Supplementary materials

Design, Synthesis, Anticancer Activity, and Solid Lipid Nanoparticle Formulation of Indole-Based Compounds as Novel Pro-Apoptotic Agents Targeting Bcl-2 Protein

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Additional Experimental Detail

1) **Table S1:** The Data of Ligand-Docking Studies on Bcl-2 anti-apoptotic protein target.

2) **Figure S1:** Standard calibration curve of 8b using HPLC-UV analysis. All data are represented as mean of three independent experiments ± SEM.

3) **Figure S2:** NMR spectra of all new compounds

Table S1: The Data of Ligand-Docking Studies on Bcl-2 anti-apoptotic protein target

Ligand name	MOE docking Scores (*S*) [a] (Kcal moL^{-1})	RMSD [b] (Å)	Ligand-target interaction description [Type; Length (Å); Angle (°); Binding Residues]
3a	-4.2200	1.7838	Hydrogen bonding ; 2.51 **Å** ; 148.0° ; Asp111-C=**O** side chain with benzimidazole (N**H**) ring π-π stacking ; 3.85 **Å** ; Tyr108 side chain with benzimidazole ring
7b	-4.7696	1.5547	Hydrogen bonding ; 2.98 **Å** ; 112.5° ; Arg146-=N**H**H side chain with 4-Me**O**
7d	-4.5808	1.7670	Hydrogen bonding ; 2.10 **Å** ; 149.9° ; Arg146-=N**H**H side chain with pyridine (**N**) ring π-Hydrogen contact ; 4.15 **Å** ; Leu137 side chain with pyridine ring π-Hydrogen contact ; 4.17 **Å** ; Leu137 side chain with pyridine ring
8a	-4.7696	1.2117	Hydrogen bonding ; 2.10 **Å** ; 158.7° ; Arg146–N**H**H side chain with NHC=**O** linker
8b	-4.8585	1.6829	Hydrogen bonding ; 2.15 **Å** ; 175.5° ; Arg146–N**H**H side chain with NHC=**O** linker
8c	-6.2460	1.7374	Hydrogen bonding ; 2.66 **Å** ; 129.0° ; Arg146–N**H**H side chain with indole (**N**H) ring π-Hydrogen interaction ; 3.33 **Å** ; Arg146-N**H** side chain with indole ring
8d	-6.1846	1.3960	Hydrogen bonding ; 2.08 **Å** ; 156.0° ; Arg146–N**H**H side chain with NHC=**O** linker Hydrogen bonding ; 2.53 **Å** ; 142.5° ; Arg146-N**H** side chain with NHC=**O** linker
8f	-5.7070	2.6217	Hydrogen bonding ; 2.30 **Å** ; 160.1° ; Arg146–N**H**H side chain with NHC=**O** linker π-Hydrogen interaction ; 3.10 **Å** ; Arg146-N**H** side chain with indole ring

