

Supporting Information

Simple synthesis of new imidazopyridinone, pyridopyrimidinone, and thiazolopyridinone derivatives and optimization of reaction parameters using response surface methodology

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Experimental Section

General

The various diamines, cysteamine hydrochloride, 1,1-bis(methylthio)-2-nitroethene, various aldehydes, 2,2-dimethyl-1,3-dioxane-4,6-dione (Meldrum's acid) and solvents were purchased from Sigma-Aldrich chemical company and were used as received without further purification. Melting points were determined with an electrothermal 9100 apparatus. Infrared (IR) spectra were recorded on a Bruker Tensor 27 spectrometer. Nuclear magnetic resonance (NMR) spectra were obtained on a Bruker DRX-300 Avance instrument (300 MHz for ^1H and 75.4 MHz for ^{13}C) with DMSO as solvent. Chemical shifts are expressed in parts per million (ppm), and coupling constant (J) are reported in hertz (Hz). Elemental analyses for C, H and N were performed using a PerkinElmer 2004 series [II] CHN elemental analyzer. Mass spectra were recorded with an Agilent 5975C VL MSD with Triple-Axis Detector operating at an ionization potential of 70 eV.

General procedure for the synthesis of product 5.

Synthesis of imidazopyridinone and pyridopyrimidinone derivatives: The mixtures of various diamines (1 mmol), 1,1-bis(methylthio)-2-nitroethene (0.165 g, 1 mmol) and 10 mL EtOH/H₂O (2:1) at 72 °C in a 50 mL flask was stirred for 6 h. After completion of the reaction (monitored by thin-layer chromatography, hexane/ethyl acetate 1:1), aromatic aldehyde (1 mmol), 2,2-dimethyl-1,3-dioxane-4,6-dione (Meldrum's acid) (0.144 g, 1 mmol) were added to the reaction mixture, and it was stirred under optimized condition for the time given in Table 4. Then, the reaction mixture was cooled to room temperature and filtered to give the crude product. The solid was washed with ethanol to give product in good yields.

Synthesis of thiazolopyridinone derivatives: The mixtures of cysteamine hydrochloride (0.113 g, 1 mmol), 1,1-bis(methylthio)-2-nitroethene (0.165 g, 1 mmol), 10 mL EtOH/H₂O (2:1), and Et₃N (140 μL , 1 mmol) at 72 °C in a 50 mL flask was stirred for 5 h. After completion of the reaction (monitored by thin-layer chromatography, hexane/ethyl acetate 1:1), aromatic aldehyde (1 mmol), 2,2-dimethyl-1,3-dioxane-4,6-dione (Meldrum's acid) (0.144 g, 1 mmol) were added to the reaction mixture, and it was stirred under optimized condition for the time given in Table 4. The reaction mixture was monitored by thin layer chromatography (hexane/ethyl acetate 1:1); after completion of the reaction, the reaction mixture was cooled to room temperature and the product (as colorless crystal) was filtered. The solid was washed with ethanol to give product in moderate yields.

The structures all of the products **5a-o** (figure 1) were deduced from their IR, Mass, ^1H NMR, and ^{13}C NMR spectra.

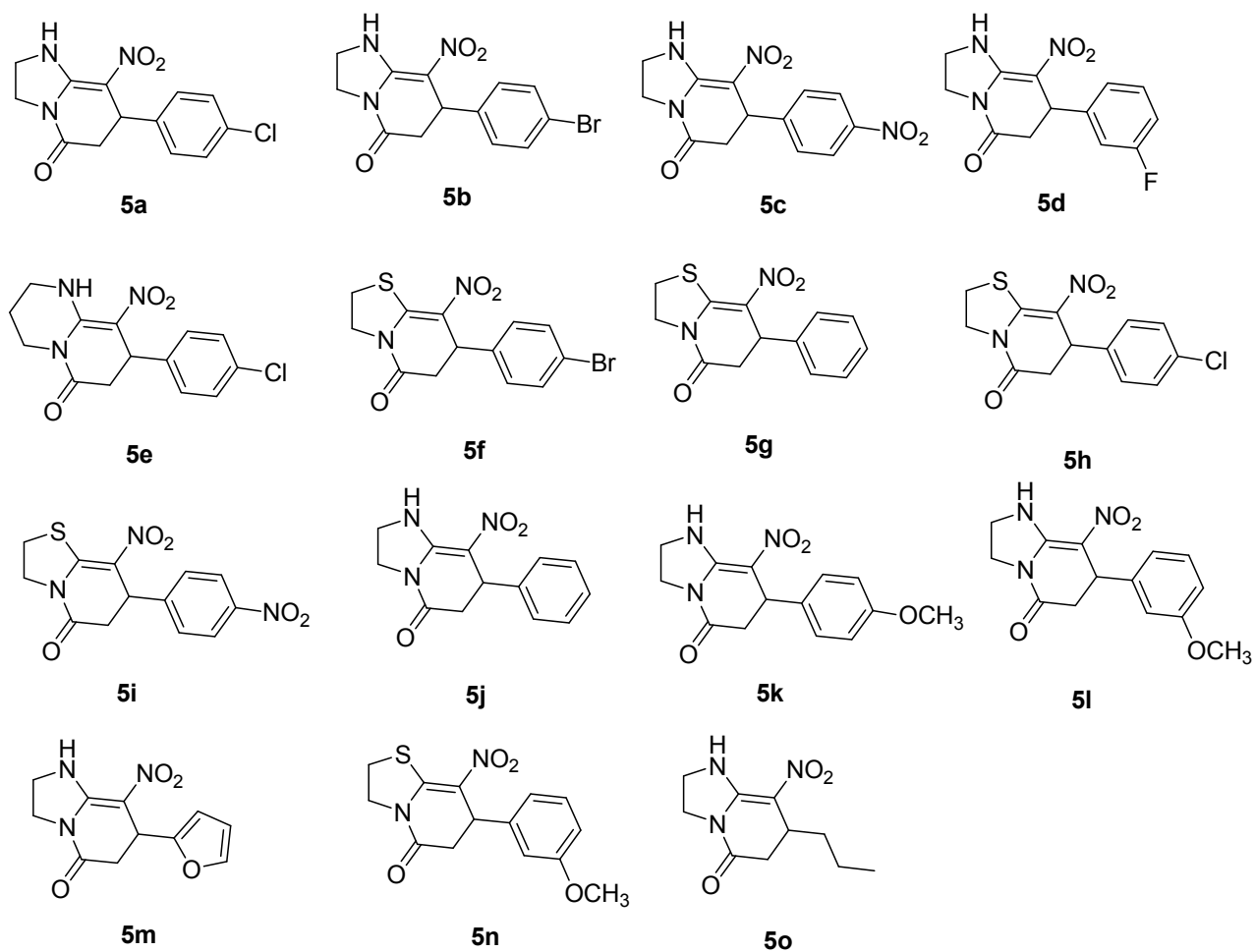
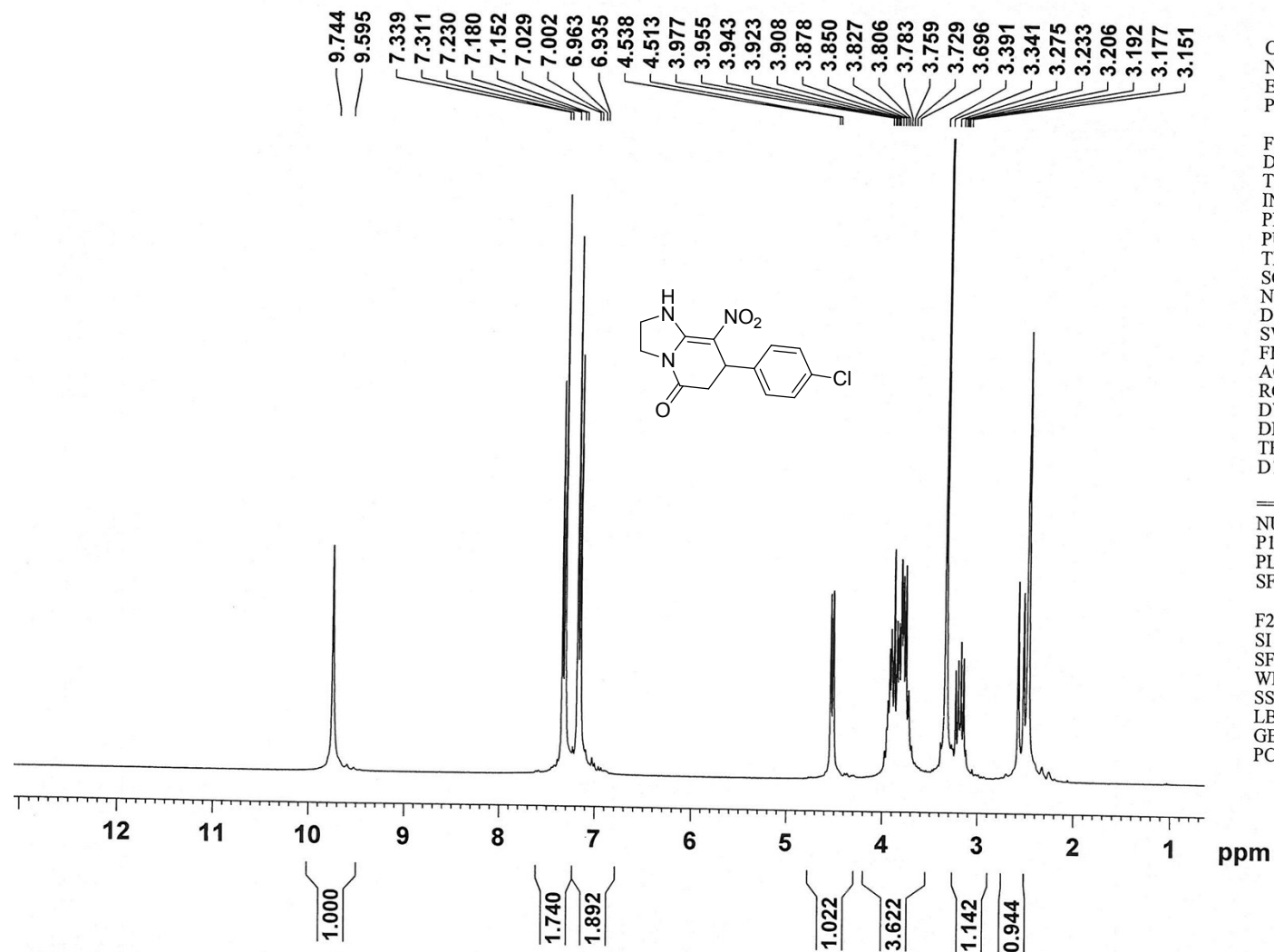


Figure 1. Structure of all products 5.

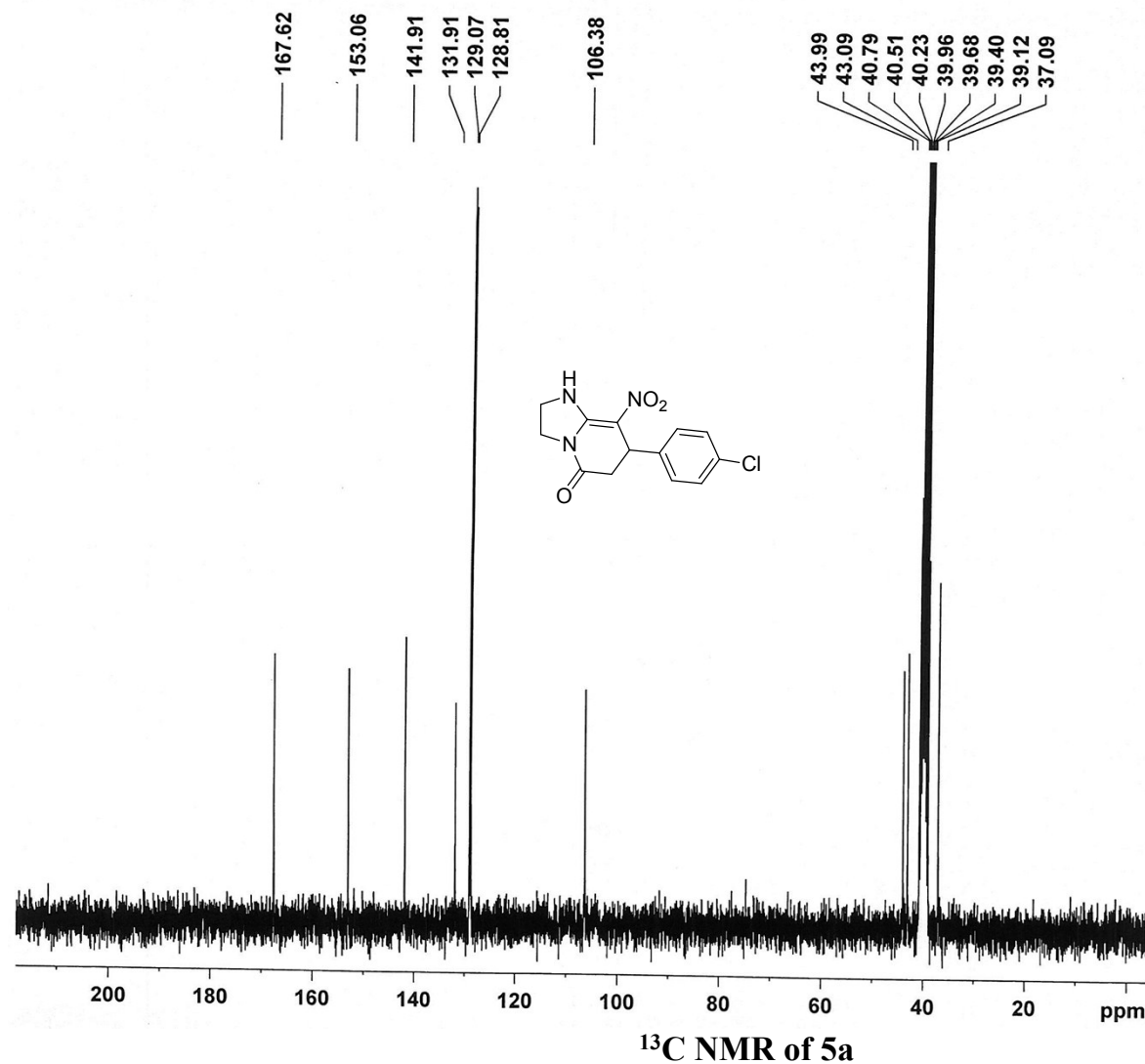
¹H NMR of 5a

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 PULPROG zg
 TD 16384
 SOLVENT DMSO
 NS 6
 DS 0
 SWH 5995.204 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 128
 DW 83.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 6.00000000 sec

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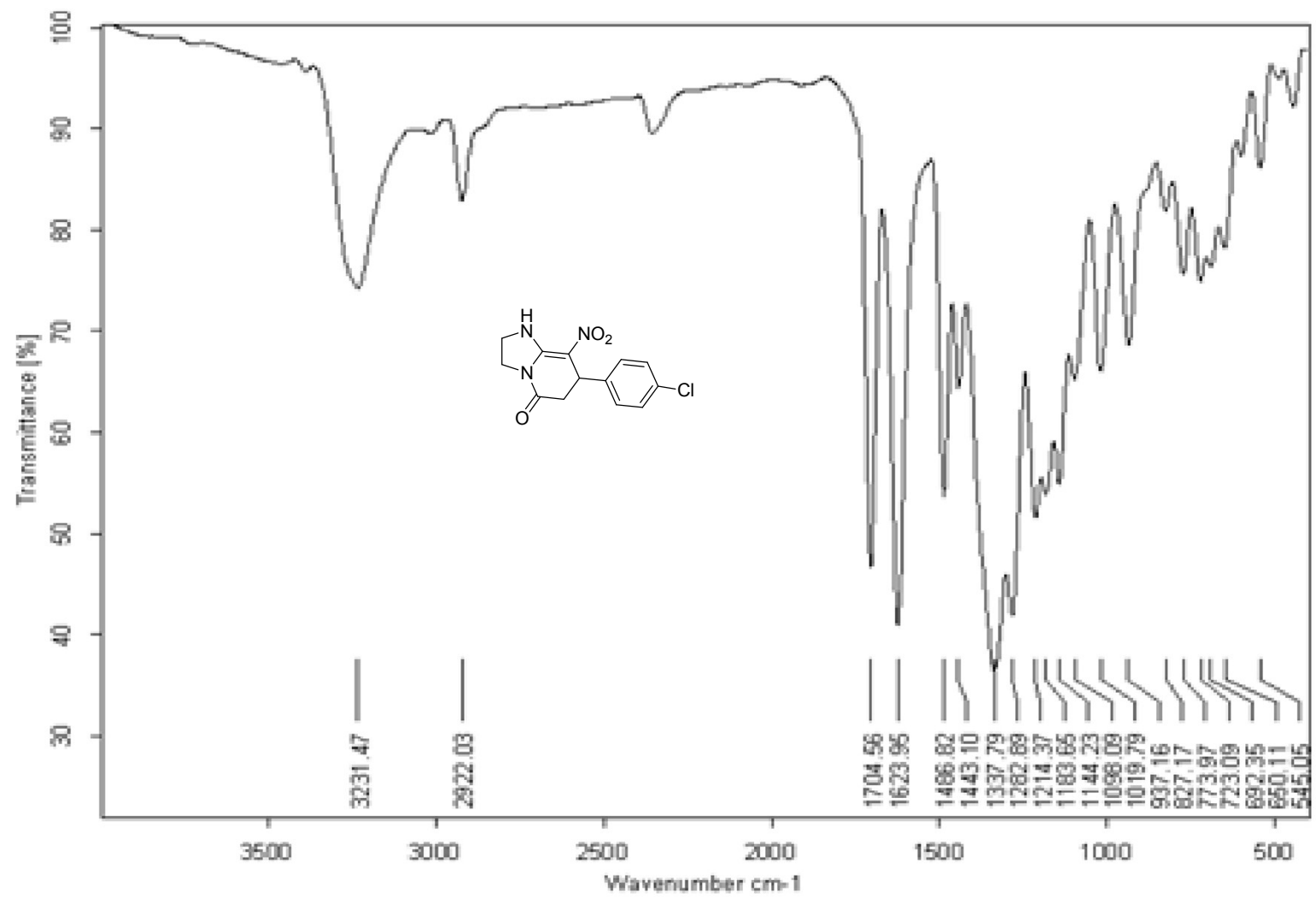
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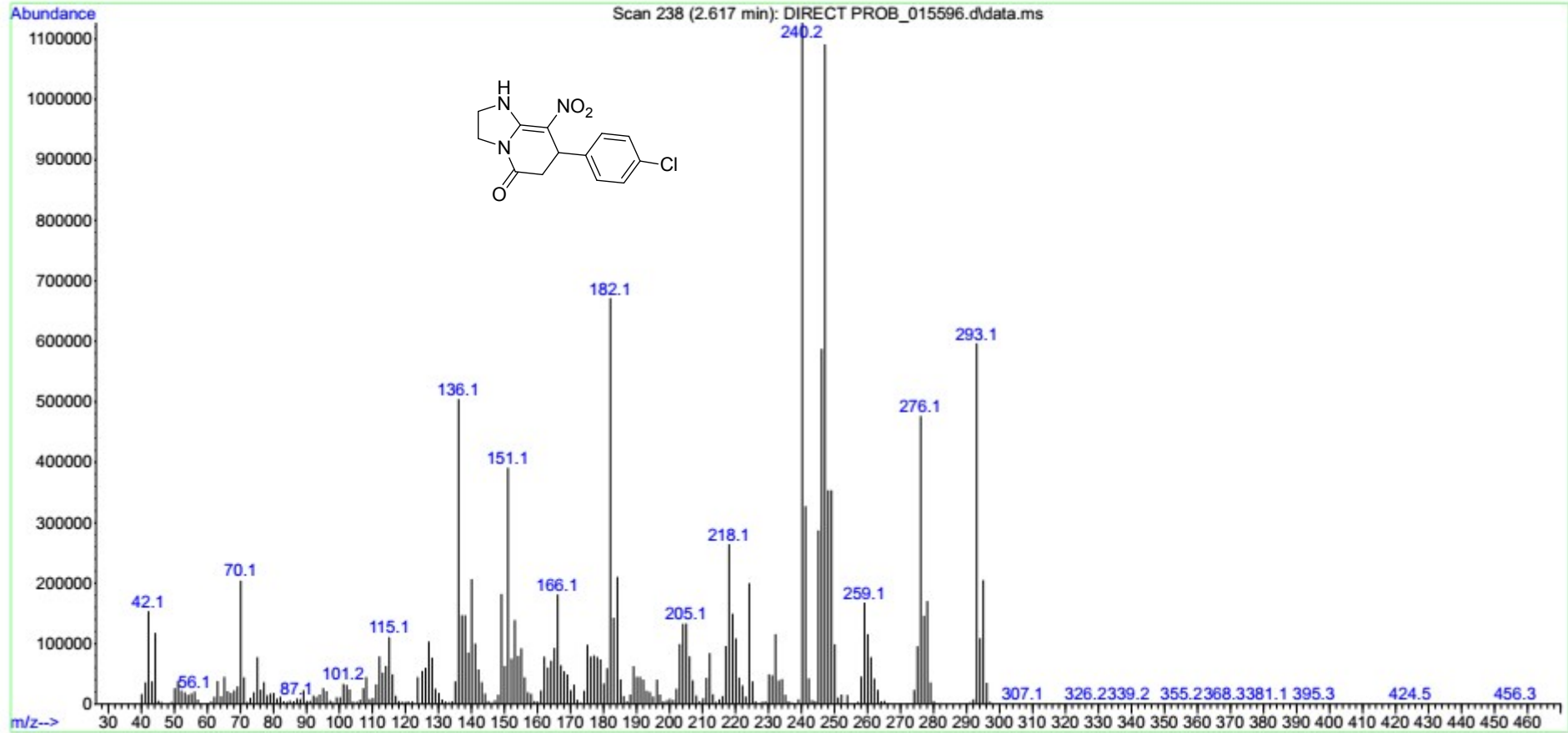
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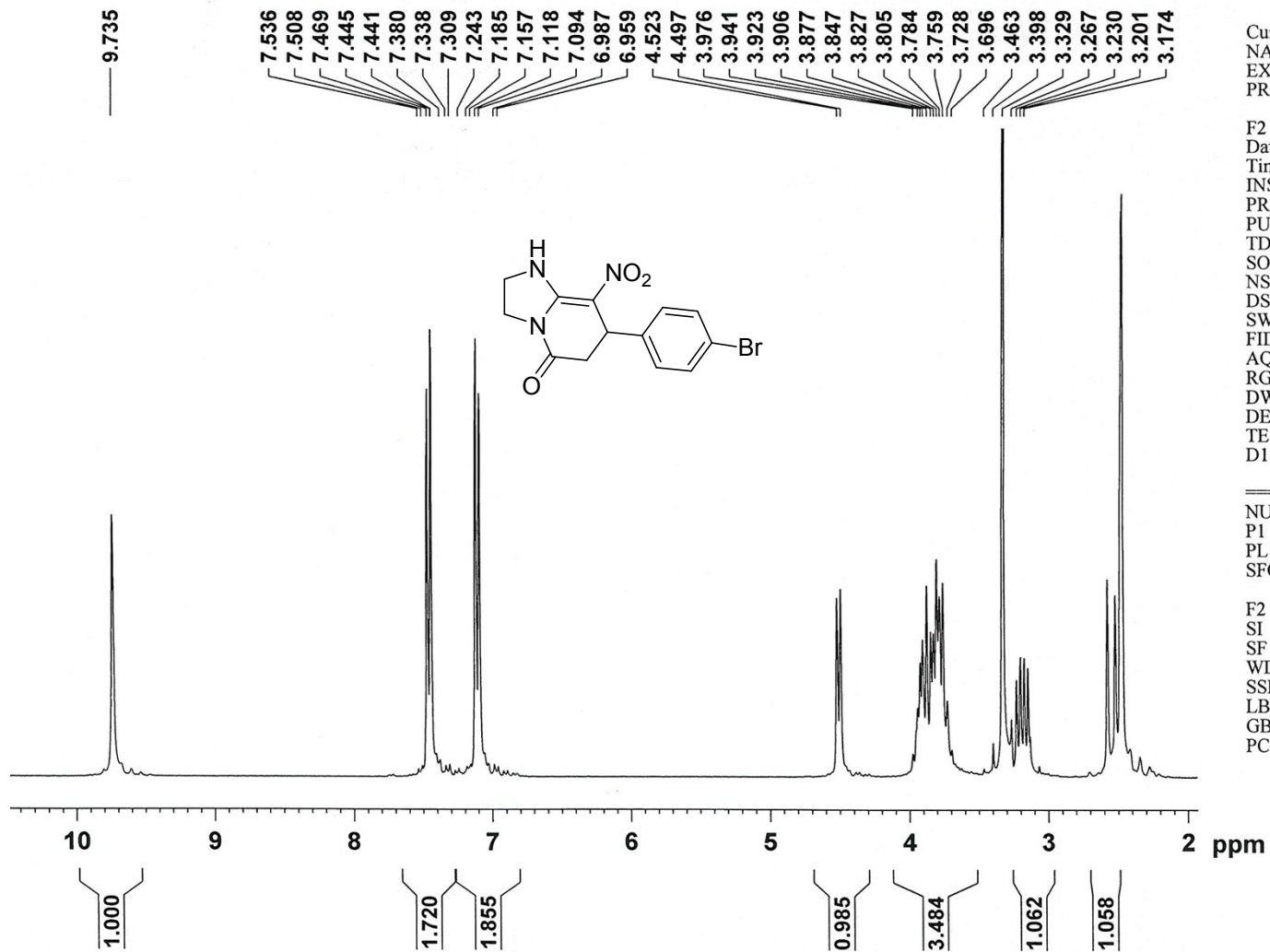
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IR of 5a



