

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

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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 CDC13
NS 20
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 134.65
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DE 6.50 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1

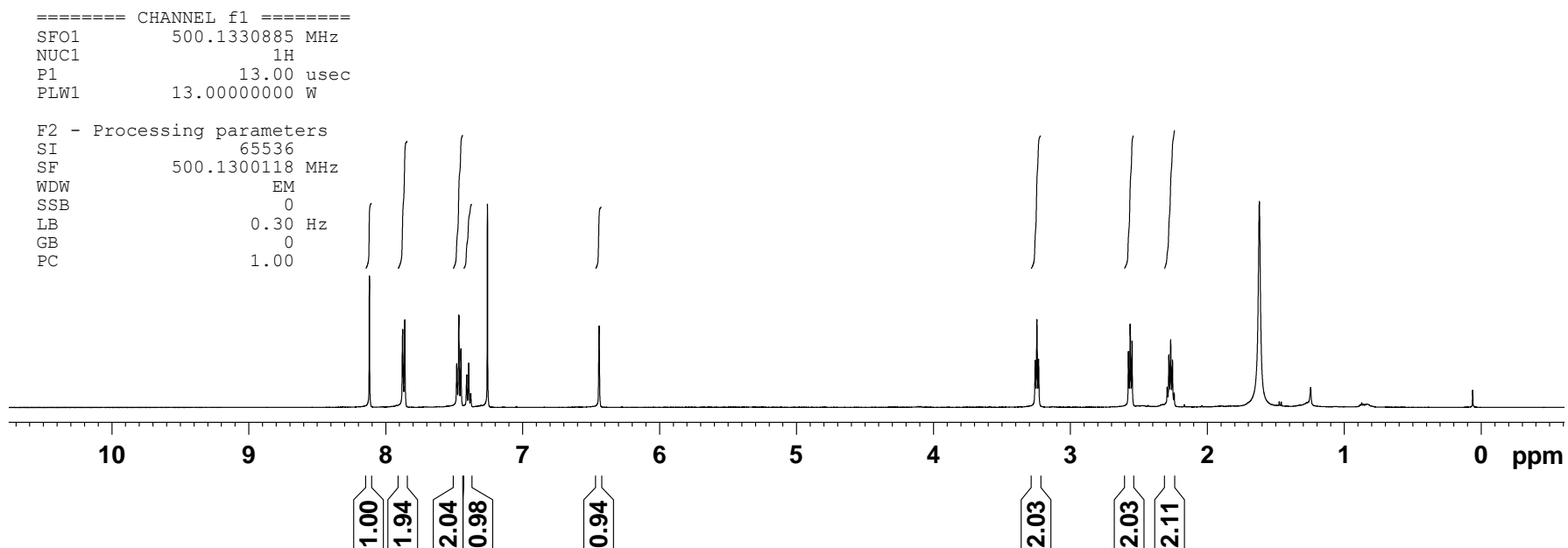
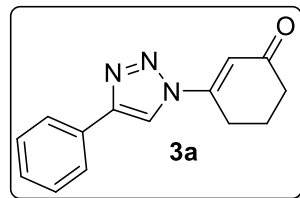


Figure S01. ¹H NMR Spectrum of 3a

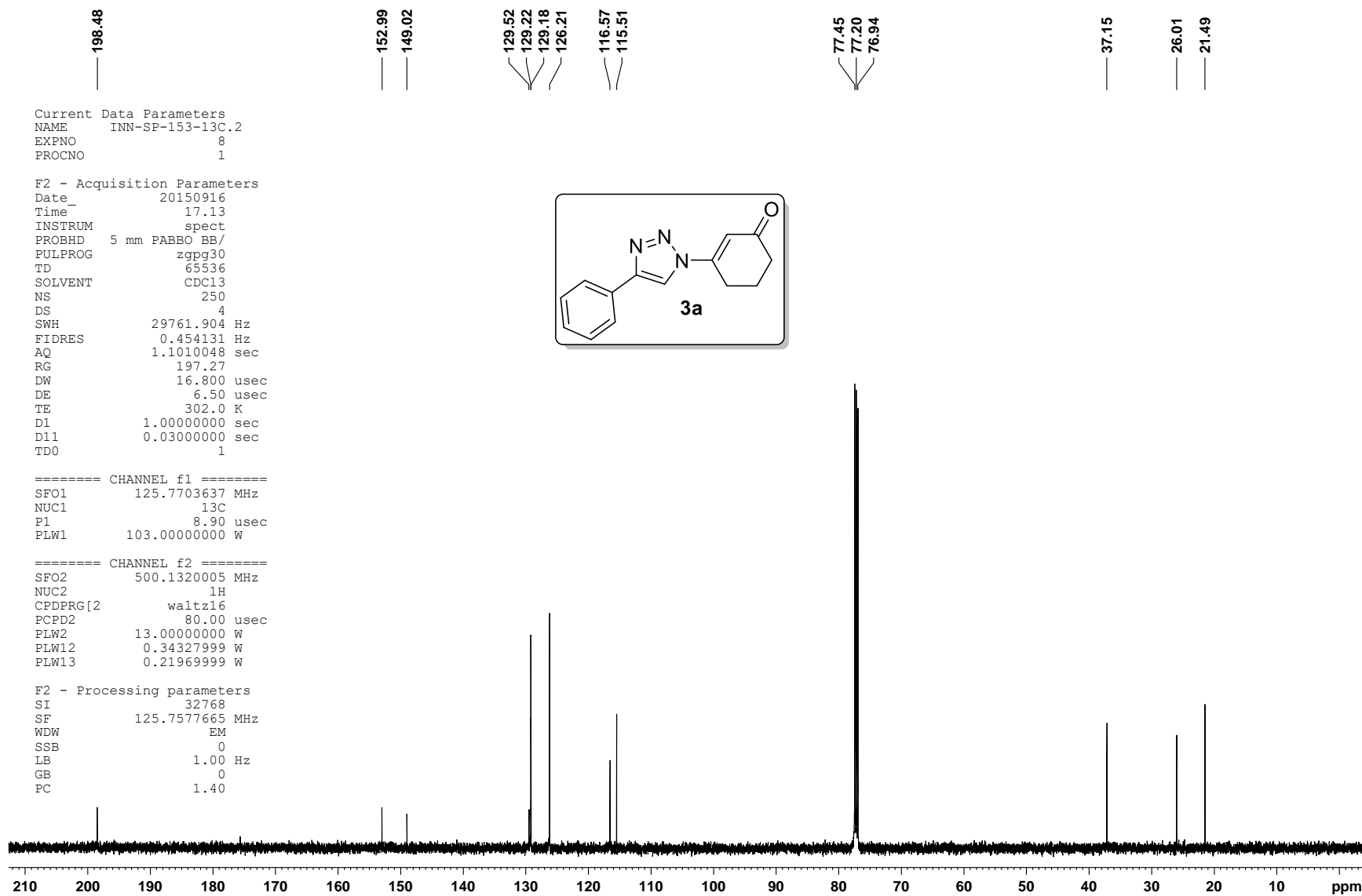


Figure S02. ¹³C NMR Spectrum of 3a

Current Data Parameters
NAME INN-SP-187-1H
EXPNO 8
PROCNO 1

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Date_ 20180427
Time_ 23.39
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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

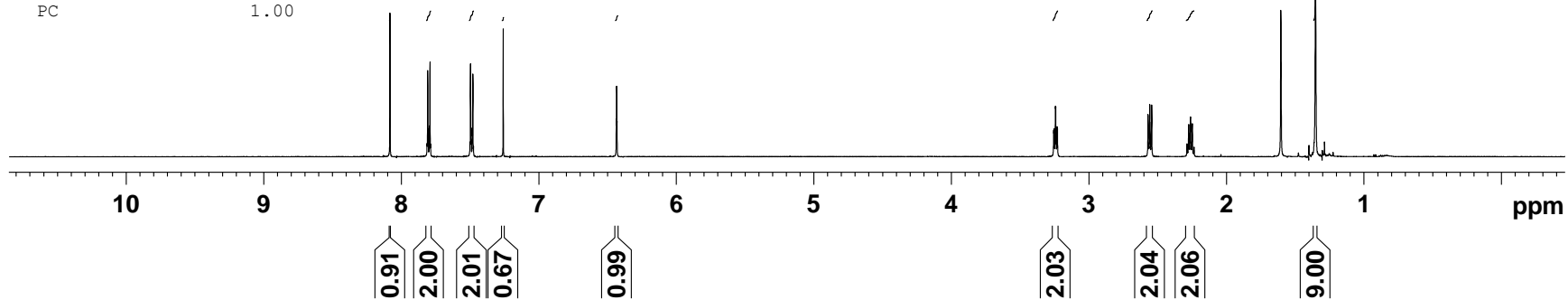
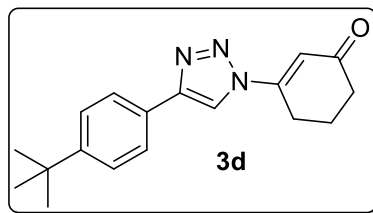


Figure S03. ¹H NMR Spectrum of 3d

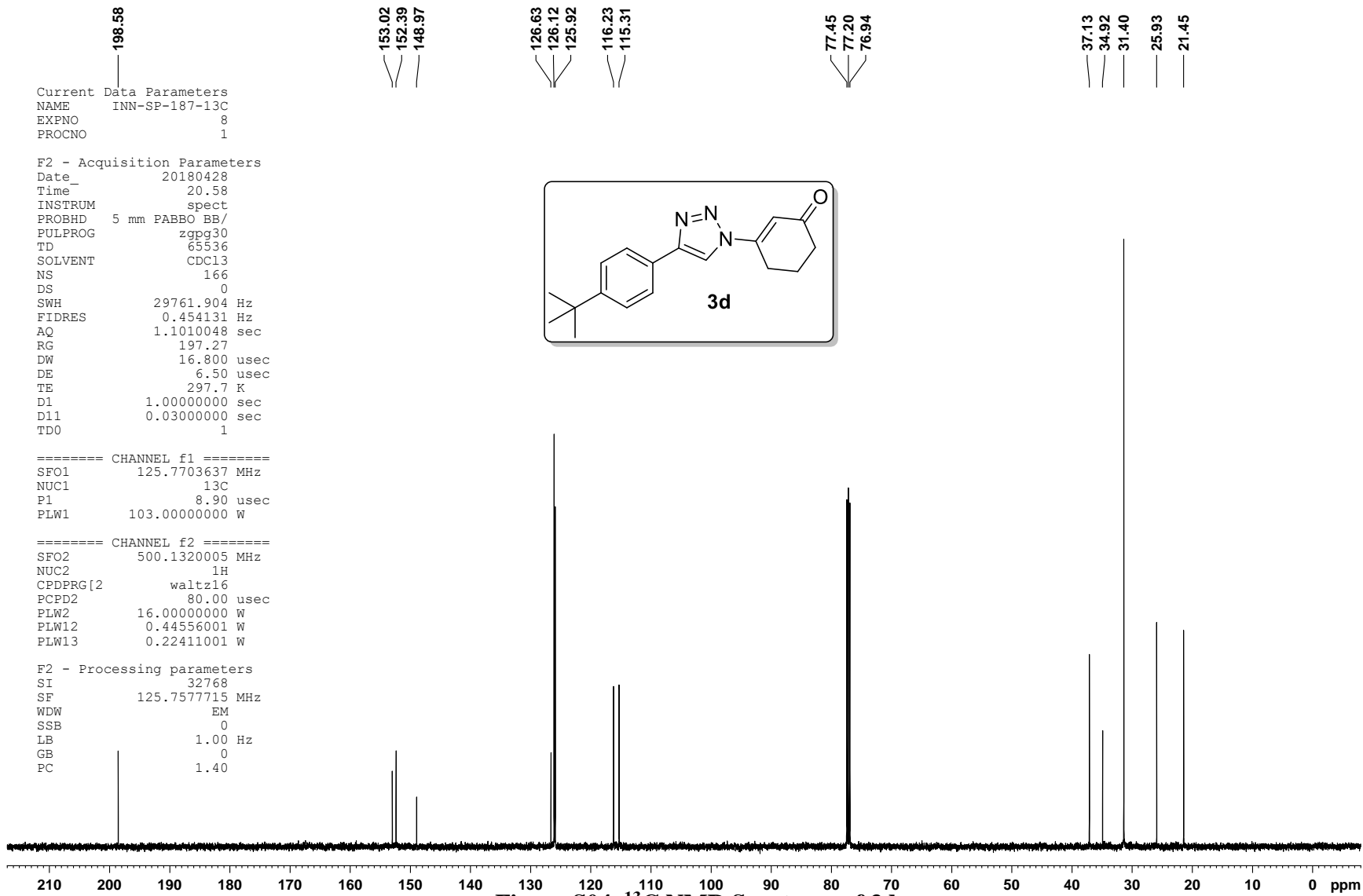
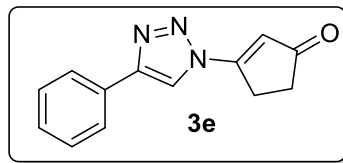


Figure S04. ¹³C NMR Spectrum of 3d

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NAME INN-SP-161-1H
EXPNO 71
PROCNO 1

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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
TDO 1



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

F2 - Processing parameters

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SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

