

Title	Synthesis and evaluation of aromatic BDSF bioisosteres on biofilm formation and colistin sensitivity in pathogenic bacteria
Authors	Gómez, Andromeda-Celeste;Horgan, Conor;Yero, Daniel;Bravo, Marc;Daura, Xavier;O'Driscoll, Michelle;Gibert, Isidre;O'Sullivan, Timothy P.
Publication date	2023-09-23
Original Citation	Gómez, A.-C., Horgan, C., Yero, D., Bravo, M., Daura, X., O'Driscoll, M., Gibert, I. and O'Sullivan, T.P. (2023) 'Synthesis and evaluation of aromatic BDSF bioisosteres on biofilm formation and colistin sensitivity in pathogenic bacteria', European Journal of Medicinal Chemistry, 261, 115819 (16 pp). https://doi.org/10.1016/j.ejmech.2023.115819 .
Type of publication	Article (peer-reviewed)
Link to publisher's version	https://doi.org/10.1016/j.ejmech.2023.115819 - 10.1016/j.ejmech.2023.115819
Rights	© 2023 The Authors. Published by Elsevier Masson SAS. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/). - http://creativecommons.org/licenses/by/4.0/
Download date	2024-06-01 06:37:00
Item downloaded from	https://hdl.handle.net/10468/15122



UCC

University College Cork, Ireland
 Coláiste na hOllscoile Corcaigh

Supplementary Data

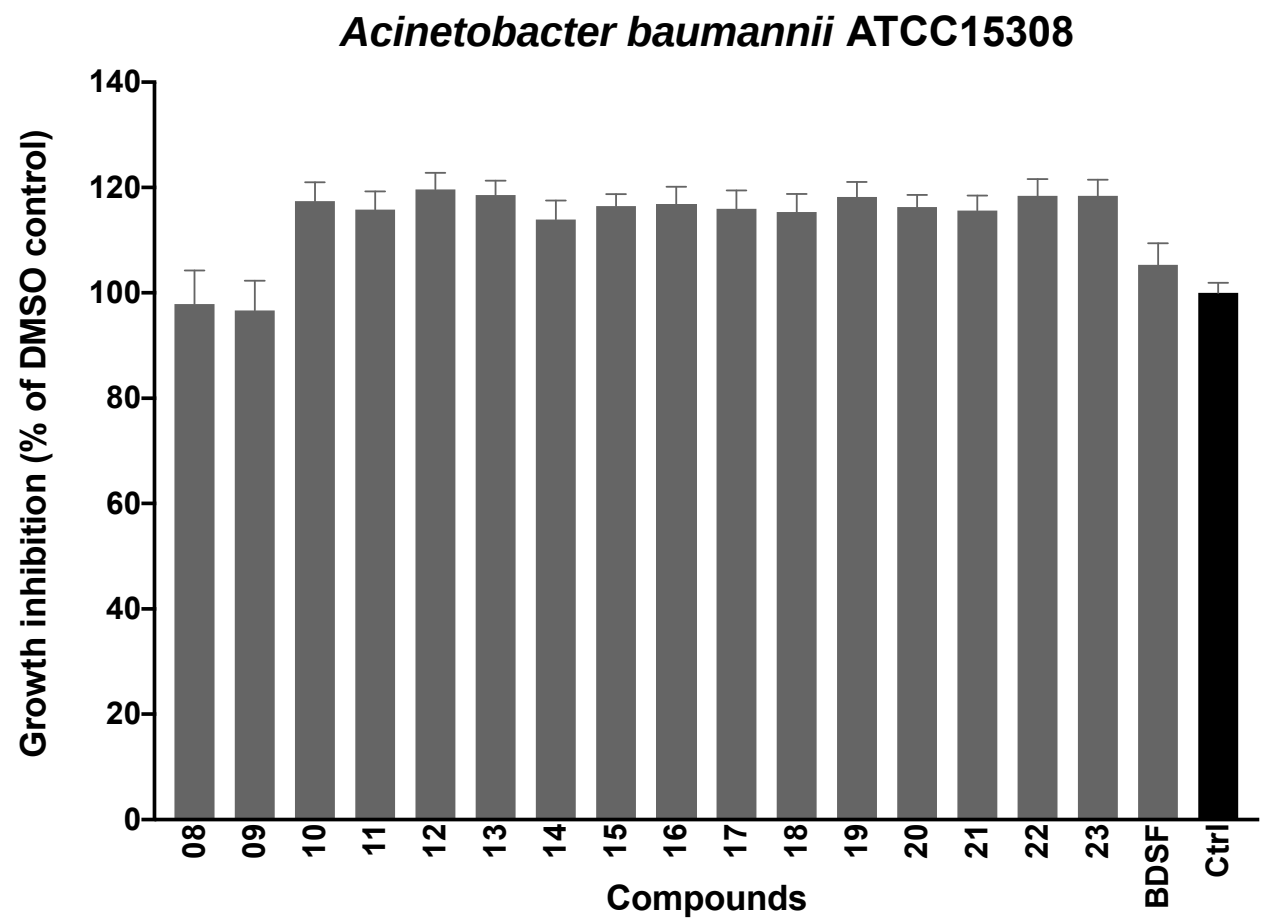
Synthesis and evaluation of aromatic BDSF bioisosteres on biofilm formation and colistin sensitivity in pathogenic bacteria

Andromeda-Celeste Gómez^{1,2*}, Conor Horgan^{3*}, Daniel Yero^{1,2}, Marc Bravo^{1,2}, Xavier Daura^{1,4,5}, Michelle O'Driscoll^{3,6,7}, Isidre Gibert^{1,2#} and Timothy P. O'Sullivan^{3,6,7#}.

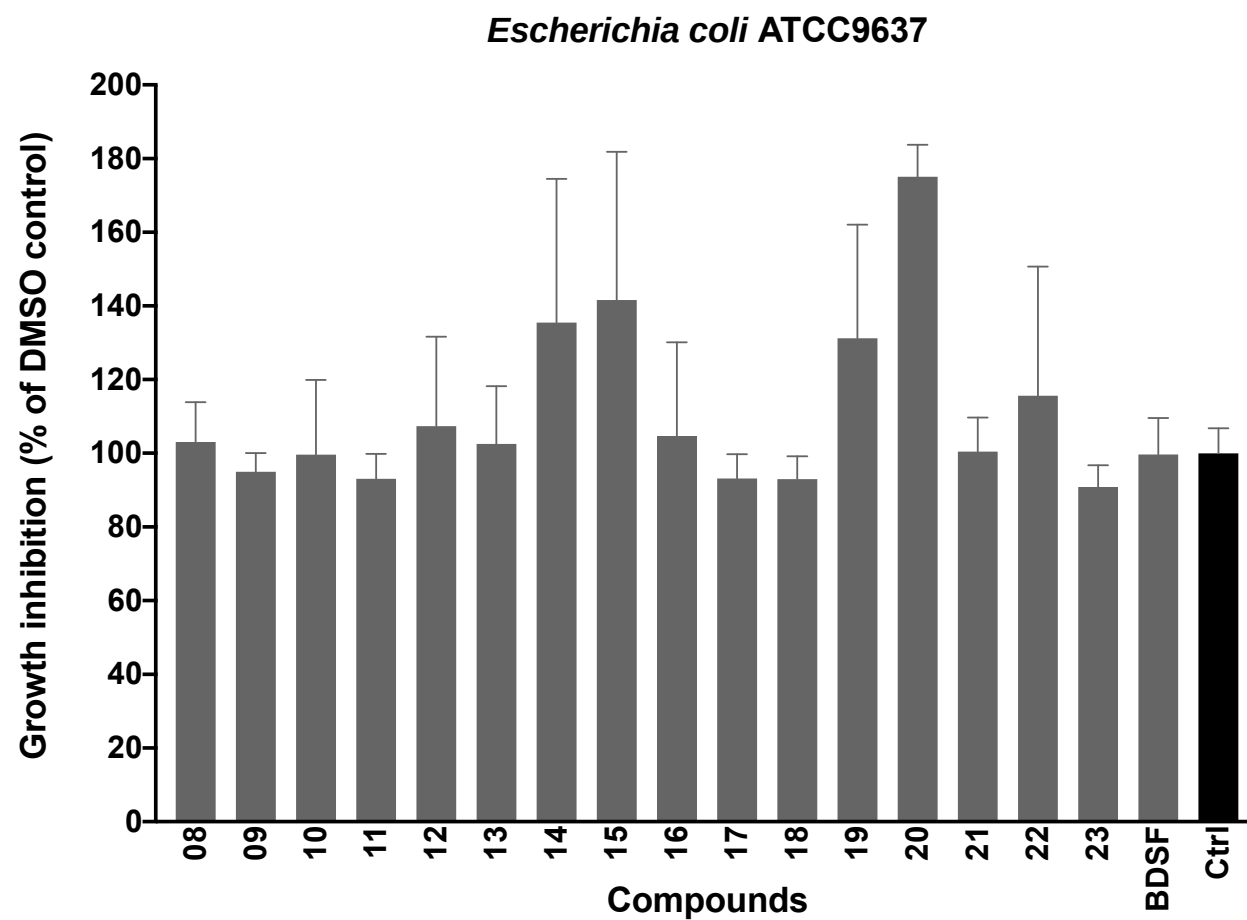
Affiliation

¹Institut de Biotecnologia i de Biomedicina, Universitat Autònoma de Barcelona, Barcelona, Spain; ²Departament de Genètica i de Microbiologia, Universitat Autònoma de Barcelona, Barcelona, Spain; ³School of Chemistry, University College Cork, Cork, Ireland; ⁴Catalan Institution for Research and Advanced Studies (ICREA), Barcelona, Spain; ⁵ CIBER de Bioingeniería, Biomateriales y Nanomedicina, Instituto de Salud Carlos III, Cerdanyola de Vallès, Spain; ⁶School of Pharmacy, University College Cork, Cork, Ireland; ⁷Analytical and Biological Chemistry Research Facility, University College Cork, Cork, Ireland.

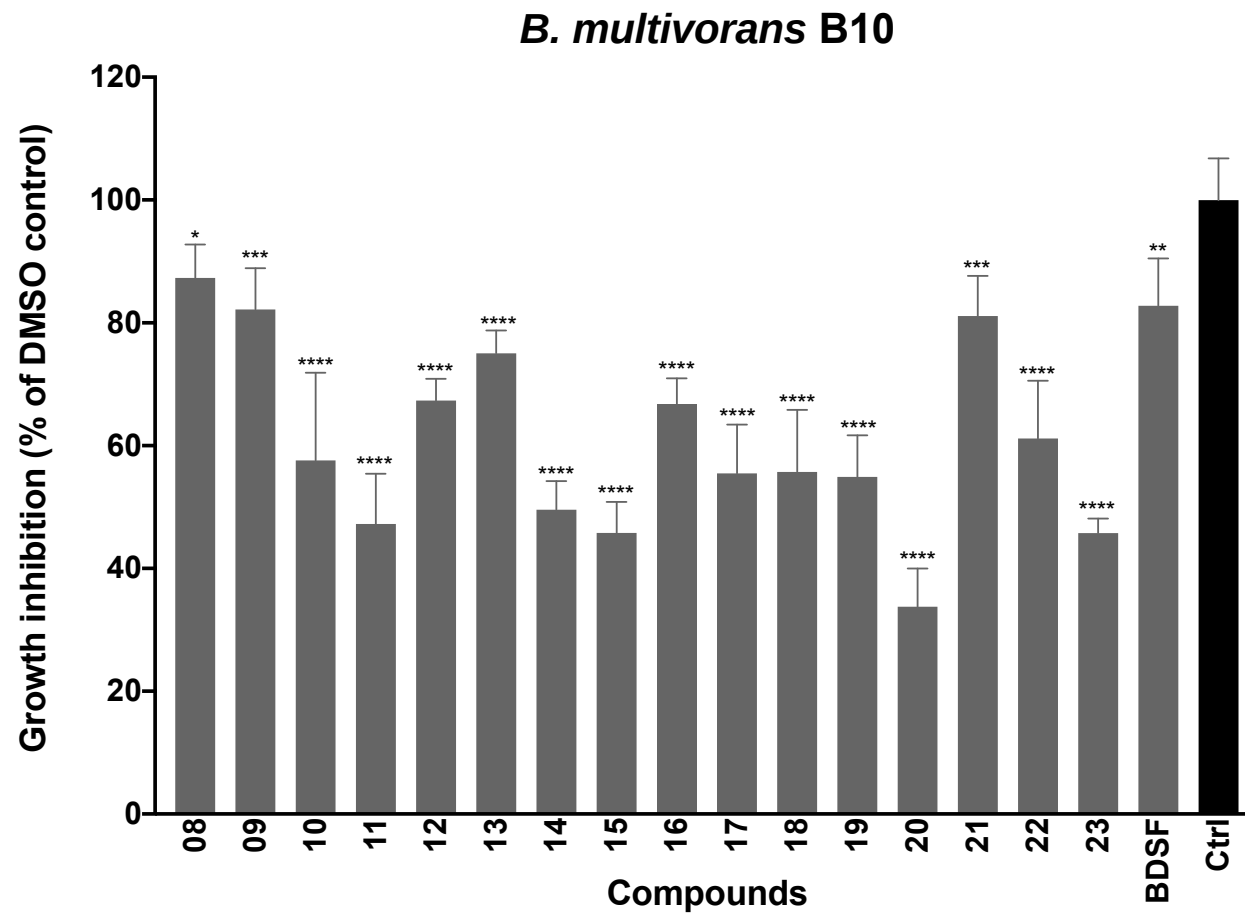
Effect of BDSF derivates on bacterial growth



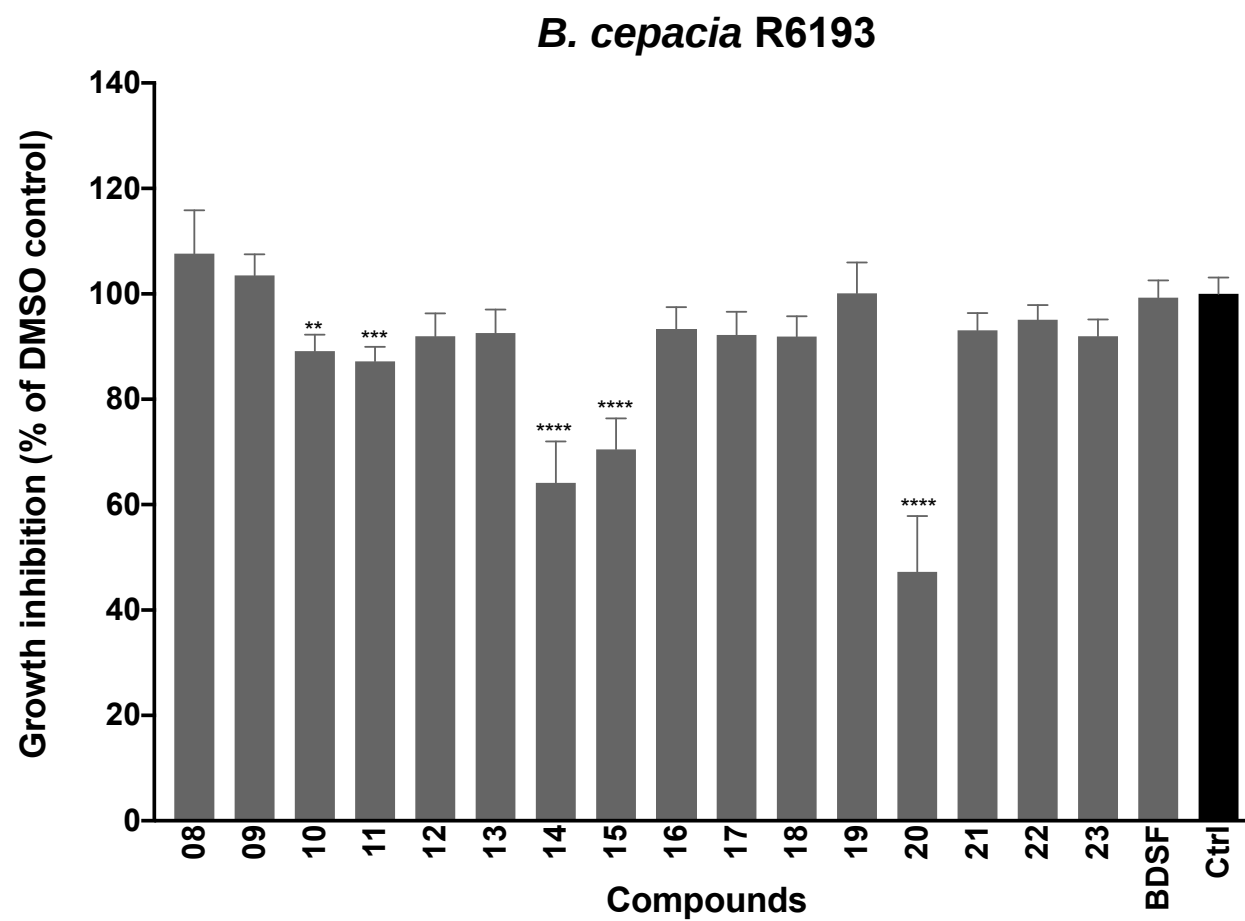
Supplementary Figure A1. Effect of sulfonamides on bacterial growth of *A. baumannii* ATCC15308.



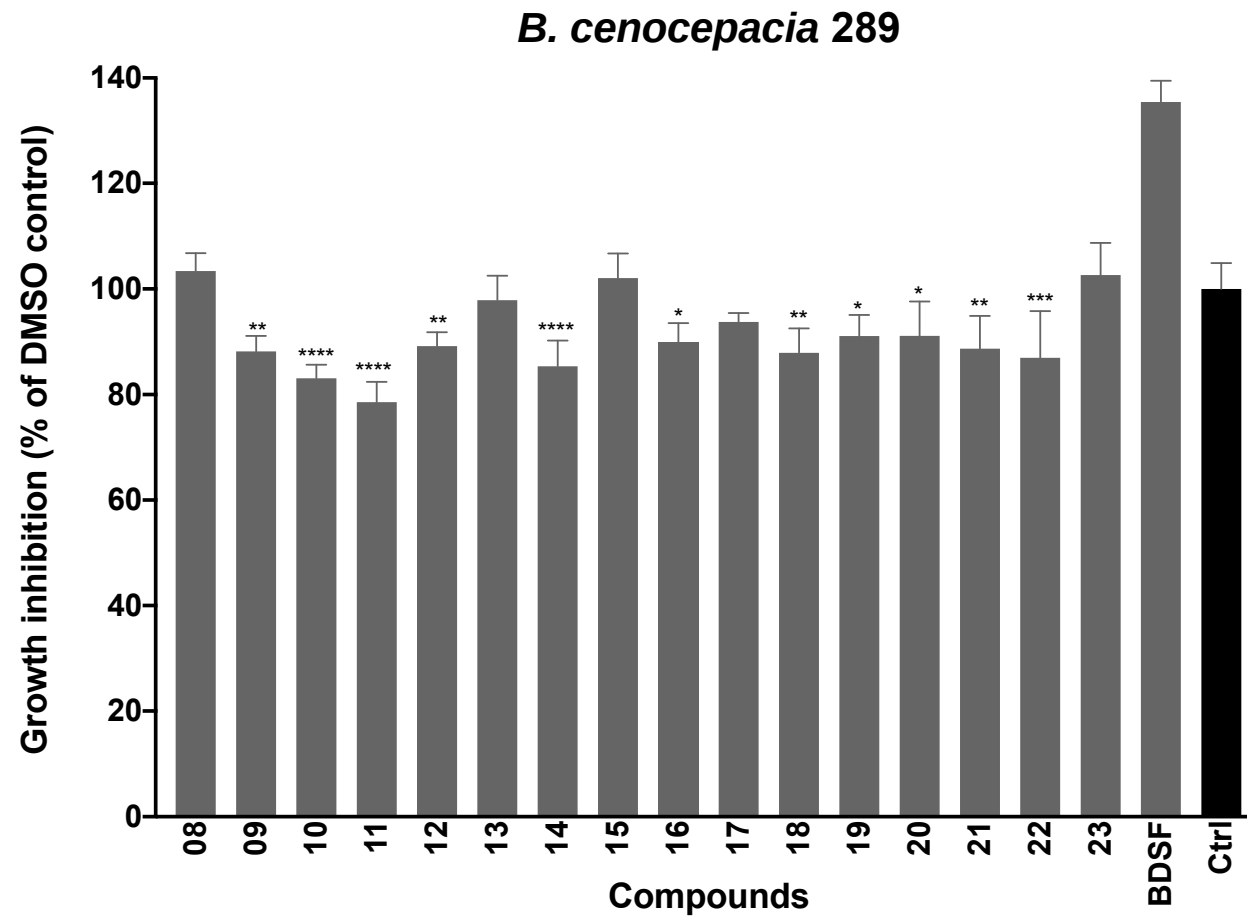
Supplementary Figure A2. Effect of sulfonamides on bacterial growth of *E. coli* ATCC9637.



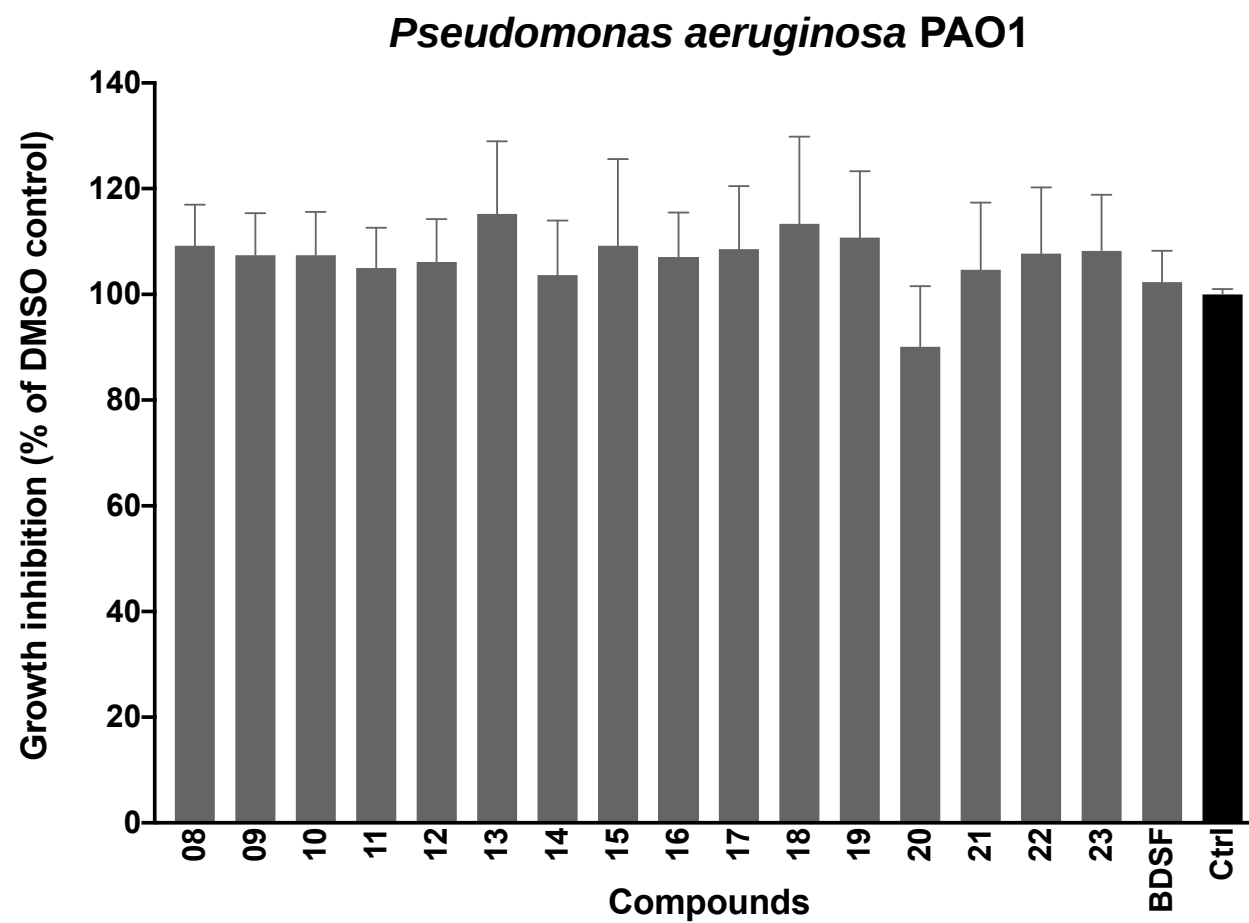
Supplementary Figure A3. Effect of sulfonamides on bacterial growth of *B. multivorans* B10 (* $p < 0.05$, ** $p < 0.01$, *** $p < 0.001$, **** $p < 0.0001$).