Mass of 5a



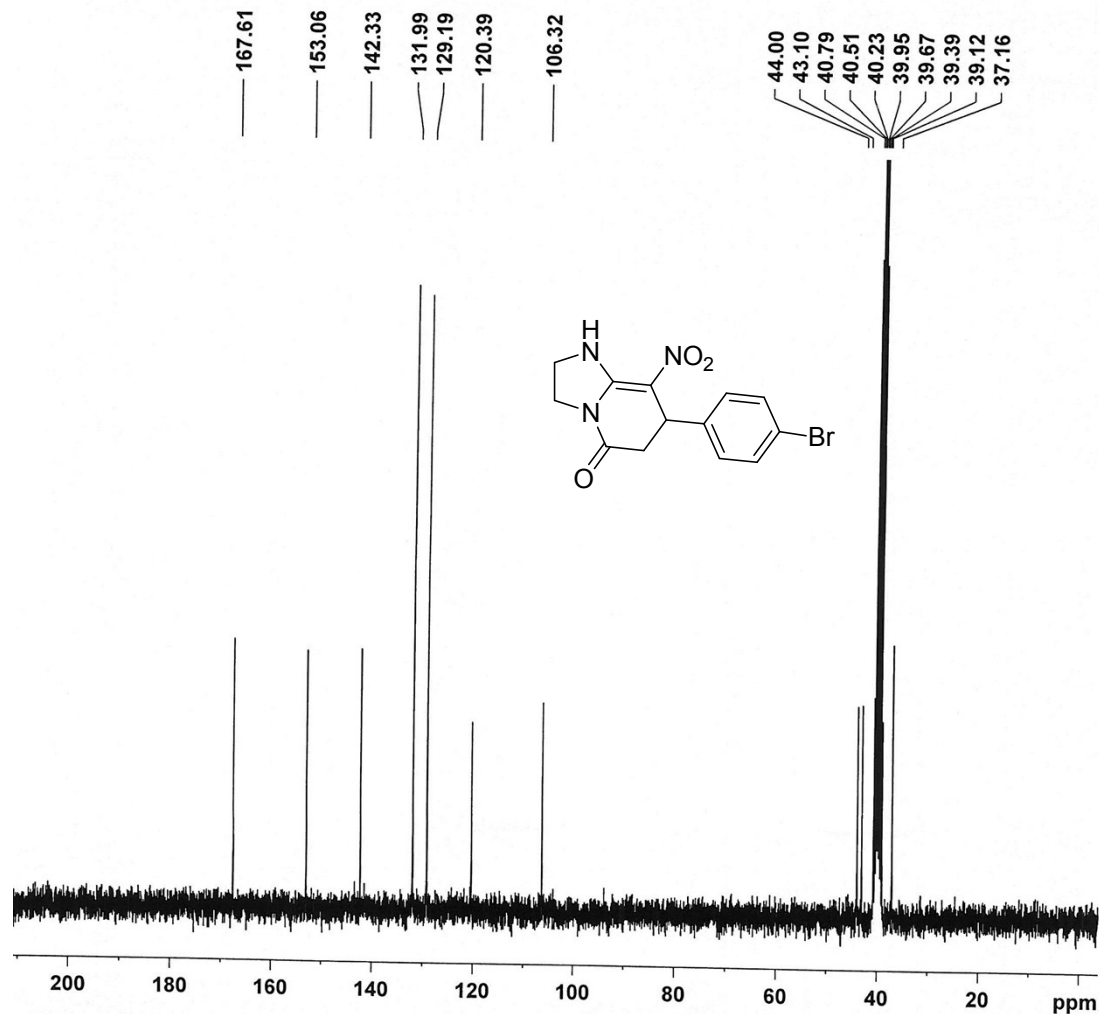
¹H NMR of 5b

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 SOLVENT DMSO
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 DS 0
 SWH 5995.204 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 128
 DW 83.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 6.00000000 sec

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 SFO1 299.8729987 MHz

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 ^{13}C NMR of 5b

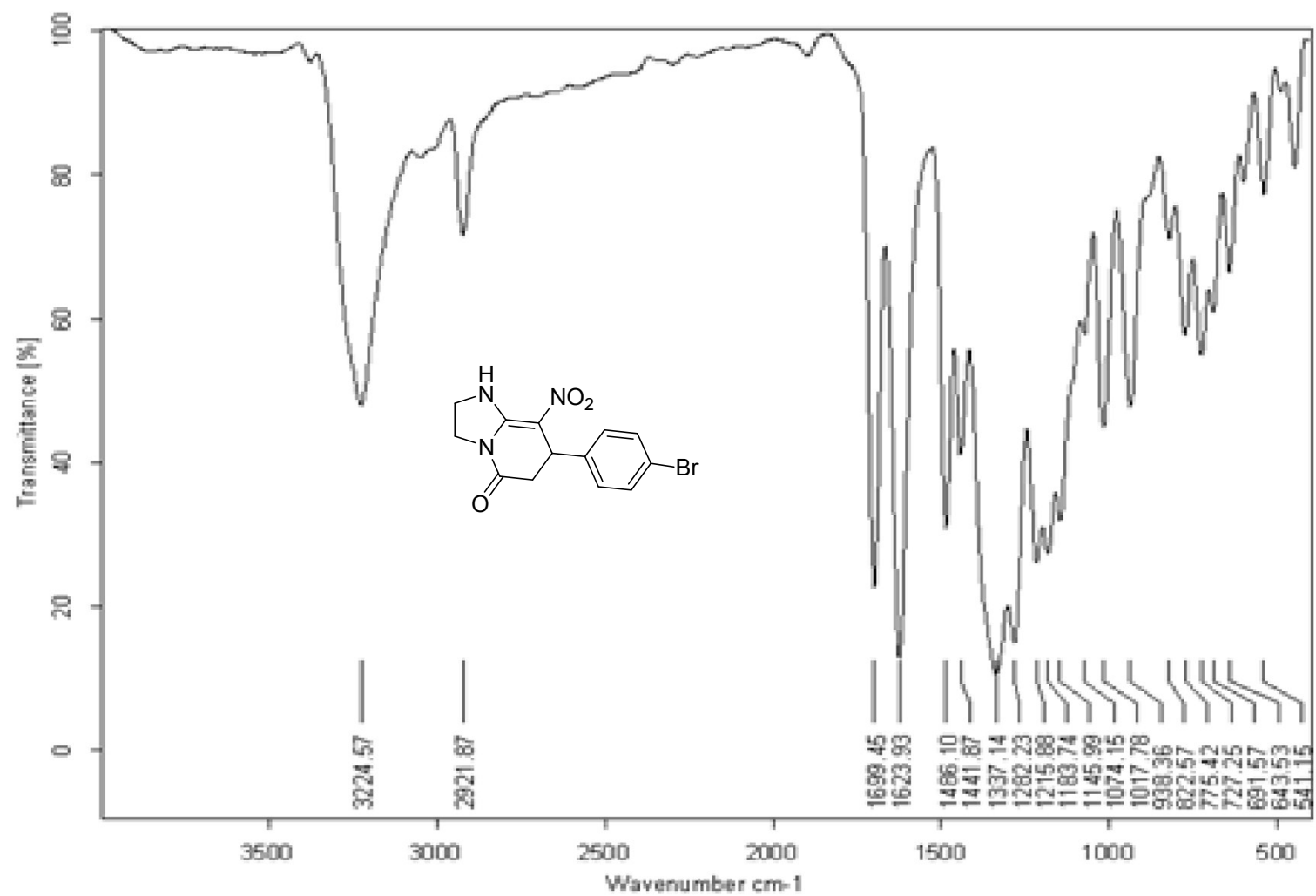
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 FIDRES 0.274439 Hz
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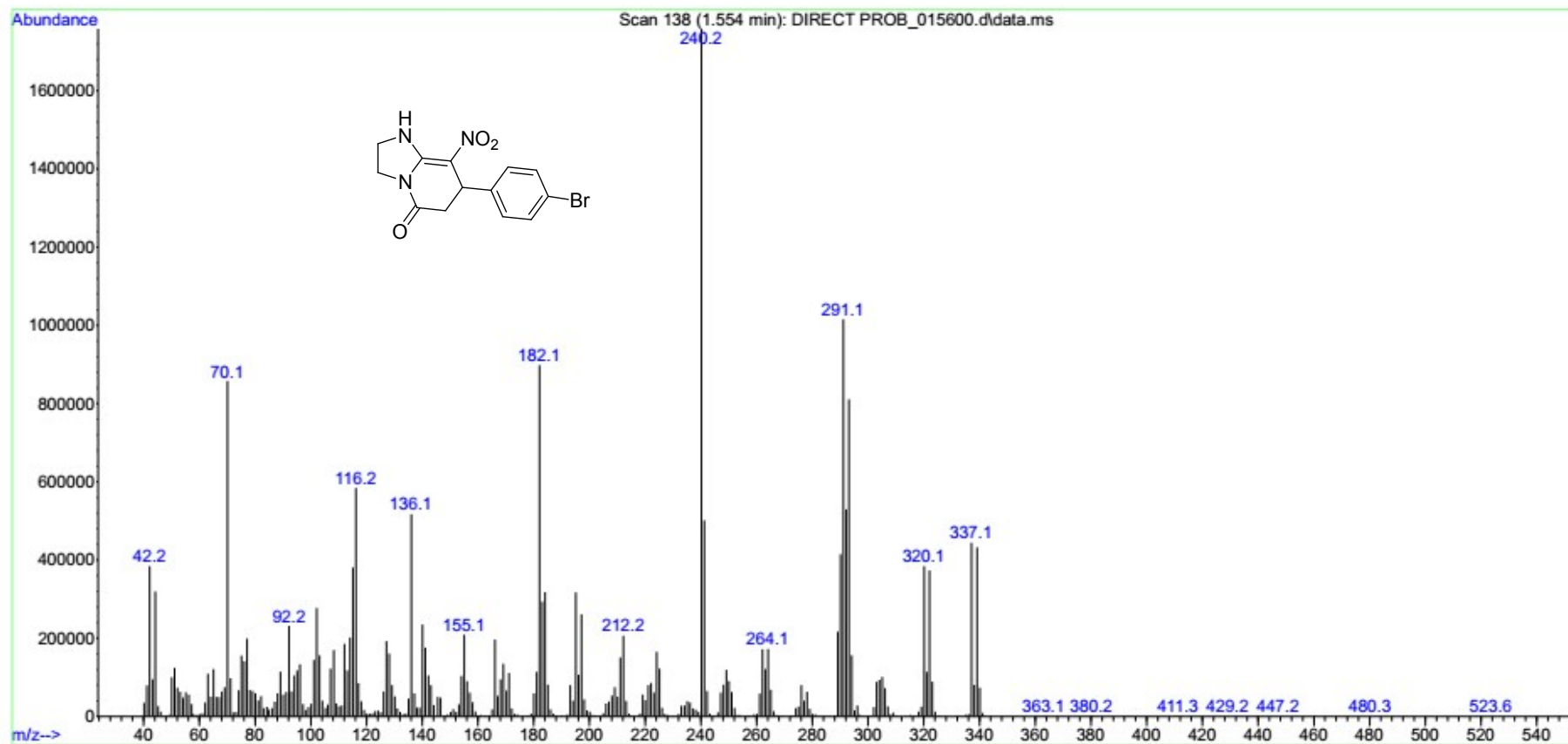
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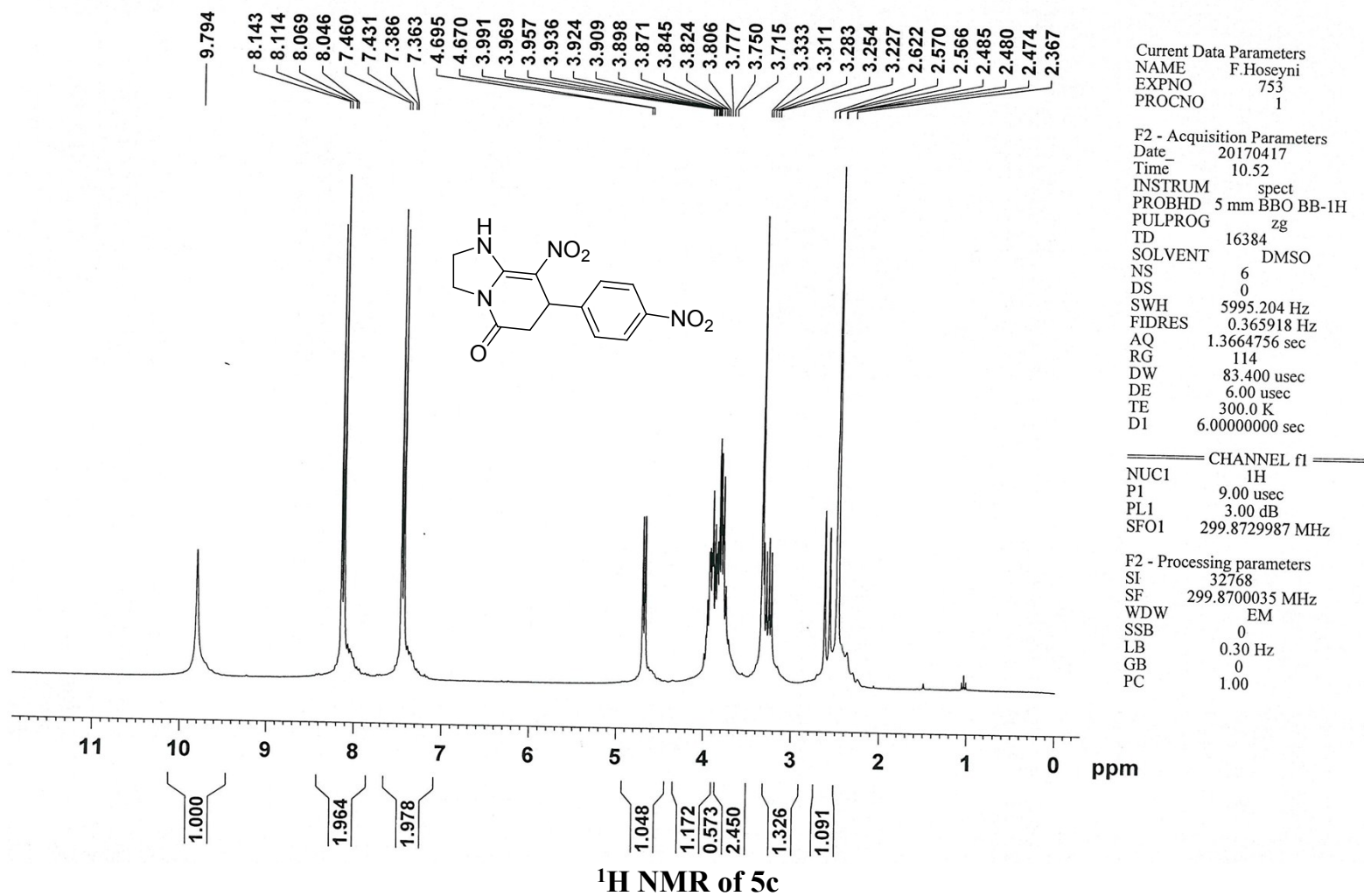
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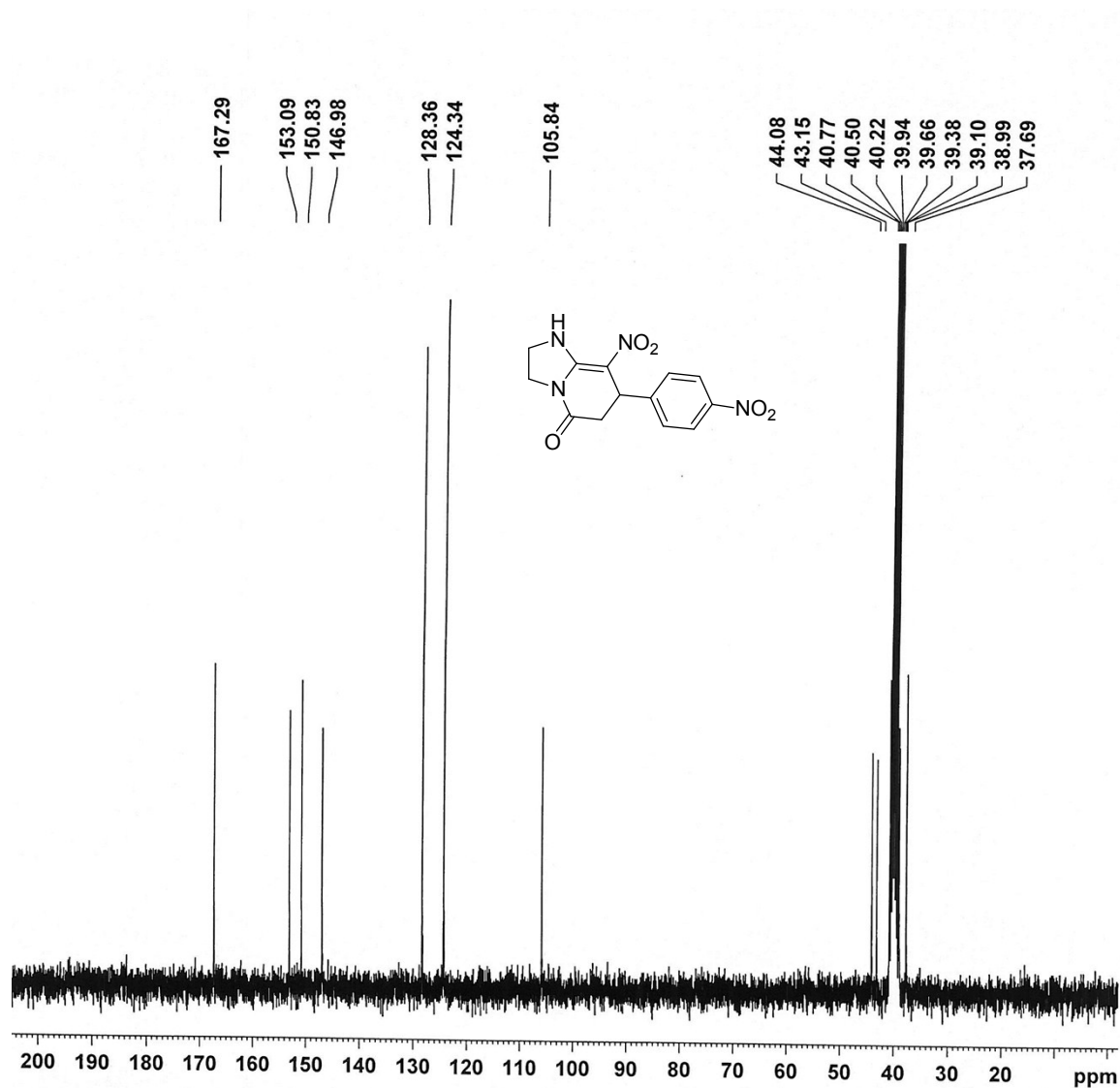


