Supporting Information

Marine-Inspired Bis-indoles Possessing Anti-proliferative Activity against Breast Cancer; Design, Synthesis and Biological Evaluation

Wagdy M. Eldehna, Ghada S. Hassan, Sara T. Al-Rashood, Hamad M. Alkahtani, Abdulrahman A. Almehizia, Ghada H. Al-Ansary

Biological Evaluations

1. Anti-proliferative action toward human breast cell lines

The two examined human breast cancer cell lines (MCF-7 and Breast MDA-MB-231), and non-tumorigenic human breast epithelial cell line (MCF-10A) have been obtained from American Type Culture Collection (ATCC). The cells were maintained in Dulbecco's modified Eagle's medium (DMEM) supplemented with 10% heat inactivated fetal calf serum (GIBCO), penicillin (100 U/ml) and streptomycin (100 μg/ml) at 37 ^{o}C in humidified atmosphere containing 5% CO_2. Cells at a concentration of 0.50 x 10^6 were grown in a 25 cm^2 flask in 5 ml of culture medium.

The anti-proliferative activity of the tested compounds was measured *in vitro* using the Sulfo-Rhodamine-B stain (SRB) assay. Briefly, Cells were inoculated in 96-well microtiter plate (5X10^4 cells/ well) for 24 h before treatment with the tested compounds to allow attachment of cell to the wall of the plate. Tested compounds were dissolved in DMSO at 1 mg/ml immediately before use and diluted to the appropriate volume just before addition to the cell culture. Different concentrations of tested compounds, doxorubicin and sorafenib were added to the cells (three wells were prepared for each individual dose). Cells were incubated with the compounds for 48 h at 37°C and in atmosphere of 5% CO_2. After 48 h cells were fixed, washed, and stained for 30 min with 0.4% (w/v) SRB dissolved in 1% acetic acid. Unbound dye was removed by four washes with 1% acetic acid, and attached stain was recovered with Tris-EDTA buffer. Color intensity was measured in an ELISA reader. The relation between percent of surviving fraction and drug concentration is plotted to get the survival curve for each cell line. The concentration required for 50% inhibition of cell viability (IC_{50}) was calculated.

2. Cell Cycle Analysis

Breast cancer MCF-7 cells were treated with bis-indoles **7e** and **9a** for 24 h (at their IC_{50} concentration), and then cells were washed twice with ice-cold phosphate buffered saline (PBS). Subsequently, the treated cells were collected by centrifugation, fixed in ice-cold 70% (*v*/*v*) ethanol, washed with PBS, re-suspended with 100 μg/mL RNase, stained with 40 μg/mL PI, and analyzed by flow cytometry using FACS Calibur (Becton Dickinson, BD, Franklin Lakes, NJ, USA). The cell cycle distributions were calculated using CellQuest software 5.1 (Becton Dickinson).

3. ELISA Immunoassay

The levels of the pro-apoptotic markers (Bax, caspase-3 and p53) as well as the anti-apoptotic marker Bcl-2 were determined using ELISA colorimetric kits per the manufacturer's instructions. Breast cancer MCF-7 cells were cultured as a monolayer in T-25 flasks and were seeded to attain 30% confluency prior to treatment. Cells were then treated separately with bis-indoles **7e** and **9a** at their IC_{50} concentrations for 48 h. At the end of treatment, cells were collected via trypsinization and centrifuged at 10,000 rpm. The pellet was then rinsed with PBS and lysed in RIPA lysis buffer at 4 °C for 45 min, then centrifuged at 14,000 rpm for 20 min to remove the cellular debris. Lysates were then collected and stored at −80 °C for later protein determination using Pierce BCA Protein Assay Kit according to manufacturer's recommendations.

The cell lysate was diluted 10 times, and 100 μL (50 mg protein) was added to the wells of four separate microtiter plates for the four ELISA kits that were pre-coated with primary antibodies specific to Bax, Bcl-2, caspase-3 and p53 proteins, respectively. A secondary biotin-linked antibody specific to the protein captured by the primary antibody was further added to bind the captured protein, forming a "sandwich" of specific antibodies around the desired protein in the cell lysate. The streptavidin-HRP complex was then used to bind the biotin-linked secondary antibody through its streptavidin portion. The HRP domain reacted with the added TMB substrate to form a colored product that measured at 450 nm by a plate reader ChroMate-4300 after the reaction was terminated *via* the addition of stop solution.

4. Annexin V-FITC Apoptosis Assay

Phosphatidylserine externalization was assayed using Annexin V-FITC/PI apoptosis detection kit (BD Biosciences, USA) according to the manufacturer's instructions. Breast cancer MCF-7 cells were cultured to a monolayer then treated with bis-indoles **7e** and **9a** at their IC_{50} concentration. Briefly, cells were then harvested *via* trypsinization, and rinsed twice in PBS followed by binding buffer. Moreover, cells were re-suspended in 100 μL of binding buffer with the addition of 1 μL of FITC-Annexin V followed by an incubation period of 30 min at 4 °C. Cells were then rinsed in binding buffer and resuspended in 150 μL of binding buffer with the addition of 1 μL of DAPI (1 μg/μL in PBS). Cells were then analyzed using the flow cytometer BD FACS Canto II and the results were interpreted with FlowJo7.6.4 software (Tree Star, Ashland, OR, USA).

5. CDK2 kinase inhibitory activity

Reaction Biology Corp. Kinase HotSpotSM service (http://www.reactionbiology.com) was used for screening of tested compounds. CDK2 Kinase inhibitory activity was assessed by the HotSpot assay platform, which contained specific kinase/substrate pairs along with required cofactors. Base reaction buffer: 20 mM Hepes (pH 7.5), 10 mM $MgCl_2$, 1 mM EGTA, 0.02% Brij35, 0.02 mg/ml BSA, 0.1 mM Na_3VO_4, 2 mM DTT, 1% DMSO. Testing compounds were dissolved in 100% DMSO to specific concentration. The serial dilution was conducted by Integra Viaflo Assist in DMSO. The reaction mixture containing the examined compound and 33P-ATP was incubated at room temperature for 2 h and radioactivity was detected by filter-binding method. Kinase activity data were expressed as the percent remaining kinase activity in test samples compared to vehicle (dimethyl sulfoxide) reactions.

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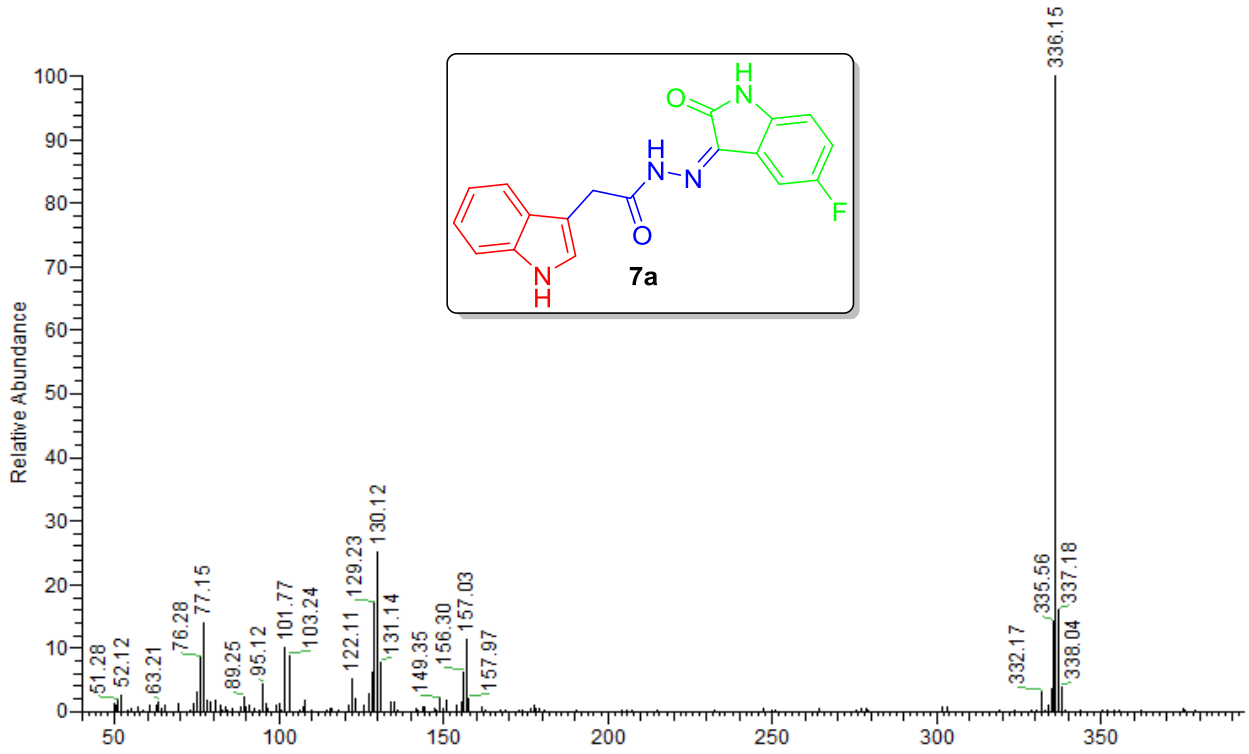

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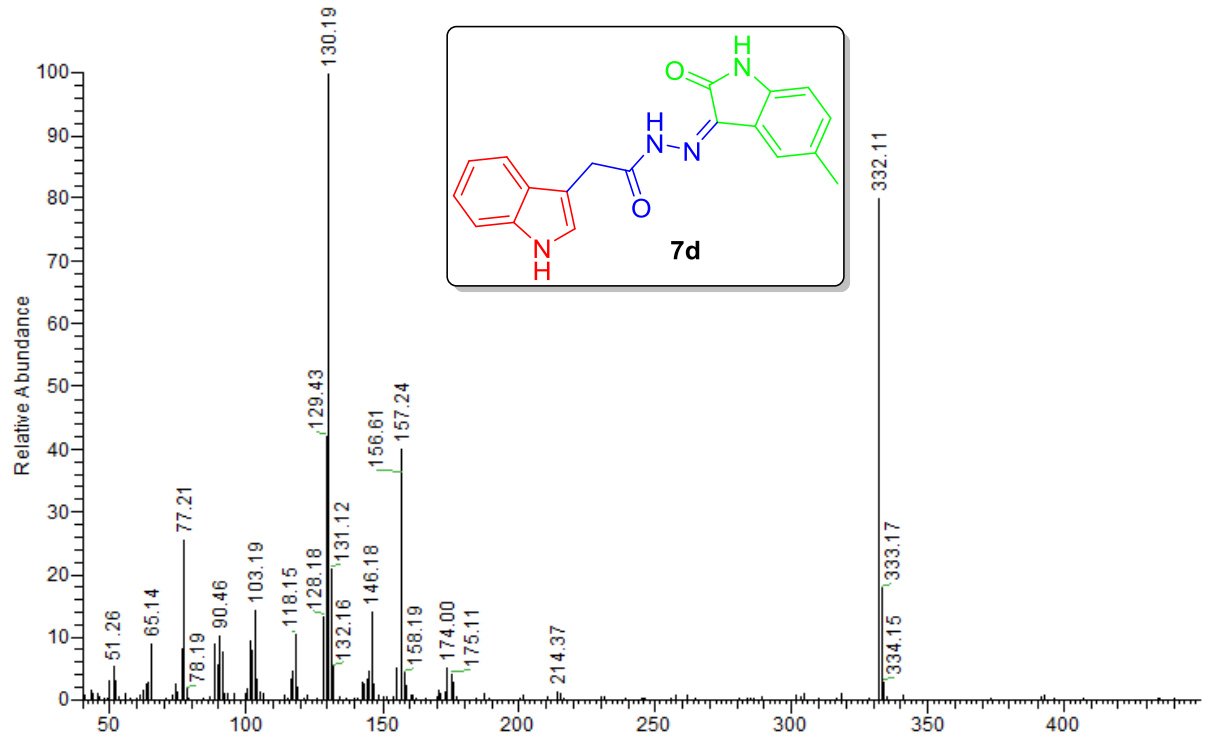

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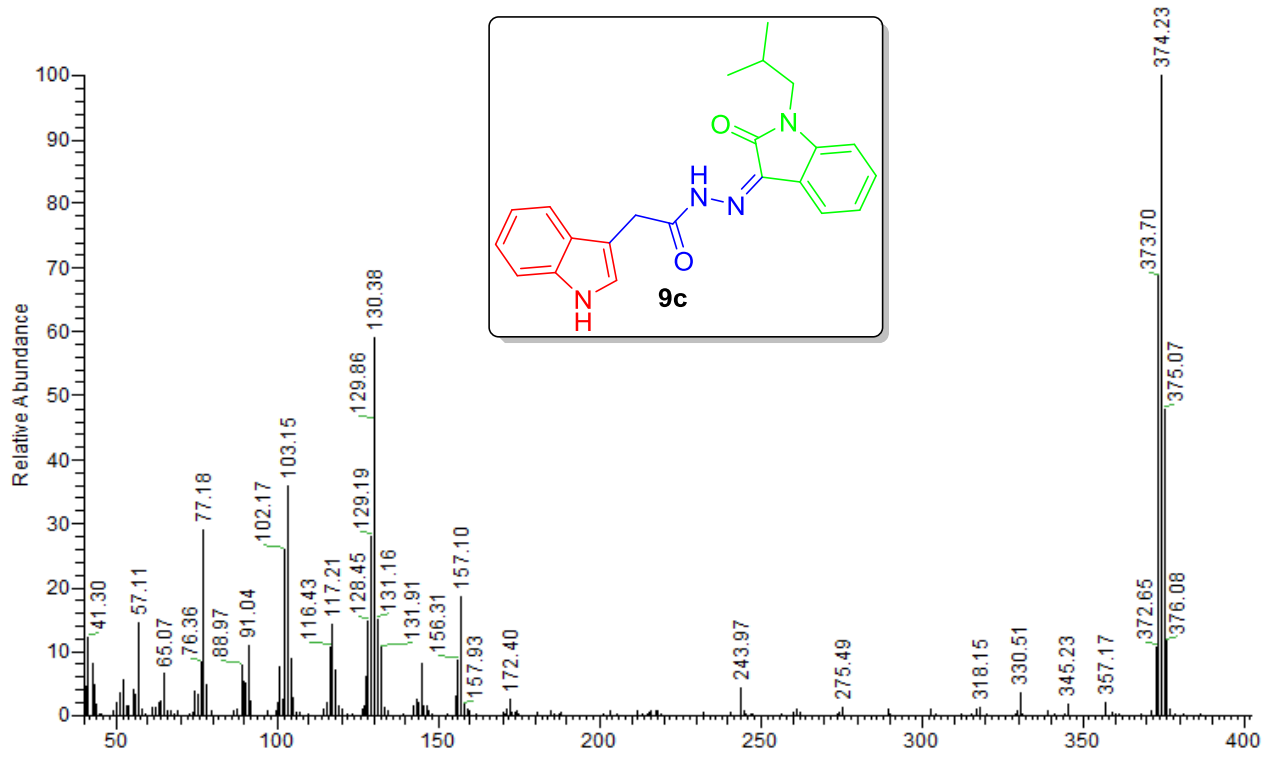

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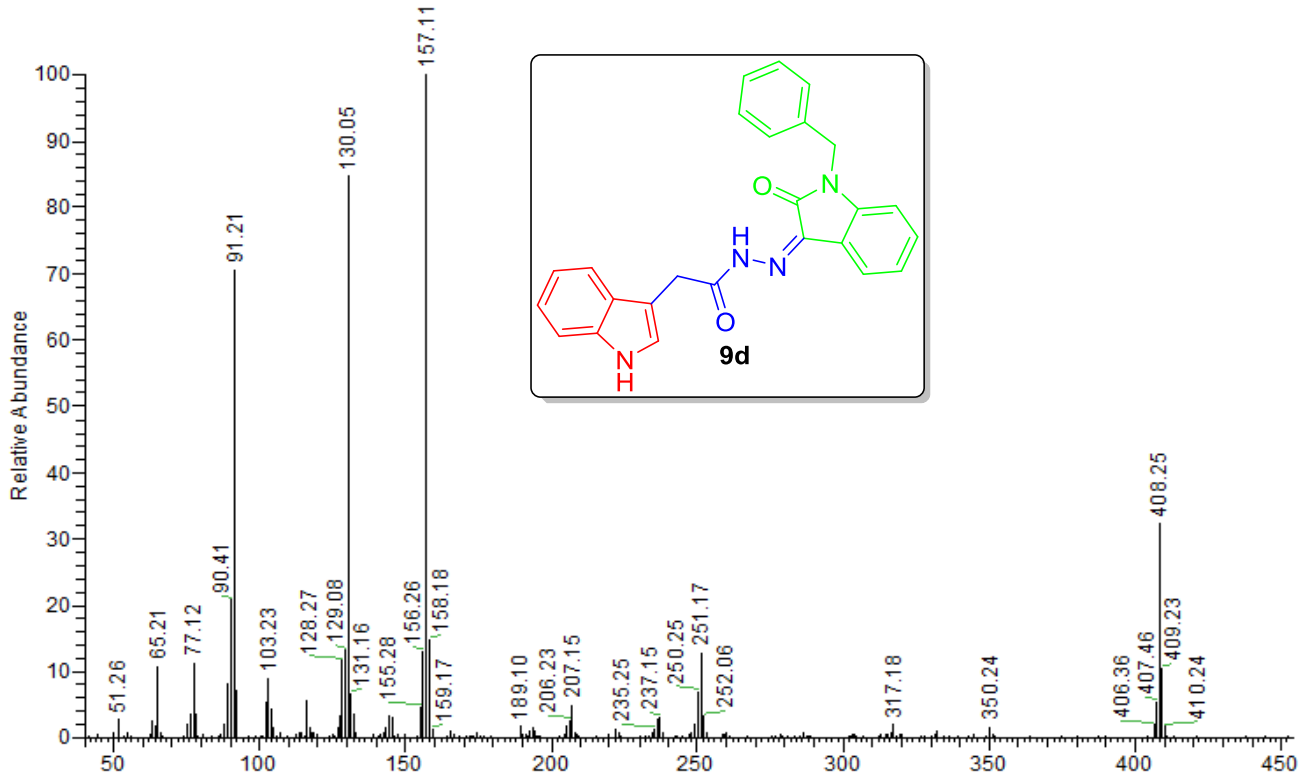

