

Supporting Information

Synthesis of Spiroimidazopyridineoxindole, Spiropyridopyrimidineoxindole and Spiropyridodiazepineoxindole Structures Based on Heterocyclic Ketene Aminals *via* a Four- Component Reaction

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The Table of Contents

Title	Page
Title, author's name, address and table of contents	1
Experimental Section; General remarks	2
Figure 1. The ^1H and ^{13}C NMR chemical shifts of 5a	2
Figure 2. Structure of all products 5	3
^1H and ^{13}C NMR and IR and Mass spectrums of 5a	4-7
^1H and ^{13}C NMR and IR and Mass spectrums of 5b	8-11
^1H and D_2O exchange and ^{13}C NMR and IR and Mass spectrums of 5c	12-16
^1H and D_2O exchange and ^{13}C NMR (in DMSO and CDCl_3) and IR spectrums of 5d	17-20
^1H and ^{13}C NMR and Mass spectrums of 5e	21-23
^1H and ^{13}C NMR spectrums of 5f	24-25
^1H and ^{13}C NMR spectrums of 5g	26-27
^1H and ^{13}C NMR spectrums of 5h	28-29
^1H and expand and ^{13}C NMR spectrums of 5i	30-32
^1H and ^{13}C NMR spectrums of 5j	33-34

Experimental Section

General remarks:

Melting points were measured on an Electrothermal 9100 apparatus. Mass spectra were recorded with an Agilent 5975C VL MSD with Triple-Axis Detector operating at an ionization potential of 70 Ev. ^1H and ^{13}C NMR spectra were measured (DMSO) with a Bruker DRX-300 AVANCE spectrometer at 300 and 75 MHz, respectively. IR spectra were recorded on a Bruker Tensor 27, $\bar{\nu}$ in cm^{-1} . All NMR spectra at room temperature were determined in $\text{DMSO-}d_6$. Chemical shifts are reported in parts per million (δ) downfield from an internal tetramethylsilane reference. Coupling constants (J values) are reported in hertz (Hz), and spin multiplicities are indicated by the following symbols: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet). All chemicals were purchased from Merck or Aldrich and were used without further purification.

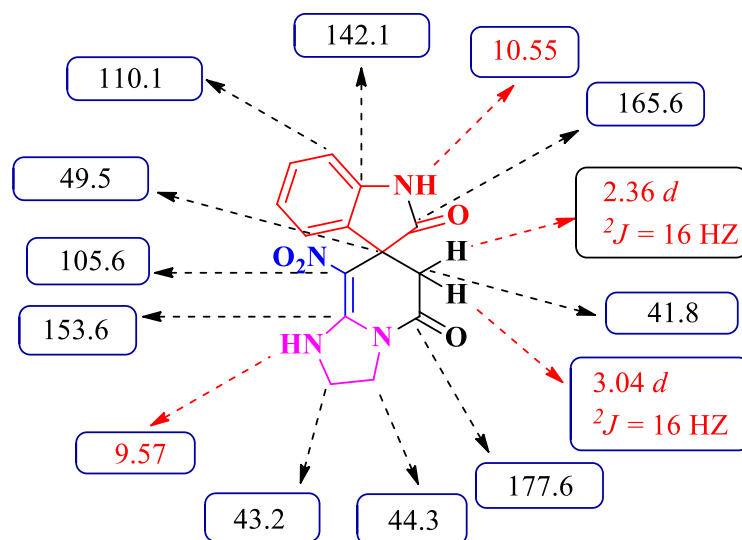


Figure 1. The ^1H and ^{13}C NMR chemical shifts of **5a**.

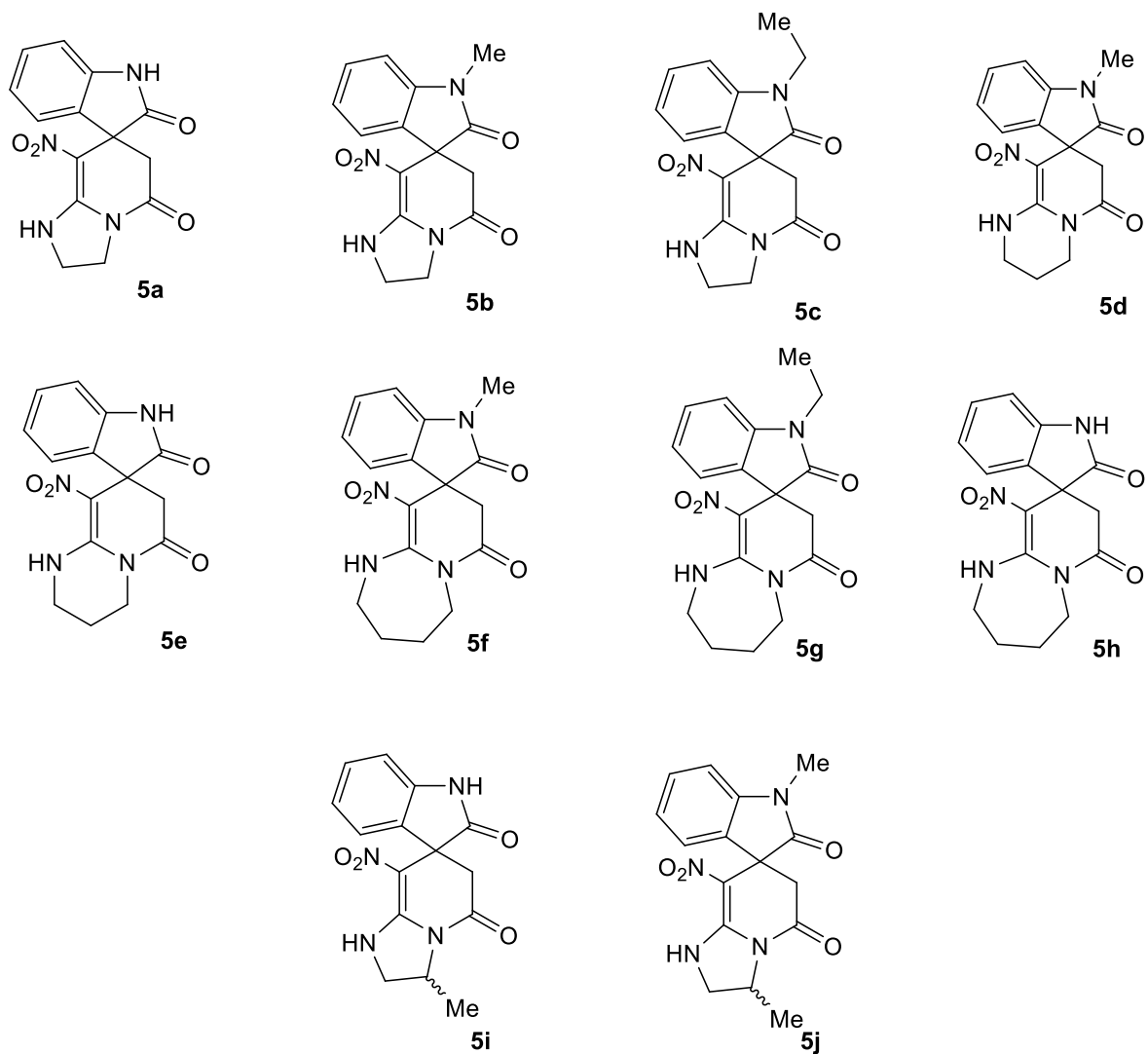
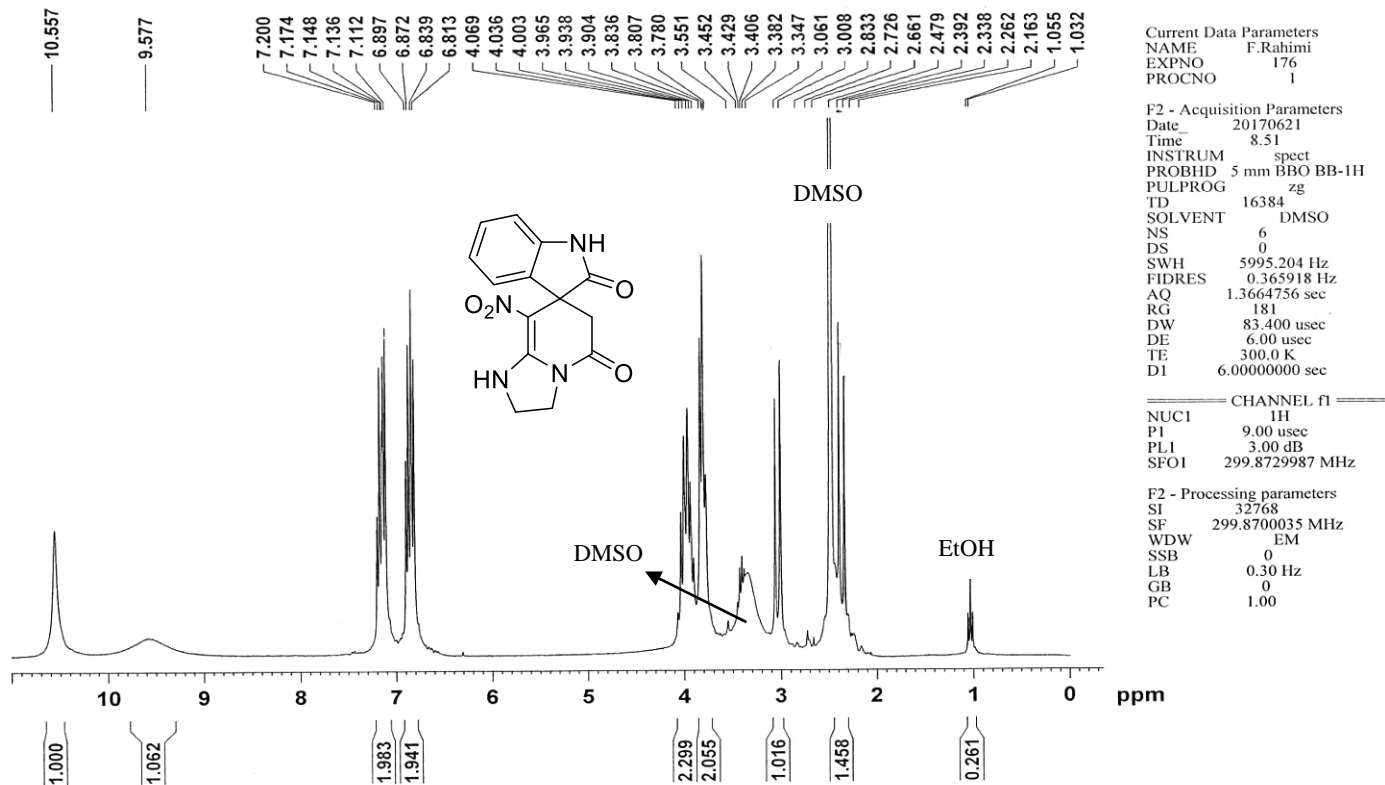


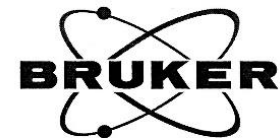
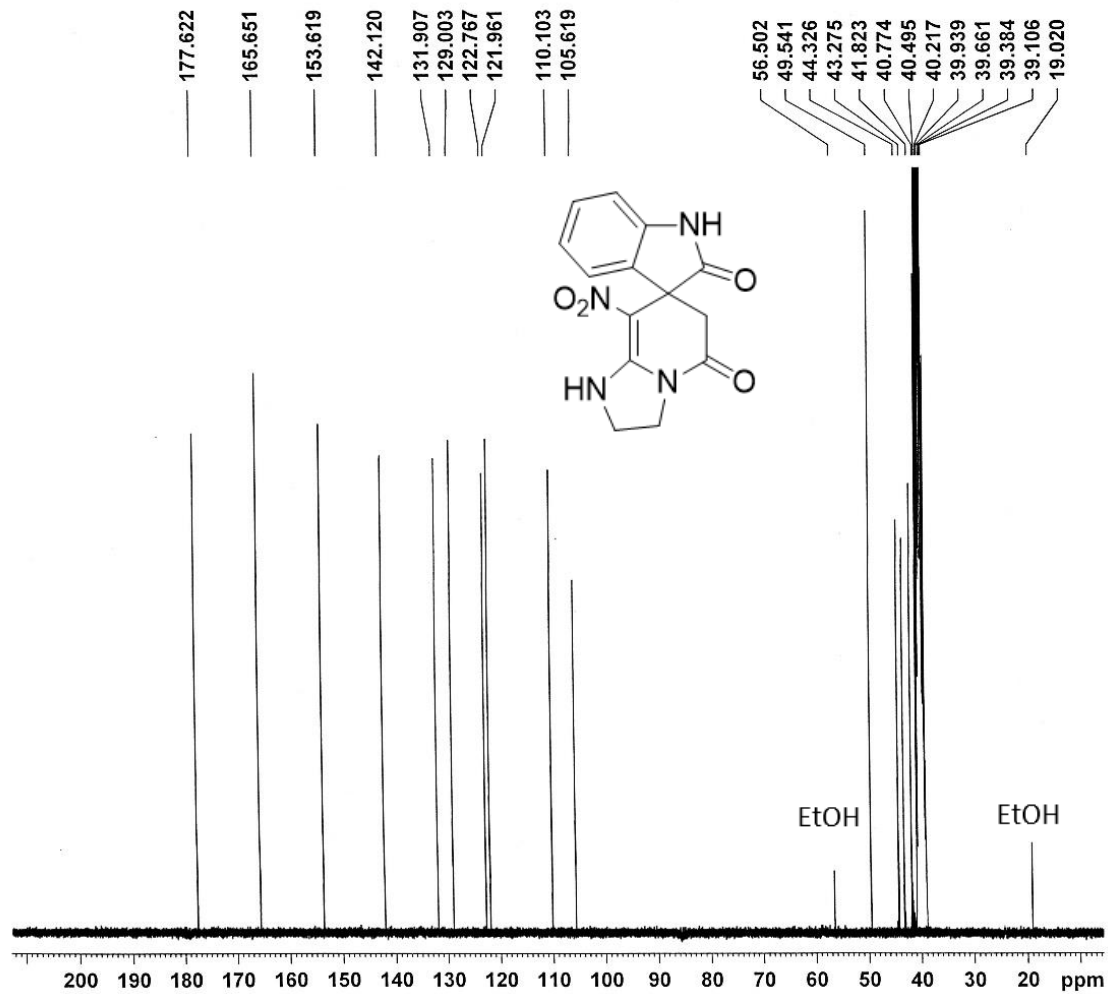
Figure 2. Structure of all products **5**

The structures of all products **5a-j** were deduced from their IR, mass, ^1H NMR, and ^{13}C NMR spectra.



