

Supplementary Information
For

Regio- and stereoselective synthesis of functionalized tetrahydrobenzochromenes and hexahydrochromenochromenones via [4+2] annulation of curcumins with nitrochromenes

Banamali Laha, Alati Suresh and Irishi N N Namboothiri*

Department of Chemistry and Indian Institute of Technology, Bombay, Mumbai 400 076
irishi@iitb.ac.in

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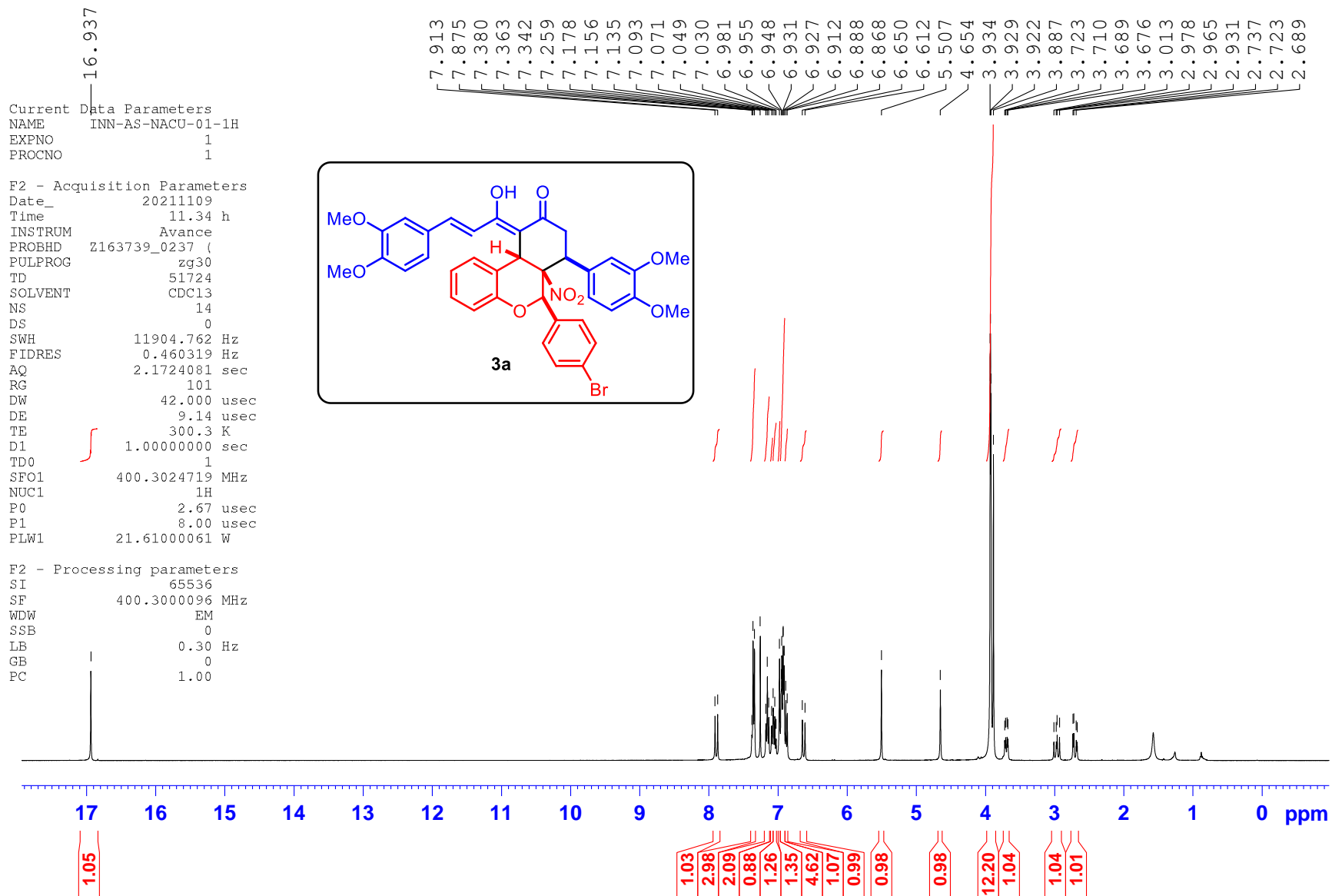


Figure S01. ¹H NMR Spectrum of 3a

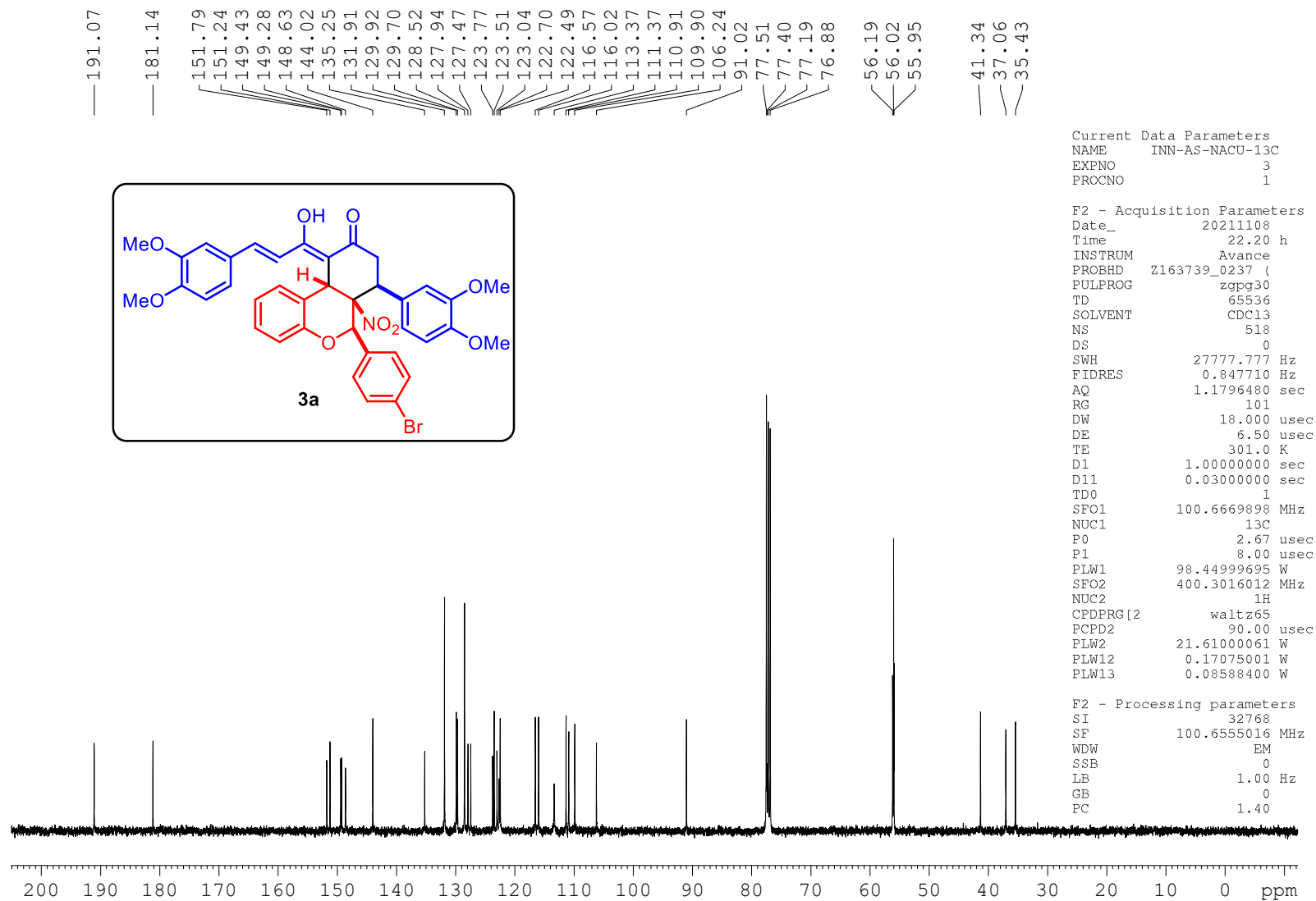


Figure S02. ¹³C NMR Spectrum of 3a

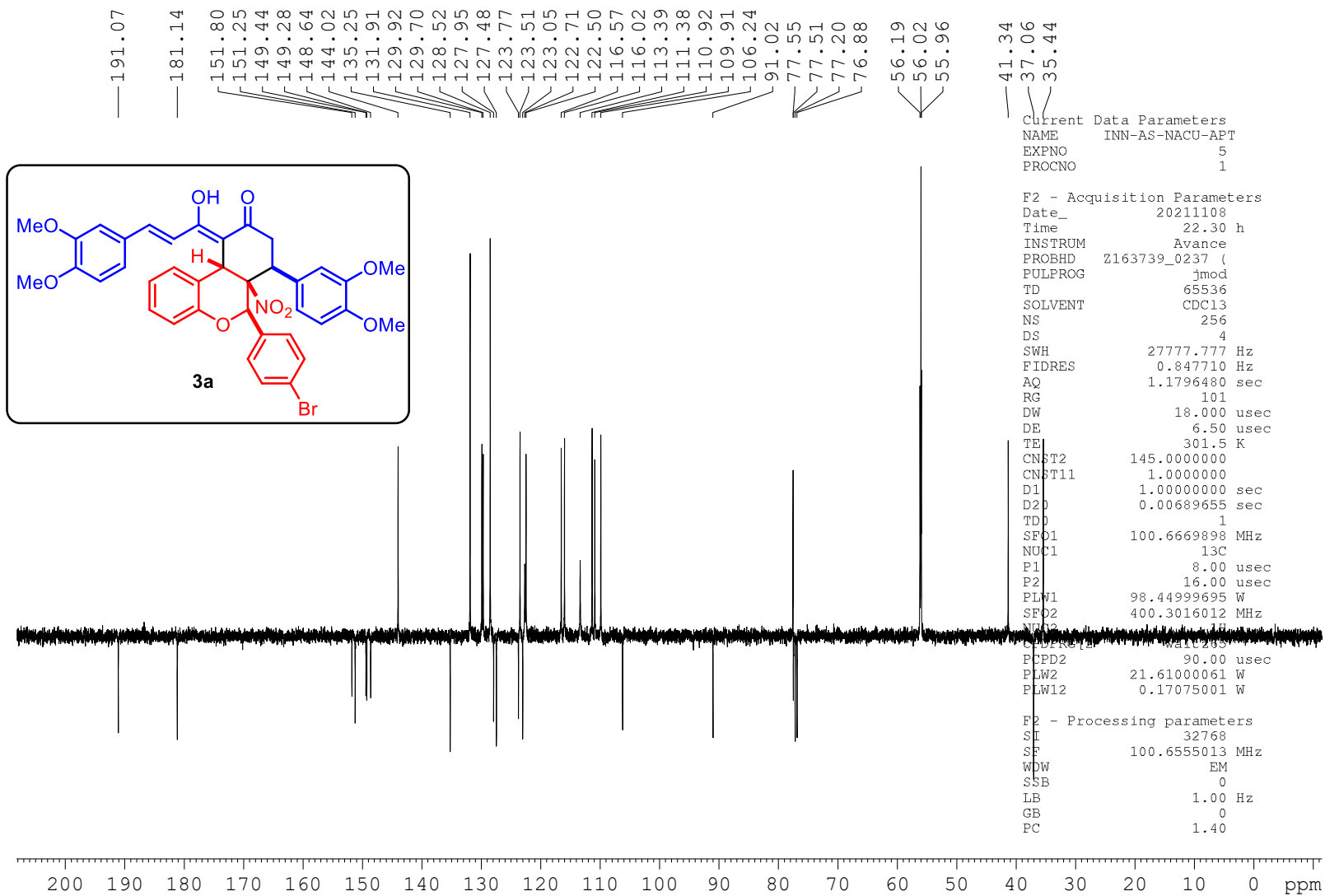


Figure S03. ¹³C-APT NMR Spectrum of **3a**

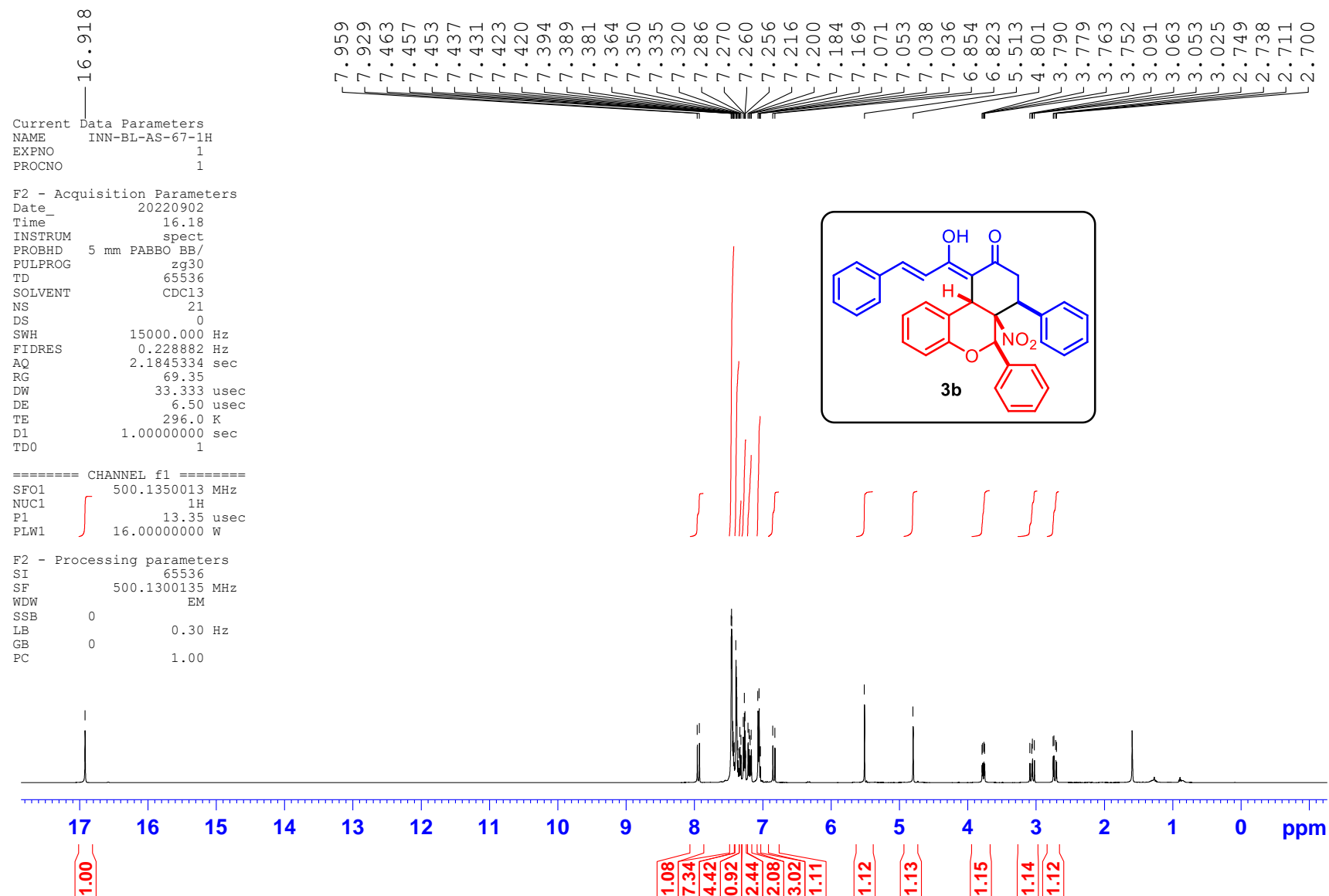


Figure S04. ¹H NMR Spectrum of 3b

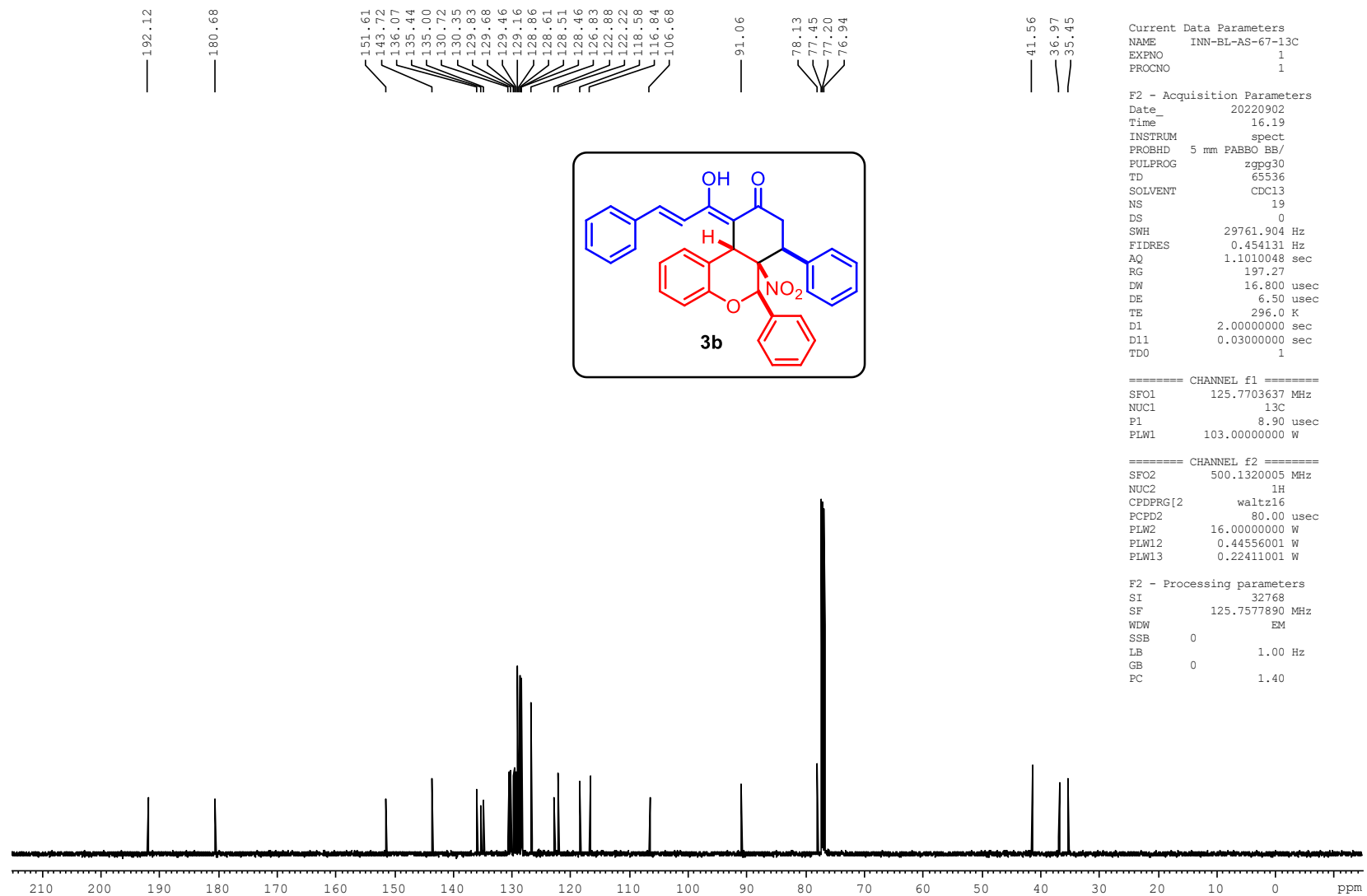


Figure S05. ¹³C NMR Spectrum of **3b**

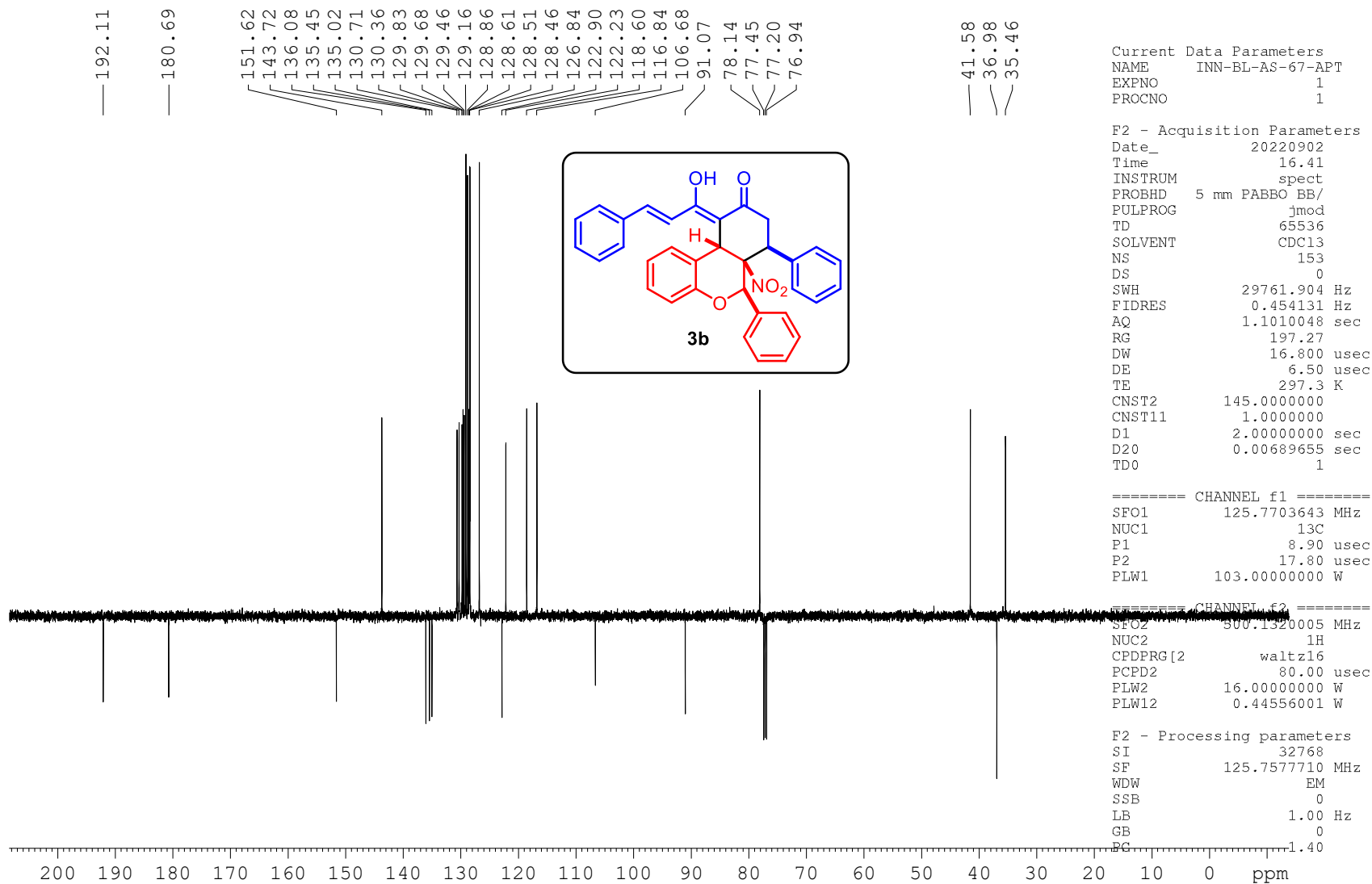


Figure S06. ¹³C-APT NMR Spectrum of 3b

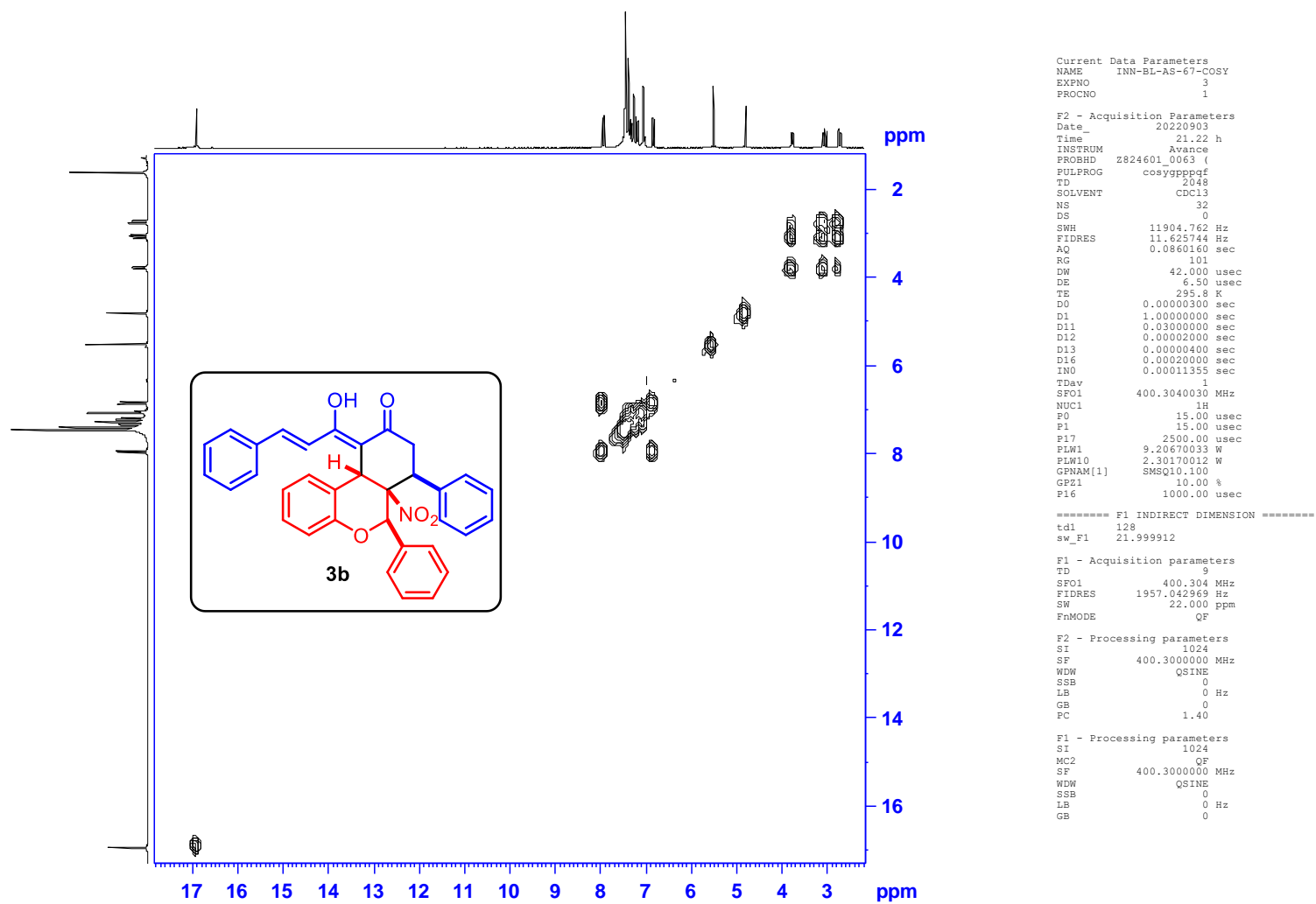


Figure S07. ^1H - ^1H COSY NMR Spectrum of 3b

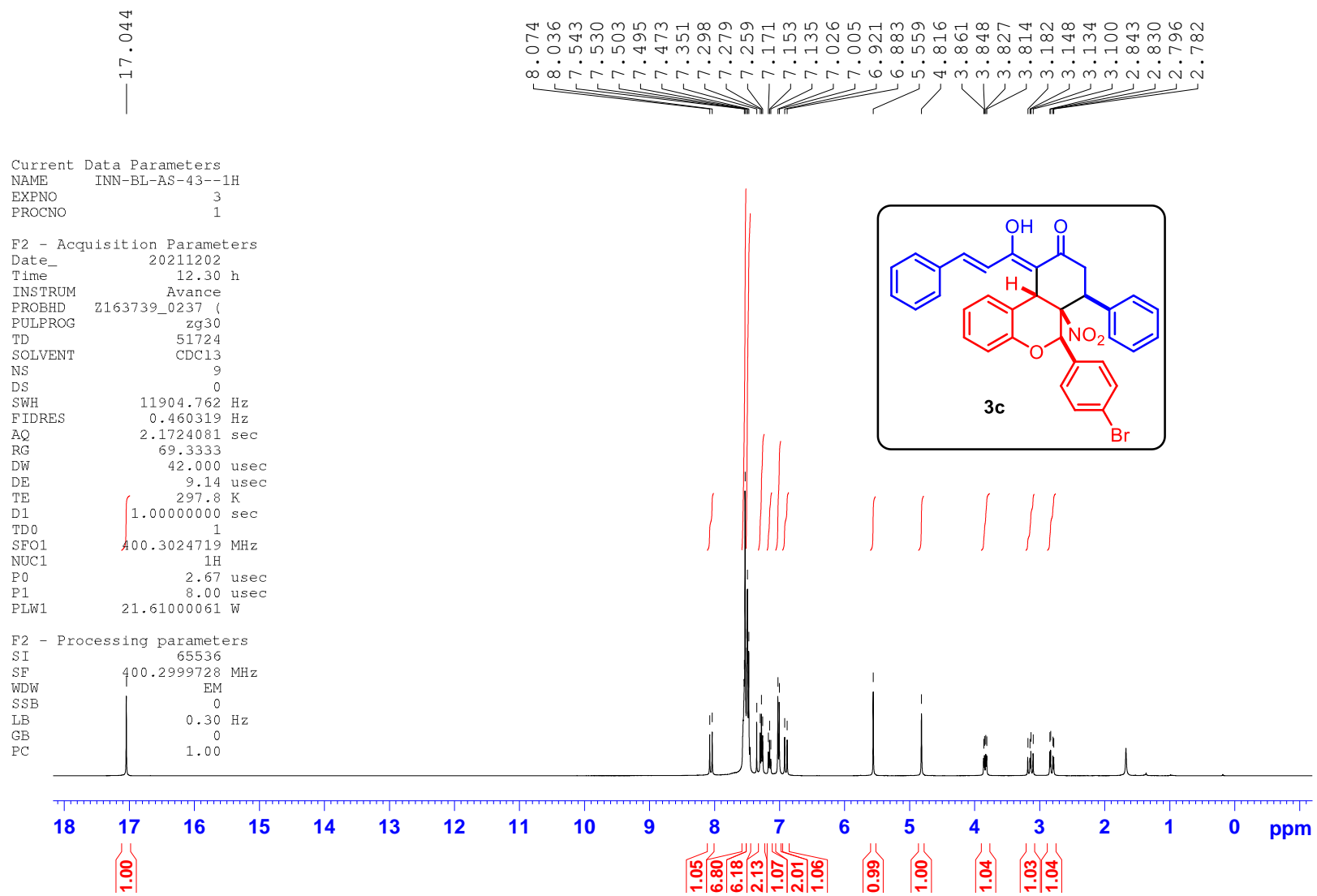
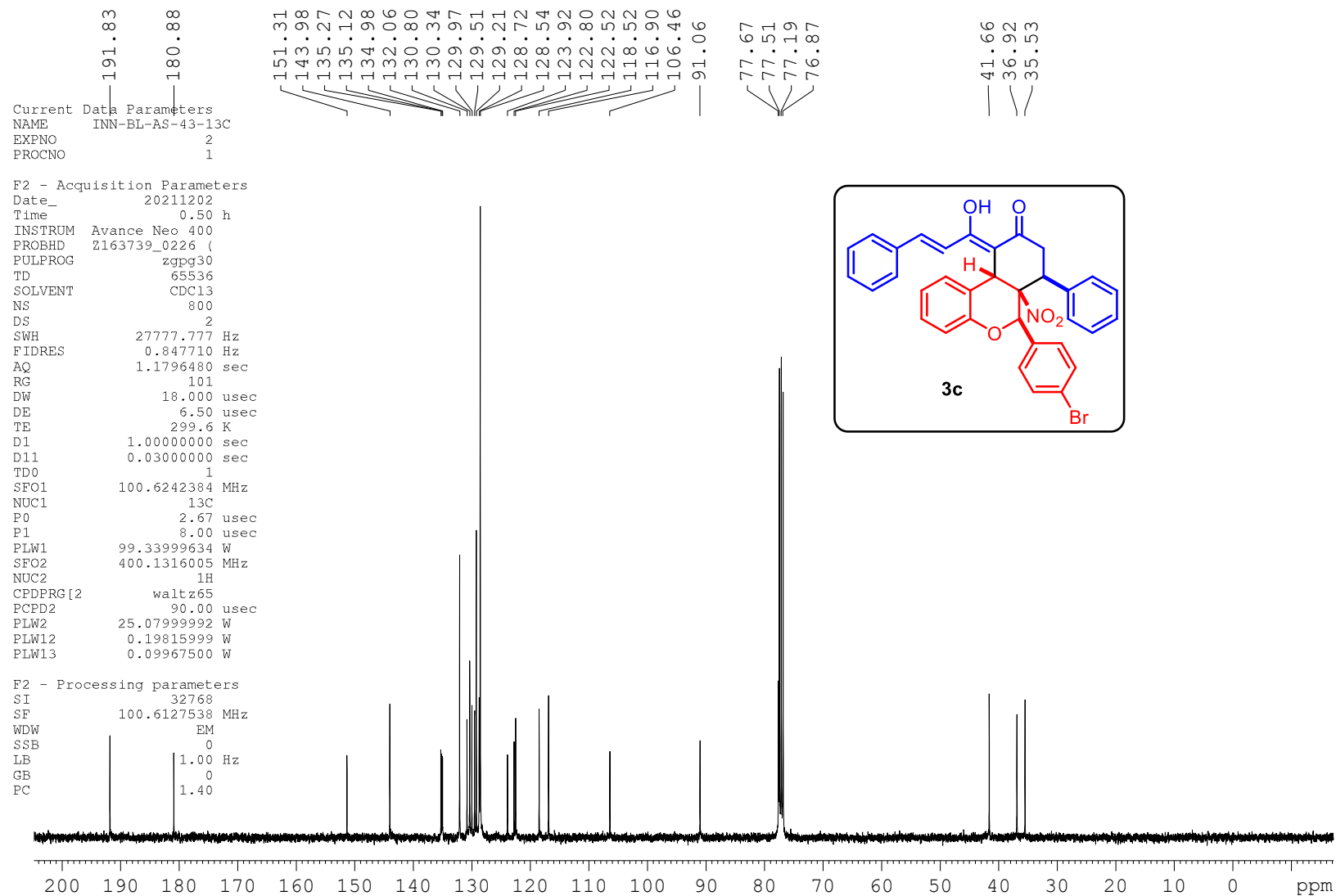


