



Supporting Information

for

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

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and Irishi N. N. Namboothiri

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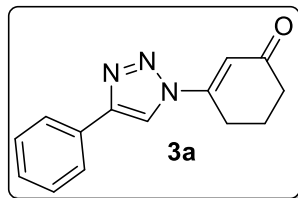
Copies of NMR spectra

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Current Data Parameters
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 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 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 =====
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 NUC1 1H
 P1 13.00 usec
 PLW1 13.00000000 W

F2 - Processing parameters
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 SF 500.1300118 MHz
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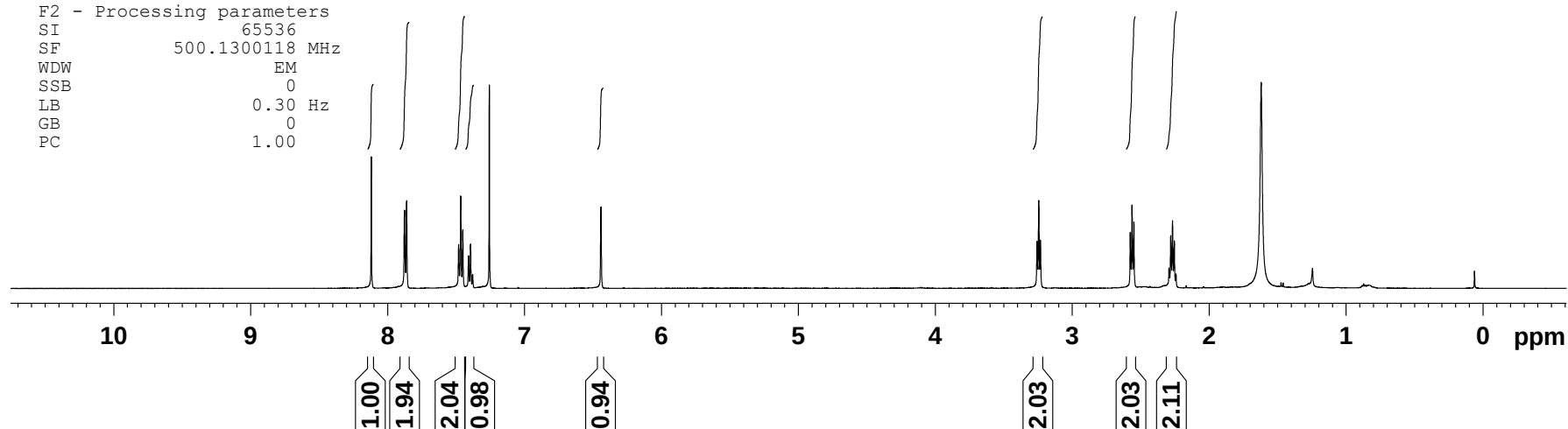


Figure S01: ¹H NMR spectrum of 3a.

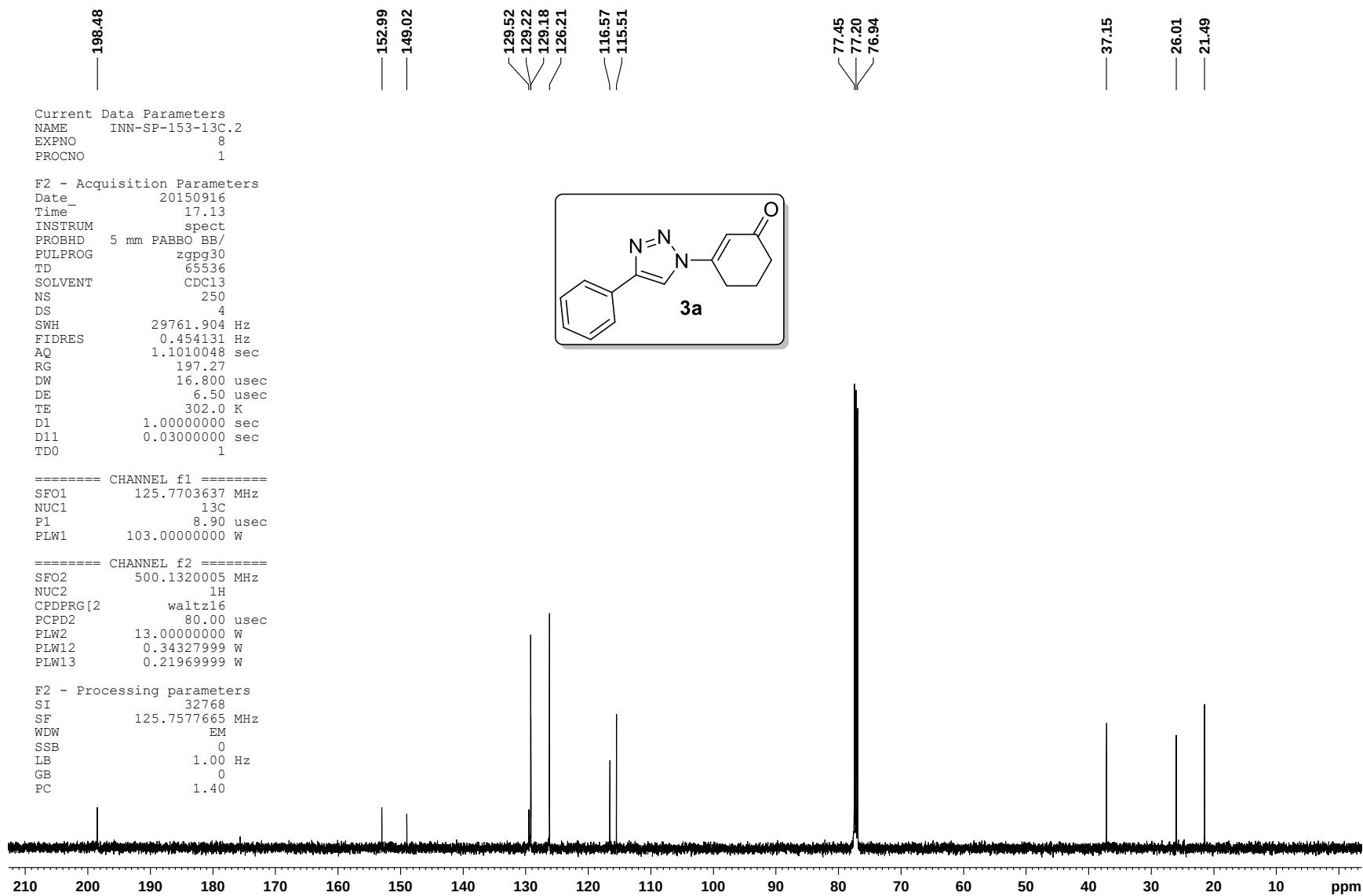


Figure S02: ^{13}C NMR spectrum of 3a.

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PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 7
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 297.4 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 500.1300130 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

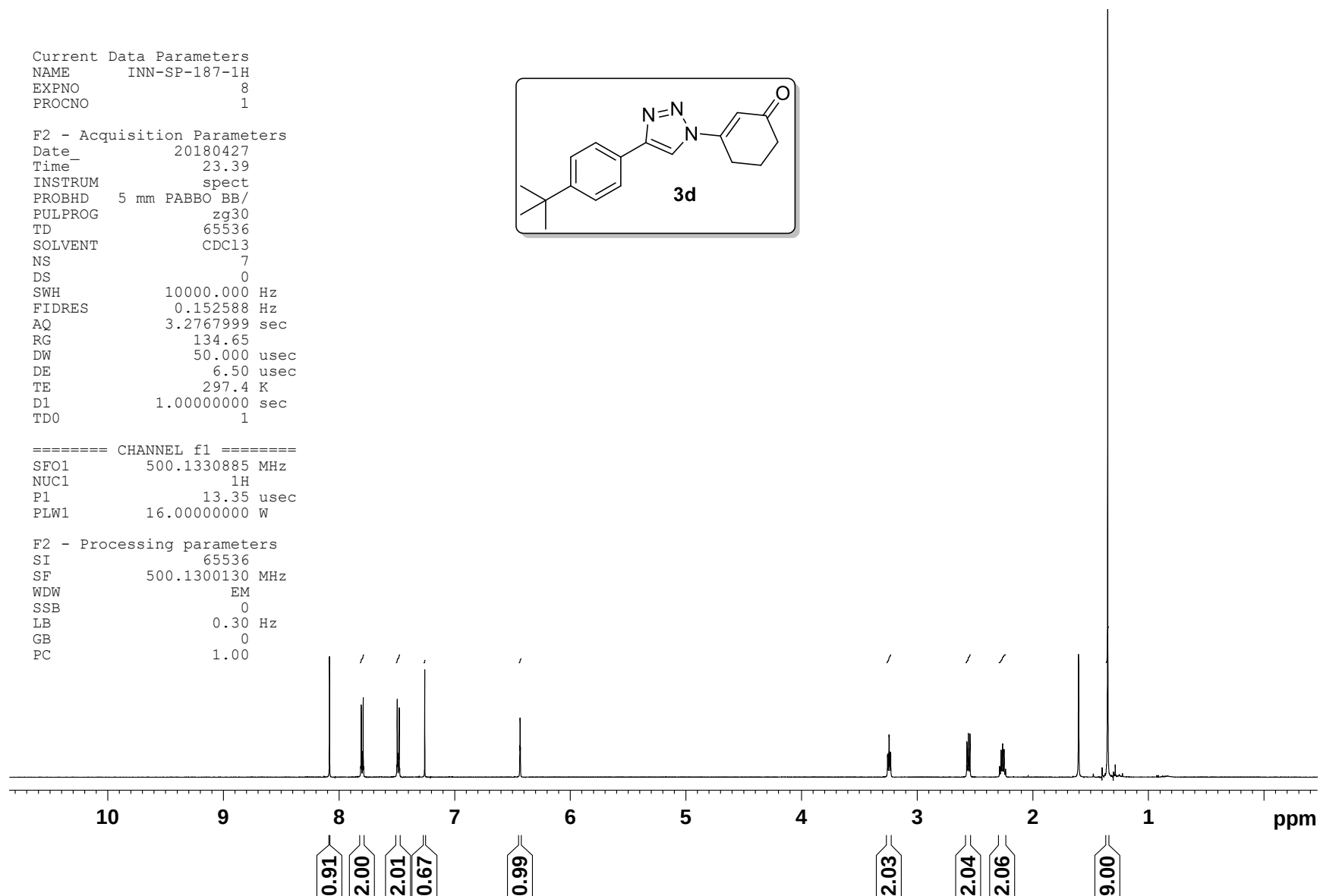
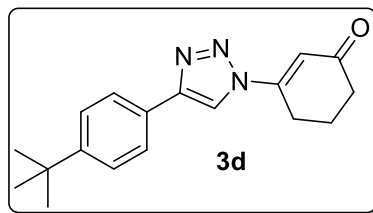


Figure S03: ^1H NMR spectrum of 3d.

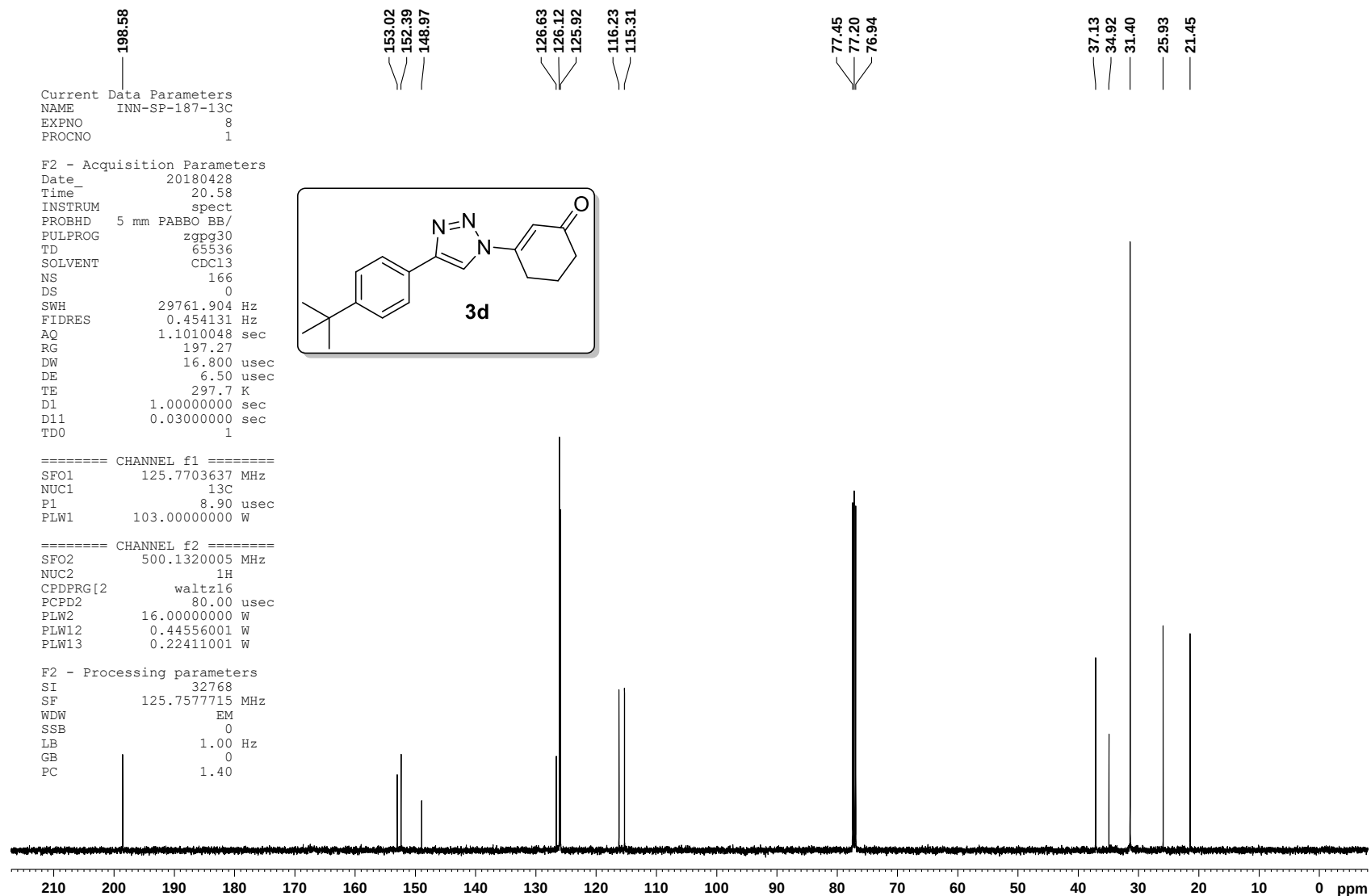
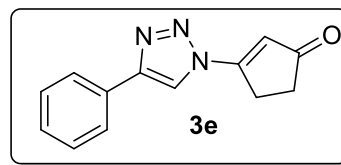


Figure S04: ^{13}C NMR spectrum of 3d.

Current Data Parameters
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 EXPNO 71
 PROCNO 1

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 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

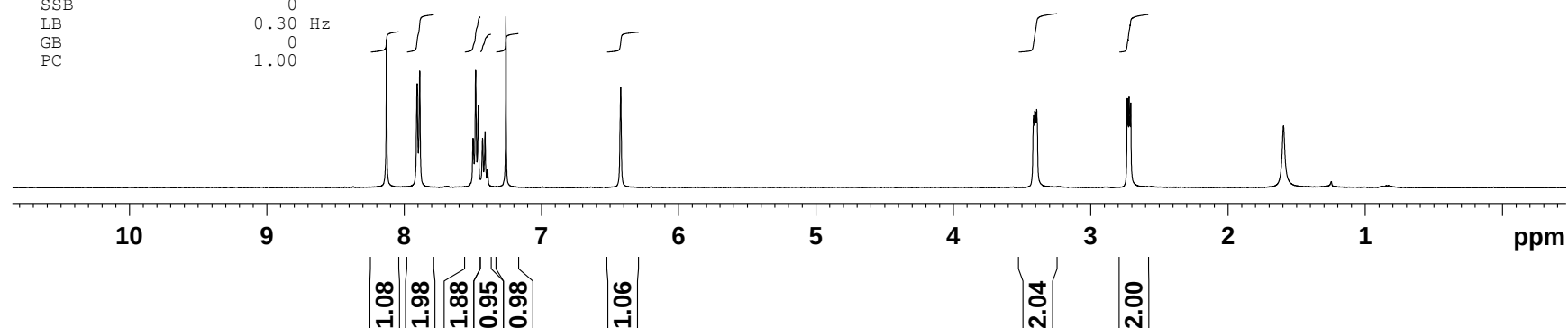


Figure S05: ¹H NMR spectrum of 3e.