¹H NMR of 5a

R1 CNMR



Current Data Parameters
 NAME F.Rahimi
 EXPNO 183
 PROCNO 1

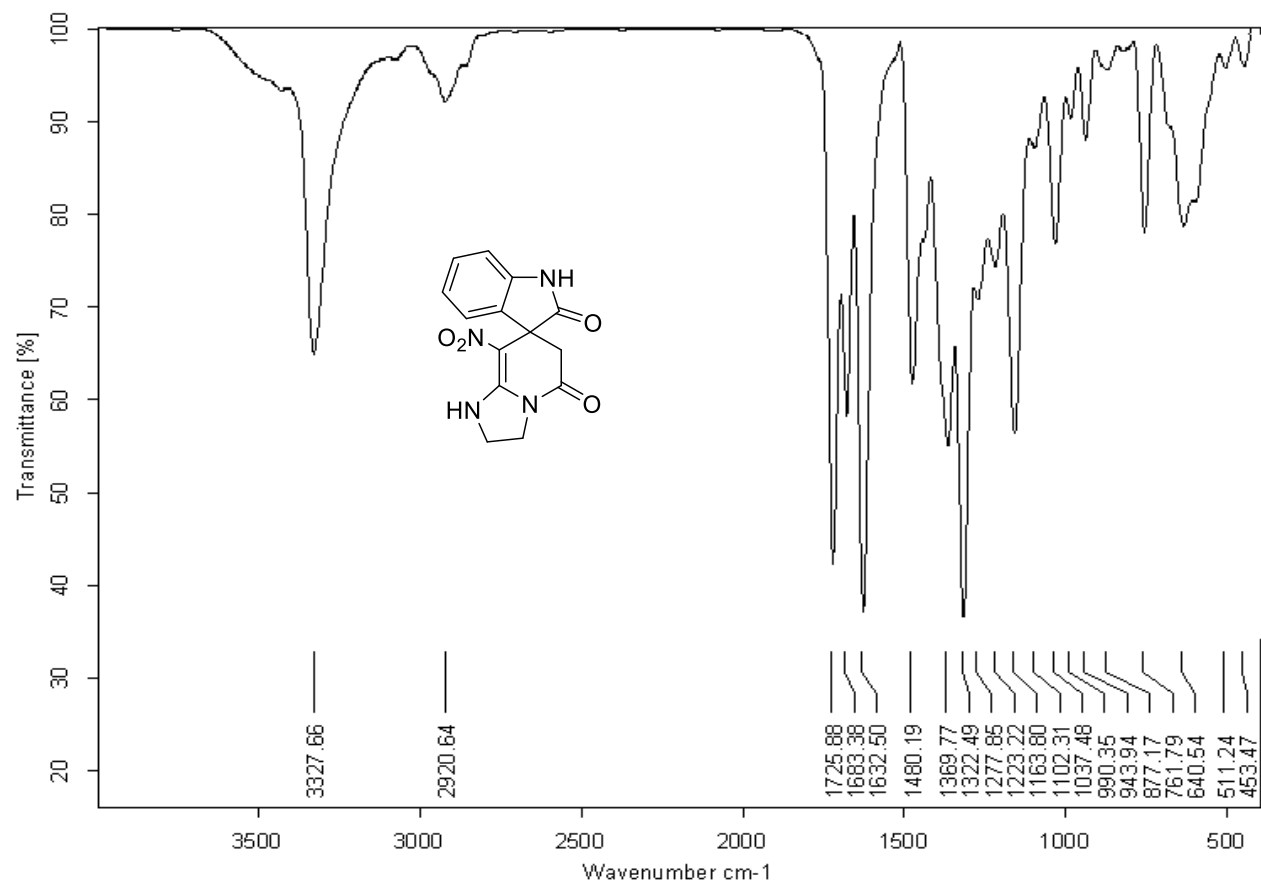
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 FIDRES 0.241437 Hz
 AQ 2.0709877 sec
 RG 32768
 DW 31.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 4.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 =====
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 P1 14.00 usec
 PL1 -6.00 dB
 SFO1 75.4102882 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

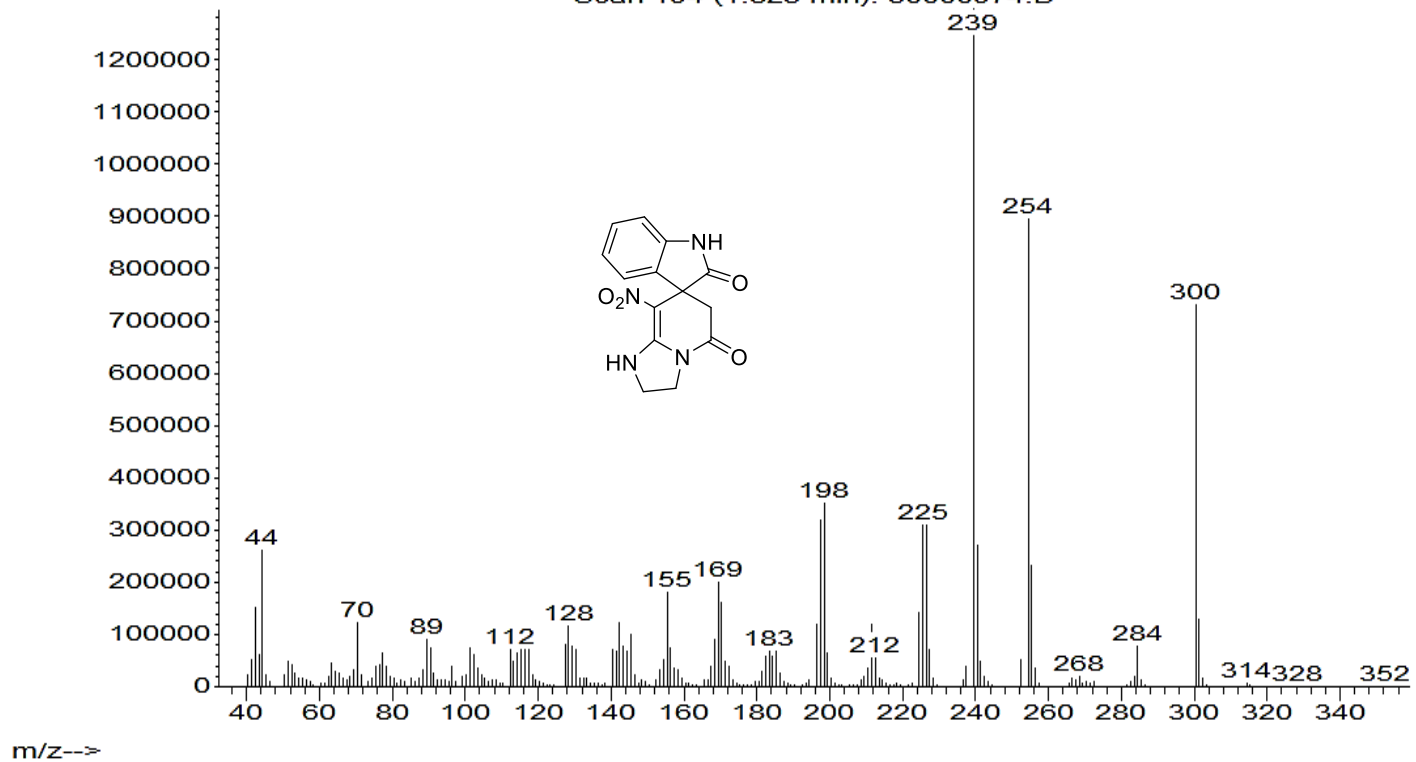
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¹³C NMR of 5a

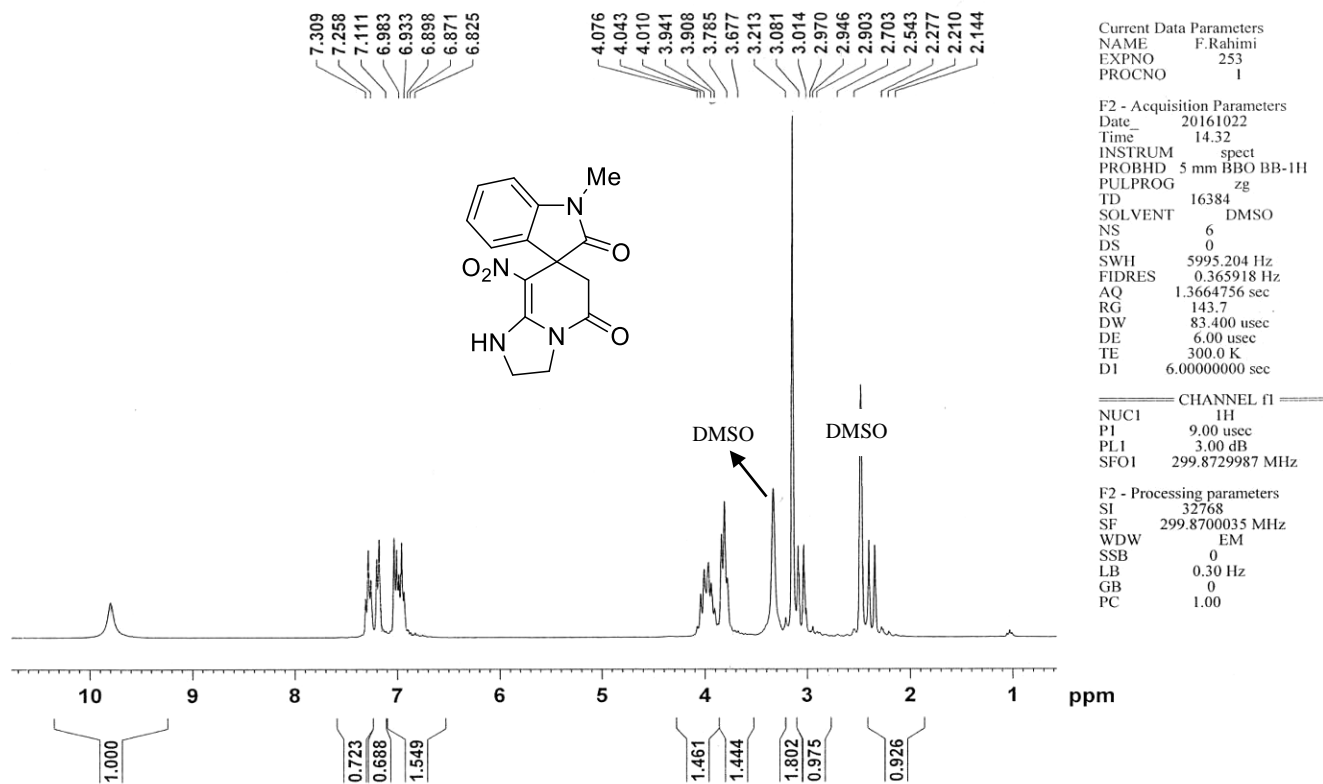
**IR of 5a**

Abundance

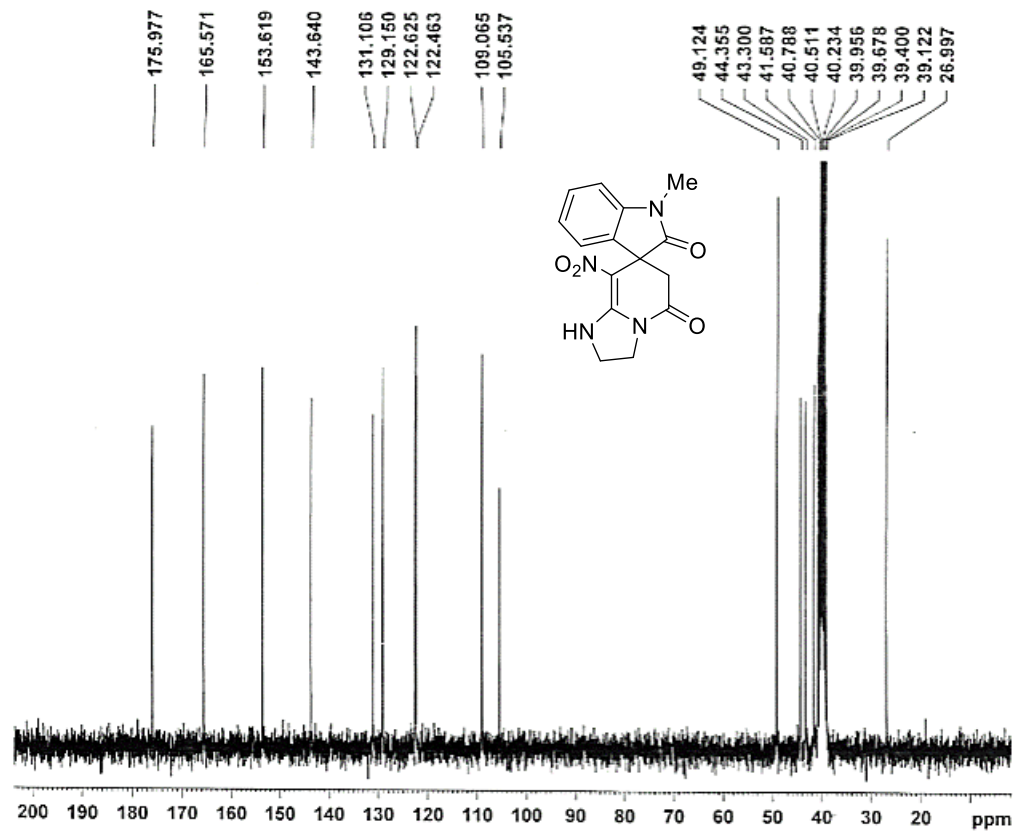
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Mass of 5a