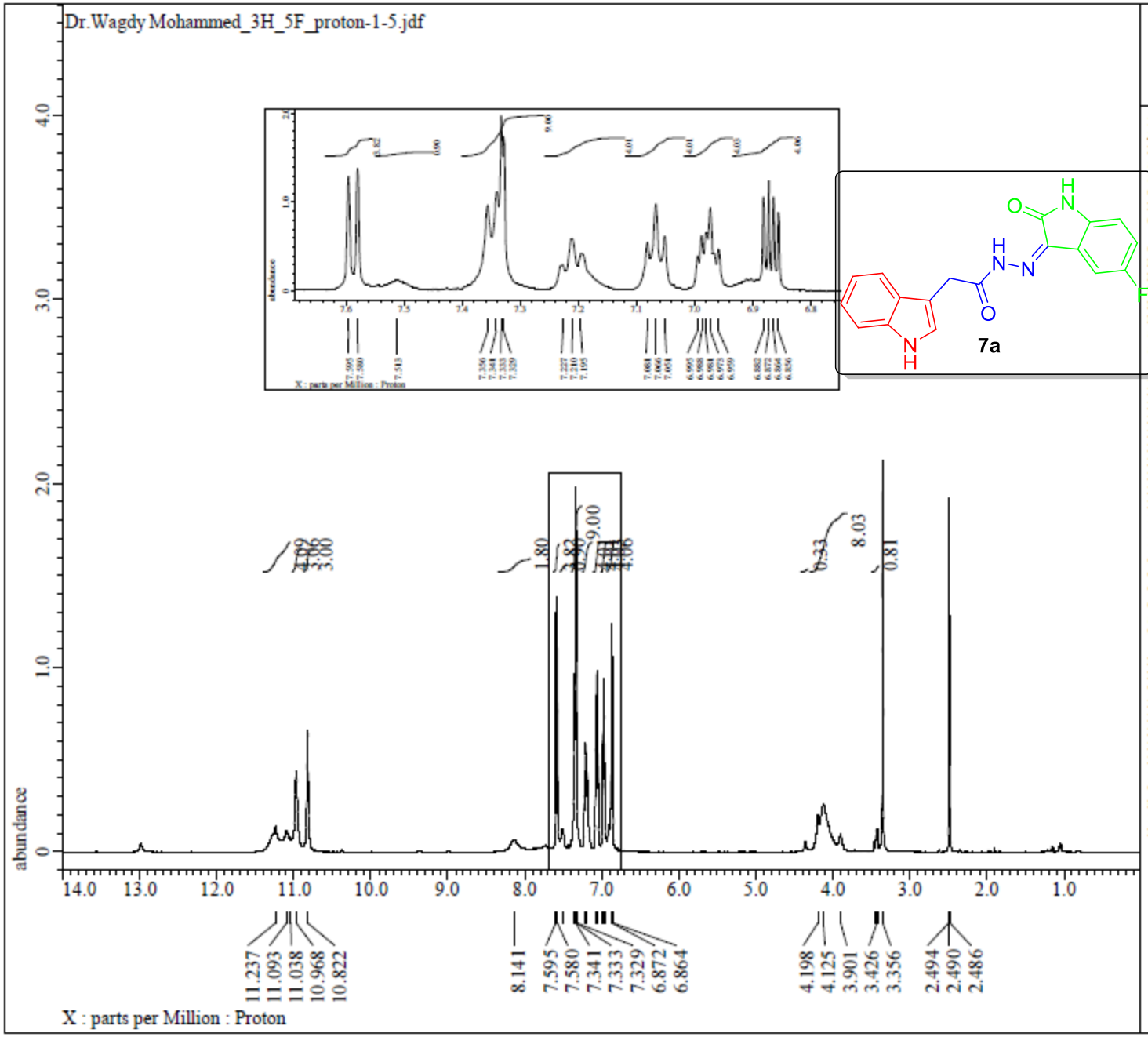

Mansoura University
JEOL ECA-500 II
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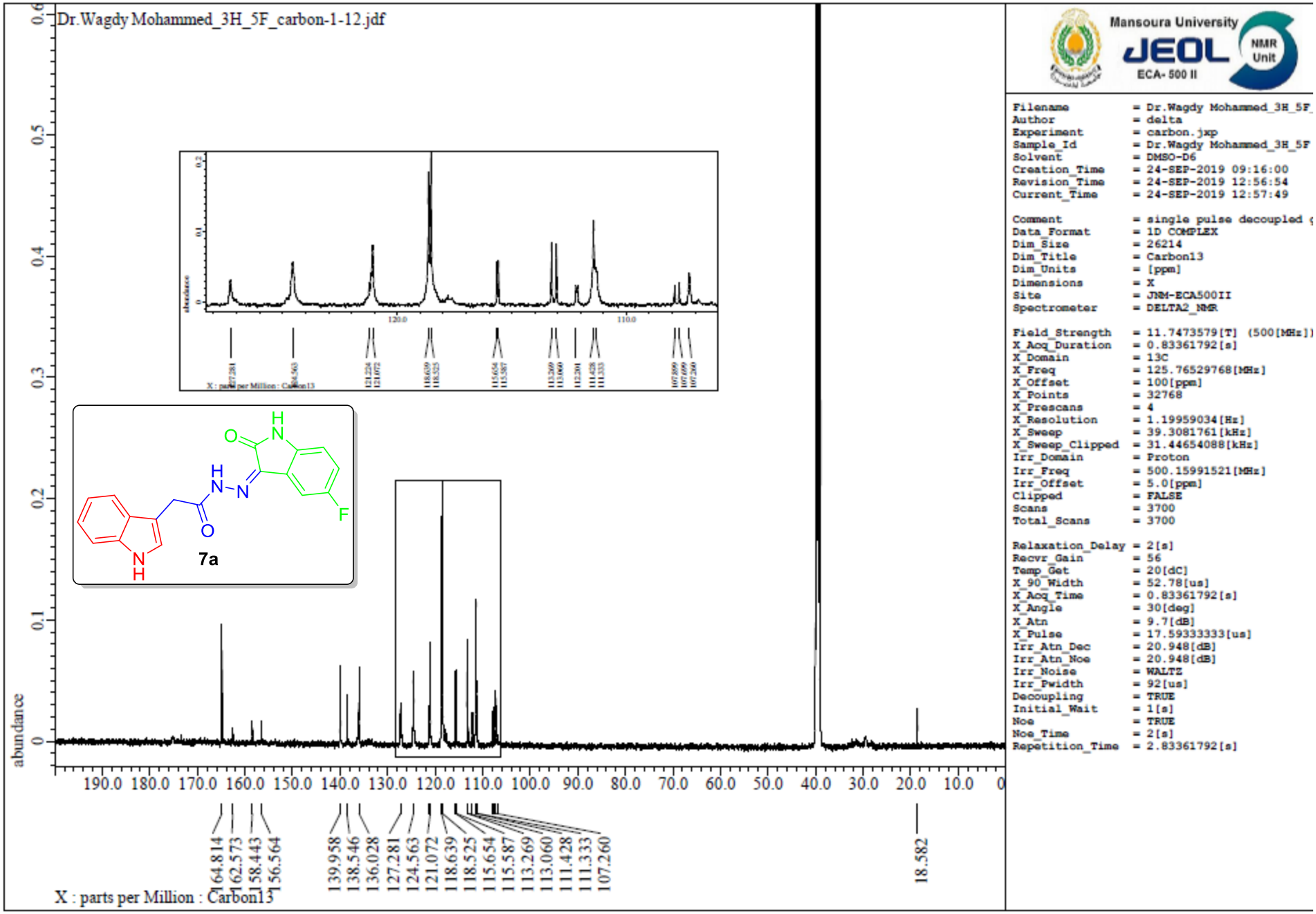
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Mansoura University
JEOL
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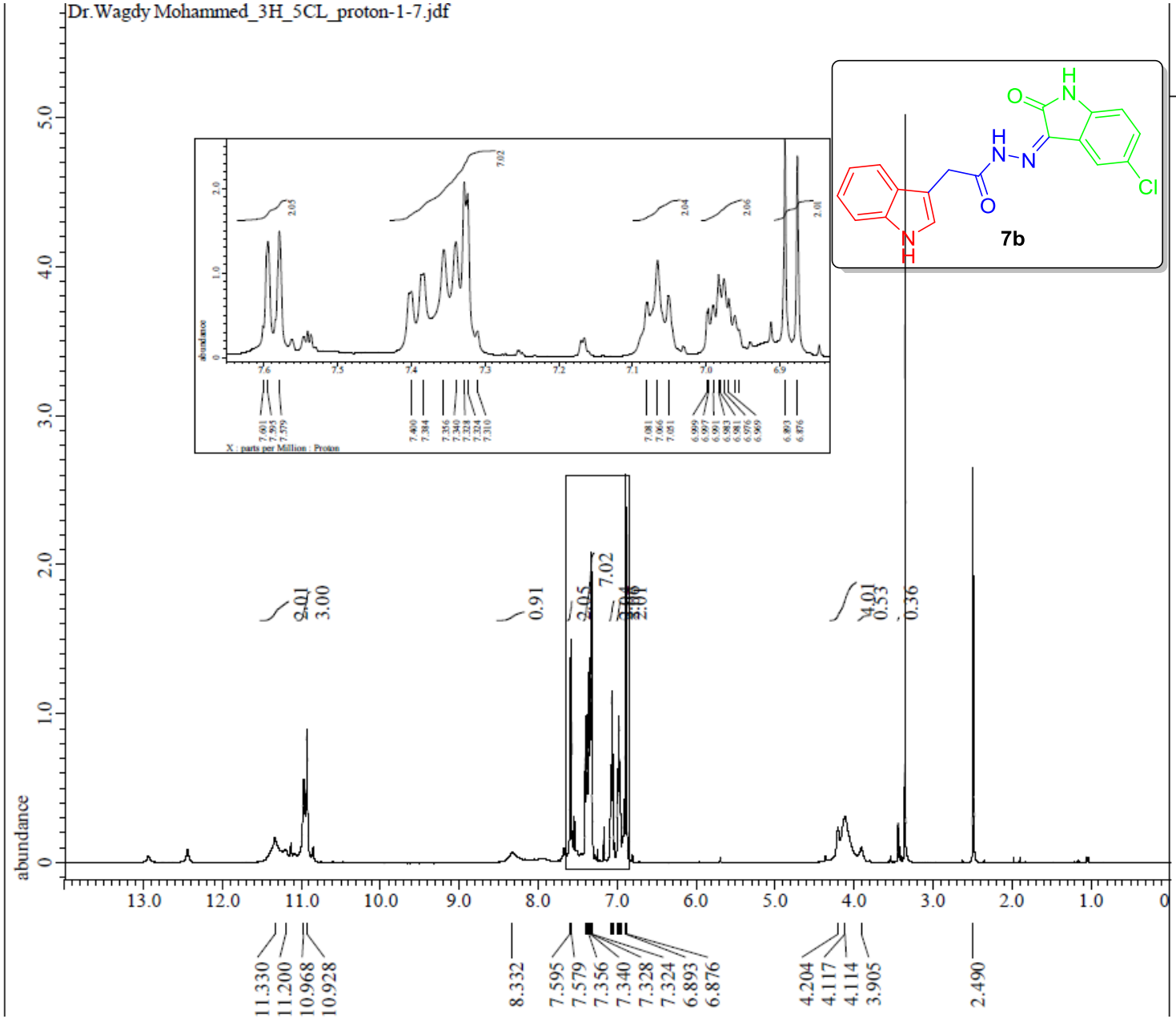

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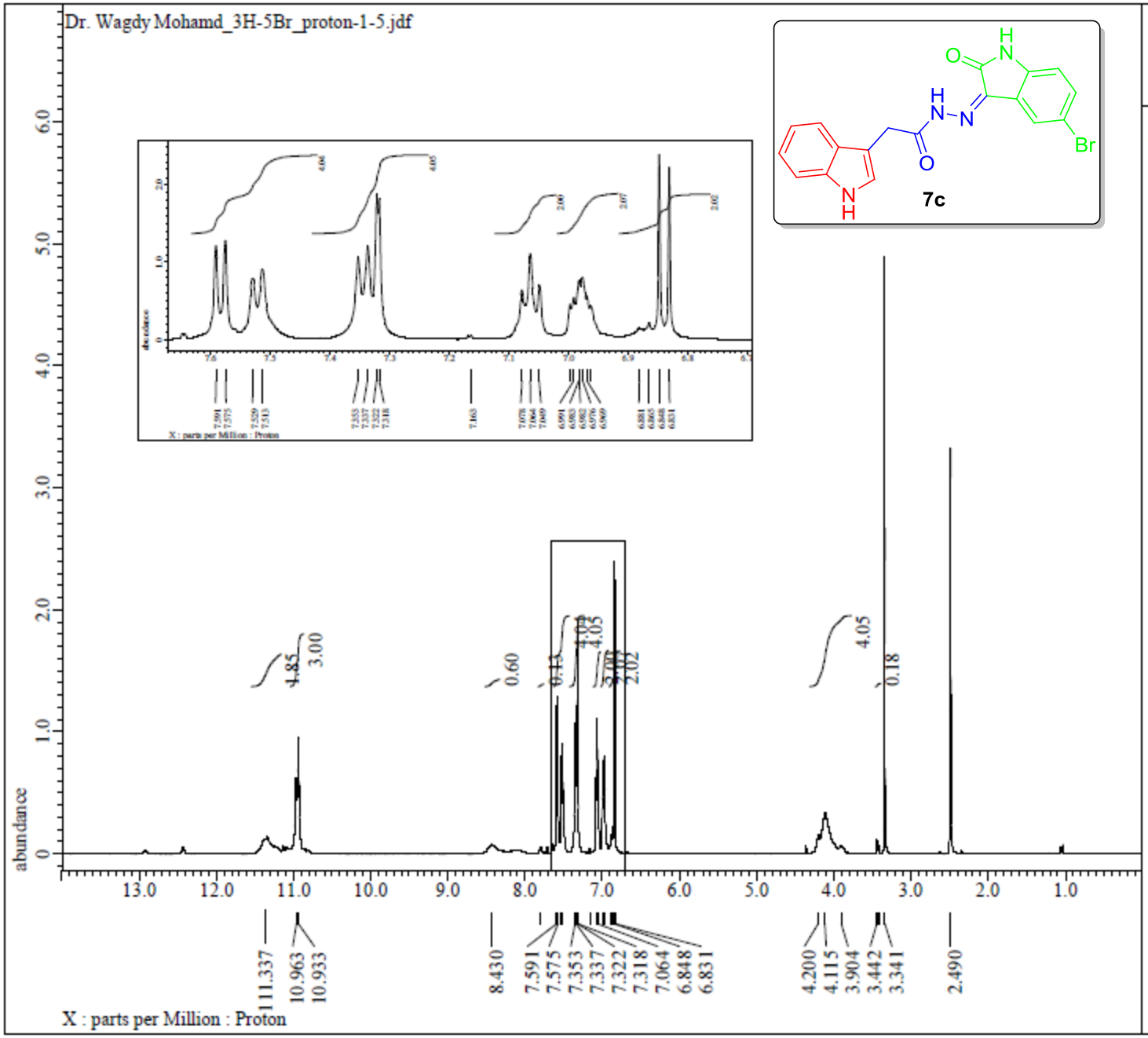

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NMR Unit

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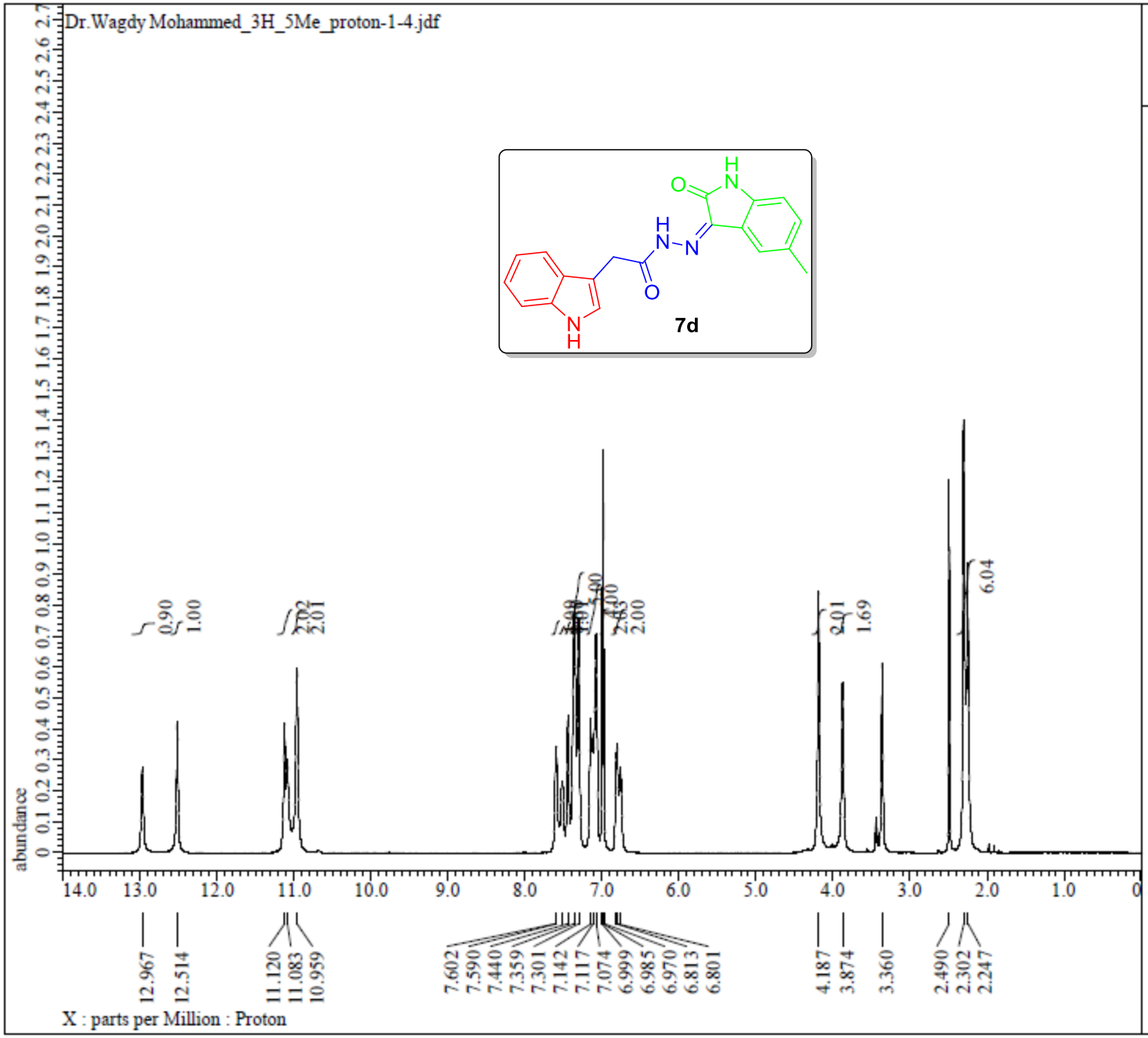