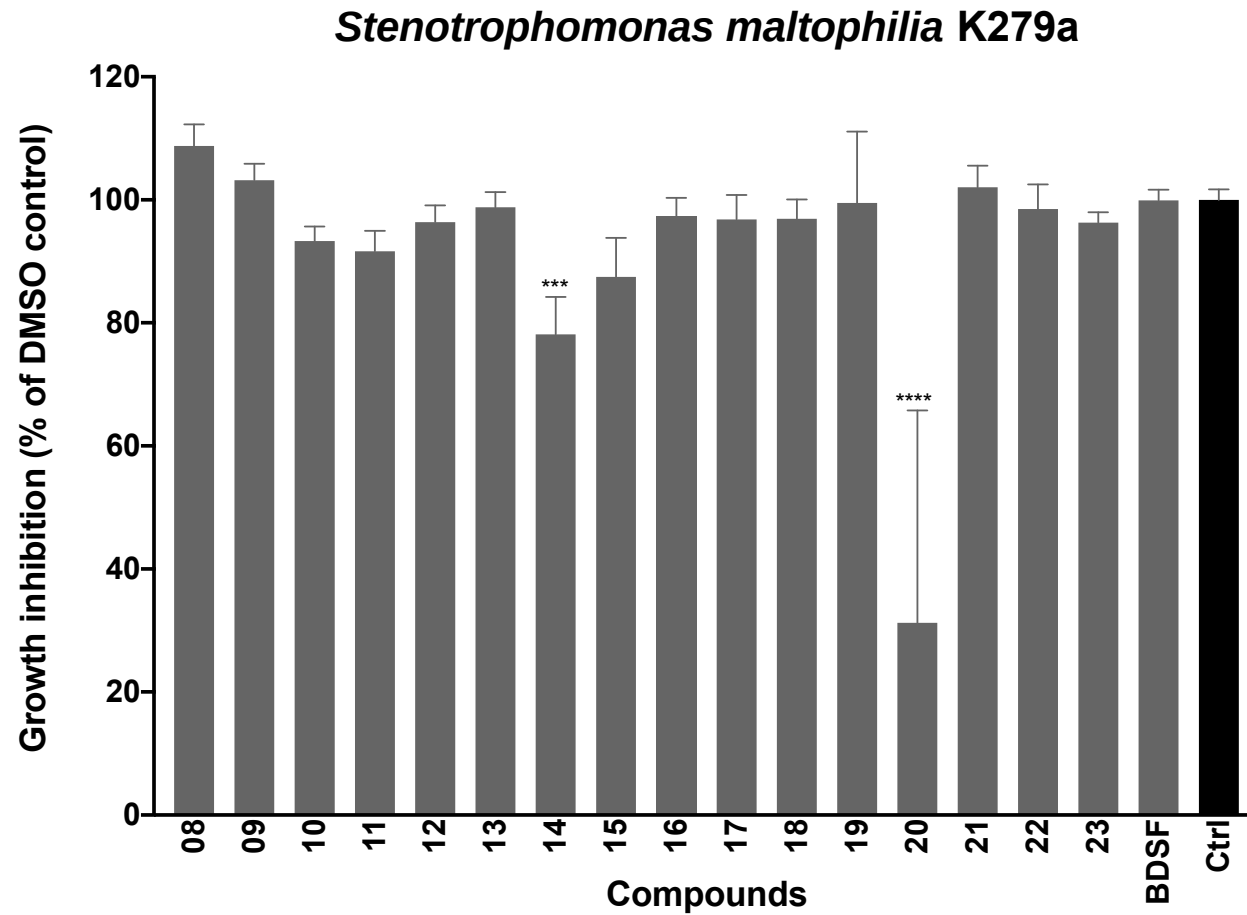
Supplementary Figure A4. Effect of sulfonamides on bacterial growth of *B. cepacia* R6193 (* $p < 0.05$, ** $p < 0.01$, *** $p < 0.001$, **** $p < 0.0001$).



Supplementary Figure A5. Effect of sulfonamides on bacterial growth of *B. cenocepacia* 289 (* $p < 0.05$, ** $p < 0.01$, *** $p < 0.001$, **** $p < 0.0001$).

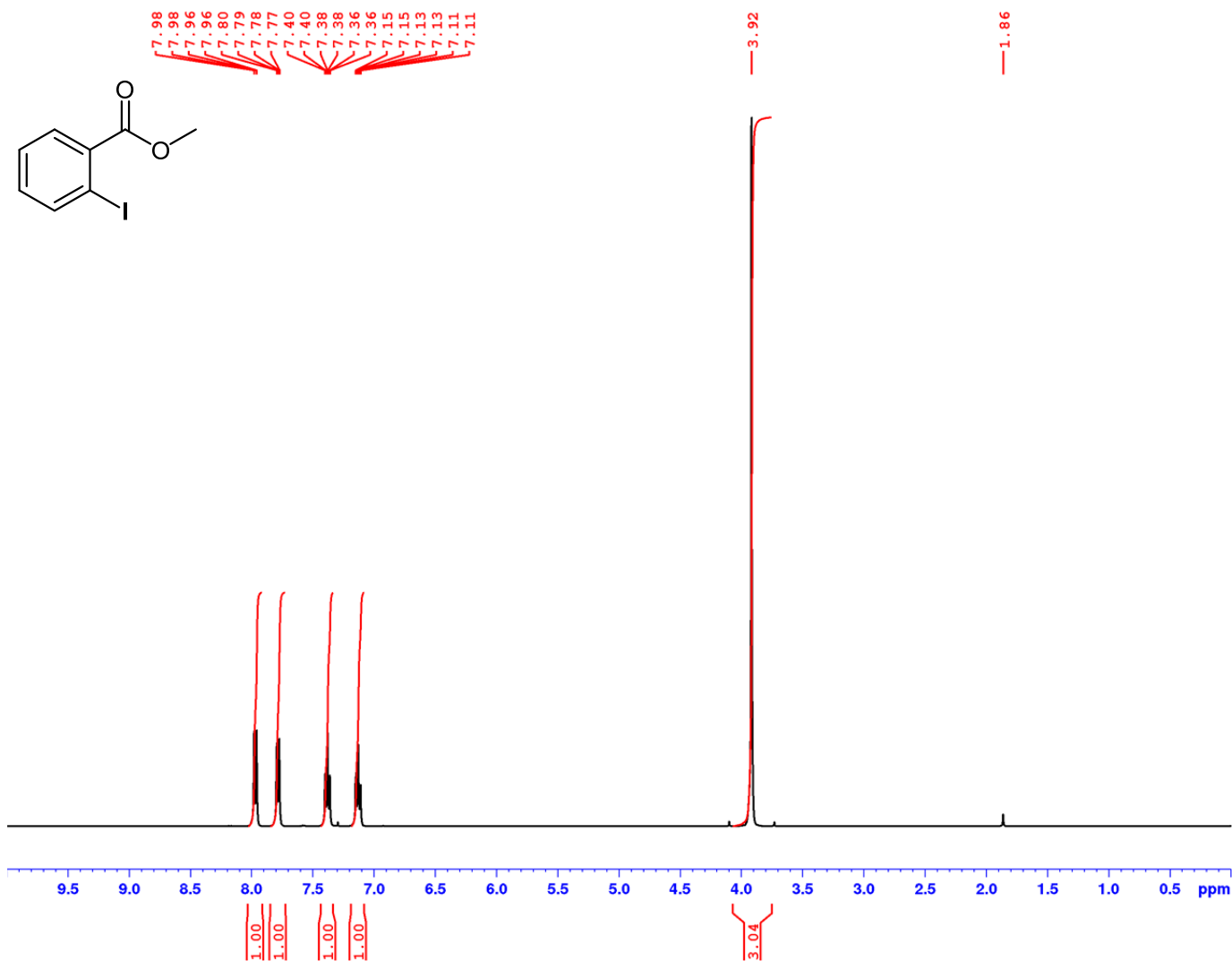


Supplementary Figure A6. Effect of sulfonamides on bacterial growth of *P. aeruginosa* PAO1.



Supplementary Figure A7. Effect of sulfonamides on bacterial growth of *S. maltophilia* K279a (* $p < 0.05$, ** $p < 0.01$, *** $p < 0.001$, **** $p < 0.0001$).

Methyl 2-Iodobenzoate (4)



Current Data Parameters
NAME 41042901
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190307
Time 11.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 131072
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.063157 Hz
AQ 7.9167490 sec
RG 35.9
DW 60.400 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 -0.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1299956 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



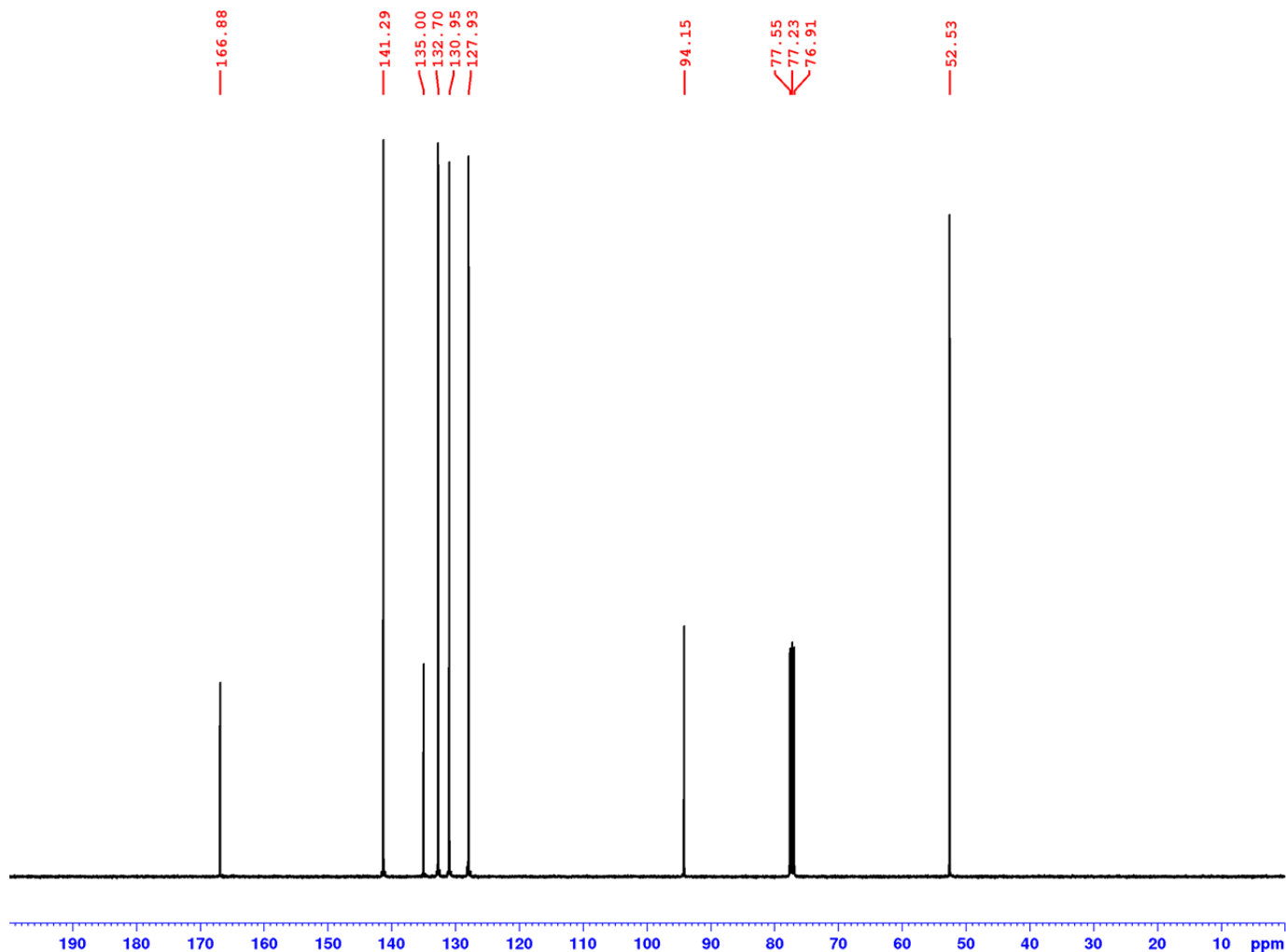
Current Data Parameters
NAME 4I042902
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190308
Time 22.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.182959 Hz
AQ 2.7328513 sec
RG 456.1
DW 20.850 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

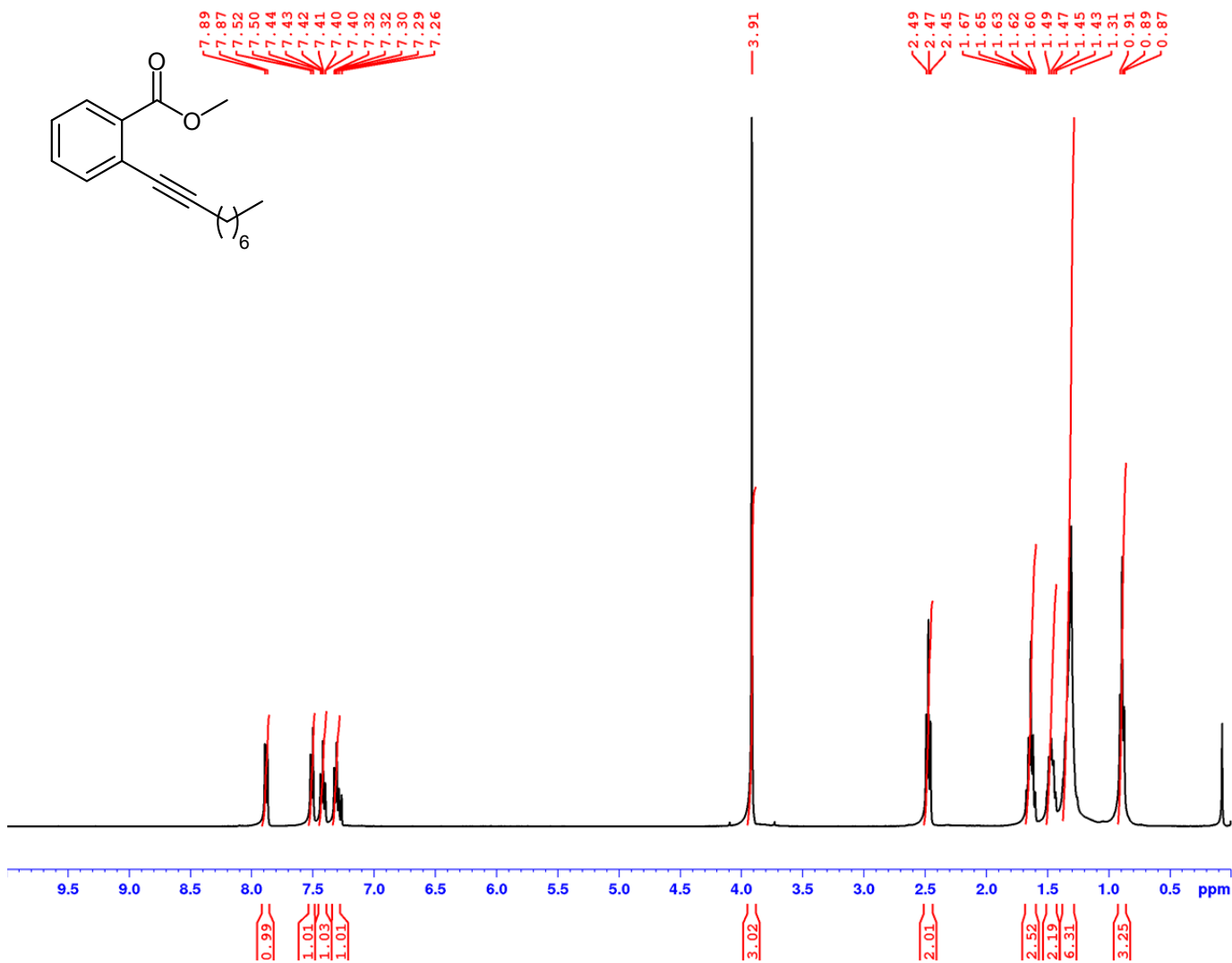
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -0.50 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -0.20 dB
PL12 17.93 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Methyl 2-(Non-1-yn-1-yl)benzoate (5)



Current Data Parameters
 NAME 4I004301
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190205
 Time 13.19
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 131072
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.063157 Hz
 AQ 7.9167490 sec
 RG 64
 DW 60.400 usec
 DE 6.00 usec
 TE 673.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.00 usec
 PL1 -0.50 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300077 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



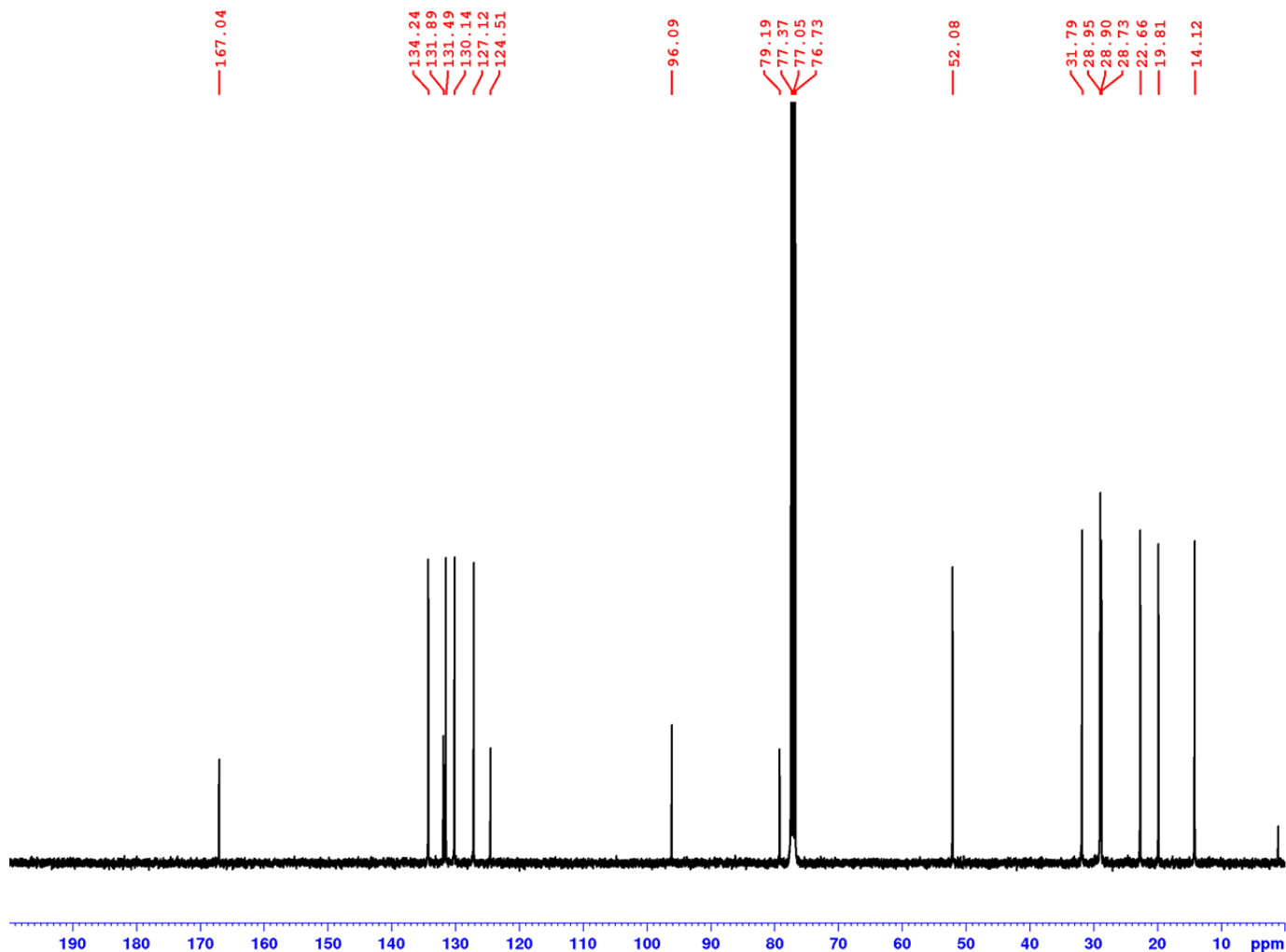
Current Data Parameters
NAME 4I004302
EXPNO 10
PROCNO 1

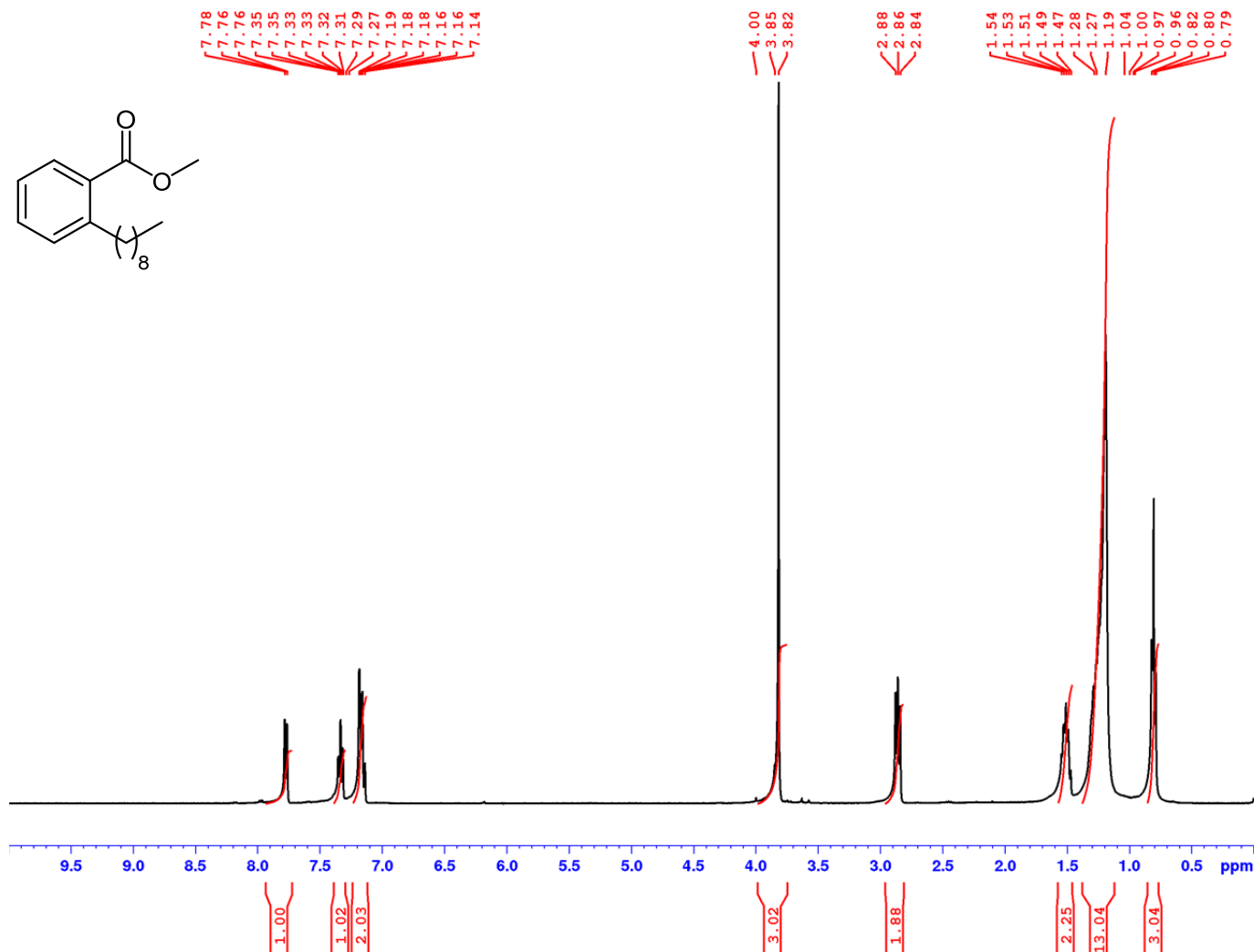
F2 - Acquisition Parameters
Date_ 20190206
Time 22.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.182959 Hz
AQ 2.7328513 sec
RG 456.1
DW 20.850 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -0.50 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -0.20 dB
PL12 17.93 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