¹H NMR of 5b



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 EXPNO 254
 PROCNO 1

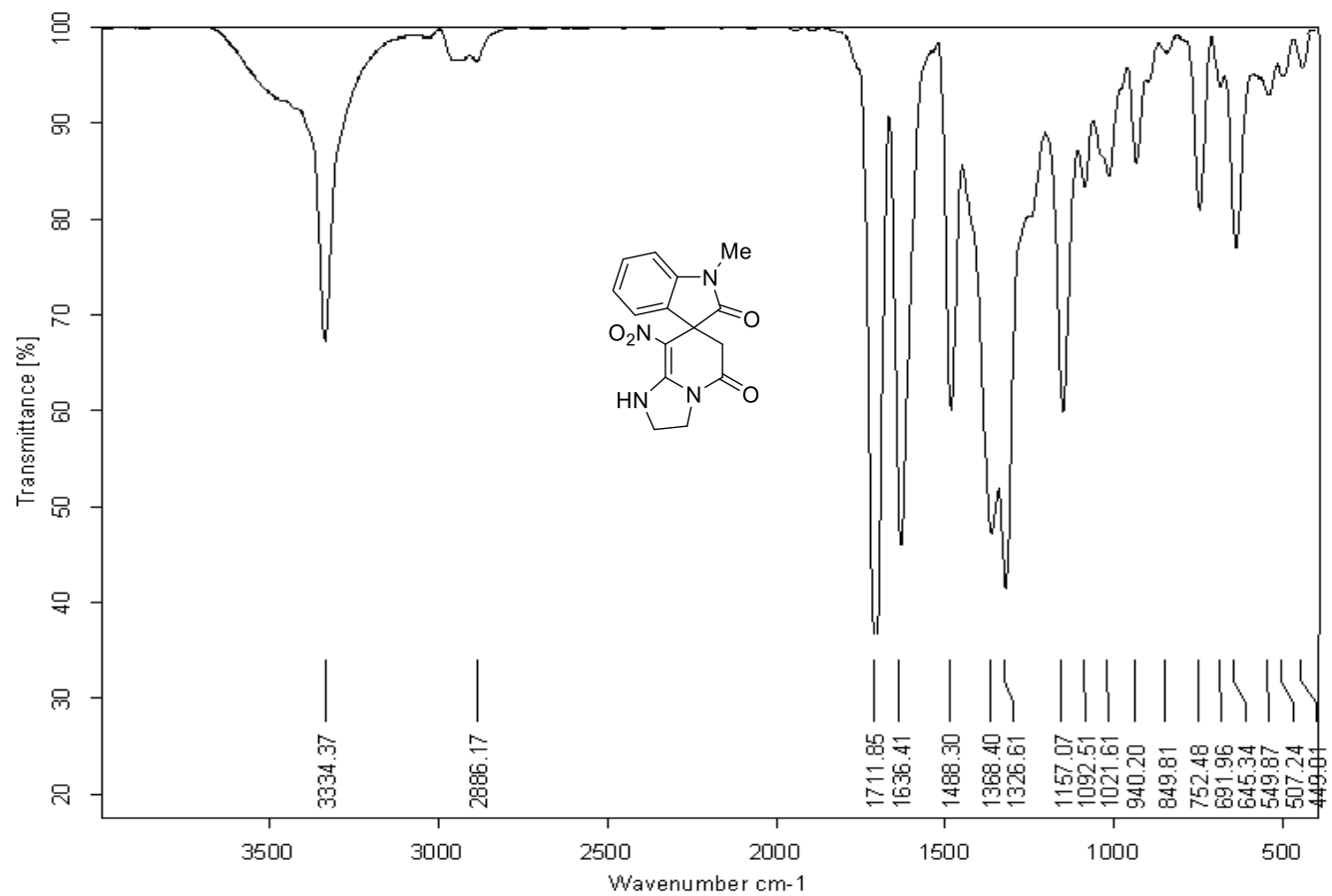
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 FIDRES 0.241437 Hz
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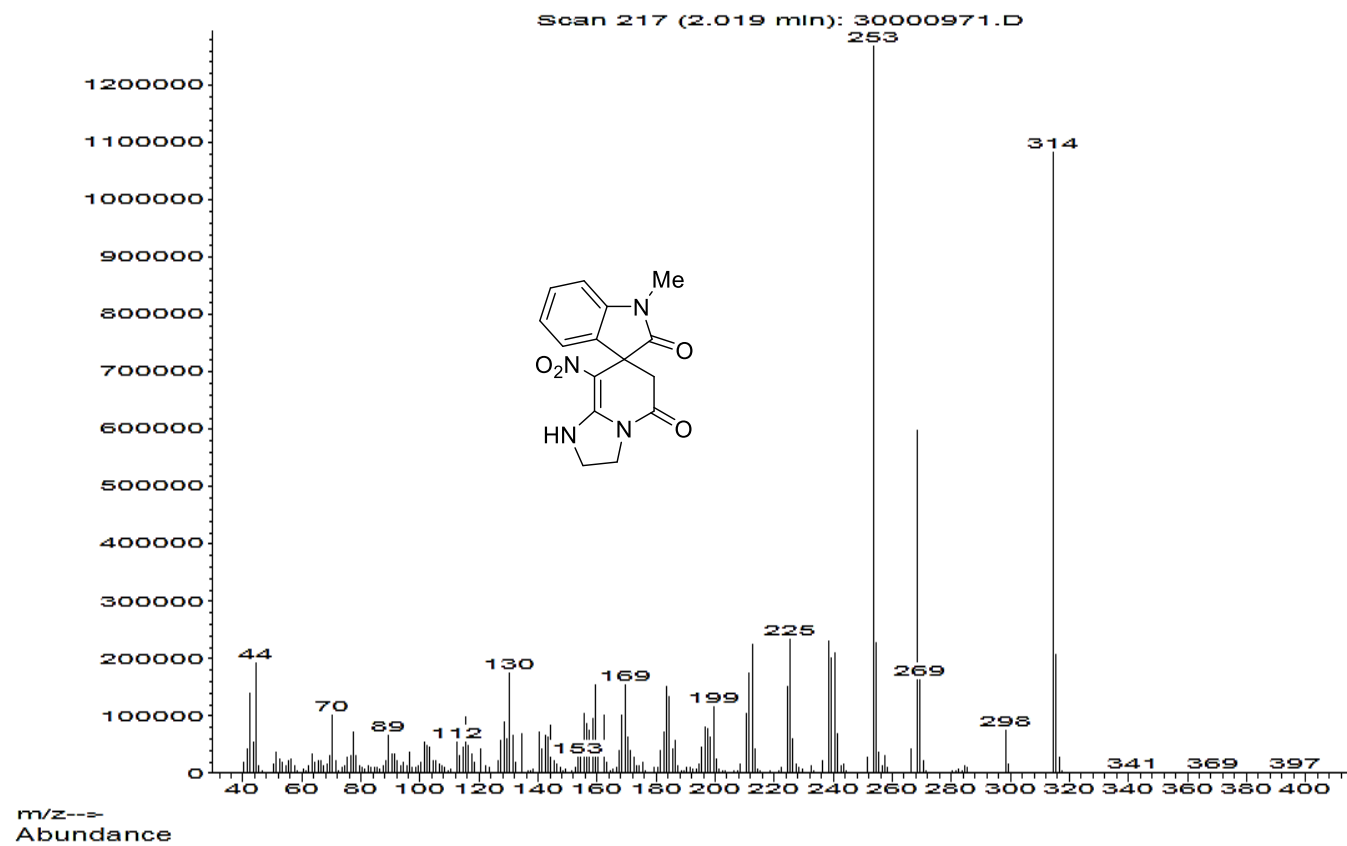
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 PCPD2 80.00 usec
 PL2 3.00 dB
 PL12 23.00 dB
 PL13 23.00 dB
 SFO2 299.8711995 MHz

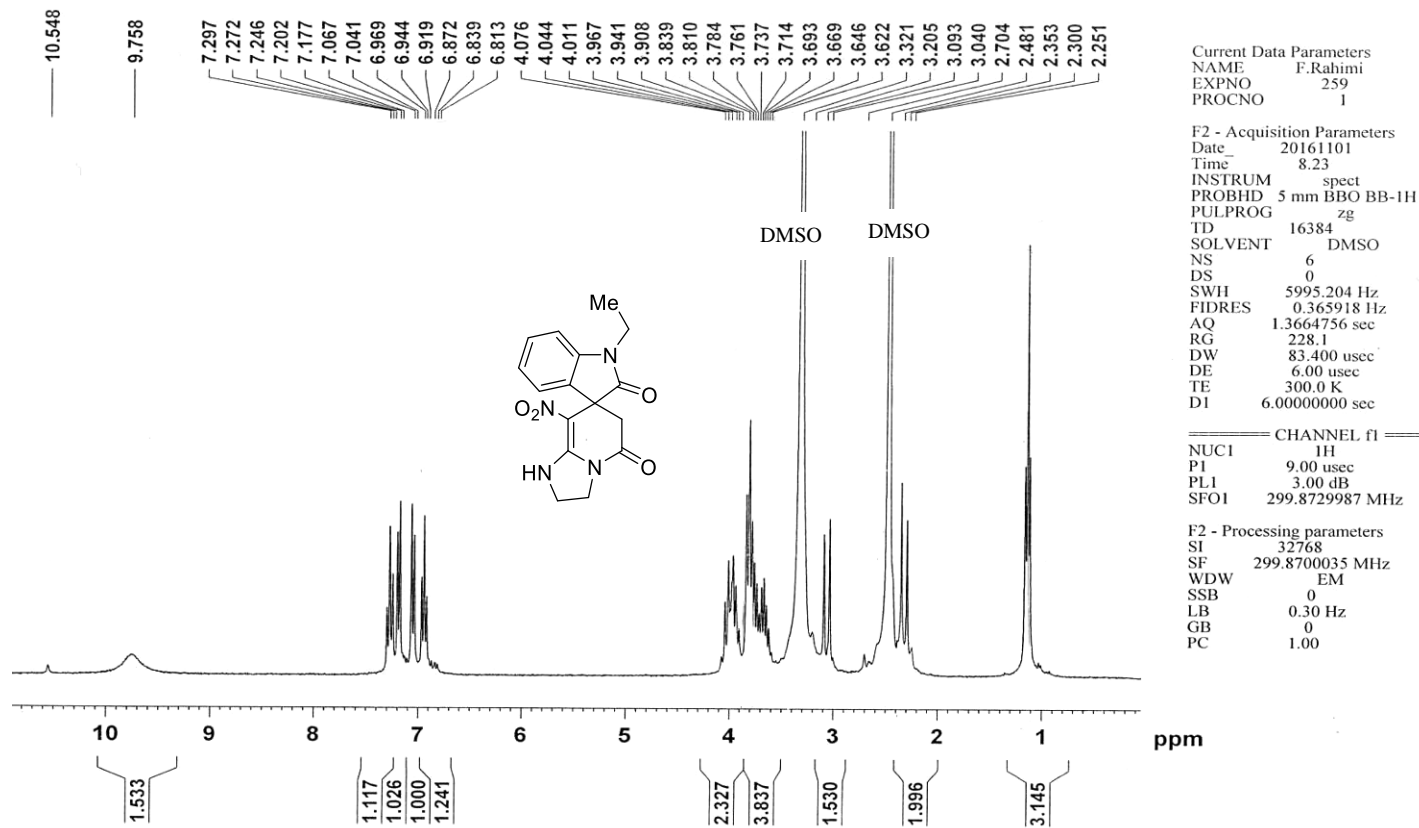
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¹³C NMR of 5b