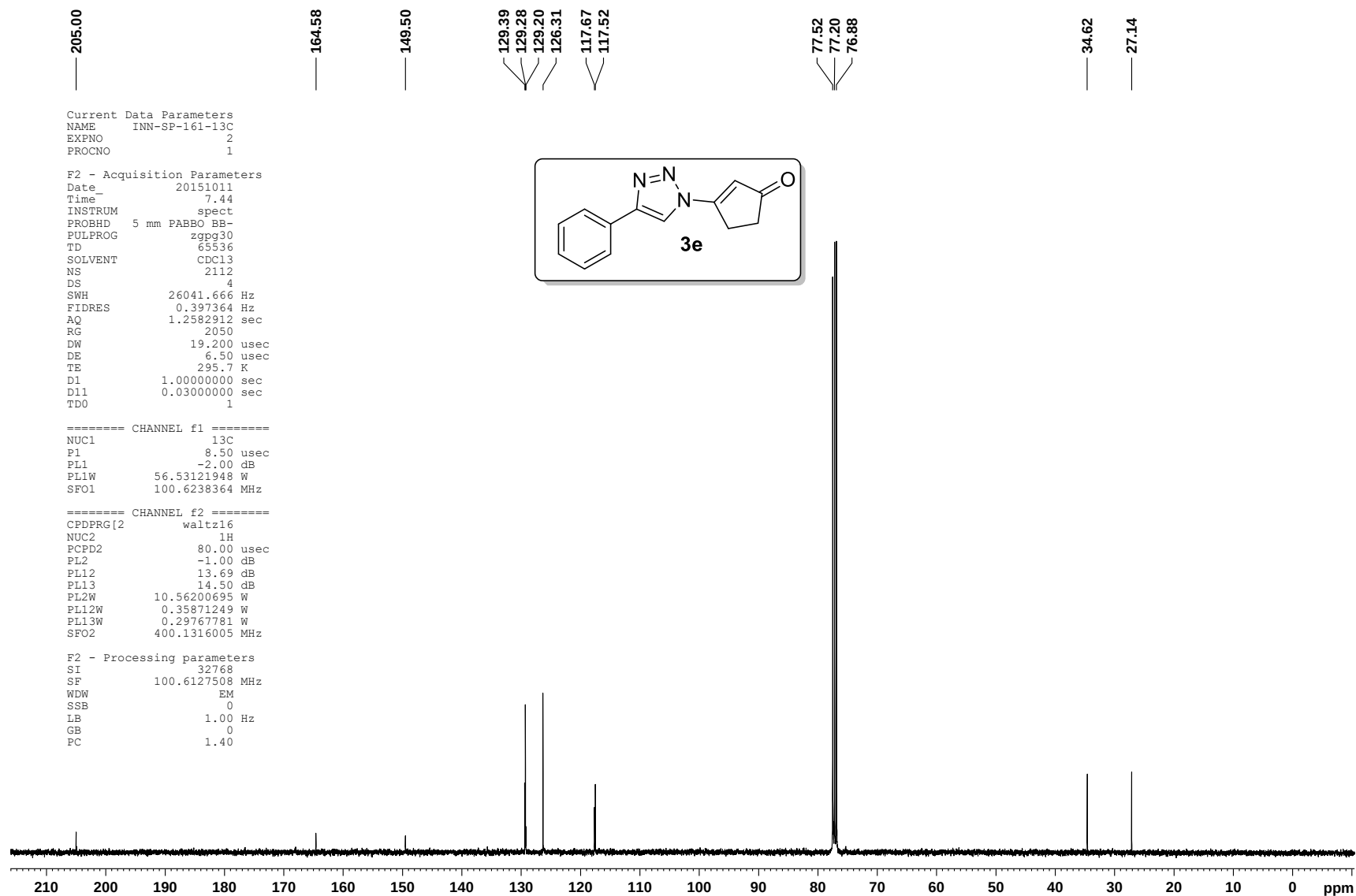
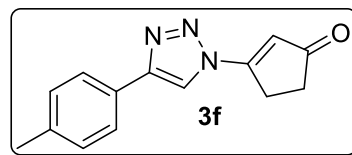


Figure S06: ^{13}C NMR spectrum of **3e**.

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

F2 - Acquisition Parameters
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 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

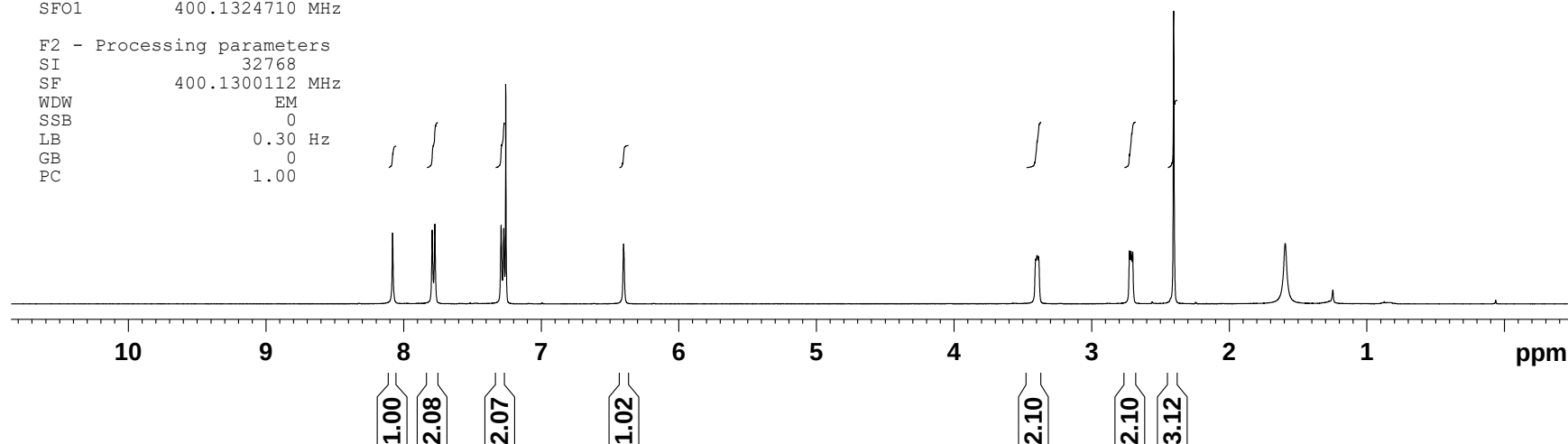


Figure S07: ¹H NMR spectrum of 3f.

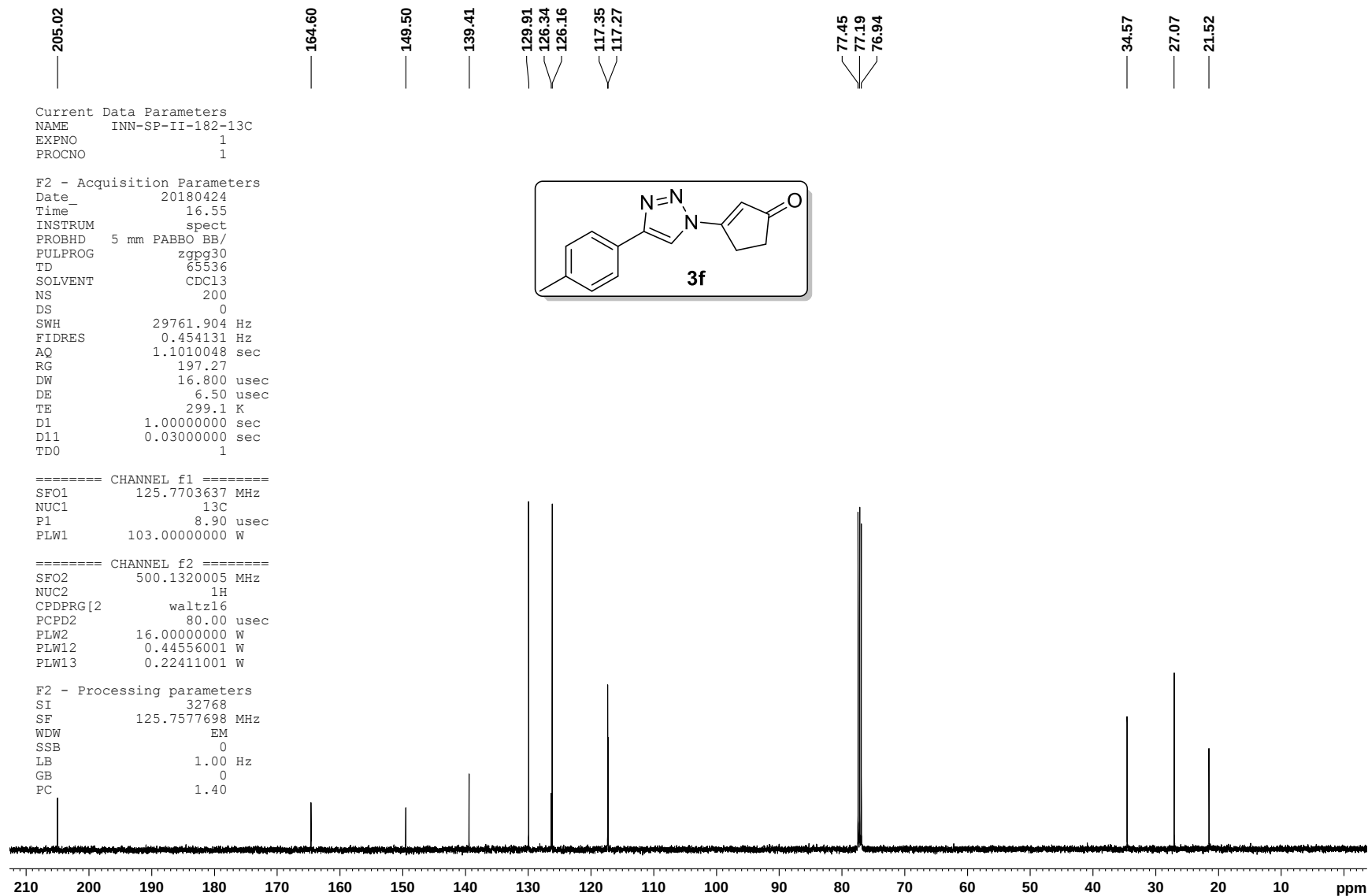


Figure S08: ^{13}C NMR spectrum of **3f**.

Current Data Parameters
NAME INN-SP-184-1H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151203
Time_ 18.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 11
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 296.9 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 500.1300124 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

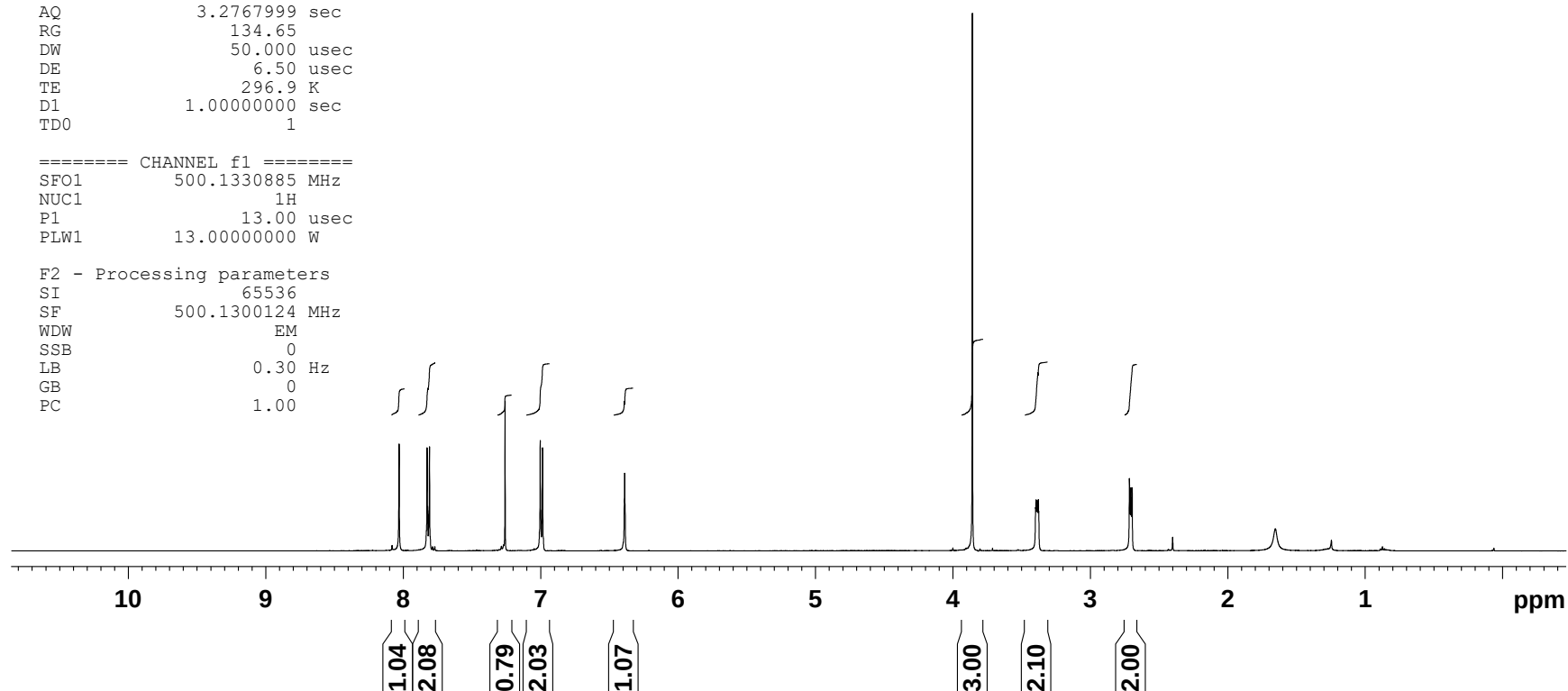
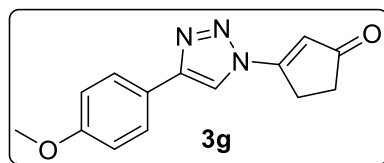


Figure S09: ^1H NMR spectrum of 3g.

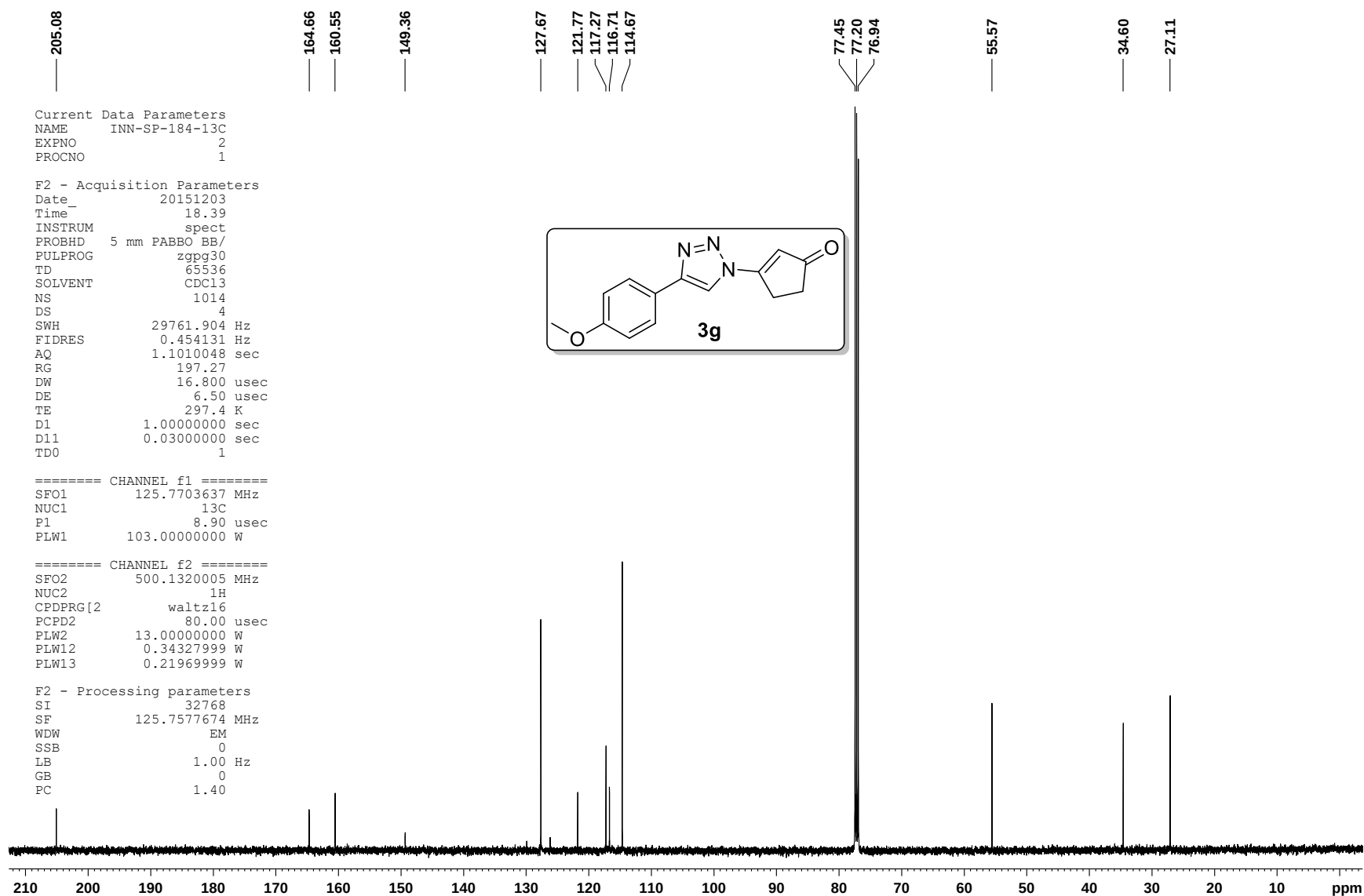


Figure S10: ^{13}C NMR spectrum of 3g.