Figure S08. ¹H NMR Spectrum of 3c



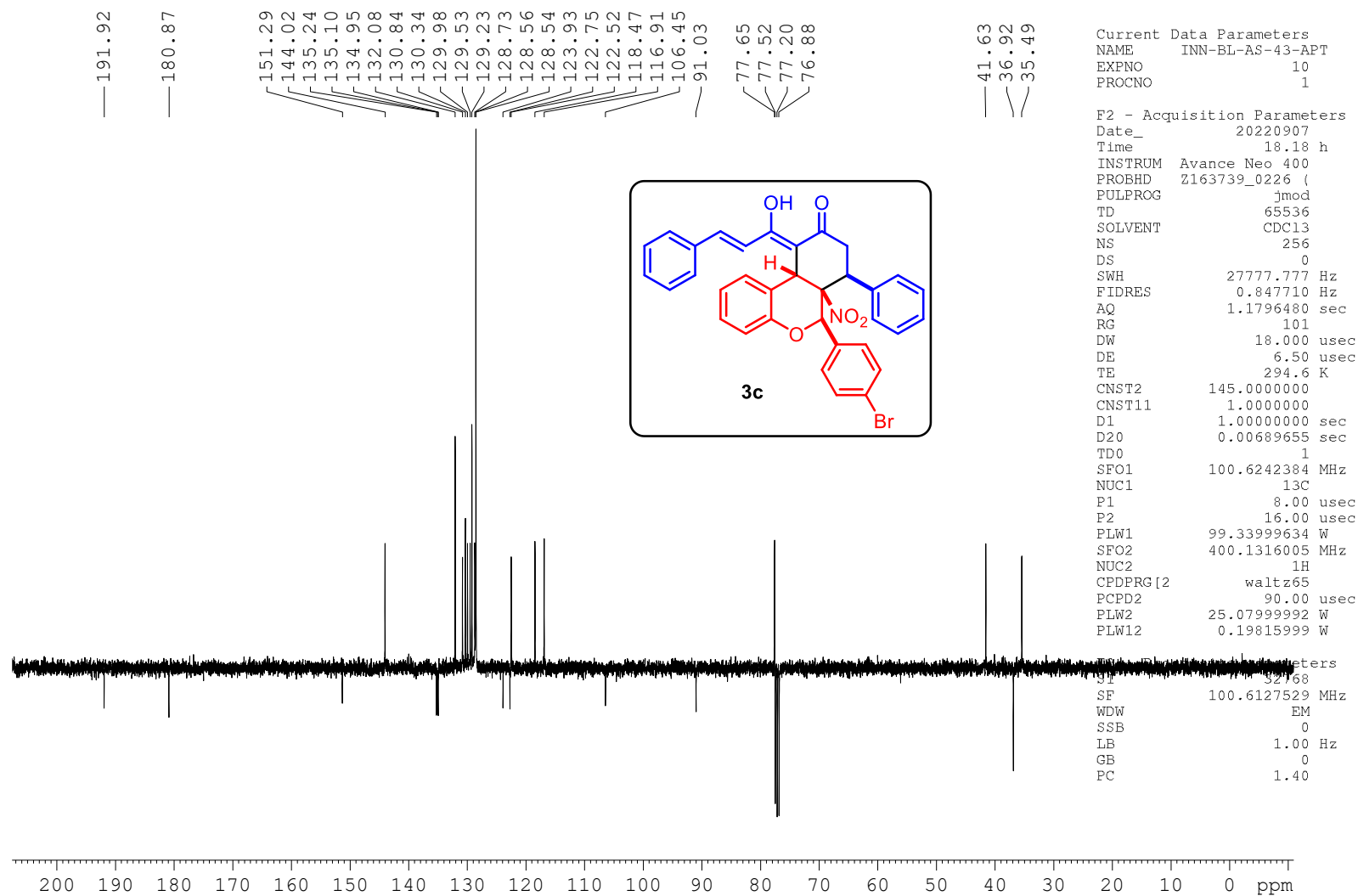


Figure S10. ¹³C-APT Spectrum of 3c

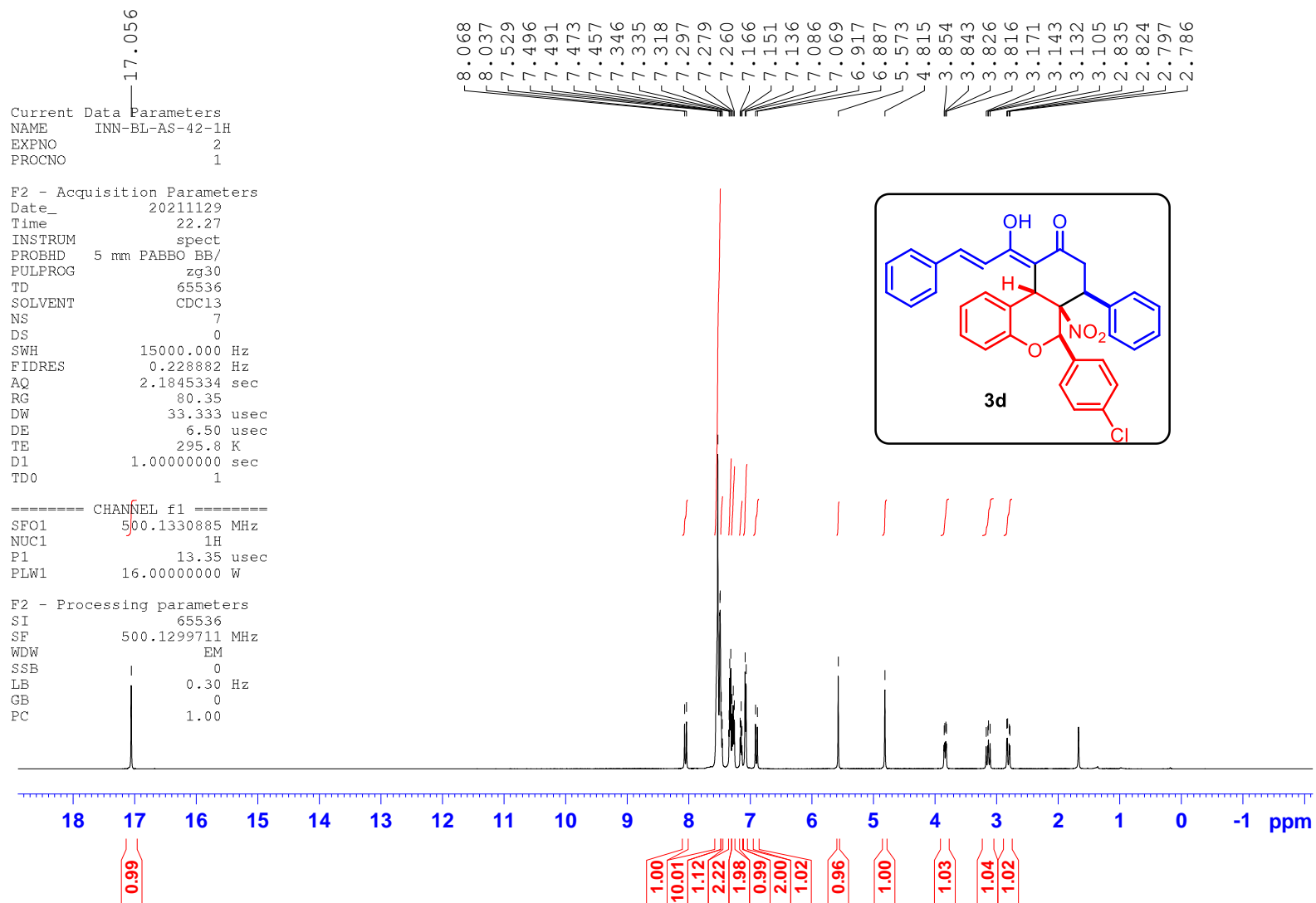


Figure S11. ¹H NMR Spectrum of **3d**

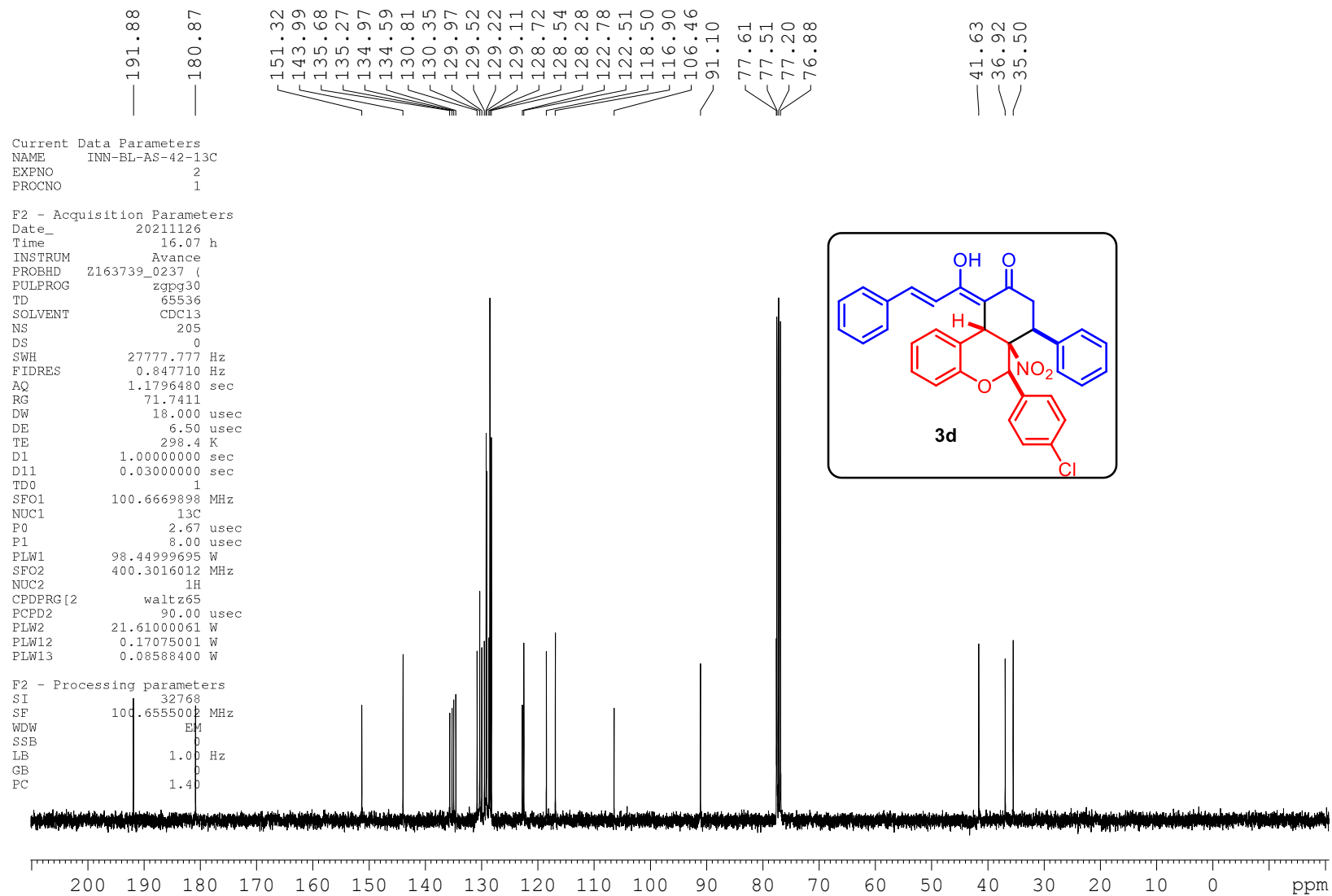


Figure S12. ¹³C NMR Spectrum of 3d

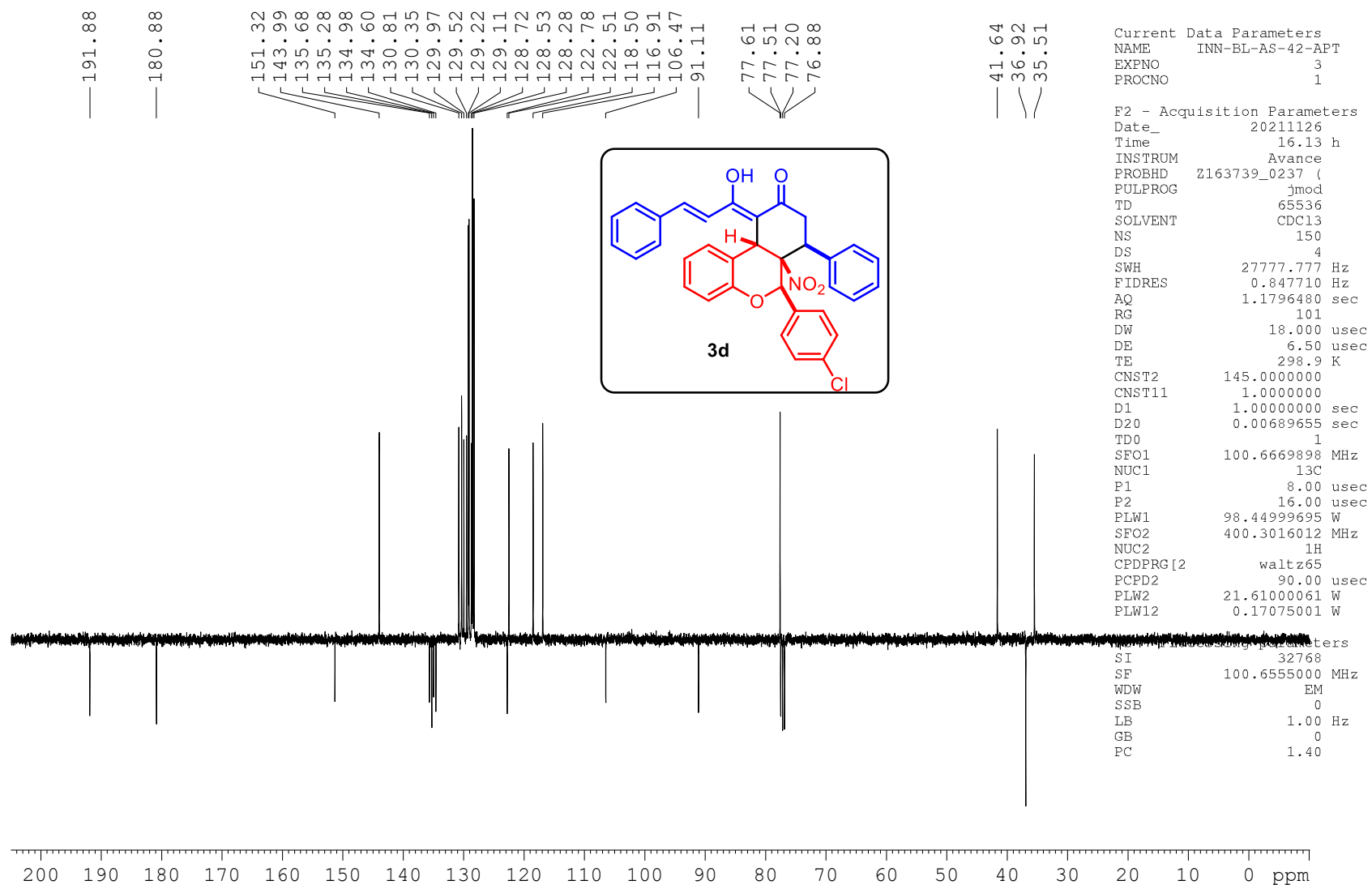


Figure S13. ¹³C-APT NMR Spectrum of 3d

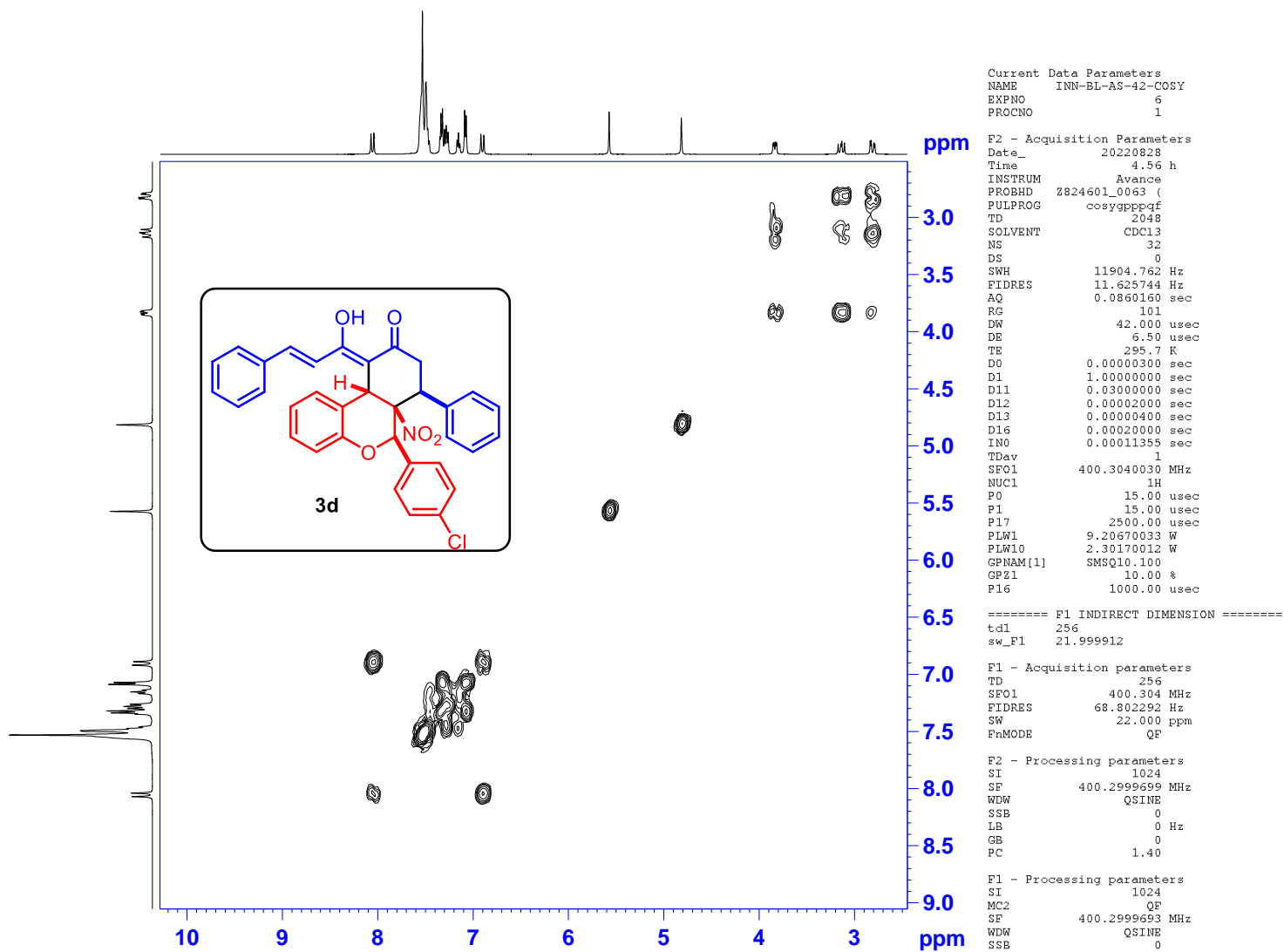
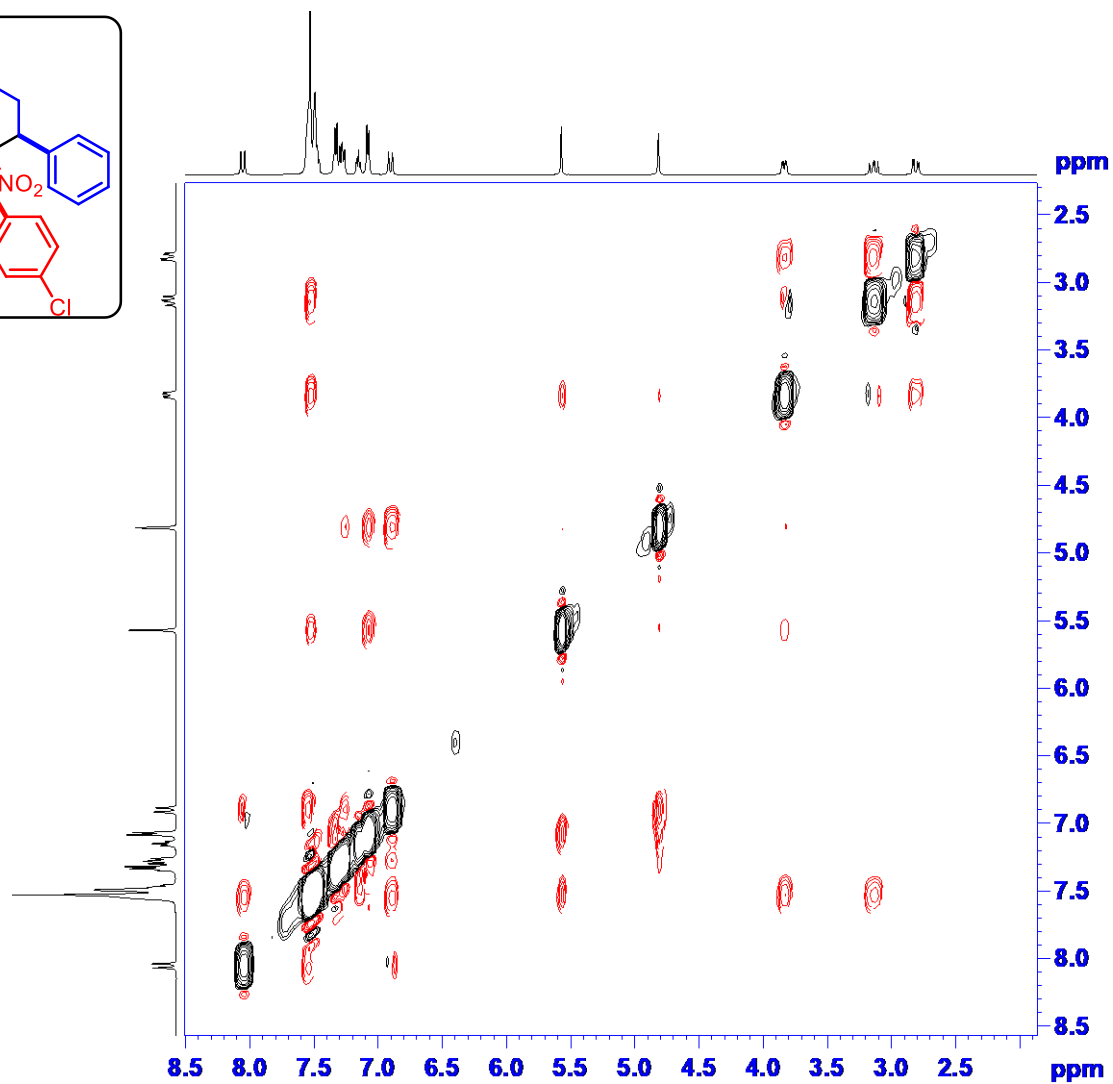
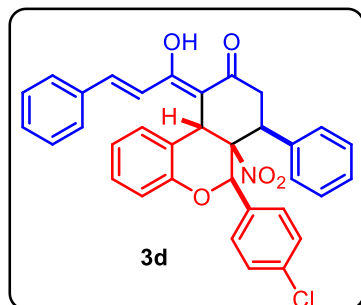


Figure S14. ^1H - ^1H COSY NMR Spectrum of 3d



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 PROCNO 1

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 TD 2048
 SOLVENT CDC13
 NS 32
 DS 0
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 FIDRES 11.625744 Hz
 AQ 0.0860160 sec
 RG 101
 DW 42.000 usec
 DE 11.45 usec
 TE 295.2 K
 D0 0.00003768 sec
 D1 1.00000000 sec
 D8 0.60000002 sec
 D16 0.00020000 sec
 IN0 0.00011355 sec
 TDav 1
 SF01 400.304030 MHz
 NUC1 1H
 P1 15.00 usec
 P2 30.00 usec
 PLW1 9.20670033 W
 GPNAM[1] SMSQ10.100
 GPZ1 40.00 %
 F16 1000.00 usec

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 sw_F1 21.999884

F1 - Acquisition parameters
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 FIDRES 68.802292 Hz
 SW 22.000 ppm
 FhMODE TPPI

F2 - Processing parameters
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 SF 400.2999696 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
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 MC2 TPPI
 SF 400.2999679 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0

Figure S15. ^1H - ^1H NOESY NMR Spectrum of 3d

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 EXPNO 18
 PROCNO 1

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 PULPROG zg30
 TD 51724
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 NS 18
 DS 0
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 FIDRES 0.460319 Hz
 AQ 2.1724081 sec
 RG 101
 DW 42.000 usec
 DE 9.14 usec
 TE 295.9 K
 D1 1.00000000 sec
 TD0 1
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 NUC1 1H
 P0 2.67 usec
 P1 8.00 usec
 PLW1 25.07999992 W

F2 - Processing parameters
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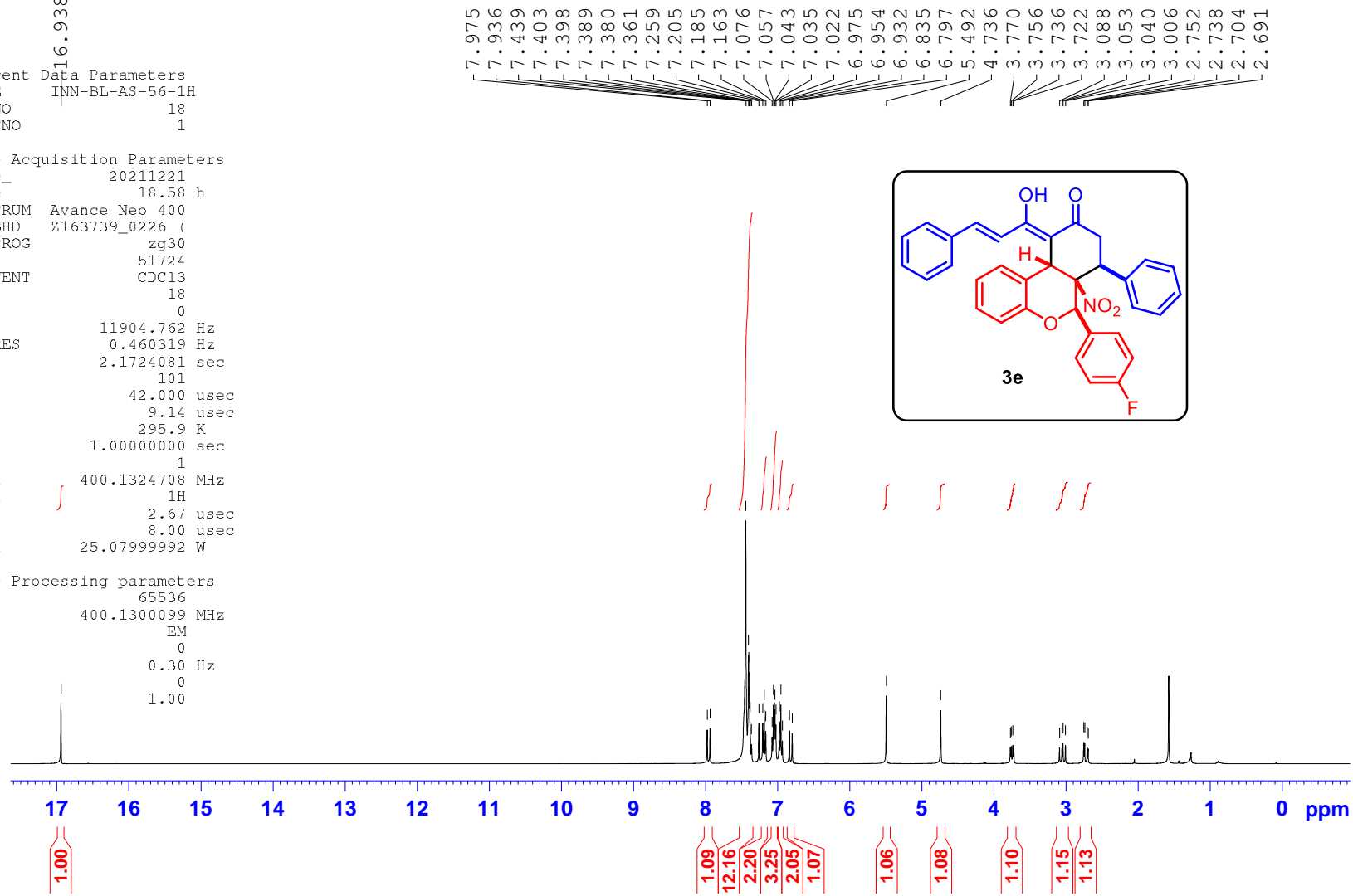


Figure S16. ¹H NMR Spectrum of 3e

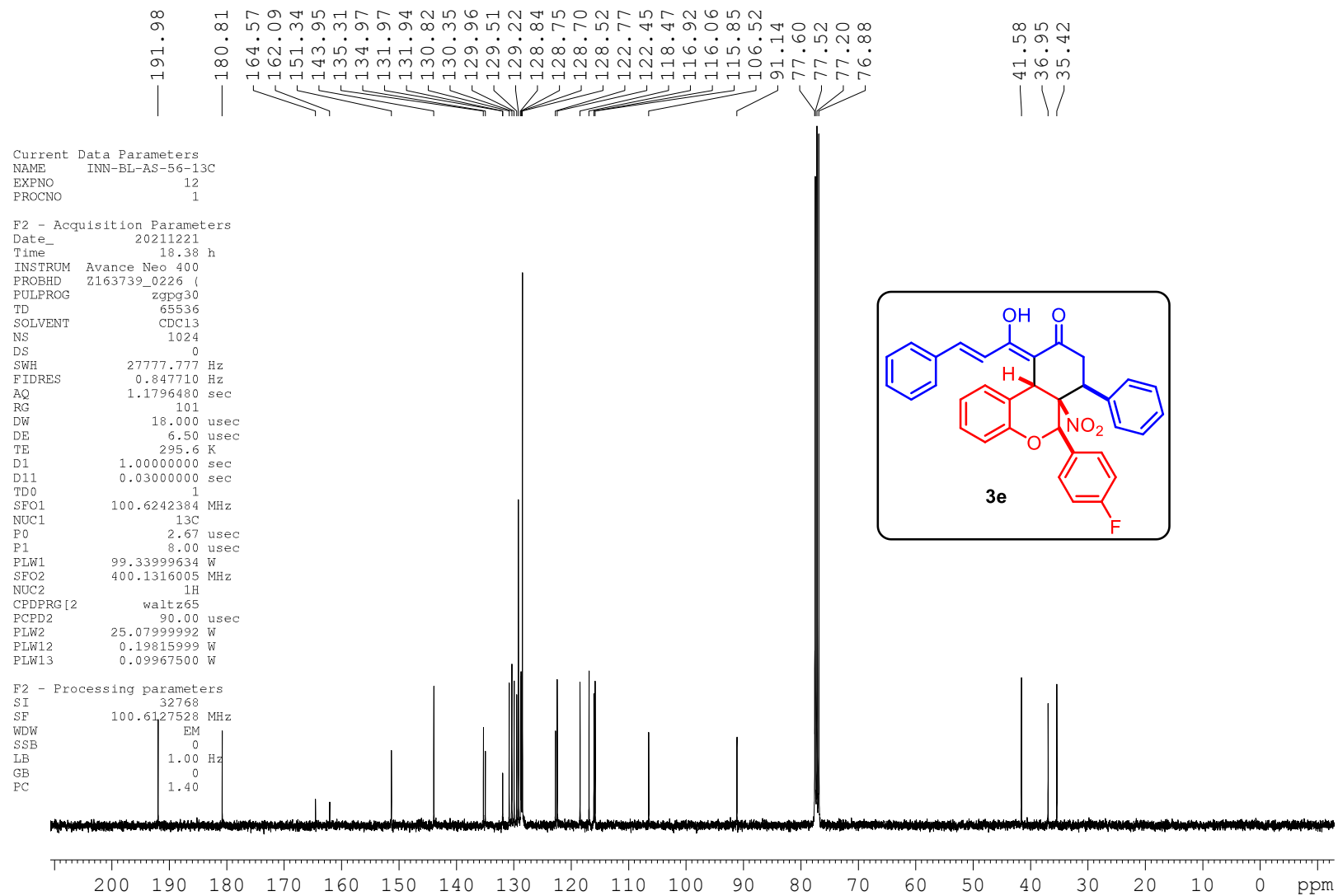


Figure S17. ^{13}C NMR Spectrum of 3e

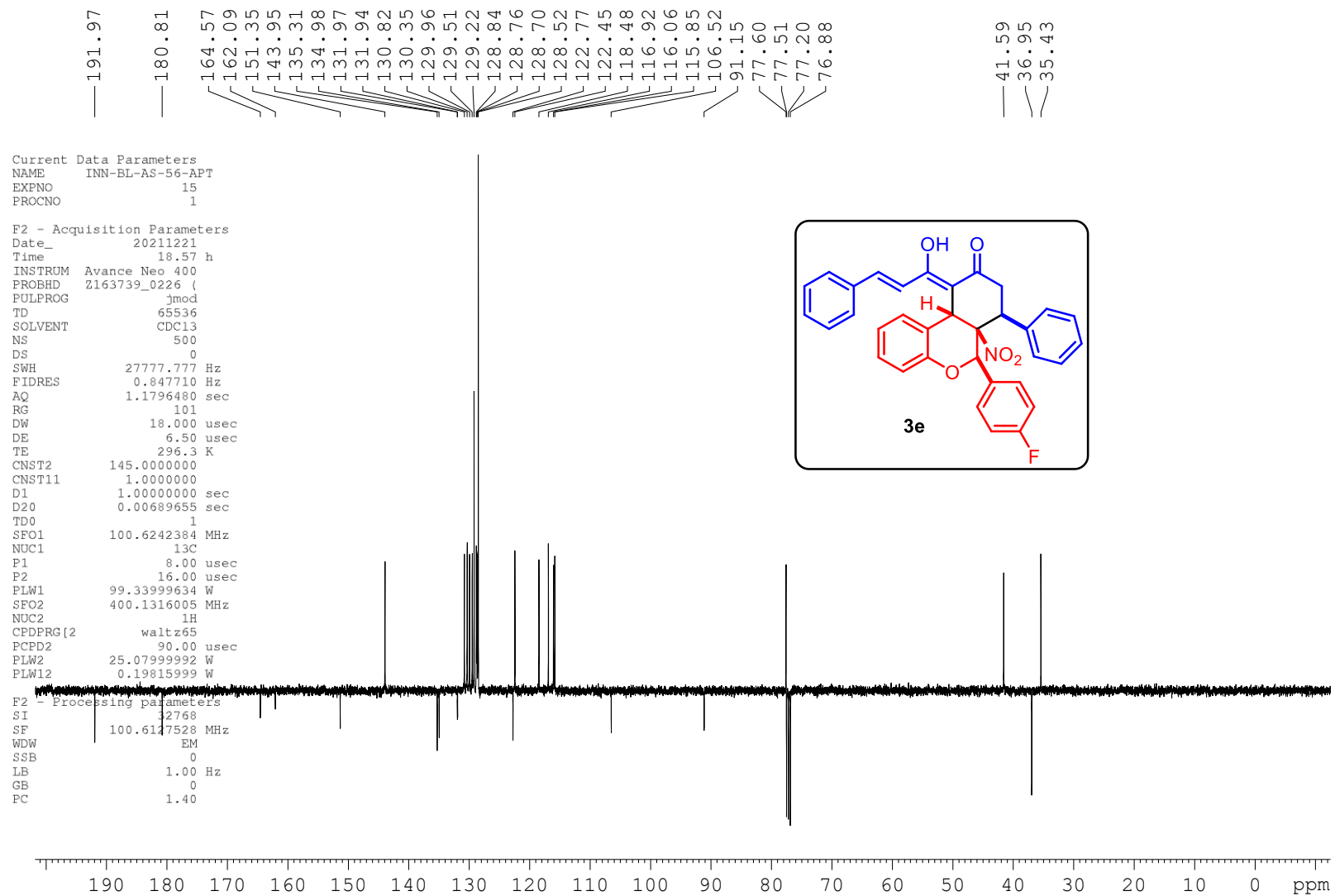


Figure S18. ¹³C-APT NMR Spectrum of 3e

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EXPNO 21
PROCNO 1

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TD 131072
SOLVENT CDC13
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DS 4
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FIDRES 2.543132 Hz
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RG 101
DW 3.000 usec
DE 6.50 usec
TE 295.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 376.4795413 MHz
NUC1 19F
P1 12.00 usec
PLW1 31.08799934 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 25.07999992 W
PLW12 0.19815999 W