**IR of 5b**

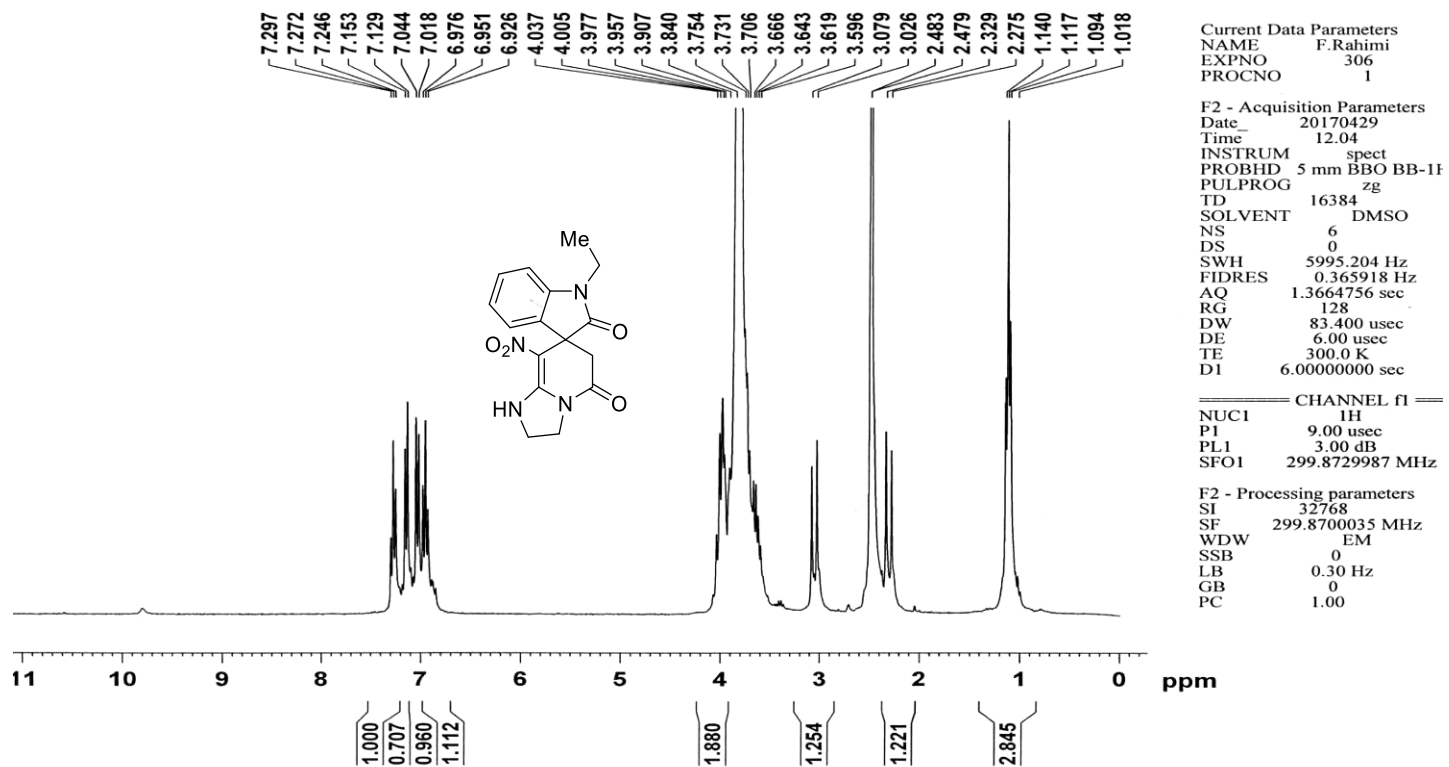


Mass of 5b

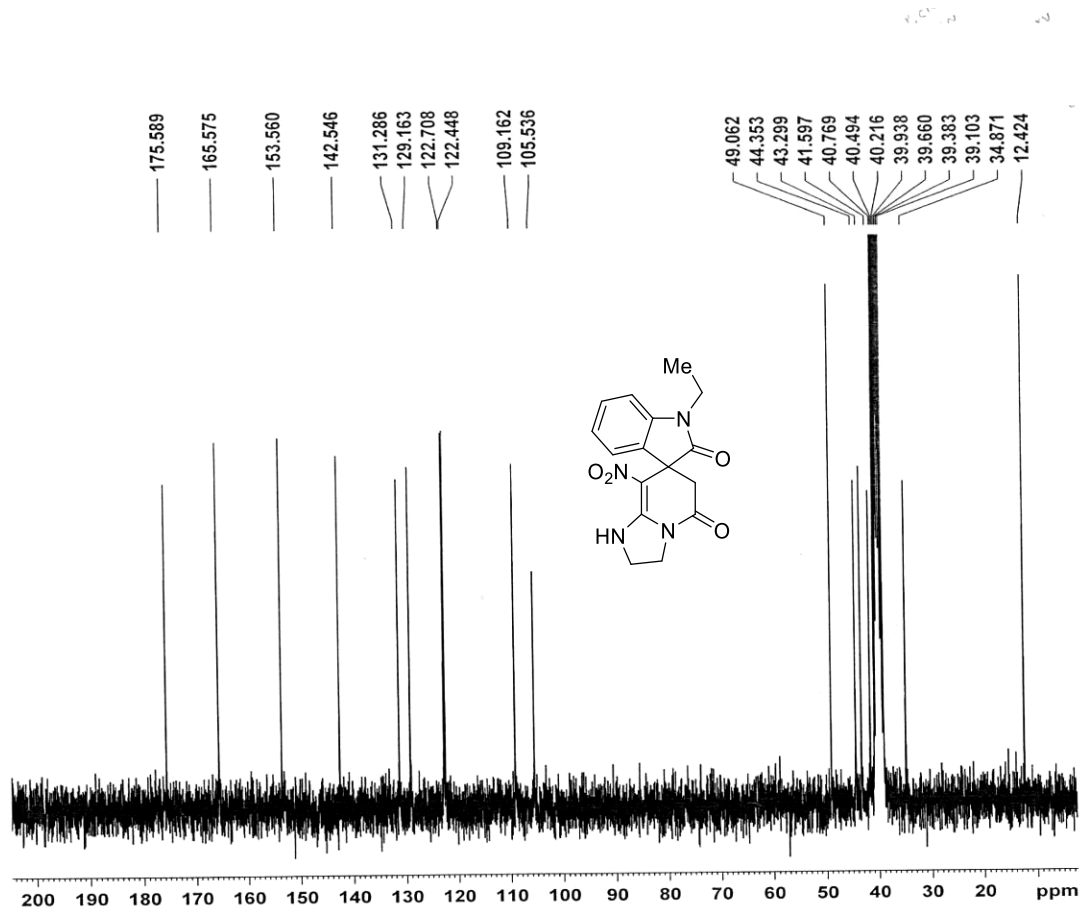


¹H NMR of 5c

c



¹H NMR with D₂O of 5c



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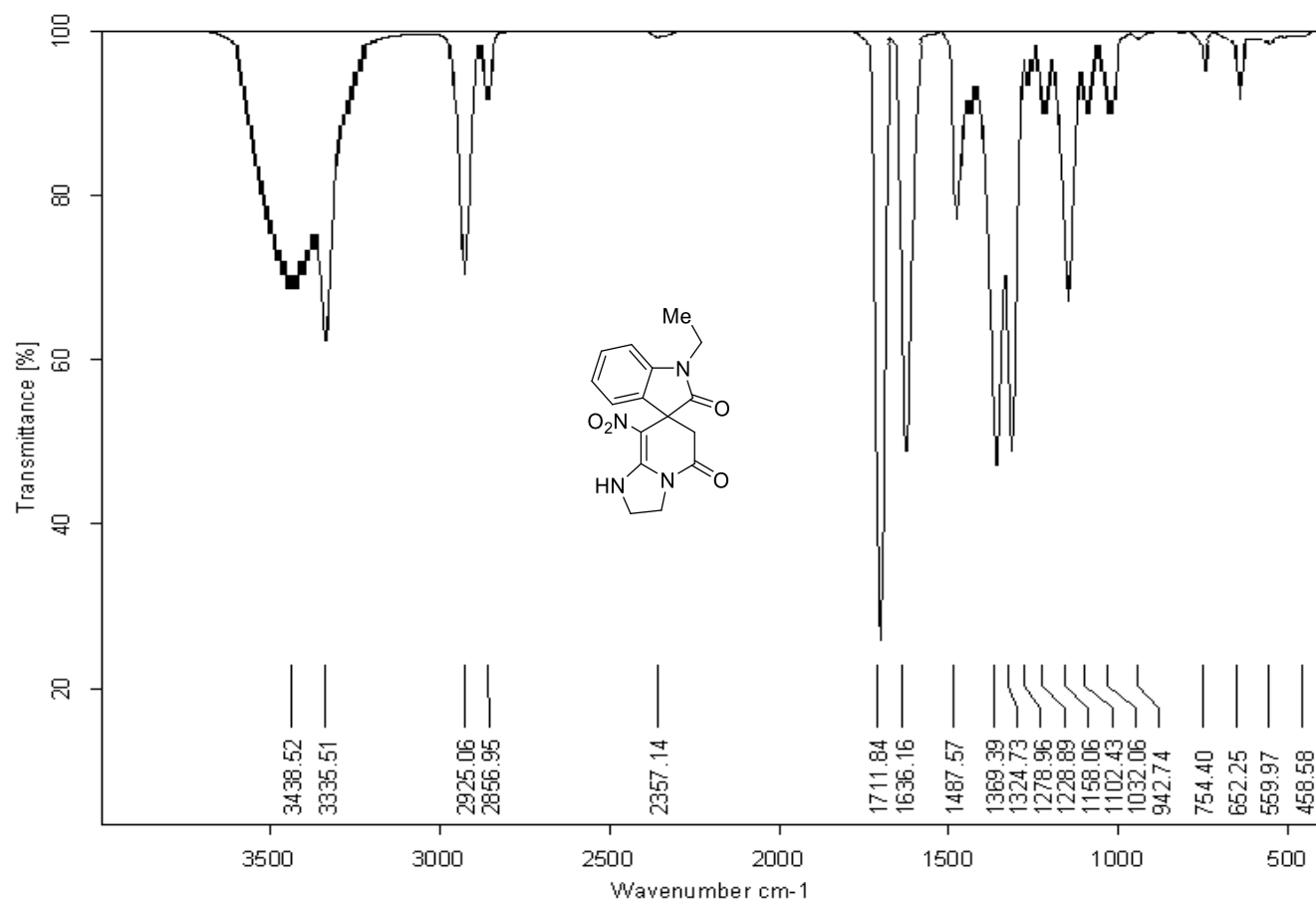
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 TD 65536
 SOLVENT DMSO
 NS 570
 DS 0
 SWH 15822.785 Hz
 FIDRES 0.241437 Hz
 AQ 2.0709877 sec
 RG 32768
 DW 31.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 4.00000000 sec
 d11 0.03000000 sec
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===== CHANNEL f1 =====
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 P1 14.00 usec
 PL1 -6.00 dB
 SFO1 75.4102882 MHz

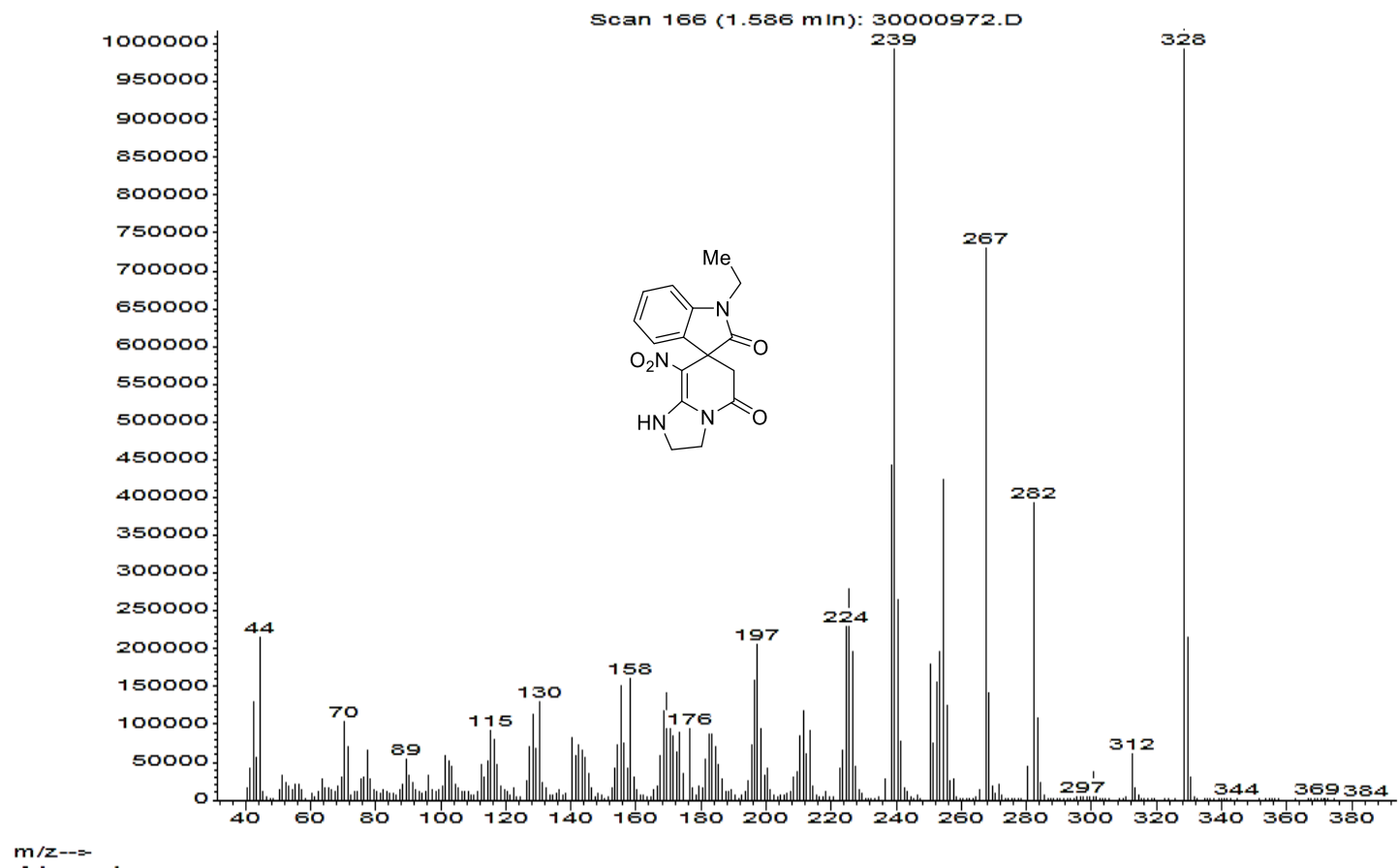
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 PL13 23.00 dB
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F2 - Processing parameters
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 WDW EM
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 LB 1.00 Hz
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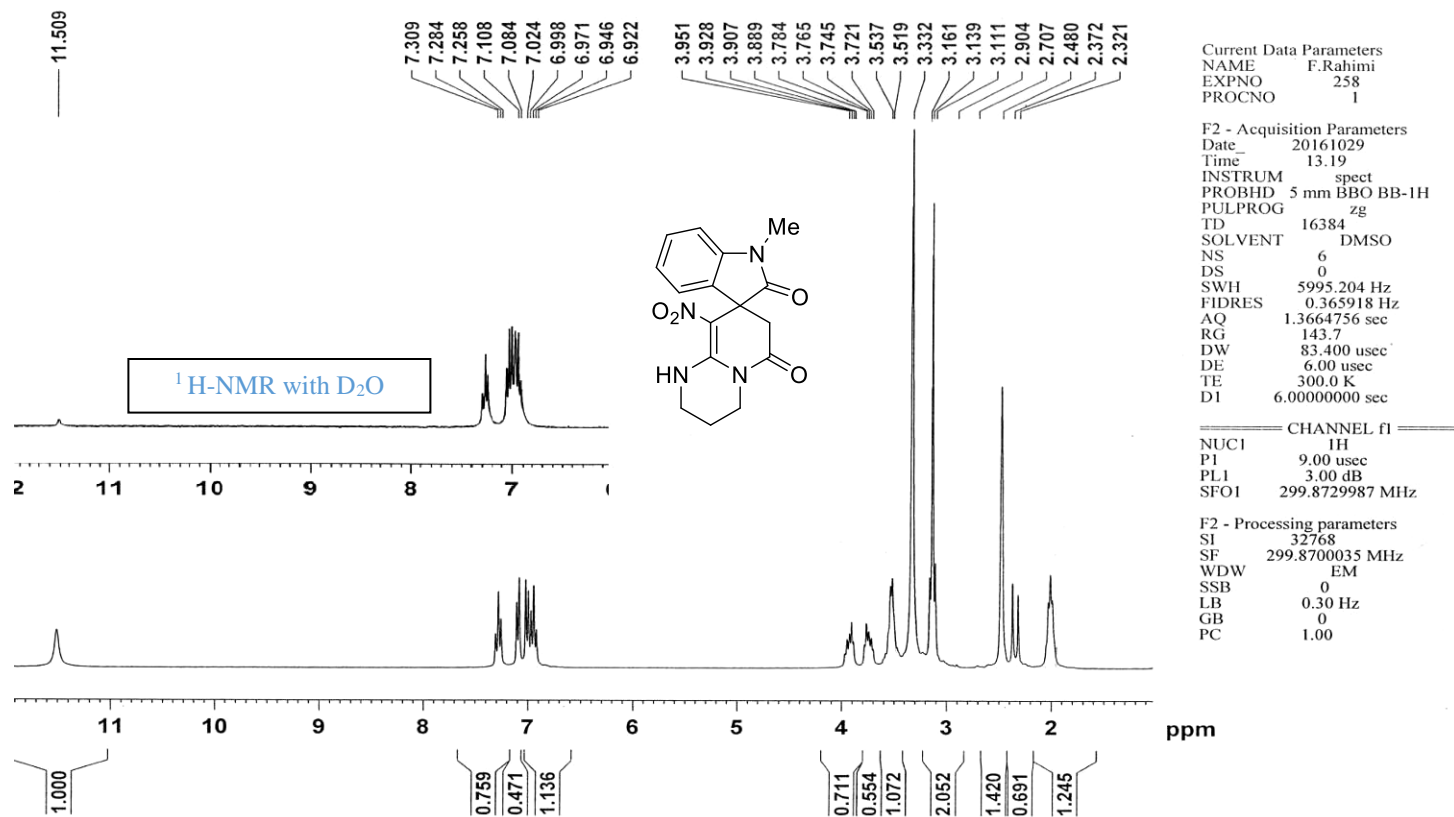
¹³C NMR of 5c



