Probing the Structural Requirements for Thiazole-Based Mimetics of Sunitinib as Potent VEGFR-2 Inhibitors

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Biological screening

In vitro antitumor testing against HepG2, HCT-116, MCF-7, HeP-2 and Hela cancer cell lines, and cytotoxicity against WI38 and WISH normal cell lines

Materials

Cell lines

Liver (HepG2), colon (HCT-116), breast (MCF-7), larynx (HeP-2) and cervix (Hela) cancer cell lines as well as lung fibroblast (WI38) and amnion epithelial (WISH) normal cell lines were obtained from American Type Culture Collection (ATCC) *via* Holding Company for Biological Products and Vaccines (VACSERA), Cairo, Egypt.

Chemical reagents

The reagents, Roswell Park Memonial Instiute (RPMI-1640) medium, 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT), DMSO, doxorubicin and sunitinib were obtained from Sigma-Aldrich co., St. Louis, USA. Fetal bovine serum was obtained from GIBCO, UK.

Procedure

Compounds **3-6** and **8-11** were screened for their *in vitro* antitumor activity against HepG2, HCT-116, MCF-7, HeP-2 and Hela cancer cell lines. In addition, compounds **3a,b**, **6g**, **8a** and **10c** were screened for their *in vitro* cytotoxicity against WI38 and WISH normal cell lines adopting MTT assay [1-3], and using doxorubicin, sunitinib as reference antitumor agent. Cells were cultured in Roswell Park Memorial Institute (RPMI) 1640 medium with 10% fetal bovine serum, penicillin (100 units/mL) and streptomycin (100 µg/mL) at 37 °C in an atmosphere of

5% CO_2 were added. Cells were placed in 96-multiwell microtiter plates (10^4 cells/well) for 24 hours at 37 °C and in an atmosphere of 5% CO_2 before treatment with the compounds to allow attachment of the cells to the wall of the plate. The tested compounds were dissolved in DMSO and diluted with phosphate buffer saline (PBS) to obtain different concentrations. Tested compounds of different concentrations were added to each well and cells were incubated with the compounds for 48 hours at 37 °C and in atmosphere of 5% CO_2. All tests were performed in triplicates. The treated cells were washed with PBS and 100 µL of 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide solution (MTT) (5 mg/mL MTT stock in PBS diluted to 1 mg/mL with 10% RPMI-1640 medium) was added. The 96-multiwell plates were read by microarray reader Perkinelmer vector 3V multilabel counter model 1420 (Perkinelmer, Boston, MA) for optical density at 490 nm [1-3]. The relative percentage cell viability was calculated from the following equation:

$$\% \text{ Cell viability} = \frac{A_{\text{treated cells}} - A_{\text{blank}}}{A_{\text{untreated cells}} - A_{\text{blank}}} \text{ X } 100$$

The relation between surviving fraction and drug concentration is plotted to get the survival curve for HepG2, HCT-116, MCF-7, HeP-2 and Hela cancer cell lines, and WI38 and WISH normal cell lines. The concentration required for 50% inhibition of cell viability (IC_{50}/µM) was obtained for each compound from the curve fitting using Sigma plot10.

In vitro kinase inhibition assay against VEGFR-2 for compounds 3a,b, 6g, 8a and 10c

In vitro kinase inhibition assay was carried out against VEGFR-2 using ELISA kit (Cat. # 40325, BPS Bioscience, USA). The procedure of the used kits was done according to the manufacturer's instructions. Briefly, compounds **3a,b**, **6g**, **8a** and **10c** and control drug, sunitinib, were made to different serial dilution. 5x kinase buffer 1, ATP and PTK substrate poly (Glu:Tyr 4:1) (10 mg/mL) were thawed. After that, the master mixture [N wells x (6 µl 5x kinase buffer 1 + 1 µl ATP (500 µM) + 1 µl PTK substrate Poly (Glu:Tyr 4:1) (10 mg/mL)+ 17 µl water)] was prepared followed by addition of 25 µl to every well. Then, 5 µl of inhibitor solution was added to each well and labeled as “test inhibitor”. For the “positive control" and “blank wells”, 5 µl of the same solution without inhibitor (inhibitor buffer) was added. 3 mL of 1x kinase buffer 1 was prepared by mixing 600 µl of 5x kinase buffer 1 with 2400 µl water was prepared. To the wells designated as "blank", 20 µl of 1x kinase buffer 1 was added. VEGFR-2

enzyme was thawed on ice. Upon first thaw, tube containing enzyme was spinned briefly to recover full content of the tube. The amount of VEGFR-2 required for the assay was calculated and the enzyme was diluted to 1 ng/µl with 1x kinase buffer 1. The reaction was initiated by adding 20 µl of diluted VEGFR-2 enzyme to the wells designated “positive control” and "test inhibitor control" and incubated at 30°C for 45 minutes. Kinase-Glo Max reagent was thawed. After the 45 minutes, 50 µl of Kinase-Glo Max reagent was added to each well. The plate was covered with aluminum foil and incubated at room temperature for 15 minutes. The luminescence was measured using the microplate reader. The values of % activity versus different concentrations of the test compound (with semi-log decrease in concentration) were then plotted using nonlinear regression analysis of sigmoidal dose-response curve, and the concentration that induces 50% inhibition of activity (IC_{50}) of VEGFR-2 were determined [4,5].

Cell cycle analysis and induction of apoptosis

Flow cytometry analysis of DNA content for cell cycle

HCT-116, MCF-7 and Hela cancer cells (2 x 10^5 cells/well) were treated with different concentrations of compound **10c**, and incubated for 24 hours at 37 ºC in an atmosphere of 5% CO_2. The cells were washed twice with ice-cold PBS, collected by centrifugation, and fixed in ice-cold 70% ethanol, washed with PBS, and then they were incubated with propidium iodide (PI) staining solution that contains 50 µg/mL PI, 0.1 mg/mL RNase A and 0.05% Triton X-100. After incubation for 1 hour at room temperature, the cells were analyzed in the dark at 37 °C by flow cytometry (Becton Dickinson FACS, San Jose, CA) [6,7]. The cell cycle distributions were determined using Cell-Quest software.

Analysis of cellular apoptosis

Annexin V-fluorescein isothiocyanate (Annexin V-FITC) is a protein that possesses high affinity to phosphatidyl serine (PS), which can be detected by staining with annexin V-FITC and counter staining with propidium iodide (PI). Apoptosis was initially induced by incubation of cells in a density of 4 x 10^6 cells/well in 100 µL of complete growing medium with addition of the tested compound **10c** (100 µL) in 96-microwell plates for 24 hours. Then, 0.5 x 10^6 cells were collected by centrifugation and resuspended in 500 µL of binding buffer. Annexin V-FITC (5 µL) along with PI (5 µL) were added, and incubated in the dark for 5 minutes at room temperature. Analysis of annexin-V-FITC binding was performed by flow cytometry (Becton Dickinson FACS, San Jose, CA) [6,7].

Caspase3/9 assay

The level of human caspase-3 was assessed using ELISA kit that was obtained from Invitrogen INC. Catalog # KHO1091 (Invitrogen, Inc., Waltham, Massachusetts, USA) in accordance with the manufacturer instructions. Also, human caspase-9 ELISA kit was obtained from DRG International, INC. Catalog # EIA-4860 (DRG International, Inc., Mountain Avenue Springfield, USA) in accordance with the manufacturer instructions. The tested compound **10c** (10 μM) was added to the cells and lysed with cell extraction buffer. After incubation at room temperature for 2 hours, wells were washed 4 times with the wash buffer, followed by addition of 100 mL of Invitrogen caspase-3 (active) or caspase-9 monoclonal antibody solution and incubated again at room temperature for another 1 hour. Wells were washed 4 times with the wash buffer, the anti-rabbit IgG horseradish peroxidase (HRP) solution (100 mL) was added, and the wells were incubated for 30 minutes at room temperature. After washing 4 times with the wash buffer, stabilized chromogen was added. Later on, the stop solution (100 mL) was added after incubation for 30 minutes. Absorbance was measured at 450 nm [8].

In vivo antitumor activity of compound 10c

In vivo antitumor screening was conducted after fulfillment of ethical statement and approval protocol for animal study from research ethical committee, Faculty of Pharmacy, Mansoura University. Evaluation of the *in vivo* antitumor activity of compound **10c** was achieved using EAC solid tumor animal model [9]. Tweny five swiss albino eight-week female mice (weighing 20-25 g) were obtained and divided into three groups (n = 5). Group 1: positive control-received equivalent volume of physiological saline; group 2: treated intraperitoneally with compound **10c** (10 mg/kg); group 3: treated intraperitoneally with doxorubicin (2 mg/kg). 7,12-Dimethylbenz[a]anthracene was used to induce breast cancer in mice. All groups were injected intraperitoneally one dose per day in a period of 20 days. Monitoring of the body weight and tumor volumes of mice was done every five days, the volume of solid tumor was monitored using a digital Vernier caliper and was calculated using the following equation:

$$\text{Tumor volume } (mm^3) = \text{Length}(mm) \times [\text{Height}(mm)]^2 \times 0.52$$

Tumor growth inhibition (%TGI) was calculated after 5,10,15 and 2 days by the formula:

$$\%\text{TGI} = \frac{1 - \frac{(Tt/T0)}{(Ct/C0)}}{1 - (\frac{C0}{Ct})} \times 100$$

Where:

Tt = median tumor volume of treated group at time t.

T0 = median tumor volume of treated group at time 0.

Ct = median tumor volume of control group at time t.

C0 = median tumor volume of control group at time 0.

At the end of the experiment, mice were sacrificed and tumors were excised, fixed in 10 % formalin solution, and embedded in paraffin.

Molecular modeling study

The molecular modeling calculations were done applying swiss dock online server [10-12]. The 3D poses was visualized by UCSF chimera software [13-15] and the 2D poses were visualized by ProteinsPlus structure-based modeling support server [16-19]. The most stable conformer of the newly synthesized analogs **3a,b**, **6g**, **8a** and **10c** was docked into the binding pocket of VEGFR-2 (PDB code: 4agd) [20,21] which was obtained from the Protein Data Bank (PDB).

HPLC purity testing

The HPLC purity for compounds **3b**, **6g**, **8a** and **10c** was tested using Knauer high performance liquid chromatography apparatus with variable-wavelength UV-visualization detecdtor operatrd at 240 nm. The mixture was separated using a shim-pack cyano column (150 mm x 4.6 mm, 5µm particle size). The composition of the mobile phase was Methanol: phosphate buffer (50: 50, v/v) adjusted at pH 4 , and programmed at flow rate of 1 mL/min with UV detection at 240 nm. Filtration of the mobile phase was carried out through 0.45 µm millipore membrane filter. Separation was performed after sonication of the mobile phase for 10 min to remove air bubbles. All determinations were performed at ambient temperature.

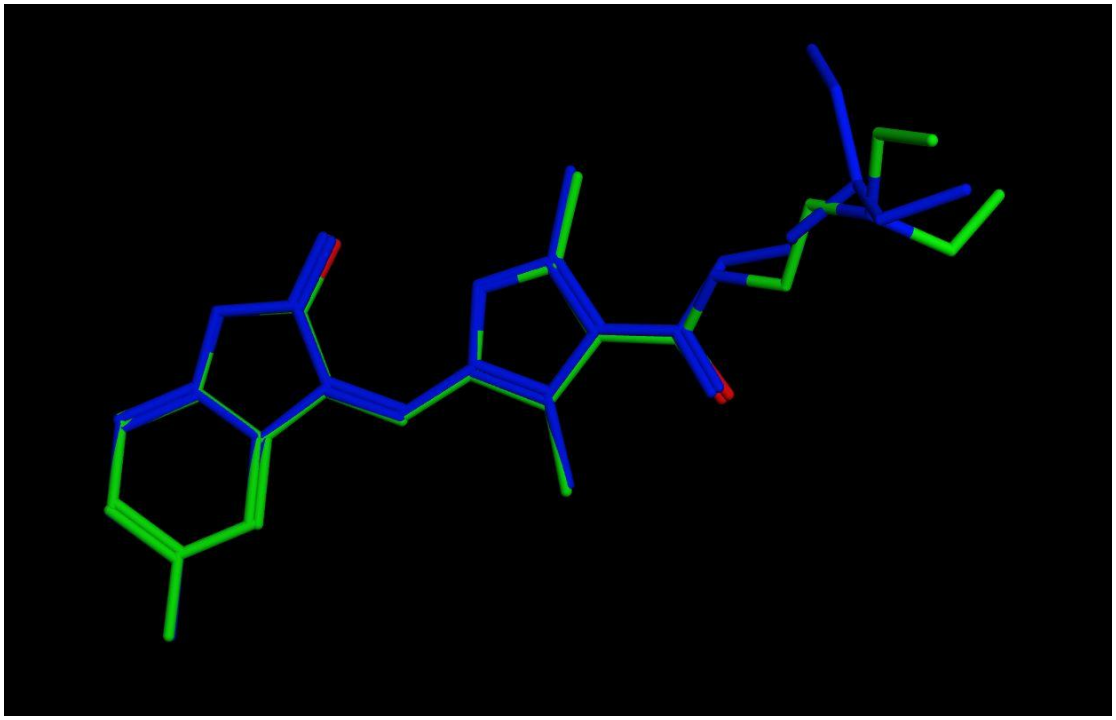


Figure S1. Superimposition of the co-crystallized sunitinib (blue) and the re-docked sunitinib (green) in the VEGFR-2 active site (RMSD = 1.05 Å).

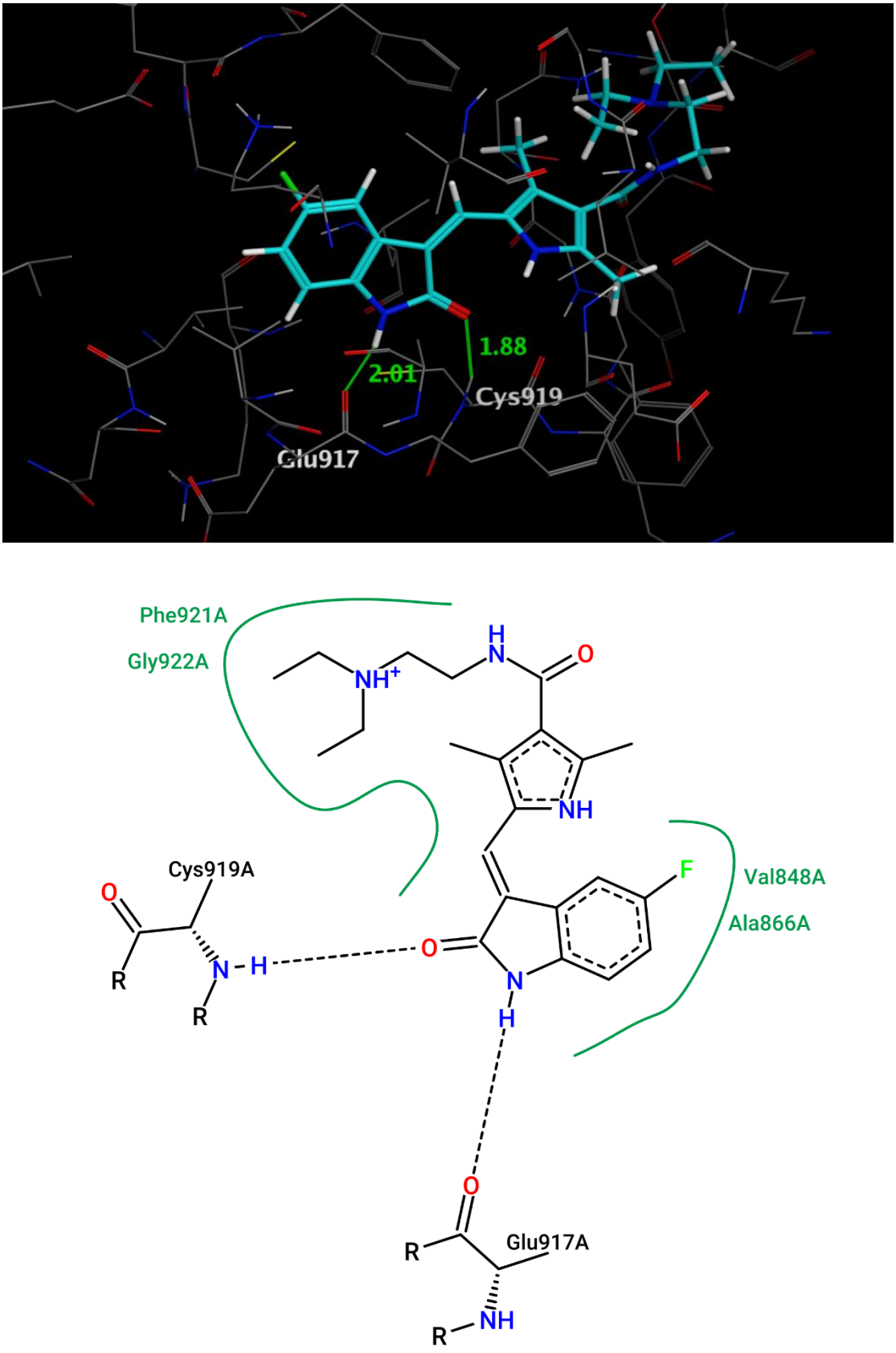


Figure S2. 3D and 2D Interaction pattern of sunitinib with the binding site of VEGFR-2.