IR of 5b



Mass of 5b



¹³C NMR of 5c

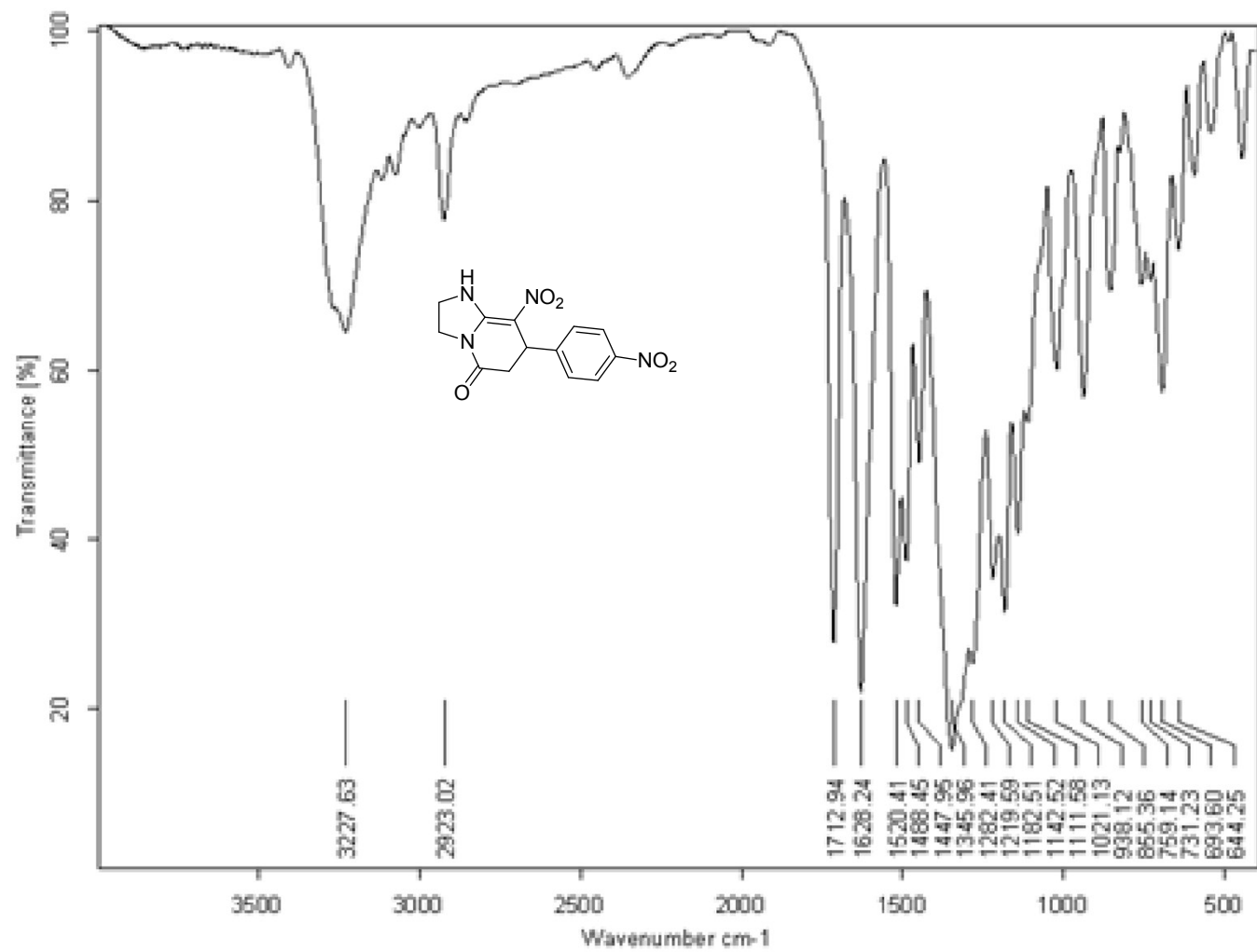
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 SOLVENT DMSO
 NS 250
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 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
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 d11 0.0300000 sec
 d12 0.0000200 sec

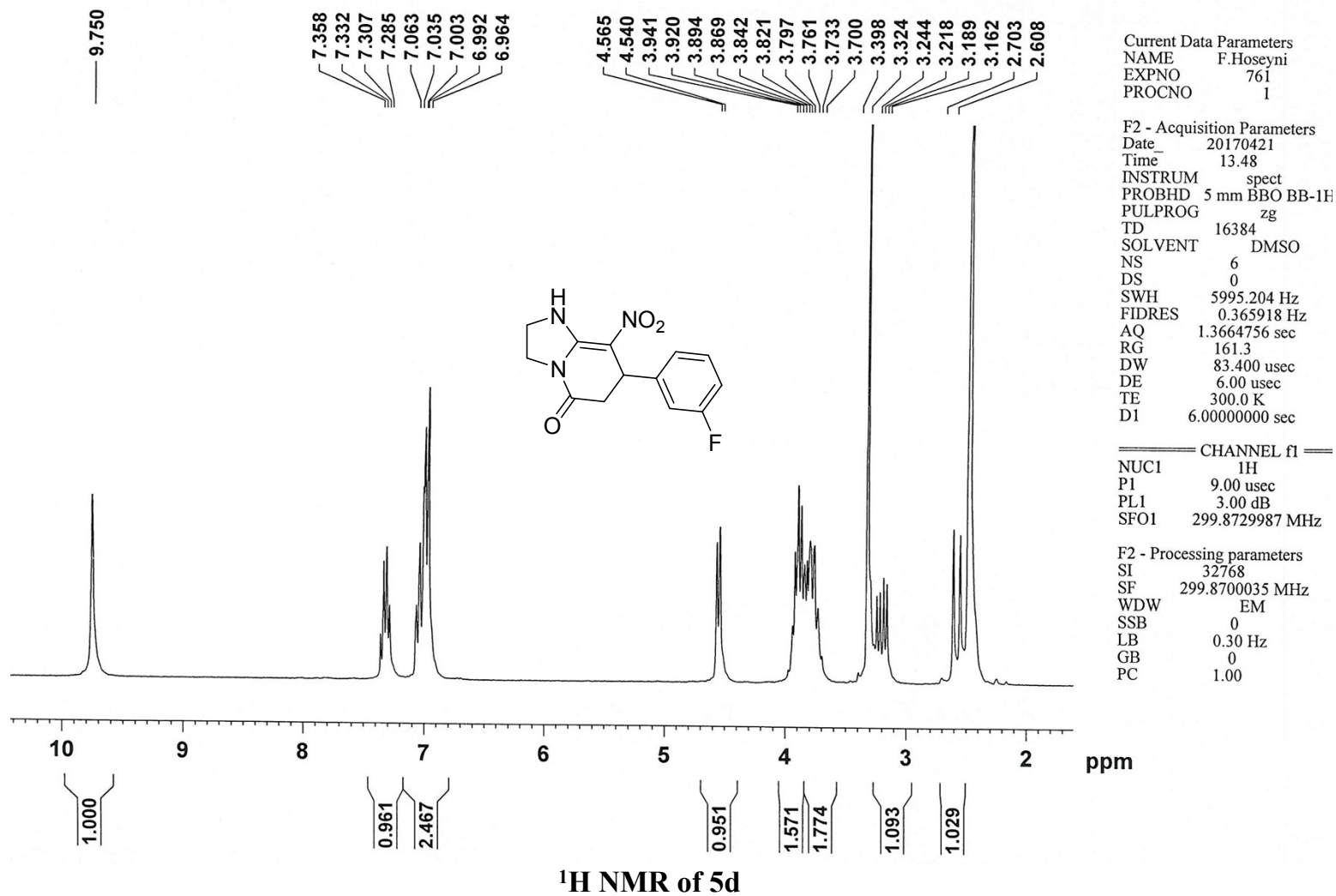
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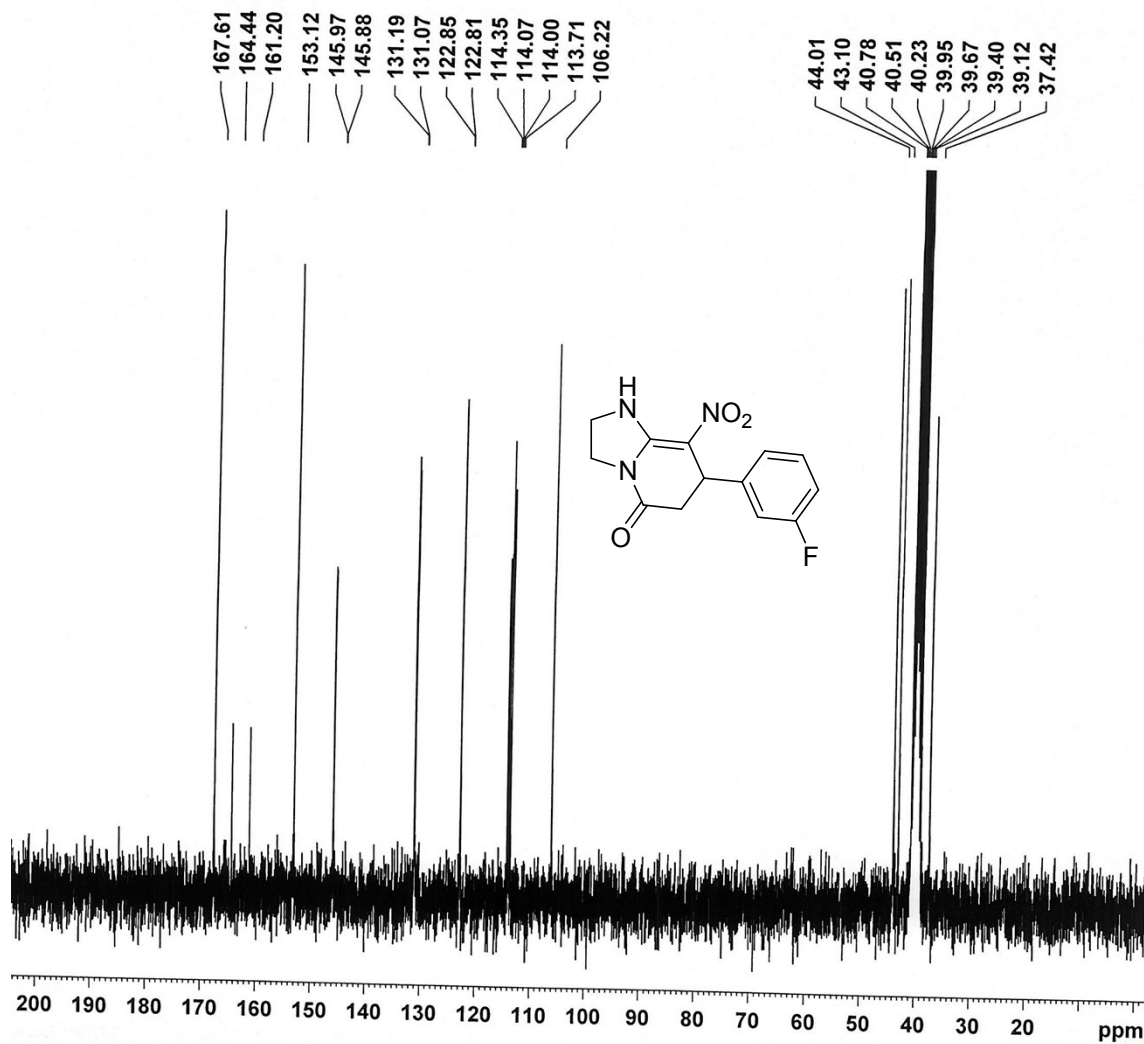
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F2 - Processing parameters
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 WDW EM
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 LB 1.00 Hz
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IR of 5c





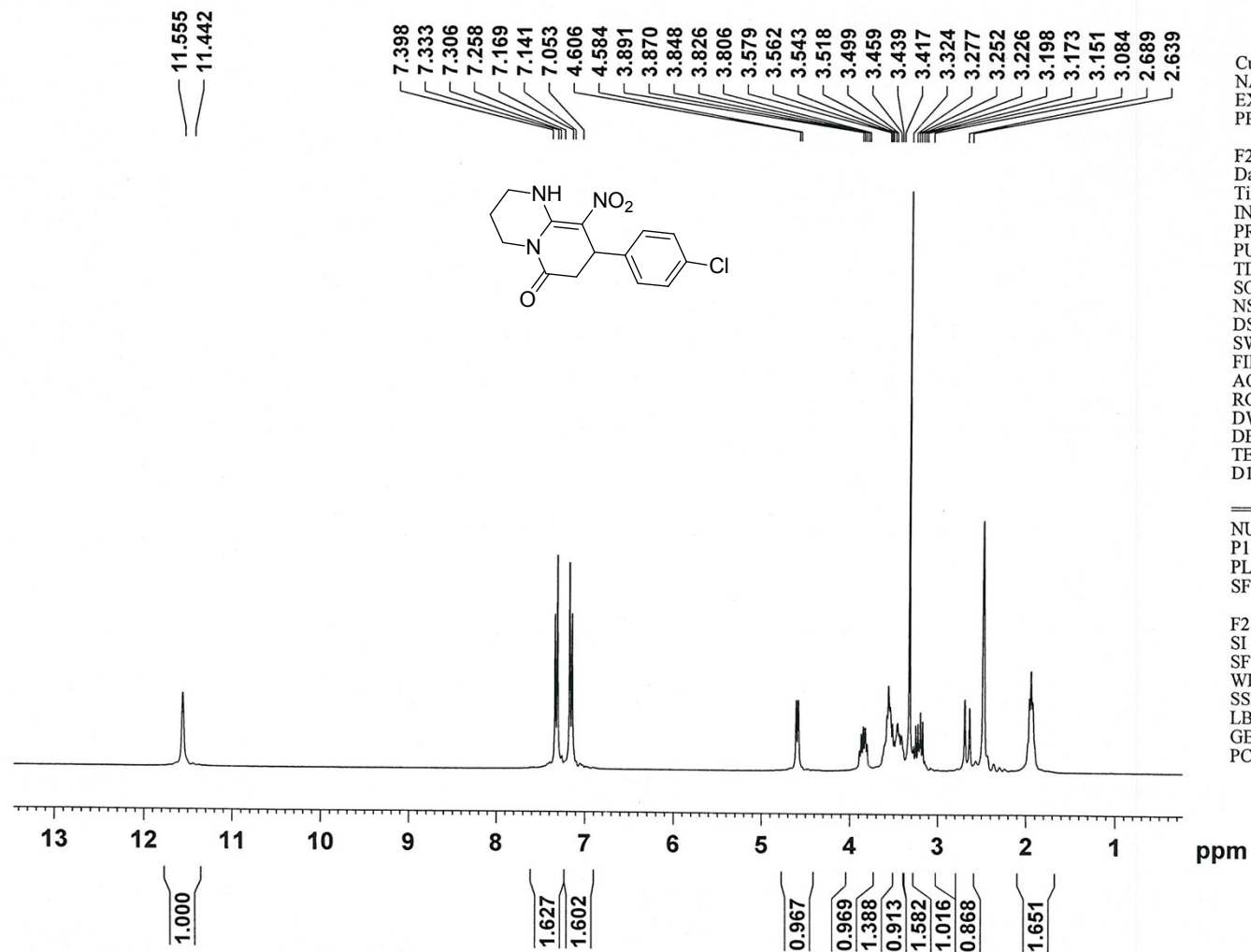
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 d11 0.0300000 sec
 d12 0.0000200 sec