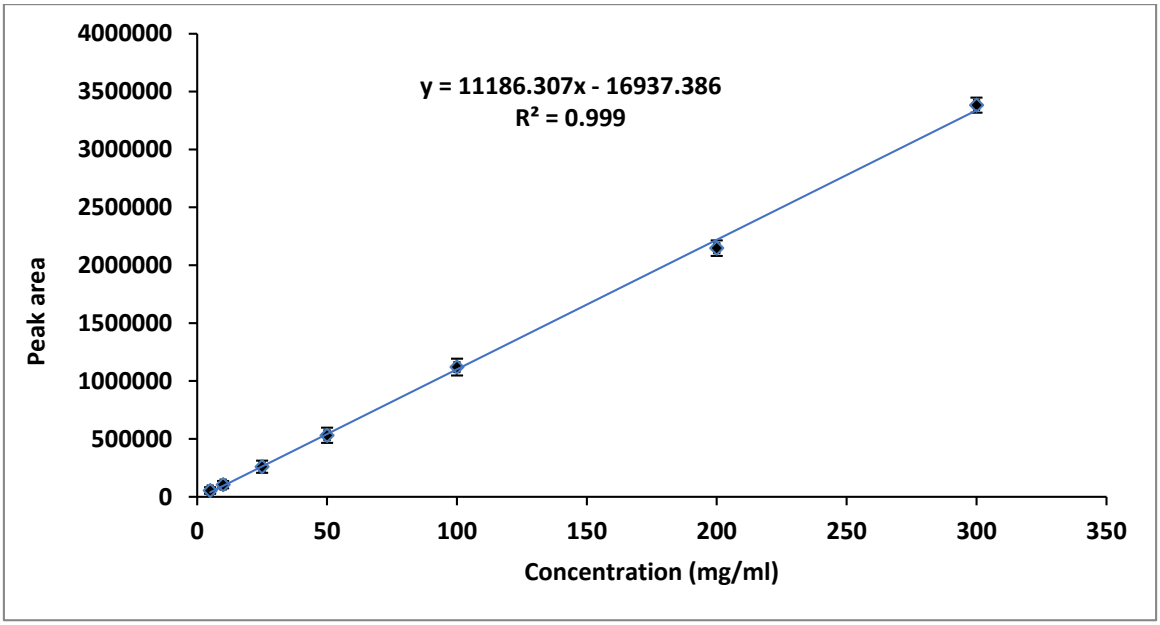
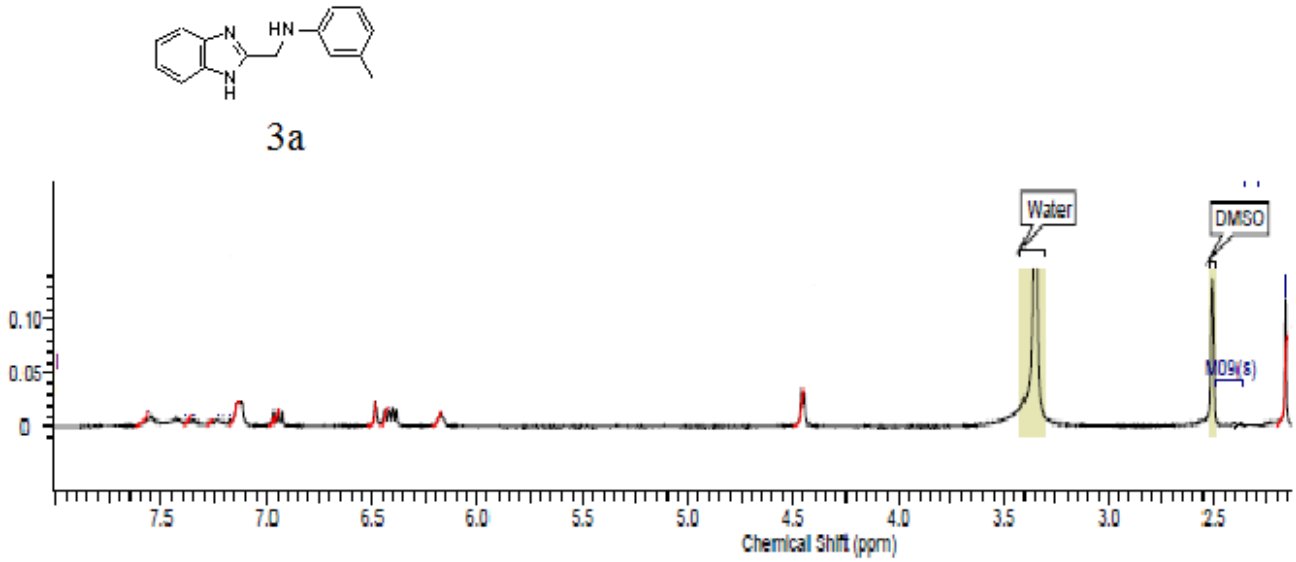
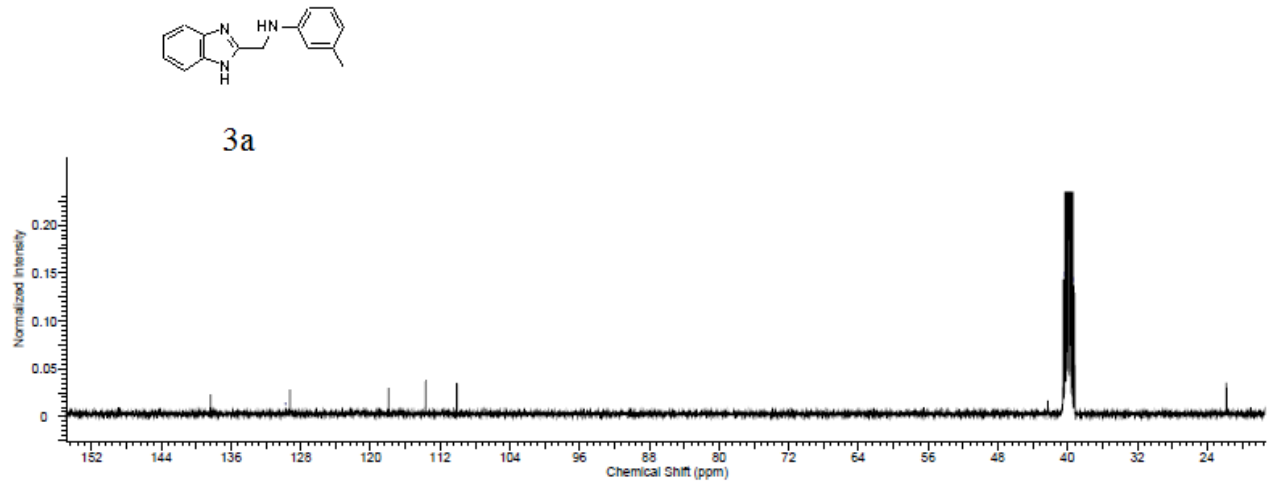
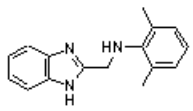


Figure S1: Standard calibration curve of 8b using HPLC-UV analysis. All data are represented as mean of three independent experiments ± SEM.

Figure S2: NMR spectra of all new compounds







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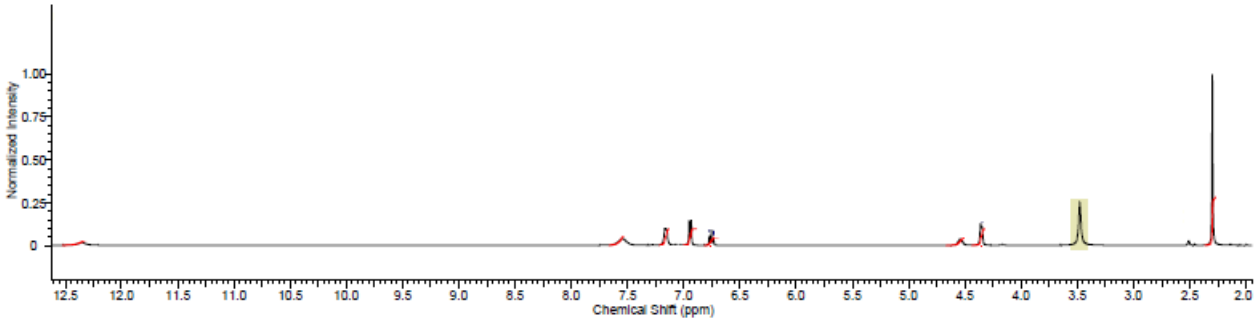