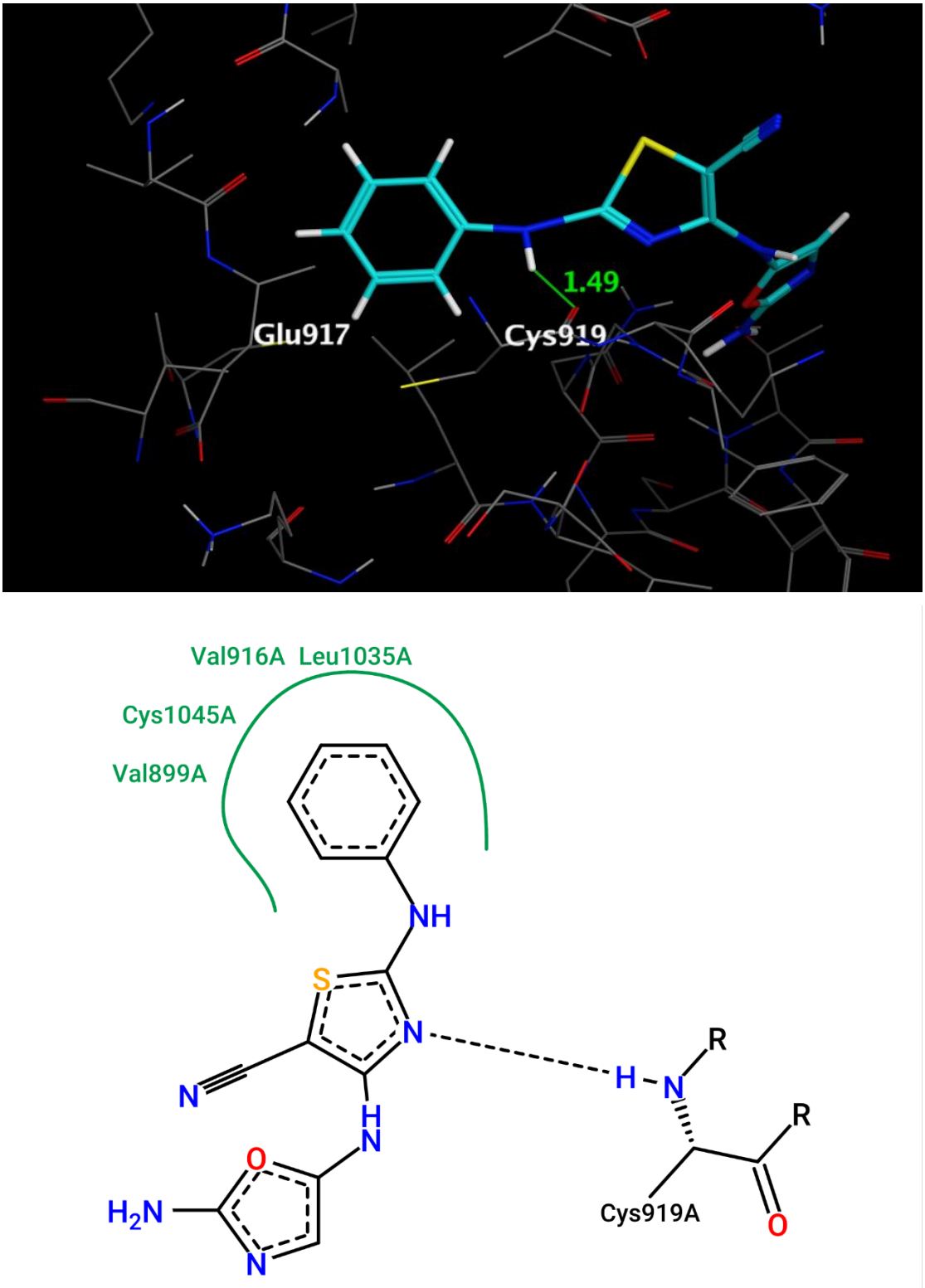


Figure S3. 3D and 2D Interaction pattern of compound **3a** with the binding site of VEGFR-2.

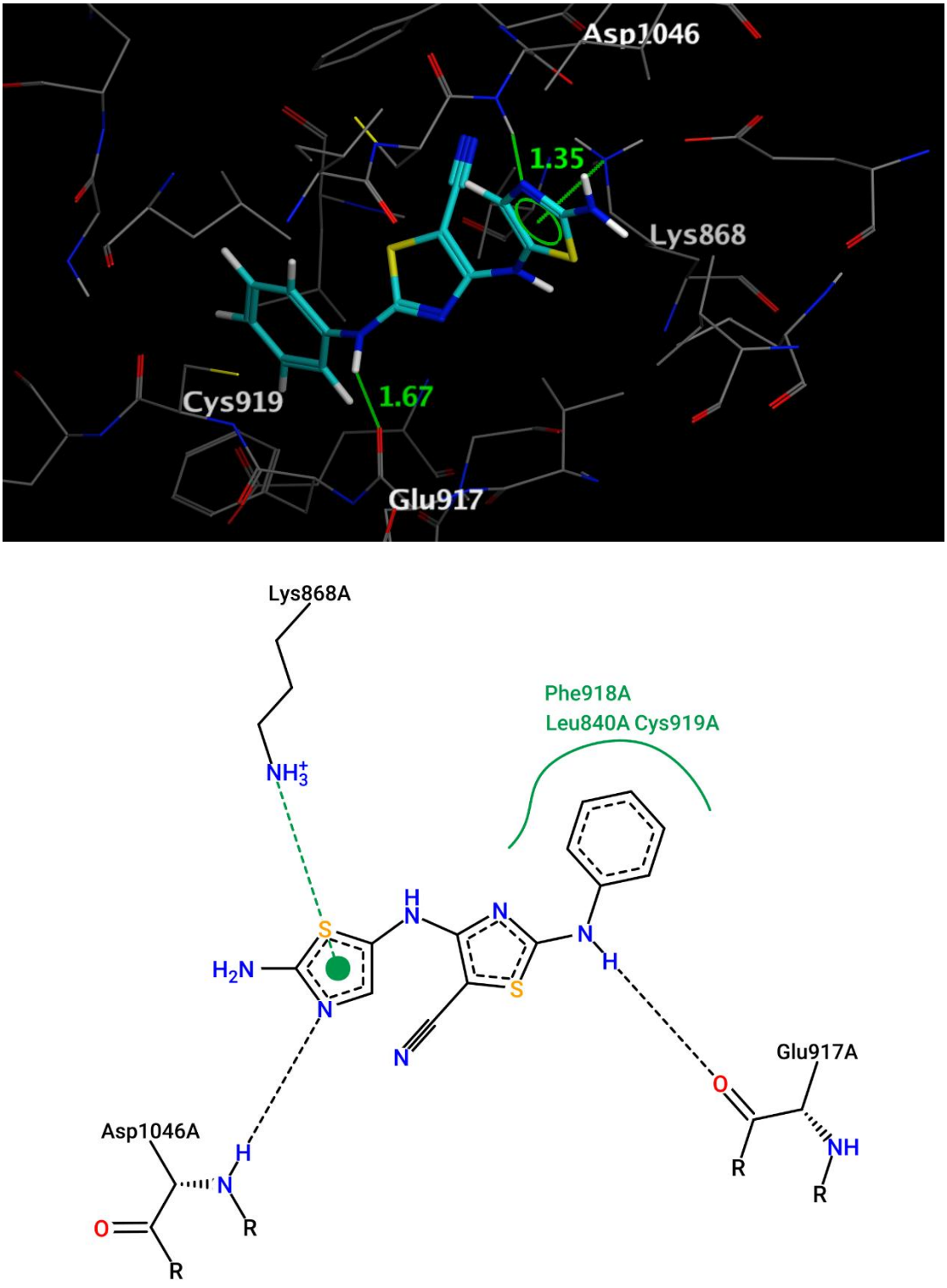
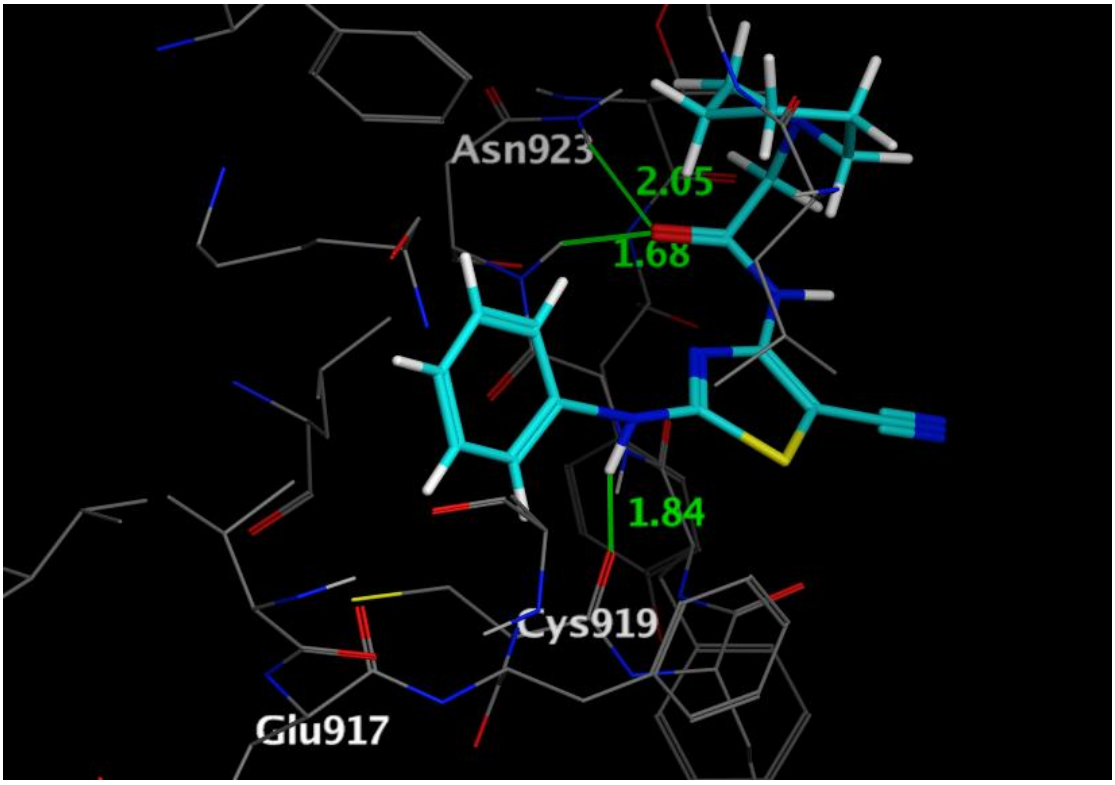


Figure S4. 3D and 2D Interaction pattern of compound **3b** with the binding site of VEGFR-2.



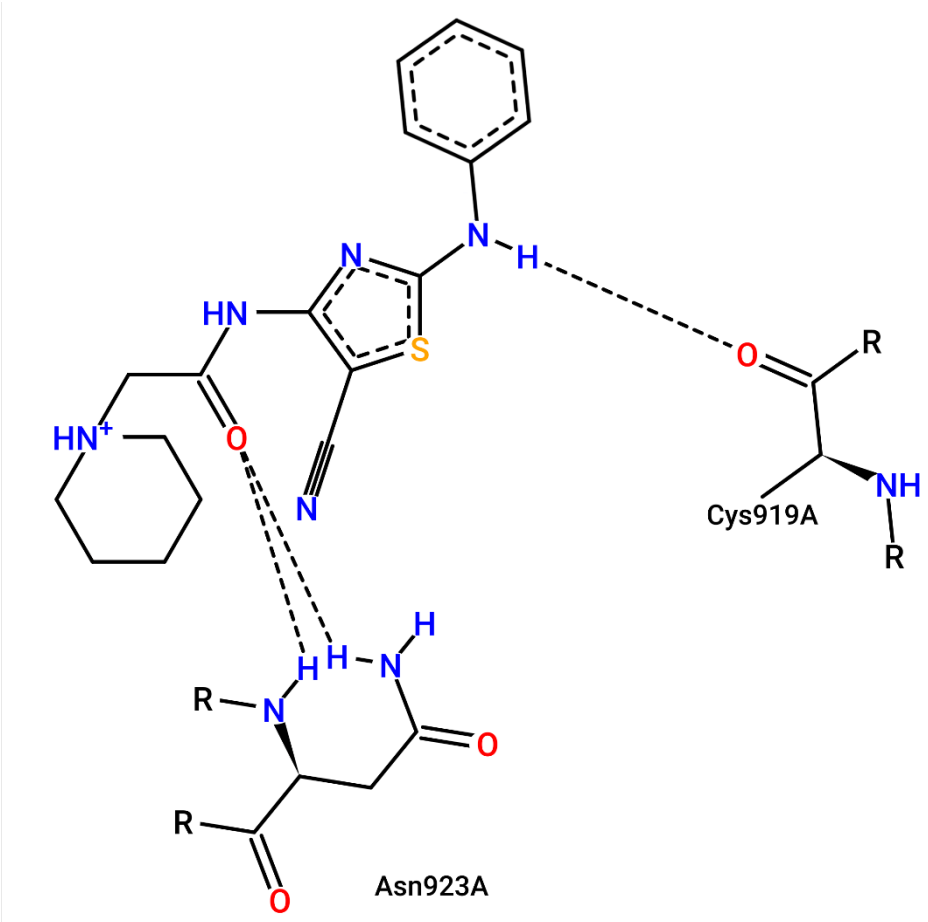


Figure S5. 3D and 2D Interaction pattern of compound **6g** with the binding site of VEGFR-2.

