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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
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Supplementary Data

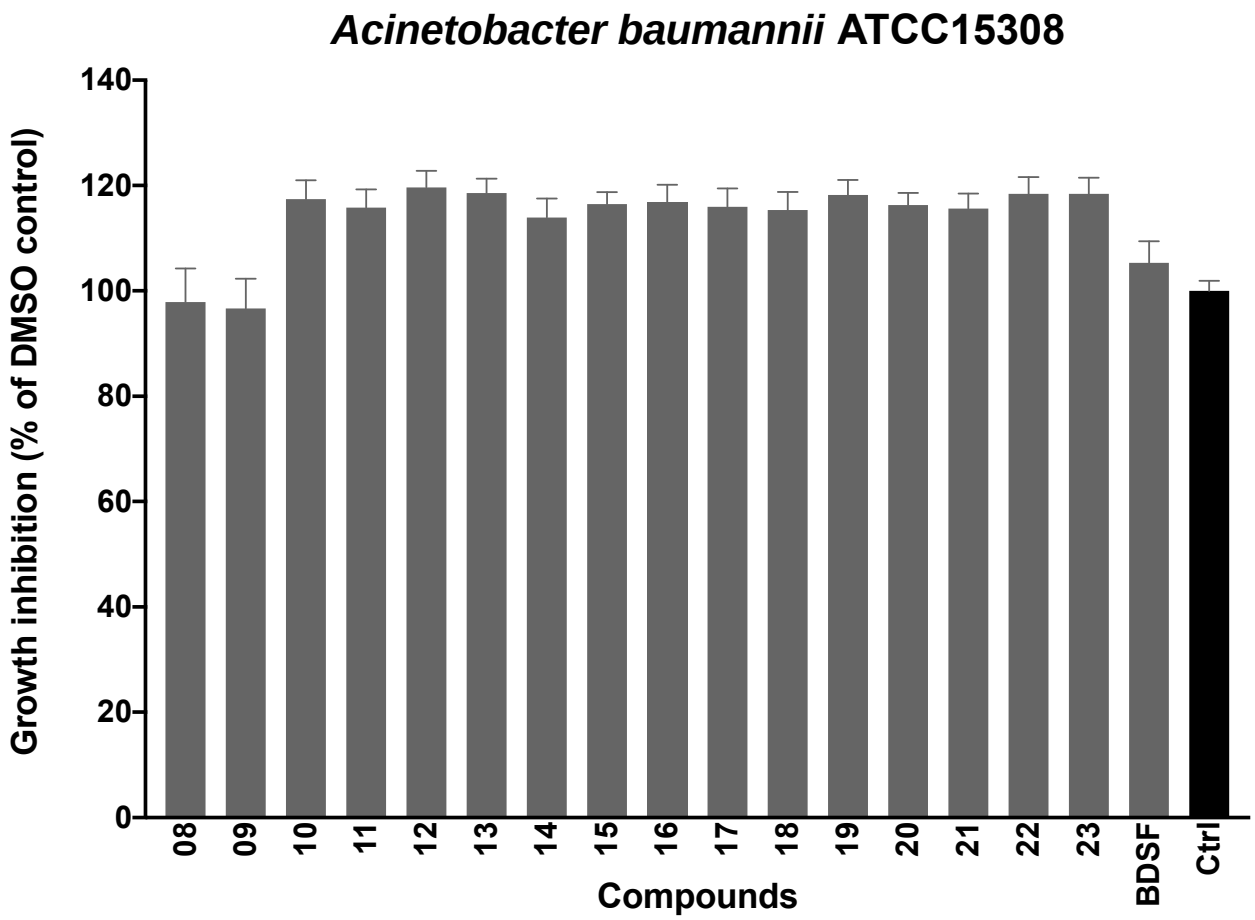
Synthesis and evaluation of aromatic BDSF bioisosteres on biofilm formation and colistin sensitivity in pathogenic bacteria

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]#.

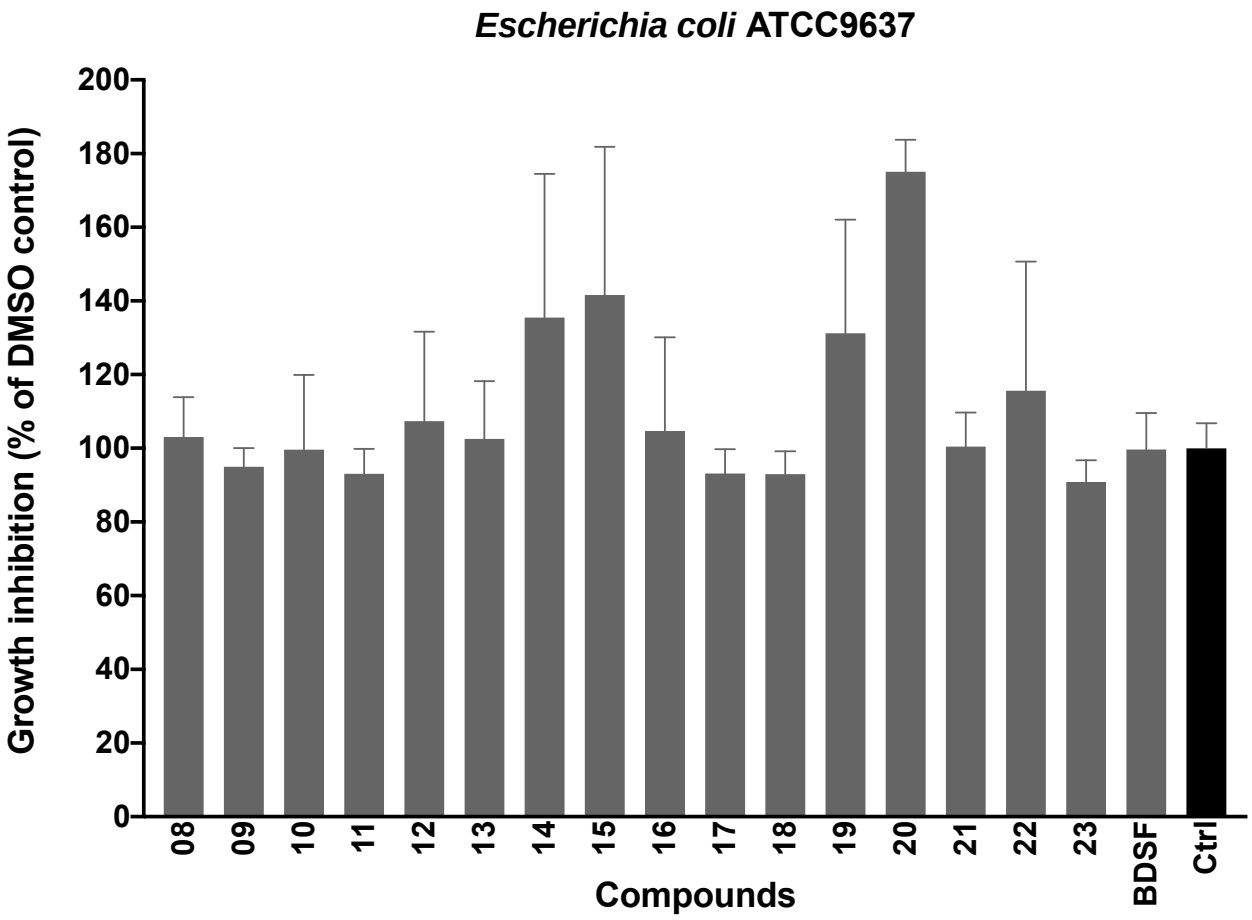
Affiliation

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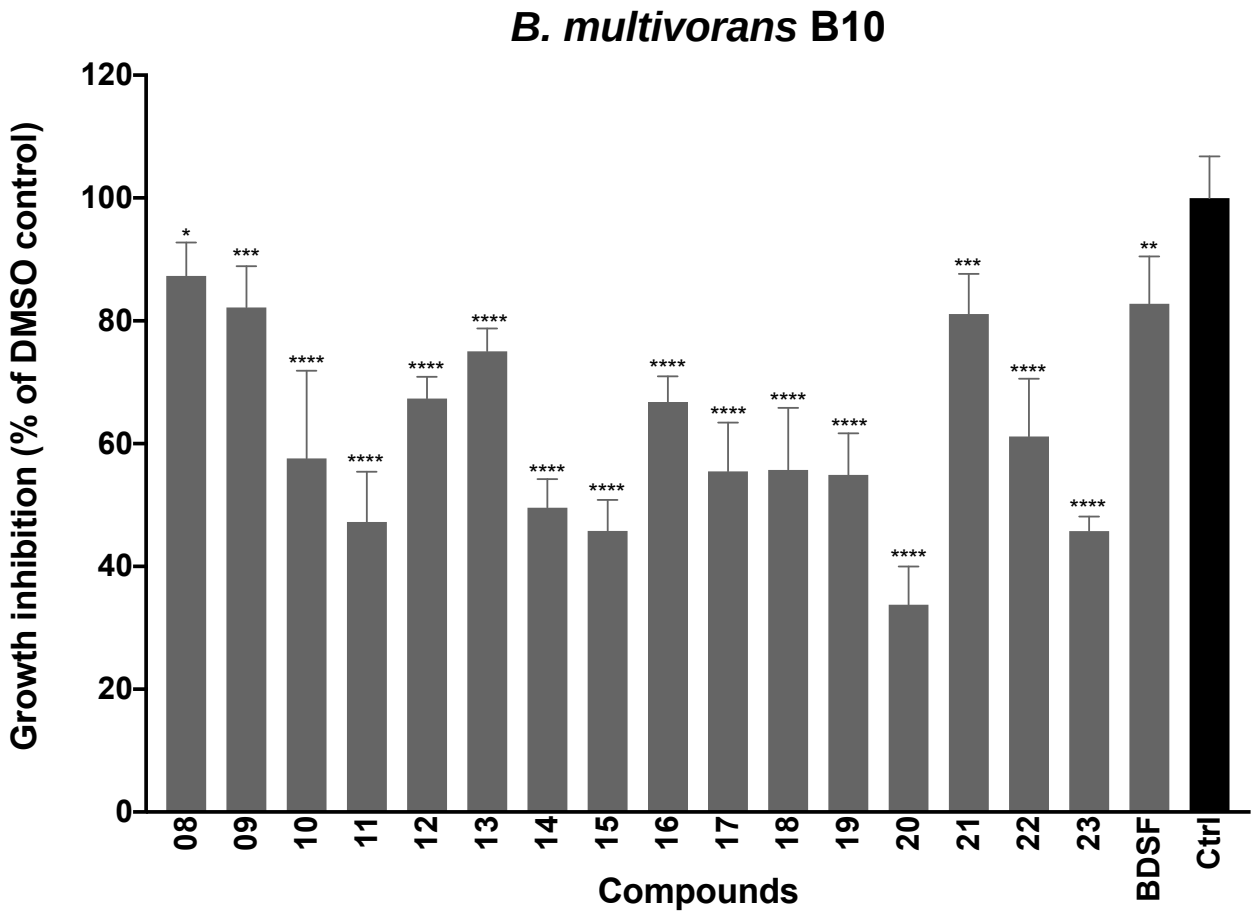
Effect of BDSF derivates on bacterial growth



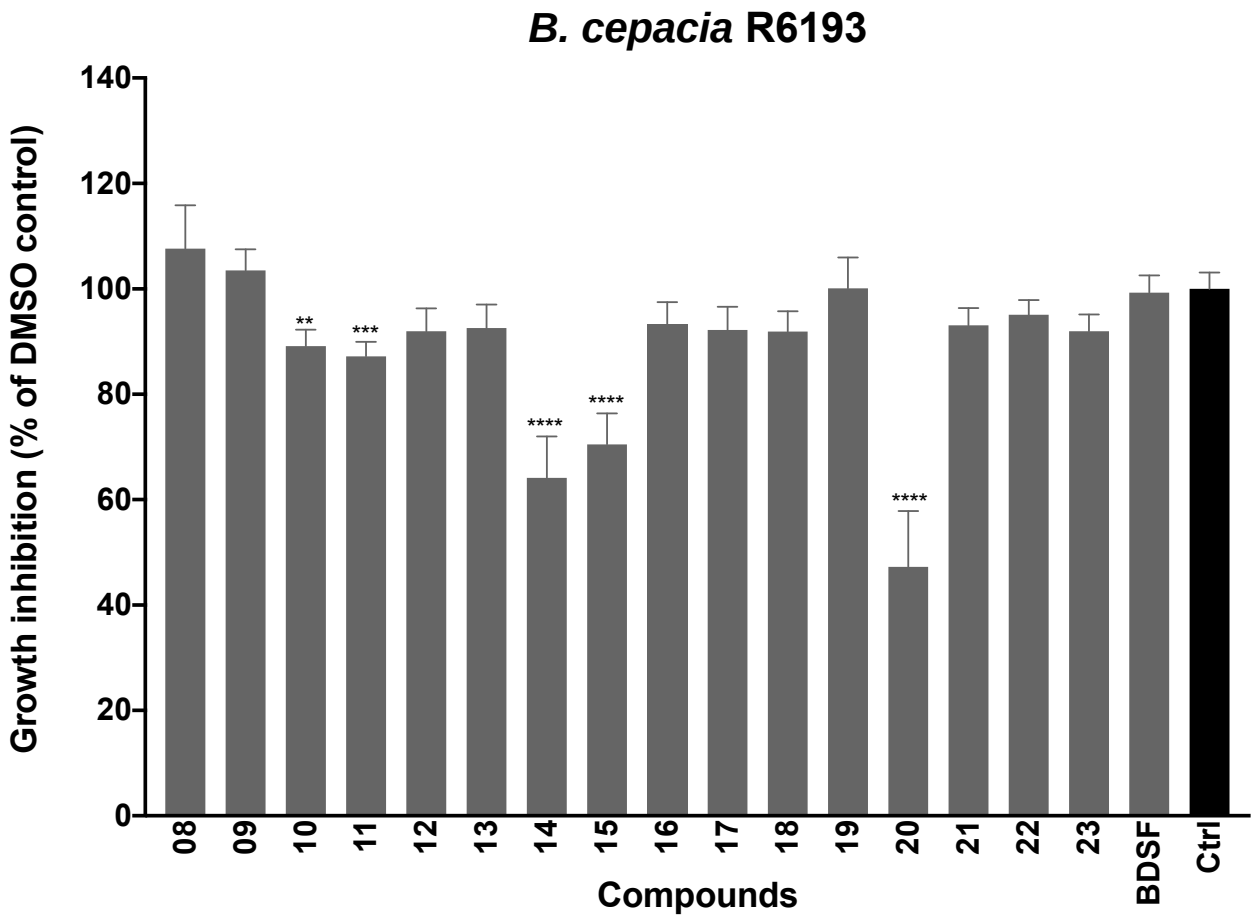
Supplementary Figure A1. Effect of sulfonamides on bacterial growth of *A. baumannii* ATCC15308.



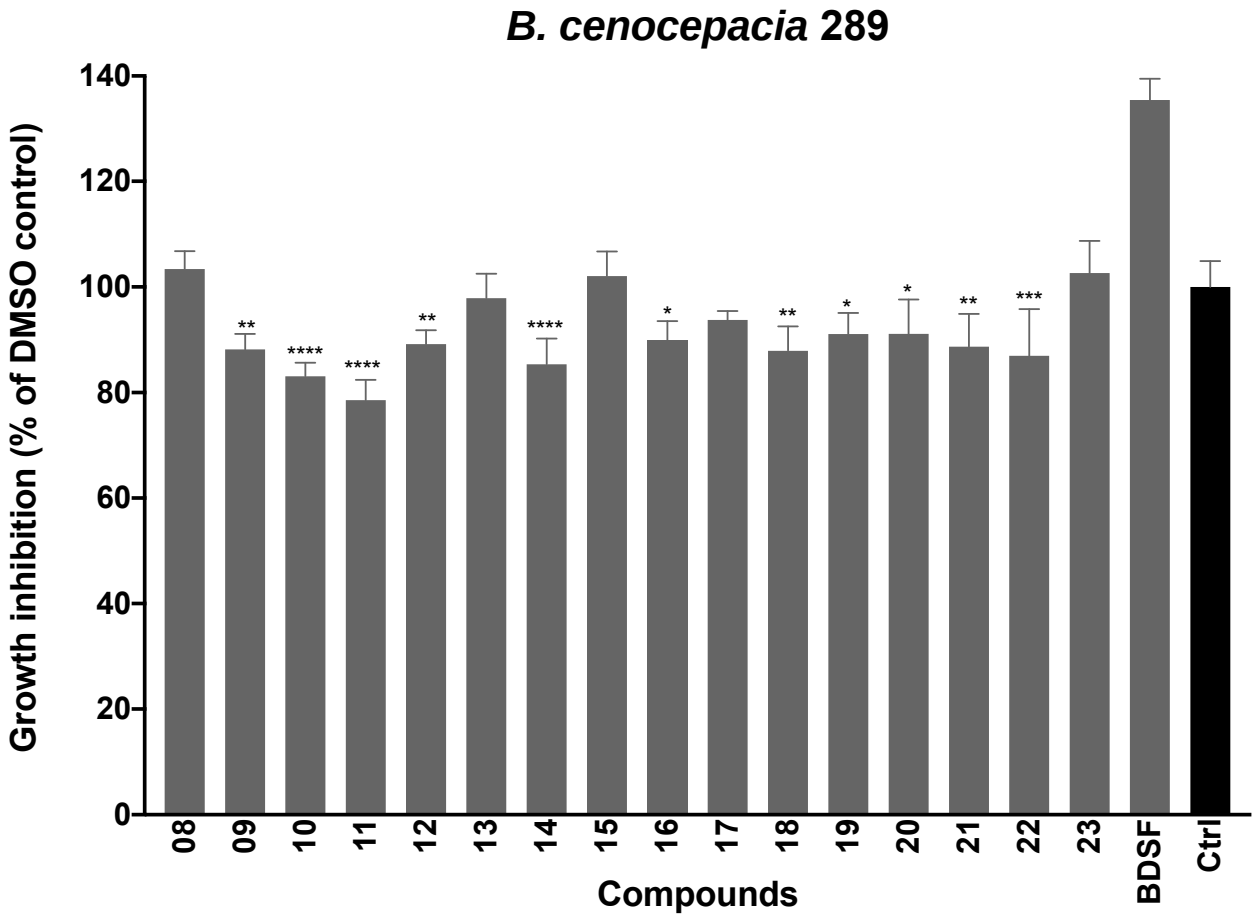
Supplementary Figure A2. Effect of sulfonamides on bacterial growth of *E. coli* ATCC9637.



