BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Synthesis of β-triazolylenones via metal-free desulfonylative alkylation of *N*-tosyl-1,2,3-triazoles

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Beilstein J. Org. Chem. **2021,** *17,* 762–770. doi:10.3762/bjoc.17.66

Copies of NMR spectra

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Current Data Parameters
NAME      INN-SP-138-6ML-1H
EXPNO                    3
PROCNO                   1

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PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     20
DS                      2
SWH            10000.000 Hz
FIDRES          0.152588 Hz
AQ             3.2767999 sec
RG                134.65
DW                50.000 usec
DE                 6.50 usec
TE                294.9 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         500.1330885 MHz
NUC1                   1H
P1                  13.00 usec
PLW1         13.00000000 W

F2 - Processing parameters
SI                  65536
SF           500.1300118 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
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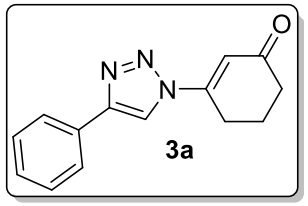

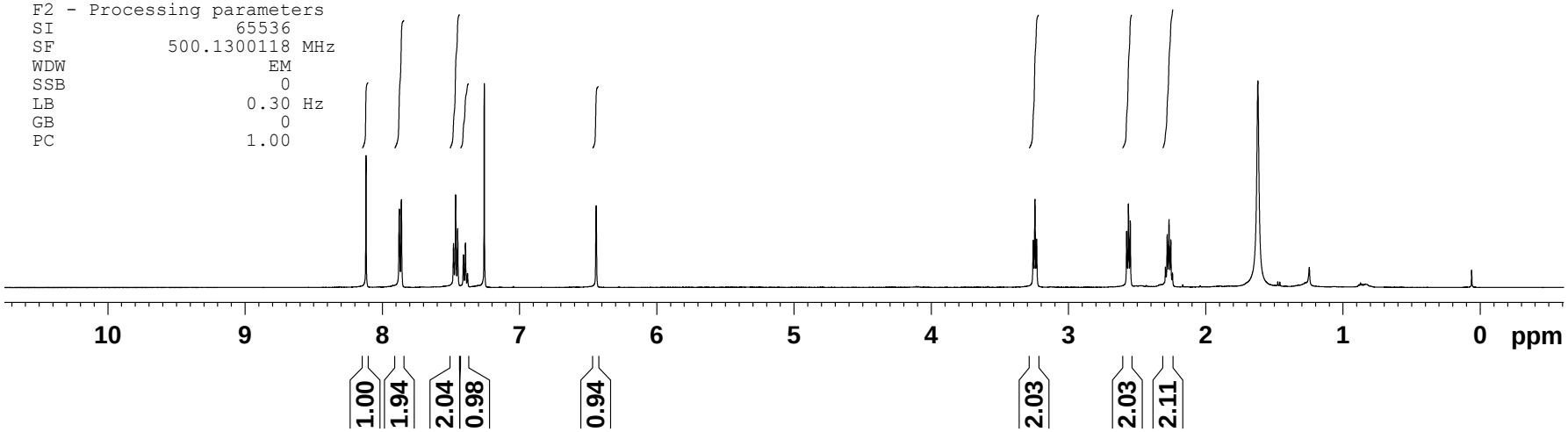

Figure S01: ^{1}H NMR spectrum of 3a.

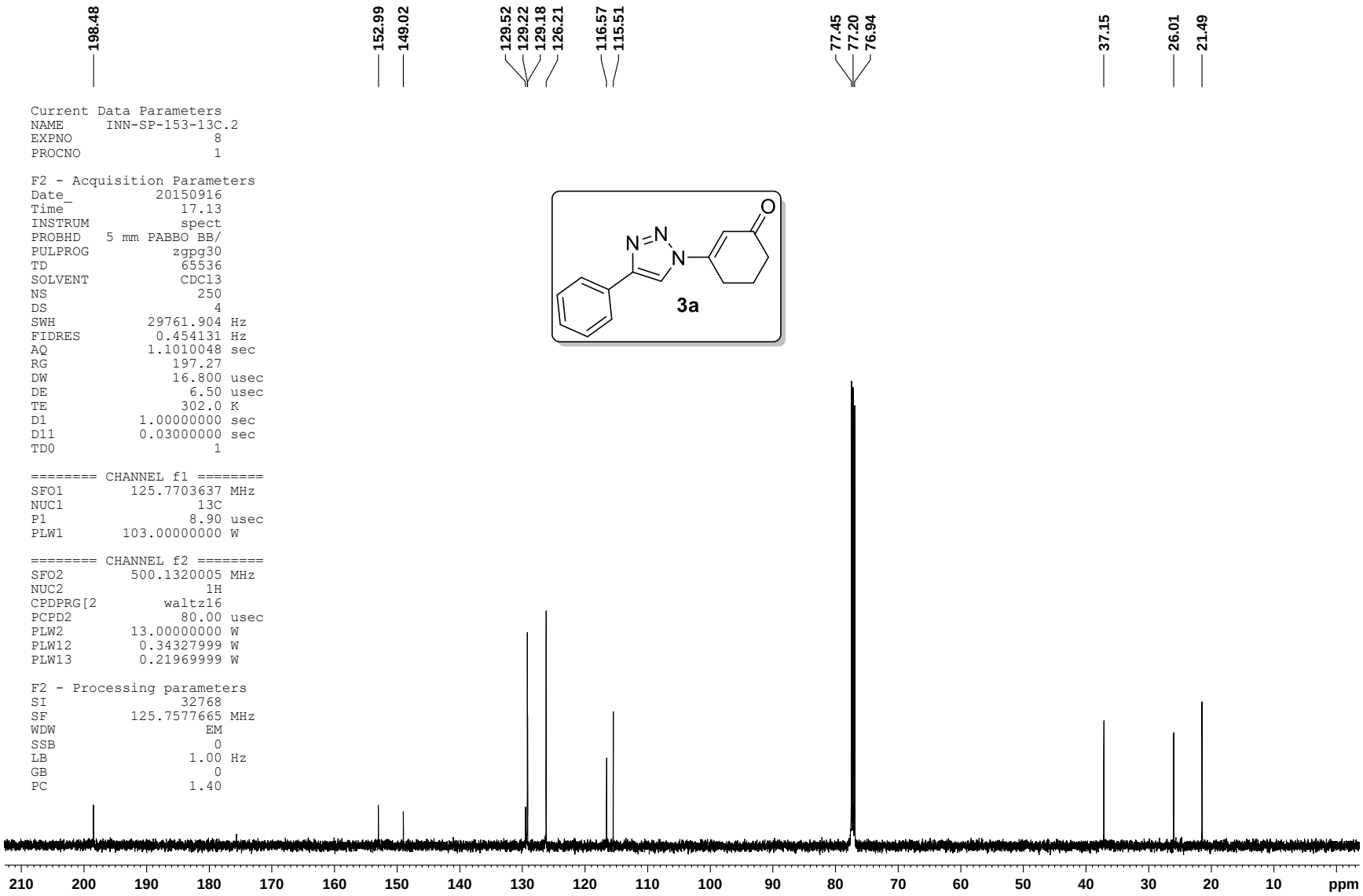

Figure S02: ^{13}C NMR spectrum of 3a.

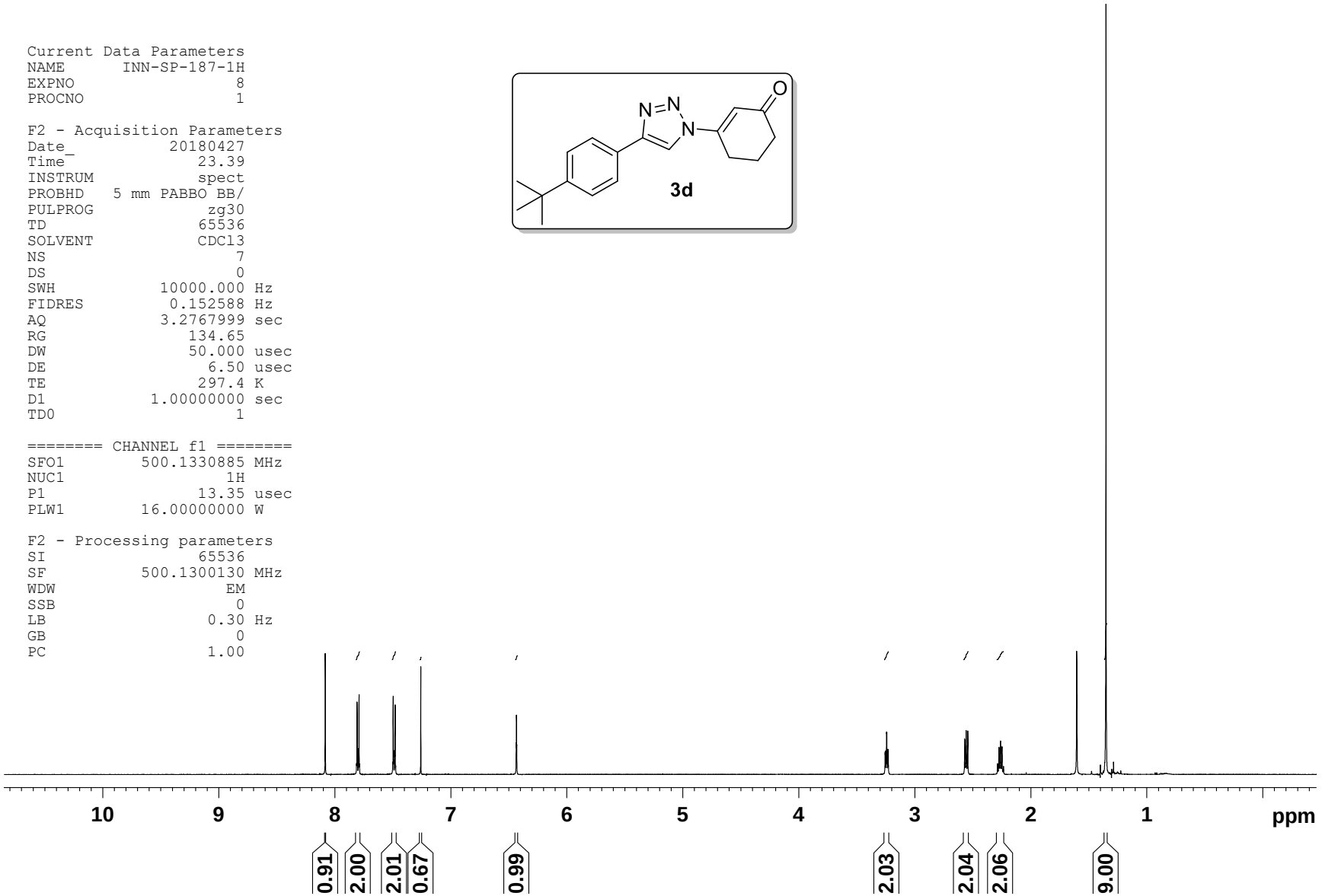

Figure S03: ^{1}H NMR spectrum of 3d.

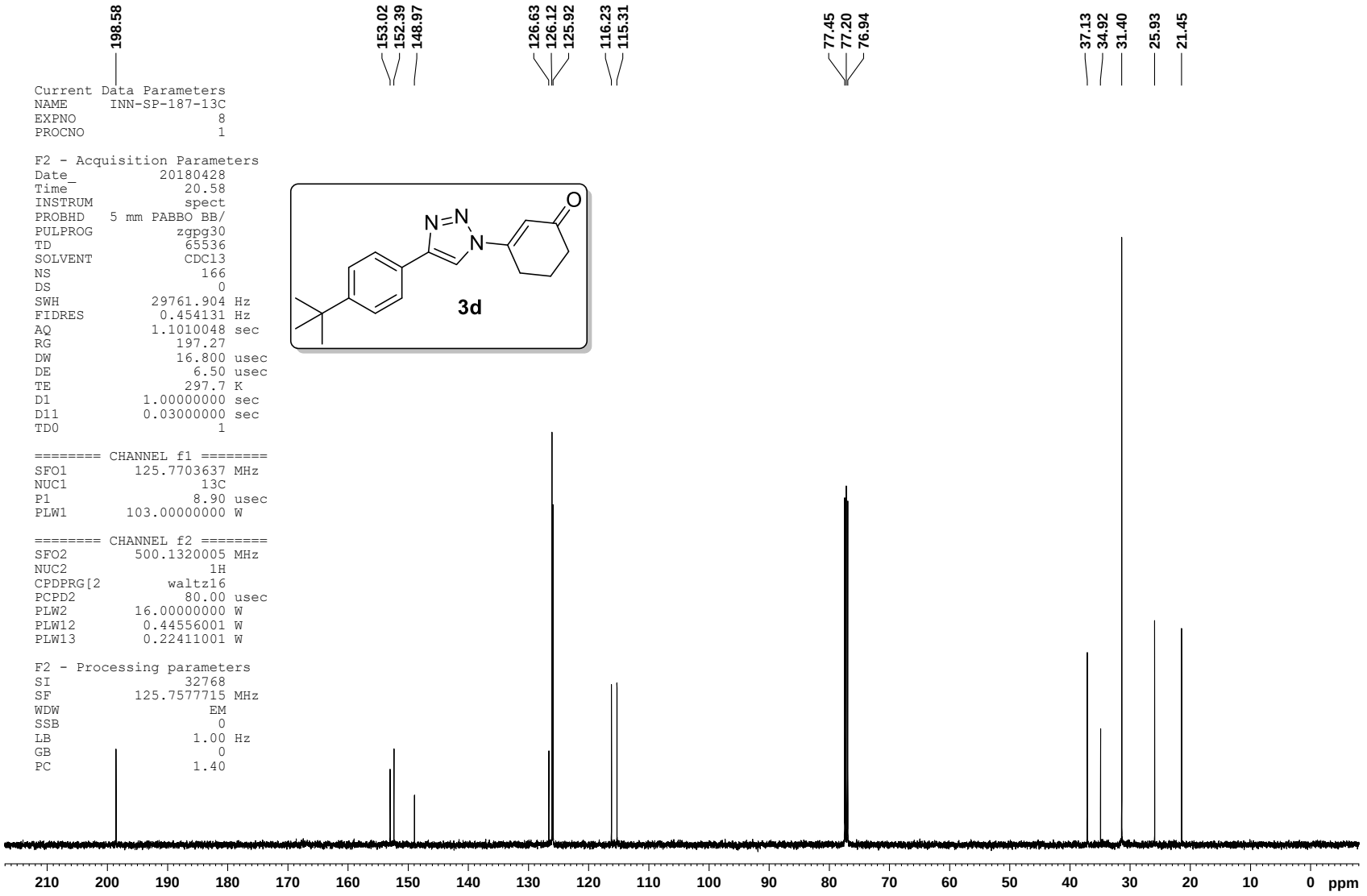

Figure S04: ^{13}C NMR spectrum of 3d.

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Current Data Parameters
NAME      INN-SP-161-1H
EXPNO                71
PROCNO                1

F2 - Acquisition Parameters
Date_           20151011
Time                7.43
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 54274
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8223.685 Hz
FIDRES          0.151522 Hz
AQ             3.2998593 sec
RG                   228
DW                60.800 usec
DE                 6.50 usec
TE                295.3 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.75 usec
PL1                -1.00 dB
PL1W        10.56200695 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300099 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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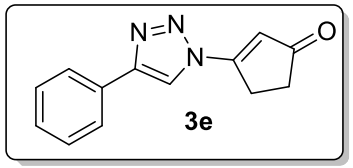

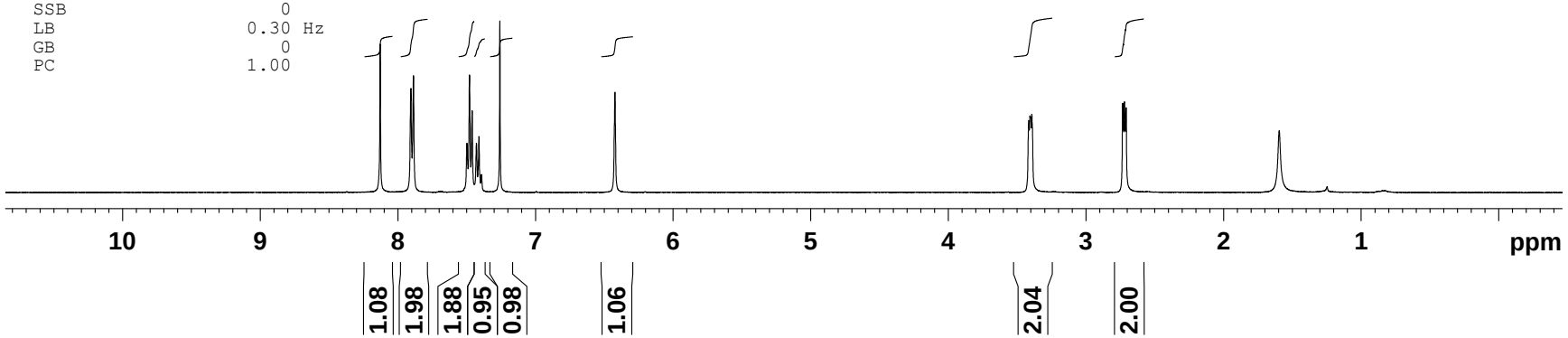

Figure S05: ^{1}H NMR spectrum of 3e.