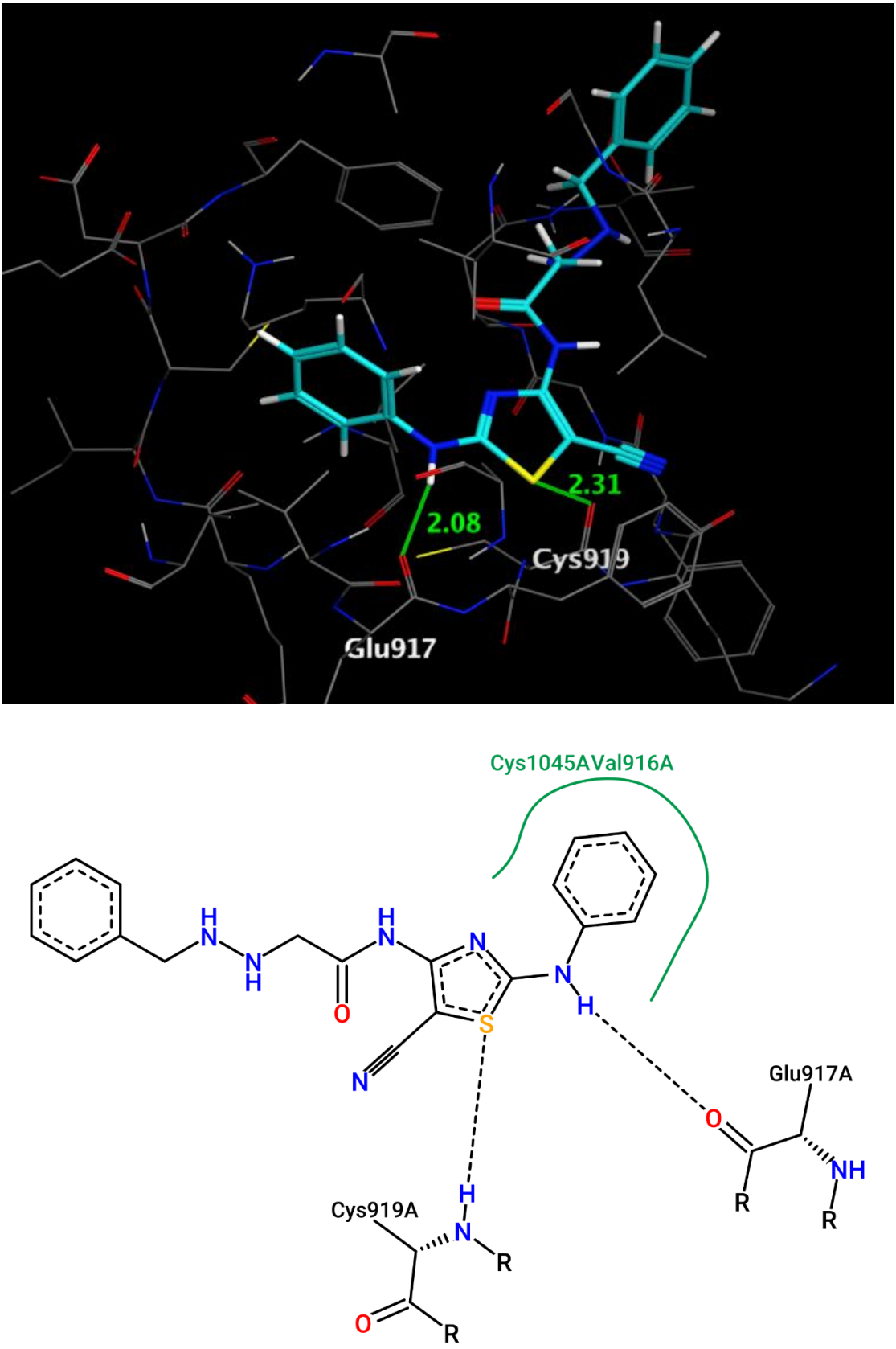


Figure S6. 3D and 2D Interaction pattern of compound **8a** with the binding site of VEGFR-2.

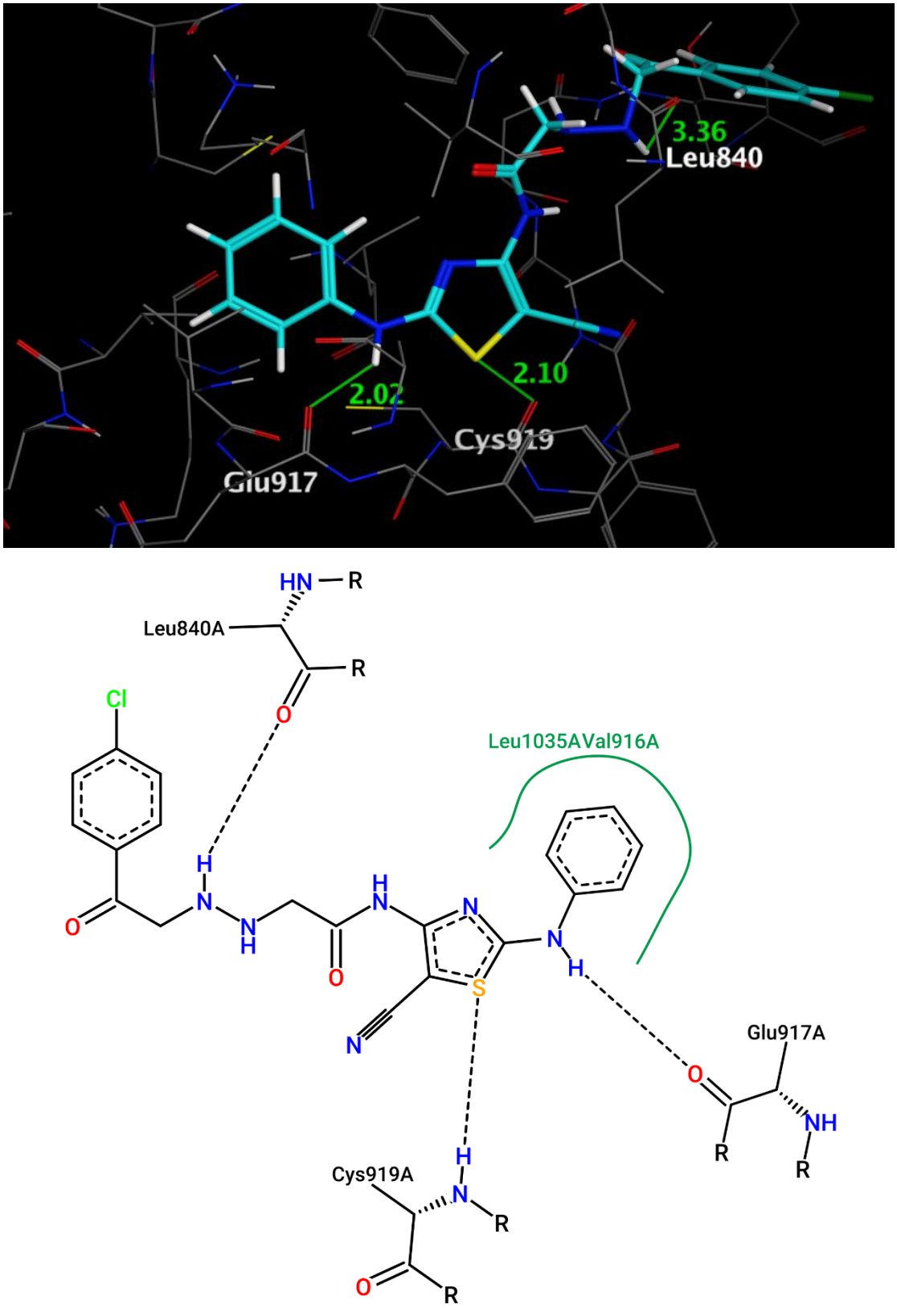


Figure S7. 3D and 2D Interaction pattern of compound **10c** with the binding site of VEGFR-2.

Table S1. Body weight of mice for control, doxorubicin, and **10c**-treated groups at 0, 5, 10, 15 and 20 days of treatment.

Group	Body weight (g)				
	day 0	**day 5**	**day 10**	**day 15**	**day 20**
Positive Control	18.20±1.068	23.00±0.707	28.20±0.860	32.60±0.509	37.00±0.707
Doxorubicin	20.00±0.707	21.60±0.927	24.40±1.030*	26.40±0.979***	28.60±0.812****
10c	19.20±0.734	23.00±1.140	27.00±0.948	30.20±0.583$^{\#\#}$	34.40±0.509$^{*\#\#\#}$

Positive control: mice with cancer implants and receiving no drug.
**** $p < 0.0001$, *** $p < 0.0005$, * $p < 0.05$ vs. Positive control group.
$p < 0.0005$, ## $p < 0.01$ vs. doxorubicin group.

Table S2. Tumor volume of the mammary gland of mice for control, doxorubicin, and **10c**-treated groups at 0, 5, 10, 15 and 20 days of treatment.

Group	Tumor volume (mm^3)				
	day 0	**day 5**	**day 10**	**day 15**	**day 20**
Positive Control	0.180±0.010	0.680±0.039	1.322±0.151	2.250±0.129	3.078±0.160
Doxorubicin	0.186±0.010	0.268±0.010****	0.368±0.014****	0.484±0.016****	0.600±0.012****
10c	0.188±0.010	0.504±0.028$^{**\#\#\#}$	0.680±0.050***	0.964±0.108$^{****\#}$	1.024±0.088$^{****\#}$

Positive control: mice with cancer implants and receiving no drug.
**** $p < 0.0001$, *** $p < 0.001$, ** $p < 0.005$ vs. Positive control group.
$p < 0.001$, # $p < 0.05$ vs. doxorubicin group.

Table S3. % Tumor Growth Inhibition (%TGI) of breast solid tumor in mice after 5, 10, 15 and 20 days of treatment with doxorubicin and compound **10c**.

Group	%TGI			
	day 5	**day 10**	**day 15**	**day 20**
Doxorubicin	84.16	84.58	86.07	86.18
10c	39.49	58.75	64.11	72.38

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Mansoura University
Faculty of Pharmacy
Research Ethics Committee

جامعة المنصورة
كلية الصيدلة
لجنة اخلاقيات البحث العلمي

السيد الأستاذ الدكتور / رئيس مجلس قسم الكيمياء الدوائية

تحية طيبة وبعد،،،

بناء علي الخطاب الوارد من سيادتكم بشأن موافقة مجلس قسمكم الموقر في ٢٠٢٢/٨/١٠ علي الطلب المقدم من أ.د / سعيد محمد بيومي - المشرف الرئيسي علي رسالة الدكتوراه الخاصة بالصيدلانية / الاء عبدالله عبدالحميد محمد – المدرس المساعد بقسم الكيمياء الدوائية لإضافة جزء خاص باجراء أبحاث علي الحيوان (الفئران المعملية) وكذلك تعديل عنوان الرسالة حتي يكون العنوان اكثر تحديدا ليتوافق مع ما تم تحضيره من مركبات وانجازه فعليا في خطة الرسالة.

عنوان الرسالة باللغة العربية والانجليزية قبل التعديل

تشييد ودراسات حاسوبية لأنظمة نيتروجينية غير متجانسة جديدة متوقع لها فعالية بيولوجية

Synthesis and *in silico* studies of certain new nitrogenous heterocyclic systems of expected biological activity

عنوان الرسالة باللغة العربية والانجليزية بعد التعديل

"تصميم وتشييد ودراسات حاسوبية لبعض مشتقات الثيازول ومشتقات الثيازول المدمجة الجديدة كمضادات محتملة للسرطان"

"Design, Synthesis and *in silico* studies of some new thiazole and fused thiazole derivatives as potential anticancer agents "

فان لجنة اخلاقيات البحث العلمي في اجتماعها بتاريخ ٢٠٢٢/٨/٢٤ قد احيطت علما بالتعديل الذي تم في عنوان الرسالة كما وافقت علي استمارة البحوث الحيوان المستوفاة بمعرفة وبتوقيع أ.د / المشرف الرئيسي وذلك بعد التأكد من توافق التجارب المقترحة مع معايير أخلاقيات البحث العلمي مع التزام المشرف الرئيسي بتقديم اسم الباحث الذي اجري جزء التجارب العملية علي الحيوان عند انهاء البحث.

وتفضلوا سيادتكم بقبول وافر الاحترام والتقدير،،،

مقرر لجنة اخلاقيات البحث العلمي
٢٩/٨/٢٠٢٢
أ.م.د / امل احمد عطوه سلام .