F2 - Processing parameters
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LB 1.00 Hz
GB 0
PC 1.00

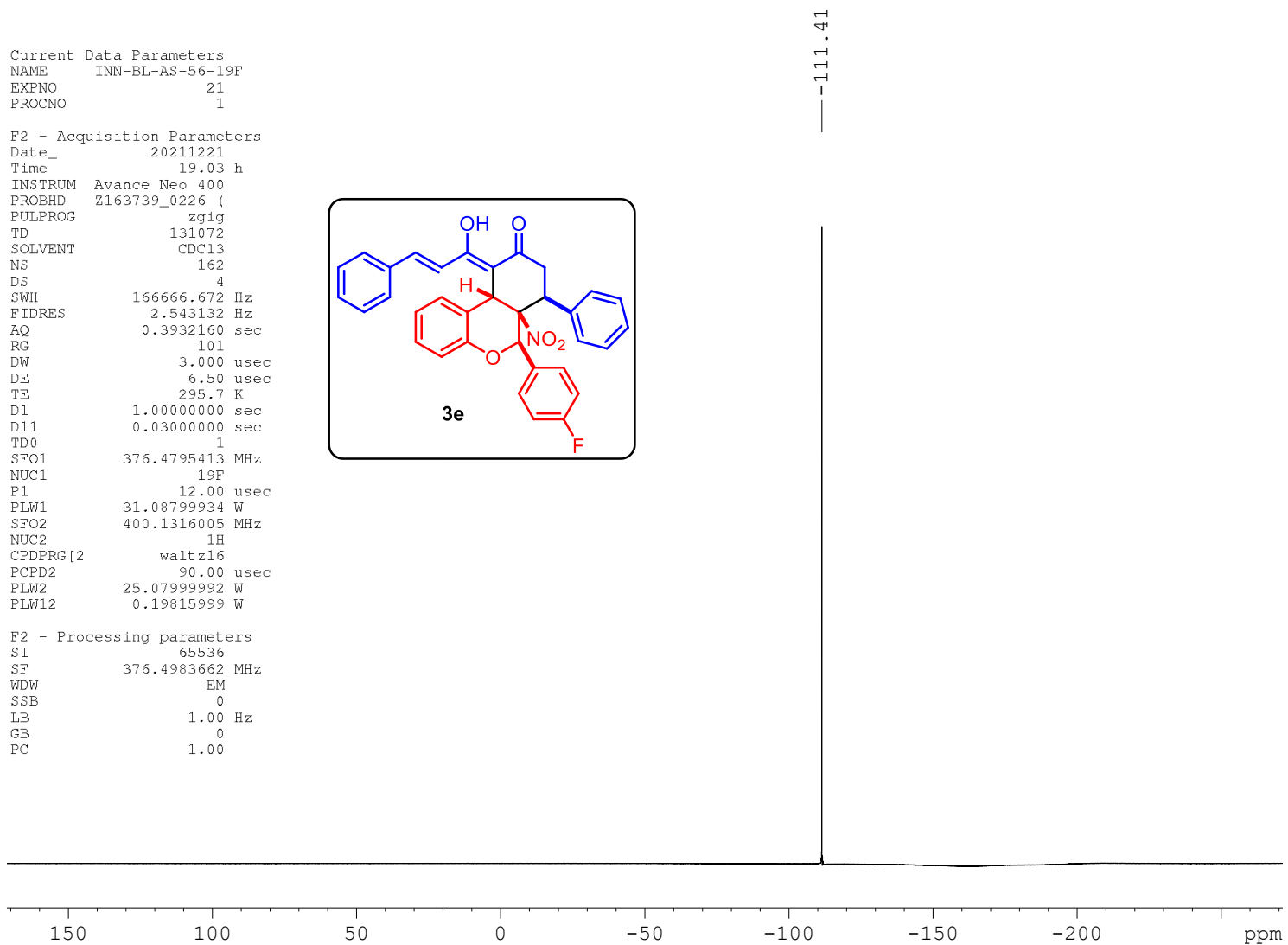
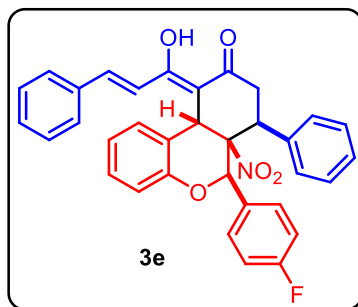