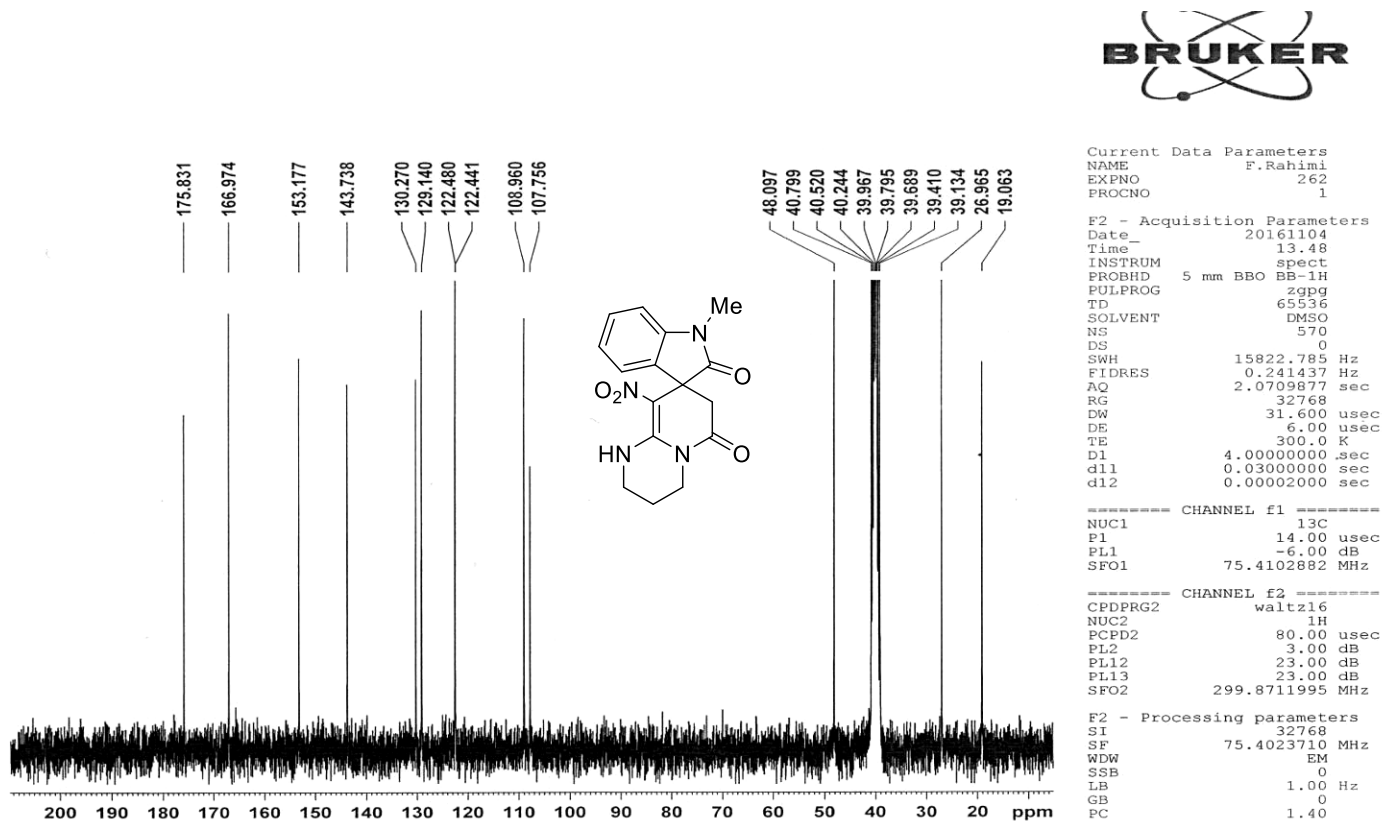
IR of 5c



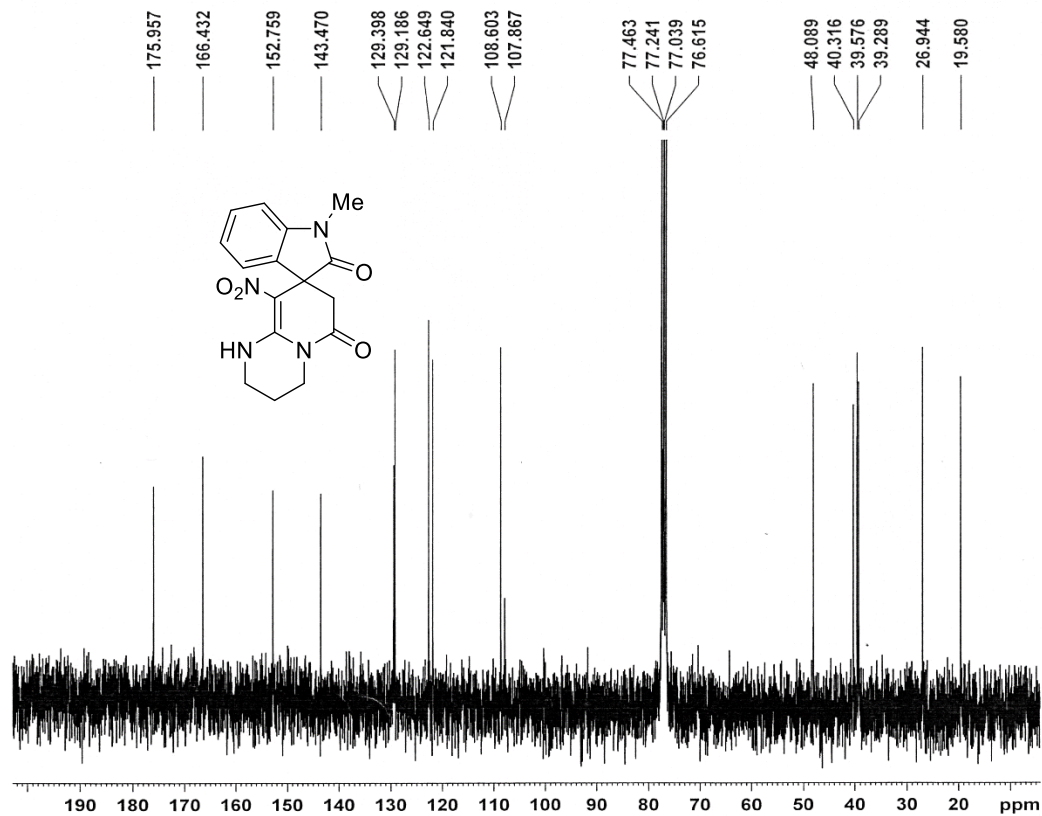
Mass of 6c

¹H NMR of 5d

In the spectrum taken in DMSO, three carbon signals are lost, but when the chloroform was used (which solves product **5d** well), the three signals appeared (two spectrums below):



¹³C NMR of **5d** (in DMSO)



¹³C NMR of 5d (in CDCl₃)

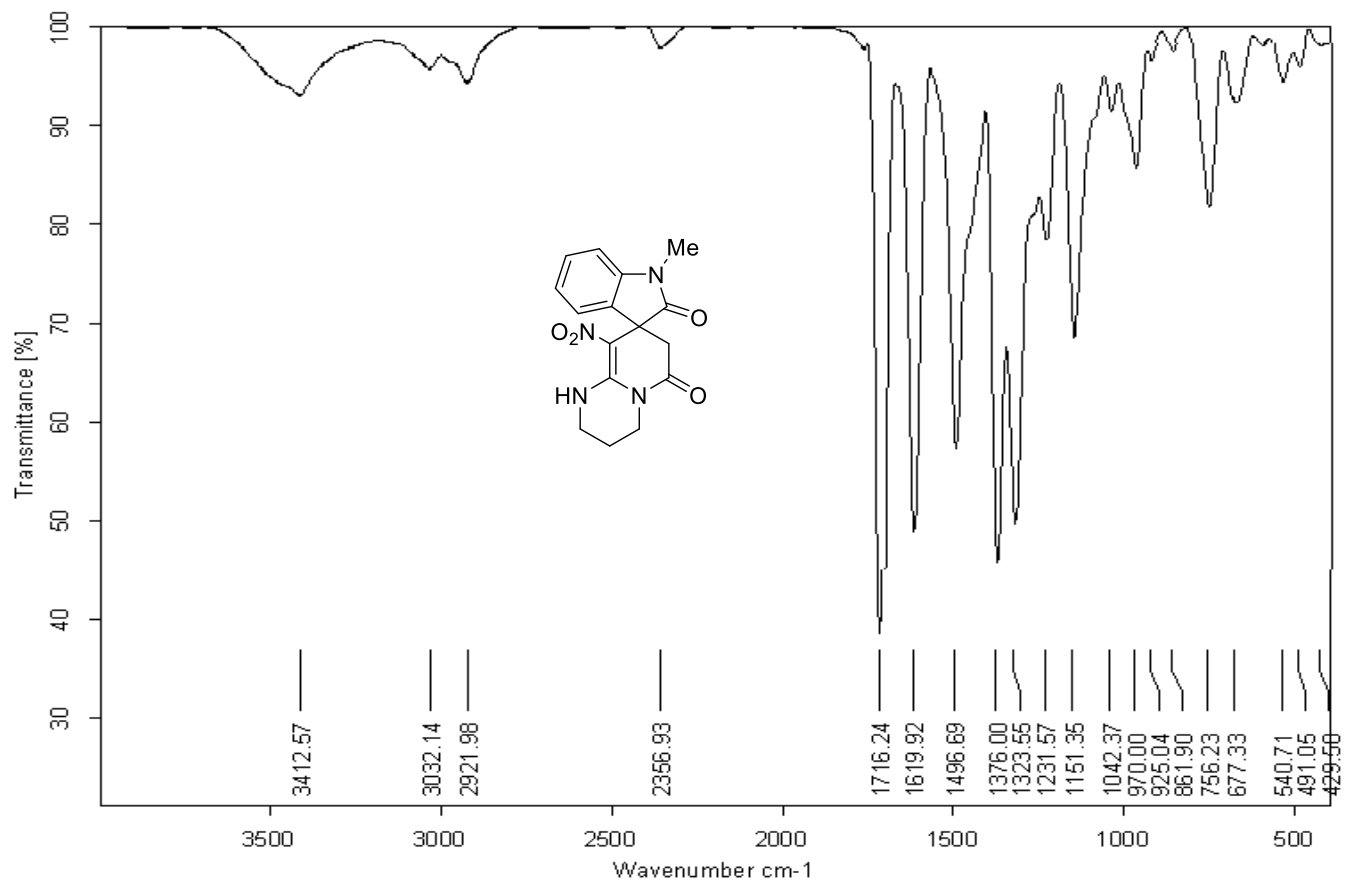
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 PULPROG zgpg
 TD 65536
 SOLVENT DMSO
 NS 1000
 DS 0
 SWH 15822.785 Hz
 FIDRES 0.241437 Hz
 AQ 2.0709877 sec
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 d11 0.03000000 sec
 d12 0.00002000 sec

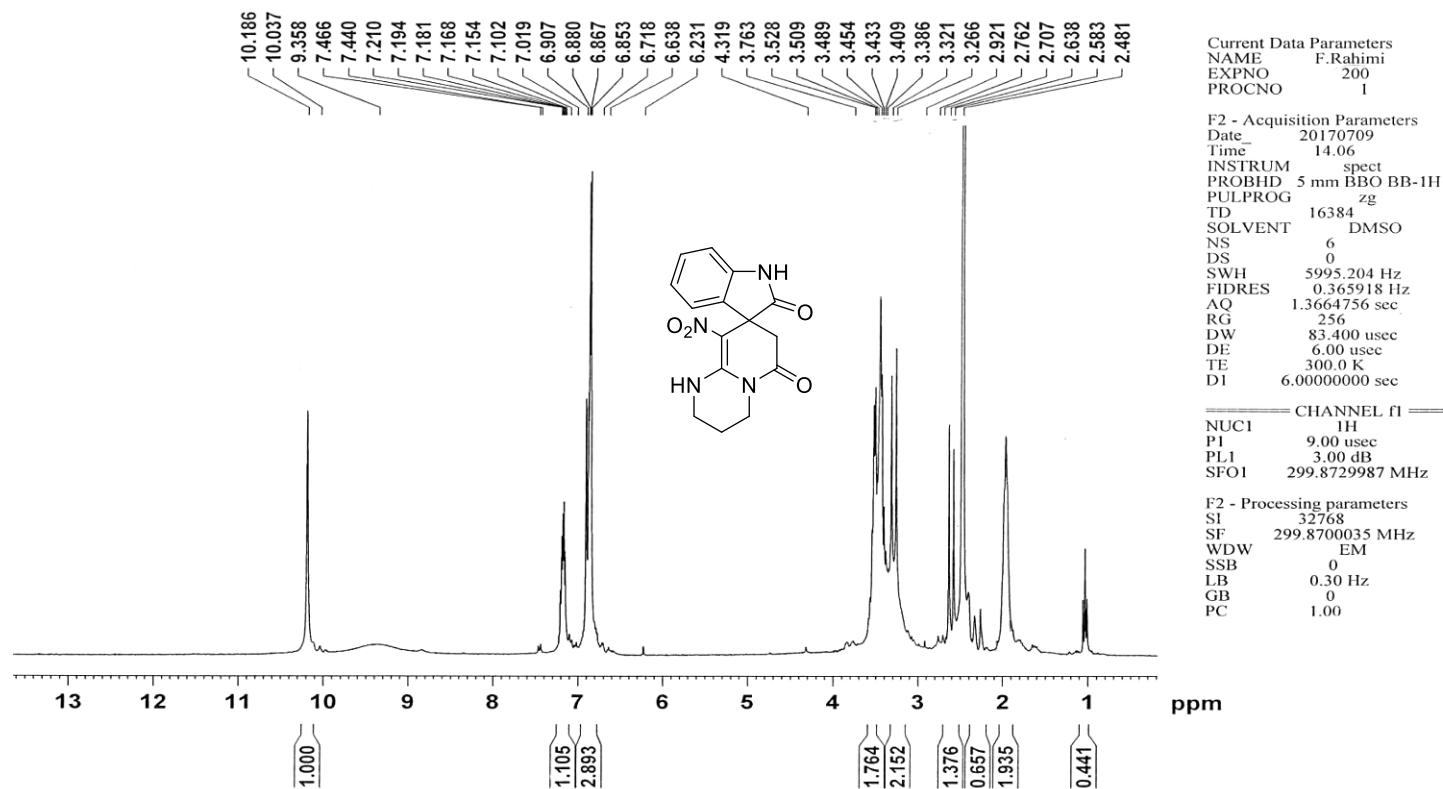
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===== CHANNEL f2 =====
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 PCPD2 80.00 usec
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 PL12 23.00 dB
 PL13 23.00 dB
 SFO2 299.8711995 MHz

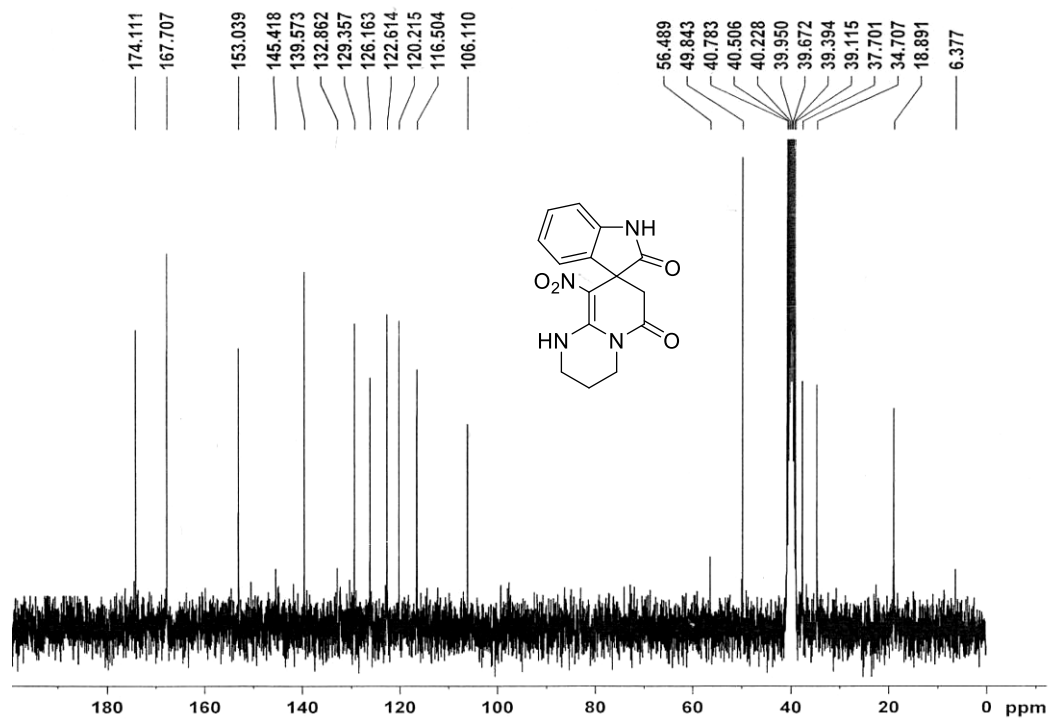
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IR of 5d