CC(=O)c1ccccc1C(C)C

```

Current Data Parameters
NAME          4I057501
EXPNO         10
PROCNO        1

F2 - Acquisition Parameters
Date_         20190315
Time          18.15
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zg30
TD            131072
SOLVENT       CDC13
NS            8
DS            2
SWH           8278.146 Hz
FIDRES        0.063157 Hz
AQ            7.9167490 sec
RG            90.5
DW            60.400 usec
DE            6.00 usec
TE            673.2 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            11.00 usec
PL1          -0.50 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI            65536
SF            400.1300384 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```



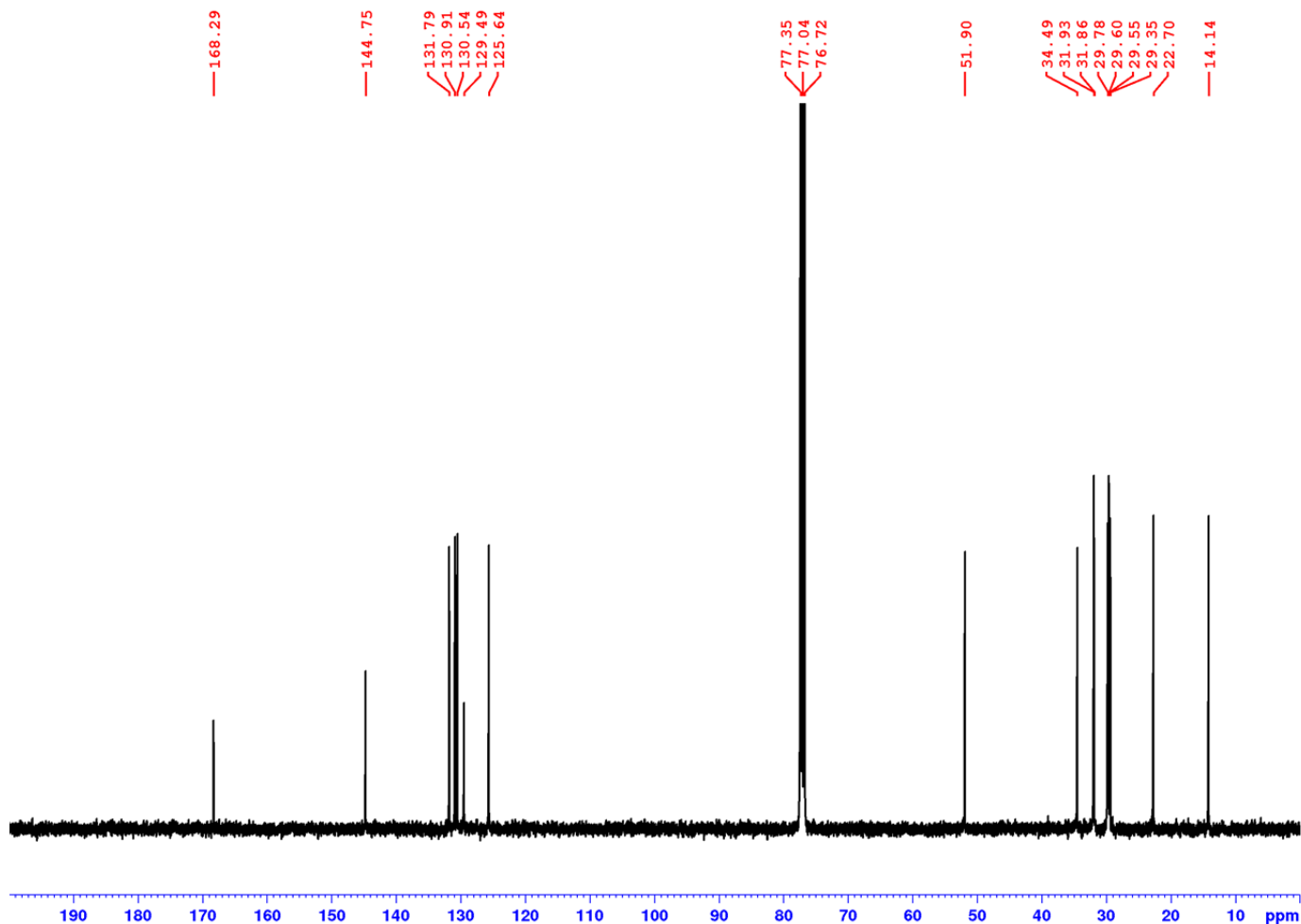
Current Data Parameters
NAME 4I057502
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190316
Time 11.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.182959 Hz
AQ 2.7328513 sec
RG 456.1
DW 20.850 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

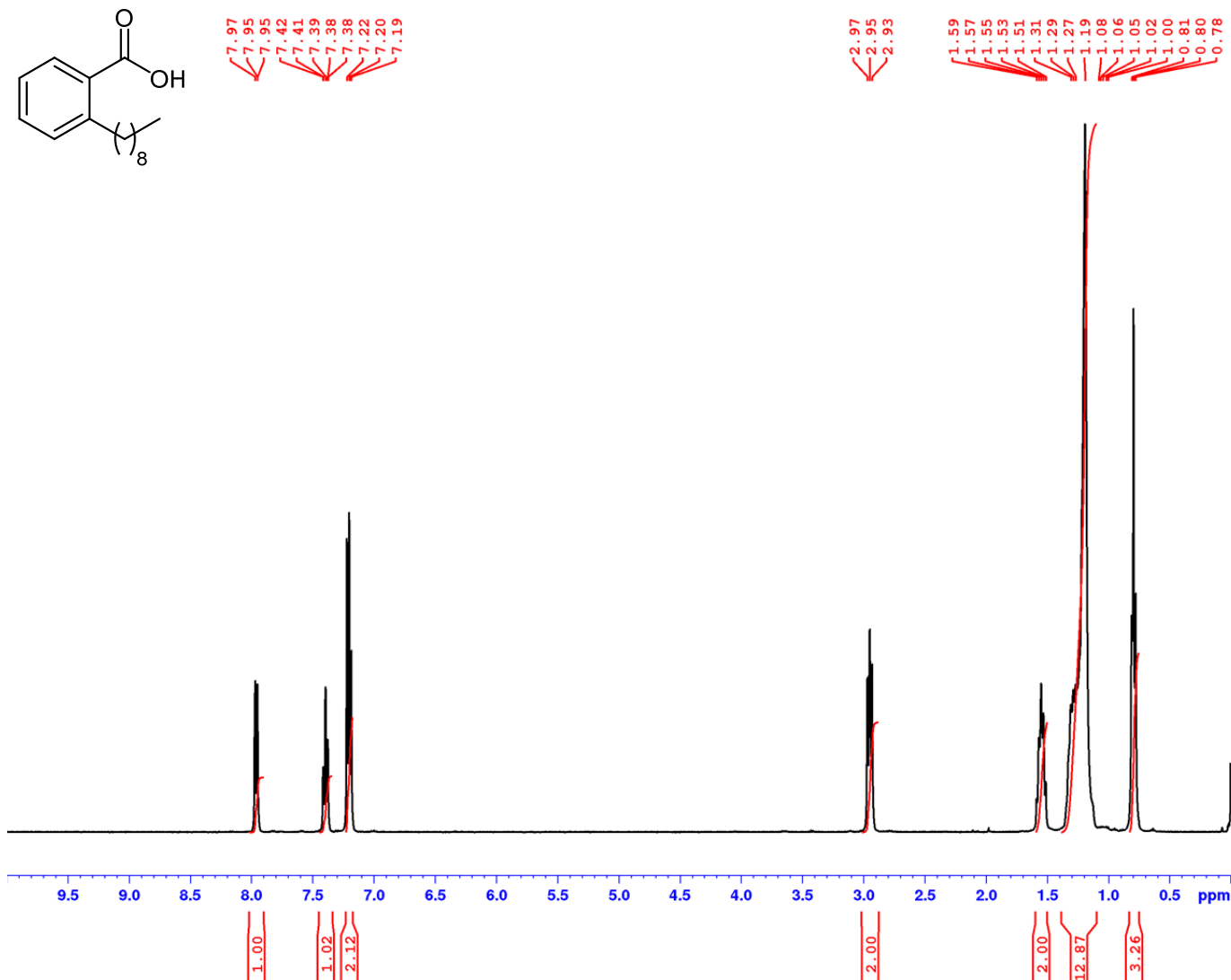
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -0.50 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -0.20 dB
PL12 17.93 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



2-Nonylbenzoic Acid (7)



Current Data Parameters
NAME 4H264601
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180802
Time 13.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 131072
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.063157 Hz
AQ 7.9167490 sec
RG 114
DW 60.400 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 -0.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300397 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



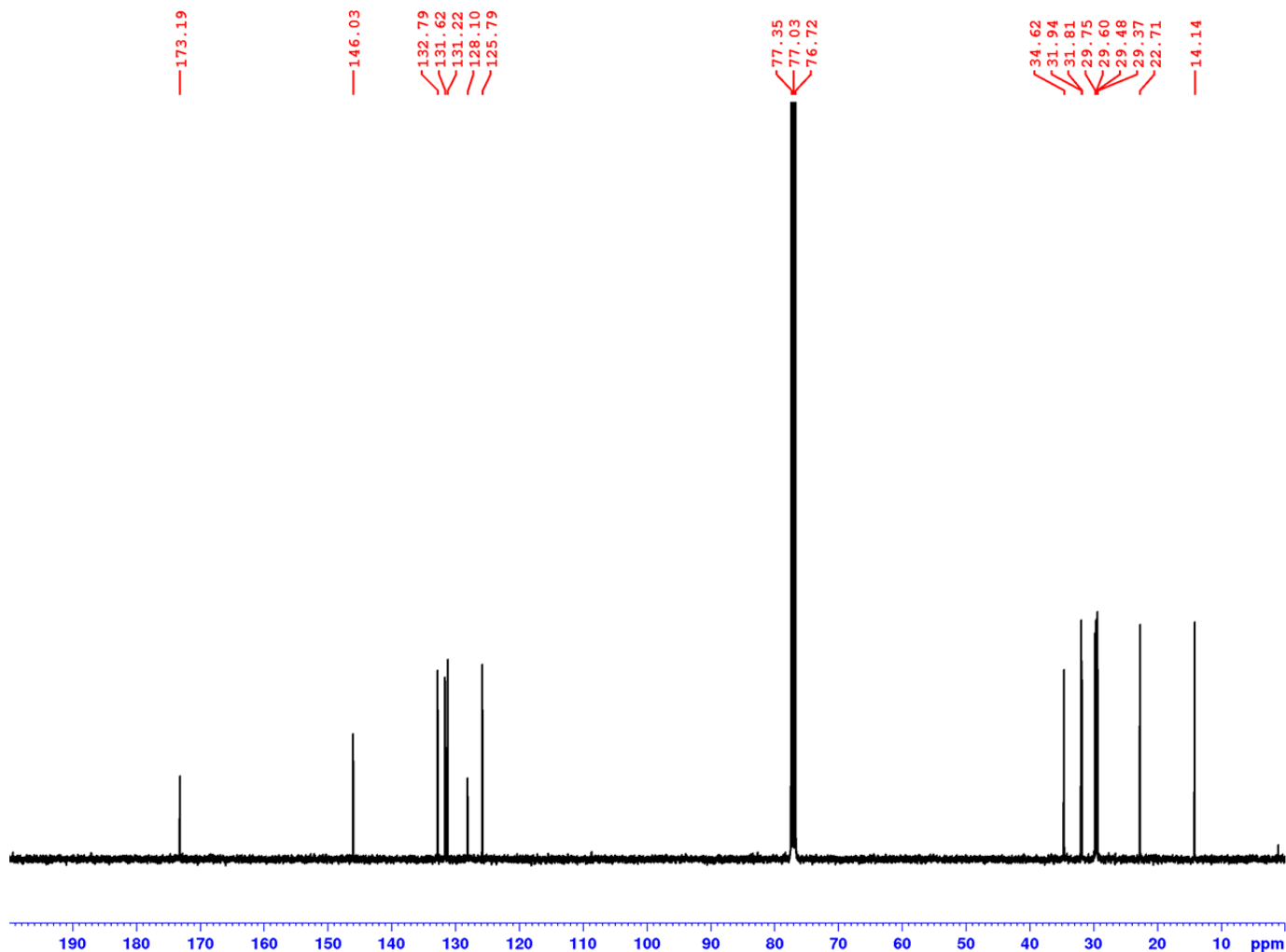
Current Data Parameters
NAME 4H264602
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180804
Time 6.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.182959 Hz
AQ 2.7328513 sec
RG 456.1
DW 20.850 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

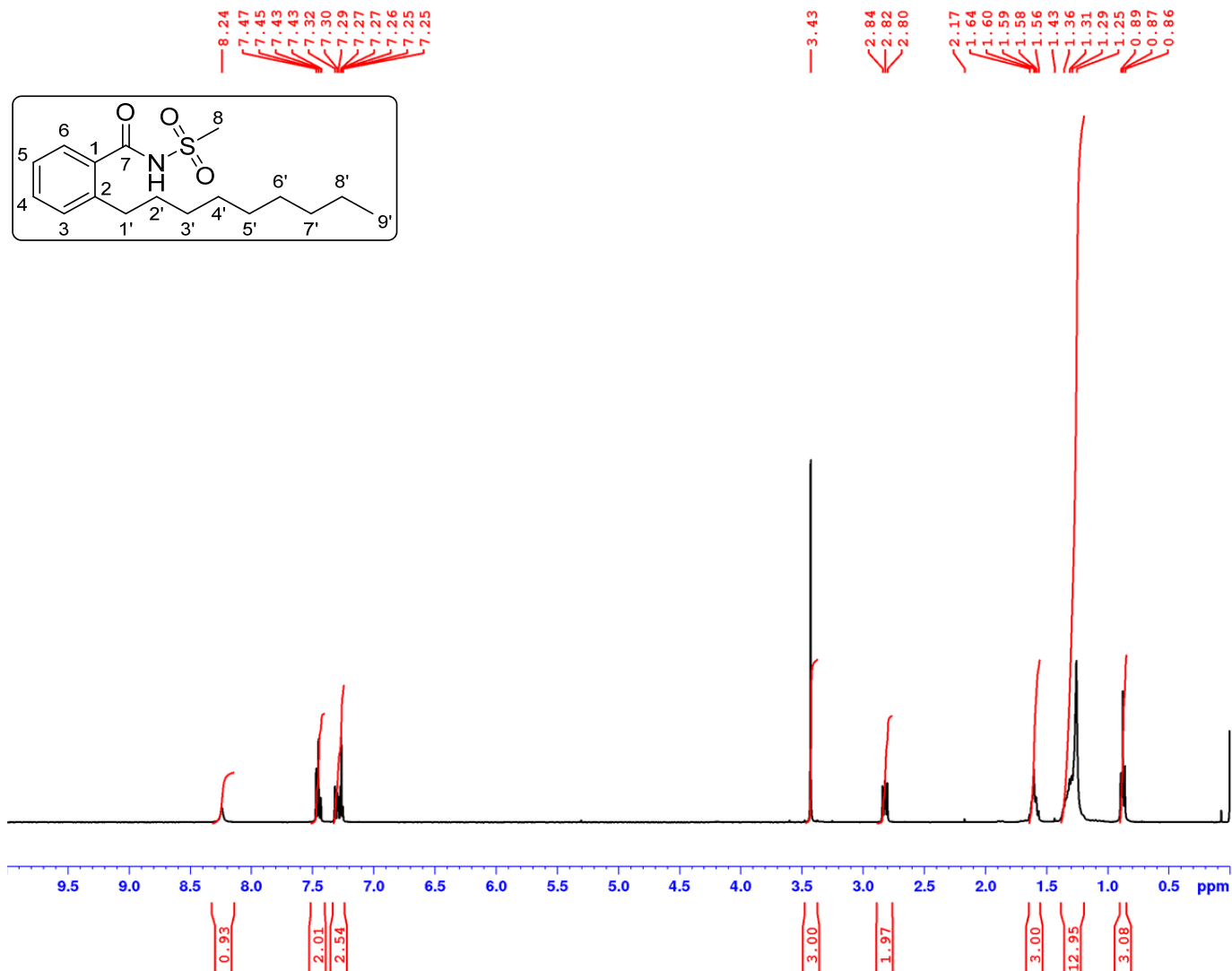
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -0.50 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -0.20 dB
PL12 17.93 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



***N*-(Methanesulfonyl)-2-nonylbenzamide (8)**



Current Data Parameters
NAME 41155401
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190612
Time 18.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 131072
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.063157 Hz
AQ 7.9167490 sec
RG 181
DW 60.400 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 -0.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300083 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



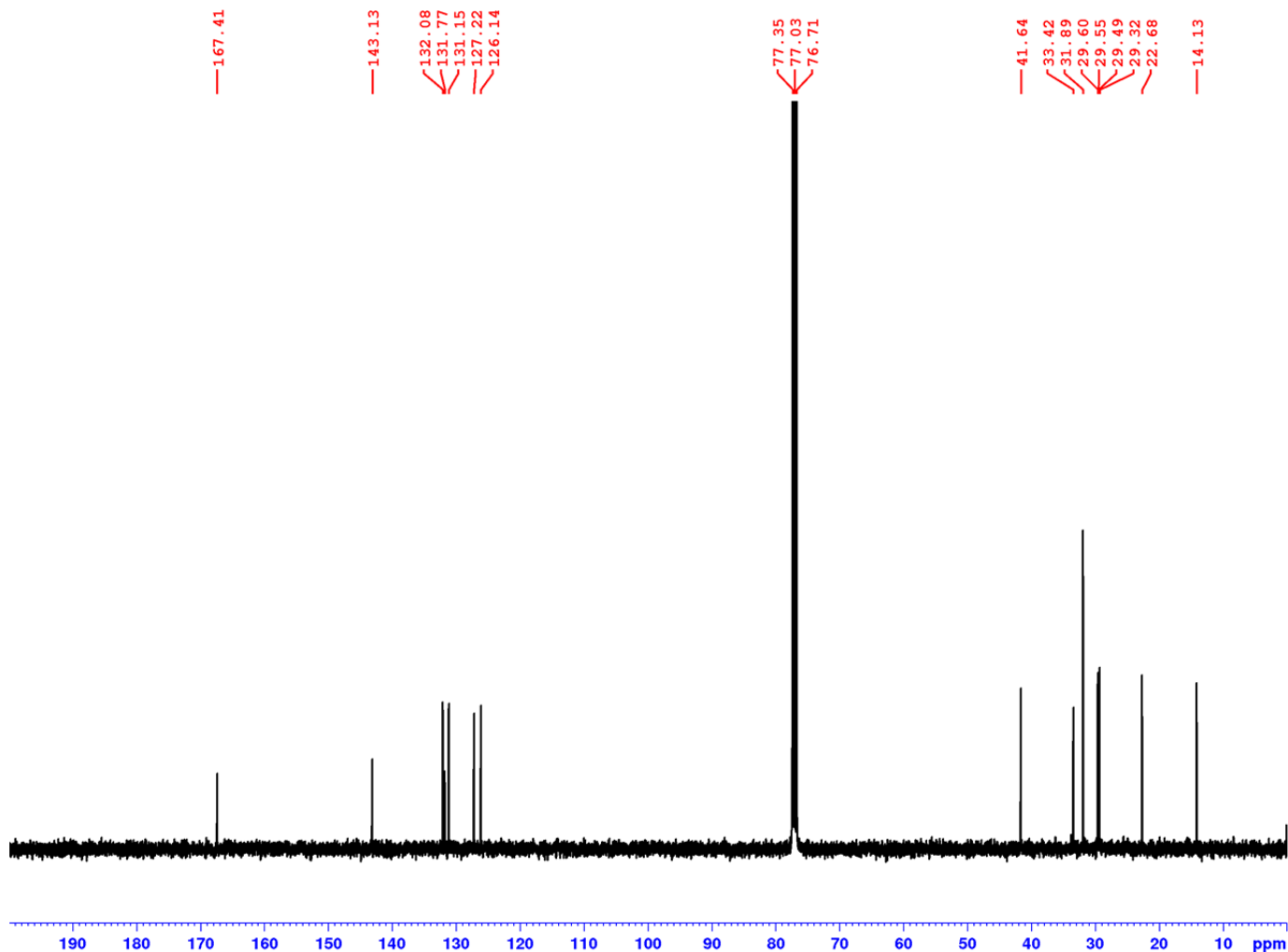
Current Data Parameters
NAME 4I155402
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190612
Time 22.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.182959 Hz
AQ 2.7328513 sec
RG 456.1