Current Data Parameters
 NAME INN-SP-III-METHOXY-TRIAVALXNE-1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180925
 Time 19.36
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 10
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 119.07
 DW 50.000 usec
 DE 6.50 usec
 TE 297.8 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 500.1300133 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

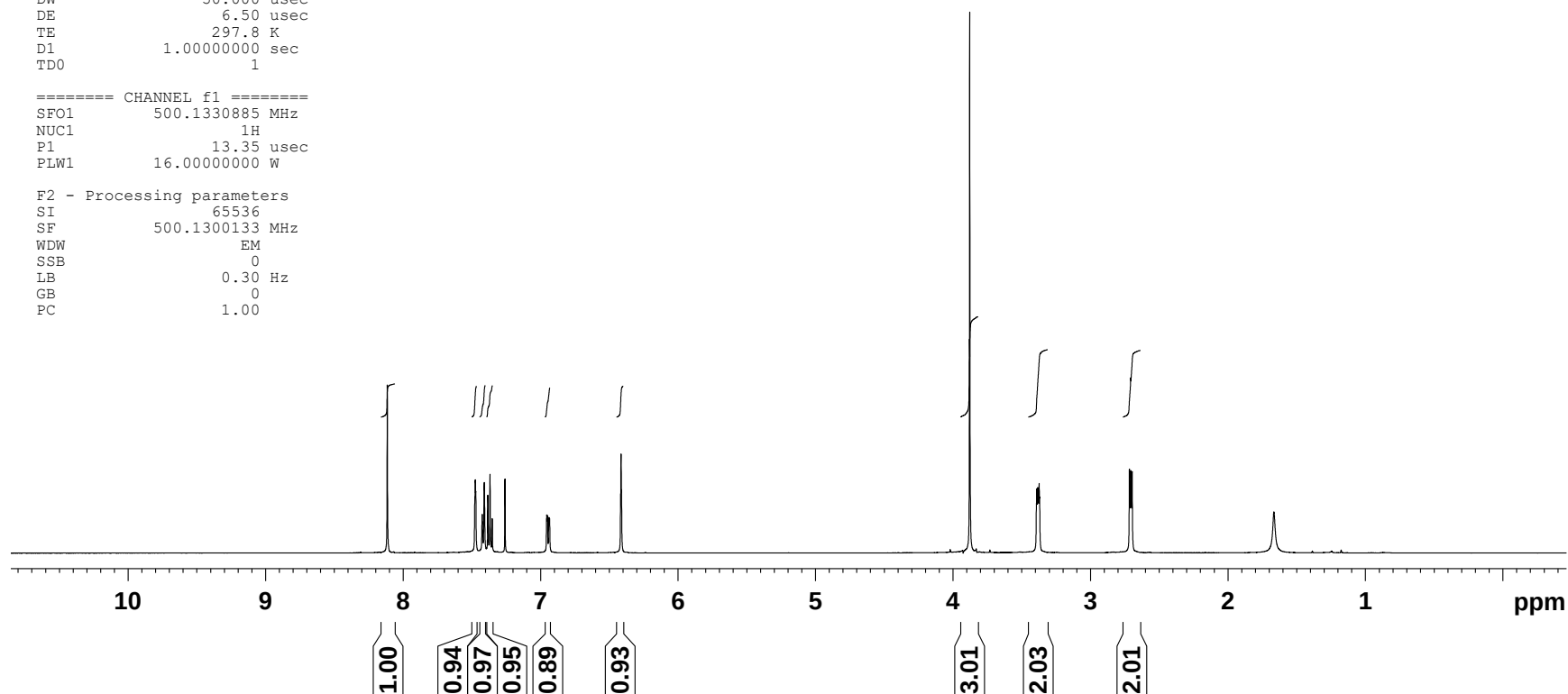
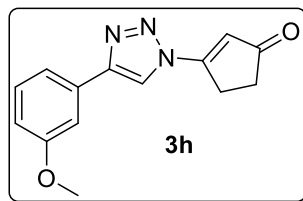


Figure S11: ¹H NMR spectrum of 3h.

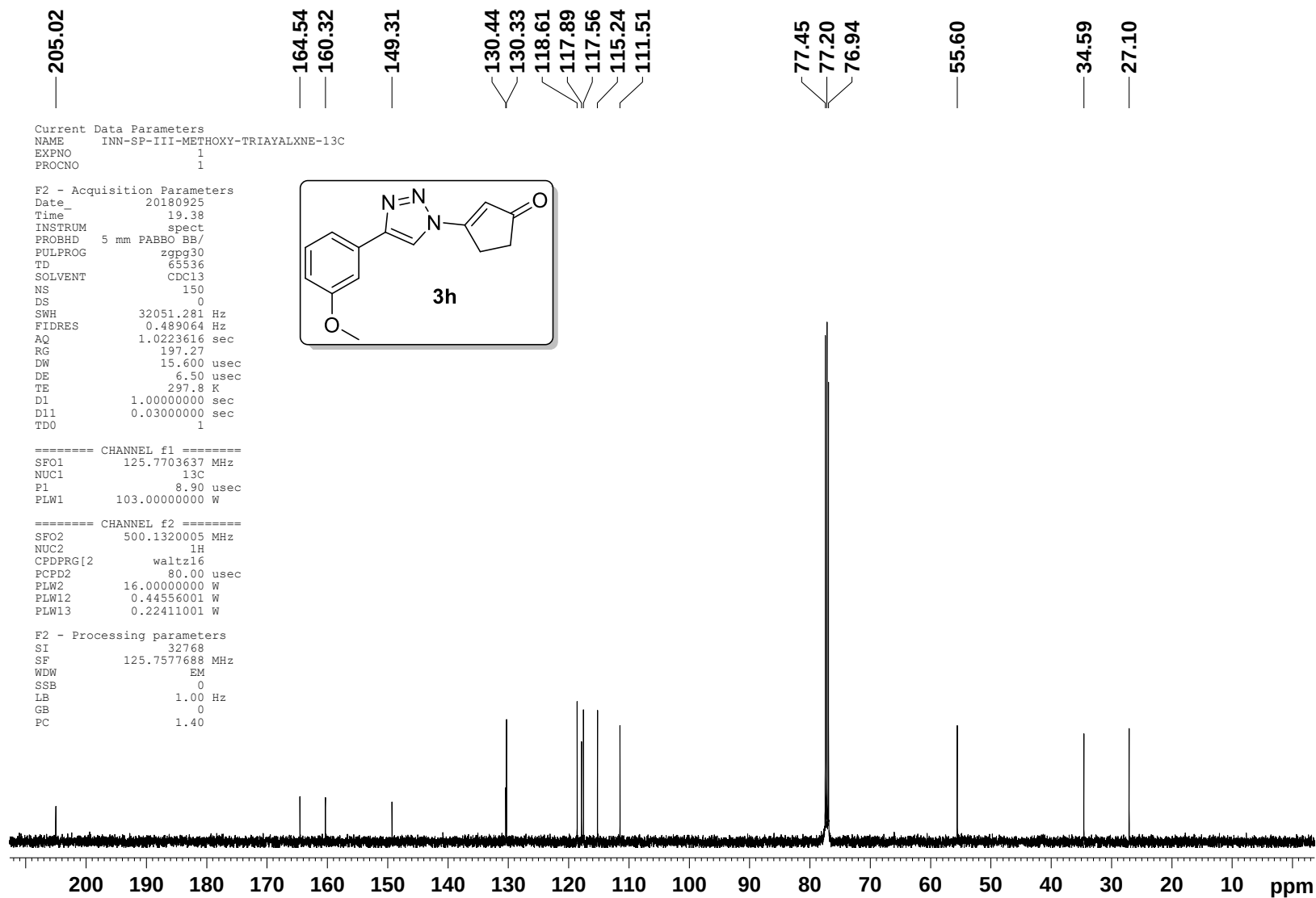


Figure S12: ^{13}C NMR spectrum of 3h.

Current Data Parameters
NAME INN-SP-186-1H
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151204
Time_ 20.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 30.72
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 500.1300123 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

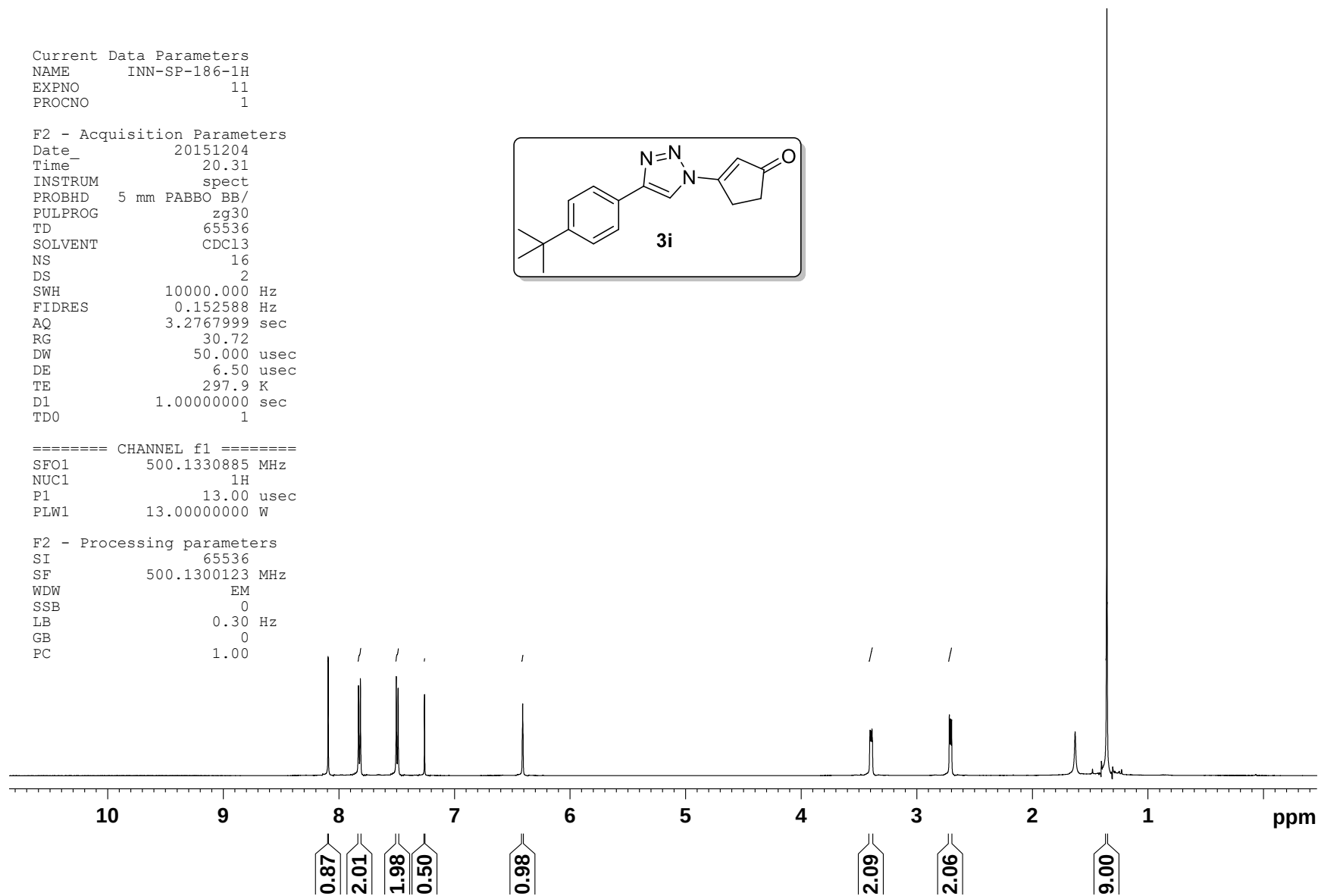
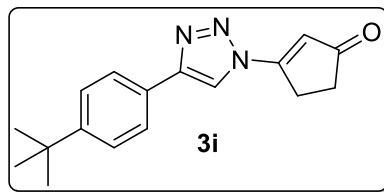


Figure S13: ¹H NMR spectrum of **3i**.

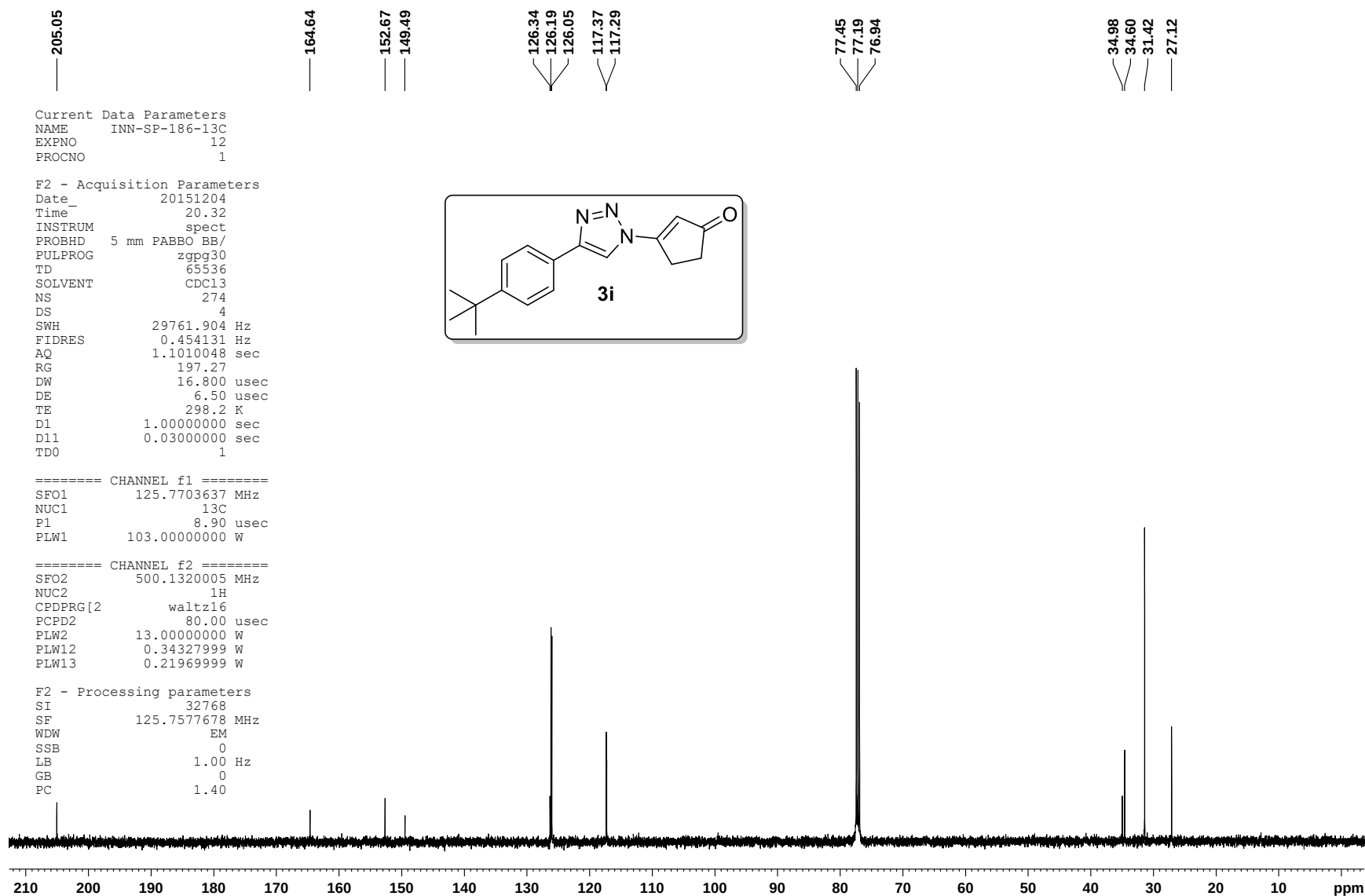
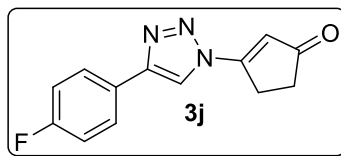


Figure S14: ^{13}C NMR spectrum of **3i**.

Current Data Parameters
 NAME INN-SP-III-89-1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180525
 Time_ 7.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 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

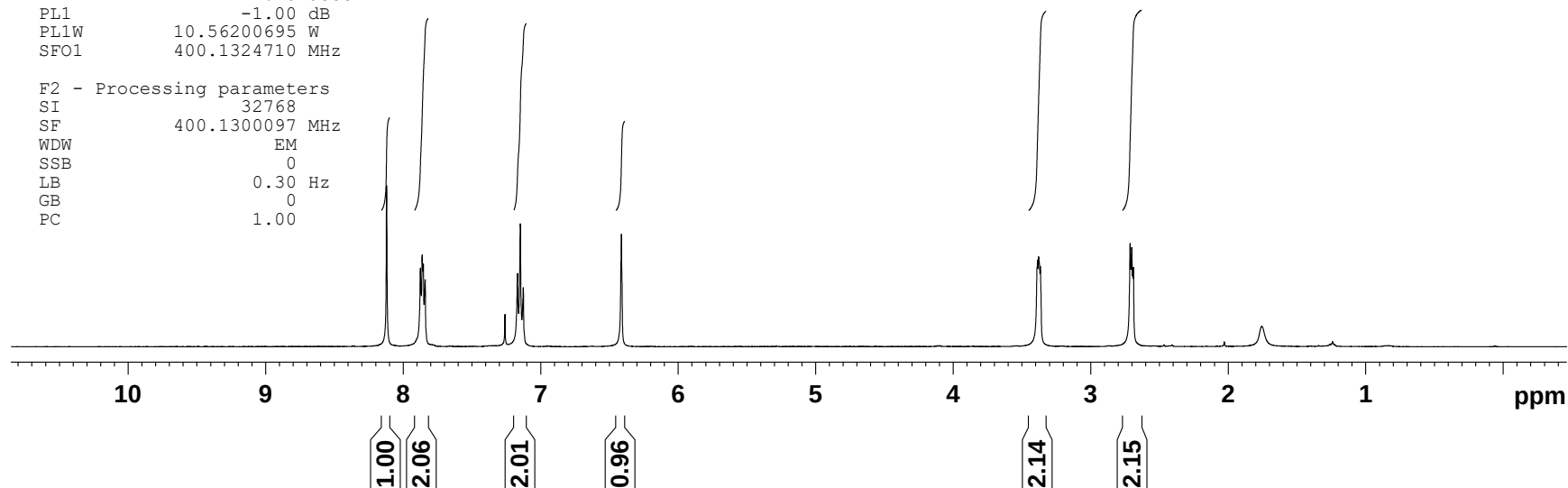


Figure S15: ¹H NMR spectrum of 3j.