¹H NMR of 5e

 ^{13}C NMR of 5e

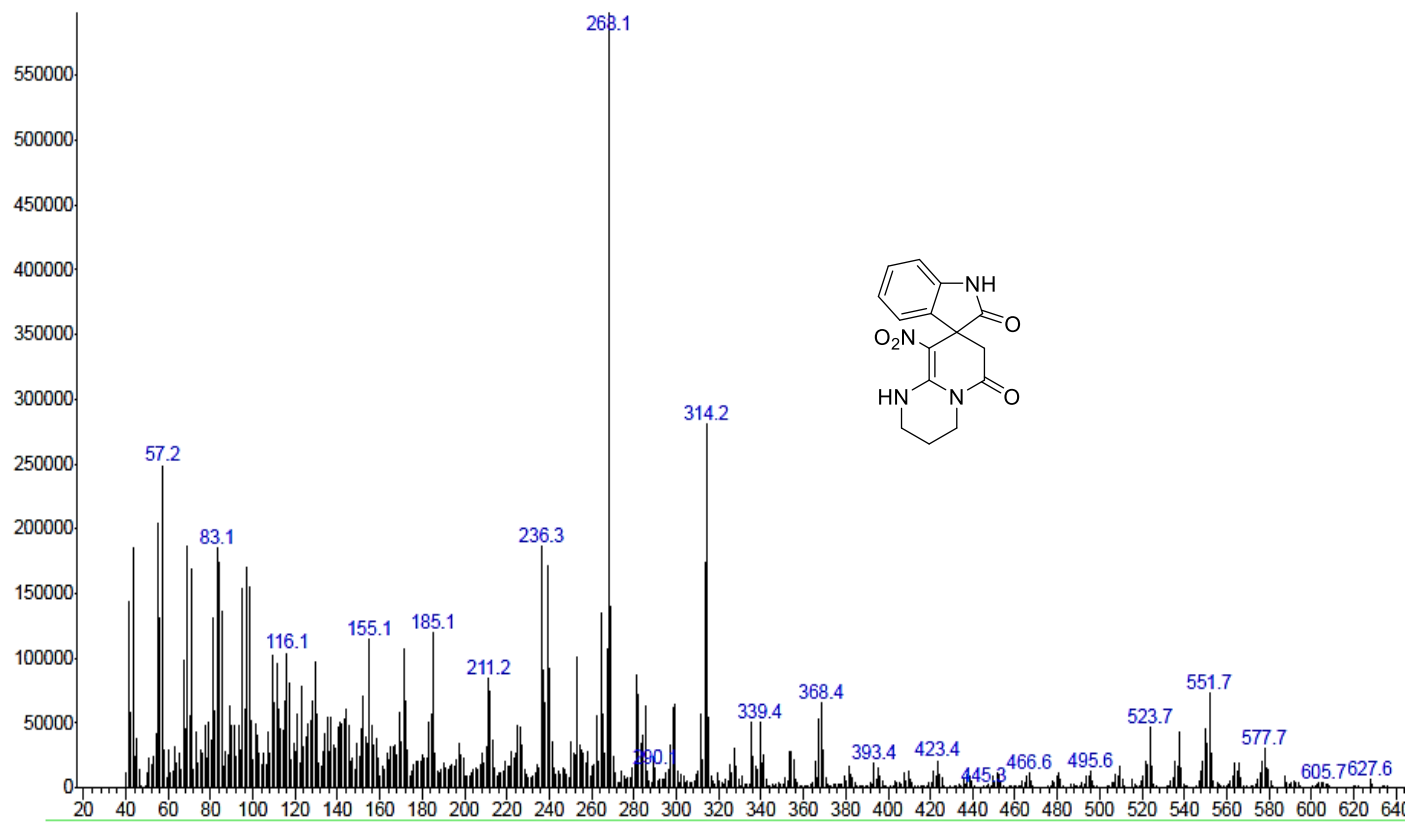
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 EXPNO 218
 PROCNO 1

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 PULPROG zgpg
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 NS 500
 DS 0
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 FIDRES 0.241437 Hz
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 D1 4.00000000 sec
 d11 0.03000000 sec
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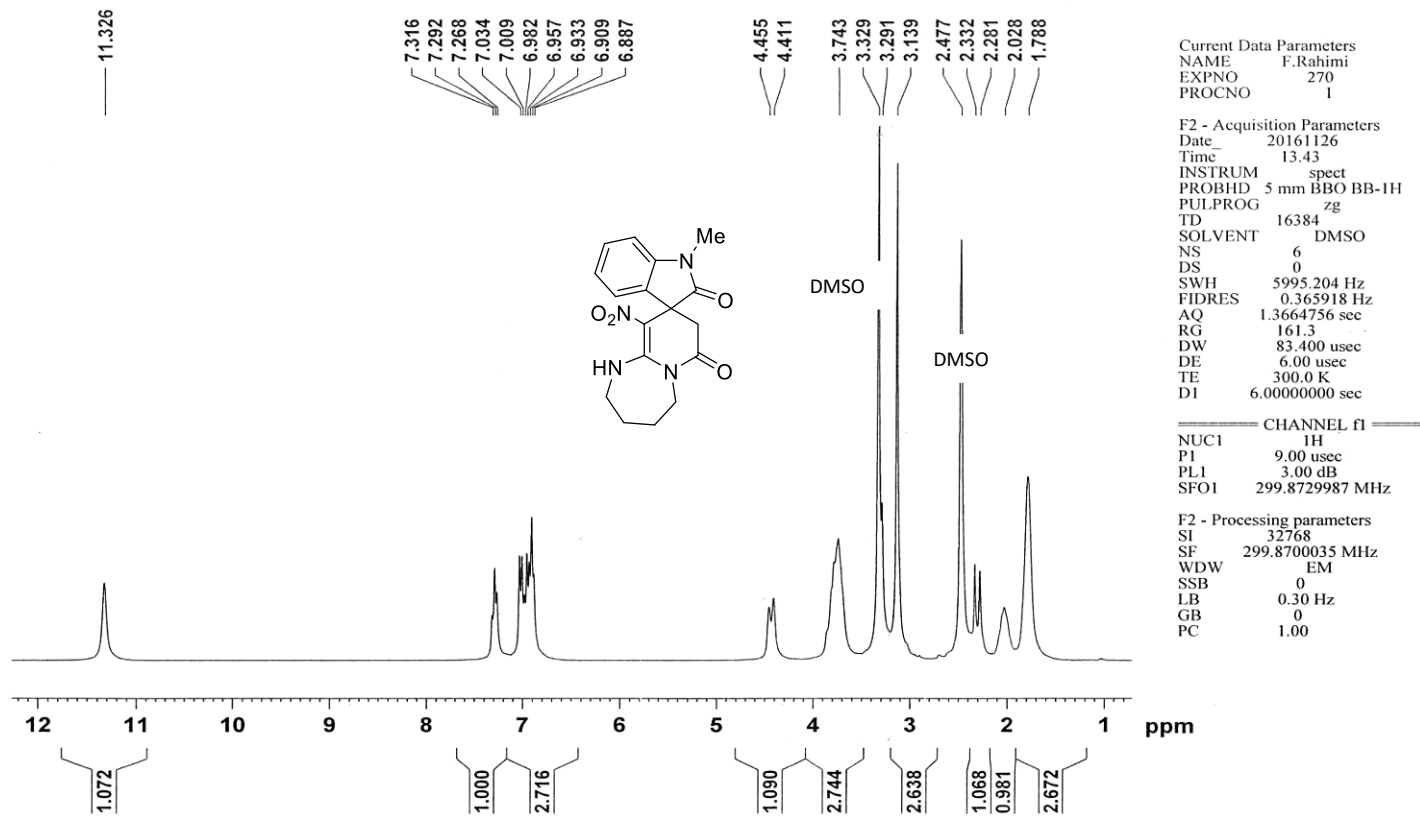
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 PL1 -6.00 dB
 SFO1 75.4102882 MHz

===== 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

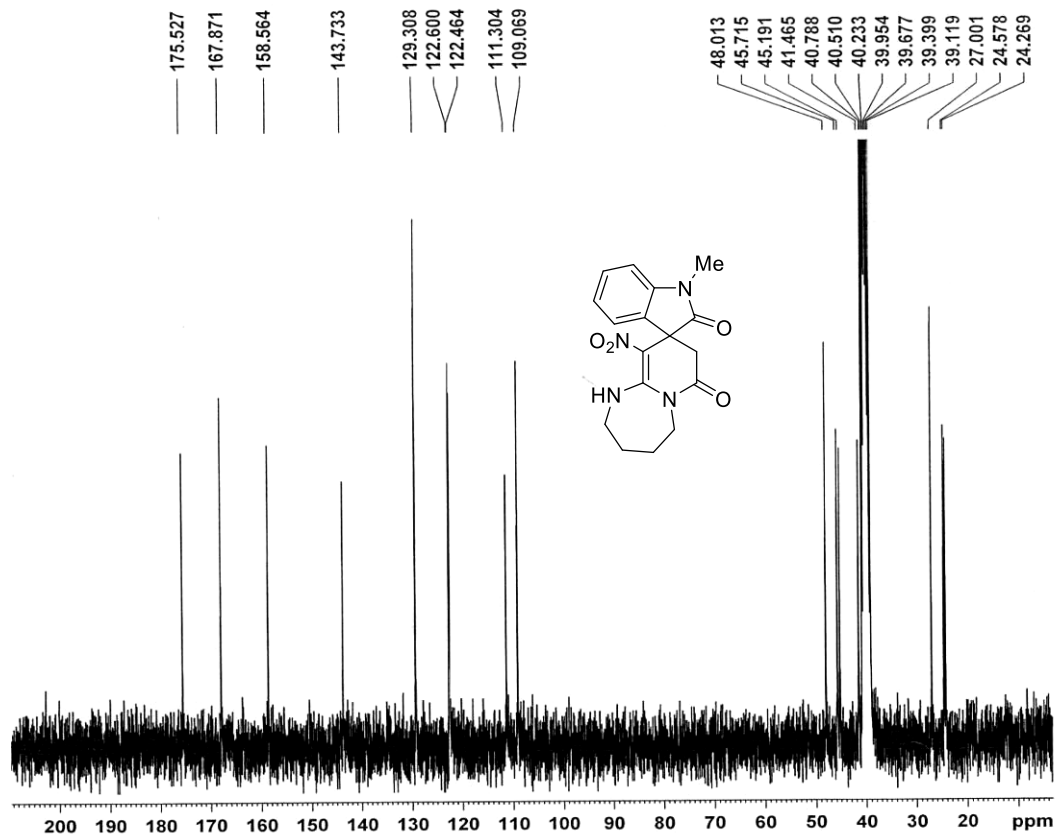
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Mass of 5e



¹H NMR of 5f



Current Data Parameters
 NAME F.Rahimi
 EXPNO 276
 PROCNO 1

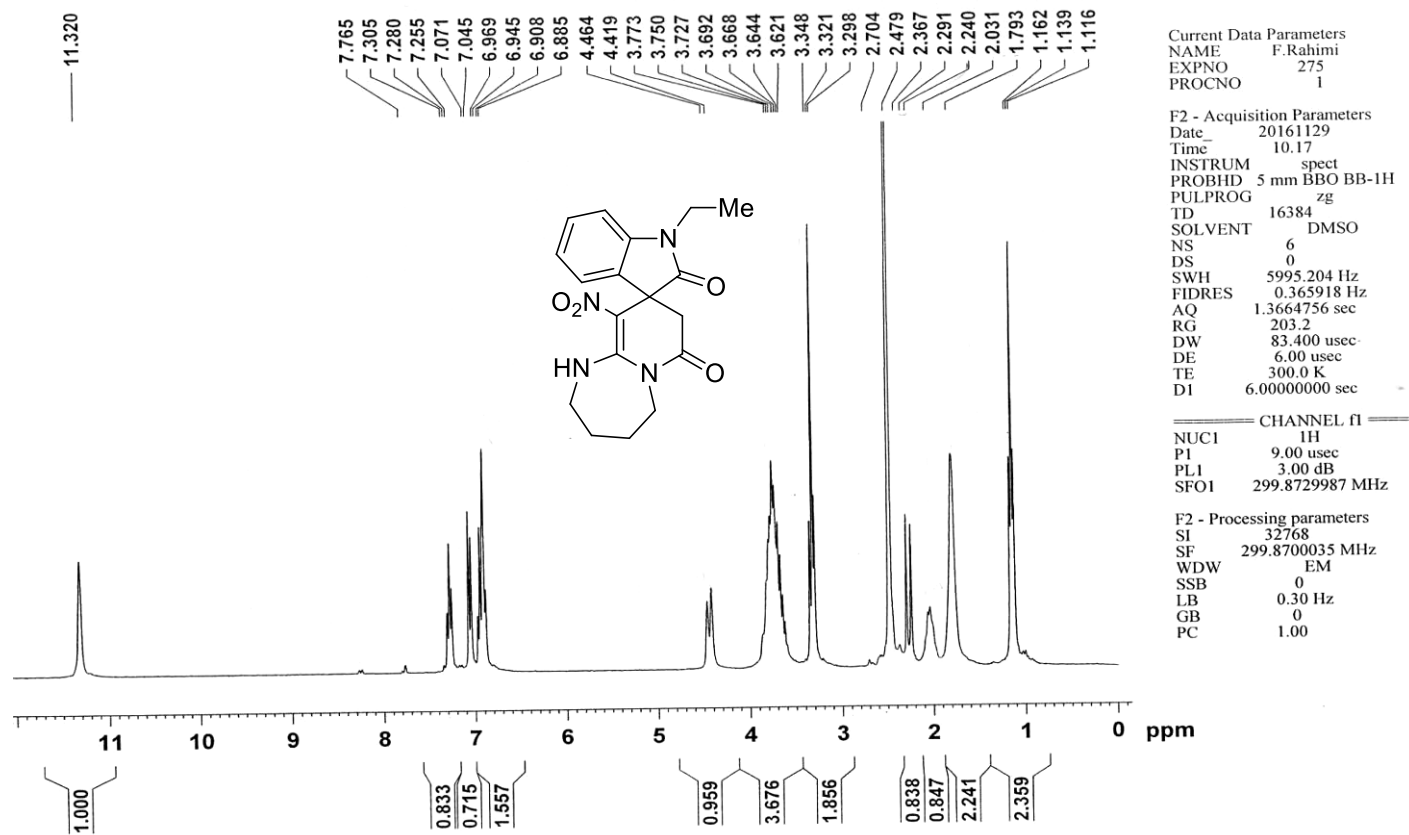
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 NS 500
 DS 0
 SWH 15822.785 Hz
 FIDRES 0.241437 Hz
 AQ 2.0709877 sec
 RG 32768
 DW 31.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 4.00000000 sec
 d11 0.03000000 sec
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===== CHANNEL f1 =====
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 PL1 -6.00 dB
 SFO1 75.4102882 MHz