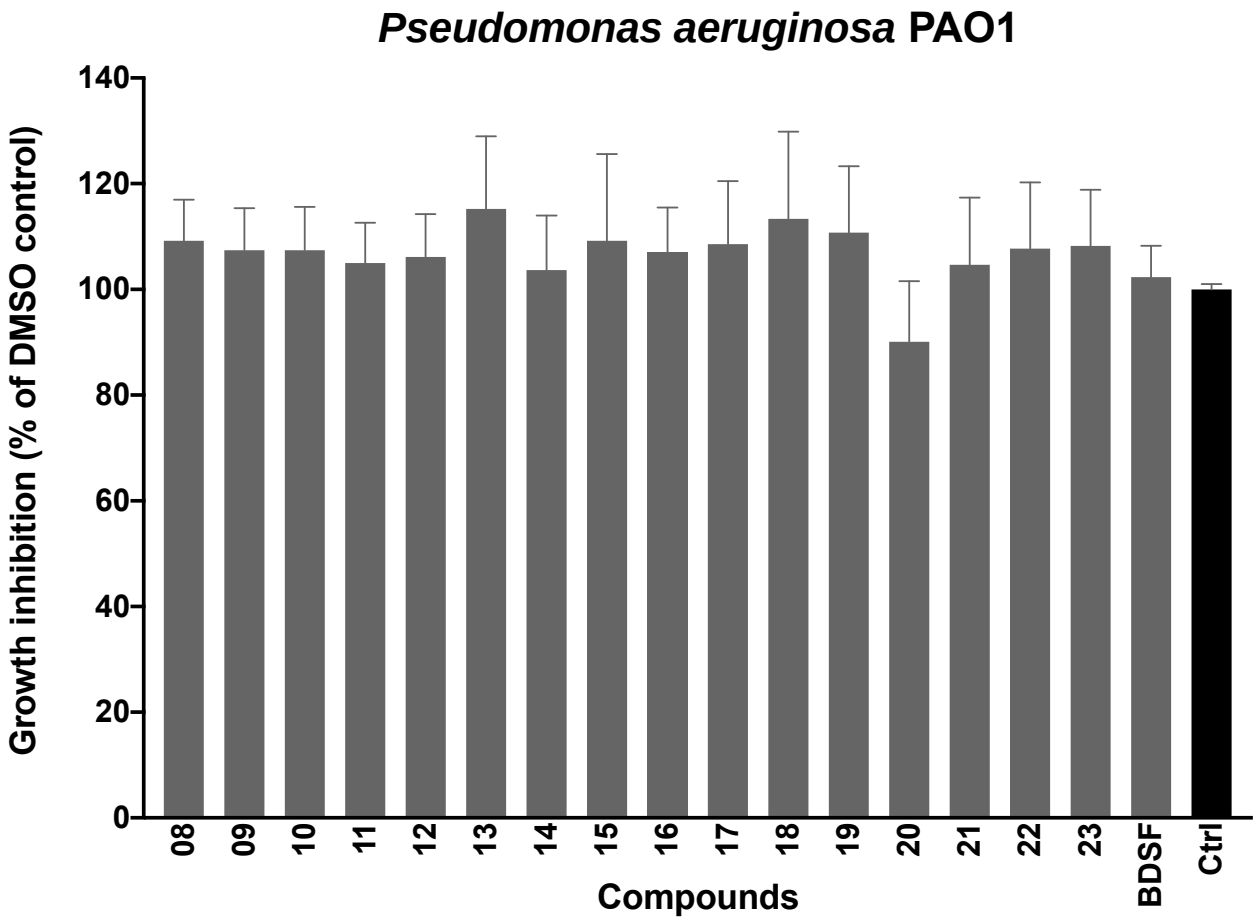
Supplementary Figure A3. Effect of sulfonamides on bacterial growth of *B. multivorans* B10 (*p < 0.05, **p < 0.01, ***p < 0.001, ****p < 0.0001).



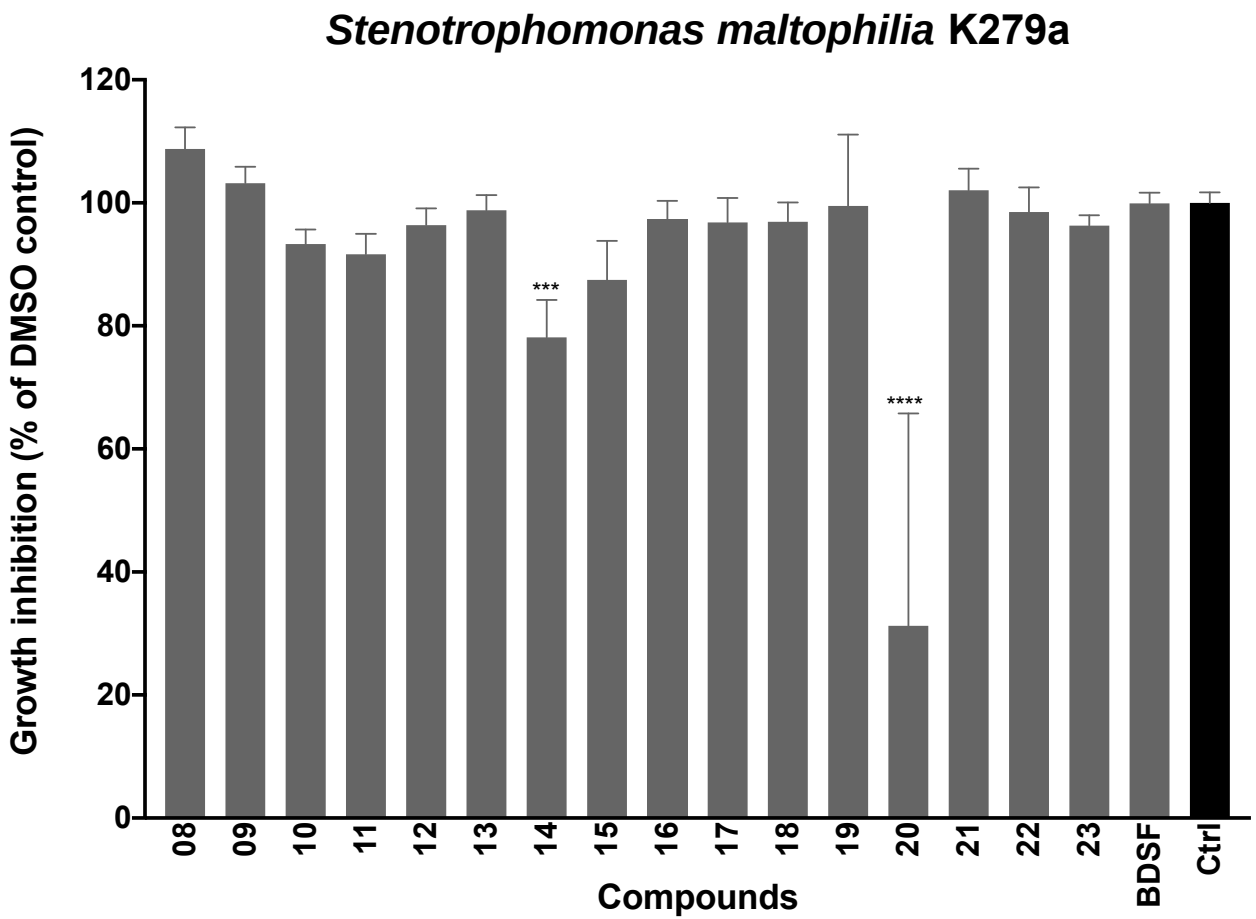
Supplementary Figure A4. Effect of sulfonamides on bacterial growth of *B. cepacia* R6193 (*p < 0.05, **p < 0.01, ***p < 0.001, ****p < 0.0001).



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).

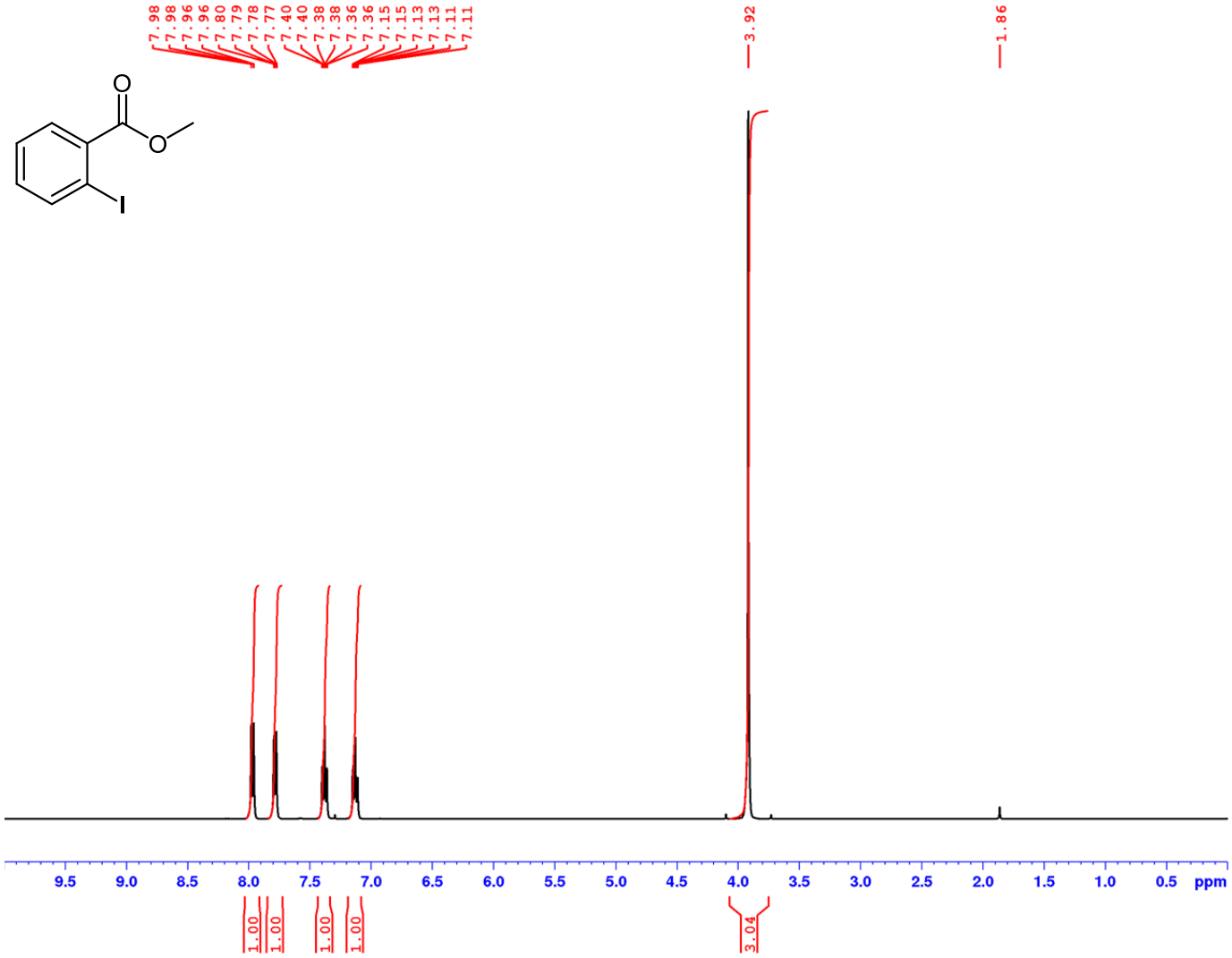


Supplementary Figure A6. Effect of sulfonamides on bacterial growth of *P. aeruginosa* PAO1.



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)

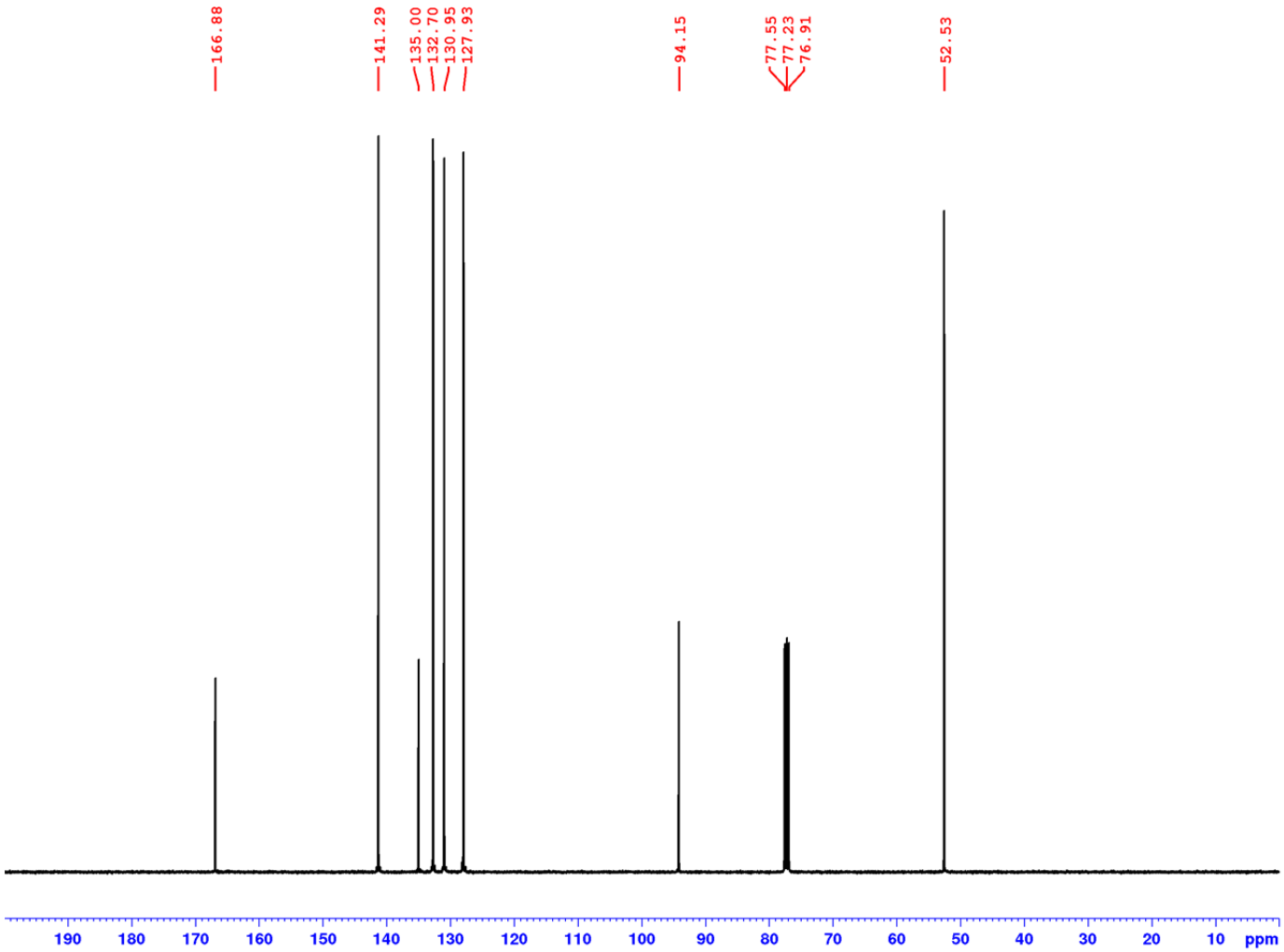



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PULPROG              zg30
TD                 131072
SOLVENT              CDCl3
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DS                       2
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FIDRES            0.063157 Hz
AQ                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
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WDW                     EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
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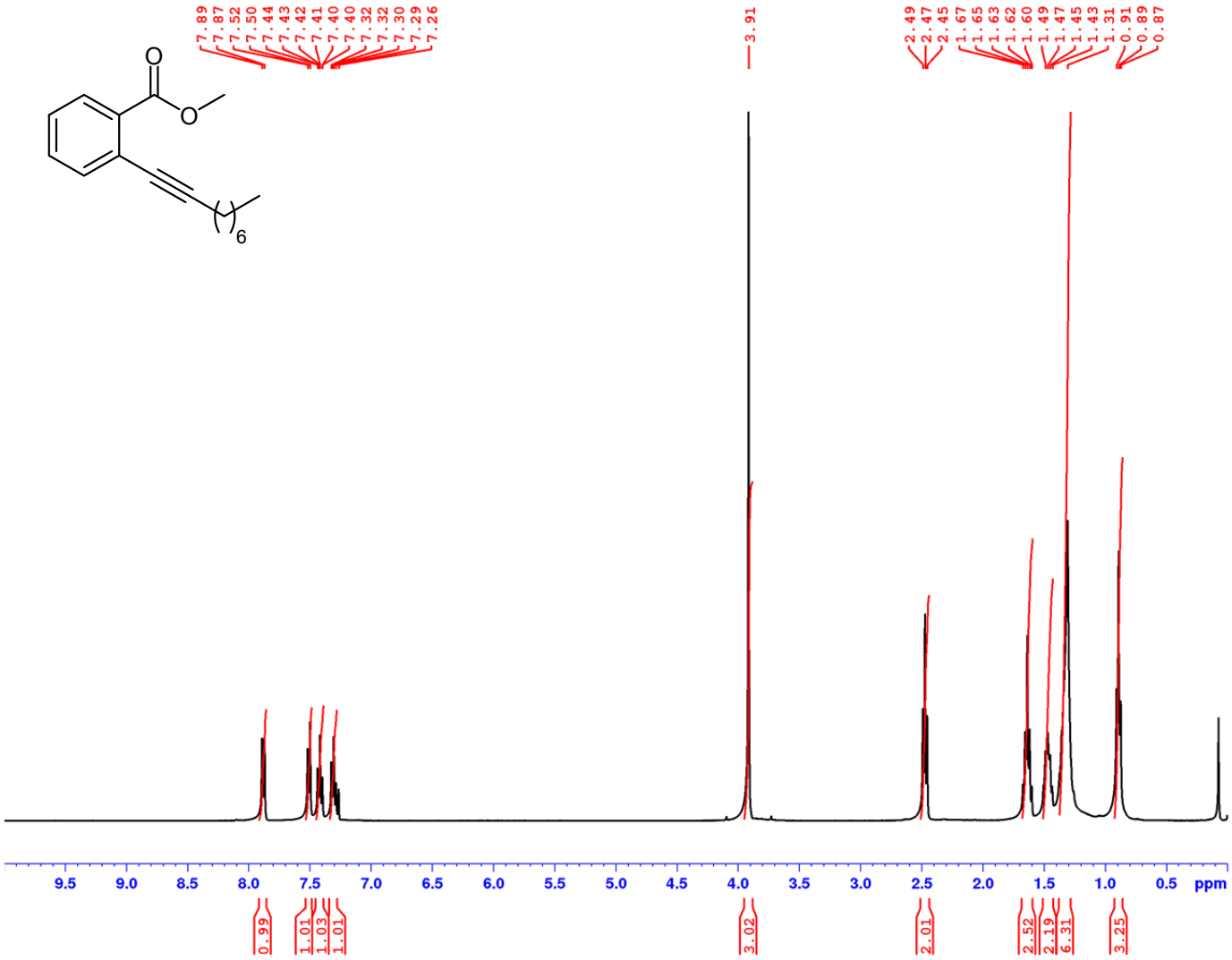
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PULPROG                zgpg30
TD                     131072
SOLVENT                  CDCl3
NS                        1024
DS                           4
SWH                  23980.814 Hz
FIDRES                0.182959 Hz
AQ                    2.7328513 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
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LB                        1.00 Hz
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PC                        1.40
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Methyl 2-(Non-1-yn-1-yl)benzoate (5)