Mansoura University
JEOL ECA-500 II
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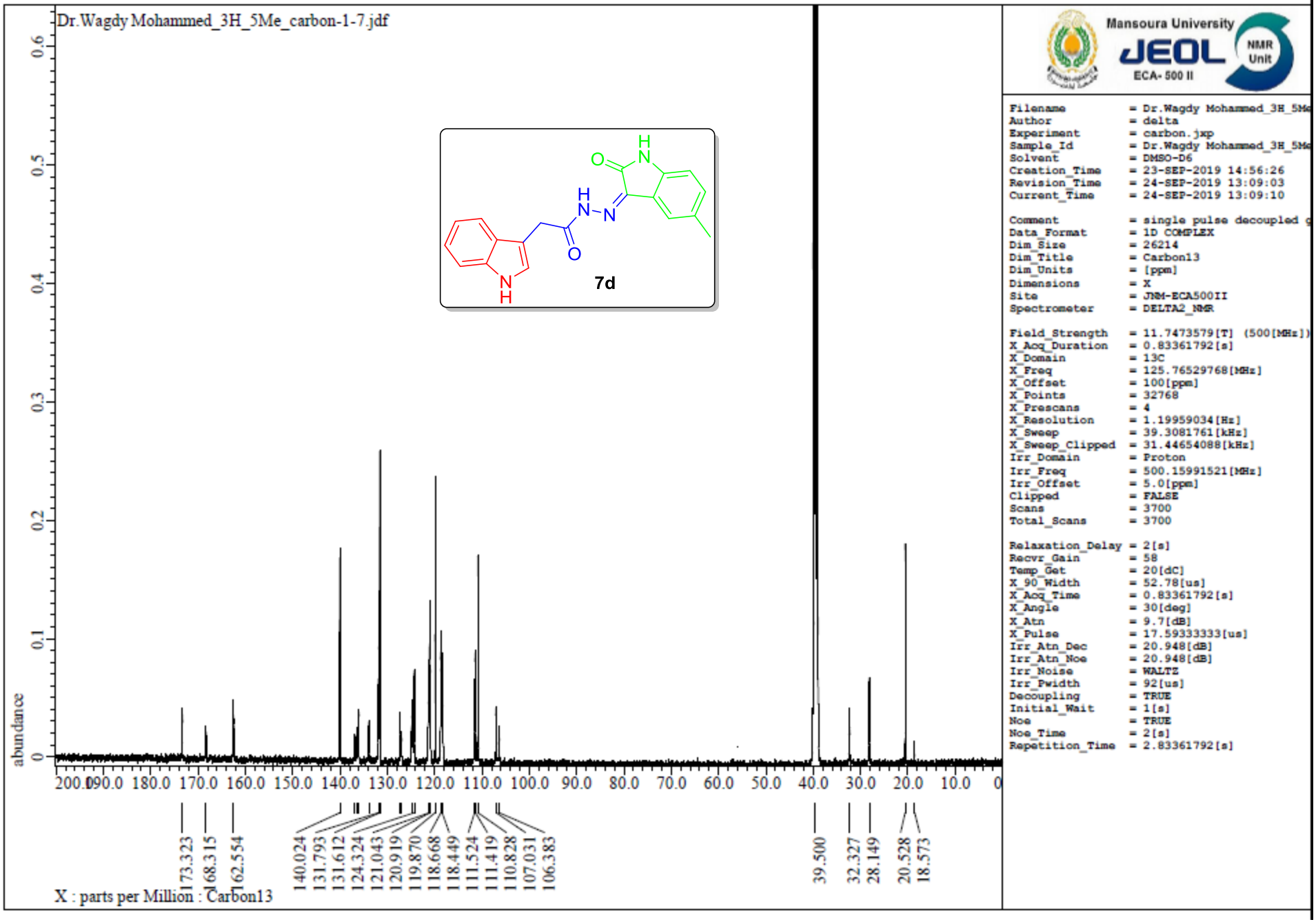
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Mansoura University
JEOL
ECA- 500 II
NMR Unit
7d
abundance
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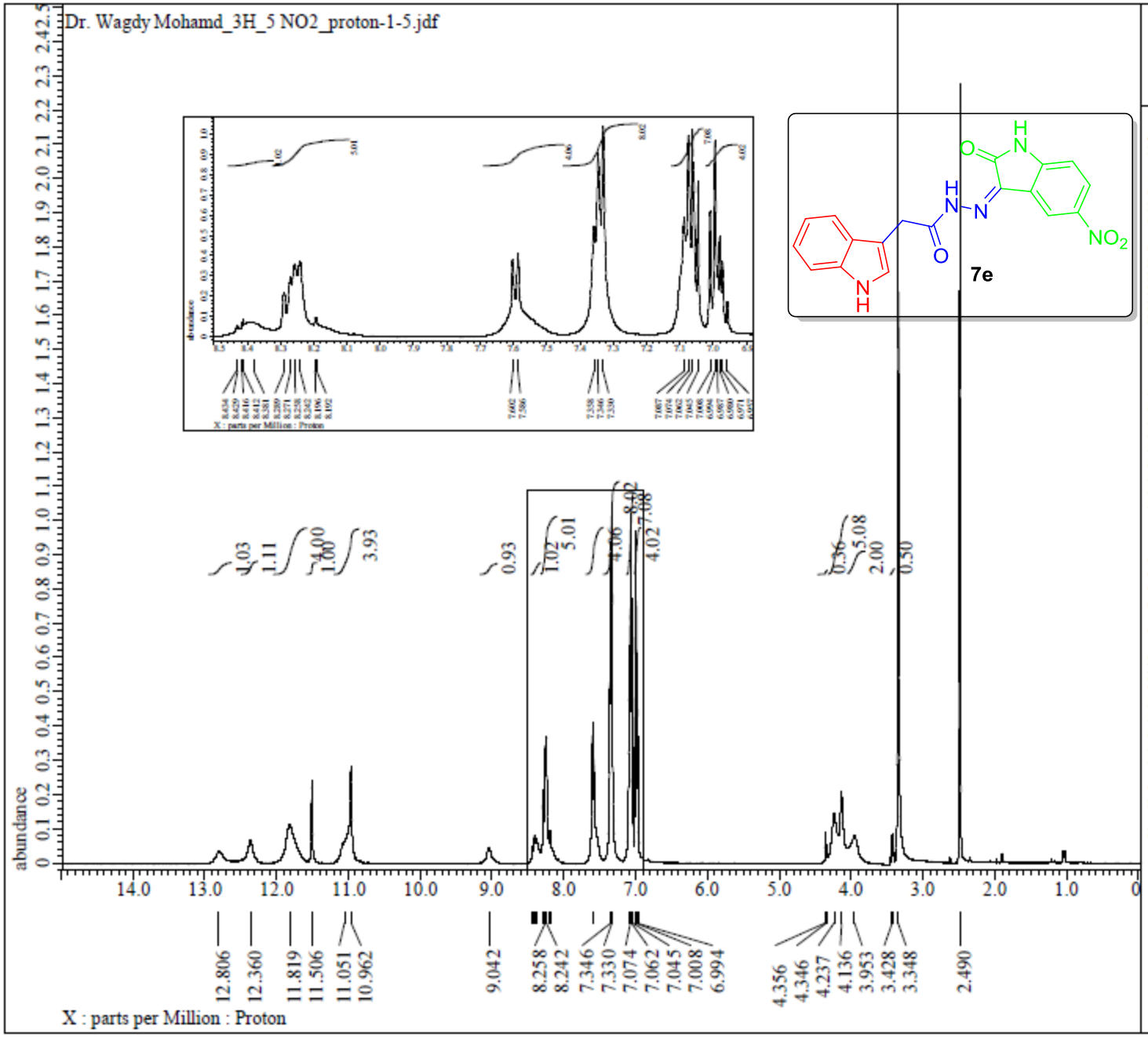

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NMR Unit

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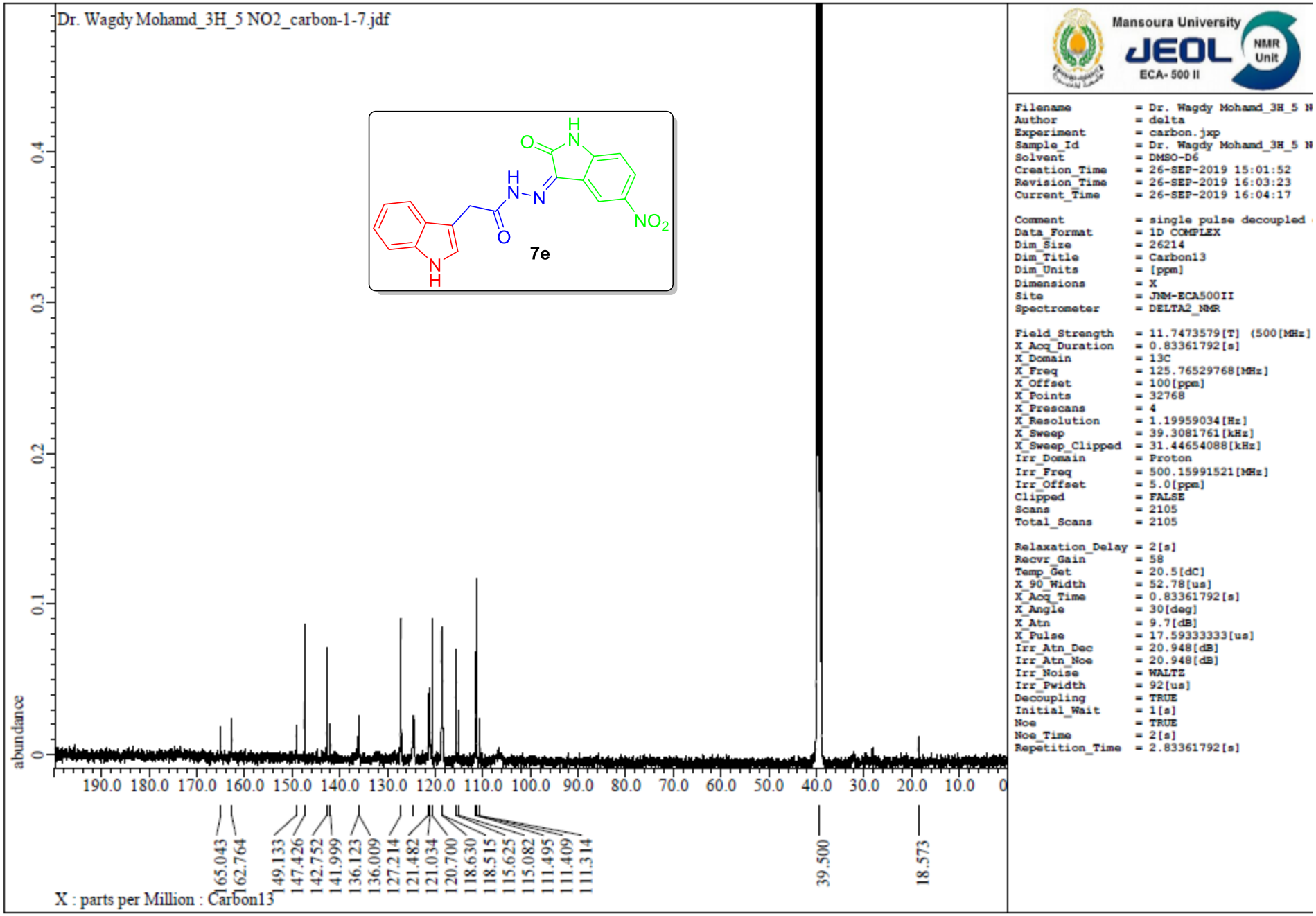
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Mansoura University
JEOL
ECA- 500 II
NMR Unit
7e
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0.4
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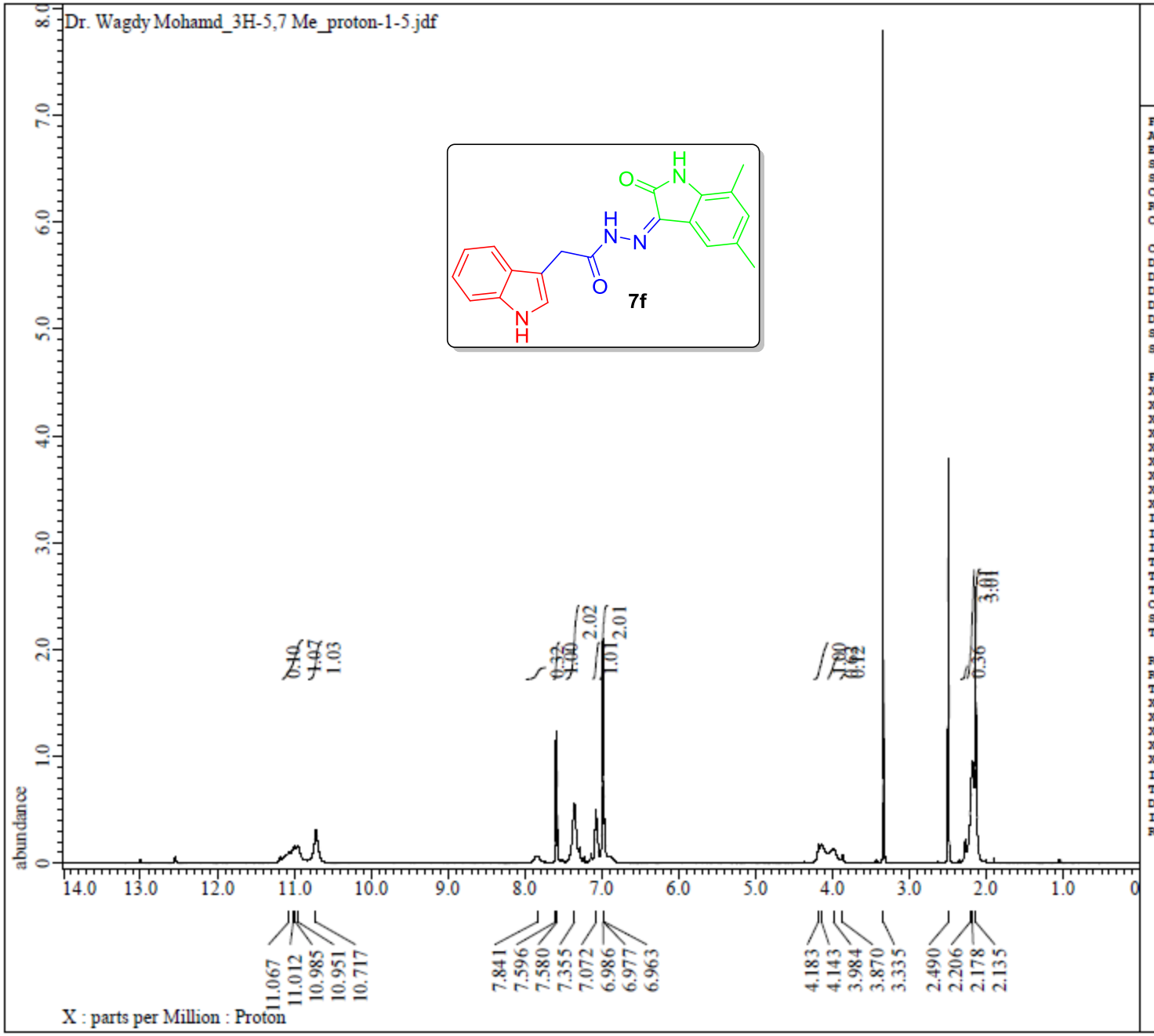
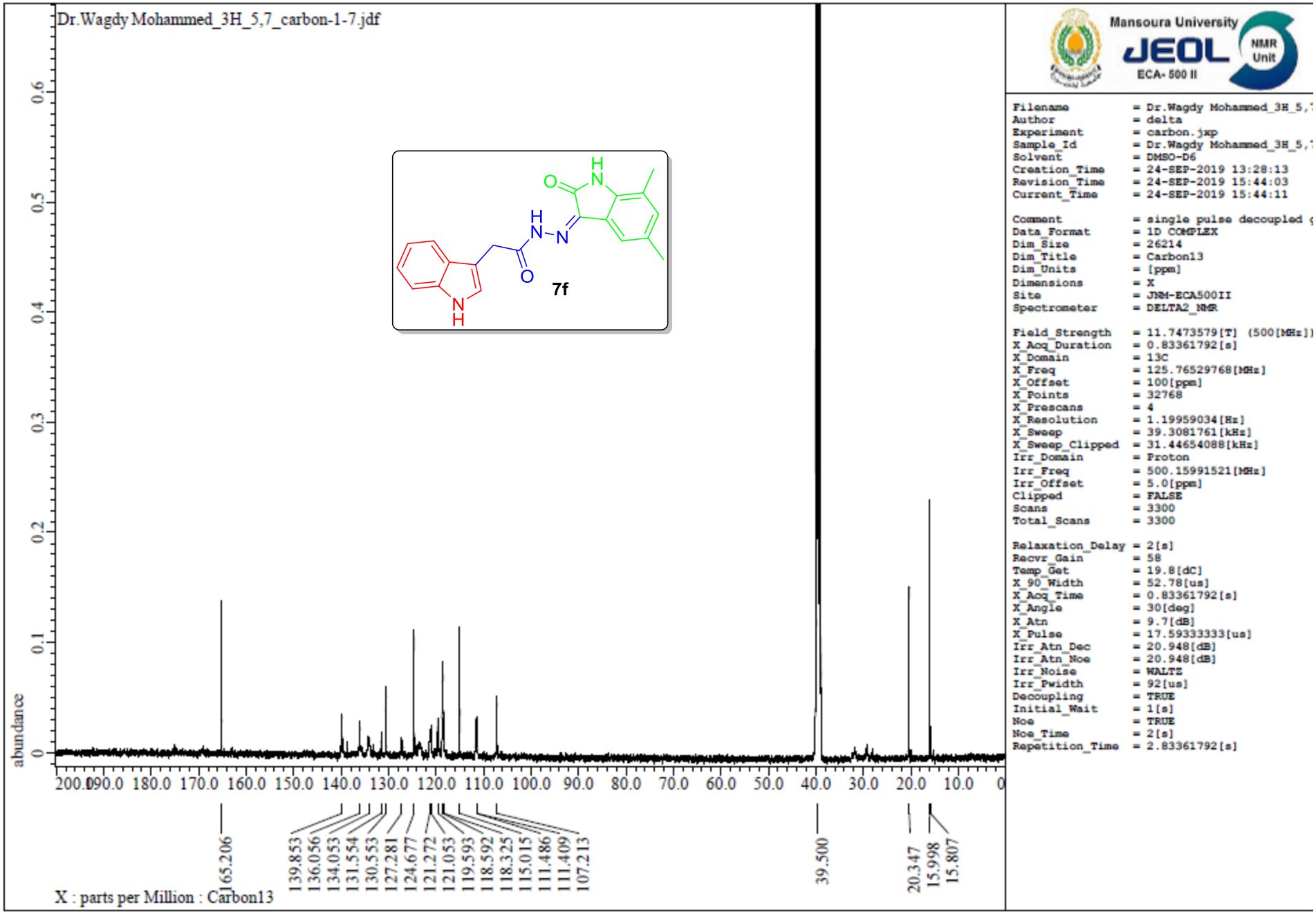
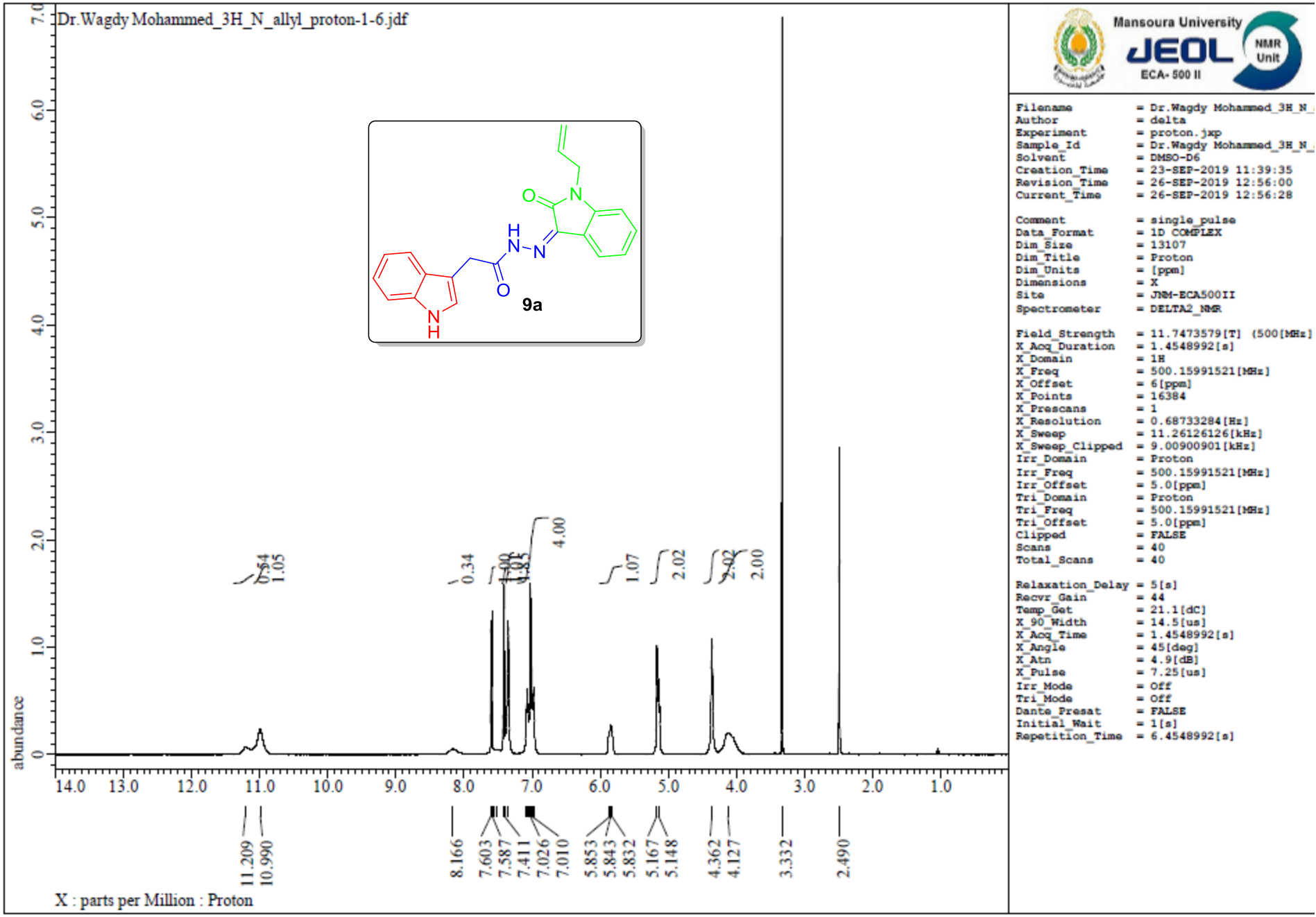
39.500
18.573
X : parts per Million : Carbon13
Filename = Dr. Wagdy Mohamd_3H_5 N
Author = delta
Experiment = carbon.jxp
Sample_Id = Dr. Wagdy Mohamd_3H_5 N
Solvent = DMSO-D6
Creation_Time = 26-SEP-2019 15:01:52
Revision_Time = 26-SEP-2019 16:03:23
Current_Time = 26-SEP-2019 16:04:17
Comment = single pulse decoupled
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 = FALSE
Scans = 2105
Total_Scans = 2105
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 20.5[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]