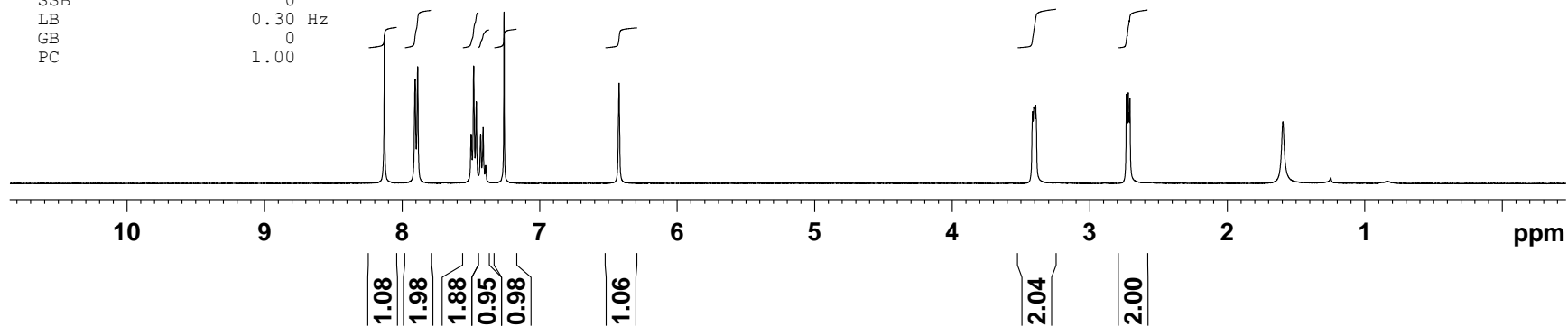


Figure S05. ¹H NMR Spectrum of 3e

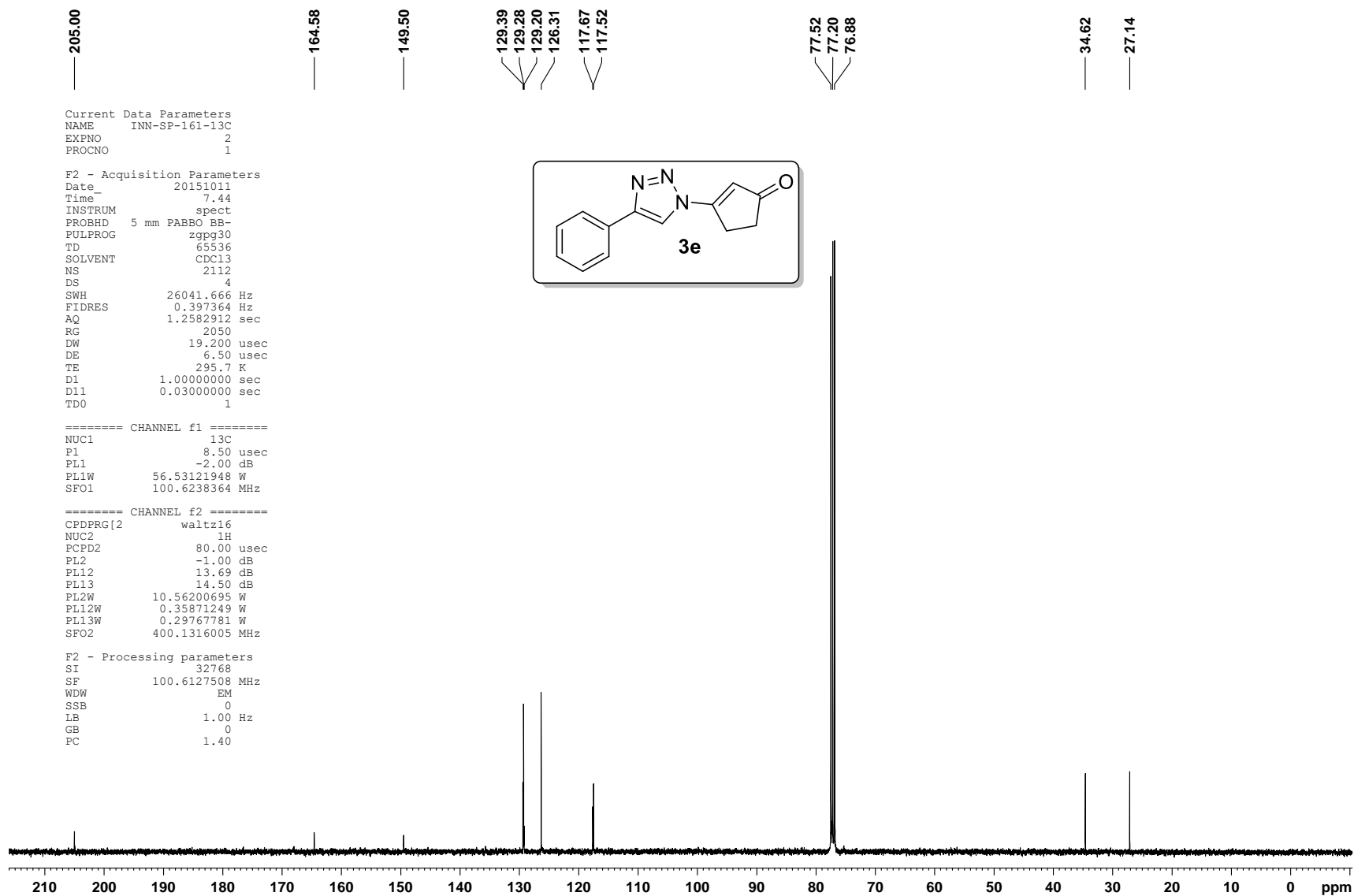


Figure S06. ¹³C NMR Spectrum of 3e

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

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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

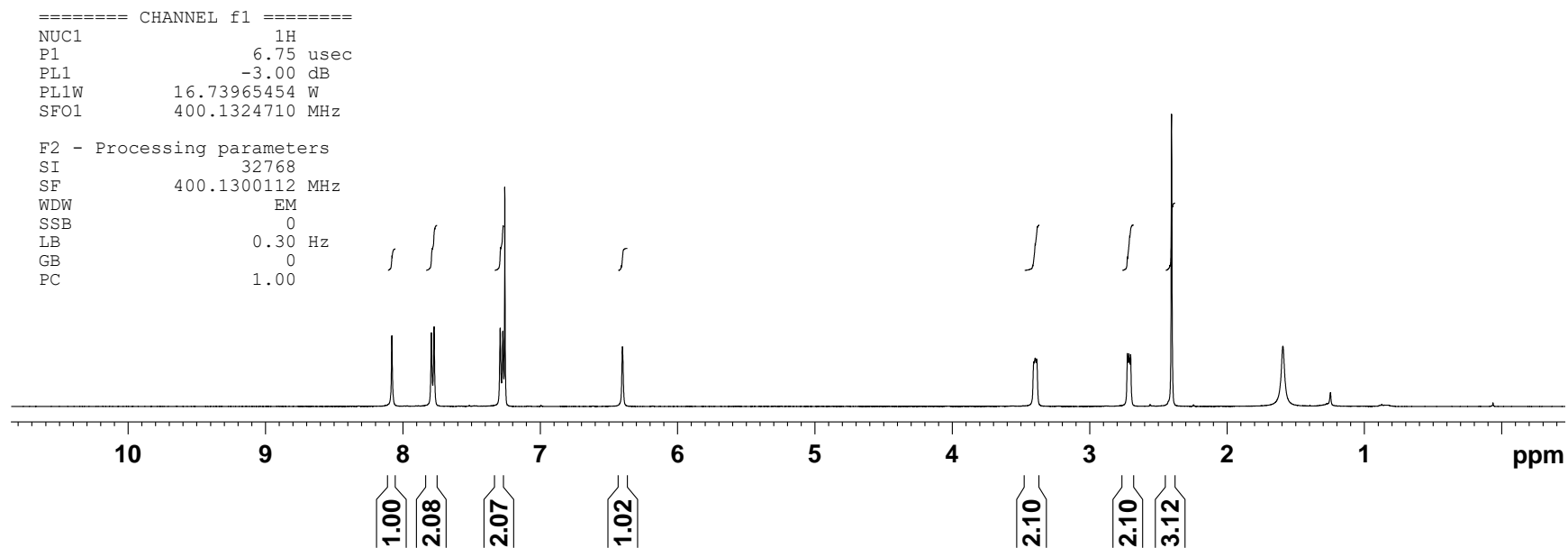
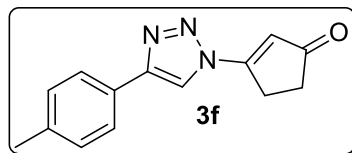


Figure S07. ¹H NMR Spectrum of 3f

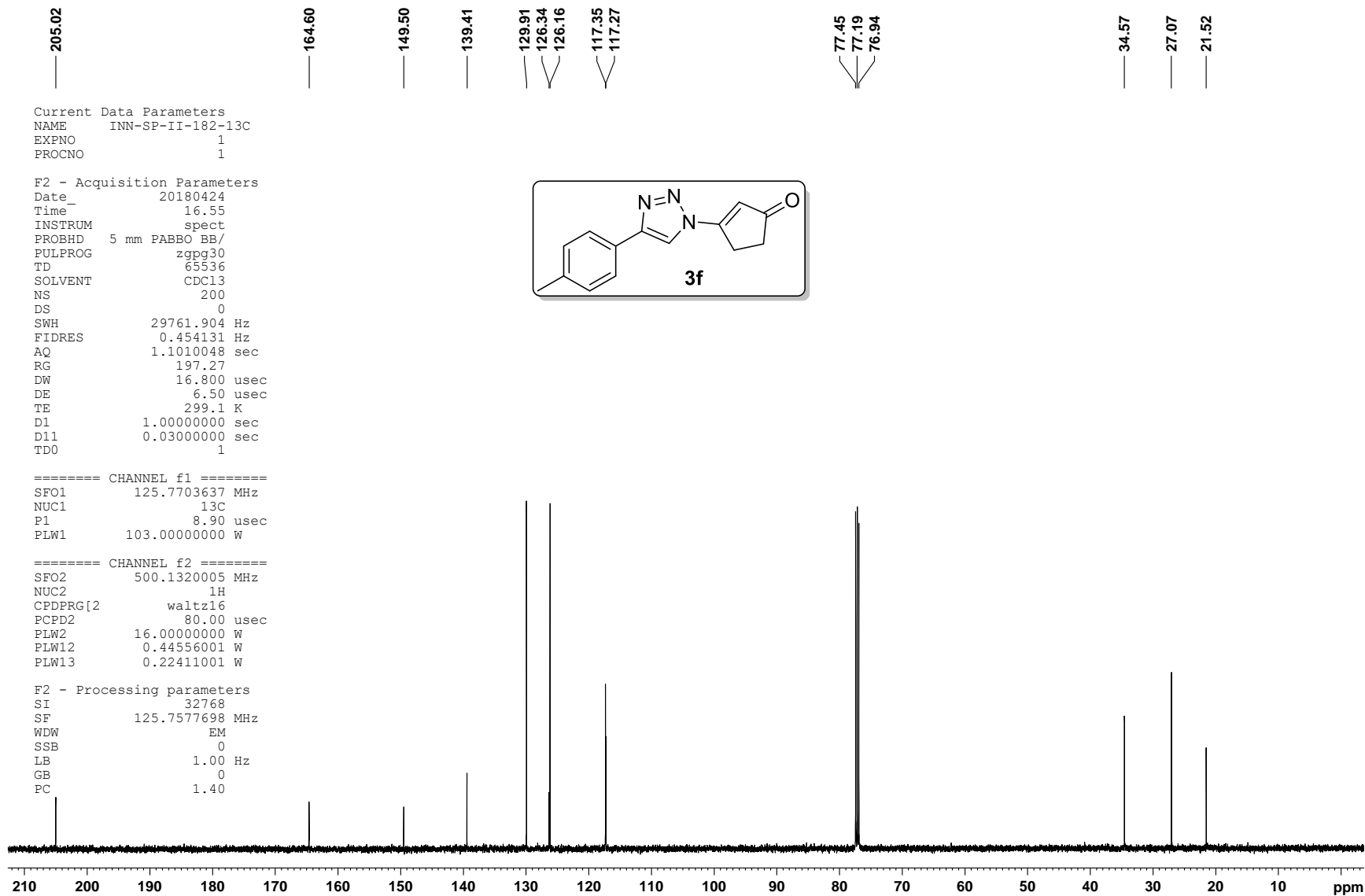


Figure S08. ¹³C NMR Spectrum of 3f

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

F2 - Acquisition Parameters
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Time_ 18.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
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

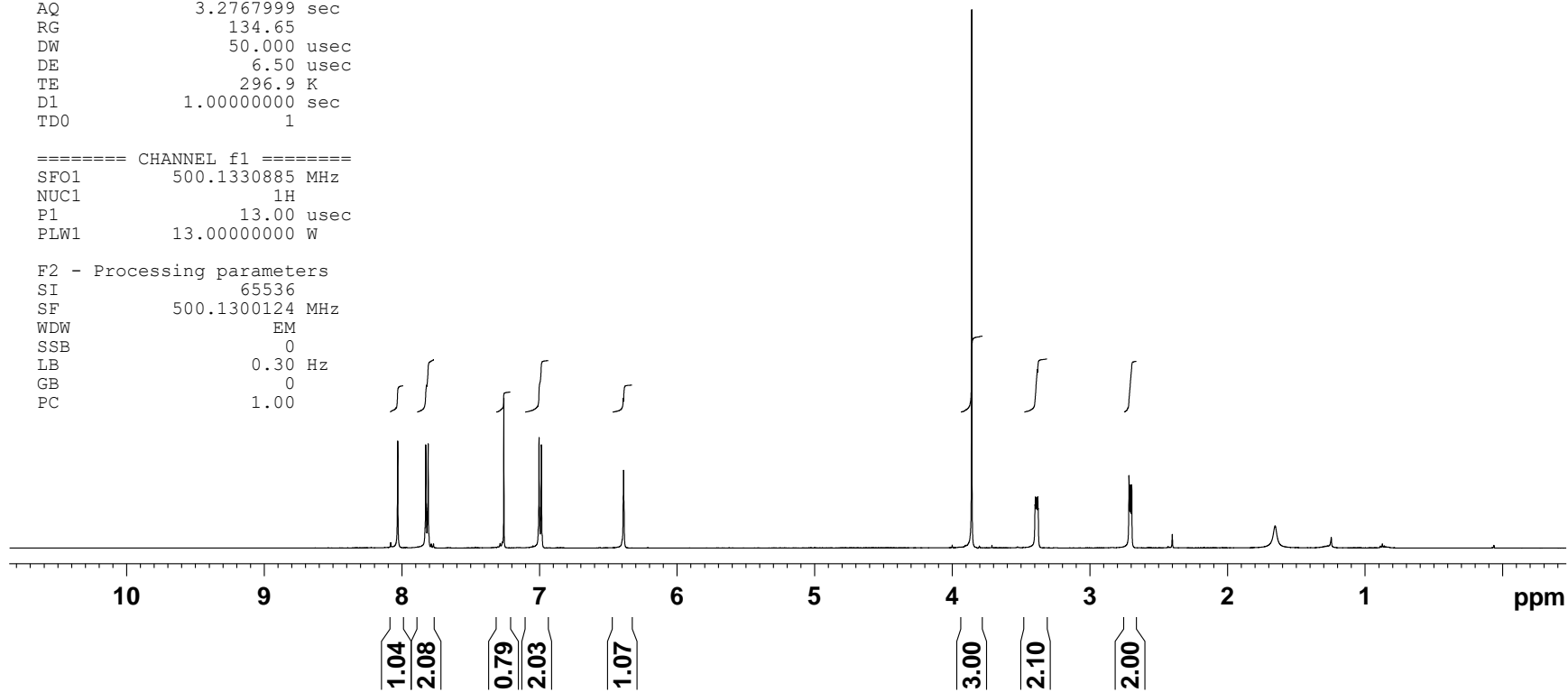
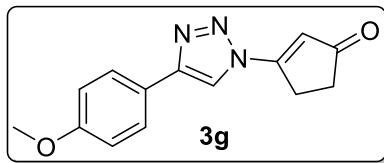