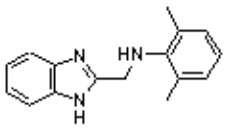

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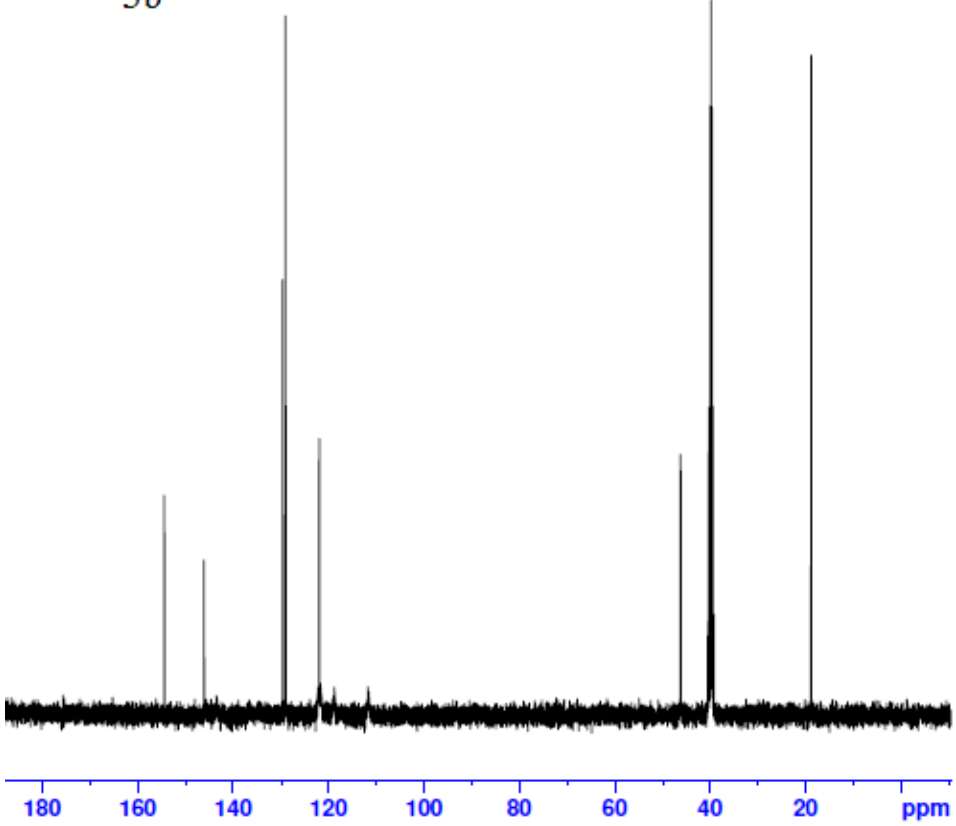

BRUKER

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DE                     6.50 usec
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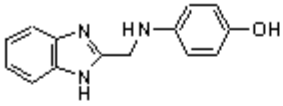

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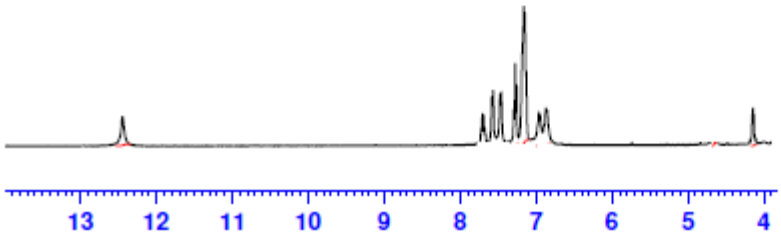


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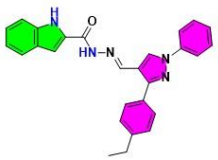

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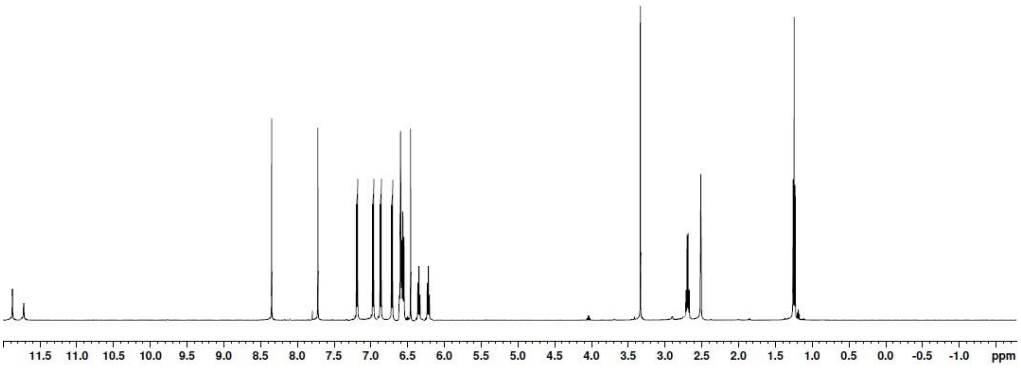