Mansoura University
JEOL ECA- 500 II
NMR Unit

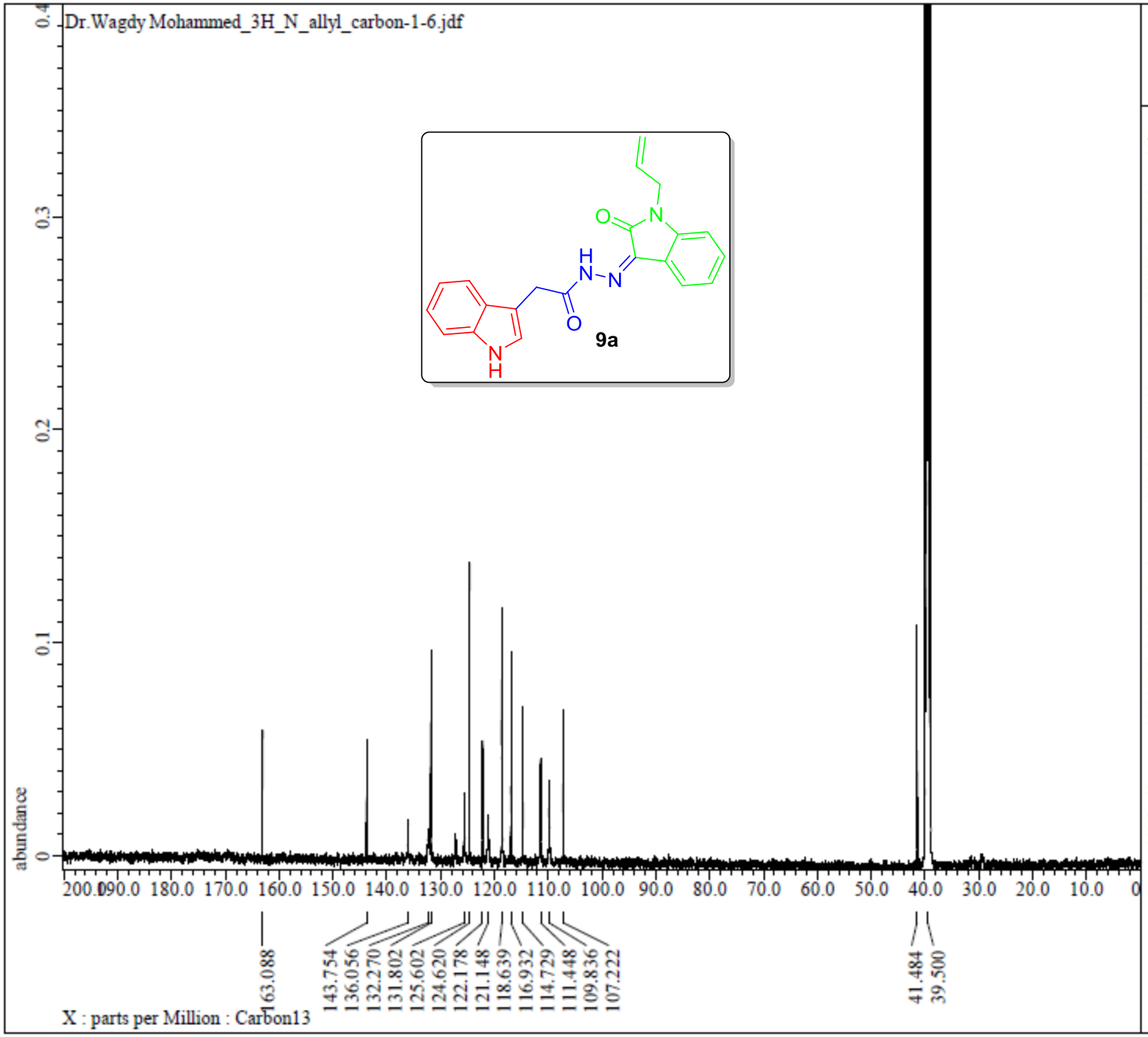
```
Filename          = Dr. Wagdy Mohamd_3H-5,7
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Dr. Wagdy Mohamd_3H-5,7
Solvent           = DMSO-D6
Creation_Time     = 17-SEP-2019 15:06:47
Revision_Time     = 17-SEP-2019 15:07:51
Current_Time      = 17-SEP-2019 15:07:58

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
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        = 46
Temp_Get          = 19.9[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]
```


Dr.Wagdy Mohammed_3H_5,7_carbon-1-7.jdf
Mansoura University
JEOL
ECA-500 II
NMR Unit
7f
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
165.206
139.853
136.056
134.053
131.554
130.553
127.281
124.677
121.272
121.053
119.593
118.592
118.325
115.015
111.486
111.409
107.213
39.500
20.347
15.998
15.807
X : parts per Million : Carbon13
Filename = Dr.Wagdy Mohammed_3H_5,7
Author = delta
Experiment = carbon.jxp
Sample_Id = Dr.Wagdy Mohammed_3H_5,7
Solvent = DMSO-D6
Creation_Time = 24-SEP-2019 13:28:13
Revision_Time = 24-SEP-2019 15:44:03
Current_Time = 24-SEP-2019 15:44:11
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 = FALSE
Scans = 3300
Total_Scans = 3300
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 19.8[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]



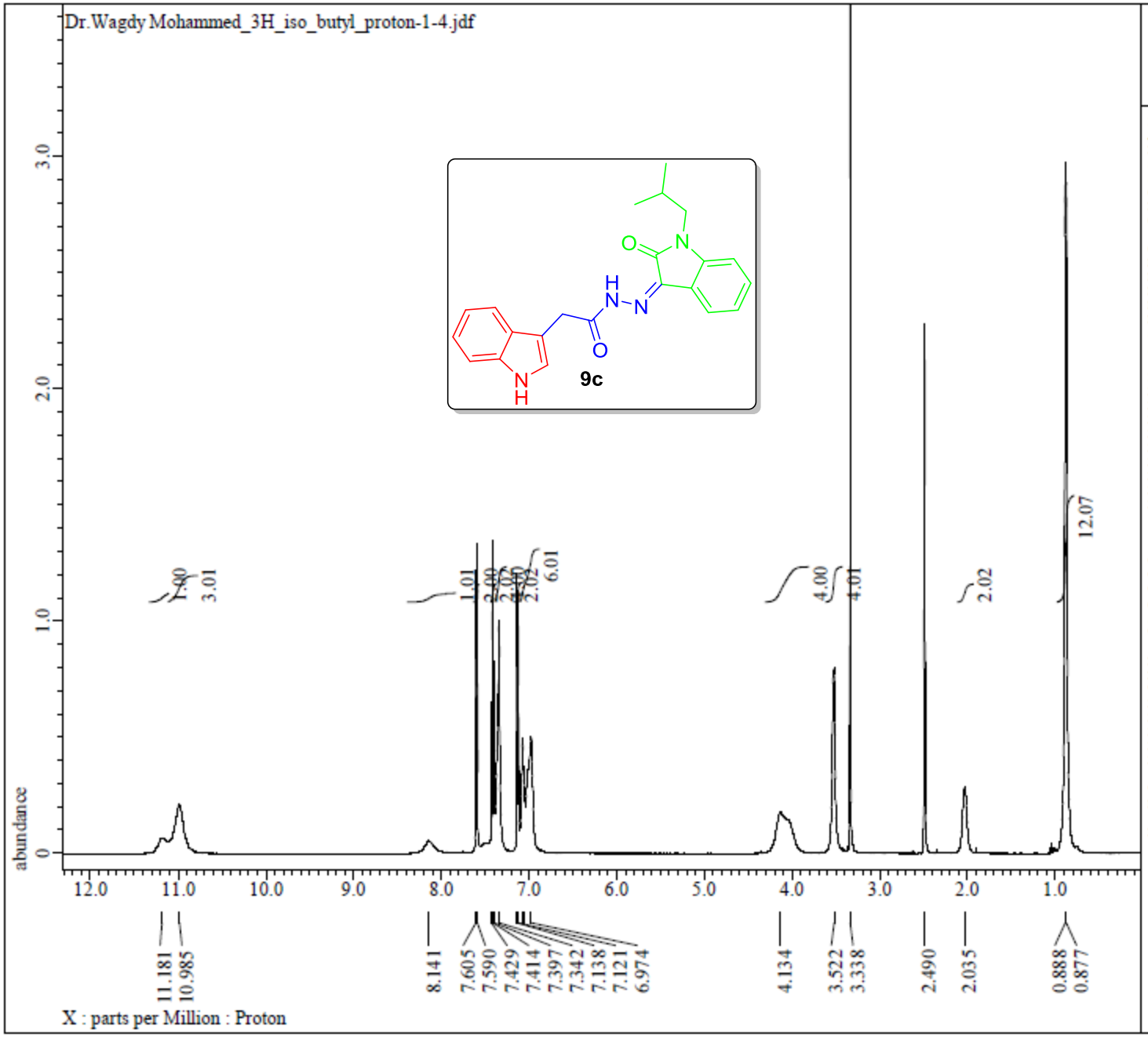
Mansoura University
JEOL ECA- 500 II NMR Unit

Filename	= Dr.Wagdy Mohammed_3H_N_
Author	= delta
Experiment	= proton.jxp
Sample_Id	= Dr.Wagdy Mohammed_3H_N_
Solvent	= DMSO-D6
Creation_Time	= 23-SEP-2019 11:39:35
Revision_Time	= 26-SEP-2019 12:56:00
Current_Time	= 26-SEP-2019 12:56:28
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	= 44
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]



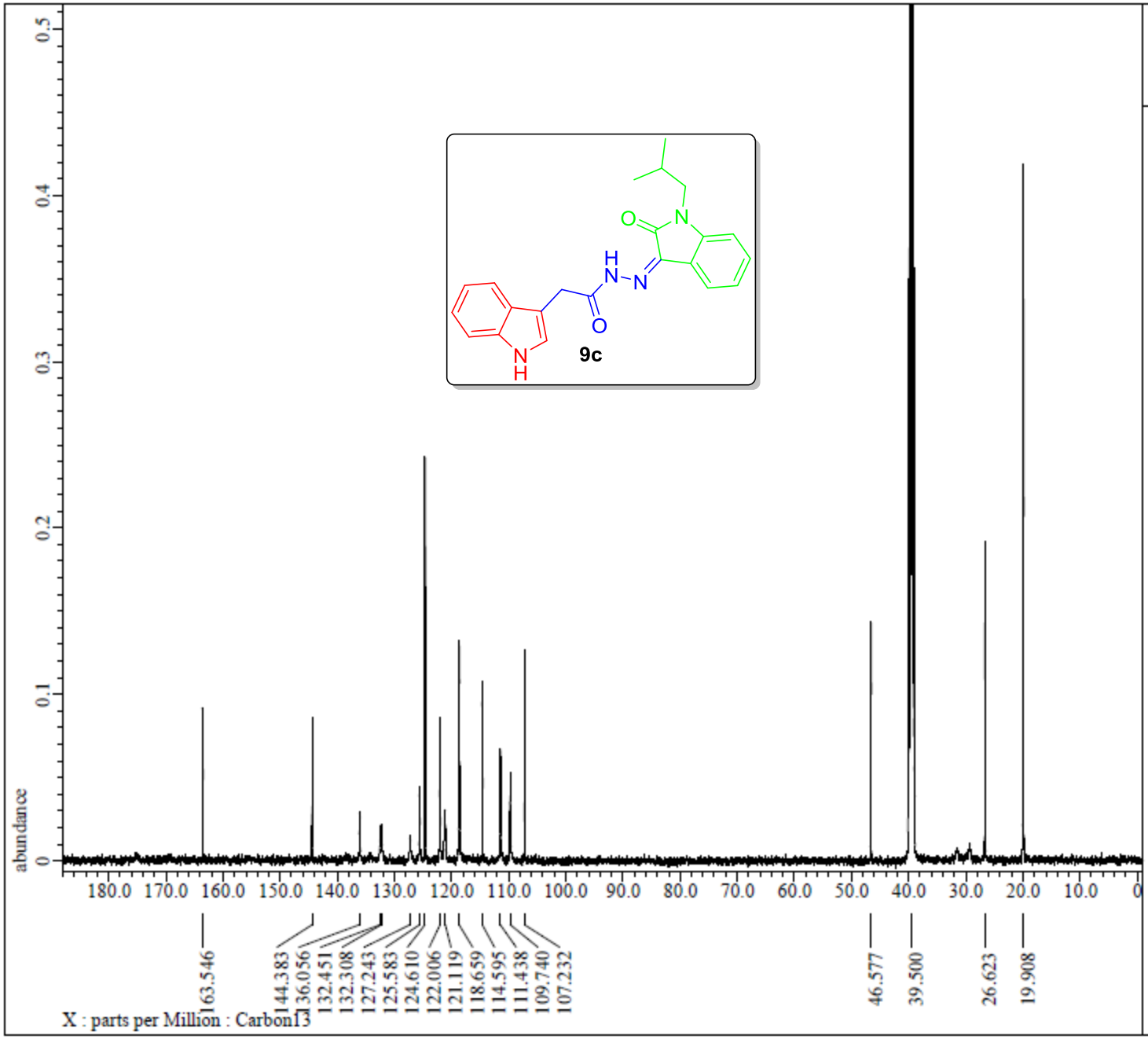
Mansoura University
JEOL ECA- 500 II
NMR Unit