Figure S09. ¹H NMR Spectrum of 3g

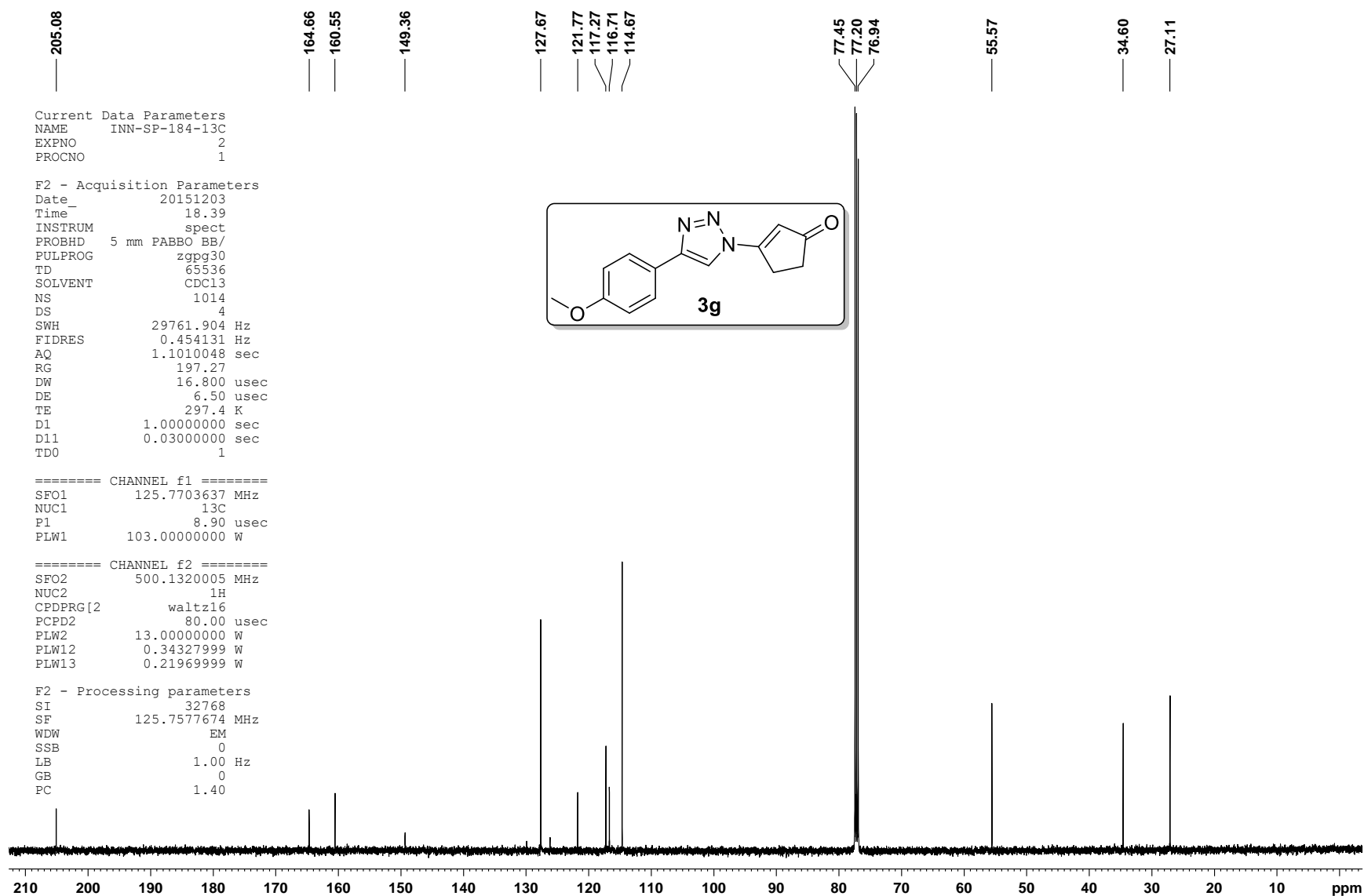


Figure S10. ¹³C NMR Spectrum of 3g

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

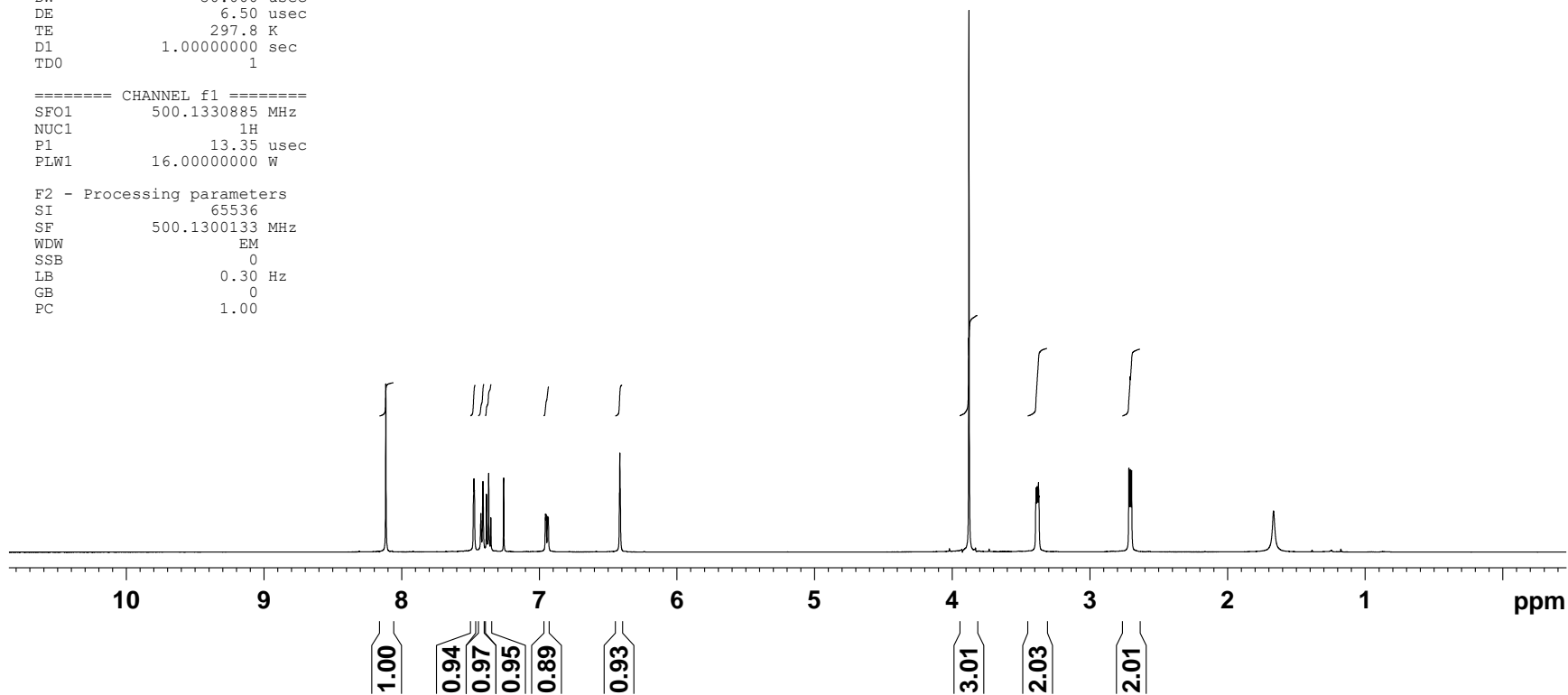
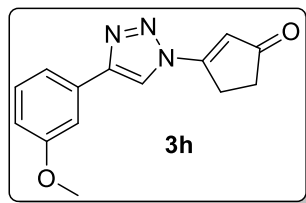


Figure S11. ¹H NMR Spectrum of 3h

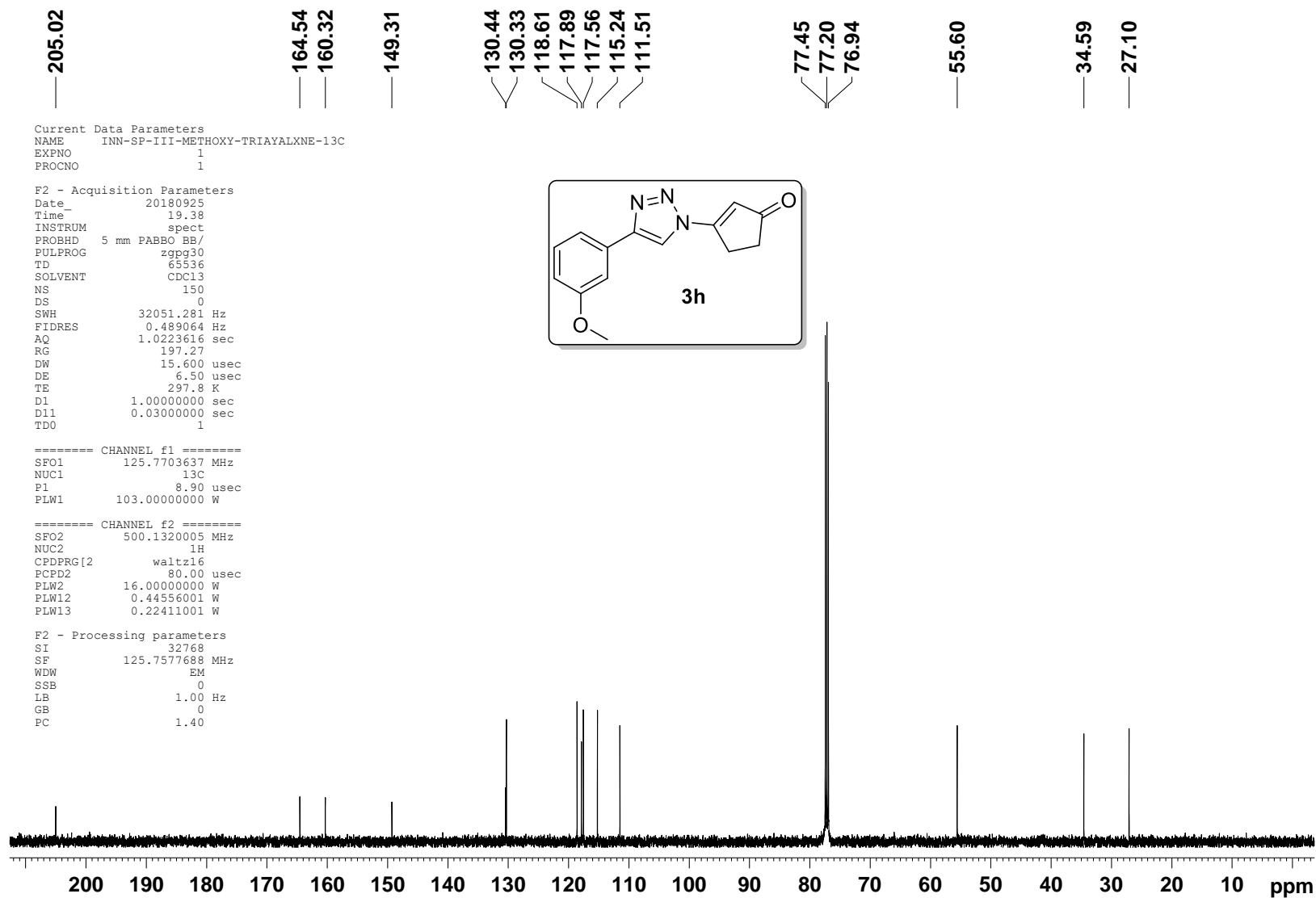
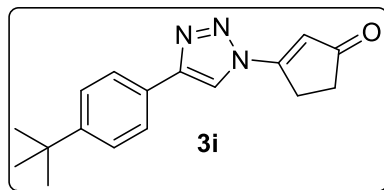