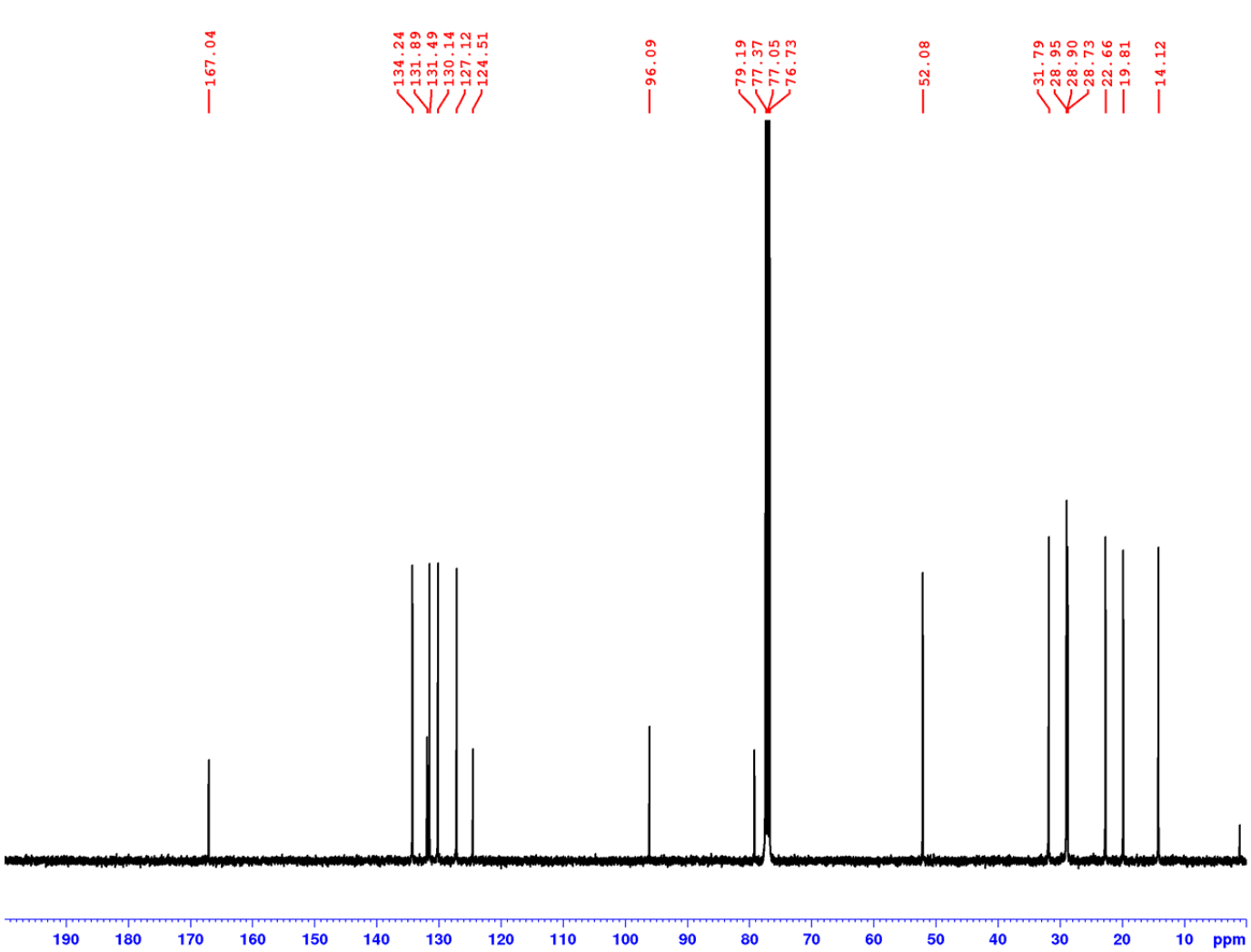
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PULPROG                  zg30
TD                     131072
SOLVENT                  CDCl3
NS                           8
DS                           2
SWH                   8278.146 Hz
FIDRES                0.063157 Hz
AQ                    7.9167490 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
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BRUKER

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PROCNO                       1

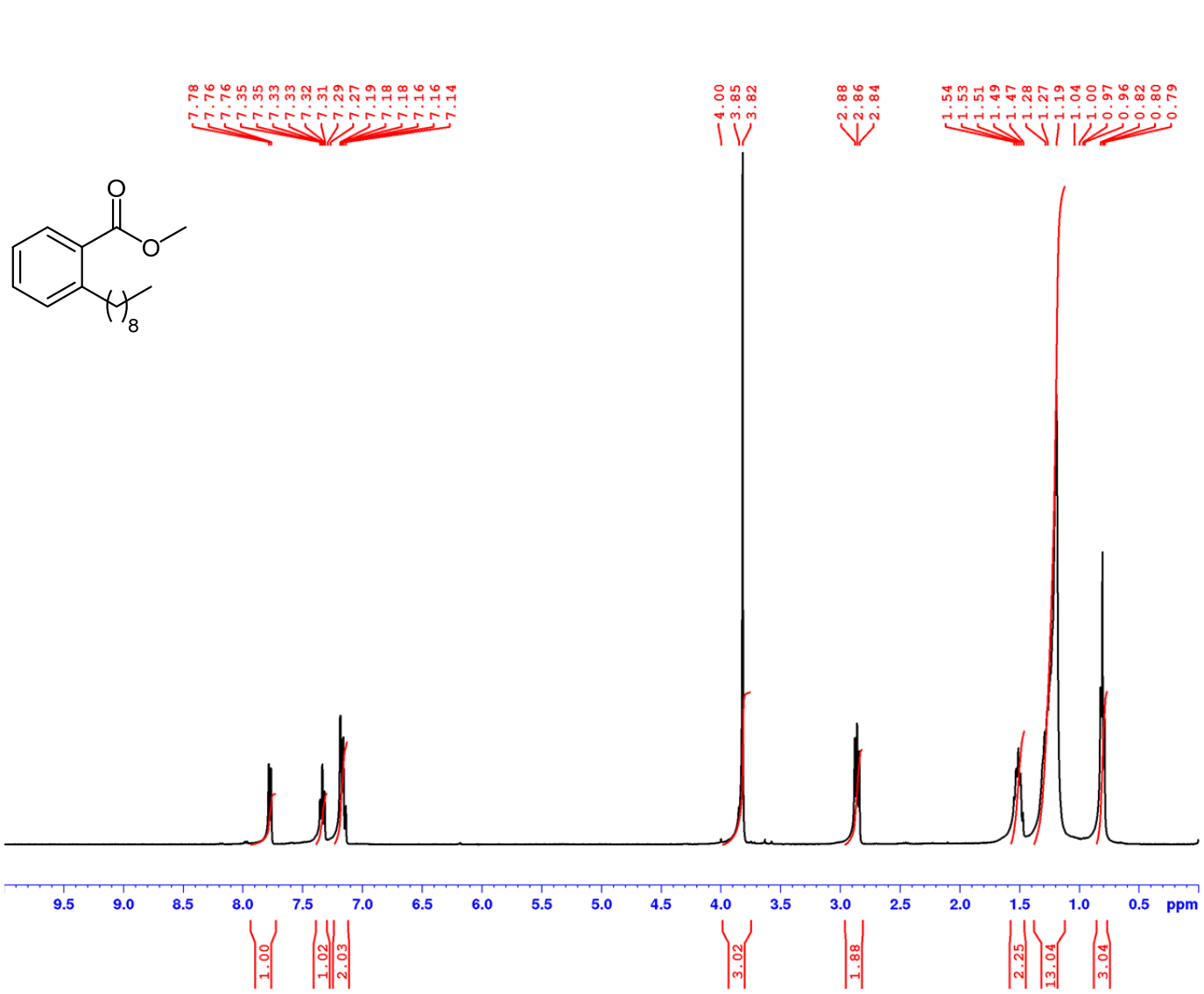
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PULPROG                 zgpg30
TD                      131072
SOLVENT                  CDCl3
NS                         1024
DS                            4
SWH                 23980.814 Hz
FIDRES               0.182959 Hz
AQ                   2.7328513 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-Nonylbenzoate (6)



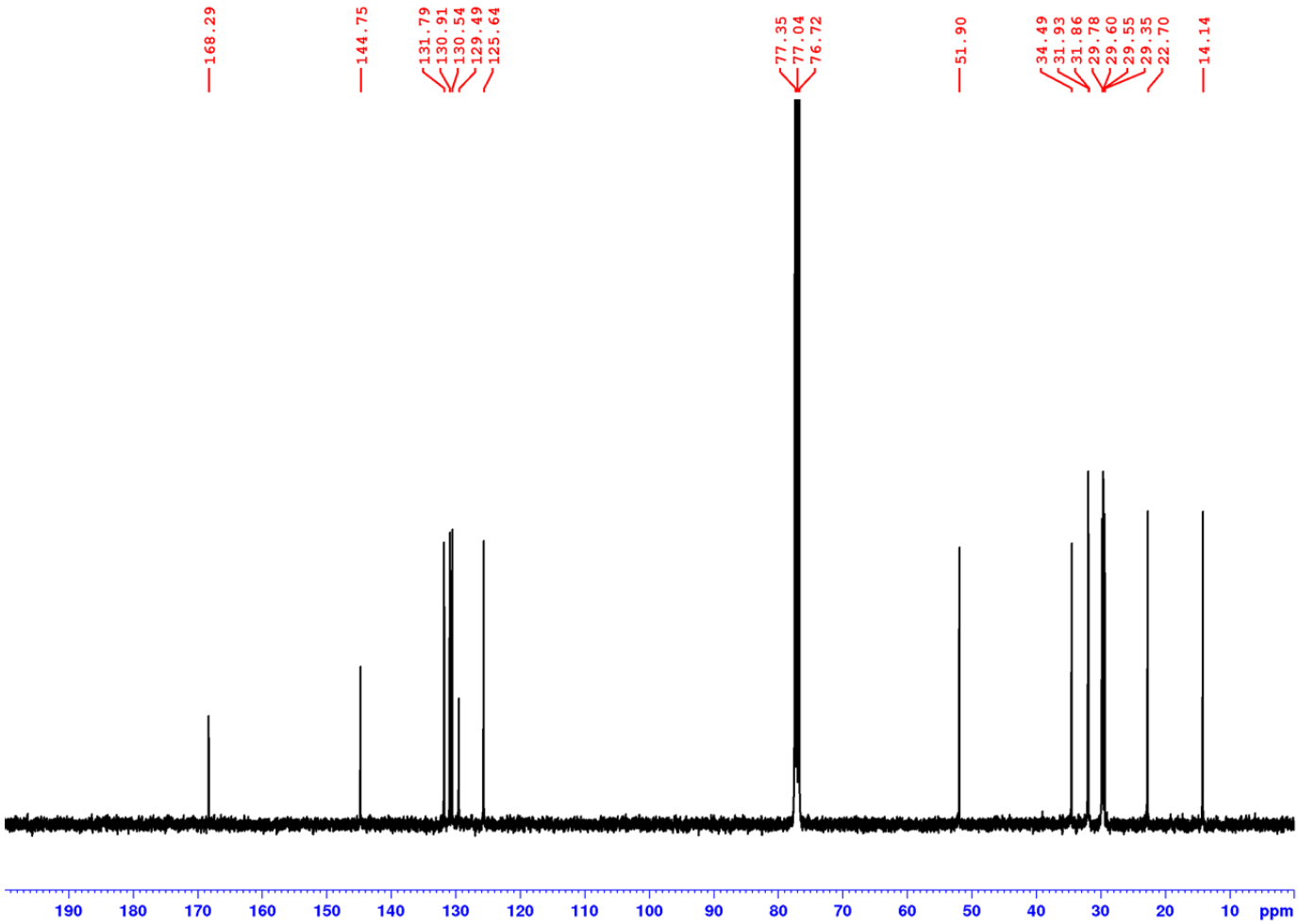
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PULPROG                  zg30
TD                     131072
SOLVENT                 CDCl3
NS                          8
DS                          2
SWH                  8278.146 Hz
FIDRES               0.063157 Hz
AQ                   7.9167490 sec
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                400.1300384 MHz
WDW                        EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
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BRUKER

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PROCNO                      1

