

Supplementary Materials

1,3,4-Oxadiazole N-Mannich Bases: Synthesis, Antimicrobial, and Anti-Proliferative Activities

Table S1. Molecular formulae, molecular weights and elemental analyses data of compounds **4a-l** and **5a-d**.

Comp. No.	Mol. Formula (Mol. Wt.)	Analysis: % Calcd. (Found)			
		C	H	N	S
4a	C ₁₇ H ₁₇ N ₃ O ₃ S (343.40)	59.46 (59.23)	4.99 (5.02)	12.24 (12.13)	9.34 (9.33)
4b	C ₁₇ H ₁₆ FN ₃ O ₃ S (361.39)	56.50 (56.44)	4.46 (4.52)	11.63 (11.60)	8.87 (8.85)
4c	C ₁₇ H ₁₆ ClN ₃ O ₃ S (377.85)	54.04 (53.88)	4.27 (4.29)	11.12 (11.02)	8.49 (8.50)
4d	C ₁₇ H ₁₆ ClN ₃ O ₃ S (377.85)	54.04 (54.0)	4.27 (4.32)	11.12 (11.04)	8.49 (8.47)
4e	C ₁₇ H ₁₆ N ₄ O ₃ S (388.40)	52.57 (52.44)	4.15 (4.22)	14.43 (14.41)	8.26 (8.12)
4f	C ₁₇ H ₁₆ N ₄ O ₃ S (388.40)	52.57 (52.50)	4.15 (4.18)	14.43 (14.43)	8.26 (8.25)
4g	C ₁₇ H ₁₆ N ₄ O ₃ S (388.40)	52.57 (52.52)	4.15 (4.23)	14.43 (14.25)	8.26 (8.22)
4h	C ₁₈ H ₁₆ F ₃ N ₃ O ₃ S (411.40)	52.55 (52.32)	3.92 (4.02)	10.21 (10.22)	7.79 (7.60)
4i	C ₁₈ H ₁₆ F ₃ N ₃ O ₃ S (411.40)	52.55 (52.48)	3.92 (3.94)	10.21 (10.15)	7.79 (7.72)
4j	C ₁₇ H ₁₅ F ₂ N ₃ O ₃ S (379.38)	53.82 (53.72)	3.99 (4.04)	11.08 (11.01)	8.45 (8.44)
4k	C ₁₇ H ₁₅ F ₂ N ₃ O ₃ S (379.38)	53.82 (53.66)	3.99 (4.12)	11.08 (10.88)	8.45 (8.45)
4l	C ₁₇ H ₁₅ Cl ₂ N ₃ O ₃ S (412.29)	49.52 (49.34)	3.67 (3.75)	10.19 (10.20)	7.78 (7.76)
5a	C ₂₁ H ₂₄ N ₄ O ₃ S (412.51)	61.14 (61.14)	5.86 (5.92)	13.58 (13.42)	7.77 (7.68)
5b	C ₂₁ H ₂₃ FN ₄ O ₃ S (430.50)	58.59 (58.44)	6.96 (6.99)	5.52 (5.38)	6.32 (6.30)
5c	C ₂₂ H ₂₆ N ₄ O ₃ S (426.53)	61.95 (61.72)	6.14 (6.30)	13.14 (13.0)	7.52 (7.48)
5d	C ₂₃ H ₂₅ F ₃ N ₄ O ₃ S (494.53)	55.86 (55.64)	5.10 (5.18)	11.33 (11.24)	6.48 (6.44)

Determination of *in vitro* antimicrobial activity (agar disc diffusion method) [1]

Sterile filter paper discs (8 mm diameter) were moistened with the compound solution in dimethyl sulfoxide of specific concentration (200 µg/disc), and the antibacterial drugs, Gentamicin sulphate and Ampicillin trihydrate (100 µg/disc) and the antifungal drug Clotrimazole (100 µg/disc), were carefully placed on agar culture plates that had been previously inoculated separately with the microorganisms. The plates were incubated at 37 °C, and the diameters of the growth inhibition zones were measured after 24 hours for bacteria and 48 hours for *C. albicans*.

Determination of the minimal inhibitory concentration (MIC) [2]

Compounds **4j**, **4l**, **5a**, **5b**, **5c**, **5d**, Gentamicin sulfate, Ampicillin trihydrate, and Clotrimazole were dissolved in dimethyl sulphoxide at a concentration of 128 µg/mL. The two-fold dilutions of the solution were prepared (128, 64, 32, ..., 0.25 µg/mL). Suspensions of the microorganisms at concentrations of 10⁶ colony-forming units per mL were inoculated in the corresponding wells. The plates were then incubated at 36°C for 24 hours. The MIC values were determined as the lowest concentrations that completely inhibited visible growth of the microorganism as detected by the unaided eye.

Determination of *in vitro* anti-proliferative activity [3,4]

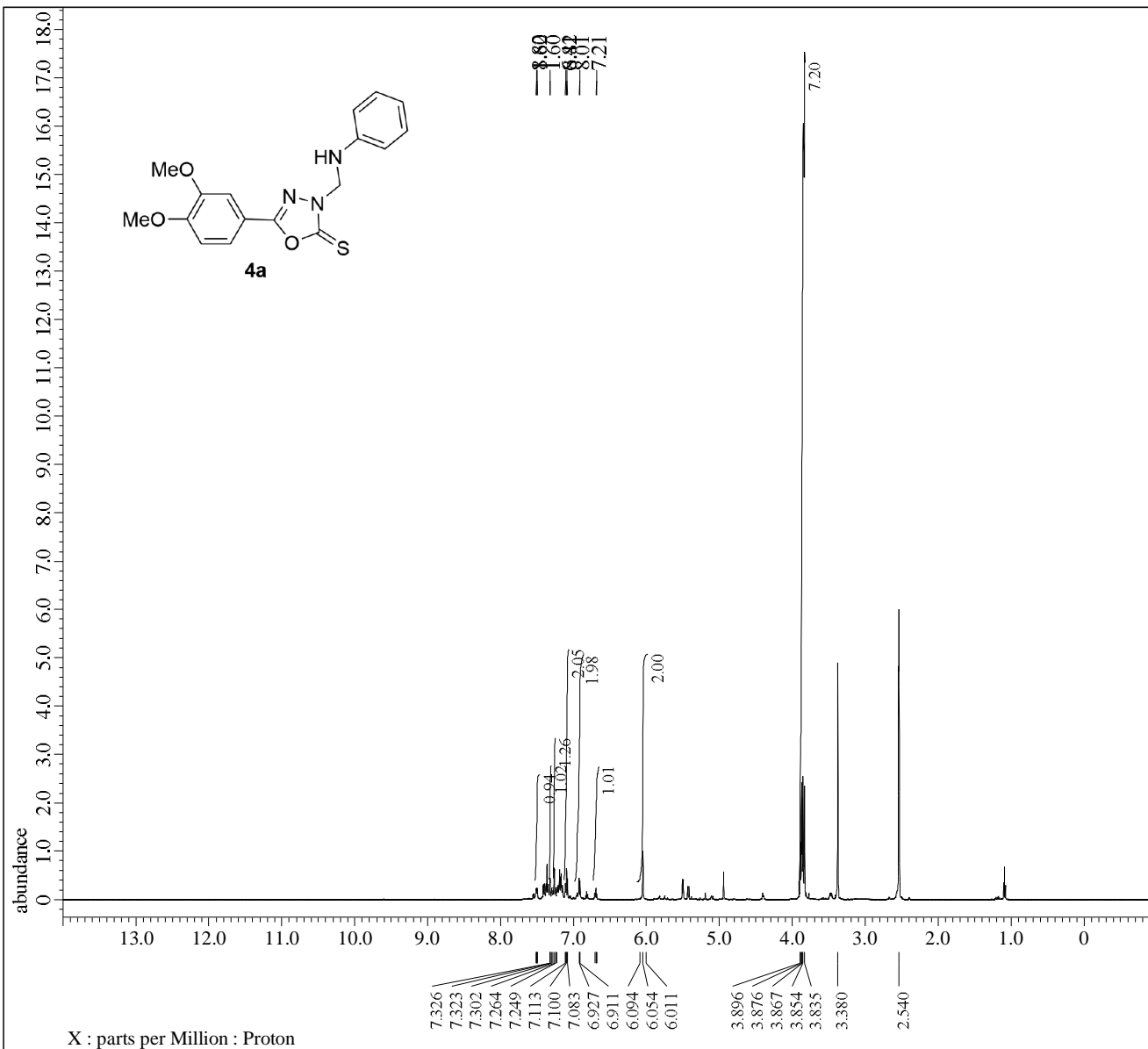
The *in vitro* anti-proliferative activity screening of compounds **4a-1** and **5a-d** was measured against three human cancer cell lines namely; prostate cancer (PC3), human colorectal cancer (HCT-116), human hepatocellular carcinoma (HePG-2), human epithelioid carcinoma (HeLa) and human breast cancer (MCF7) cell lines using the standard MTT assay. PC3, HCT-116, HePG-2, HeLa and MCF7 cells (3000 cells per well) were cultured and seeded into 96-well plates and the plates were incubated for 24 hours. The cells were then treated with compounds **4a-1**, **5a-d** and Doxorubicin at different concentrations in DMSO (0.1 µM to 100 µM) at 37 °C in an atmosphere of 5% CO₂ for 48 hours. Freshly prepared MTT was added to each well at a terminal concentration of 5 µg/mL and incubated with cells at 37 °C for 4 hours. The formazan crystals were dissolved in 100 µL of DMSO in each well, and the absorbency at 492 nm (for absorbance of MTT formazan) and 630 nm (for the reference wavelength) was measured with an enzyme linked immunosorbent assay (ELISA) reader (ChroMate-4300, FL, USA). All compounds were tested three times in each of the cell lines. The IC₅₀ values were calculated according to the equation for Boltzmann sigmoidal concentration response curve using the nonlinear regression fitting models (Graph Pad, Prism Version 5). The results reported are means of

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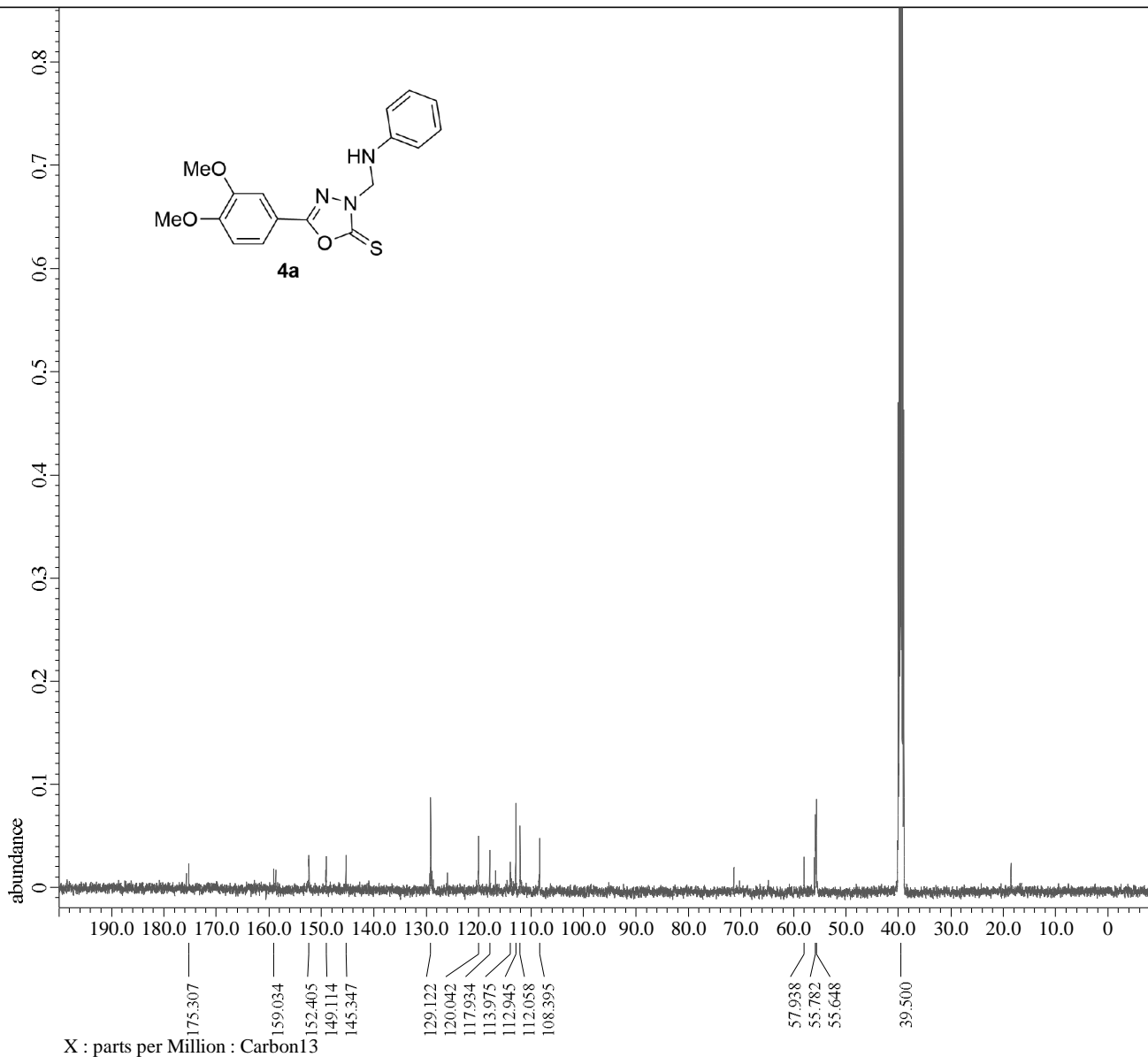
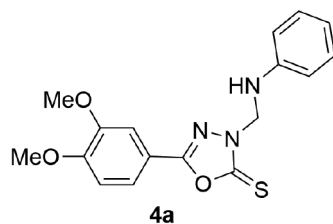
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X : parts per Million : Proton



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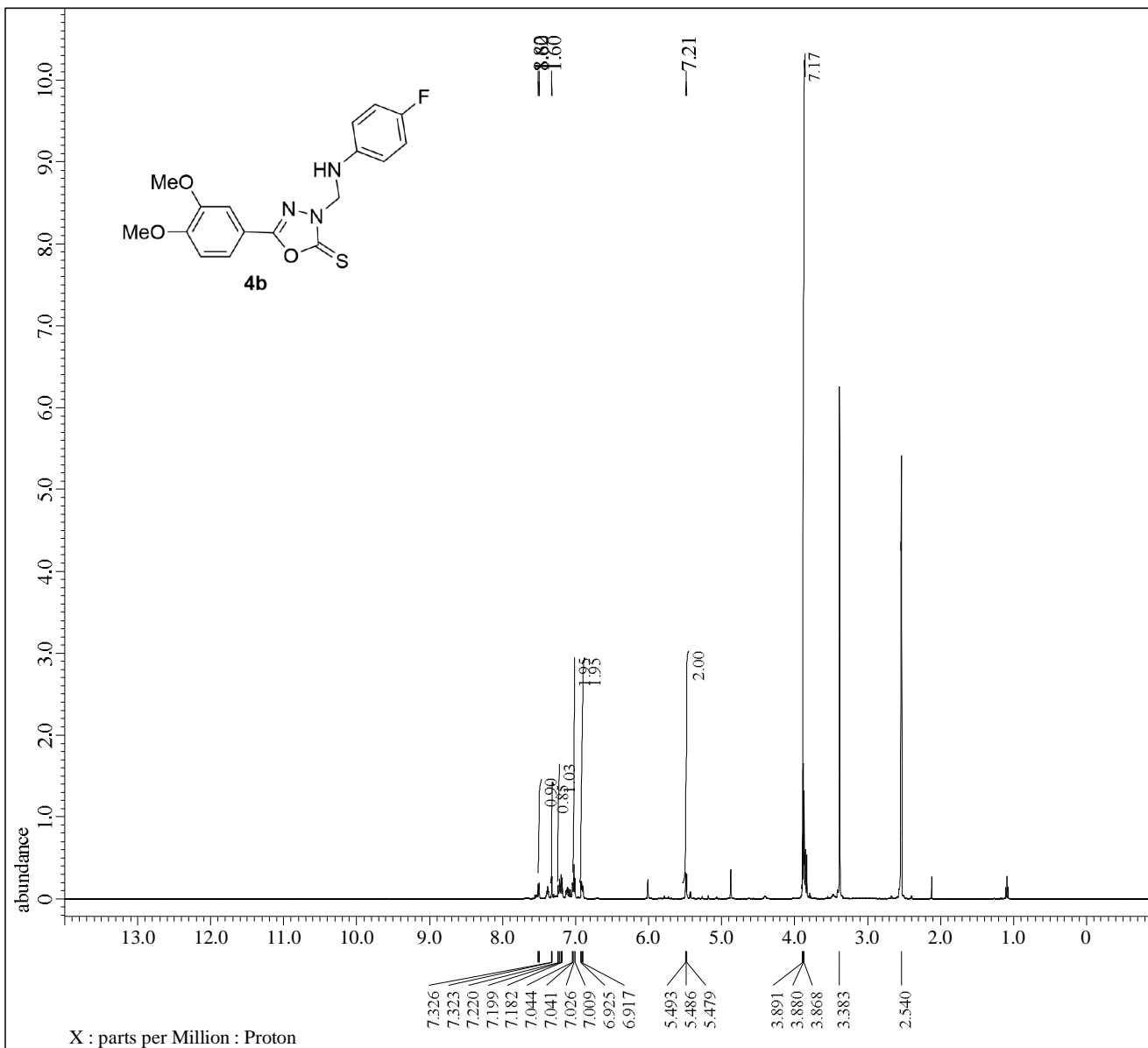
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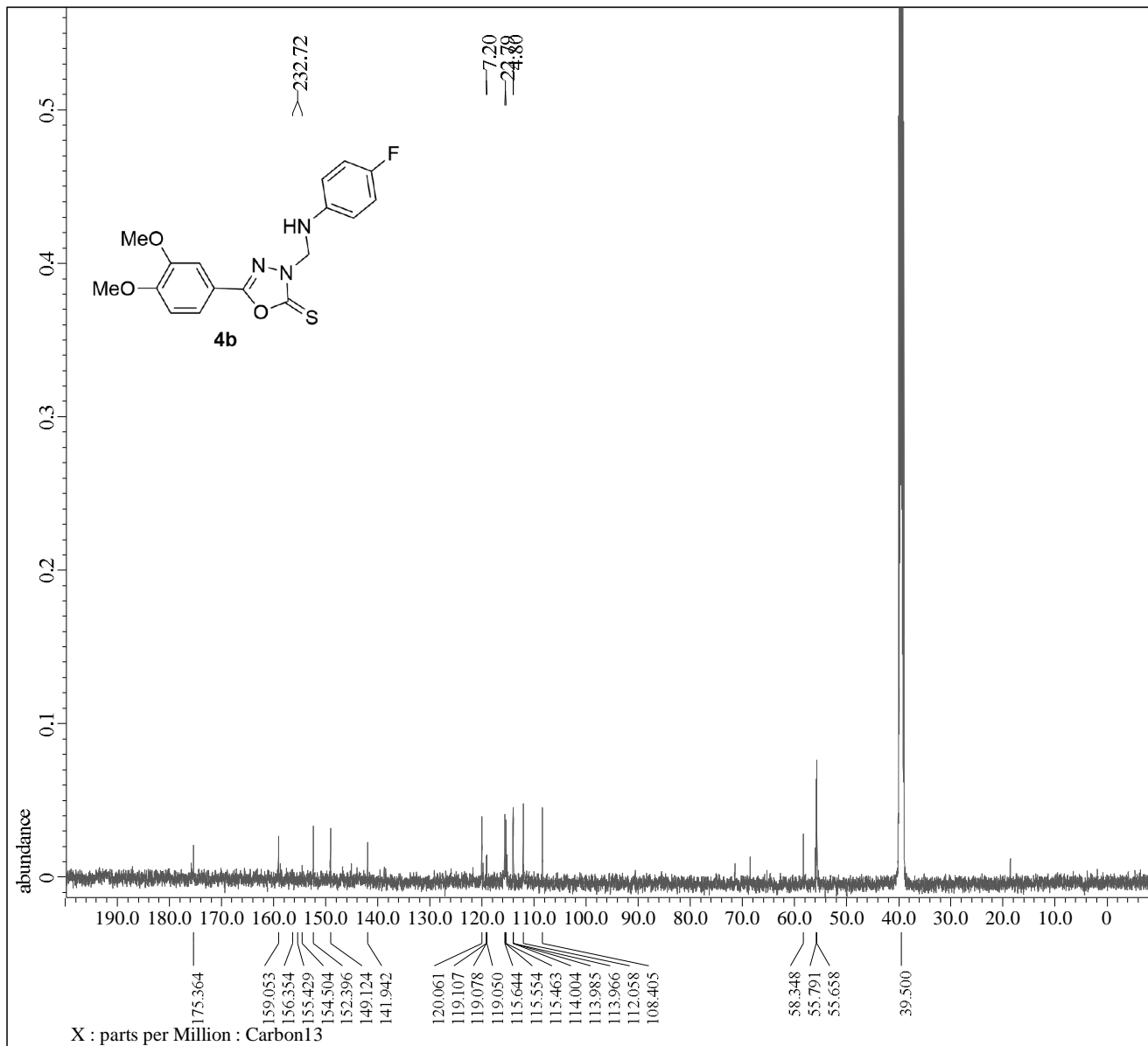