Figure S12. ¹³C NMR Spectrum of 3h

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

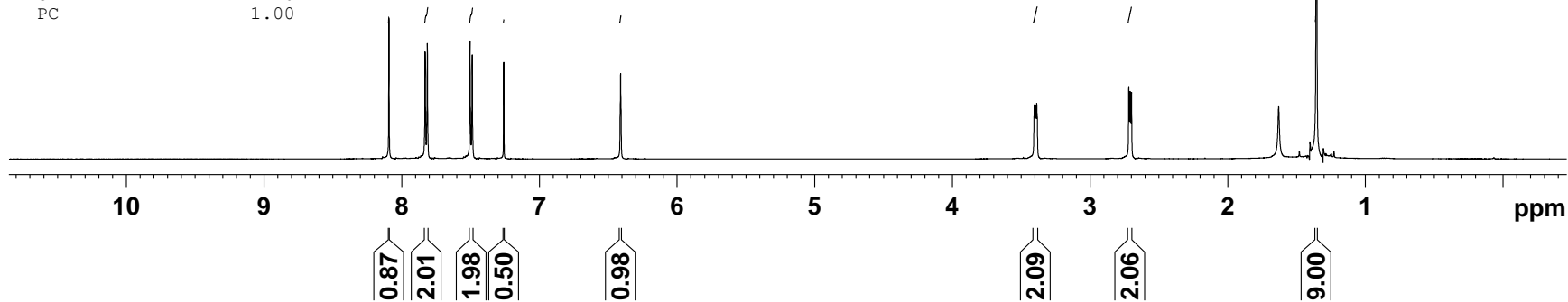


Figure S13. ¹H NMR Spectrum of 3i

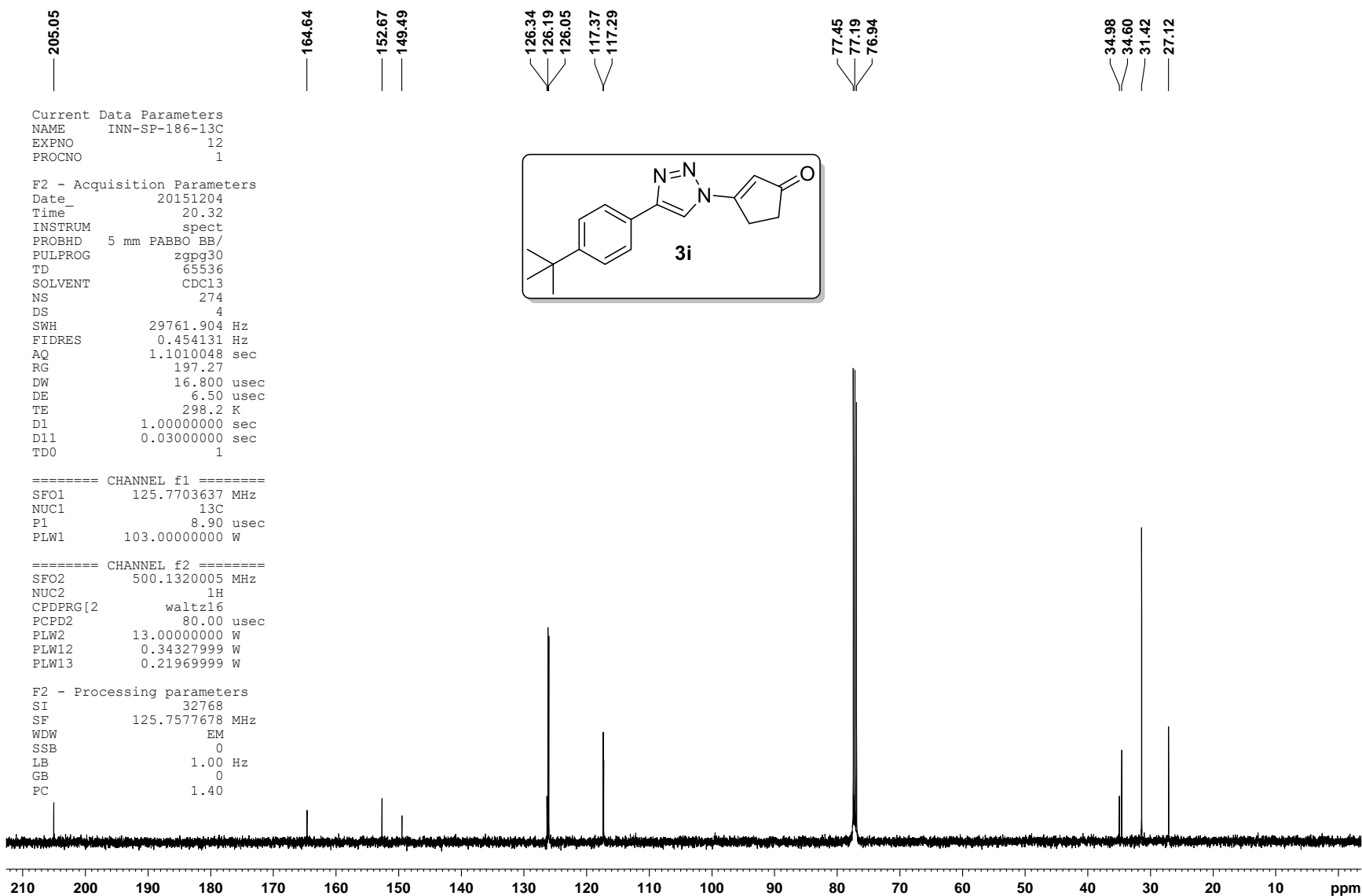


Figure S14. ¹³C NMR Spectrum of 3i

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

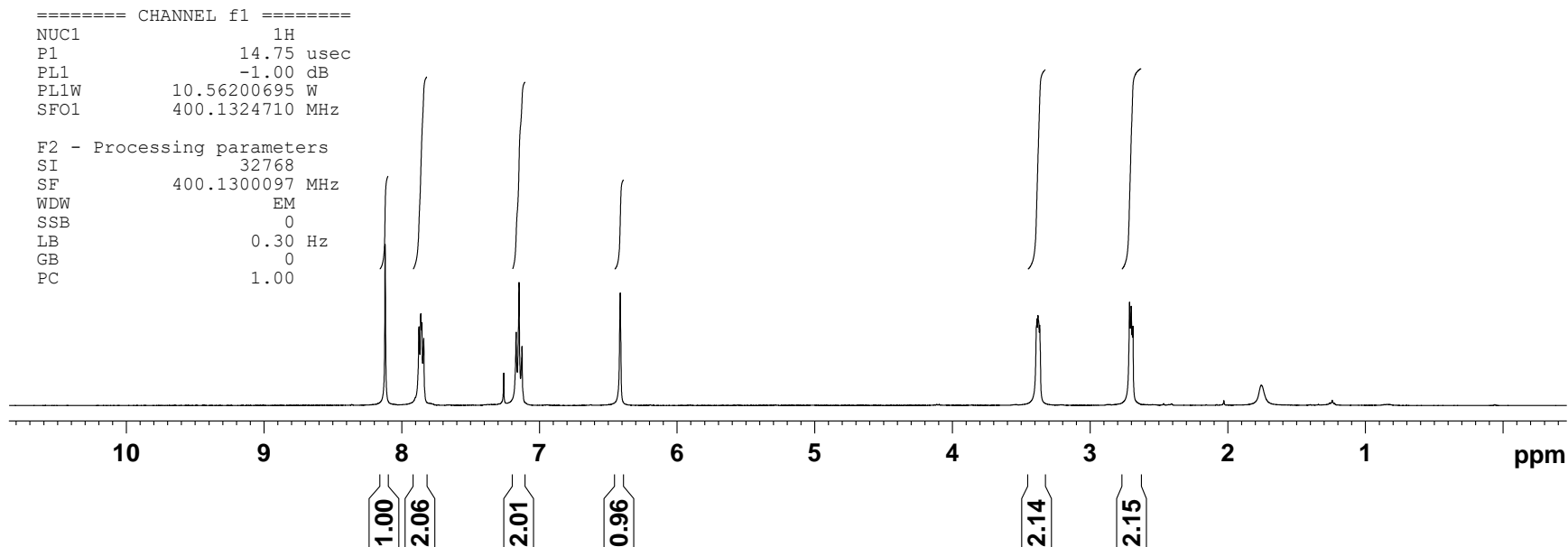
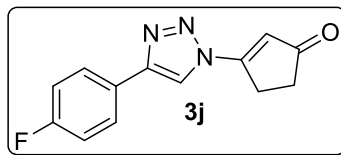


Figure S15. ¹H NMR Spectrum of 3j

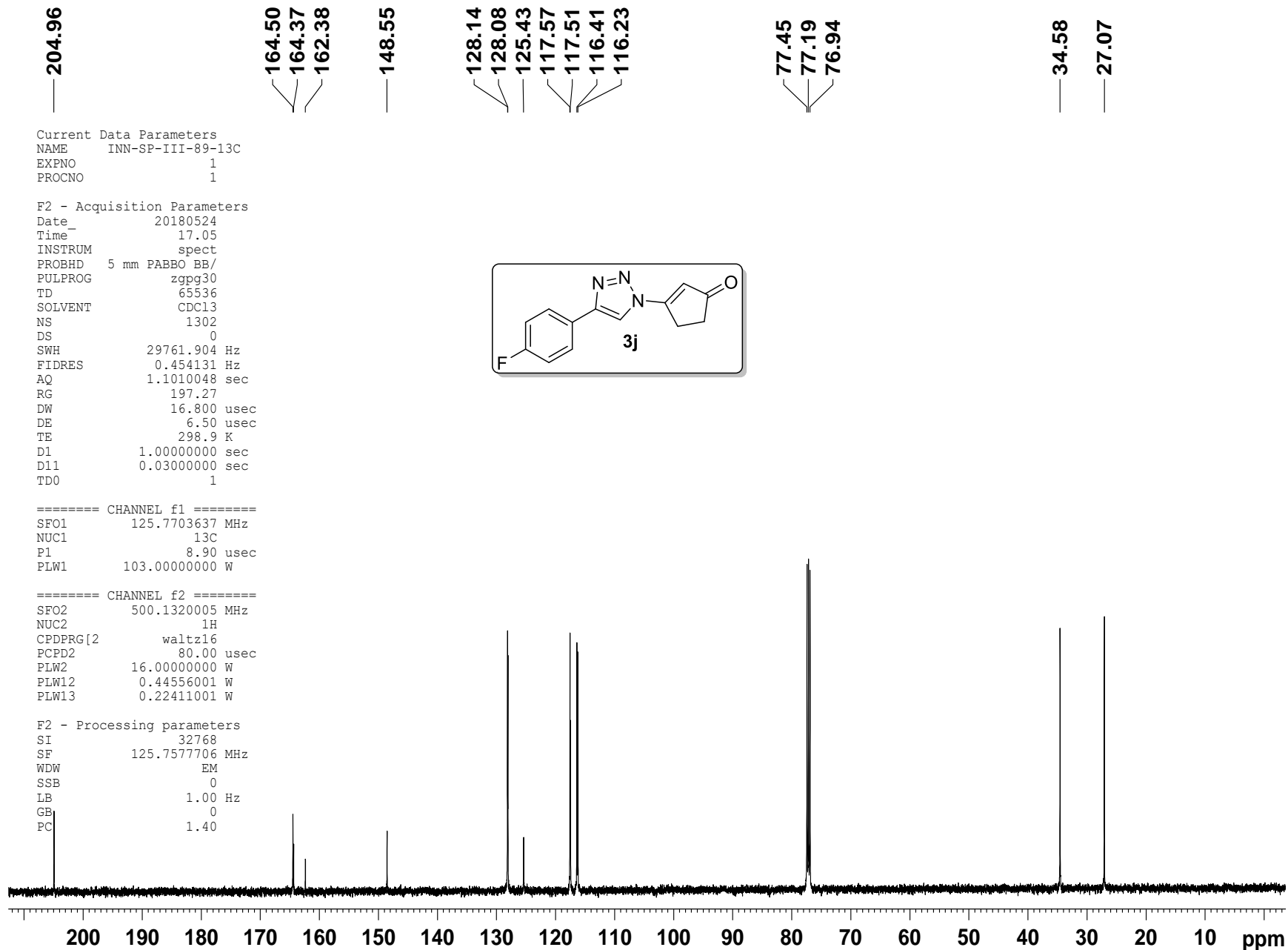


Figure S16. ¹³C NMR Spectrum of 3j

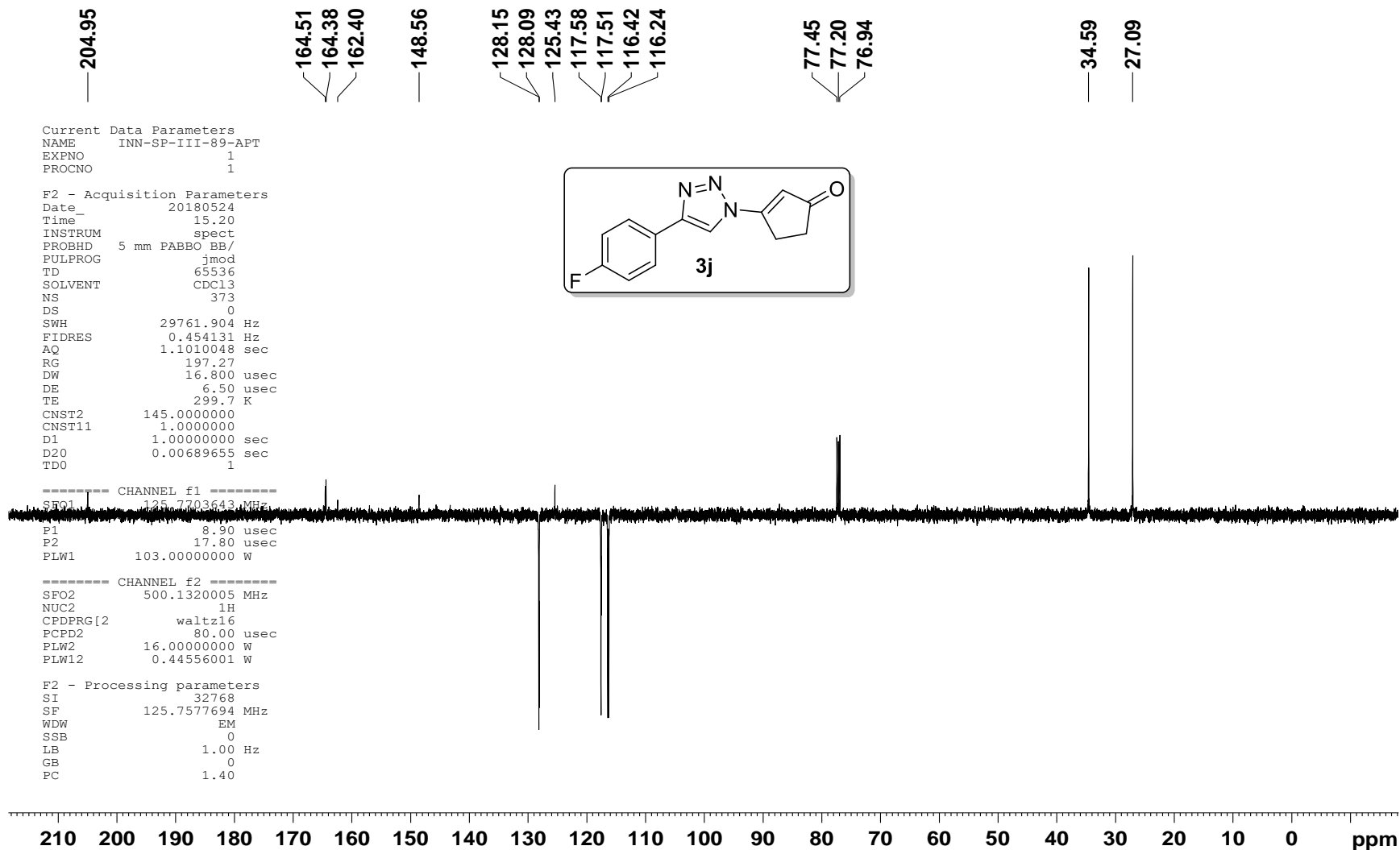


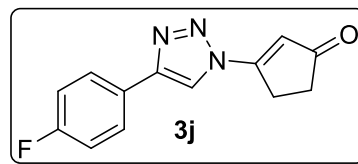
Figure S17. ¹³C-APT NMR Spectrum of 3j

Current Data Parameters
NAME INN-SP-III-89-19F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180524
Time_ 15.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
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