Figure S19. ¹⁹F NMR Spectrum of 3e

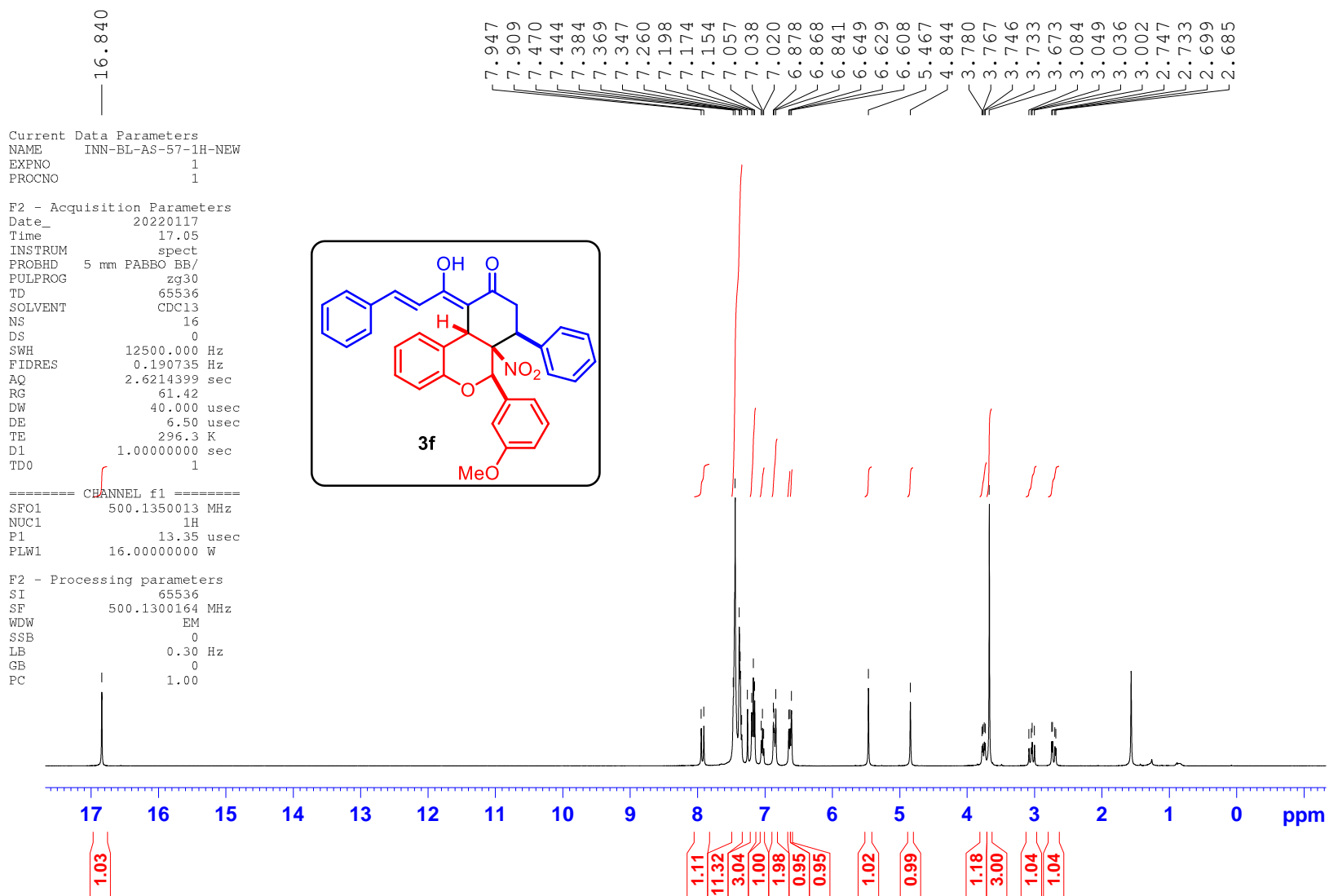


Figure S20. ¹H NMR Spectrum of 3f

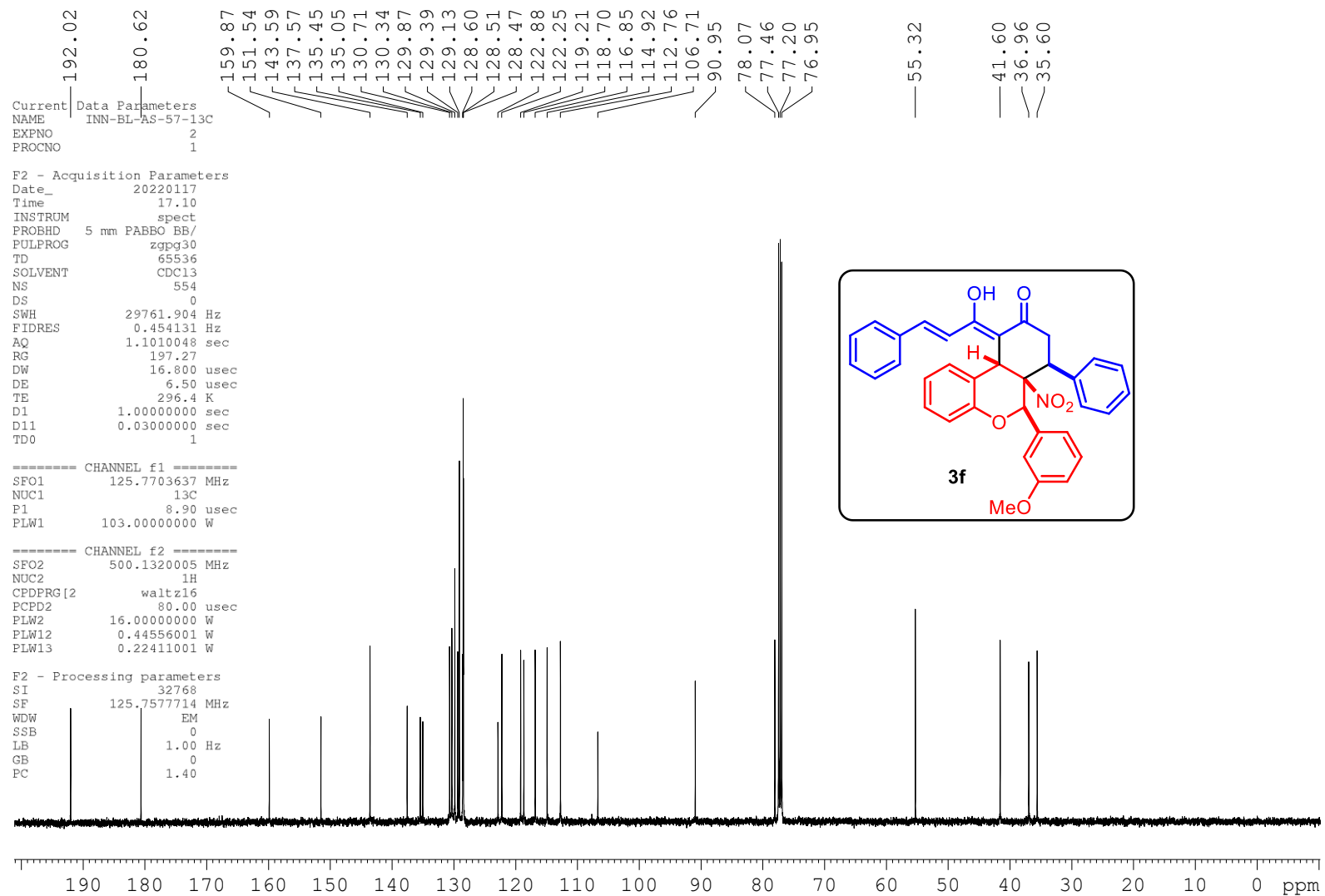


Figure S21. ¹³C NMR Spectrum of 3f

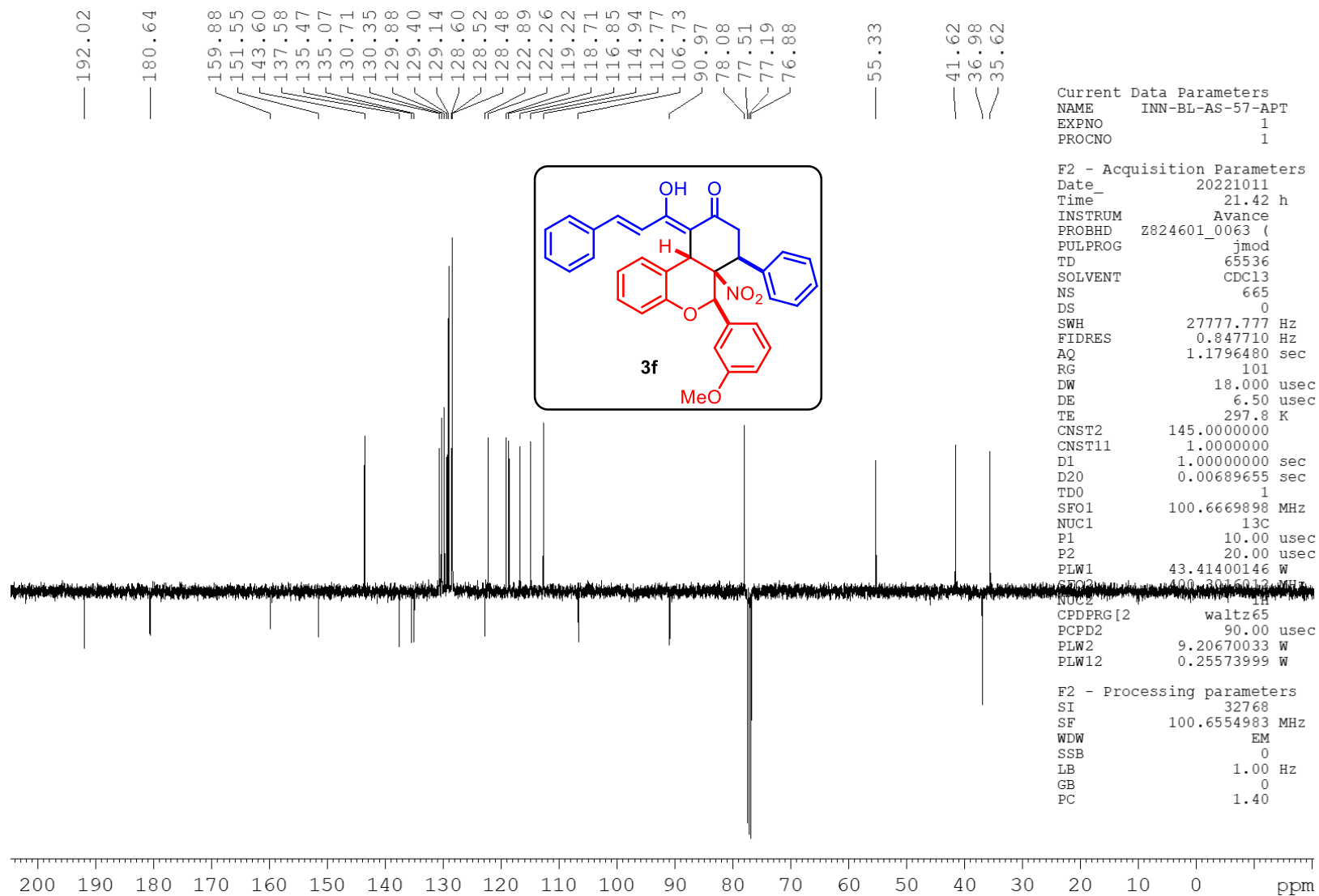


Figure S22. ¹³C-APT Spectrum of **3f**

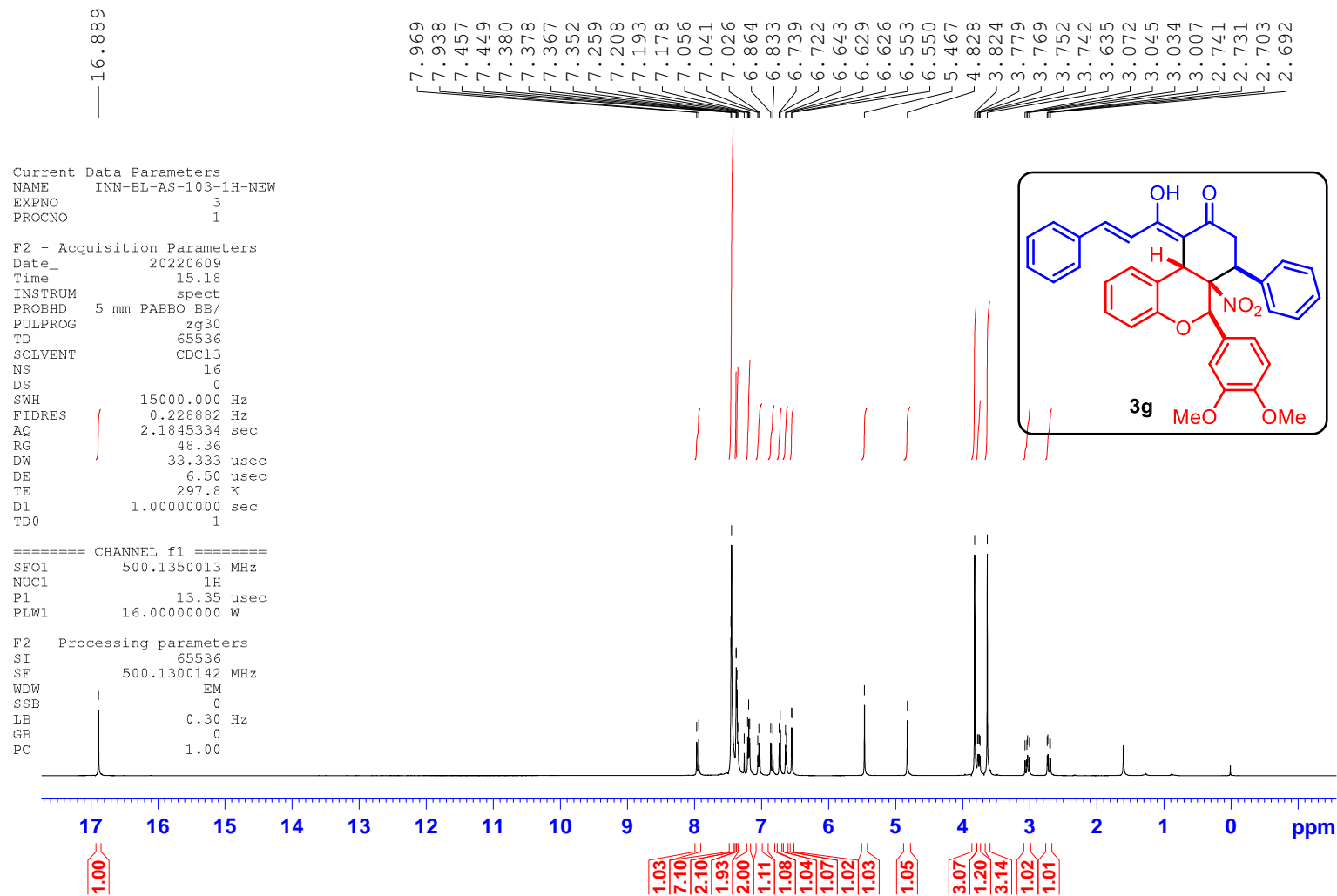


Figure S23. ¹H NMR Spectrum of 3g

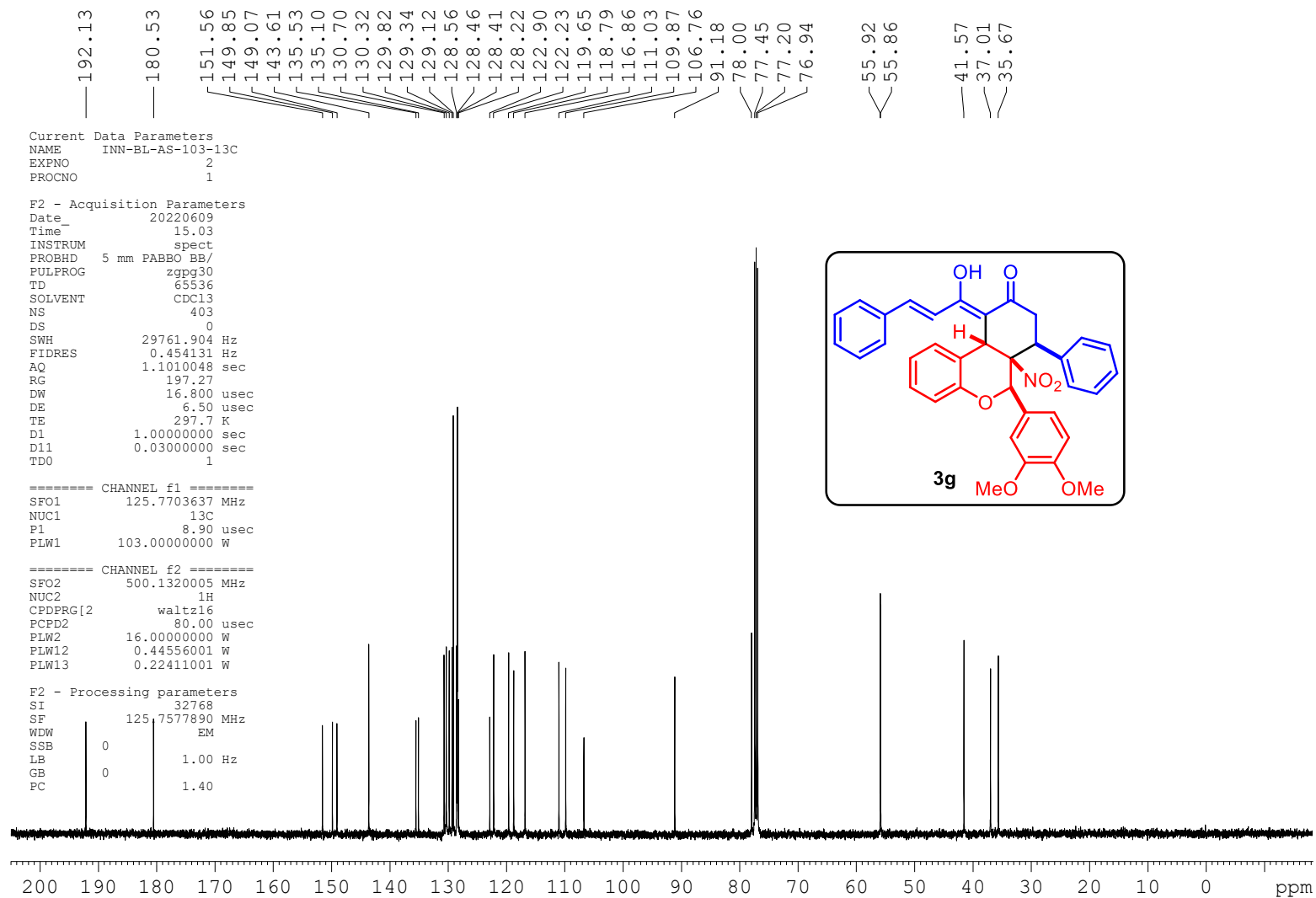


Figure S24. ¹³C NMR Spectrum of 3g

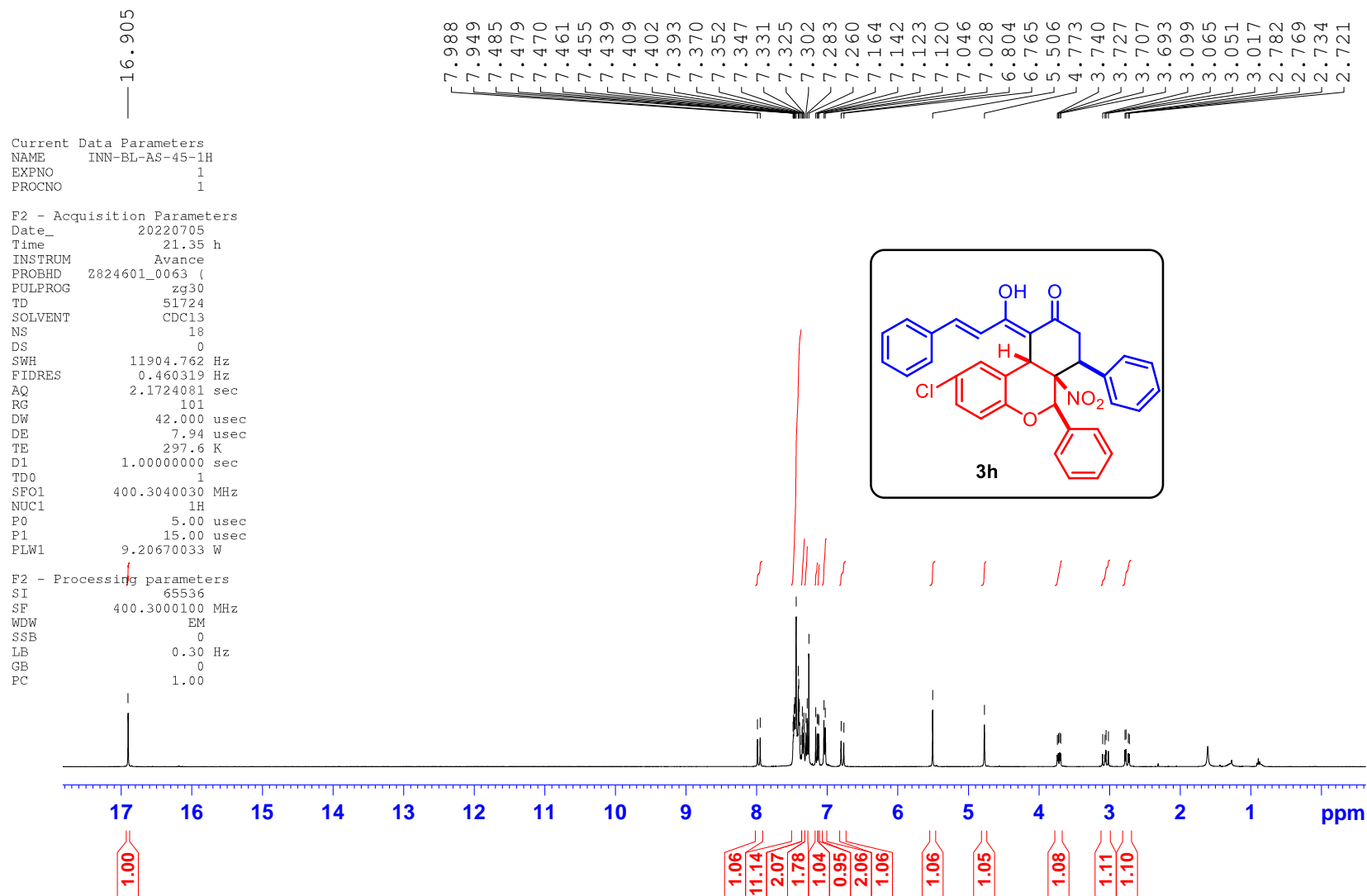


Figure S25. ¹H NMR Spectrum of 3h

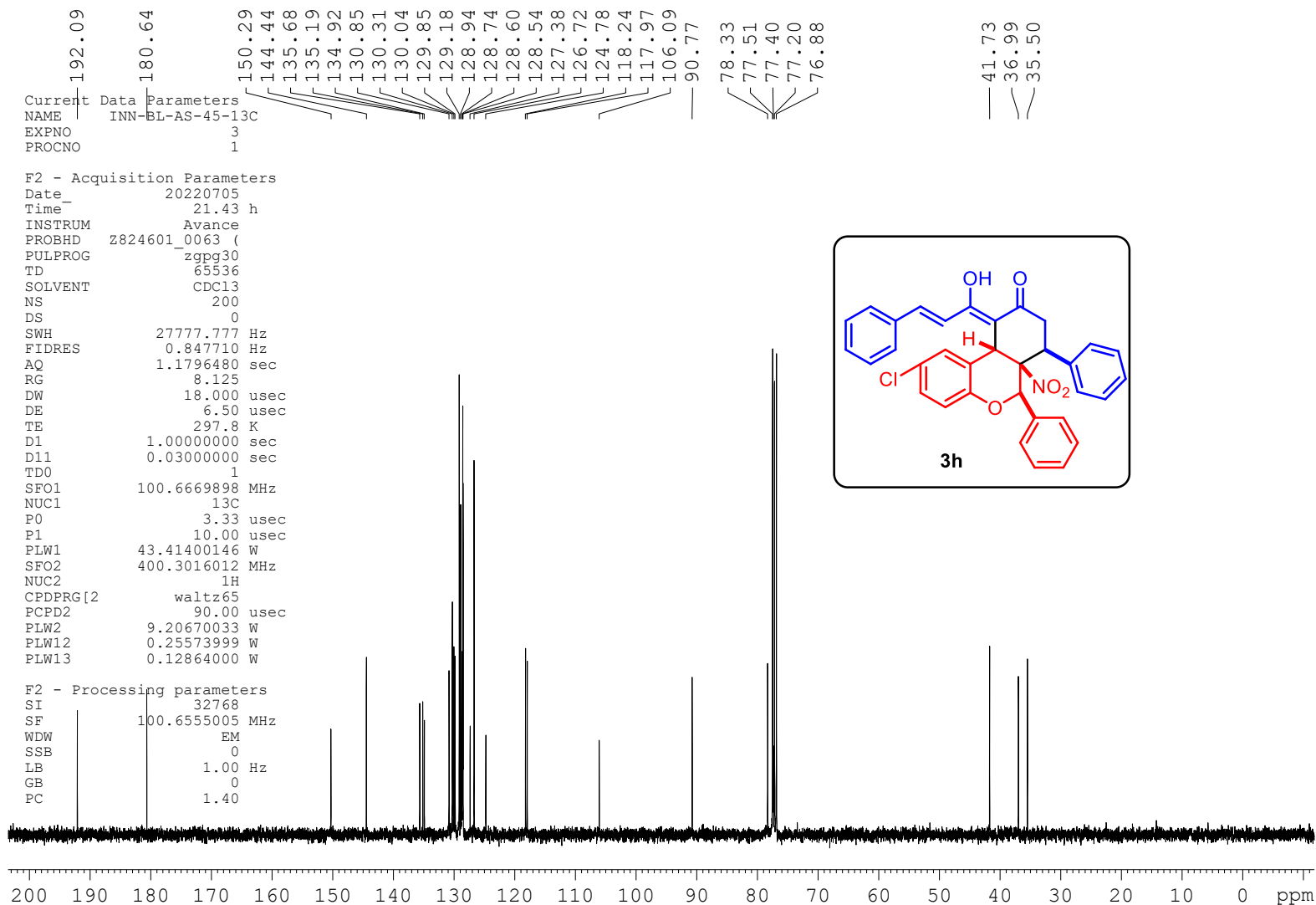


Figure S26. ¹³C NMR Spectrum of 3h

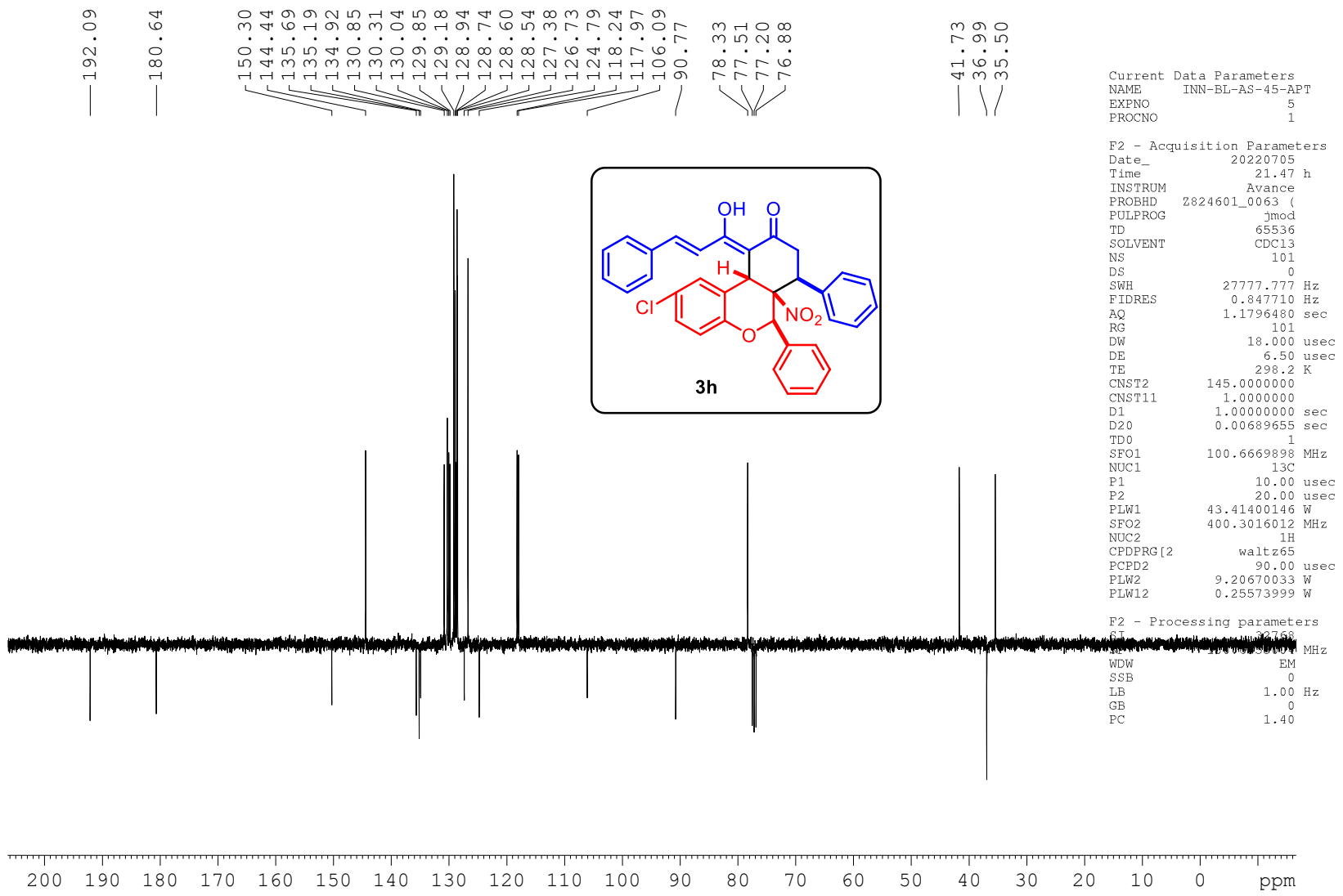


Figure S27. ¹³C-APT NMR Spectrum of 3h

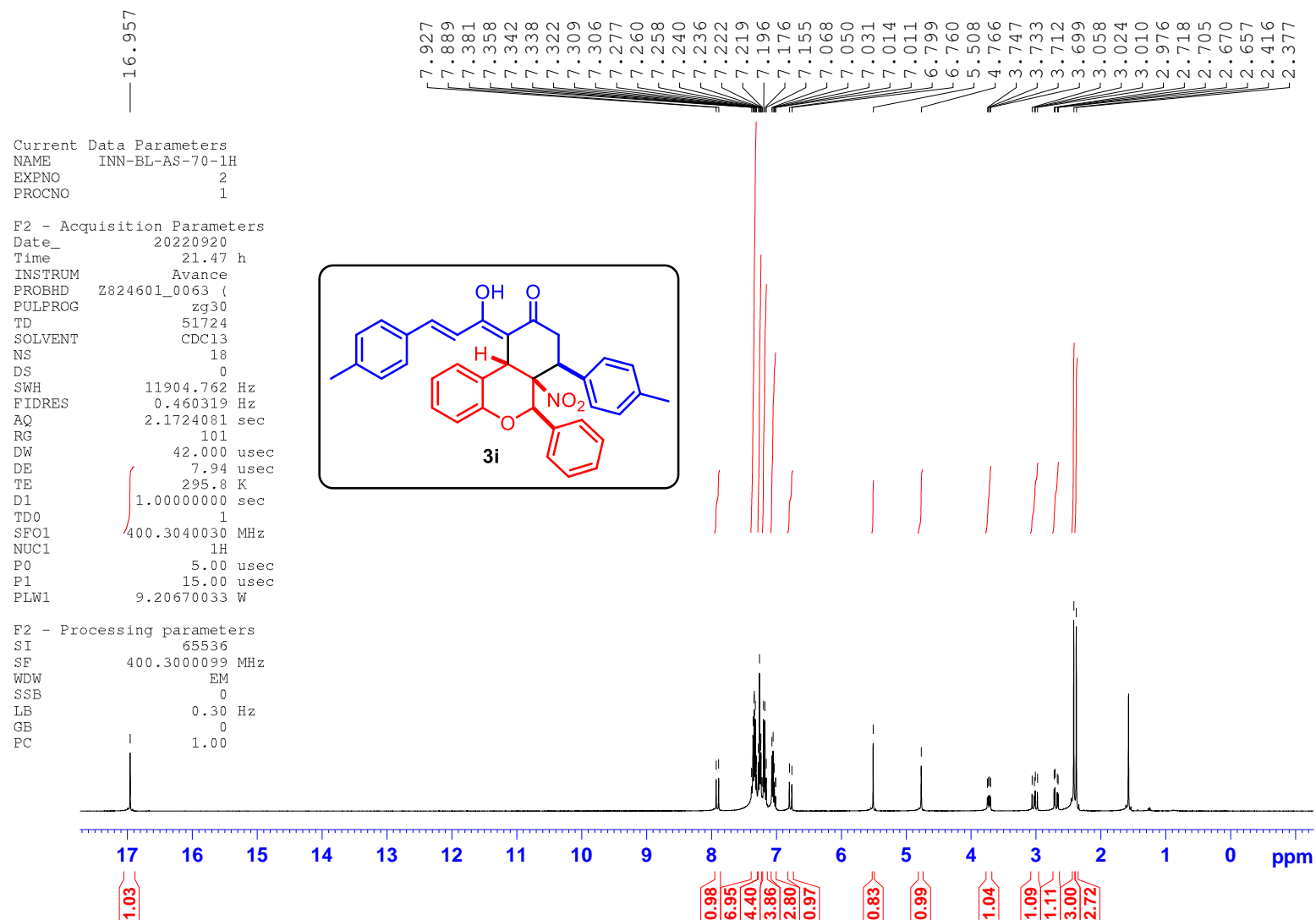


Figure S28. ¹H NMR Spectrum of 3i

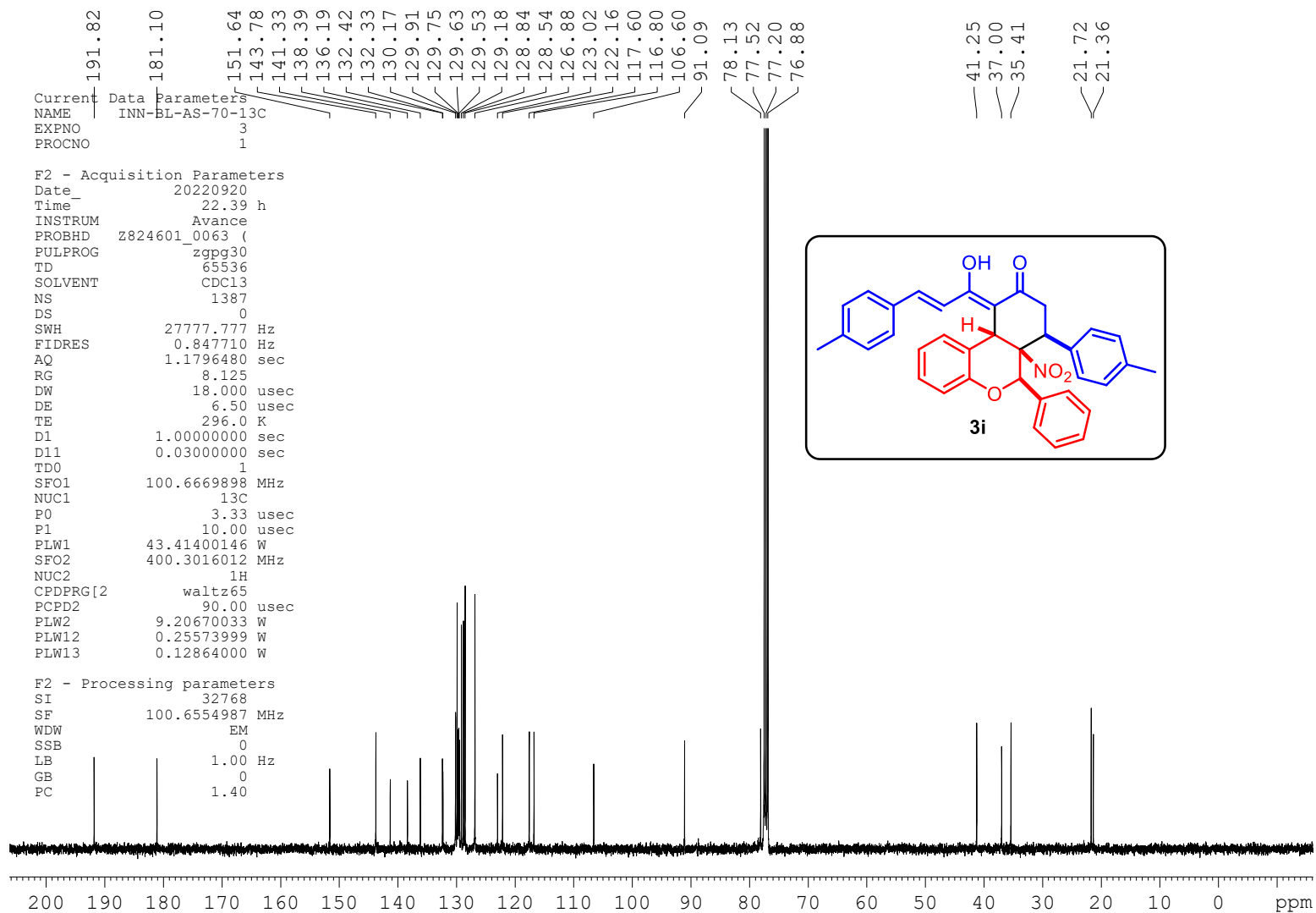


Figure S29. ¹³C NMR Spectrum of **3i**

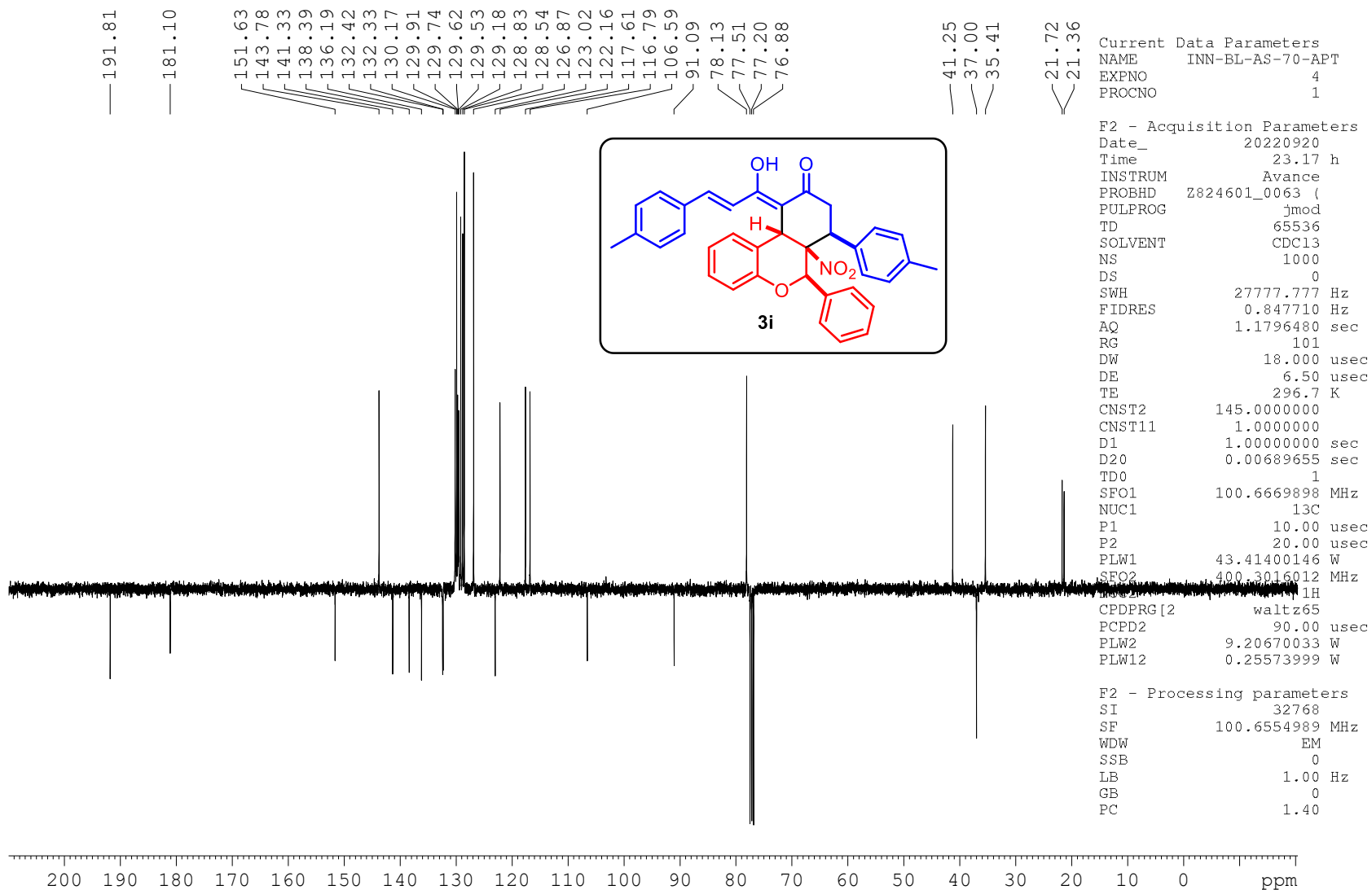


Figure S30. ¹³C-APT Spectrum of 3i

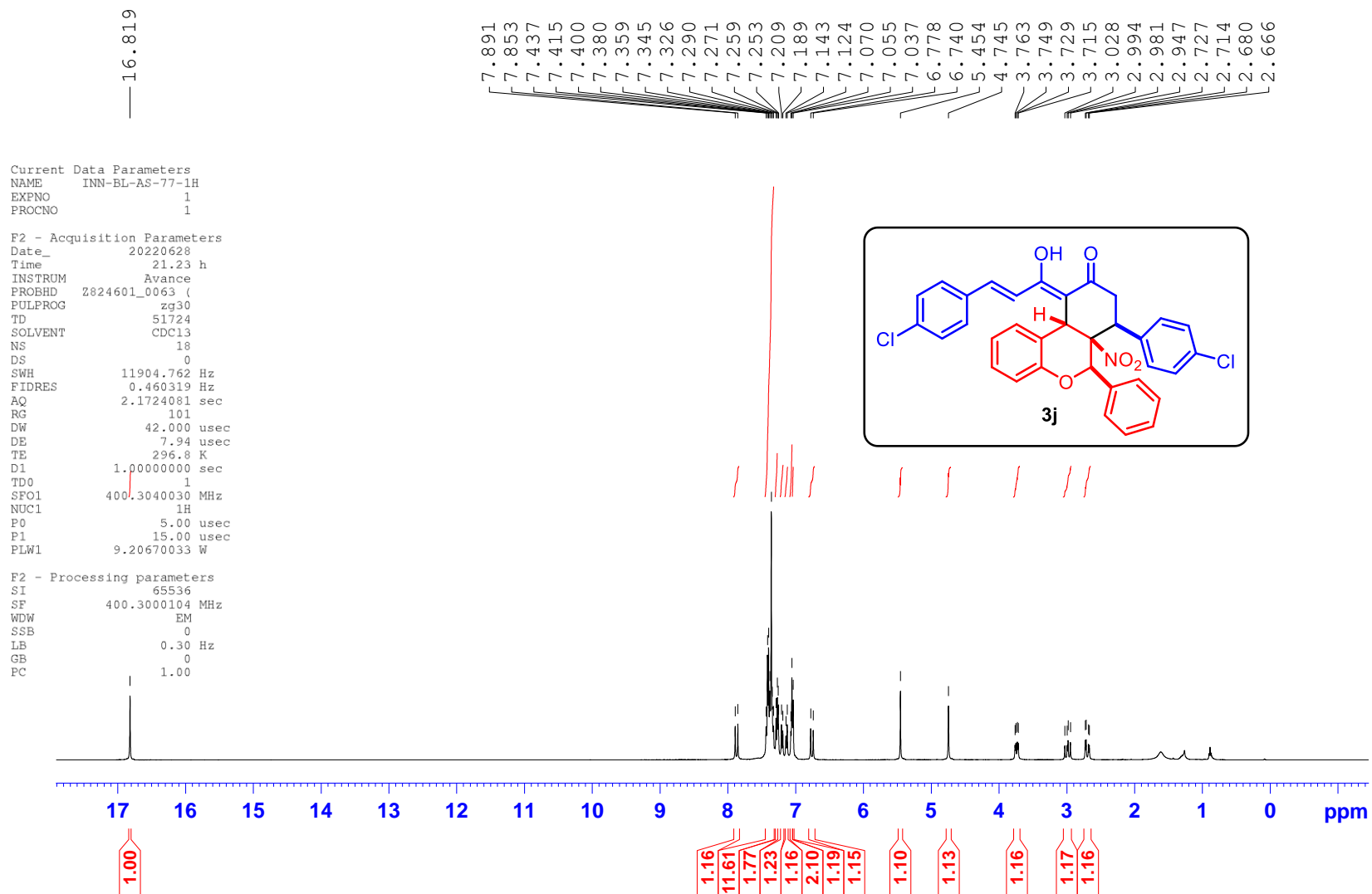


Figure S31. ¹H NMR Spectrum of 3j

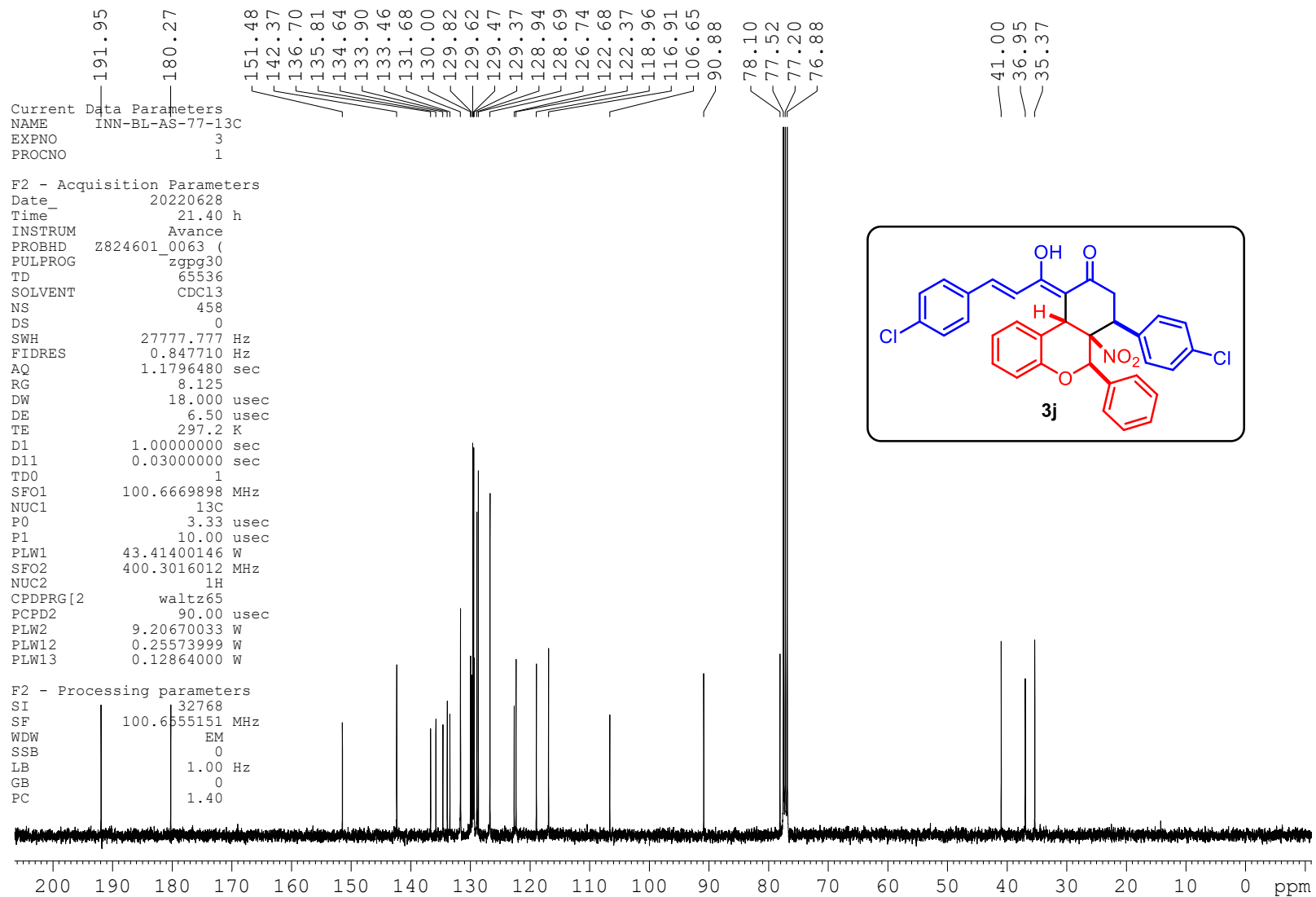


Figure S32. ^{13}C NMR Spectrum of 3j

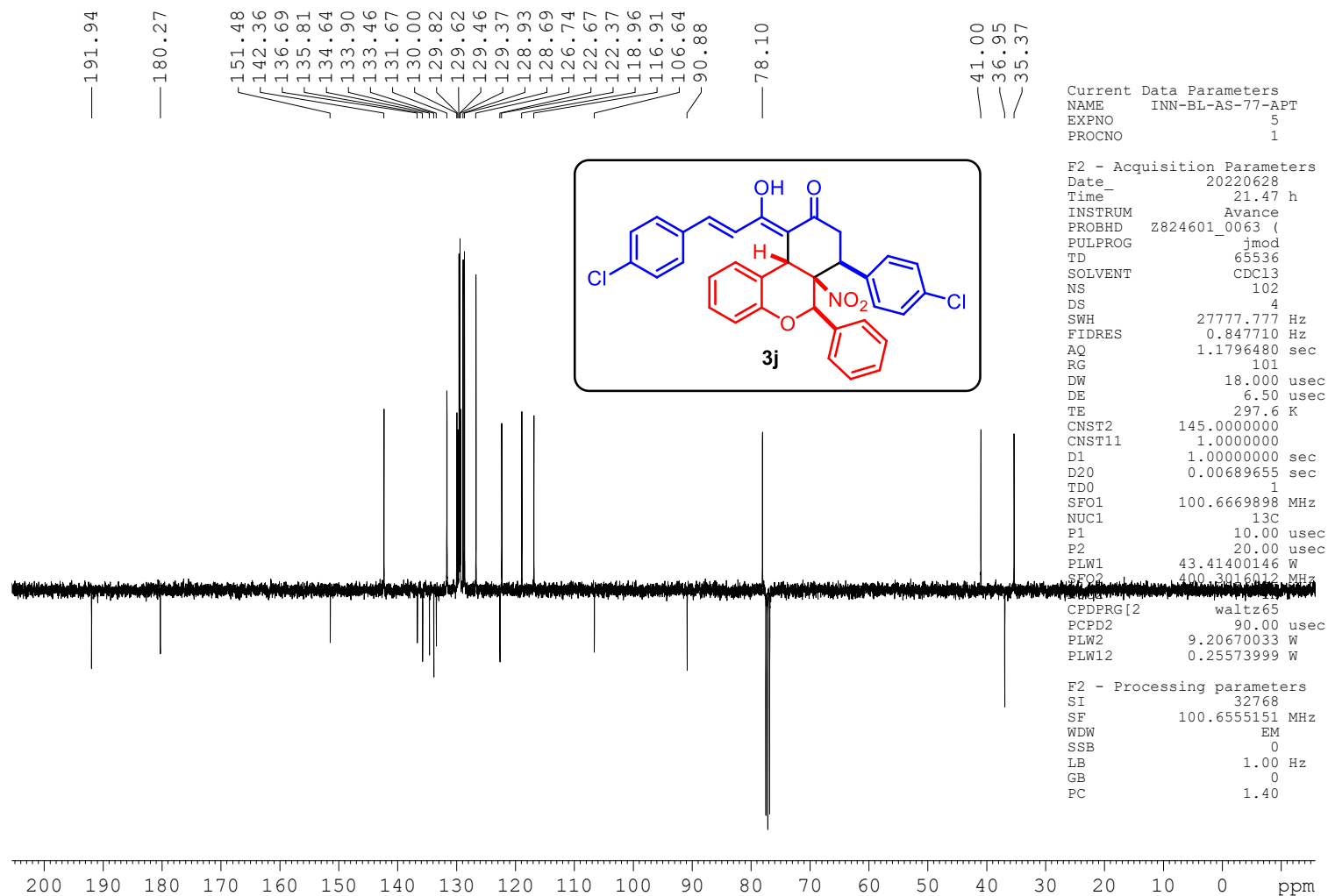


Figure S33. ¹³C-APT Spectrum of **3j**

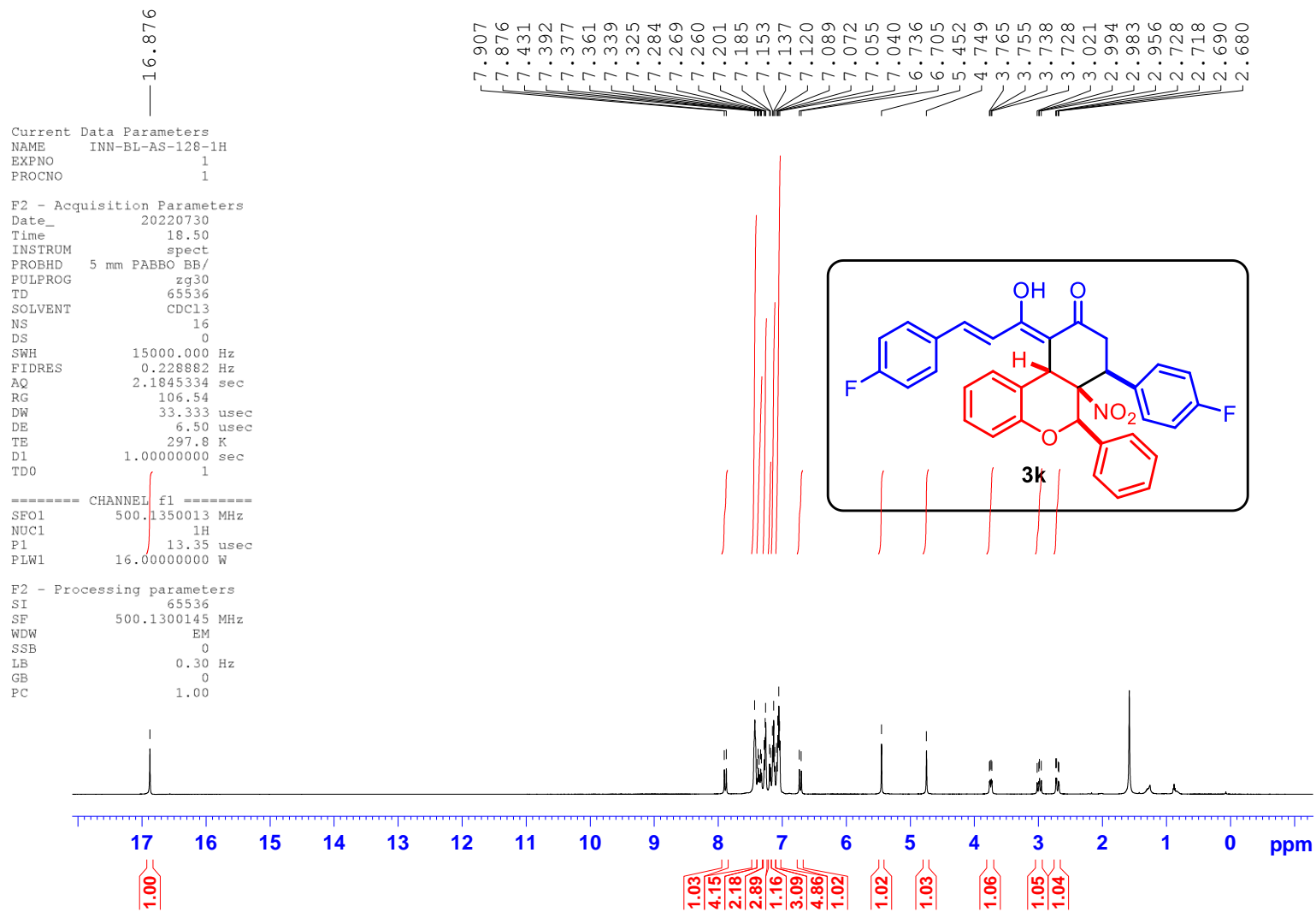


Figure S34. ¹H NMR Spectrum of 3k

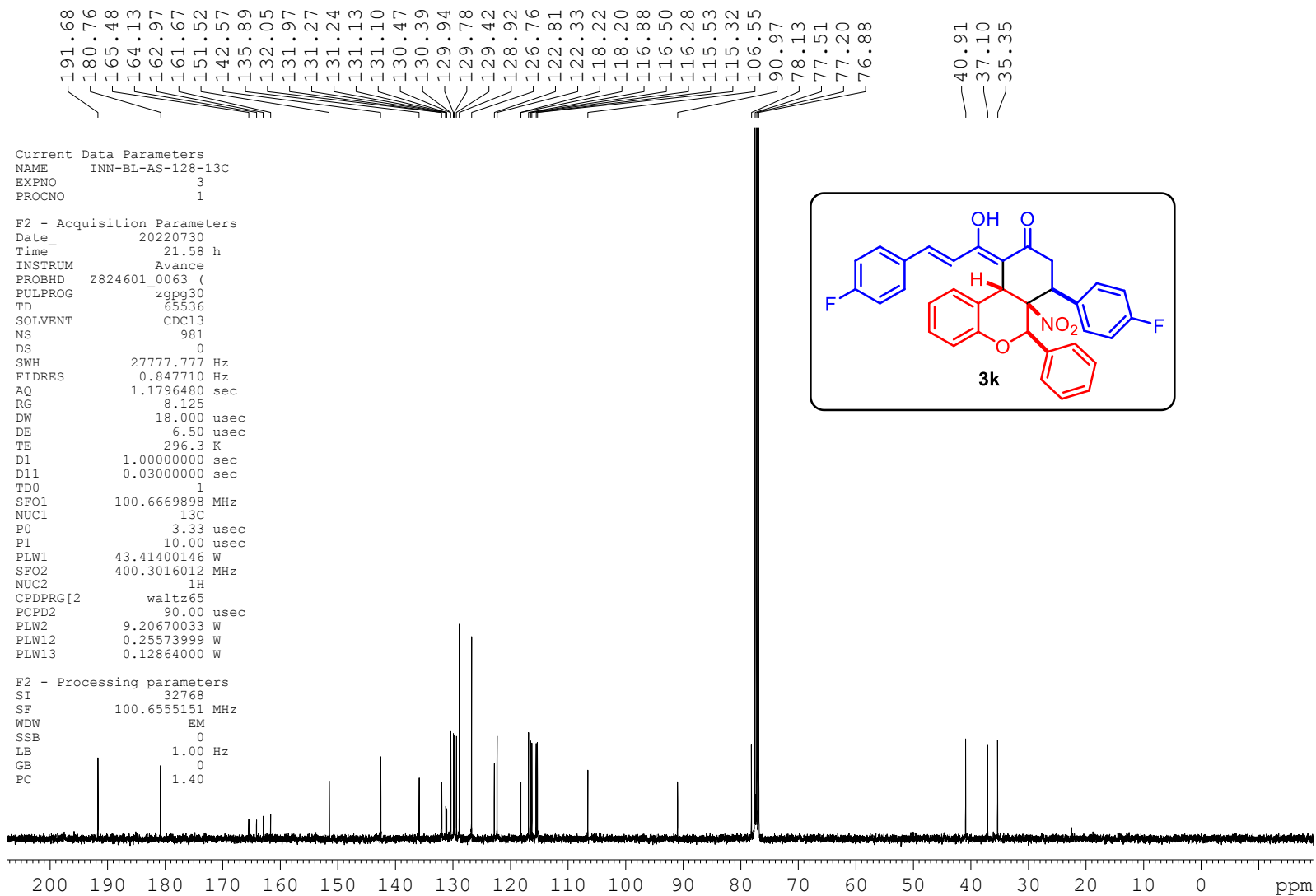


Figure S35. ¹³C NMR Spectrum of 3k

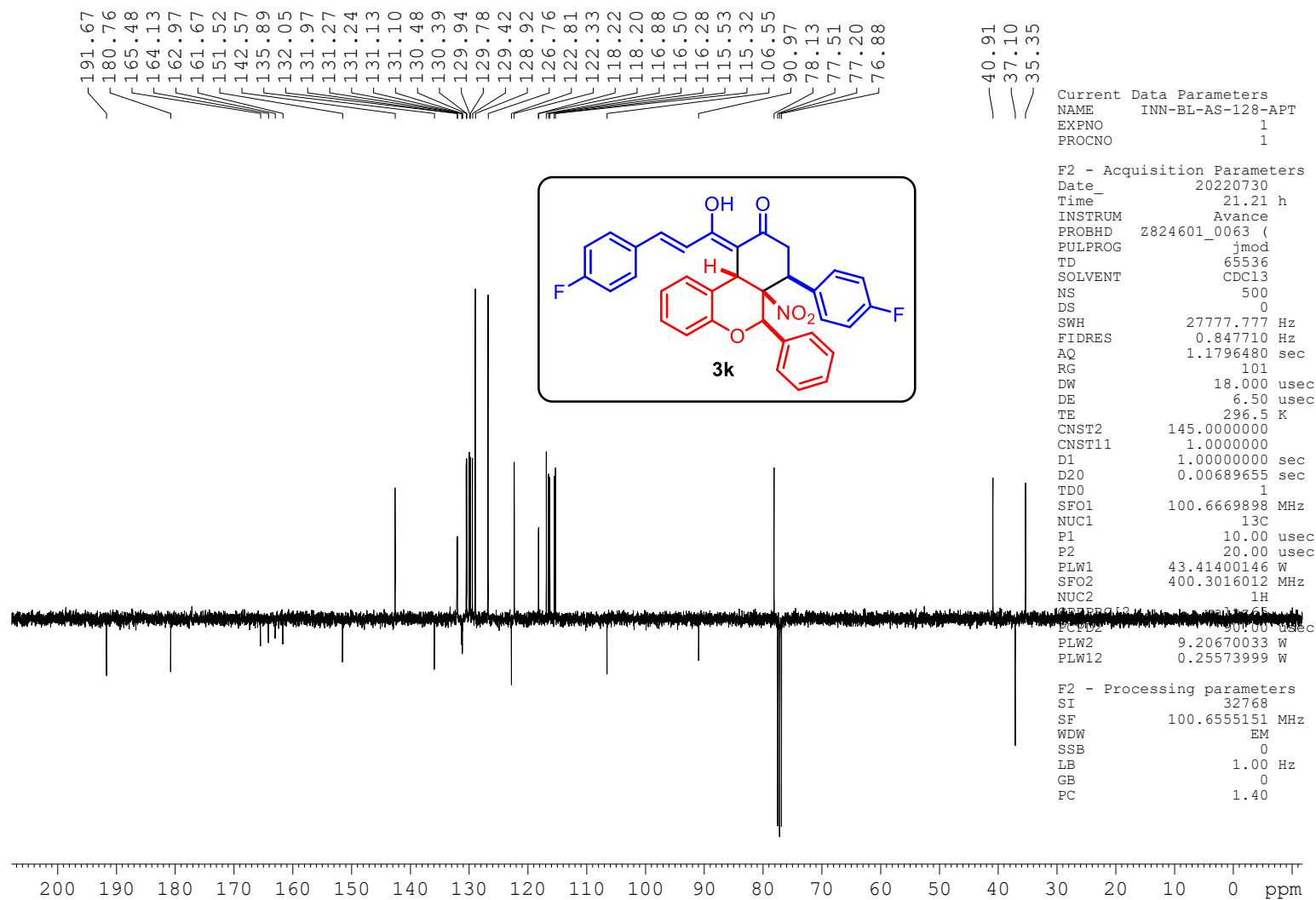


Figure S36. ¹³C-APT NMR Spectrum of 3k

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EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