==== CHANNEL f1 =====
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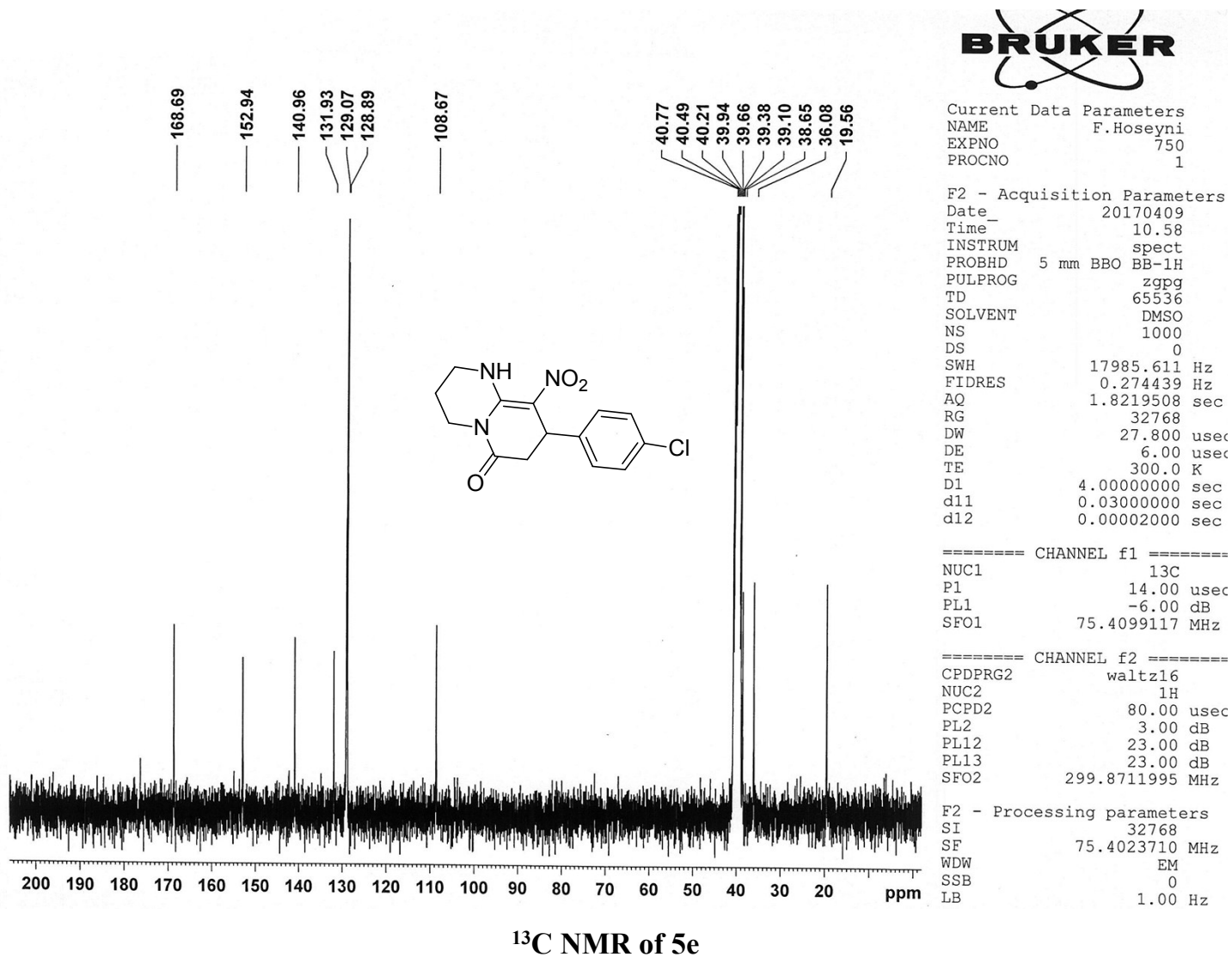
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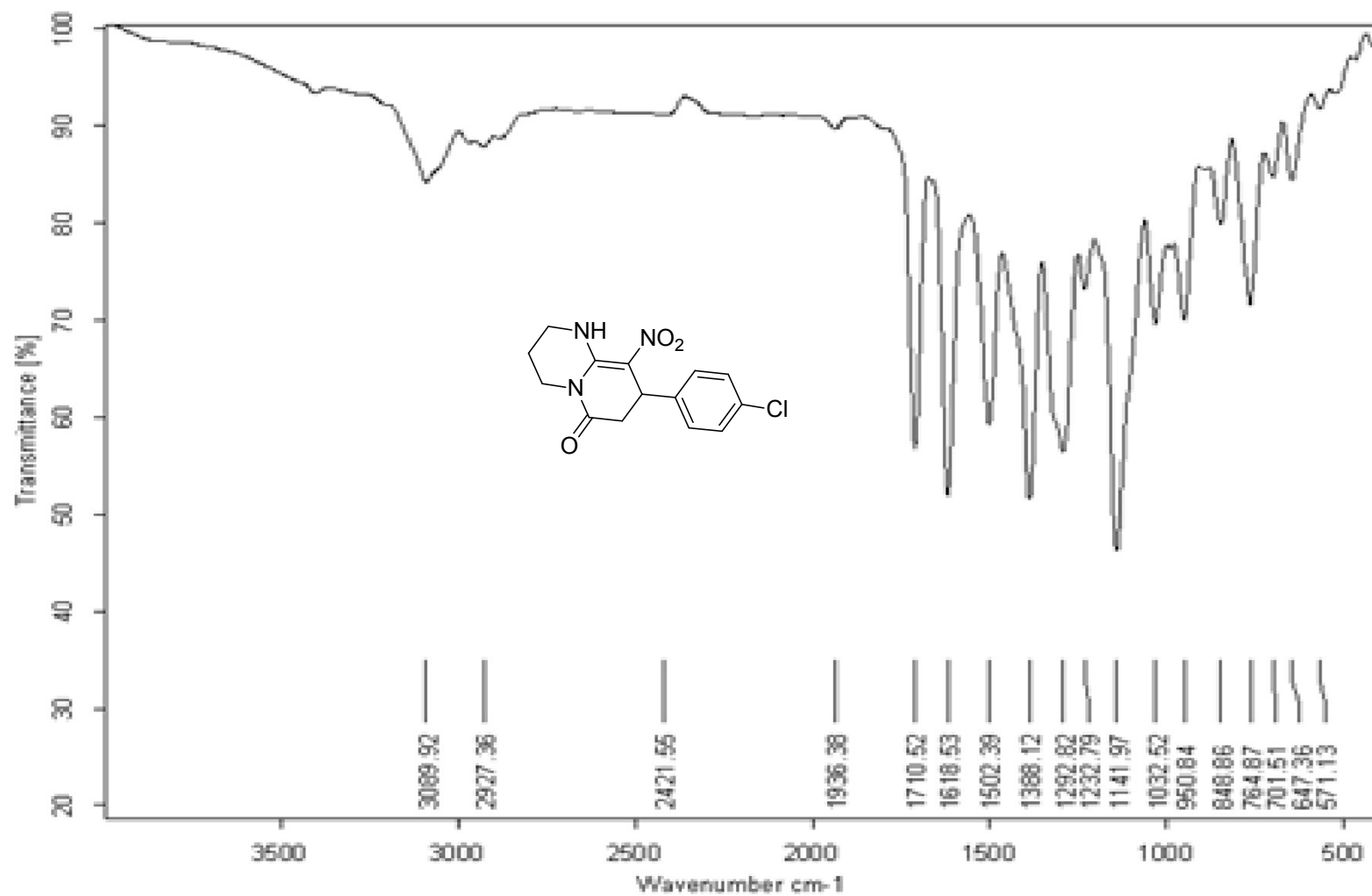
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 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 181
 DW 83.400 usec
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CHANNEL f1
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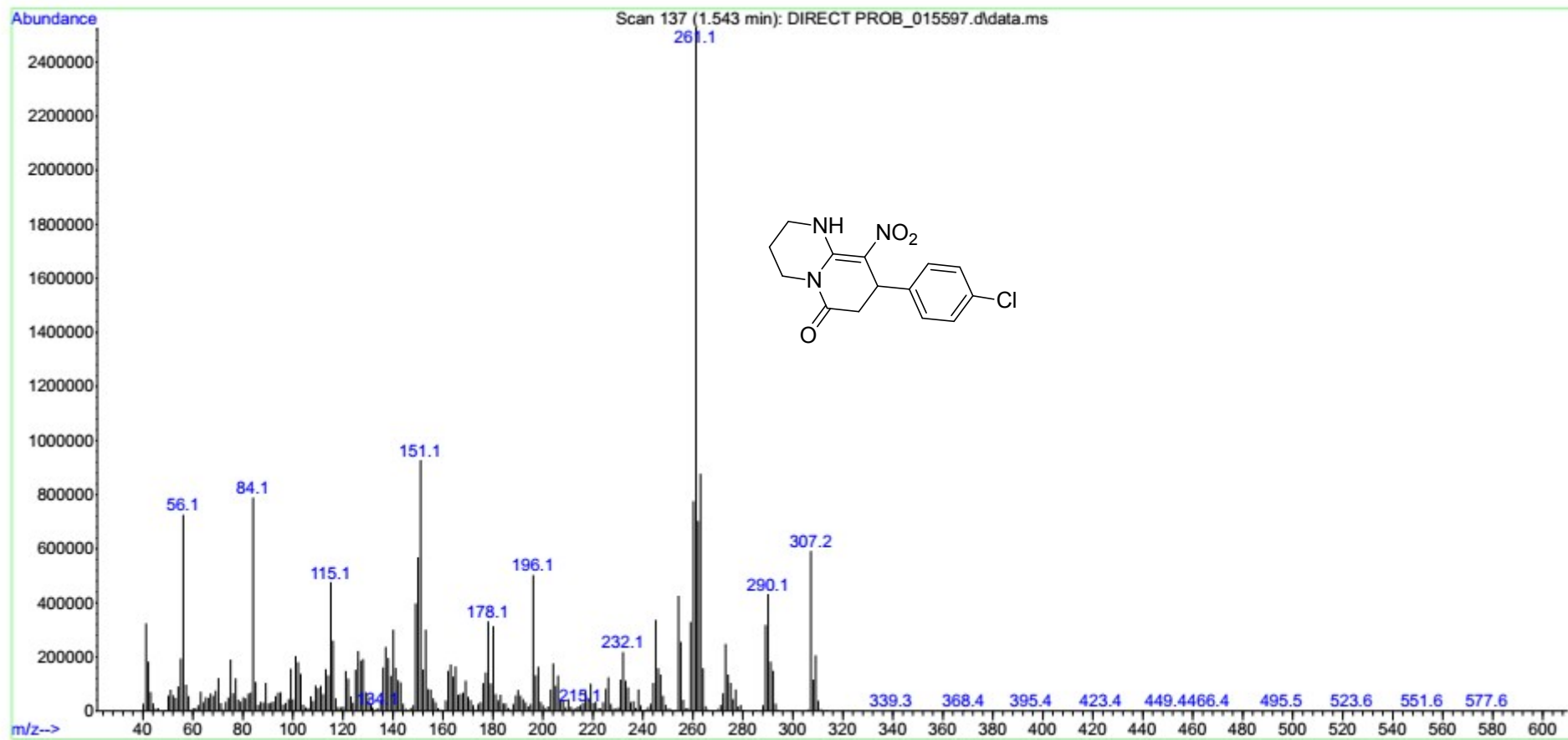
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¹H NMR of 5e

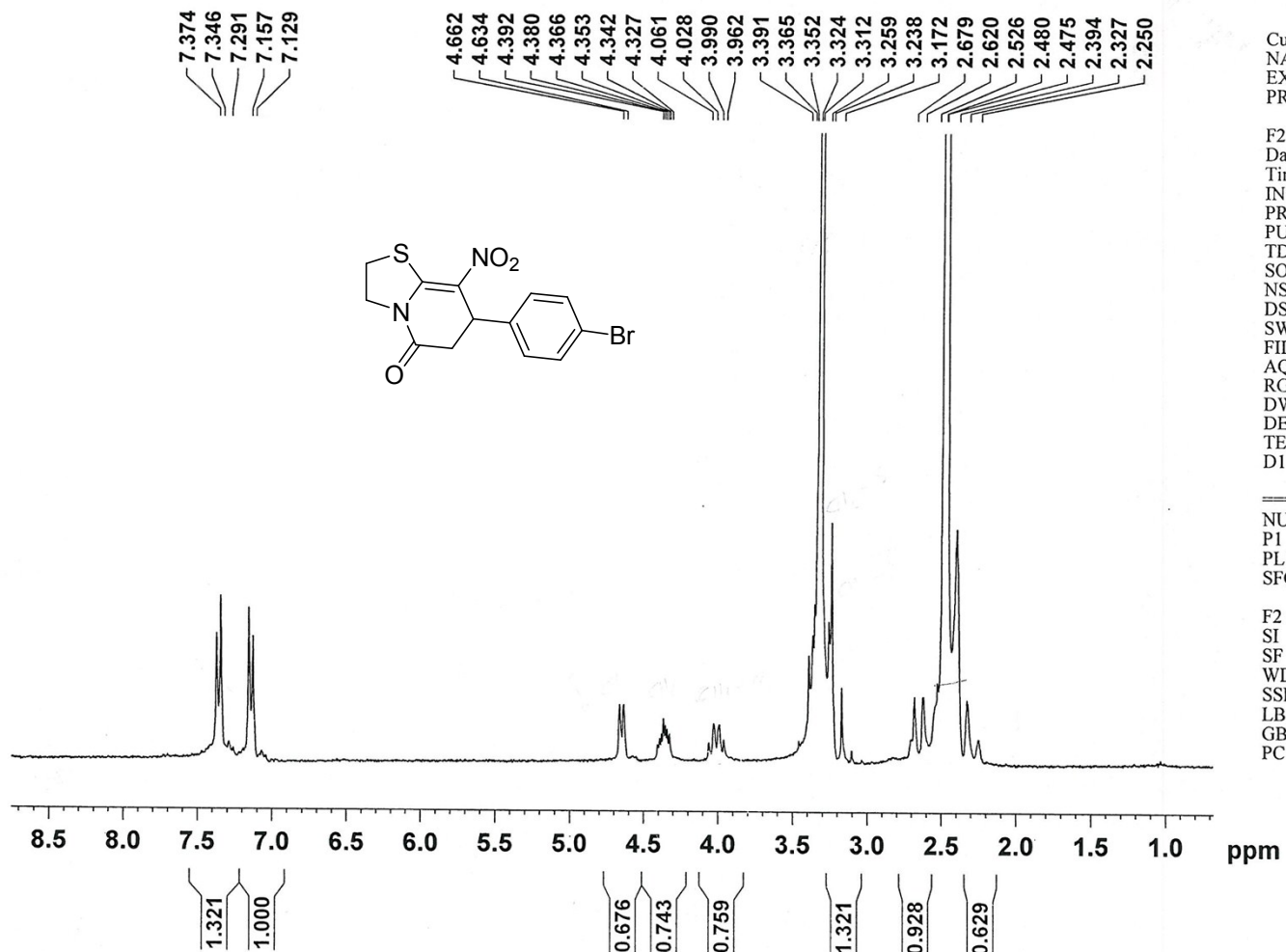




IR of 5e



Mass of 5e



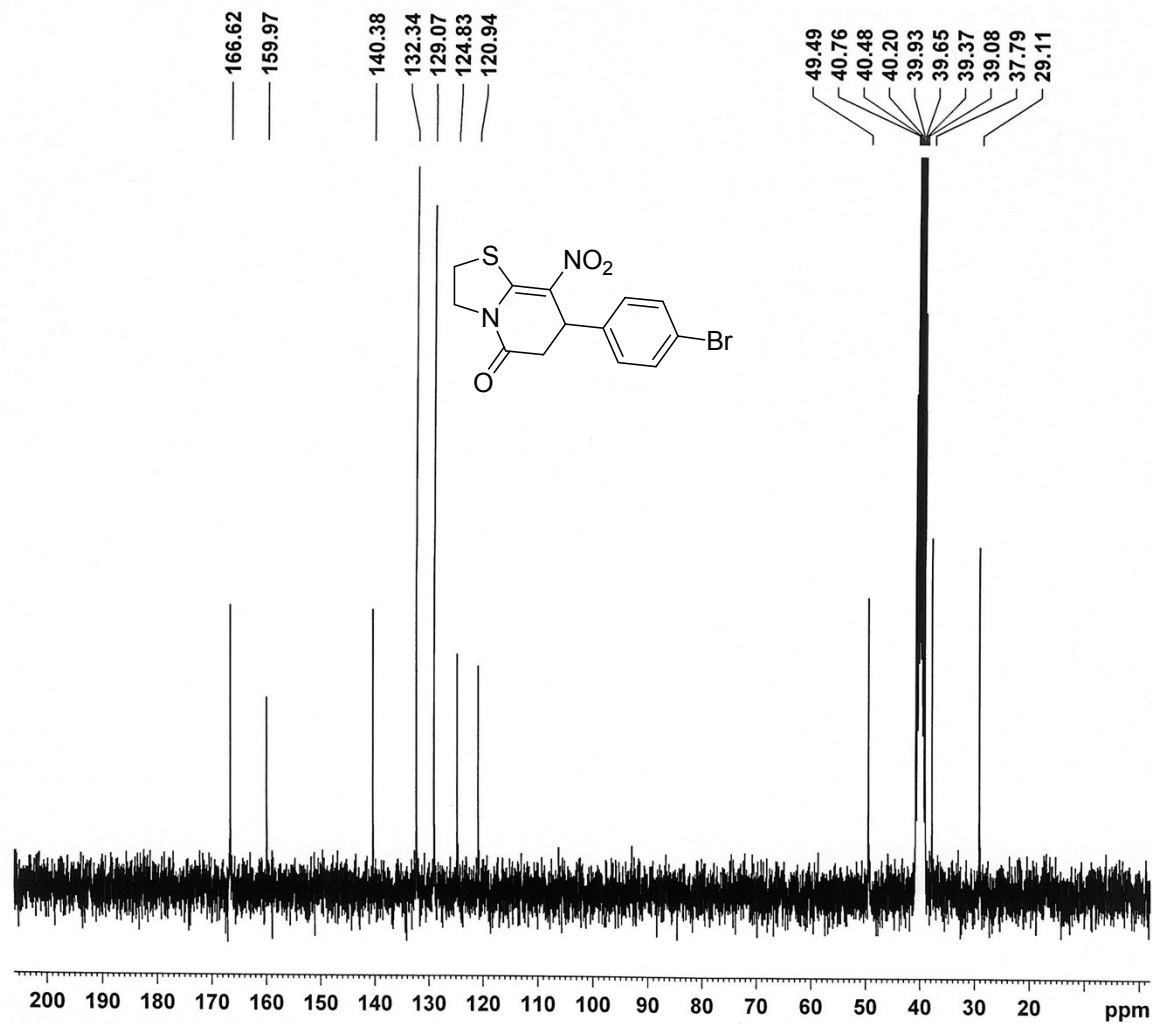
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 D1 6.00000000 sec

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F2 - Processing parameters
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¹H NMR of 5f