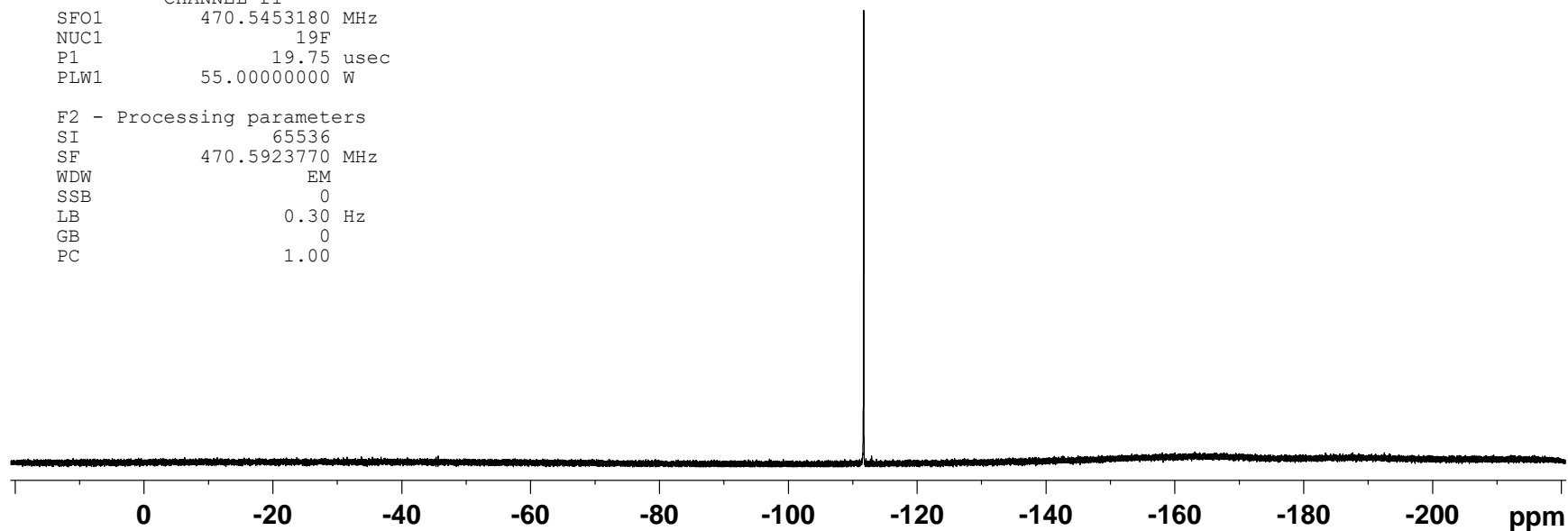


Figure S18. ¹⁹F NMR Spectrum of 3j

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

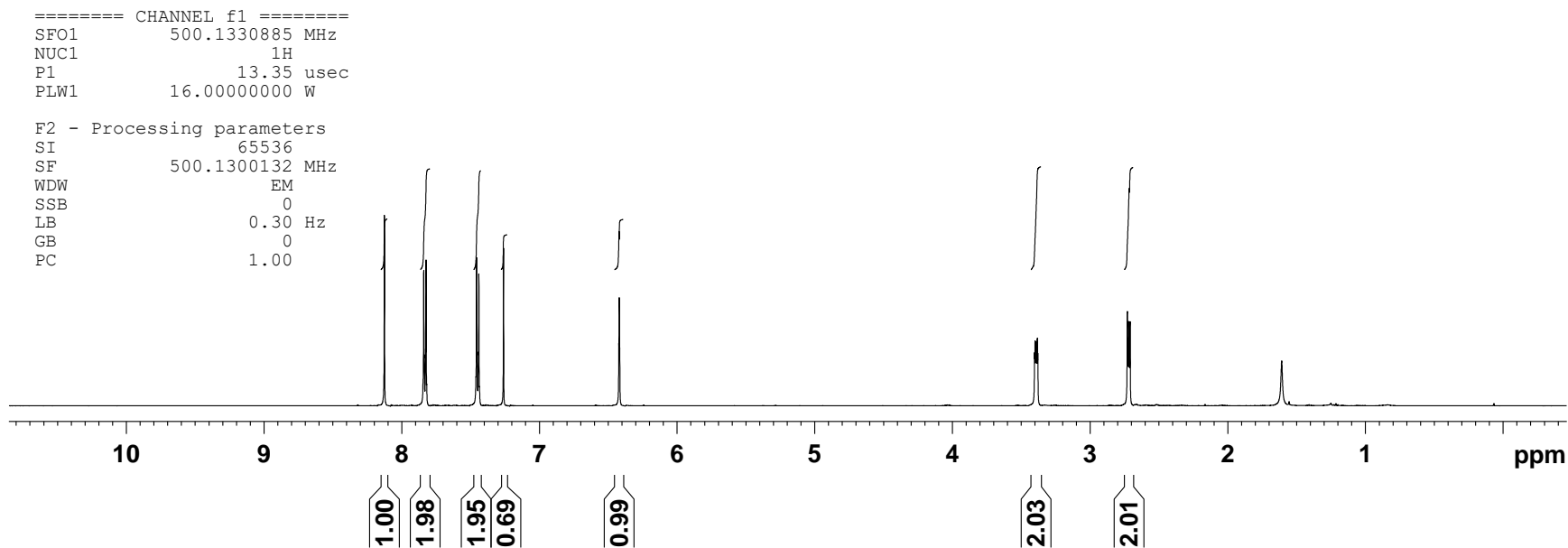
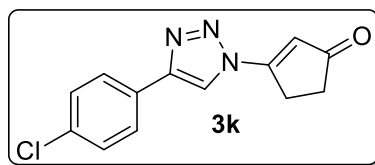


Figure S19. ¹H NMR Spectrum of 3k

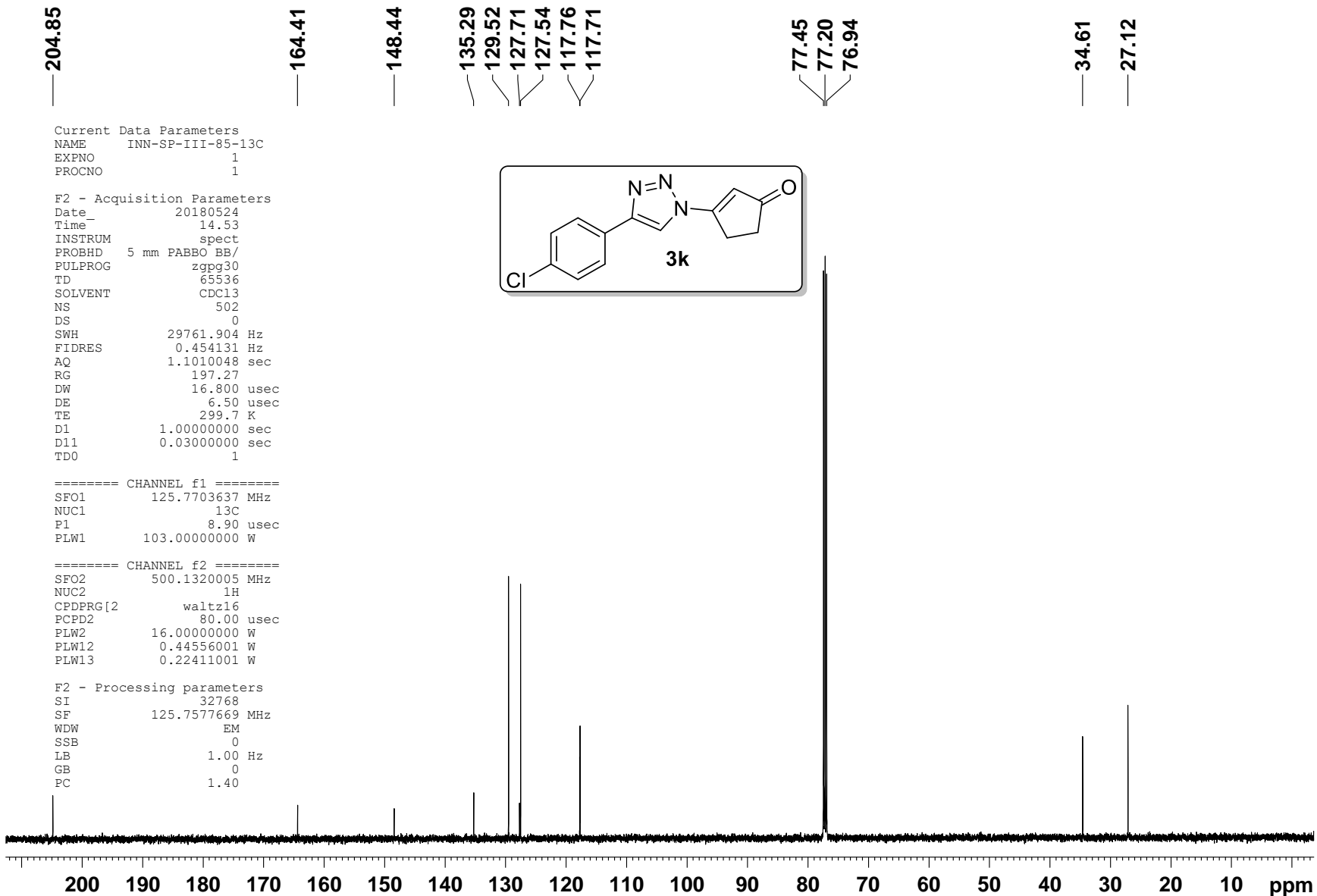


Figure S20. ¹³C NMR Spectrum of 3k

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

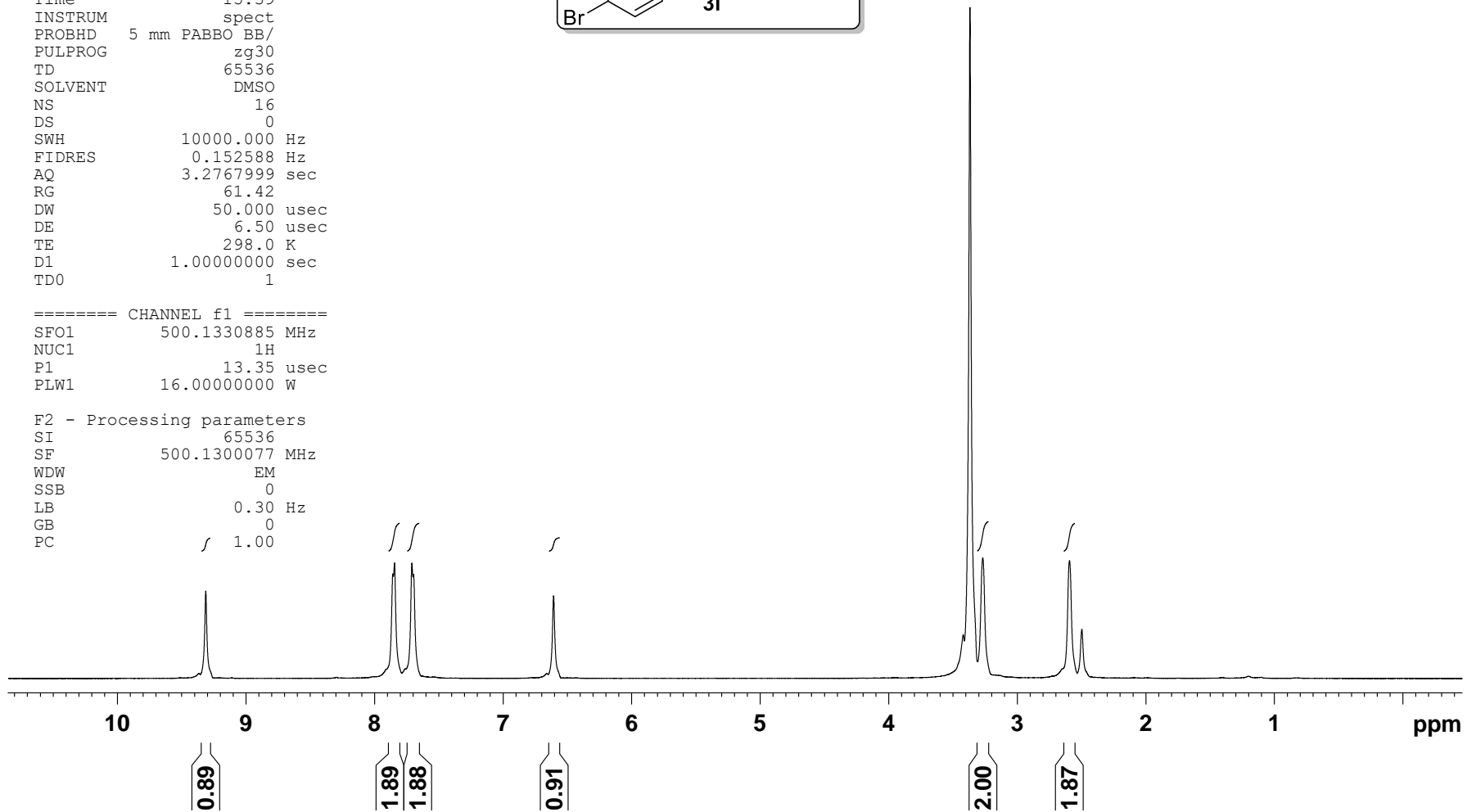
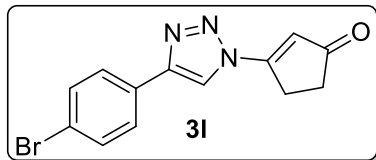