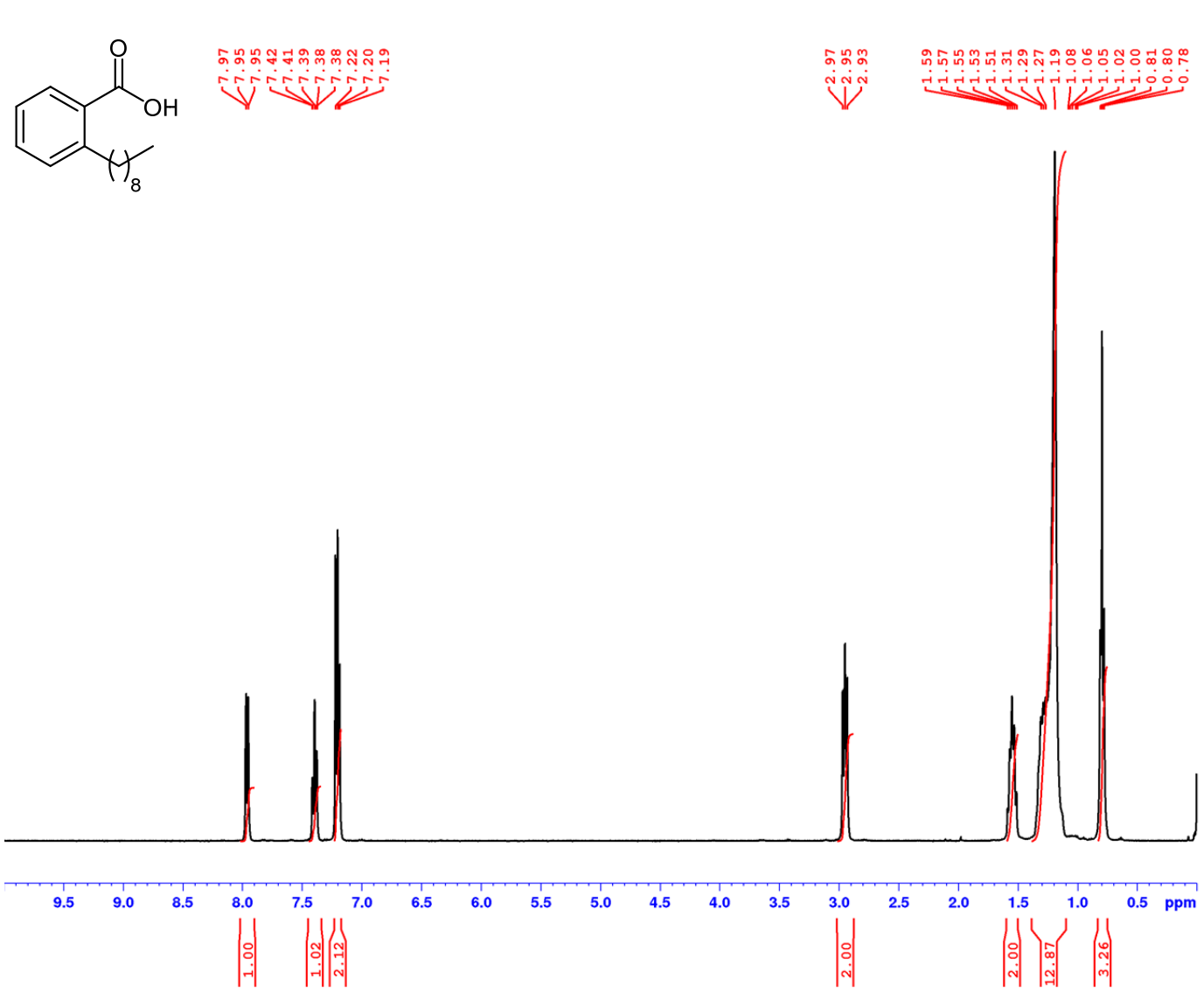
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PULPROG             zgpg30
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SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               23980.814 Hz
FIDRES             0.182959 Hz
AQ                 2.7328513 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
```

2-Nonylbenzoic Acid (7)



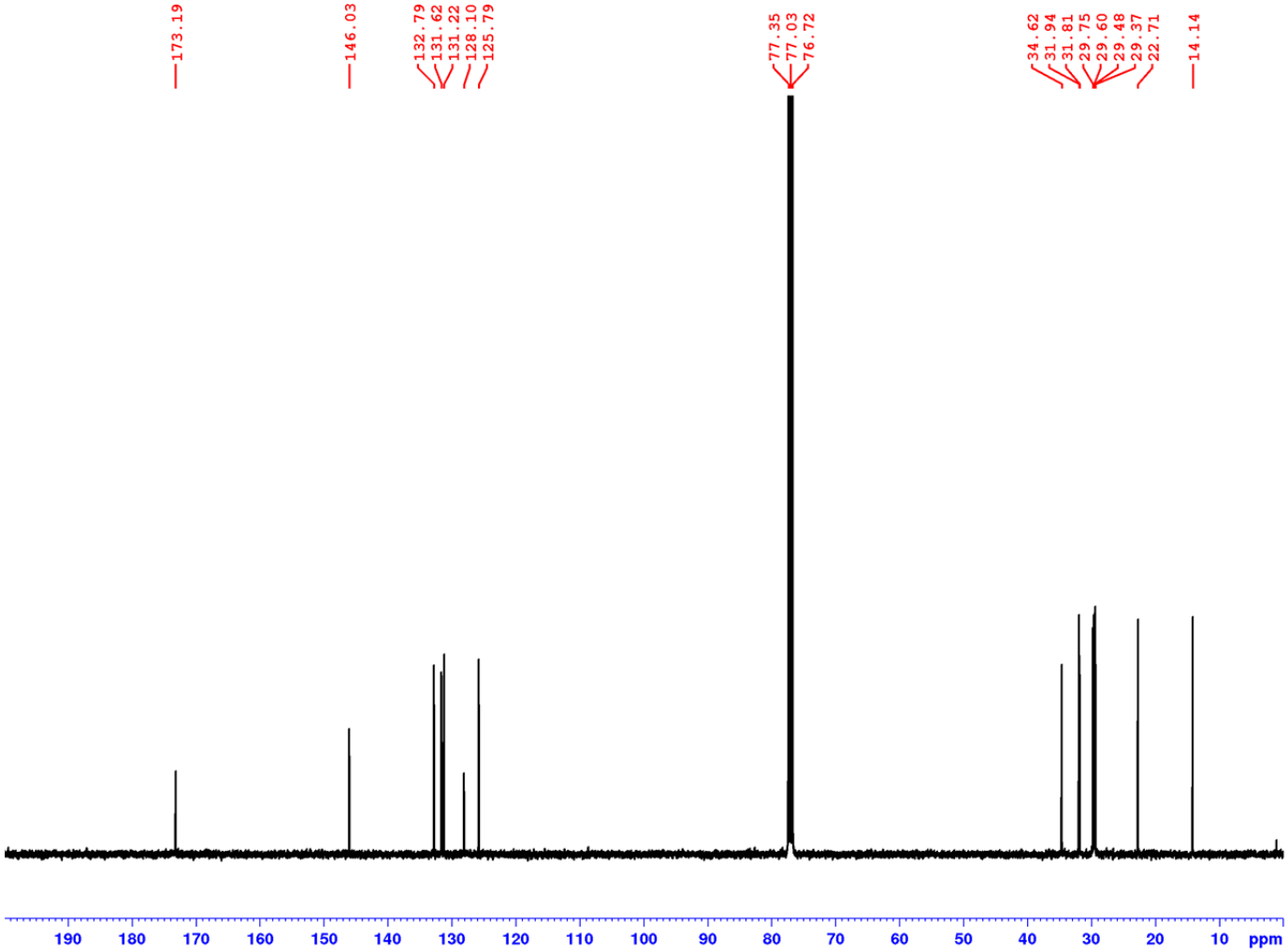
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PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                   131072
SOLVENT                CDCl3
NS                         8
DS                         2
SWH                 8278.146 Hz
FIDRES              0.063157 Hz
AQ                  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
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GB                 0
PC                     1.00
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BRUKER

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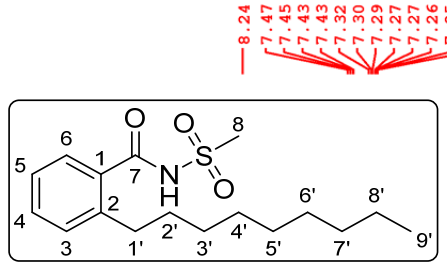
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TD                      131072
SOLVENT                   CDCl3
NS                        1024
DS                           4
SWH                  23980.814 Hz
FIDRES                0.182959 Hz
AQ                    2.7328513 sec
RG                        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
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N-(Methanesulfonyl)-2-nonylbenzamide (8)

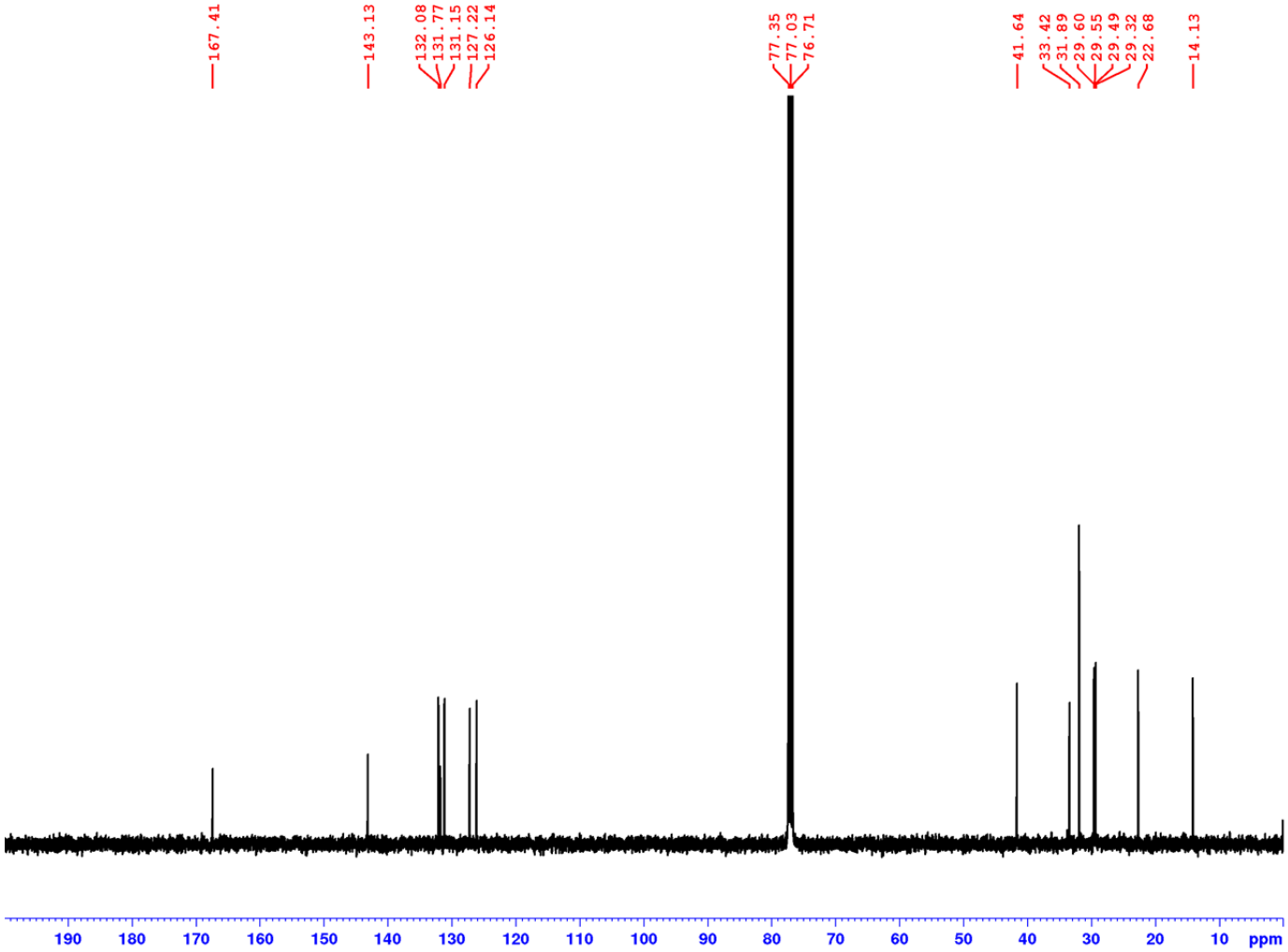



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PULPROG                  zg30
TD                     131072
SOLVENT                  CDCl3
NS                           8
DS                           2
SWH                 8278.146 Hz
FIDRES              0.063157 Hz
AQ                  7.9167490 sec
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
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GB           0
PC                       1.00
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BRUKER

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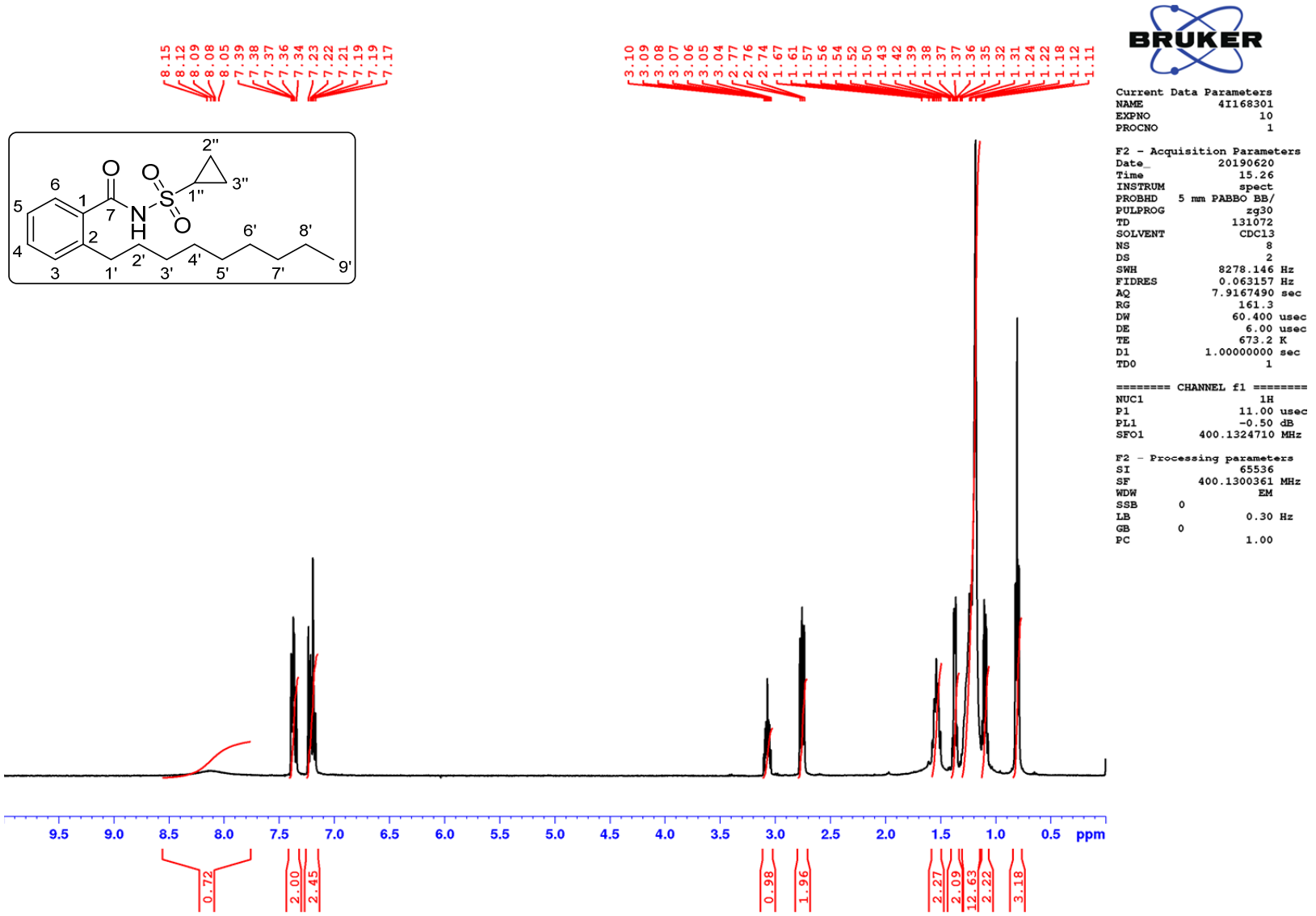
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PULPROG                zgpg30
TD                     131072
SOLVENT                  CDCl3
NS                         1024
DS                            4
SWH                23980.814 Hz
FIDRES              0.182959 Hz
AQ                  2.7328513 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)



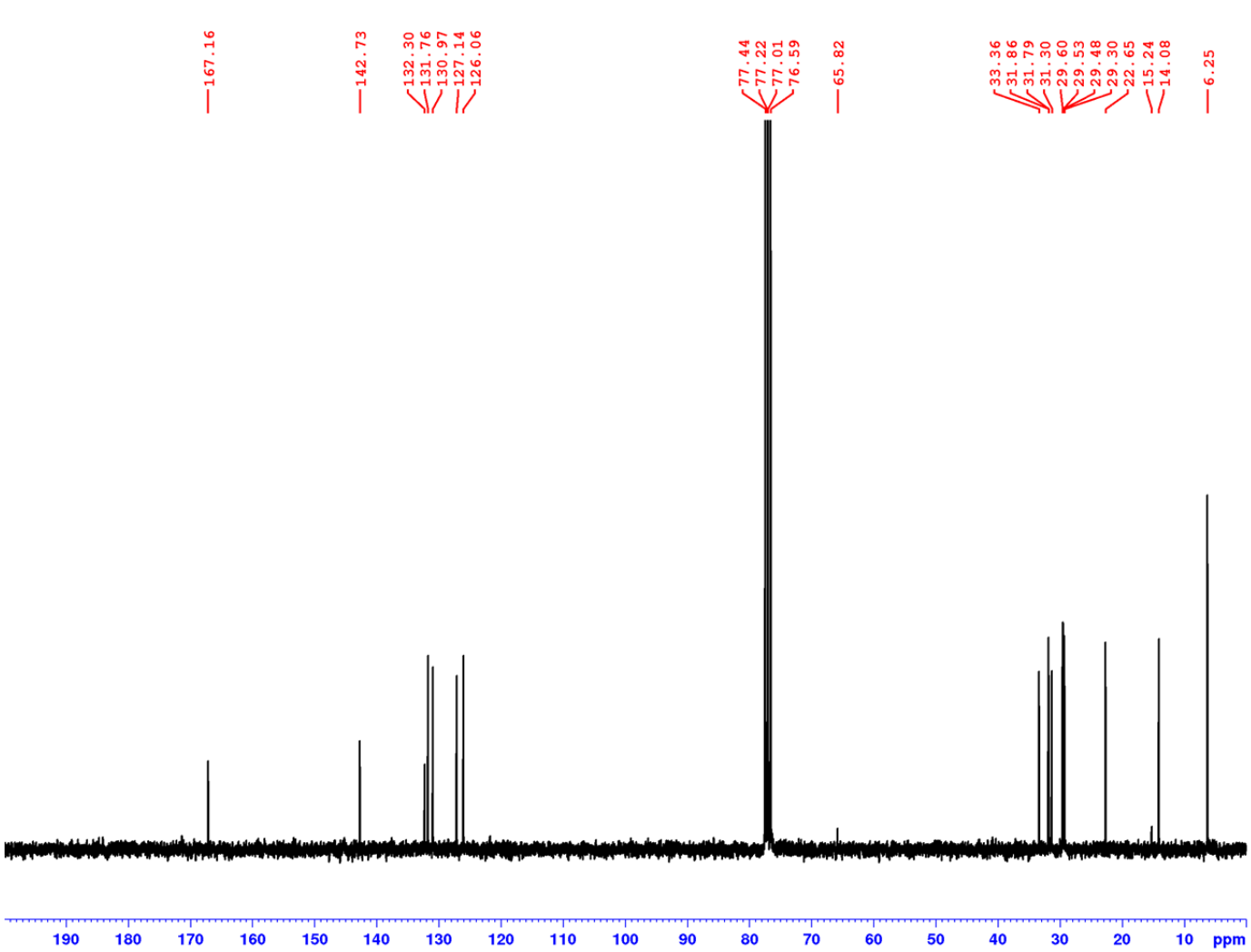
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PULPROG                 zg30
TD                    131072
SOLVENT                 CDCl3
NS                          8
DS                          2
SWH                  8278.146 Hz
FIDRES               0.063157 Hz
AQ                   7.9167490 sec
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
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BRUKER

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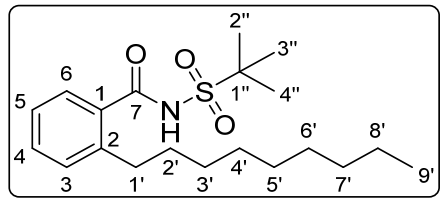
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NS                    1024
DS                       4
SWH              18115.941 Hz
FIDRES            0.276427 Hz
AQ                1.8087935 sec
RG                   209.37
DW                  27.600 usec
DE                  11.35 usec
TE                  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
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N-(*tert*-Butylsulfonyl)-2-nonylbenzamide (10)

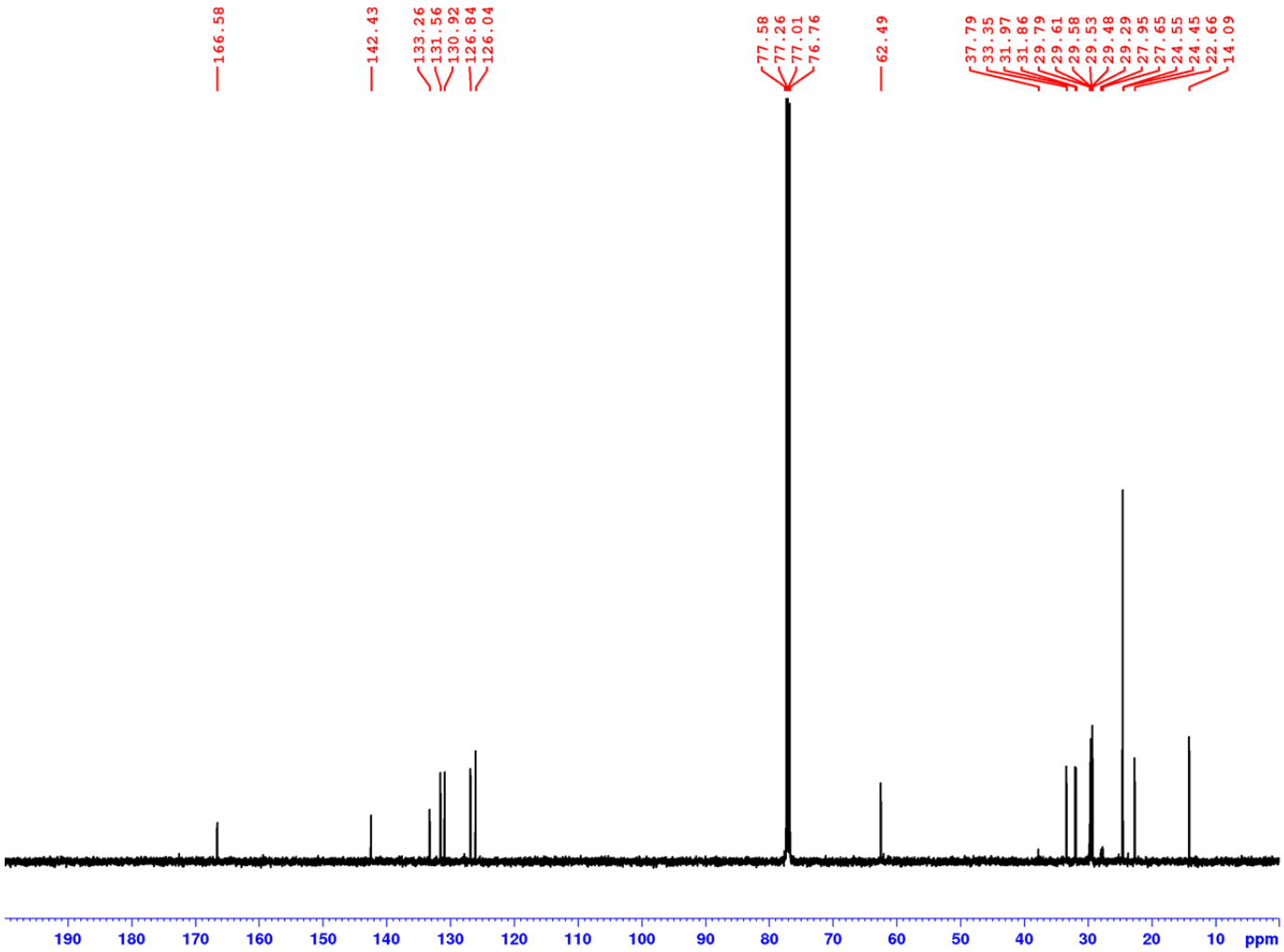



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PULPROG                 zg30
TD                    131072
SOLVENT                CDCl3
NS                         16
DS                          2
SWH                10330.578 Hz
FIDRES             0.078816 Hz
AQ                 6.3438849 sec
RG                        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
```



