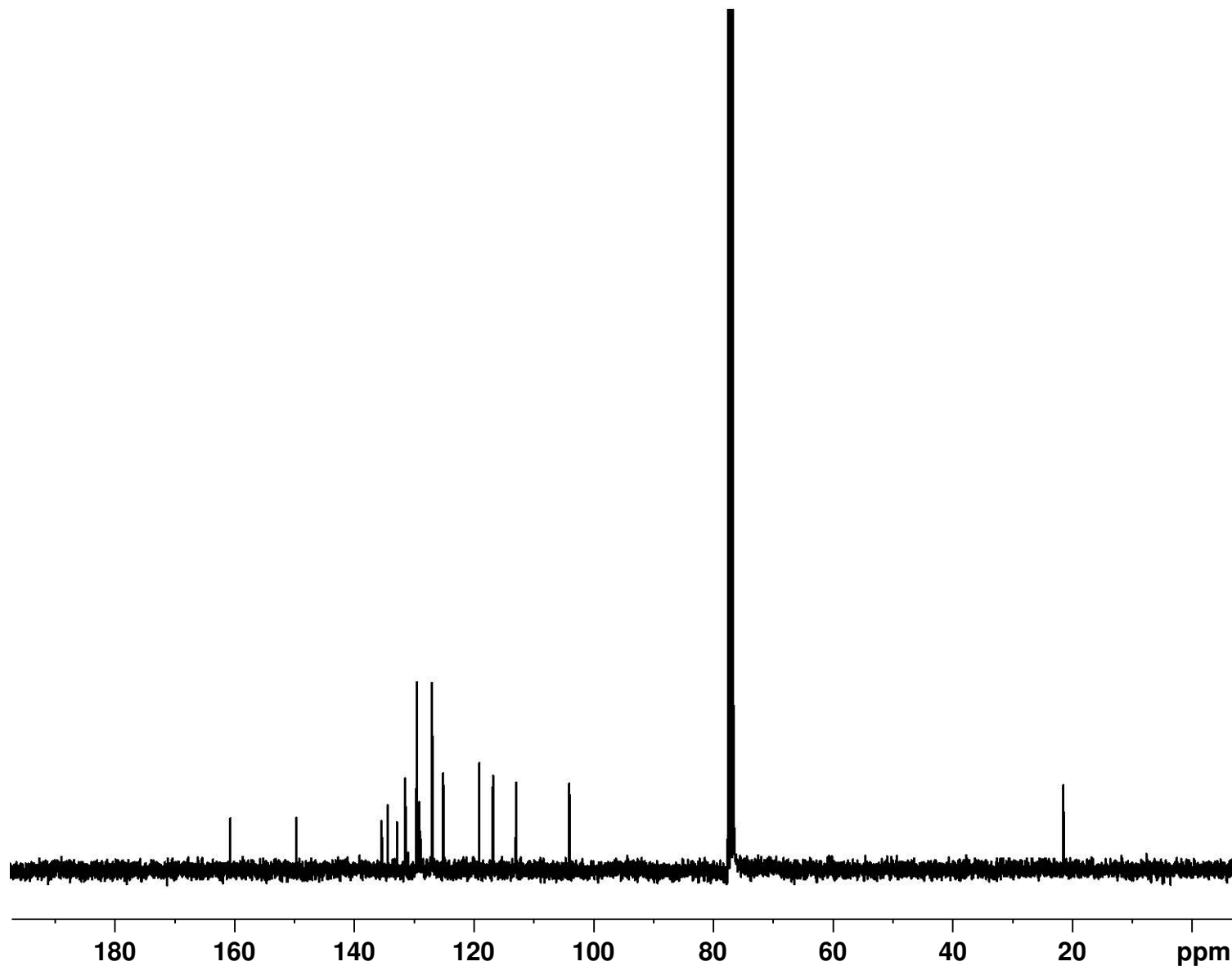
SFO1 75.4897560 MHz
NUC1 13C
P1 12.00 usec
PLW1 10.00000000 W