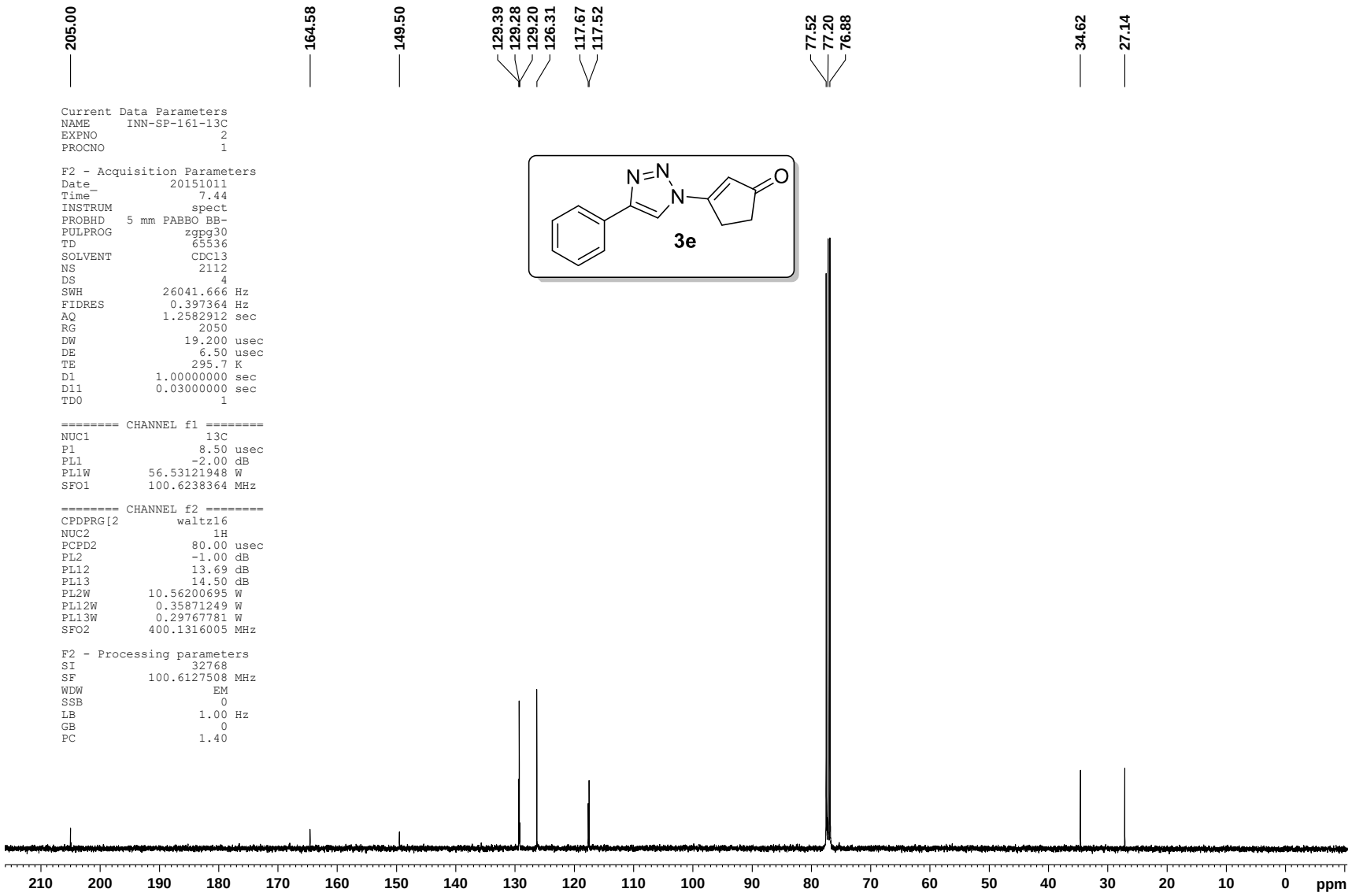

Figure S06: ^{13}C NMR spectrum of 3e.

```
Current Data Parameters
NAME      INN-SR-182-1H
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_           20151129
Time               4.10
INSTRUM           spect
PROBHD   5 mm SEI 1H/D-
PULPROG            zg30
TD                54274
SOLVENT           CDCl3
NS                   20
DS                    0
SWH            8223.685 Hz
FIDRES         0.151522 Hz
AQ            3.2998593 sec
RG                  287
DW               60.800 usec
DE                6.50 usec
TE               295.7 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1                6.75 usec
PL1              -3.00 dB
PL1W       16.73965454 W
SFO1       400.1324710 MHz

F2 - Processing parameters
SI                32768