BRUKER

```
Current Data Parameters
NAME                 Y325702
EXPNO                     10
PROCNO                     1

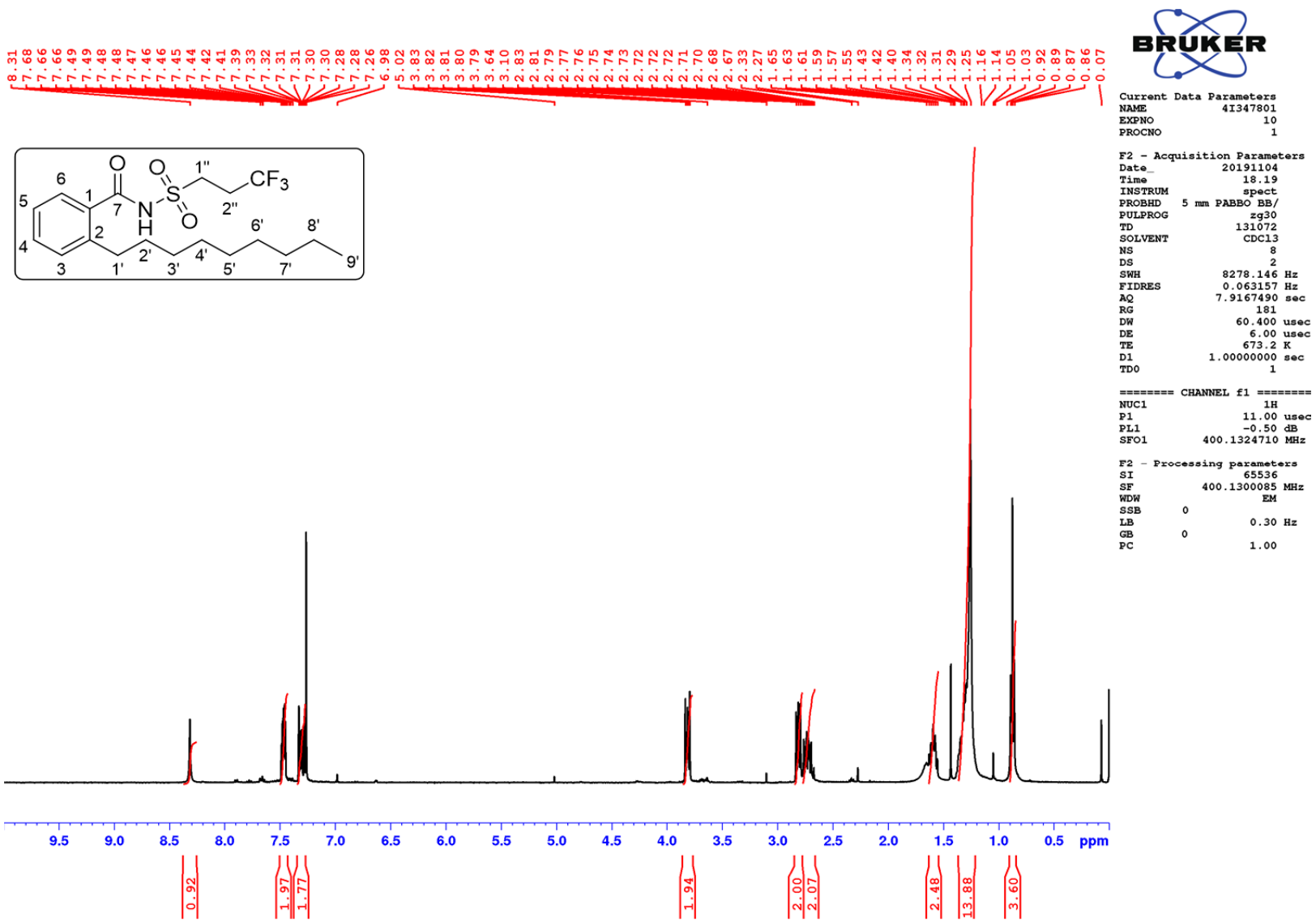
F2 - Acquisition Parameters
Date_              20220118
Time                   1.52
INSTRUM               spect
PROBHD   5 mm PAQNP 1H/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               29761.904 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
CPDPRG[2             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)



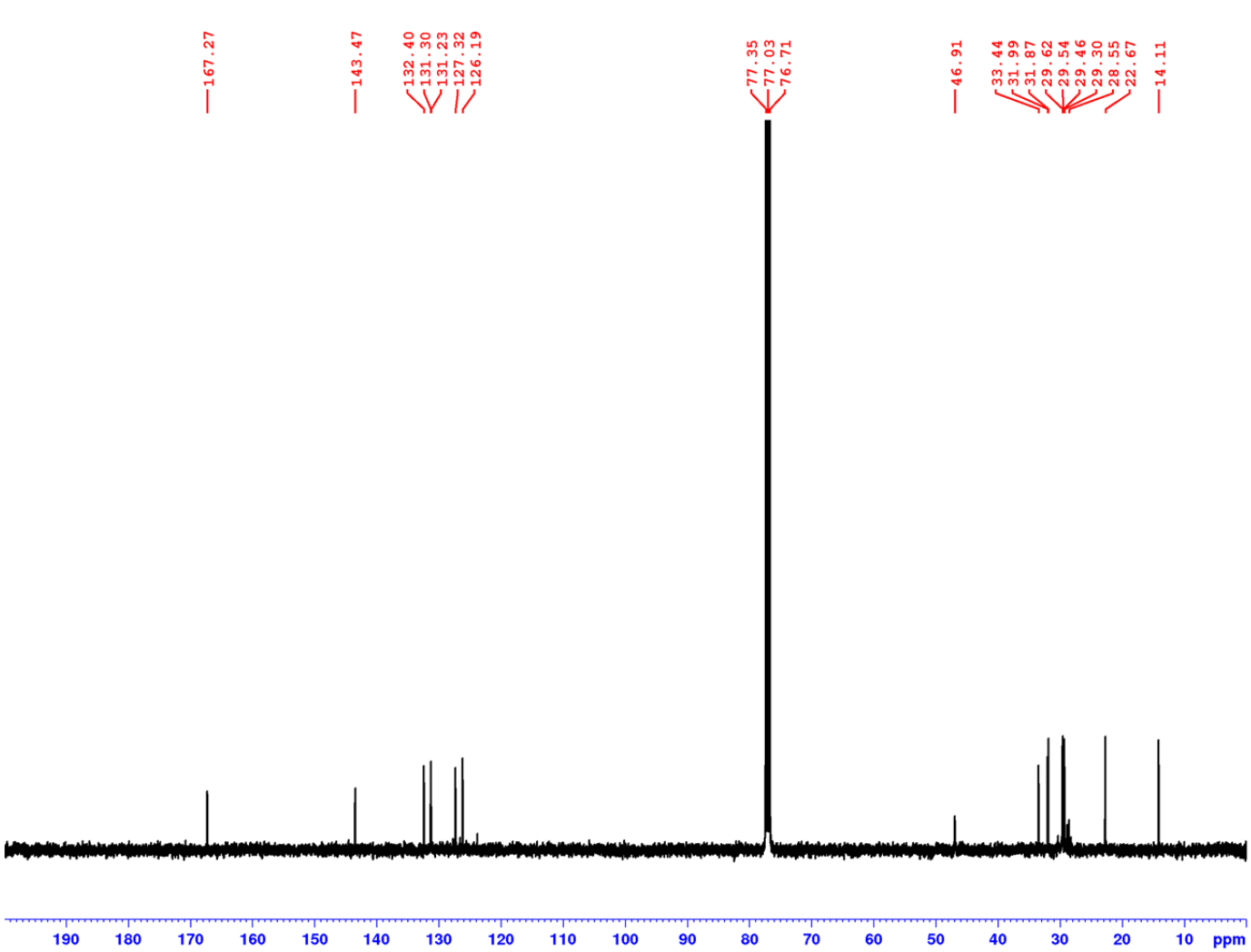
BRUKER

```
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
```



BRUKER

```
Current Data Parameters
NAME                 4I347802
EXPNO                      10
PROCNO                      1

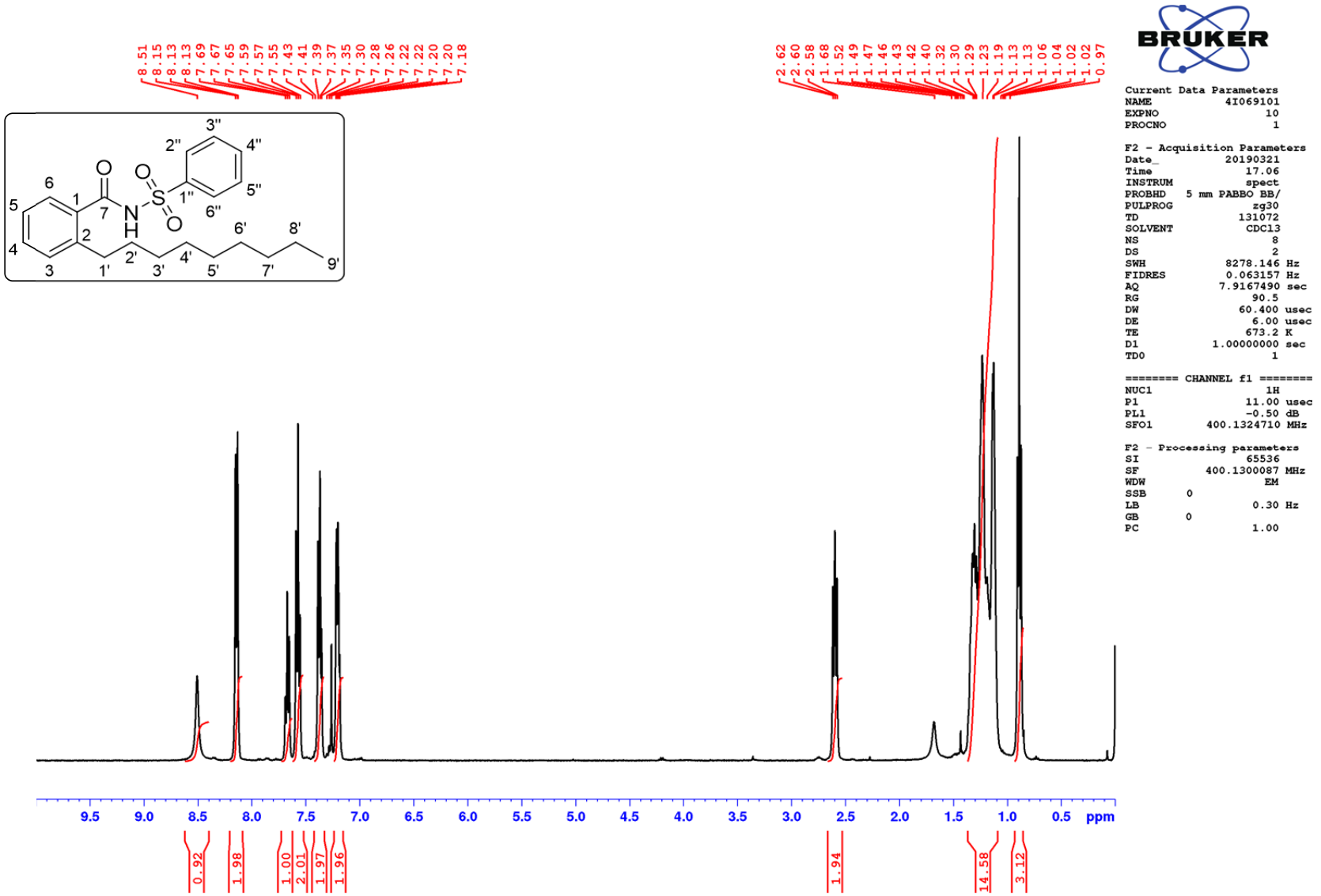
F2 - Acquisition Parameters
Date_               20191105
Time                   22.12
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                  131072
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH                23980.814 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)



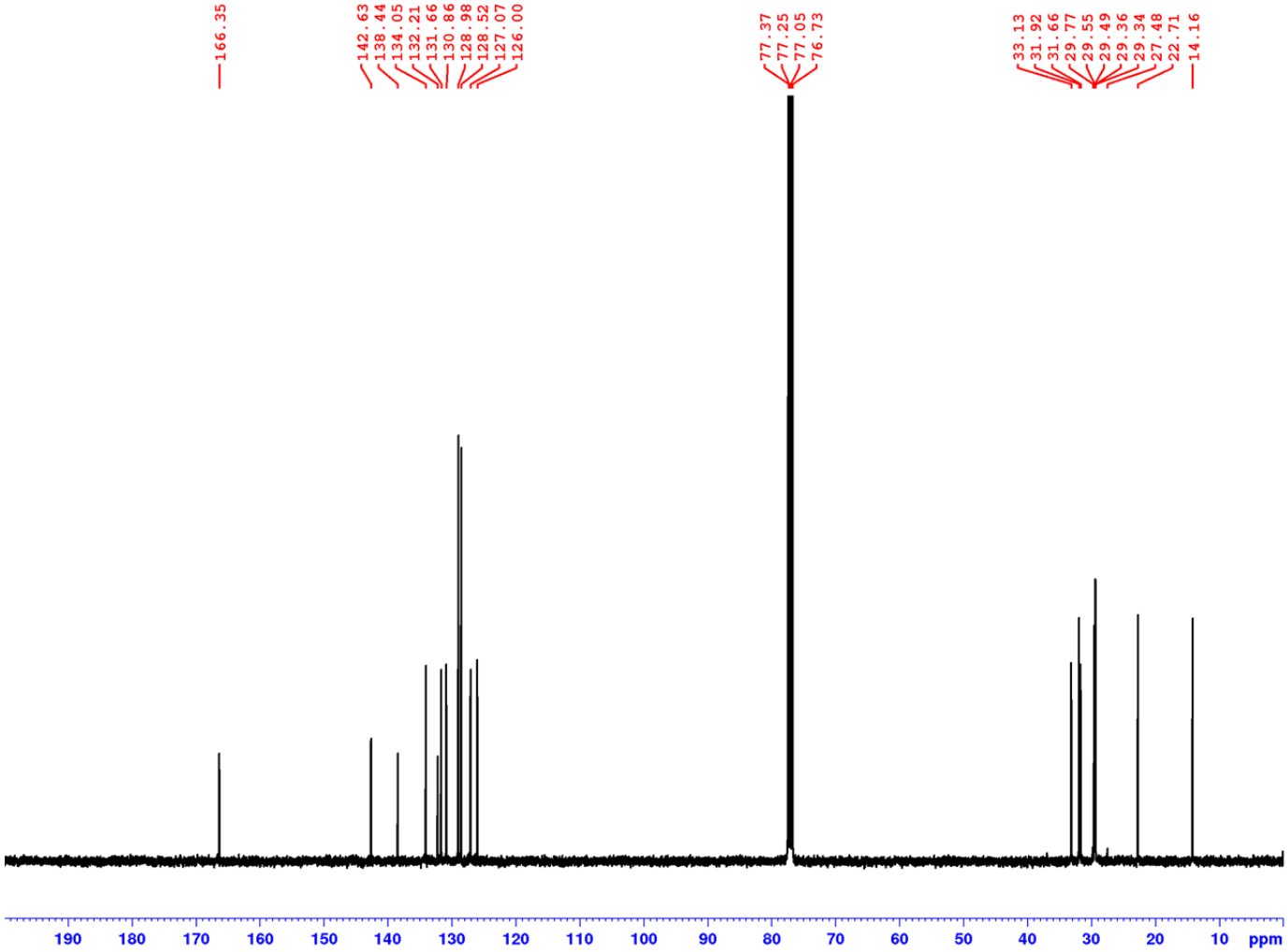
BRUKER

```
Current Data Parameters
NAME                 4I069101
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
```



BRUKER

```
Current Data Parameters
NAME                  4I069102
EXPNO                       10
PROCNO                       1

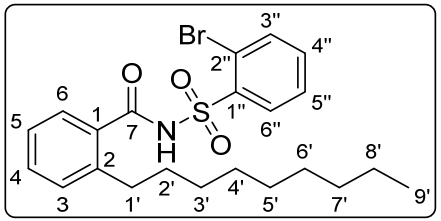
F2 - Acquisition Parameters
Date_                 20190323
Time                      4.32
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                      131072
SOLVENT                   CDCl3
NS                        1024
DS                           4
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 ========
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-(2-Bromobenzenesulfonyl)-2-nonylbenzamide (13)



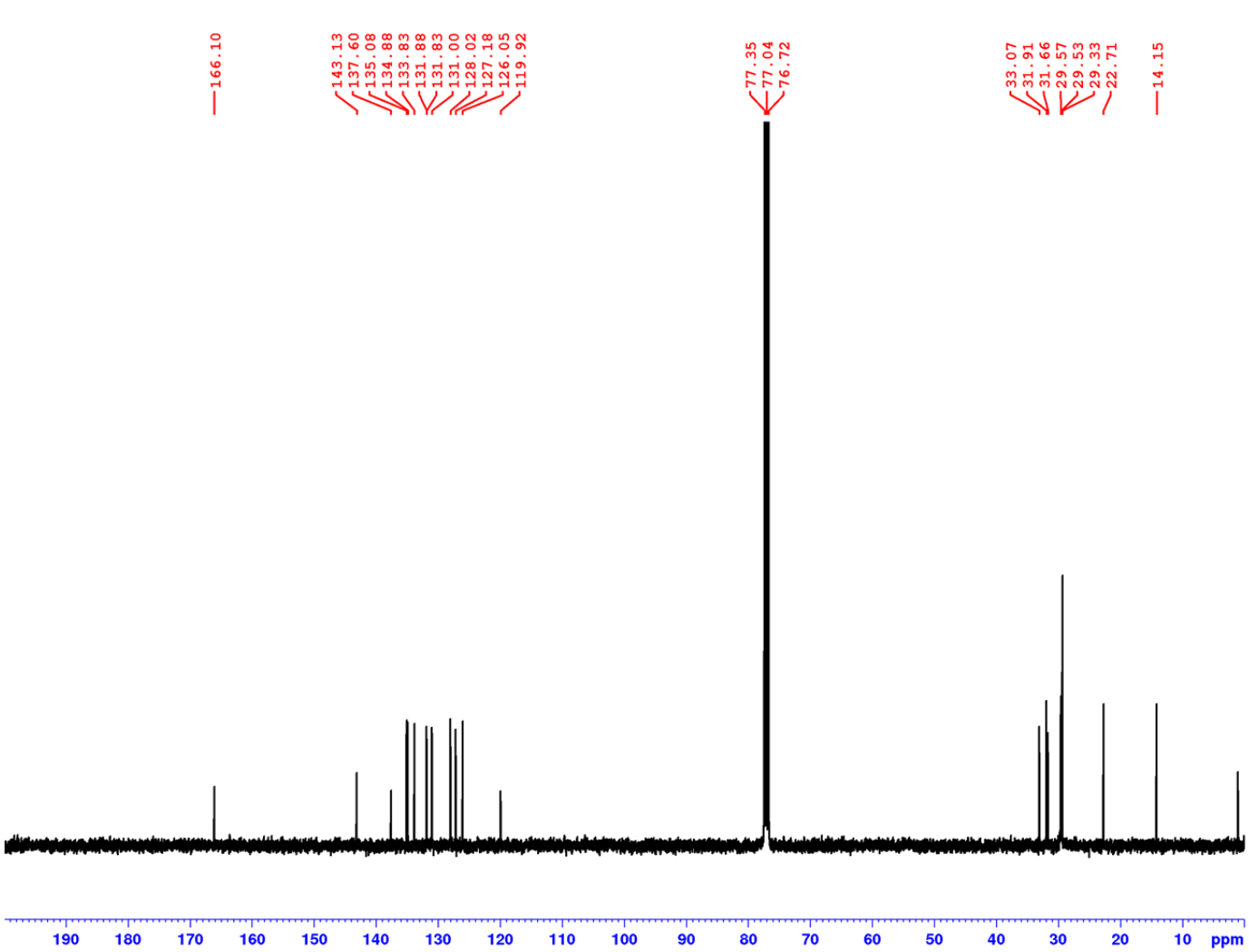
BRUKER

```
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
```



BRUKER

```
Current Data Parameters
NAME                  4H349502
EXPNO                       10
PROCNO                       1

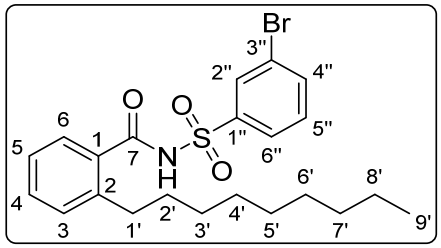
F2 - Acquisition Parameters
Date_                20181011
Time                     3.50
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                      131072
SOLVENT                  CDCl3
NS                        1024
DS                           4
SWH                  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 ========
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-Bromobenzenesulfonyl)-2-nonylbenzamide (14)