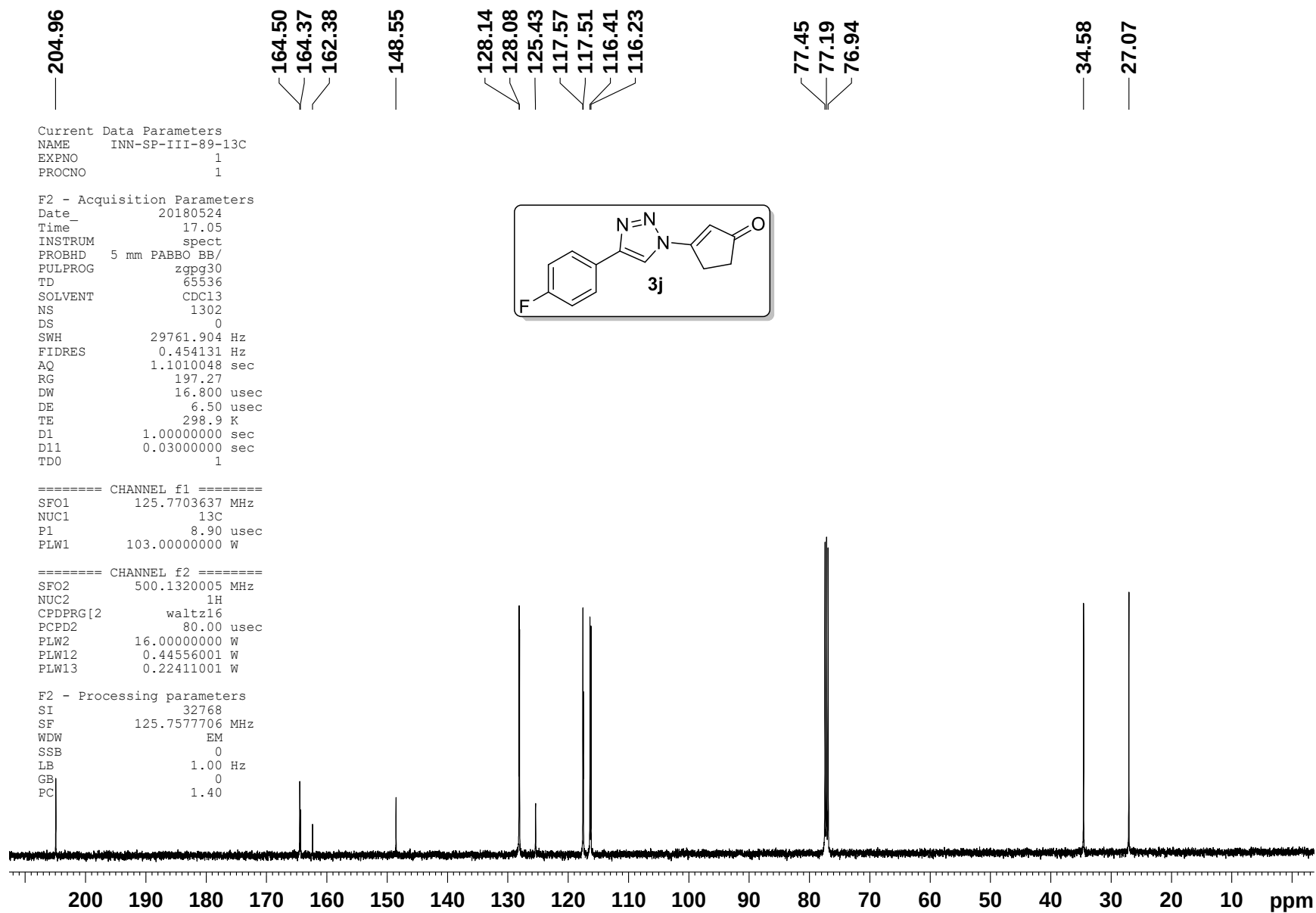


Figure S16: ^{13}C NMR spectrum of **3j**.

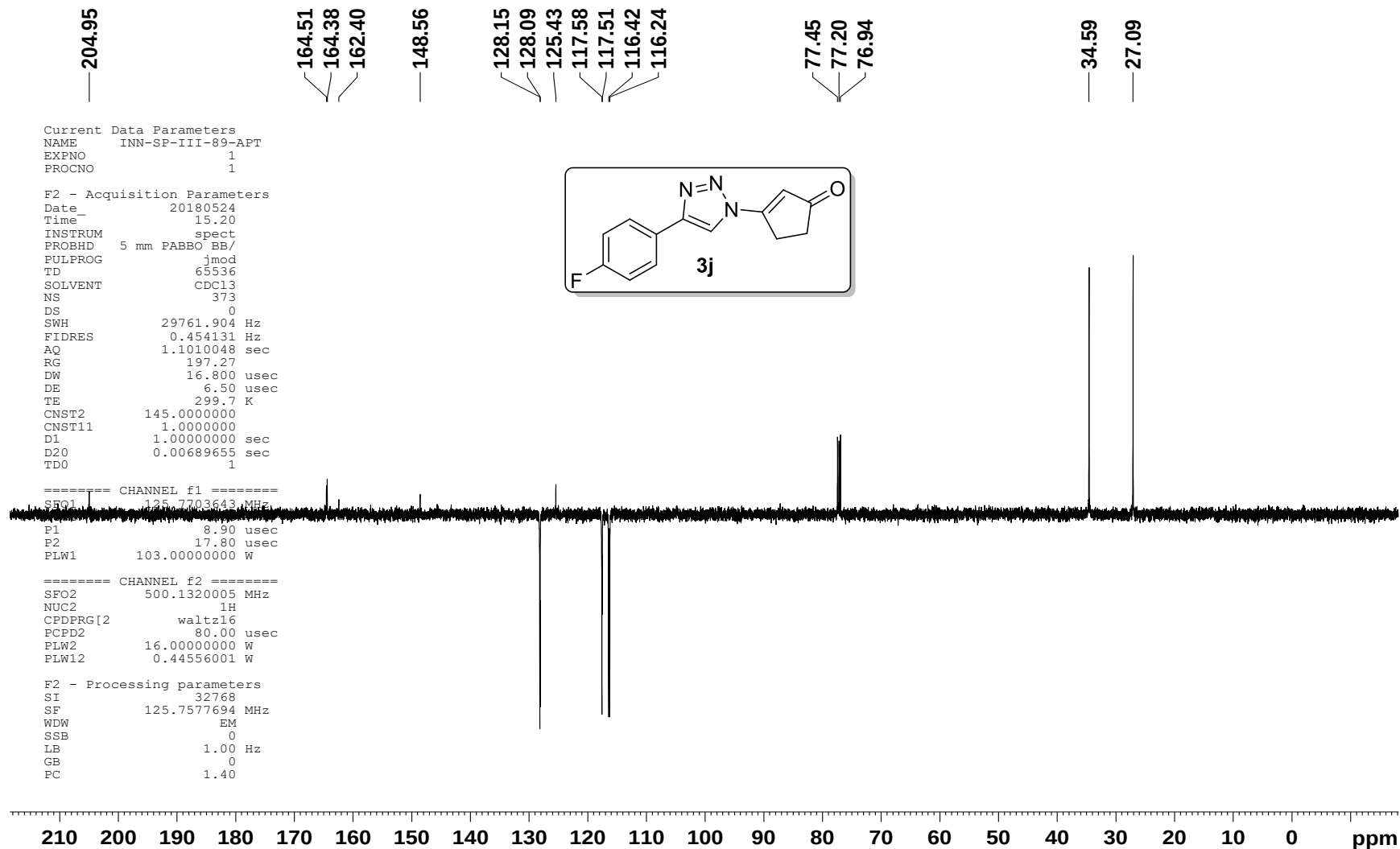


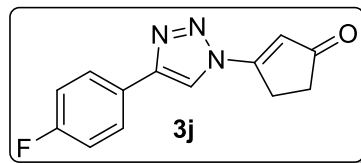
Figure S17: ¹³C-APT NMR spectrum of 3j.

Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time_ 15.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgflqn
TD 131072
SOLVENT CDC13
NS 13
DS 0
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767168 sec
RG 197.27
DW 4.400 usec
DE 6.50 usec
TE 299.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 470.5453180 MHz
NUC1 19F
P1 19.75 usec
PLW1 55.00000000 W

F2 - Processing parameters
SI 65536
SF 470.5923770 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



-111.65

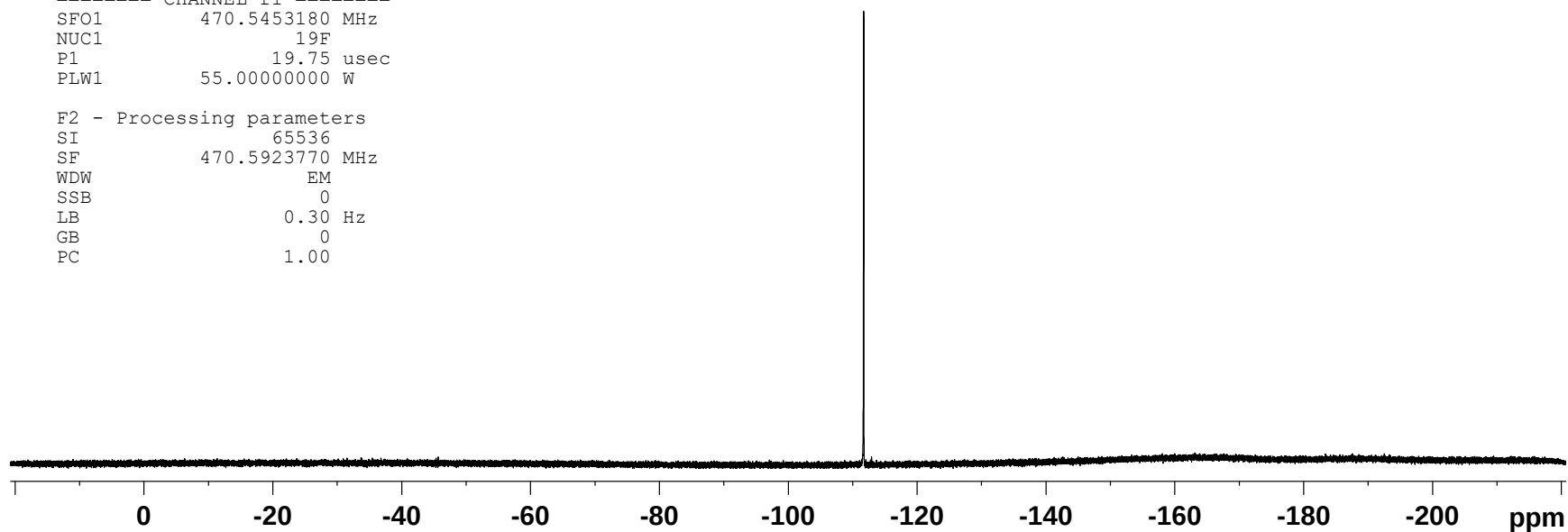
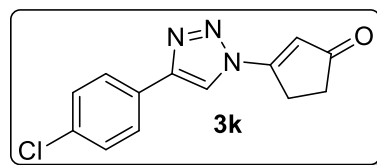


Figure S18: ¹⁹F NMR spectrum of 3j.

Current Data Parameters
 NAME INN-SP-III-85-1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180524
 Time_ 13.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 9
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 177.33
 DW 50.000 usec
 DE 6.50 usec
 TE 300.1 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 500.1300132 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

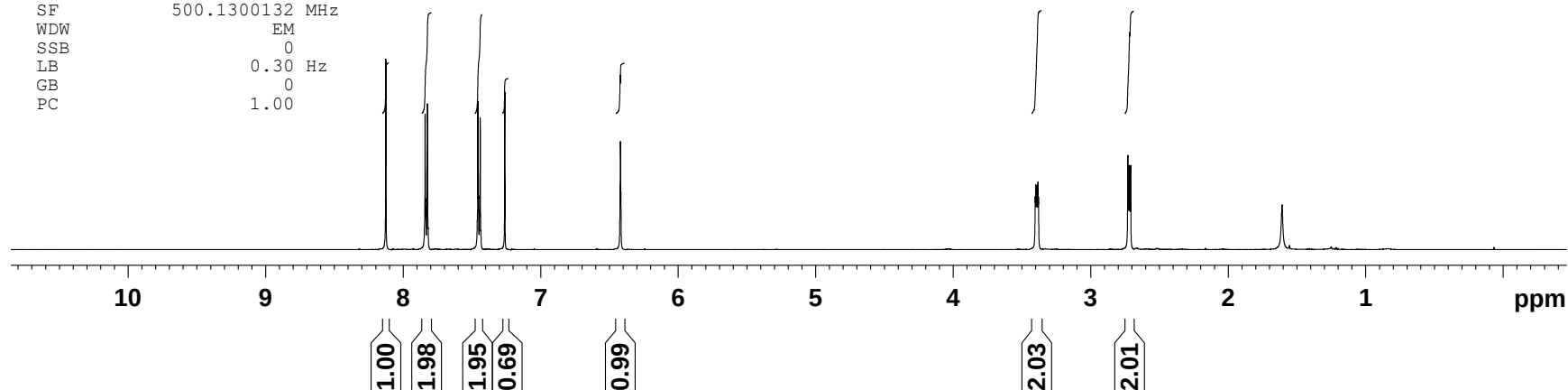


Figure S19: ¹H NMR spectrum of 3k.

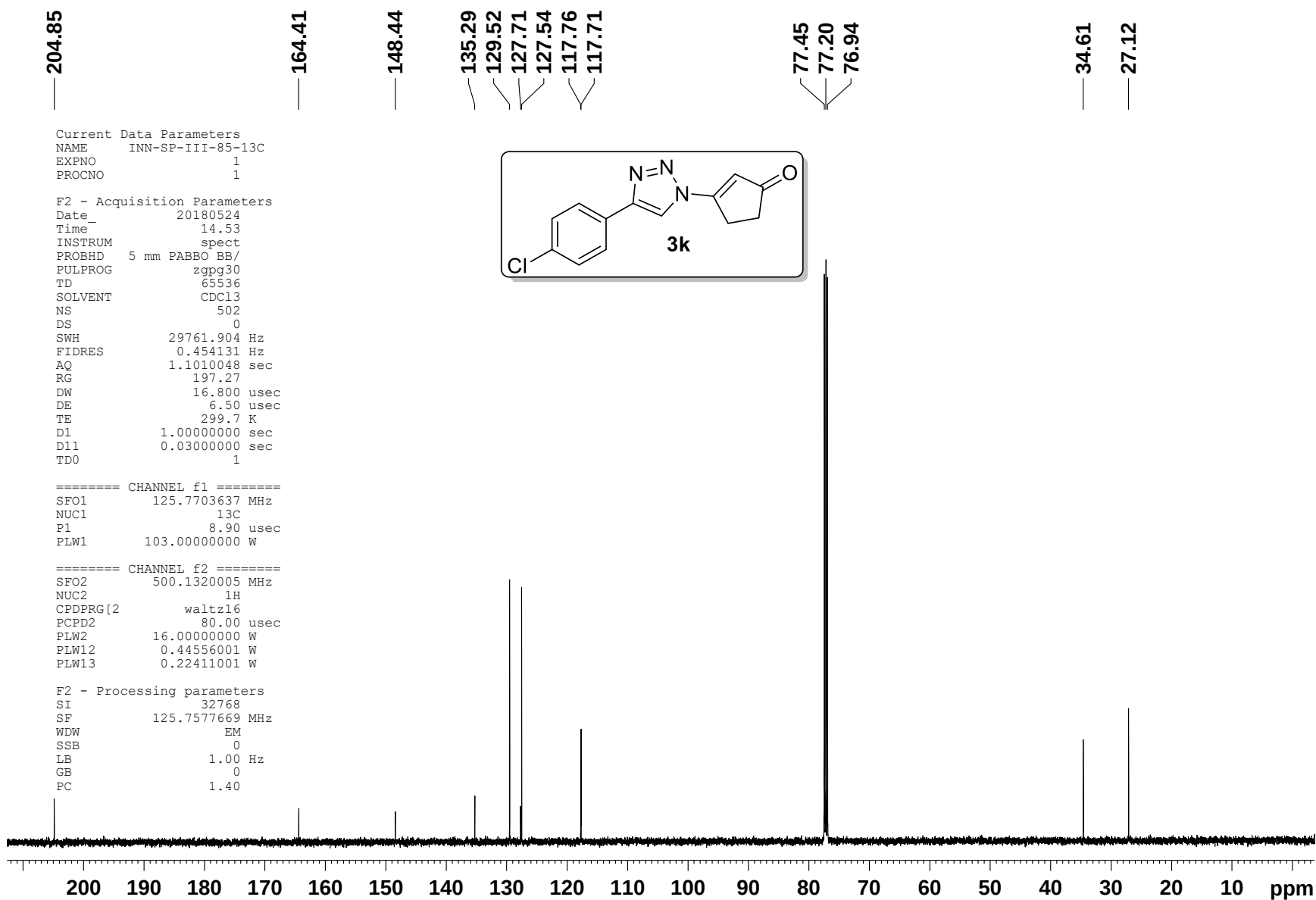


Figure S20: ^{13}C NMR spectrum of 3k.