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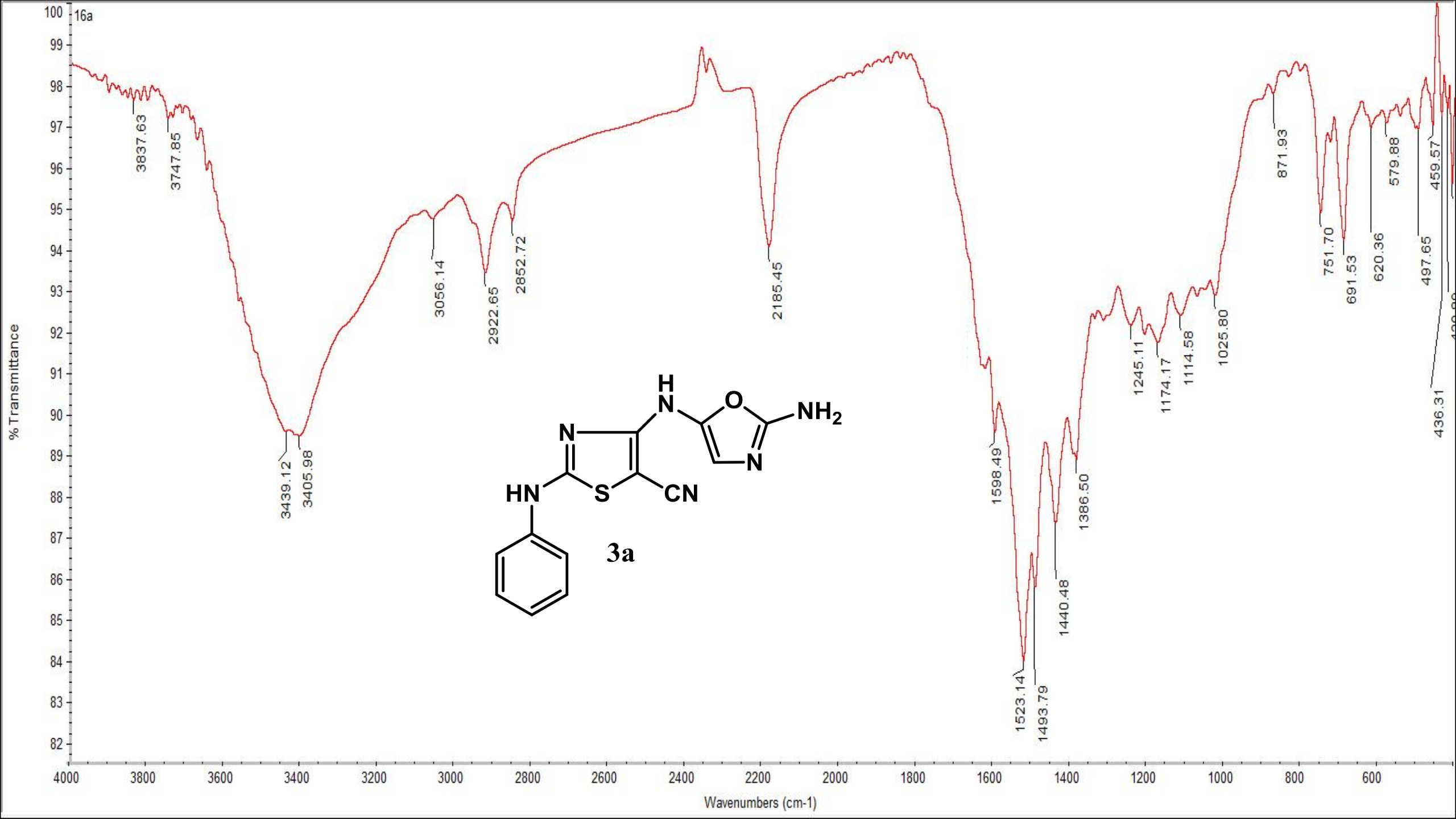
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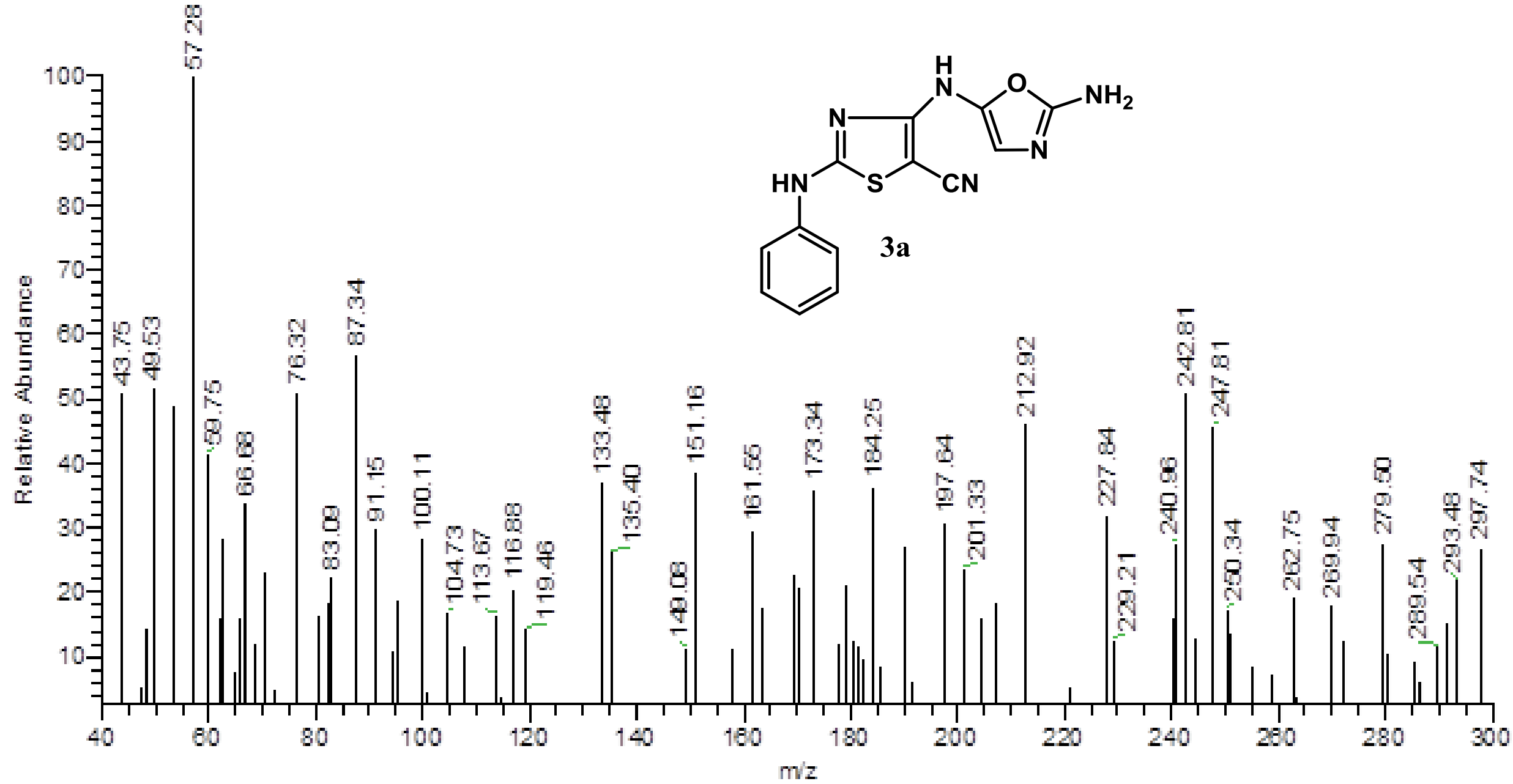
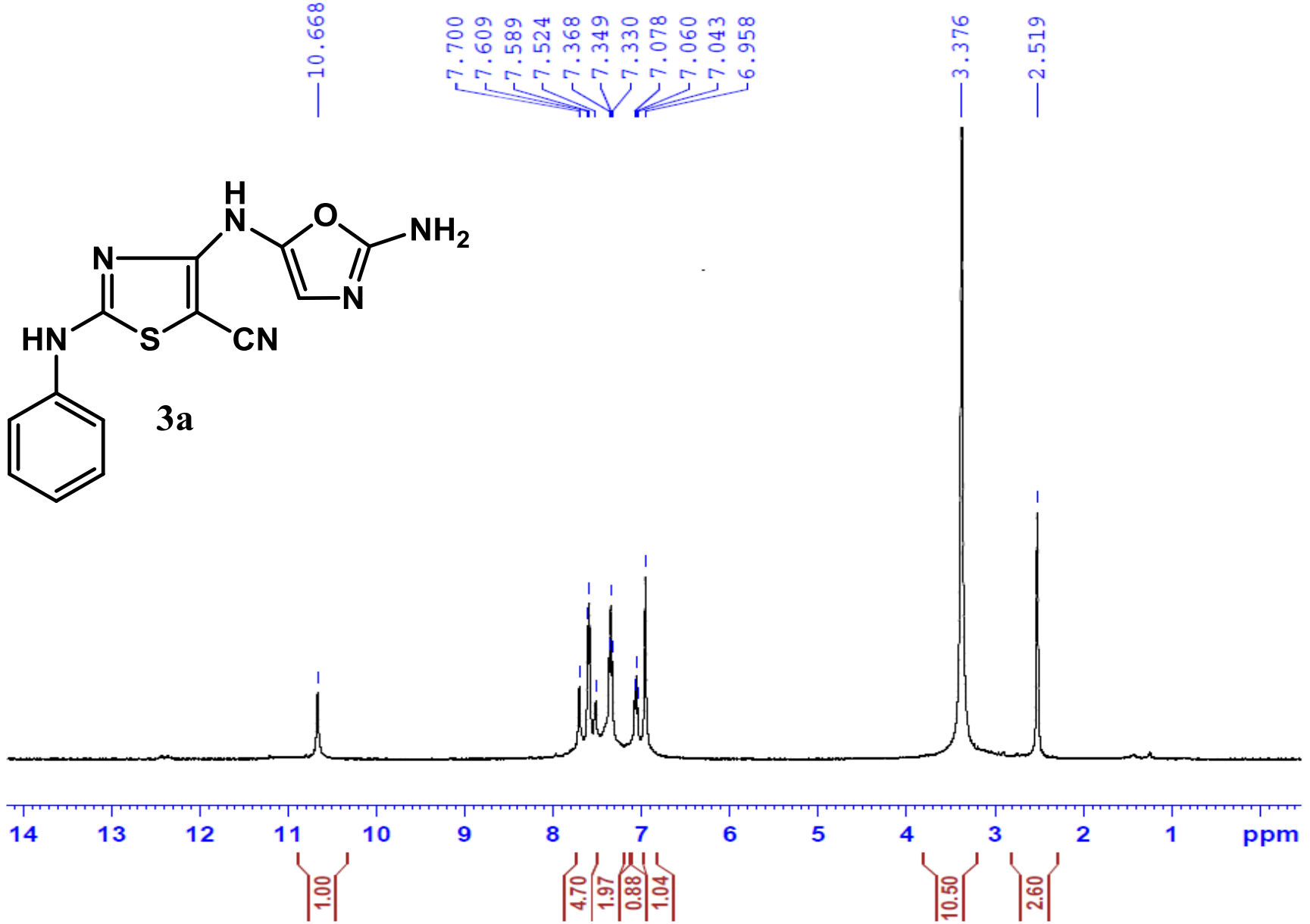
3a

alaa-16a #148 RT: 2.49 AV: 1 SB: 6 2.79 , 2.48-2.54 NL: 6.36E2
T: + cEI Full ms [40.00-1000.00]



3a

Alaa Abdullah-2-HNMR-DMSO-AF



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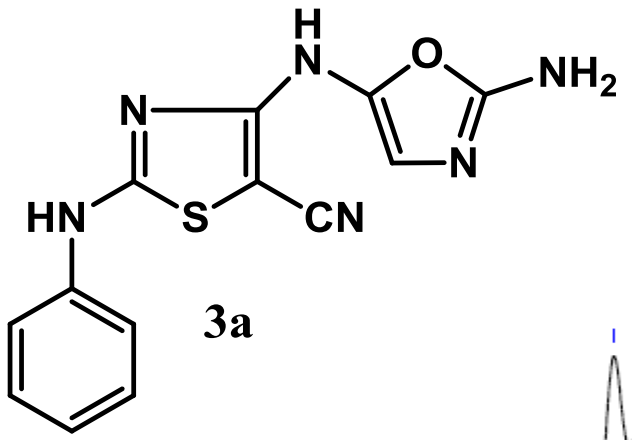
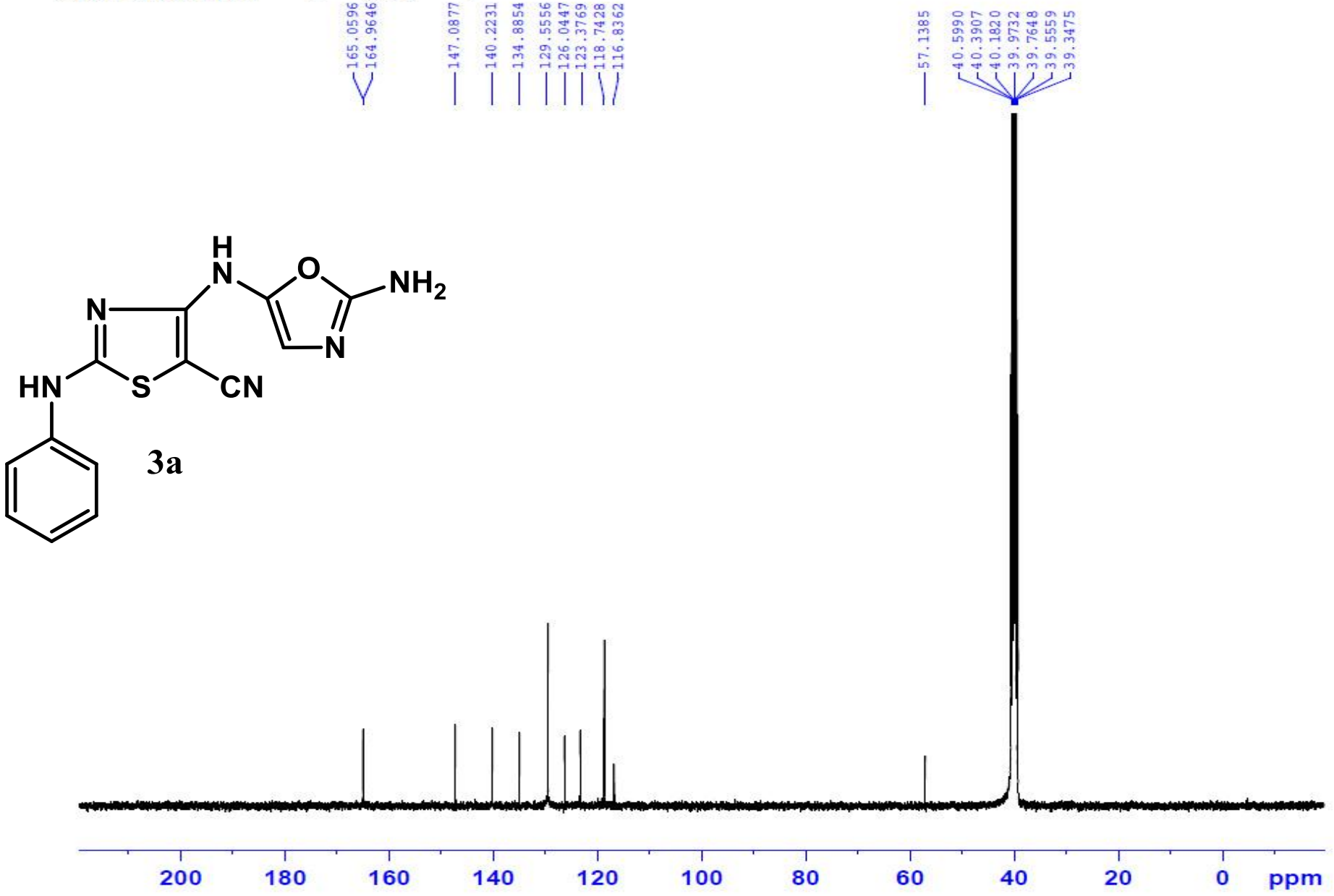
```
Current Data Parameters
NAME      Alaa Abdullah-2-HNMR-
EXPNO                       10
PROCNO                       1

F2 - Acquisition Parameters
Date_              20220510
Time                 14.44 h
INSTRUM                spect
PROBHD    Z108618_0945 (
PULPROG                 zg30
TD                     65536
SOLVENT                 DMSO
NS                        16
DS                         2
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                  4.0894465 sec
RG                     158.72
DW                     62.400 usec
DE                      6.50 usec
TE                     295.3 K
D1                  1.00000000 sec
TD0                        1
SFO1              400.2024712 MHz
NUC1                       1H
P1                     13.50 usec
PLW1              13.00000000 W

F2 - Processing parameters
SI                     65536
SF                400.2000000 MHz
WDW                       EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

Alaa Abdullah-2-HNMR-DMSO-AF



3a

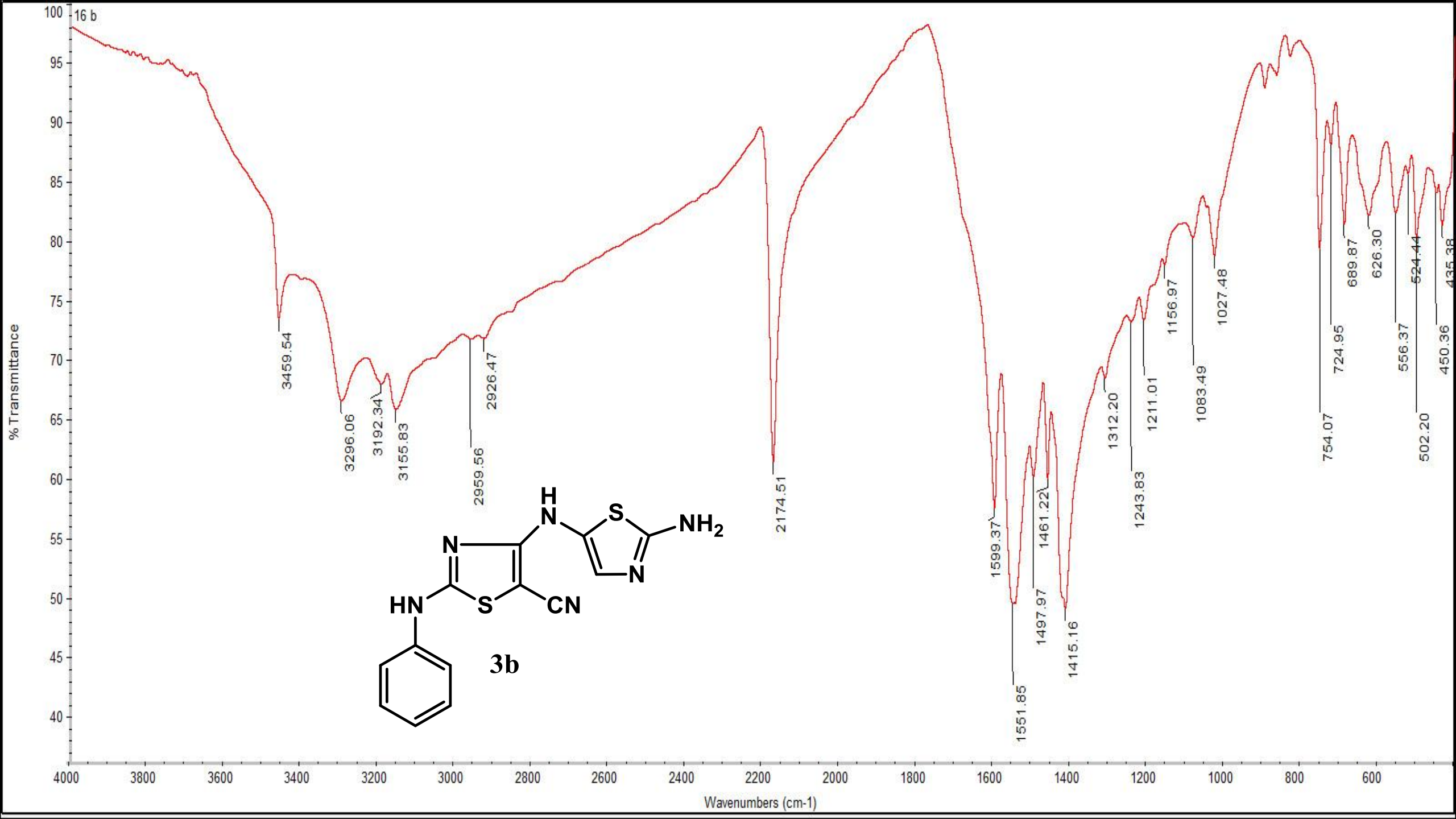
Alaa Abdullah - 2 - C13 - T

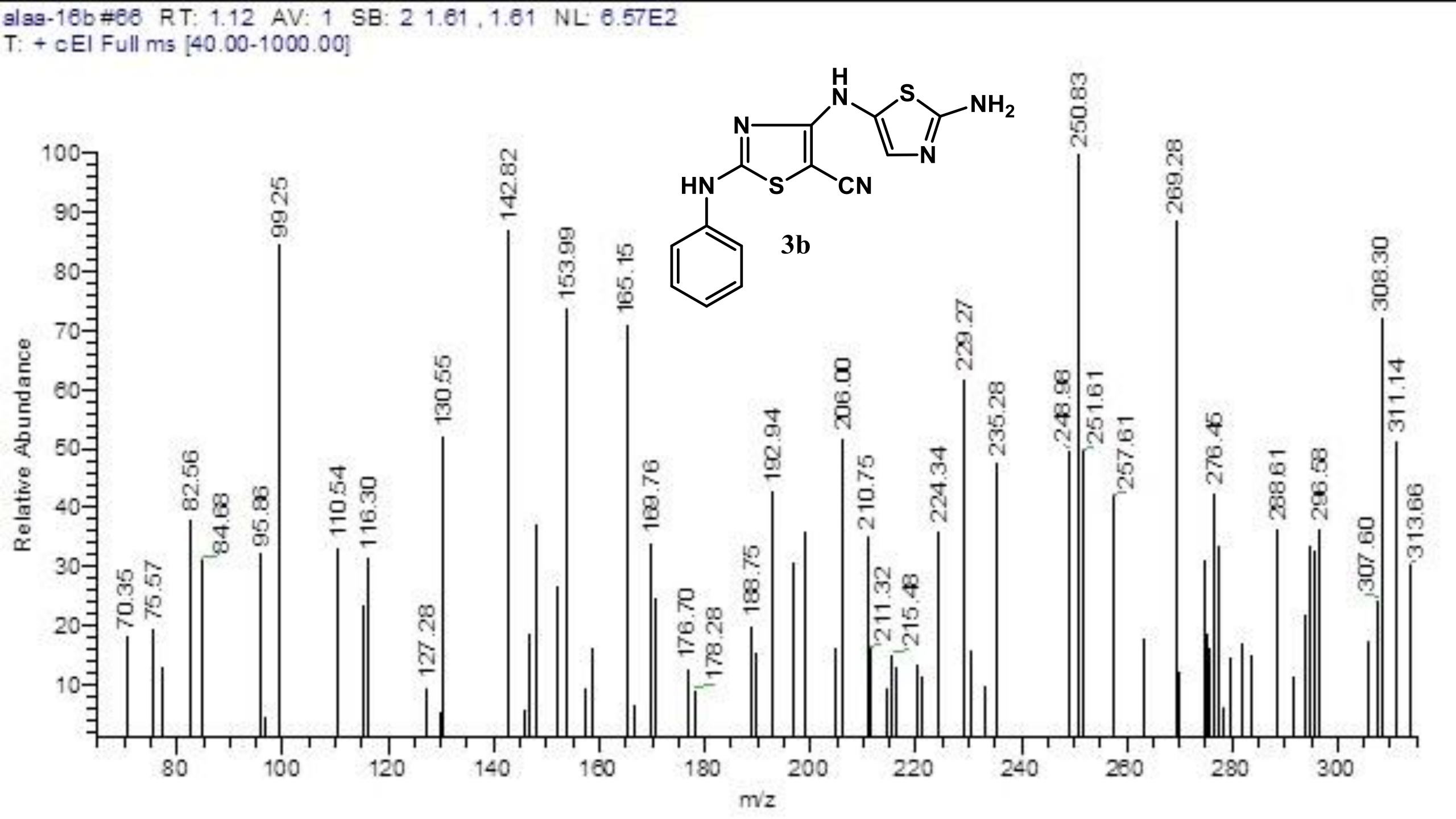


3a

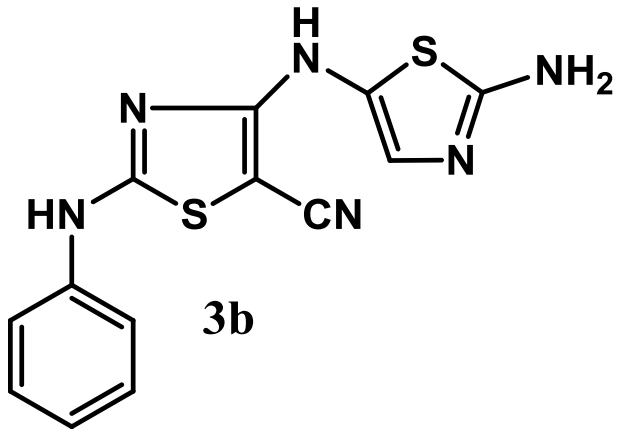
Faculty of Pharmacy