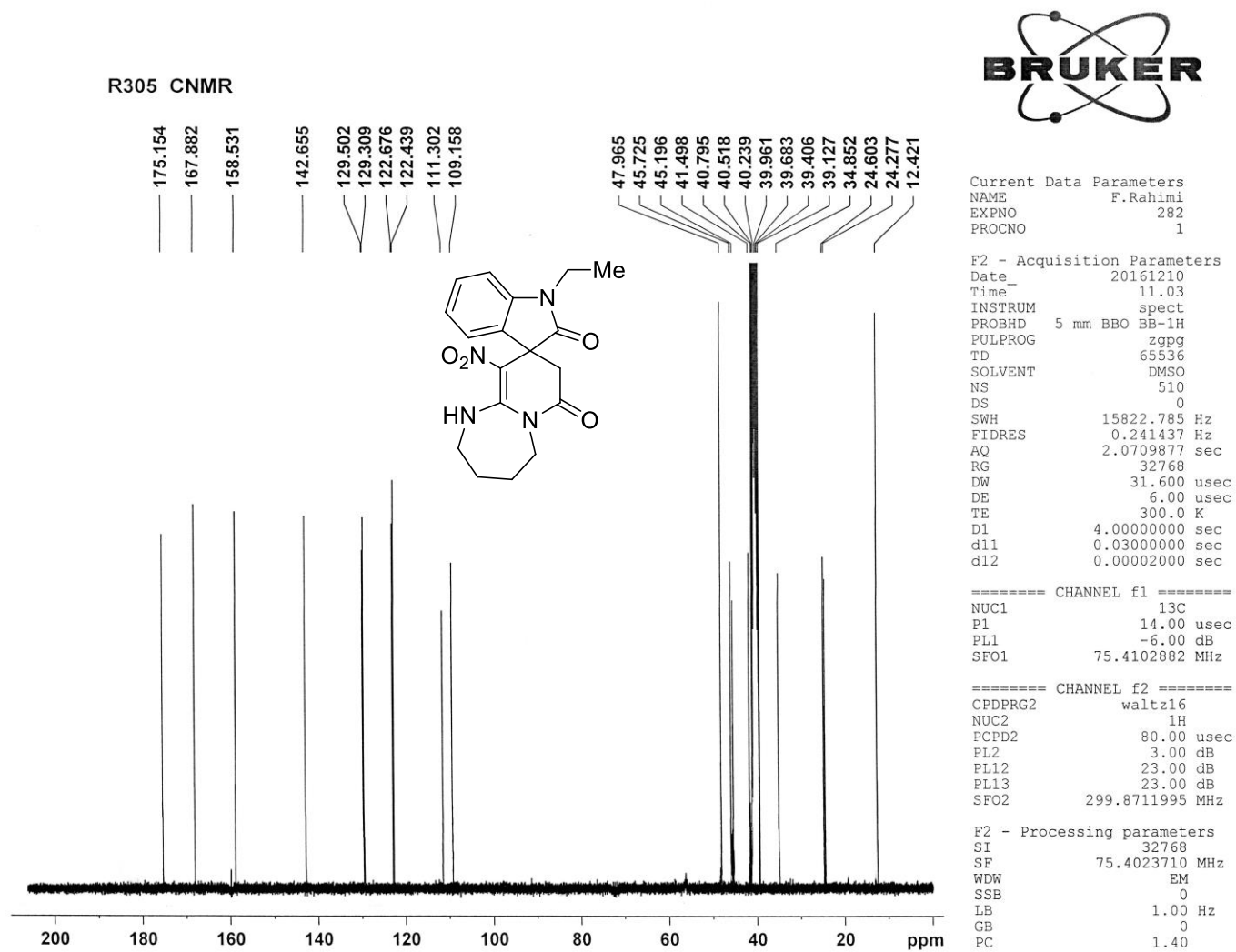
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 PL2 3.00 dB
 PL12 23.00 dB
 PL13 23.00 dB
 SFO2 299.8711995 MHz

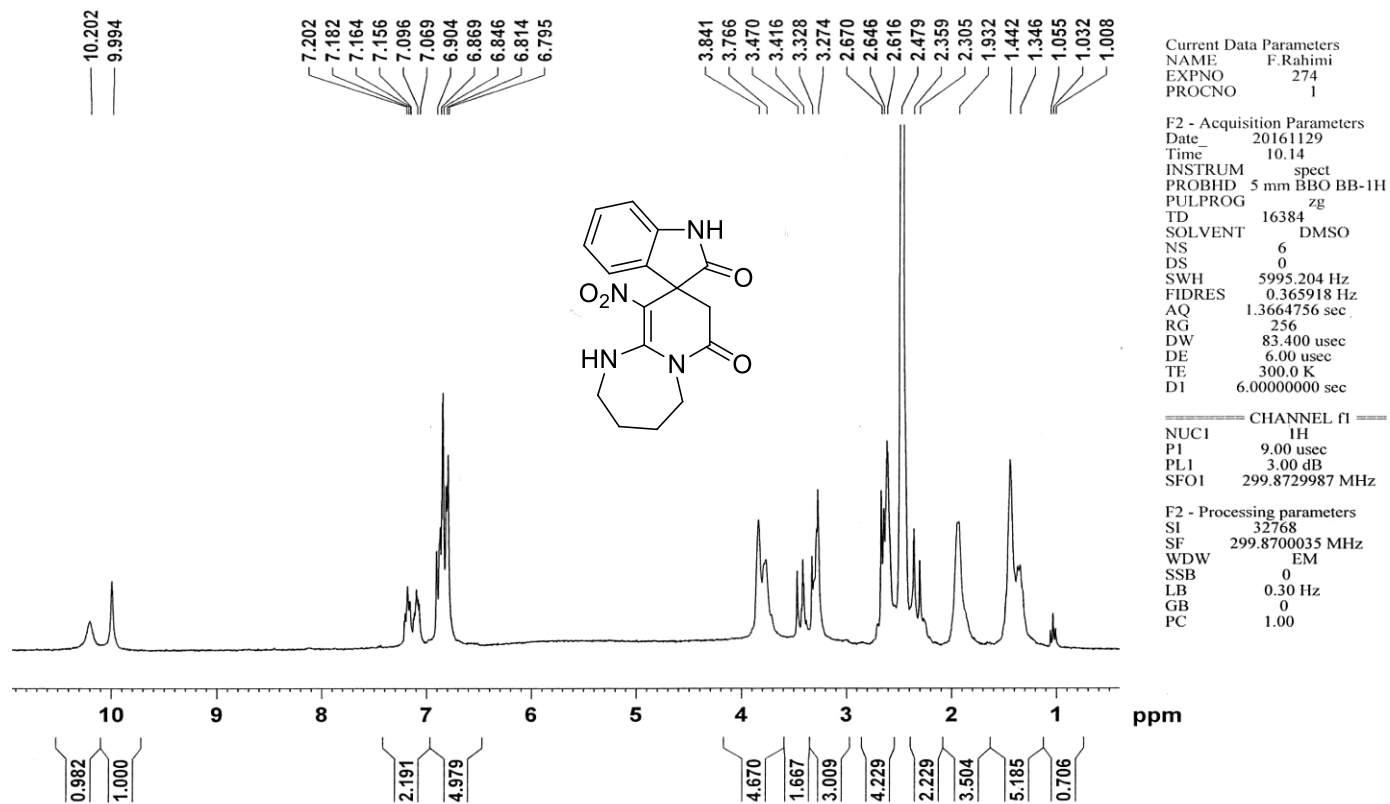
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¹³C NMR of 5f