===== CHANNEL f2 =====

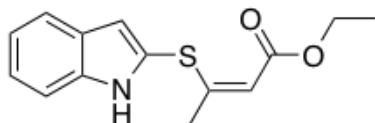
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.21333000 W
PLW13 0.17280000 W

F2 - Processing parameters

SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



ethyl (Z)-3-((1H-indol-2-yl)thio)but-2-enoate (19)



Current Data Parameters

NAME SR-03-329
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

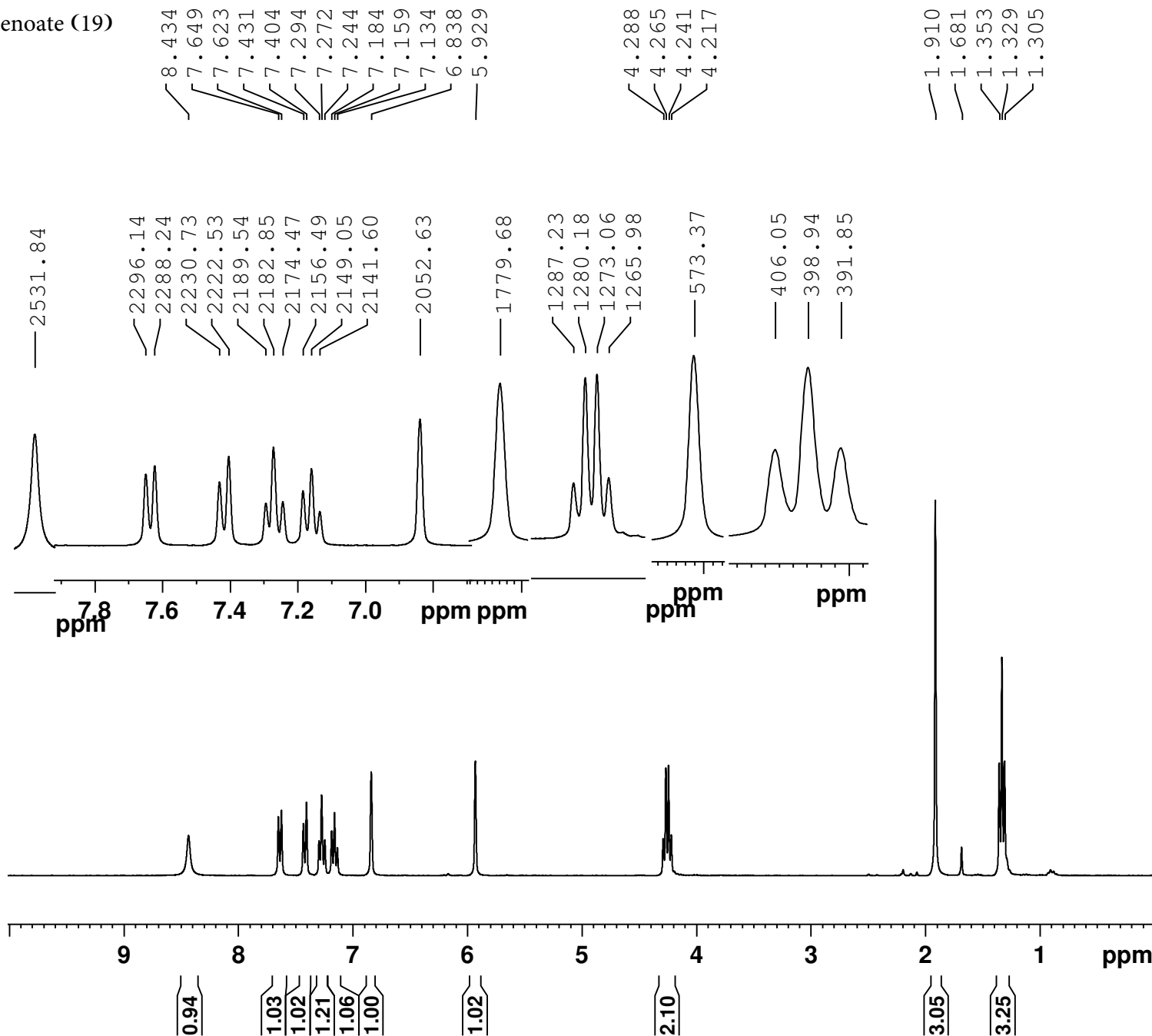
Date_ 20180822
Time 15.16
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 31.623
DW 81.920 usec
DE 6.50 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====