```
Current Data Parameters
NAME      Alaa Abdullah - 2 - C13 - T
EXPNO                 10
PROCNO                 1

P2 - Acquisition Parameters
Date_           20220517
Time                6.58 h
INSTRUM            spect
PROBHD   Z108618_0945 (
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 2100
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                197.77
DW                20.800 usec
DE                 6.50 usec
TE                296.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1
SFO1          100.6404331 MHz
NUC1                13C
P1                 10.00 usec
PLW1          47.00000000 W
SFO2          400.2016008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2          13.00000000 W
PLW12          0.29249999 W
PLW13          0.14713000 W

P2 - Processing parameters
SI                 32768
SF            100.6303700 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


16 b
% Transmittance
Wavenumbers (cm-1)
3459.54
3296.06
3192.34
3155.83
2959.56
2926.47
2174.51
1599.37
1551.85
1497.97
1461.22
1415.16
1312.20
1243.83
1211.01
1156.97
1083.49
1027.48
754.07
724.95
689.87
626.30
556.37
524.44
502.20
450.36
435.38
H
N
S
NH2
N
N
HN
S
CN
3b


alaa-16b #66 RT: 1.12 AV: 1 SB: 2 1.61 , 1.61 NL: 6.57E2
T: + cEI Full ms [40.00-1000.00]
Relative Abundance
m/z
3b
70.35
75.57
82.56
84.68
95.86
99.25
110.54
116.30
127.28
130.55
142.82
153.99
165.15
169.76
176.70
178.28
188.75
192.94
206.00
210.75
211.32
215.48
224.34
229.27
235.28
248.98
250.83
251.61
257.61
269.28
276.45
288.61
296.58
307.60
308.30
311.14
313.66