SF          400.1300112 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
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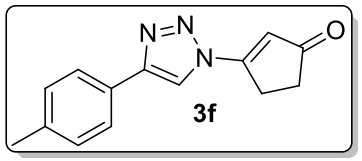

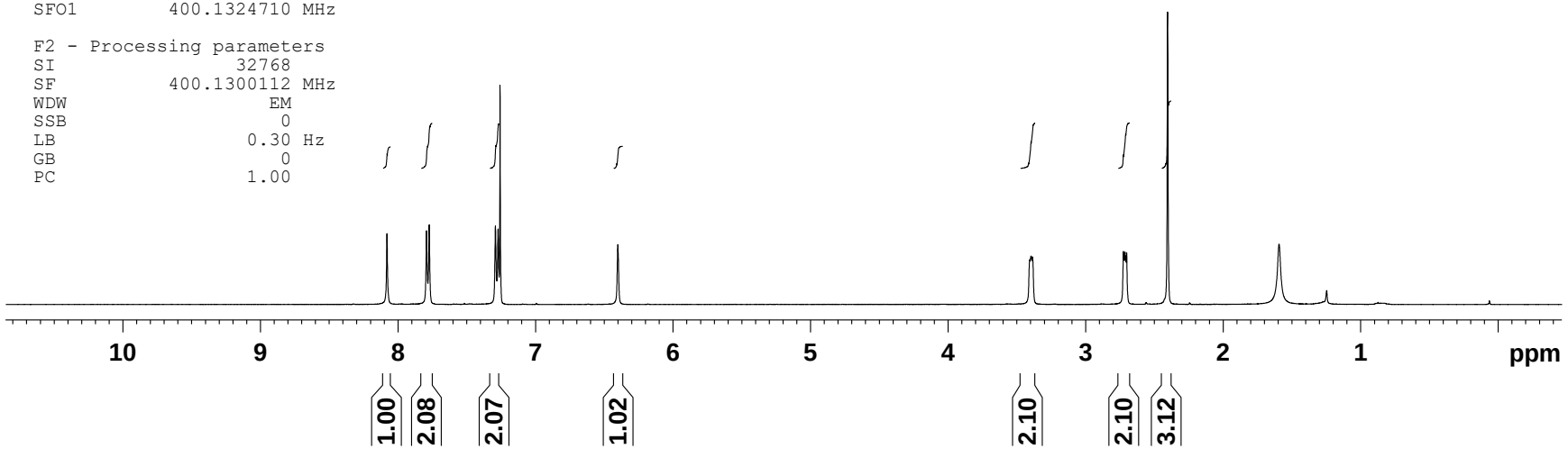

Figure S07: ^{1}H NMR spectrum of 3f.

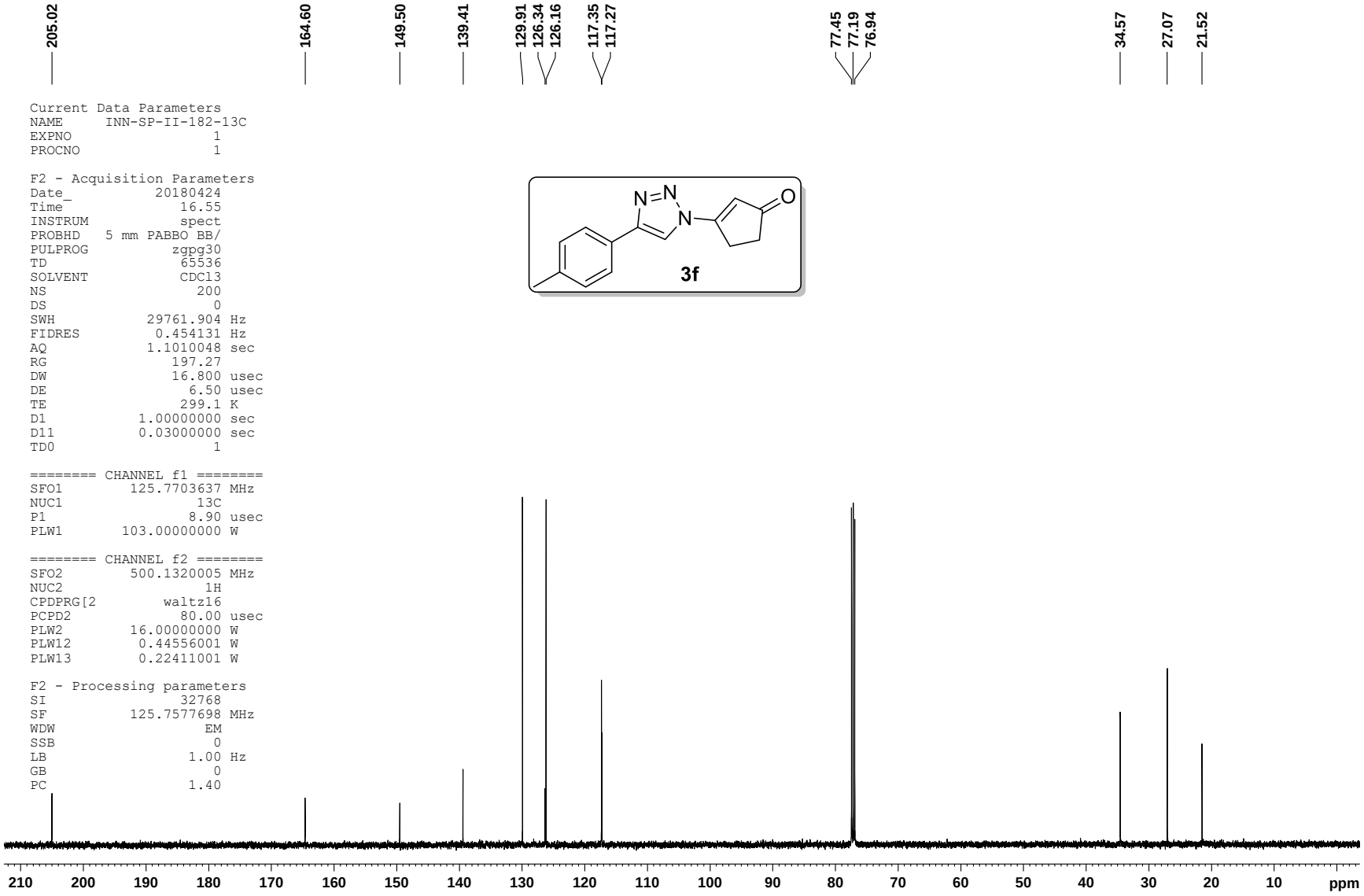

Figure S08: ^{13}C NMR spectrum of 3f.

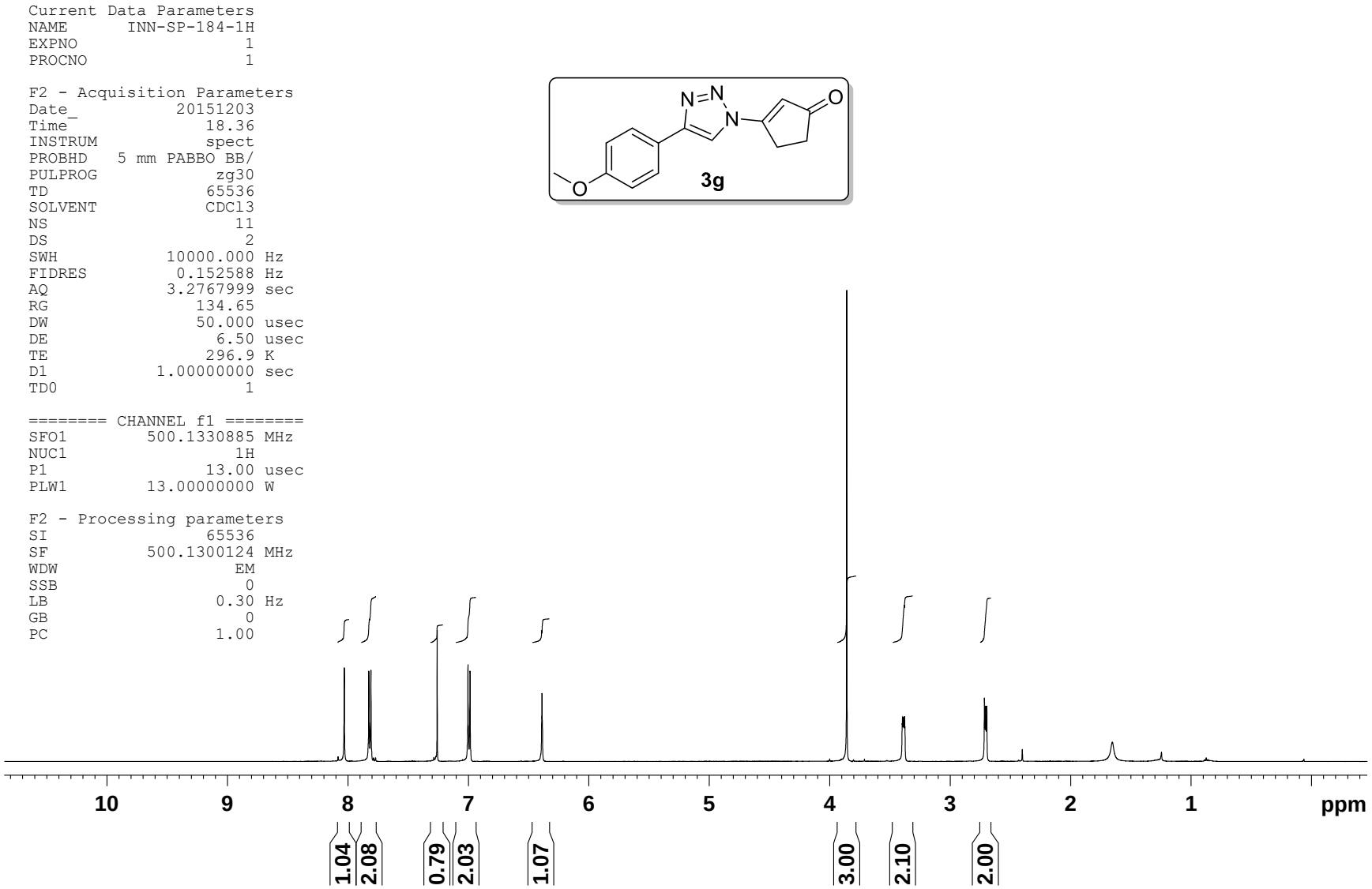

Figure S09: ^{1}H NMR spectrum of 3g.

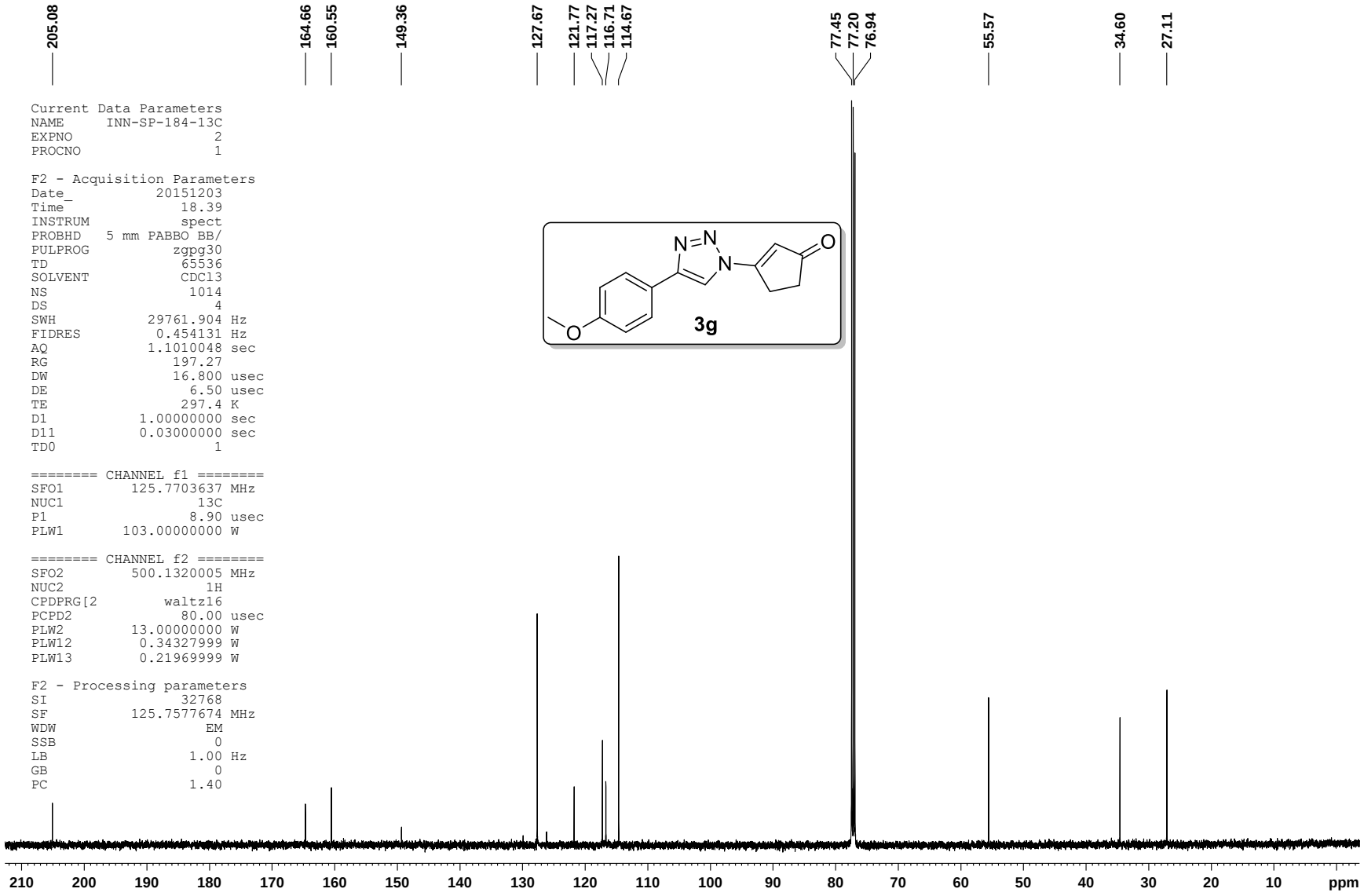

Figure S10: ^{13}C NMR spectrum of 3g.

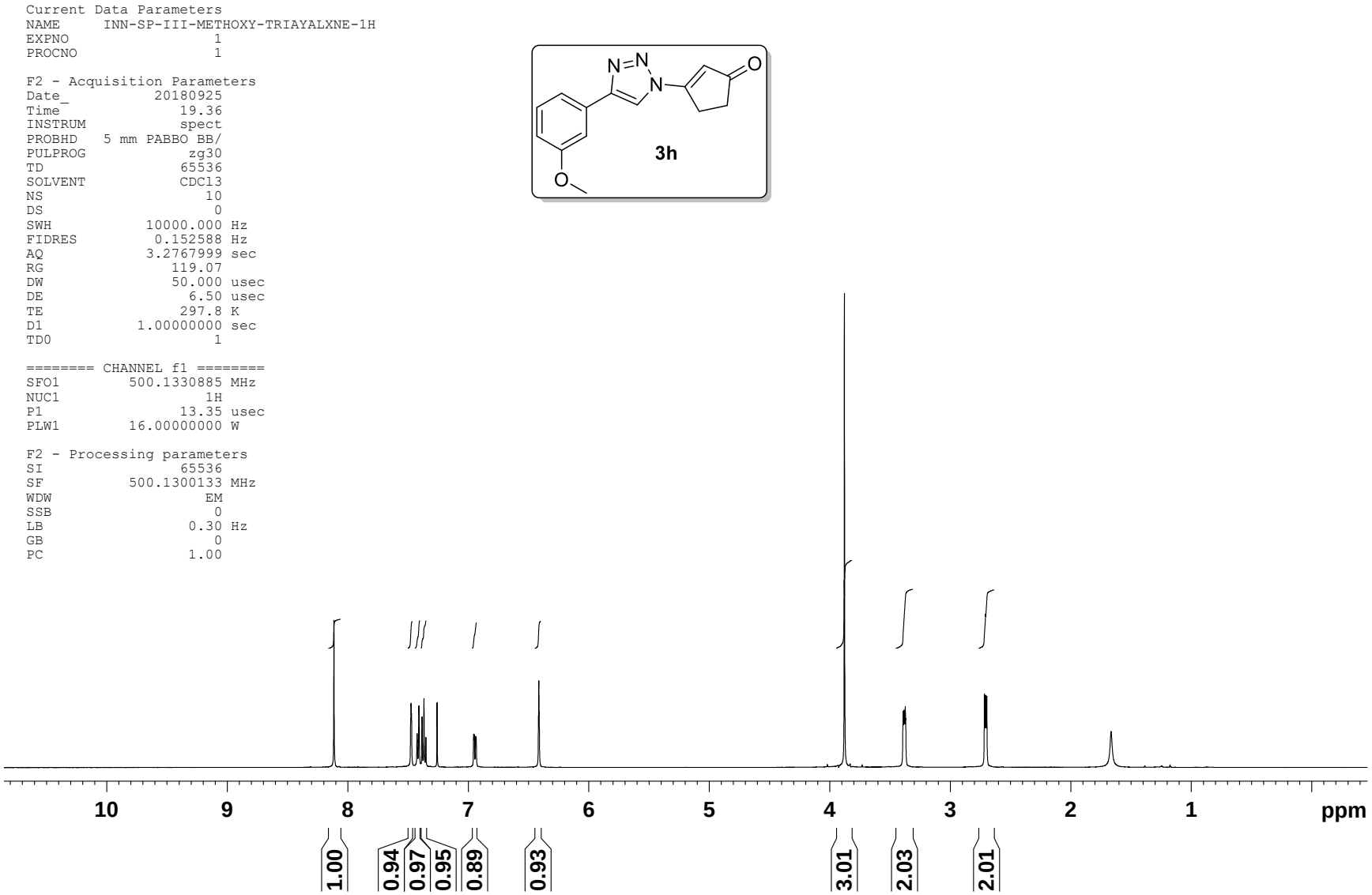

Figure S11: ^{1}H NMR spectrum of 3h.

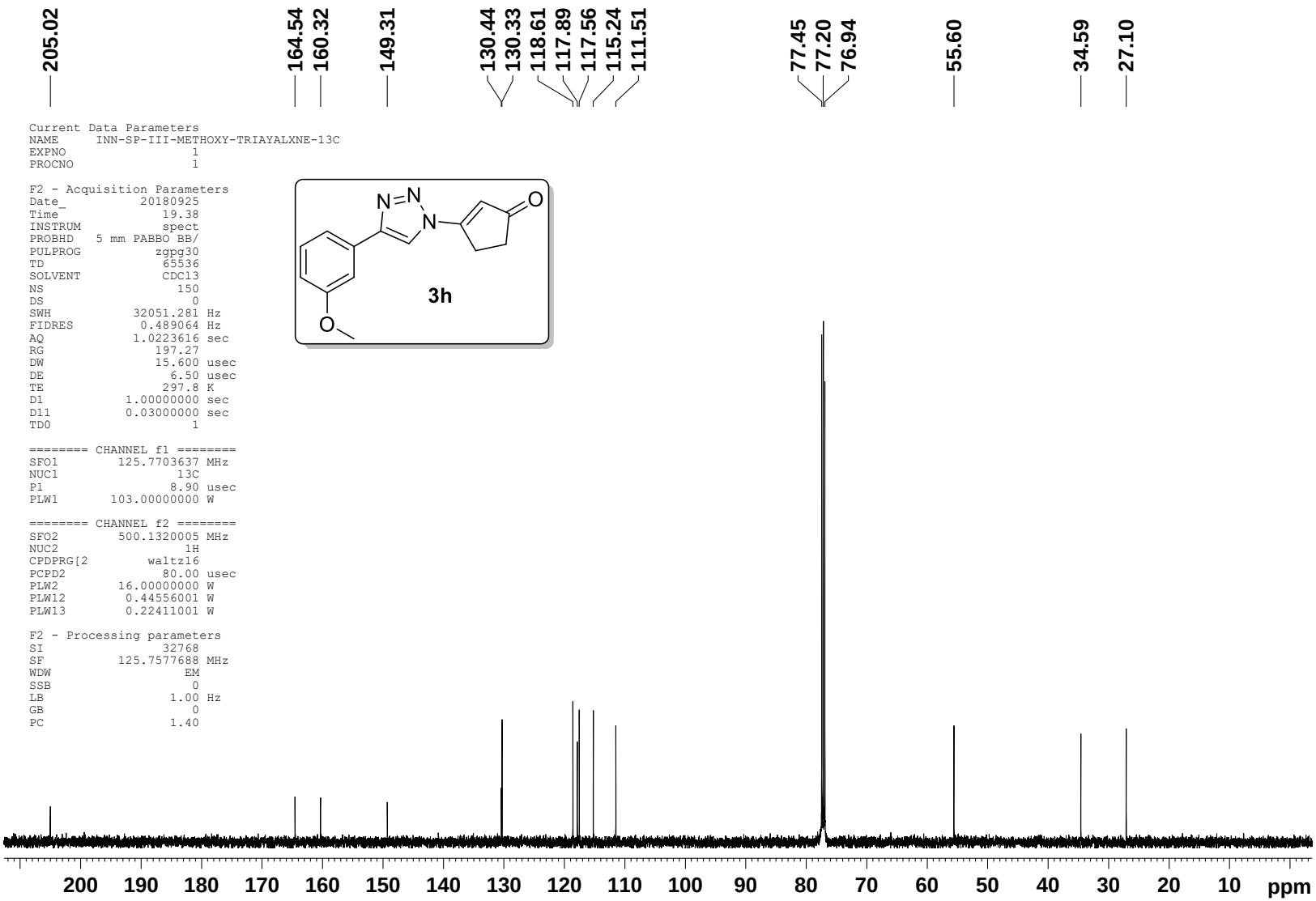

Figure S12: ^{13}C NMR spectrum of 3h.

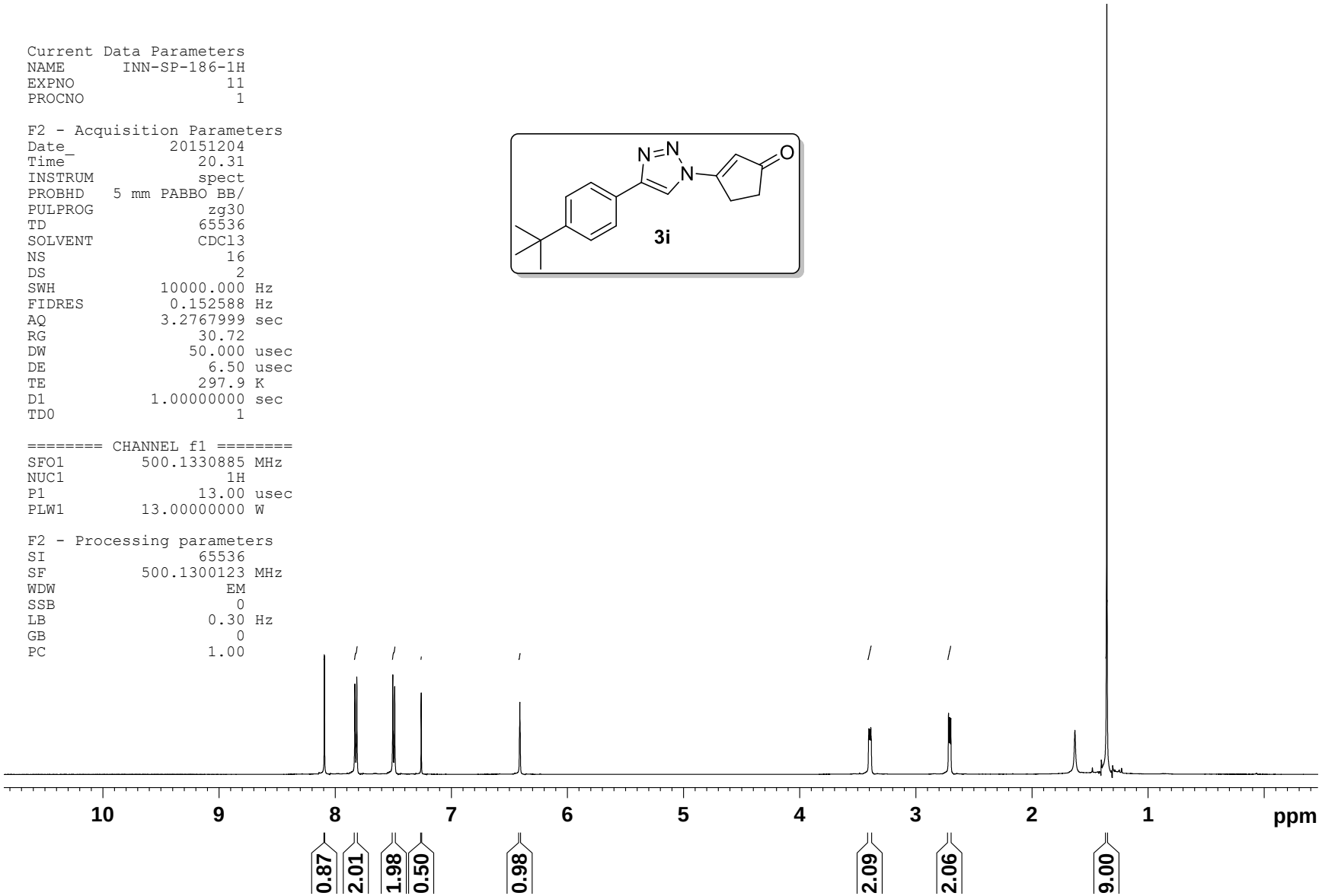

Figure S13: ^{1}H NMR spectrum of 3i.

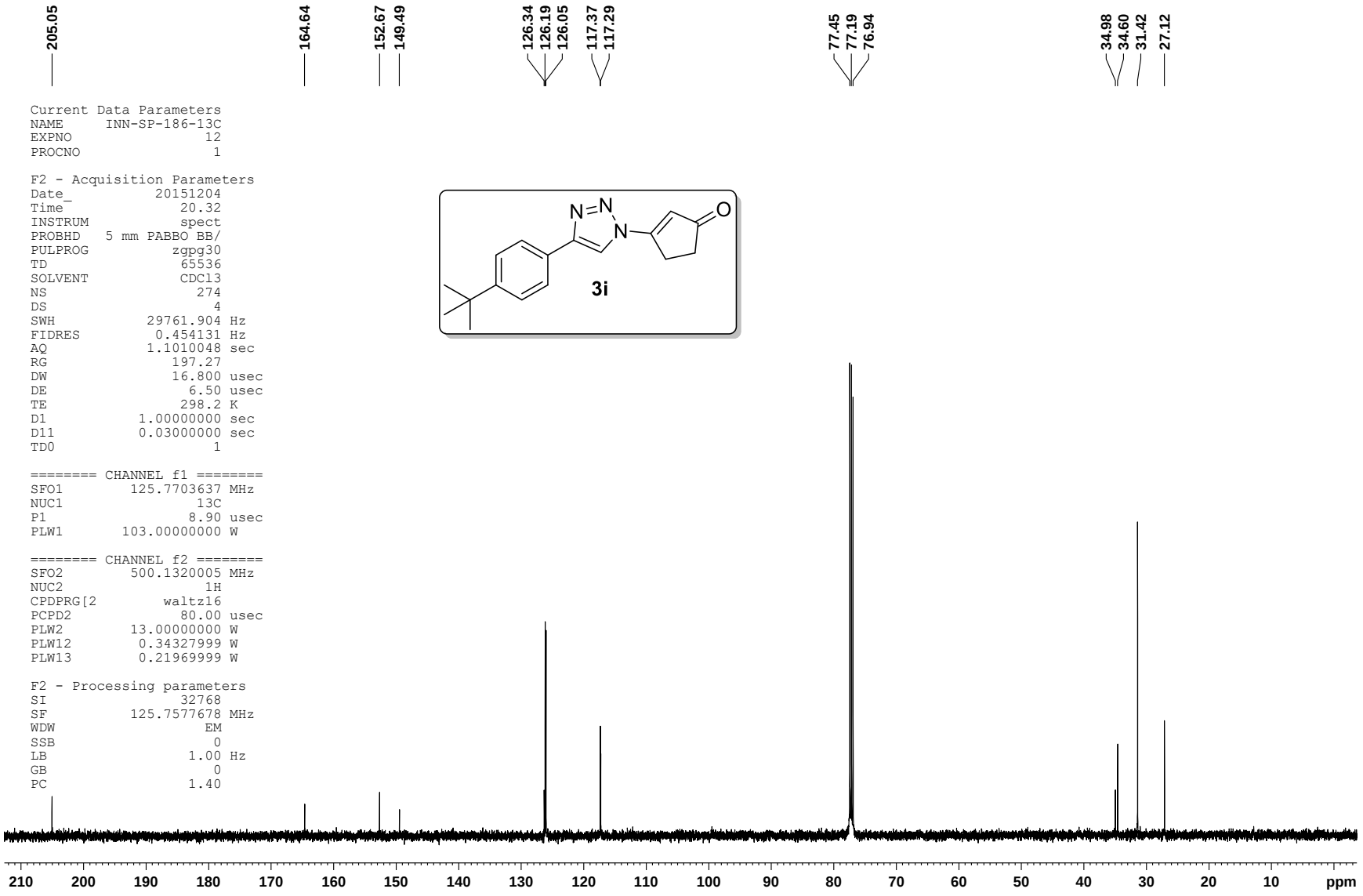

Figure S14: ^{13}C NMR spectrum of 3i.