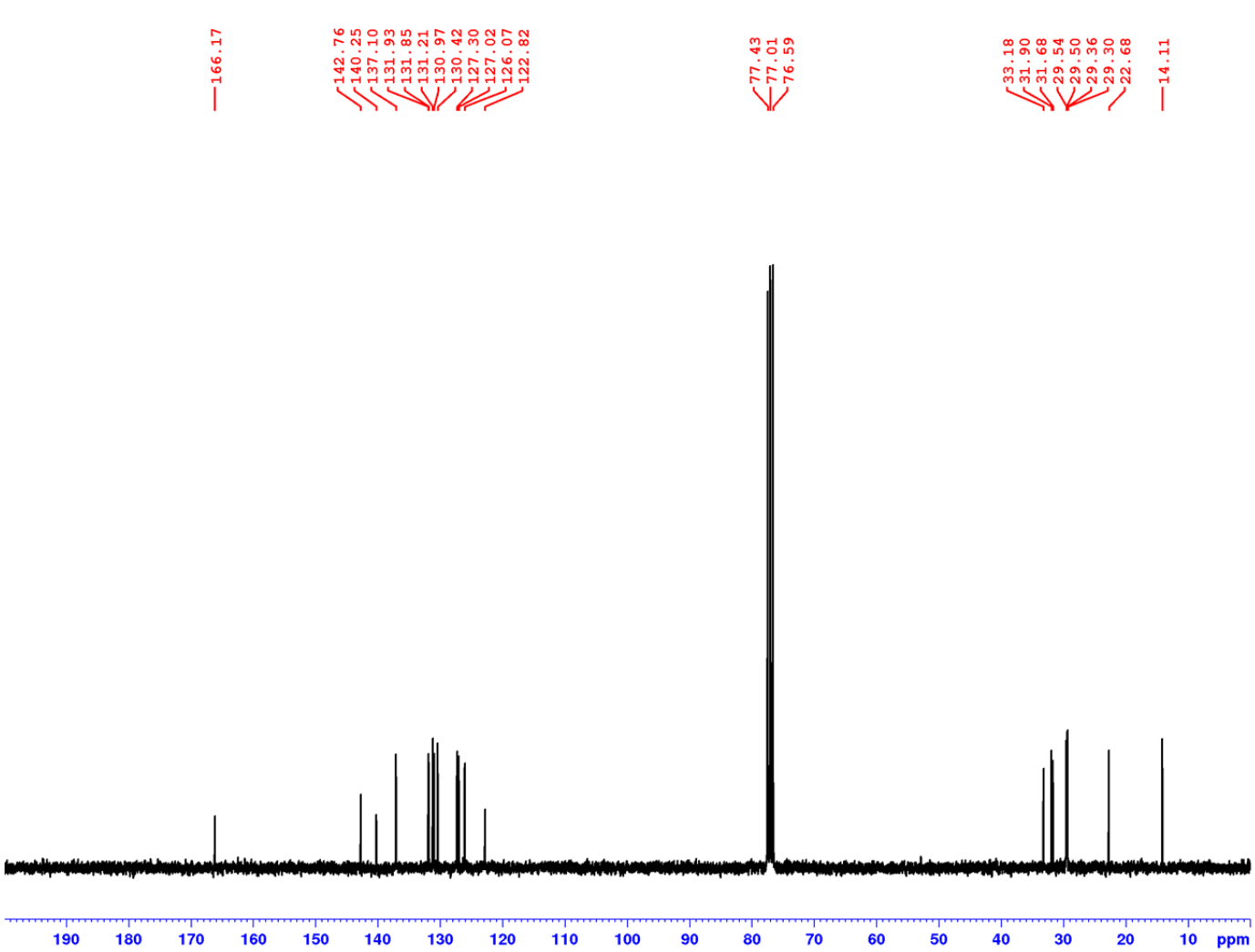
BRUKER

```
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
```



BRUKER

```
Current Data Parameters
NAME                  W334602
EXPNO                      10
PROCNO                      1

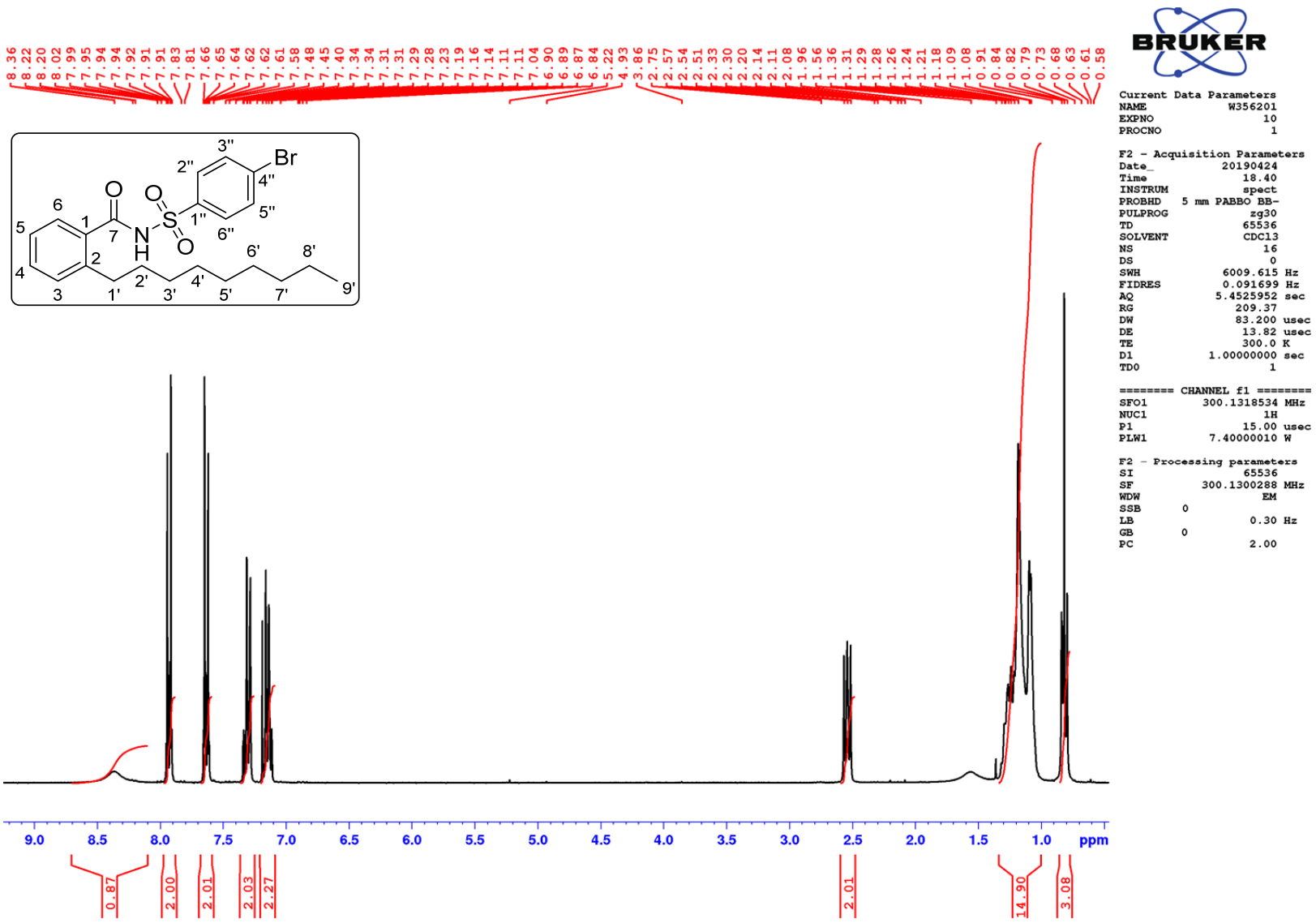
F2 - Acquisition Parameters
Date_               20190419
Time                    5.39
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1024
DS                          4
SWH                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
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-Bromobenzene)sulfonyl)-2-nonylbenzamide (15)



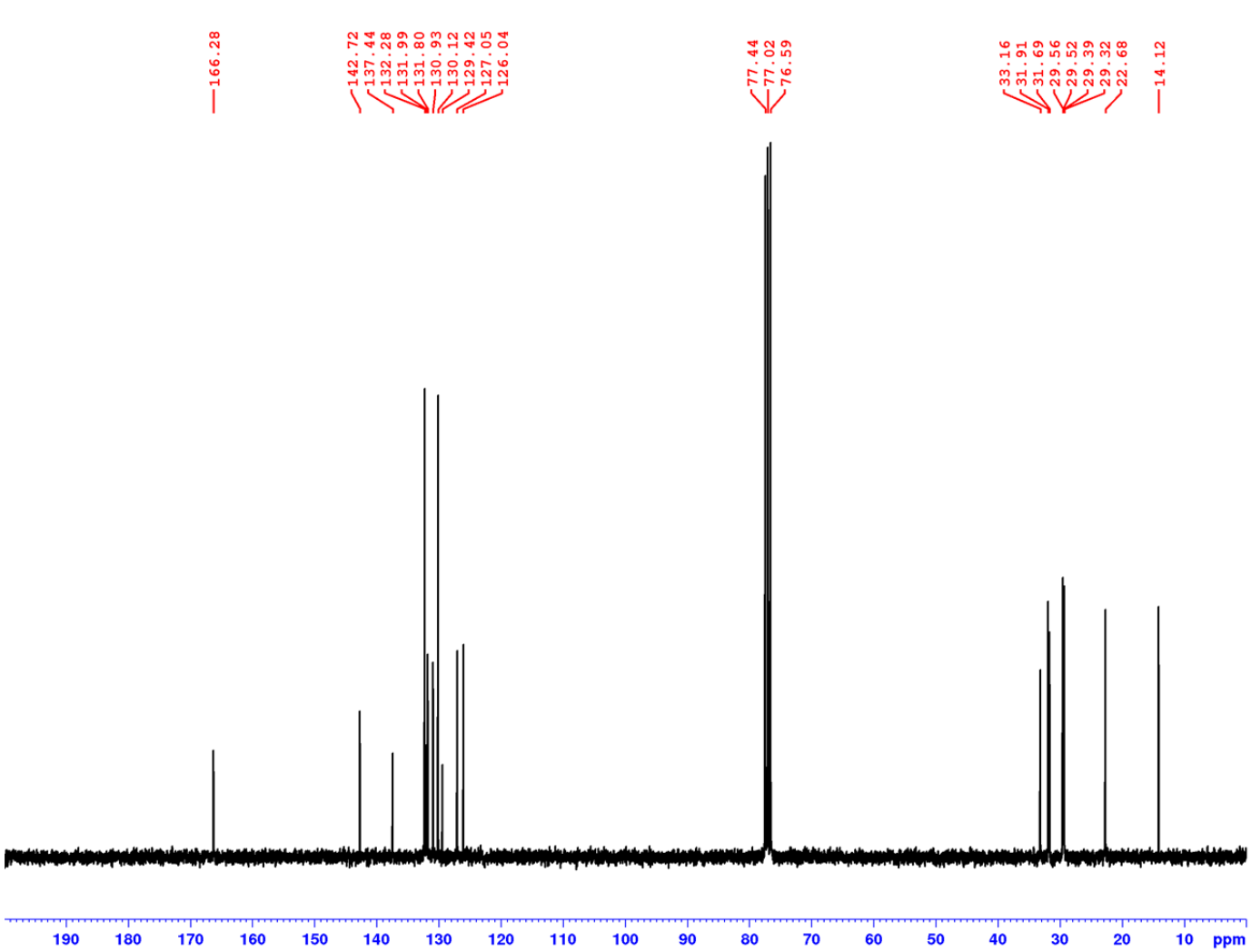
BRUKER

```
Current Data Parameters
NAME                  W356201
EXPNO                      10
PROCNO                      1

F2 - Acquisition Parameters
Date_               20190424
Time                   18.40
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             300.1300288 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    2.00
```



BRUKER

```
Current Data Parameters
NAME                 W356202
EXPNO                     10
PROCNO                     1

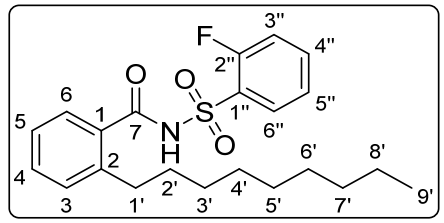
F2 - Acquisition Parameters
Date_              20190426
Time                   4.42
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               18115.941 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
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-(2-Fluorobenzenesulfonyl)-2-nonylbenzamide (16)

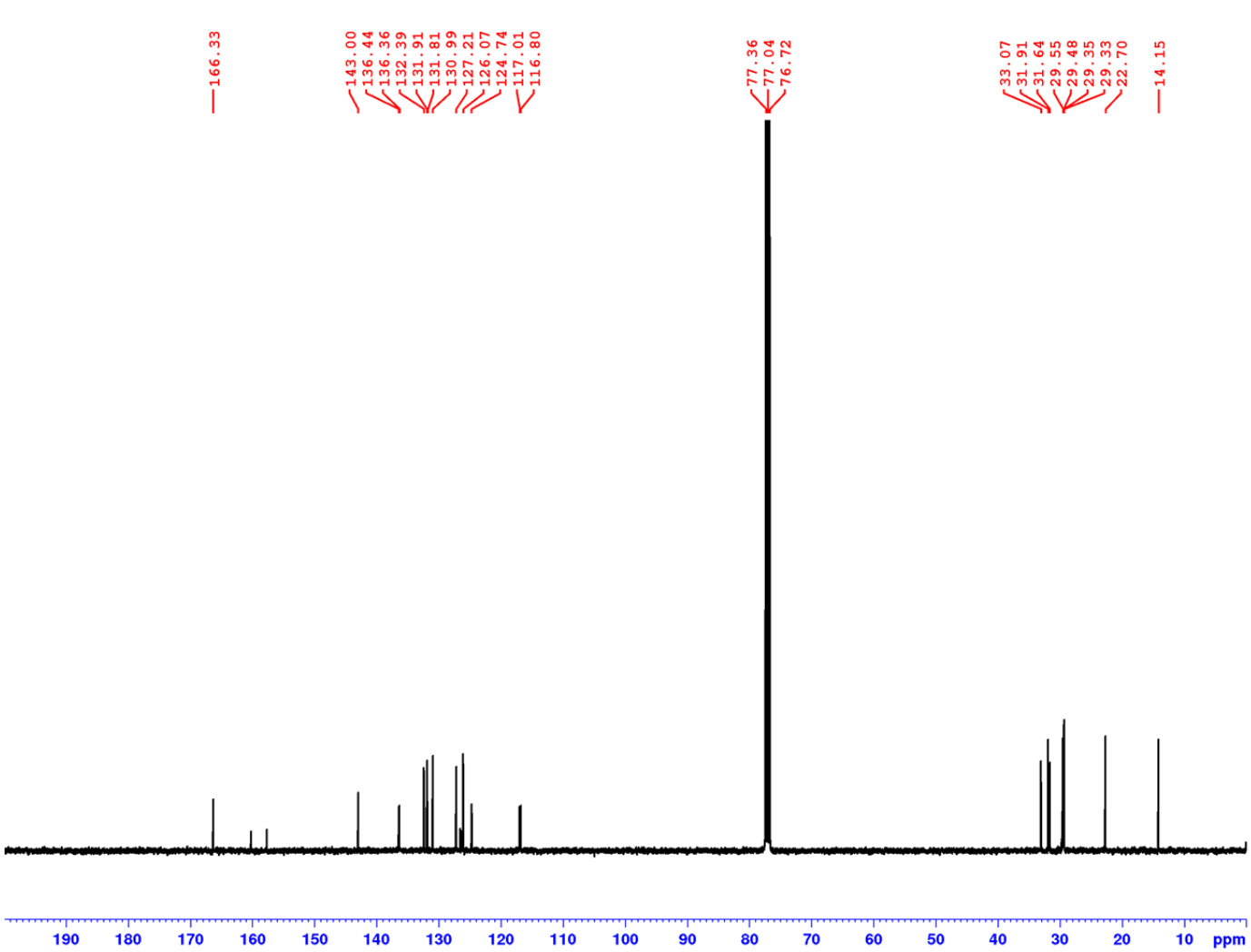



```
Current Data Parameters
NAME                  4I086101
EXPNO                       10
PROCNO                       1

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
```



BRUKER

```
Current Data Parameters
NAME                4I088102
EXPNO                     10
PROCNO                     1

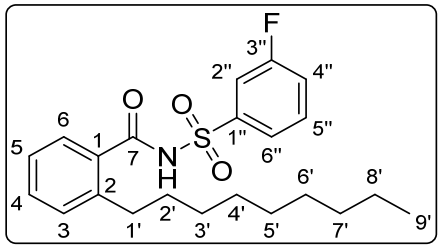
F2 - Acquisition Parameters
Date_              20190404
Time                  22.50
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                  131072
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               23980.814 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)

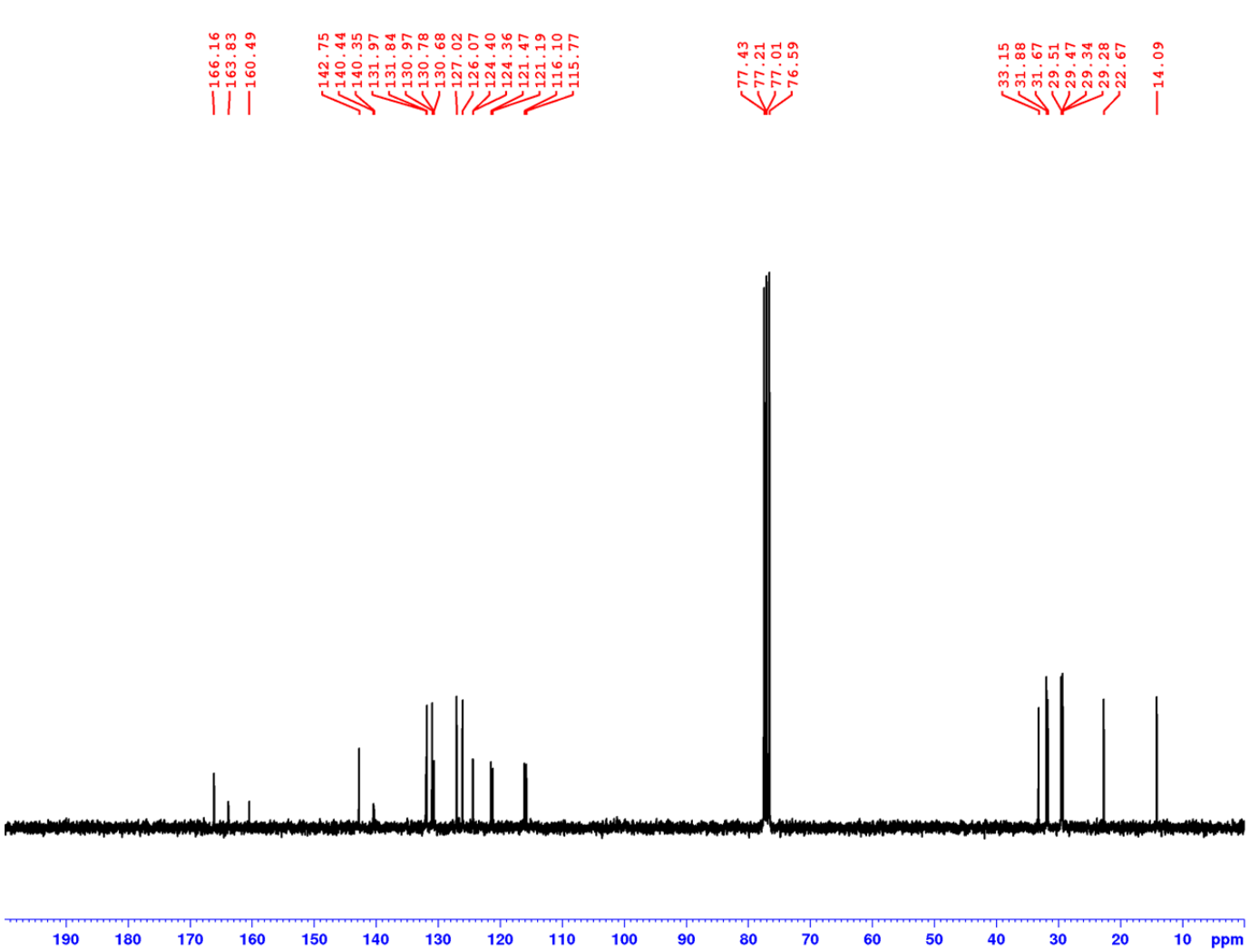