¹³C NMR of 5f

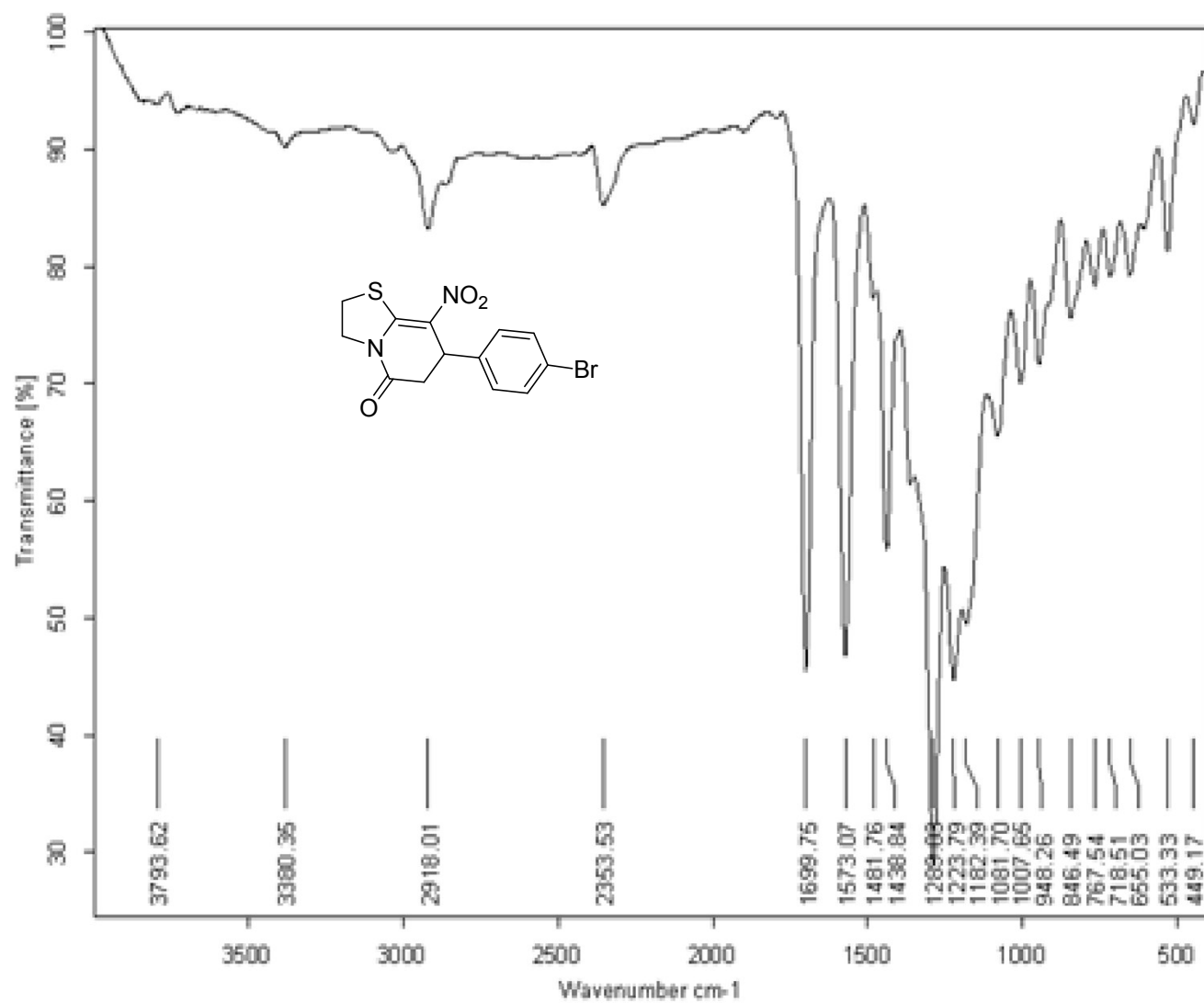
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 FIDRES 0.274439 Hz
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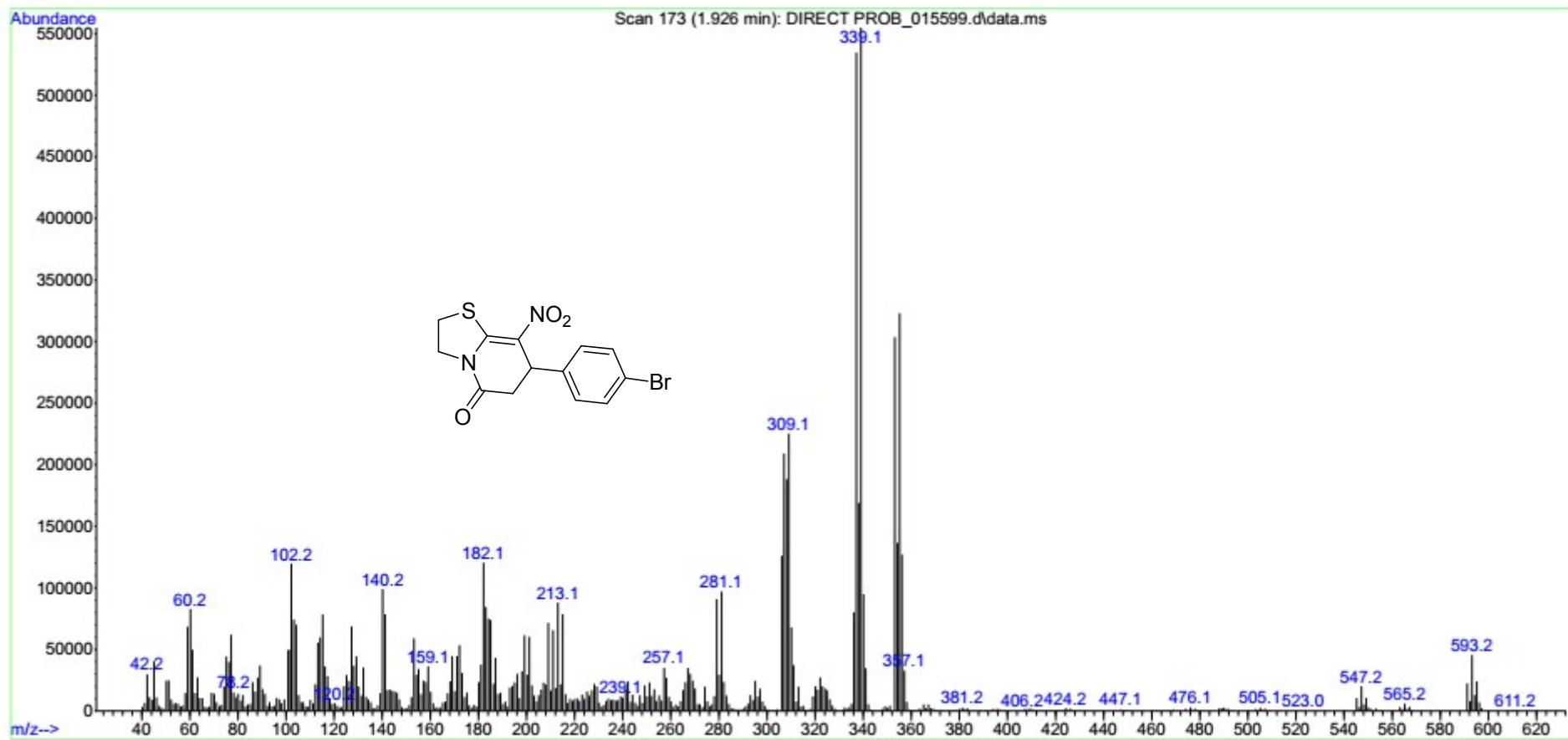
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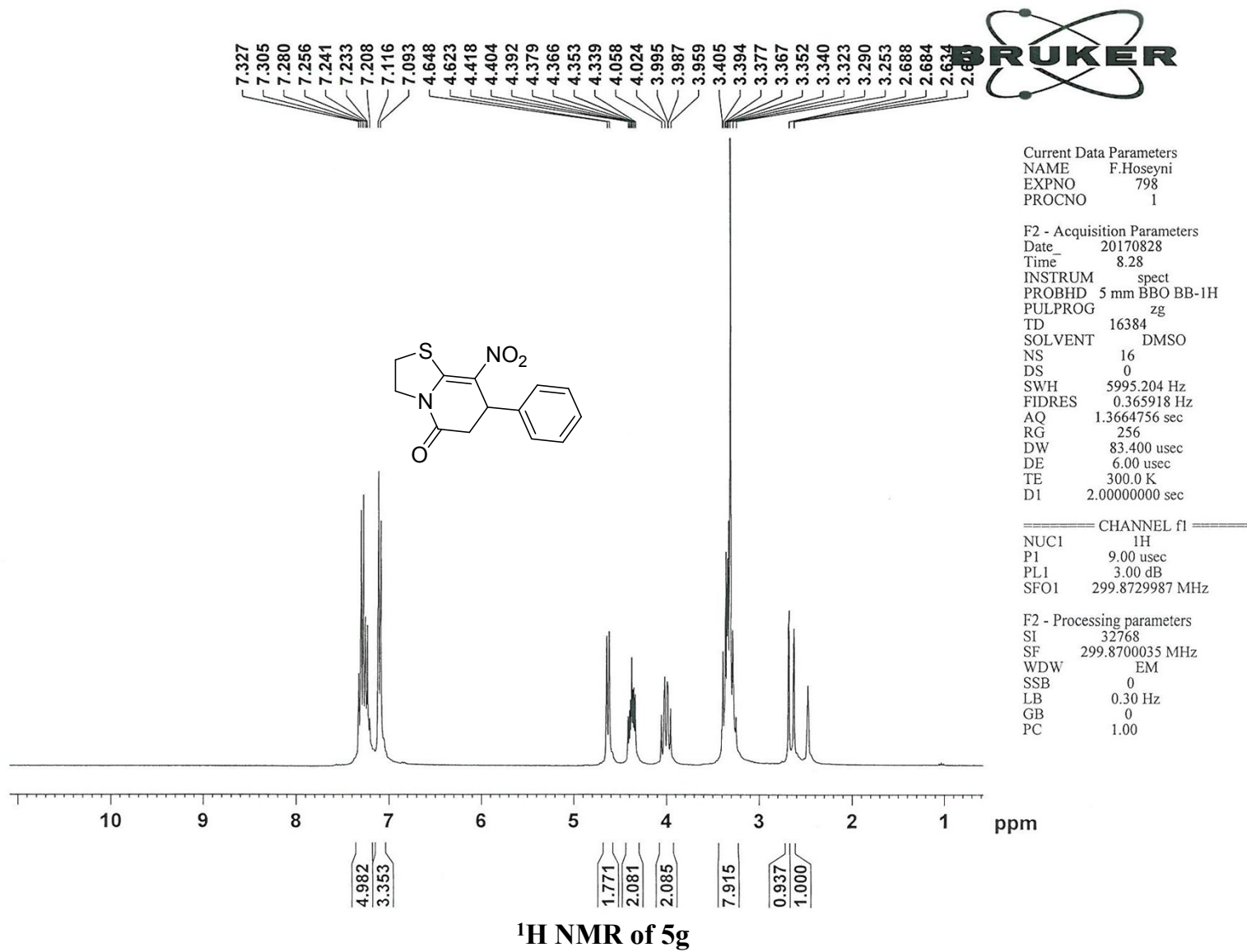
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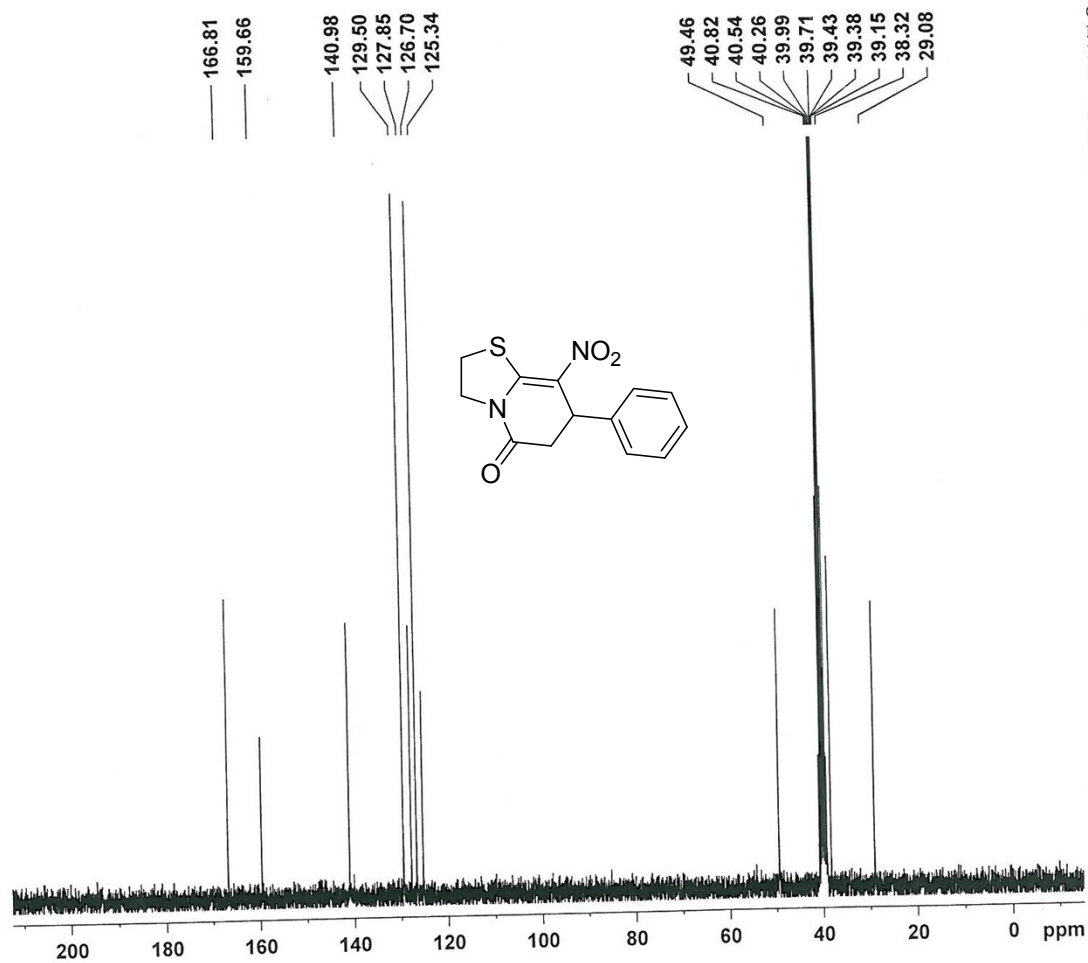
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IR of 5f





 ^{13}C NMR of 5g

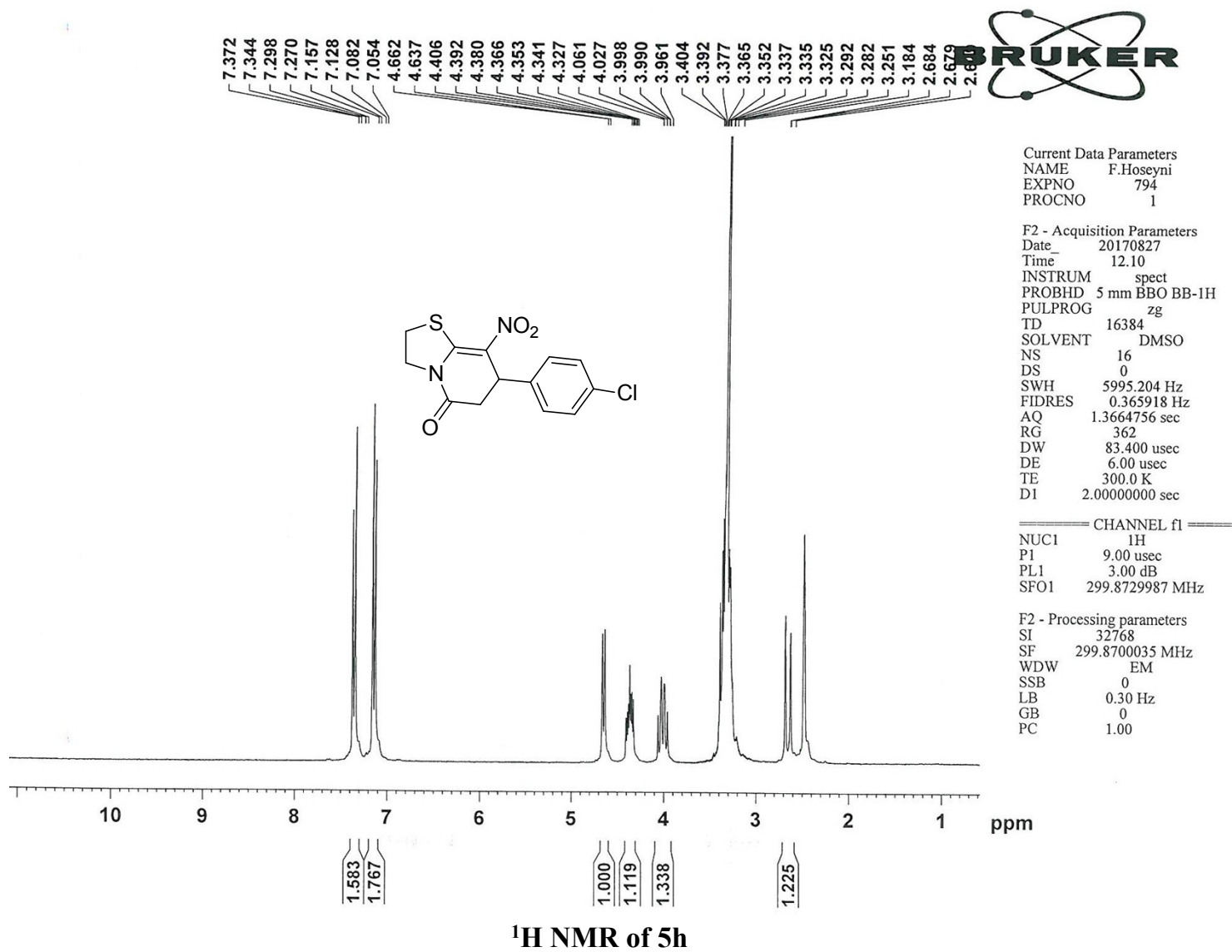
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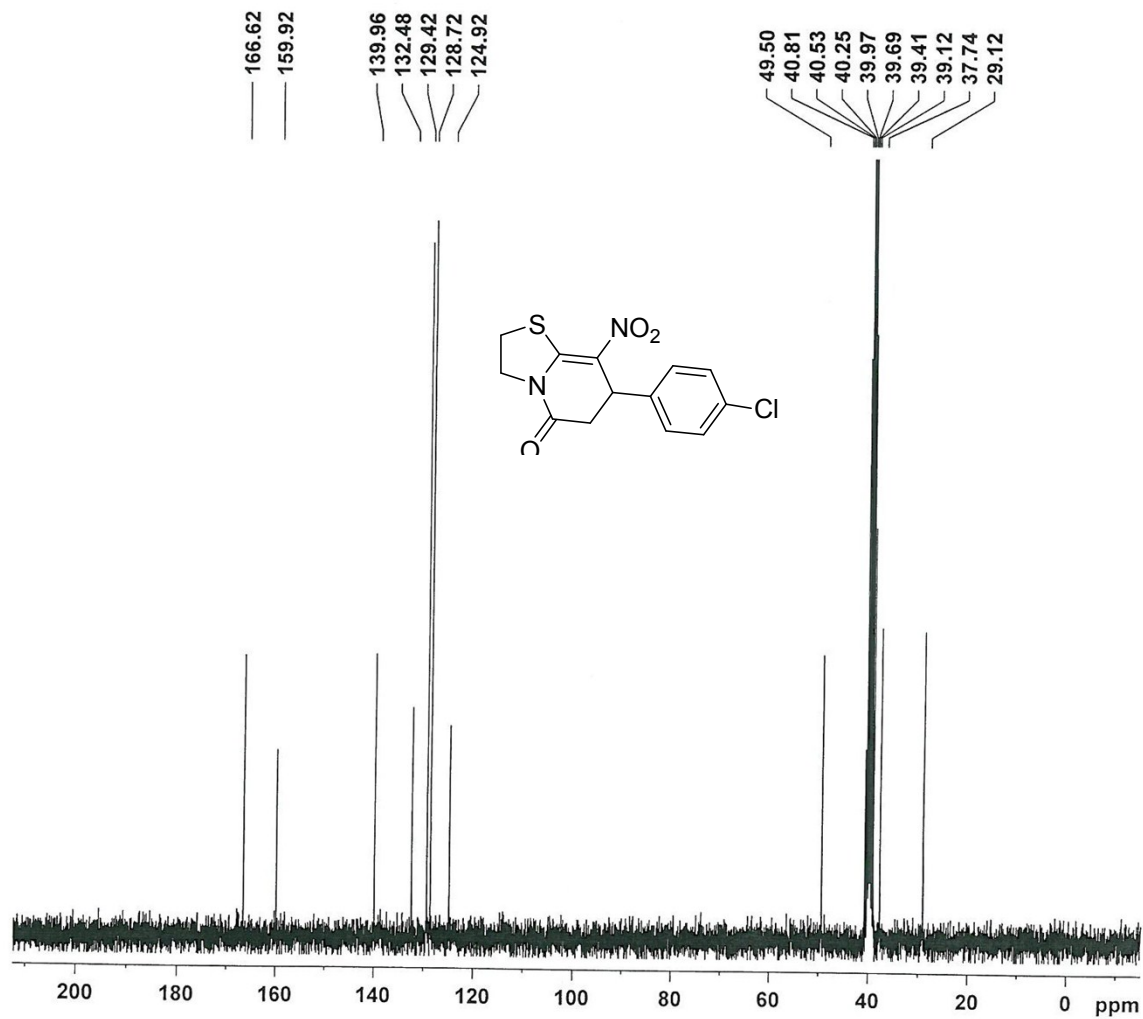
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 RG 32768
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 DE 6.00 usec
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===== CHANNEL f1 =====
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 SFO1 75.4099117 MHz