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SOLVENT CDC13
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FIDRES 2.543132 Hz
AQ 0.3932160 sec
RG 101
DW 3.000 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
TDO 1
SFO1 376.4795413 MHz
NUC1 19F
P1 12.00 usec
PLW1 31.08799934 W

F2 - Processing parameters

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SF 376.4983662 MHz
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LB 1.00 Hz
GB 0
PC 1.00

-108.69
-113.46

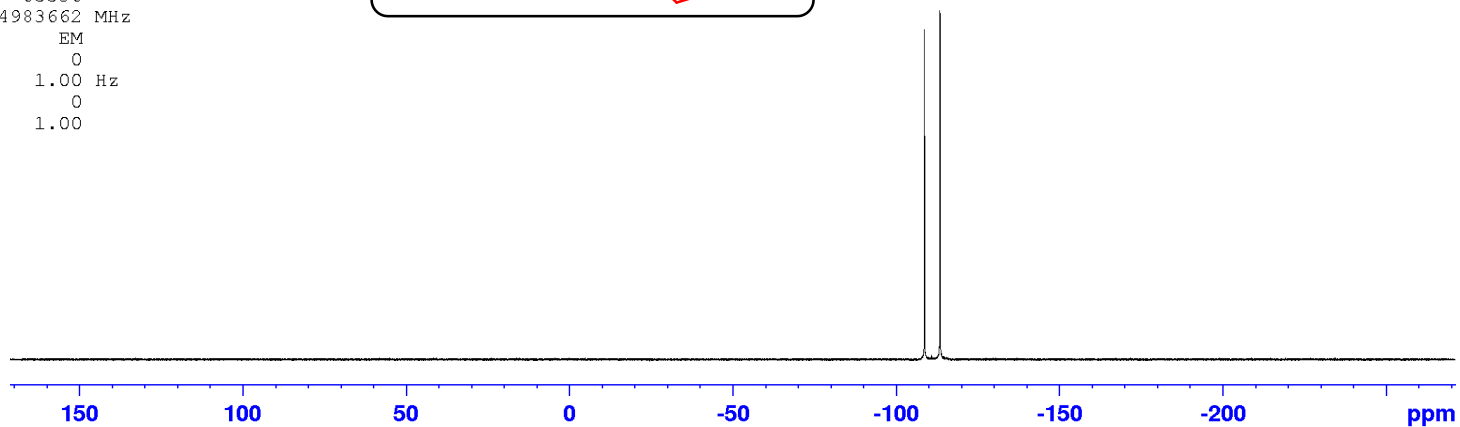
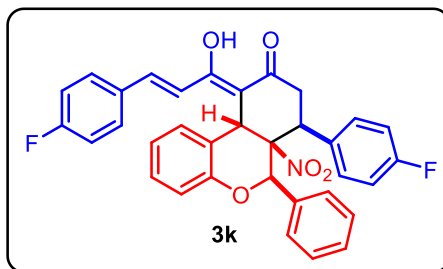


Figure S37. ¹⁹F NMR Spectrum of 3k

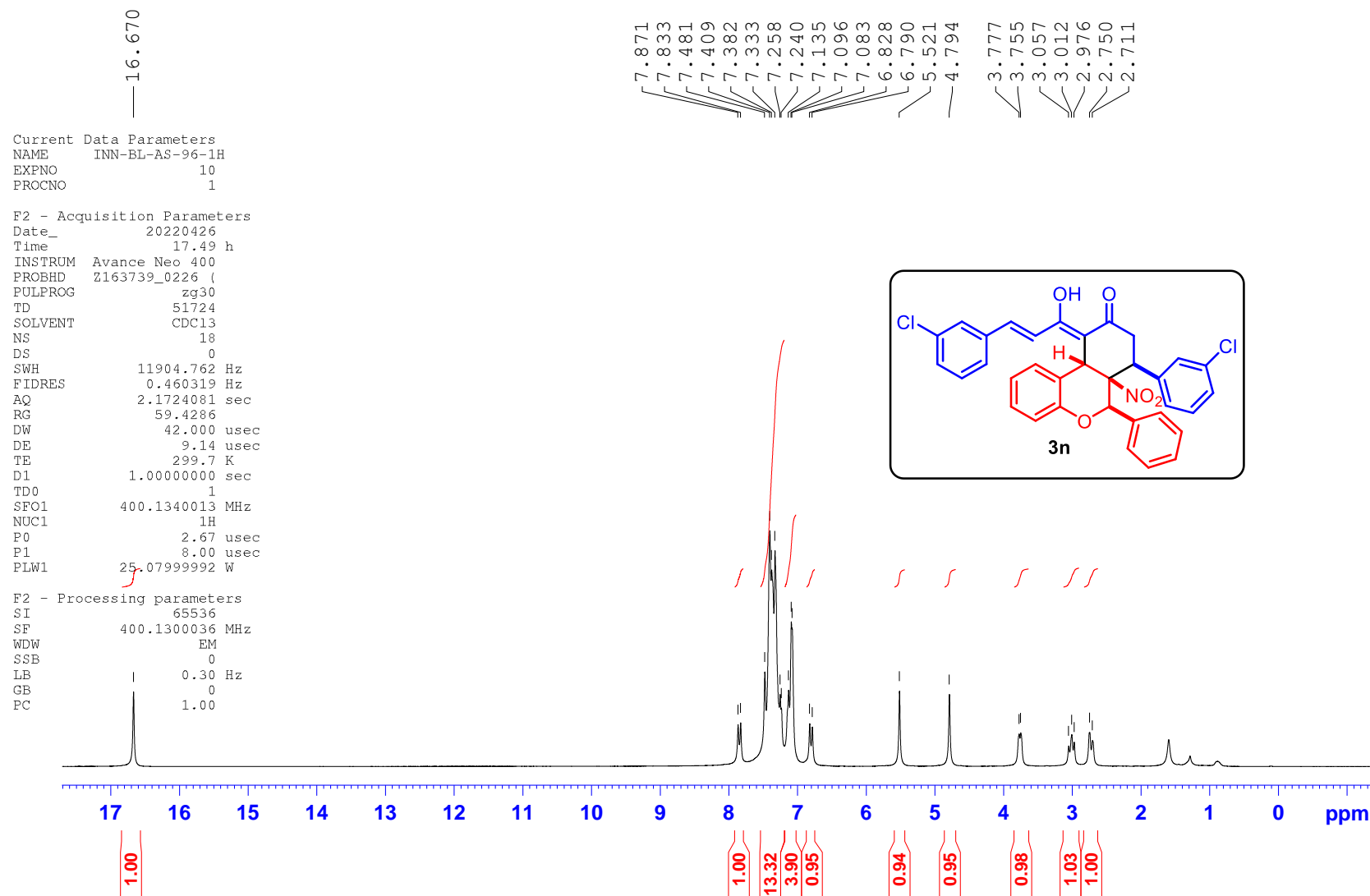


Figure S38. ¹H NMR Spectrum of 3n

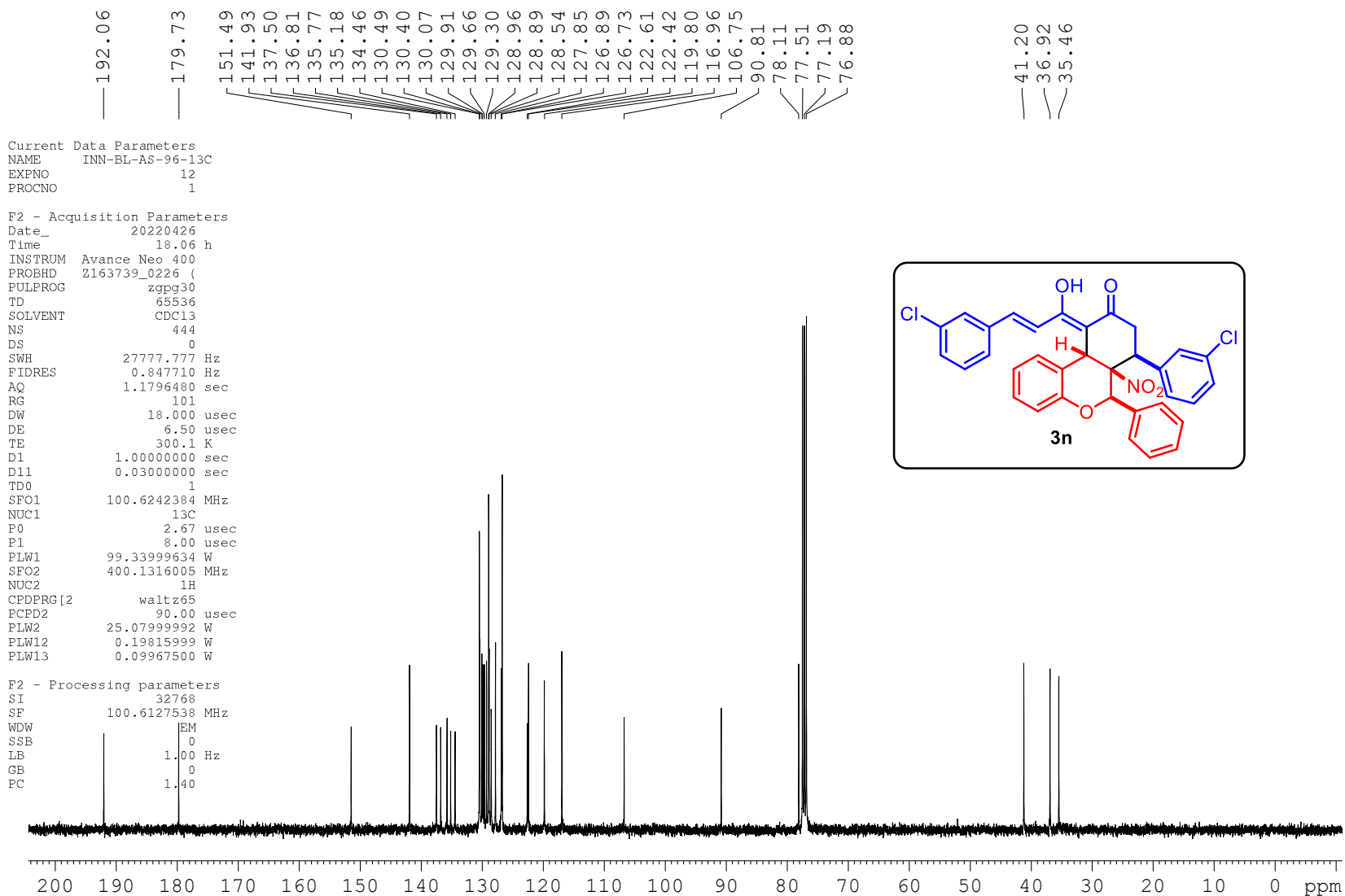


Figure S39. ¹³C NMR Spectrum of 3n

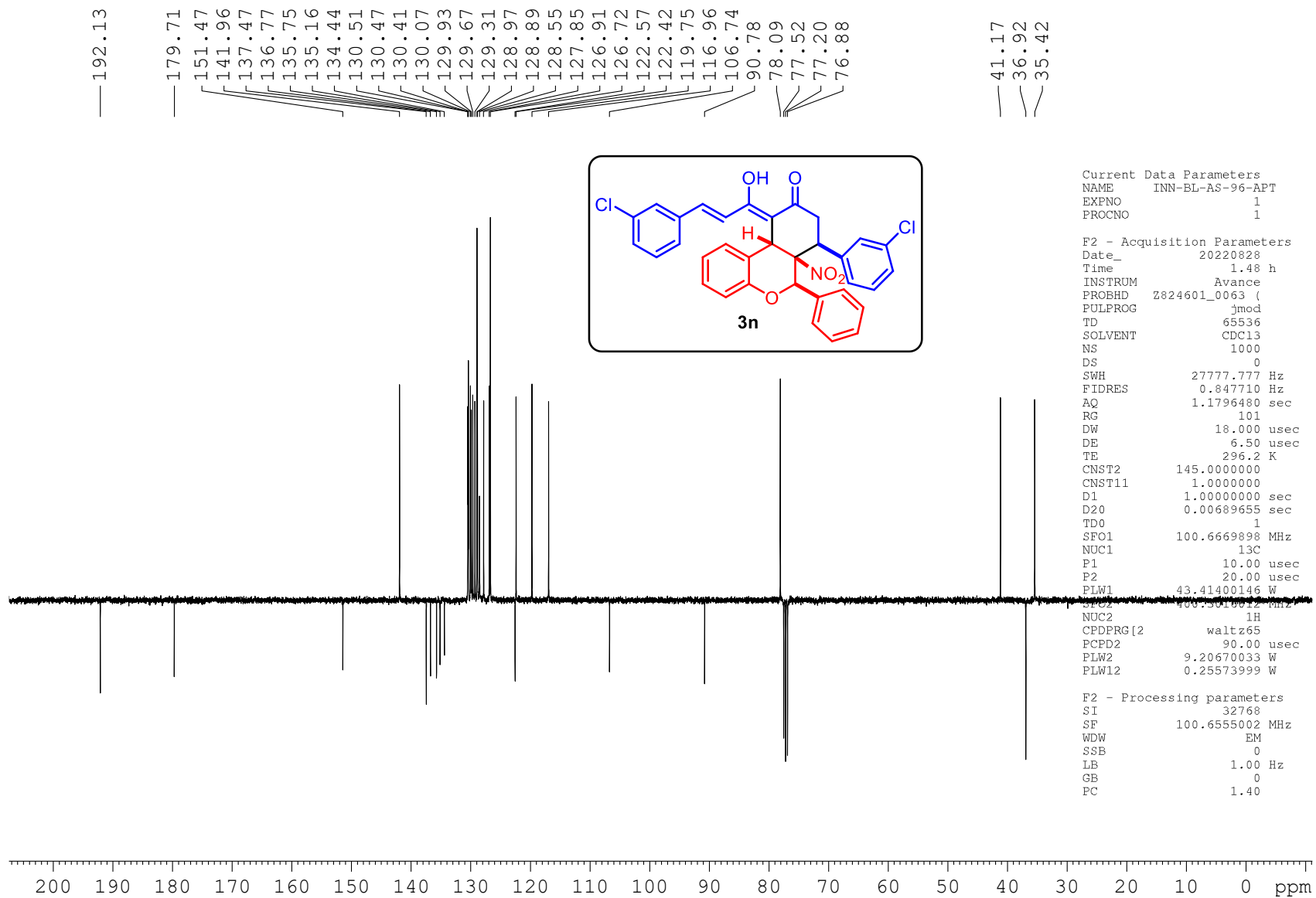


Figure S40. ¹³C-APT NMR Spectrum of **3n**

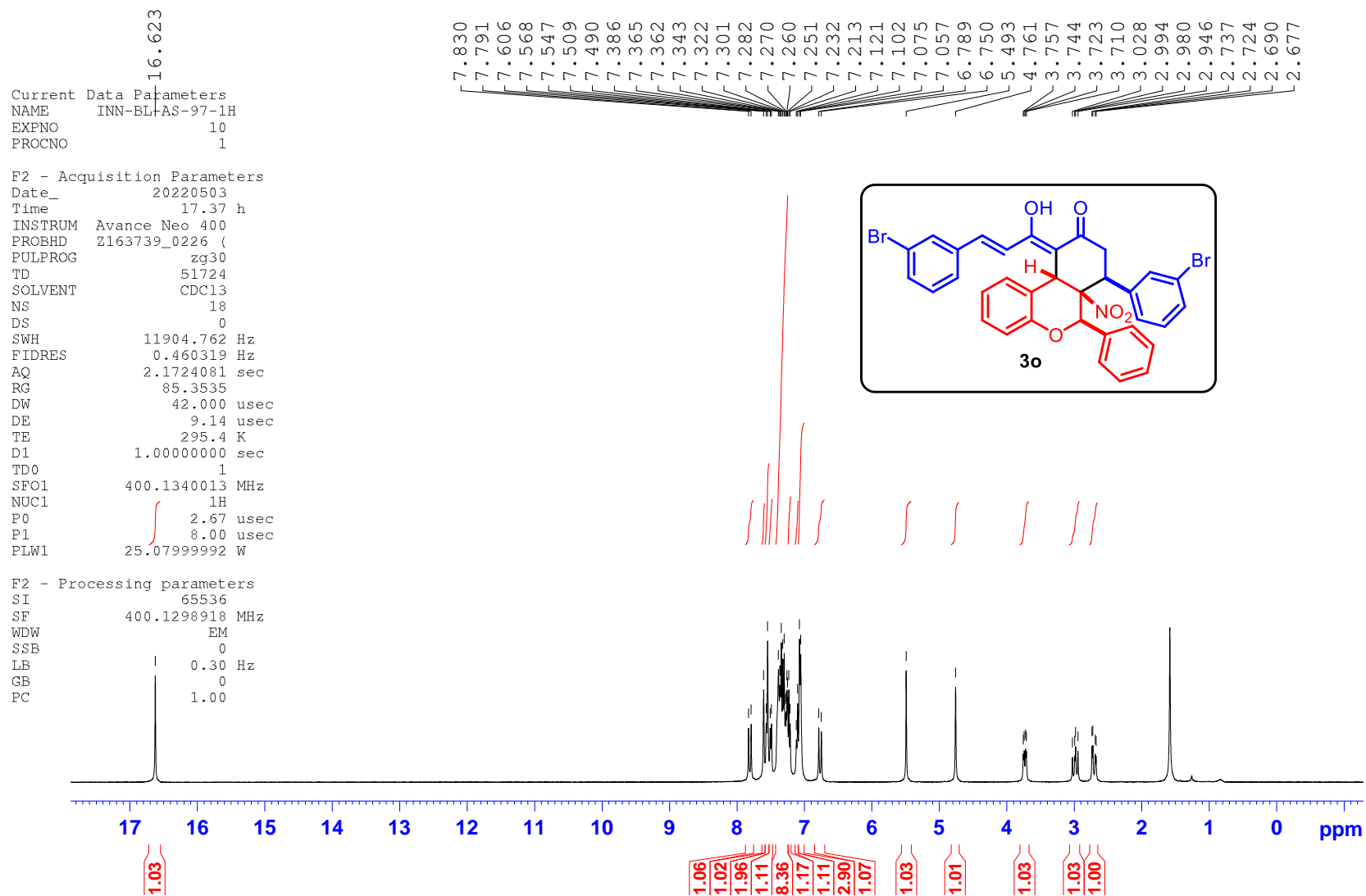


Figure S41. ¹H NMR Spectrum of 3o

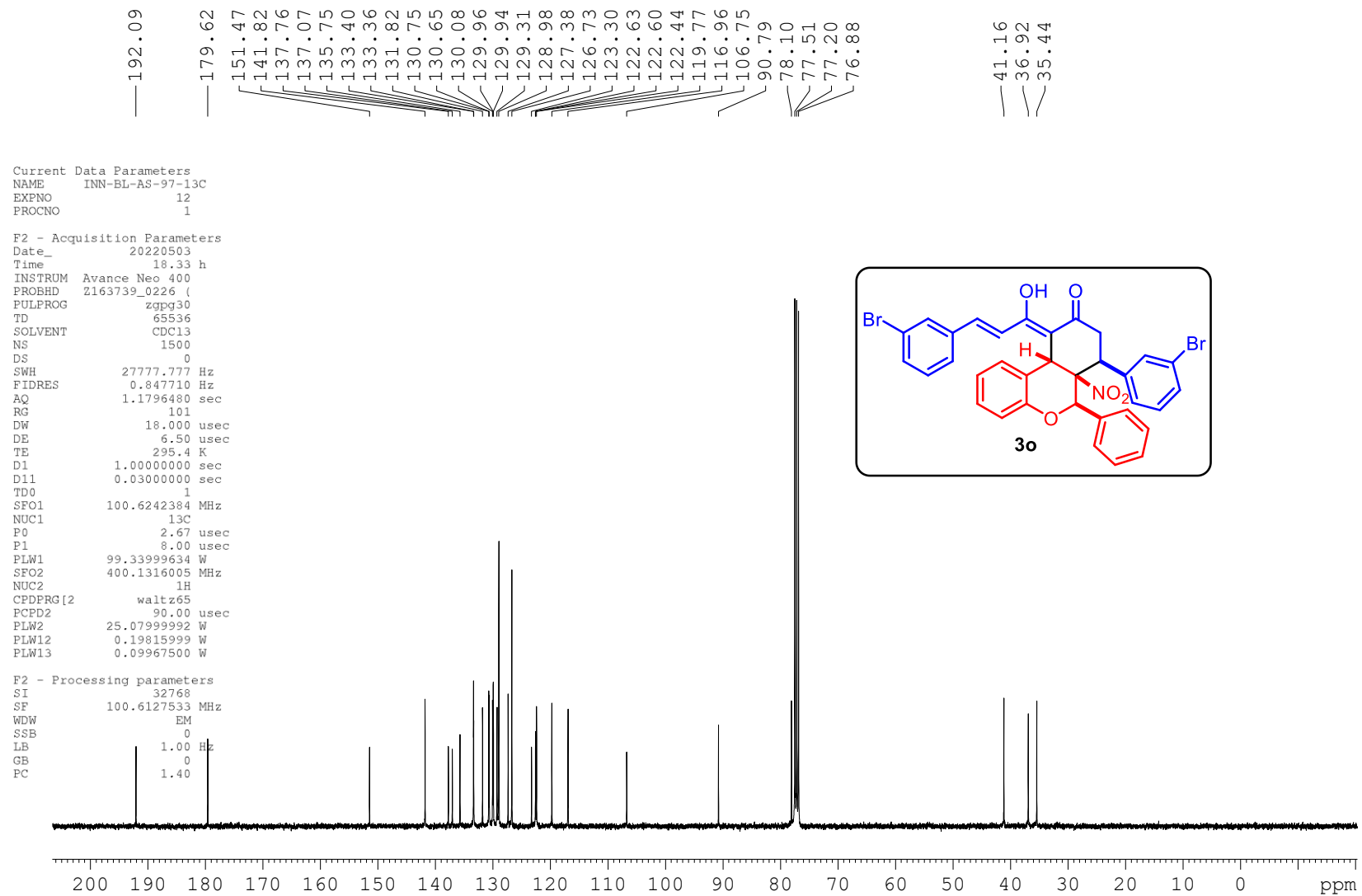


Figure S42. ¹³C NMR Spectrum of 3o

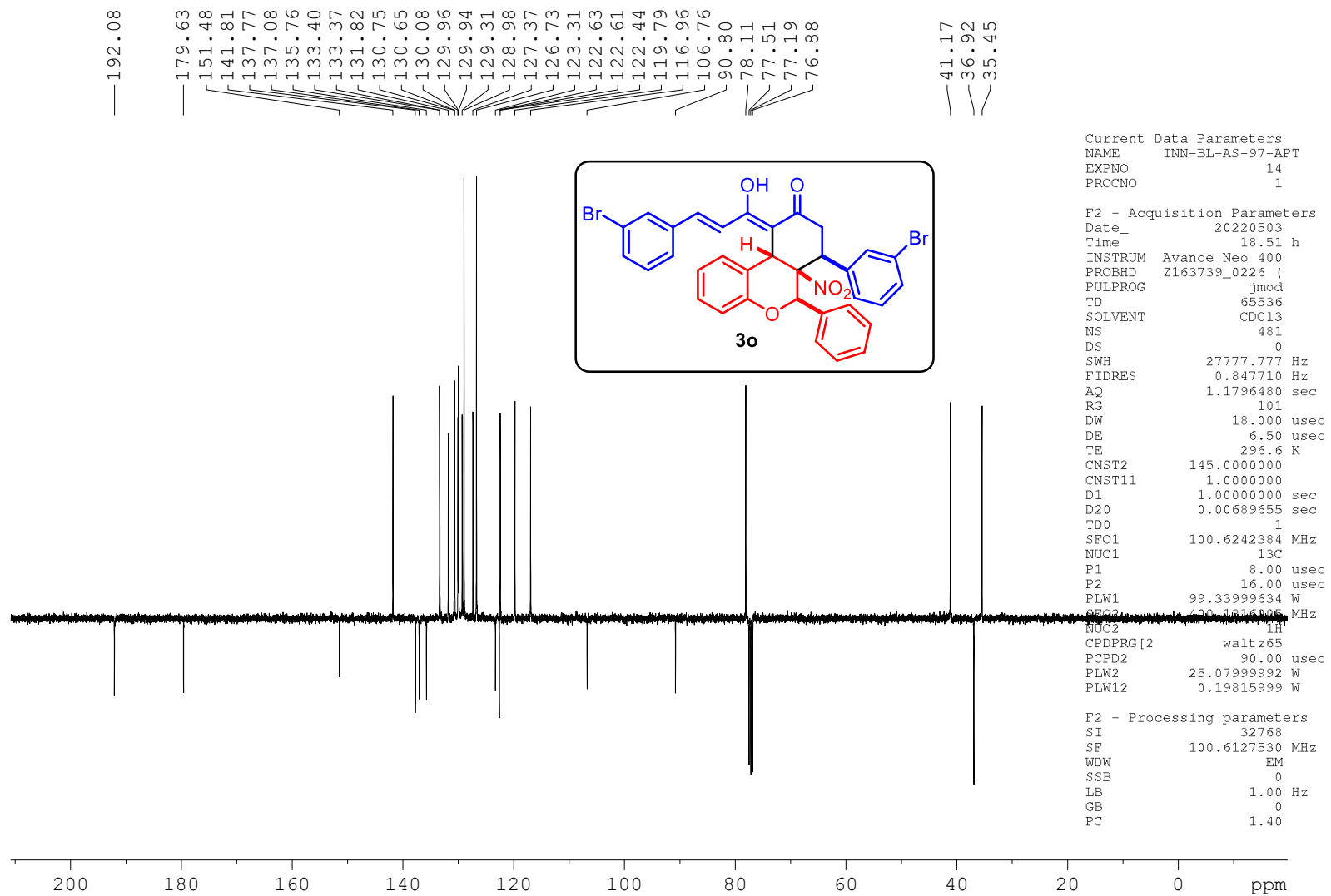


Figure S43. ¹³C-APT NMR Spectrum of **3o**

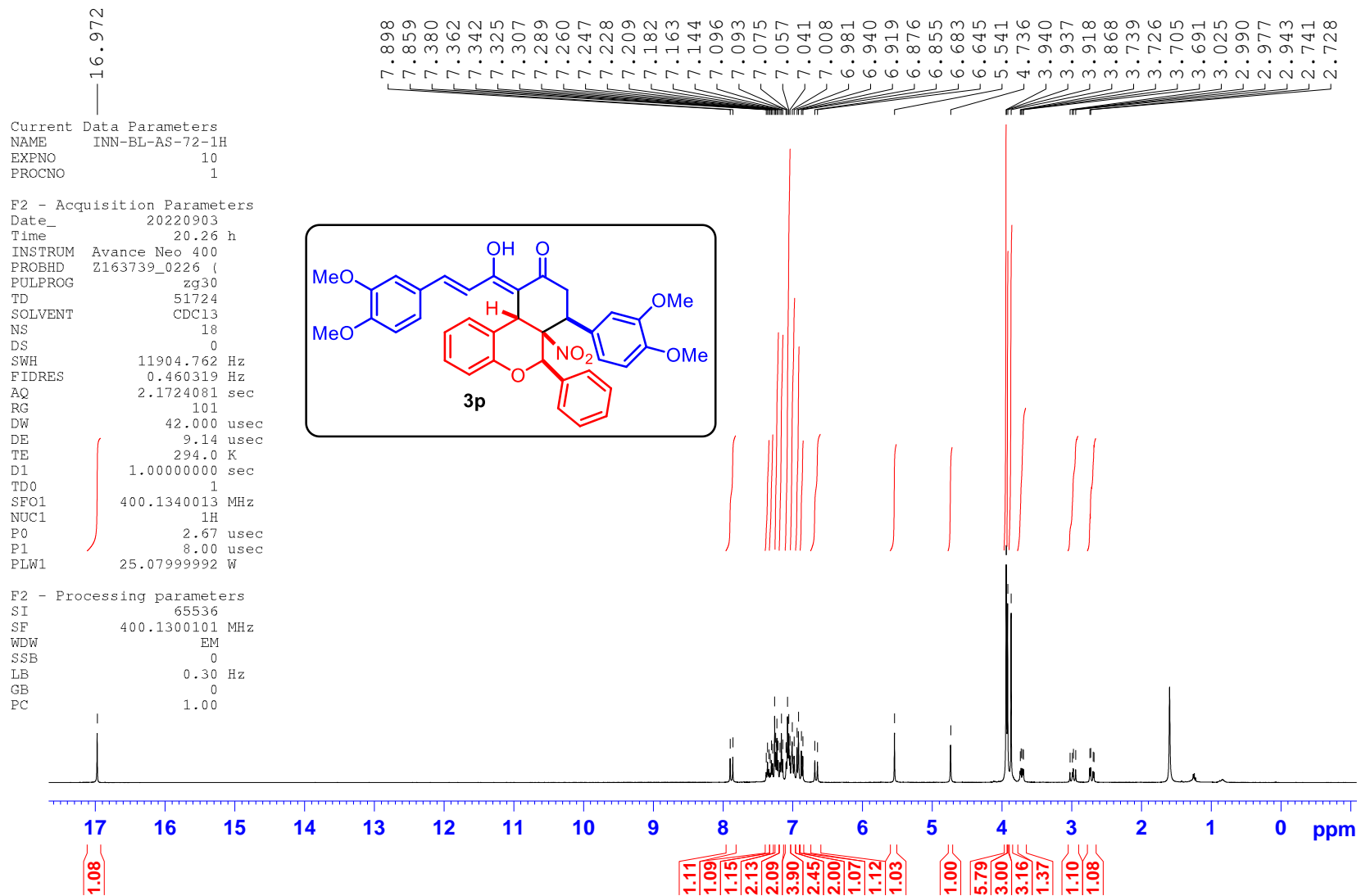


Figure S44. ¹H NMR Spectrum of 3p

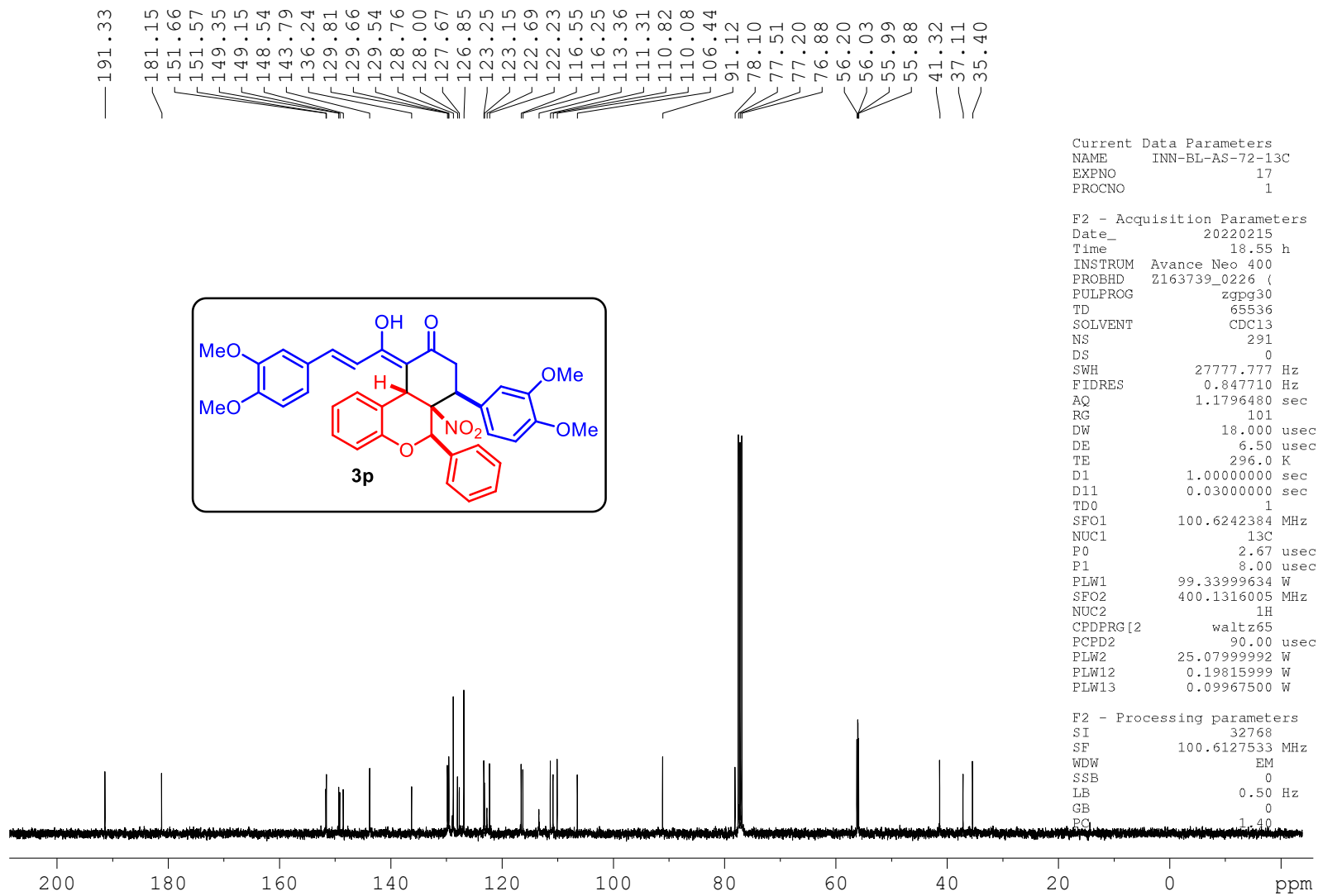


Figure S45. ¹³C NMR Spectrum of 3p

INN-BL-AS-105-1H

16.891
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EXPNO 10
PROCNO 1

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TD 51724
SOLVENT CDC13
NS 18
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FIDRES 0.460319 Hz
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RG 101
DW 42.000 usec
DE 9.14 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1
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P0 2.67 usec
P1 8.00 usec
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F2 - Processing parameters
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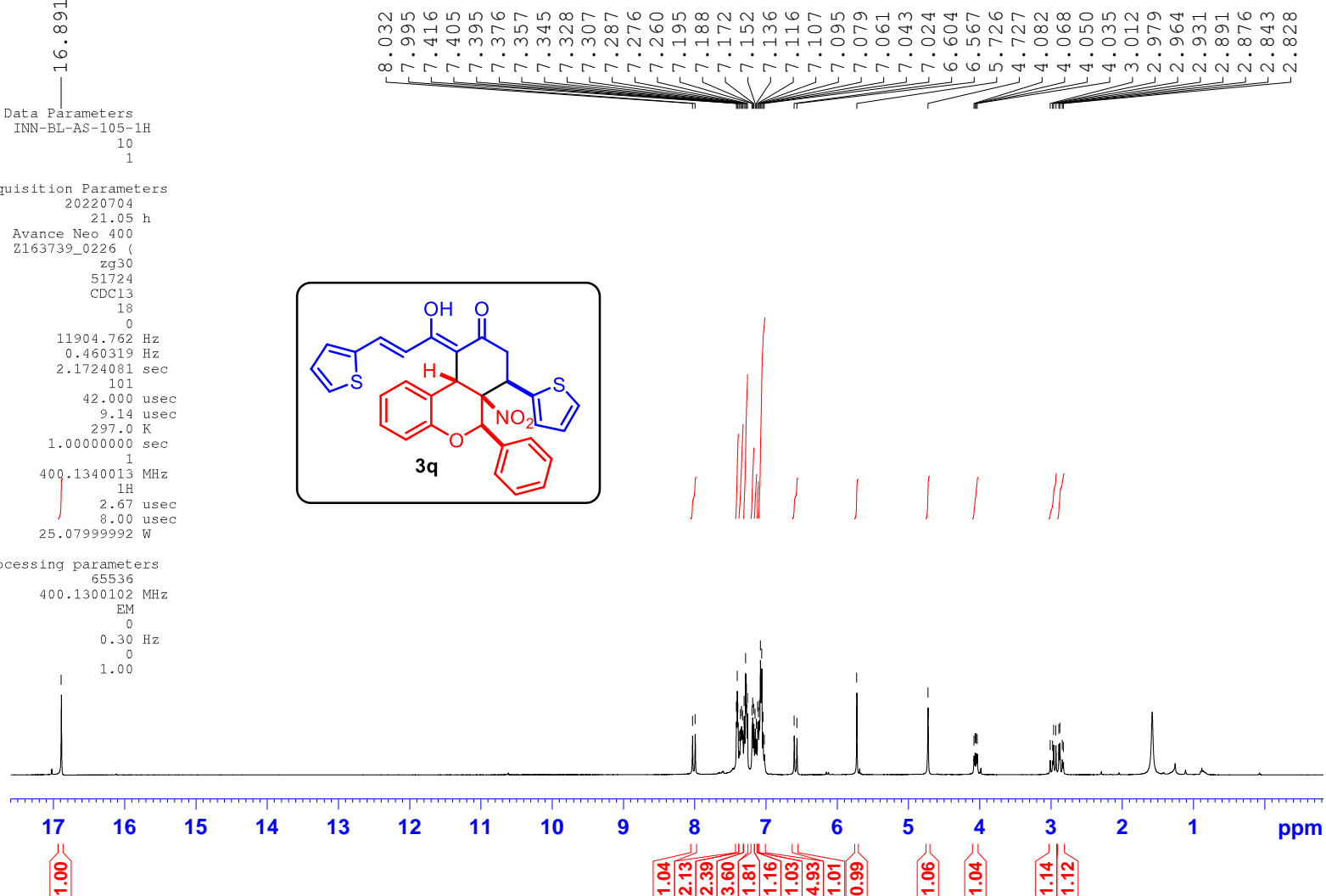
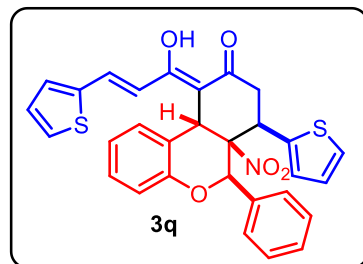