```
Current Data Parameters
NAME                  W303601
EXPNO                      10
PROCNO                      1

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
```



BRUKER

```
Current Data Parameters
NAME                  W303602
EXPNO                      10
PROCNO                      1

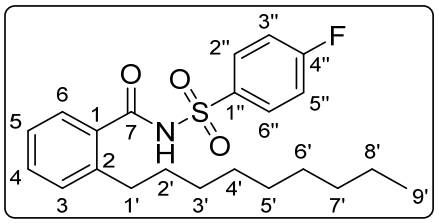
F2 - Acquisition Parameters
Date_               20190404
Time                   23.25
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               18115.941 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
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-Fluorobenzenesulfonyl)-2-nonylbenzamide (18)



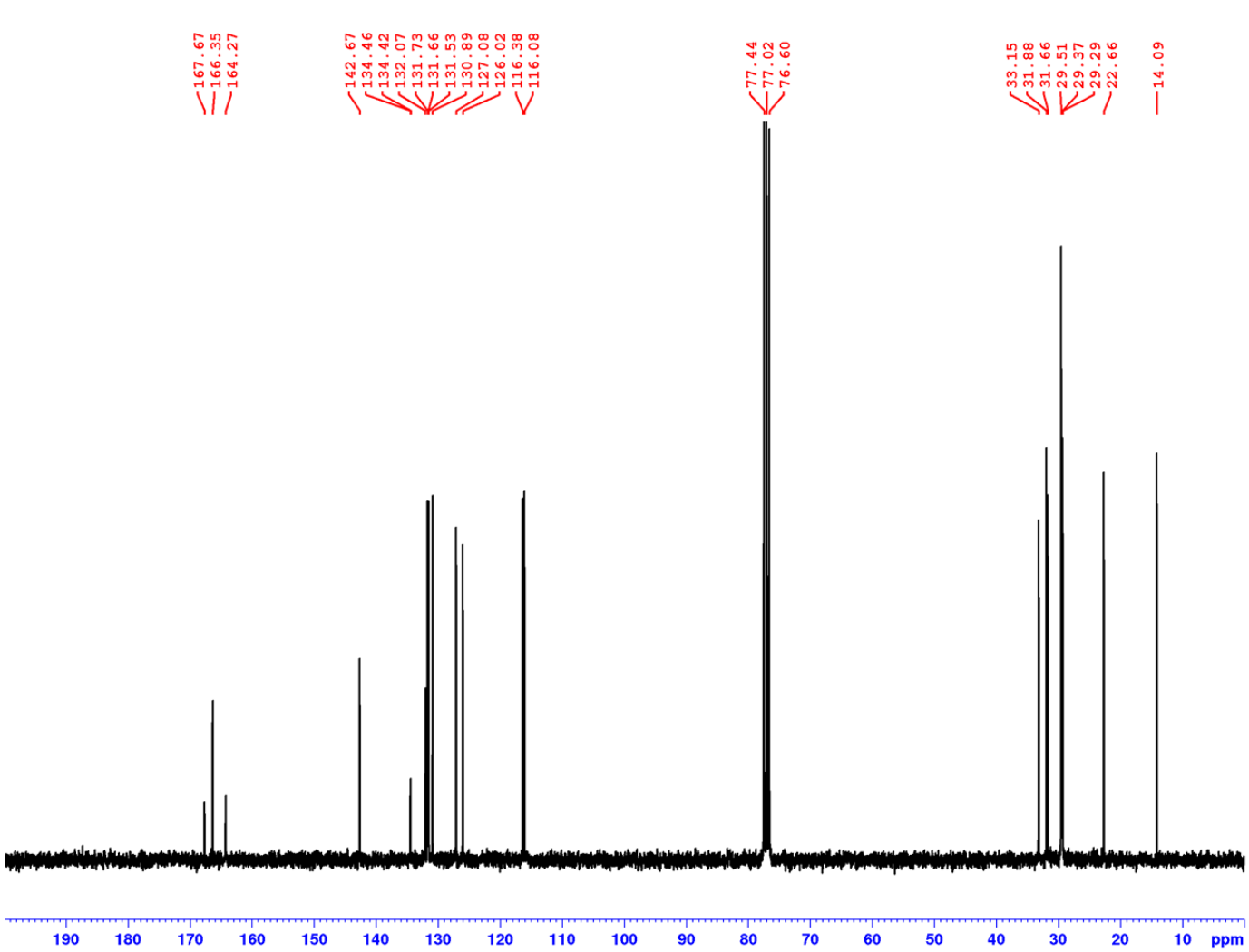
BRUKER

```
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
```



BRUKER

```
Current Data Parameters
NAME                  W313802
EXPNO                      10
PROCNO                      1

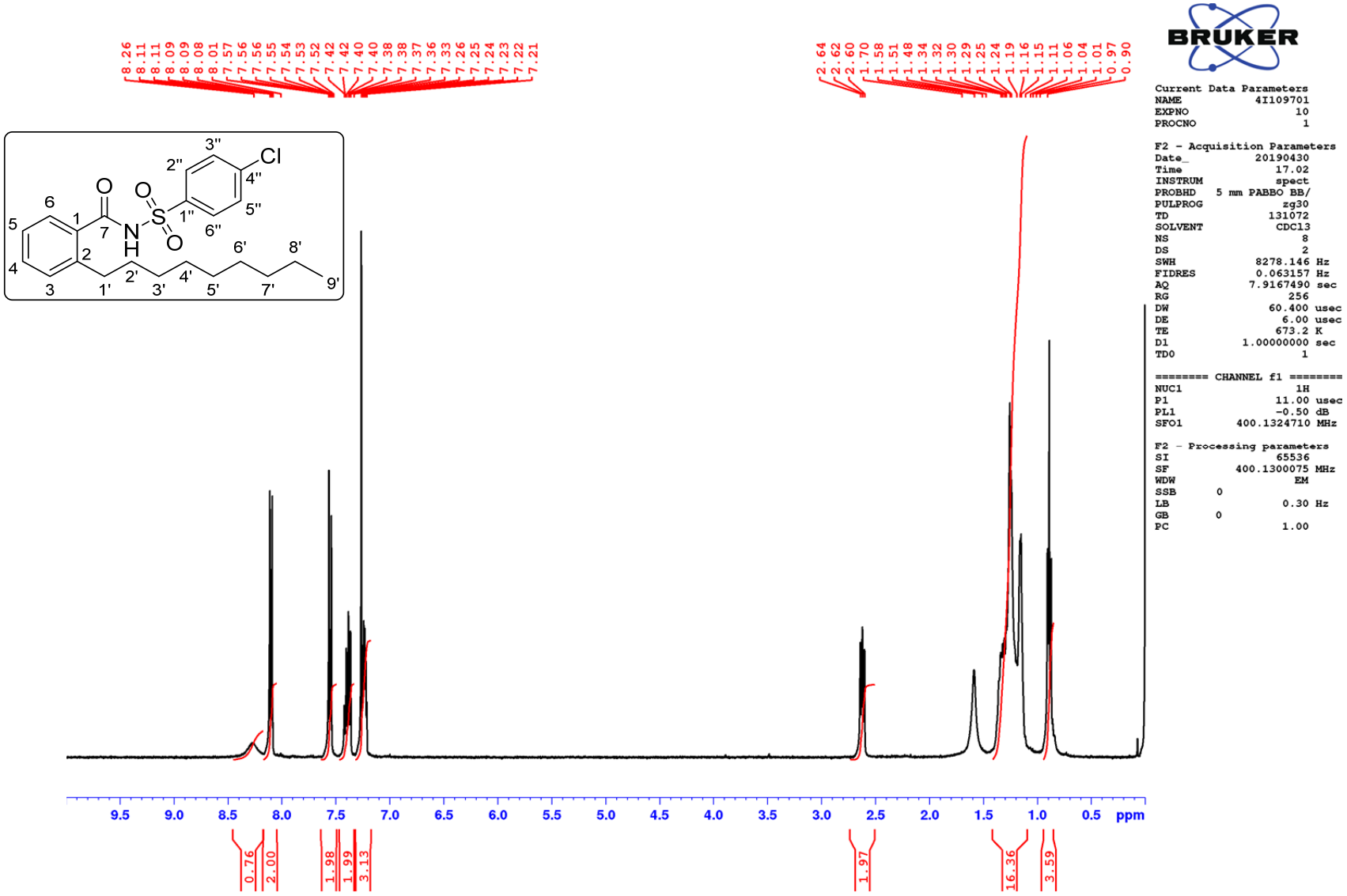
F2 - Acquisition Parameters
Date_               20190410
Time                    4.00
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1024
DS                          4
SWH                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
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-Chlorobenzenesulfonyl)-2-nonylbenzamide (19)



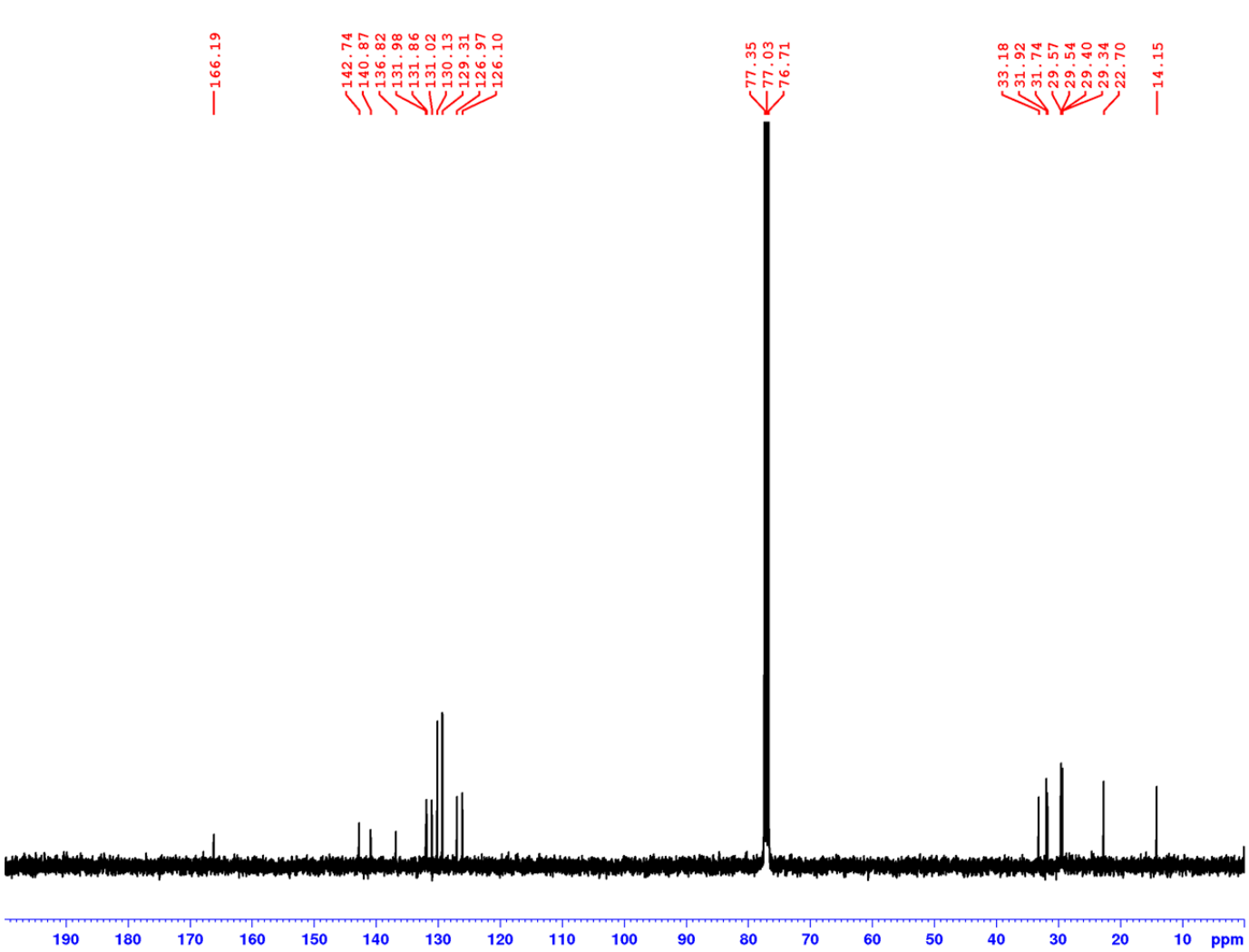
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```
Current Data Parameters
NAME                  4I109701
EXPNO                       10
PROCNO                       1

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
```



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```
Current Data Parameters
NAME                  4I109702
EXPNO                       10
PROCNO                       1

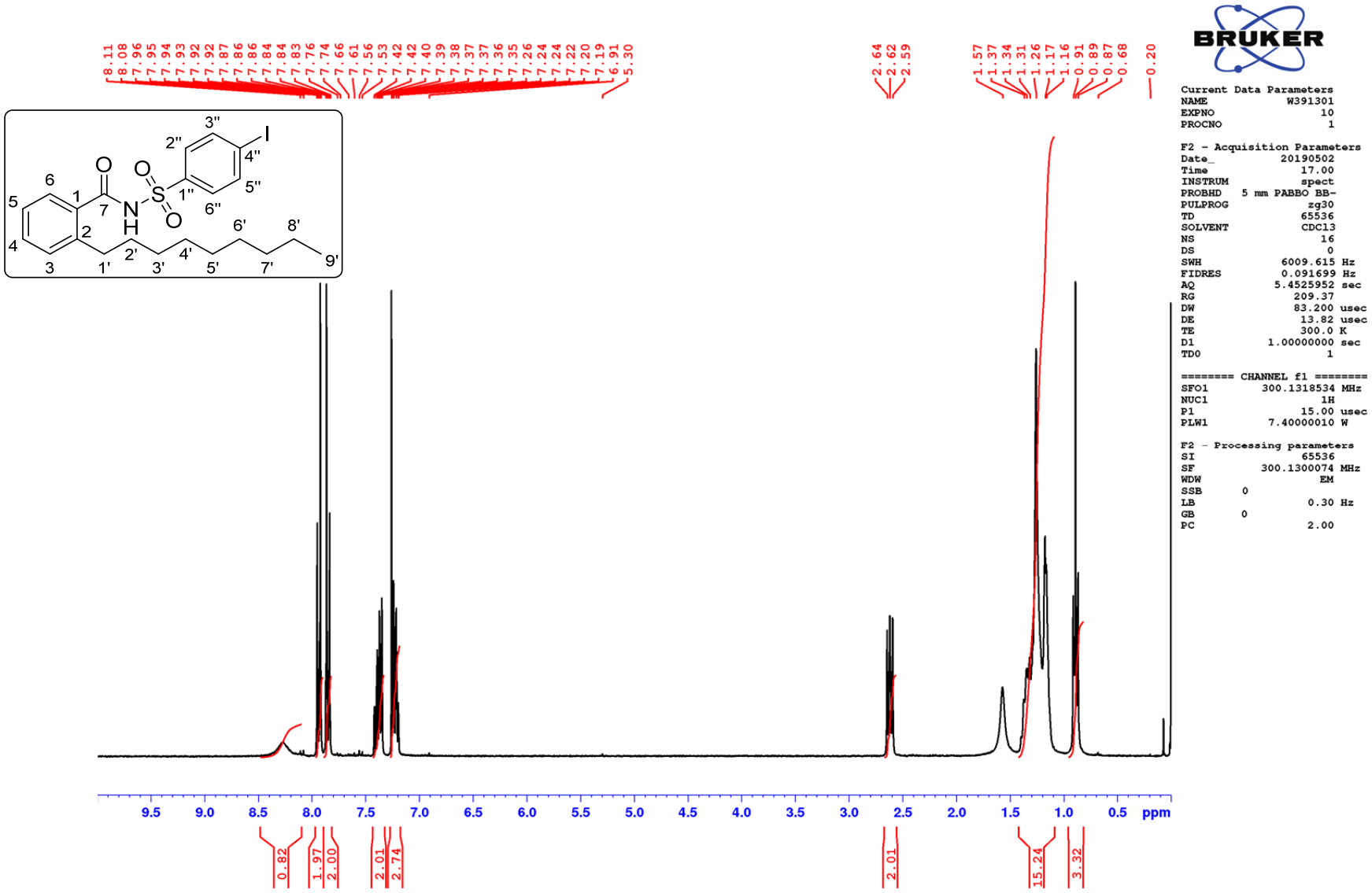
F2 - Acquisition Parameters
Date_               20190430
Time                    22.13
INSTRUM                 spect
PROBHD   5 mm PABBO BB/
PULPROG                 zgpg30
TD                      131072
SOLVENT                 CDCl3
NS                        1024
DS                           4
SWH                 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 ========
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-(4-Iodobenzenesulfonyl)-2-nonylbenzamide (20)