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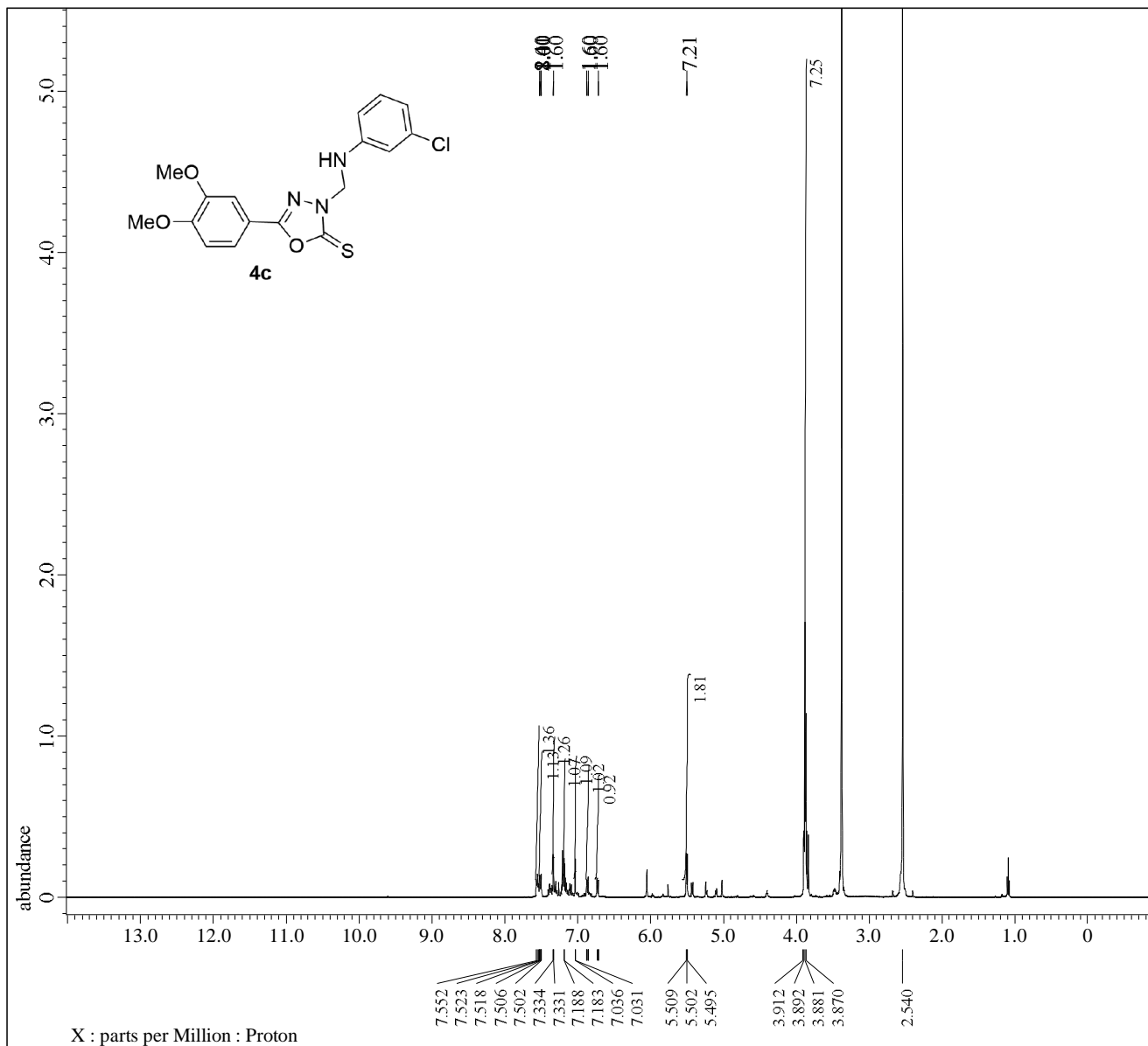


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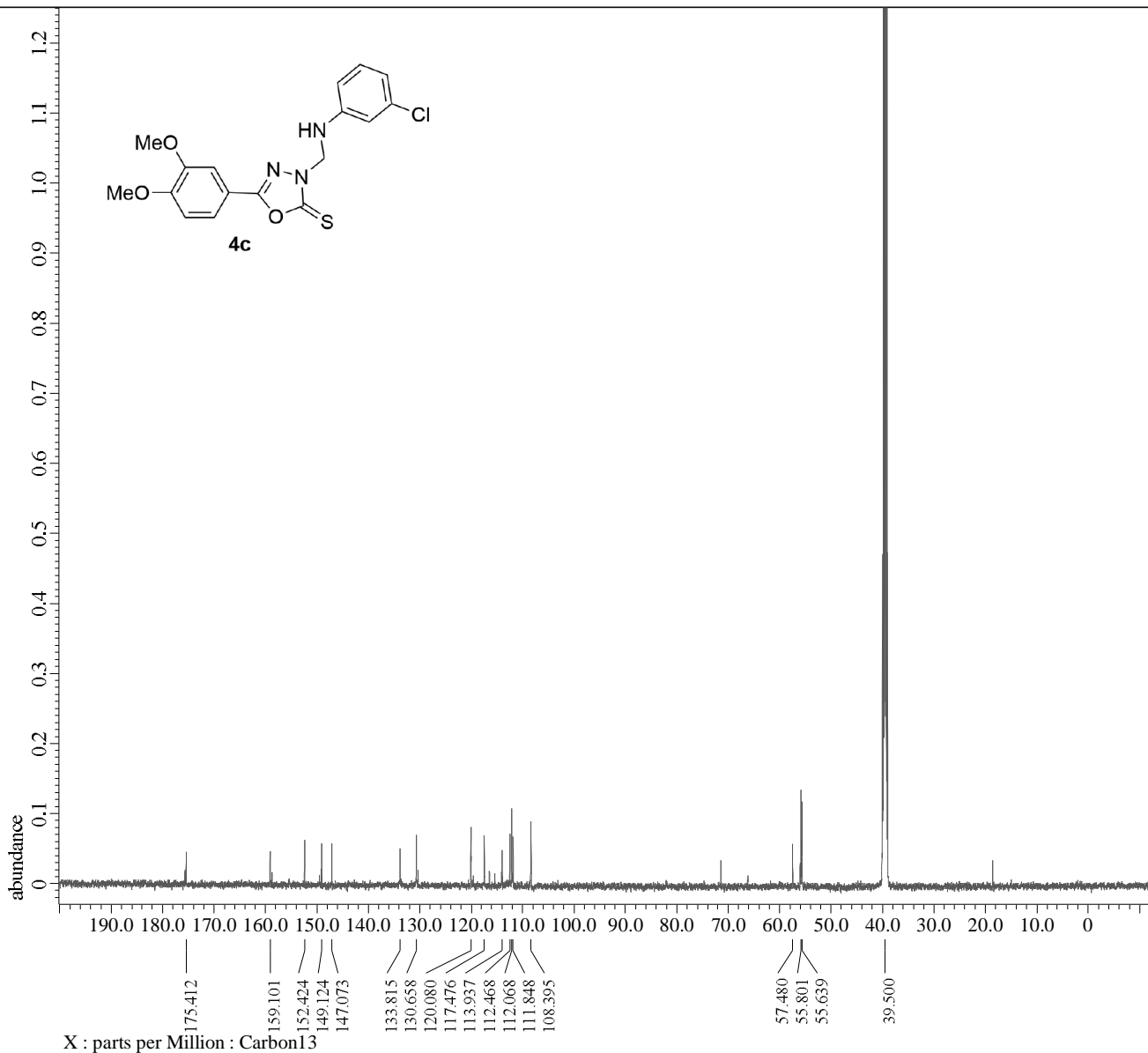
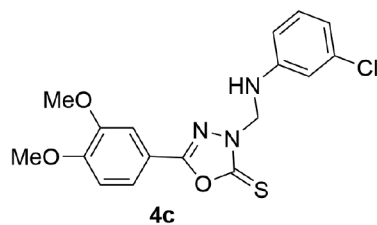
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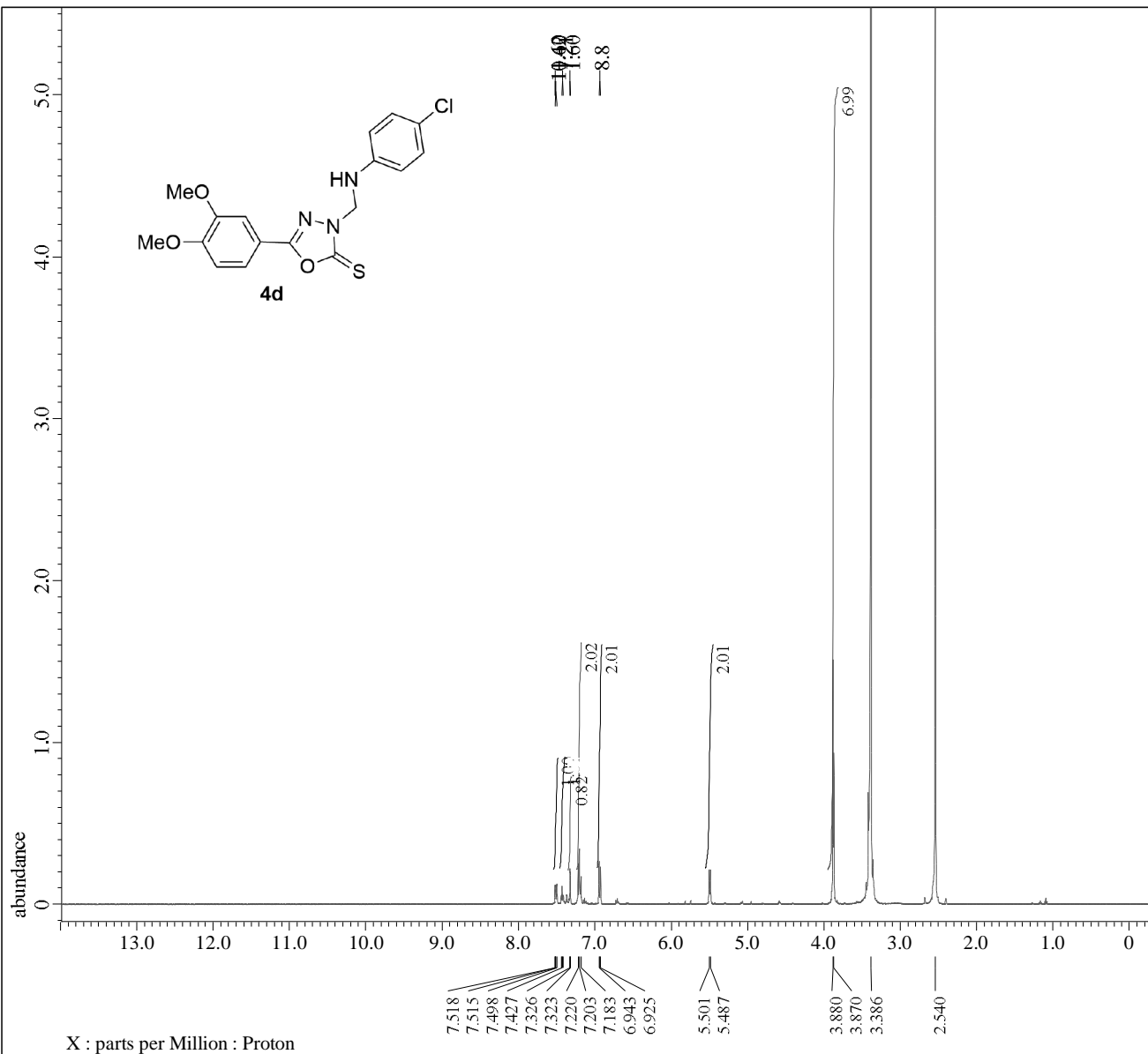
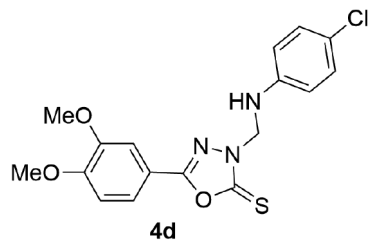
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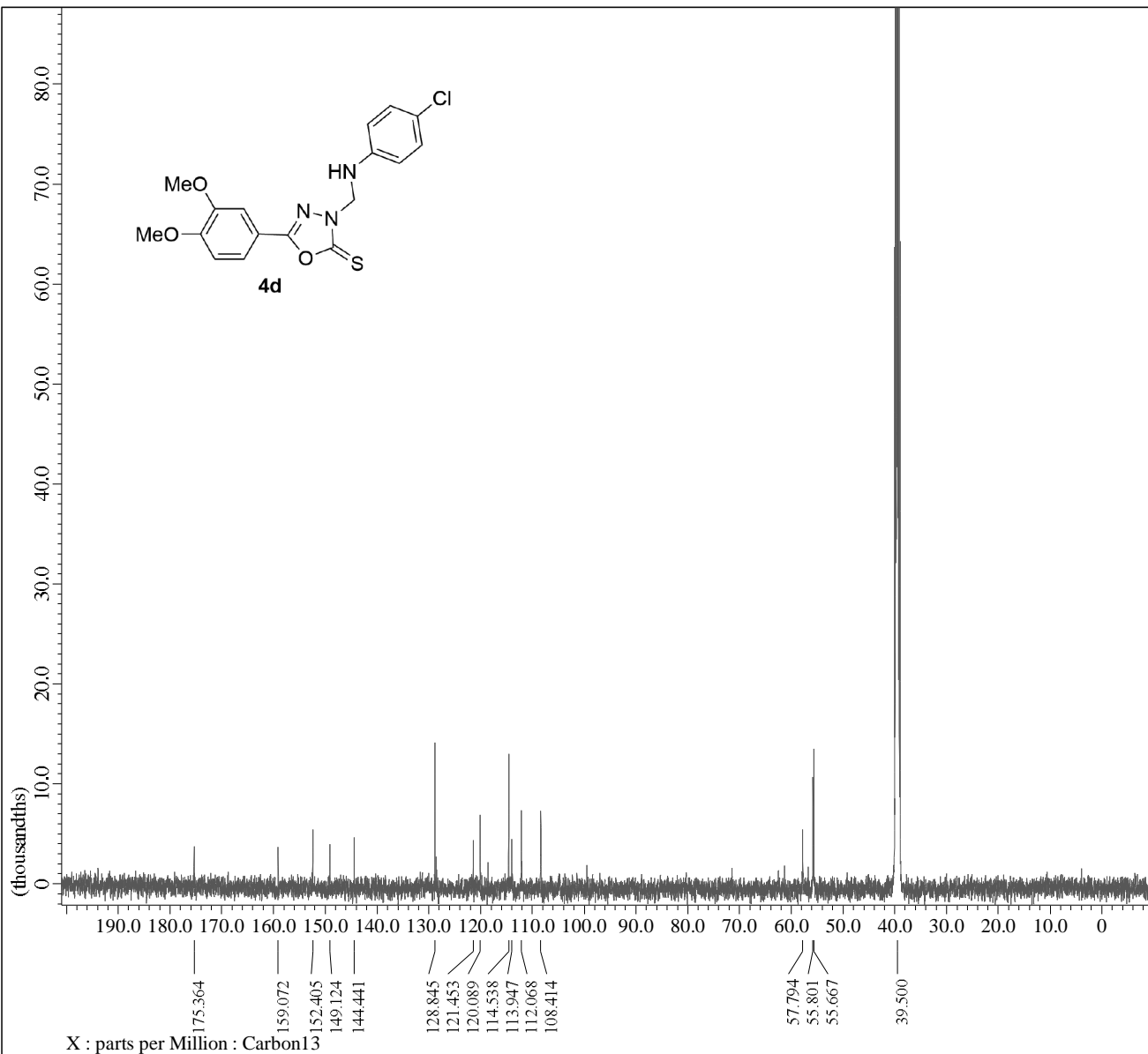
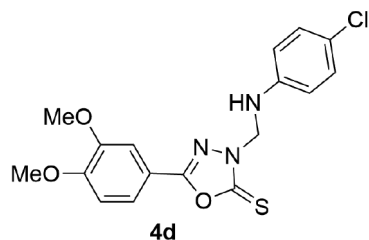