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EXPNO                   1
PROCNO                  1

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INSTRUM            spect
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PULPROG             zg30
TD                 54274
SOLVENT            CDCl3
NS                     6
DS                     0
SWH             8223.685 Hz
FIDRES          0.151522 Hz
AQ             3.2998593 sec
RG                   128
DW                60.800 usec
DE                 6.50 usec
TE                297.4 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.75 usec
PL1               -1.00 dB
PL1W        10.56200695 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300097 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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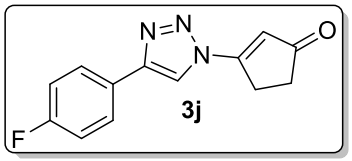

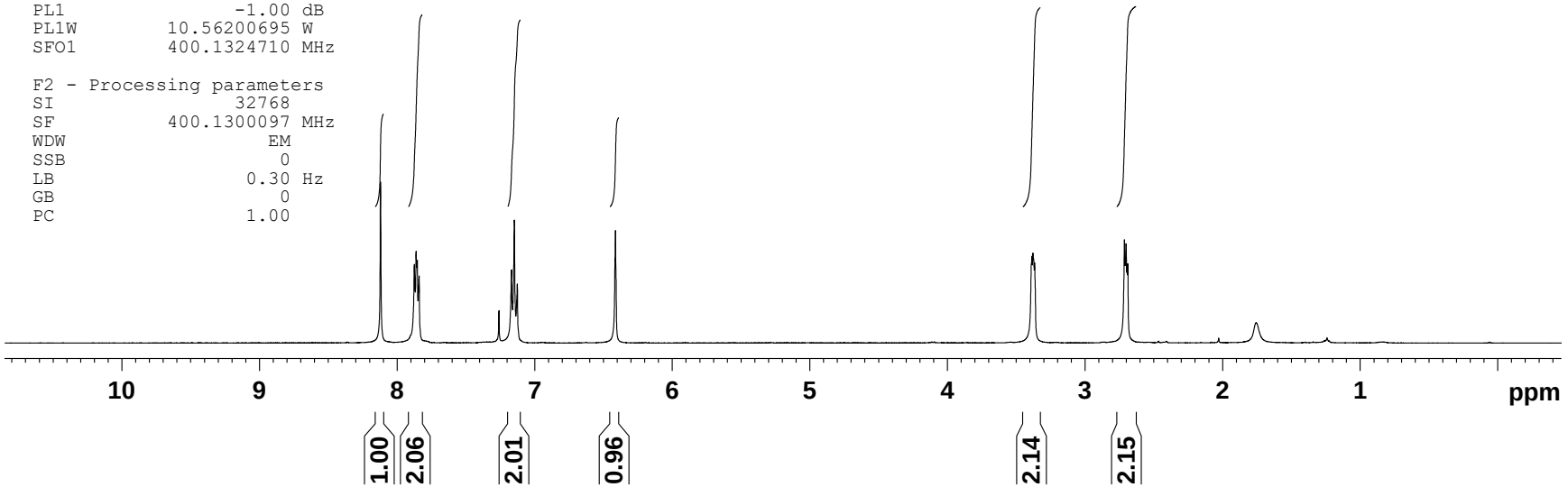

Figure S15: ^{1}H NMR spectrum of 3j.

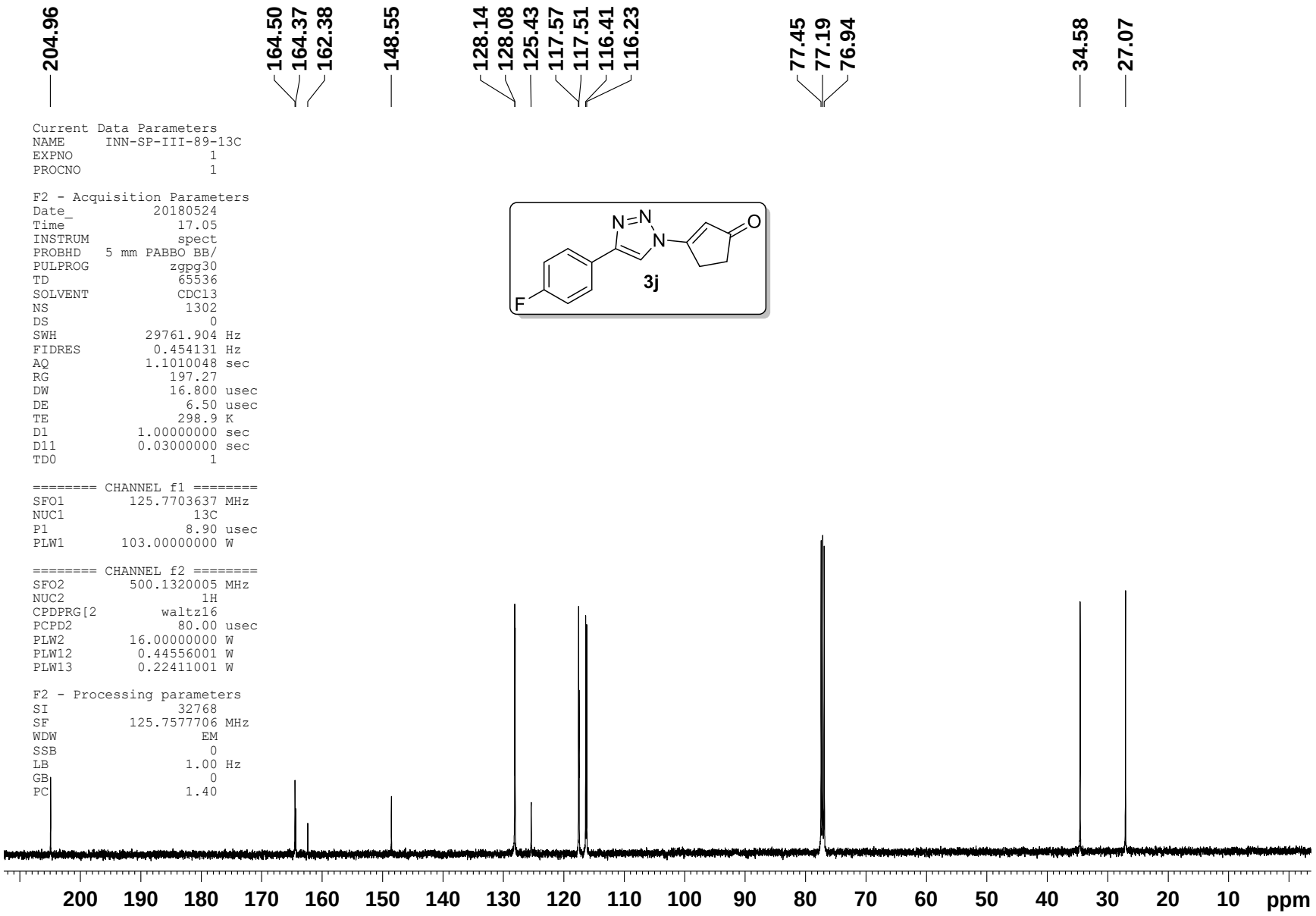

Figure S16: ^{13}C NMR spectrum of 3j.

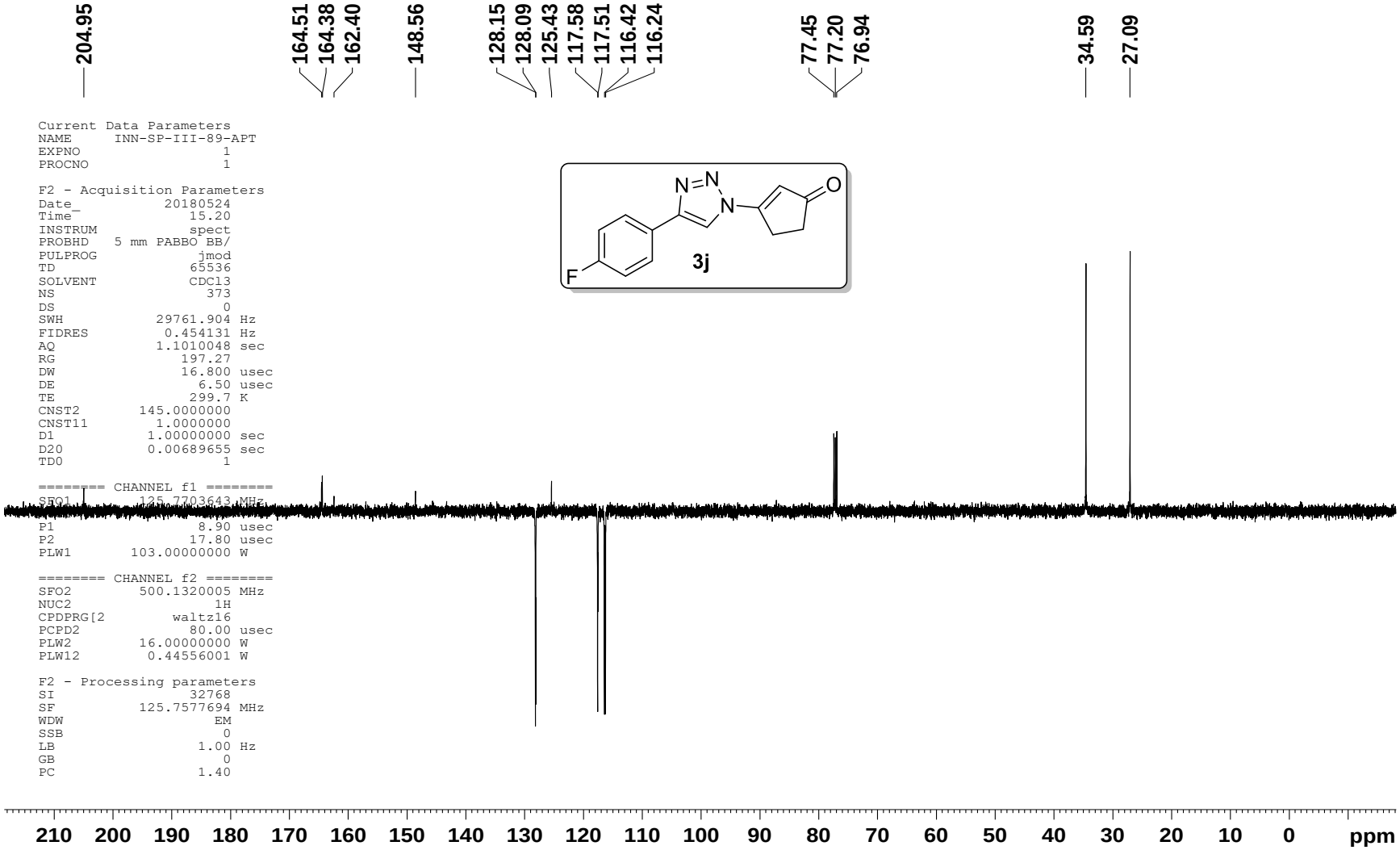

Figure S17: ^{13}C-APT NMR spectrum of 3j.

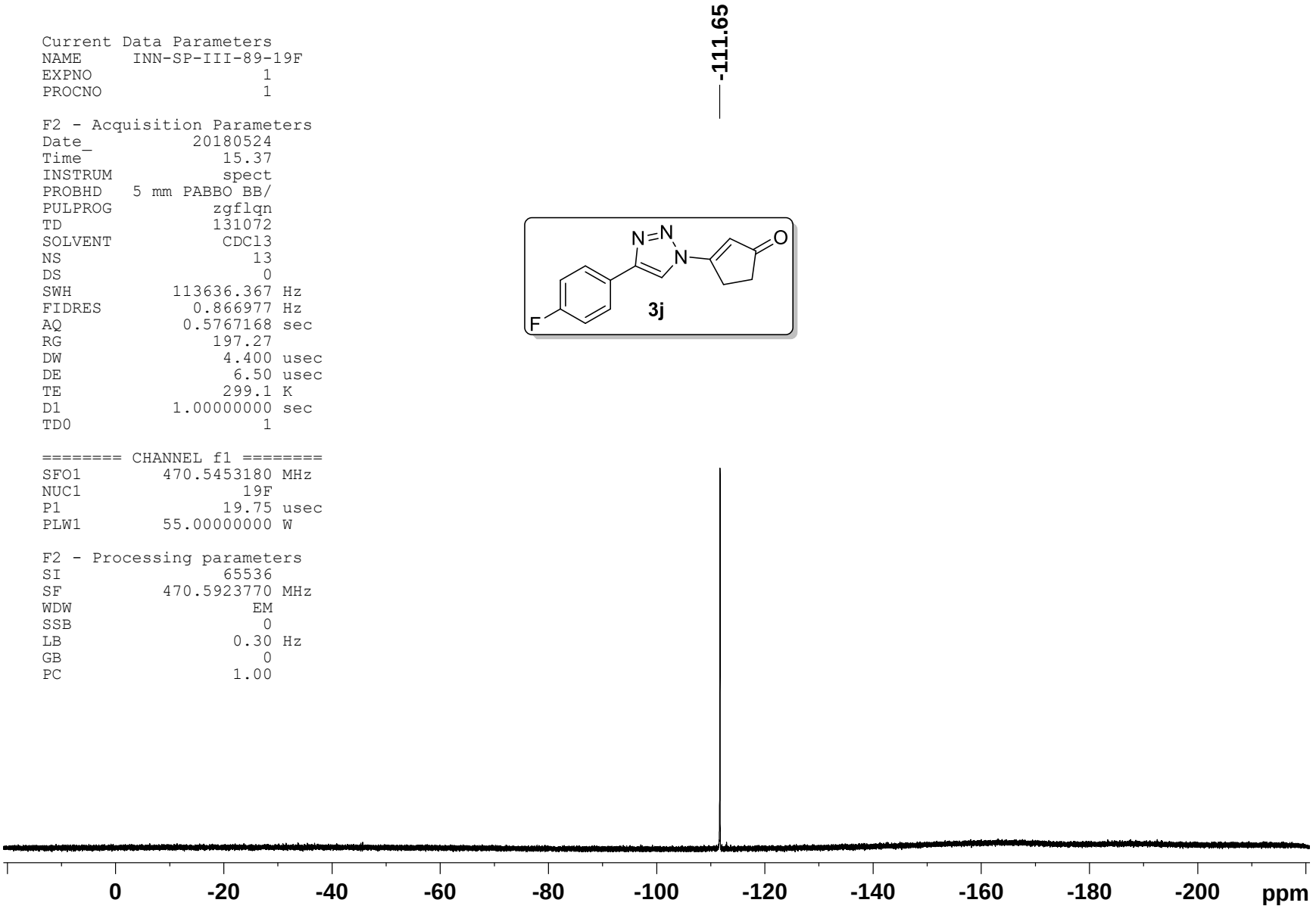

Figure S18: ^{19}F NMR spectrum of 3j.

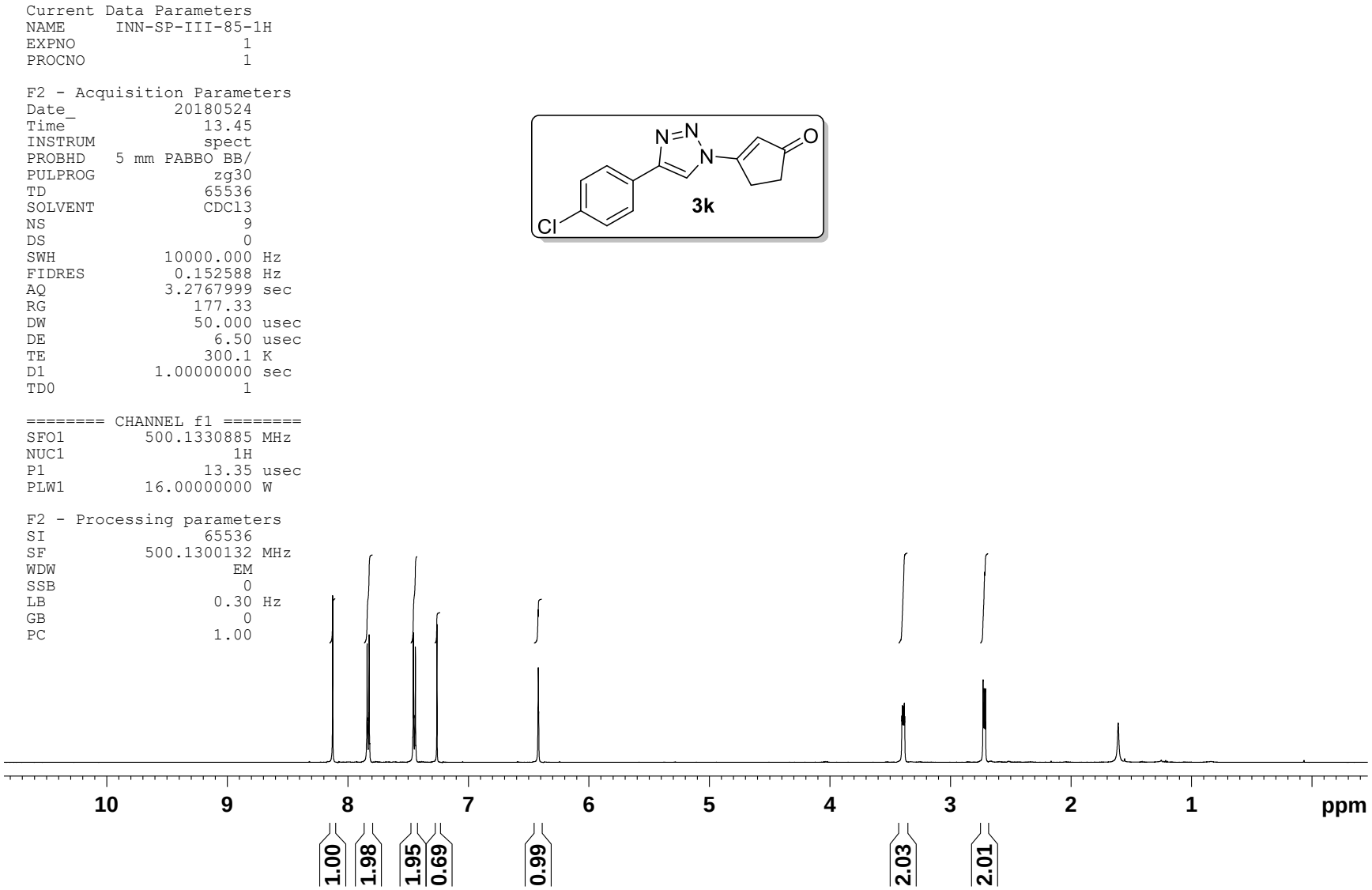

Figure S19: ^{1}H NMR spectrum of 3k.

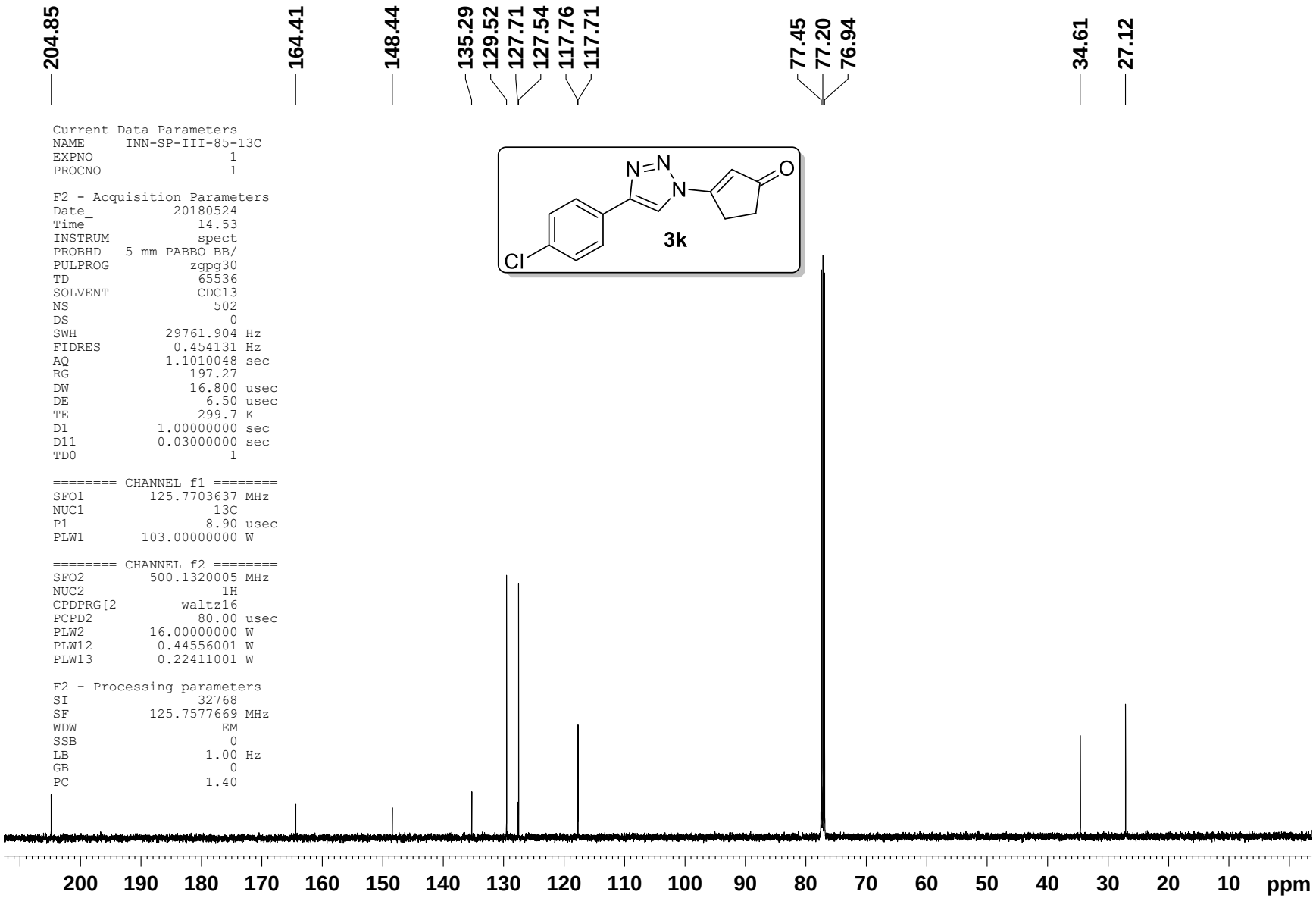

Figure S20: ^{13}C NMR spectrum of 3k.

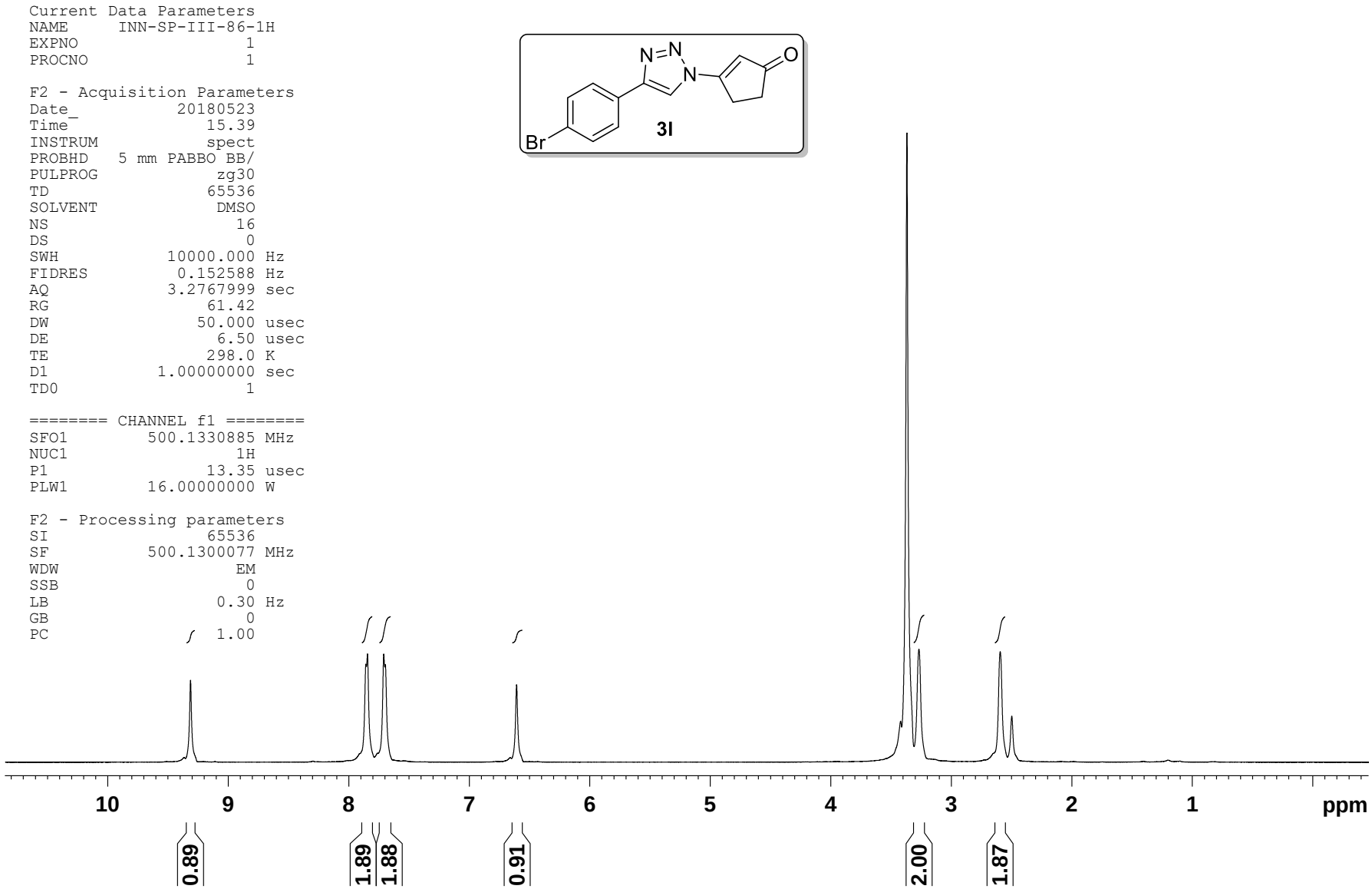

Figure S21: ^{1}H NMR spectrum of 3l.

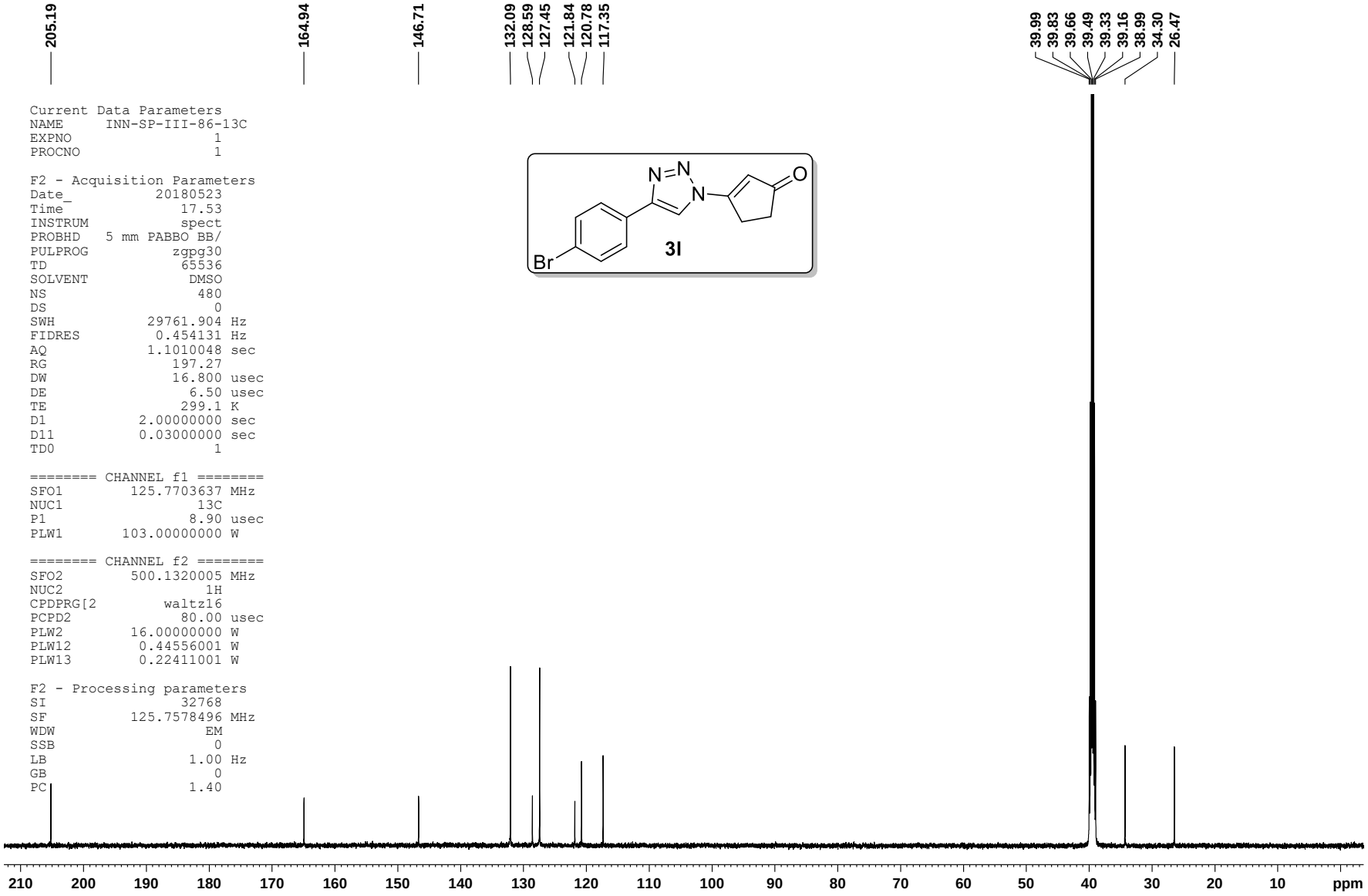

Figure S22: ^{13}C NMR spectrum of 3l.

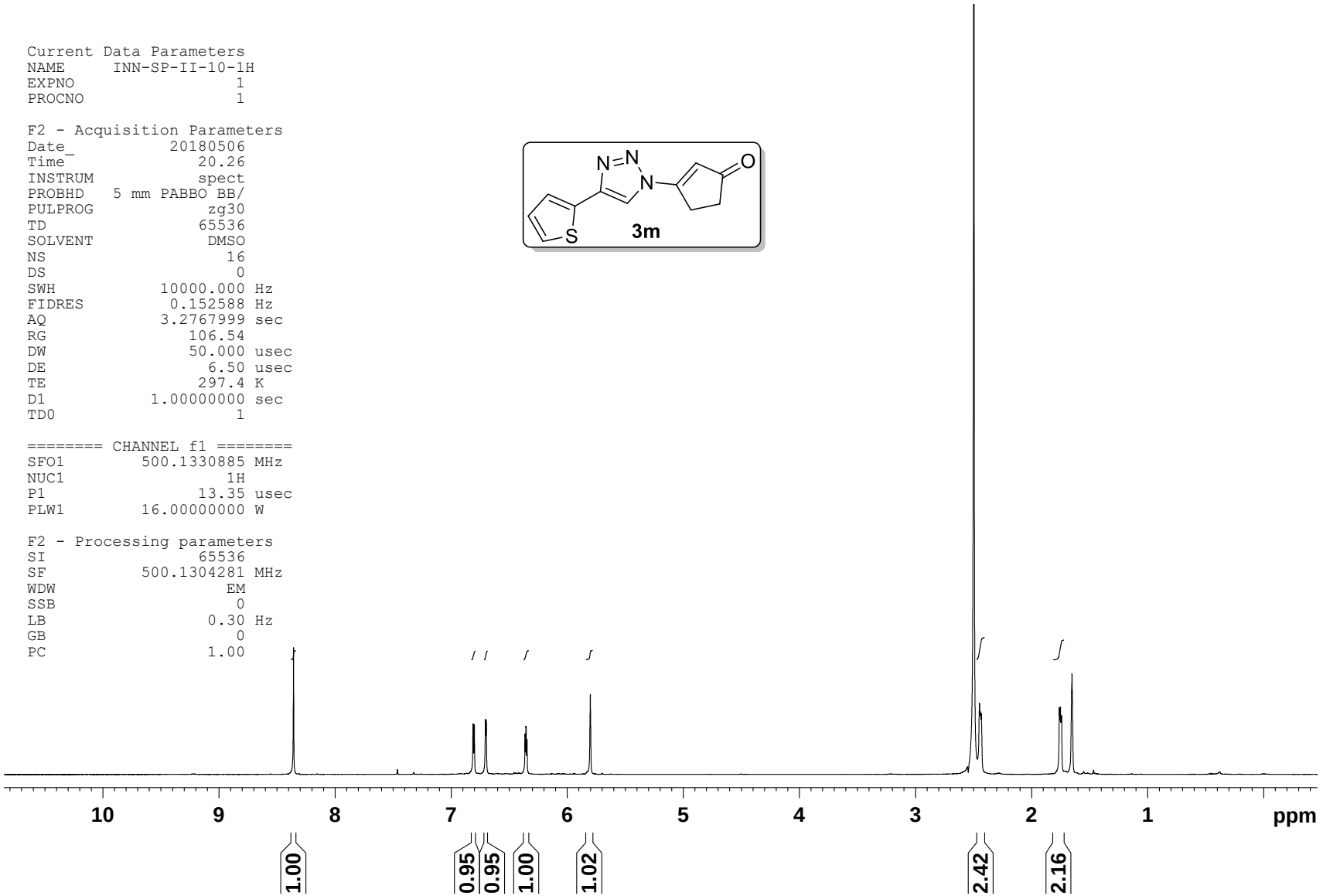

Figure S23: ^{1}H NMR spectrum of 3m.

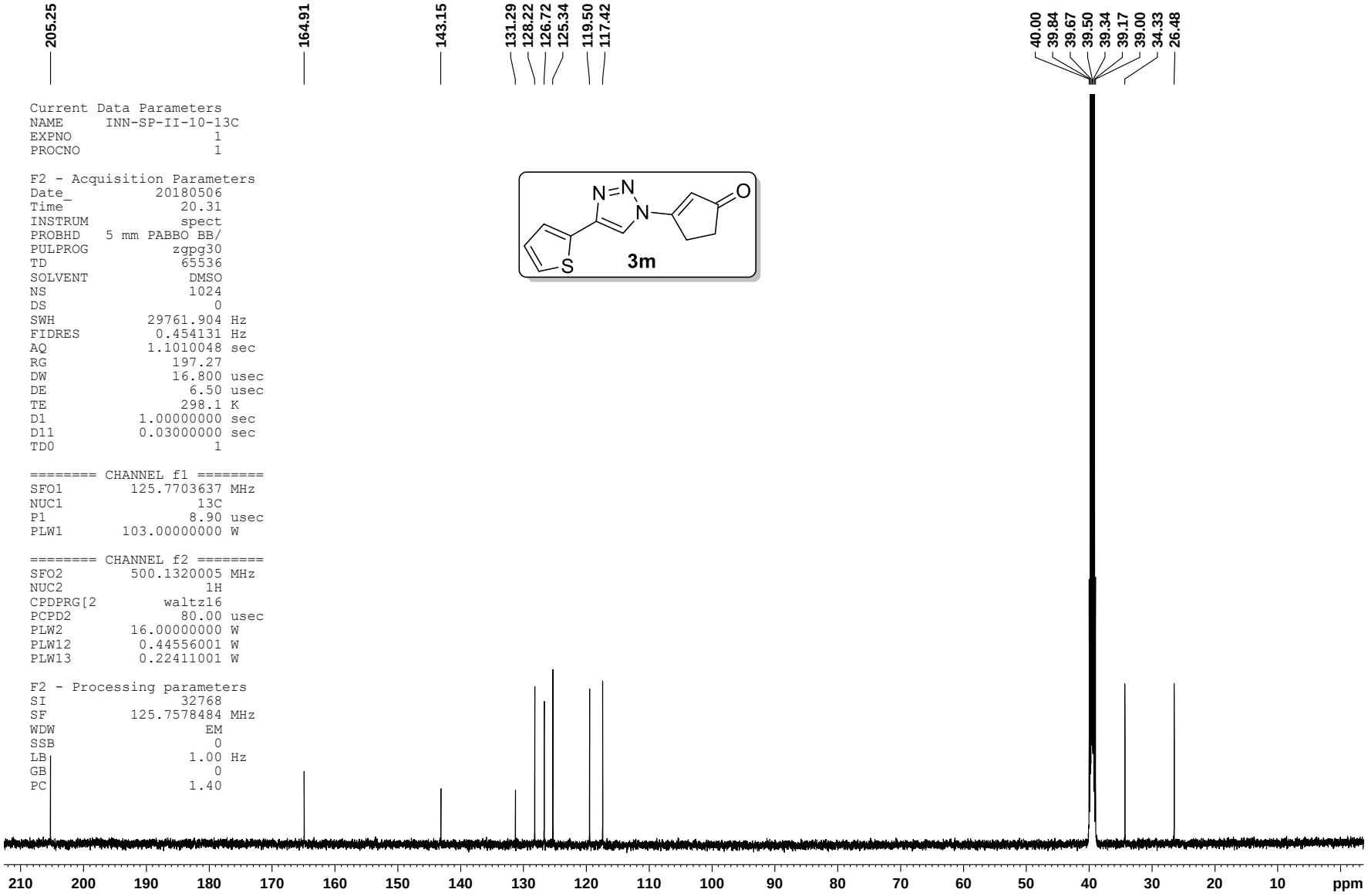

Figure S24: ^{13}C NMR spectrum of 3m.