Alaa Abdullah-2-HNMR-DMSO-AF



3b

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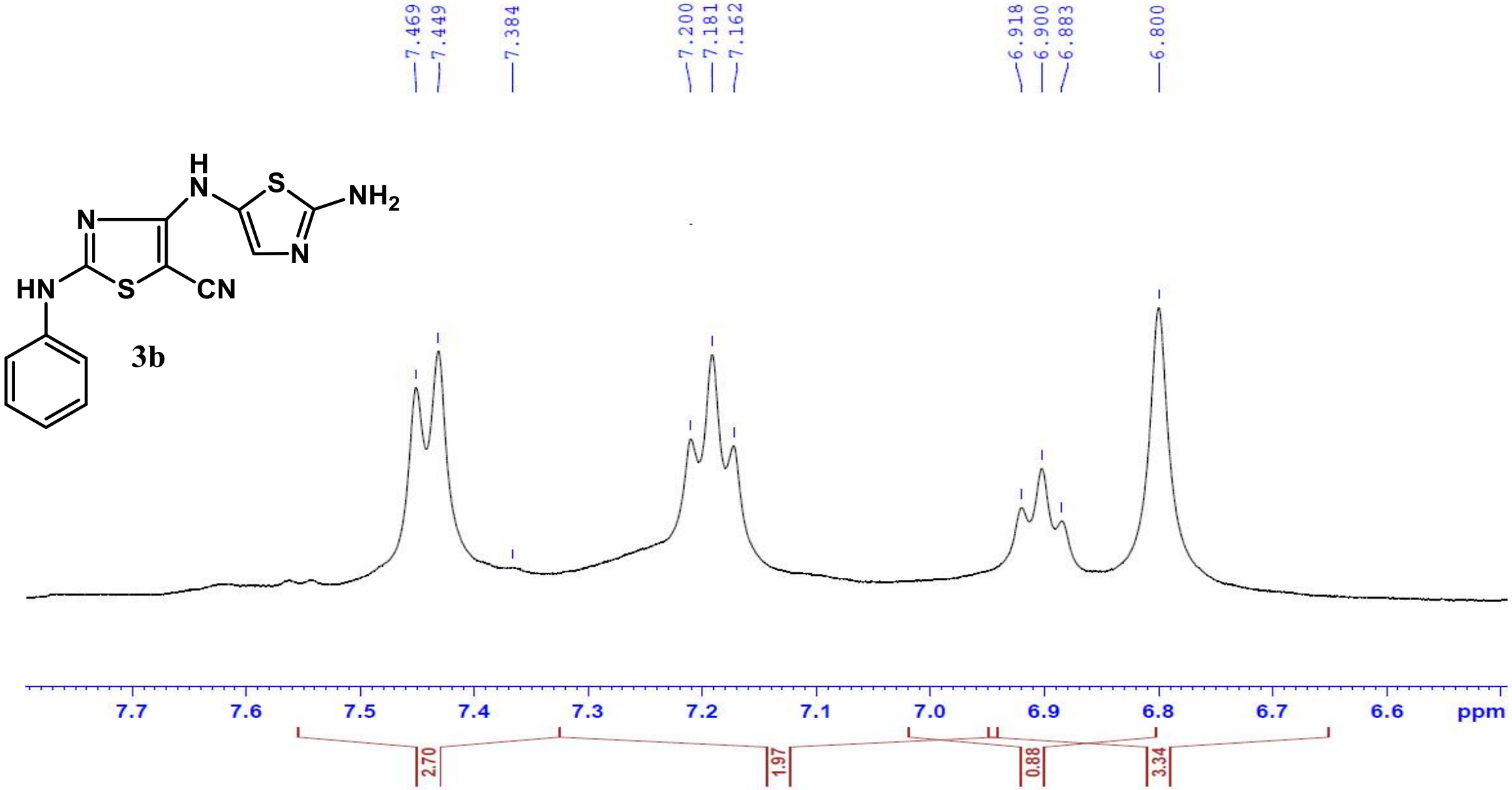
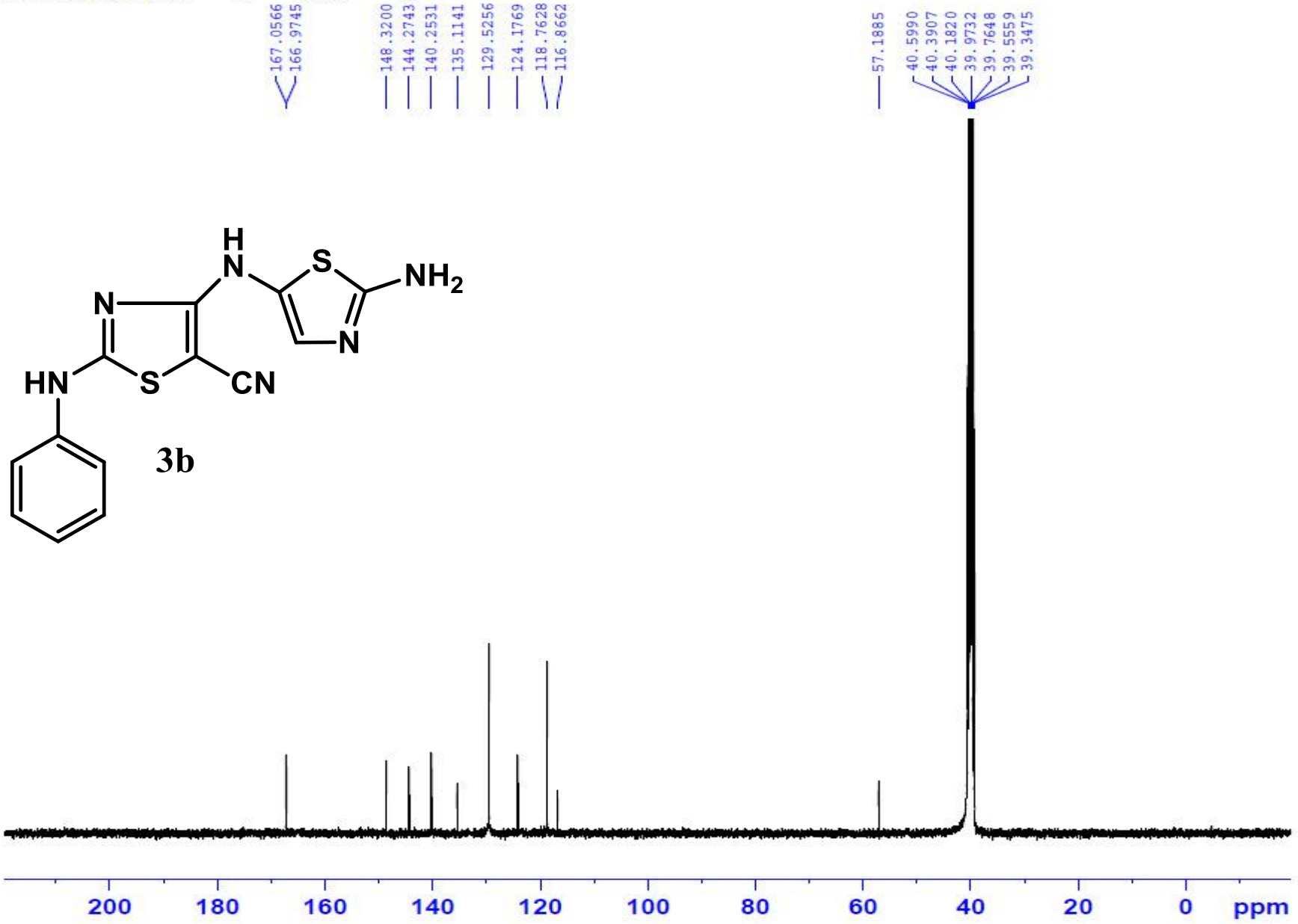
```
Current Data Parameters
NAME      Alaa Abdullah-2-HNMR-
EXPNO                       10
PROCNO                       1

F2 - Acquisition Parameters
Date_              20220510
Time                 14.44 h
INSTRUM              spect
PROBHD    Z108618_0945 (
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH               8012.820 Hz
FIDRES            0.244532 Hz
AQ                4.0894465 sec
RG                   158.72
DW                   62.400 usec
DE                    6.50 usec
TE                   295.3 K
D1             1.00000000 sec
TD0                     1
SFO1           400.2024712 MHz
NUC1                   1H
P1                   13.50 usec
PLW1           13.00000000 W

F2 - Processing parameters
SI                  65536
SF             400.2000000 MHz
WDW                    EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

Alaa Abdullah-2-HNMR-DMSO-AF

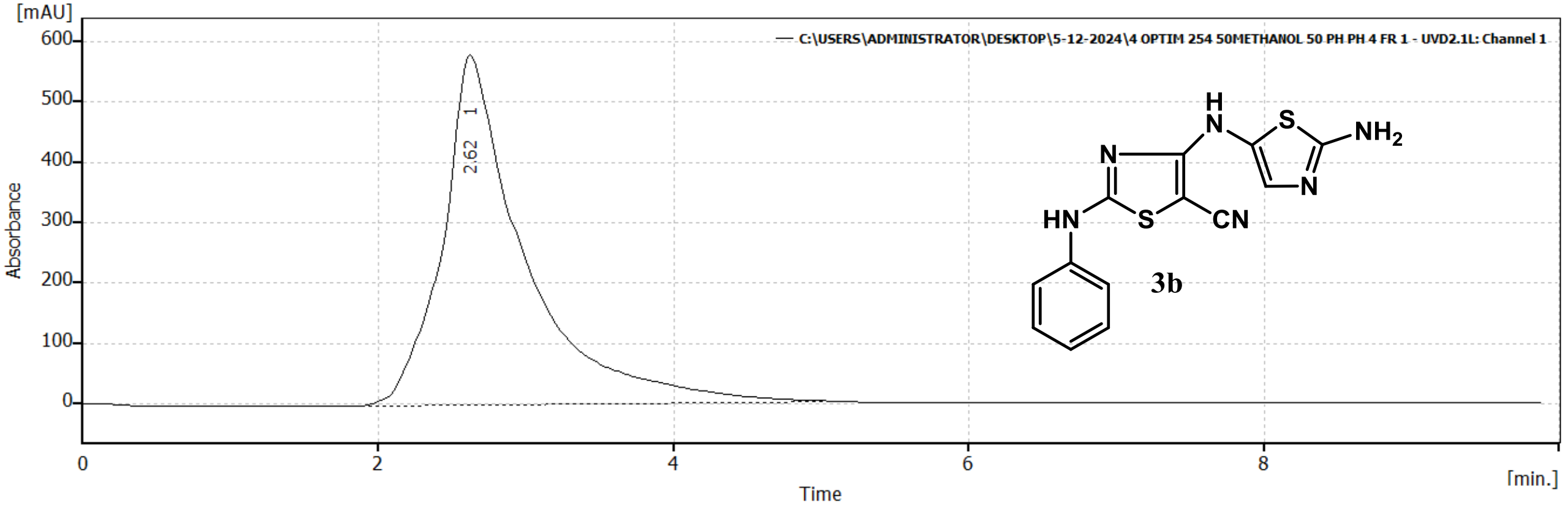


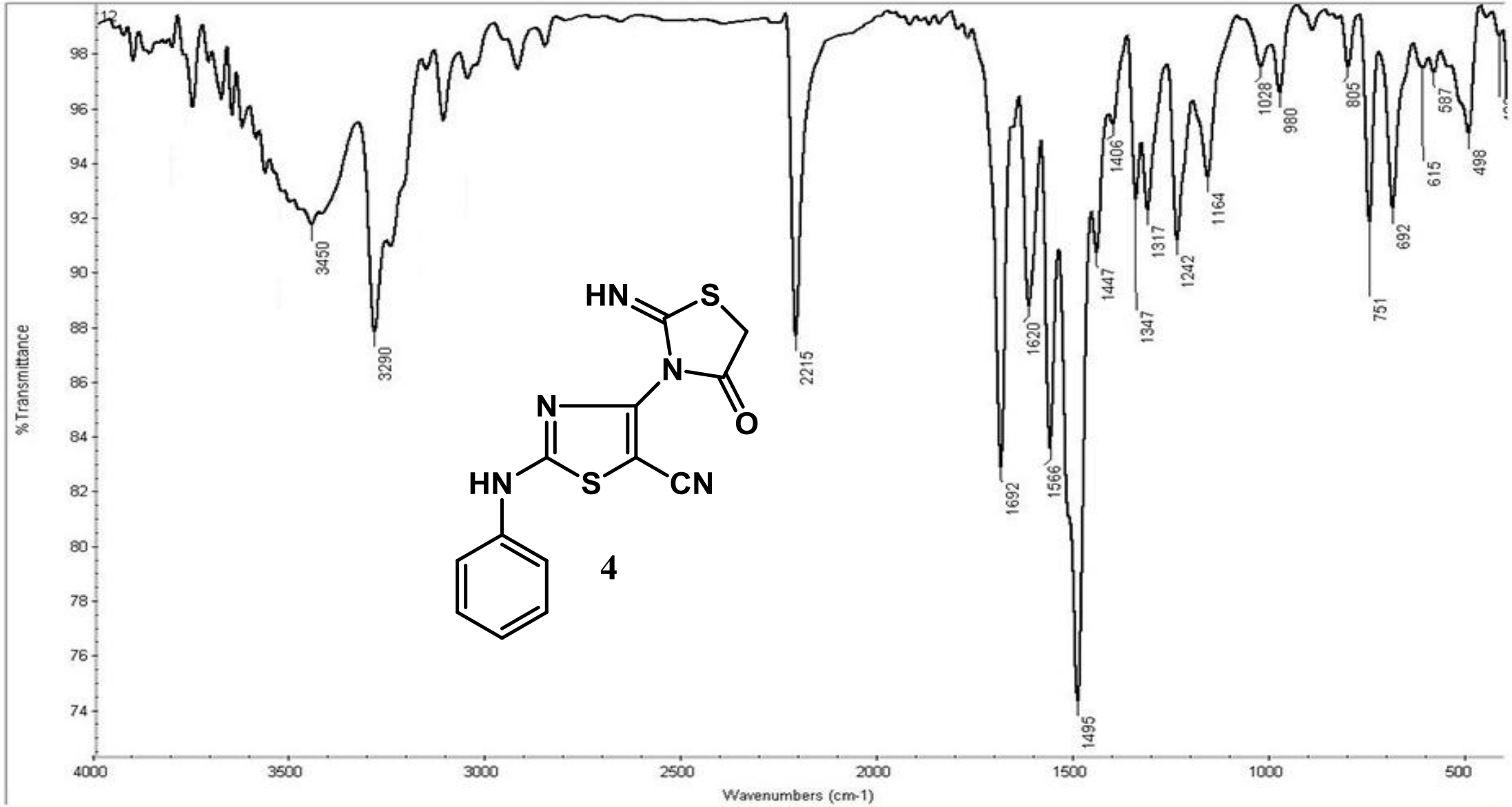
Alaa Abdullah - 2 - C13 - T



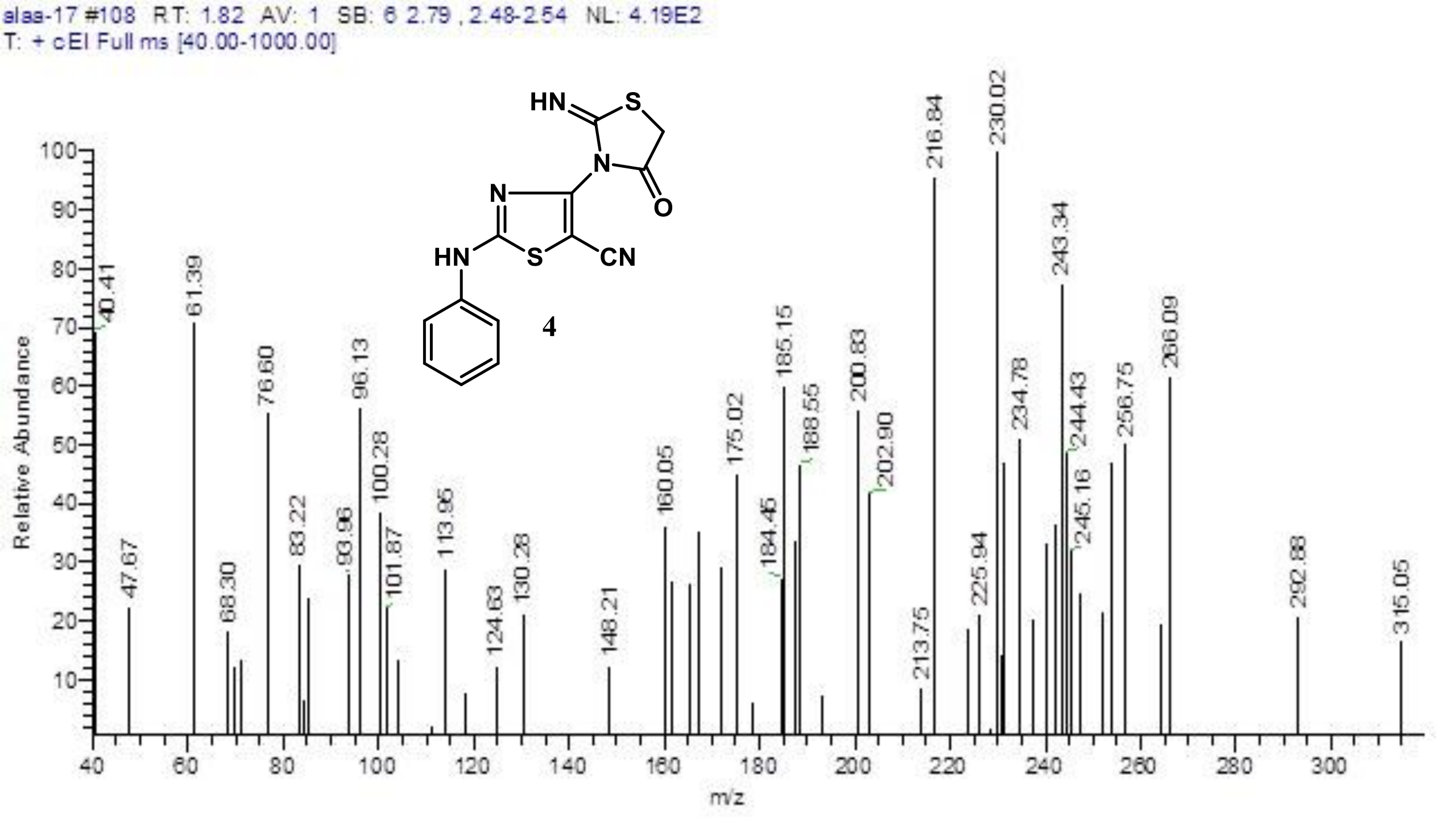
3b


```
Current Data Parameters
NAME      Alaa Abdullah - 2 - C13 - T
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220517
Time                6.58 h
INSTRUM            spect
PROBHD   Z108618_0945 (
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                  2100
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                 197.77
DW                 20.800 usec
DE                  6.50 usec
TE                296.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6404331 MHz
NUC1                 13C
P1                 10.00 usec
PLW1          47.00000000 W
SFO2          400.2016008 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          13.00000000 W
PLW12          0.29249999 W
PLW13          0.14713000 W

F2 - Processing parameters
SI                 32768
SF            100.6303700 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

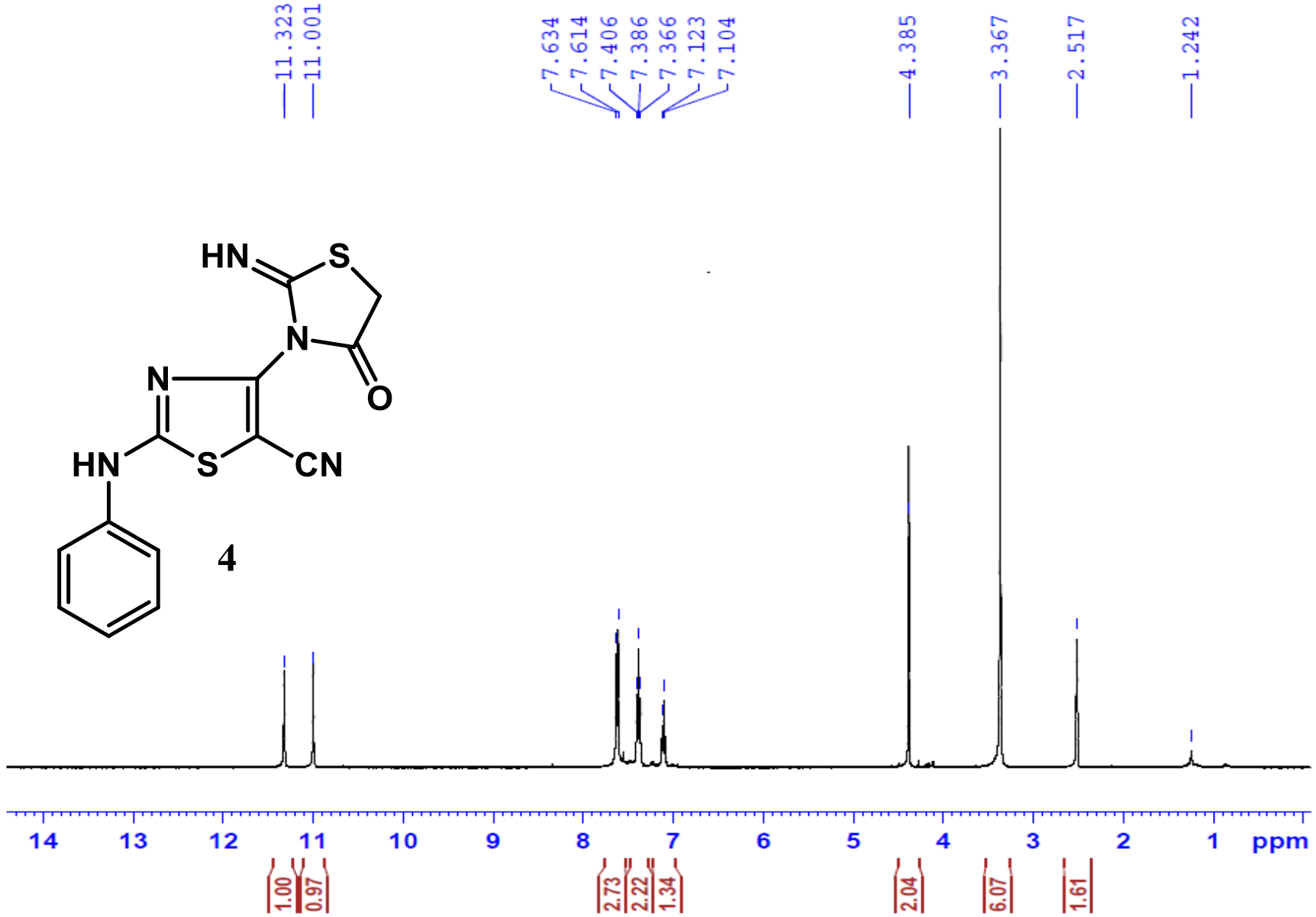

[mAU]
600
500
400
300
200
100
0
Absorbance
C:\USERS\ADMINISTRATOR\DESKTOP\5-12-2024\4 OPTIM 254 50METHANOL 50 PH PH 4 FR 1 - UVD2.1L: Channel 1
2.62
1
0
2
4
6
8
Time
[min.]
H
N
S
NH2
N
N
HN
S
CN
3b