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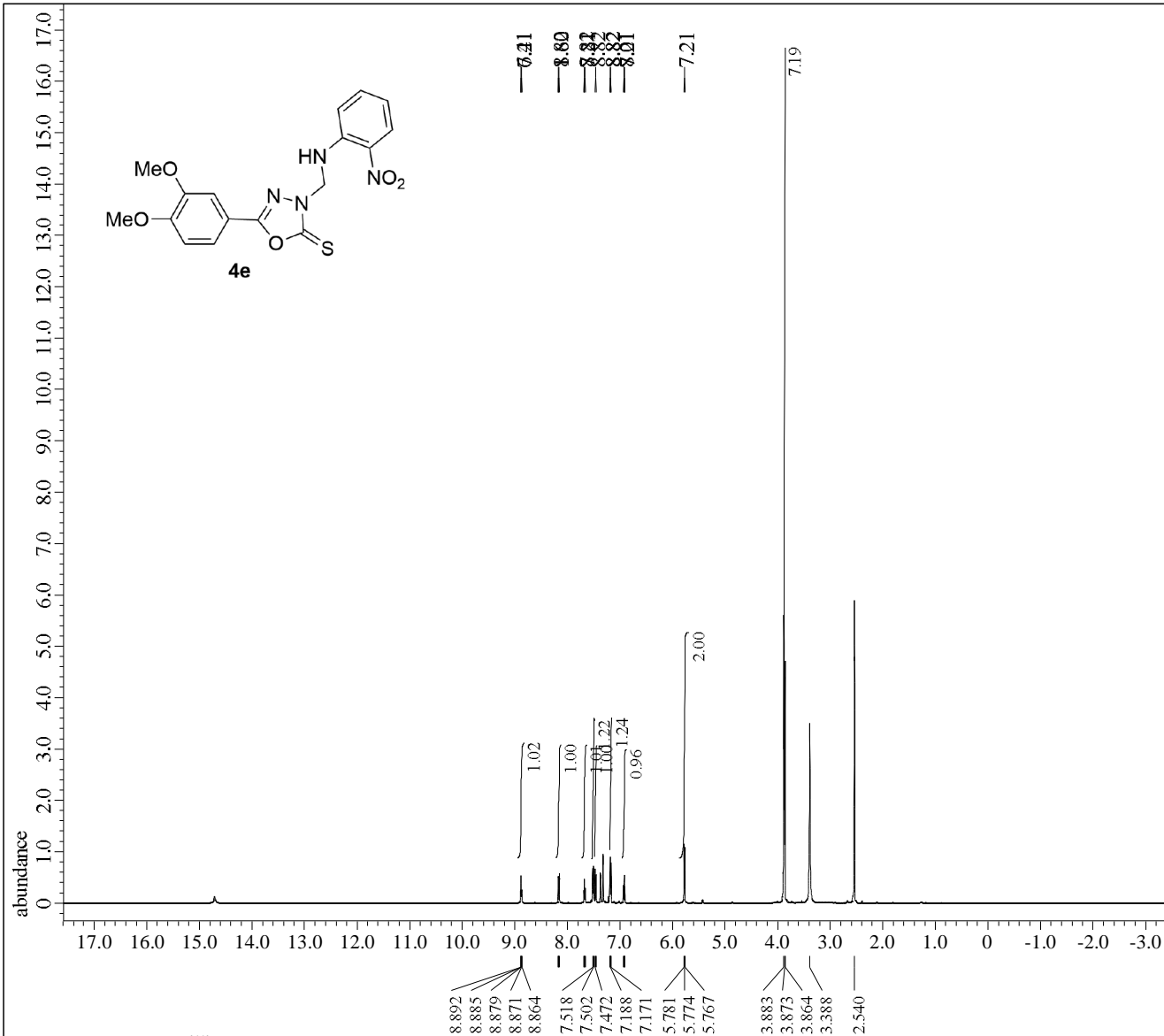
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 Initial_Wait = 1[s]
 Repetition_Time = 6.24780544[s]



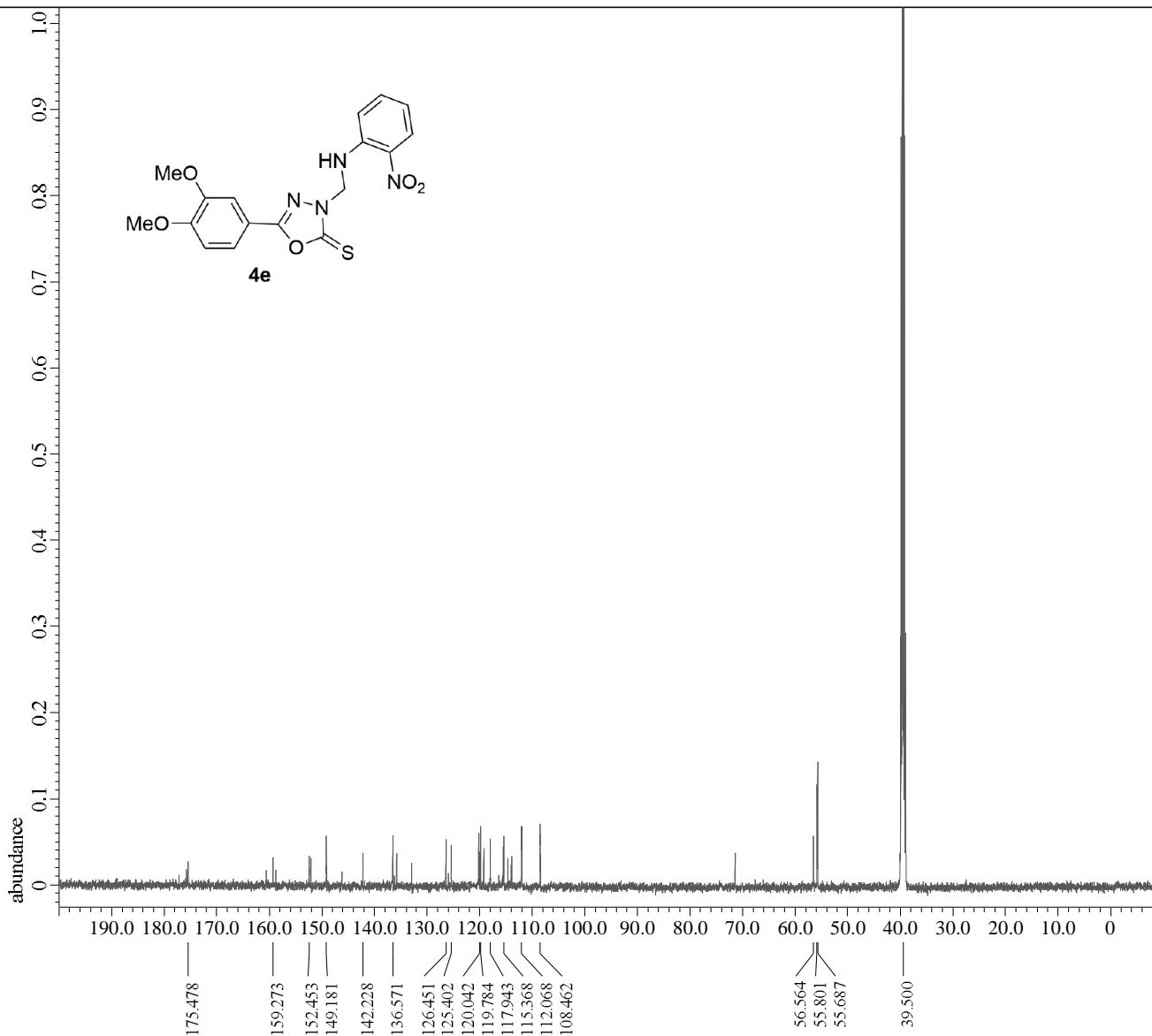
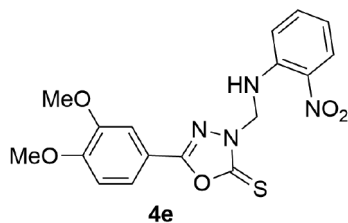
X : parts per Million : Proton

Filename = Prof.DR Ali Elemam_DM_8_ca
 Author = delta
 Experiment = carbon.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_8
 Solvent = DMSO-D6
 Creation_Time = 25-JAN-2021 17:23:30
 Revision_Time = 5-FEB-2021 08:20:39
 Current_Time = 5-FEB-2021 08:23:10

Comment = single pulse decoupled gat
 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 = 1024
 Total_Scans = 1024

Relaxation_Delay = 2[s]
 Recvr_Gain = 58
 Temp_Get = 20.1[dC]
 X_90_Width = 32.3[us]
 X_Acq_Time = 0.83361792[s]
 X_Angle = 30[deg]
 X_Atn = 10[dB]
 X_Pulse = 10.76666667[us]
 Irr_Atn_Dec = 17.693[dB]
 Irr_Atn_Noise = 17.693[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]

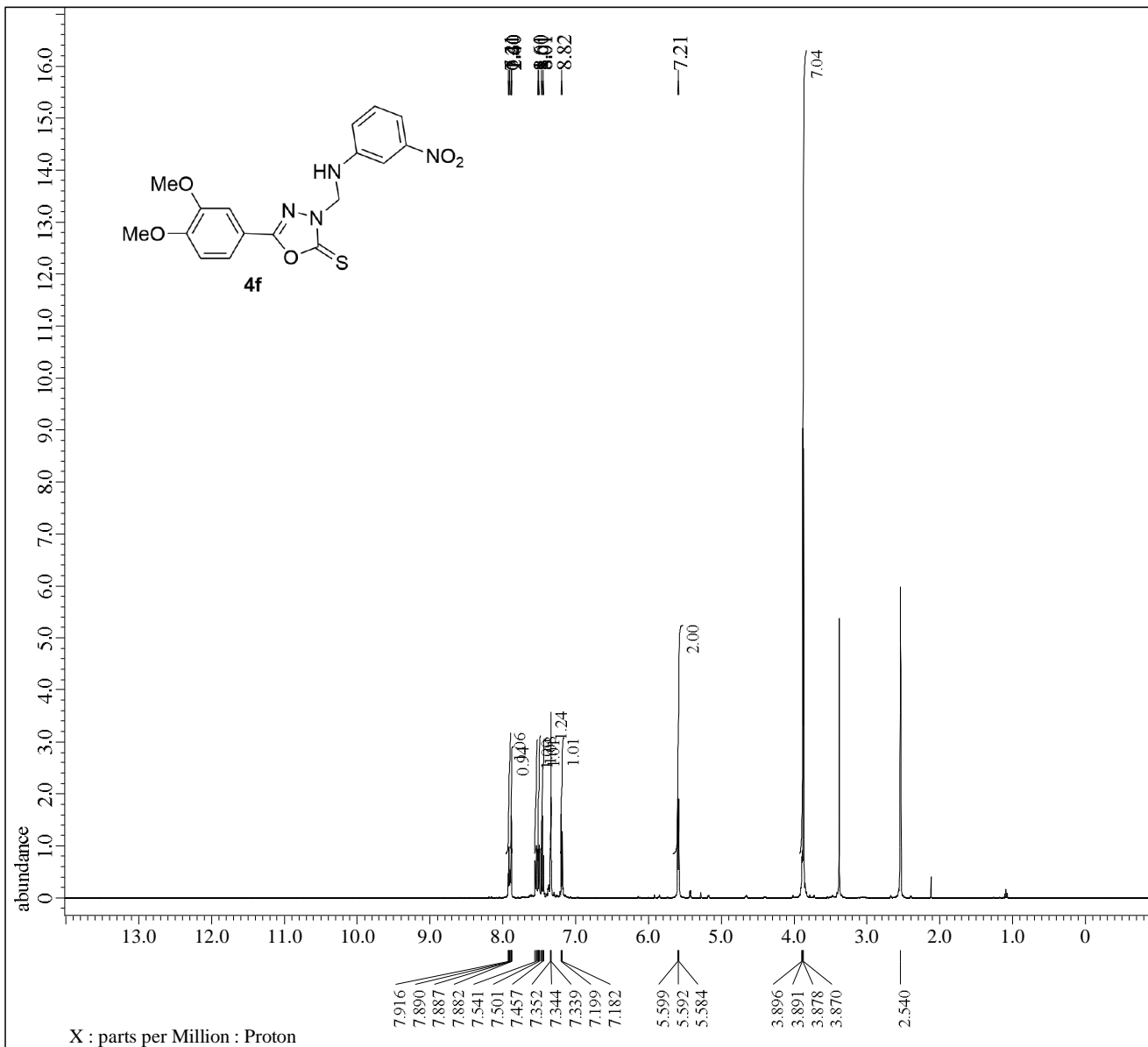


Filename = Prof.DR Ali Elemam_DM_9_pr
 Author = delta
 Experiment = proton.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_9
 Solvent = DMSO-D6
 Creation_Time = 30-DEC-2020 12:04:05
 Revision_Time = 6-FEB-2021 08:22:16
 Current_Time = 6-FEB-2021 08:23:07

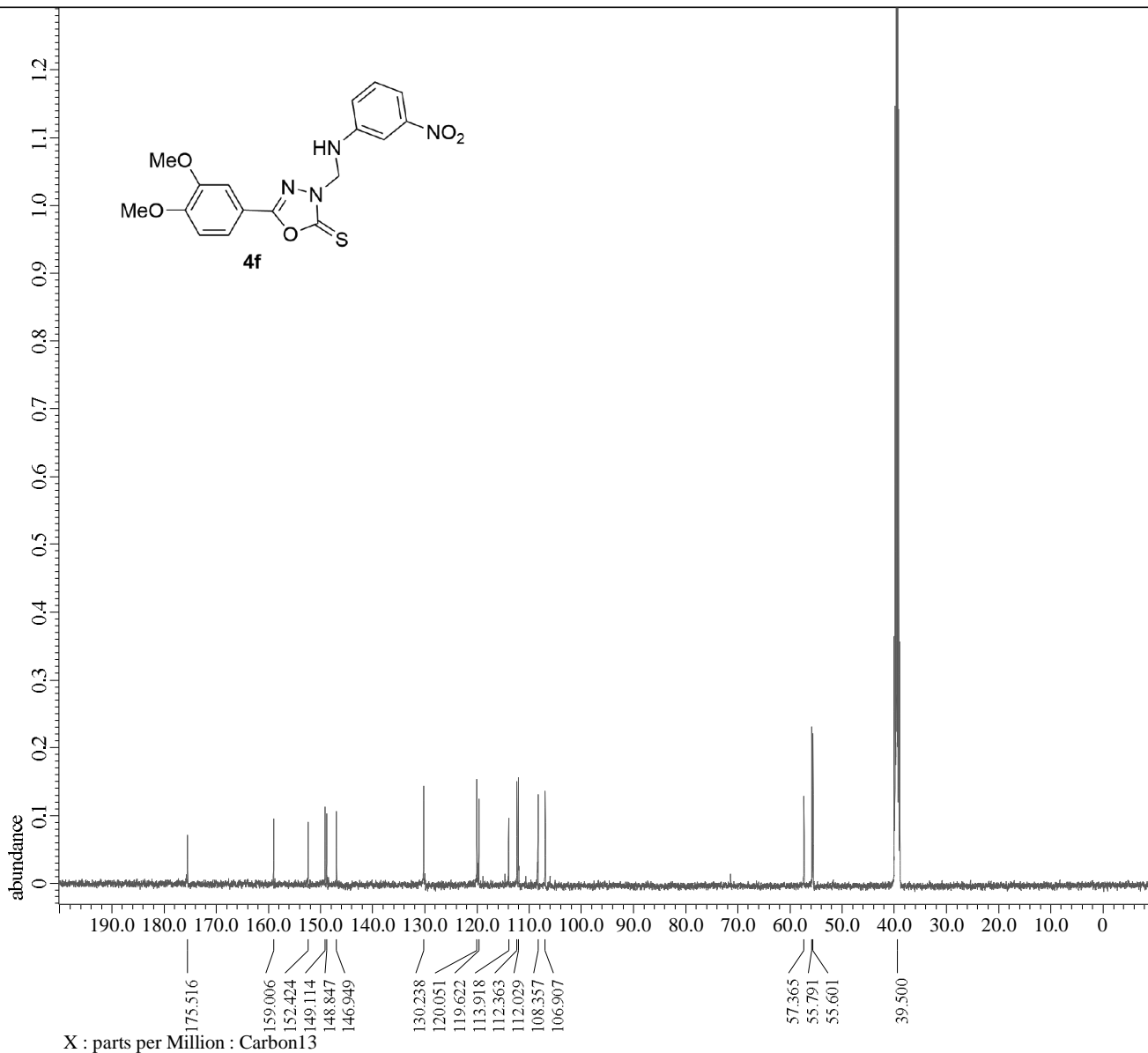
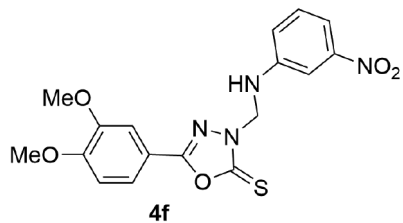
Comment = single_pulse
 Data_Format = 1D_COMPLEX
 Dim_Size = 13107
 Dim_Title = Proton
 Dim_Units = [ppm]
 Dimensions = X
 Site = JNM-ECA500II
 Spectrometer = DELTA2_NMR

Field_Strength = 11.7473579[T] (500[MHz])
 X_Acq_Duration = 1.24780544[s]
 X_Domain = 1H
 X_Freq = 500.15991521[MHz]
 X_Offset = 7.0[ppm]
 X_Points = 16384
 X_Prescans = 1
 X_Resolution = 0.80140699[Hz]
 X_Sweep = 13.1302521[kHz]
 X_Sweep_Clippped = 10.50420168[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 = 50
 Temp_Get = 18.3[dC]
 X_90_Width = 16[us]
 X_Acq_Time = 1.24780544[s]
 X_Angle = 45[deg]
 X_Atn = 2.5[dB]
 X_Pulse = 8[us]
 Irr_Mode = Off
 Tri_Mode = Off
 Dante_Presat = FALSE
 Initial_Wait = 1[s]
 Repetition_Time = 6.24780544[s]