```
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EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180417
Time                15.41
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PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      0
SWH             10000.000 Hz
FIDRES           0.152588 Hz
AQ               3.2767999 sec
RG                  134.65
DW                  50.000 usec
DE                    6.50 usec
TE                  298.2 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          500.1330885 MHz
NUC1                   1H
P1                  13.35 usec
PLW1          16.00000000 W

F2 - Processing parameters
SI                  65536
SF            500.1300131 MHz
WDW                    EM
SSB                     0
LB                   0.10 Hz
GB                      0
PC                   1.00
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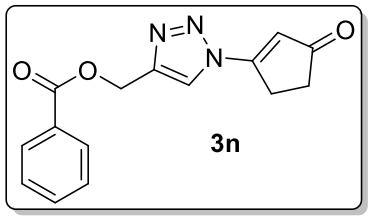


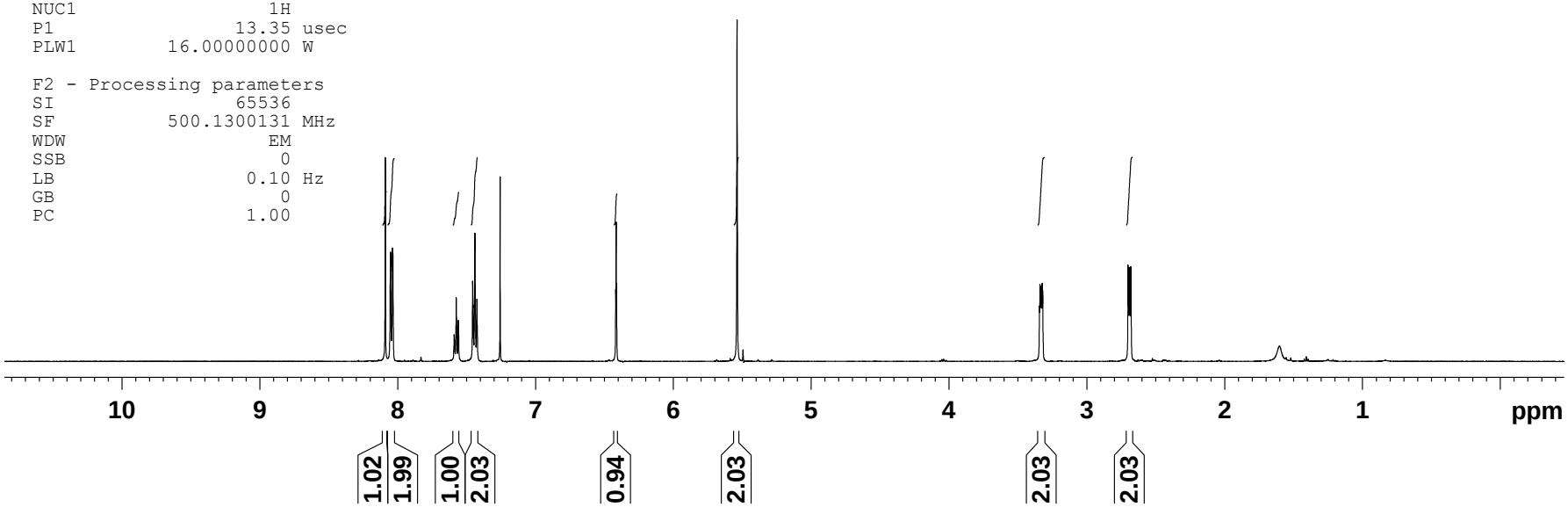


Figure S25: ^{1}H NMR spectrum of 3n.