% 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
3450
3290
2215
1692
1620
1566
1495
1447
1406
1347
1317
1242
1164
1028
980
805
751
692
615
587
498
HN
S
N
O
N
HN
S
CN

4


alaa-17 #108 RT: 1.82 AV: 1 SB: 6 2.79 , 2.48-2.54 NL: 4.19E2
T: + cEI Full ms [40.00-1000.00]
HN
S
N
N
O
HN
S
CN
4
Relative Abundance
m/z
40.41
47.67
61.39
68.30
76.60
83.22
93.96
96.13
100.28
101.87
113.95
124.63
130.28
148.21
160.05
175.02
184.45
185.15
188.55
200.83
202.90
213.75
216.84
225.94
230.02
234.78
243.34
244.43
245.16
256.75
266.09
292.88
315.05

Alaa Abdullah-12-HNMR-DMSO-AF



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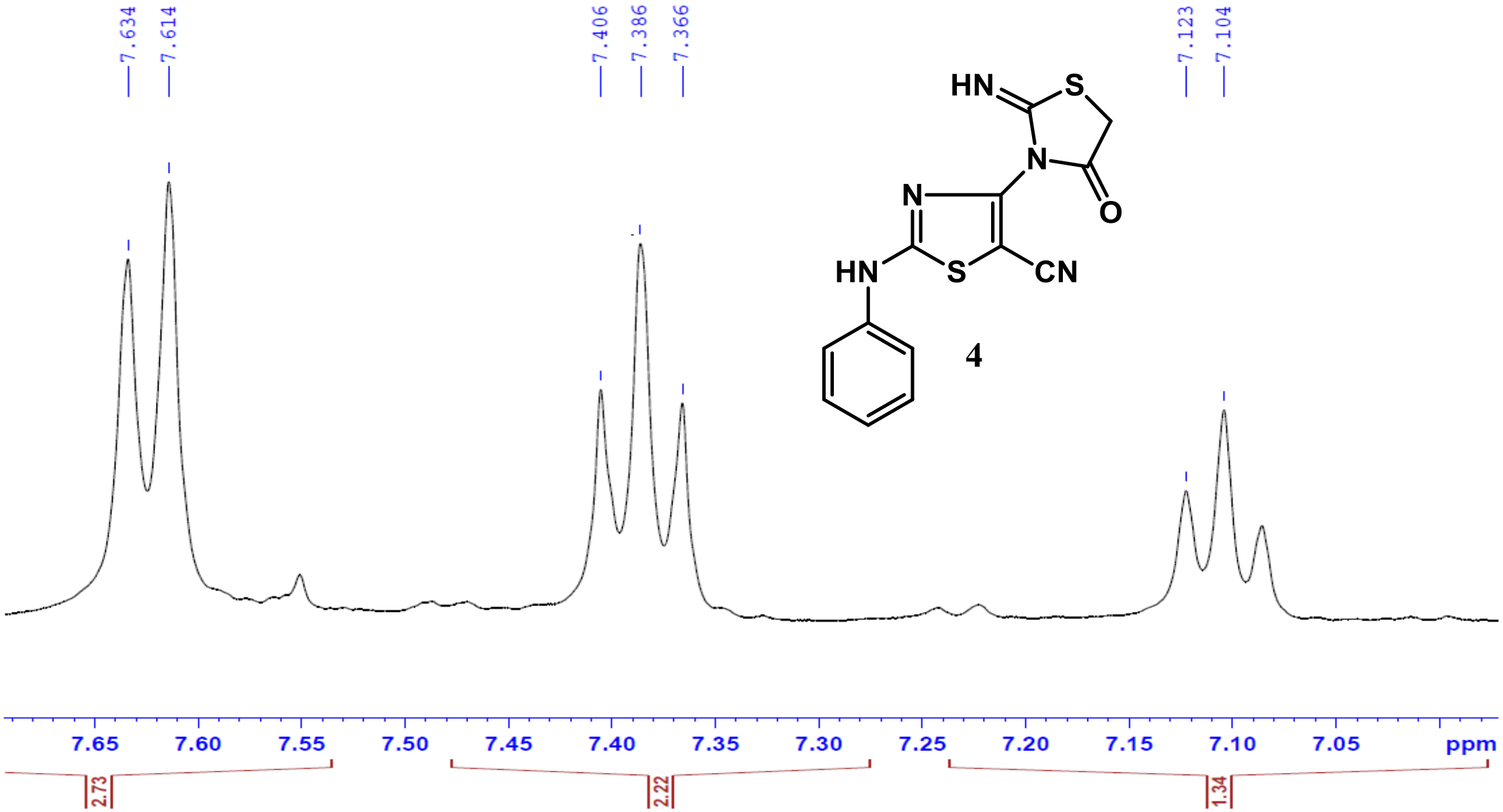
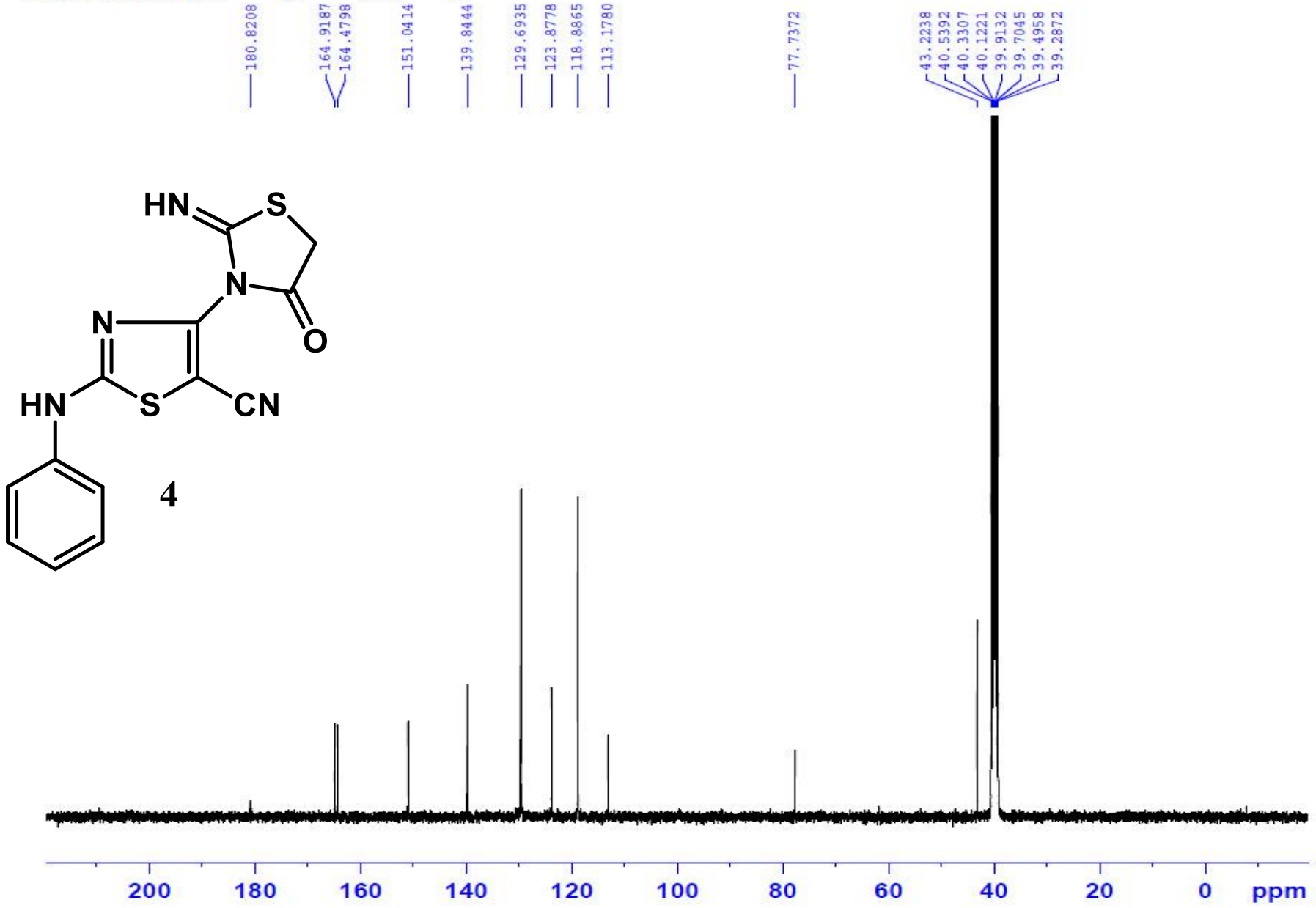
```
Current Data Parameters
NAME      Alaa Abdullah-12-HNMR
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_              20220510
Time                15.42 h
INSTRUM              spect
PROBHD    Z108618_0945 (
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH               8012.820 Hz
FIDRES            0.244532 Hz
AQ                4.0894465 sec
RG                   176.72
DW                   62.400 usec
DE                    6.50 usec
TE                   295.3 K
D1                1.00000000 sec
TD0                       1
SFO1           400.2024712 MHz
NUC1                     1H
P1                   13.50 usec
PLW1           13.00000000 W

F2 - Processing parameters
SI                    65536
SF             400.2000000 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

Alaa Abdullah-12-HNMR-DMSO-AF



Alaa Abdullah - 12 - C13 - T



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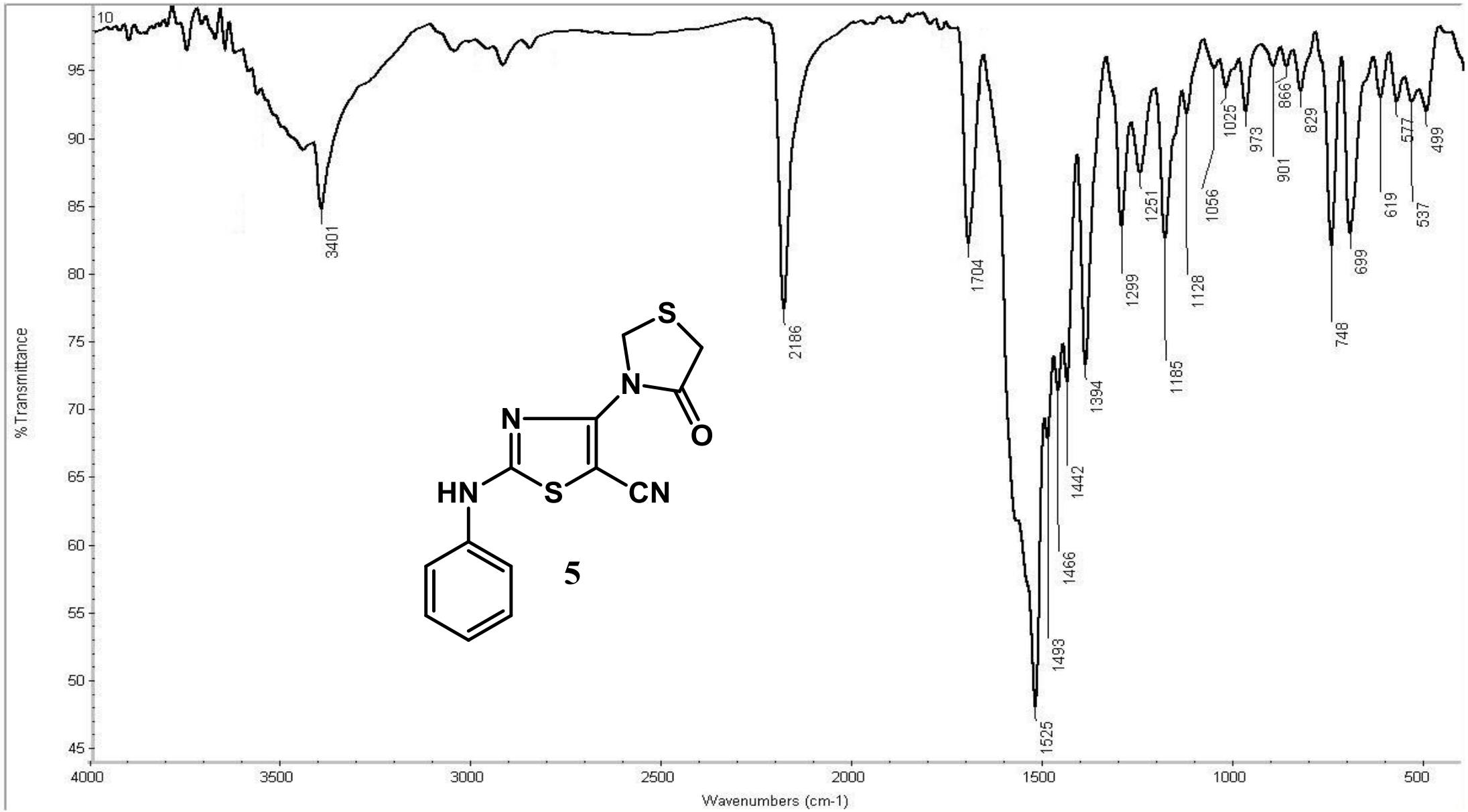
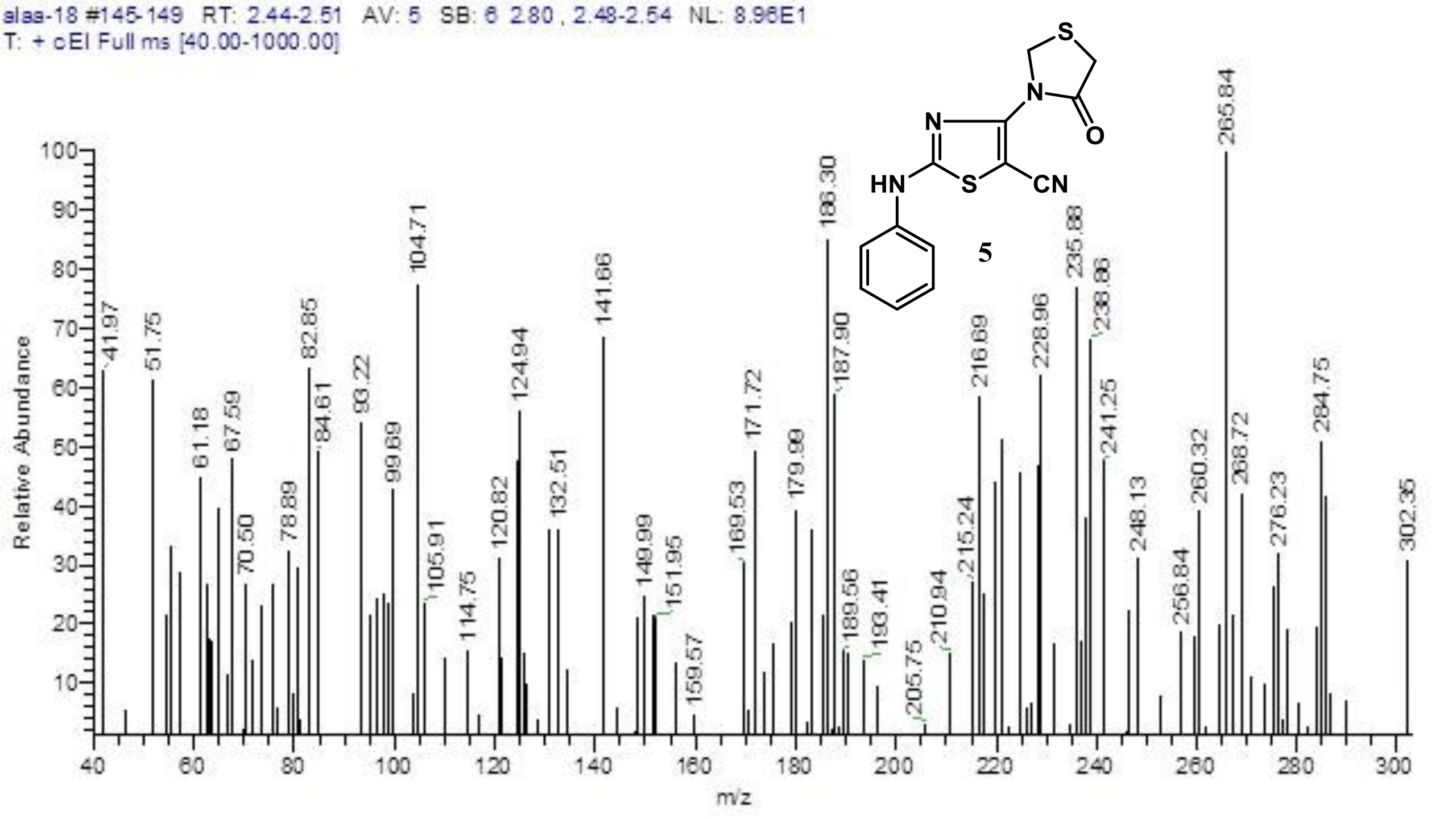
Current Data Parameters
NAME Alaa Abdullah - 12 - C13 - T
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220516
Time 18.36 h
INSTRUM spect
PROBHD Z108618_0945 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2100
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 197.77
DW 20.800 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6404331 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W
SFO2 400.2016008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.29249999 W
PLW13 0.14713000 W

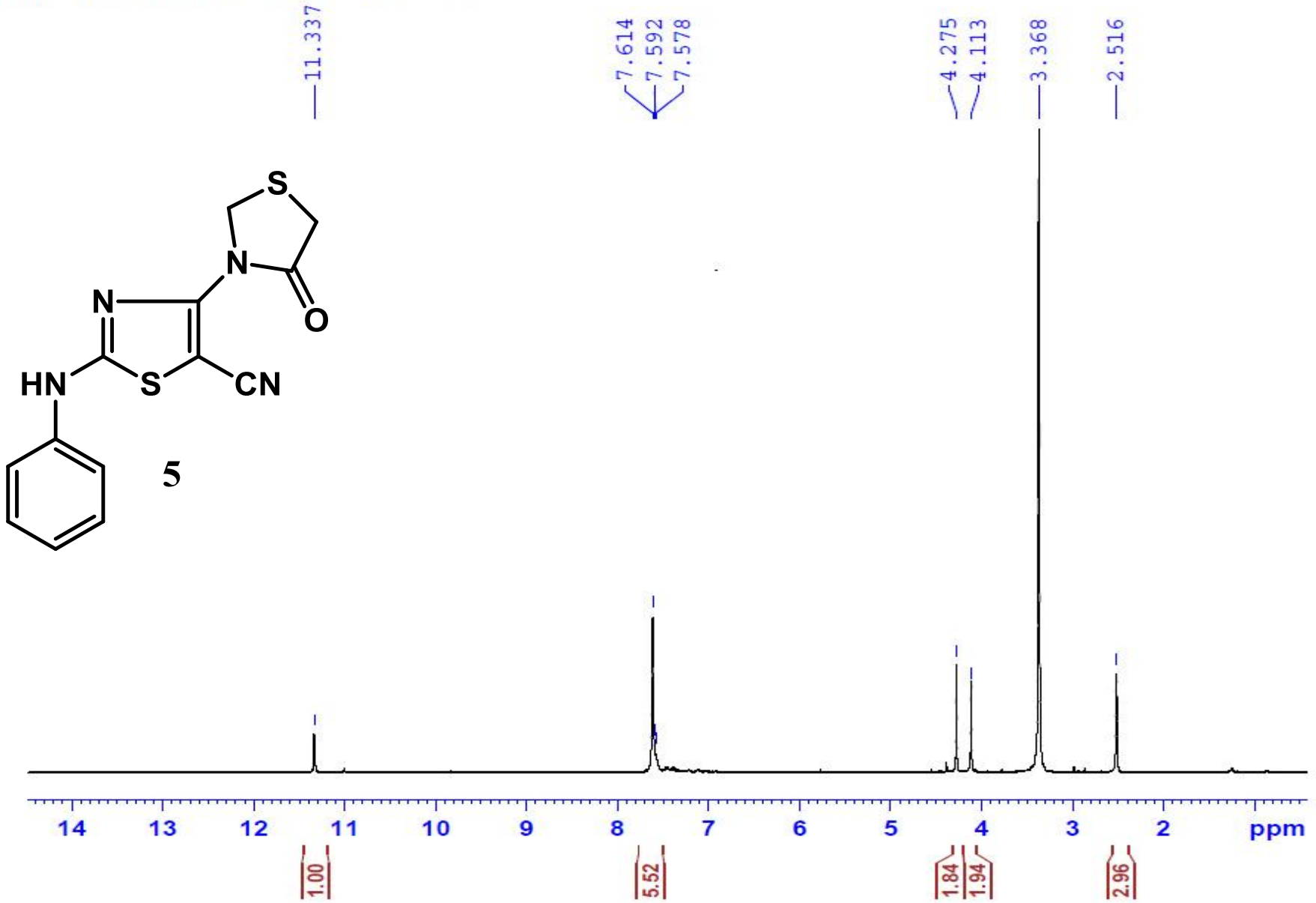
F2 - Processing parameters
SI 32768
SF 100.6303700 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


10
% Transmittance
Wavenumbers (cm-1)
4000
3500
3000
2500
2000
1500
1000
500
95
90
85
80
75
70
65
60
55
50
45
3401
2186
1704
1525
1493
1466
1442
1394
1299
1251
1185
1128
1056
1025
973
901
866
829
748
699
619
577
537
499
S
N
O
N
HN
S
CN

5


alaa-18 #145-149 RT: 2.44-2.51 AV: 5 SB: 6 2.80 , 2.48-2.54 NL: 8.96E1
T: + cEI Full ms [40.00-1000.00]
Relative Abundance
m/z
5
41.97
51.75
61.18
67.59
70.50
78.89
82.85
84.61
93.22
99.69
104.71
105.91
114.75
120.82
124.94
132.51
141.66
149.99
151.95
159.57
169.53
171.72
179.99
186.30
187.90
189.56
193.41
205.75
210.94
215.24
216.69
228.96
235.88
238.86
241.25
248.13
256.84
260.32
265.84
268.72
276.23
284.75
302.35

Alaa Abdullah-11-HNMR-DMSO-AF



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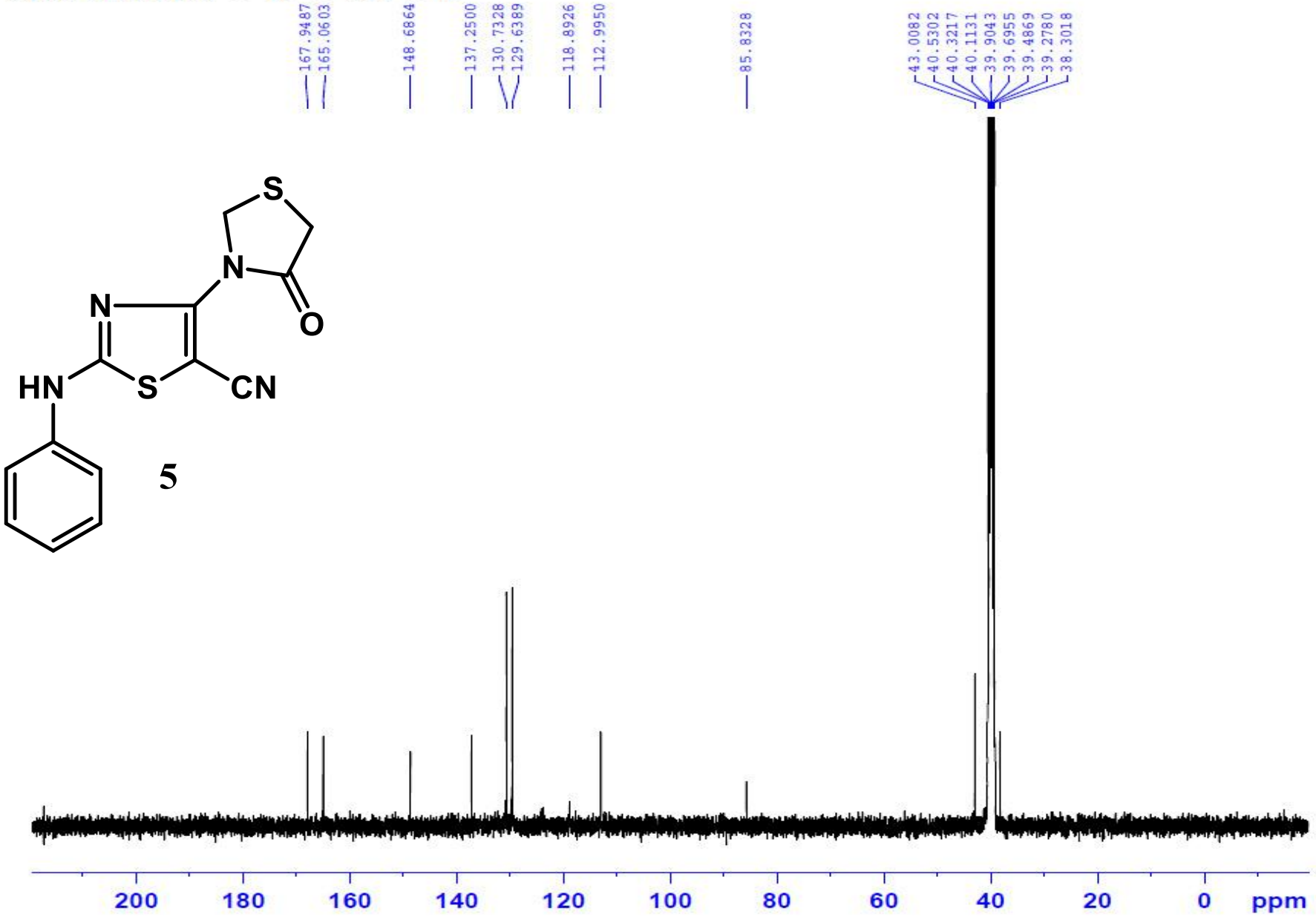
```
Current Data Parameters
NAME      Alaa Abdullah-11-HNMR
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220510
Time              15.37 h
INSTRUM           spect
PROBHD    Z108618_0945 (
PULPROG             zg30
TD                65536
SOLVENT            DMSO
NS                    16
DS                     2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                176.72
DW                62.400 usec
DE                 6.50 usec
TE                295.4 K
D1             1.00000000 sec
TD0                    1
SFO1         400.2024712 MHz
NUC1                  1H
P1                13.50 usec
PLW1          13.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2000000 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