DW 20.850 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

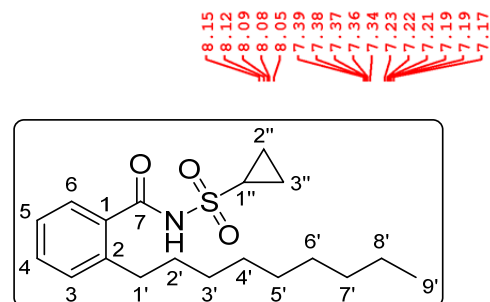
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -0.50 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -0.20 dB
PL12 17.93 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



N-(Cyclopropanesulfonyl)-2-nonylbenzamide (9)

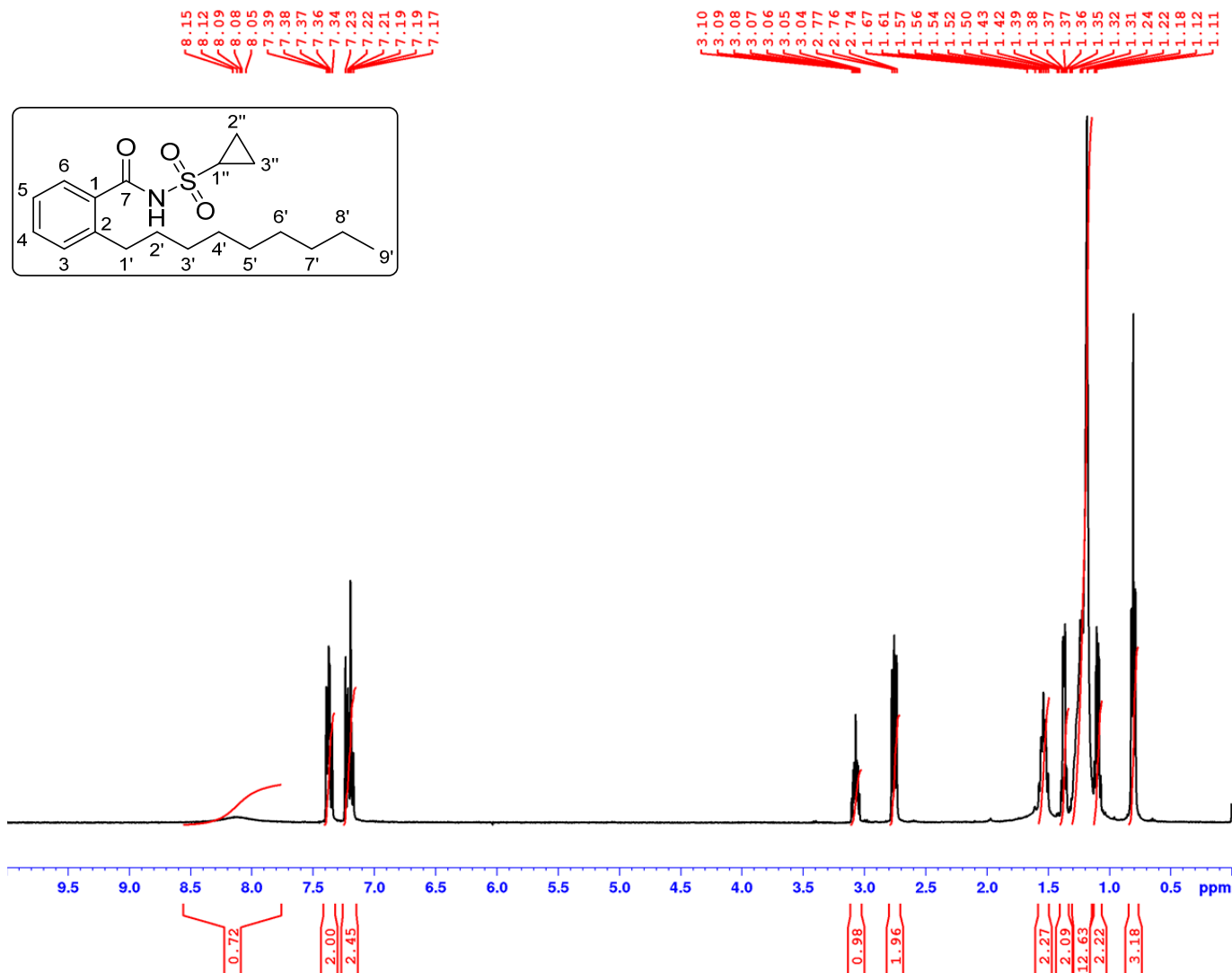


Current Data Parameters
NAME 4I168301
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190620
Time 15.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 131072
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.063157 Hz
AQ 7.9167490 sec
RG 161.3
DW 60.400 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 -0.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300361 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





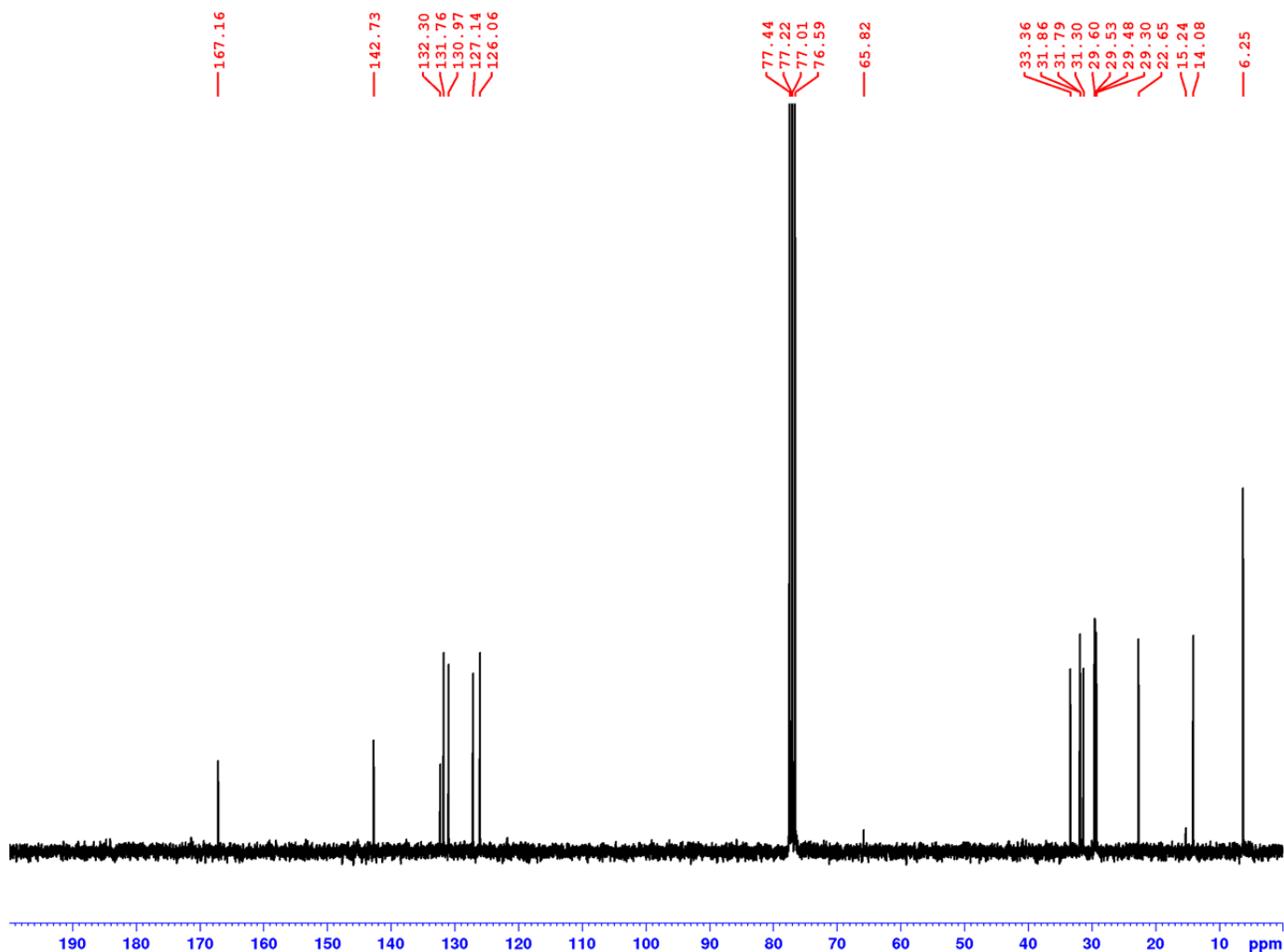
Current Data Parameters
NAME W549302
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190618
Time 21.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 209.37
DW 27.600 usec
DE 11.35 usec
TE 300.0 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1

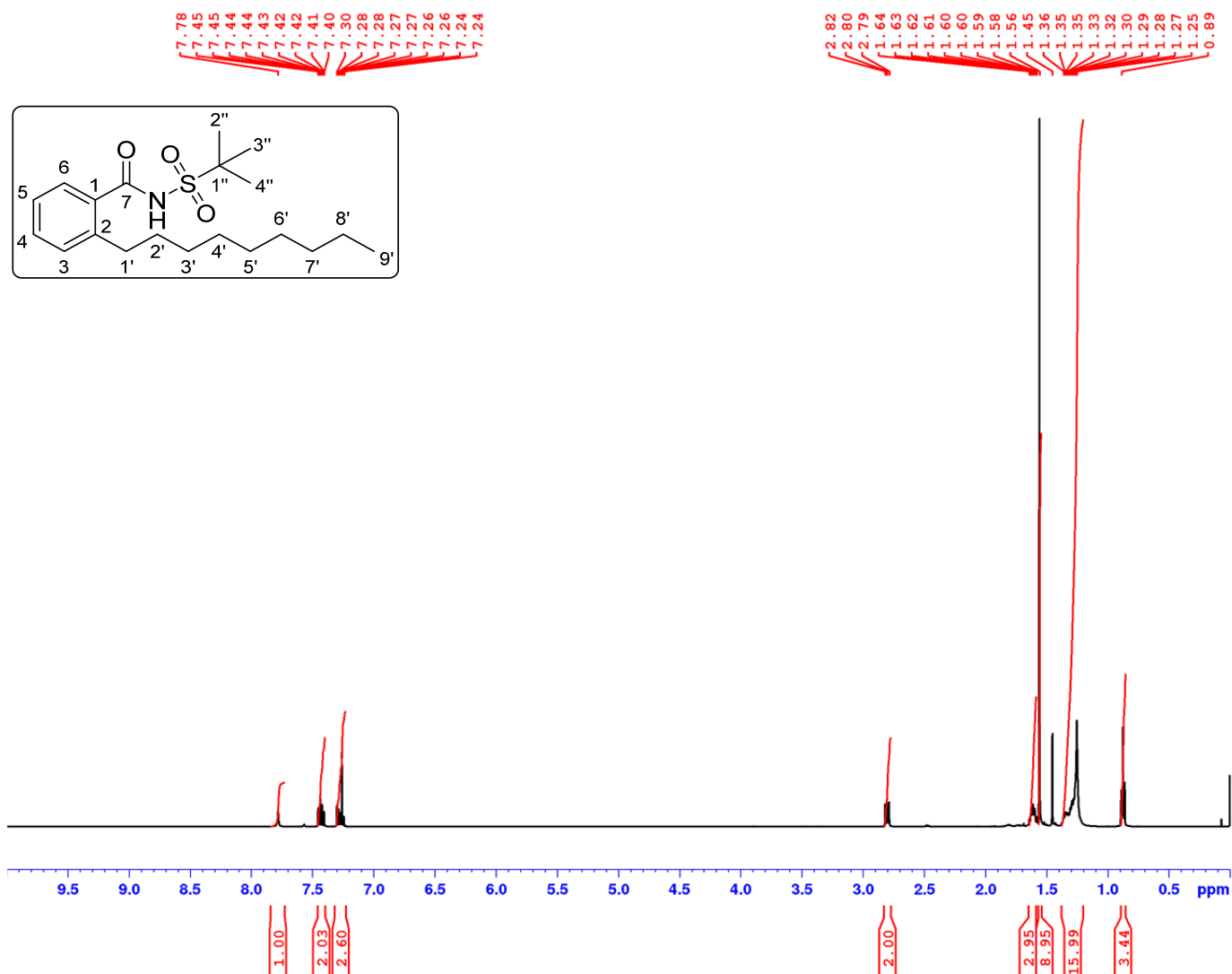
===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 10.00 usec
PLW1 35.00000000 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.40000010 W
PLW12 0.20556000 W
PLW13 0.16650000 W

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



N-(*tert*-Butylsulfonyl)-2-nonylbenzamide (10)



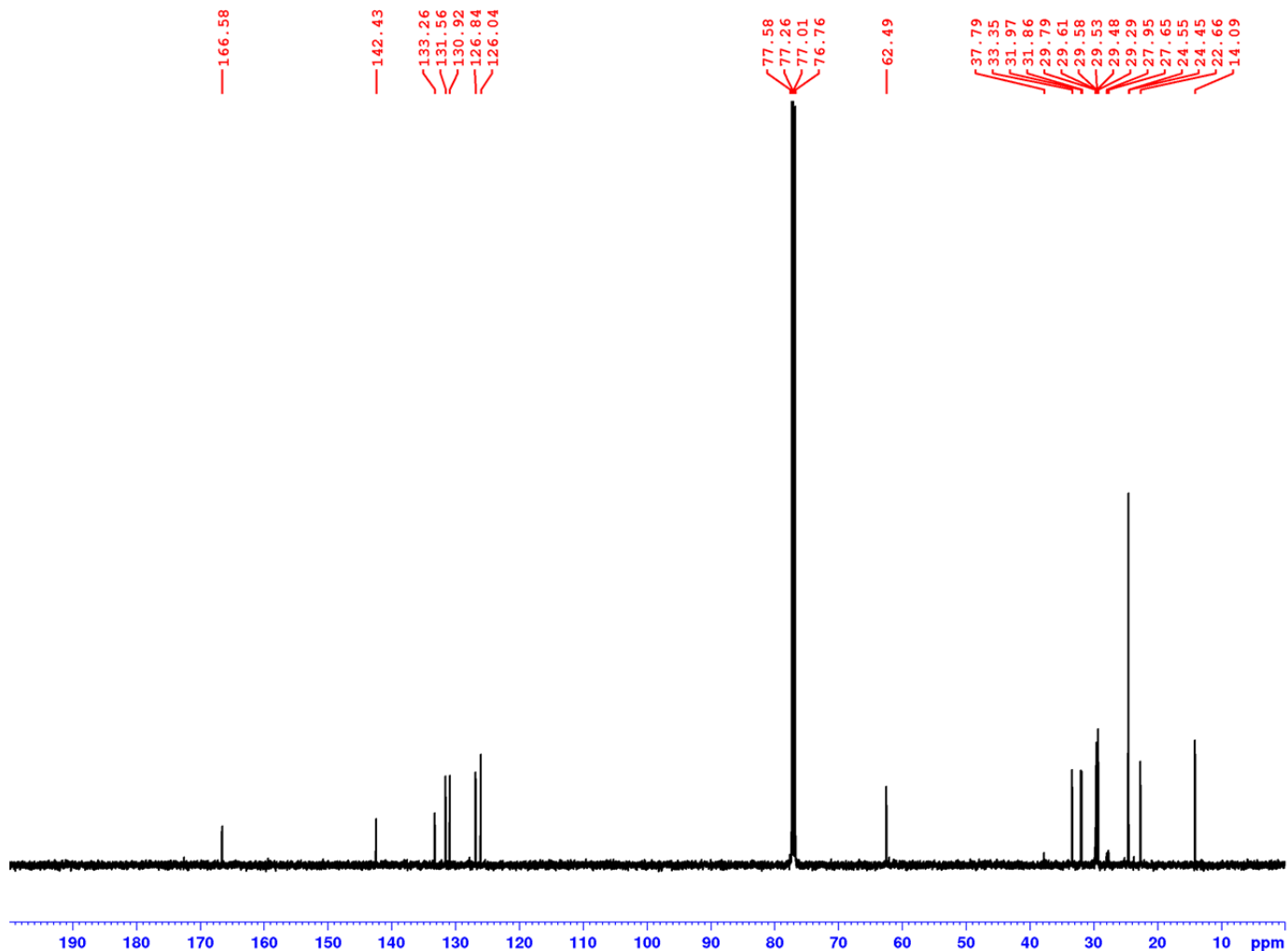
BRUKER

Current Data Parameters
NAME Y325701
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220118
Time 1.13
INSTRUM spect
PROBHD 5 mm PAQNP 1H/
PULPROG zg30
TD 131072
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.078816 Hz
AQ 6.3438849 sec
RG 228
DW 48.400 usec
DE 12.58 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 12.00 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 131072
SF 500.1300112 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME Y325702
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220118
Time 1.52
INSTRUM spect
PROBHD 5 mm PAQNP 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 125.7703643 MHz
NUC1 13C
P1 10.00 usec
PLW1 87.00000000 W

===== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 28.00000000 W
PLW12 0.63000000 W
PLW13 0.40320000 W

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2-Nonyl-N-(3,3,3-trifluoropropanesulfonyl)benzamide (11)

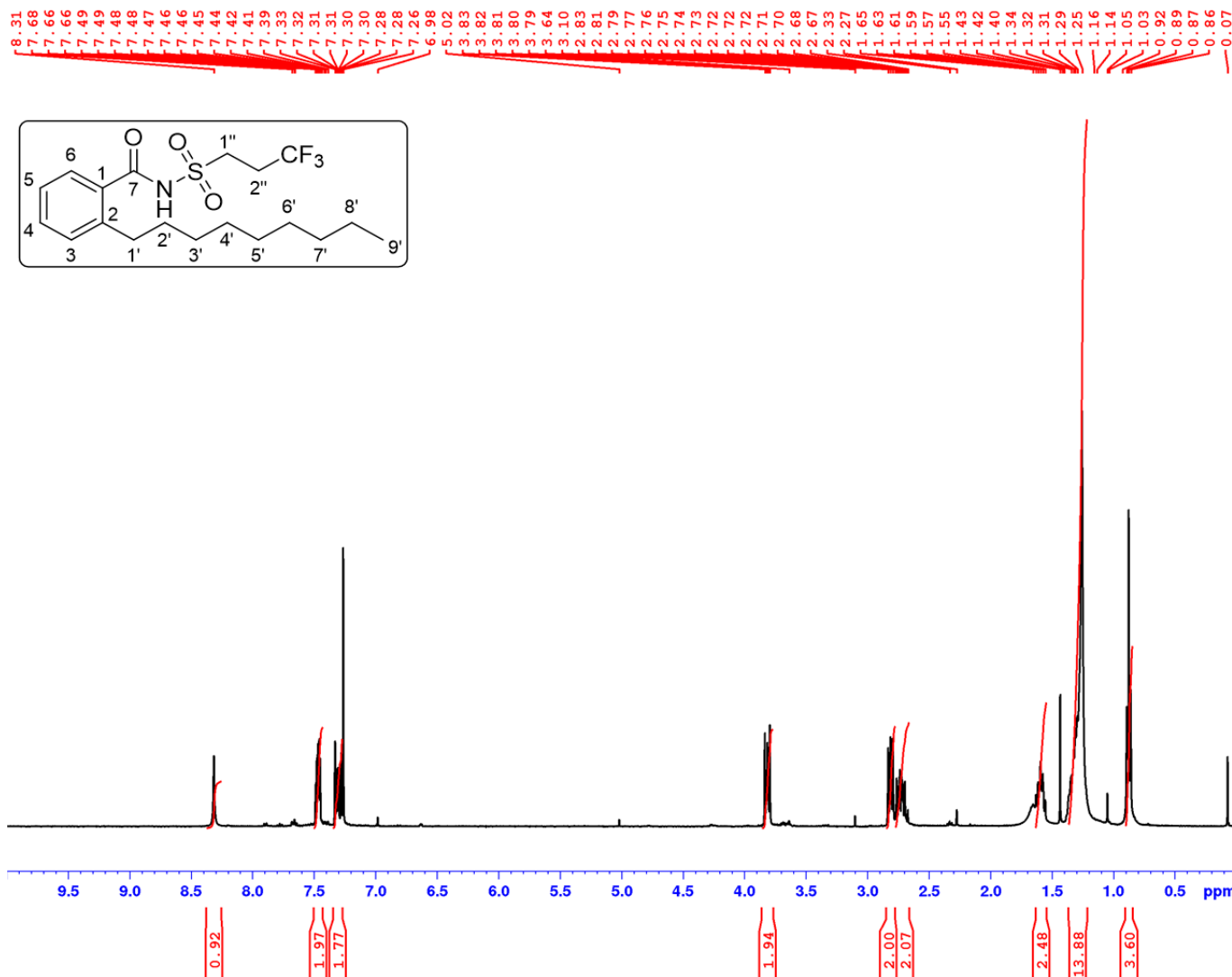


Current Data Parameters
 NAME 4I347801
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191104
 Time 18.19
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 131072
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.063157 Hz
 AQ 7.9167490 sec
 RG 181
 DW 60.400 usec
 DE 6.00 usec
 TE 673.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.00 usec
 PL1 -0.50 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300085 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





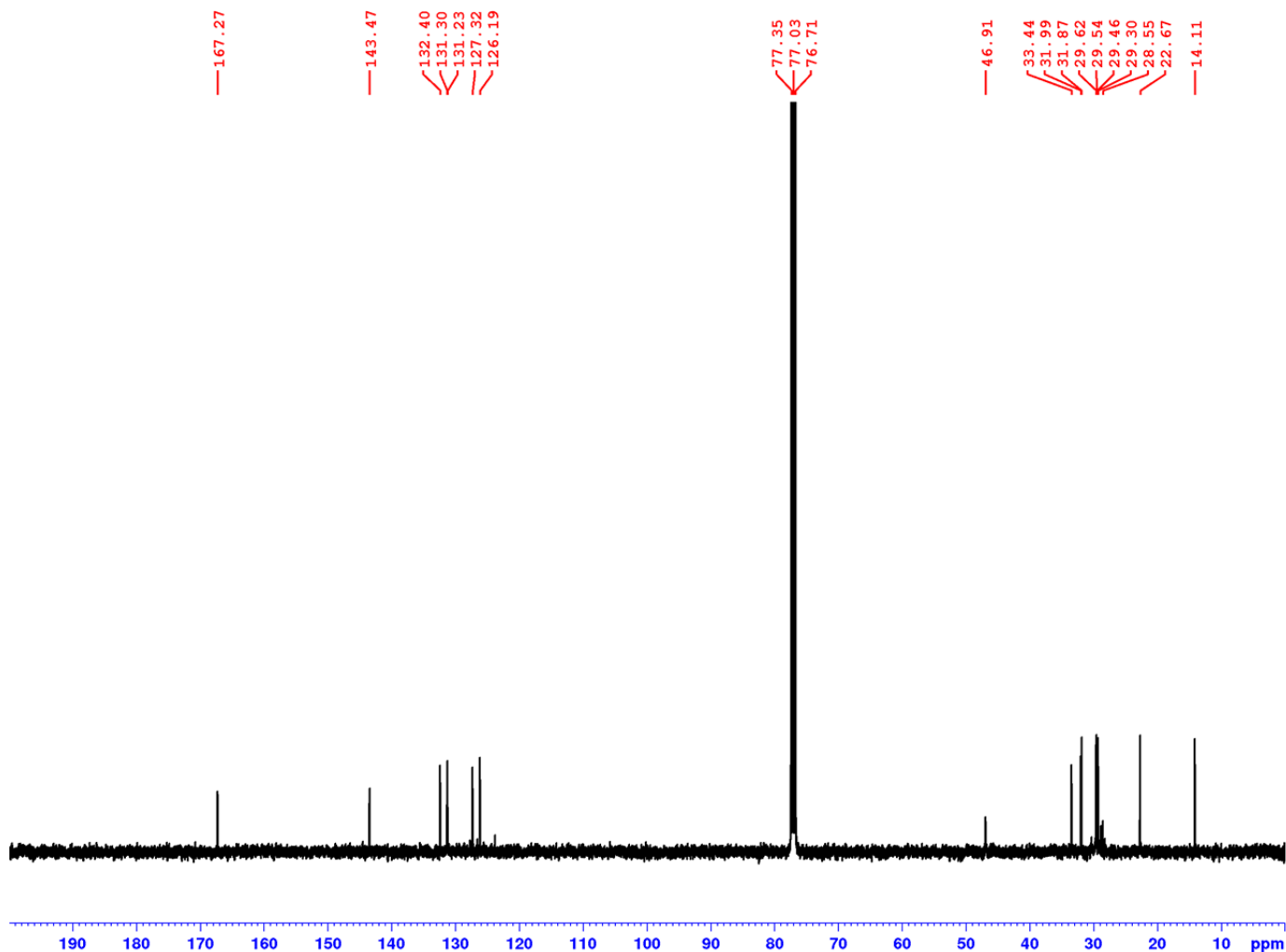
Current Data Parameters