Figure S21. ¹H NMR Spectrum of 3I

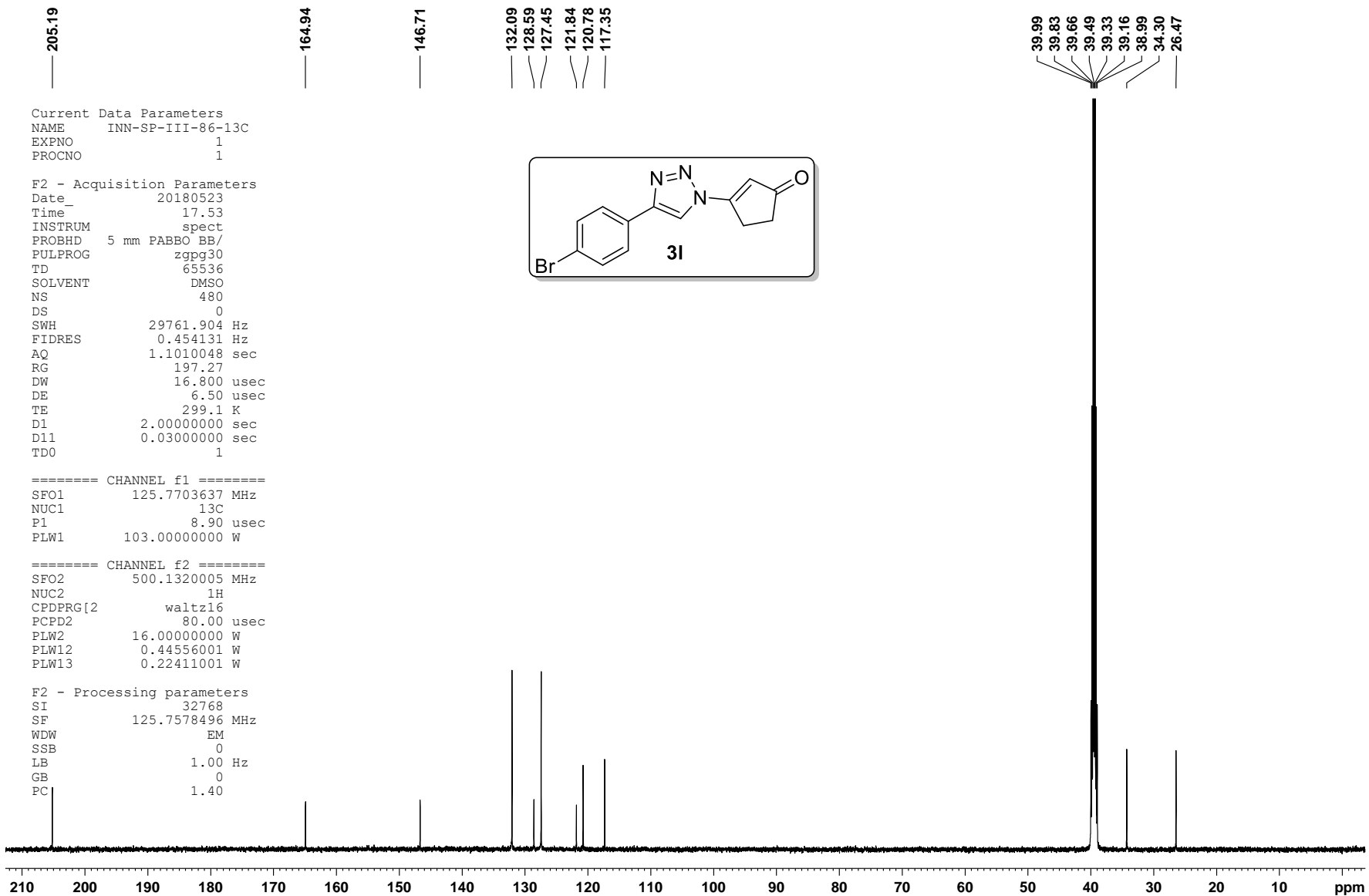


Figure S22. ¹³C NMR Spectrum of 3l

Current Data Parameters
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EXPNO 1
PROCNO 1

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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 1.0000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 13.35 usec
PLW1 16.0000000 W

F2 - Processing parameters
SI 65536
SF 500.1304281 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

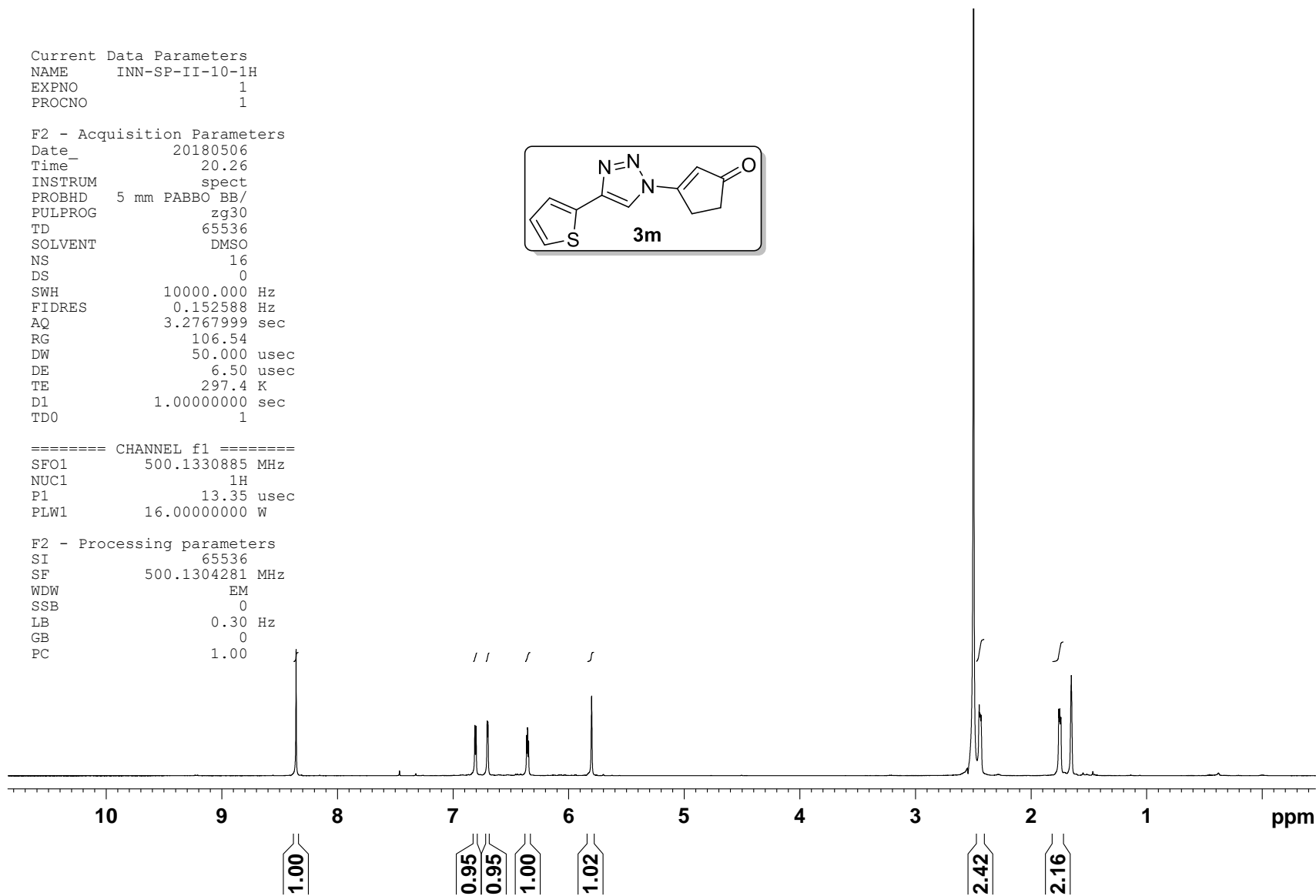
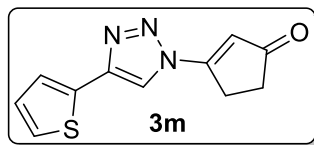


Figure S23. ¹H NMR Spectrum of 3m

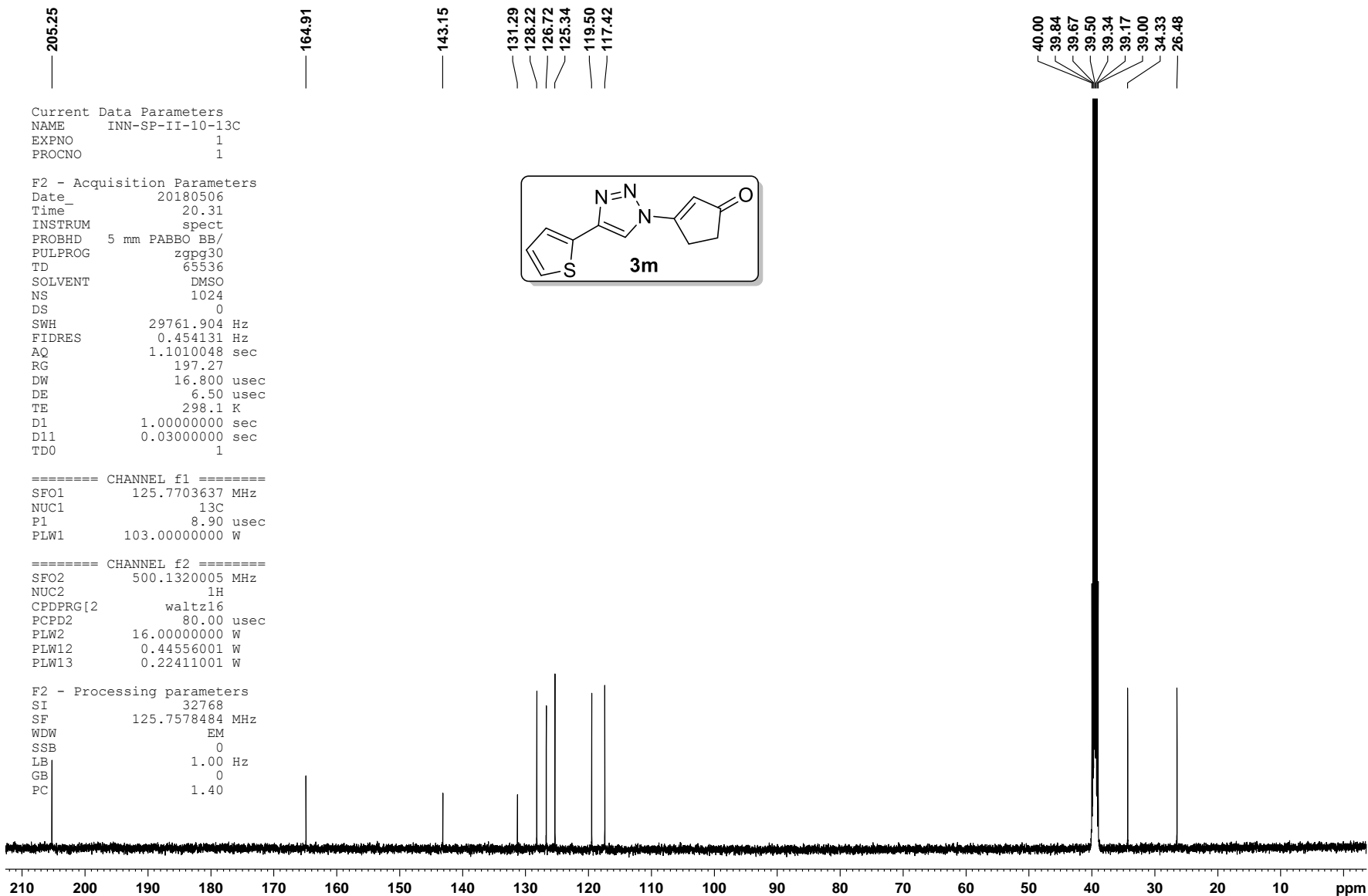
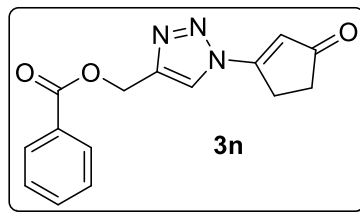


Figure S24. ¹³C NMR Spectrum of 3m

Current Data Parameters
NAME INN-SP-II-104-1H
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180417
Time_ 15.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
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