Figure S46. ¹H NMR Spectrum of 3q

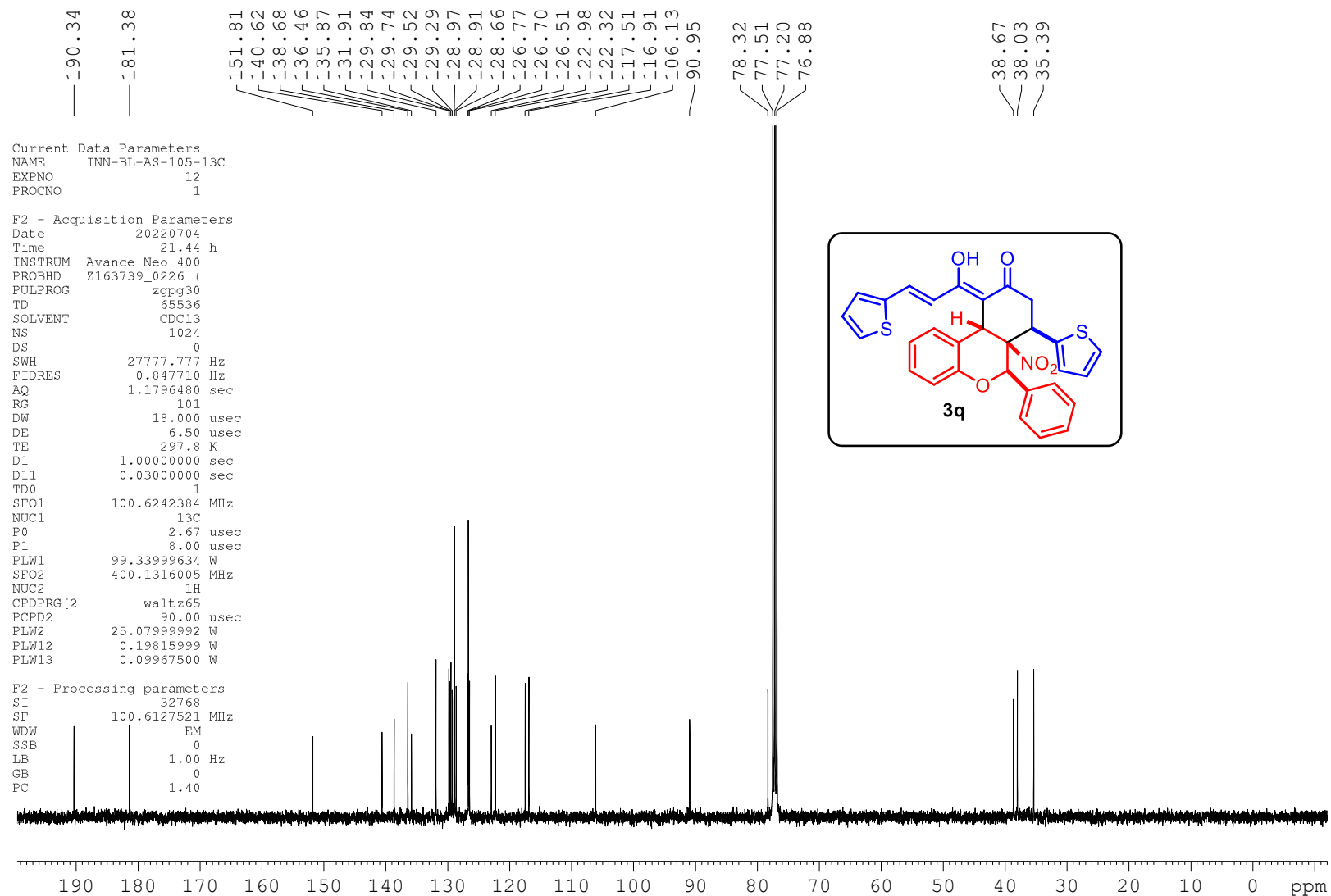


Figure S47. ¹³C NMR Spectrum of 3q

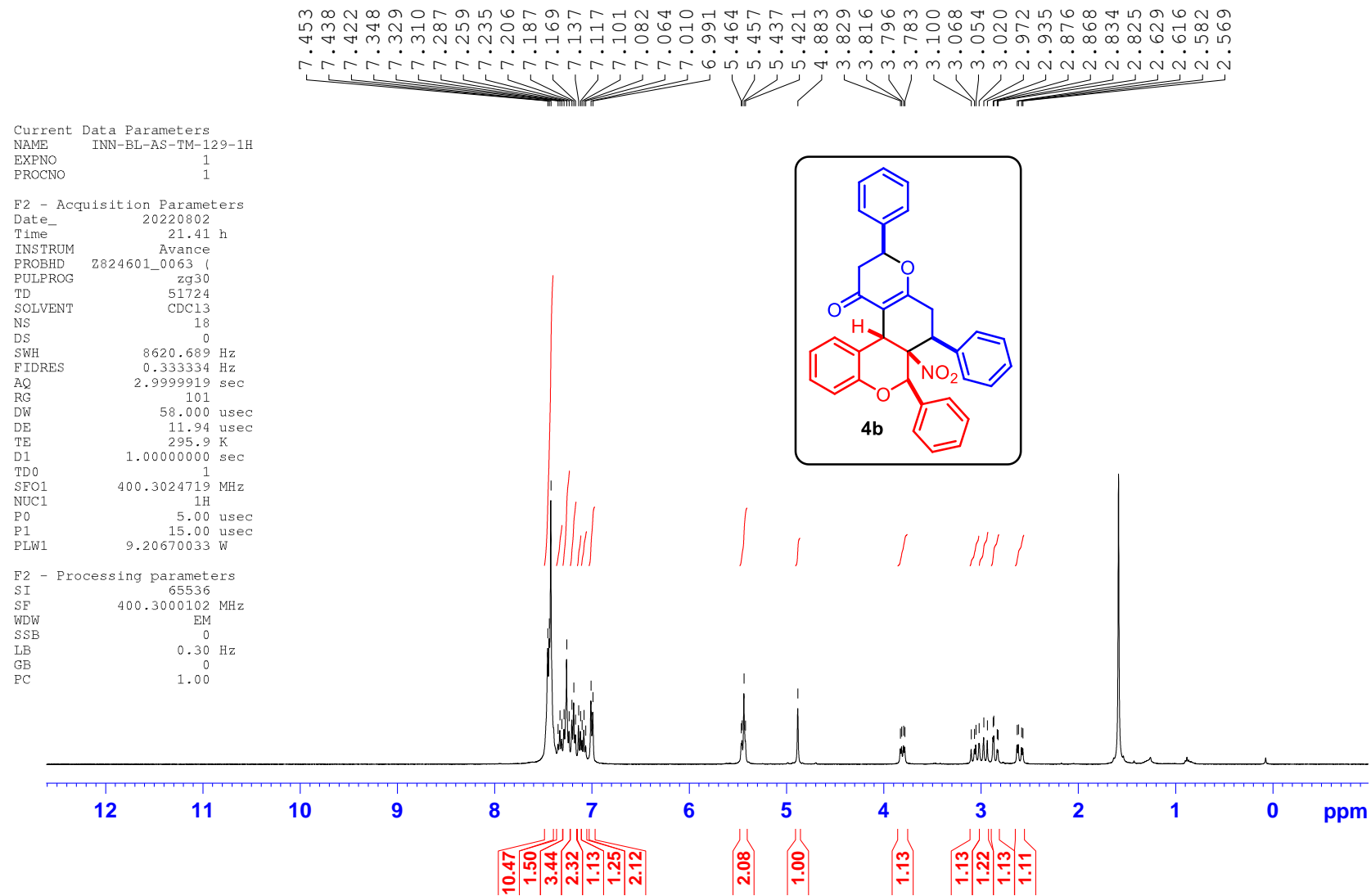


Figure S48. ¹H NMR Spectrum of 4b

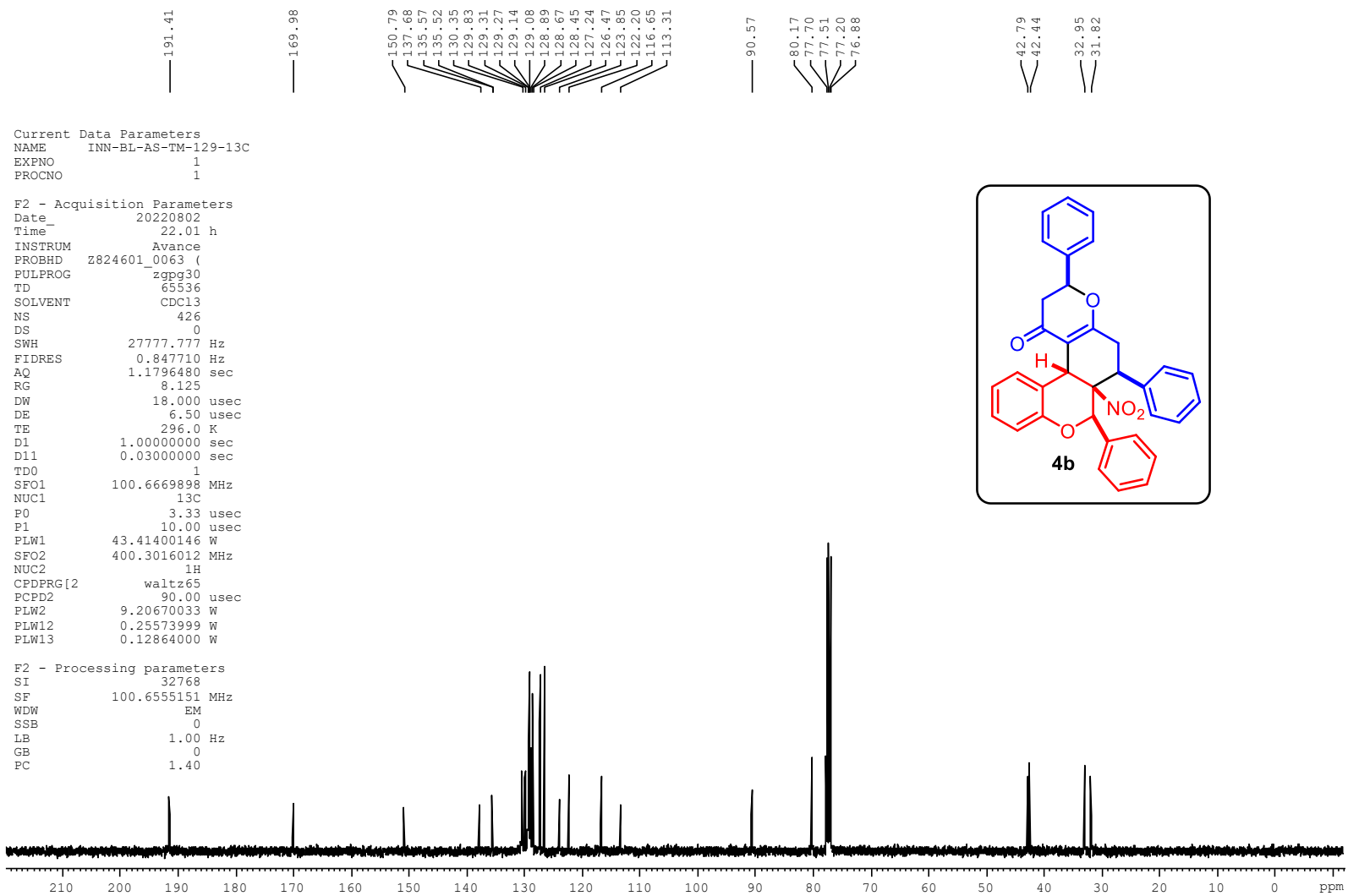


Figure S49. ¹³C NMR Spectrum of 4b

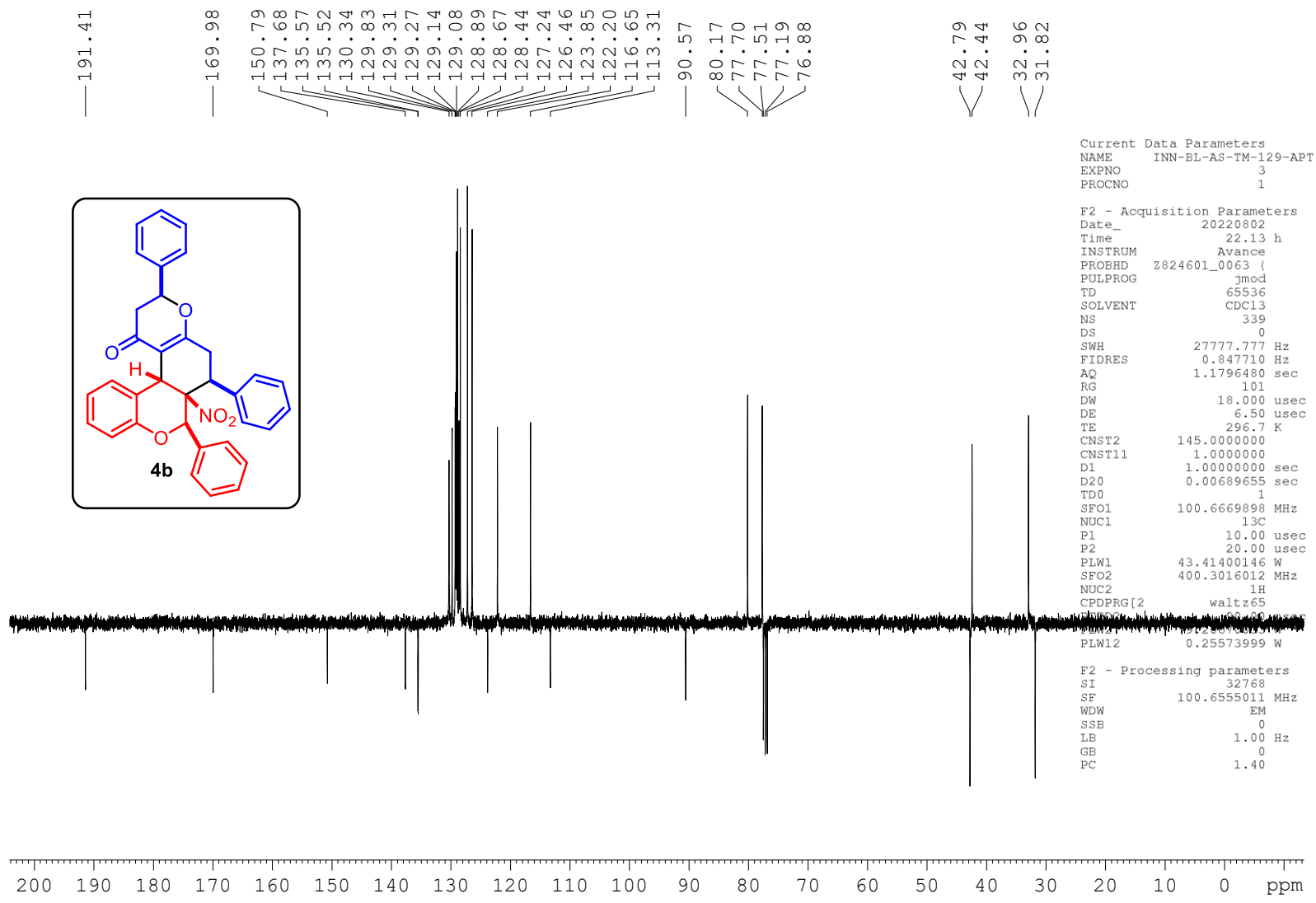


Figure S50. ¹³C-APT NMR Spectrum of 4b

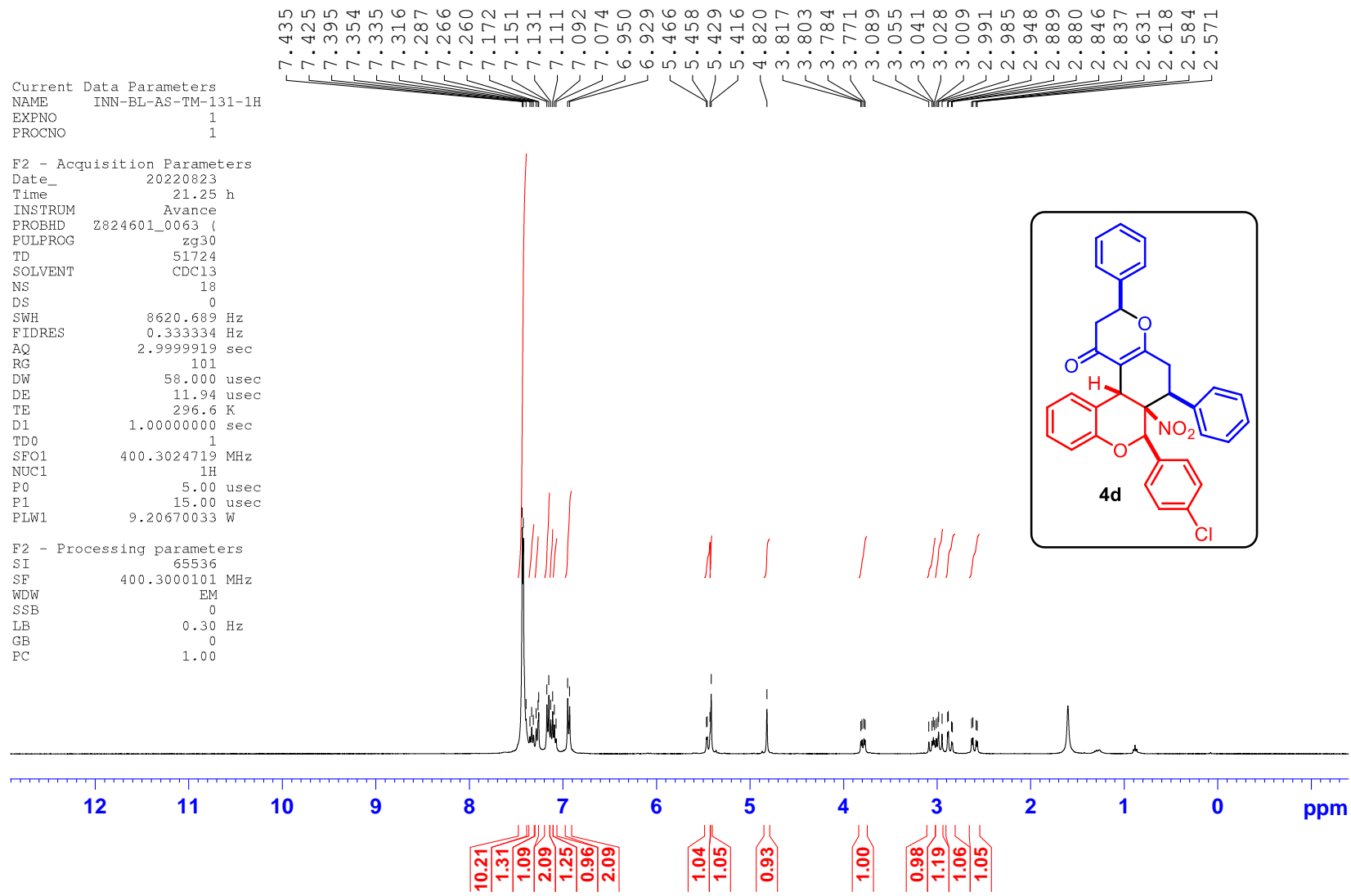


Figure S51. ¹H NMR Spectrum of 4d

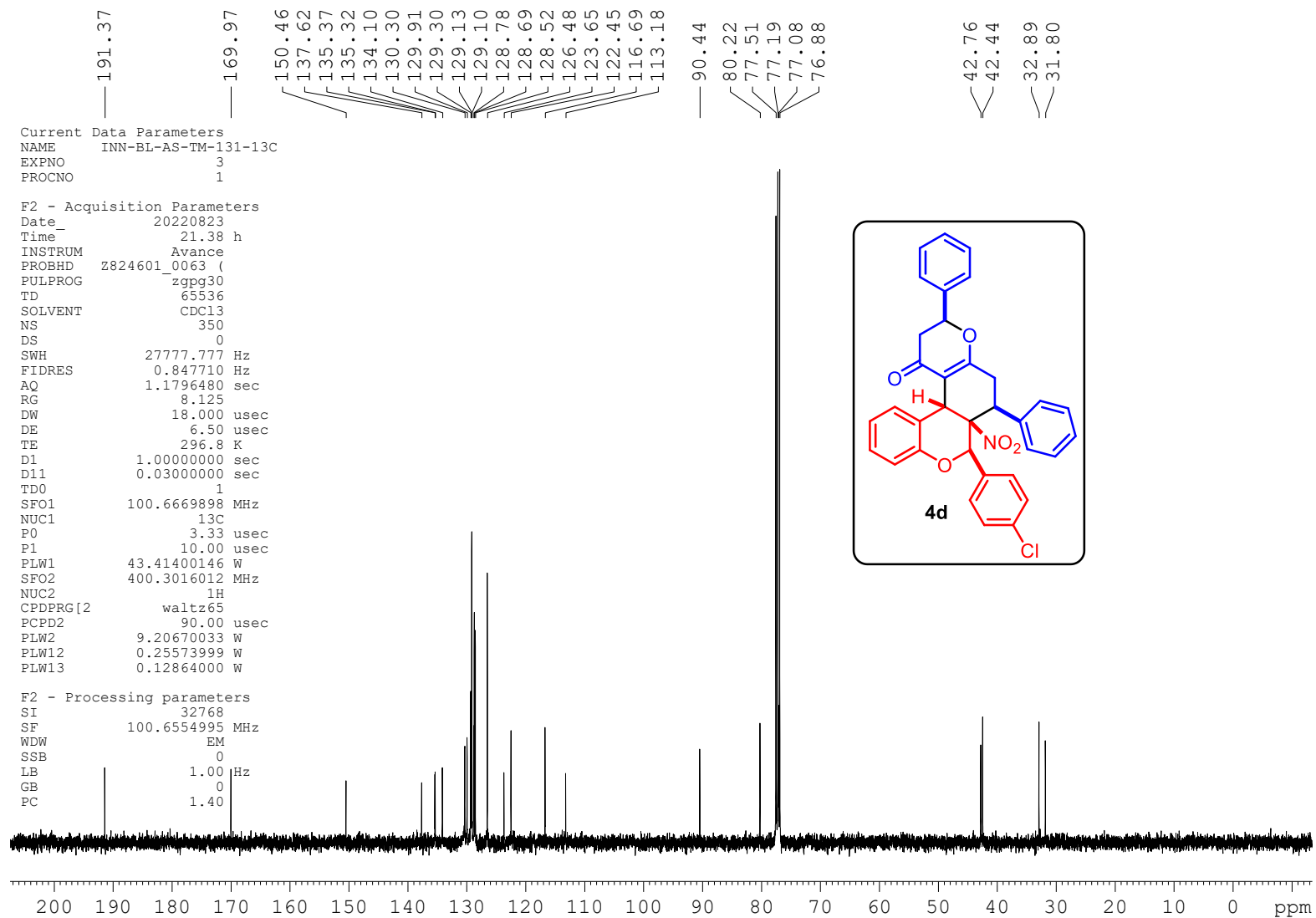


Figure S52. ¹³C NMR Spectrum of 4d

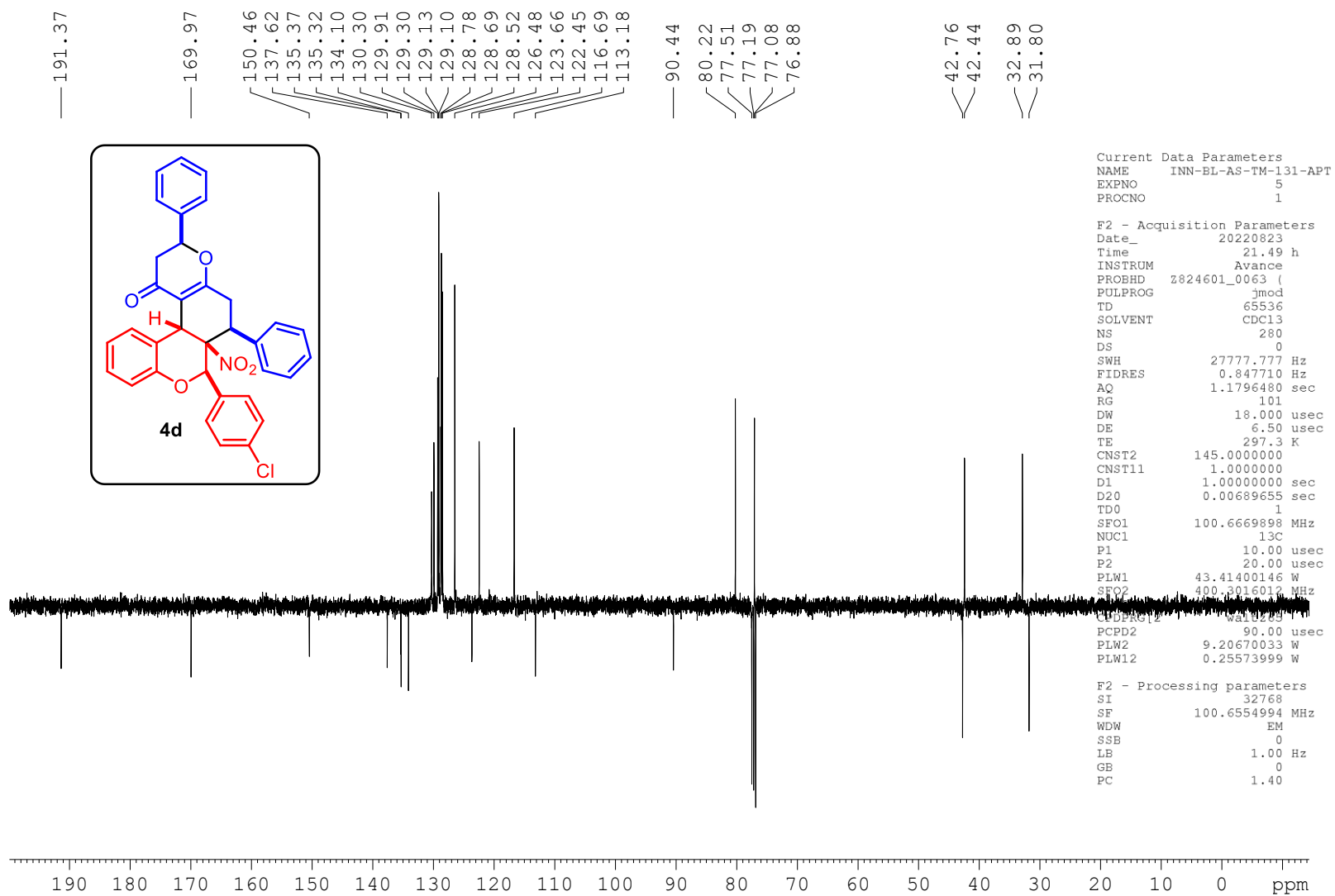


Figure S53. ¹³C-APT NMR Spectrum of 4d

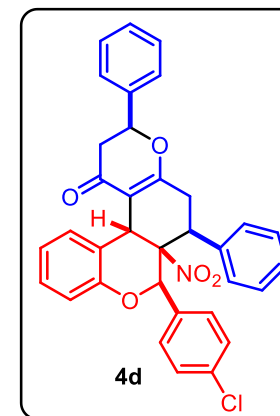
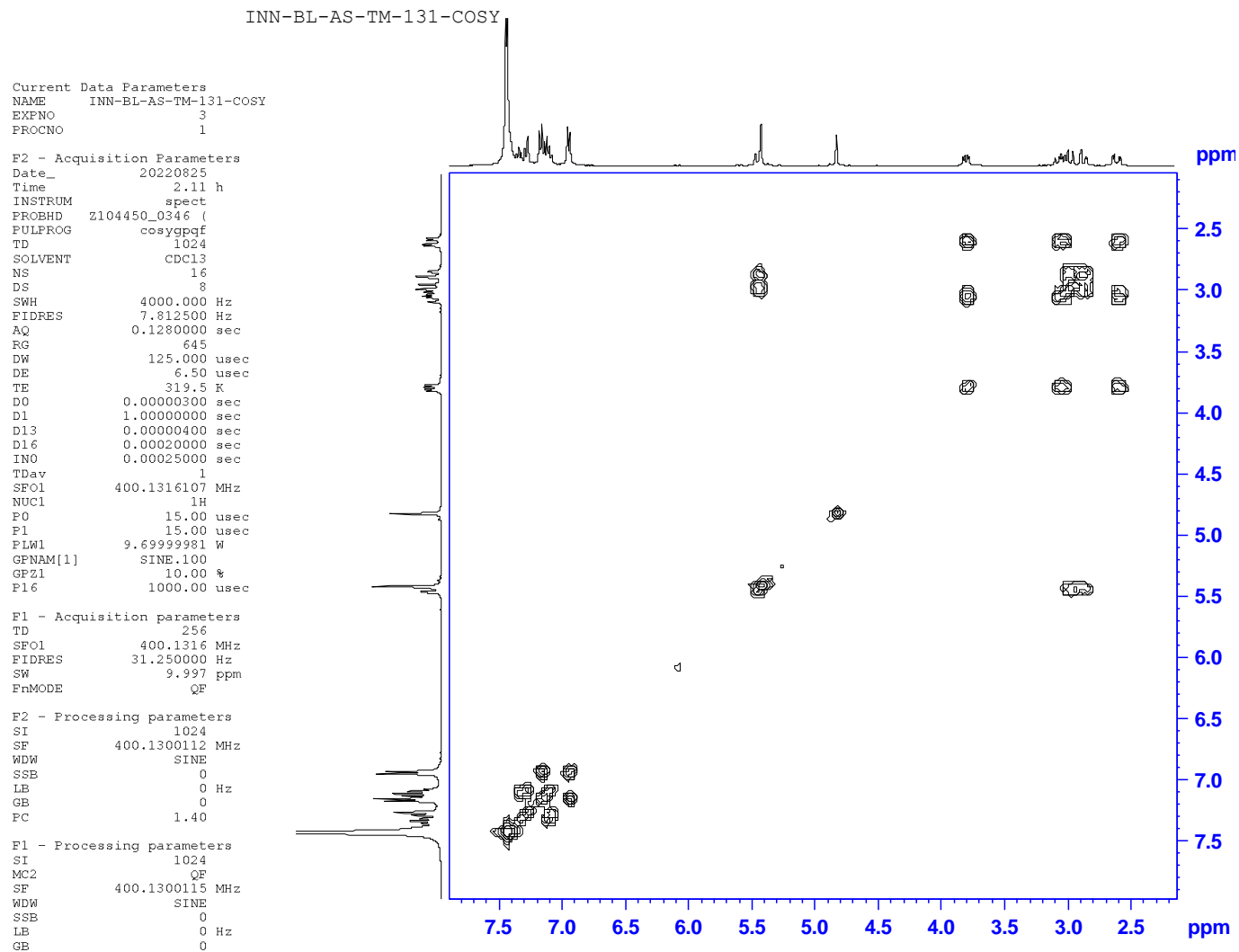