NAME 4I347802
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191105
Time 22.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.182959 Hz
AQ 2.7328513 sec
RG 812.7
DW 20.850 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

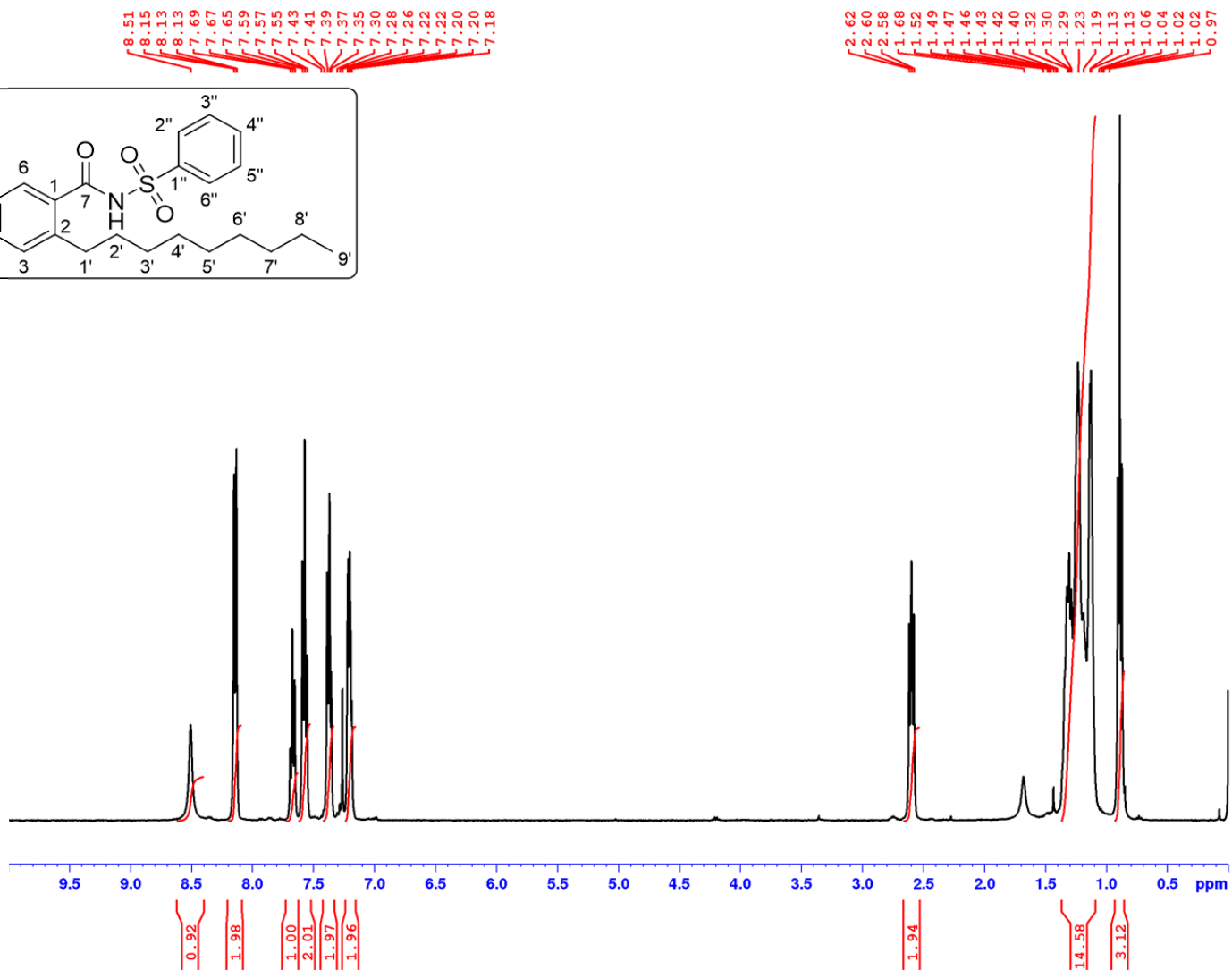
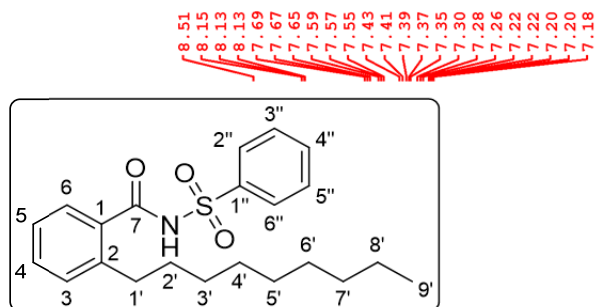
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -0.50 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -0.20 dB
PL12 17.93 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



***N*-(Benzenesulfonyl)-2-nonylbenzamide (12)**

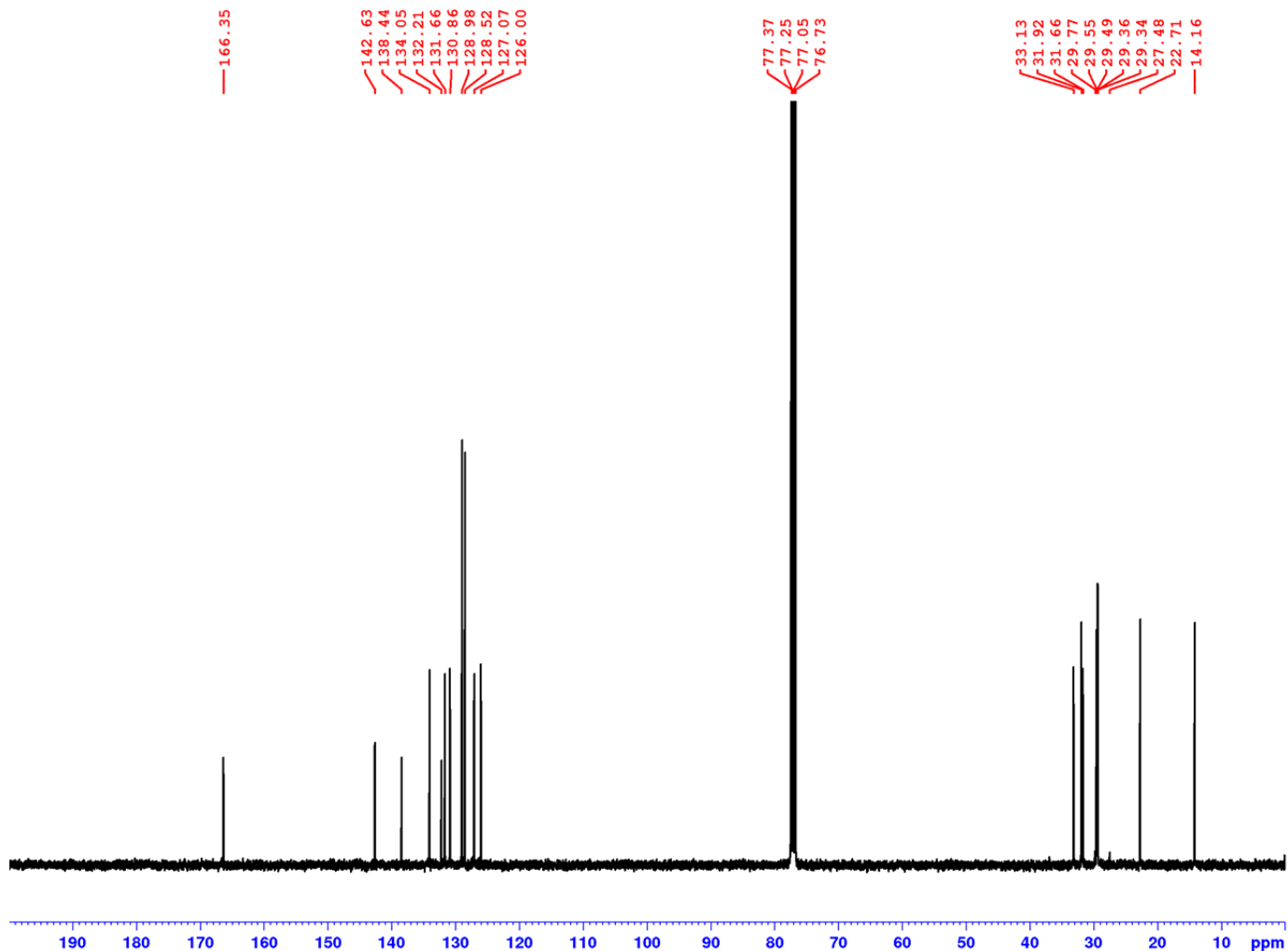


Current Data Parameters
NAME 41069101
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190321
Time 17.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 131072
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.063157 Hz
AQ 7.9167490 sec
RG 90.5
DW 60.400 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 -0.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300087 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME 4I069102
 EXPNO 10
 PROCNO 1

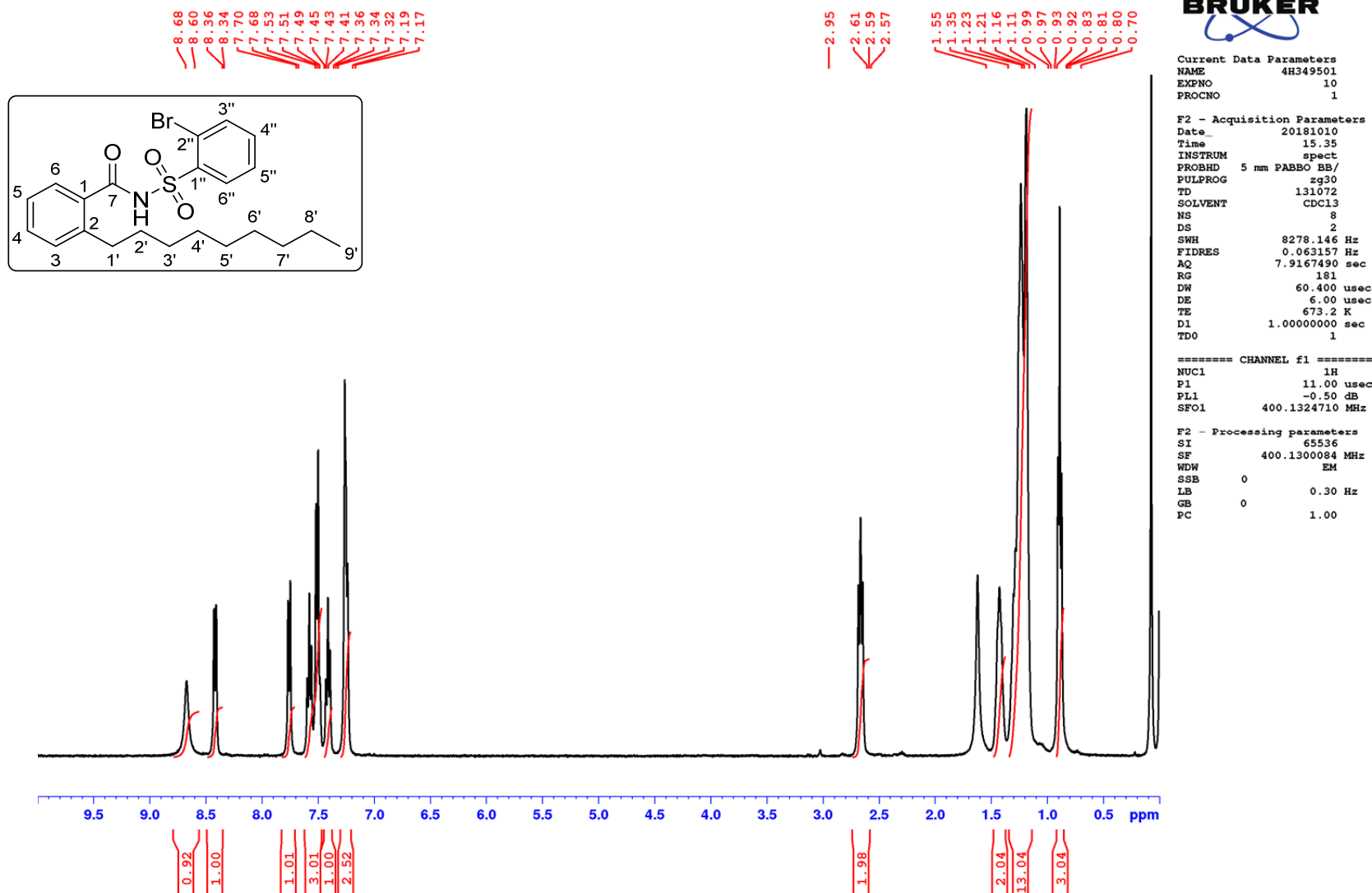
F2 - Acquisition Parameters
 Date_ 20190323
 Time 4.32
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 131072
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.182959 Hz
 AQ 2.7328513 sec
 RG 456.1
 DW 20.850 usec
 DE 6.50 usec
 TE 673.2 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -0.50 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -0.20 dB
 PL12 17.93 dB
 PL13 19.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

N-(2-Bromobenzenesulfonyl)-2-nonylbenzamide (13)



Current Data Parameters
NAME 4H349501
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181010
Time 15.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 131072
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.063157 Hz
AQ 7.9167490 sec
RG 181
DW 60.400 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 -0.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



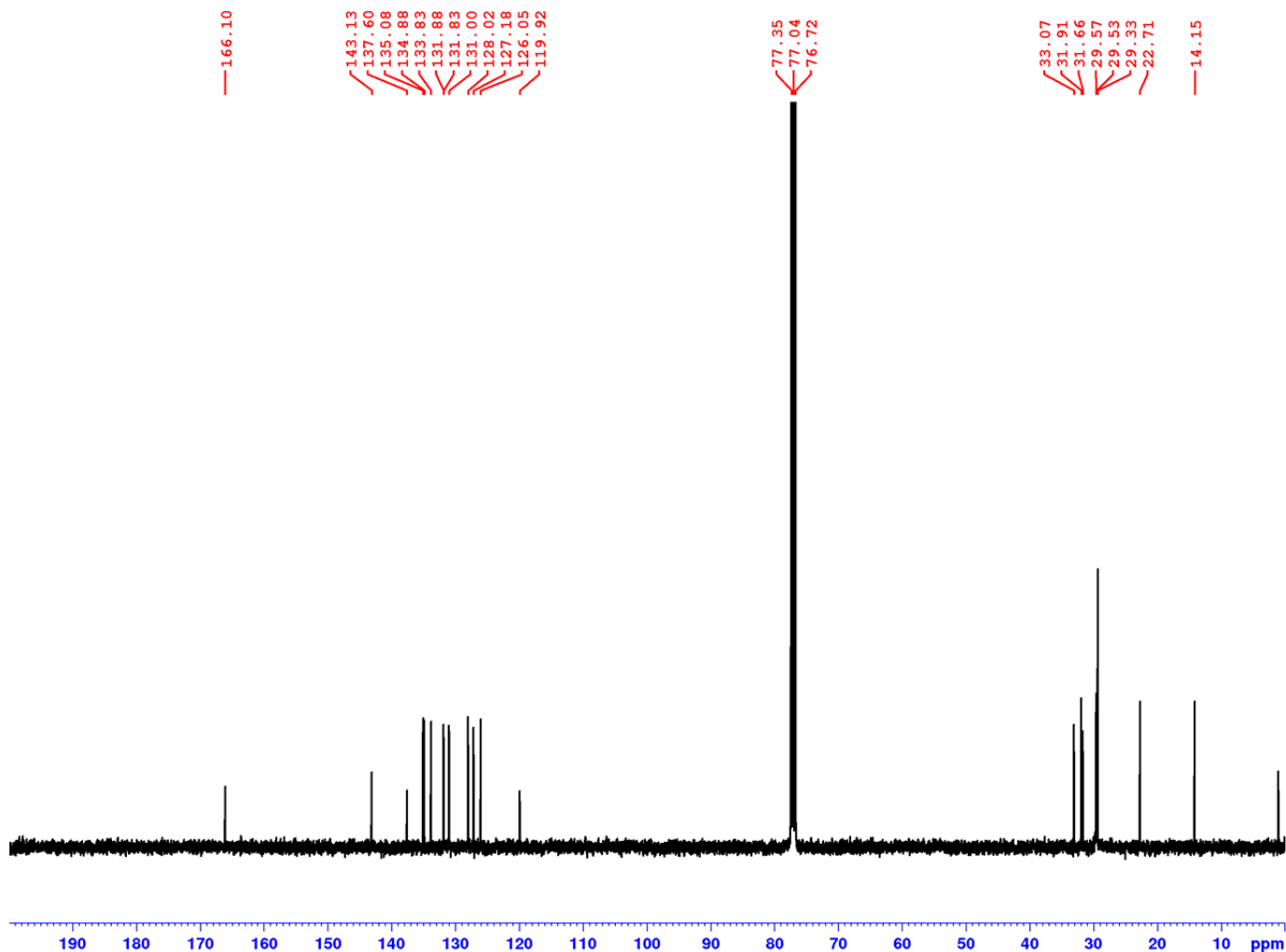
Current Data Parameters
NAME 4H349502
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181011
Time 3.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.182959 Hz
AQ 2.7328513 sec
RG 456.1
DW 20.850 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

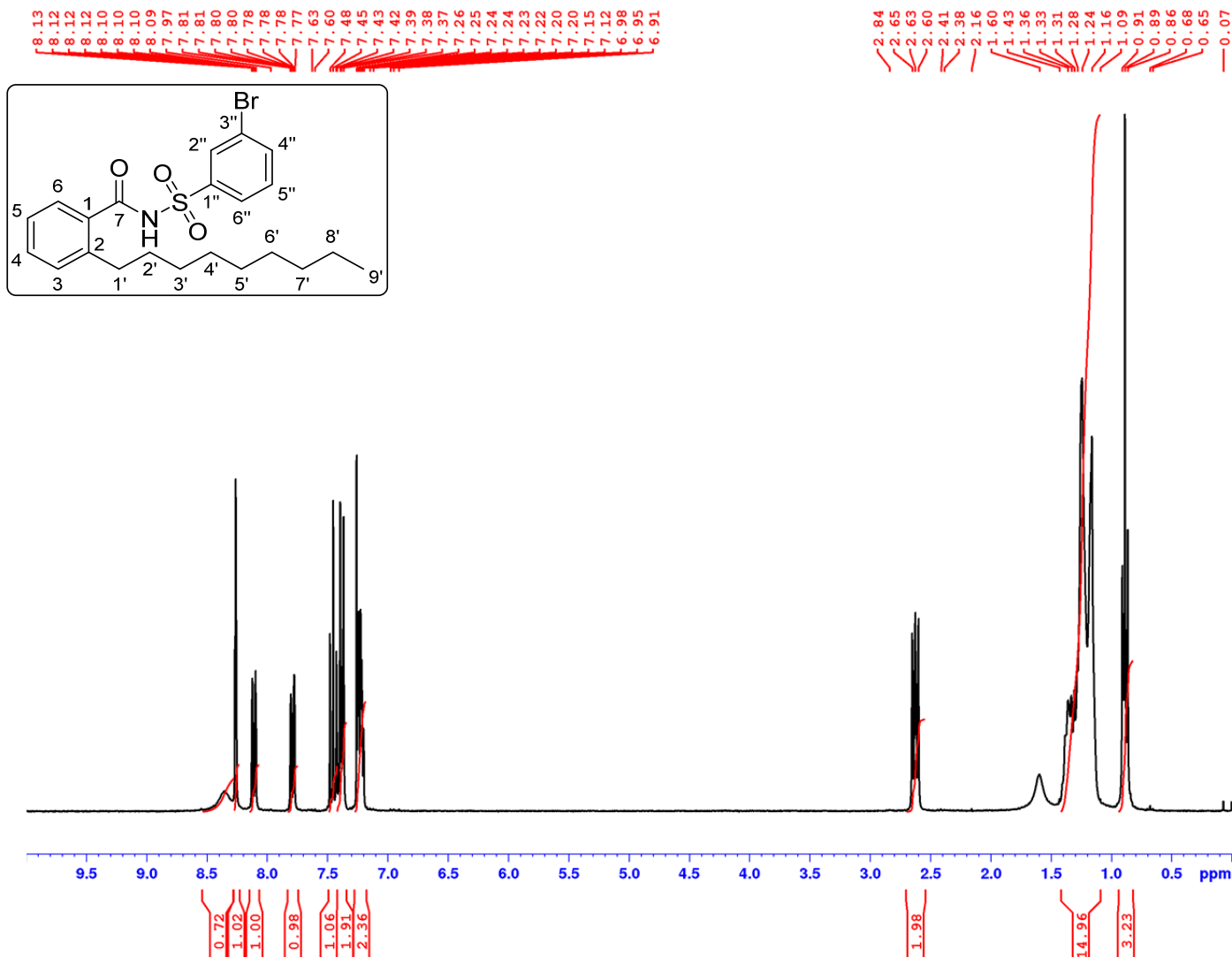
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -0.50 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -0.20 dB
PL12 17.93 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



N-(3-Bromobenzenesulfonyl)-2-nonylbenzamide (14)



BRUKER

Current Data Parameters
NAME W334601
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190418
Time 14.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 209.37
DW 83.200 usec
DE 13.82 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 15.00 usec
PLW1 7.40000010 W

F2 - Processing parameters
SI 65536
SF 300.1300076 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00



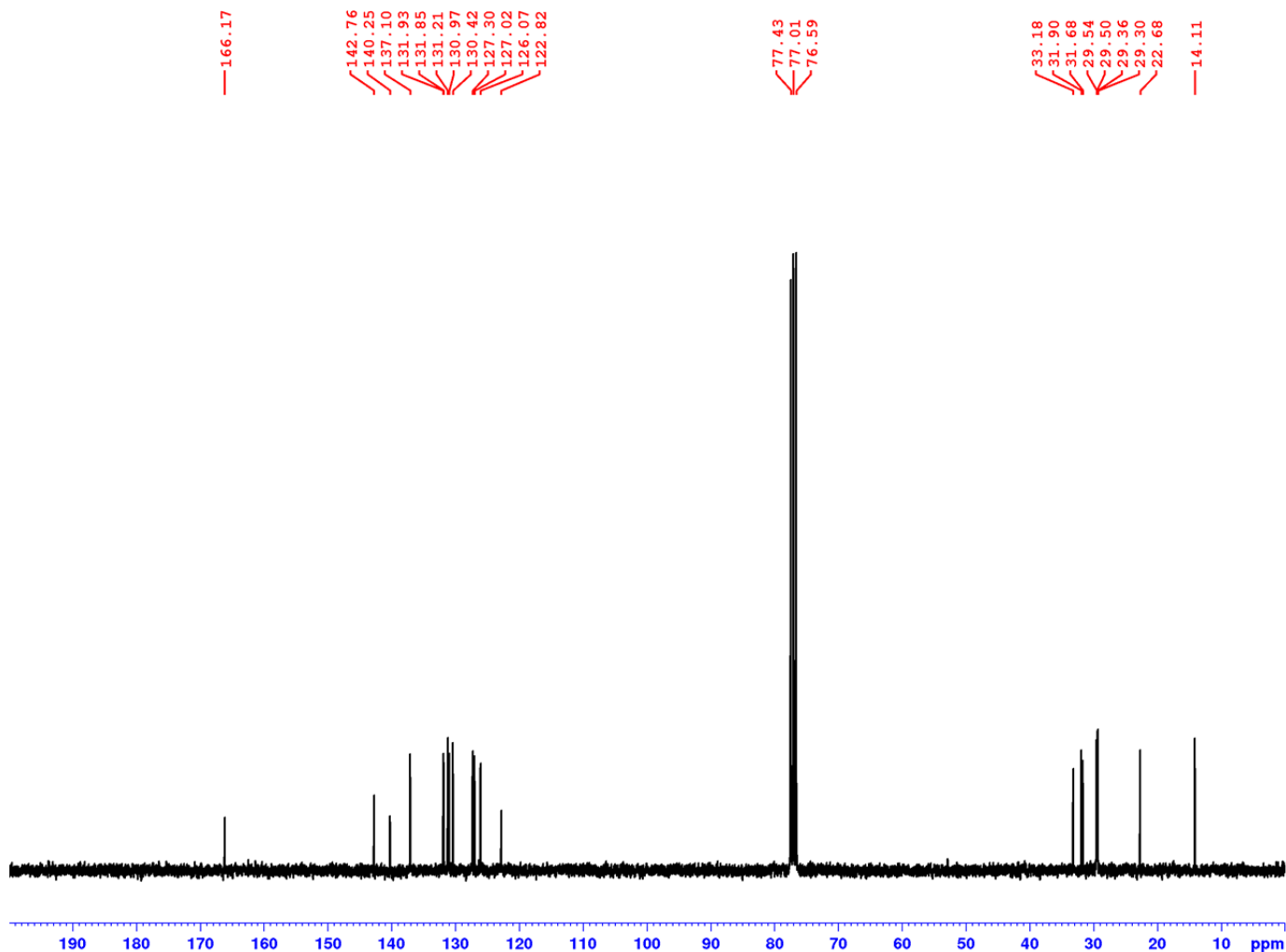