Filename	= Dr.Wagdy Mohammed_3H_N_
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= Dr.Wagdy Mohammed_3H_N_
Solvent	= DMSO-D6
Creation_Time	= 24-SEP-2019 00:07:16
Revision_Time	= 24-SEP-2019 12:47:45
Current_Time	= 24-SEP-2019 12:48:40
Comment	= single pulse decoupled
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	= FALSE
Scans	= 3700
Total_Scans	= 3700
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 18.6[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]



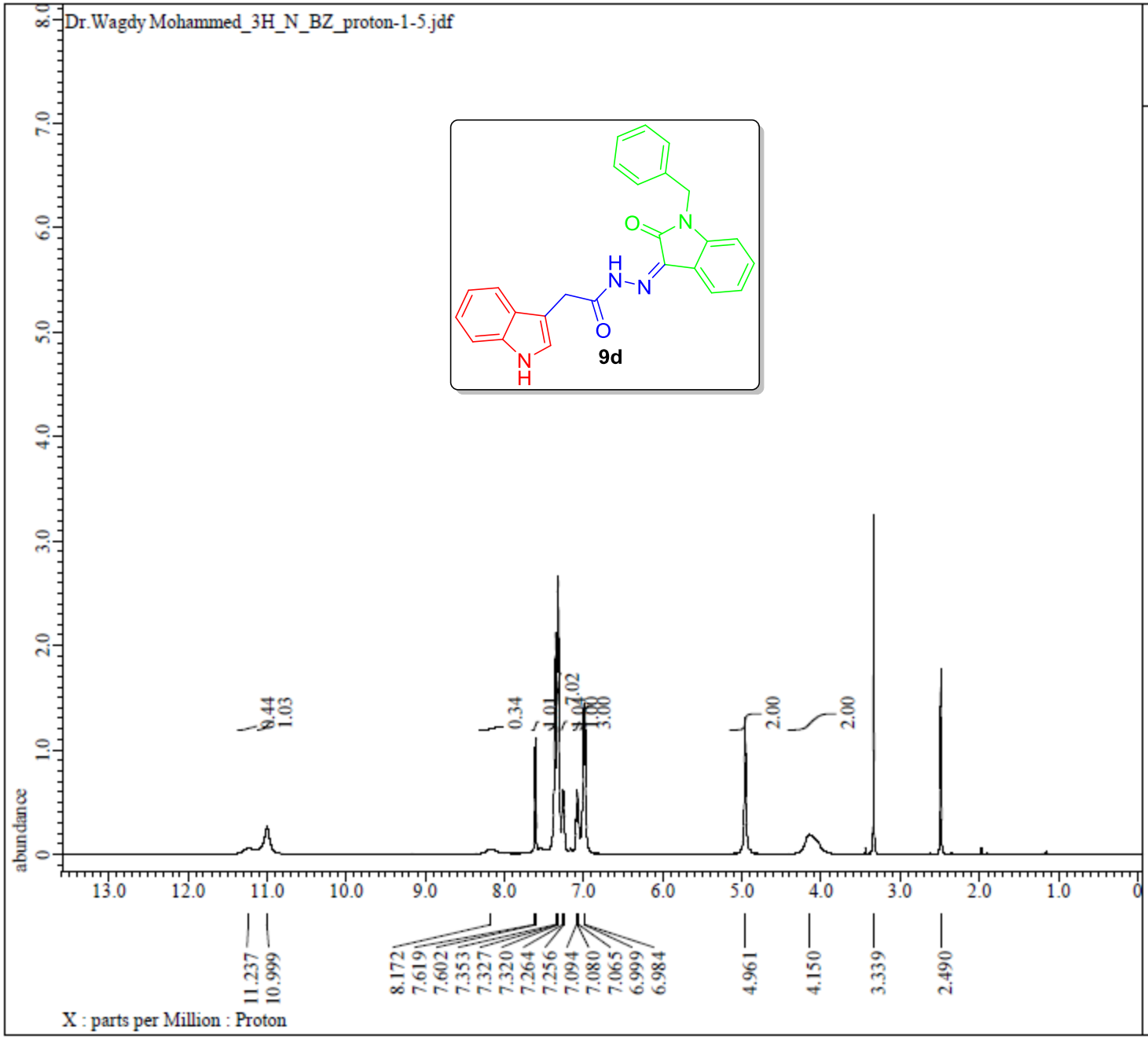
Mansoura University
JEOL ECA- 500 II NMR Unit

```
Filename          = Dr.Wagdy Mohammed_3H_iso
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Dr.Wagdy Mohammed_3H_iso
Solvent           = DMSO-D6
Creation_Time     = 23-SEP-2019 13:21:15
Revision_Time     = 24-SEP-2019 15:51:53
Current_Time      = 24-SEP-2019 15:52:30

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        = 42
Temp_Get          = 20.3[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]
```



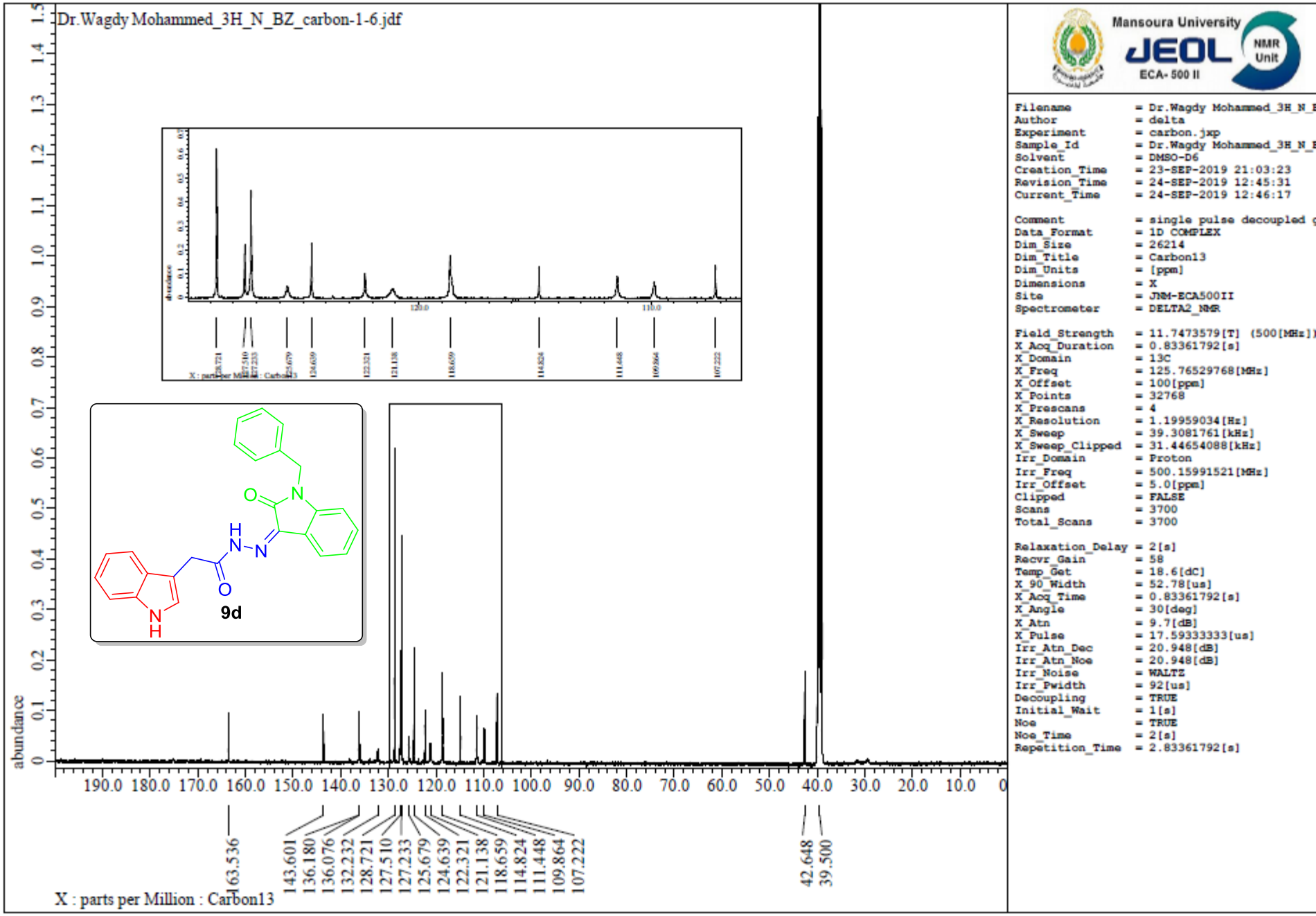
Mansoura University
JEOL
ECA- 500 II
NMR Unit

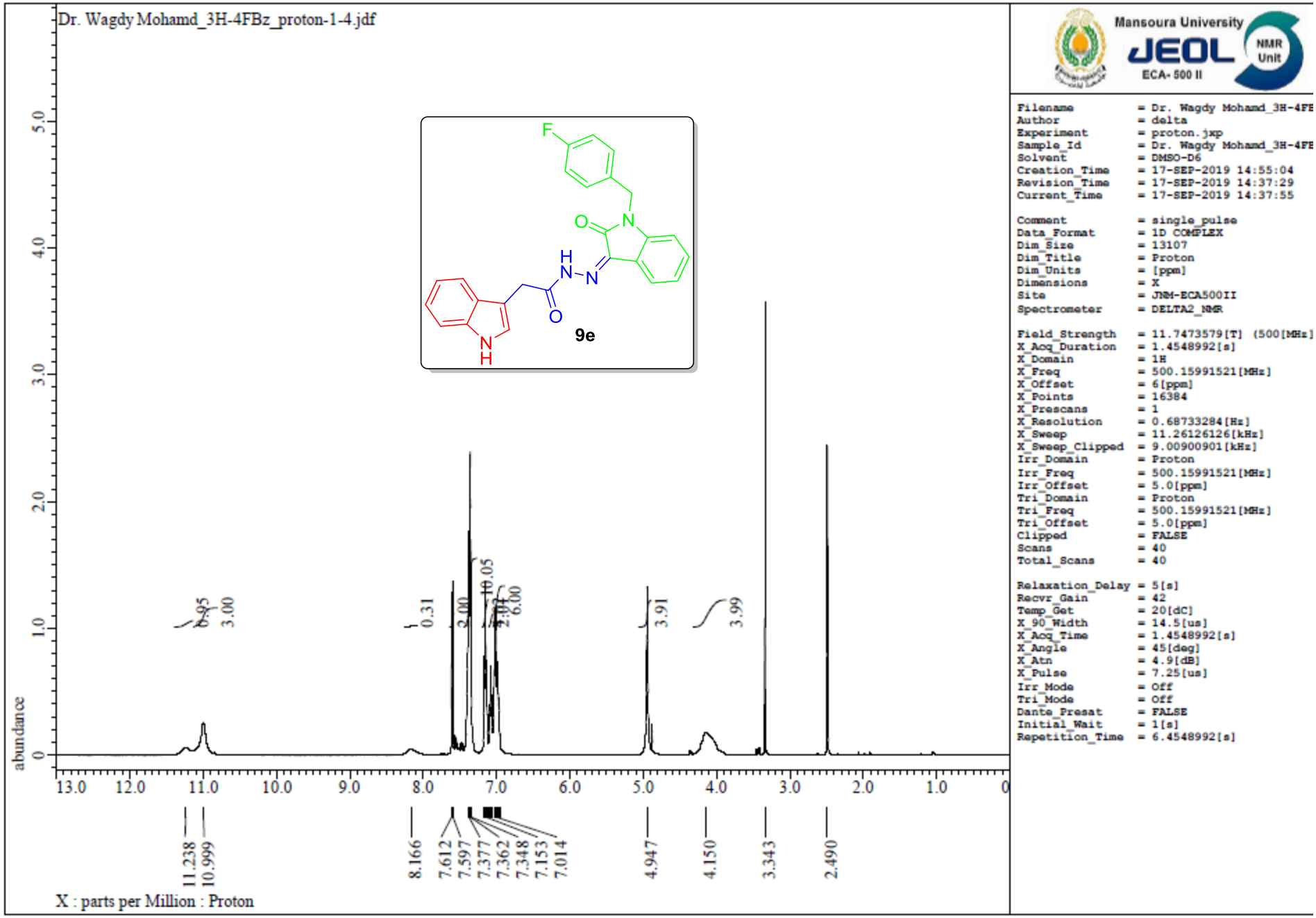
```
Filename          = Dr.Wagdy Mohammed_3H_isa
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Dr.Wagdy Mohammed_3H_isa
Solvent           = DMSO-D6
Creation_Time     = 25-SEP-2019 02:48:45
Revision_Time     = 25-SEP-2019 09:25:27
Current_Time      = 25-SEP-2019 09:28:42

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           = FALSE
Scans             = 3700
Total_Scans       = 3700

Relaxation_Delay  = 2[s]
Recvr_Gain        = 56
Temp_Get          = 18.8[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]
```