Figure S54. ^1H - ^1H COSY NMR Spectrum of 4d

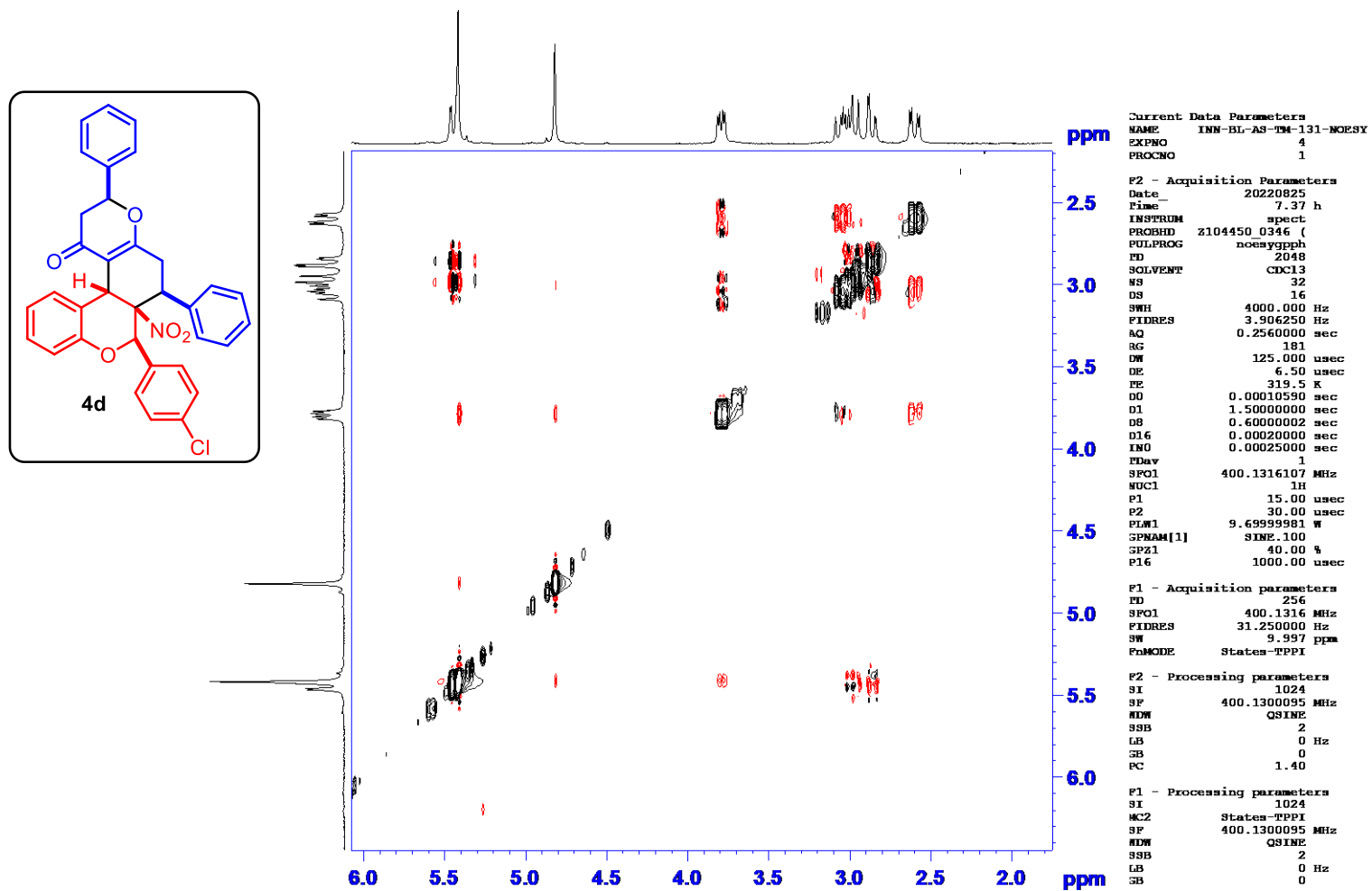


Figure S55. ^1H - ^1H NOESY NMR Spectrum of 4d

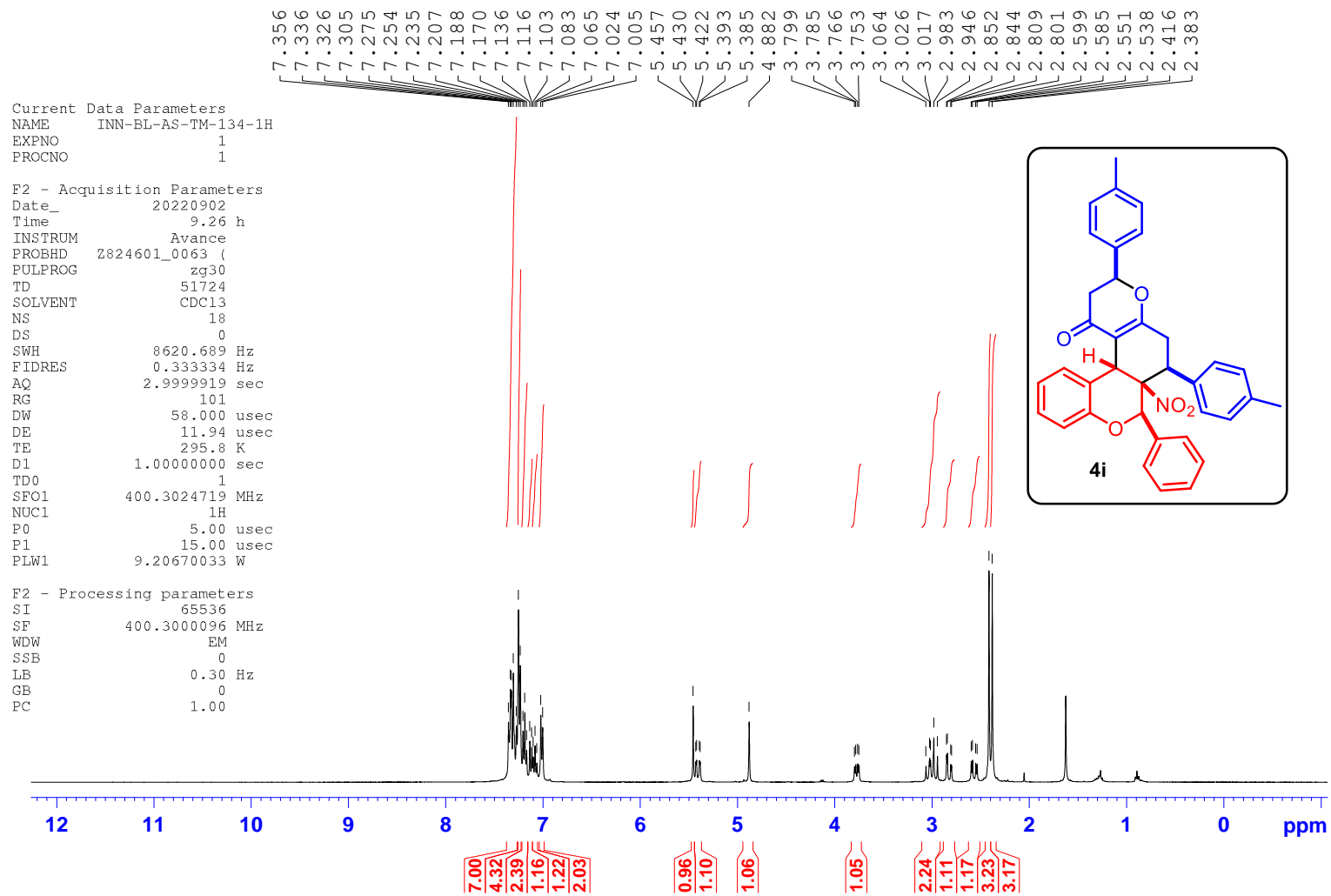


Figure S56. ¹H NMR Spectrum of 4i

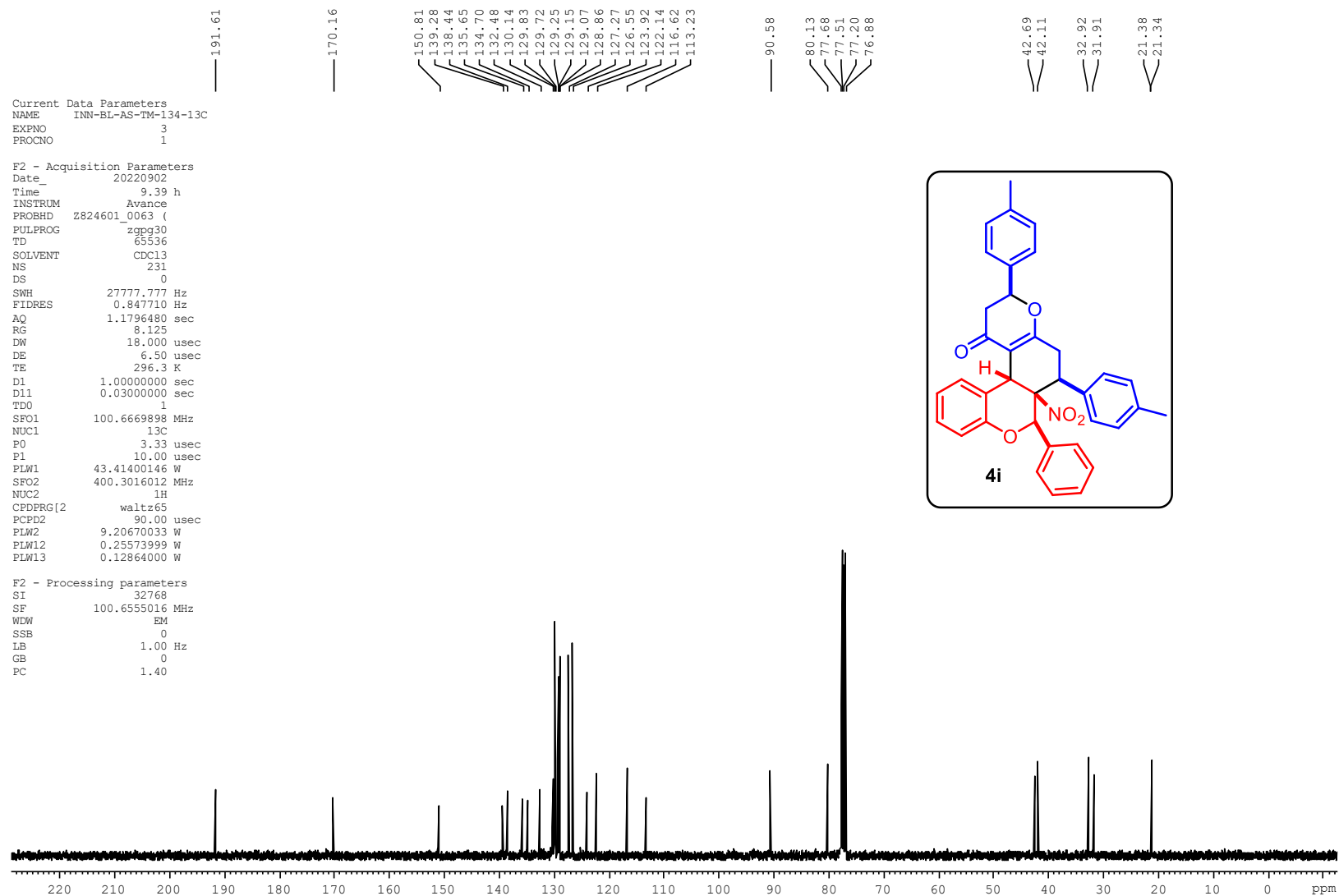


Figure S57. ¹³C NMR Spectrum of 4i

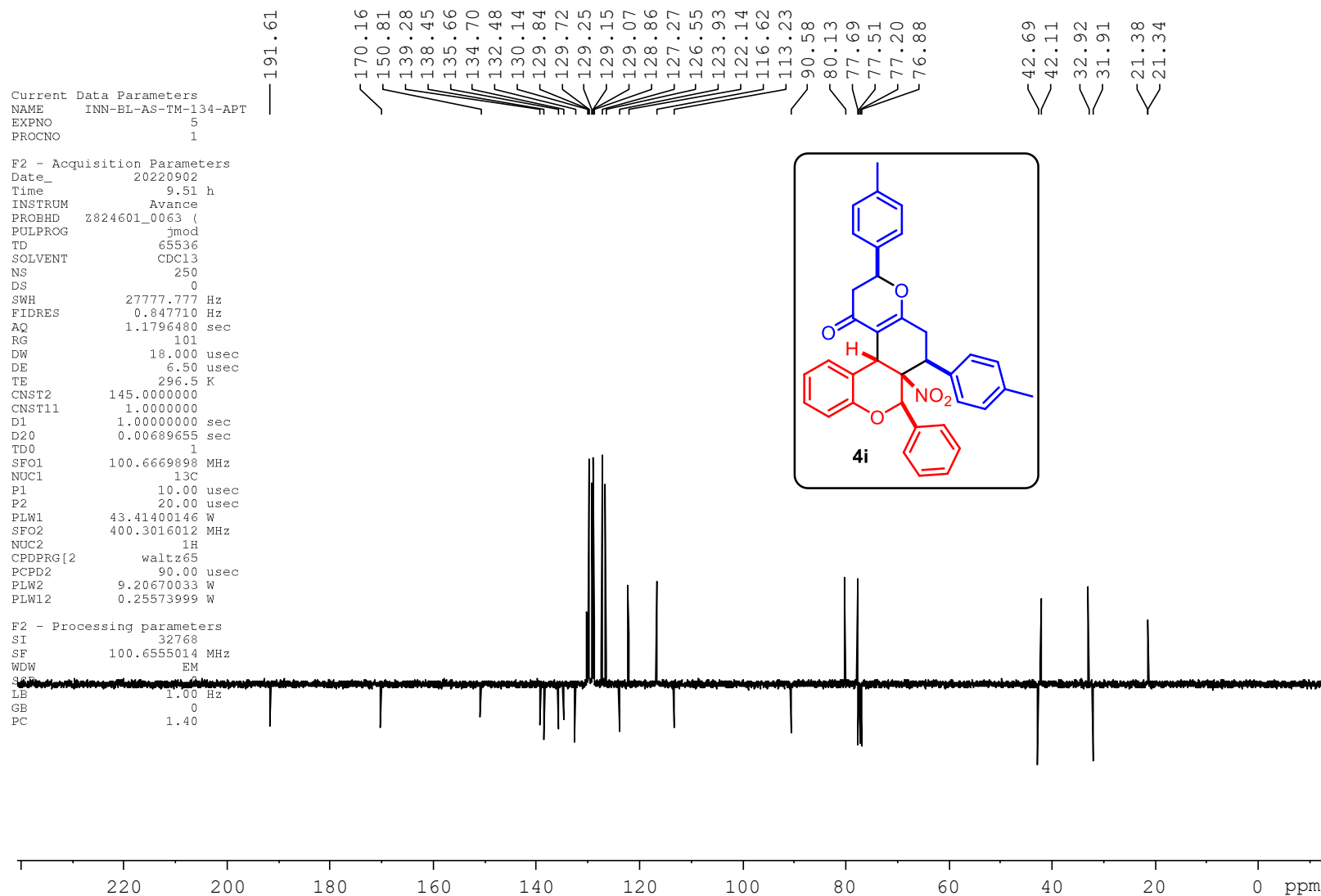


Figure S58. ¹³C-APT NMR Spectrum of **4i**

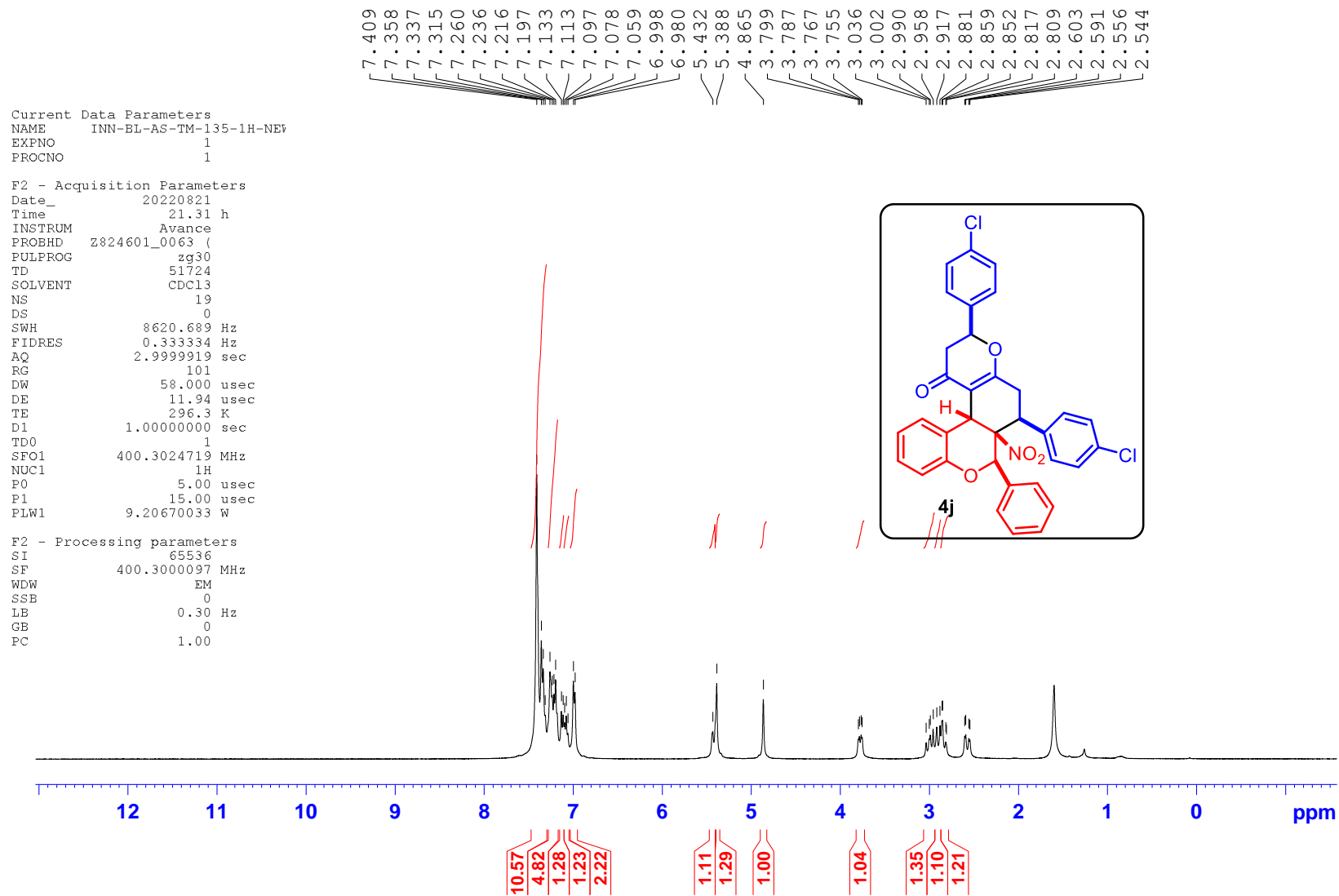
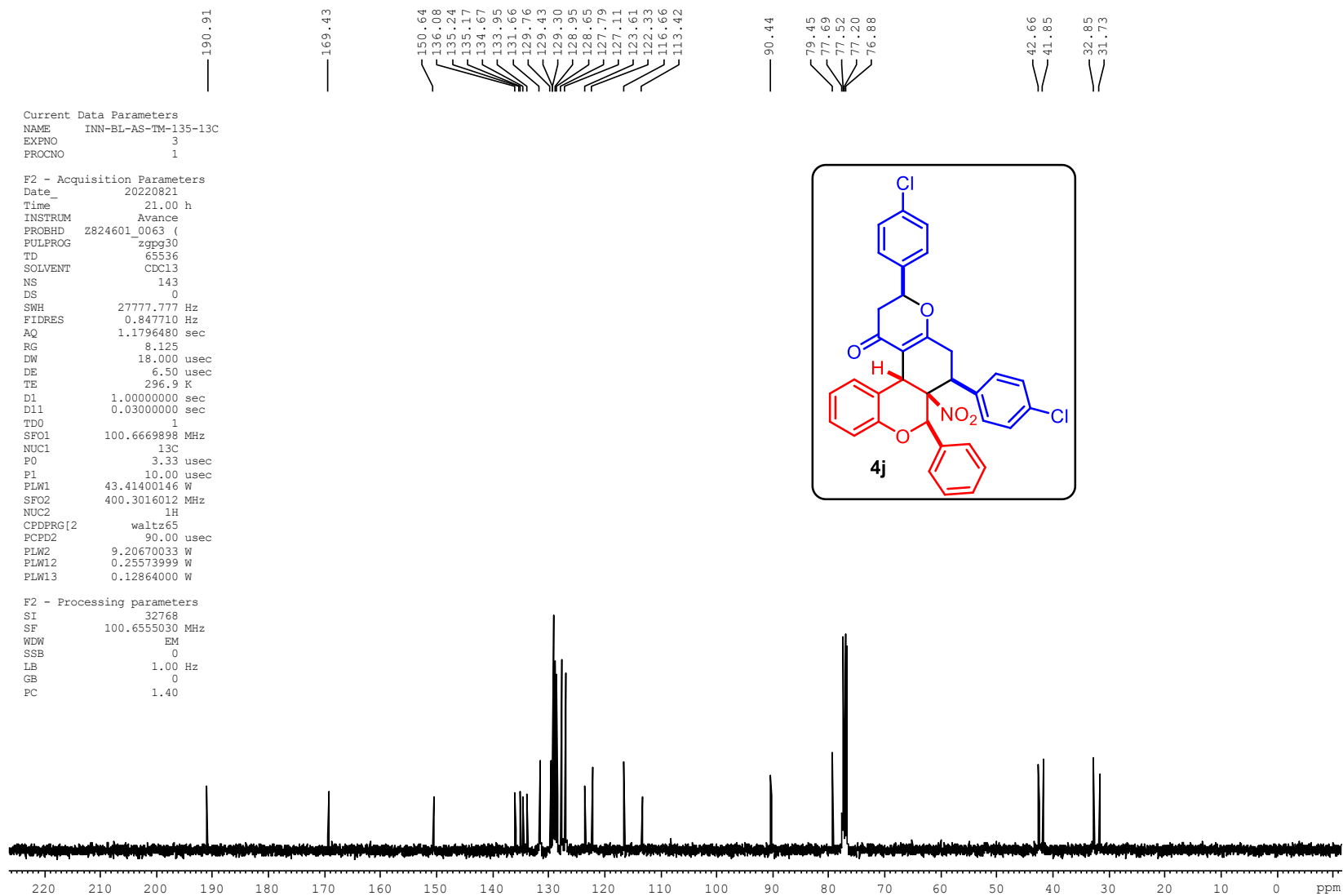