X : parts per Million : Proton



Filename = Prof.DR Ali Elemam_DM_9_ca
 Author = delta
 Experiment = carbon.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_9
 Solvent = DMSO-D6
 Creation_Time = 25-JAN-2021 18:19:54
 Revision_Time = 5-FEB-2021 03:37:02
 Current_Time = 5-FEB-2021 03:47:42

Comment = single pulse decoupled gat
 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 = 1024
 Total_Scans = 1024

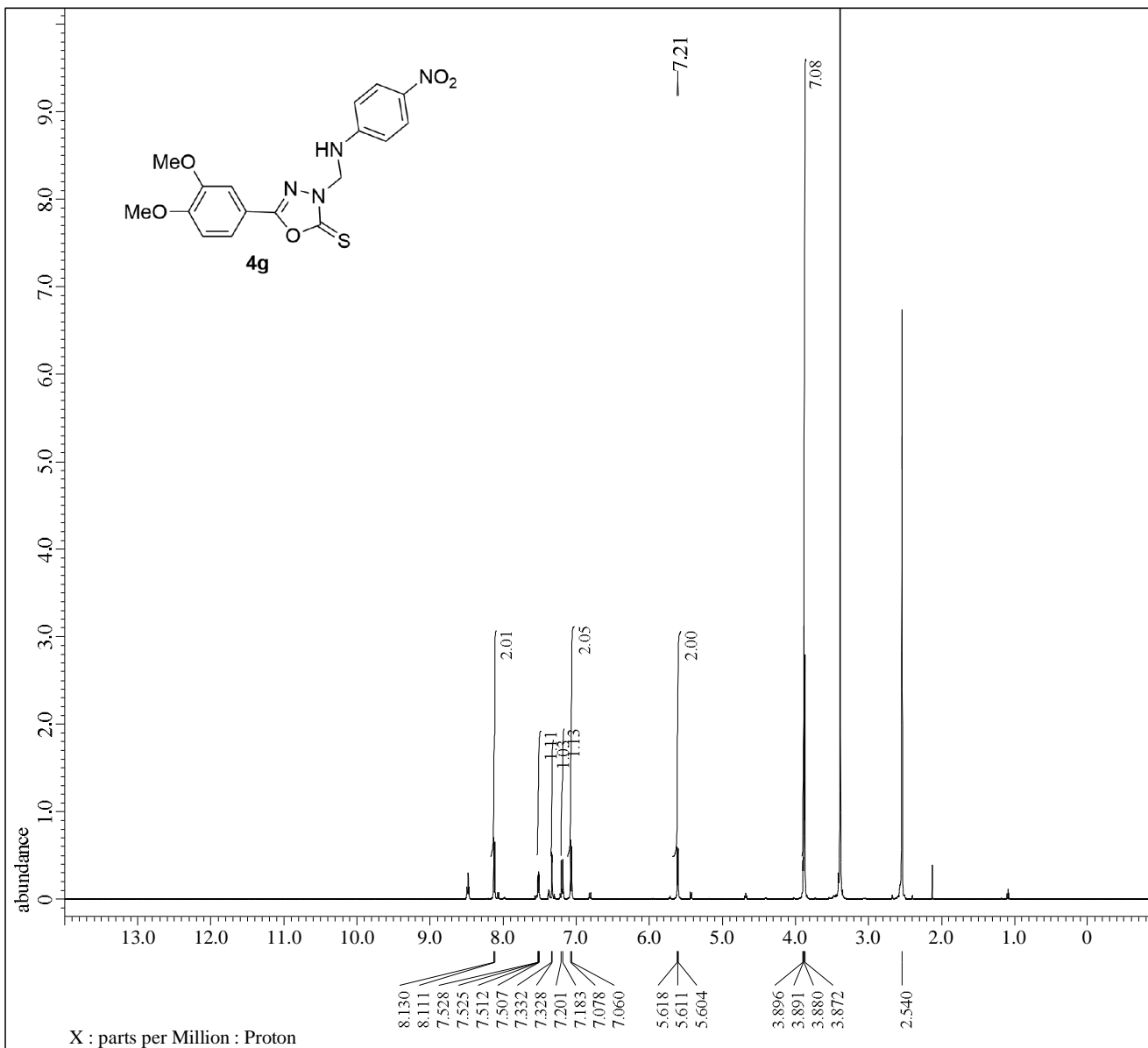
Relaxation_Delay = 2[s]
 Recvr_Gain = 58
 Temp_Get = 19.6[dC]
 X_90_Width = 32.3[us]
 X_Acq_Time = 0.83361792[s]
 X_Angle = 30[deg]
 X_Atn = 10[dB]
 X_Pulse = 10.76666667[us]
 Irr_Atn_Dec = 17.693[dB]
 Irr_Atn_Noise = 17.693[dB]
 Irr_Noise = WALTZ
 Irr_Pwidth = 92[us]
 Decoupling = TRUE
 Initial_Wait = 1[s]
 Noe = TRUE
 Noe_Time = 2[s]
 Repetition_Time = 2.83361792[s]

Filename = Prof.DR Ali Elemam_DM_10_p
 Author = delta
 Experiment = proton.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_10
 Solvent = DMSO-D6
 Creation_Time = 30-DEC-2020 12:13:04
 Revision_Time = 6-FEB-2021 08:54:27
 Current_Time = 6-FEB-2021 08:55:41

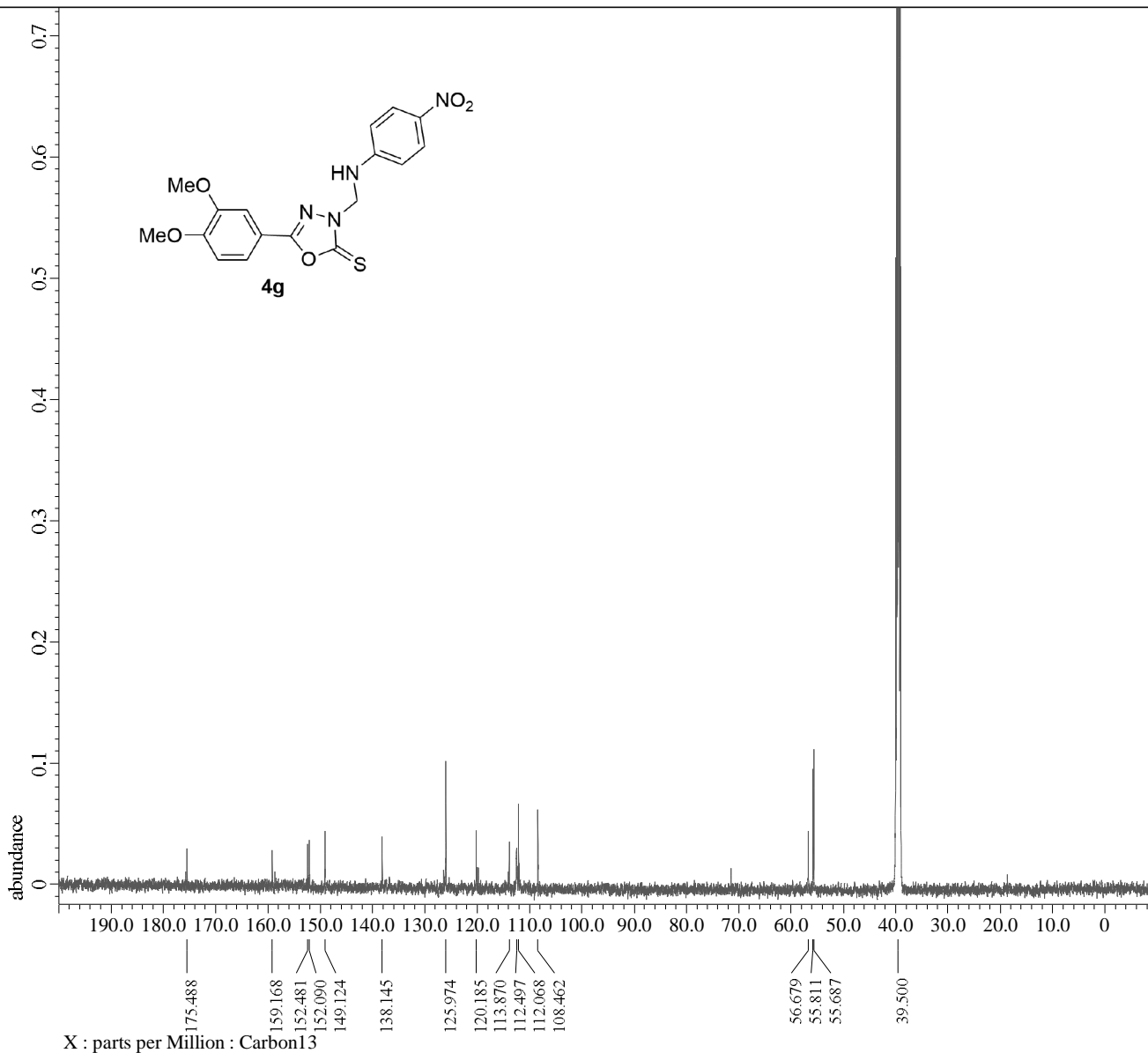
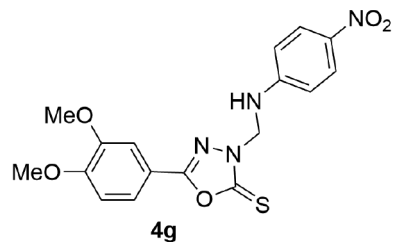
Comment = single_pulse
 Data_Format = 1D COMPLEX
 Dim_Size = 13107
 Dim_Title = Proton
 Dim_Units = [ppm]
 Dimensions = X
 Site = JNM-ECA500II
 Spectrometer = DELTA2_NMR

Field_Strength = 11.7473579[T] (500[MHz])
 X_Acq_Duration = 1.24780544[s]
 X_Domain = 1H
 X_Freq = 500.15991521[MHz]
 X_Offset = 7.0[ppm]
 X_Points = 16384
 X_Prescans = 1
 X_Resolution = 0.80140699[Hz]
 X_Sweep = 13.1302521[kHz]
 X_Sweep_Clipped = 10.50420168[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 = 50
 Temp_Get = 18.3[dC]
 X_90_Width = 16[us]
 X_Acq_Time = 1.24780544[s]
 X_Angle = 45[deg]
 X_Atn = 2.5[dB]
 X_Pulse = 8[us]
 Irr_Mode = Off
 Tri_Mode = Off
 Dante_Presat = FALSE
 Initial_Wait = 1[s]
 Repetition_Time = 6.24780544[s]



X : parts per Million : Proton



Filename = Prof.DR Ali Elemam_DM_10_c
 Author = delta
 Experiment = carbon.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_10
 Solvent = DMSO-D6
 Creation_Time = 25-JAN-2021 21:09:57
 Revision_Time = 5-FEB-2021 04:11:51
 Current_Time = 5-FEB-2021 04:13:33

Comment = single pulse decoupled gat
 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 = 1024
 Total_Scans = 1024

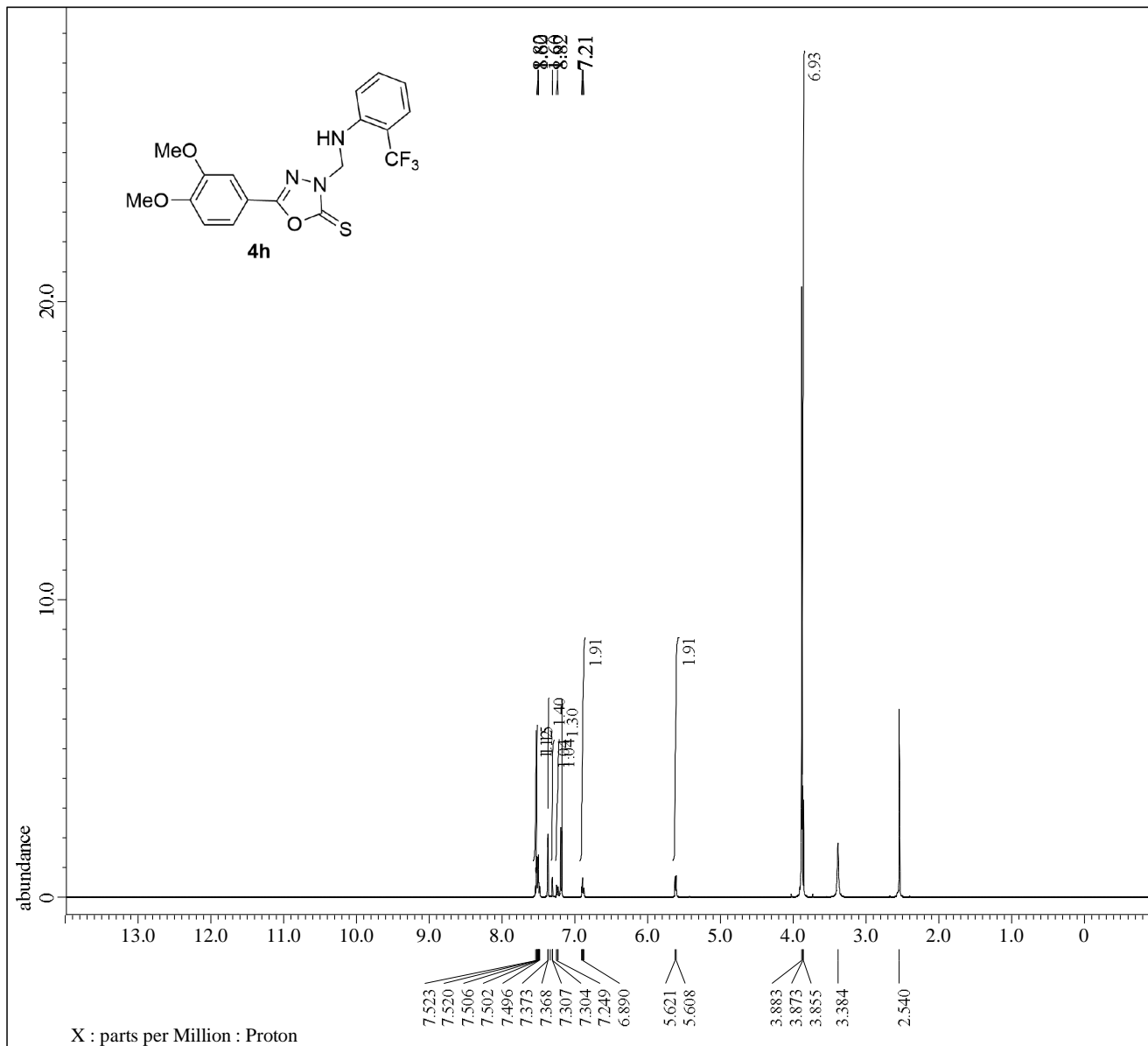
Relaxation_Delay = 2[s]
 Recvr_Gain = 58
 Temp_Get = 19.7[dC]
 X_90_Width = 32.3[us]
 X_Acq_Time = 0.83361792[s]
 X_Angle = 30[deg]
 X_Atn = 10[dB]
 X_Pulse = 10.76666667[us]
 Irr_Atn_Dec = 17.693[dB]
 Irr_Atn_Noe = 17.693[dB]
 Irr_Noise = WALTZ
 Irr_Pwidth = 92[us]
 Decoupling = TRUE
 Initial_Wait = 1[s]
 Noe = TRUE
 Noe_Time = 2[s]
 Repetition_Time = 2.83361792[s]

Filename = Prof.DR Ali Elemam_DM_12_p
 Author = delta
 Experiment = proton.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_12
 Solvent = DMSO-D6
 Creation_Time = 30-DEC-2020 14:22:18
 Revision_Time = 6-FEB-2021 09:38:13
 Current_Time = 6-FEB-2021 09:38:30

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 = 1.24780544[s]
 X_Domain = 1H
 X_Freq = 500.15991521[MHz]
 X_Offset = 7.0[ppm]
 X_Points = 16384
 X_Prescans = 1
 X_Resolution = 0.80140699[Hz]
 X_Sweep = 13.1302521[kHz]
 X_Sweep_Clippped = 10.50420168[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 = 50
 Temp_Get = 19.2[dC]
 X_90_Width = 16[us]
 X_Acq_Time = 1.24780544[s]
 X_Angle = 45[deg]
 X_Atn = 2.5[dB]
 X_Pulse = 8[us]
 Irr_Mode = Off
 Tri_Mode = Off
 Dante_Preset = FALSE
 Initial_Wait = 1[s]
 Repetition_Time = 6.24780544[s]