Current Data Parameters
NAME INN-SP-III-86-1H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180523
Time_ 15.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 61.42
DW 50.000 usec
DE 6.50 usec
TE 298.0 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 500.1300077 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

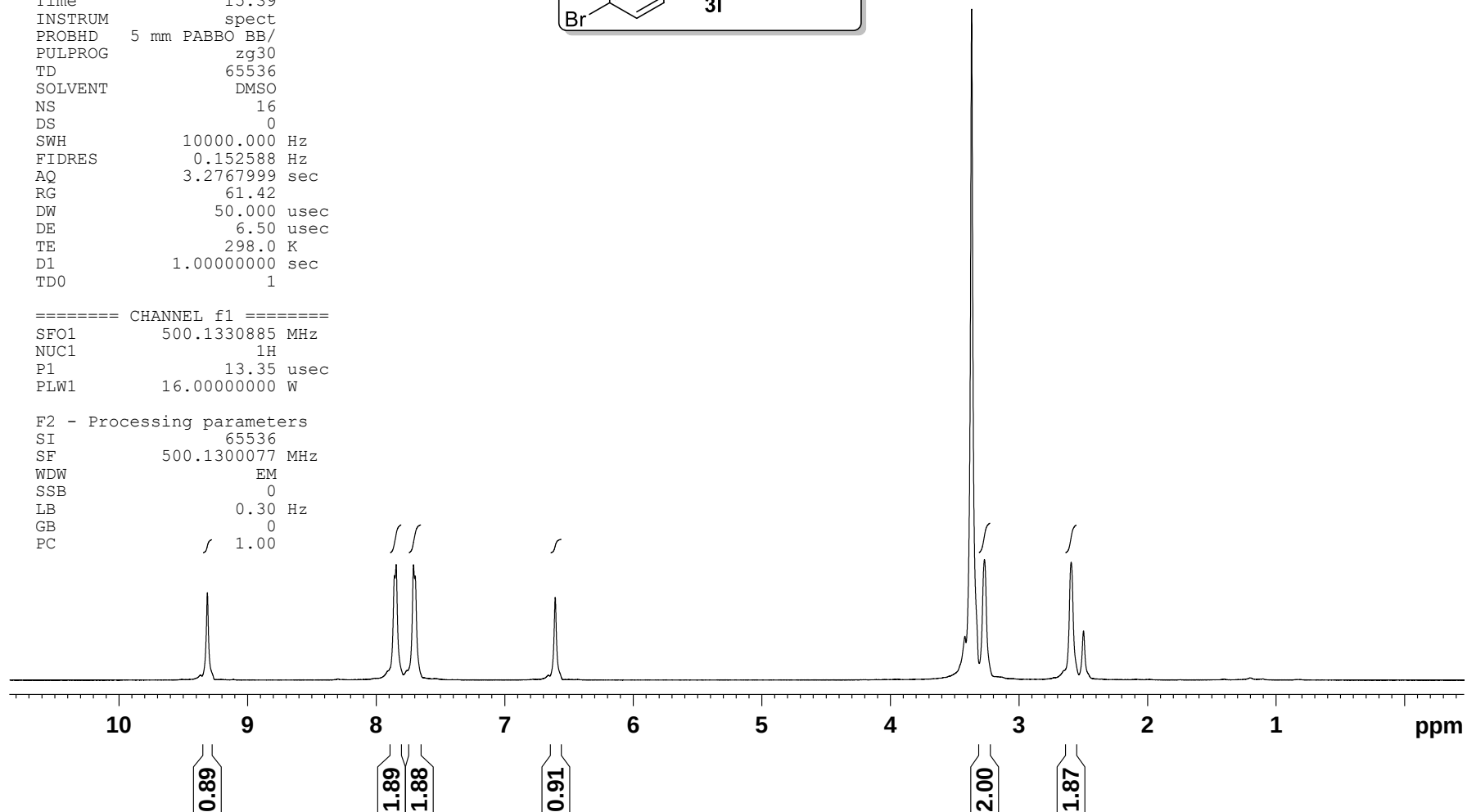
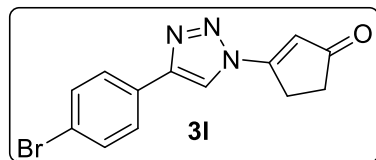


Figure S21: ¹H NMR spectrum of 3I.

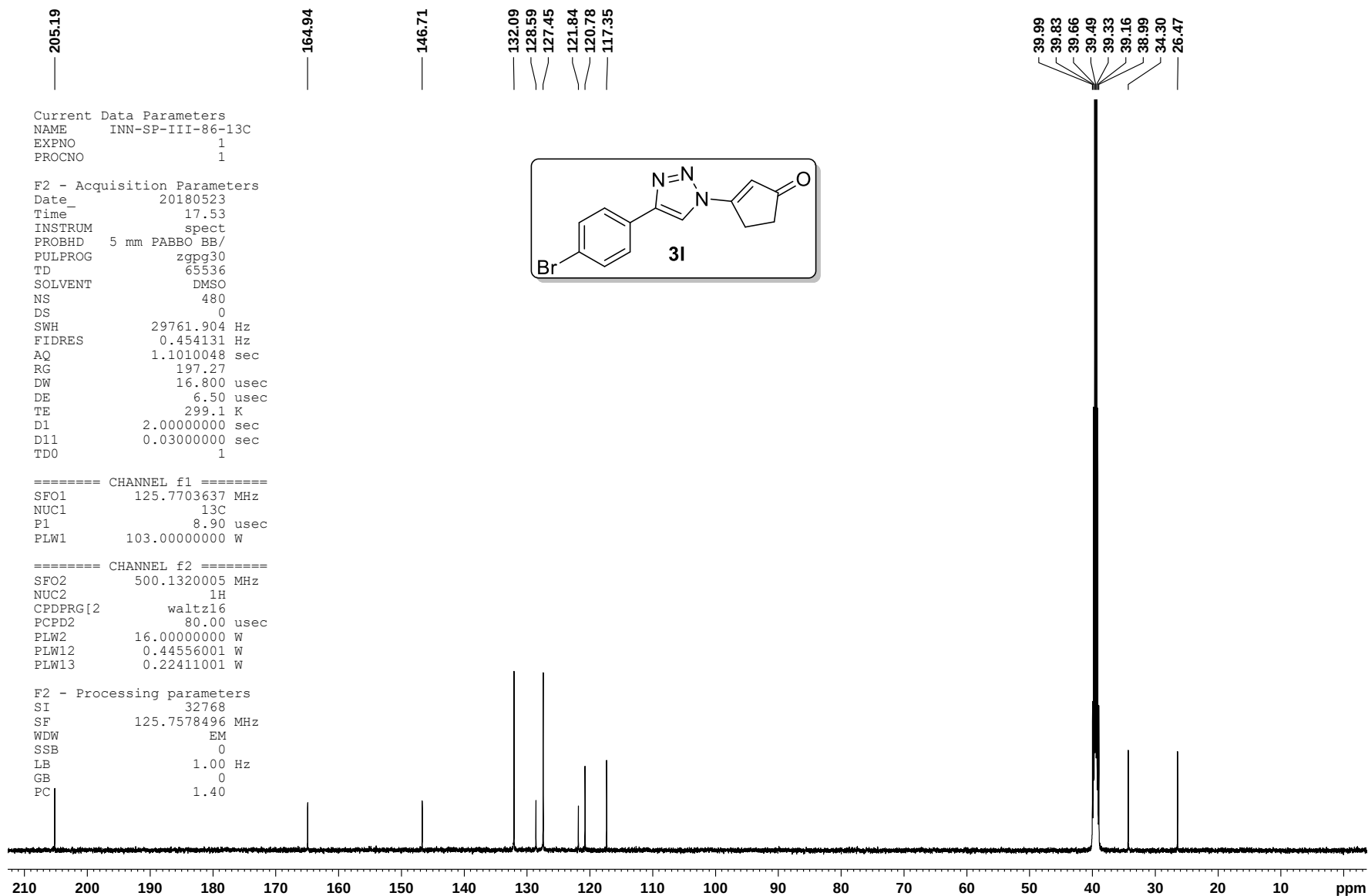


Figure S22: ^{13}C NMR spectrum of **3l**.

Current Data Parameters
NAME INN-SP-II-10-1H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180506
Time_ 20.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 106.54
DW 50.000 usec
DE 6.50 usec
TE 297.4 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 500.1304281 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

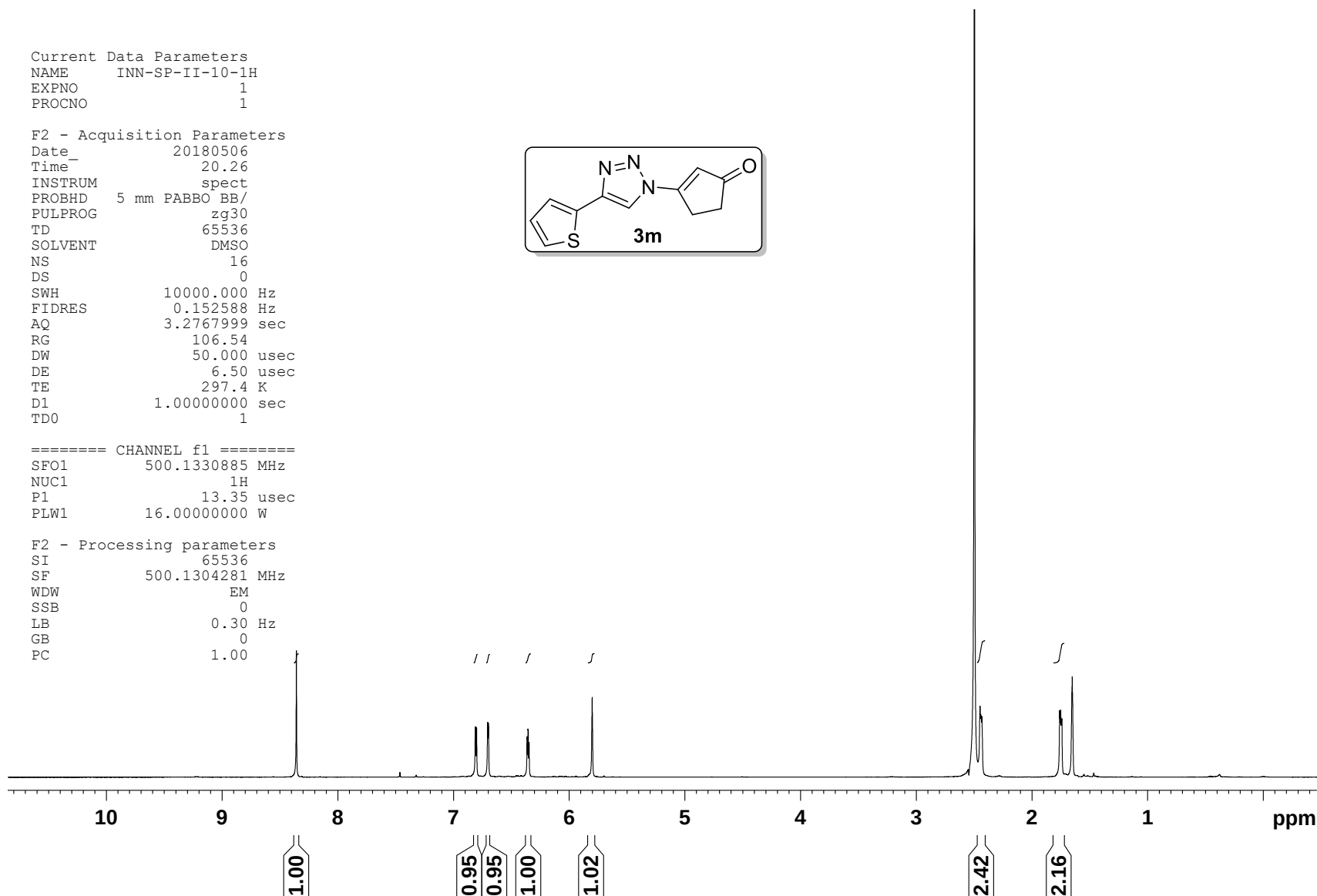
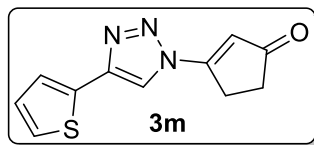


Figure S23: ¹H NMR spectrum of 3m.

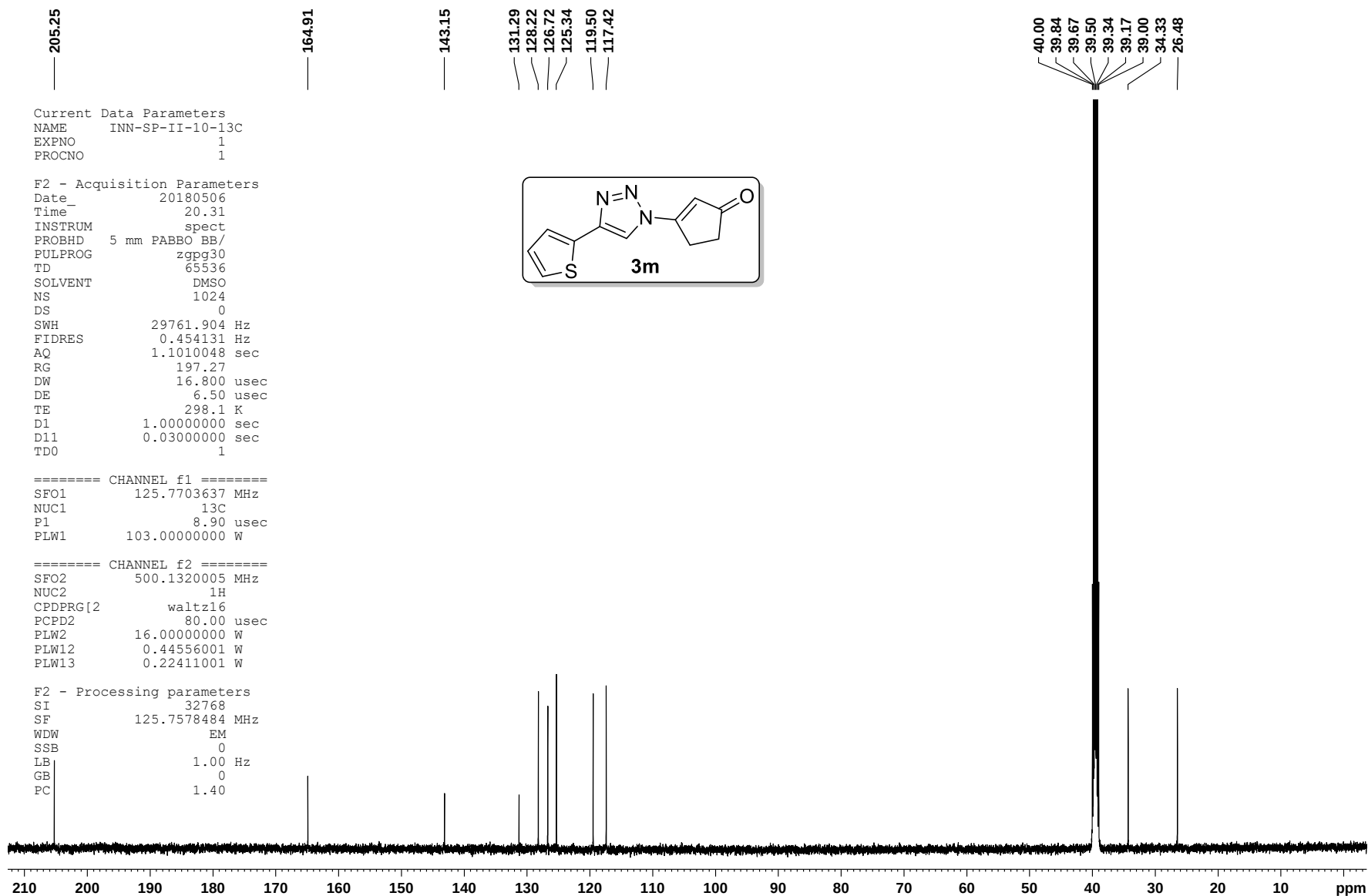


Figure S24: ^{13}C NMR spectrum of 3m.