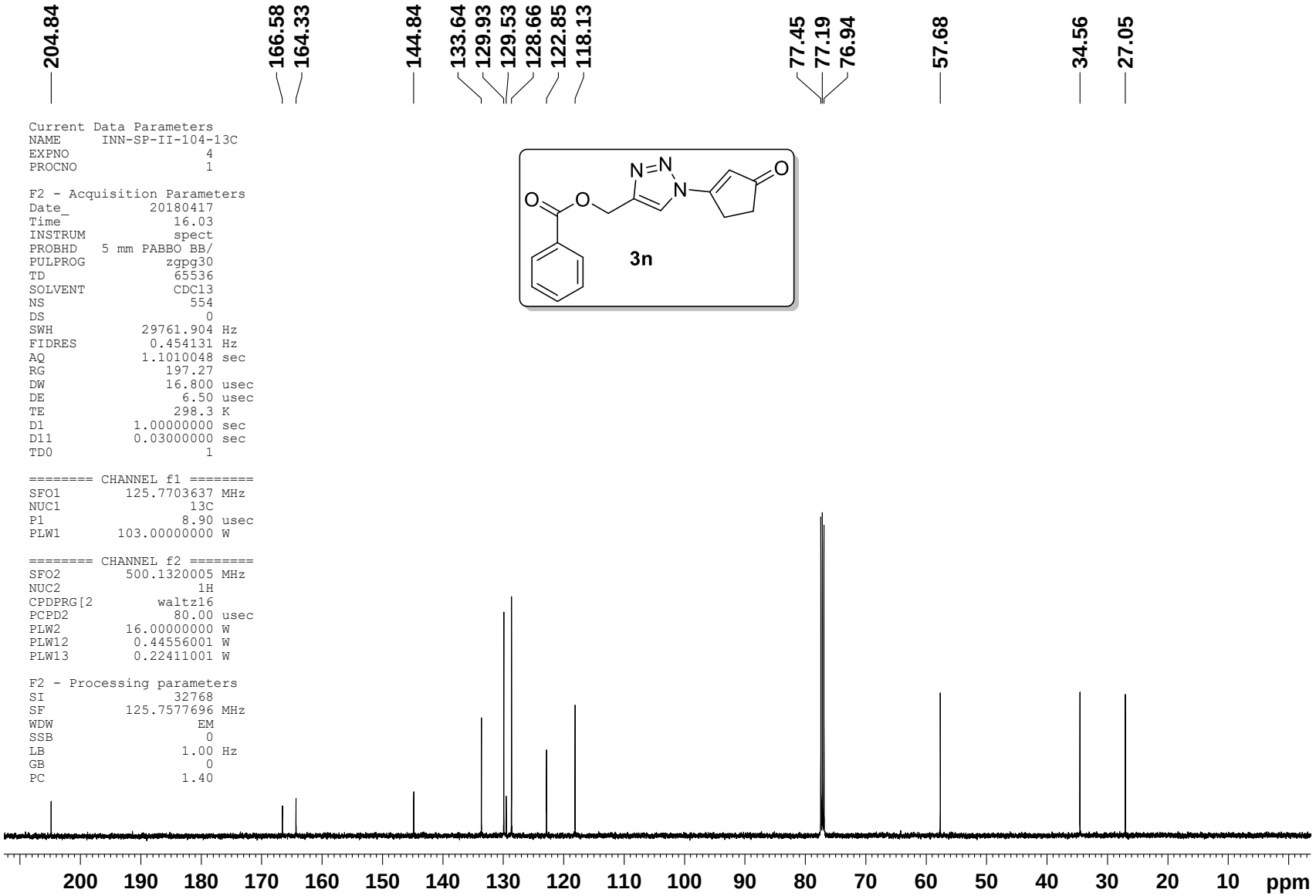


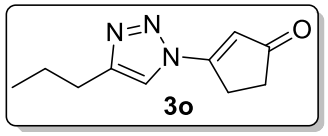
Figure S26: ^{13}C NMR spectrum of 3n.

```
Current Data Parameters
NAME      INN-SP-II-126-1H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170210
Time              17.11
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   10
DS                    2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ            3.2767999 sec
RG               106.54
DW               50.000 usec
DE                6.50 usec
TE               297.9 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        500.1330885 MHz
NUC1                1H
P1                13.00 usec
PLW1        13.00000000 W

F2 - Processing parameters
SI                65536
SF          500.1300131 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



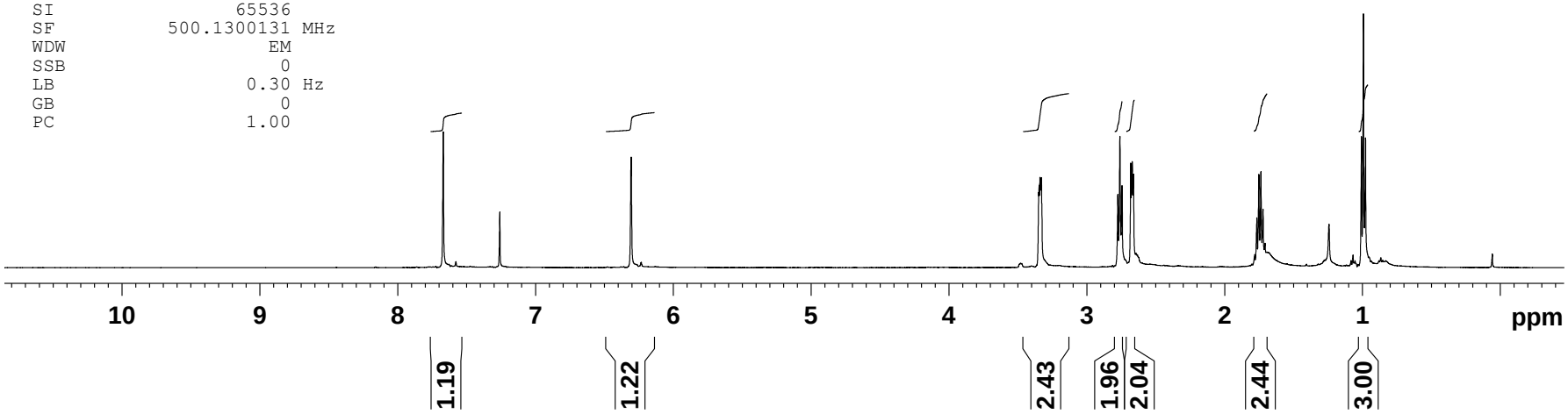


Figure S27: ^{1}H NMR spectrum of 3o.

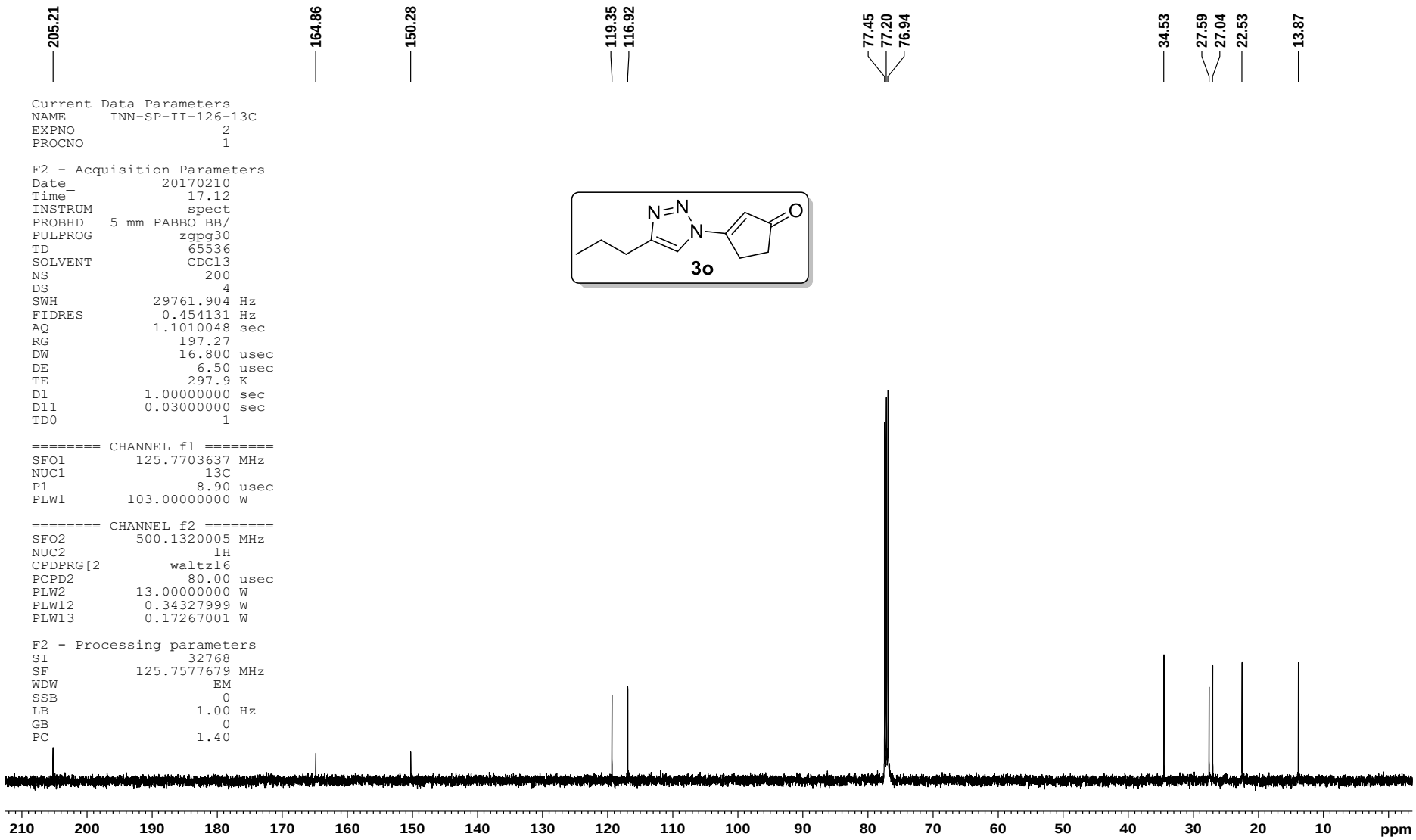


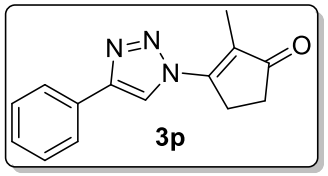
Figure S28: ^{13}C NMR spectrum of 3o.

```
Current Data Parameters
NAME      INN-SP-III-81-1H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180605
Time               5.33
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 54274
SOLVENT            CDCl3
NS                     7
DS                     0
SWH             8223.685 Hz
FIDRES          0.151522 Hz
AQ              3.2998593 sec
RG                   228
DW                60.800 usec
DE                 6.50 usec
TE                513.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.75 usec
PL1               -1.00 dB
PL1W        10.56200695 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300102 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



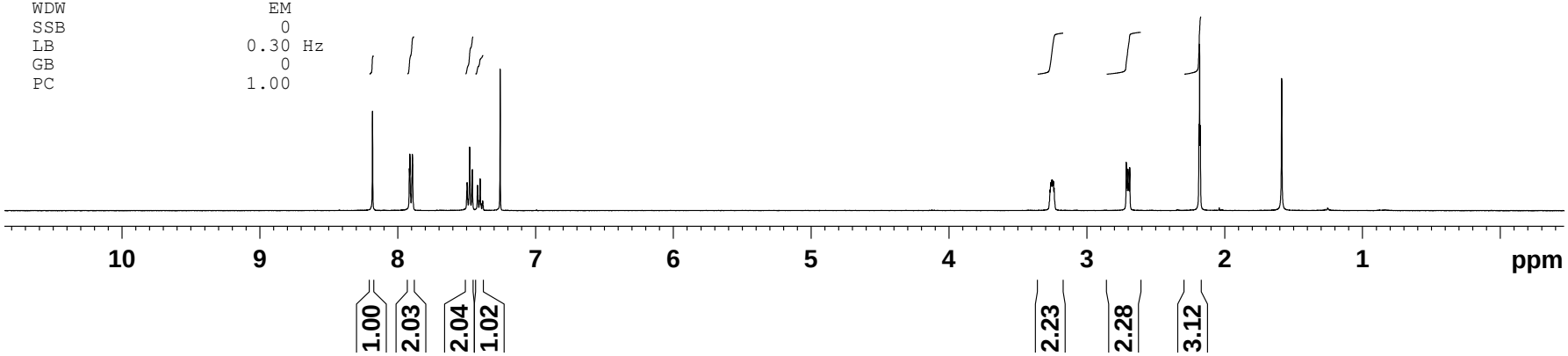


Figure S29: ^{1}H NMR spectrum of 3p.

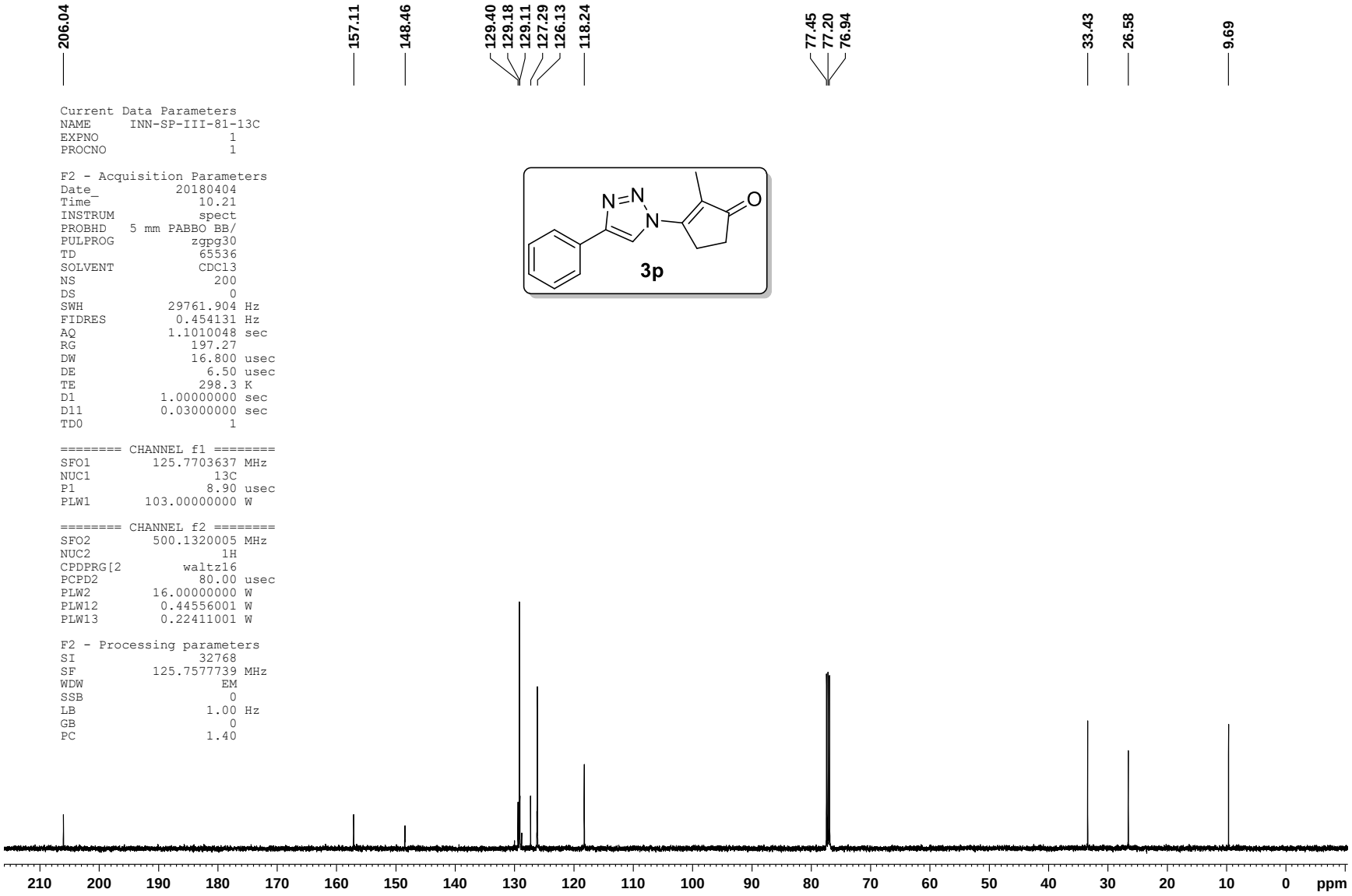


Figure S30: ^{13}C NMR spectrum of 3p.