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X_Pulse           = 7.25[us]
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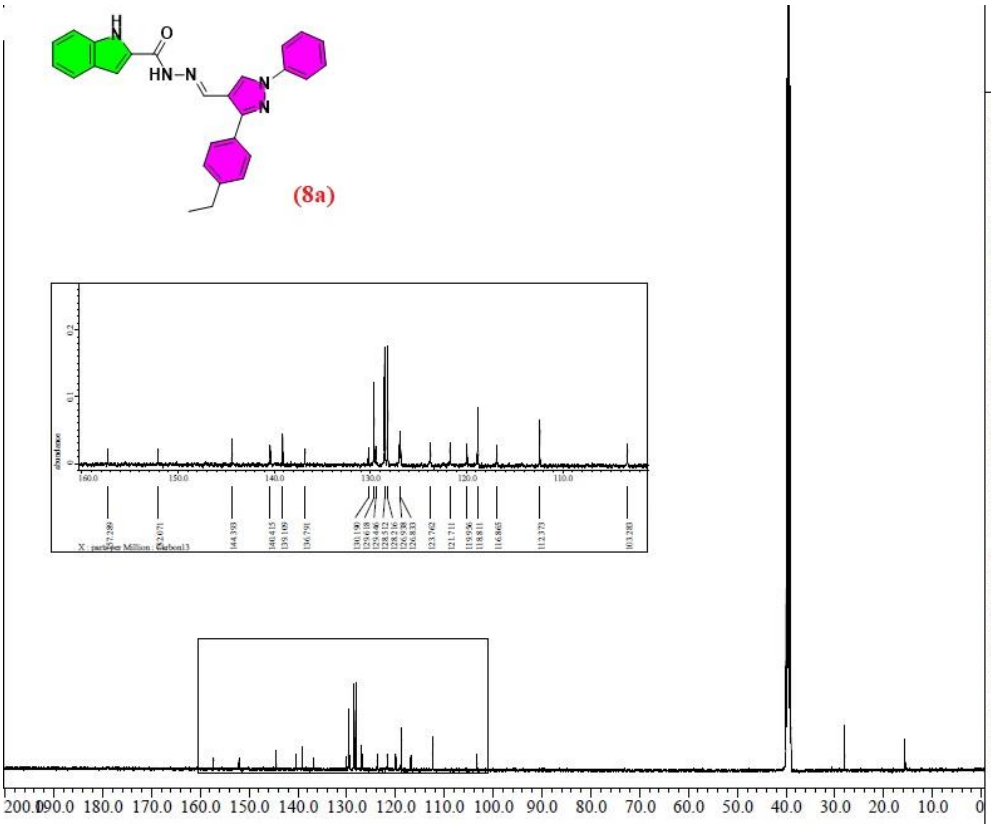
(8a)



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Spectrometer      = DELTA2_NMR

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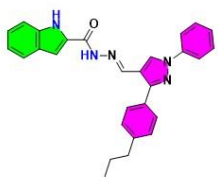

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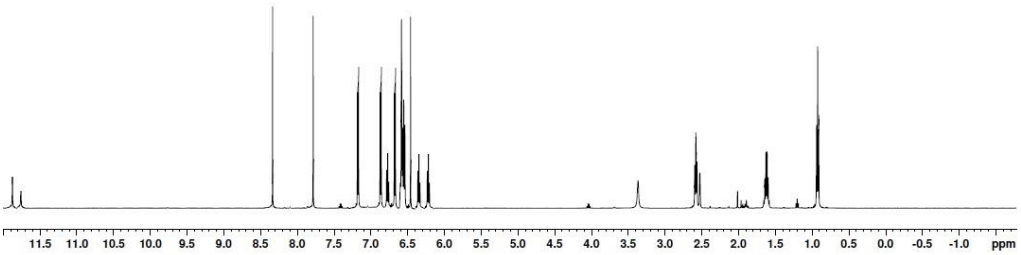

Mansoura University JEOL NMR Unit ECA-500 II

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X_Sweep_Clipped     = 9.00900901[kHz]
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Irr_Freq            = 500.15991521[MHz]
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X_Pulse             = 7.25[us]
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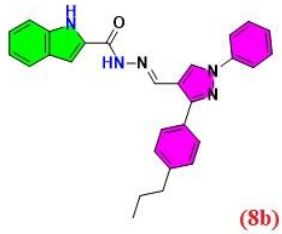

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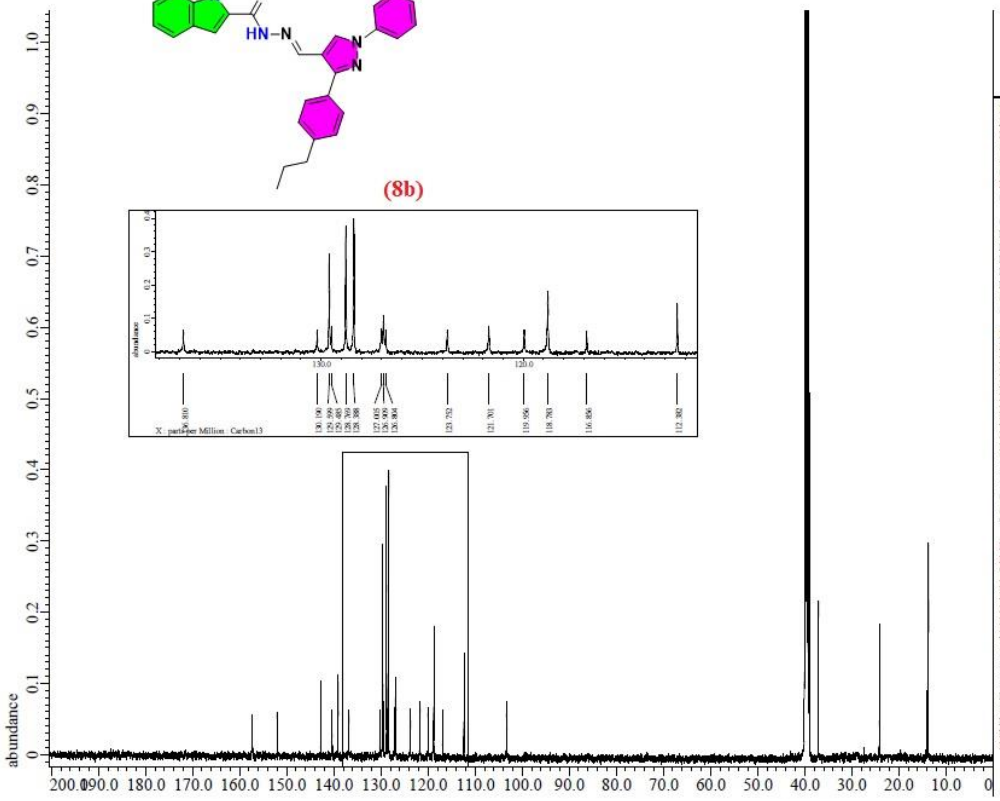