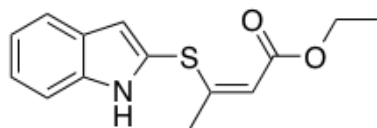
SFO1 300.1818536 MHz
NUC1 1H
P1 12.00 usec
PLW1 10.00000000 W

F2 - Processing parameters

SI 65536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ethyl (Z)-3-((1H-indol-2-yl)thio)but-2-enoate (19)



— 166.44
— 158.31
— 137.59
— 128.21
— 123.57
— 123.39
— 120.88
— 120.44
— 113.31
— 112.88
— 111.12

— 60.22

— 24.05

— 14.39

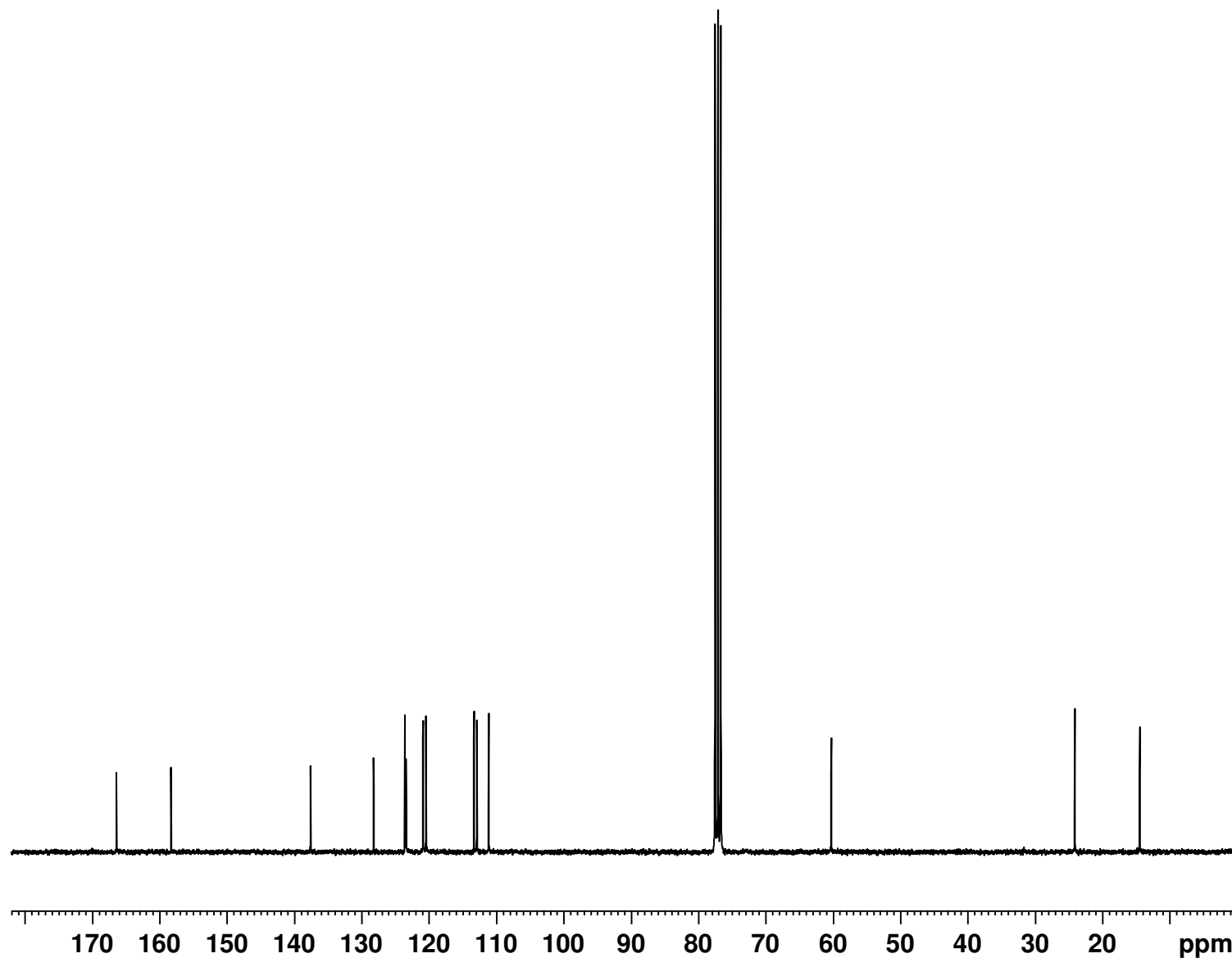
Current Data Parameters
NAME SR-03-329
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180822
Time 15.22
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10240
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 199.526
DW 20.480 usec
DE 6.50 usec
TE 293.7 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001200 sec
D40 0.02898005 sec
L4 40
L5 57
P32 90.00 usec
TD0 1