===== CHANNEL f2 =====
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 PCPD2 80.00 usec
 PL2 3.00 dB
 PL12 23.00 dB
 PL13 23.00 dB
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F2 - Processing parameters
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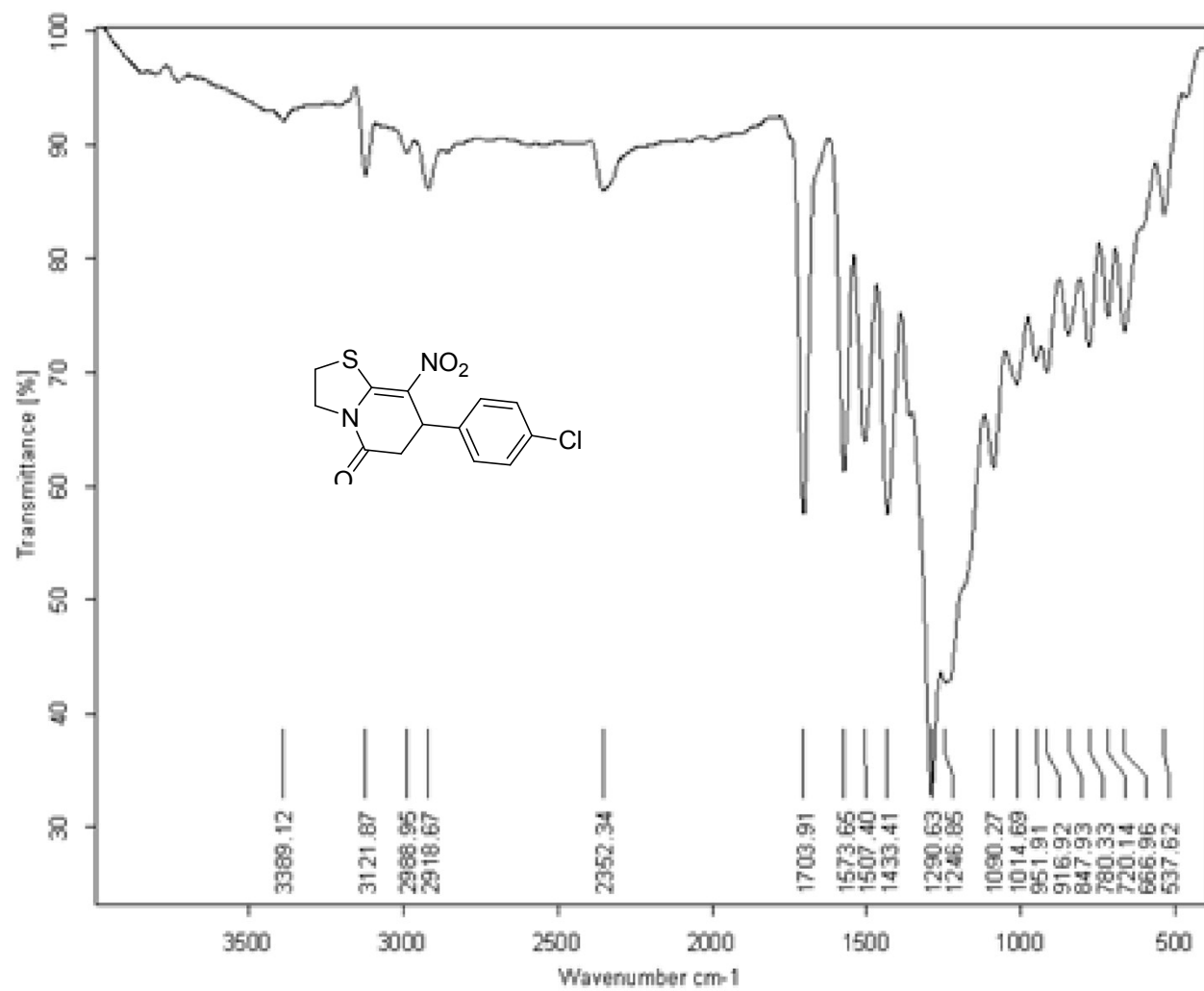
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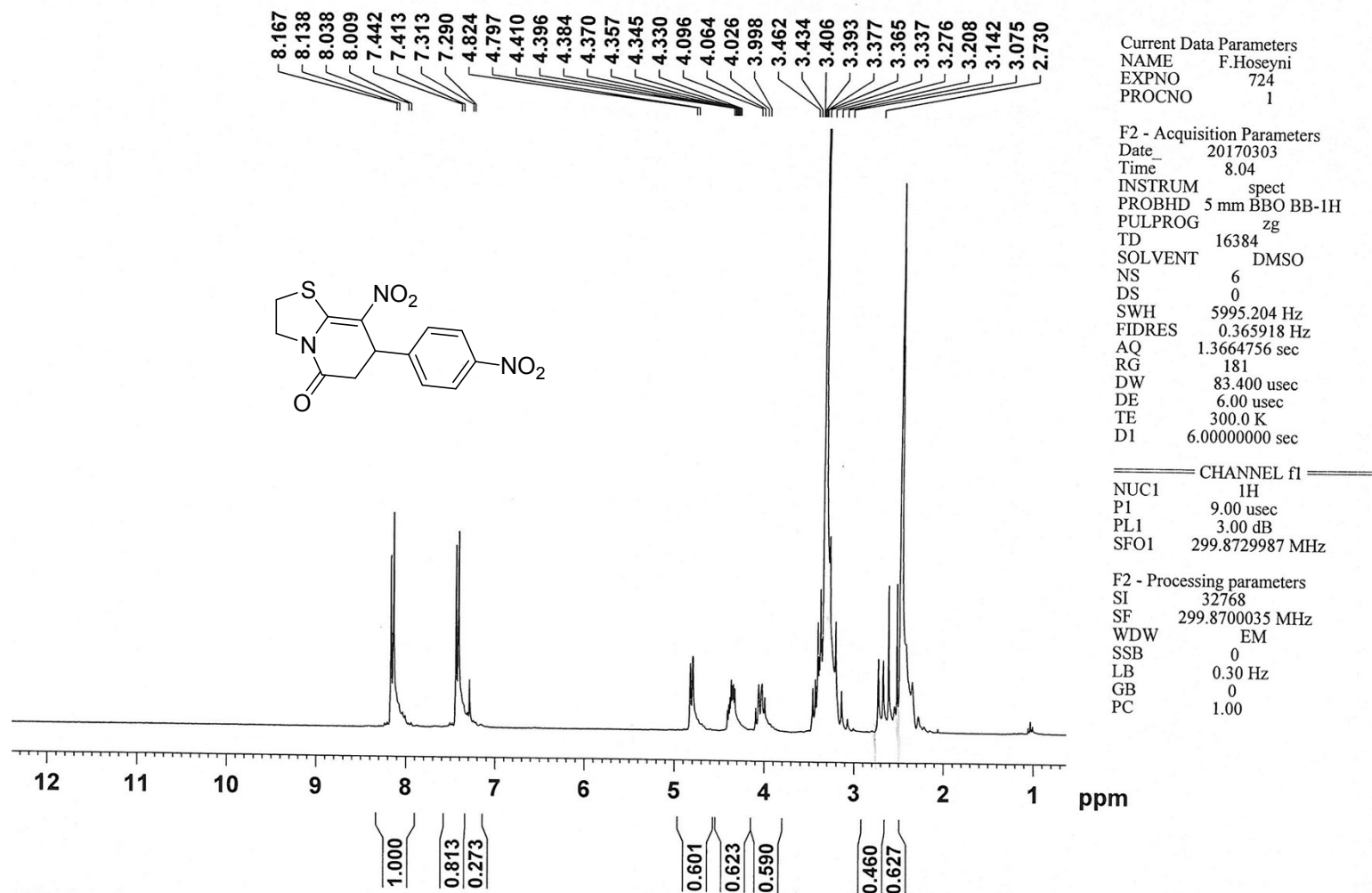
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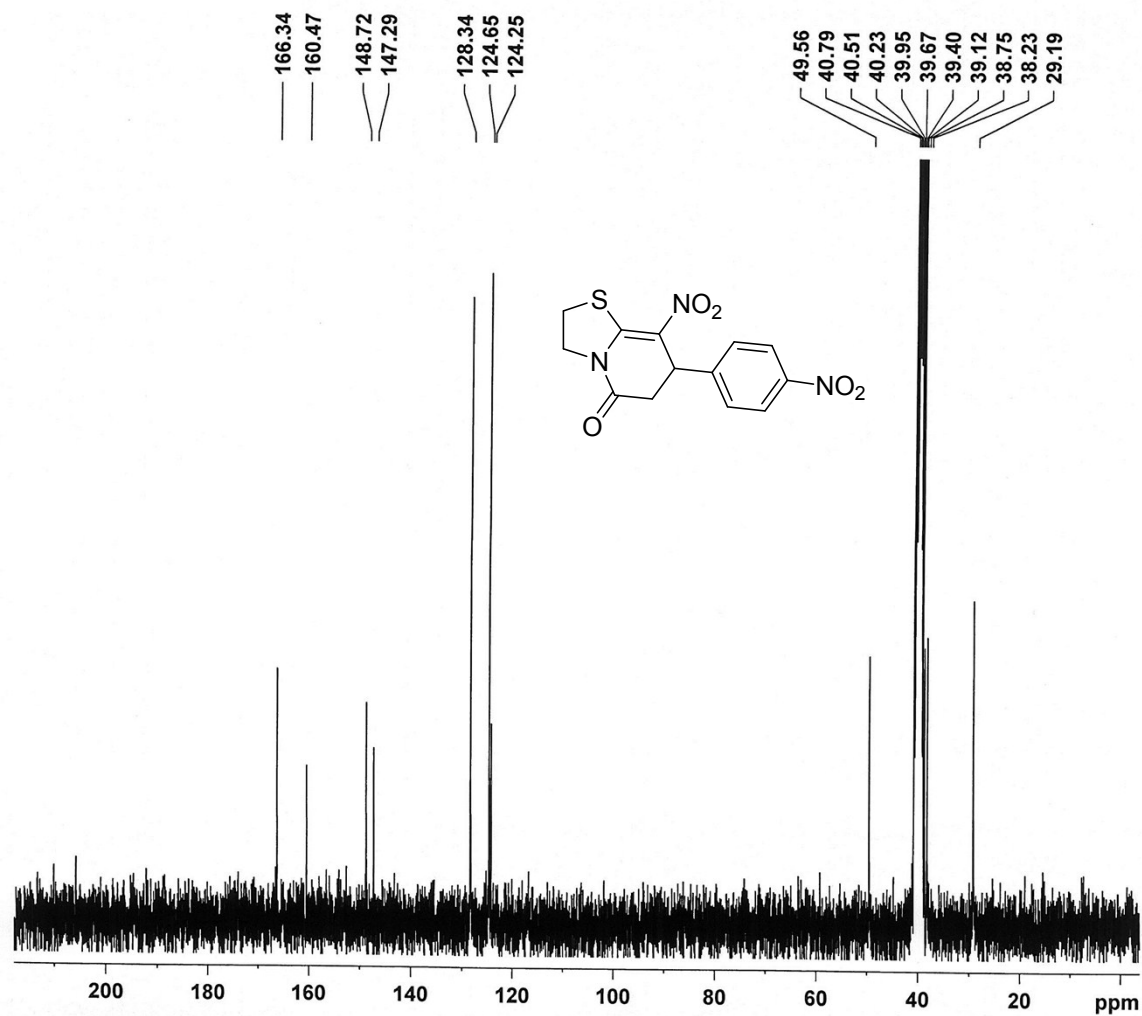
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 PL12 23.00 dB
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 SFO2 299.8711995 MHz

F2 - Processing parameters
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IR of 5h

¹H NMR of 5i



BRUKER

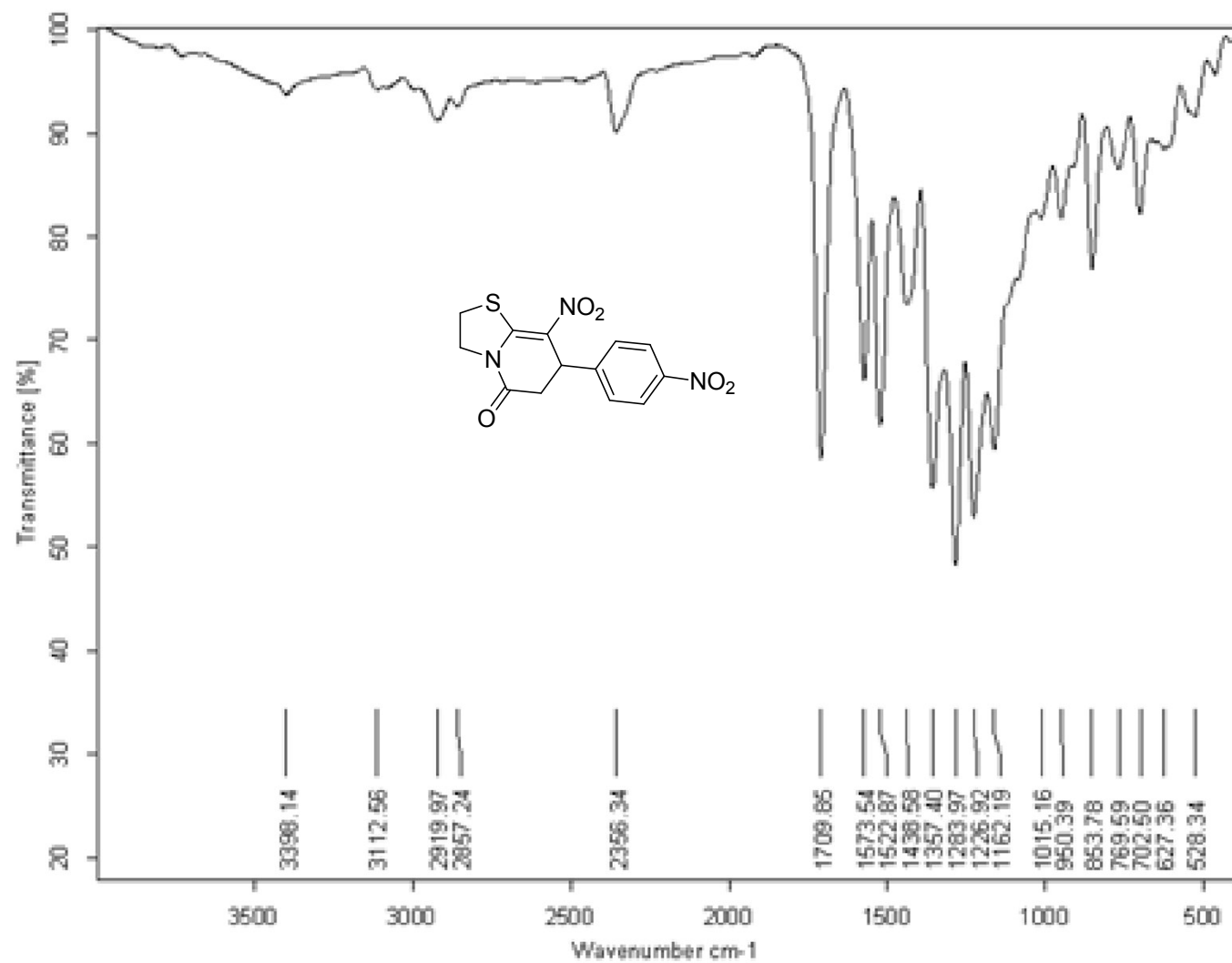
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FIDRES 0.274439 Hz
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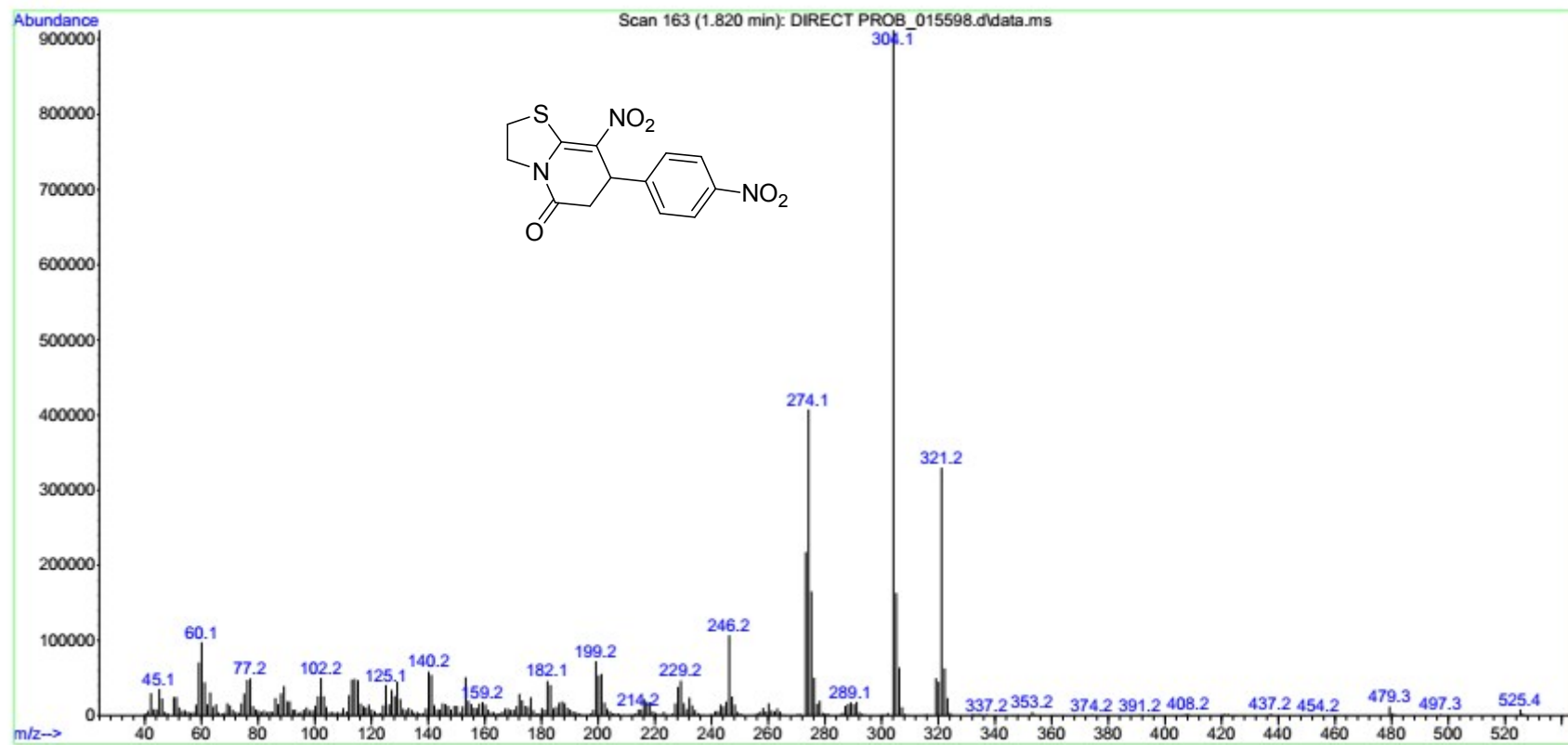
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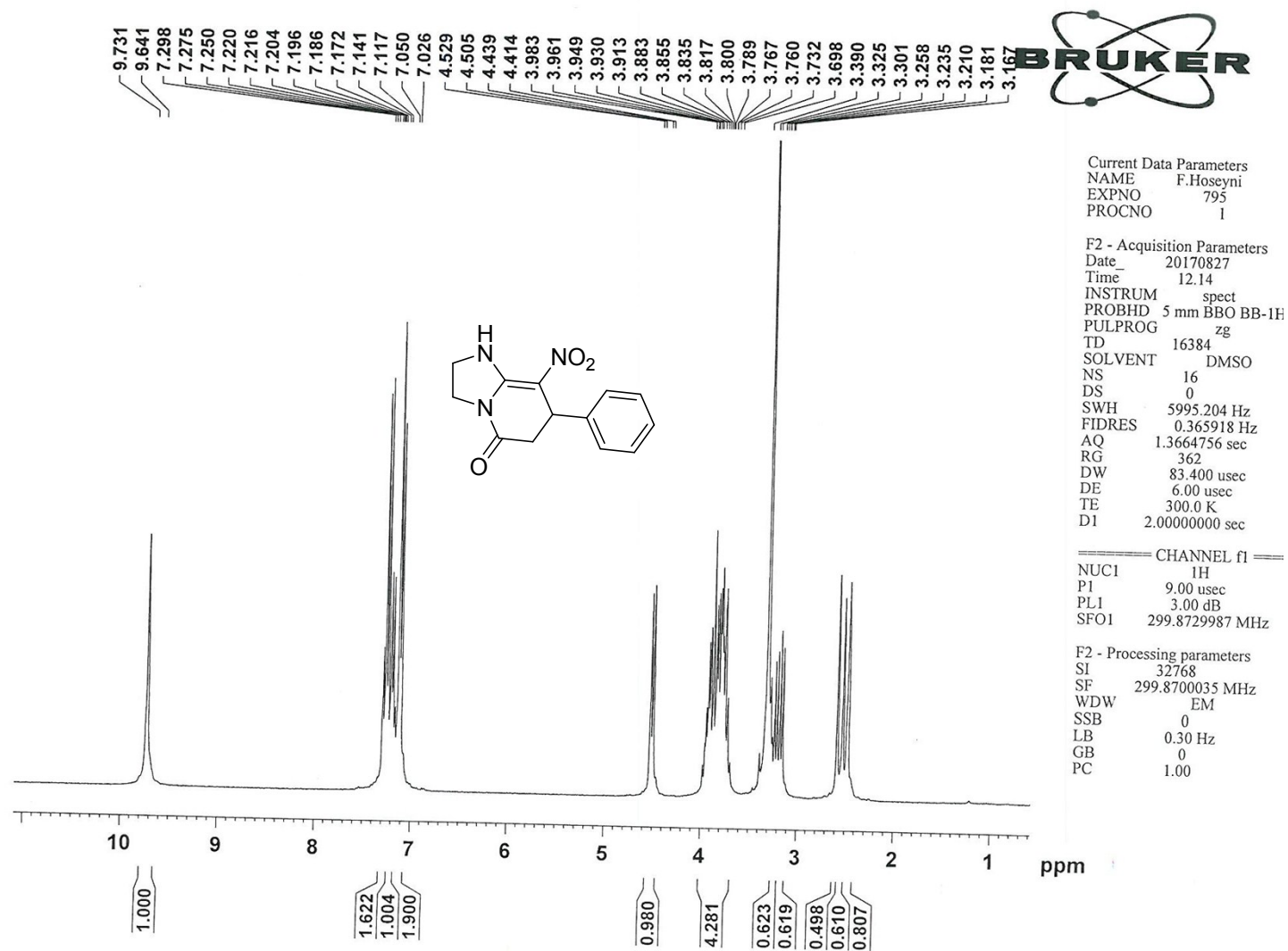
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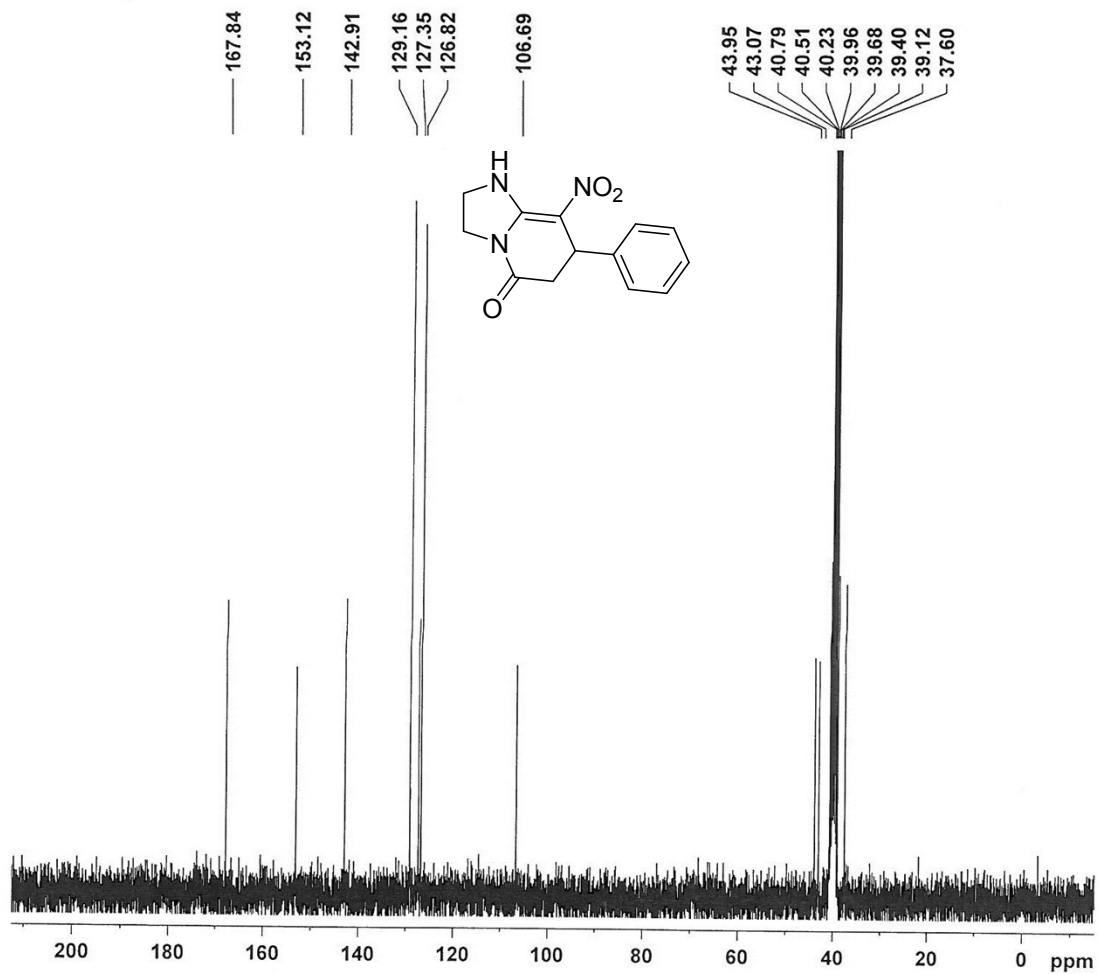