Current Data Parameters
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 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
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 Time_ 15.41
 INSTRUM spect
 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

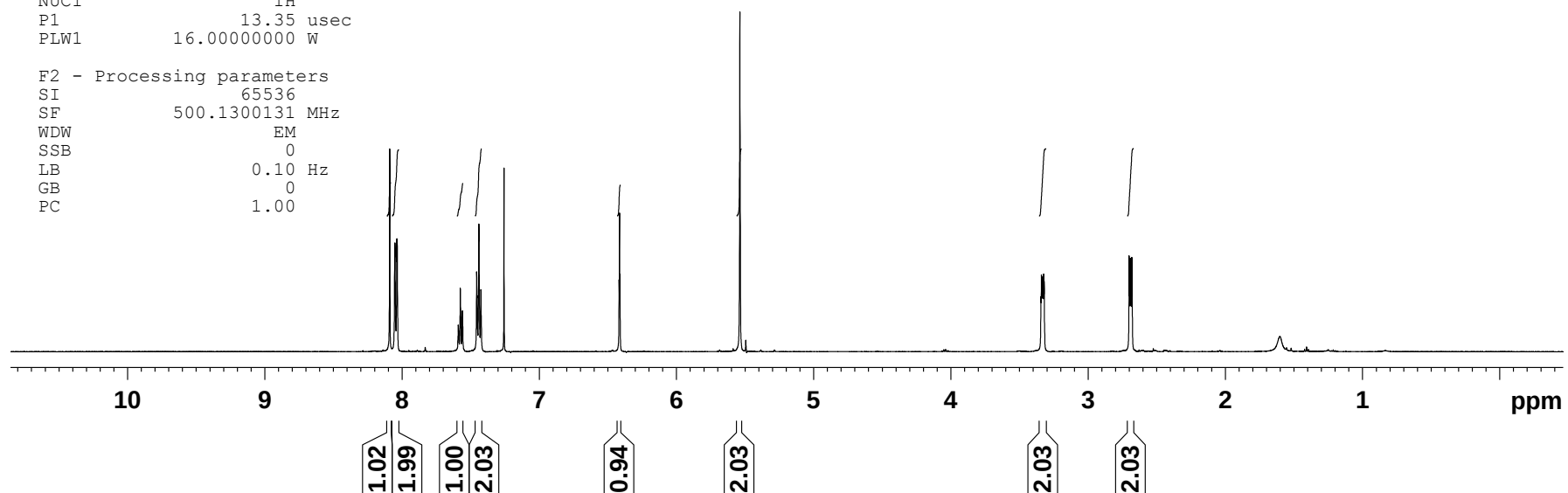
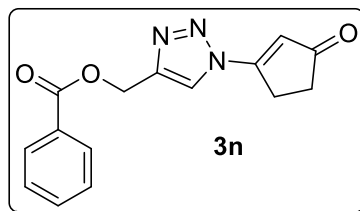


Figure S25: ¹H NMR spectrum of 3n.

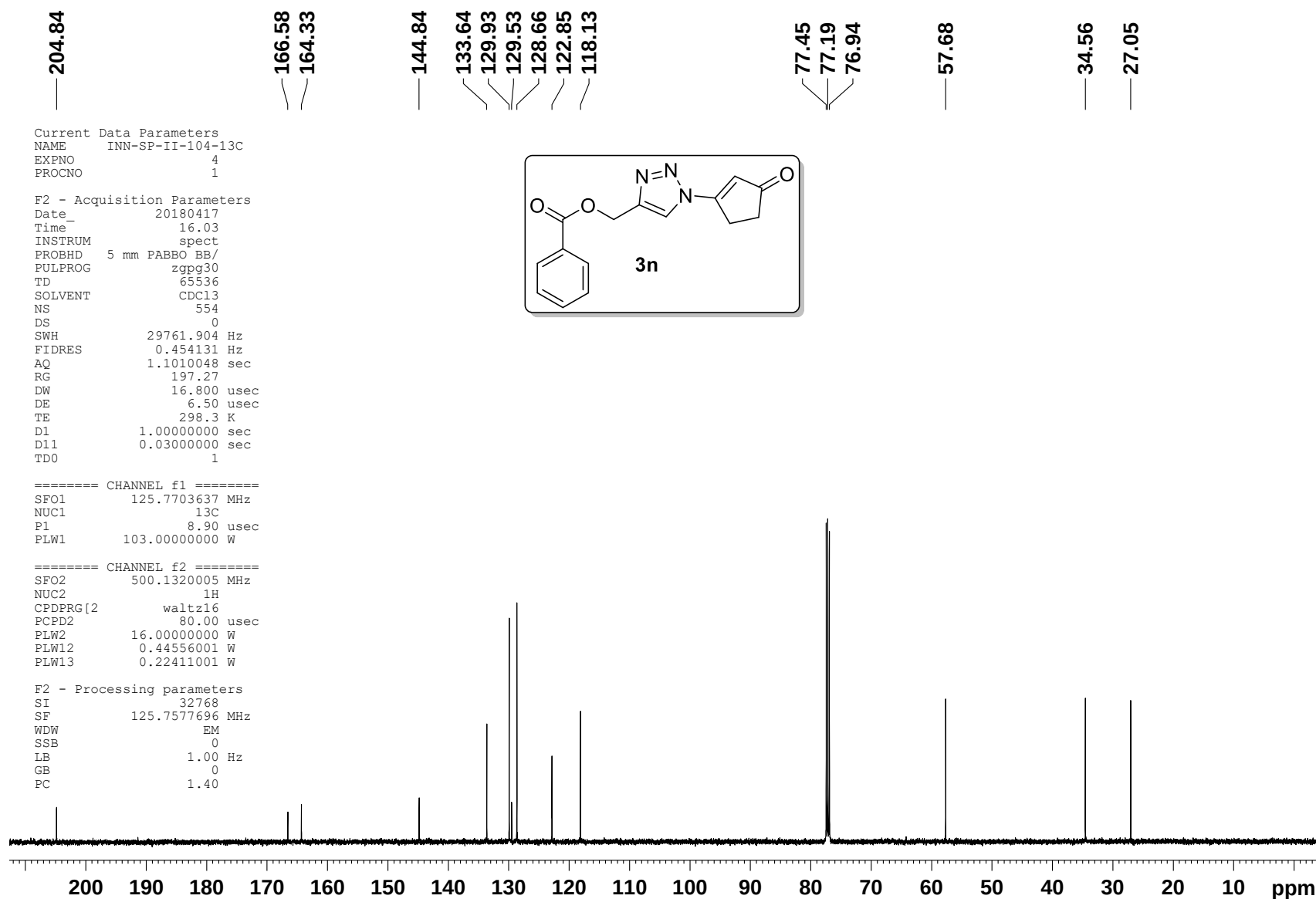


Figure S26: ^{13}C NMR spectrum of **3n**.

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

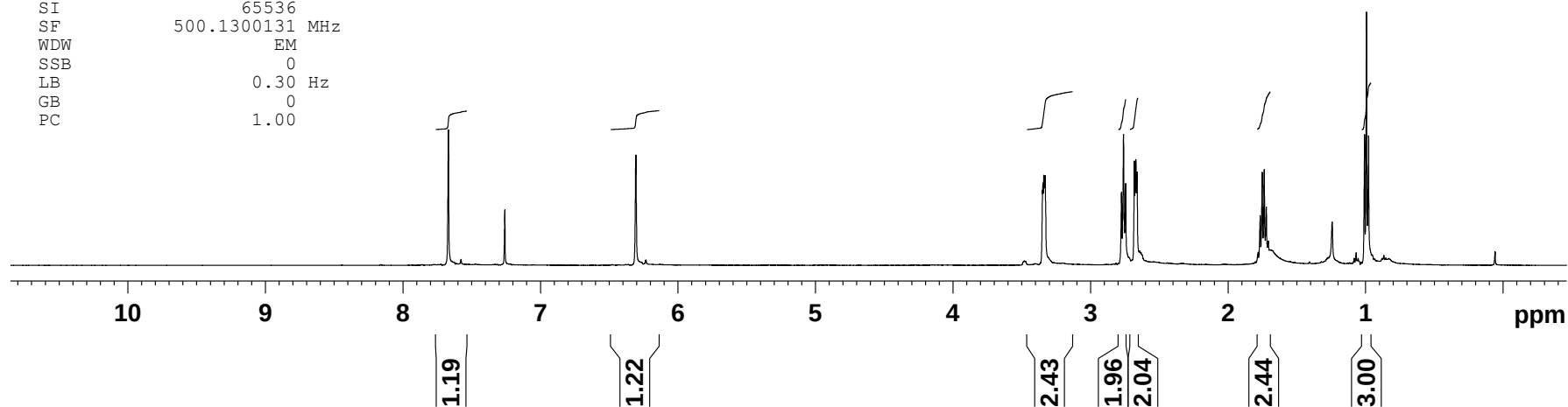
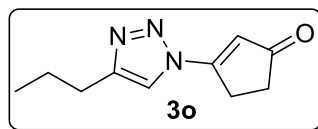


Figure S27: ^1H NMR spectrum of 3o.

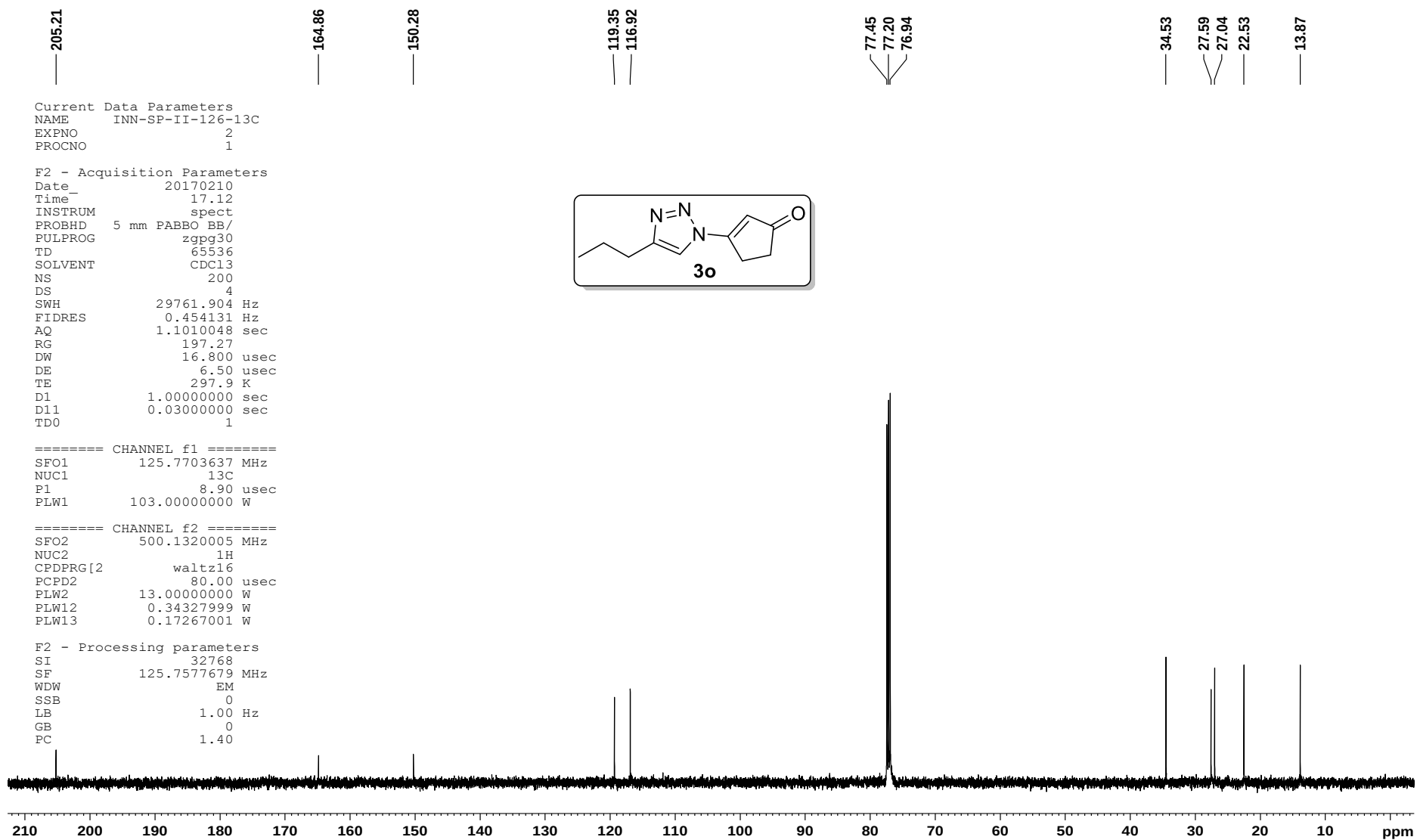
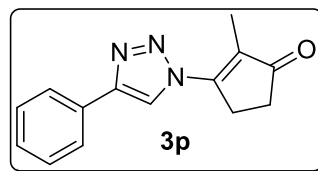


Figure S28: ^{13}C NMR spectrum of **3o**.

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

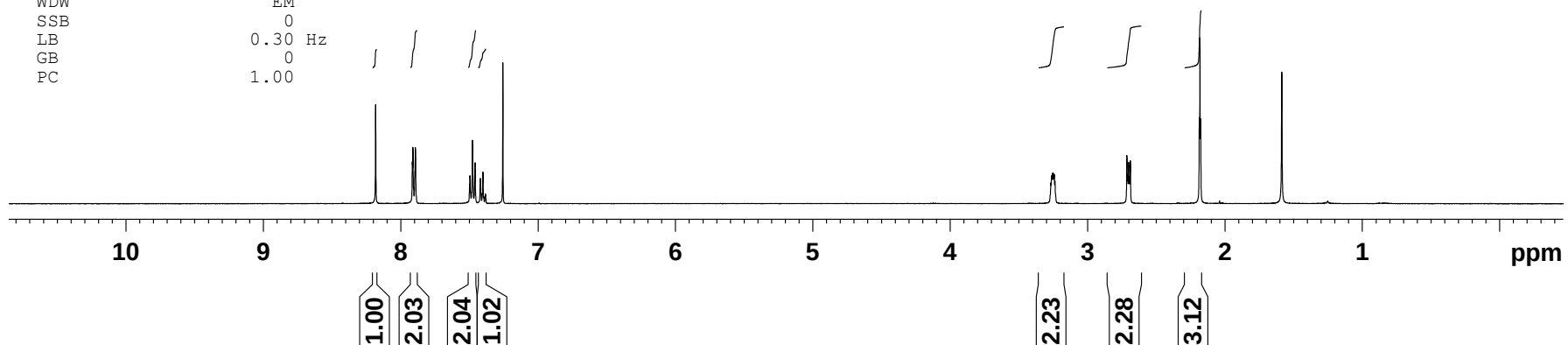


Figure S29: ¹H NMR spectrum of 3p.

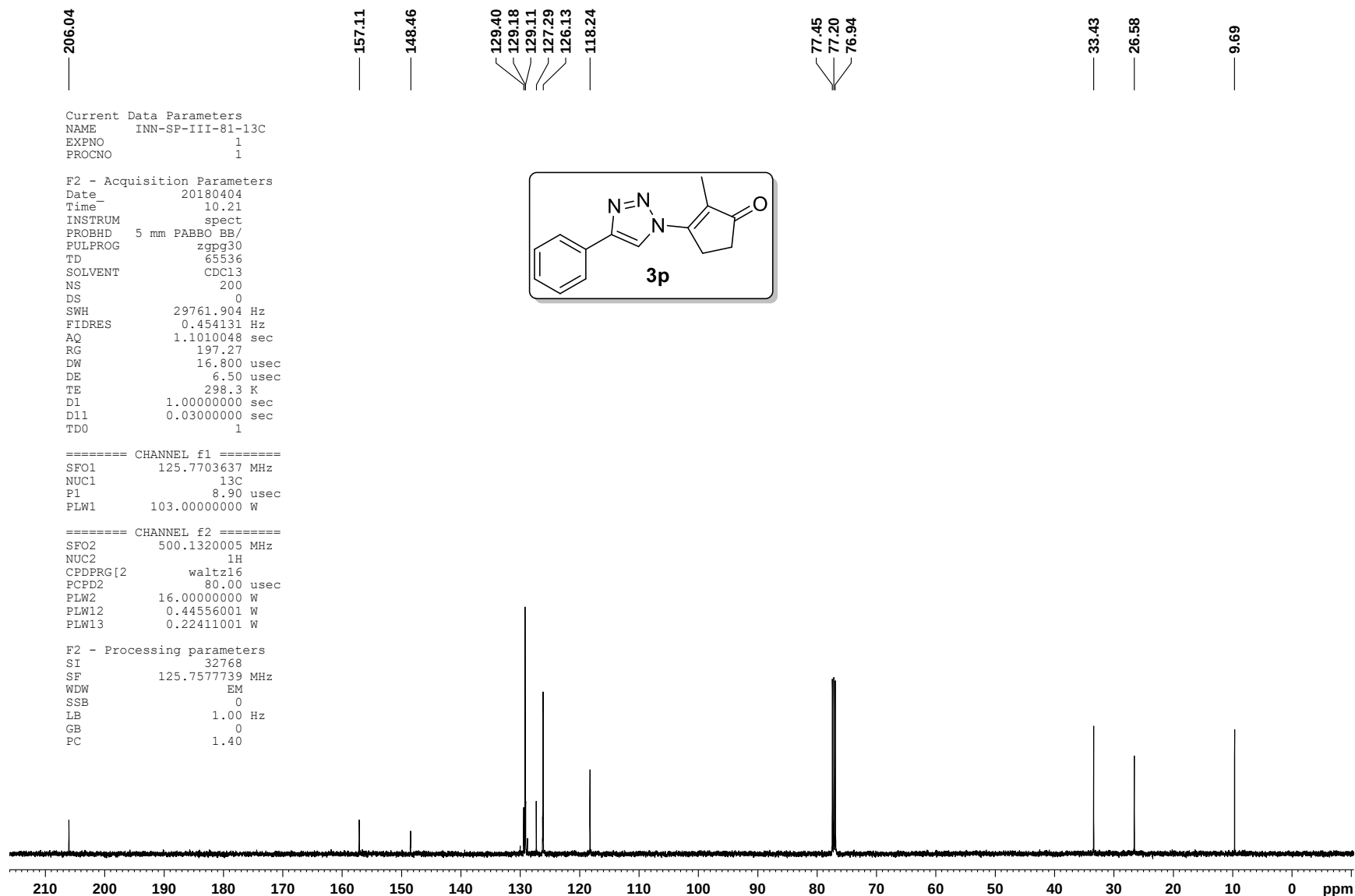


Figure S30: ^{13}C NMR spectrum of 3p.