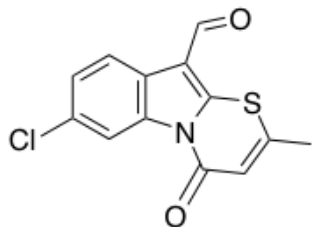
===== CHANNEL f1 =====
SFO1 75.4821746 MHz
NUC1 13C
P1 12.00 usec
PLW1 10.00000000 W

===== CHANNEL f2 =====
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.21333000 W
PLW13 0.17280000 W

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7-chloro-2-methyl-4-oxo-4H-[1,3]thiazino[3,2-a]indole-10-carbaldehyde (33)

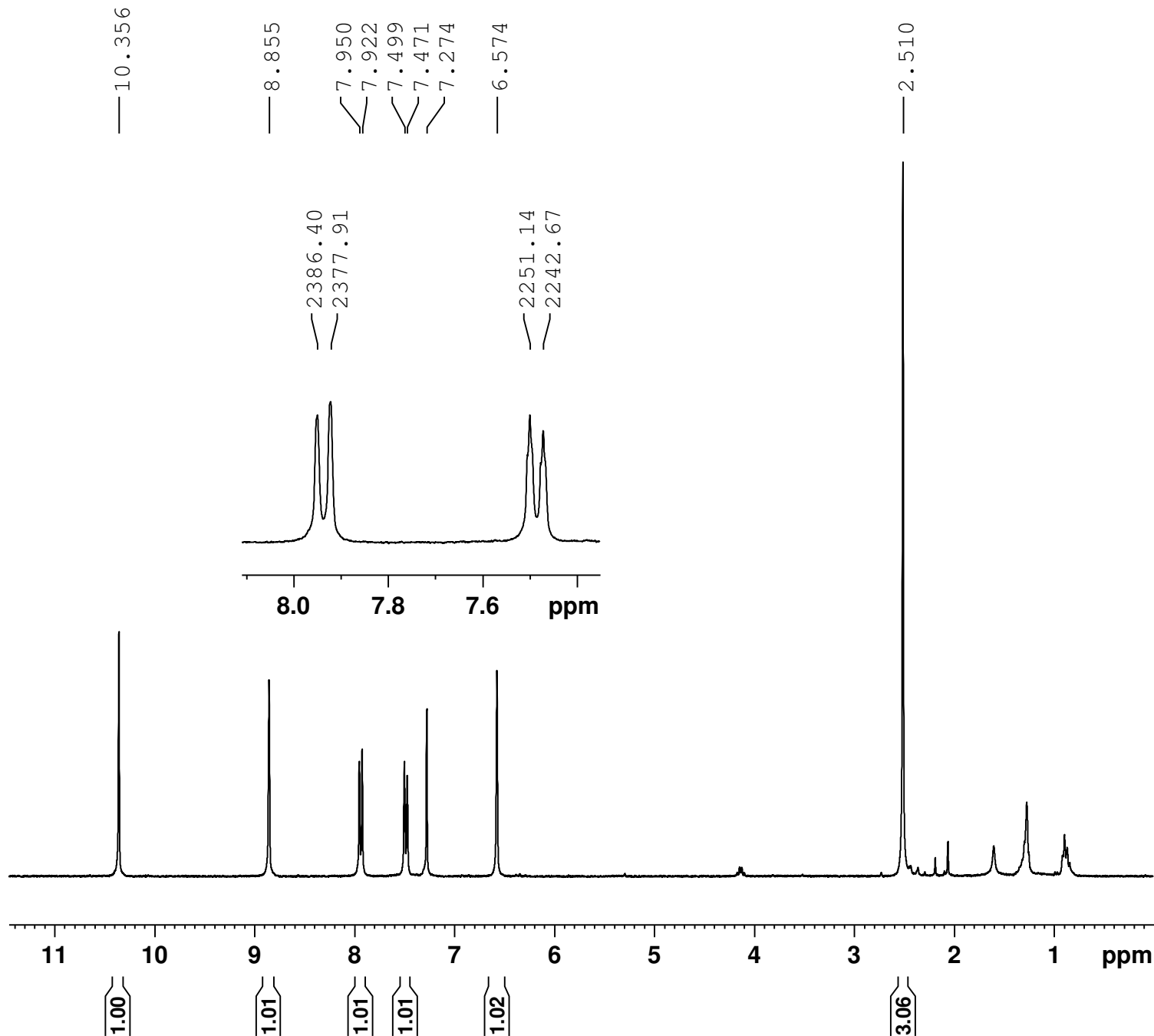


Current Data Parameters
NAME SR-04-444
EXPNO 4
PROCNO 1

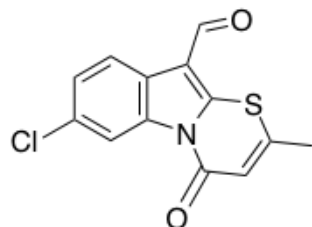
F2 - Acquisition Parameters
Date_ 20190207
Time 12.10
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 102.854
DW 81.920 usec
DE 6.50 usec
TE 293.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1818536 MHz
NUC1 1H
P1 12.00 usec
PLW1 10.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



7-chloro-2-methyl-4-oxo-4H-[1,3]thiazino[3,2-a]indole-10-carbaldehyde (33)