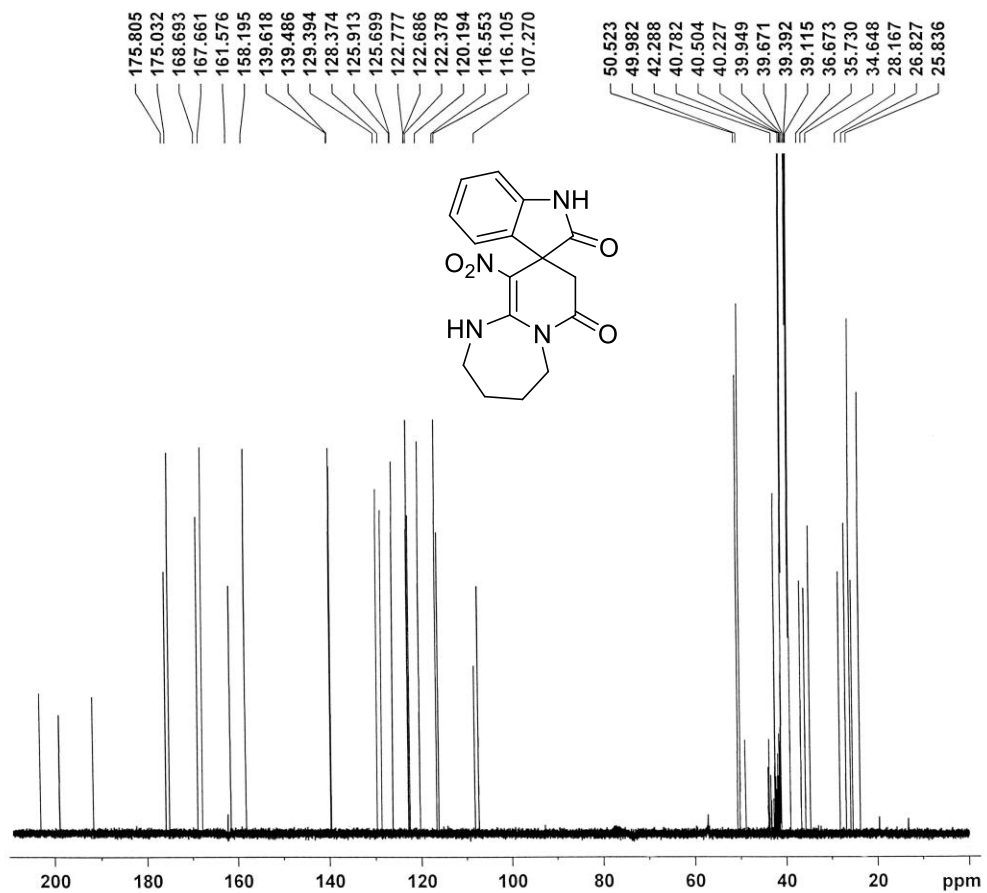


¹H NMR of 5g





R234/3 CNMR



Current Data Parameters
 NAME F. Rahimi
 EXPNO 281
 PROCNO 1

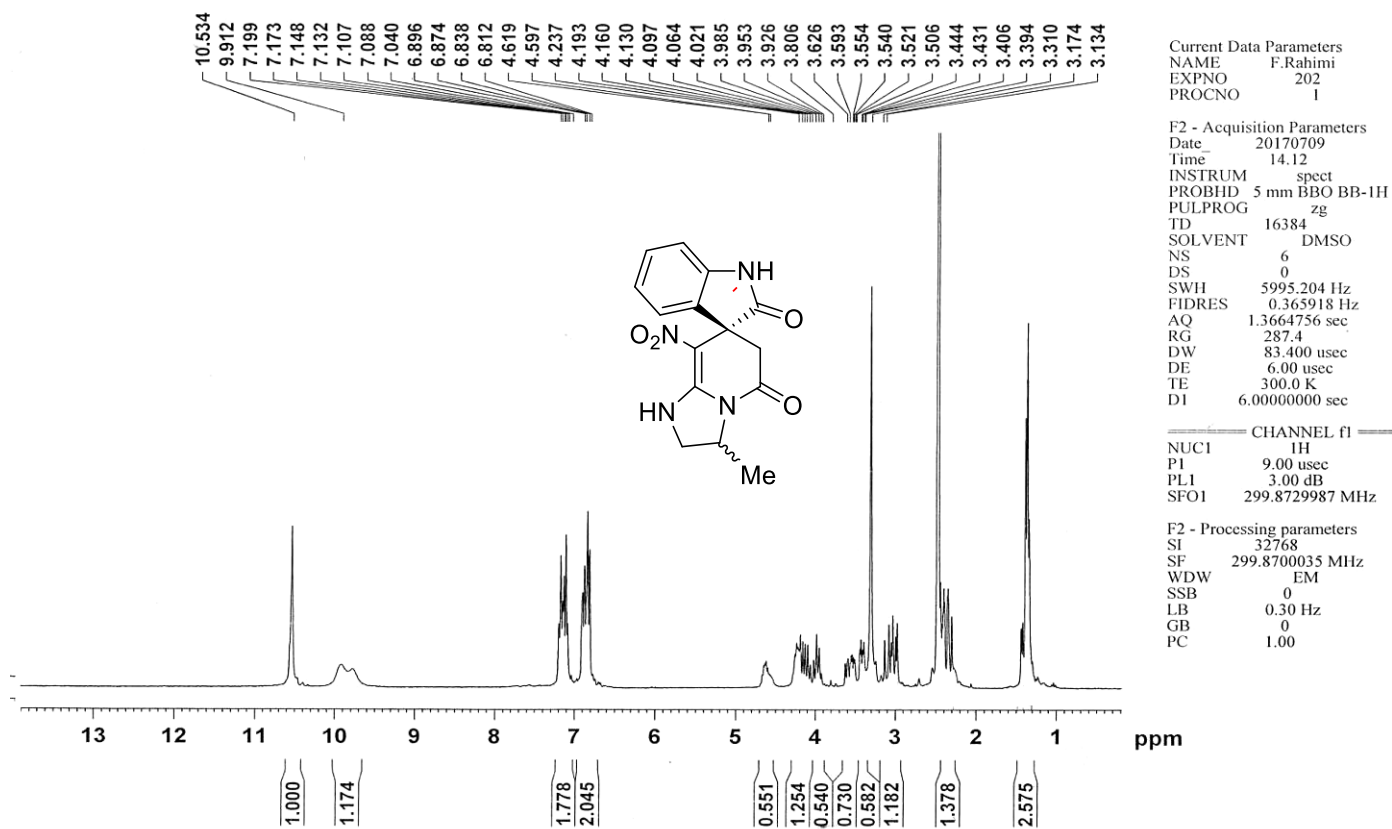
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 FIDRES 0.241437 Hz
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 RG 32768
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 TE 300.0 K
 D1 4.0000000 sec
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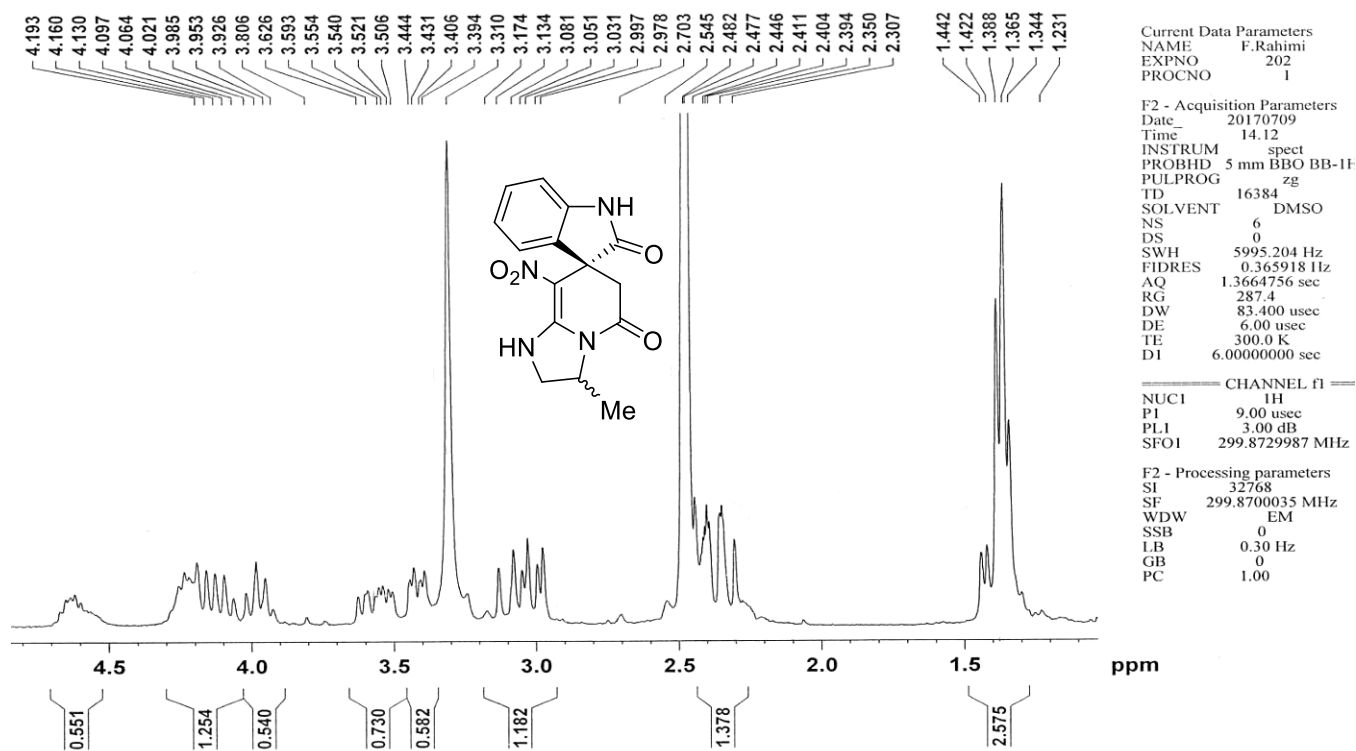
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 PL12 23.00 dB
 PL13 23.00 dB
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F2 - Processing parameters
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 WDW EM
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 GB 0
 PC 1.40

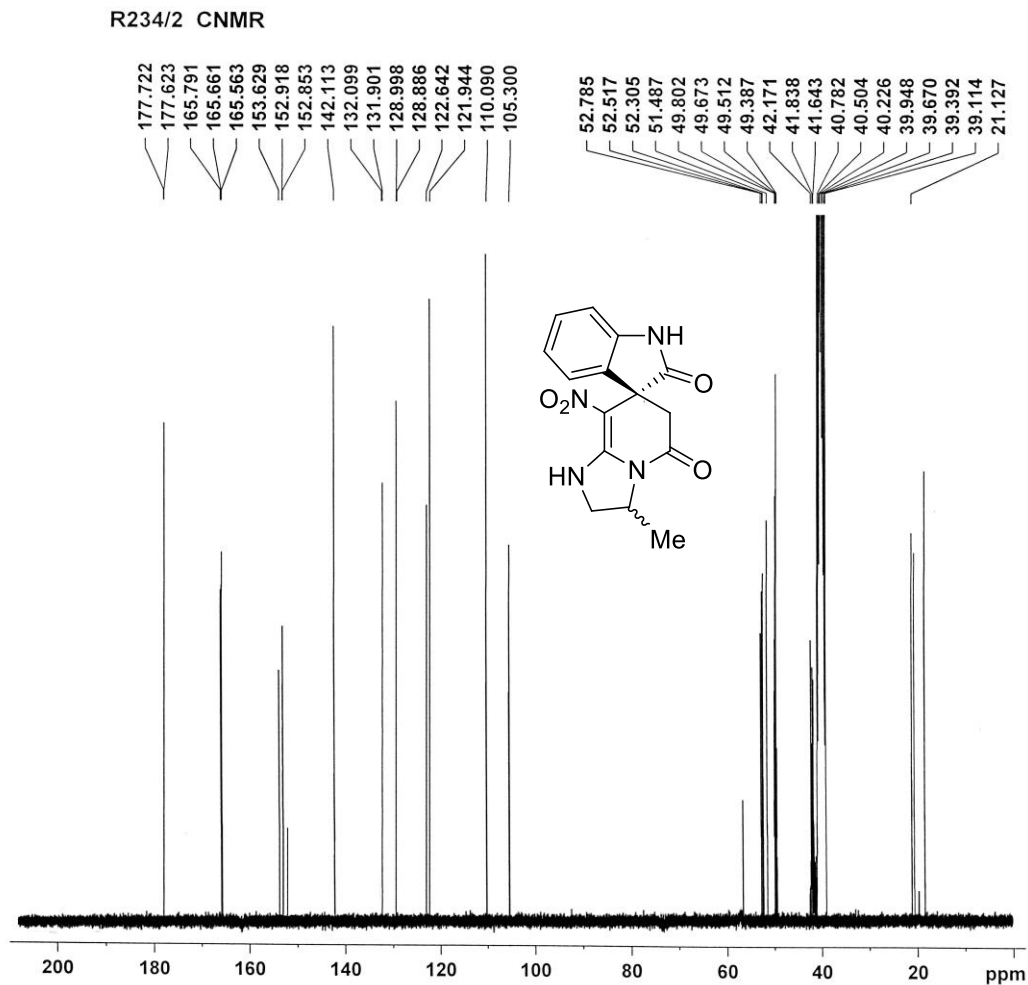
¹³C NMR of 5h



¹H NMR of 5i



¹H expand of 5i



Current Data Parameters
 NAME F.Rahimi
 EXPNO 217
 PROCNO 1

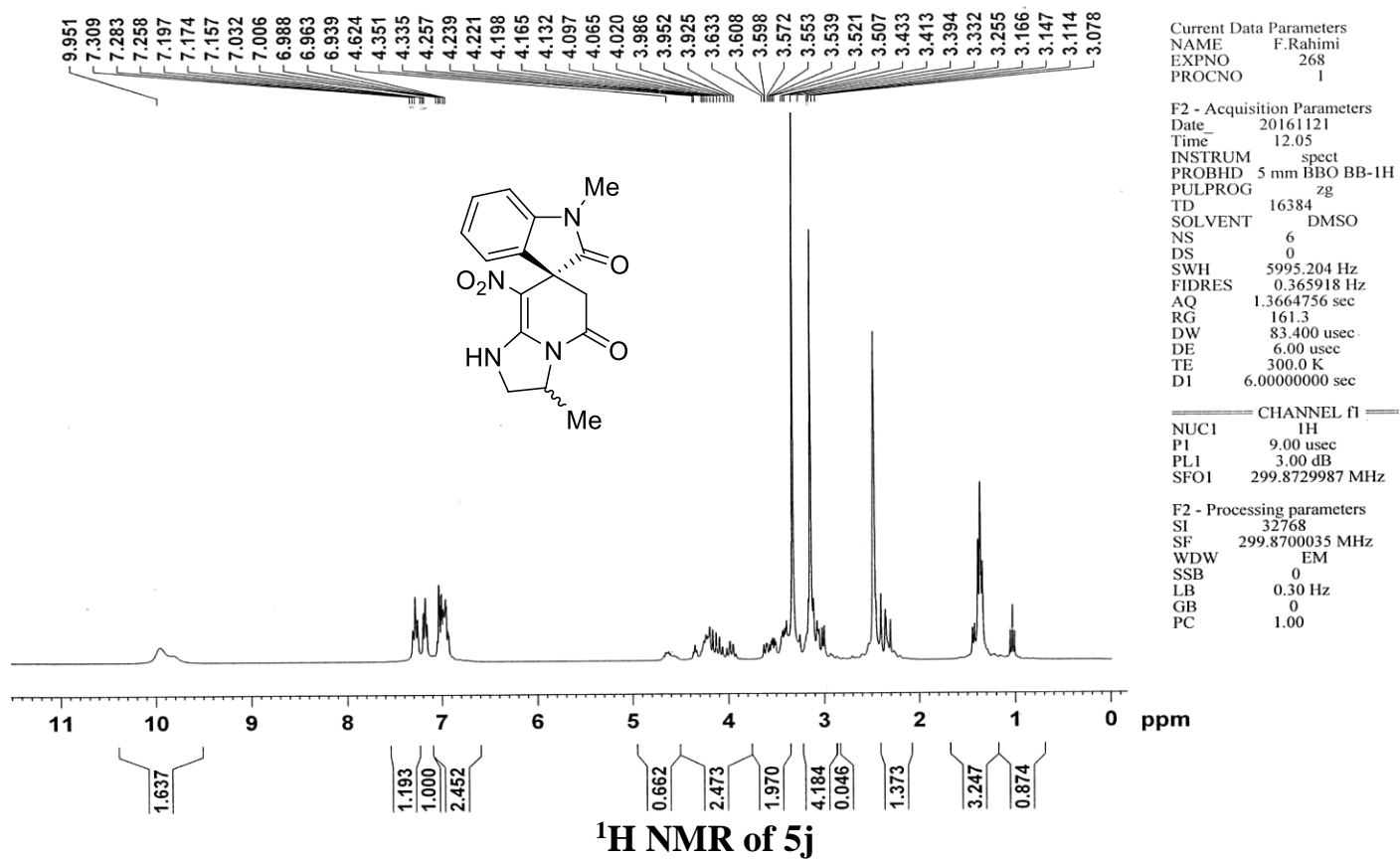
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 DS 0
 SWH 15822.785 Hz
 FIDRES 0.241437 Hz
 AQ 2.0709877 sec
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 DW 31.600 usec
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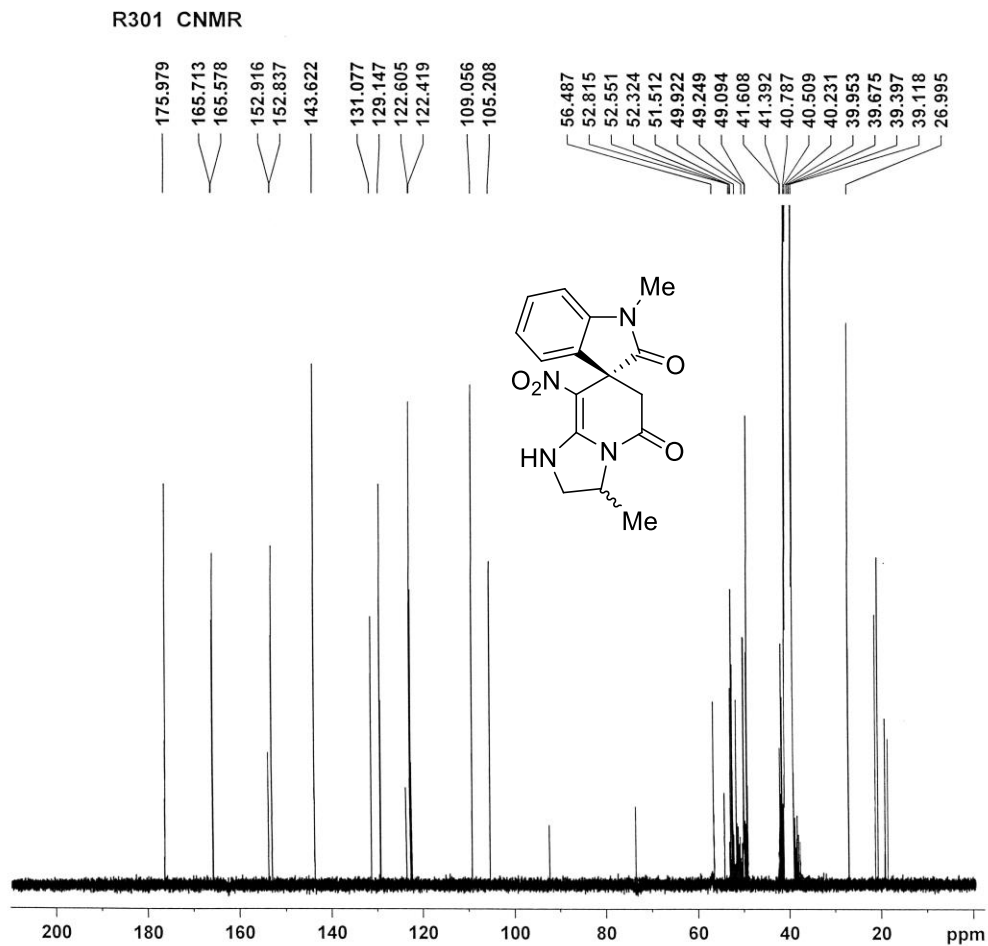
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 PL2 3.00 dB
 PL12 23.00 dB
 PL13 23.00 dB
 SFO2 299.8711995 MHz

F2 - Processing parameters
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 SSB 0
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 GB 0
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¹³C NMR of 5i





Current Data Parameters
 NAME F.Rahimi
 EXPNO 269
 PROCNO 1

F2 - Acquisition Parameters
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 SOLVENT DMSO
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 FIDRES 0.241437 Hz
 AQ 2.0709877 sec
 RG 32768
 DW 31.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 4.0000000 sec
 d11 0.0300000 sec
 d12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 14.00 usec
 PL1 -6.00 dB
 SFO1 75.4102882 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
 PC 1.40

^{13}C NMR of 5j