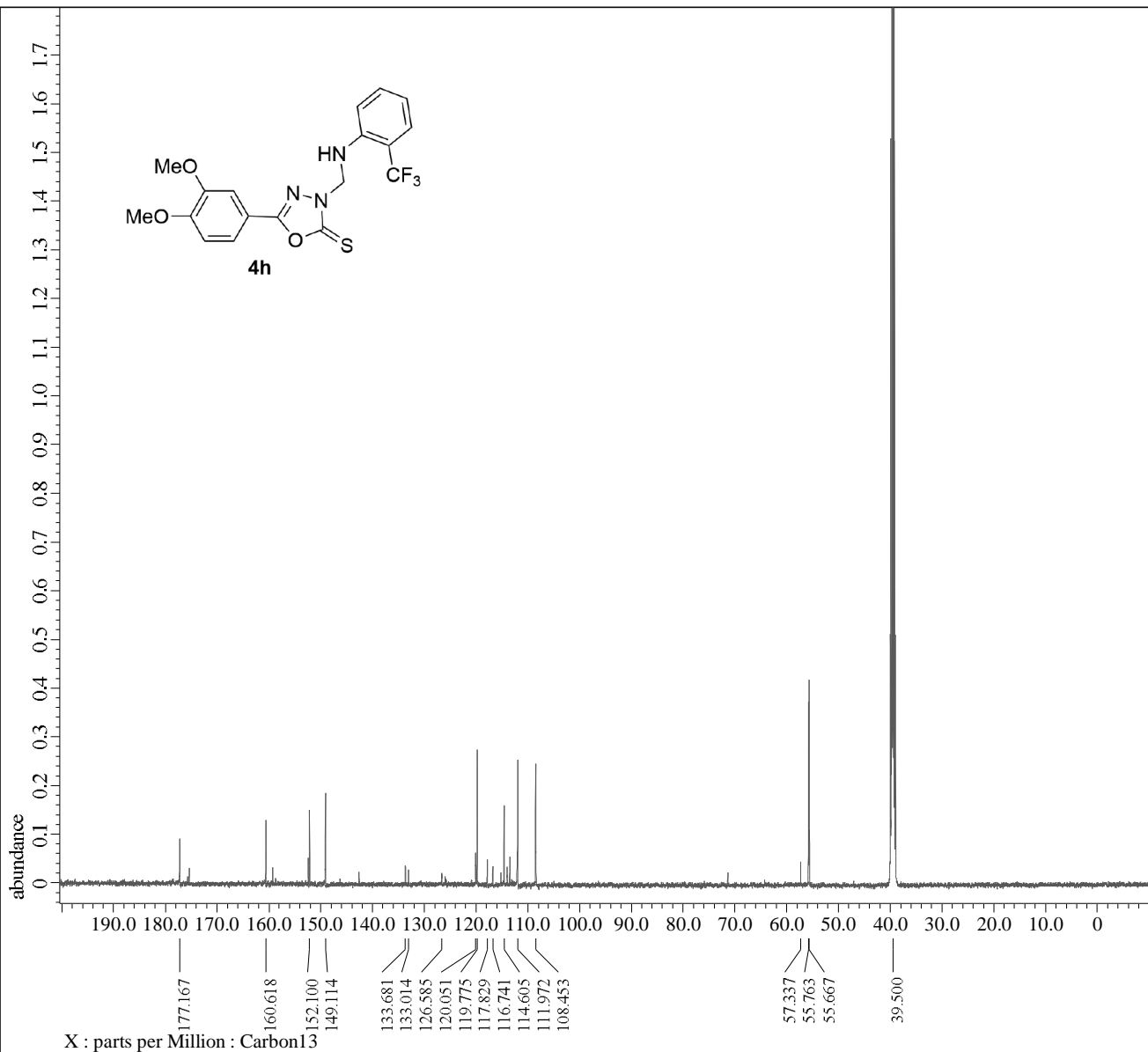


Filename = Prof.DR Ali Elemam_DM_12_c
 Author = delta
 Experiment = carbon.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_12
 Solvent = DMSO-D6
 Creation_Time = 25-JAN-2021 23:04:23
 Revision_Time = 5-FEB-2021 04:27:37
 Current_Time = 5-FEB-2021 04:30:28

Comment = single pulse decoupled gat
 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 = 1024
 Total_Scans = 1024

Relaxation_Delay = 2[s]
 Recvr_Gain = 58
 Temp_Get = 19.6[dC]
 X_90_Width = 32.3[us]
 X_Acq_Time = 0.83361792[s]
 X_Angle = 30[deg]
 X_Atn = 10[dB]
 X_Pulse = 10.76666667[us]
 Irr_Atn_Dec = 17.693[dB]
 Irr_Atn_Noe = 17.693[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]

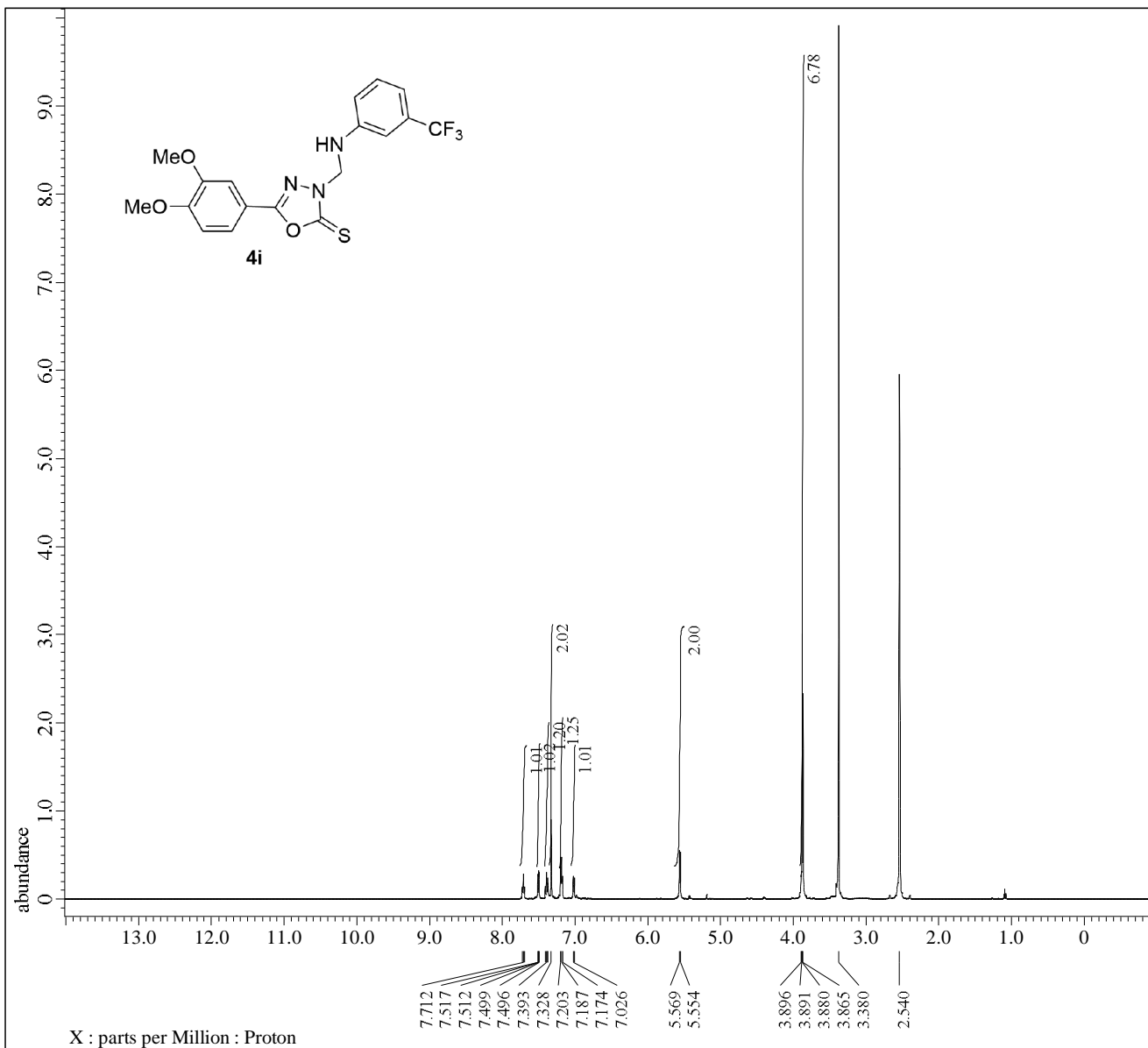


Filename = Prof.DR Ali Elemam_DM_13_p
 Author = delta
 Experiment = proton.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_13
 Solvent = DMSO-D6
 Creation_Time = 30-DEC-2020 14:31:19
 Revision_Time = 6-FEB-2021 09:42:39
 Current_Time = 6-FEB-2021 09:44:24

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 = 1.24780544[s]
 X_Domain = 1H
 X_Freq = 500.15991521[MHz]
 X_Offset = 7.0[ppm]
 X_Points = 16384
 X_Prescans = 1
 X_Resolution = 0.80140699[Hz]
 X_Sweep = 13.1302521[kHz]
 X_Sweep_Clippped = 10.50420168[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 = 50
 Temp_Get = 19.2[dC]
 X_90_Width = 16[us]
 X_Acq_Time = 1.24780544[s]
 X_Angle = 45[deg]
 X_Atn = 2.5[dB]
 X_Pulse = 8[us]
 Irr_Mode = Off
 Tri_Mode = Off
 Dante_Presat = FALSE
 Initial_Wait = 1[s]
 Repetition_Time = 6.24780544[s]



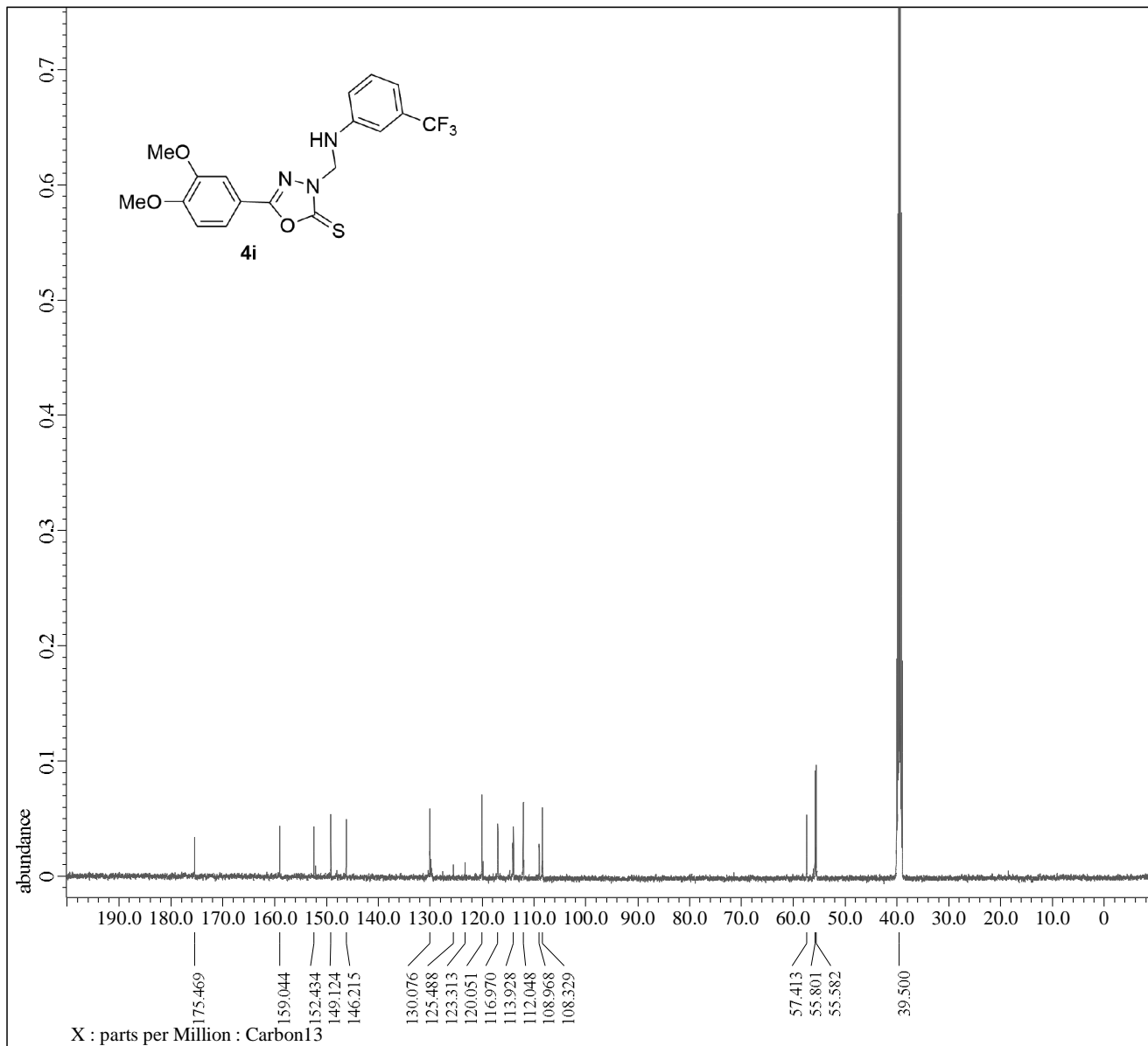
X : parts per Million : Proton

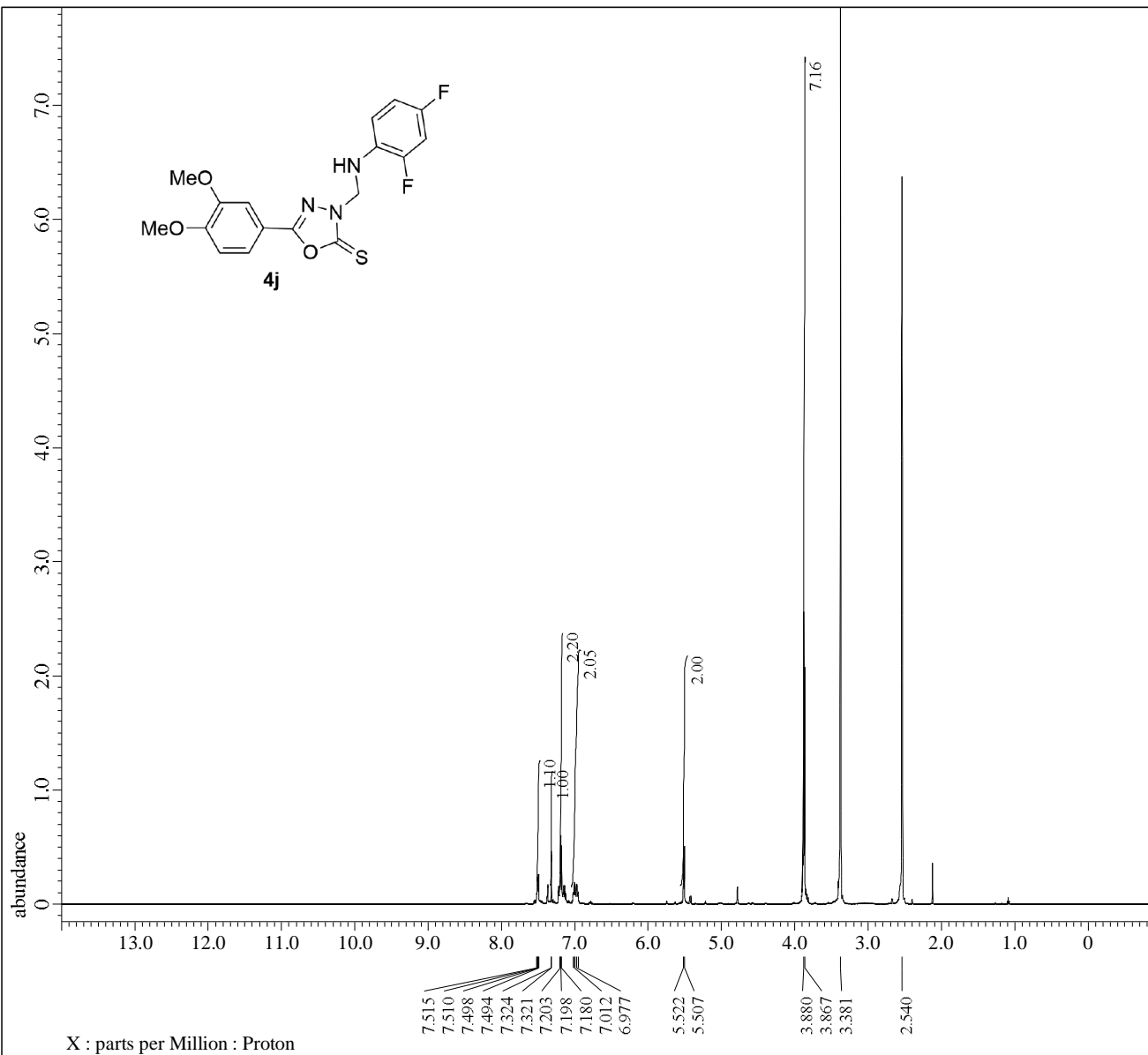
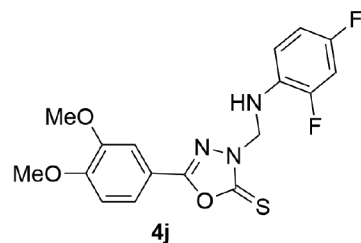
Filename = Prof.DR Ali Elemam_DM_13_c
 Author = delta
 Experiment = carbon.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_13
 Solvent = DMSO-D6
 Creation_Time = 3-FEB-2021 20:42:59
 Revision_Time = 5-FEB-2021 04:40:24
 Current_Time = 5-FEB-2021 04:40:50

Comment = single pulse decoupled gat
 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 = 1850
 Total_Scans = 1850

Relaxation_Delay = 2[s]
 Recvr_Gain = 60
 Temp_Get = 20.4[dC]
 X_90_Width = 32.3[us]
 X_Acq_Time = 0.83361792[s]
 X_Angle = 30[deg]
 X_Atn = 10[dB]
 X_Pulse = 10.76666667[us]
 Irr_Atn_Dec = 17.693[dB]
 Irr_Atn_NoE = 17.693[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]





Filename = Prof.DR Ali Elemam_DM_15_p
 Author = delta
 Experiment = proton.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_15
 Solvent = DMSO-D6
 Creation_Time = 30-DEC-2020 13:00:20
 Revision_Time = 6-FEB-2021 10:22:51
 Current_Time = 6-FEB-2021 10:24:11

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 = 1.24780544[s]
 X_Domain = 1H
 X_Freq = 500.15991521[MHz]
 X_Offset = 7.0[ppm]
 X_Points = 16384
 X_Prescans = 1
 X_Resolution = 0.80140699[Hz]
 X_Sweep = 13.1302521[kHz]
 X_Sweep_Clippped = 10.50420168[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