183.15

158.87

150.10

138.11

135.62

130.59

126.46

124.63

117.87

117.64

116.35

114.84

22.71

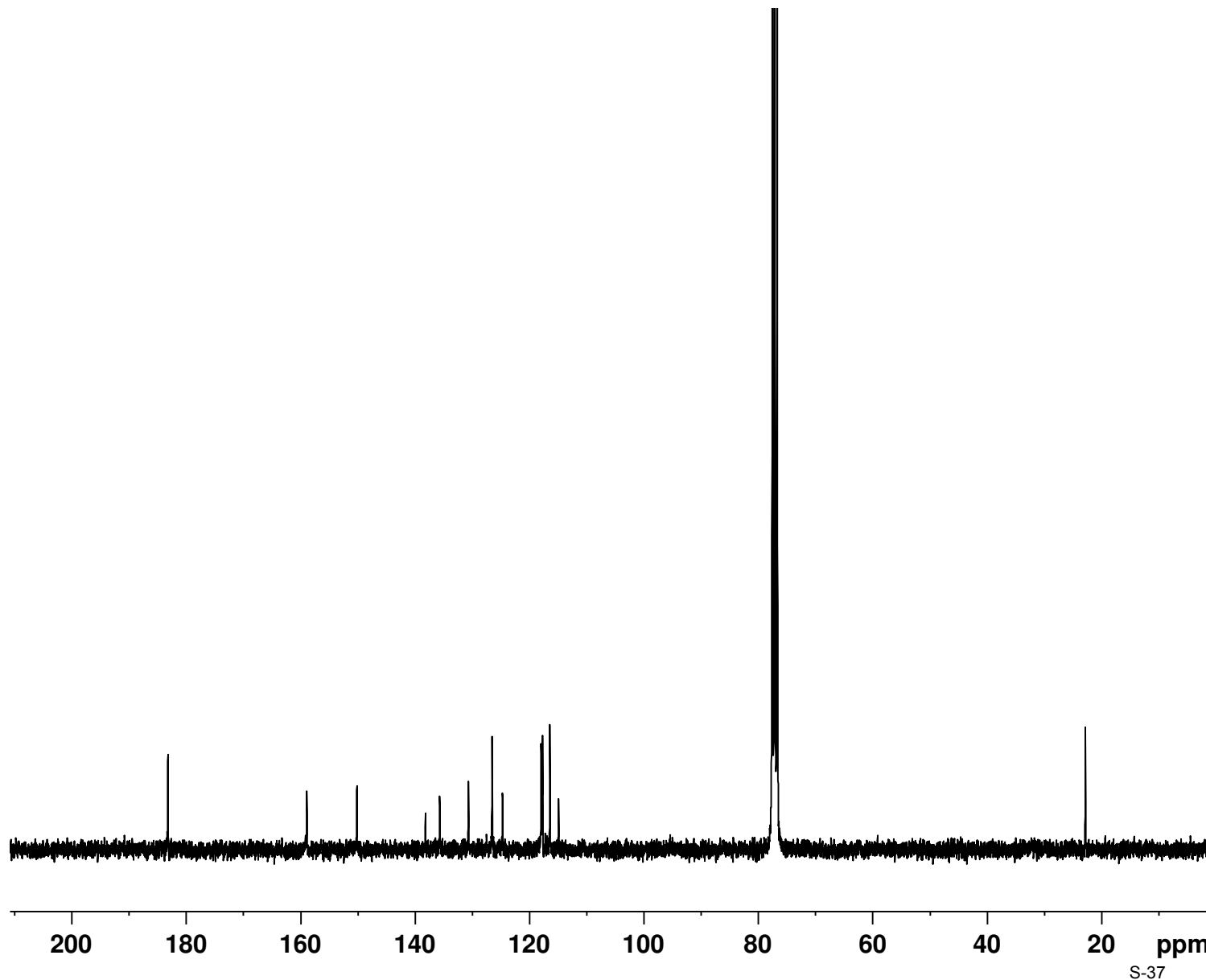
Current Data Parameters
NAME SR-04-444
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190128
Time 17.43
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 10240
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 199.526
DW 20.480 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001200 sec
D40 0.02898005 sec
L4 40
L5 57
P32 90.00 usec
TD0 1

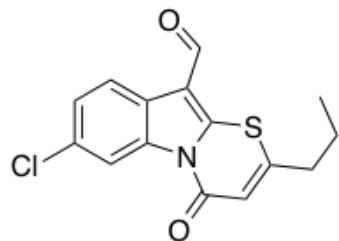
===== CHANNEL f1 =====
SFO1 75.4897560 MHz
NUC1 13C
P1 12.00 usec
PLW1 10.00000000 W

===== CHANNEL f2 =====
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.21333000 W
PLW13 0.17280000 W

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7-chloro-4-oxo-2-propyl-4H-[1,3]thiazino[3,2-a]indole-10-carbaldehyde (34)