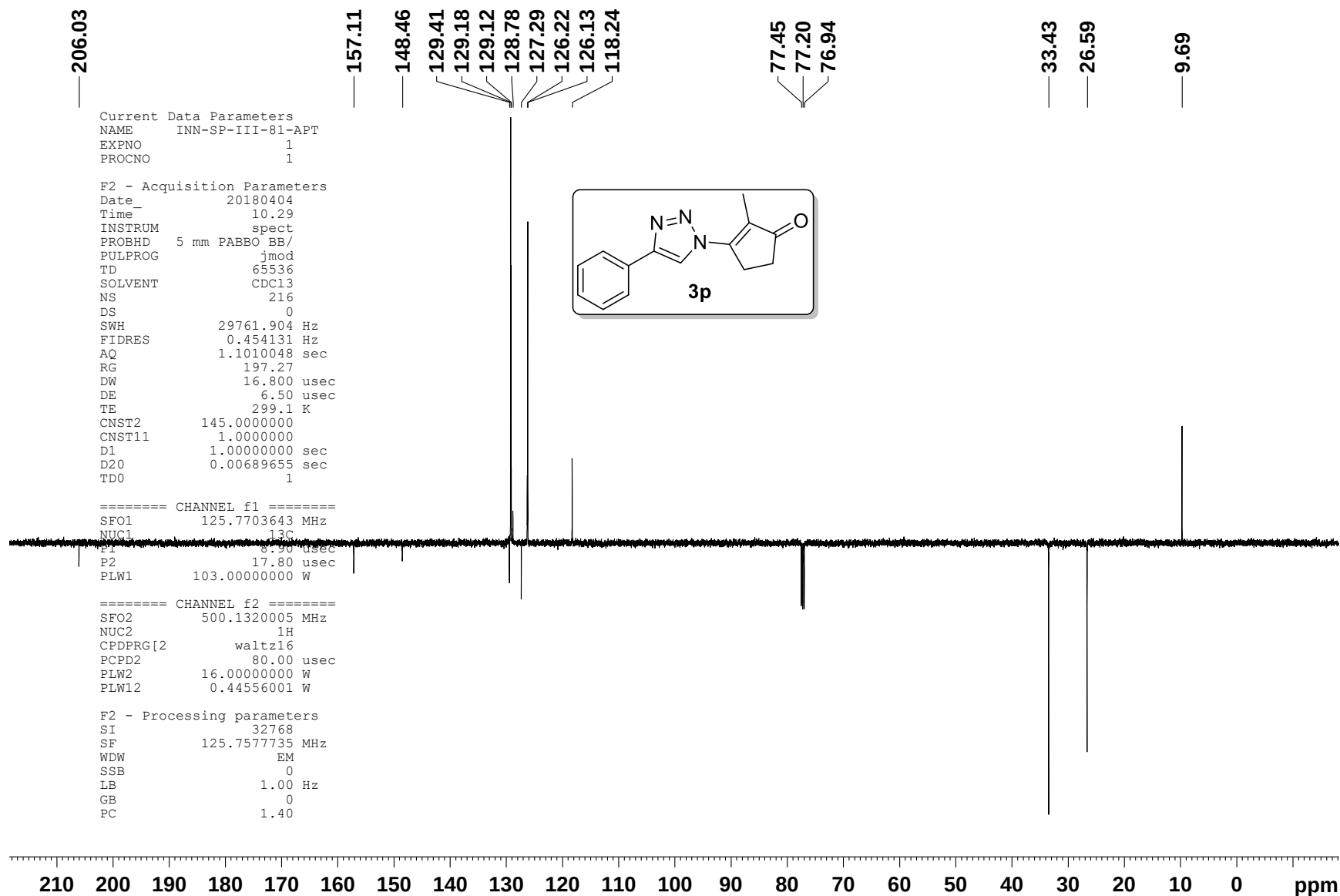


Figure S31: ¹³C-APT NMR spectrum of 3p.

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

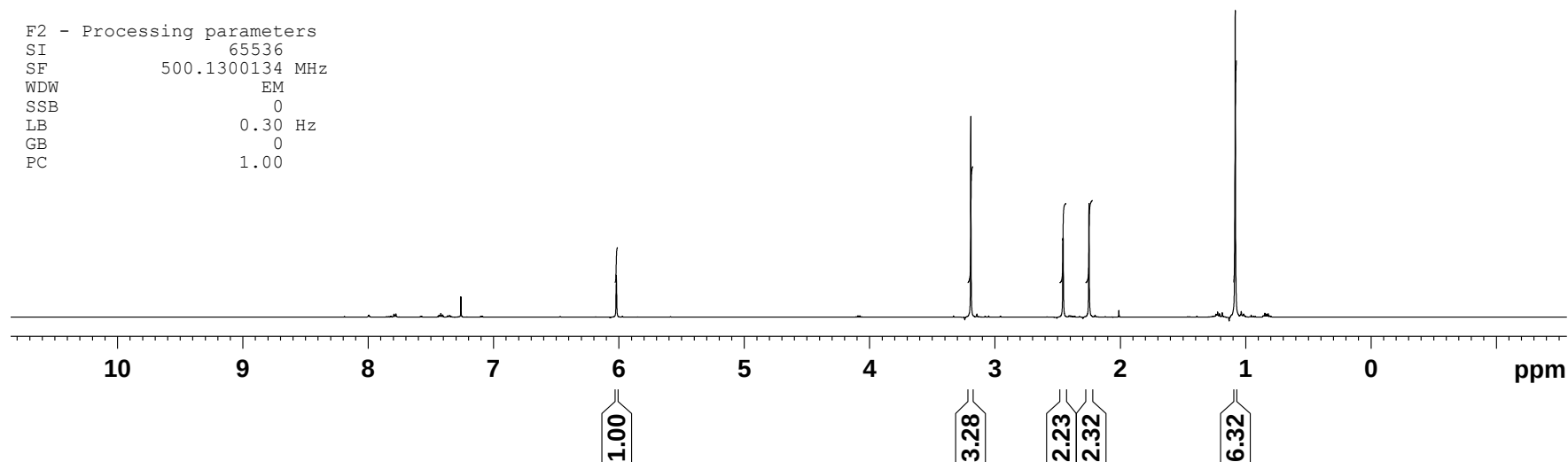
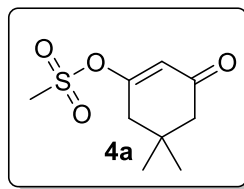


Figure S32: ¹H NMR spectrum of 4a.

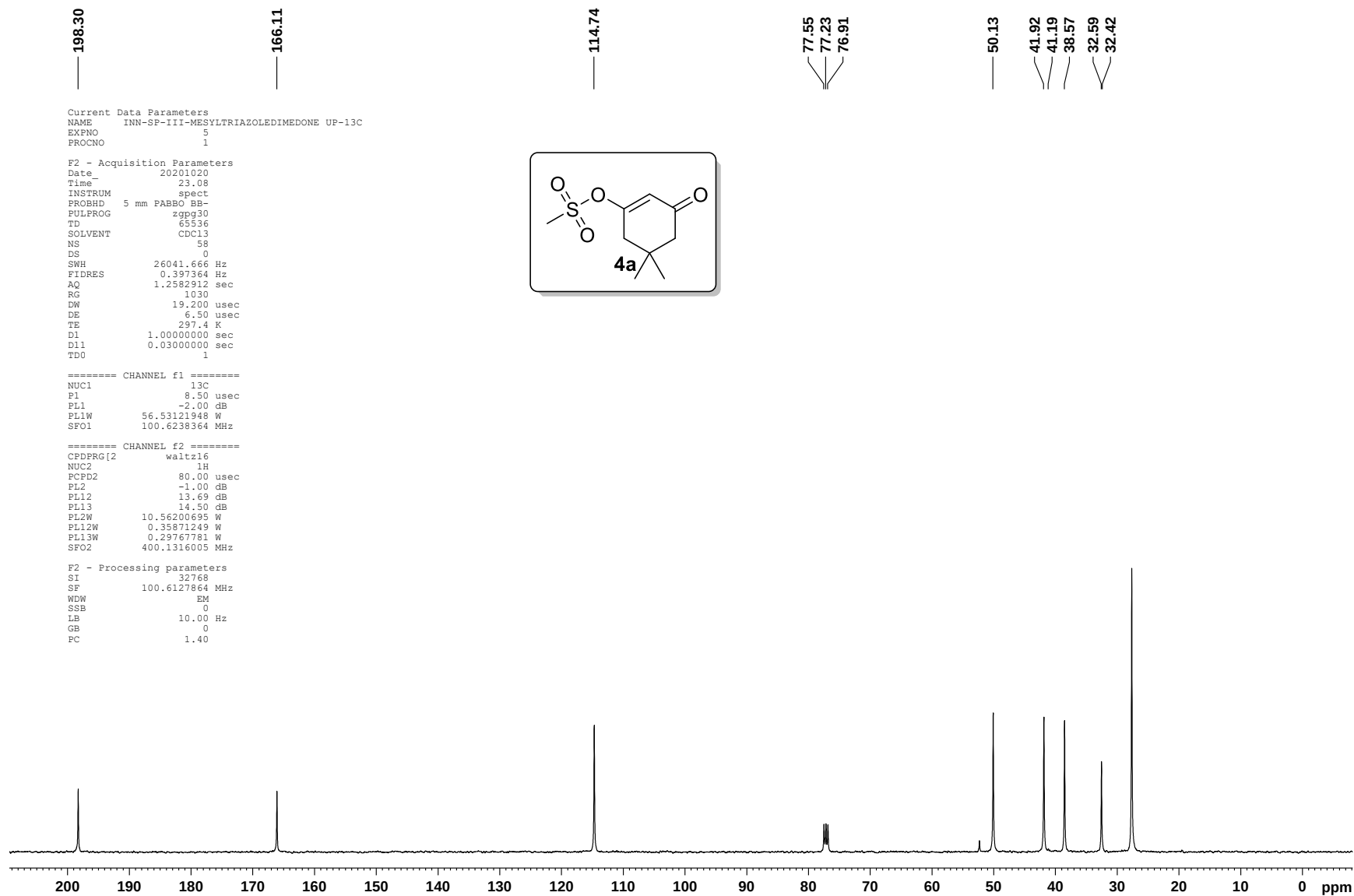


Figure S33: ¹³C NMR spectrum of 4a.

Current Data Parameters
 NAME INN-SP-III-161-INT
 EXPNO 16
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210303
 Time_ 13.49 h
 INSTRUM Avance
 PROBHD Z163739_0237 (
 PULPROG zg30
 TD 51724
 SOLVENT DMSO
 NS 18
 DS 0
 SWH 8620.689 Hz
 FIDRES 0.333334 Hz
 AQ 2.9999919 sec
 RG 32
 DW 58.000 usec
 DE 13.14 usec
 TE 296.7 K
 D1 1.00000000 sec
 TD0 1
 SF01 400.3024719 MHz
 NUC1 1H
 P0 2.67 usec
 P1 8.00 usec
 PLW1 21.61000061 W

F2 - Processing parameters
 SI 65536
 SF 400.3000037 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

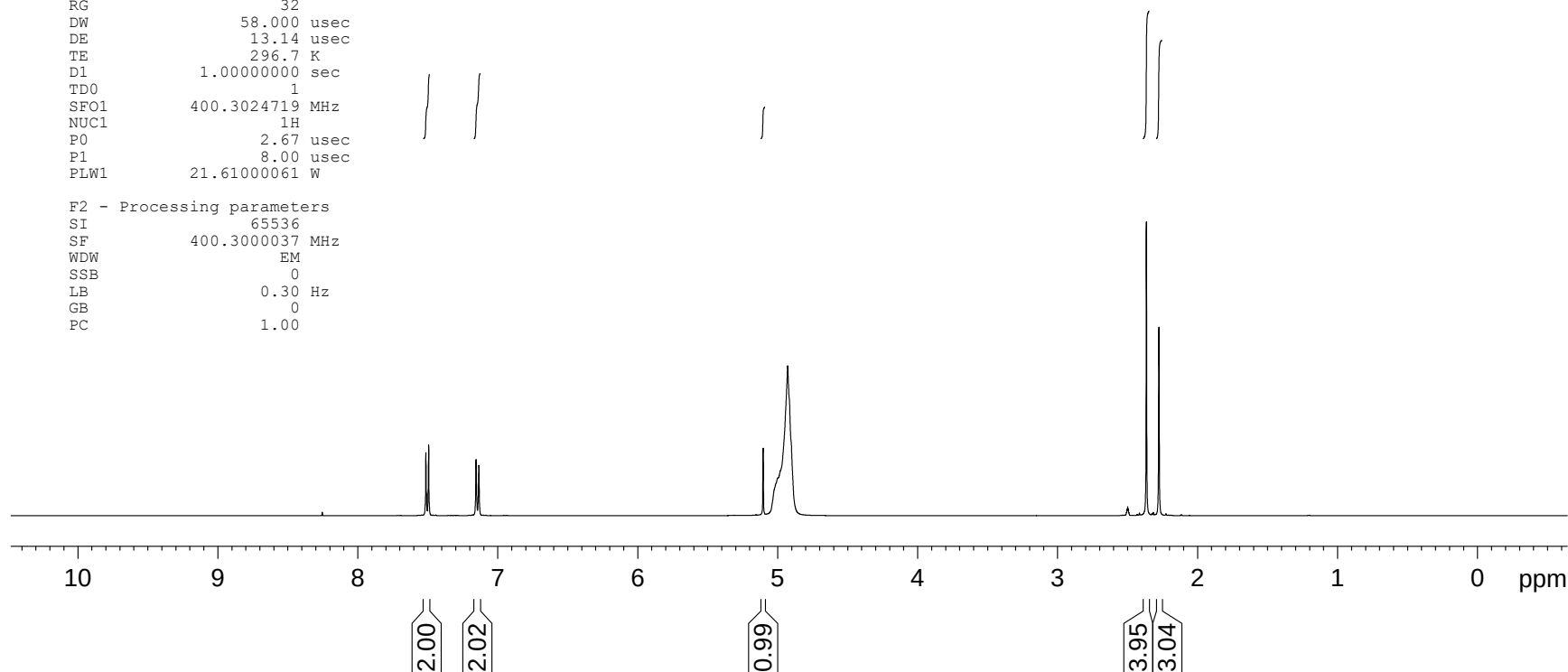
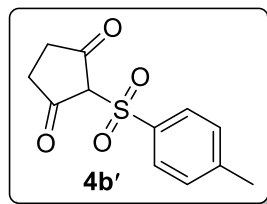


Figure S34: ¹H NMR spectrum of 4b'.

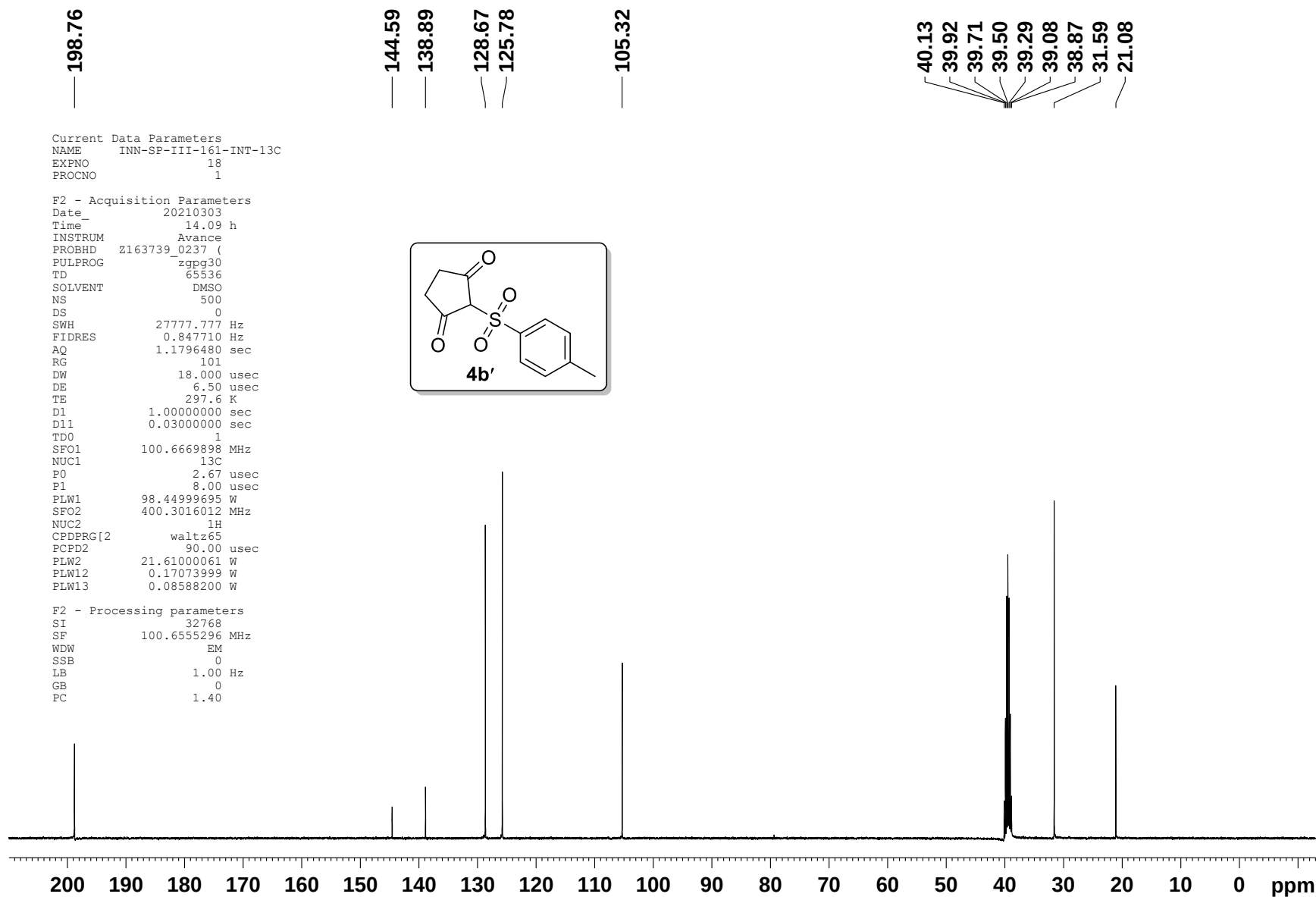


Figure S35: ^{13}C NMR spectrum of 4b'.