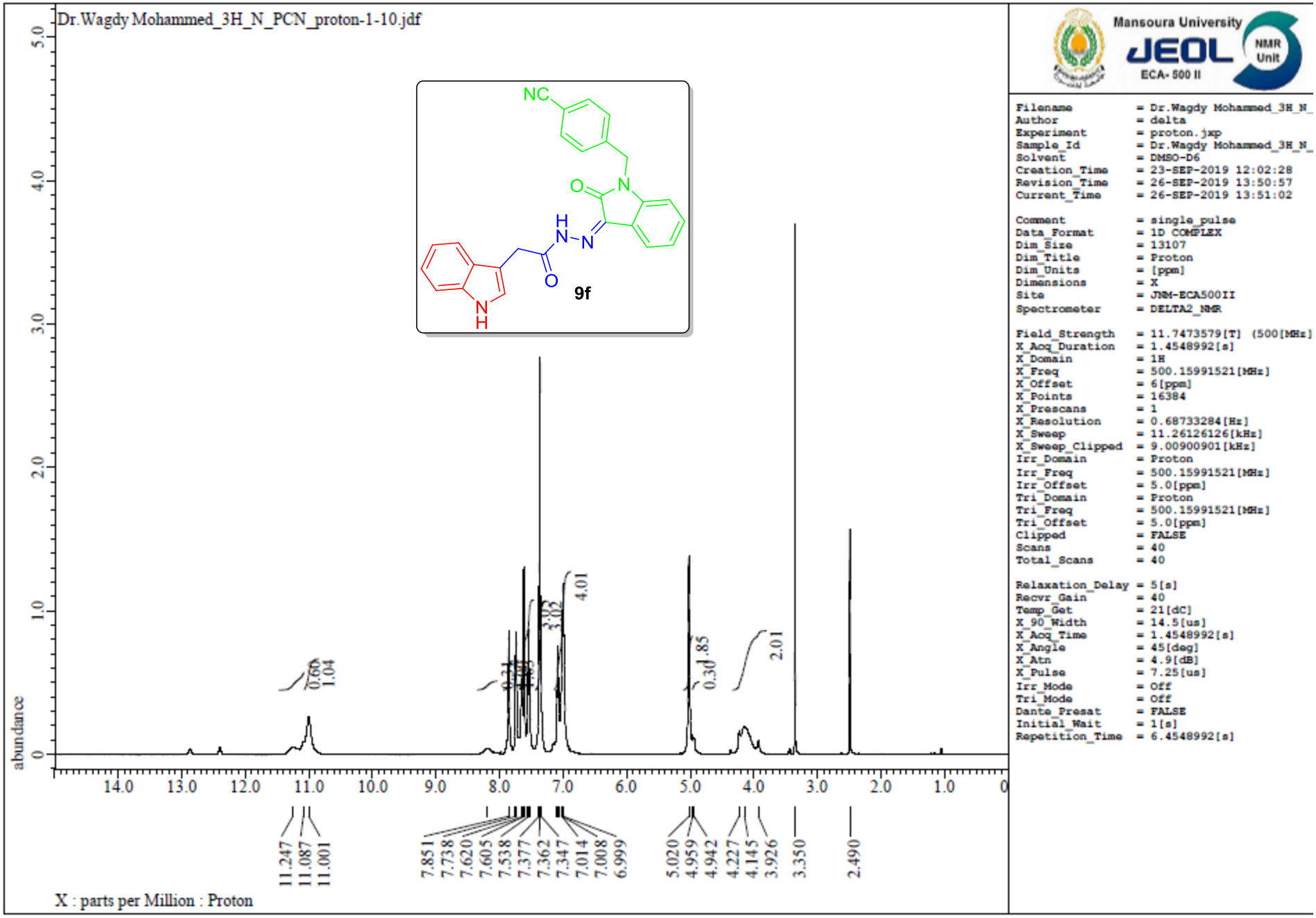


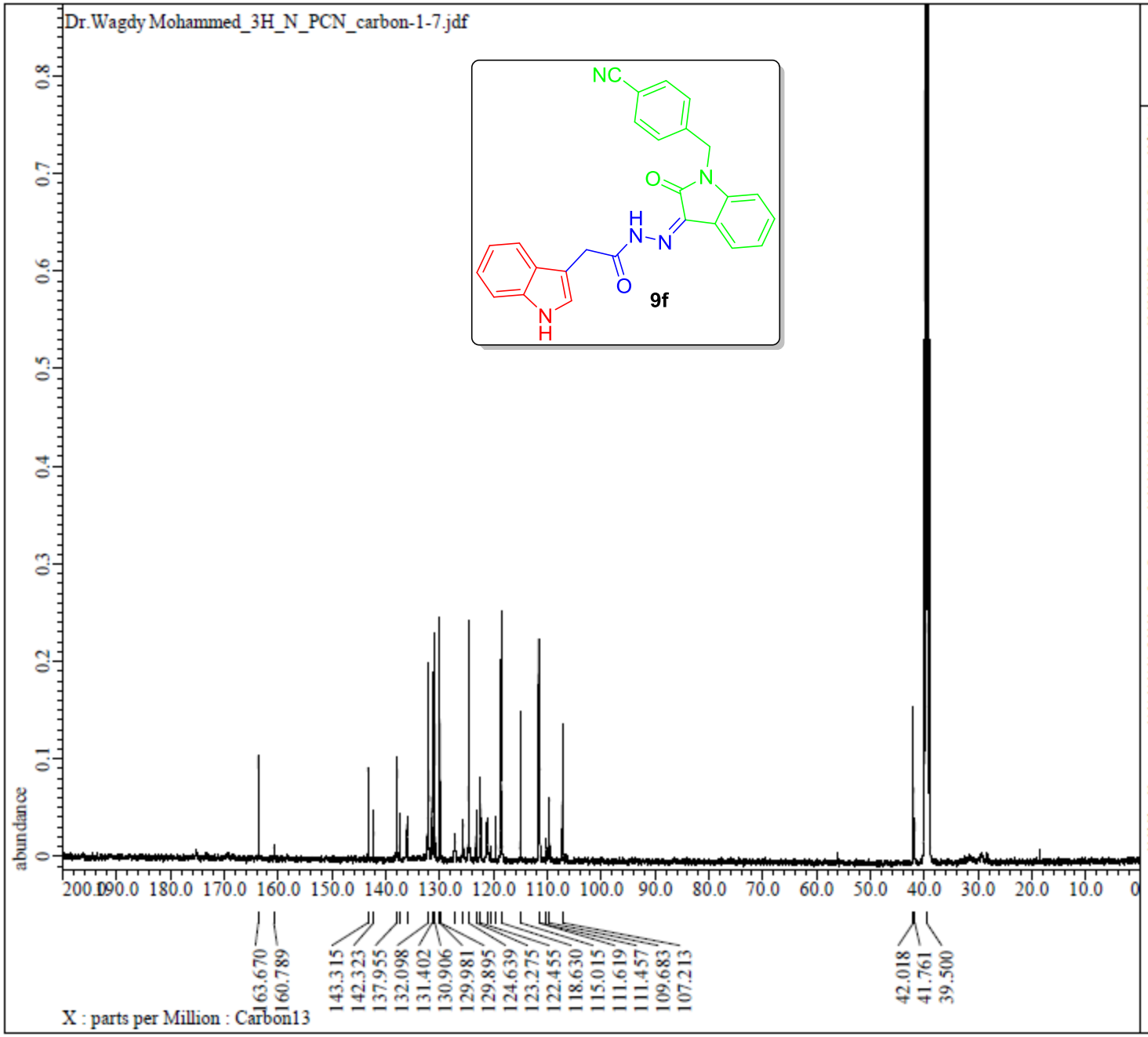
Mansoura University
JEOL ECA- 500 II
NMR Unit

```
Filename          = Dr.Wagdy Mohammed_3H_N_
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Dr.Wagdy Mohammed_3H_N_
Solvent           = DMSO-D6
Creation_Time     = 23-SEP-2019 11:28:22
Revision_Time     = 25-SEP-2019 10:35:45
Current_Time      = 25-SEP-2019 10:35:51

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        = 42
Temp_Get          = 21.5[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]
```


Dr.Wagdy Mohammed_3H_N_BZ_carbon-1-6.jdf
Mansoura University
JEOL
ECA-500 II
NMR Unit
Filename = Dr.Wagdy Mohammed_3H_N_B
Author = delta
Experiment = carbon.jxp
Sample_Id = Dr.Wagdy Mohammed_3H_N_B
Solvent = DMSO-D6
Creation_Time = 23-SEP-2019 21:03:23
Revision_Time = 24-SEP-2019 12:45:31
Current_Time = 24-SEP-2019 12:46:17
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 = FALSE
Scans = 3700
Total_Scans = 3700
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 18.6[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]
9d
abundance
163.536
143.601
136.180
136.076
132.232
128.721
127.510
127.233
125.679
124.639
122.321
121.138
118.659
114.824
111.448
109.864
107.222
42.648
39.500
X : parts per Million : Carbon13

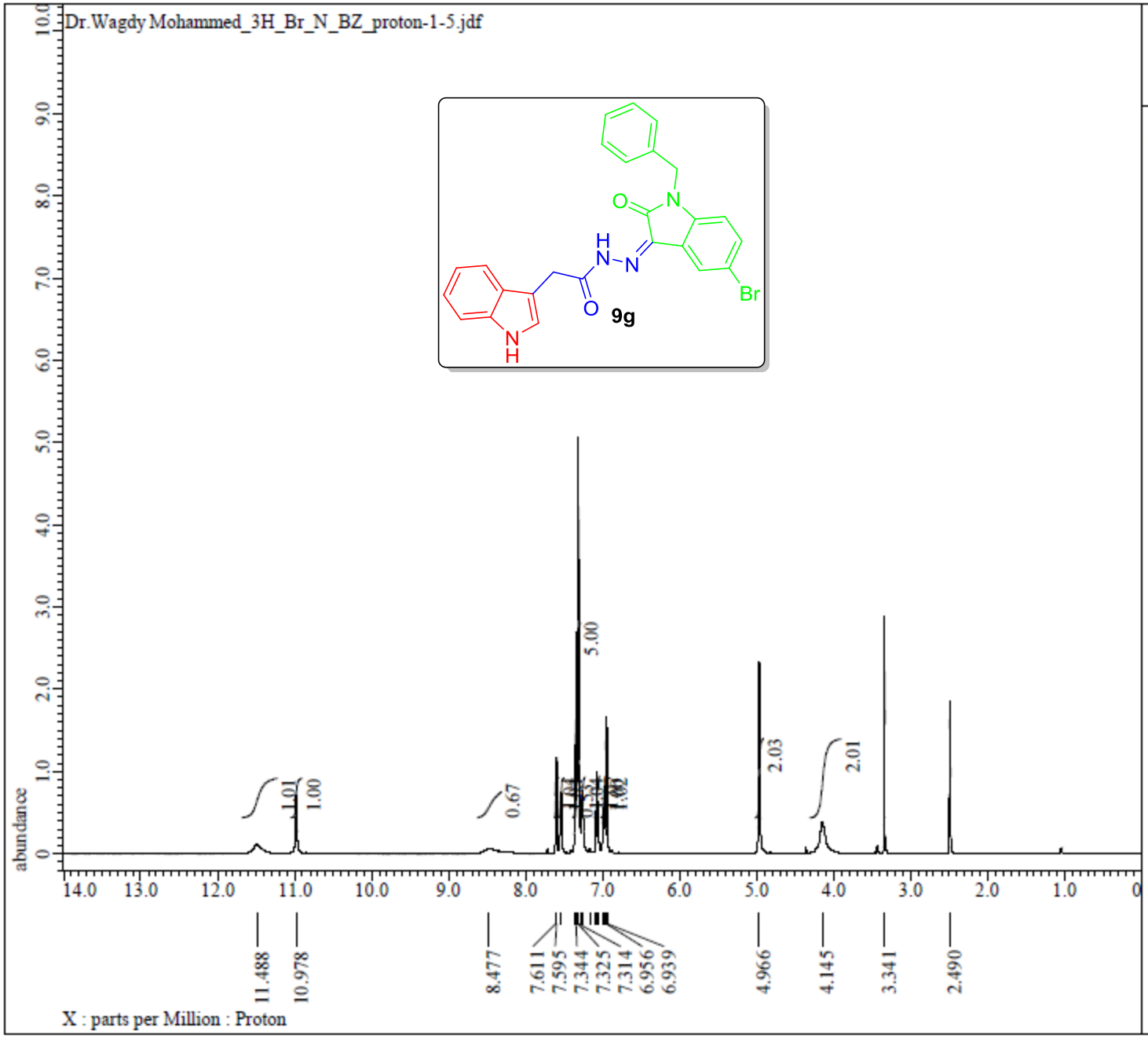

Dr. Wagdy Mohamd_3H-4FBz_proton-1-4.jdf
Mansoura University
JEOL
ECA- 500 II
NMR Unit
F
O
N
H
N
N
O
N
H
9e
abundance
0.95
3.00
0.31
3.00
10.05
2.04
6.00
3.91
3.99
11.238
10.999
8.166
7.612
7.597
7.377
7.362
7.348
7.153
7.014
4.947
4.150
3.343
2.490
X : parts per Million : Proton
Filename = Dr. Wagdy Mohamd_3H-4FB
Author = delta
Experiment = proton.jxp
Sample_Id = Dr. Wagdy Mohamd_3H-4FB
Solvent = DMSO-D6
Creation_Time = 17-SEP-2019 14:55:04
Revision_Time = 17-SEP-2019 14:37:29
Current_Time = 17-SEP-2019 14:37:55
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 = 42
Temp_Get = 20[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]


Dr.Wagdy Mohammed_3H_N_PCN_proton-1-10.jdf
Mansoura University
JEOL
ECA- 500 II
NMR Unit
NC
O
N
H
N
N
O
N
H
9f
Filename = Dr.Wagdy Mohammed_3H_N_
Author = delta
Experiment = proton.jxp
Sample_Id = Dr.Wagdy Mohammed_3H_N_
Solvent = DMSO-D6
Creation_Time = 23-SEP-2019 12:02:28
Revision_Time = 26-SEP-2019 13:50:57
Current_Time = 26-SEP-2019 13:51:02
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 = 40
Temp_Get = 21[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]
abundance
0.66
1.04
4.01
3.02
3.02
0.85
0.30
2.01
11.247
11.087
11.001
7.851
7.738
7.620
7.605
7.538
7.377
7.362
7.347
7.014
7.008
6.999
5.020
4.959
4.942
4.227
4.145
3.926
3.350
2.490
X : parts per Million : Proton



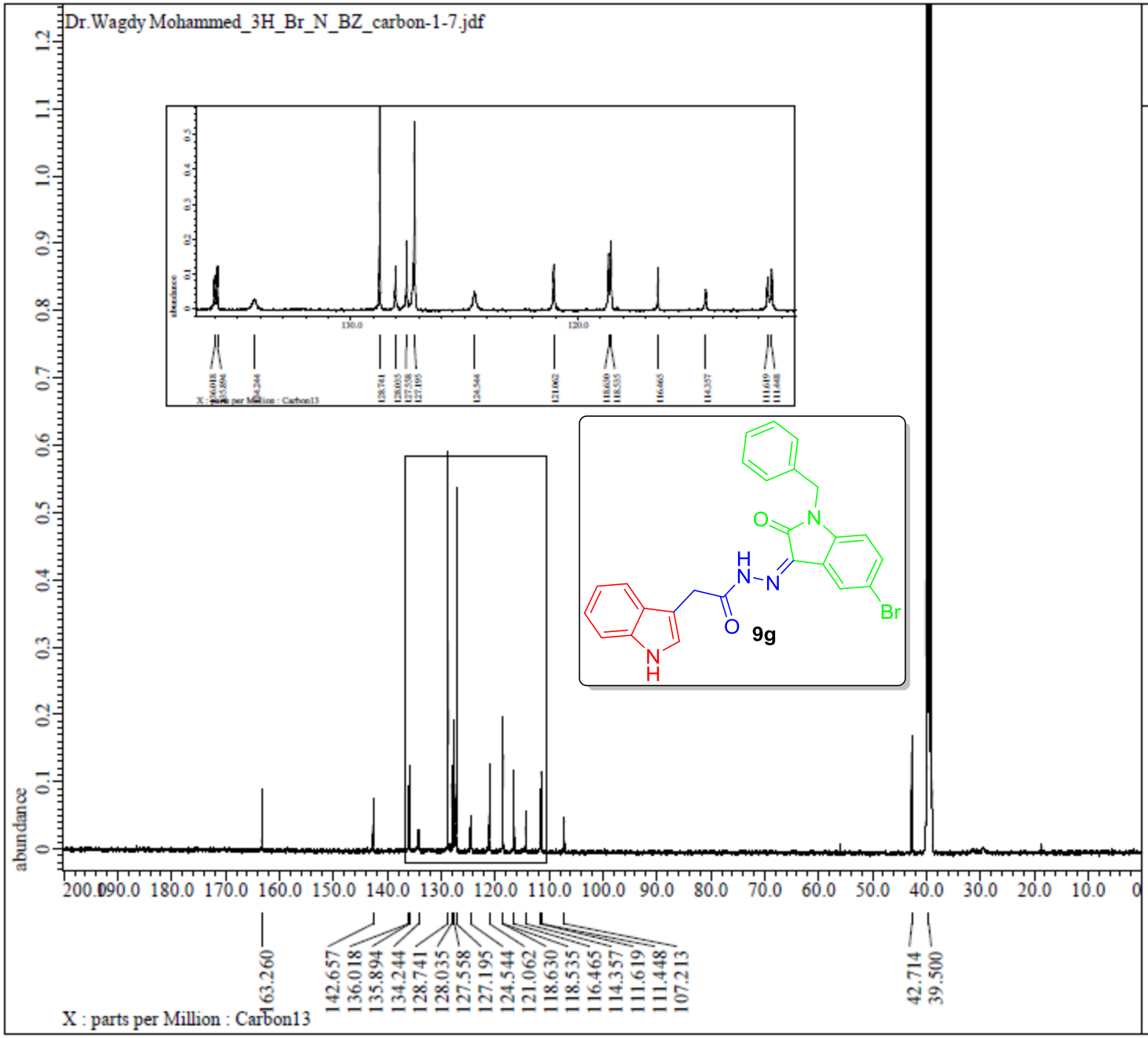
Mansoura University
JEOL
ECA- 500 II
NMR Unit

Filename	= Dr.Wagdy Mohammed_3H_N_P
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= Dr.Wagdy Mohammed_3H_N_P
Solvent	= DMSO-D6
Creation_Time	= 24-SEP-2019 06:14:19
Revision_Time	= 24-SEP-2019 12:59:14
Current_Time	= 24-SEP-2019 13:00:02
Comment	= single pulse decoupled c
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	= 3700
Total_Scans	= 3700
Relaxation_Delay	= 2[s]
Recvr_Gain	= 58
Temp_Get	= 19.7[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]



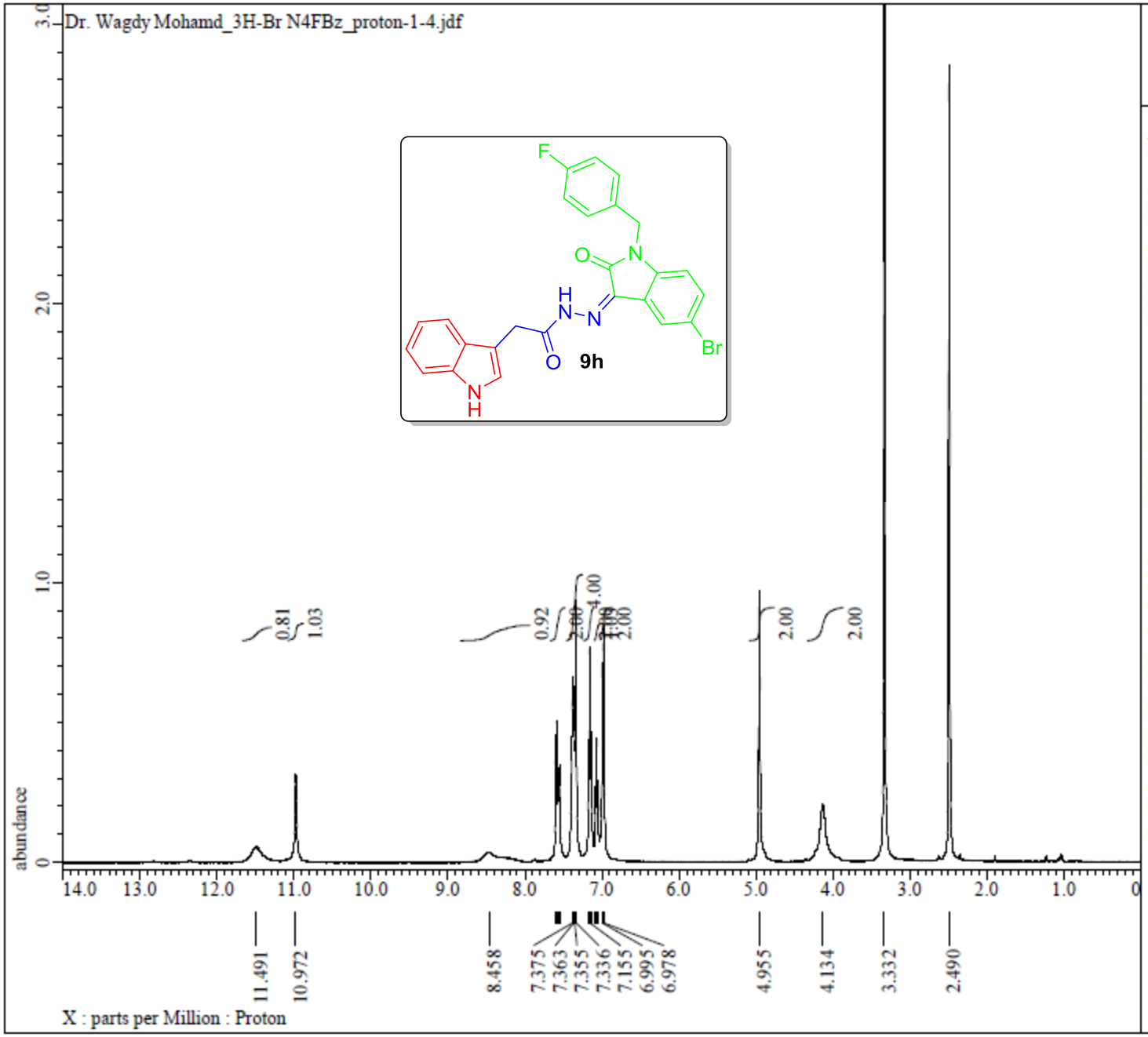
Mansoura University
JEOL ECA- 500 II
NMR Unit