IR of 5i



Mass of 5i

¹H NMR of 5j

¹³C NMR of 5j

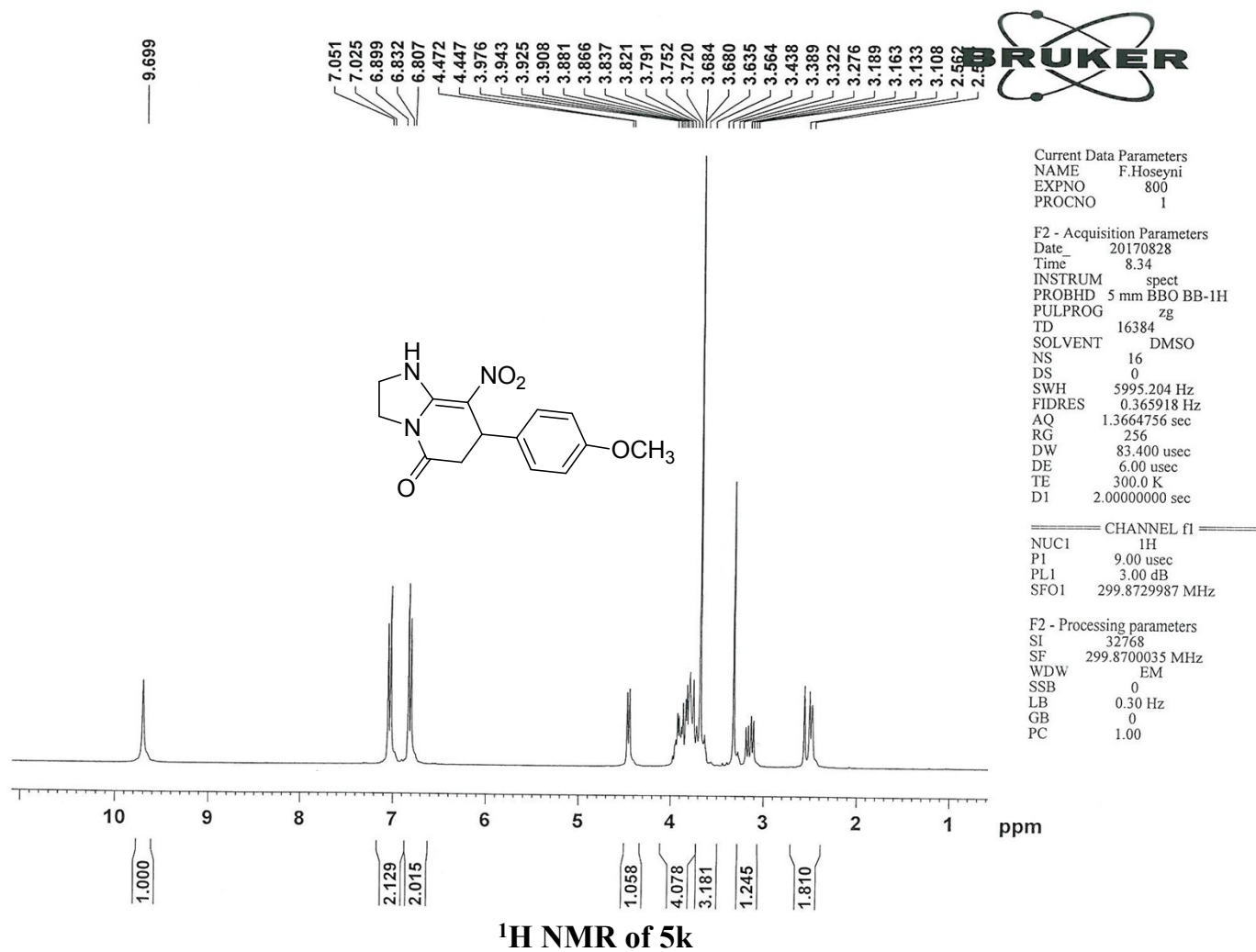
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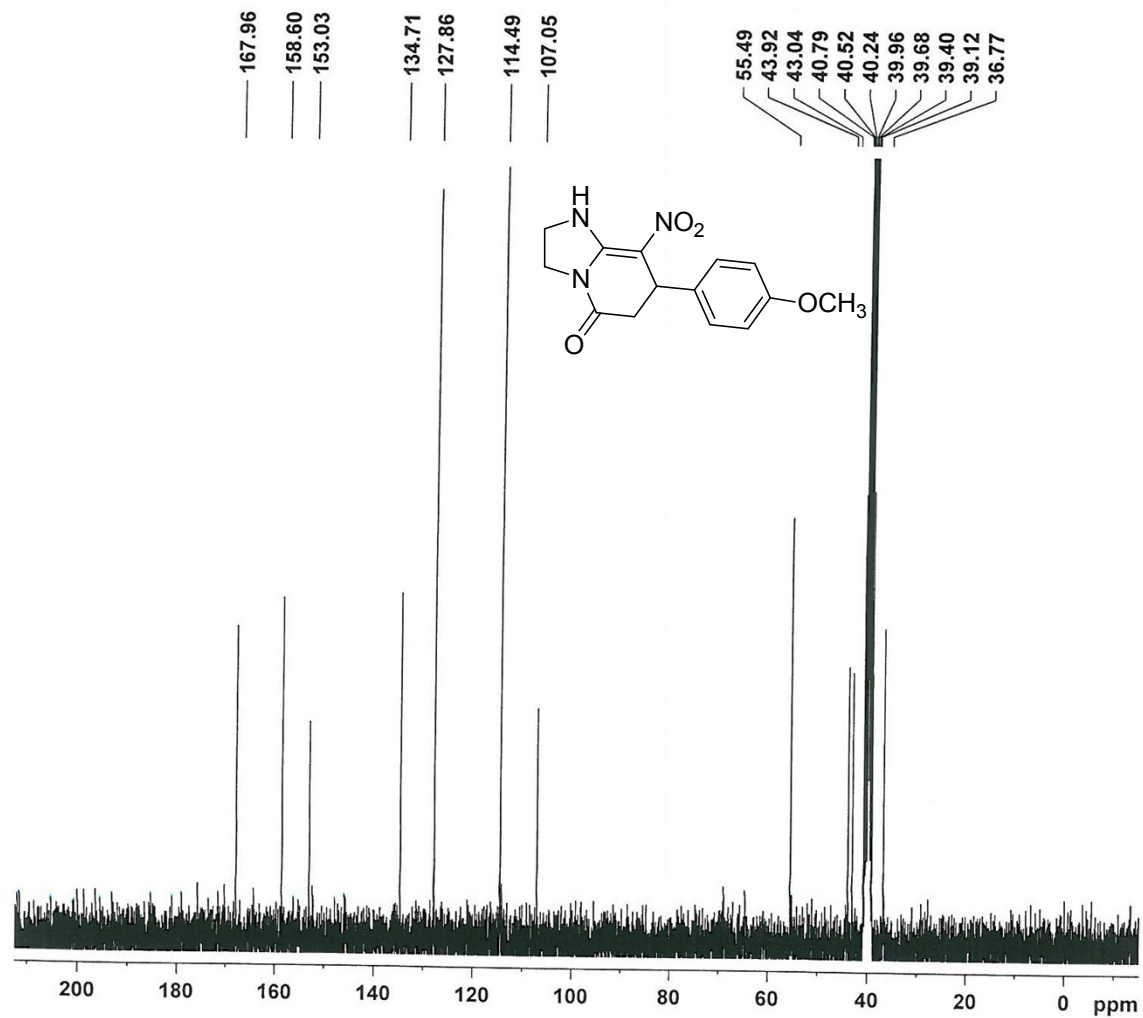
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 DS 0
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 32768
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 14.00 usec
 PL1 -6.00 dB
 SFO1 75.4099117 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 3.00 dB
 PL12 23.00 dB
 PL13 23.00 dB
 SFO2 299.8711995 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4023710 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0





Current Data Parameters
 NAME F.Hoseyni
 EXPNO 807
 PROCNO 1

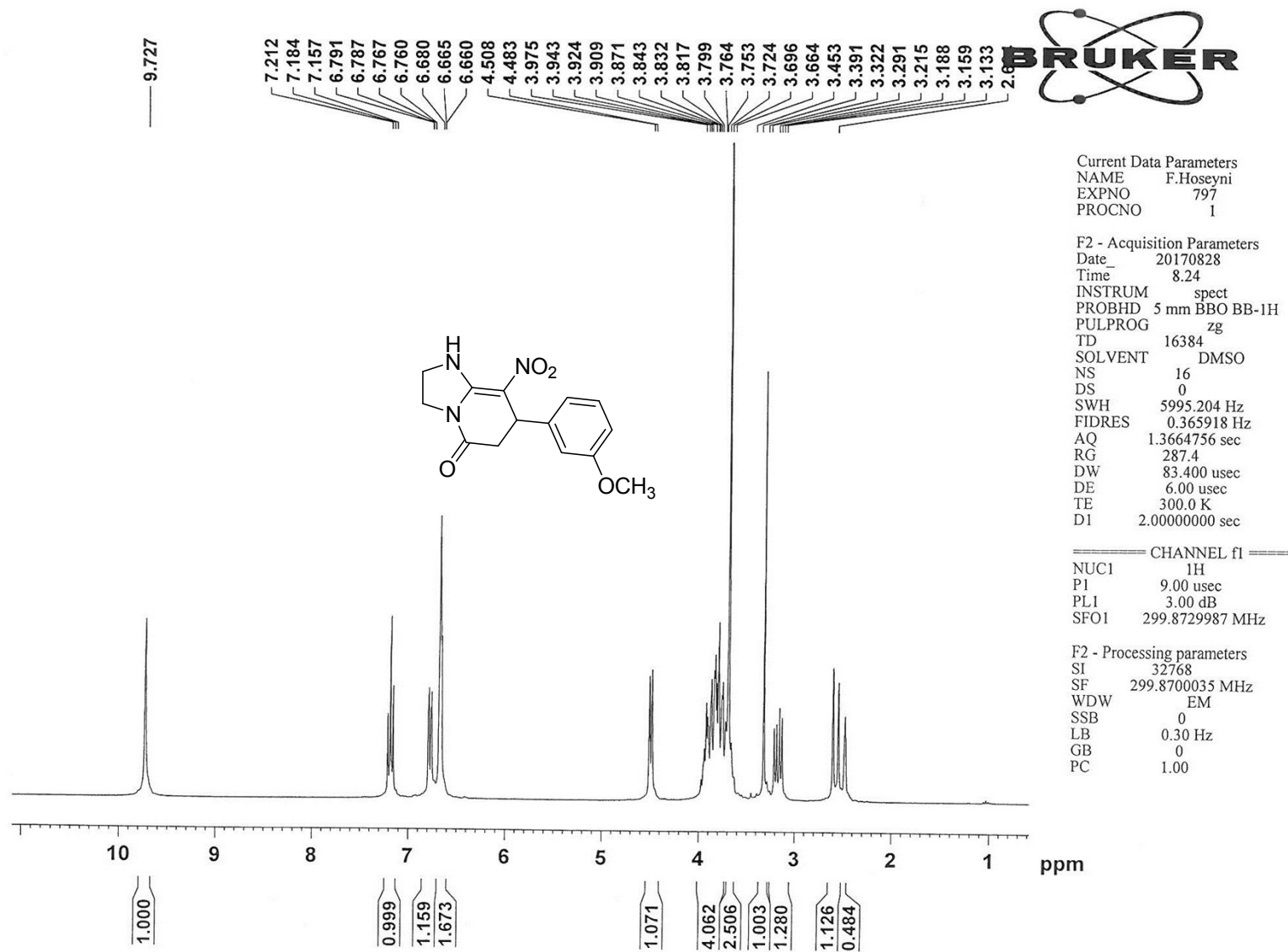
F2 - Acquisition Parameters
 Date_ 20170831
 Time_ 13.15
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg
 TD 65536
 SOLVENT DMSO
 NS 2000
 DS 0
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 32768
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 d12 0.0000200 sec

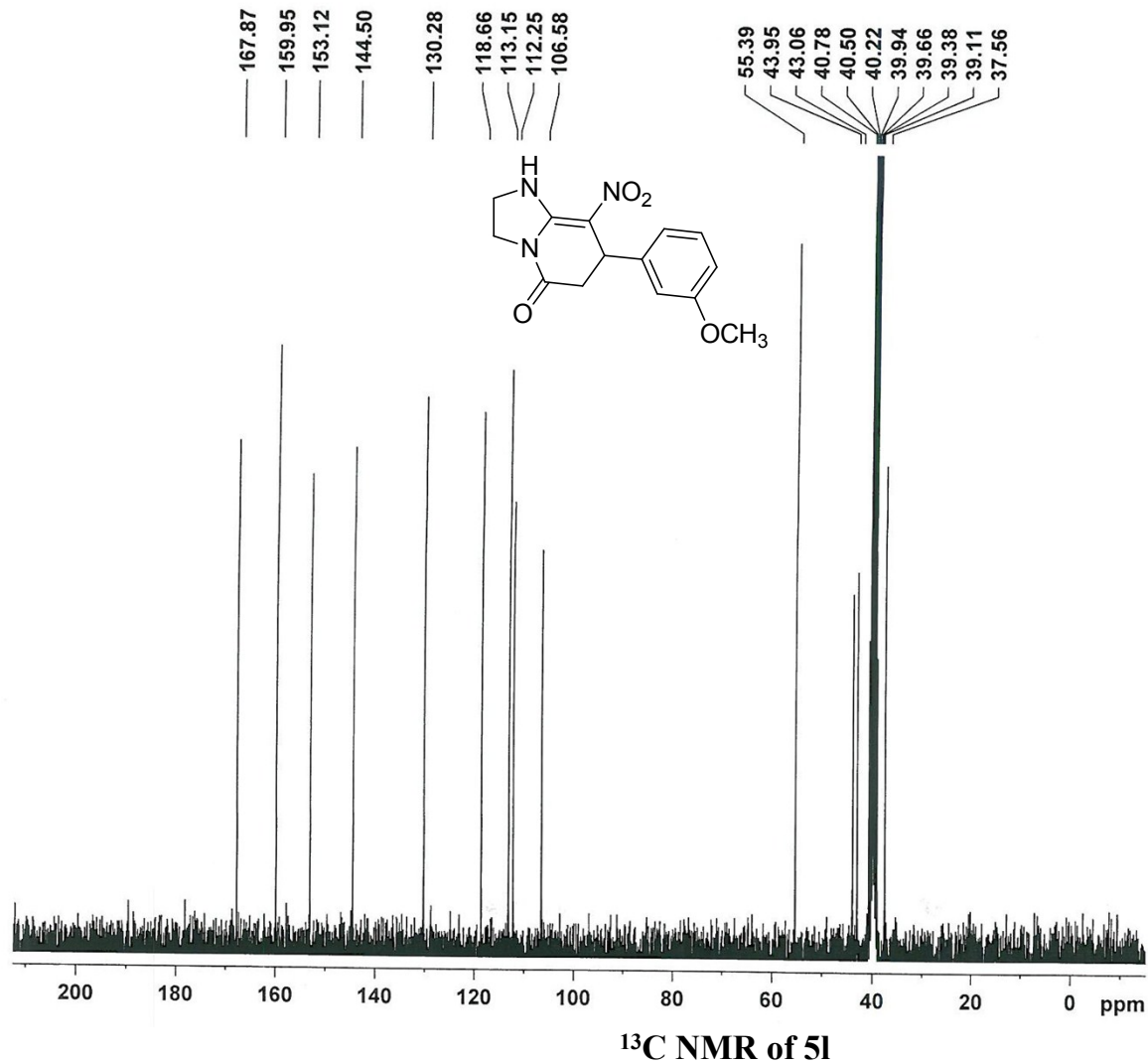
==== CHANNEL f1 =====
 NUC1 13C
 P1 14.00 usec
 PL1 -6.00 dB
 SFO1 75.4099117 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 3.00 dB
 PL12 23.00 dB
 PL13 23.00 dB
 SFO2 299.8711995 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4023710 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GR ^