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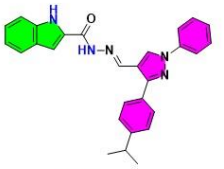

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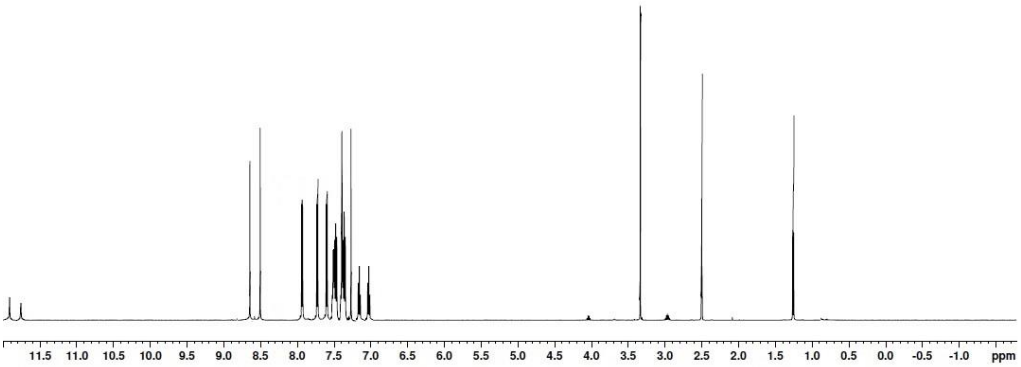

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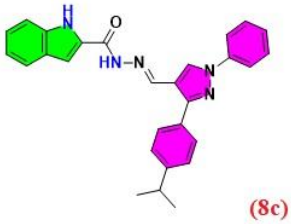

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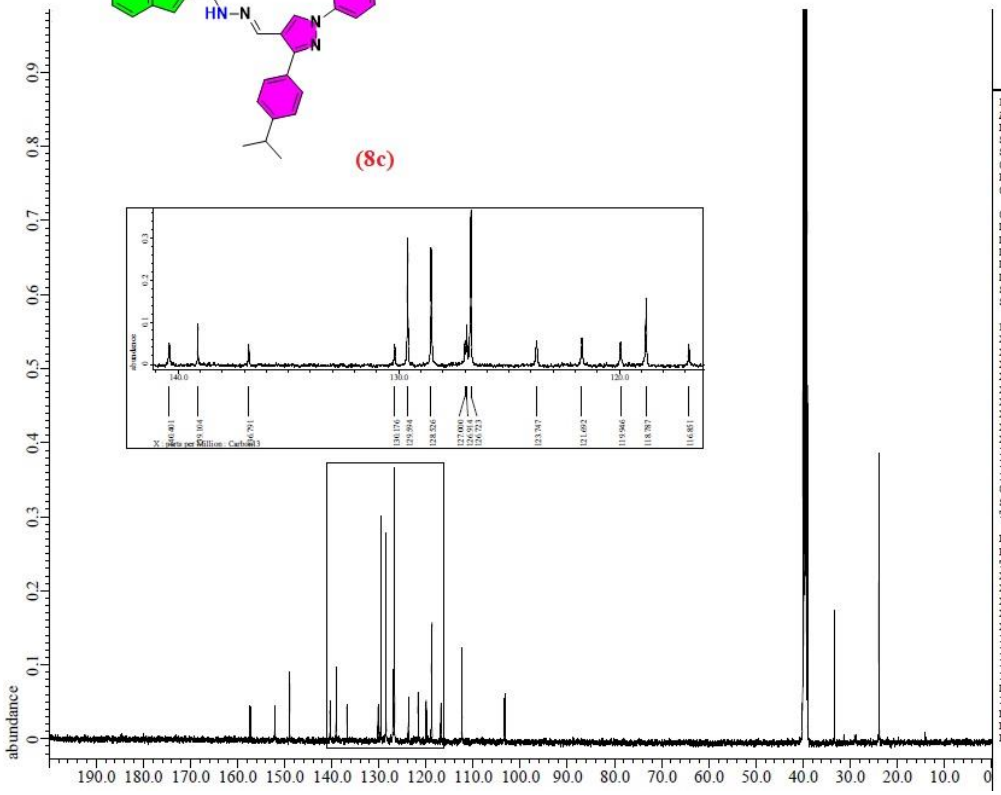

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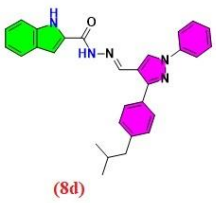
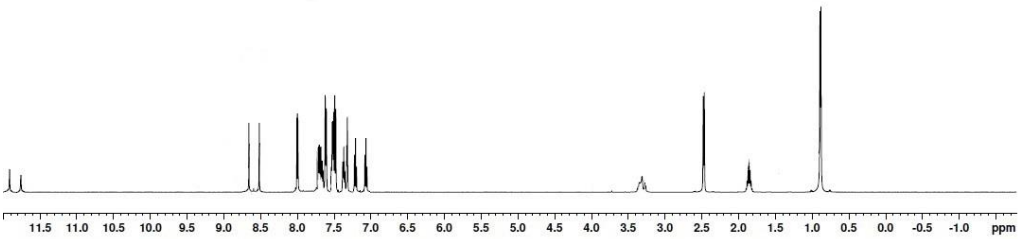
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = TRUE
Scans             = 1750
Total_Scans       = 1750