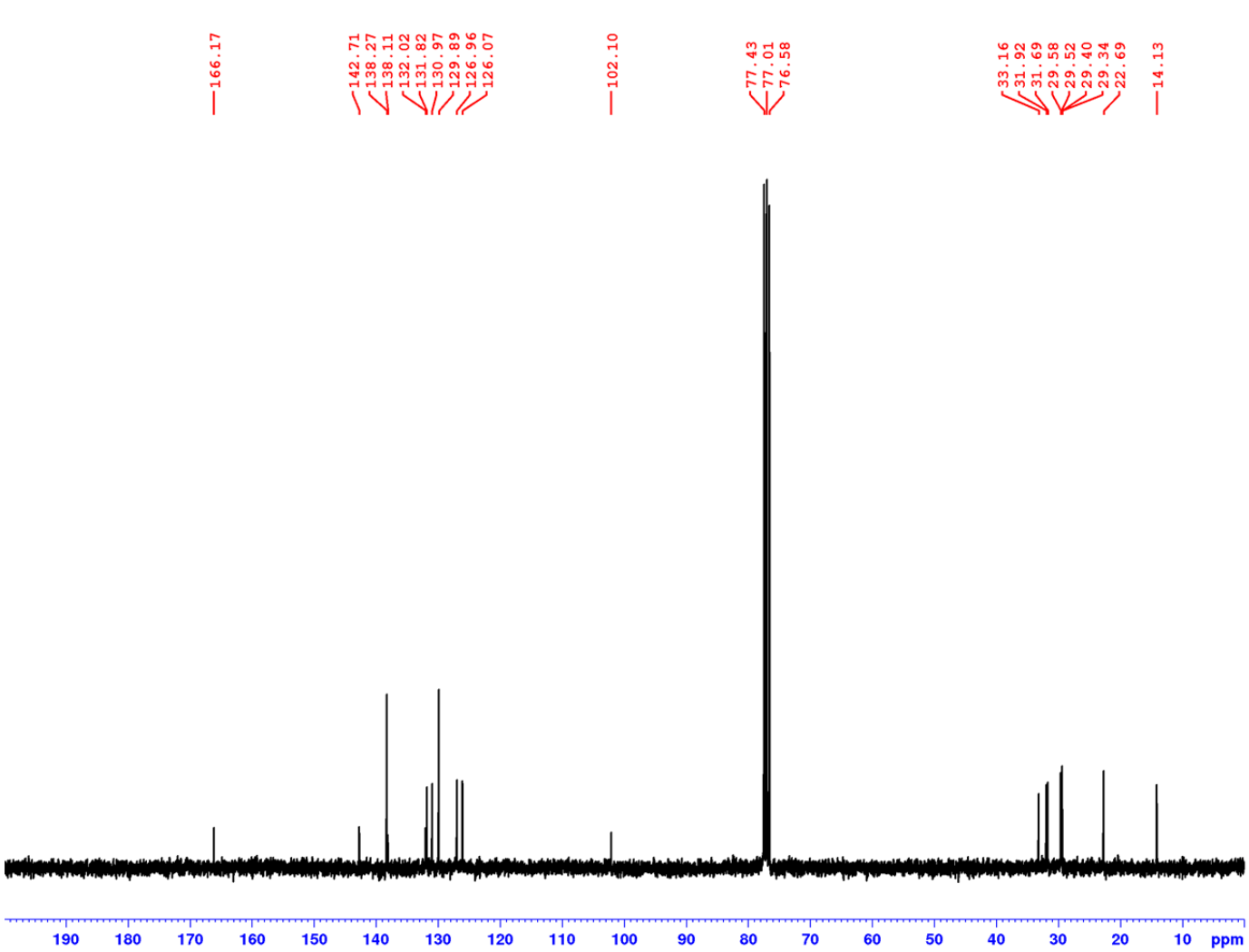



```
Current Data Parameters
NAME                  W391301
EXPNO                      10
PROCNO                      1

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
```



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```
Current Data Parameters
NAME                  W391302
EXPNO                      10
PROCNO                      1

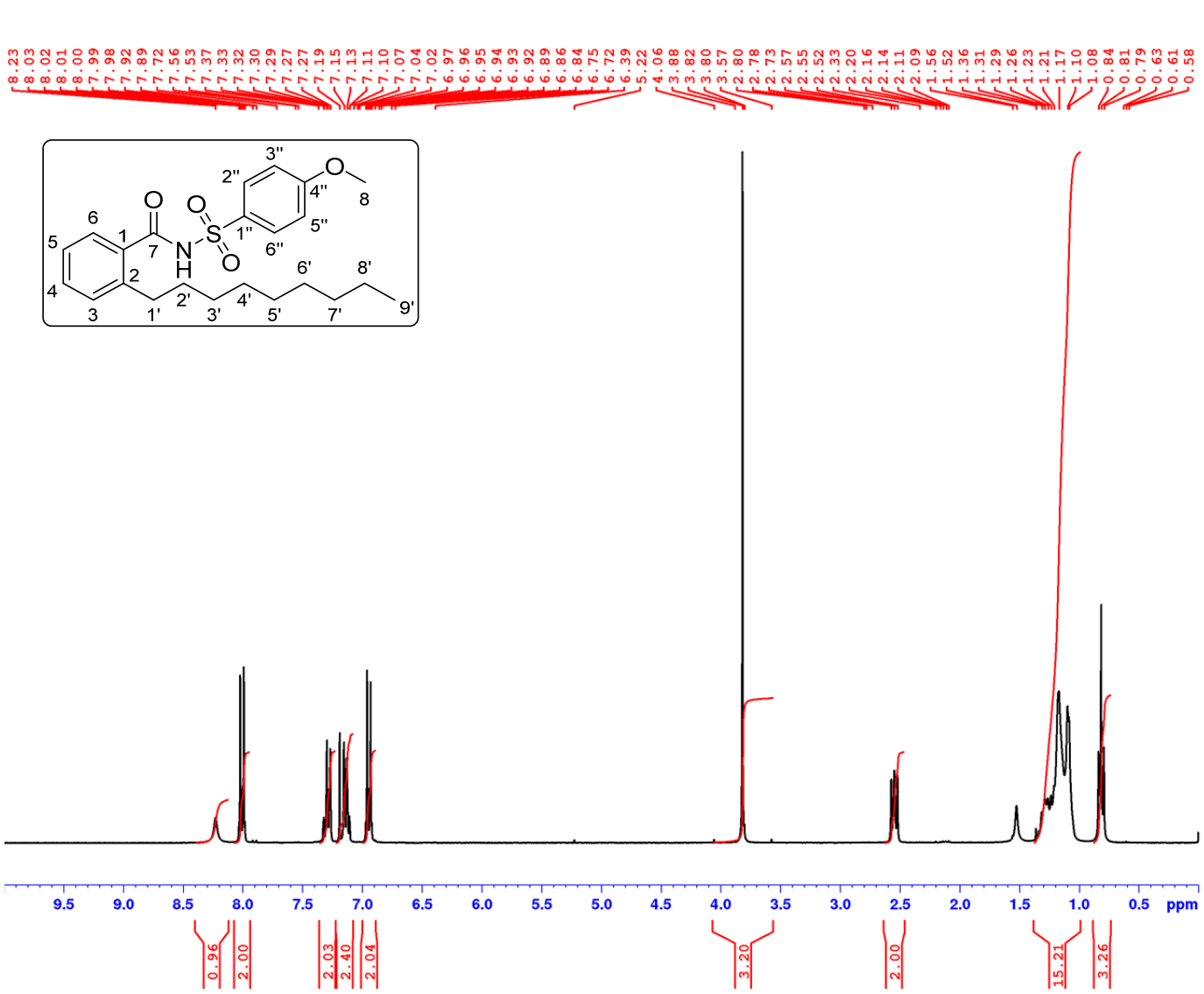
F2 - Acquisition Parameters
Date_                20190507
Time                     1.59
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1024
DS                          4
SWH                 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
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-Methoxybenzenesulfonyl)-2-nonylbenzamide (21)

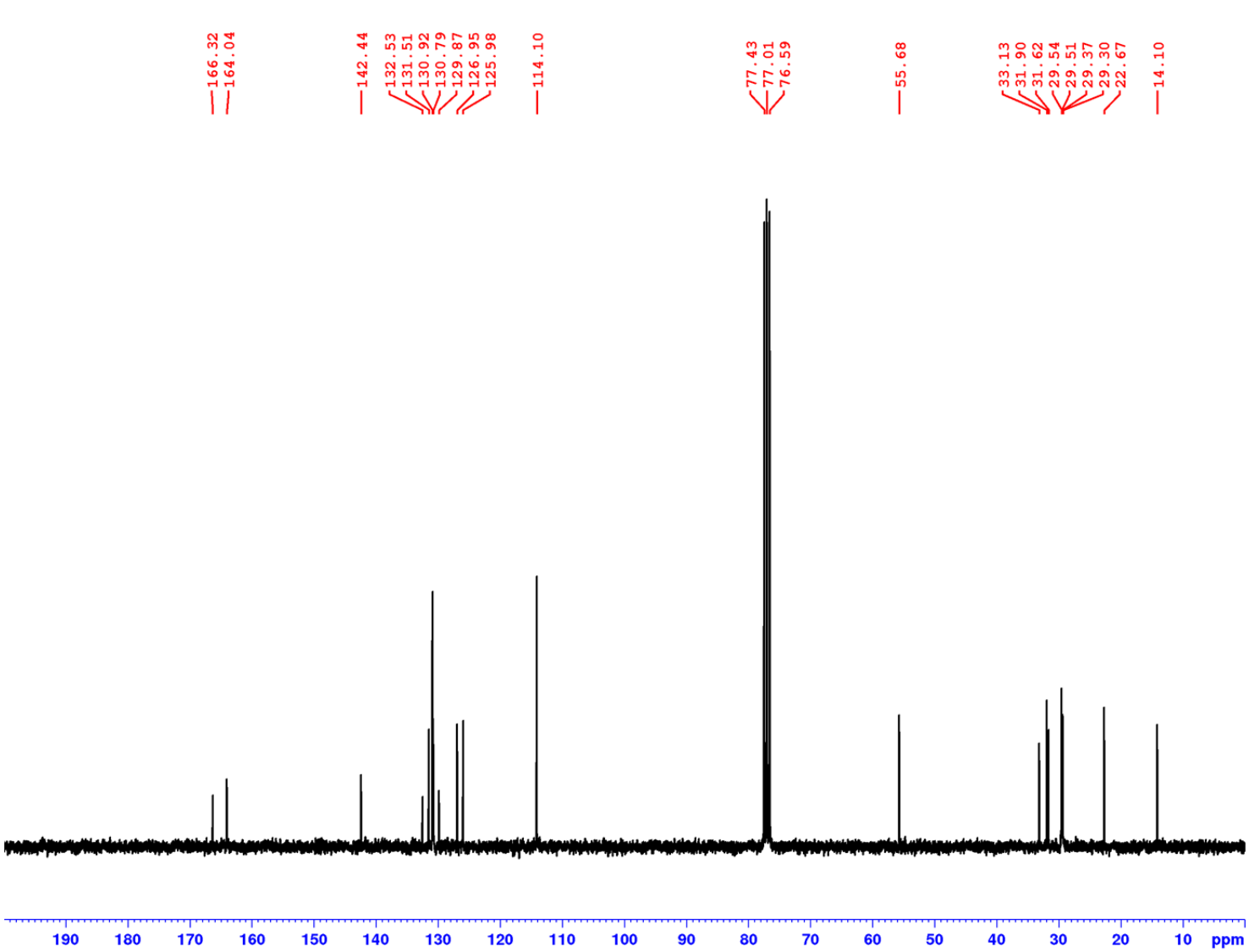



```
Current Data Parameters
NAME                  W529601
EXPNO                      10
PROCNO                      1

F2 - Acquisition Parameters
Date_               20190606
Time                   18.42
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             300.1300284 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    2.00
```



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Current Data Parameters
NAME W529602
EXPNO 10
PROCNO 1

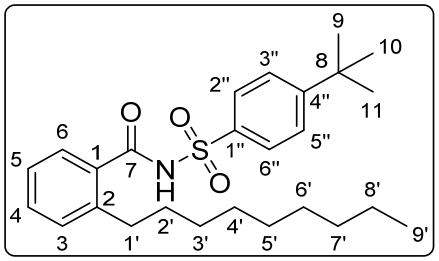
F2 - Acquisition Parameters
Date_ 20190607
Time 1.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 209.37
DW 27.600 usec
DE 11.35 usec
TE 300.0 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1

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

======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
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)

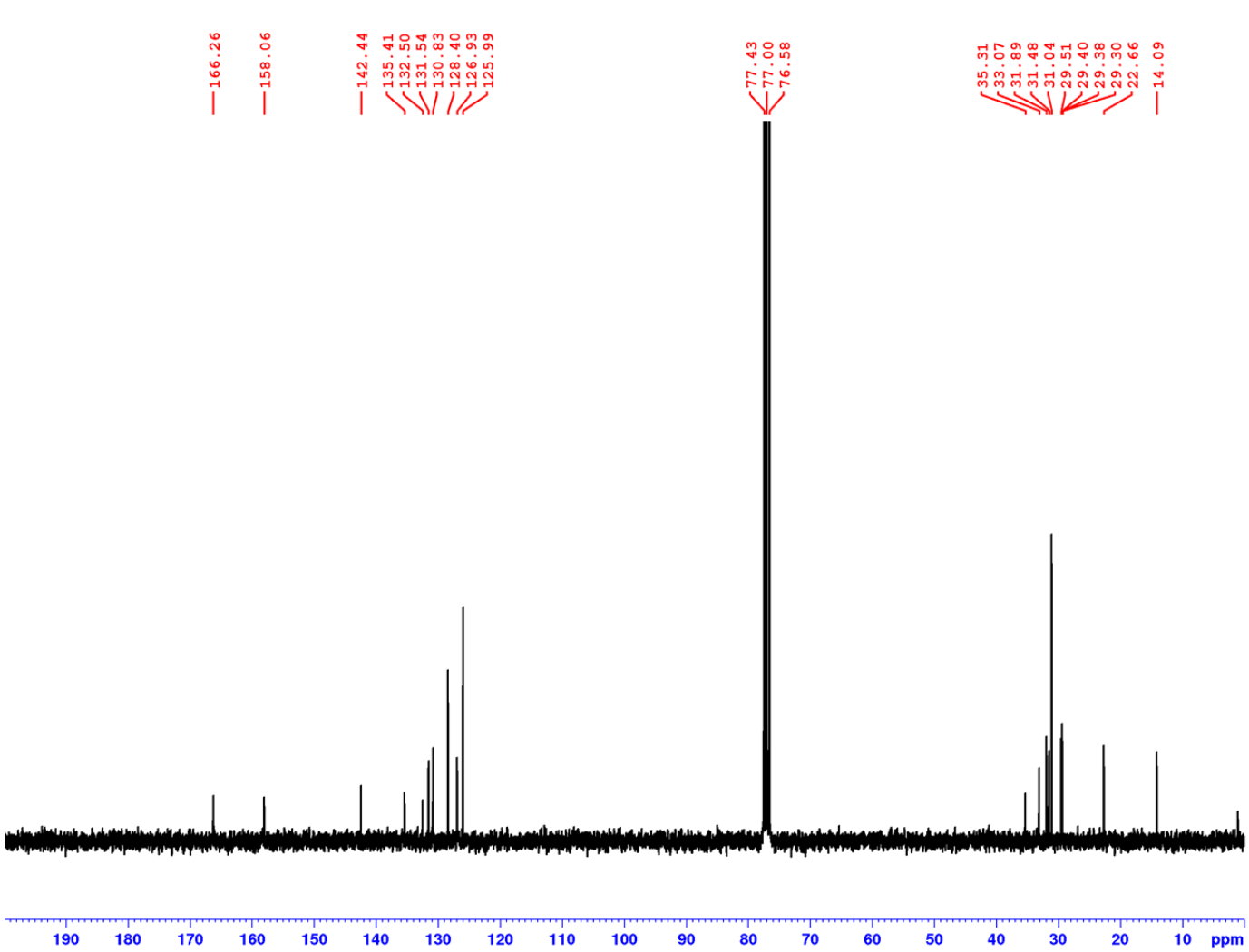



```
Current Data Parameters
NAME                  W529701
EXPNO                      10
PROCNO                      1

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
```



BRUKER

```
Current Data Parameters
NAME                 W529702
EXPNO                     10
PROCNO                     1

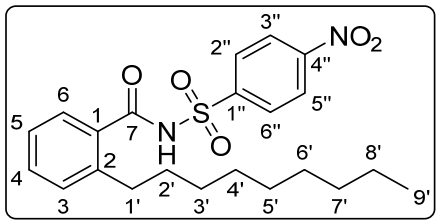
F2 - Acquisition Parameters
Date_              20190606
Time                  19.46
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               18115.941 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
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-Nitrobenzenesulfonyl)-2-nonylbenzamide (23)

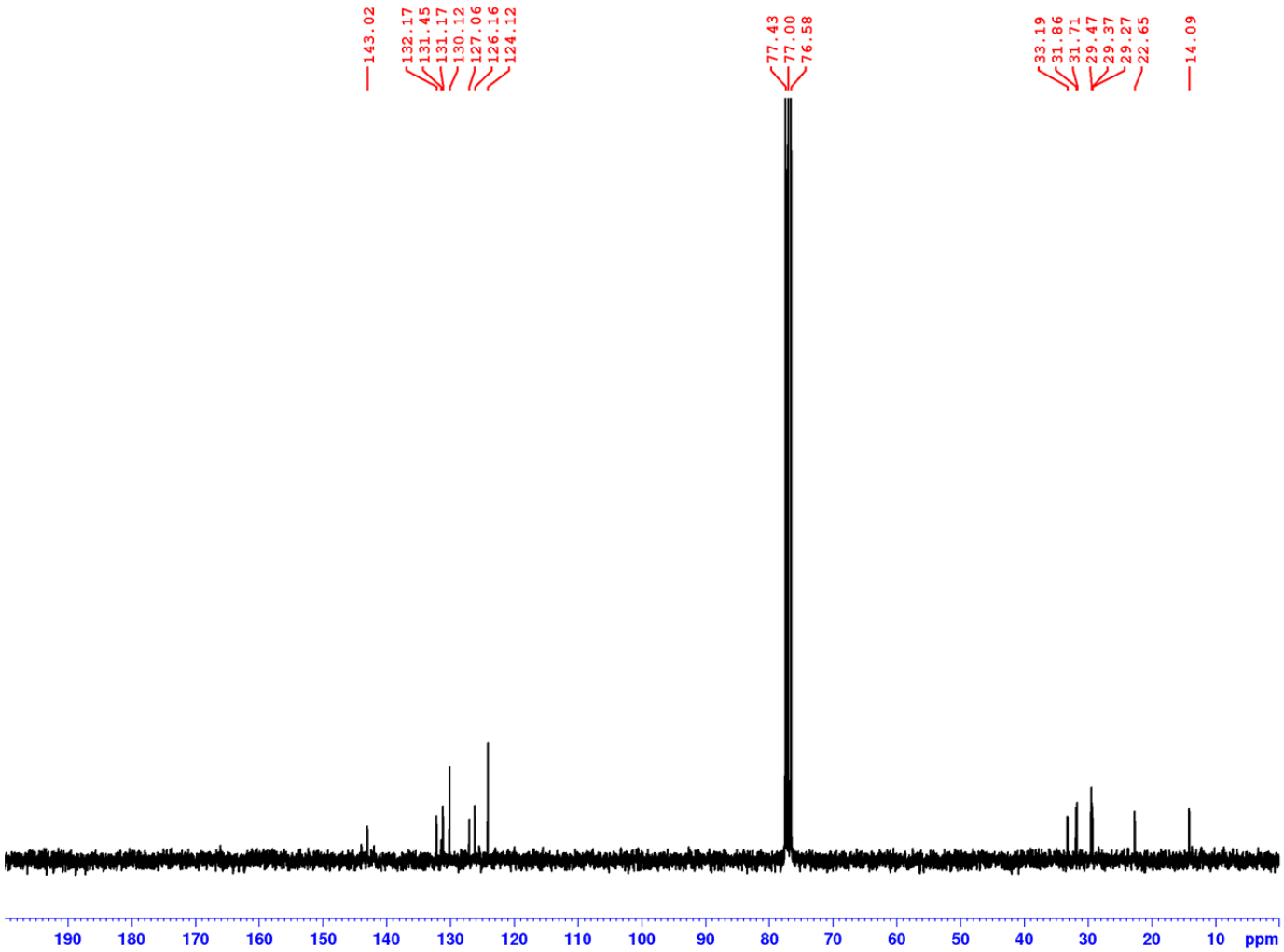



```
Current Data Parameters
NAME                  W634401
EXPNO                      10
PROCNO                      1

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
```



BRUKER

```
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                 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
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
```