¹³C NMR of 5k

¹H NMR of 5I



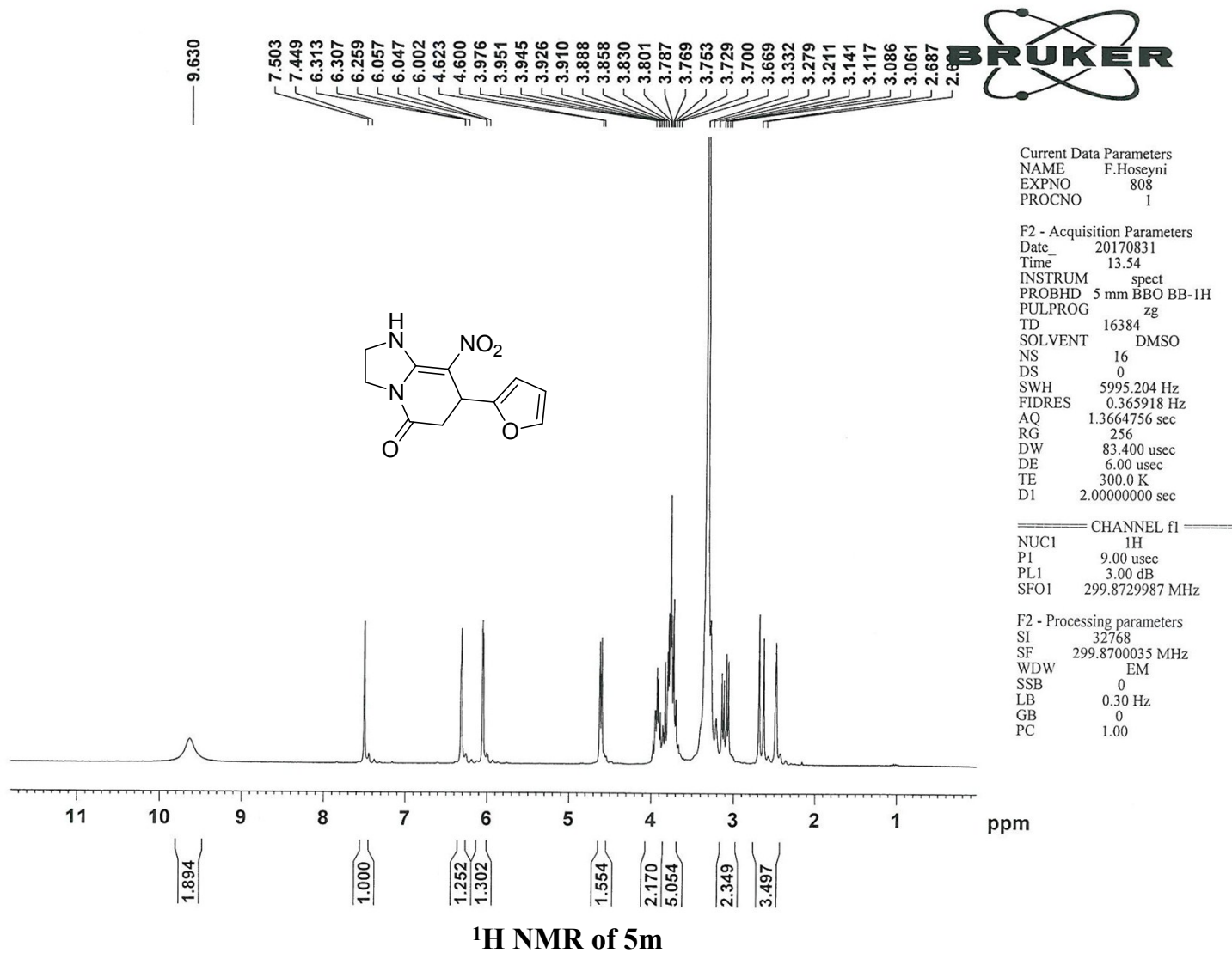
Current Data Parameters
 NAME F.Hoseyni
 EXPNO 804
 PROCNO 1

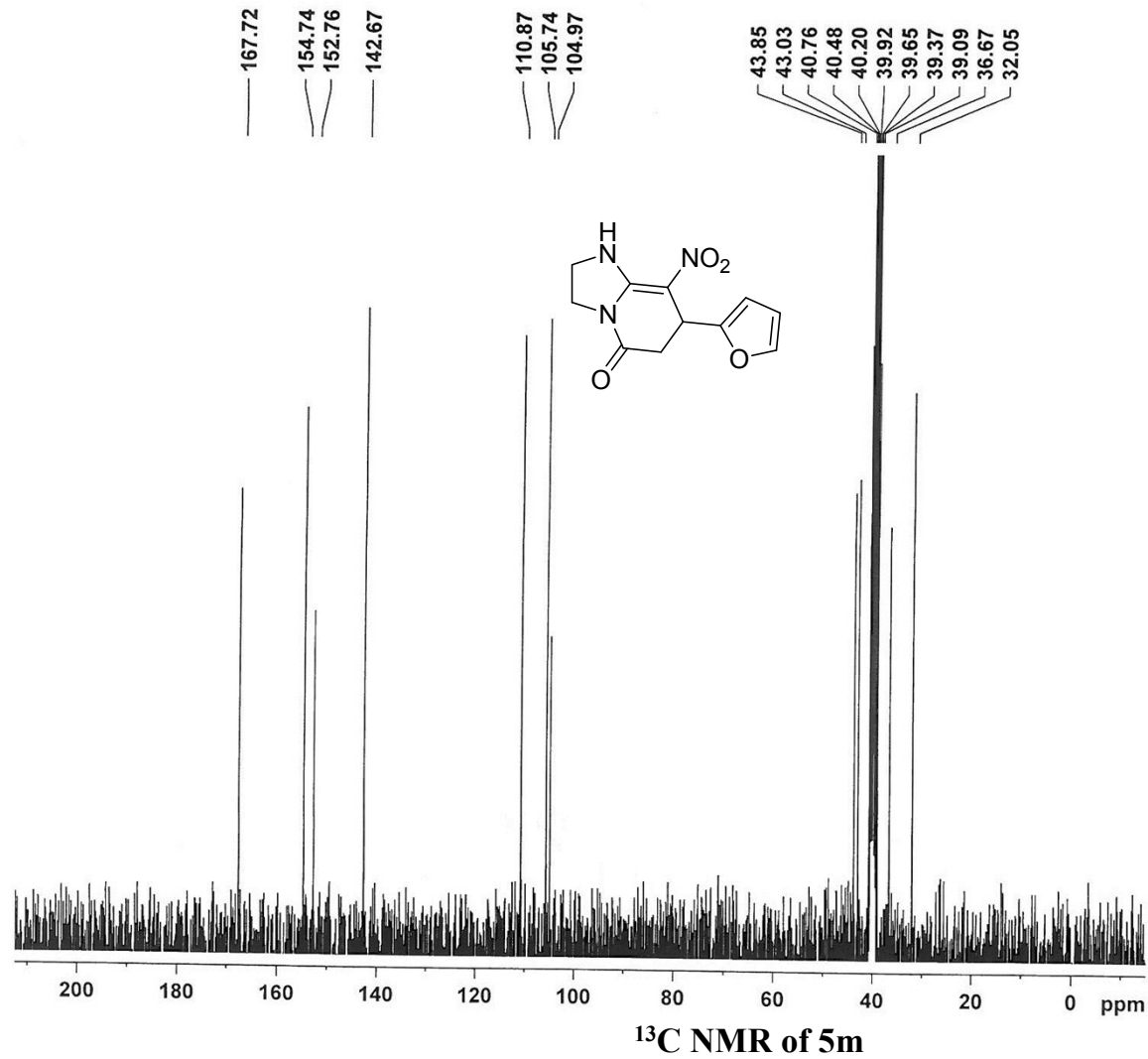
F2 - Acquisition Parameters
 Date_ 20170831
 Time_ 9.06
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg
 TD 65536
 SOLVENT DMSO
 NS 850
 DS 0
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 32768
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 d12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 14.00 usec
 PL1 -6.00 dB
 SFO1 75.4099117 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 3.00 dB
 PL12 23.00 dB
 PL13 23.00 dB
 SFO2 299.8711995 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4023710 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz





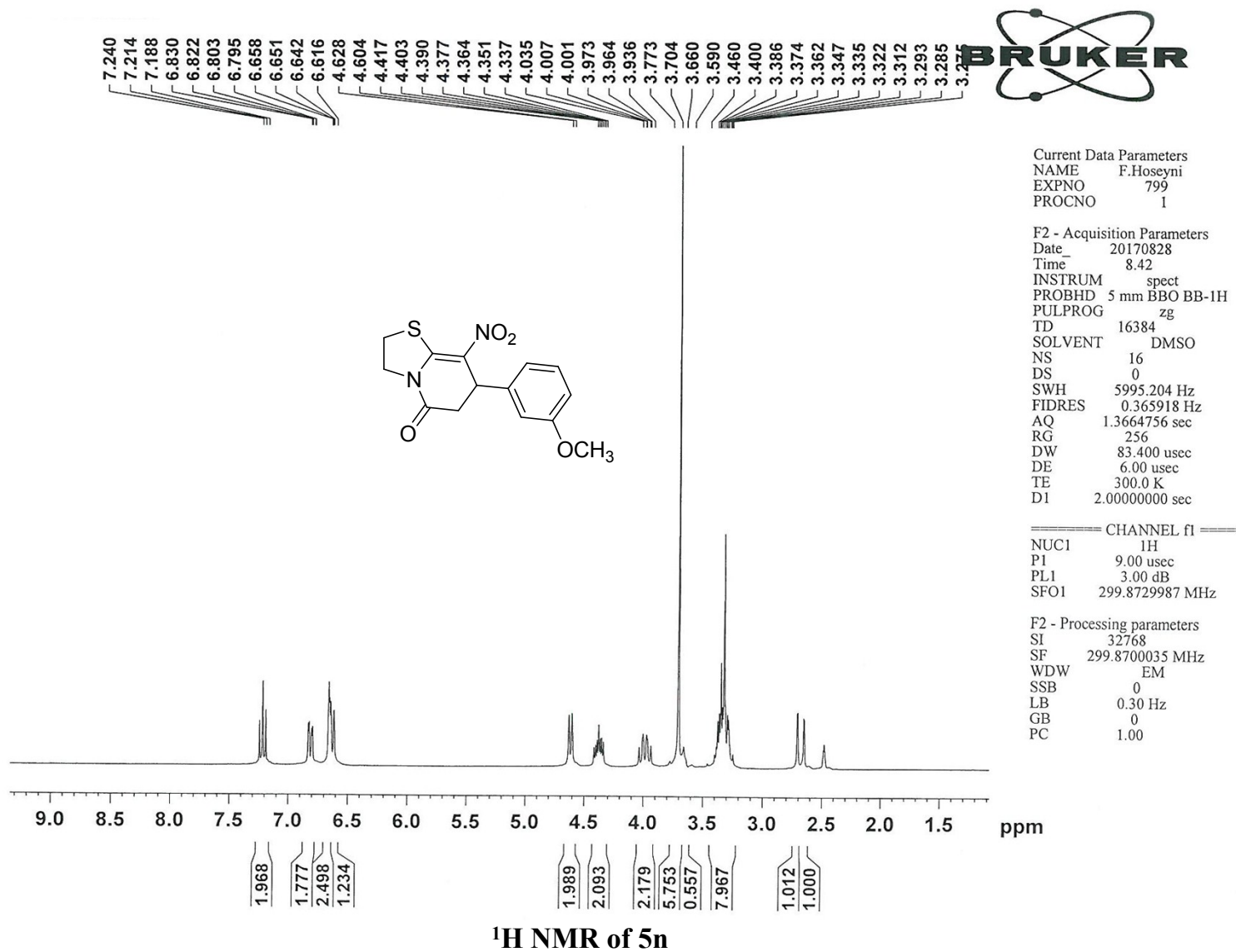
Current Data Parameters
 NAME F.Hoseyni
 EXPNO 810
 PROCNO 1

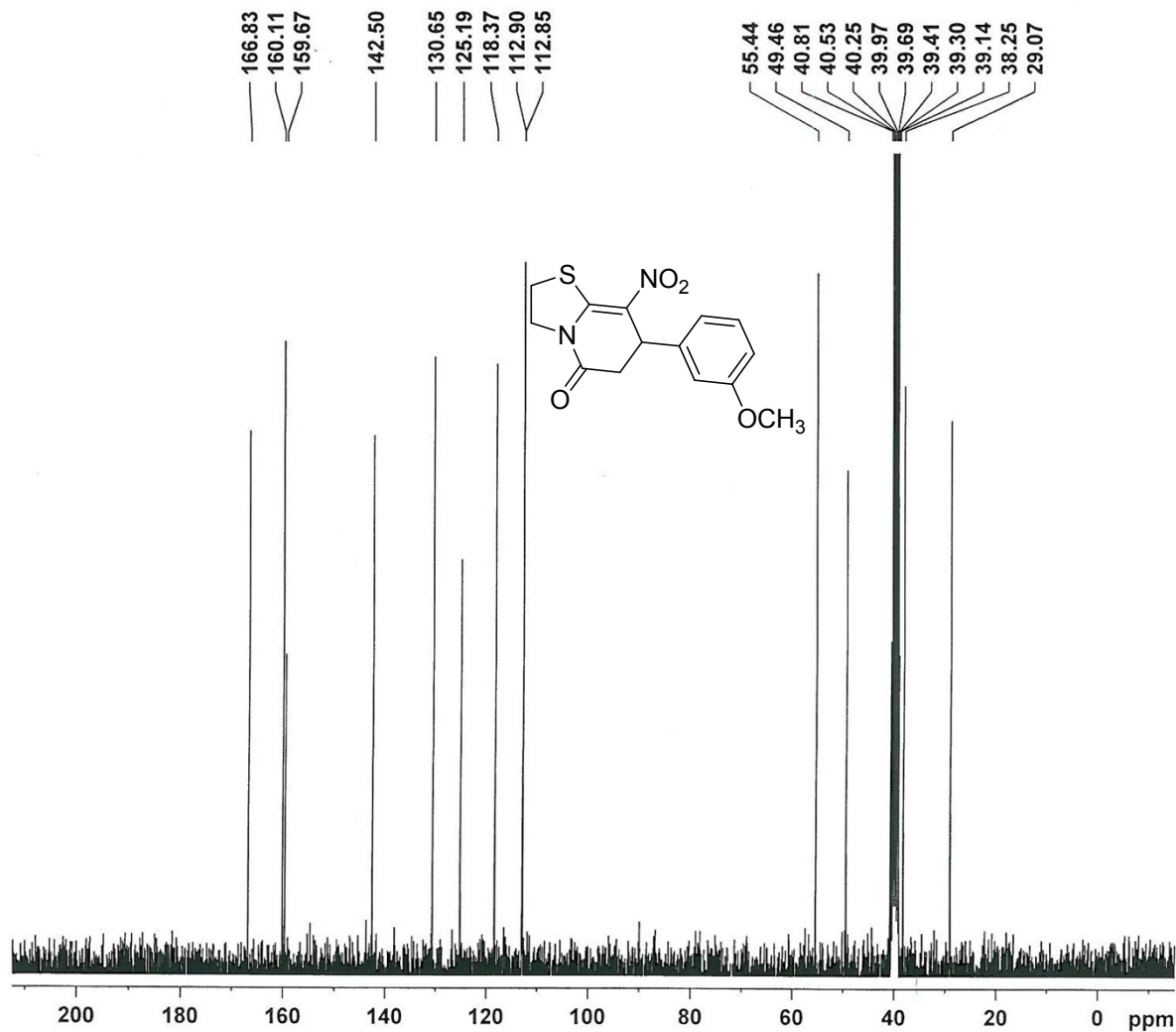
F2 - Acquisition Parameters
 Date_ 20170902
 Time_ 8.58
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg
 TD 65536
 SOLVENT DMSO
 NS 751
 DS 0
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 32768
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 14.00 usec
 PL1 -6.00 dB
 SFO1 75.4099117 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 3.00 dB
 PL12 23.00 dB
 PL13 23.00 dB
 SFO2 299.8711995 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4023710 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz



 ^{13}C NMR of 5n

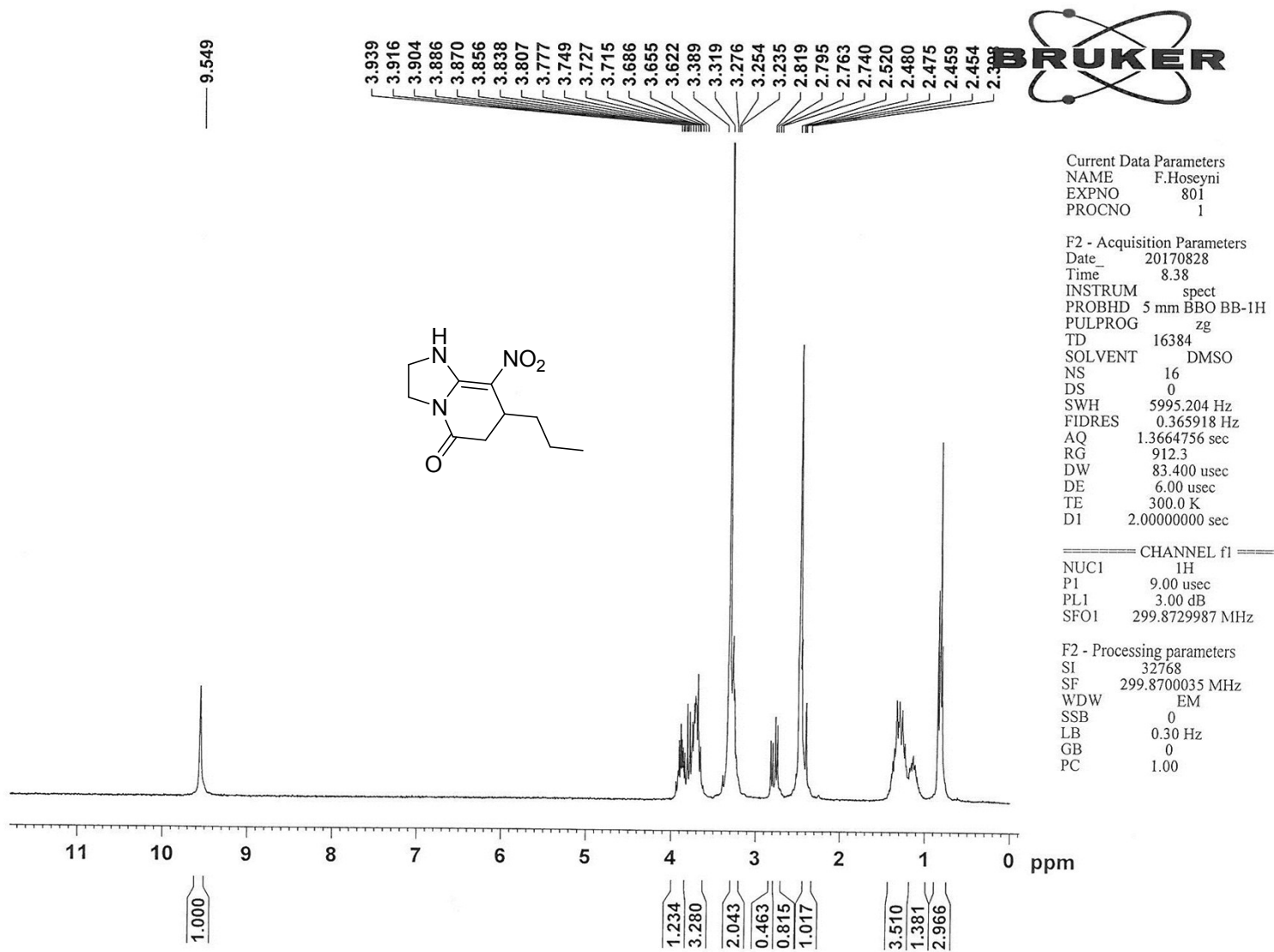
Current Data Parameters
 NAME F.Hoseyni
 EXPNO 806
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170831
 Time_ 11.02
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg
 TD 65536
 SOLVENT DMSO
 NS 850
 DS 0
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 32768
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 d12 0.00002000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 14.00 usec
 PL1 -6.00 dB
 SFO1 75.4099117 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 3.00 dB
 PL12 23.00 dB
 PL13 23.00 dB
 SFO2 299.8711995 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4023710 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0

¹H NMR of 5o