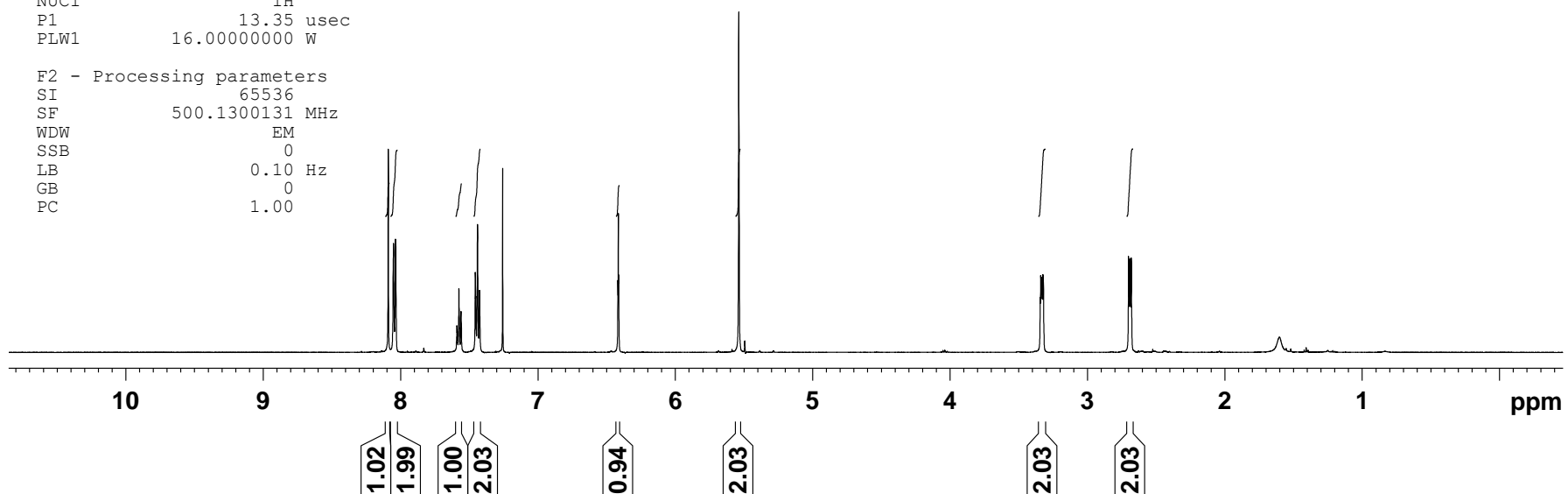


Figure S25. ¹H NMR Spectrum of 3n

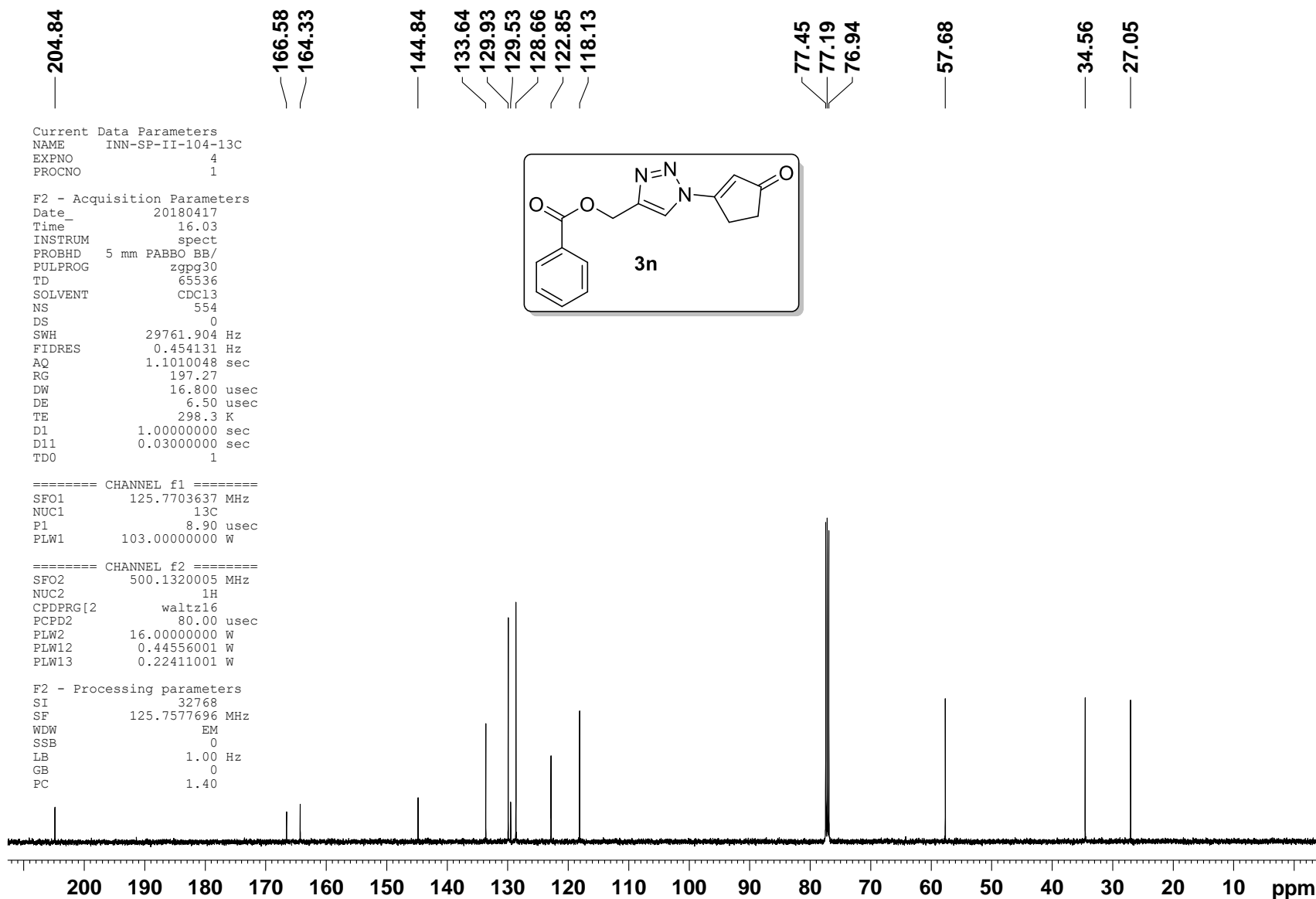
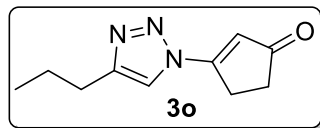


Figure S26. ¹³C NMR Spectrum of 3n

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 CDC13
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



=====
SFO1 500.1330885 MHz
NUC1 1H
P1 13.000 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

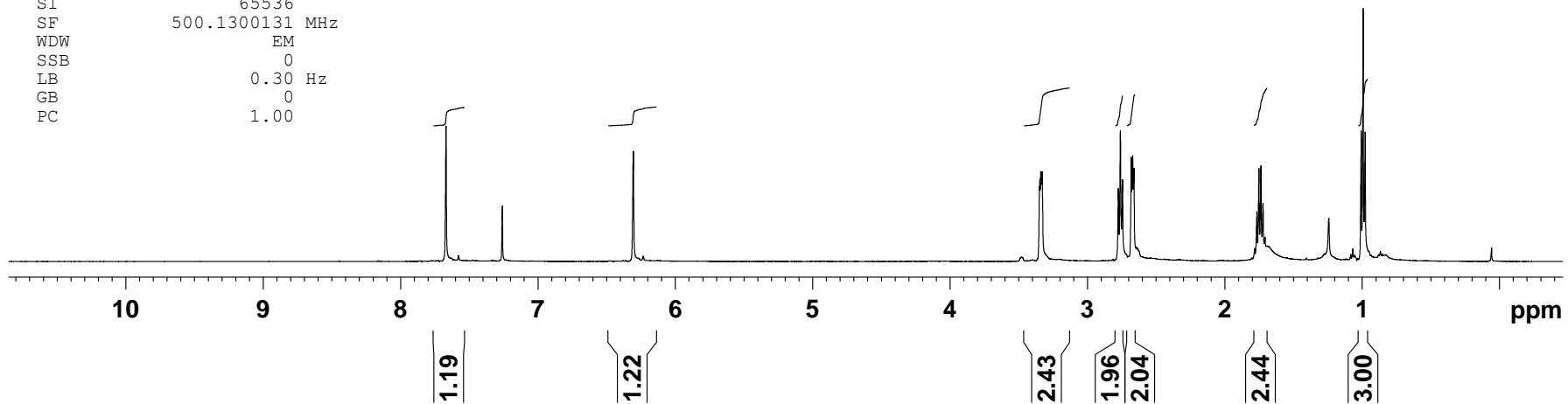


Figure S27. ¹H NMR Spectrum of 3o

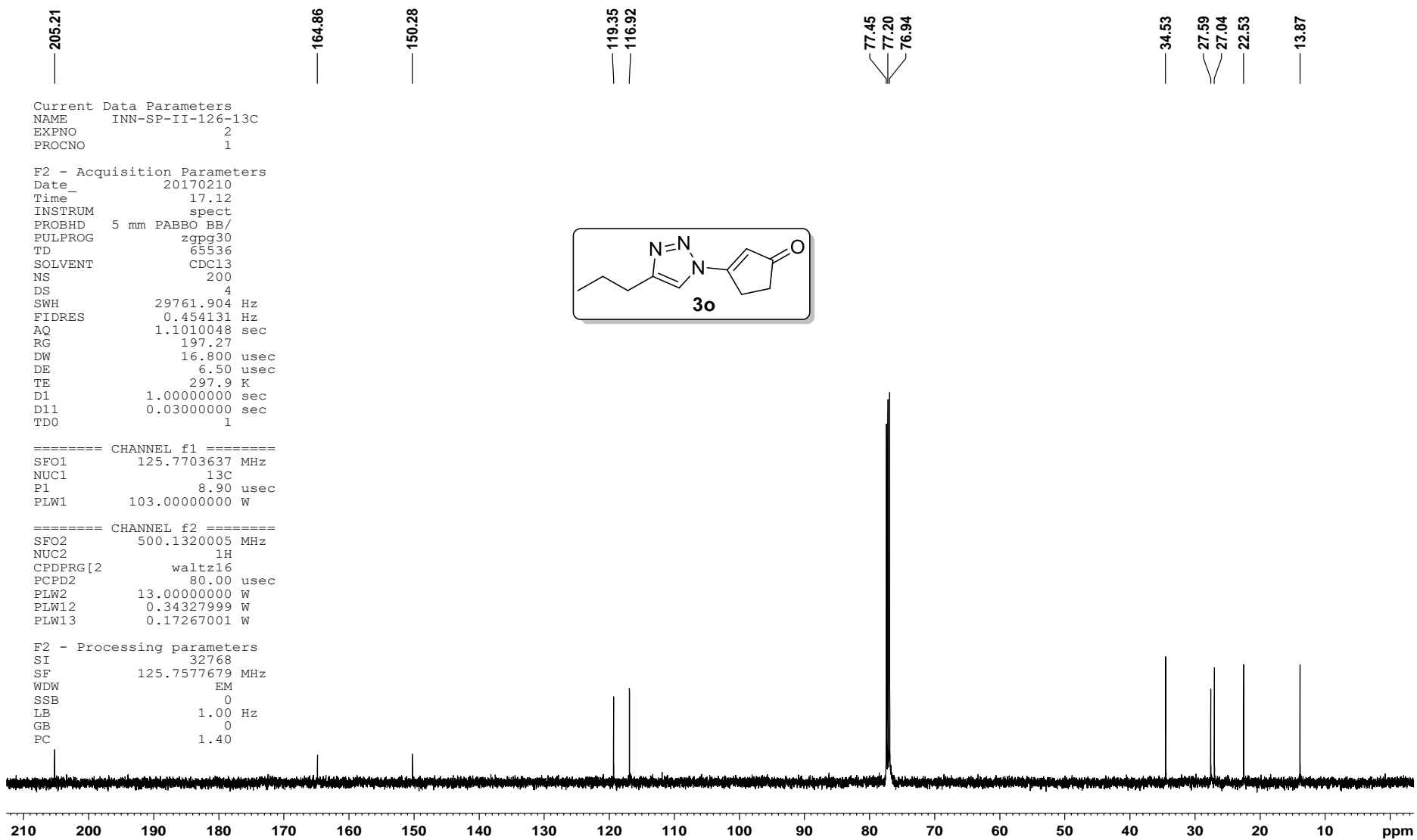
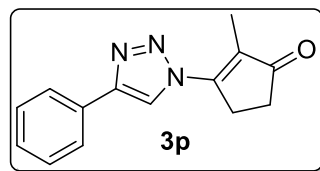


Figure S28. ¹³C NMR Spectrum of 3o

Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20180605
Time_ 5.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 54274
SOLVENT CDC13
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