Relaxation_Delay  = 2[s]
Recvr_Gain        = 58
Temp_Get          = 21.5[dC]
X_90_Width        = 52.78[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 9.7[dB]
X_Pulse           = 17.59333333[us]
Irr_Atn_Dec       = 20.948[dB]
Irr_Atn_Noe       = 20.948[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```



(8d)



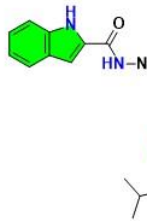
Mansoura University JEOL NMR Unit ECA-500 II

```
Filename          = Manar Nagy_9_proton-1-9
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Manar Nagy_9
Solvent           = DMSO-D6
Creation_Time     = 29-JUL-2019 11:07:21
Revision_Time     = 29-JUL-2019 11:10:03
Current_Time      = 29-JUL-2019 11:11:10

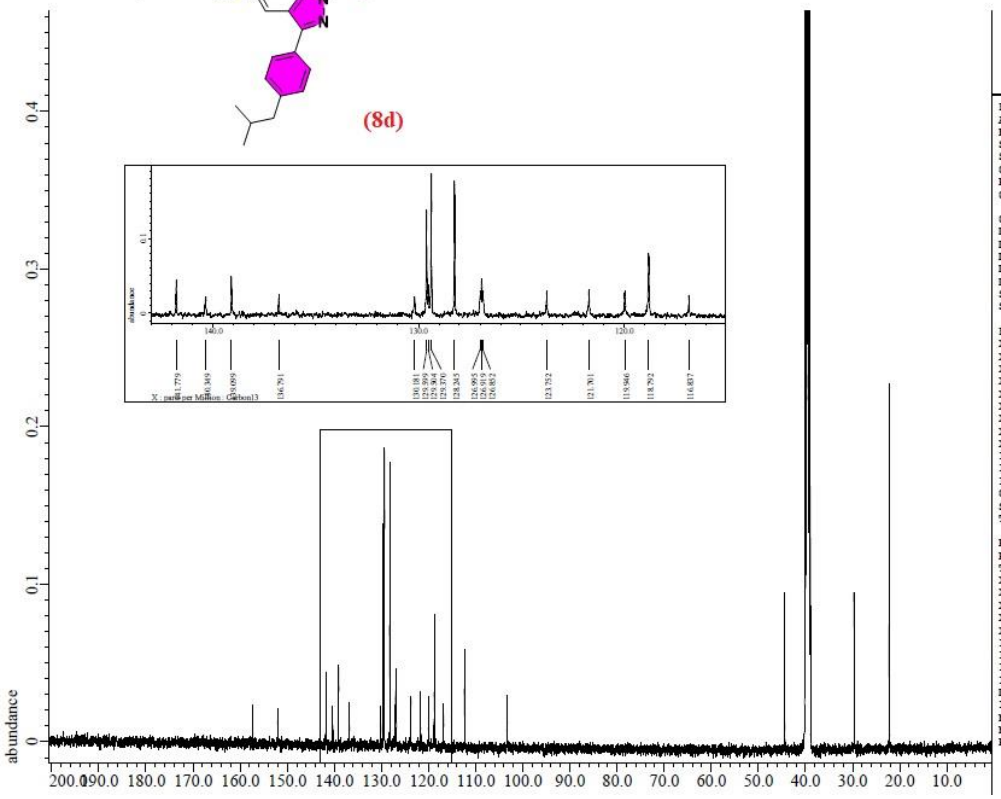
Comment           = single pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500II
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T]  (500[MHz])
X_Acq_Duration    = 1.4548992[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 6[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.68733284[Hz]
X_Sweep           = 11.26126126[kHz]
X_Sweep_Clipped   = 9.00900901[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 40
Total_Scans       = 40

Relaxation_Delay  = 5[s]
Recvr_Gain        = 36
Temp_Get          = 21.1[dC]
X_90_Width        = 14.5[us]
X_Acq_Time        = 1.4548992[s]
X_Angle           = 45[deg]
X_Atn             = 4.9[dB]
X_Pulse           = 7.25[us]
Irr_Mode          = Off
Tri_Mode          = Off
DanTe_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.4548992[s]
```



(8d)