Current Data Parameters
NAME W334602
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190419
Time 5.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 209.37
DW 27.600 usec
DE 11.35 usec
TE 300.0 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1

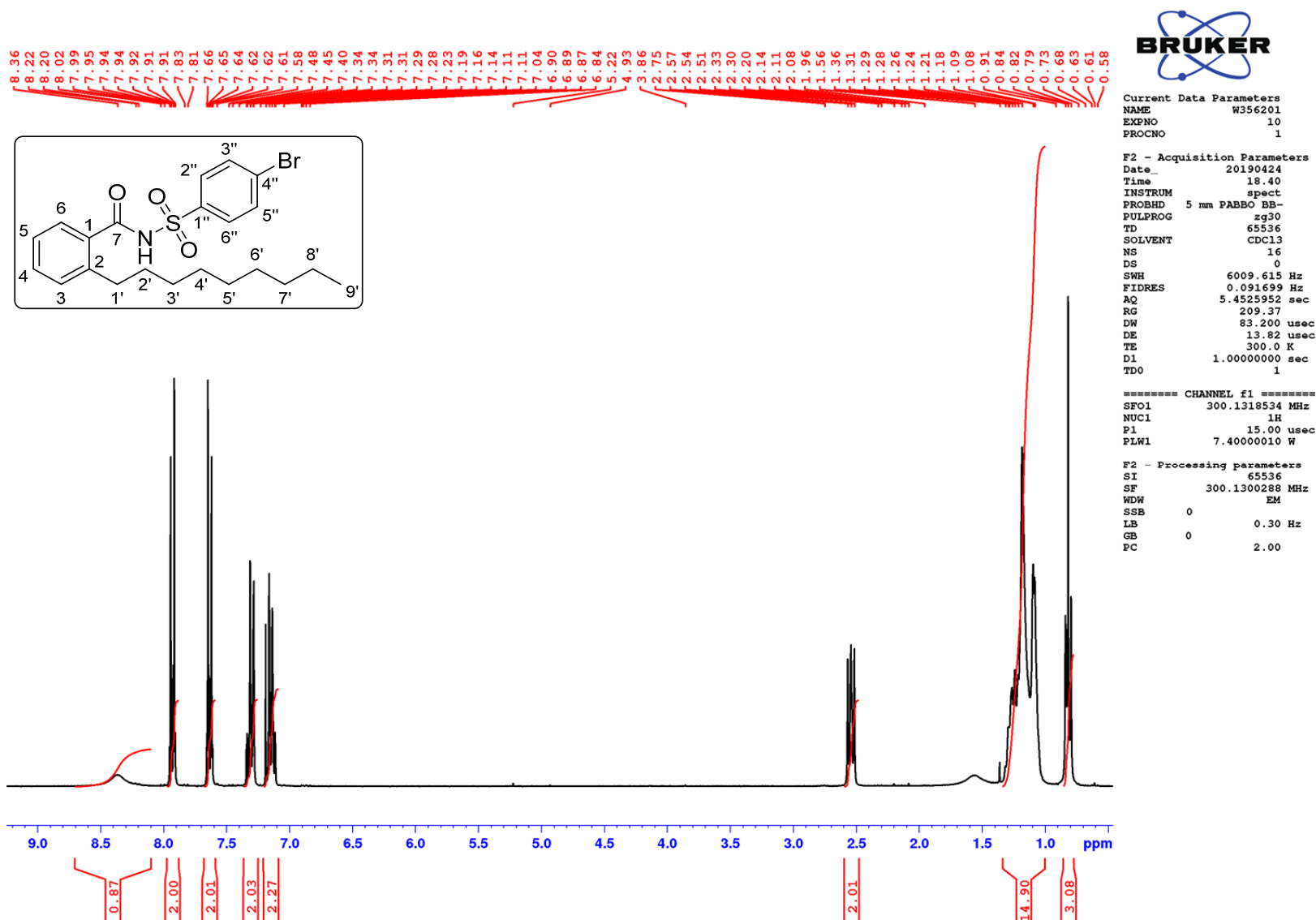
===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 10.00 usec
PLW1 35.00000000 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.40000010 W
PLW12 0.20556000 W
PLW13 0.16650000 W

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



N-(4-Bromobenzene)sulfonyl)-2-nonylbenzamide (15)





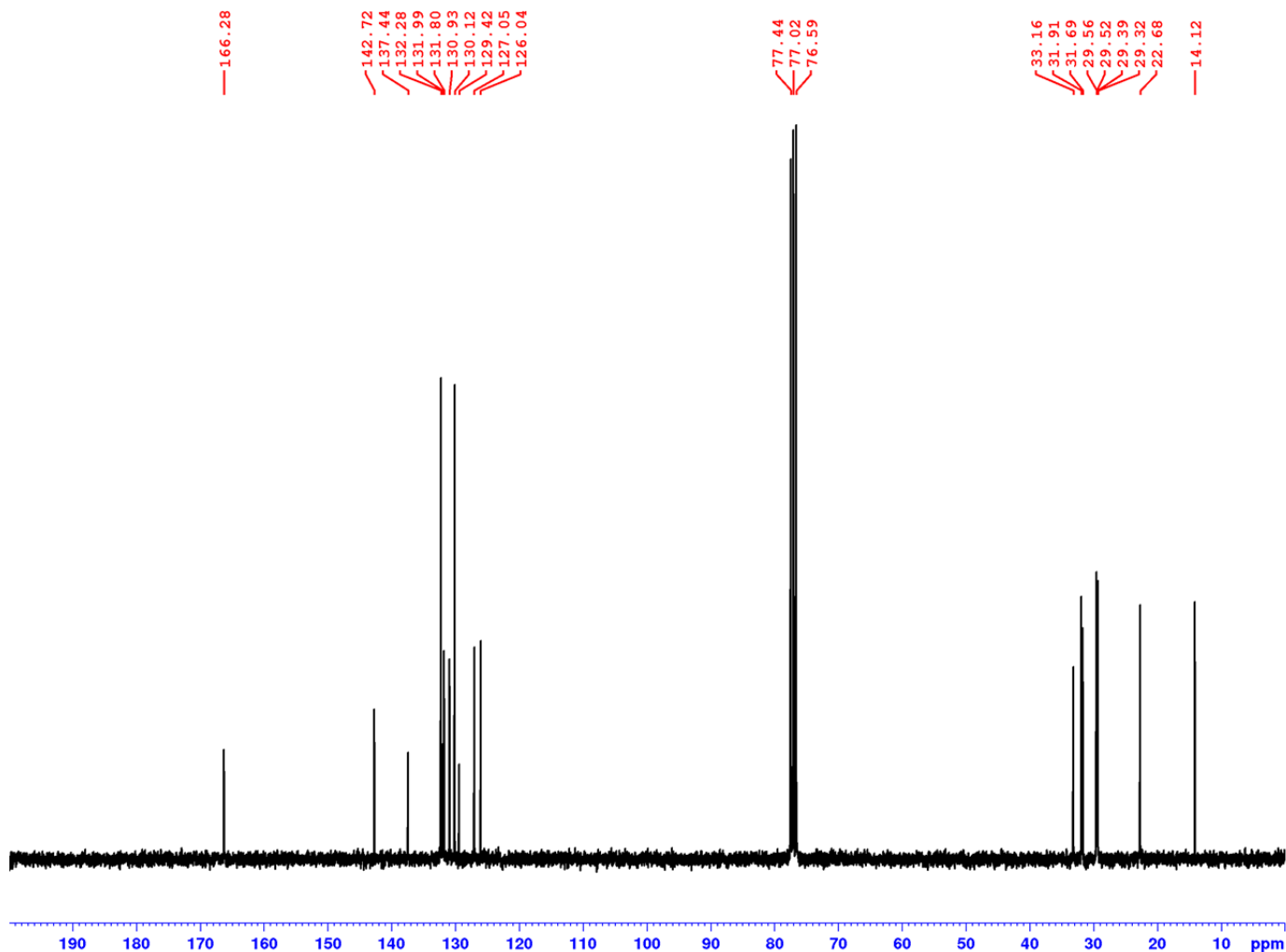
Current Data Parameters
NAME W356202
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190426
Time 4.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 209.37
DW 27.600 usec
DE 11.35 usec
TE 300.0 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1

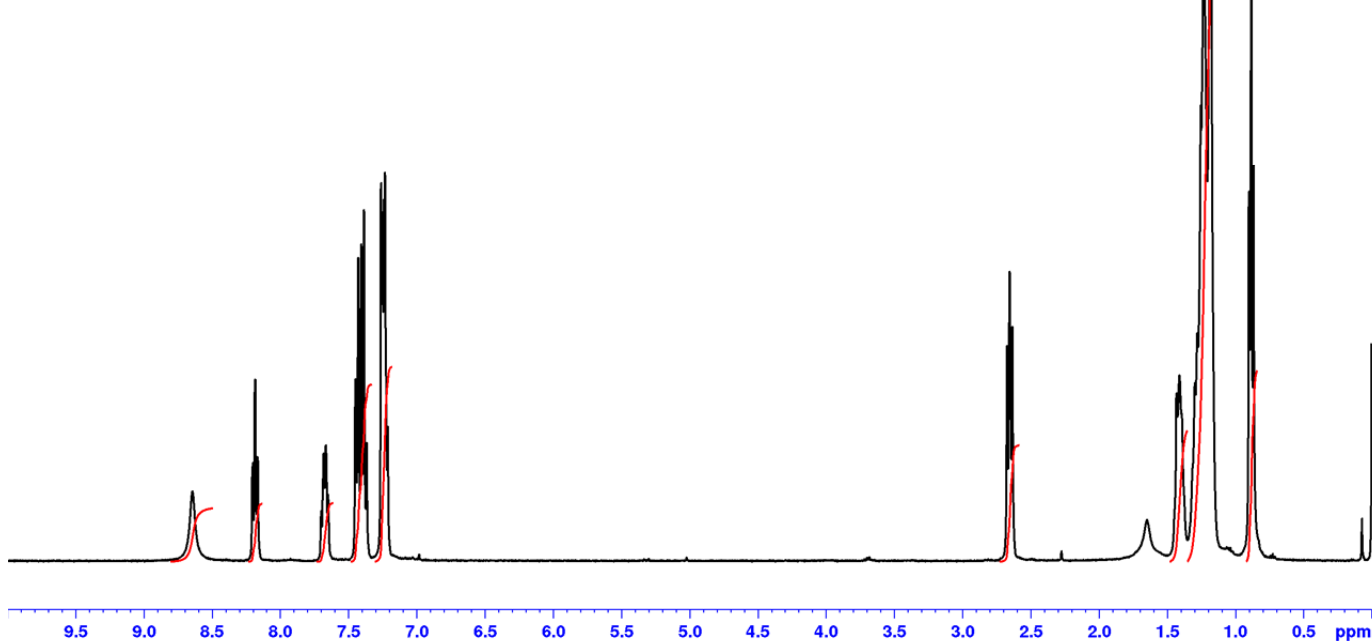
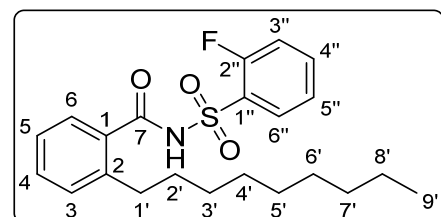
===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 10.00 usec
PLW1 35.00000000 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.40000010 W
PLW12 0.20556000 W
PLW13 0.16650000 W

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



N-(2-Fluorobenzenesulfonyl)-2-nonylbenzamide (16)



Current Data Parameters
NAME 41086101
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190402
Time 18.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 131072
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.063157 Hz
AQ 7.9167490 sec
RG 128
DW 60.400 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 -0.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300085 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



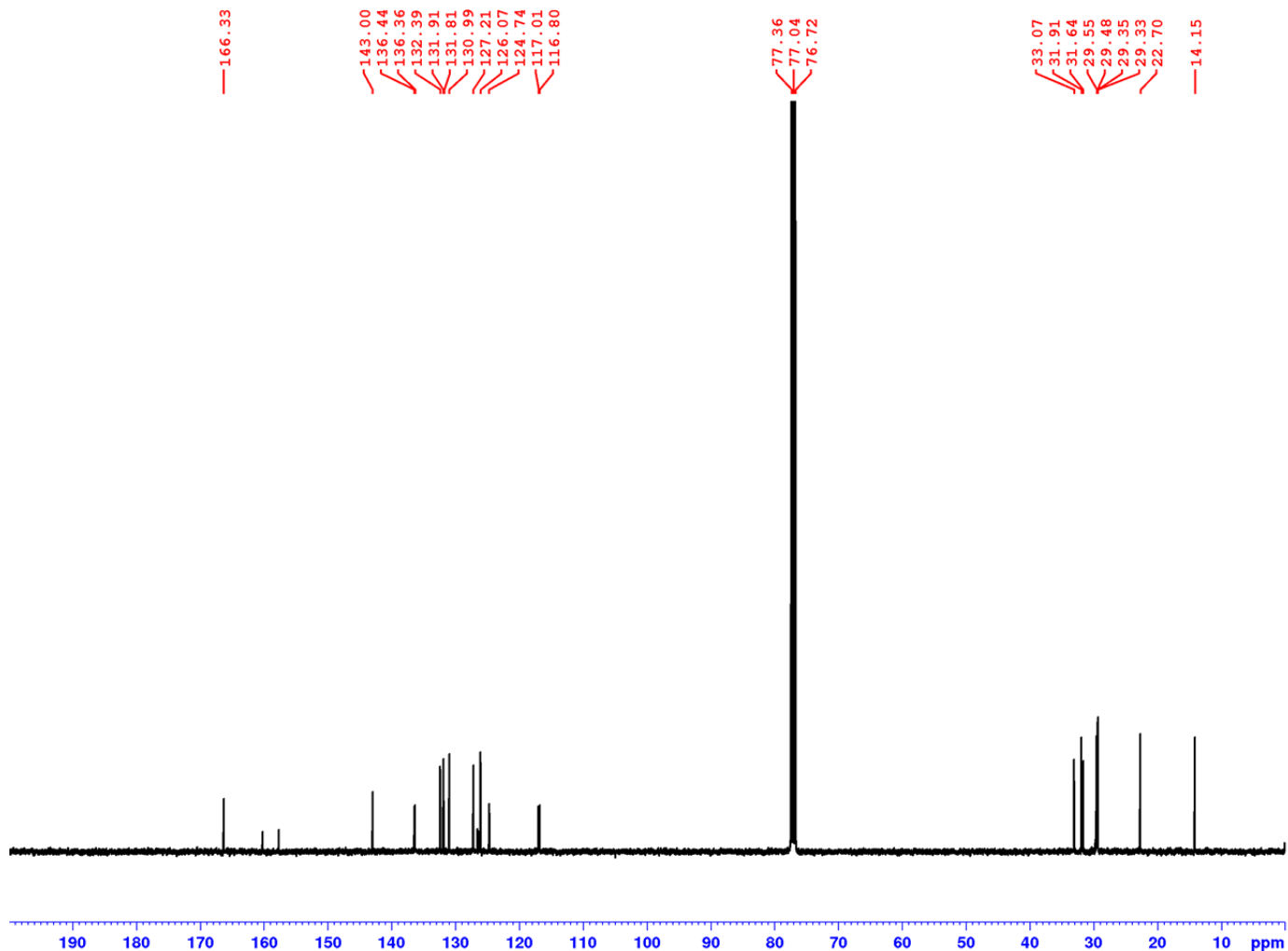
Current Data Parameters
NAME 4I088102
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190404
Time 22.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.182959 Hz
AQ 2.7328513 sec
RG 456.1
DW 20.850 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

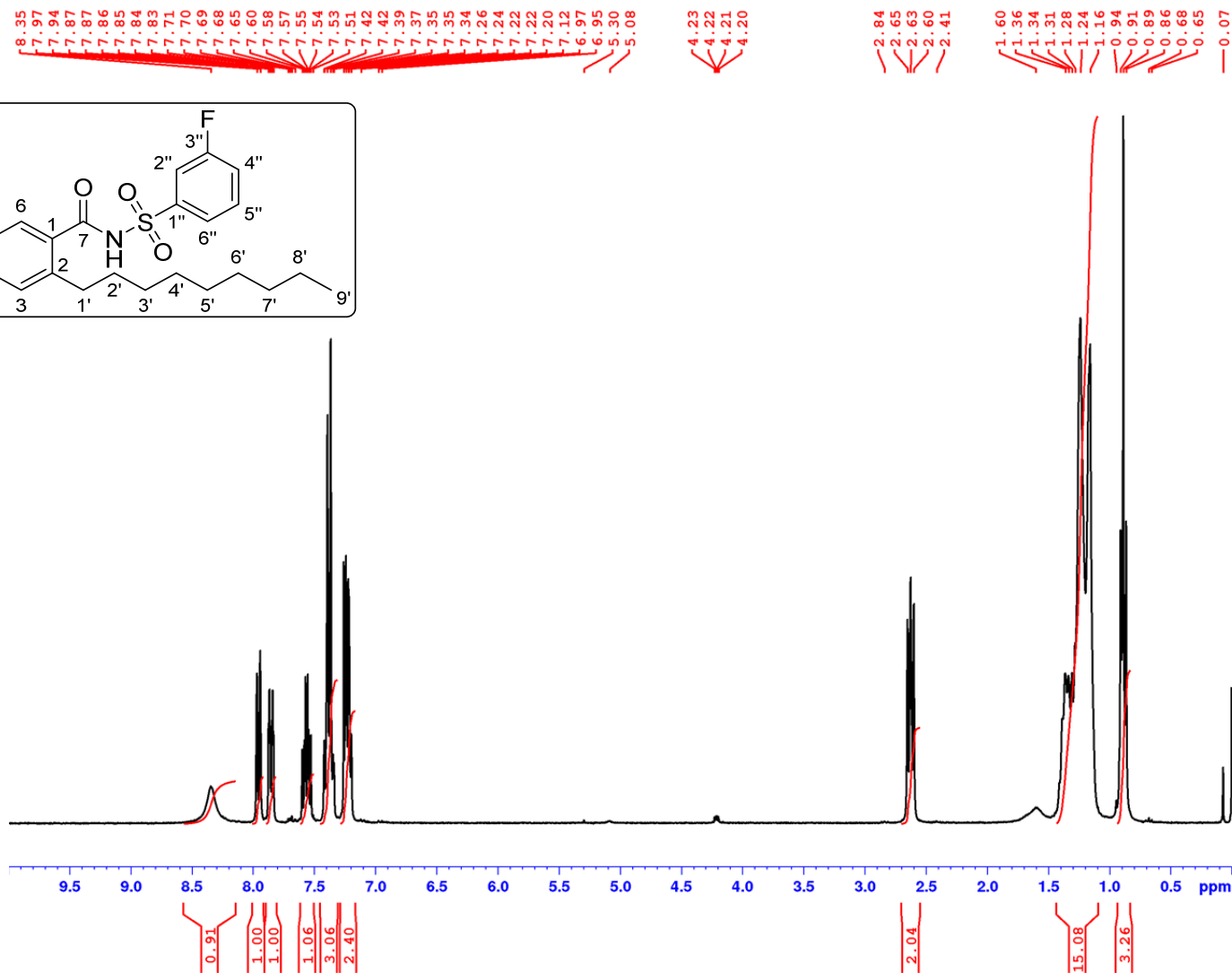
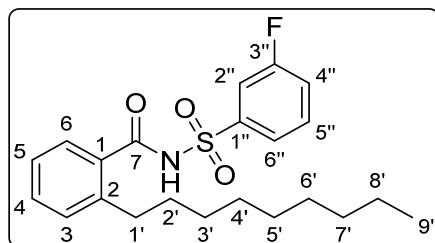
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -0.50 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -0.20 dB
PL12 17.93 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



N-(3-Fluorobenzenesulfonyl)-2-nonylbenzamide (17)



Current Data Parameters
NAME W303601
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190404
Time 17.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 209.37
DW 83.200 usec
DE 13.82 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 15.00 usec
PLW1 7.40000010 W

F2 - Processing parameters
SI 65536
SF 300.1300075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00



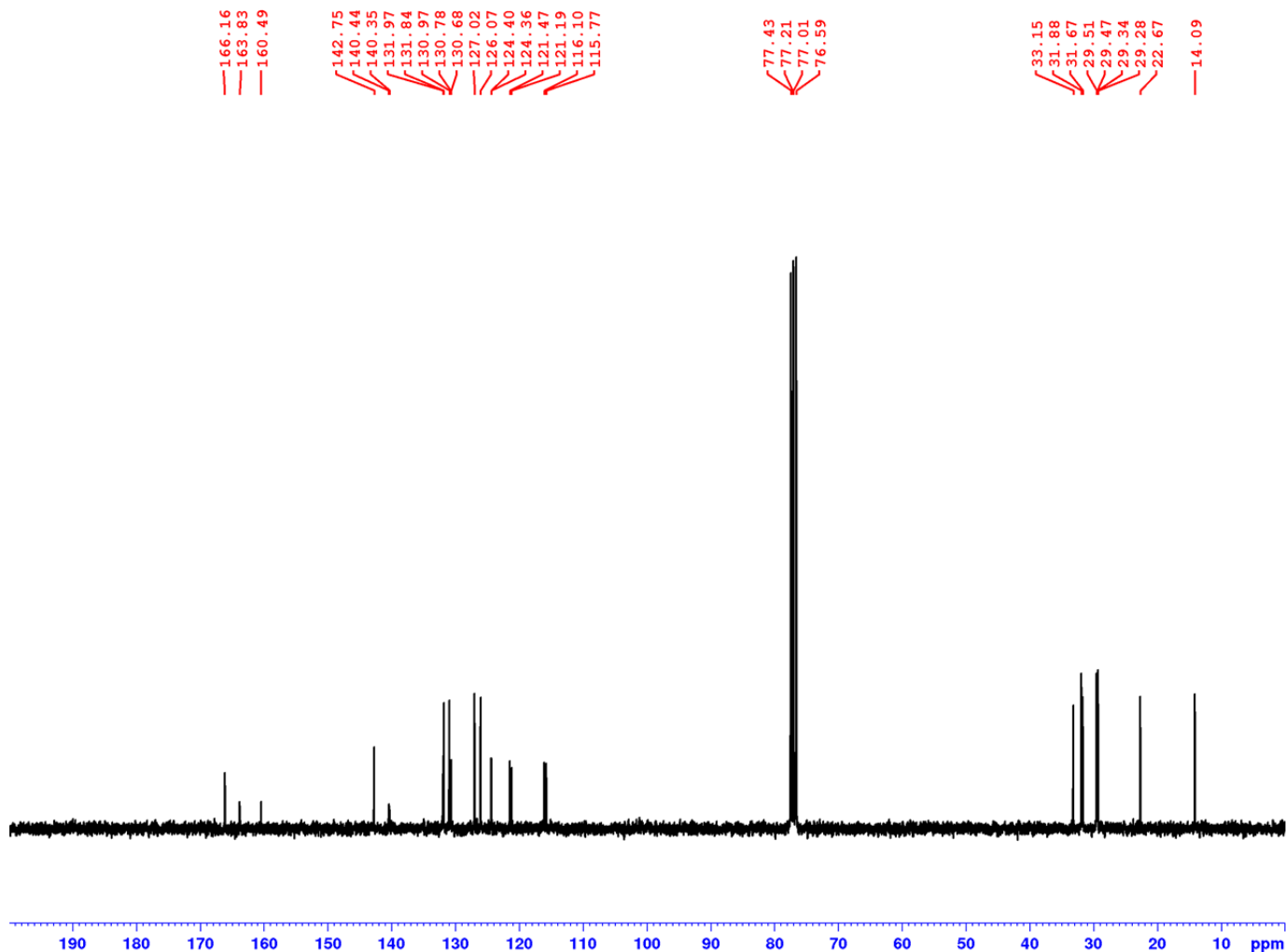
Current Data Parameters
NAME W303602
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190404
Time 23.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 209.37
DW 27.600 usec
DE 11.35 usec
TE 300.0 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1