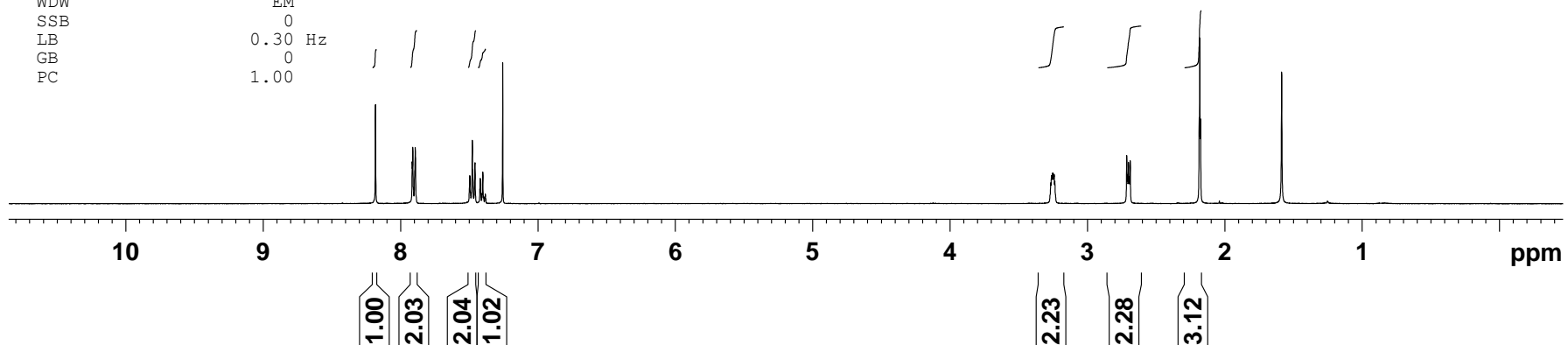


Figure S29. ¹H NMR Spectrum of 3p

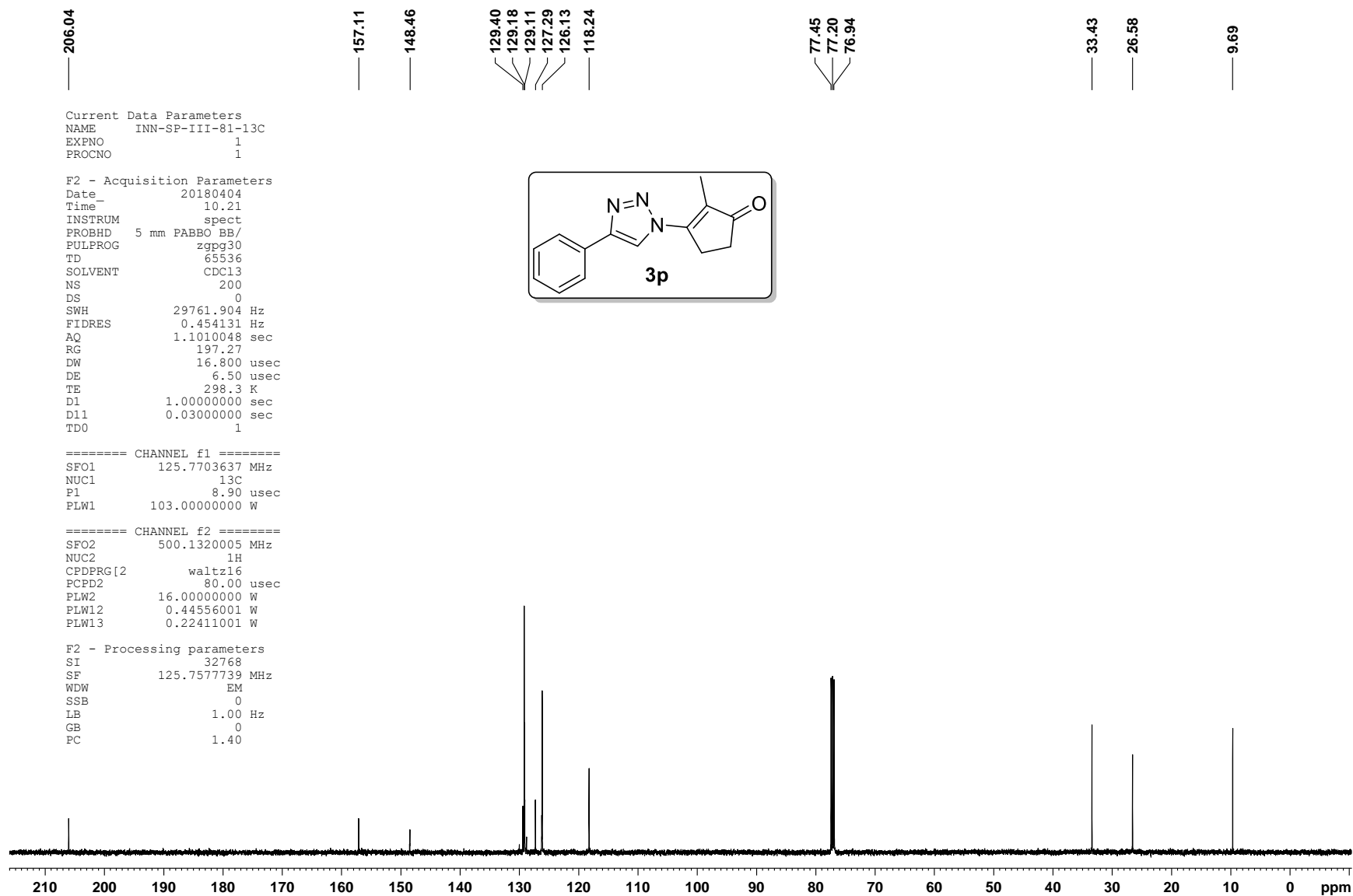


Figure S30. ^{13}C NMR Spectrum of 3p

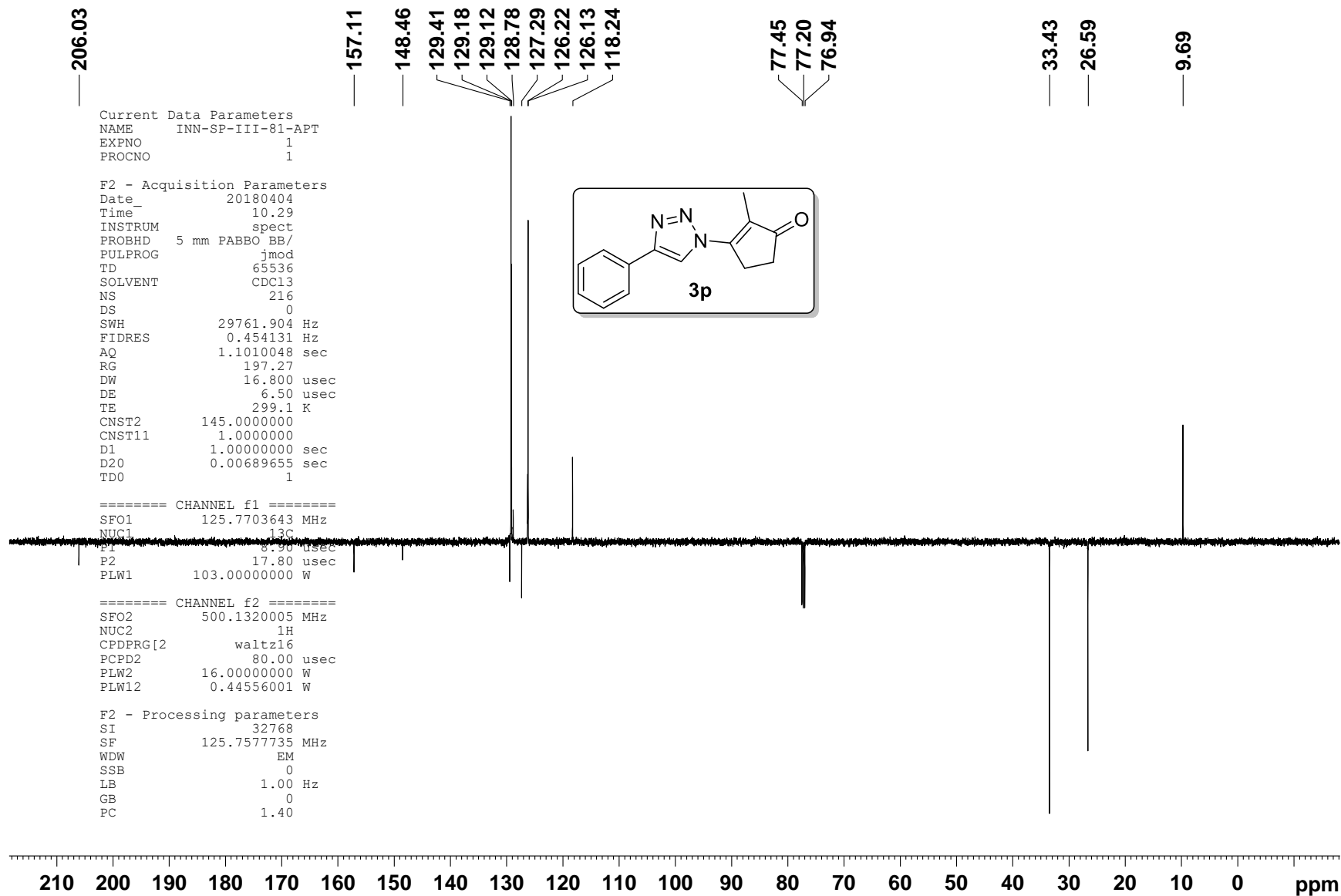
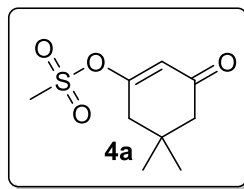


Figure S31. ¹³C-APT NMR Spectrum of 3p

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 CDC13
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

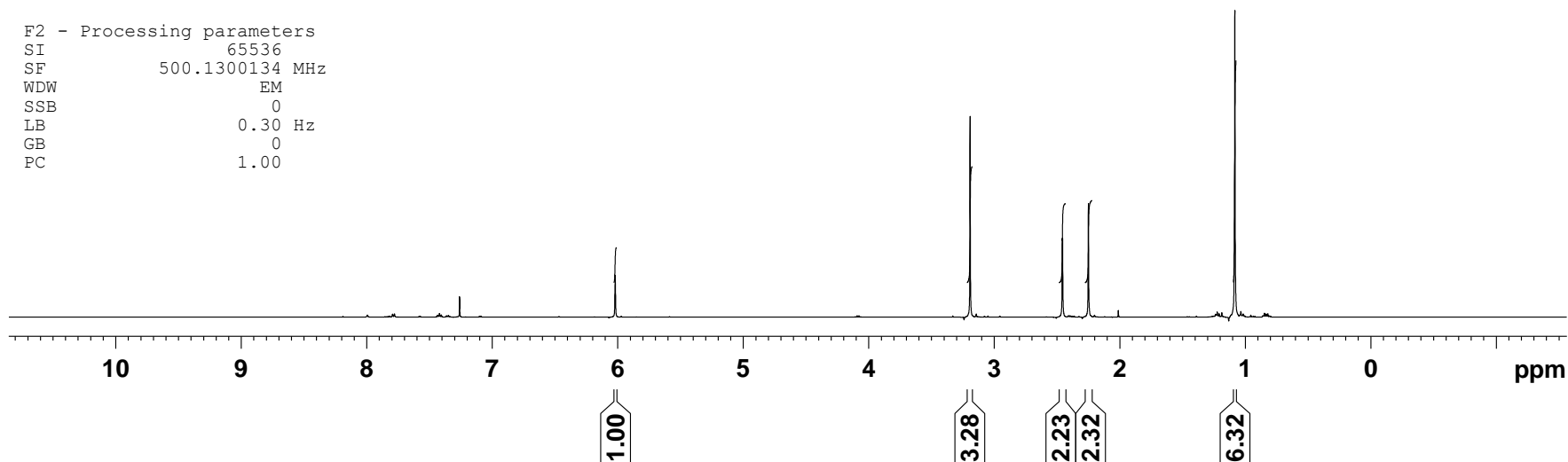


Figure S32. ¹H NMR Spectrum of 4a

198.30

166.11

114.74

77.55
77.23
76.91

50.13

41.92

41.19

38.57

32.59

32.42

Current Data Parameters
 NAME INN-SP-III-MESYLTRIAZOLEDIMEDONE UP-13C
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201020
 Time_ 23.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 58
 DS 0
 SNH 26041.666 Hz
 FIDRES 0.397364 Hz
 AQ 1.2582912 sec
 RG 1030
 DW 19.200 usec
 DE 6.50 usec
 TE 297.4 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.00 dB
 PL1W 56.53121948 W
 SFO1 100.6238364 MHz

==== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 13.69 dB
 PL13 14.50 dB
 PL2W 10.56200695 W
 PL12W 0.35871249 W
 PL13W 0.29767781 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127864 MHz
 WDW EM
 SSB 0
 LB 10.00 Hz
 GB 0
 FC 1.40

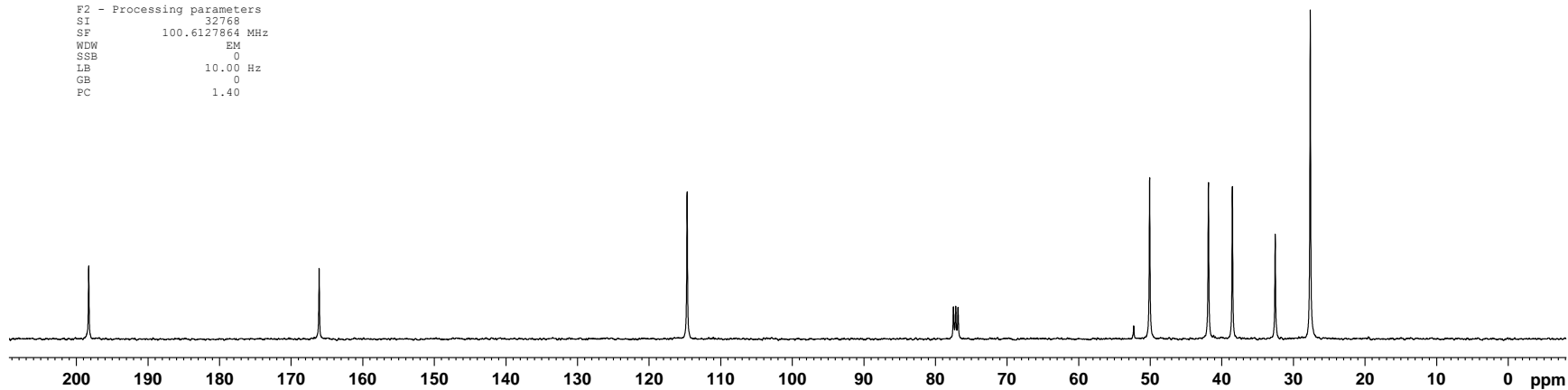
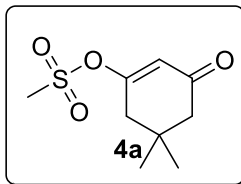


Figure S33. ¹³C NMR Spectrum of 4a

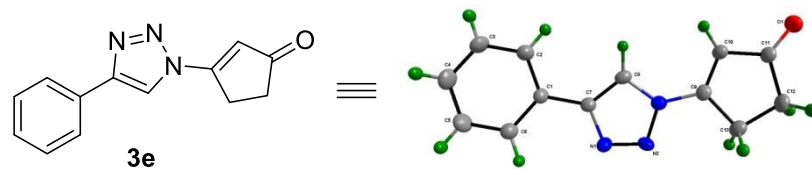


Figure S34. ORTEP diagram of 3e

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)

2 Θ range for data collection/ $^{\circ}$	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