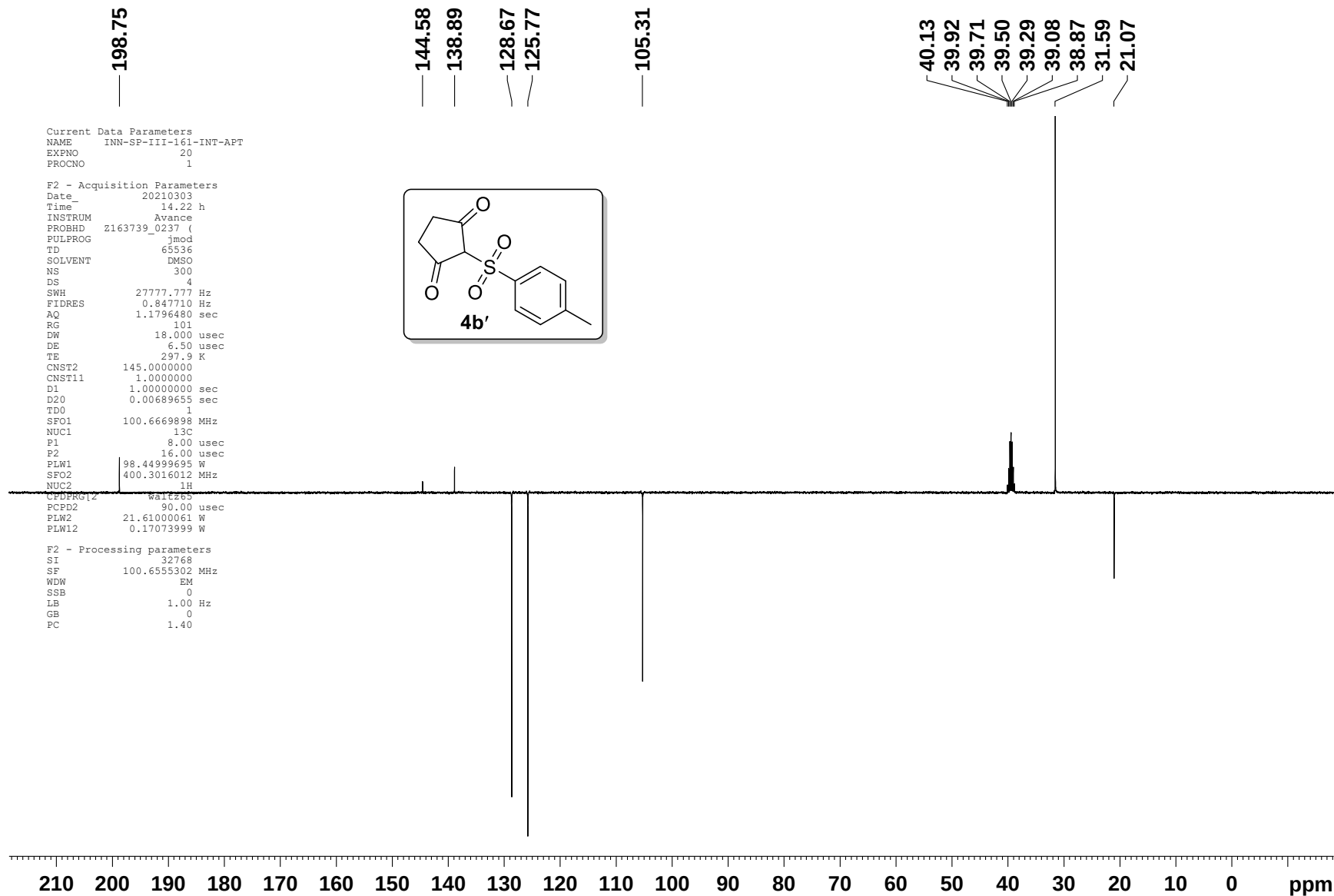


Figure S36: ¹³C-APT NMR spectrum of 4b'.

Current Data Parameters
 NAME INN-SP-III-BA-CYCLOPENTENINT-1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210314
 Time 22.24
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 13
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 157.24
 DW 50.000 usec
 DE 6.50 usec
 TE 295.5 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.130885 MHz
 NUC1 1H
 P1 13.35 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300140 MHz
 WDW EM
 SSB 0
 LB 0.56 Hz
 GB 0
 PC 1.00

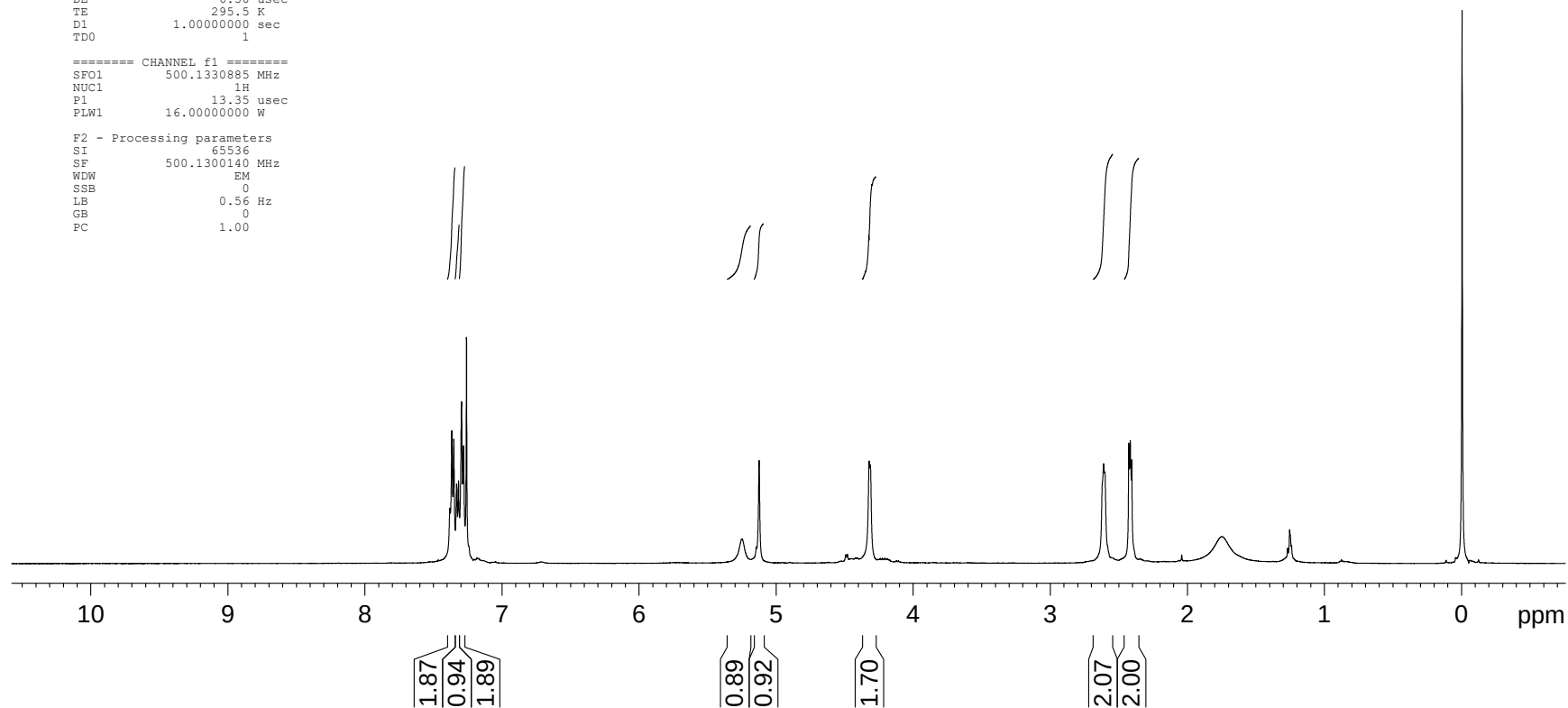
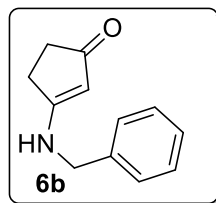


Figure S37: ¹H NMR spectrum of 6b.

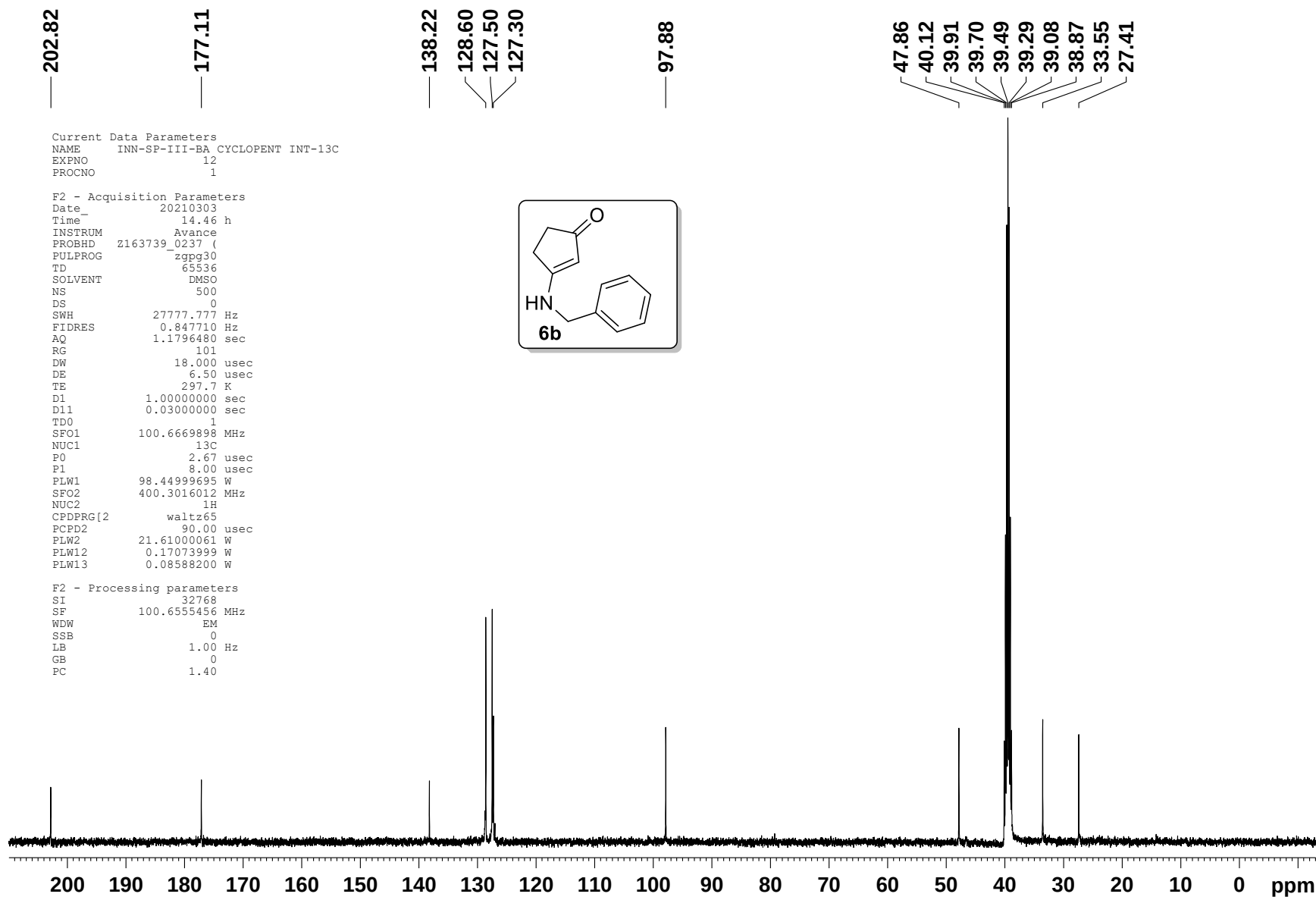


Figure S38: ¹³C NMR spectrum of 6b.

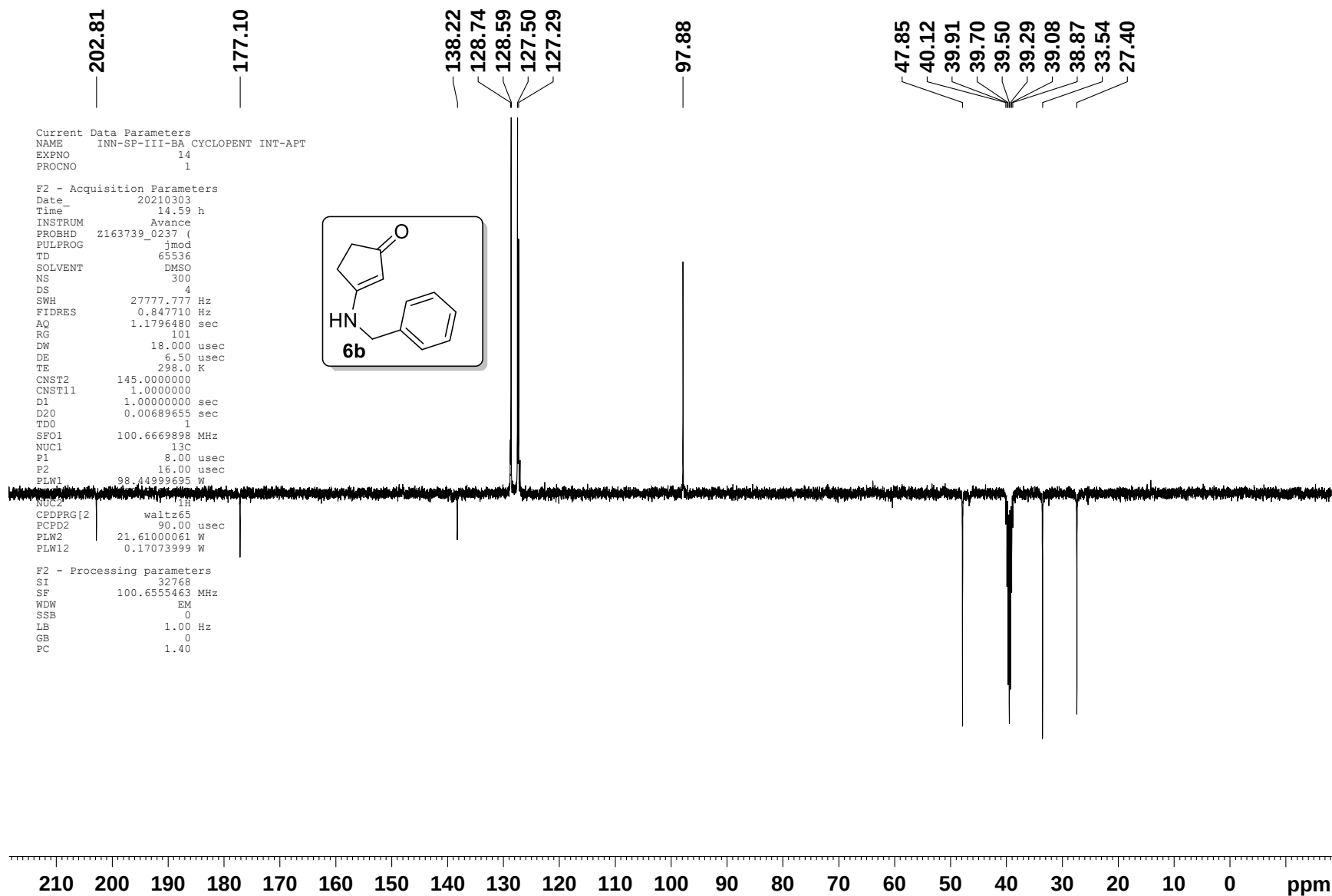


Figure S39: ¹³C-APT NMR spectrum of 6b.

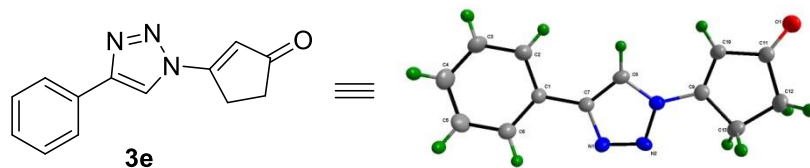


Figure S40: ORTEP diagram of 3e.

Table S1: Crystal table of 3e.

Identification code	Reflection List
Empirical formula	C ₁₃ H ₁₁ N ₃ O
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} /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)
2θ 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 [$R_{\text{int}} = 0.0876$, $R_{\text{sigma}} = 0.1717$]
Data/restraints/parameters	1881/0/154
Goodness-of-fit on F^2	0.960
Final R indexes [$I\geq 2\sigma(I)$]	$R_1 = 0.0511$, $wR_2 = 0.1082$
Final R indexes [all data]	$R_1 = 0.1056$, $wR_2 = 0.1493$
Largest diff. peak/hole / e $\text{\AA}^{-3}$	0.58/-0.69