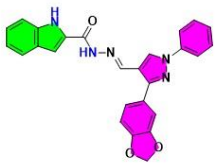
Mansoura University JEOL NMR Unit ECA-500 II

```
Filename          = Manar Nagy_6_carbon-1-7.
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Manar Nagy_6
Solvent           = DMSO-D6
Creation_Time     = 18-AUG-2019 15:56:13
Revision_Time     = 19-AUG-2019 09:16:56
Current_Time      = 19-AUG-2019 09:17:01

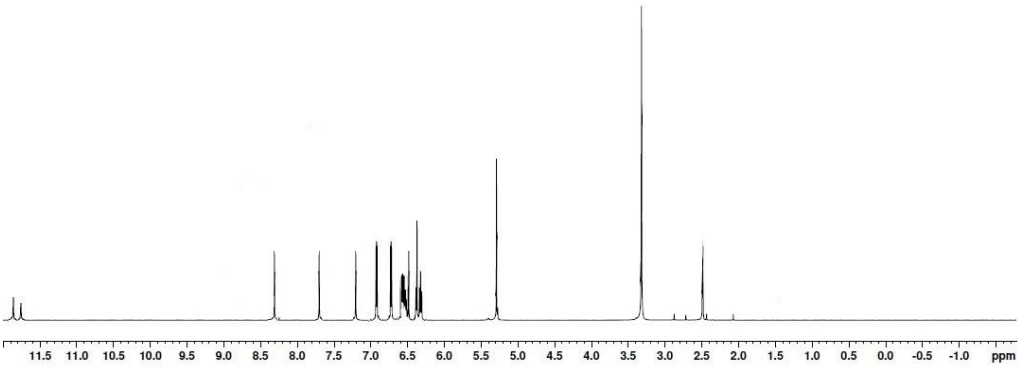
Comment           = single pulse decoupled g
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500II
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T]  (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = TRUE
Scans             = 2500
Total_Scans       = 2500

Relaxation_Delay  = 2[s]
Recvr_Gain        = 58
Temp_Get          = 20[dC]
X_90_Width        = 52.78[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 9.7[dB]
X_Pulse           = 17.59333333[us]
Irr_Atn_Dec       = 20.948[dB]
Irr_Atn_Noe       = 20.948[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```



(8e)



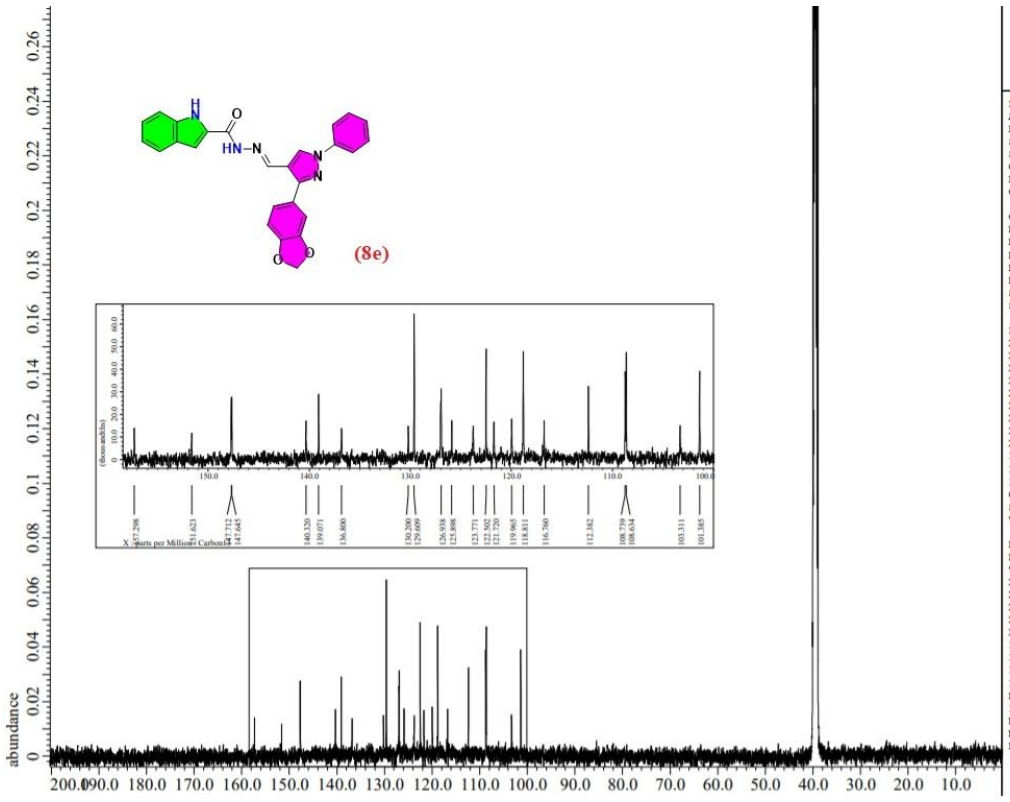
Mansoura University JEOL NMR Unit ECA-500 II

```
Filename          = Manar Nagy10_proton-1-10
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Manar Nagy_10
Solvent           = DMSO-D6
Creation_Time     = 30-JUL-2019 11:47:21
Revision_Time     = 30-JUL-2019 14:10:03
Current_Time      = 30-JUL-2019 14:11:10

Comment           = single pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500II
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T]  (500[MHz]
X_Acq_Duration    = 1.4548992[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 6[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.68733284[Hz]
X_Sweep           = 11.26126126[kHz]
X_Sweep_Clipped   = 9.00900901[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 40
Total_Scans       = 40

Relaxation_Delay  = 5[s]
Recvr_Gain        = 36
Temp_Get          = 21.1[dC]
X_90_Width        = 14.5[us]
X_Acq_Time        = 1.4548992[s]
X_Angle           = 45[deg]
X_Atn             = 4.9[dB]
X_Pulse           = 7.25[us]
Irr_Mode          = Off
Tri_Mode          = Off
DanTe_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.4548992[s]
```



(8e)

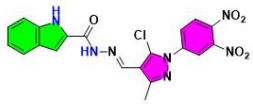
Mansoura University JEOL NMR Unit ECA-500 II

```
Filename          = Manar Nagy_8_carbon-1-1
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Manar Nagy_8
Solvent           = DMSO-D6
Creation_Time     = 18-AUG-2019 20:20:43
Revision_Time     = 19-AUG-2019 09:09:26
Current_Time      = 19-AUG-2019 09:10:27