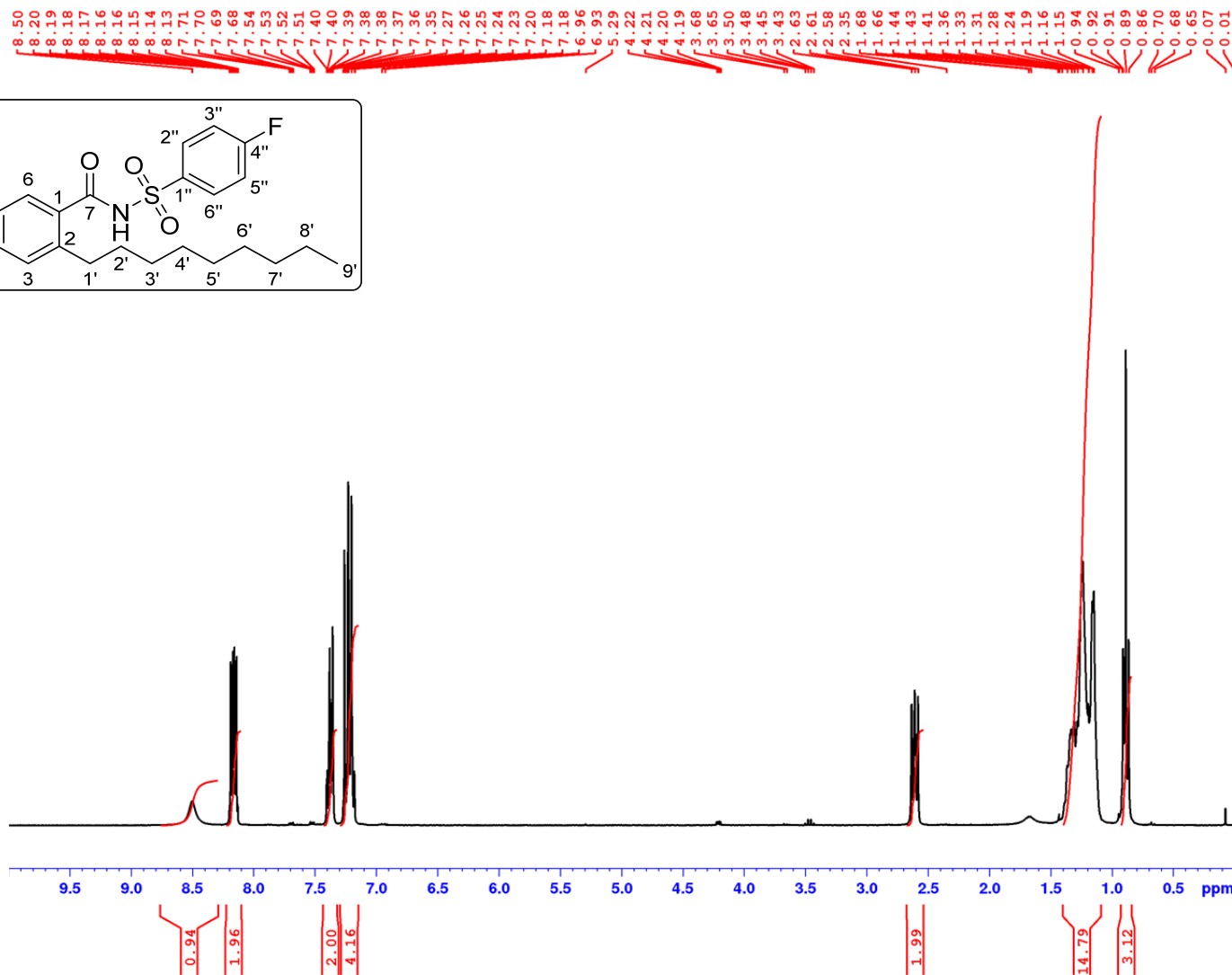
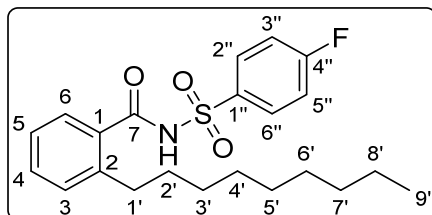
===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 10.00 usec
PLW1 35.00000000 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.40000010 W
PLW12 0.20556000 W
PLW13 0.16650000 W

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



N-(4-Fluorobenzenesulfonyl)-2-nonylbenzamide (18)



Current Data Parameters
NAME W313801
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190409
Time 11.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 209.37
DW 83.200 usec
DE 13.82 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 15.00 usec
PLW1 7.40000010 W

F2 - Processing parameters
SI 65536
SF 300.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00



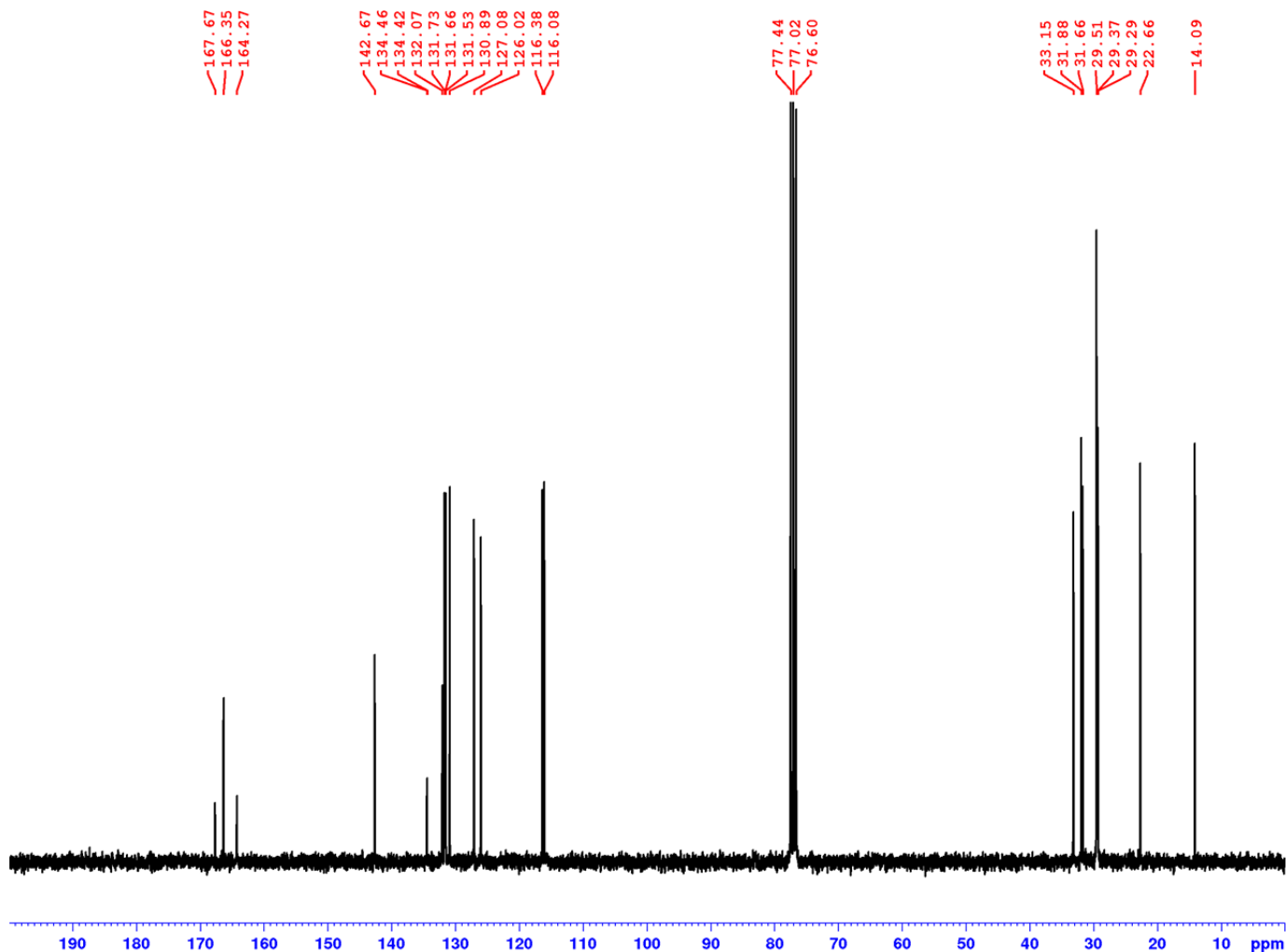
Current Data Parameters
NAME W313802
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190410
Time 4.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 209.37
DW 27.600 usec
DE 11.35 usec
TE 300.0 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1

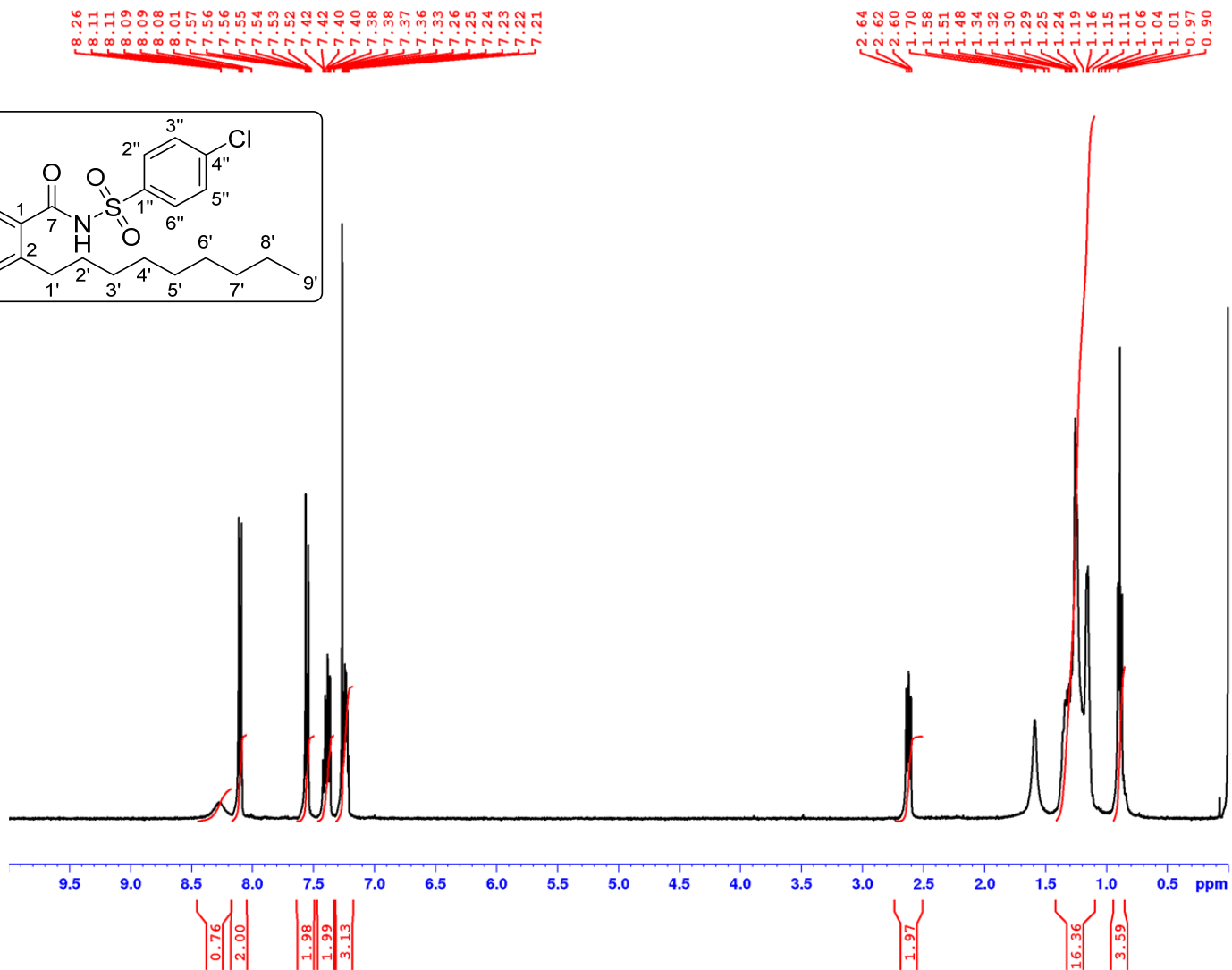
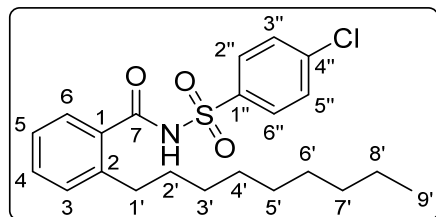
===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 10.00 usec
PLW1 35.00000000 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.40000010 W
PLW12 0.20556000 W
PLW13 0.16650000 W

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



N-(4-Chlorobenzenesulfonyl)-2-nonylbenzamide (19)

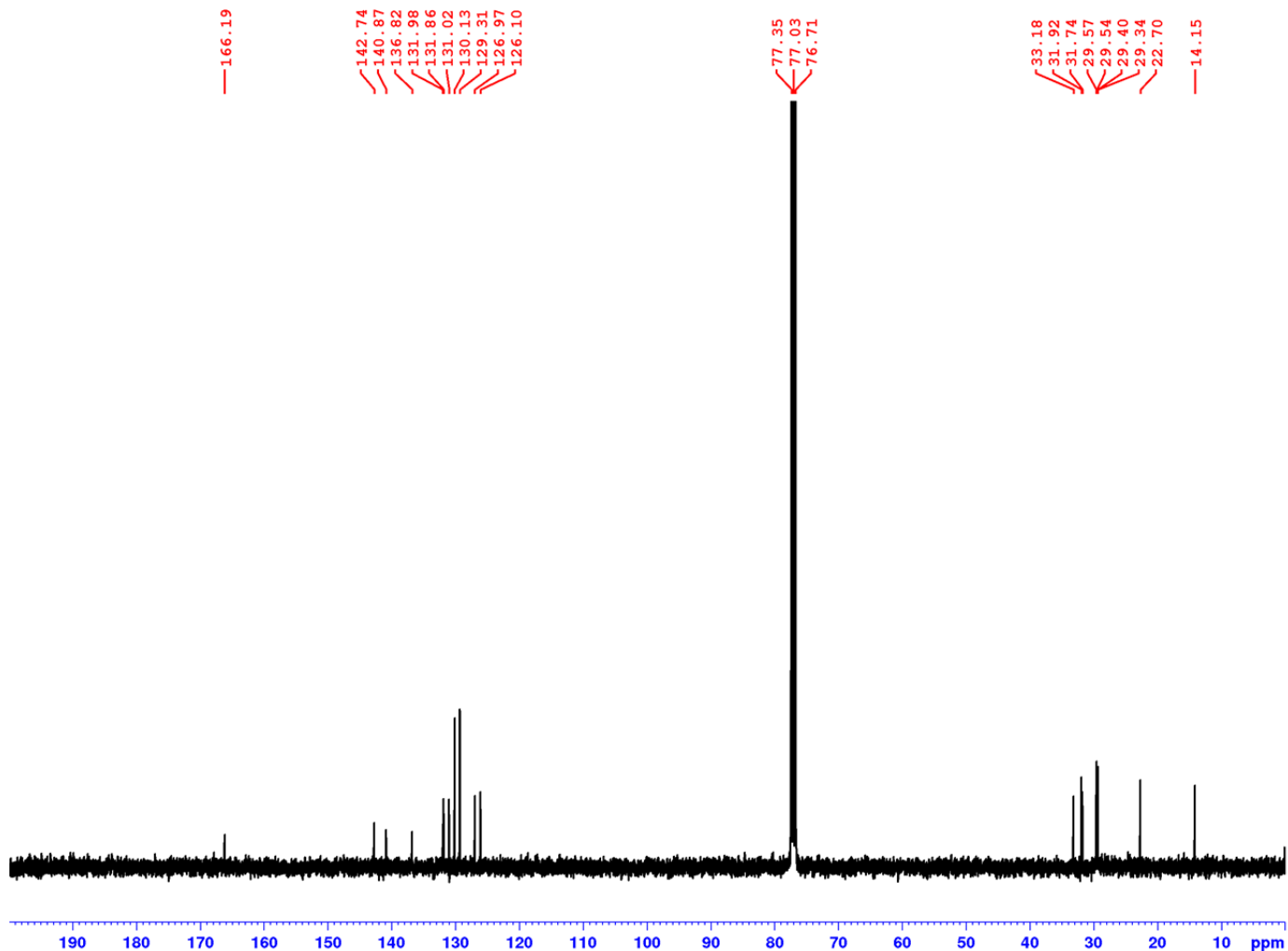


Current Data Parameters
NAME 41109701
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190430
Time 17.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 131072
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.063157 Hz
AQ 7.9167490 sec
RG 256
DW 60.400 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 -0.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 4I109702
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190430
Time 22.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.182959 Hz
AQ 2.7328513 sec
RG 456.1
DW 20.850 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -0.50 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -0.20 dB
PL12 17.93 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N-(4-Iodobenzenesulfonyl)-2-nonylbenzamide (20)

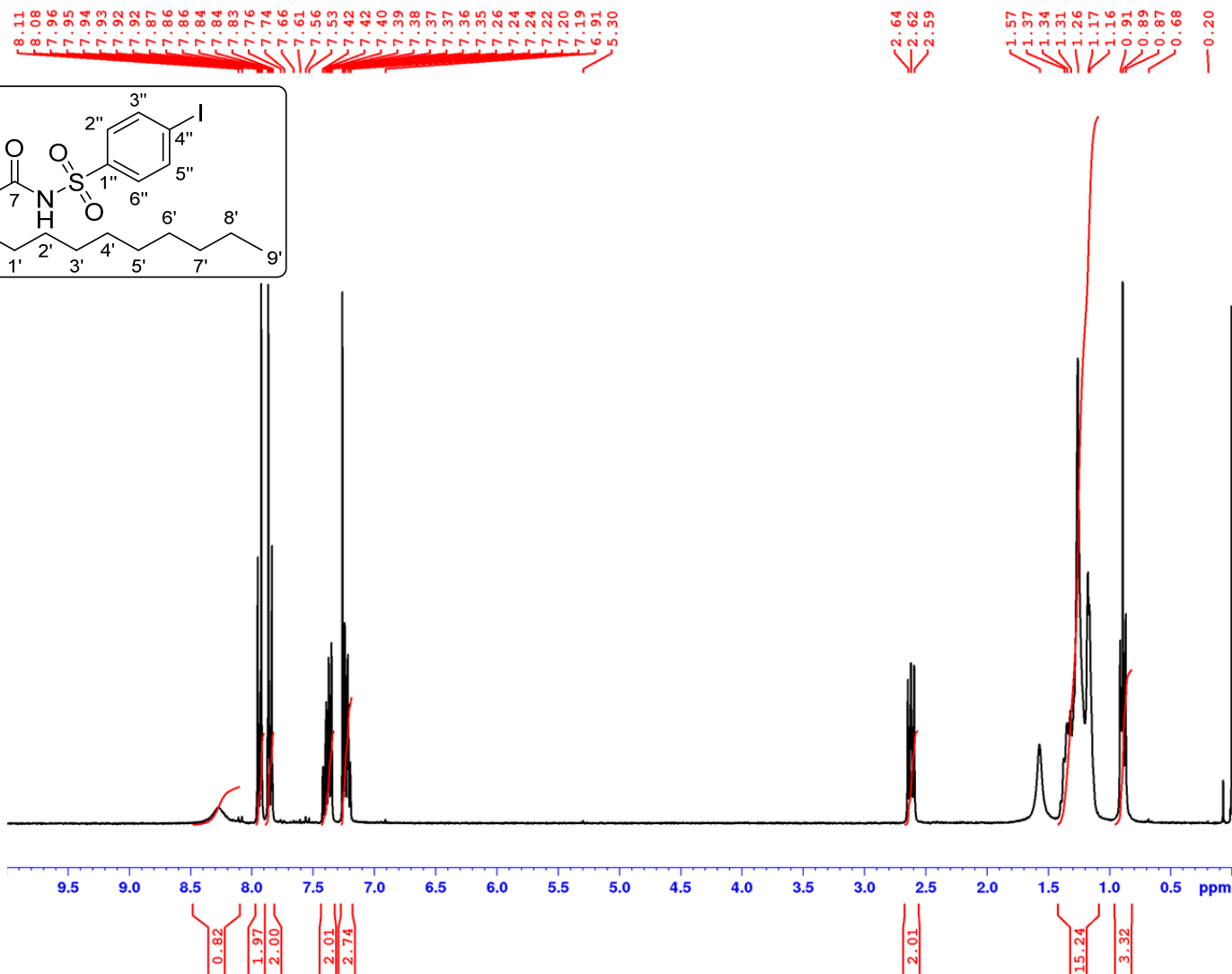


Current Data Parameters
NAME W391301
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190502
Time 17.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 209.37
DW 83.200 usec
DE 13.82 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 15.00 usec
PLW1 7.40000010 W

F2 - Processing parameters
SI 65536
SF 300.1300074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00





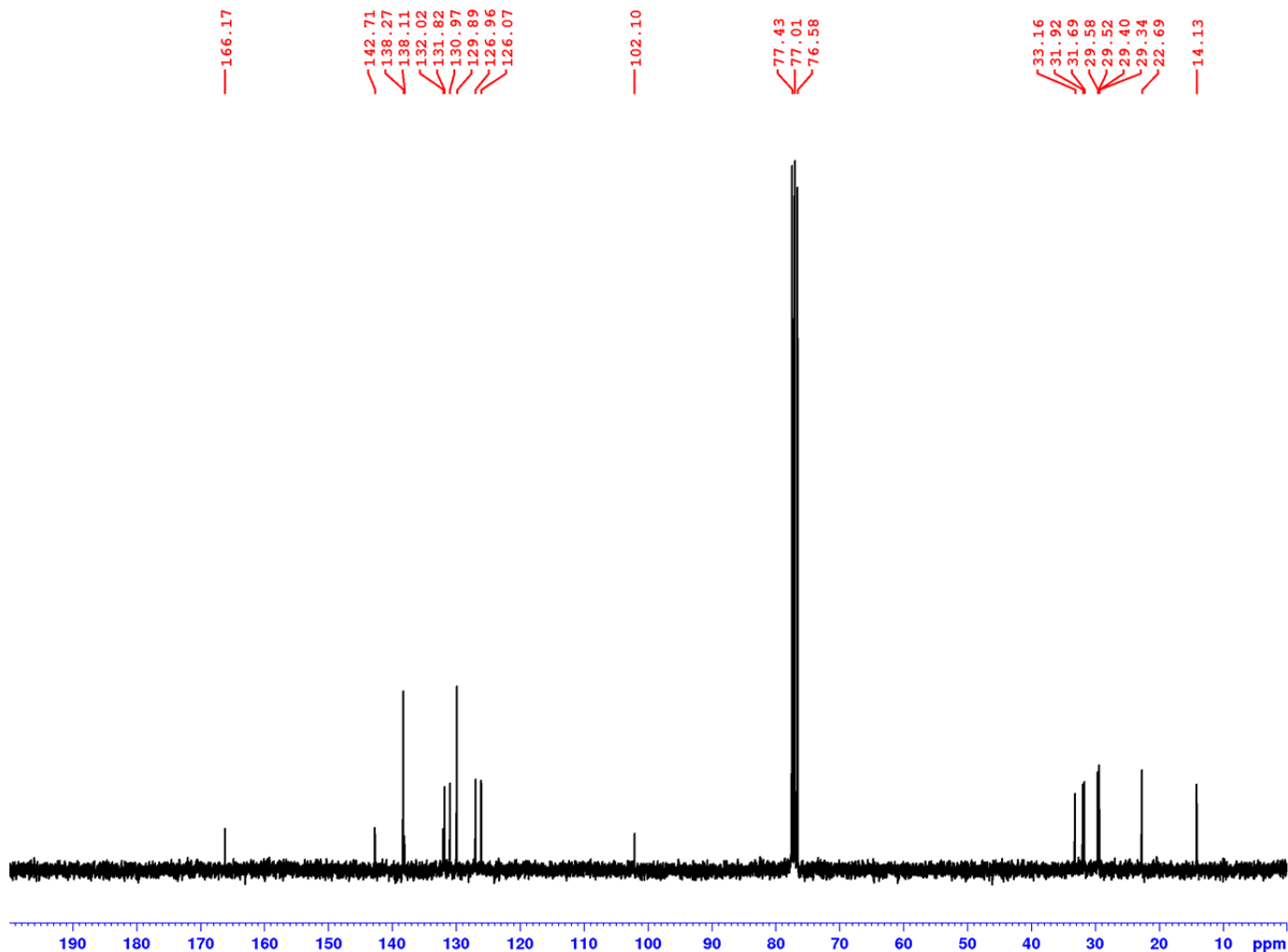
Current Data Parameters
NAME W391302
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190507
Time 1.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 209.37
DW 27.600 usec
DE 11.35 usec
TE 300.0 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1