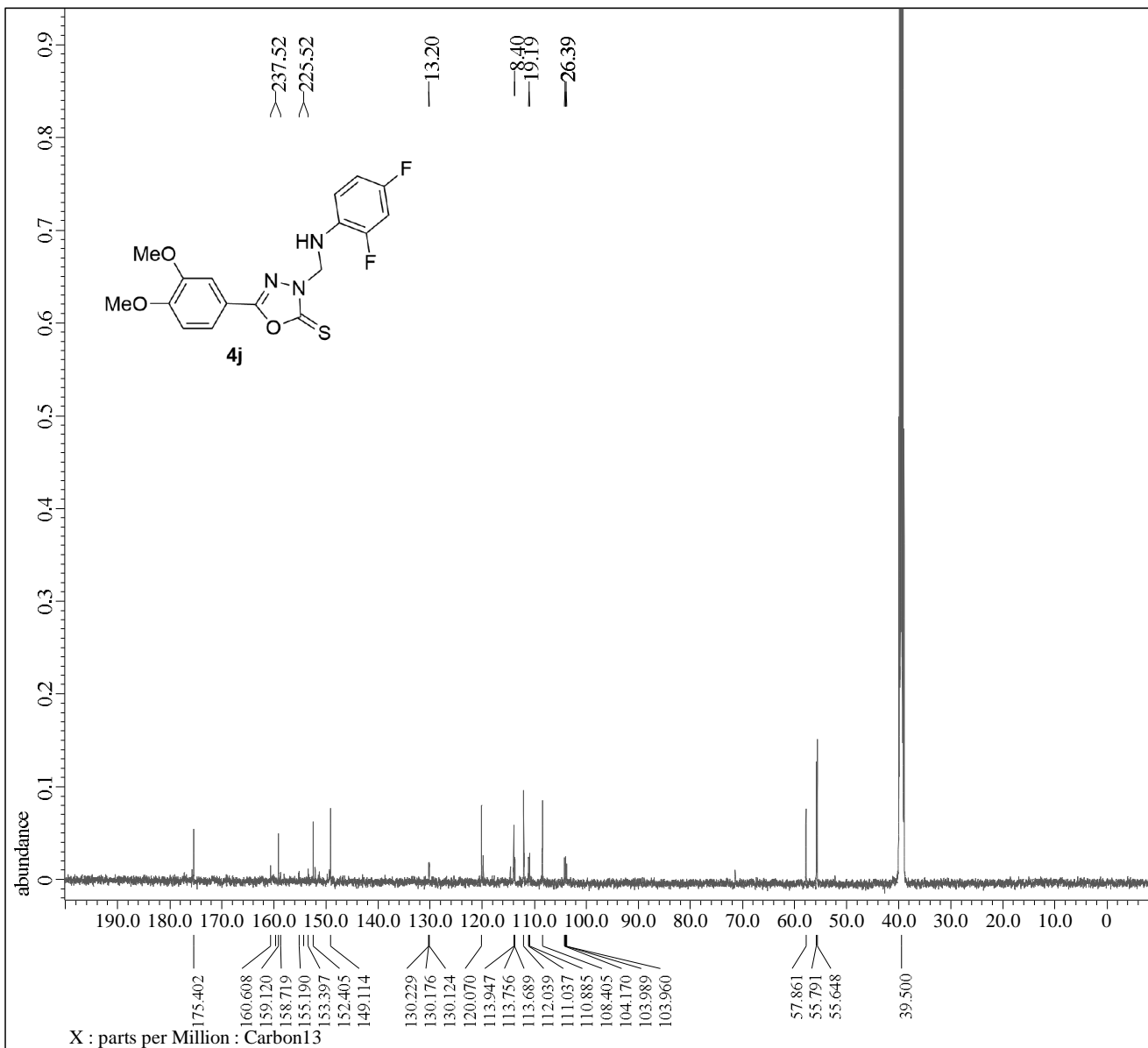
Relaxation_Delay = 5[s]
 Recvr_Gain = 50
 Temp_Get = 18.4[dC]
 X_90_Width = 16[us]
 X_Acq_Time = 1.24780544[s]
 X_Angle = 45[deg]
 X_Atn = 2.5[dB]
 X_Pulse = 8[us]
 Irr_Mode = Off
 Tri_Mode = Off
 Dante_Preset = FALSE
 Initial_Wait = 1[s]
 Repetition_Time = 6.24780544[s]

Filename = Prof.DR Ali Elemam_DM_15_c
 Author = delta
 Experiment = carbon.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_15
 Solvent = DMSO-D6
 Creation_Time = 26-JAN-2021 01:54:58
 Revision_Time = 5-FEB-2021 05:09:19
 Current_Time = 5-FEB-2021 05:10:08

Comment = single pulse decoupled gat
 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_Clippped = 31.44654088[kHz]
 Irr_Domain = Proton
 Irr_Freq = 500.15991521[MHz]
 Irr_Offset = 5.0[ppm]
 Clipped = FALSE
 Scans = 1024
 Total_Scans = 1024

Relaxation_Delay = 2[s]
 Recvr_Gain = 58
 Temp_Get = 20.1[dC]
 X_90_Width = 32.3[us]
 X_Acq_Time = 0.83361792[s]
 X_Angle = 30[deg]
 X_Atn = 10[dB]
 X_Pulse = 10.76666667[us]
 Irr_Atn_Dec = 17.693[dB]
 Irr_Atn_Noie = 17.693[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]

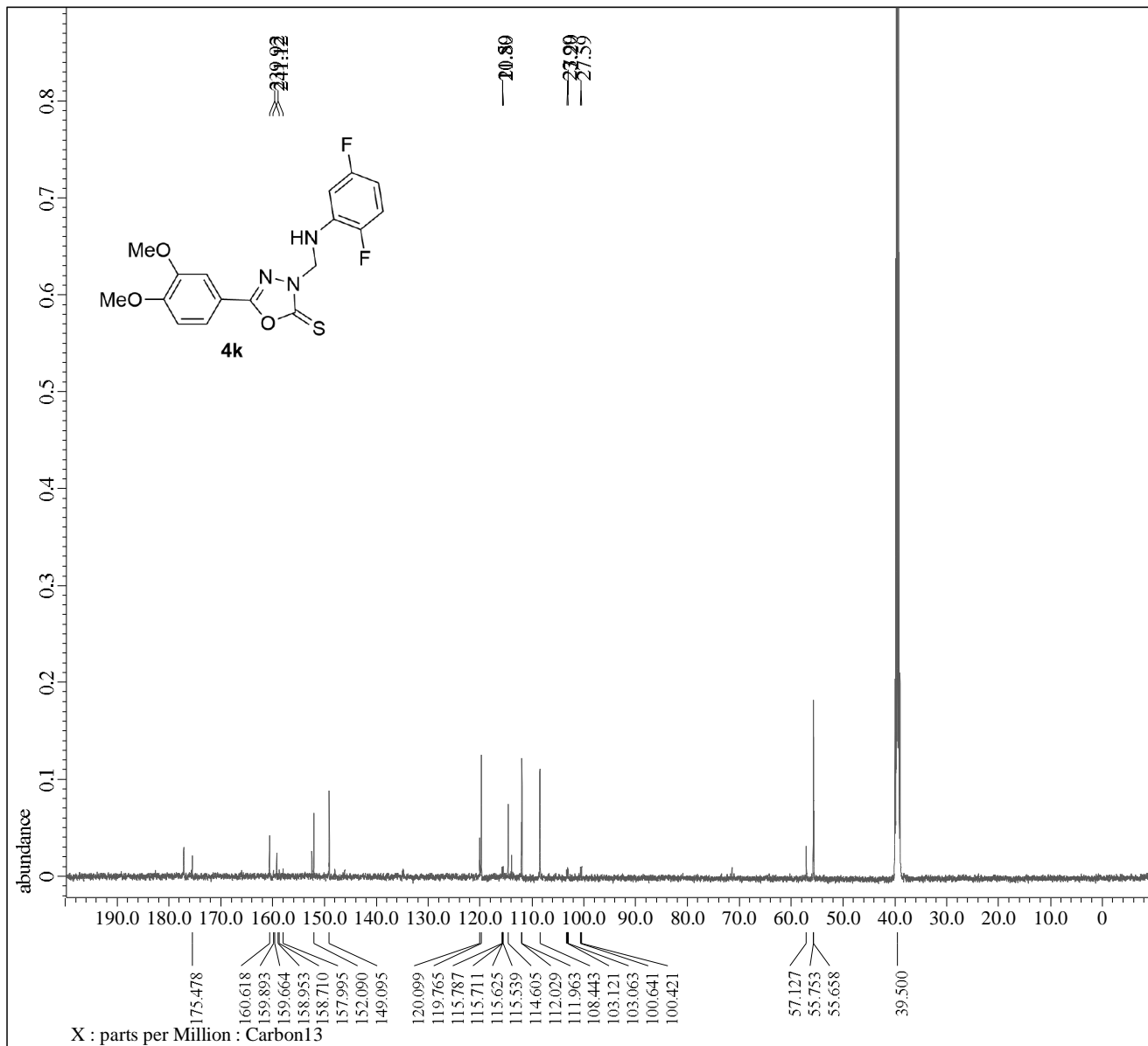


Filename = Prof.DR Ali Elemam_DM_16_c
 Author = delta
 Experiment = carbon.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_16
 Solvent = DMSO-D6
 Creation_Time = 26-JAN-2021 02:51:44
 Revision_Time = 5-FEB-2021 05:52:07
 Current_Time = 5-FEB-2021 05:53:46

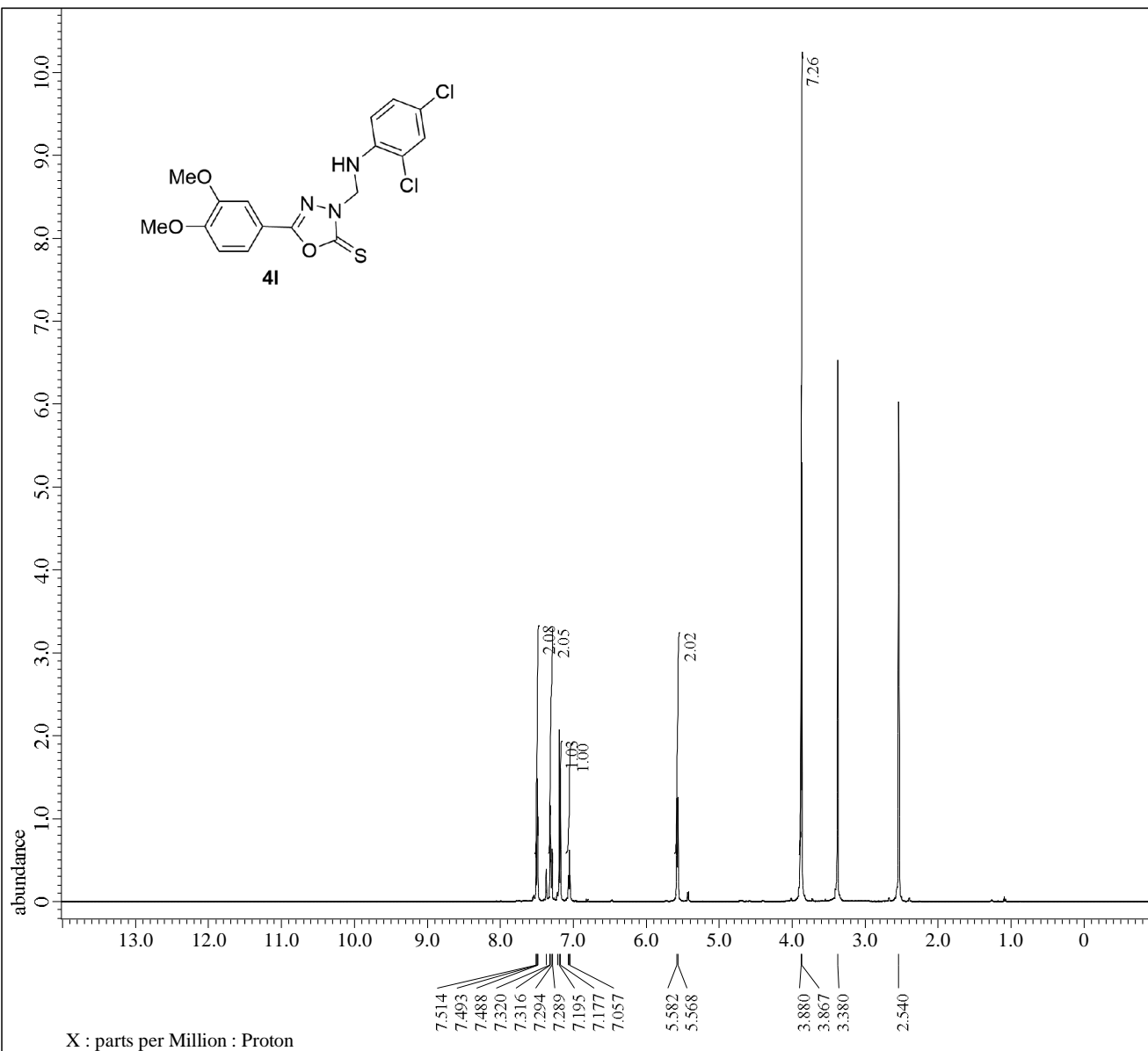
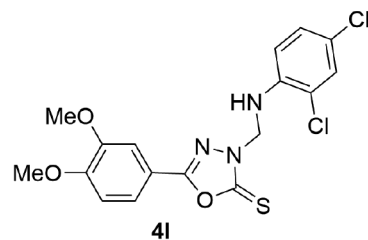
Comment = single pulse decoupled gat
 Data_Format = 1D COMPLEX
 Dim_Size = 26214
 Dim_Title = Carbon13
 Dim_Units = [ppm]
 Dimensions = X
 Site = JNM-ECA500II
 Spectrometer = DELTA2_NMR

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_Clippped = 31.44654088[kHz]
 Irr_Domain = Proton
 Irr_Freq = 500.15991521[MHz]
 Irr_Offset = 5.0[ppm]
 Clipped = FALSE
 Scans = 1024
 Total_Scans = 1024

Relaxation_Delay = 2[s]
 Recvr_Gain = 60
 Temp_Get = 20[dc]
 X_90_Width = 32.3[us]
 X_Acq_Time = 0.83361792[s]
 X_Angle = 30[deg]
 X_Atn = 10[db]
 X_Pulse = 10.76666667[us]
 Irr_Atn_Dec = 17.693[db]
 Irr_Atn_Noie = 17.693[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]



X : parts per Million : Carbon13

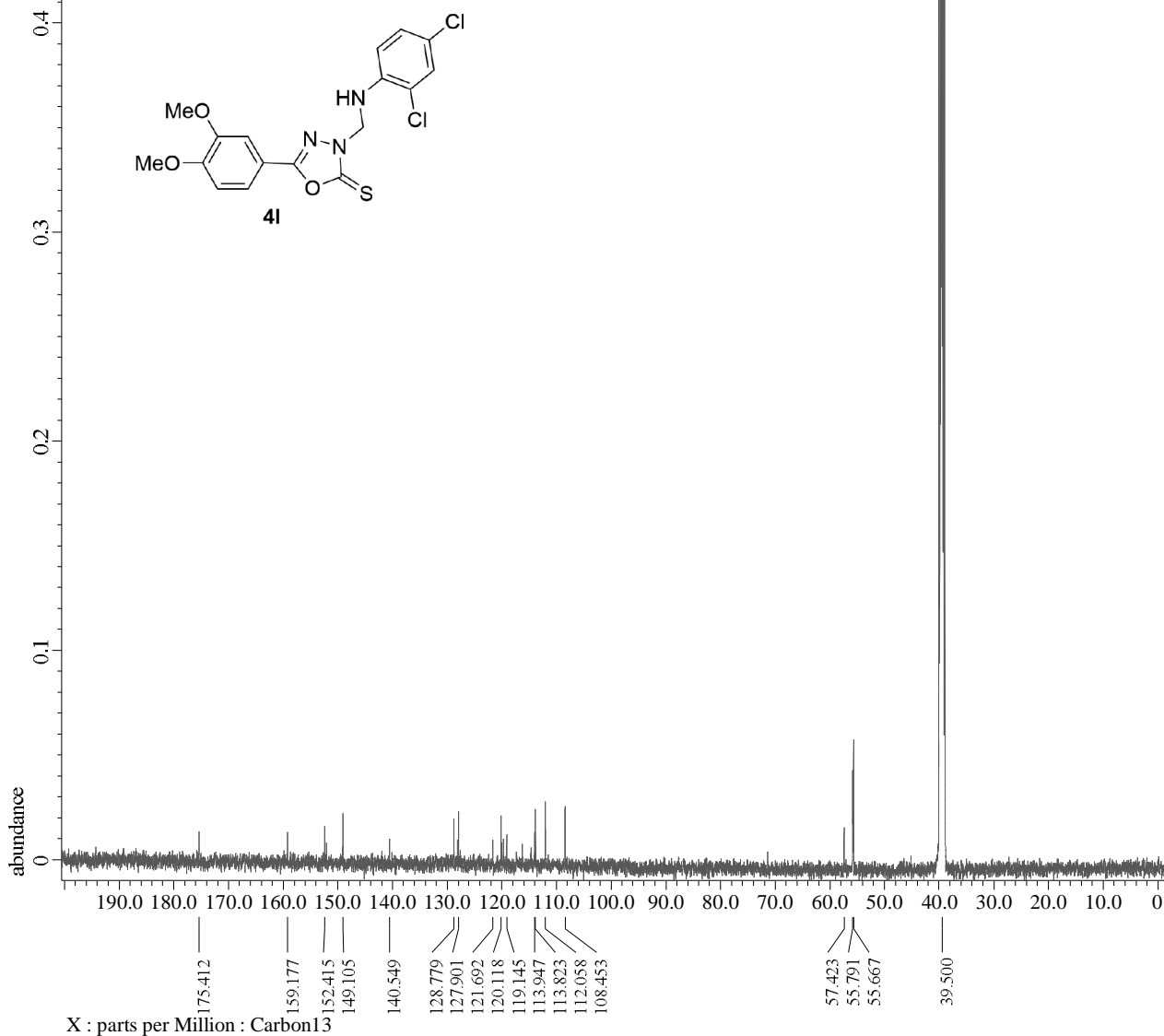
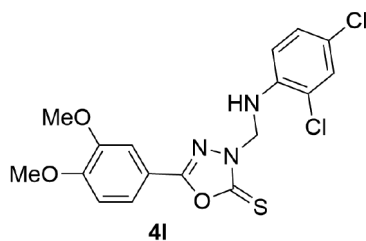


Filename = Prof.DR Ali Elemam_DM_14_p
 Author = delta
 Experiment = proton.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_14
 Solvent = DMSO-D6
 Creation_Time = 30-DEC-2020 14:40:18
 Revision_Time = 6-FEB-2021 10:07:38
 Current_Time = 6-FEB-2021 10:08:05

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 = 1.24780544[s]
 X_Domain = 1H
 X_Freq = 500.15991521[MHz]
 X_Offset = 7.0[ppm]
 X_Points = 16384
 X_Prescans = 1
 X_Resolution = 0.80140699[Hz]
 X_Sweep = 13.1302521[kHz]
 X_Sweep_Clipped = 10.50420168[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 = 50
 Temp_Get = 18.8[dC]
 X_90_Width = 16[us]
 X_Acq_Time = 1.24780544[s]
 X_Angle = 45[deg]
 X_Atn = 2.5[dB]
 X_Pulse = 8[us]
 Irr_Mode = Off
 Tri_Mode = Off
 Dante_Preset = FALSE
 Initial_Wait = 1[s]
 Repetition_Time = 6.24780544[s]