Current Data Parameters
 NAME SR-04-445
 EXPNO 1
 PROCNO 1

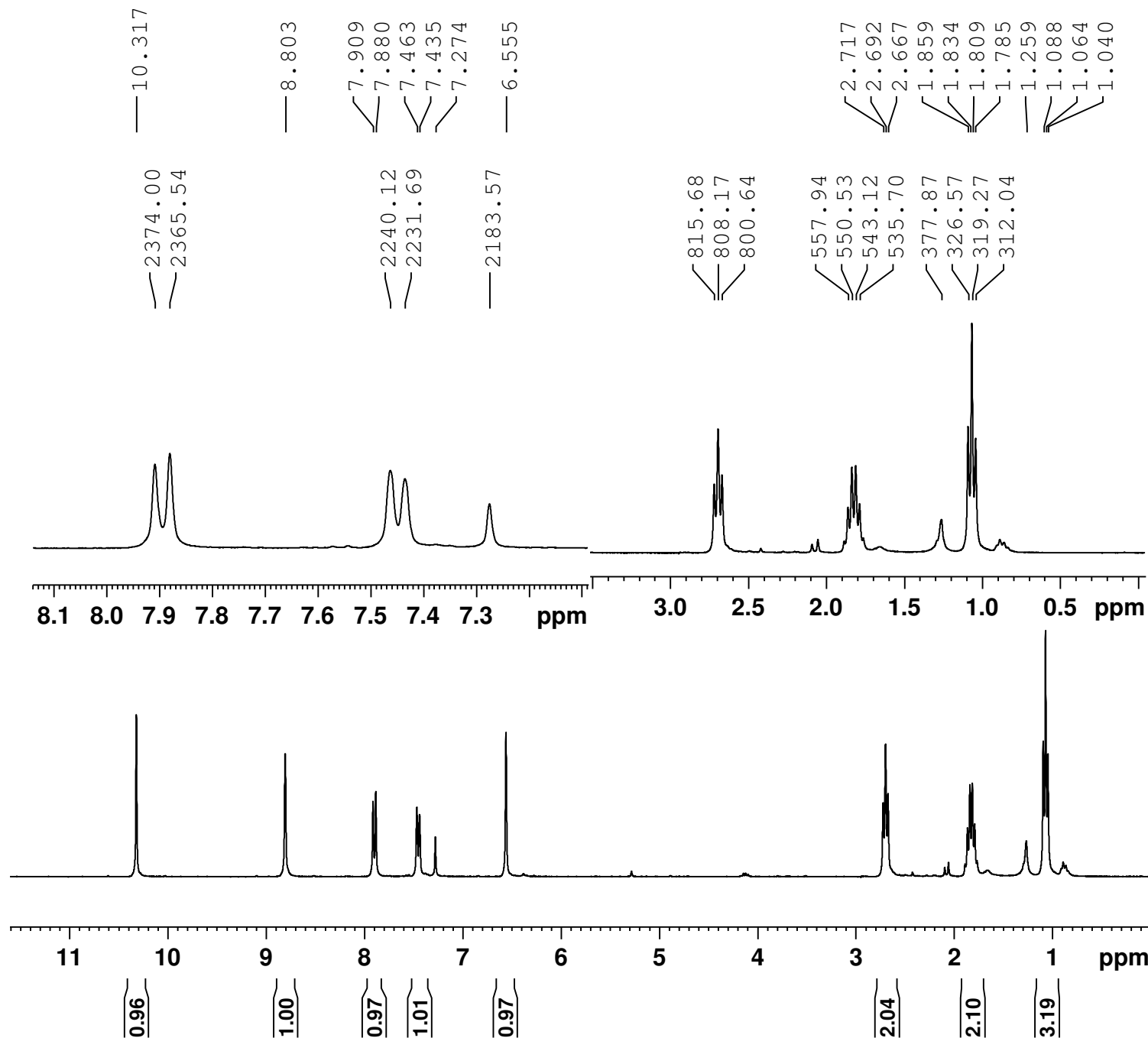
F2 - Acquisition Parameters

Date_ 20190129
 Time 13.34
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 31.623
 DW 81.920 usec
 DE 6.50 usec
 TE 295.4 K
 D1 1.00000000 sec
 TD0 1

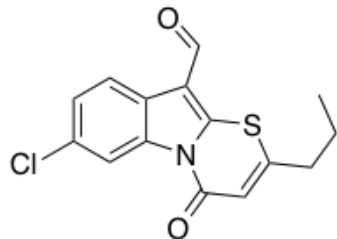
===== CHANNEL f1 =====
 SFO1 300.1818536 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 10.00000000 W

F2 - Processing parameters

SI 65536
 SF 300.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



7-chloro-4-oxo-2-propyl-4H-[1,3]thiazino[3,2-a]indole-10-carbaldehyde (34)



Current Data Parameters
NAME SR-04-445
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190129
Time 13.43
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2762
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 199.526
DW 20.480 usec
DE 6.50 usec
TE 295.4 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001200 sec
D40 0.02898005 sec
L4 40
L5 57
P32 90.00 usec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4897560 MHz
NUC1 13C
P1 12.00 usec
PLW1 10.00000000 W

===== CHANNEL f2 =====
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.21333000 W
PLW13 0.17280000 W

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