Filename	= Dr.Wagdy Mohammed_3H_Br
Author	= delta
Experiment	= proton.jxp
Sample_Id	= Dr.Wagdy Mohammed_3H_Br
Solvent	= DMSO-D6
Creation_Time	= 23-SEP-2019 11:51:01
Revision_Time	= 17-OCT-2019 14:15:57
Current_Time	= 17-OCT-2019 14:16:04
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
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	= 42
Temp_Get	= 21[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]



Mansoura University
JEOL ECA- 500 II NMR Unit

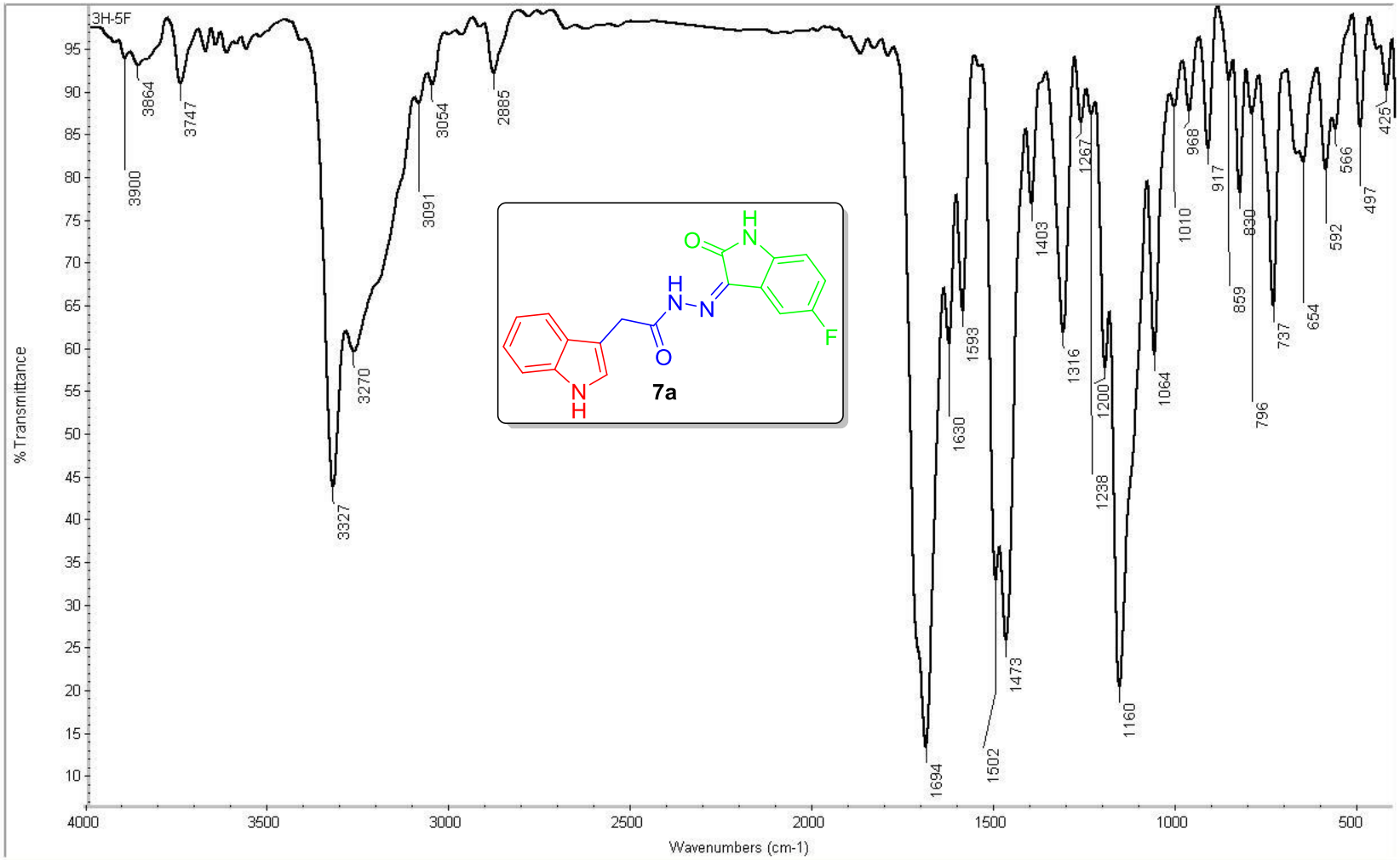
```
Filename          = Dr.Wagdy Mohammed_3H_Br
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Dr.Wagdy Mohammed_3H_Br
Solvent           = DMSO-D6
Creation_Time     = 24-SEP-2019 03:09:35
Revision_Time     = 24-SEP-2019 12:51:49
Current_Time      = 24-SEP-2019 12:52:22

Comment           = single pulse decoupled
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             = 3700
Total_Scans       = 3700

Relaxation_Delay  = 2[s]
Recvr_Gain        = 58
Temp_Get          = 18.9[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         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

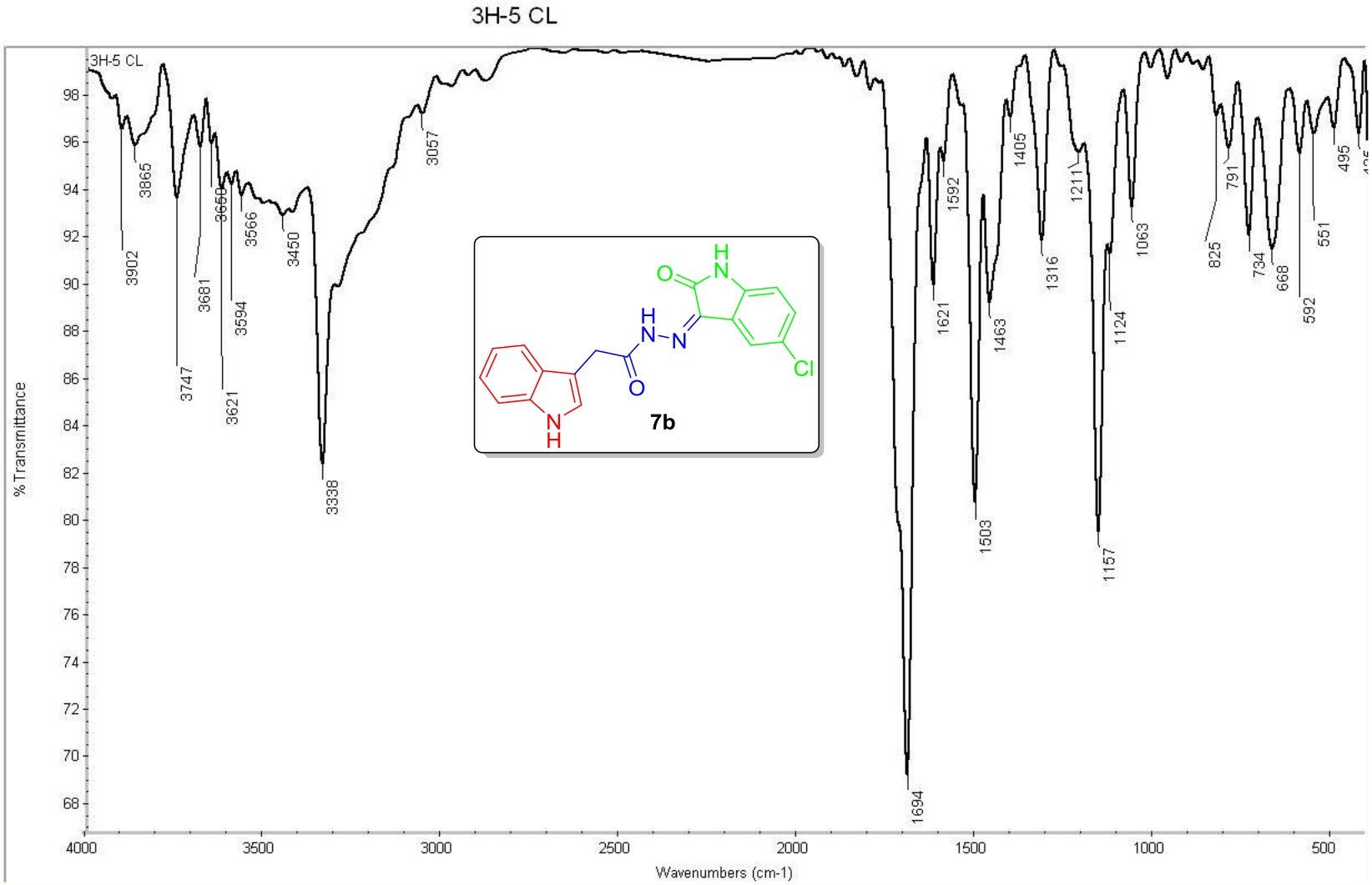


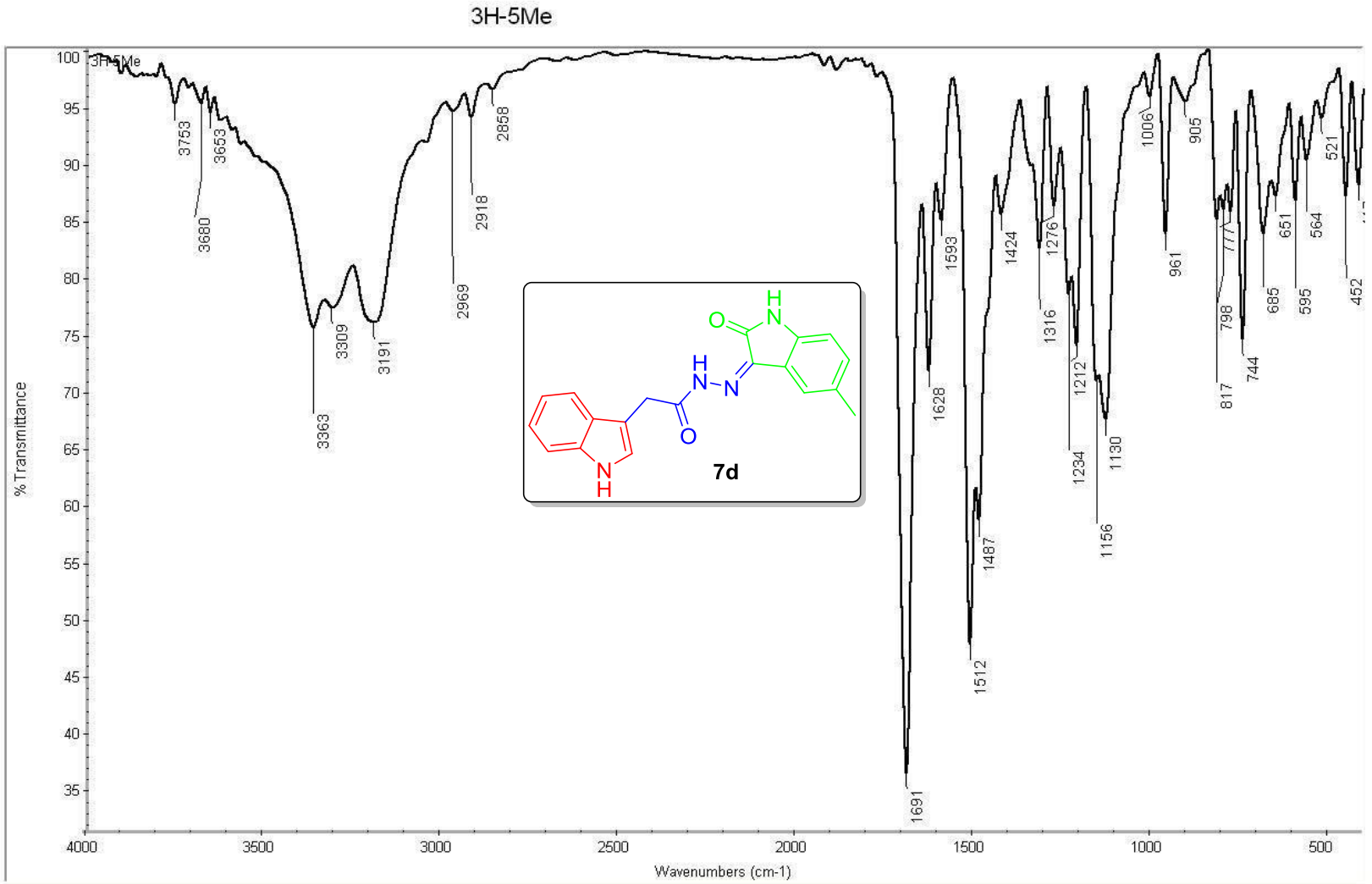
Mansoura University
JEOL
ECA- 500 II
NMR Unit

Filename	= Dr. Wagdy Mohamd_3H-Br
Author	= delta
Experiment	= proton.jxp
Sample_Id	= Dr. Wagdy Mohamd_3H-Br
Solvent	= DMSO-D6
Creation_Time	= 17-SEP-2019 15:23:50
Revision_Time	= 17-SEP-2019 15:55:40
Current_Time	= 17-SEP-2019 15:55:46
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	= 48
Temp_Get	= 20[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]

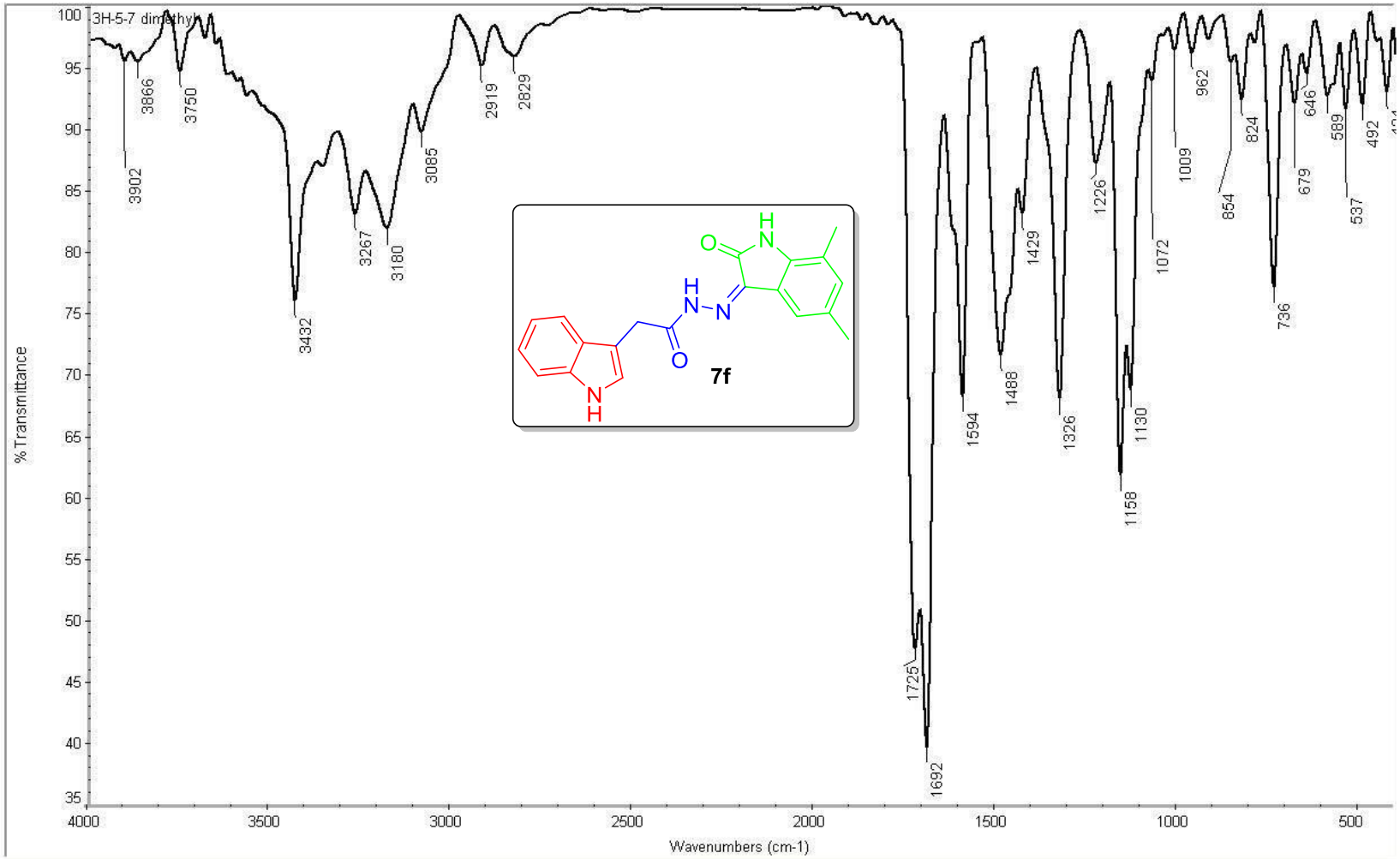
3H-5F

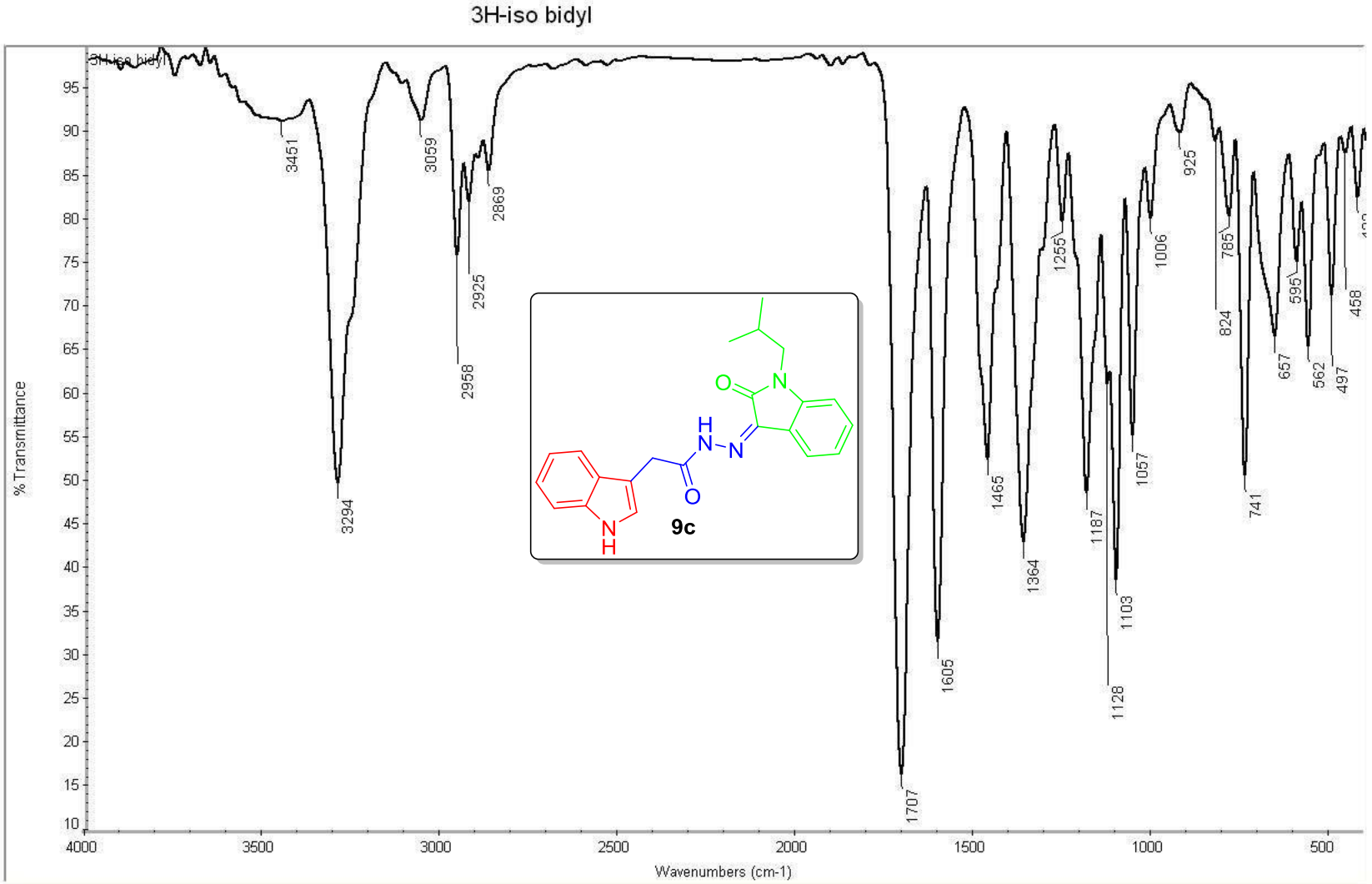

3H-5F
% Transmittance
Wavenumbers (cm-1)
4000
3500
3000
2500
2000
1500
1000
500
3900
3864
3747
3327
3270
3091
3054
2885
1694
1630
1593
1502
1473
1403
1316
1267
1238
1200
1160