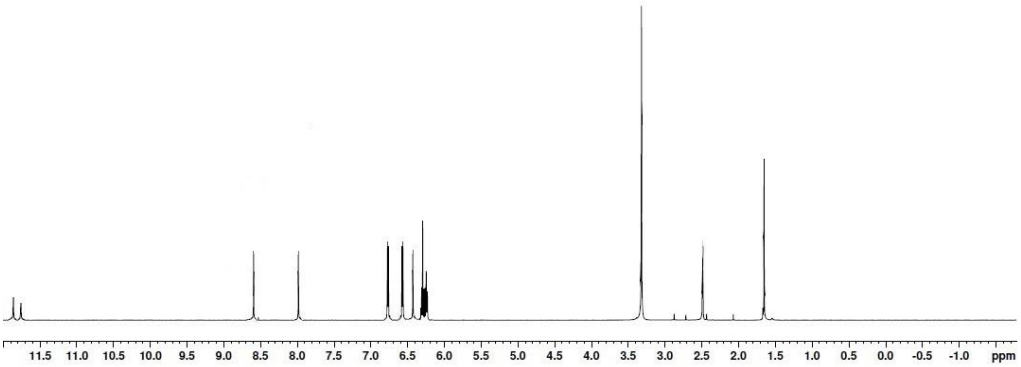
Comment           = single pulse decoupled
Data_Format       = 1D REAL
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500II
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T]  (500[MHz]
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = TRUE
Scans             = 2500
Total_Scans       = 2500

Relaxation_Delay  = 2[s]
Recvr_Gain        = 58
Temp_Get          = 18.3[dC]
X_90_Width        = 52.78[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 9.7[dB]
X_Pulse           = 17.59333333[us]
Irr_Atn_Dec       = 20.948[dB]
Irr_Atn_Noe       = 20.948[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```



(8f)



Mansoura University JEOL NMR Unit ECA-500 II

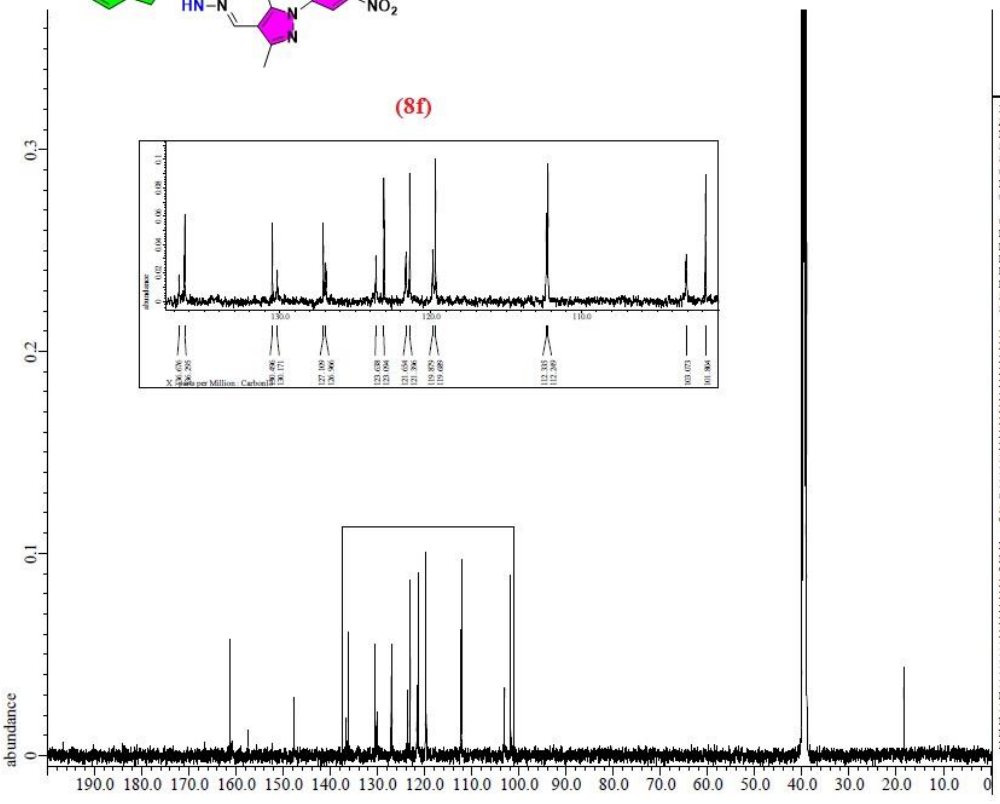
```
Filename          = Manar Nagy10_proton-1-11
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Manar Nagy_11
Solvent           = DMSO-D6
Creation_Time     = 30-JUL-2019 15:03:21
Revision_Time     = 30-JUL-2019 15:10:47
Current_Time      = 30-JUL-2019 15:11:10

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500II
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T]  (500[MHz])
X_Acq_Duration    = 1.4548992[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 6[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.68733284[Hz]
X_Sweep           = 11.26126126[kHz]
X_Sweep_Clipped   = 9.00900901[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 40
Total_Scans       = 40

Relaxation_Delay  = 5[s]
Recvr_Gain        = 36
Temp_Get          = 21.1[dC]
X_90_Width        = 14.5[us]
X_Acq_Time        = 1.4548992[s]
X_Angle           = 45[deg]
X_Atn             = 4.9[dB]
X_Pulse           = 7.25[us]
Irr_Mode          = Off
Tri_Mode          = Off
DanTe_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.4548992[s]
```

(8f)



Mansoura University JEOL NMR Unit ECA-500 II

```
Filename          = Manar Nagy_11_carbon-1-1
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Manar Nagy_11
Solvent           = DMSO-D6
Creation_Time     = 10-SEP-2019 13:58:07
Revision_Time     = 15-SEP-2019 15:04:31
Current_Time      = 15-SEP-2019 15:05:11

Comment           = single pulse decoupled g
Data_Format       = 1D REAL
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500II
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T]  (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = TRUE
Scans             = 2402
Total_Scans       = 2402

Relaxation_Delay  = 2[s]
Recvr_Gain        = 58
Temp_Get          = 19.9[dC]
X_90_Width        = 52.78[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 9.7[dB]
X_Pulse           = 17.59333333[us]
Irr_Atn_Dec       = 20.948[dB]
Irr_Atn_Noe       = 20.948[dB]
Irr_Noise         = WALTS
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```