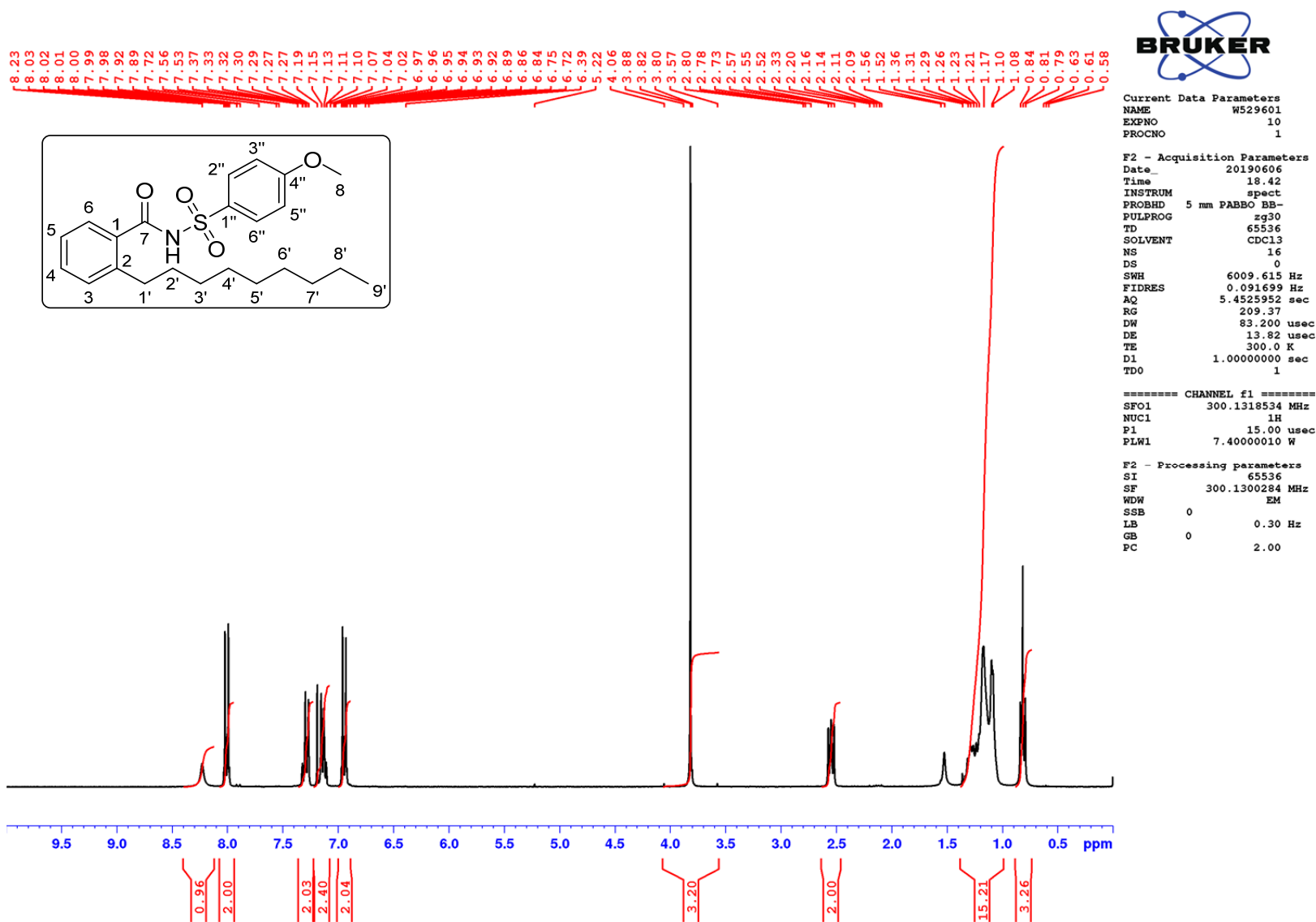
===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 10.00 usec
PLW1 35.00000000 W

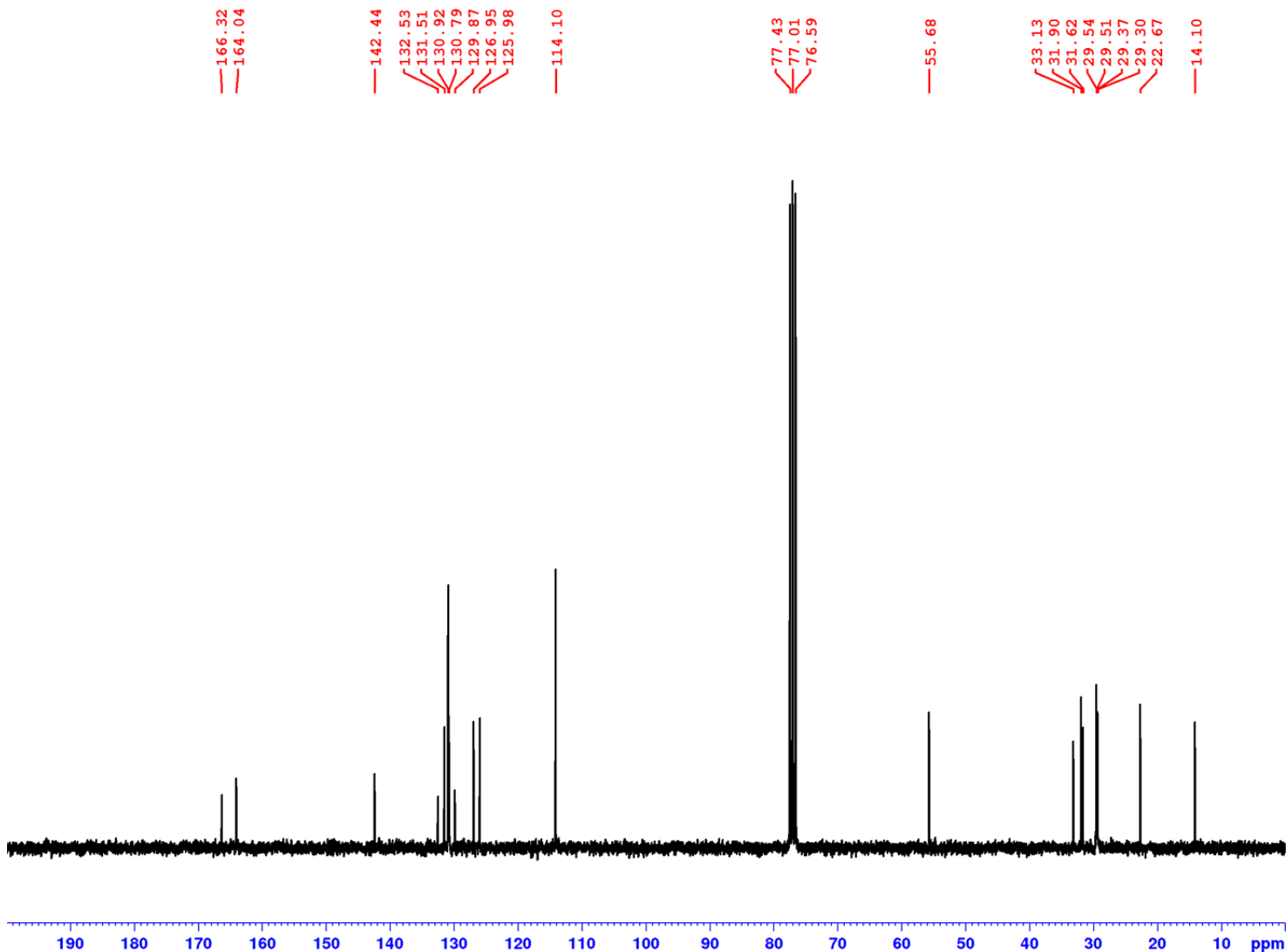
===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.40000010 W
PLW12 0.20556000 W
PLW13 0.16650000 W

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



N-(4-Methoxybenzenesulfonyl)-2-nonylbenzamide (21)





Current Data Parameters
 NAME W529602
 EXPNO 10
 PROCNO 1

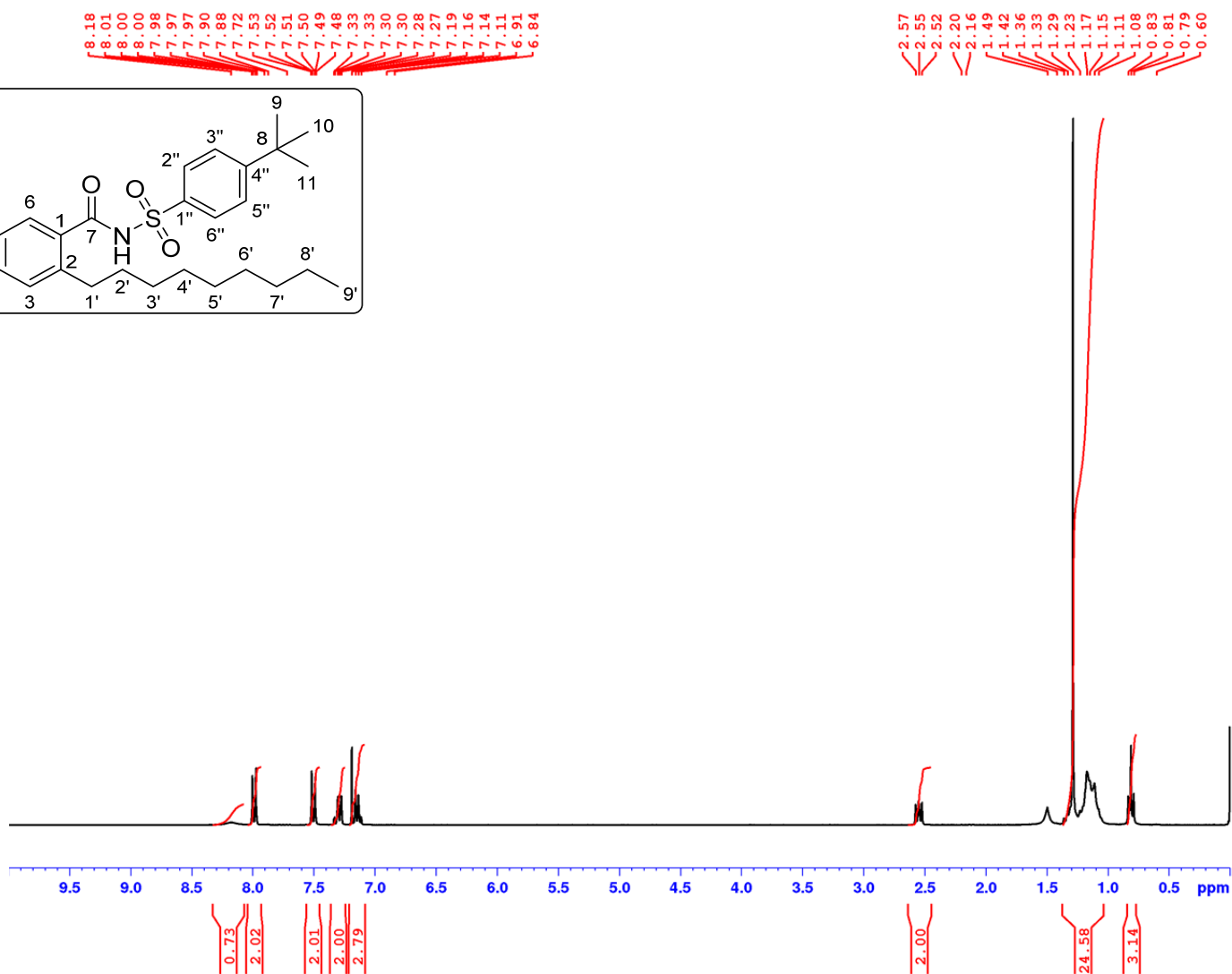
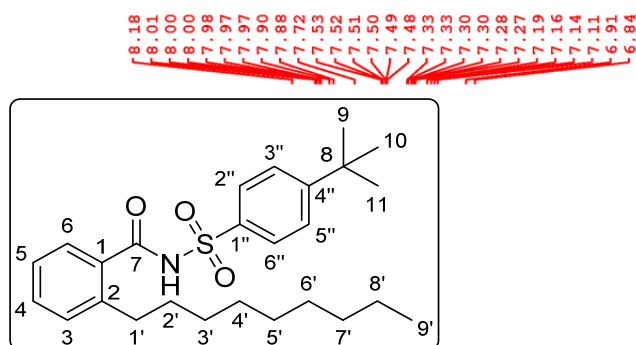
F2 - Acquisition Parameters
 Date_ 20190607
 Time 1.42
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 18115.941 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 209.37
 DW 27.600 usec
 DE 11.35 usec
 TE 300.0 K
 D1 0.50000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 75.4752949 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 35.00000000 W

===== CHANNEL f2 =====
 SFO2 300.1312005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 7.40000010 W
 PLW12 0.20556000 W
 PLW13 0.16650000 W

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

N-(4-*tert*-Butylbenzenesulfonyl)-2-nonylbenzamide (22)



Current Data Parameters
NAME W529701
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190606
Time 18.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 209.37
DW 83.200 usec
DE 13.82 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 15.00 usec
PLW1 7.40000010 W

F2 - Processing parameters
SI 65536
SF 300.1300283 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00



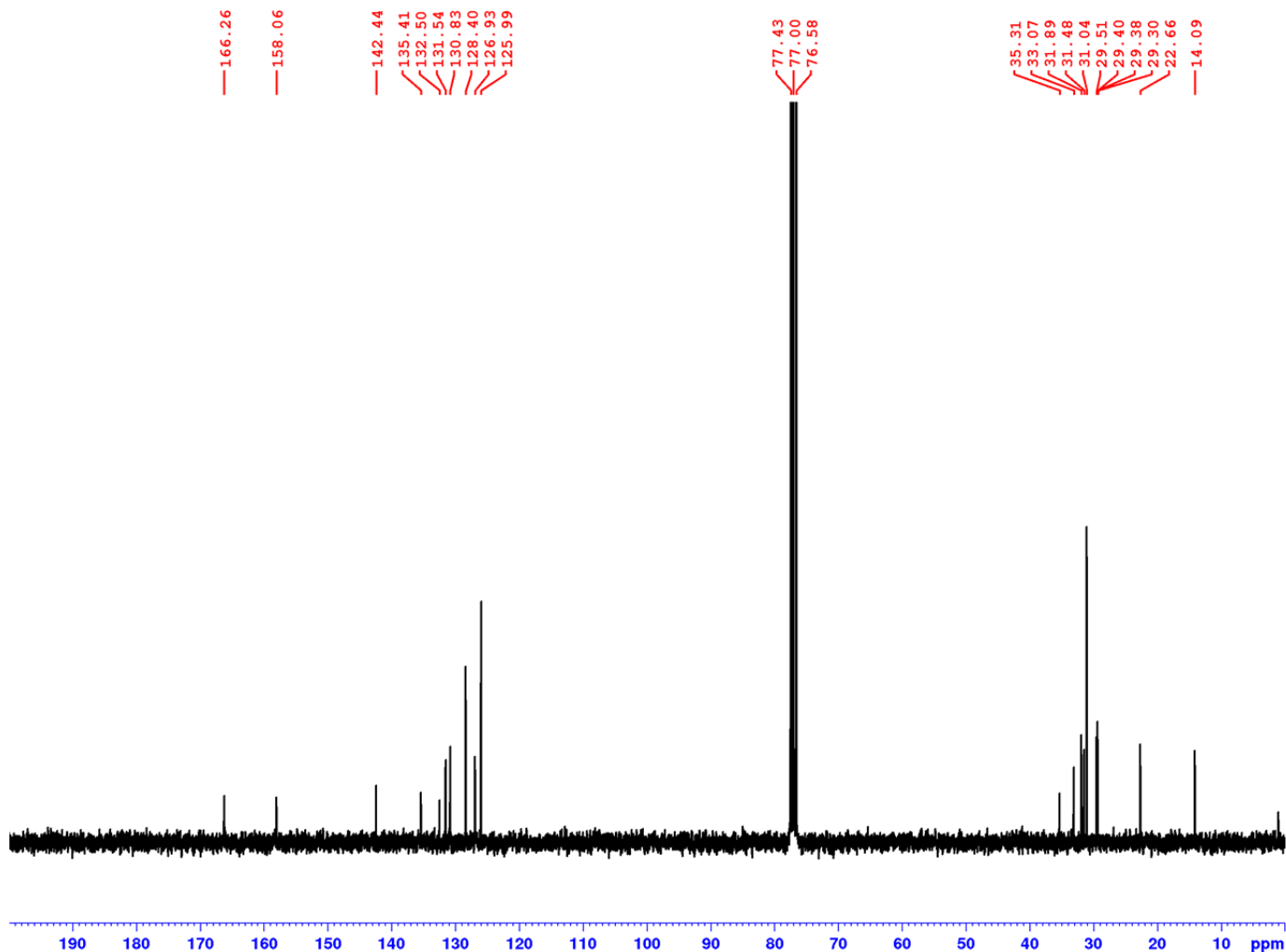
Current Data Parameters
NAME W529702
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190606
Time 19.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 209.37
DW 27.600 usec
DE 11.35 usec
TE 300.0 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1

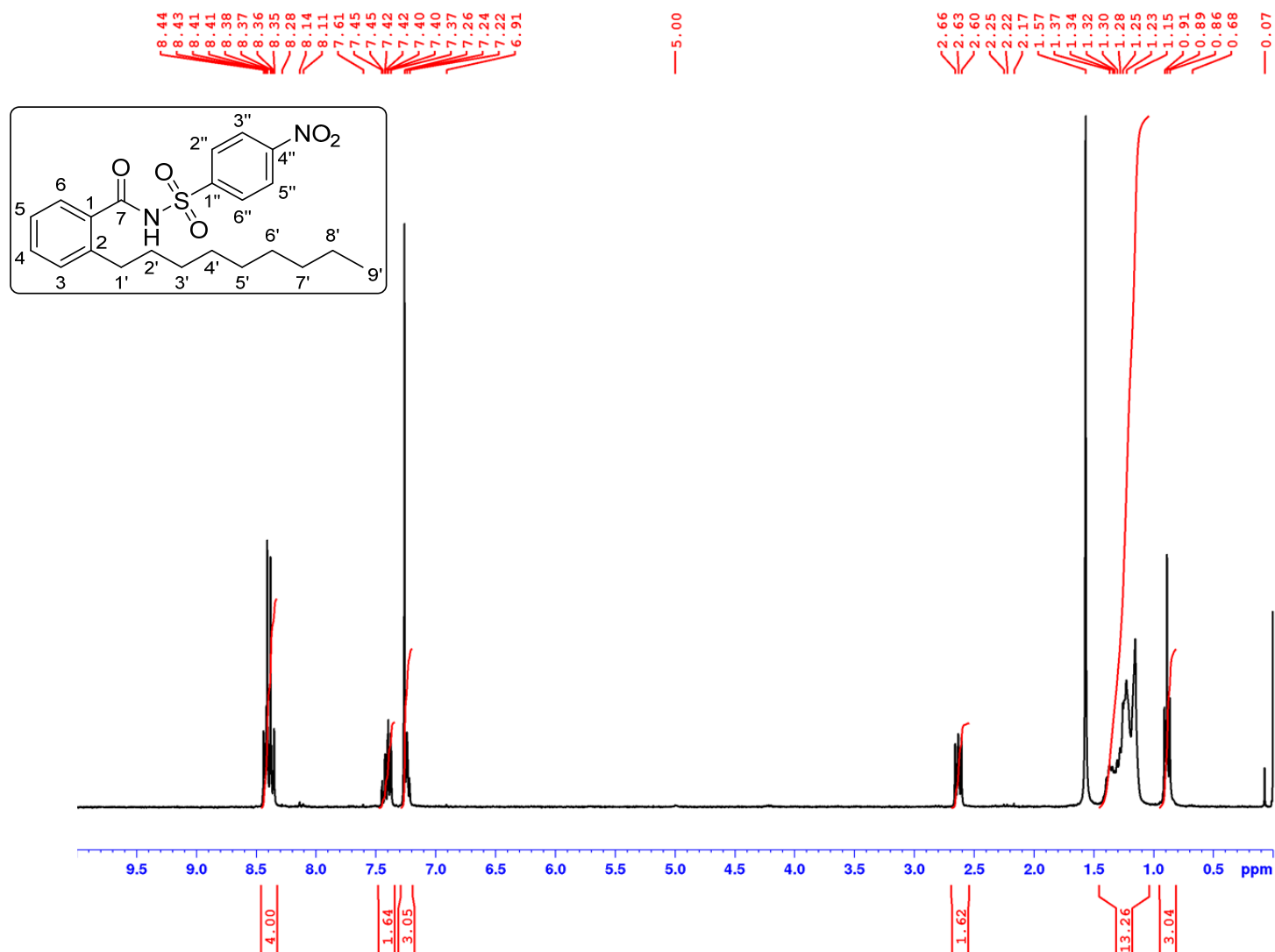
===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 10.00 usec
PLW1 35.00000000 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.40000010 W
PLW12 0.20556000 W
PLW13 0.16650000 W

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



N-(4-Nitrobenzenesulfonyl)-2-nonylbenzamide (23)



Current Data Parameters
NAME W634401
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190809
Time 15.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 209.37
DW 83.200 usec
DE 13.82 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 15.00 usec
PLW1 7.40000010 W

F2 - Processing parameters
SI 65536
SF 300.1300072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00



Current Data Parameters
NAME W634402
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190812
Time 22.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 209.37
DW 27.600 usec
DE 11.35 usec
TE 300.0 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 10.00 usec
PLW1 35.00000000 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.40000010 W
PLW12 0.20556000 W
PLW13 0.16650000 W

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