Figure S59. ¹H NMR Spectrum of 4j



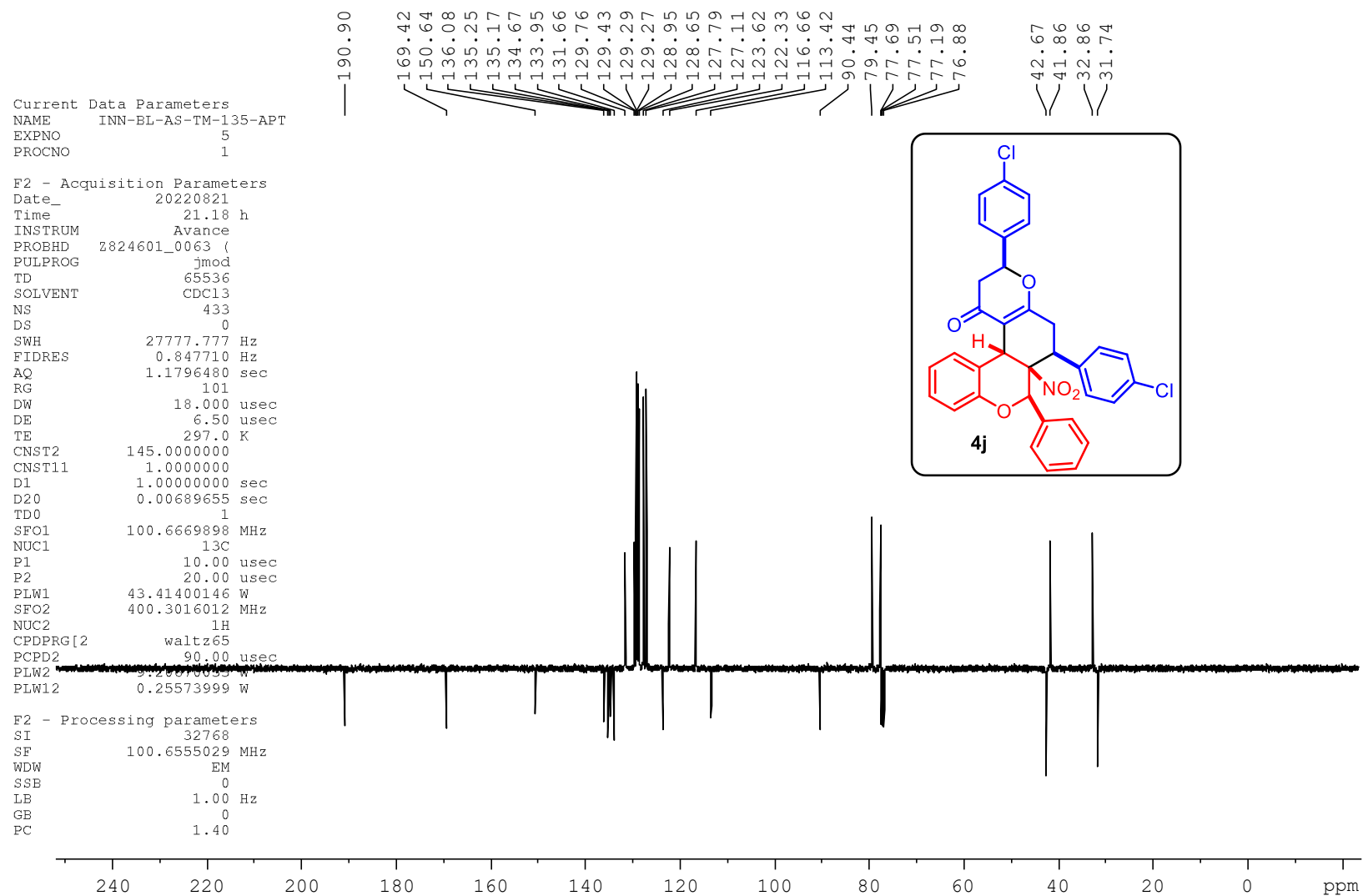


Figure S61. ¹³C-APT NMR Spectrum of 4j

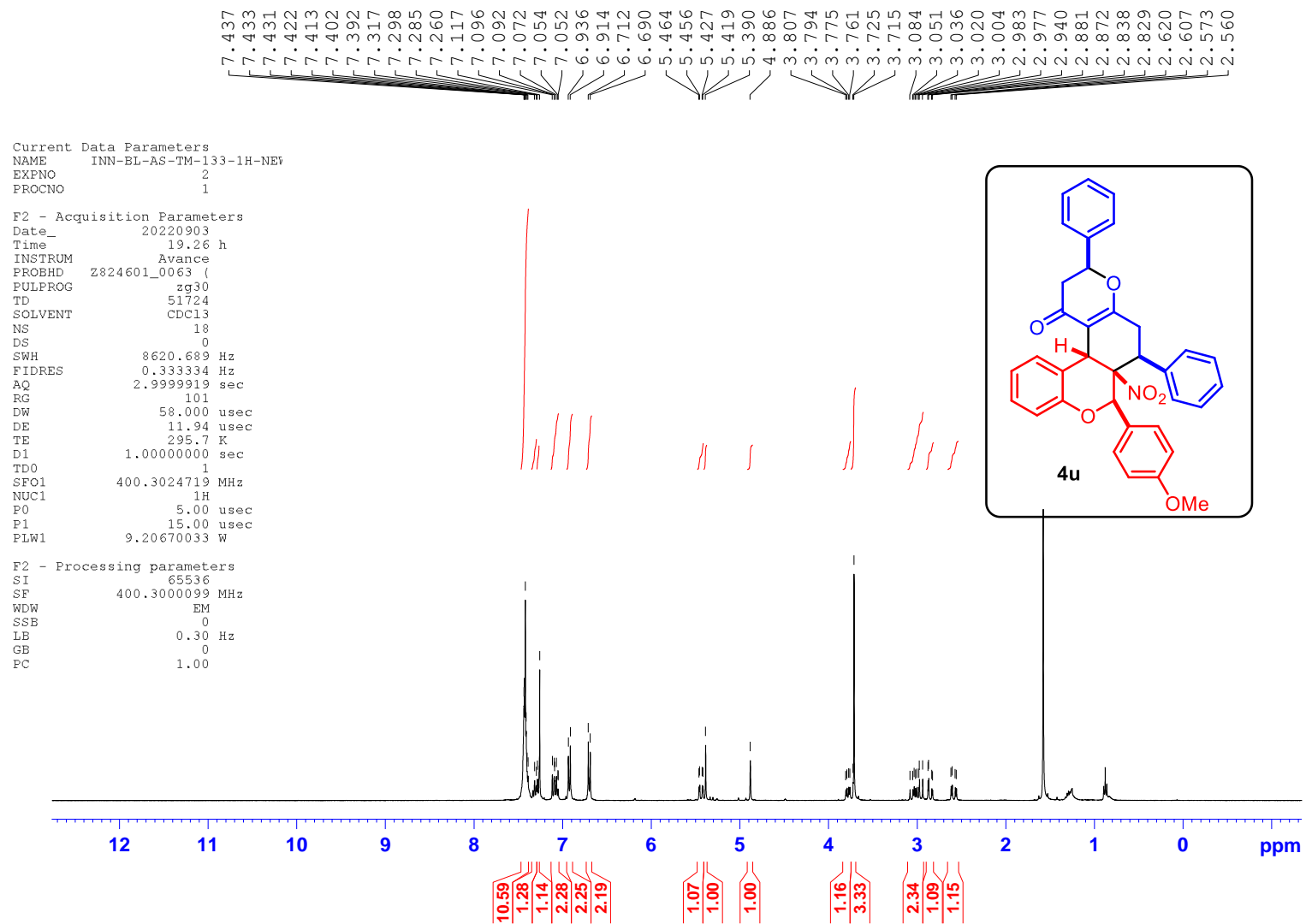


Figure S62. ¹H NMR Spectrum of 4u

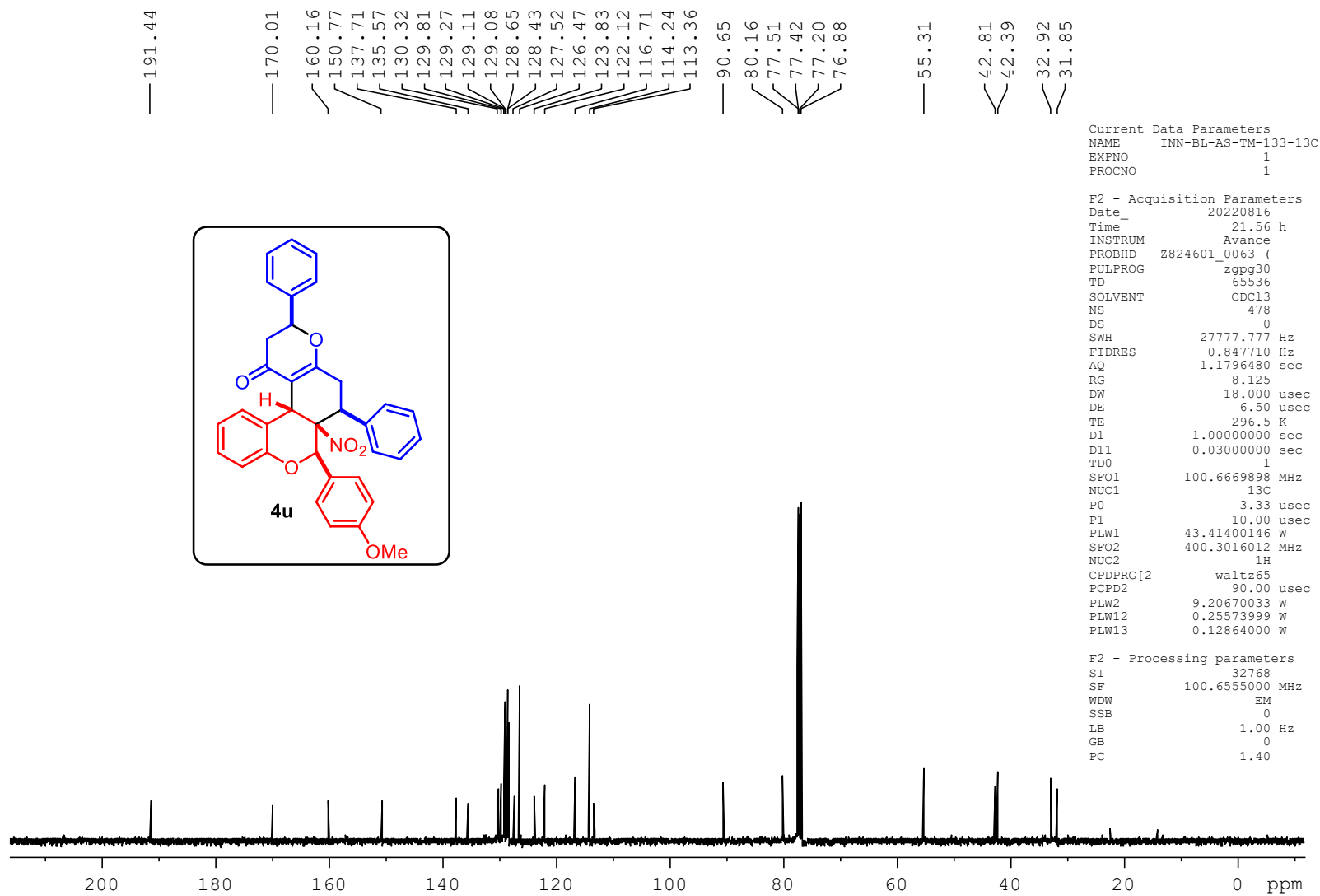


Figure S63. ¹³C NMR Spectrum of 4u

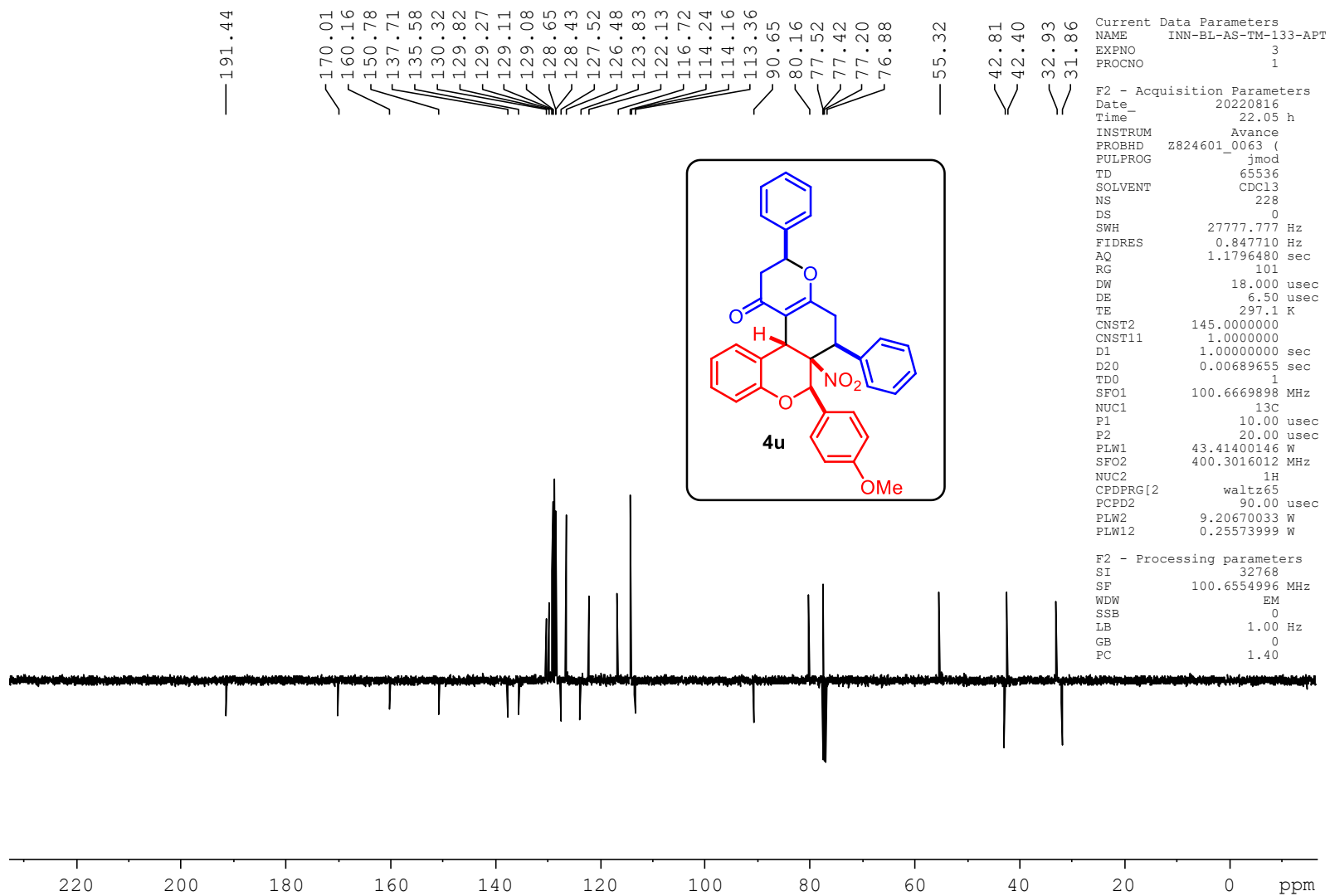


Figure S64. ¹³C-APT NMR Spectrum of 4u

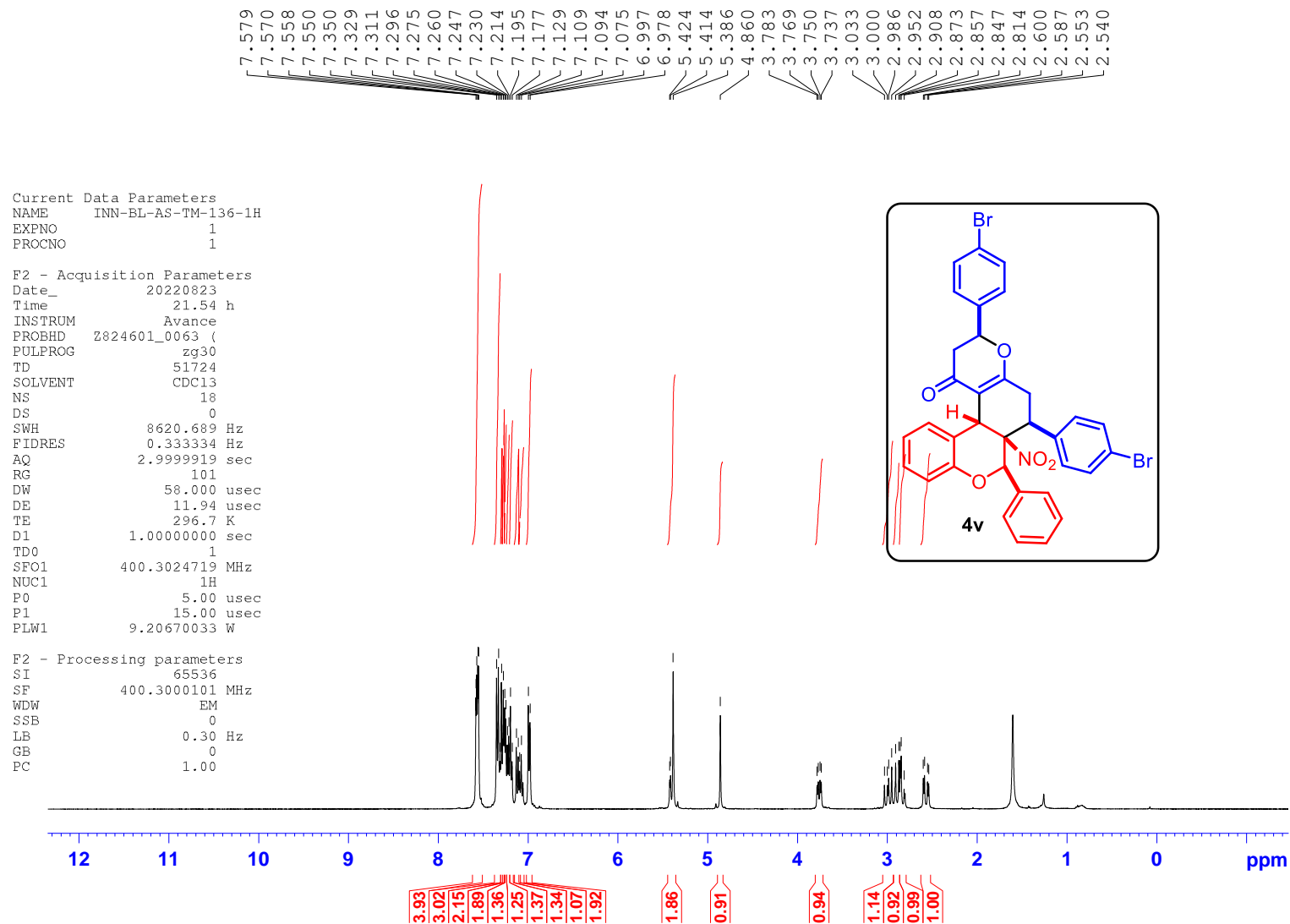


Figure S65. ¹H NMR Spectrum of 4v

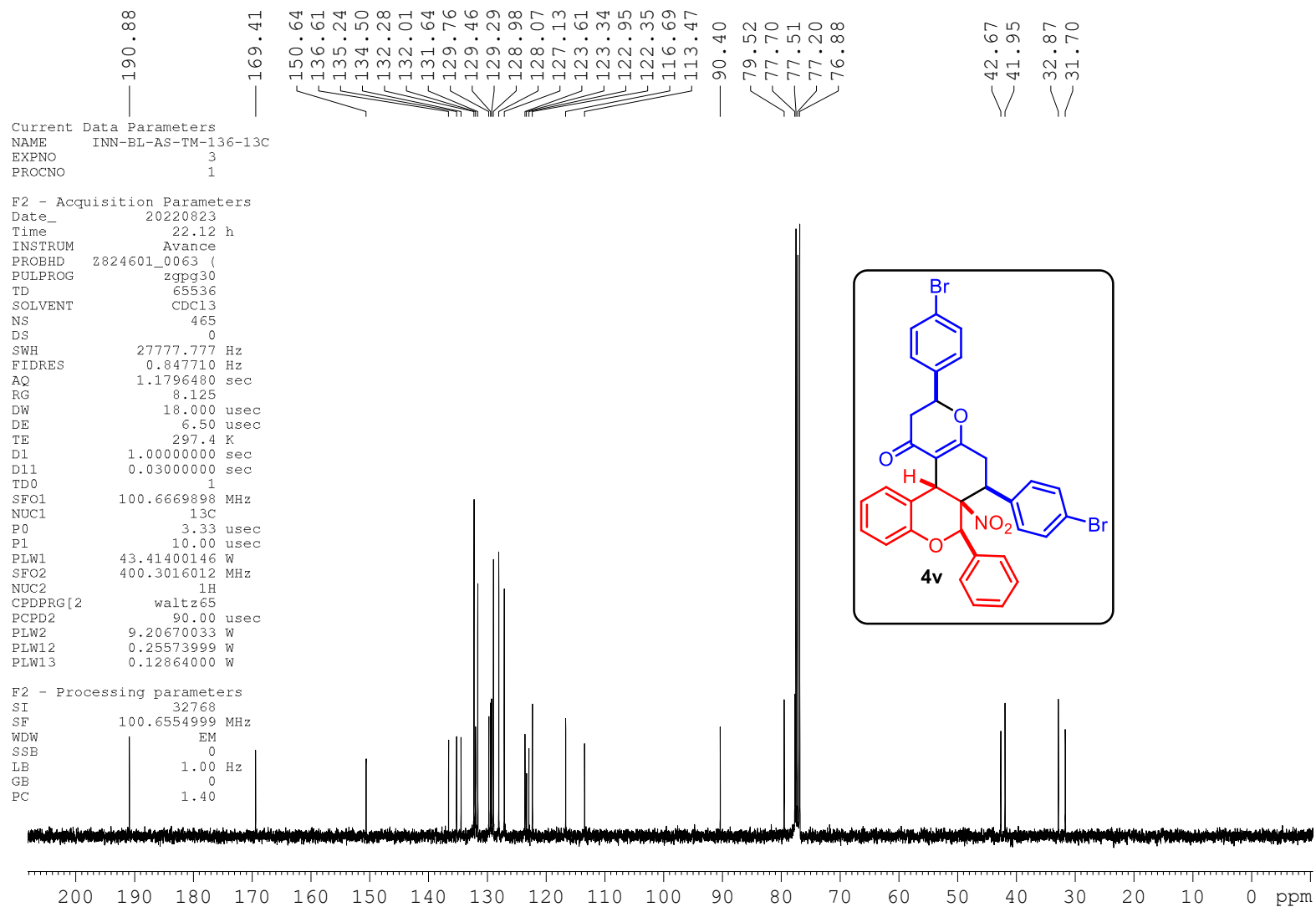


Figure S66. ^{13}C NMR Spectrum of 4v

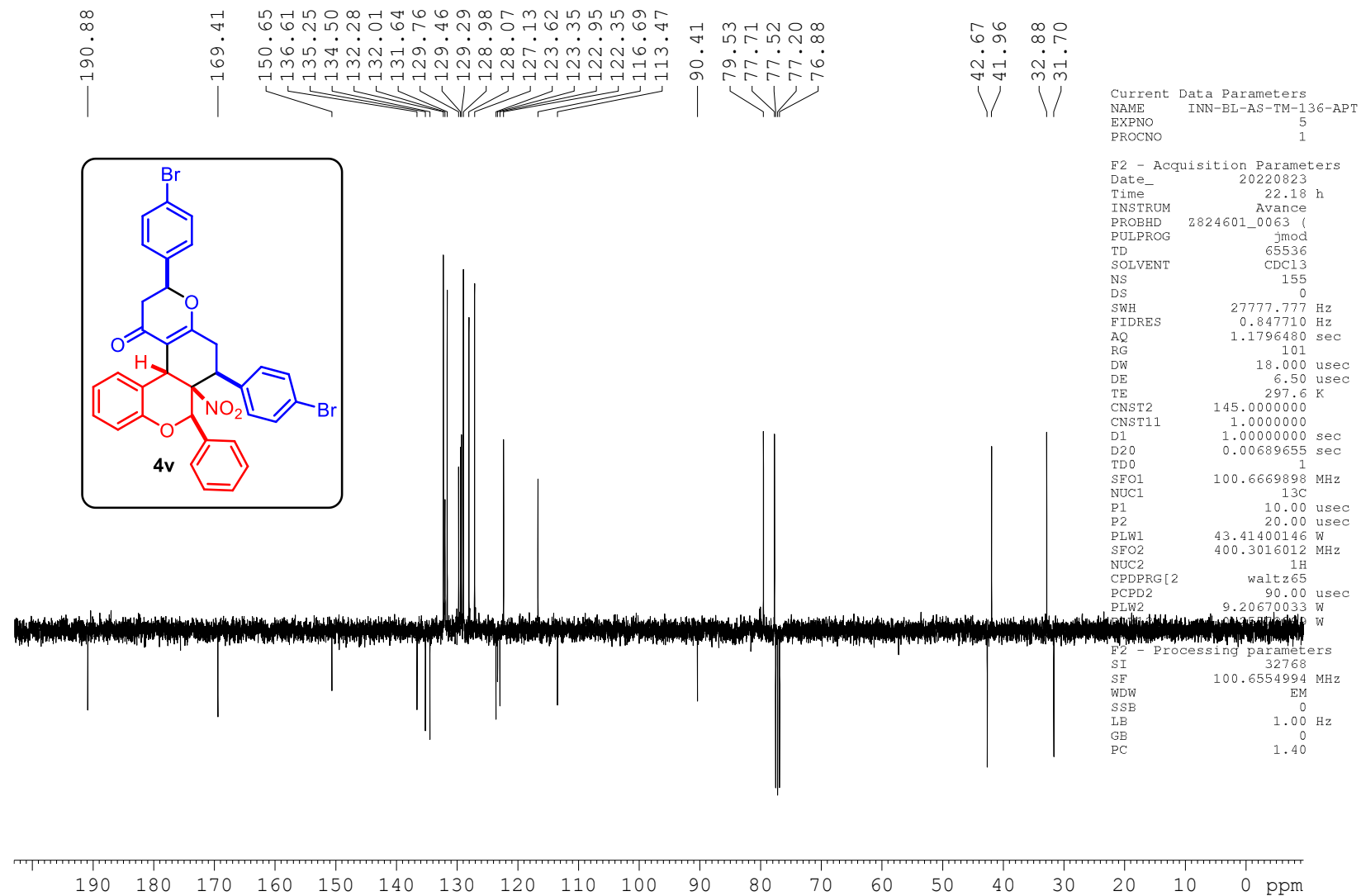


Figure S67. ¹³C-APT NMR Spectrum of 4v

Current Data Parameters
 NAME INN-BL-AS-TM-130-1H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220730
 Time 20.39 h
 INSTRUM Avance
 PROBHD Z824601_0063 (
 PULPROG zg30
 TD 51724
 SOLVENT CDC13
 NS 14
 DS 0
 SWH 11904.762 Hz
 FIDRES 0.460319 Hz
 AQ 2.1724081 sec
 RG 101
 DW 42.000 usec
 DE 7.94 usec
 TE 296.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.3040030 MHz
 NUC1 1H
 P0 5.00 usec
 P1 15.00 usec
 PLW1 9.20670033 W

F2 - Processing parameters
 SI 65536
 SF 400.3000535 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

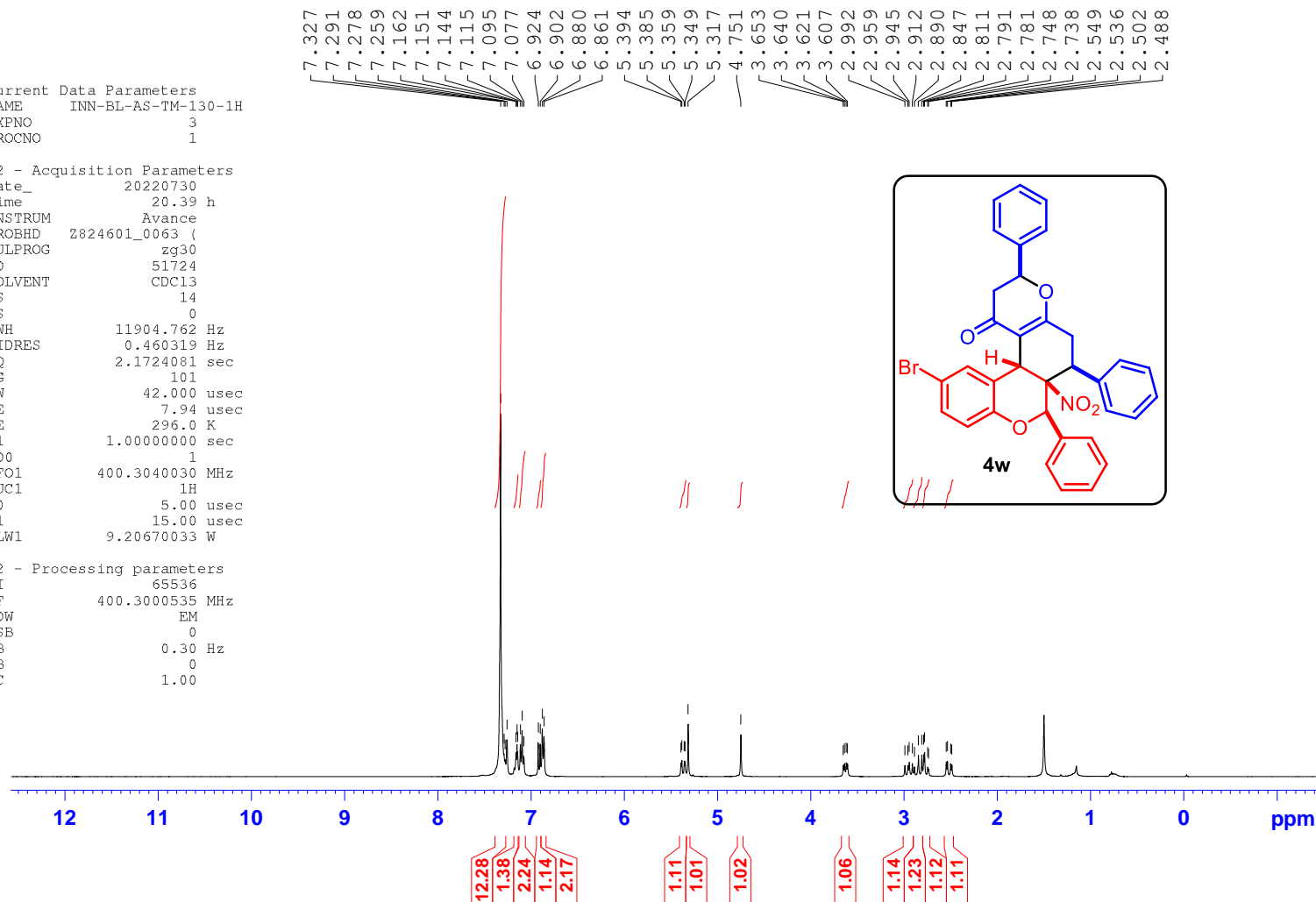


Figure S68. ¹H NMR Spectrum of 4w

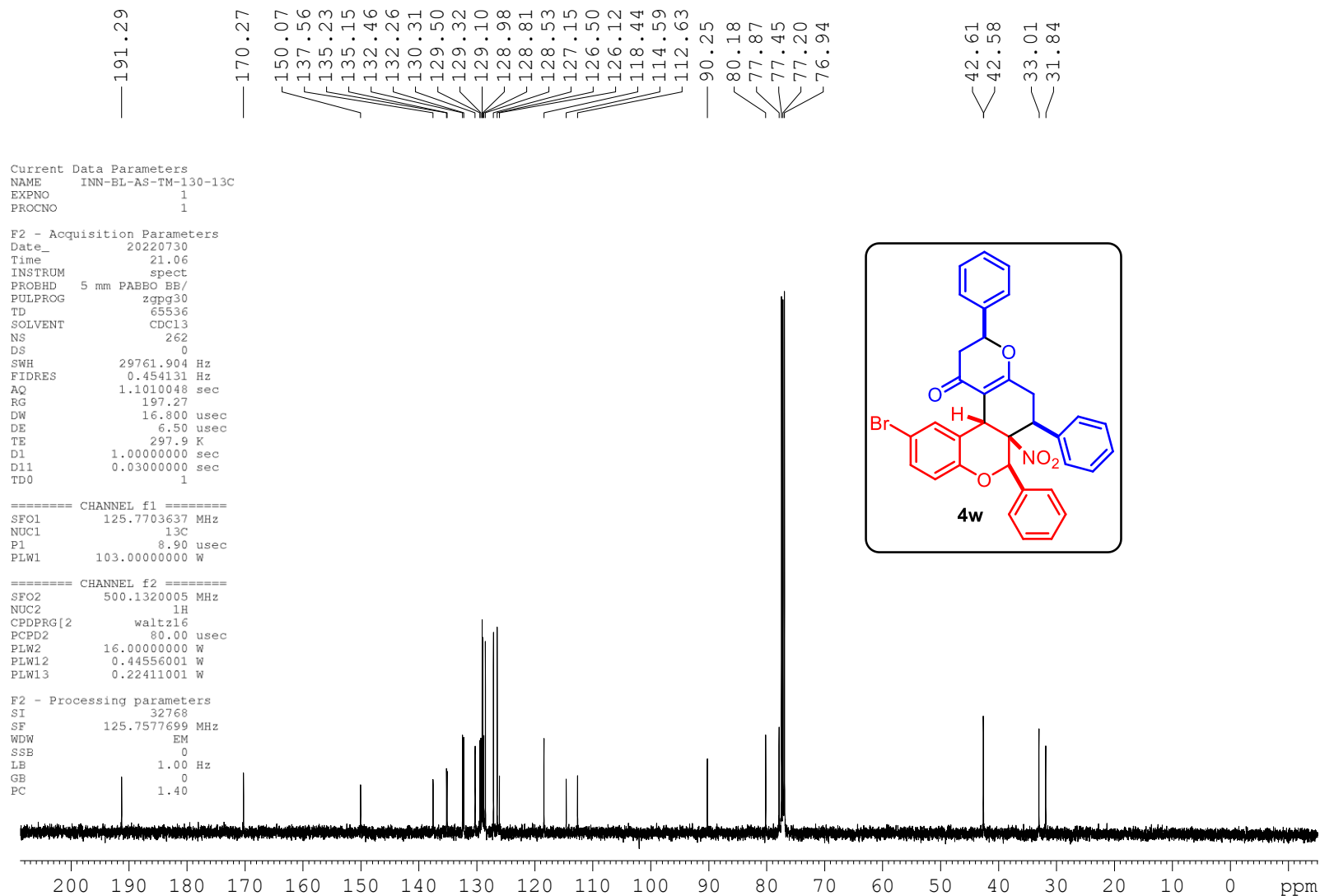


Figure S69. ^{13}C NMR Spectrum of 4w

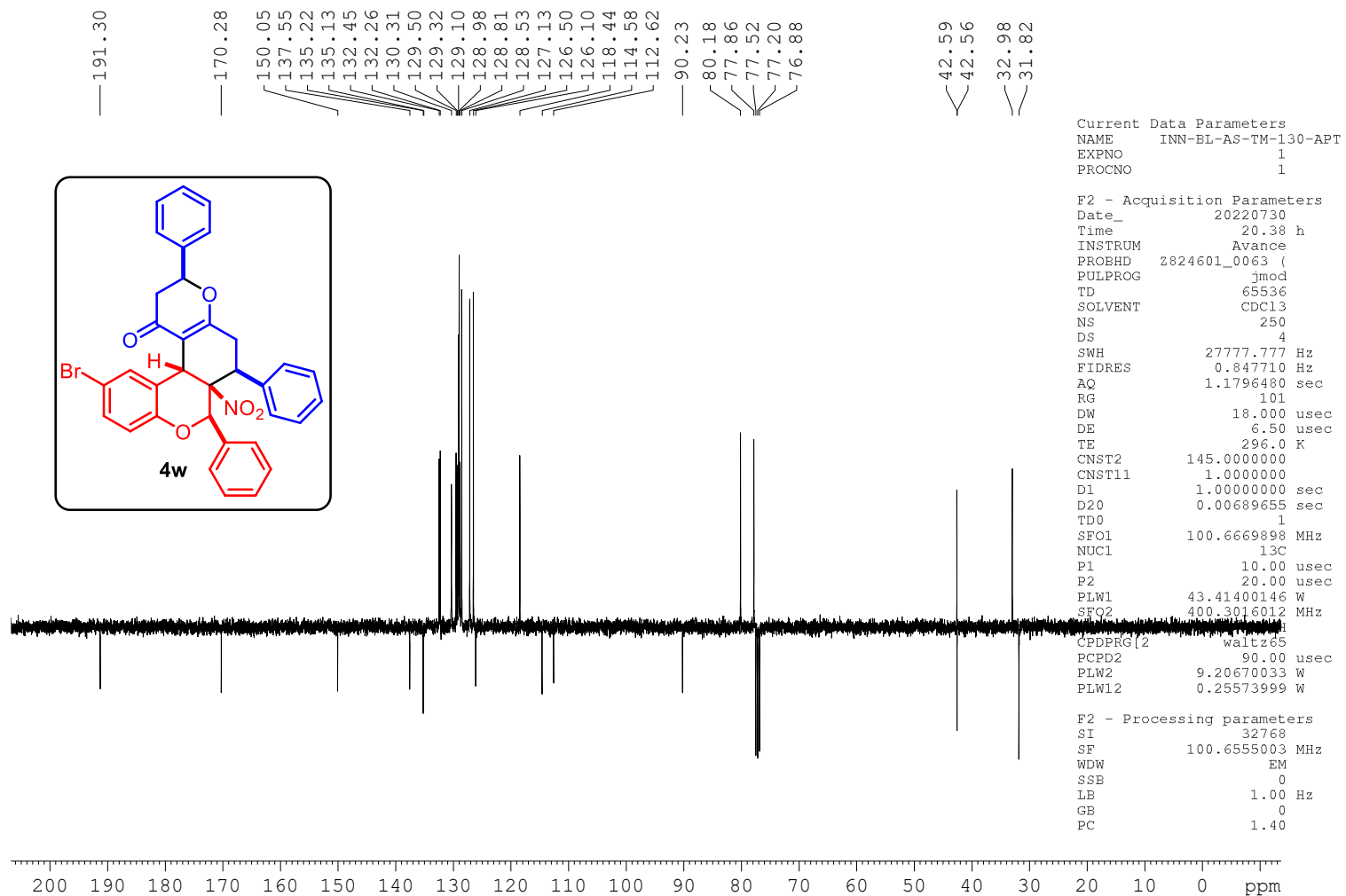
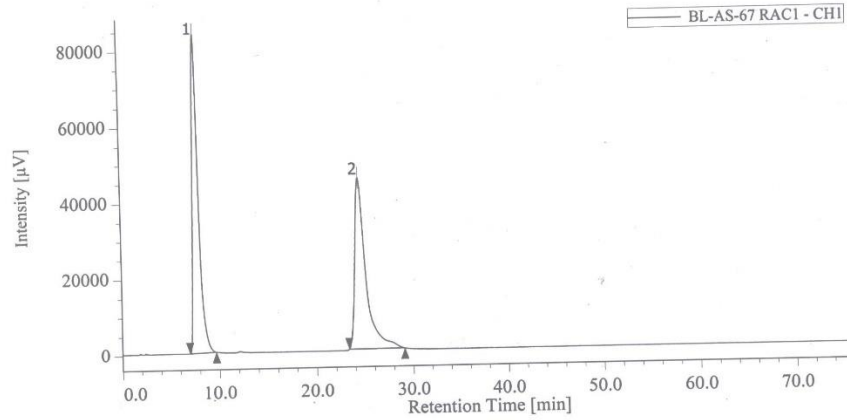


Figure S70. ¹³C-APT NMR Spectrum of 4w

Chromatogram



Chromatogram Information

User Name Administrator
 Date Modified 2/1/2022 6:32:04 AM
 Description
 HPLC System Name JASCO LC-4000
 Injection Date 2/1/2022 5:16:20 AM
 Volume 1.00 [µL]
 Sample # 1
 Project Name sivasankar
 Acquisition Time 110.0 [min]
 Acquisition Sequence BL-AS-67 RAC1
 Control Method BL-2%-1F-360NM
 Peak ID Table
 Calibration Method
 Additional Information

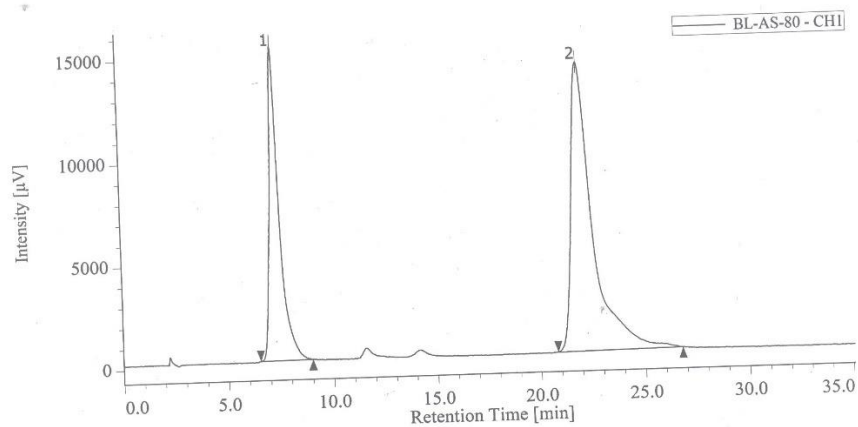
Channel & Peak Information Table

Chromatogram Name BL-AS-67 RAC1-CH1
 Sample Name
 Channel Name CH1
 Sampling Interval 500 [msec]
 Peak Method (Manual)

#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	1	7.858	3545073	83703	50.070	65.075	N/A	876	11.809	1.235	
2	Unknown	1	24.542	3535139	44922	49.930	34.925	N/A	3072	N/A	1.839	

Figure S71. HPLC profile of racemic 3b

Chromatogram



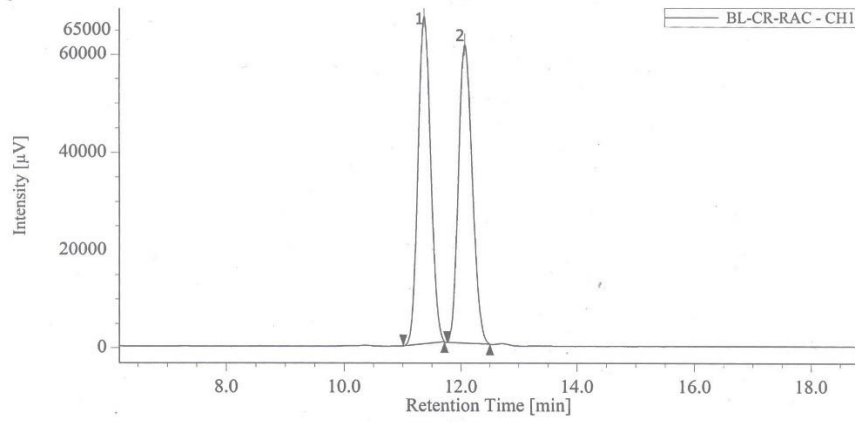
Chromatogram Information
 User Name Administrator
 Date Modified 3/2/2022 9:13:26 PM
 Description JASCO LC-4000
 HPLC System Name 3/2/2022 8:30:06 PM
 Injection Date 2.00 [µL]
 Volume 1
 Sample # sivasankar
 Project Name 110.0 [min]
 Acquisition Time BL-AS-80
 Acquisition Sequence BL-2%-1F-360NM
 Control Method
 Peak ID Table
 Calibration Method
 Additional Information

Channel & Peak Information Table
 Chromatogram Name BL-AS-80-CH1
 Sample Name CH1
 Channel Name 500 [msec]
 Sampling Interval (Manual)
 Peak Method

#	Peak Name	GH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	1	7.367	497122	15278	33.342	52.186	N/A	1642	12.887	1.257	
2	Unknown	1	22.033	993866	13999	66.658	47.814	N/A	3212	N/A	1.937	

Figure S72. HPLC profile of enantioenriched 3b'

Chromatogram



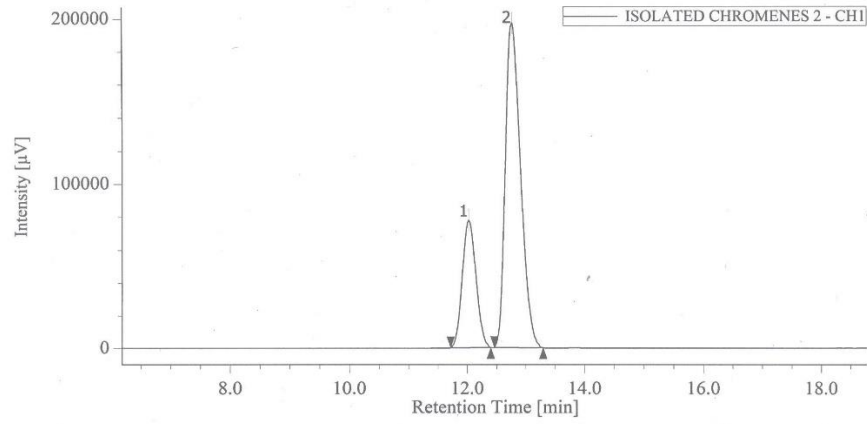
Chromatogram Information
 User Name Administrator
 Date Modified 2/24/2022 3:58:13 AM
 Description
 HPLC System Name JASCO LC-4000
 Injection Date 2/23/2022 10:06:09 PM
 Volume 2.00 [µL]
 Sample # 1
 Project Name sivasankar
 Acquisition Time 110.0 [min]
 Acquisition Sequence BL-CR-RAC
 Control Method BL-2%-1F-360NM
 Peak ID Table
 Calibration Method
 Additional Information

Channel & Peak Information Table
 Chromatogram Name BL-CR-RAC-CH1
 Sample Name
 Channel Name CH1
 Sampling Interval 500 [msec]
 Peak Method (Manual)

#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	1	11.367	1018666	66882	50.091	52.327	N/A	12532	1.648	1.074	
2	Unknown	1	12.067	1014956	60932	49.909	47.673	N/A	11720	N/A	1.159	

Figure S73. HPLC profile of racemic 2b

Chromatogram



Chromatogram Information
 User Name Administrator
 Date Modified 2/24/2022 10:02:38 PM
 Description
 HPLC System Name JASCO LC-4000
 Injection Date 2/24/2022 8:58:08 PM
 Volume 2.00 [µL]
 Sample # 1
 Project Name sivasankar
 Acquisition Time 110.0 [min]
 Acquisition Sequence ISOLATED CHROM 2
 Control Method BL-2%-1F-360NM
 Peak ID Table
 Calibration Method
 Additional Information

Channel & Peak Information Table
 Chromatogram Name ISOLATED CHROMENES 2-CH1
 Sample Name
 Channel Name CH1
 Sampling Interval 500 [msec]
 Peak Method (Manual)

#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	1	12.025	1259654	77574	26.149	28.301	N/A	12206	1.604	1.086	
2	Unknown	1	12.758	3557493	196526	73.851	71.699	N/A	11245	N/A	1.326	

Figure S74. HPLC profile of enantioenriched 2b'