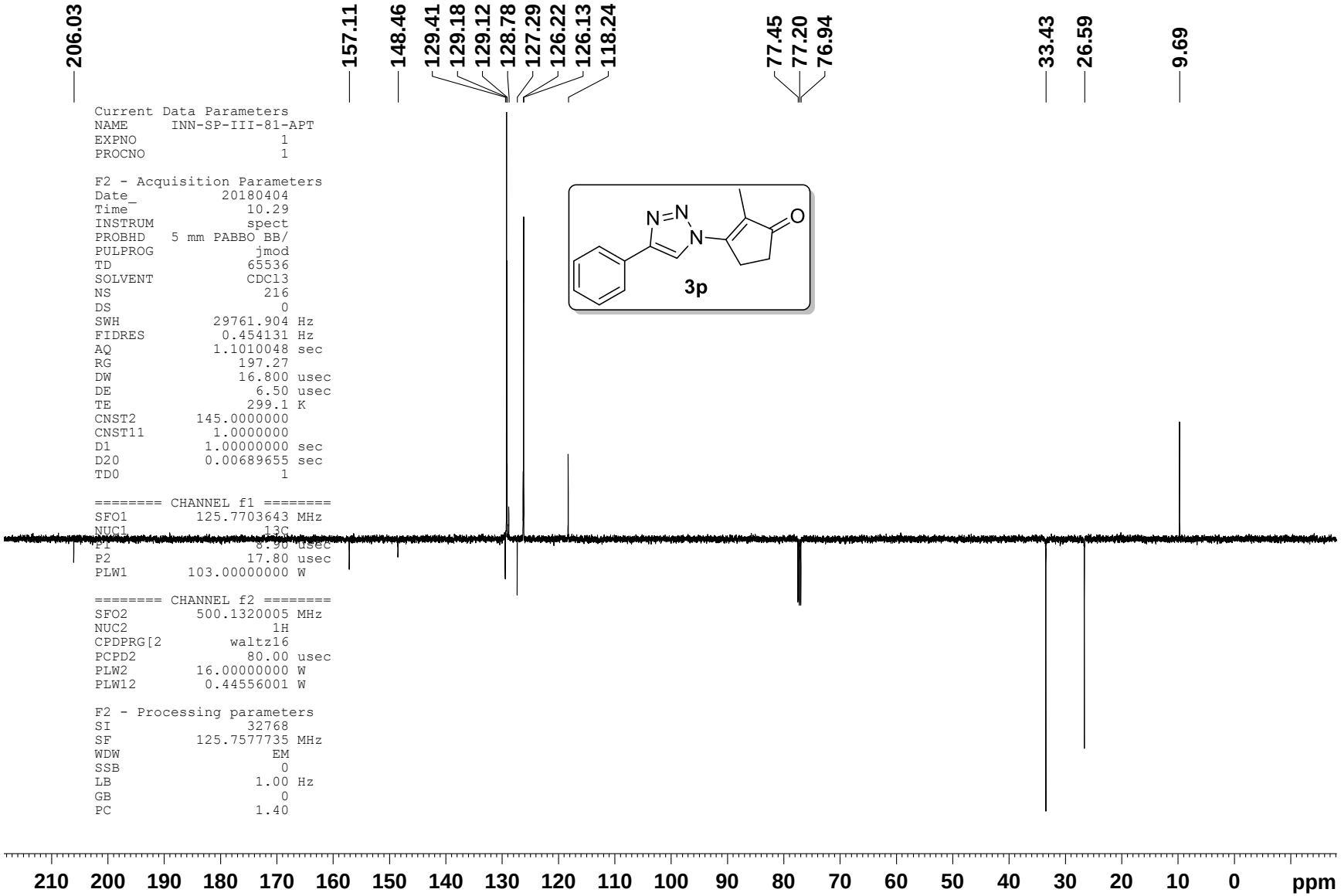


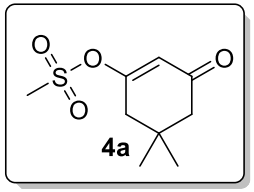
Figure S31: ^{13}C-APT NMR spectrum of 3p.

```
Current Data Parameters
NAME      IIN-SP-III-BTN-1H
EXPNO                  15
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190308
Time_               23.36
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     25
DS                      0
SWH             10000.000 Hz
FIDRES              0.152588 Hz
AQ              3.2767999 sec
RG                  30.72
DW                 50.000 usec
DE                   6.50 usec
TE                  296.7 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          500.1330885 MHz
NUC1                   1H
P1                  13.35 usec
PLW1          16.00000000 W

F2 - Processing parameters
SI                  65536
SF            500.1300134 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



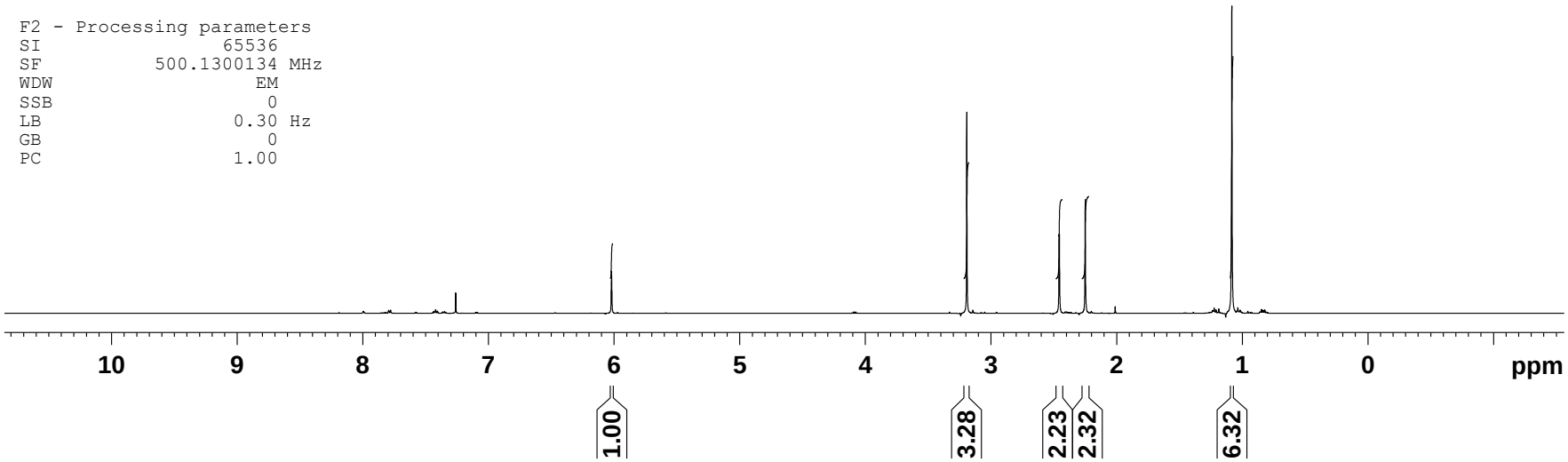


Figure S32: ^{1}H NMR spectrum of 4a.

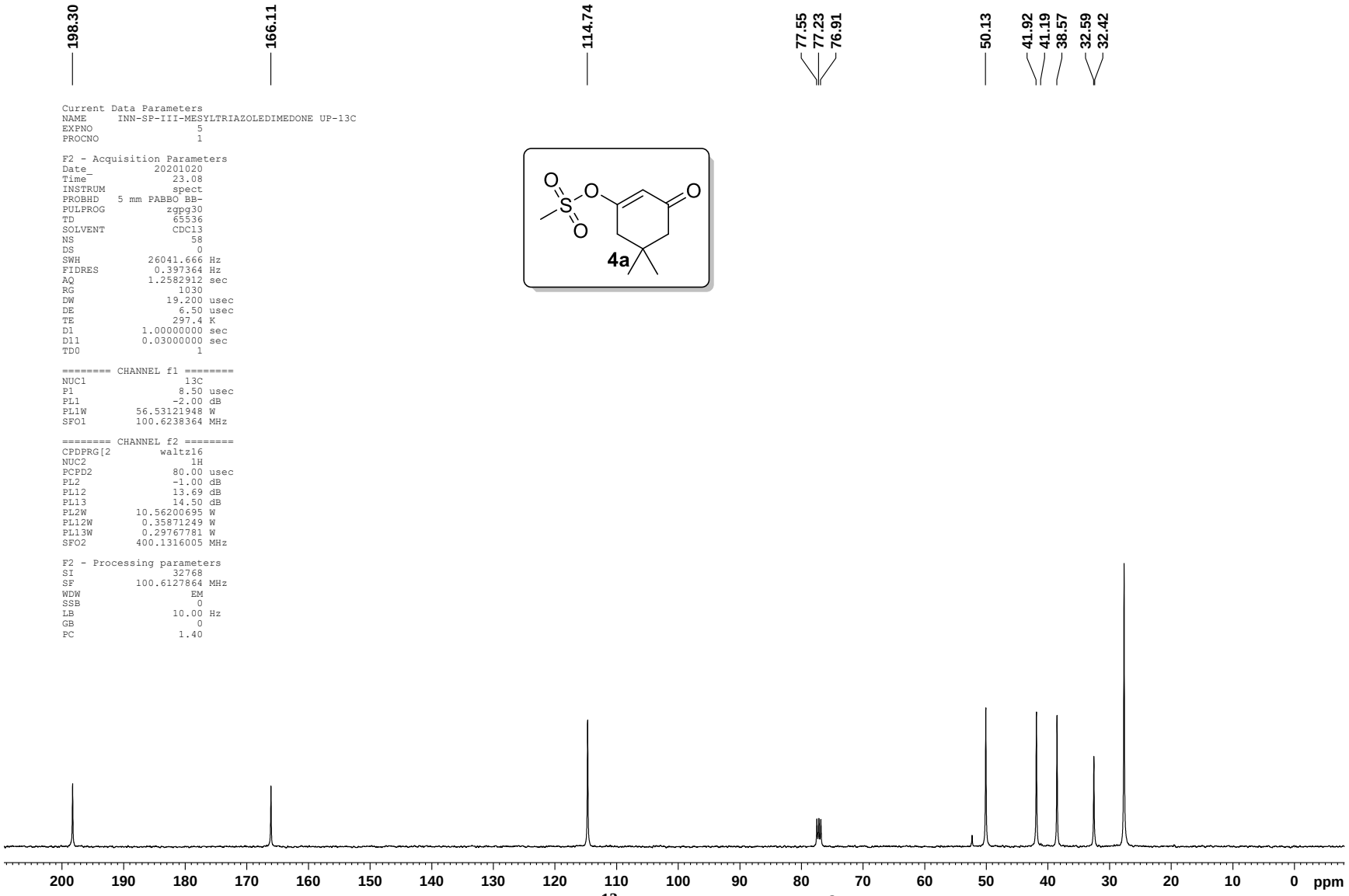


Figure S33: ^{13}C NMR spectrum of 4a.

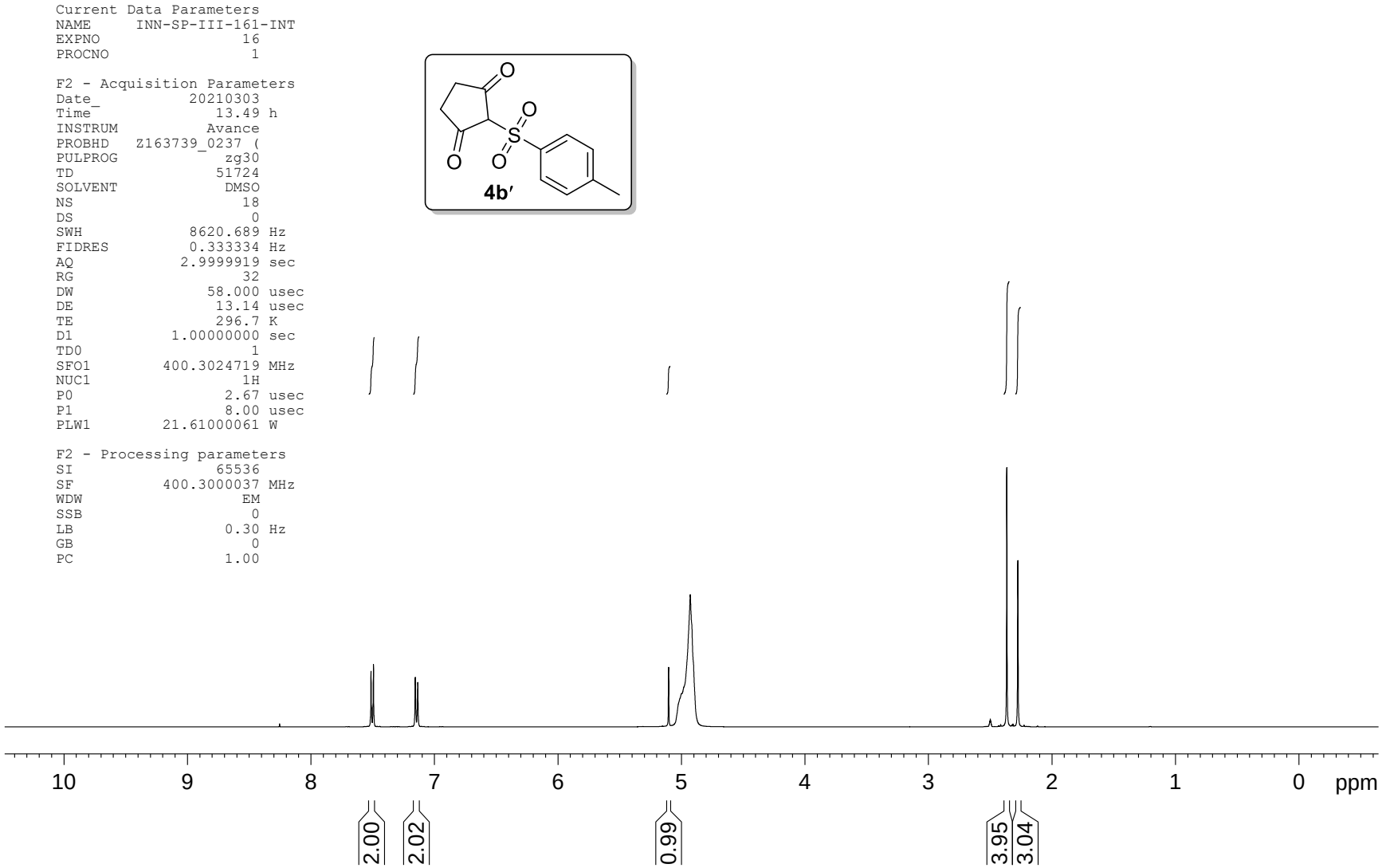


Figure S34: ^{1}H NMR spectrum of 4b'.

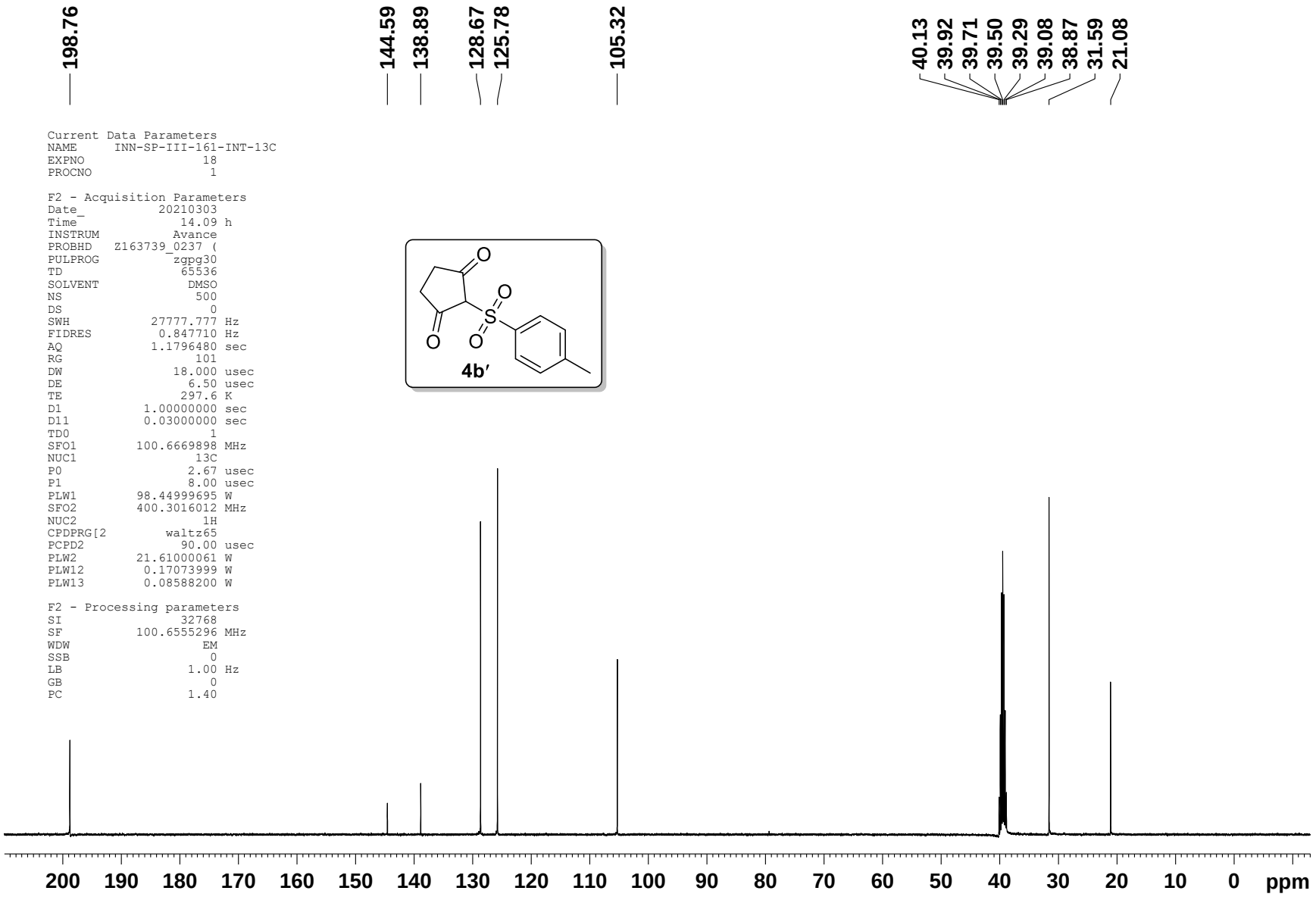


Figure S35: ^{13}C NMR spectrum of 4b'.

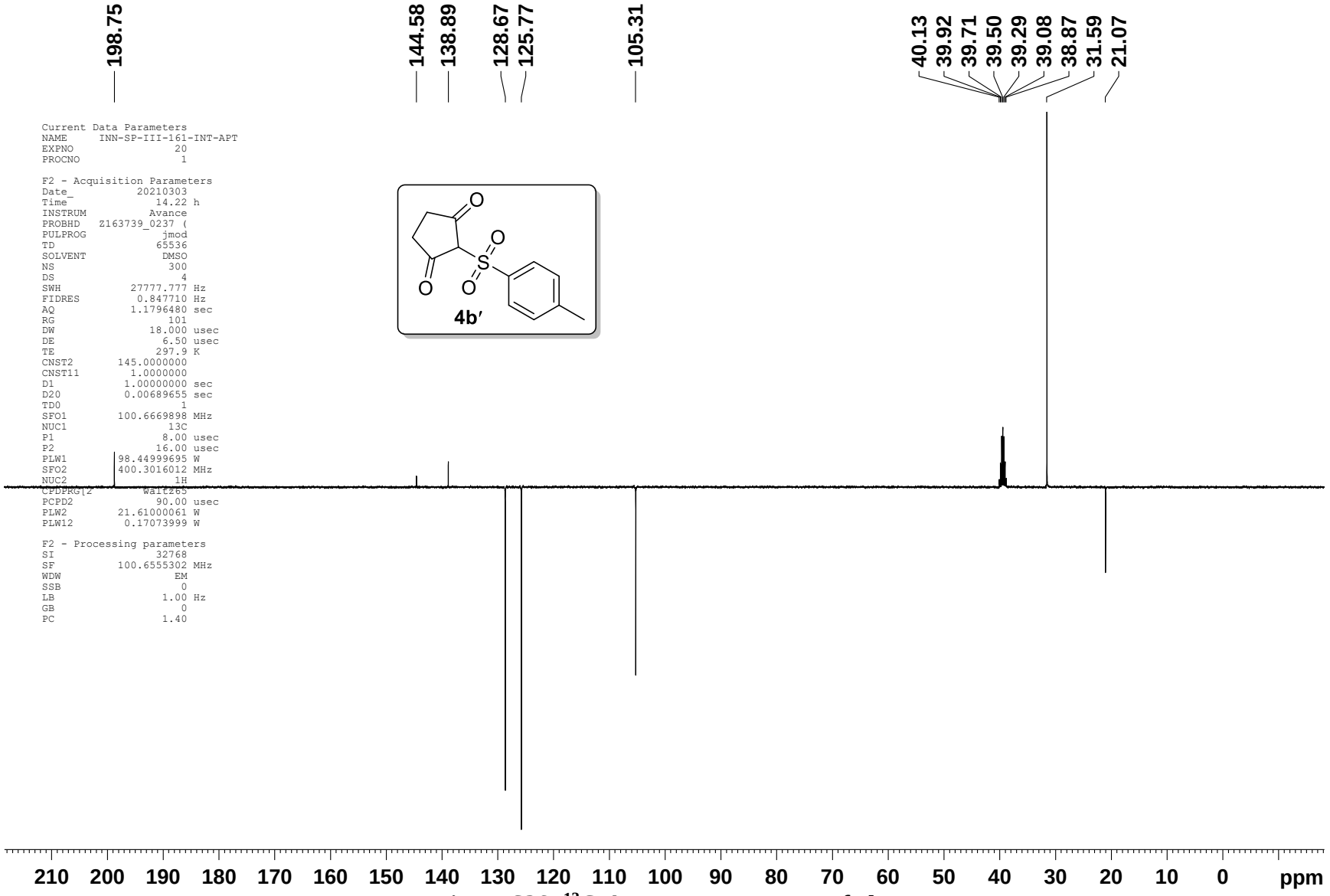


Figure S36: ^{13}C-APT NMR spectrum of 4b'.

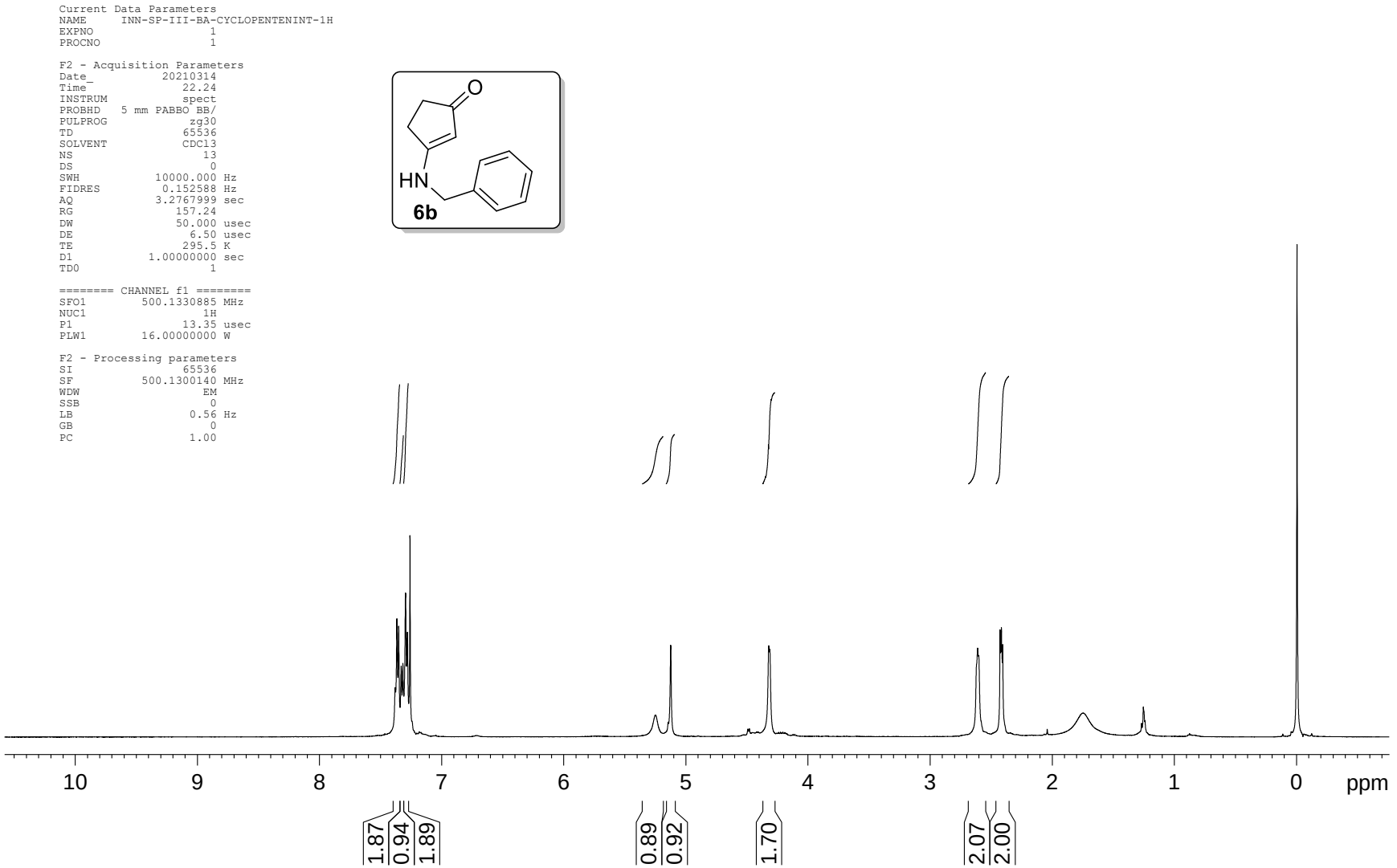


Figure S37: ^{1}H NMR spectrum of 6b.

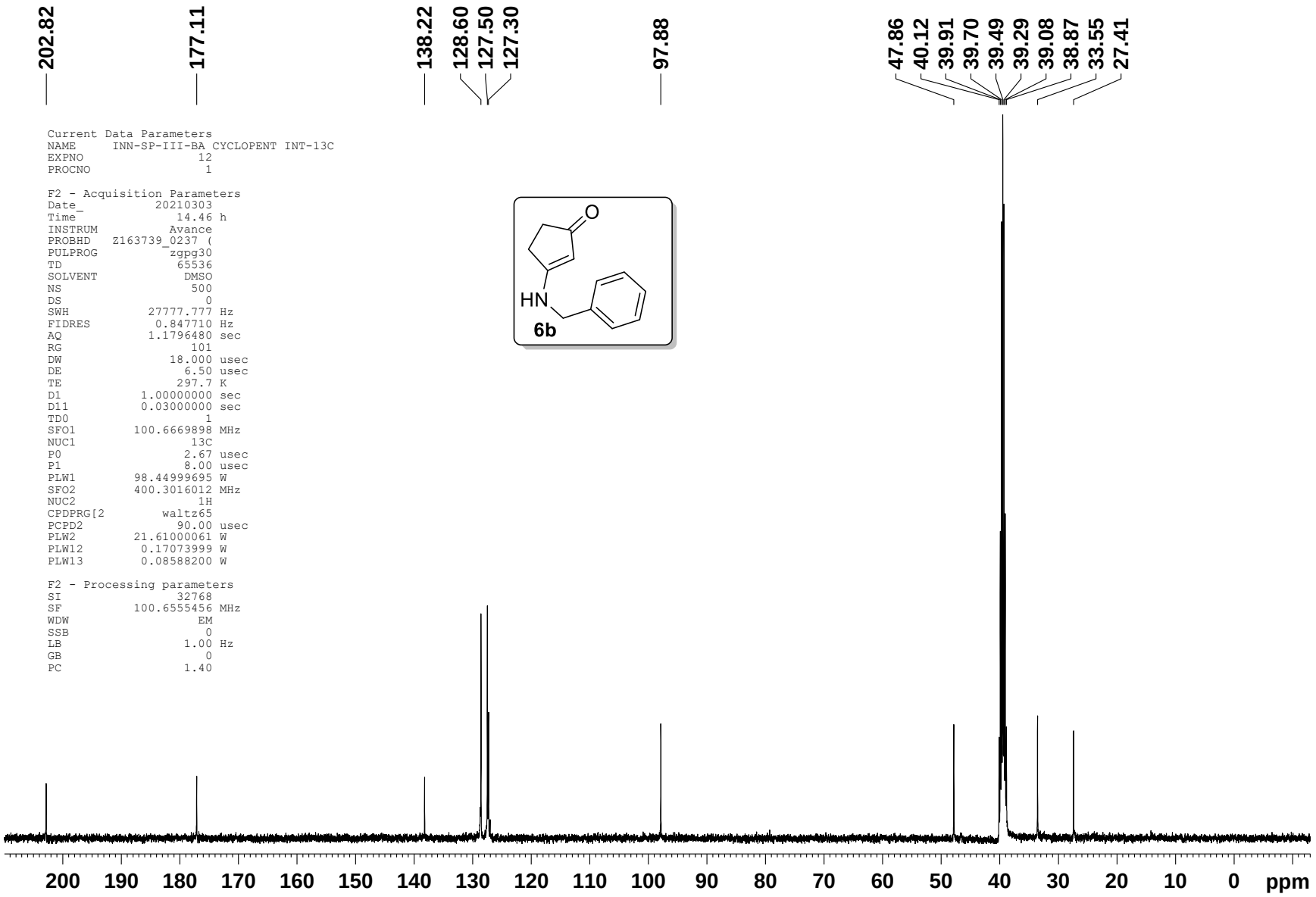


Figure S38: ^{13}C NMR spectrum of 6b.

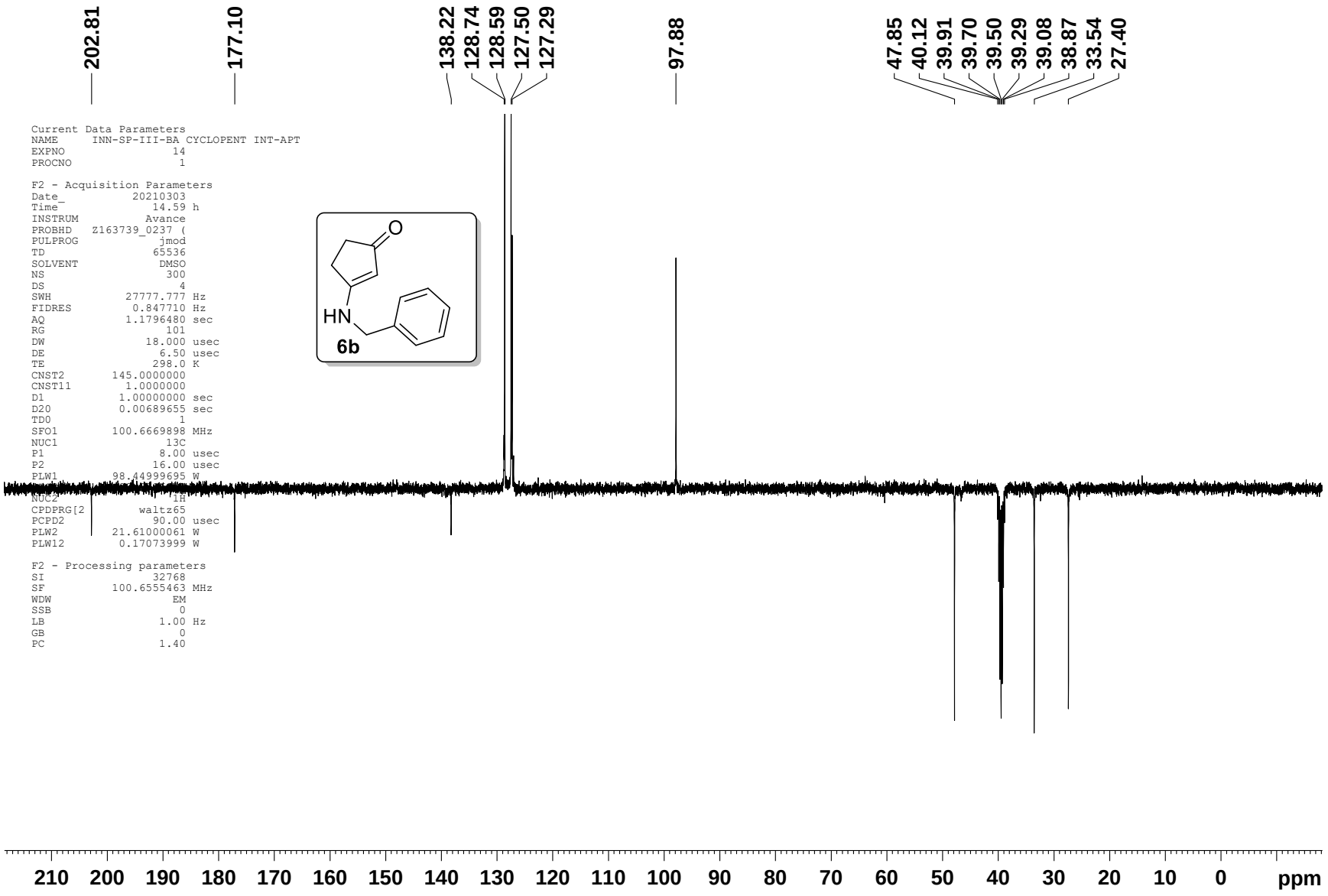


Figure S39: ^{13}C-APT NMR spectrum of 6b.

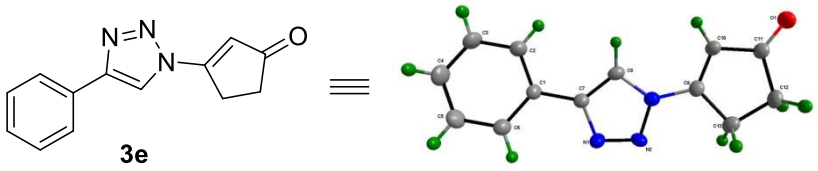


Figure S40: ORTEP diagram of 3e.

Table S1: Crystal table of 3e.

Identification code	Reflection List
Empirical formula	$C_{13}H_{11}N_3O$
Formula weight	225:25
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	5.890
b/Å	24.263
c/Å	7.661
α/°	90
β/°	99.67
γ/°	90
Volume/Å^3	1079.3
Z	4
ρ_{calc}g/cm^3	1.386
μ/mm^{-1}	0.092
F(000)	472.0
Crystal size/mm^3	0.230 × 0.110 × 0.050
Radiation	MoKα (λ = 0.71073)
2□ range for data collection/°	6.354 to 49.992

Index ranges	$? \leq \eta \leq ?, ? \leq \kappa \leq ?, ? \leq \lambda \leq ?$
Reflections collected	1881
Independent reflections	1881 [R_{int} = 0.0876, R_{sigma} = 0.1717]
Data/restraints/parameters	1881/0/154
Goodness-of-fit on F^2	0.960
Final R indexes [I>=2σ (I)]	R_1 = 0.0511, wR_2 = 0.1082
Final R indexes [all data]	R_1 = 0.1056, wR_2 = 0.1493
Largest diff. peak/hole / e $Å^{-3}$	0.58/-0.69