Filename = Prof.DR Ali Elemam_DM_14_c
 Author = delta
 Experiment = carbon.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_14
 Solvent = DMSO-D6
 Creation_Time = 3-FEB-2021 22:18:44
 Revision_Time = 5-FEB-2021 04:46:58
 Current_Time = 5-FEB-2021 04:48:17

Comment = single pulse decoupled gat
 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_Clippped = 31.44654088[kHz]
 Irr_Domain = Proton
 Irr_Freq = 500.15991521[MHz]
 Irr_Offset = 5.0[ppm]
 Clipped = FALSE
 Scans = 1850
 Total_Scans = 1850

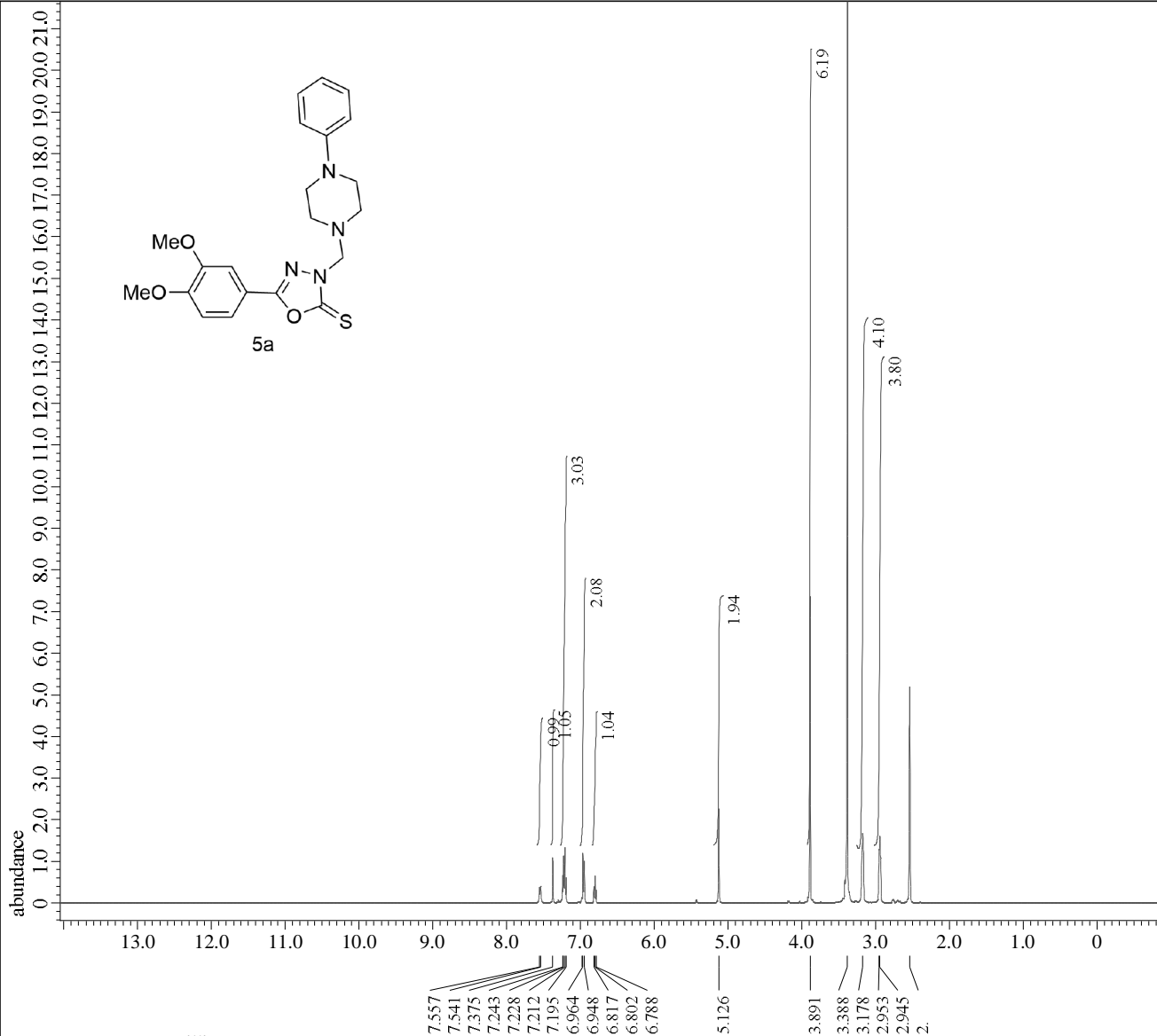
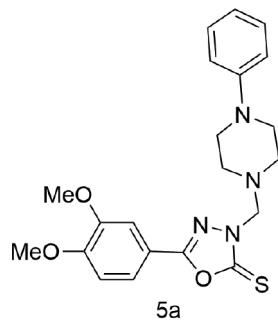
Relaxation_Delay = 2[s]
 Recvr_Gain = 58
 Temp_Get = 19.8[dC]
 X_90_Width = 32.3[us]
 X_Acq_Time = 0.83361792[s]
 X_Angle = 30[deg]
 X_Atn = 10[dB]
 X_Pulse = 10.76666667[us]
 Irr_Atn_Dec = 17.693[dB]
 Irr_Atn_Noe = 17.693[dB]
 Irr_Noise = WALTZ
 Irr_Pwidth = 92[us]
 Decoupling = TRUE
 Initial_Wait = 1[s]
 Noe = TRUE
 Noe_Time = 2[s]
 Repetition_Time = 2.83361792[s]

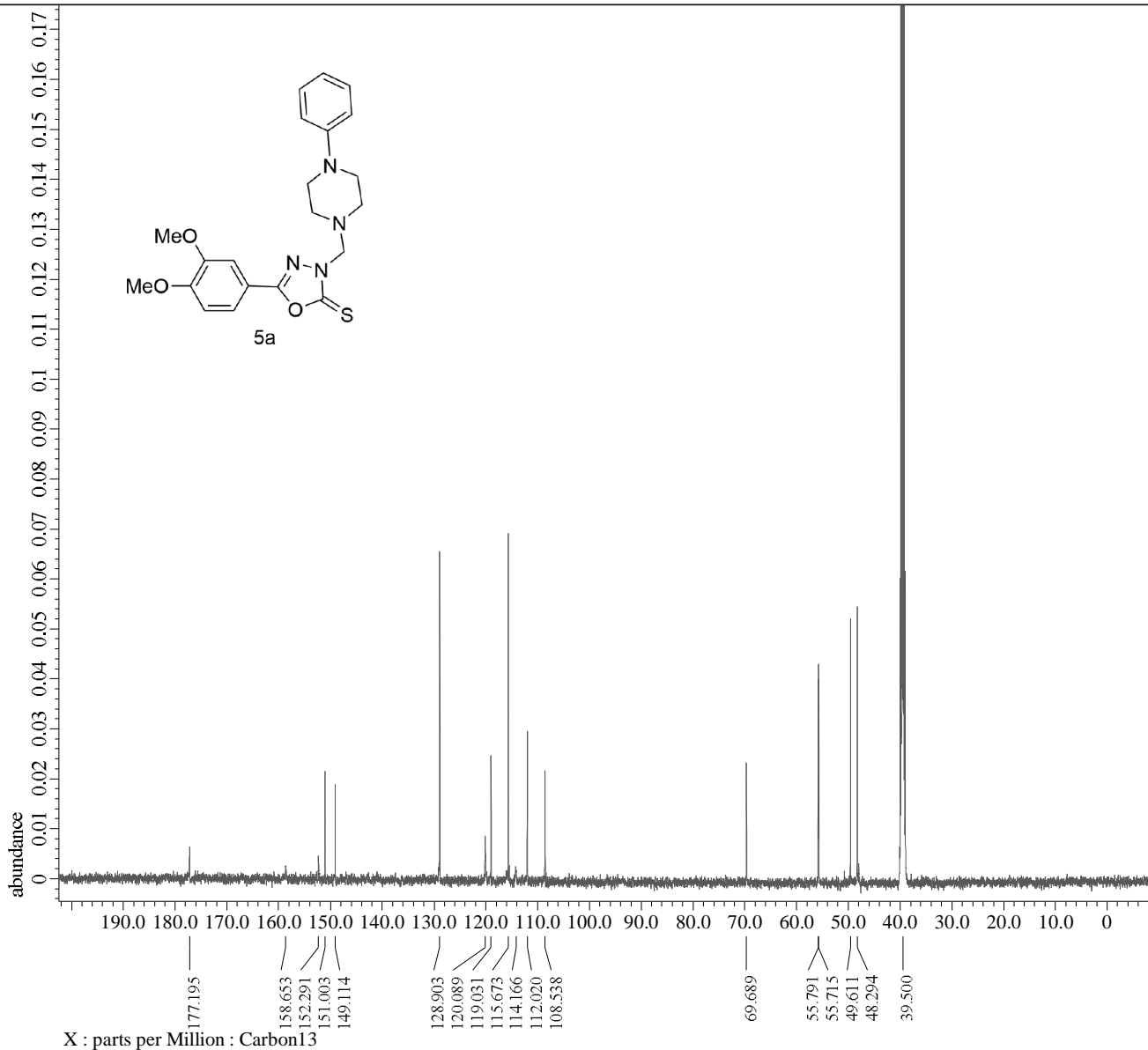
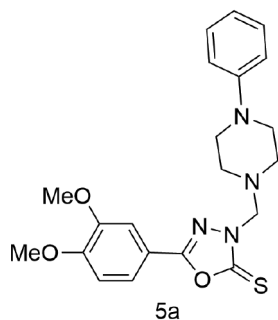
Filename = Prof.DR Ali Elemam_DM_1_pr
 Author = delta
 Experiment = proton.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_1
 Solvent = DMSO-D6
 Creation_Time = 14-DEC-2020 11:41:11
 Revision_Time = 5-FEB-2021 23:12:44
 Current_Time = 5-FEB-2021 23:13:51

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 = 1.24780544[s]
 X_Domain = 1H
 X_Freq = 500.15991521[MHz]
 X_Offset = 7.0[ppm]
 X_Points = 16384
 X_Prescans = 1
 X_Resolution = 0.80140699[Hz]
 X_Sweep = 13.1302521[kHz]
 X_Sweep_Clipped = 10.50420168[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 = 50
 Temp_Get = 18.9[dC]
 X_90_Width = 16[us]
 X_Acq_Time = 1.24780544[s]
 X_Angle = 45[deg]
 X_Atn = 2.5[dB]
 X_Pulse = 8[us]
 Irr_Mode = Off
 Tri_Mode = Off
 Dante_Preset = FALSE
 Initial_Wait = 1[s]
 Repetition_Time = 6.24780544[s]



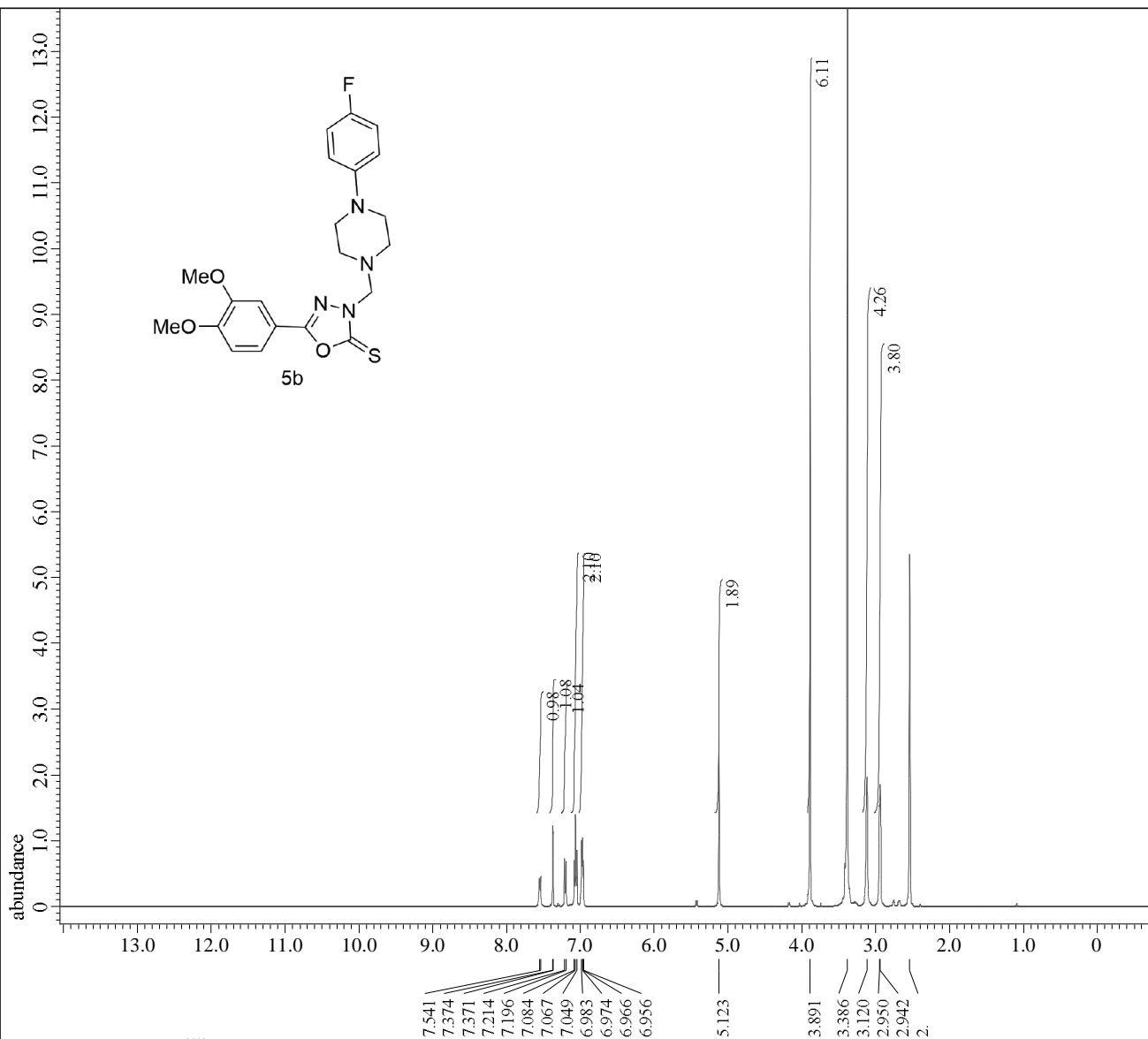
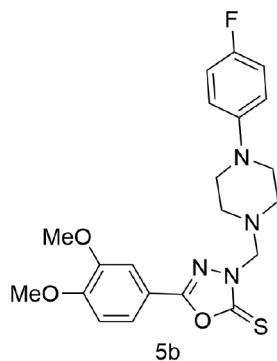


Filename = Prof.DR Ali Elemam_DM_1_ca
 Author = delta
 Experiment = carbon.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_1
 Solvent = DMSO-D6
 Creation_Time = 21-DEC-2020 19:28:08
 Revision_Time = 5-FEB-2021 08:35:11
 Current_Time = 5-FEB-2021 08:36:32

Comment = single pulse decoupled gat
 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_Clippped = 31.44654088[kHz]
 Irr_Domain = Proton
 Irr_Freq = 500.15991521[MHz]
 Irr_Offset = 5.0[ppm]
 Clipped = FALSE
 Scans = 1500
 Total_Scans = 1500

Relaxation_Delay = 2[s]
 Recvr_Gain = 50
 Temp_Get = 20.3[dC]
 X_90_Width = 32.3[us]
 X_Acq_Time = 0.83361792[s]
 X_Angle = 30[deg]
 X_Atn = 10[dB]
 X_Pulse = 10.76666667[us]
 Irr_Atn_Dec = 17.693[dB]
 Irr_Atn_Noie = 17.693[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]



Filename = Prof.DR Ali Elemam_DM_2_pr
 Author = delta
 Experiment = proton.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_2
 Solvent = DMSO-D6
 Creation_Time = 14-DEC-2020 11:50:57
 Revision_Time = 5-FEB-2021 23:19:09
 Current_Time = 5-FEB-2021 23:19:16

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 = 1.24780544[s]
 X_Domain = 1H
 X_Freq = 500.15991521[MHz]
 X_Offset = 7.0[ppm]
 X_Points = 16384
 X_Prescans = 1
 X_Resolution = 0.80140699[Hz]
 X_Sweep = 13.1302521[kHz]
 X_Sweep_Clippped = 10.50420168[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