1064
1010
968
917
890
859
796
737
654
592
566
497
425
7a

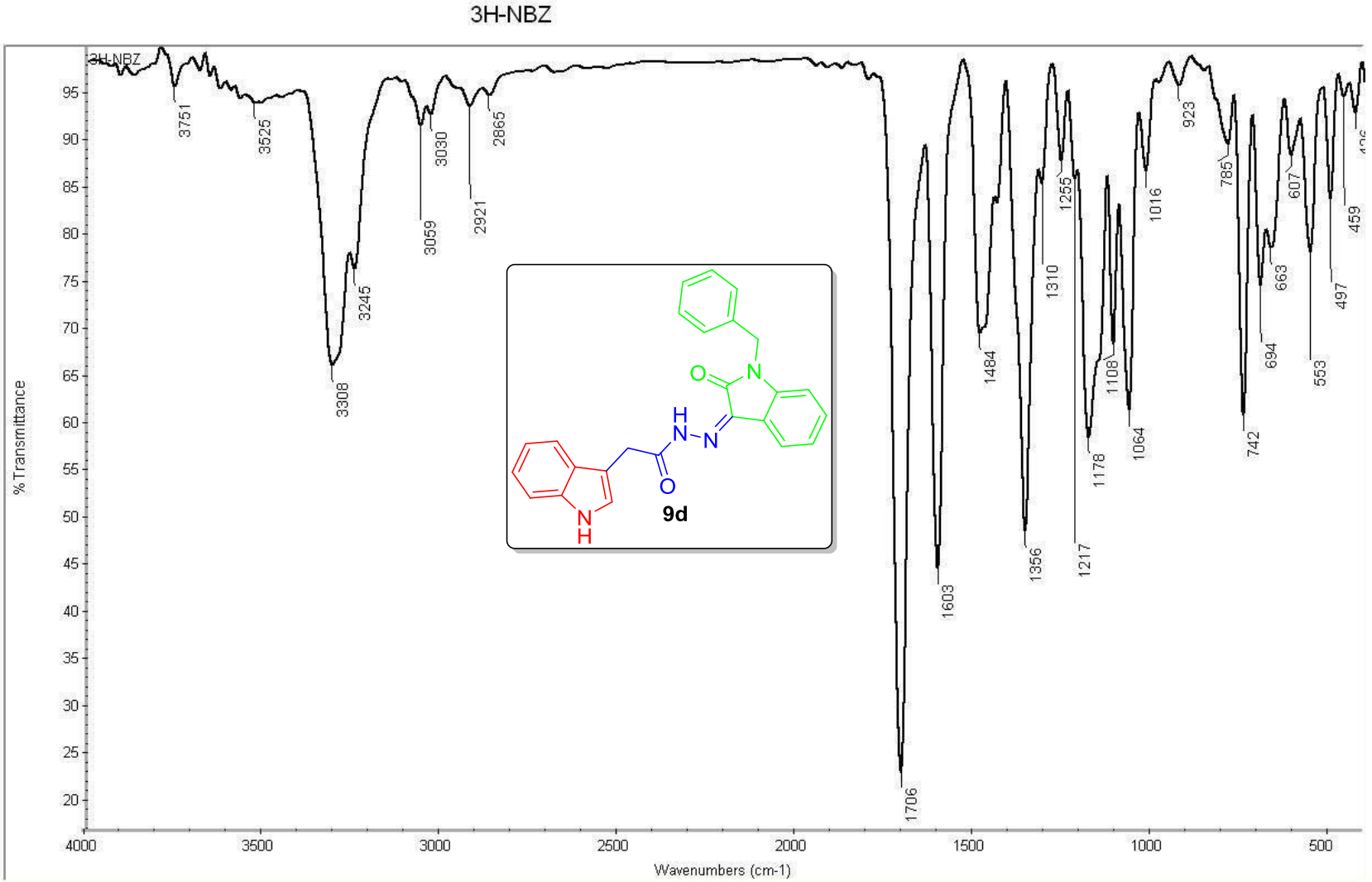

3H-5 CL
3H-5 CL
% Transmittance
Wavenumbers (cm-1)
4000
3500
3000
2500
2000
1500
1000
500
98
96
94
92
90
88
86
84
82
80
78
76
74
72
70
68
3902
3865
3747
3681
3660
3621
3594
3566
3450
3338
3057
1694
1621
1592
1503
1463
1405
1316
1211
1157
1124
1063
825
791
734
668
592
551
495
H
O
N
H
N-N
O
Cl
N
H
7b

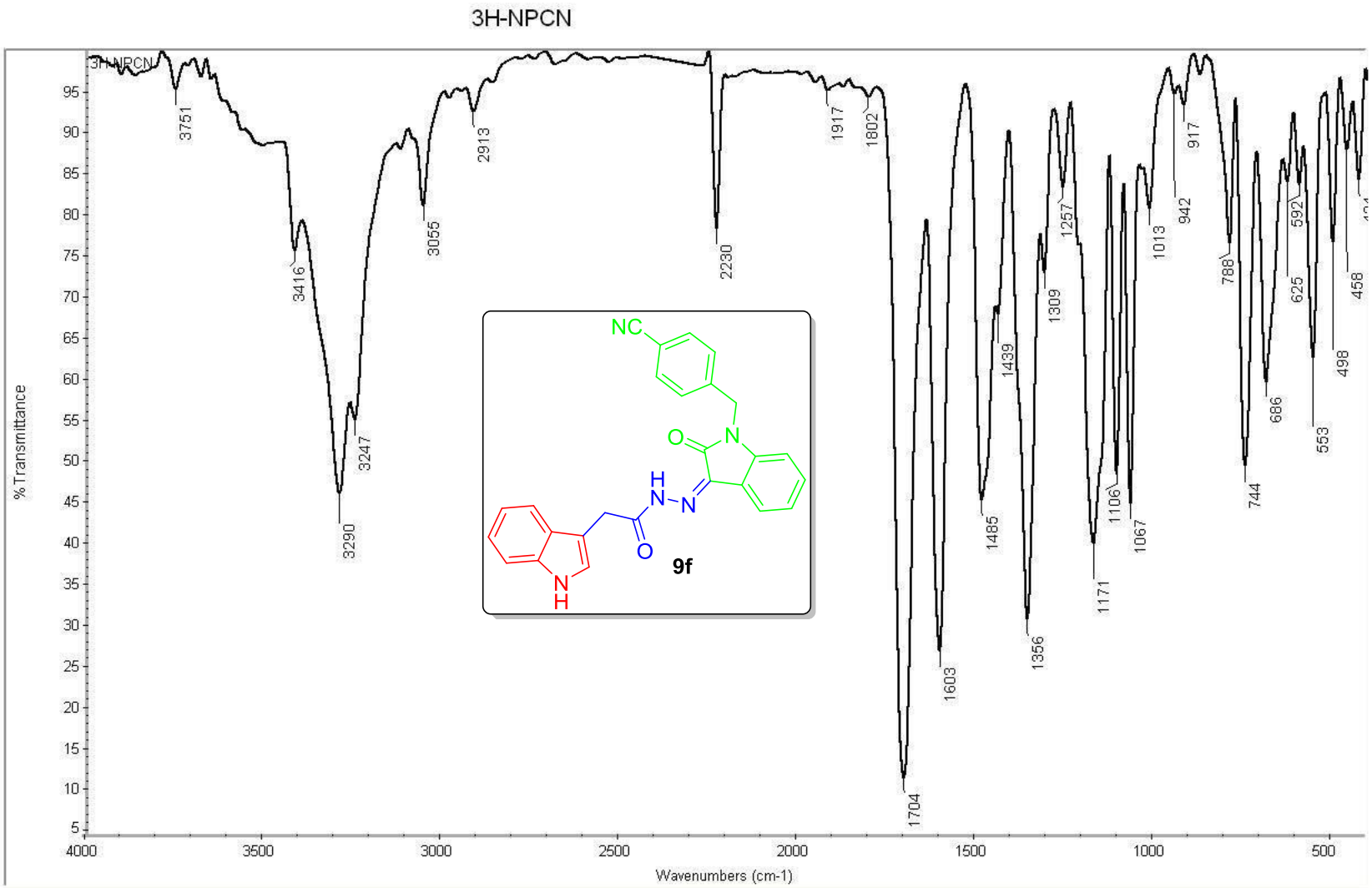

3H-5Me
3H-5Me
% Transmittance
Wavenumbers (cm-1)
100
95
90
85
80
75
70
65
60
55
50
45
40
35
4000
3500
3000
2500
2000
1500
1000
500
3753
3680
3653
3363
3309
3191
2969
2918
2858
1691
1628
1593
1512
1487
1424
1316
1276
1234
1212
1156
1130
1006
961
905
817
798
777
744
685
651
595
564
521
452
7d

3H-5-7 dimethyl

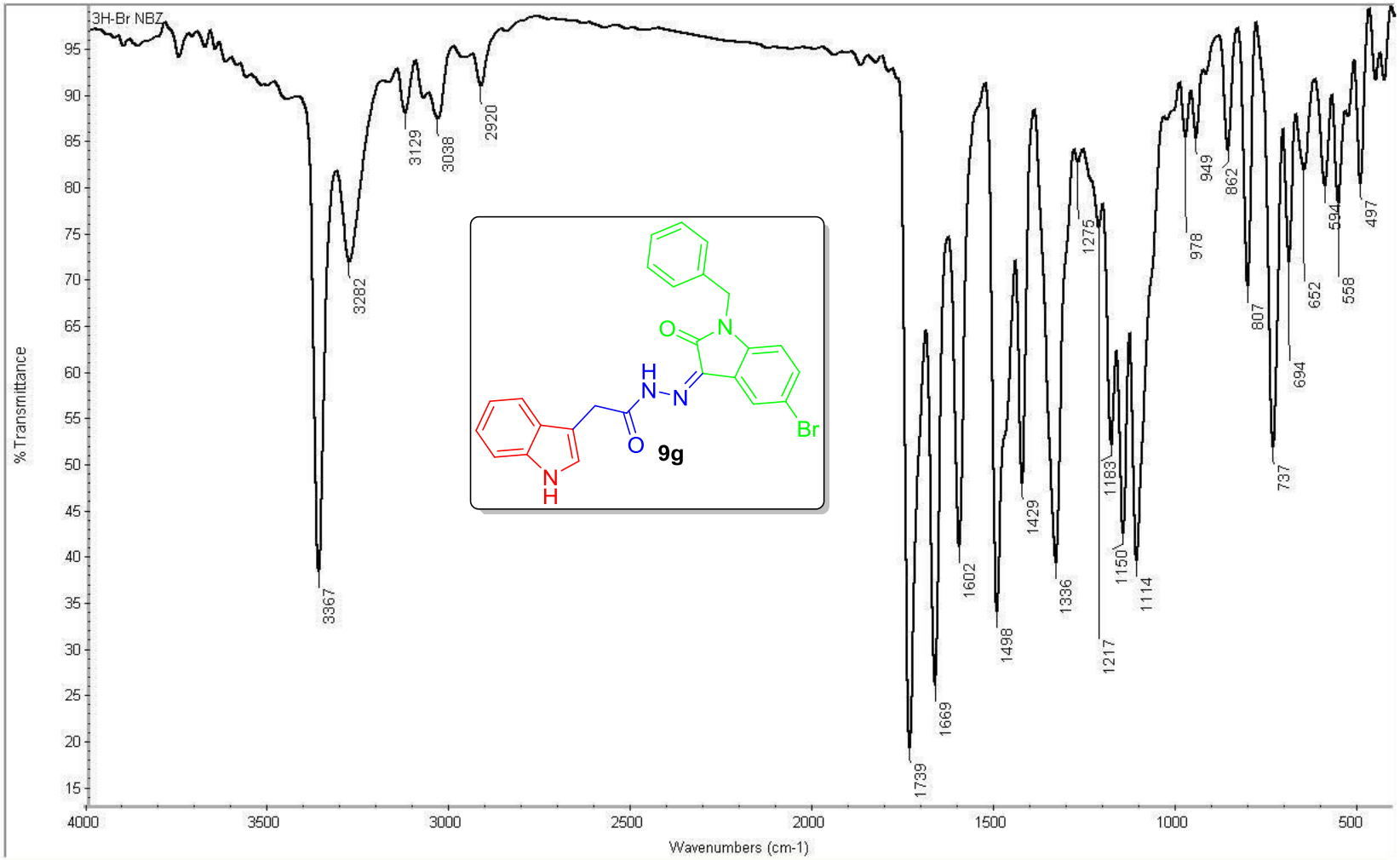



3H-iso bidyl
3H-iso bidyl
% Transmittance
Wavenumbers (cm-1)
4000
3500
3000
2500
2000
1500
1000
500
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
3451
3294
3059
2958
2925
2869
1707
1605
1465
1364
1255
1187
1128
1103
1057
1006
925
824
785
741
657
595
562
497
458
O
N
H
N
N
O
H
9c


3H-NBZ
3H-NBZ
%Transmittance
Wavenumbers (cm-1)
4000
3500
3000
2500
2000
1500
1000
500
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
3751
3525
3308
3245
3059
3030
2921
2865
1706
1603
1484
1356
1310
1255
1217
1178
1108
1064
1016
923
785
742
694
663
607
553
497
459
O
N
H
N
N
O
H
N
9d


3H-NPCN
3H-NPCN
% Transmittance
Wavenumbers (cm-1)
3751
3416
3290
3247
3055
2913
2230
1917
1802
1704
1603
1485
1439
1356
1309
1257
1171
1106
1067
1013
942
917
788
744
686
625
592
553
498
458
NC
O
N
H
N
N
O
H
N
9f

3H-Br NBZ


3H-Br NBZ
% Transmittance
Wavenumbers (cm-1)
4000
3500
3000
2500
2000
1500
1000
500
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
3367
3282
3129
3038
2920
1739
1669
1602
1498
1429
1336
1275
1217
1183
1150
1114
978
949
862
807
737
694
652
594
558
497
O
N
H
N
N
O
Br
H
9g