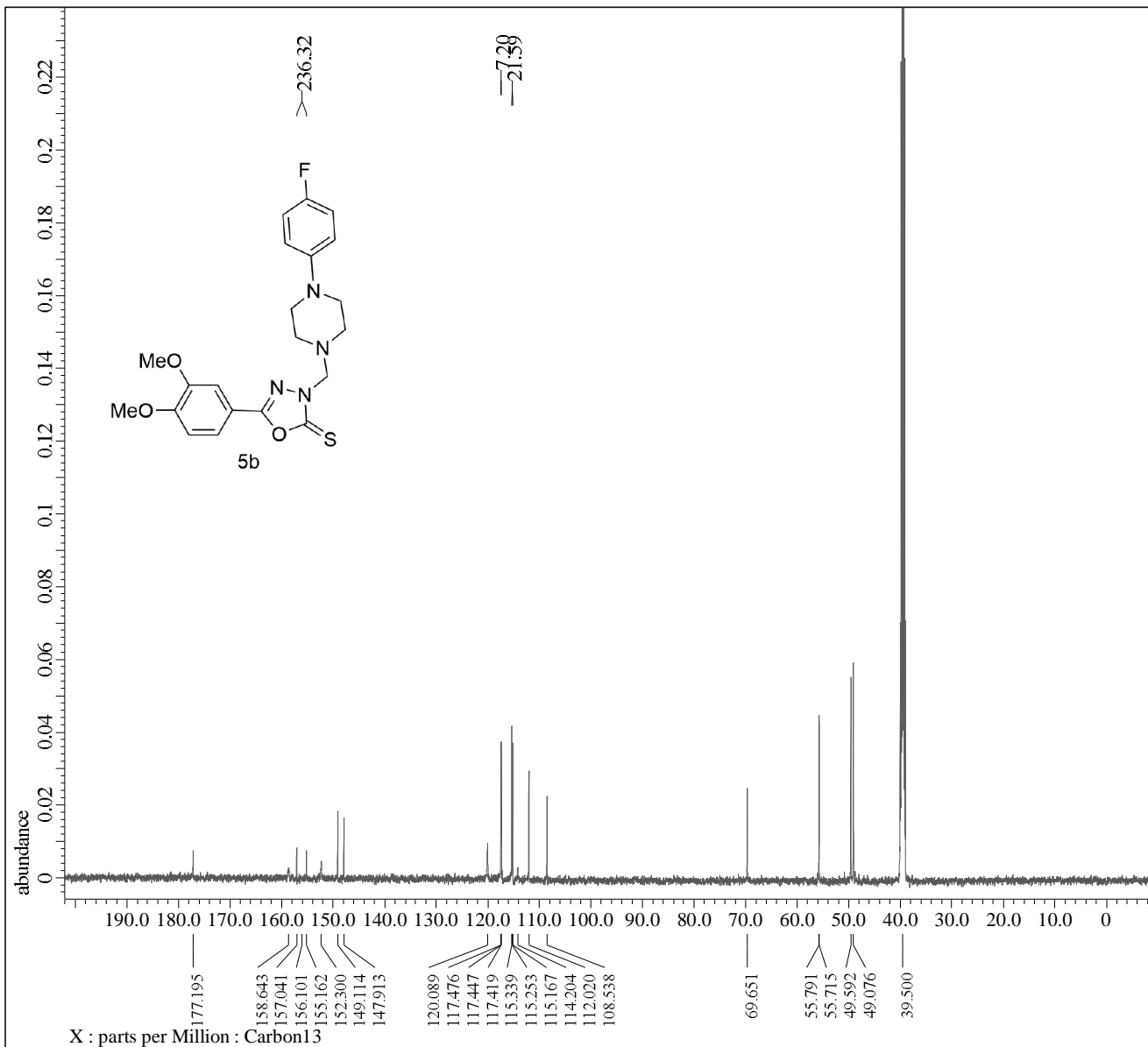
Relaxation_Delay = 5[s]
 Recvr_Gain = 50
 Temp_Get = 19[dc]
 X_90_Width = 16[us]
 X_Acq_Time = 1.24780544[s]
 X_Angle = 45[deg]
 X_Atn = 2.5[dB]
 X_Pulse = 8[us]
 Irr_Mode = Off
 Tri_Mode = Off
 Dante_Preset = FALSE
 Initial_Wait = 1[s]
 Repetition_Time = 6.24780544[s]

Filename = Prof.DR Ali Elemam_DM_2_ca
 Author = delta
 Experiment = carbon.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_2
 Solvent = DMSO-D6
 Creation_Time = 21-DEC-2020 20:44:41
 Revision_Time = 5-FEB-2021 08:45:38
 Current_Time = 5-FEB-2021 08:49:17

Comment = single pulse decoupled gat
 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 = 1500
 Total_Scans = 1500

Relaxation_Delay = 2[s]
 Recvr_Gain = 50
 Temp_Get = 19.9[dC]
 X_90_Width = 32.3[us]
 X_Acq_Time = 0.83361792[s]
 X_Angle = 30[deg]
 X_Atn = 10[dB]
 X_Pulse = 10.76666667[us]
 Irr_Atn_Dec = 17.693[dB]
 Irr_Atn_Noe = 17.693[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]

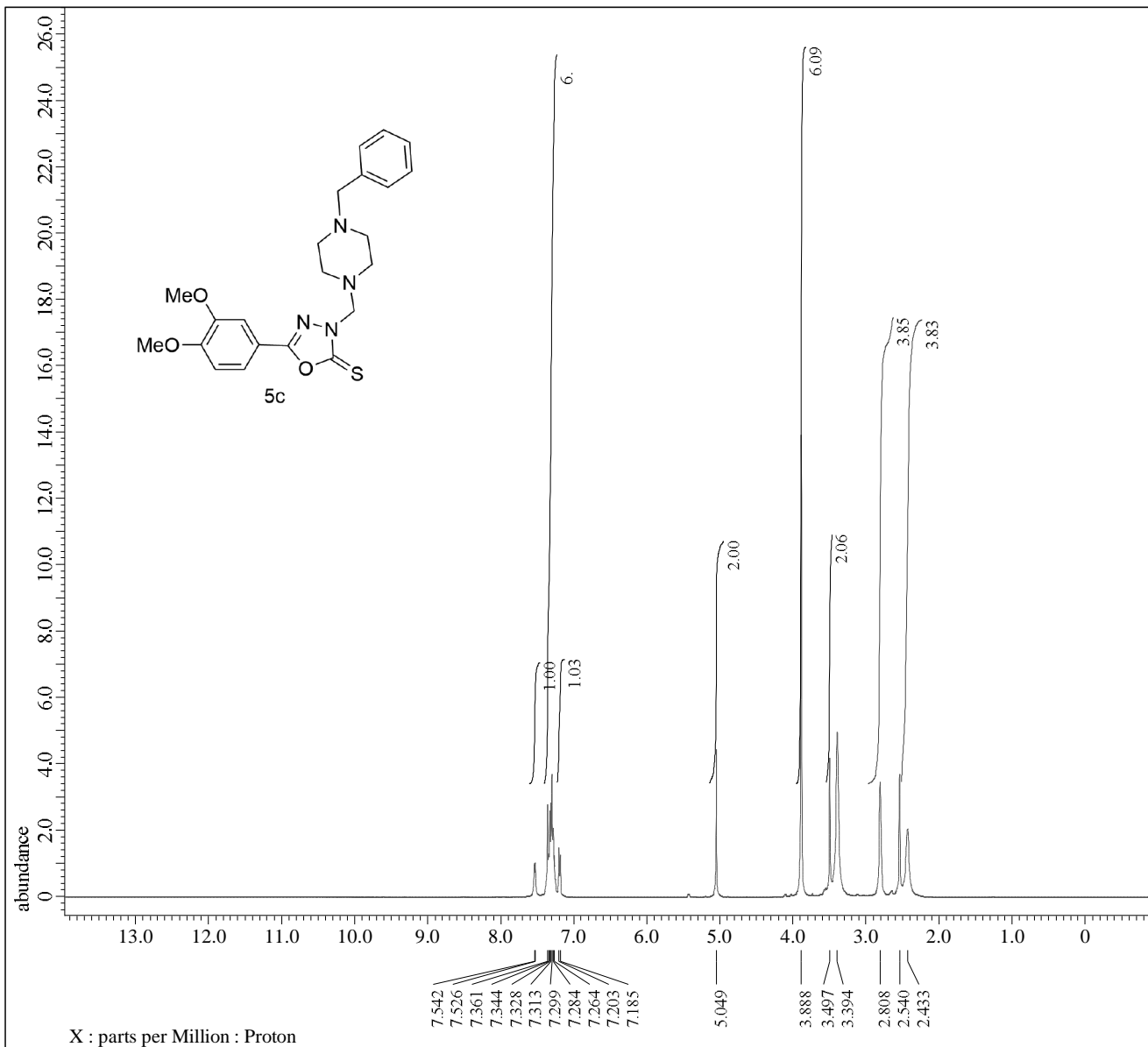


Filename = Prof.DR Ali Elemam_DM_3_pr
 Author = delta
 Experiment = proton.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_3
 Solvent = DMSO-D6
 Creation_Time = 14-DEC-2020 12:02:59
 Revision_Time = 5-FEB-2021 23:22:48
 Current_Time = 5-FEB-2021 23:23:09

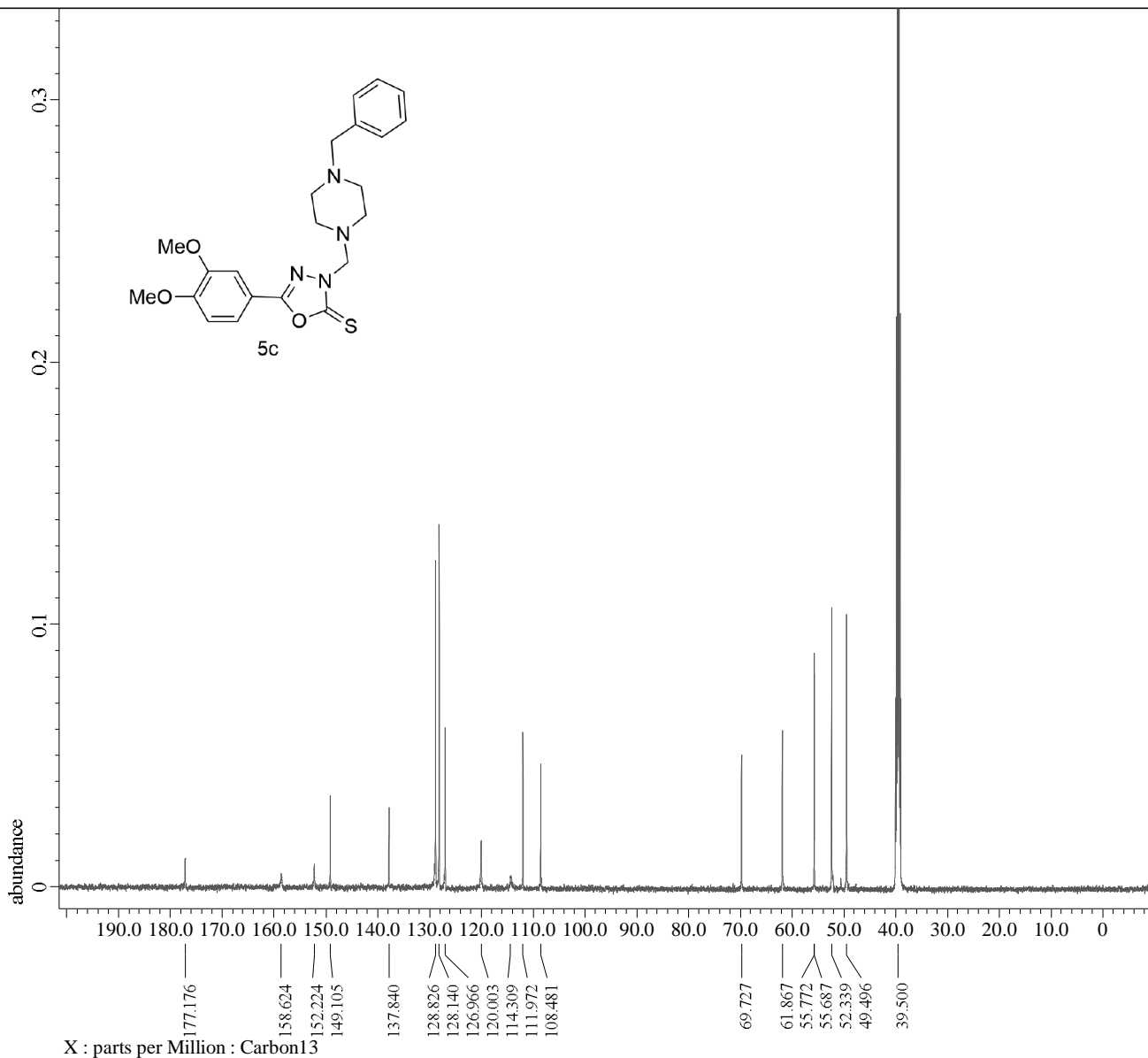
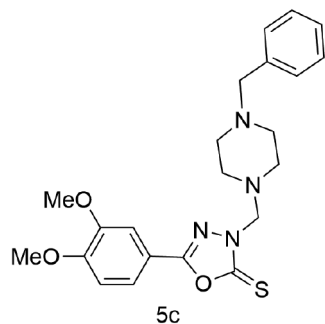
Comment = single_pulse
 Data_Format = 1D COMPLEX
 Dim_Size = 13107
 Dim_Title = Proton
 Dim_Units = [ppm]
 Dimensions = X
 Site = JNM-ECA500II
 Spectrometer = DELTA2_NMR

Field_Strength = 11.7473579[T] (500[MHz])
 X_Acq_Duration = 1.24780544[s]
 X_Domain = 1H
 X_Freq = 500.15991521[MHz]
 X_Offset = 7.0[ppm]
 X_Points = 16384
 X_Prescans = 1
 X_Resolution = 0.80140699[Hz]
 X_Sweep = 13.1302521[kHz]
 X_Sweep_Clippped = 10.50420168[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 = TRUE
 Scans = 40
 Total_Scans = 40

Relaxation_Delay = 5[s]
 Recvr_Gain = 50
 Temp_Get = 18.7[dC]
 X_90_Width = 16[us]
 X_Acq_Time = 1.24780544[s]
 X_Angle = 45[deg]
 X_Atn = 2.5[dB]
 X_Pulse = 8[us]
 Irr_Mode = Off
 Tri_Mode = Off
 Dante_Preset = FALSE
 Initial_Wait = 1[s]
 Repetition_Time = 6.24780544[s]



X : parts per Million : Proton

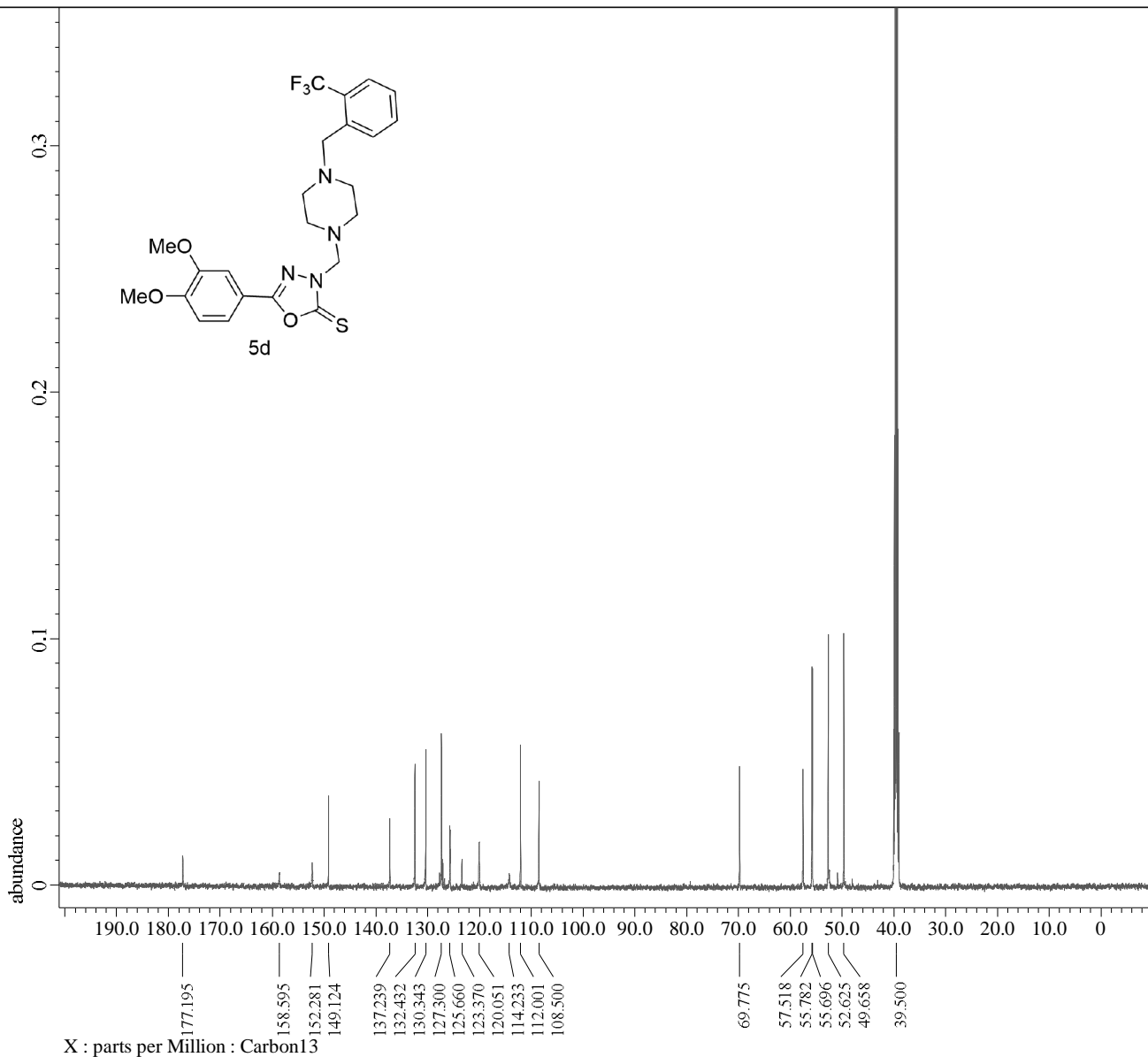
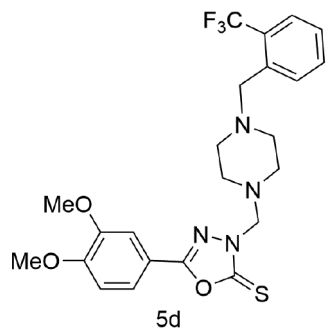


Filename = Prof.DR Ali Elemam_DM_3_ca
 Author = delta
 Experiment = carbon.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_3
 Solvent = DMSO-D6
 Creation_Time = 21-DEC-2020 22:01:52
 Revision_Time = 5-FEB-2021 08:52:07
 Current_Time = 5-FEB-2021 08:53:24

Comment = single pulse decoupled gat
 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 = 1500
 Total_Scans = 1500

Relaxation_Delay = 2[s]
 Recvr_Gain = 50
 Temp_Get = 20.1[dc]
 X_90_Width = 32.3[us]
 X_Acq_Time = 0.83361792[s]
 X_Angle = 30[deg]
 X_Atn = 10[db]
 X_Pulse = 10.76666667[us]
 Irr_Atn_Dec = 17.693[db]
 Irr_Atn_Noie = 17.693[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]



Filename = Prof.DR Ali Elemam_DM_4_ca
 Author = delta
 Experiment = carbon.jxp
 Sample_Id = Prof.DR Ali Elemam_DM_4
 Solvent = DMSO-D6
 Creation_Time = 22-DEC-2020 08:58:10
 Revision_Time = 5-FEB-2021 09:06:07
 Current_Time = 5-FEB-2021 09:07:41

Comment = single pulse decoupled gat
 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 = 1500
 Total_Scans = 1500

Relaxation_Delay = 2[s]
 Recvr_Gain = 50
 Temp_Get = 18.9[dC]
 X_90_Width = 32.3[us]
 X_Acq_Time = 0.83361792[s]
 X_Angle = 30[deg]
 X_Atn = 10[dB]
 X_Pulse = 10.76666667[us]
 Irr_Atn_Dec = 17.693[dB]
 Irr_Atn_Noie = 17.693[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]