Alaa Abdullah - 11 - C13 - T



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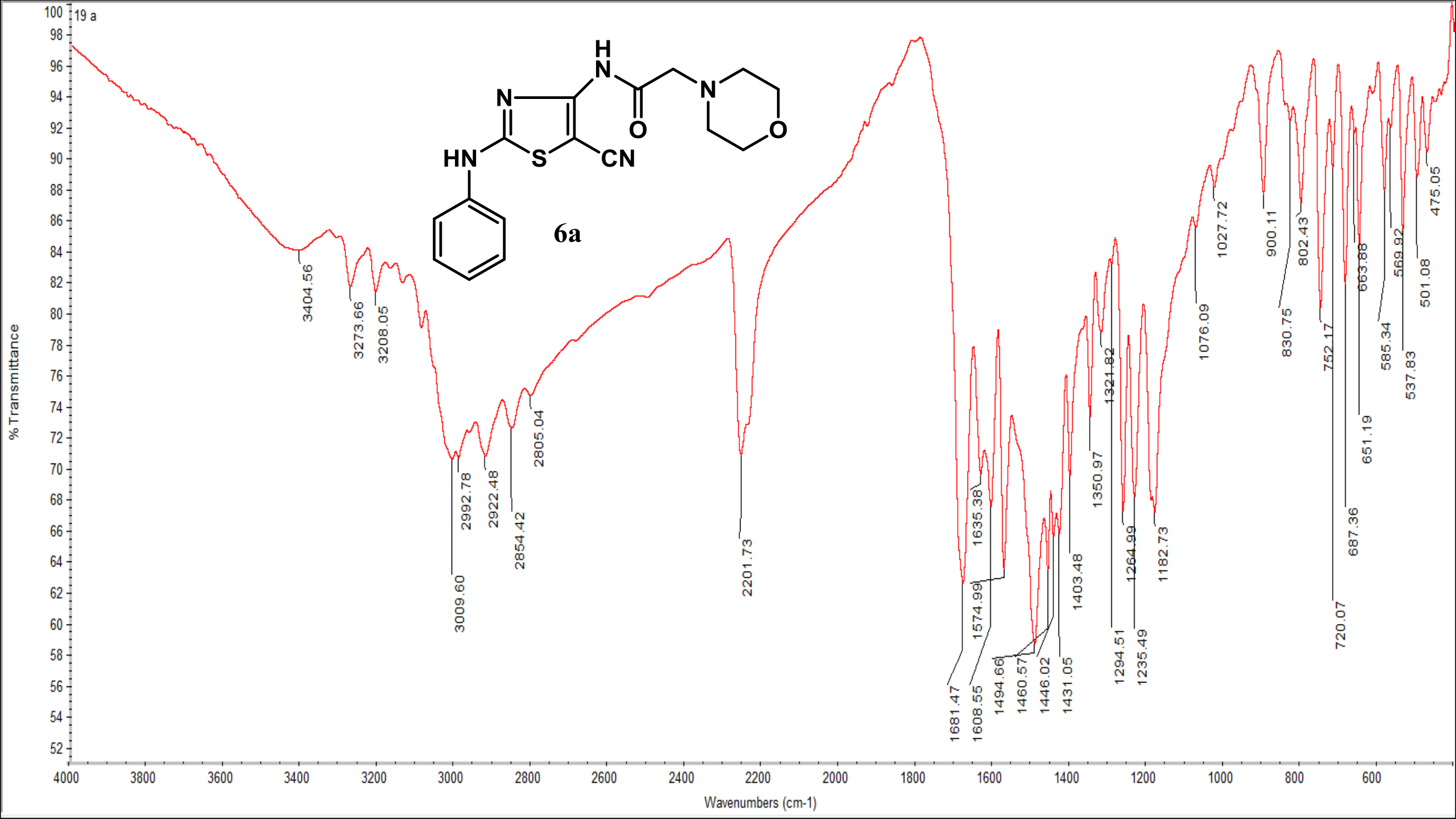
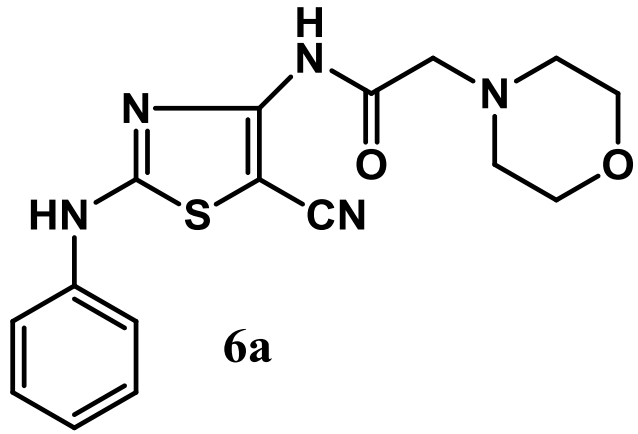
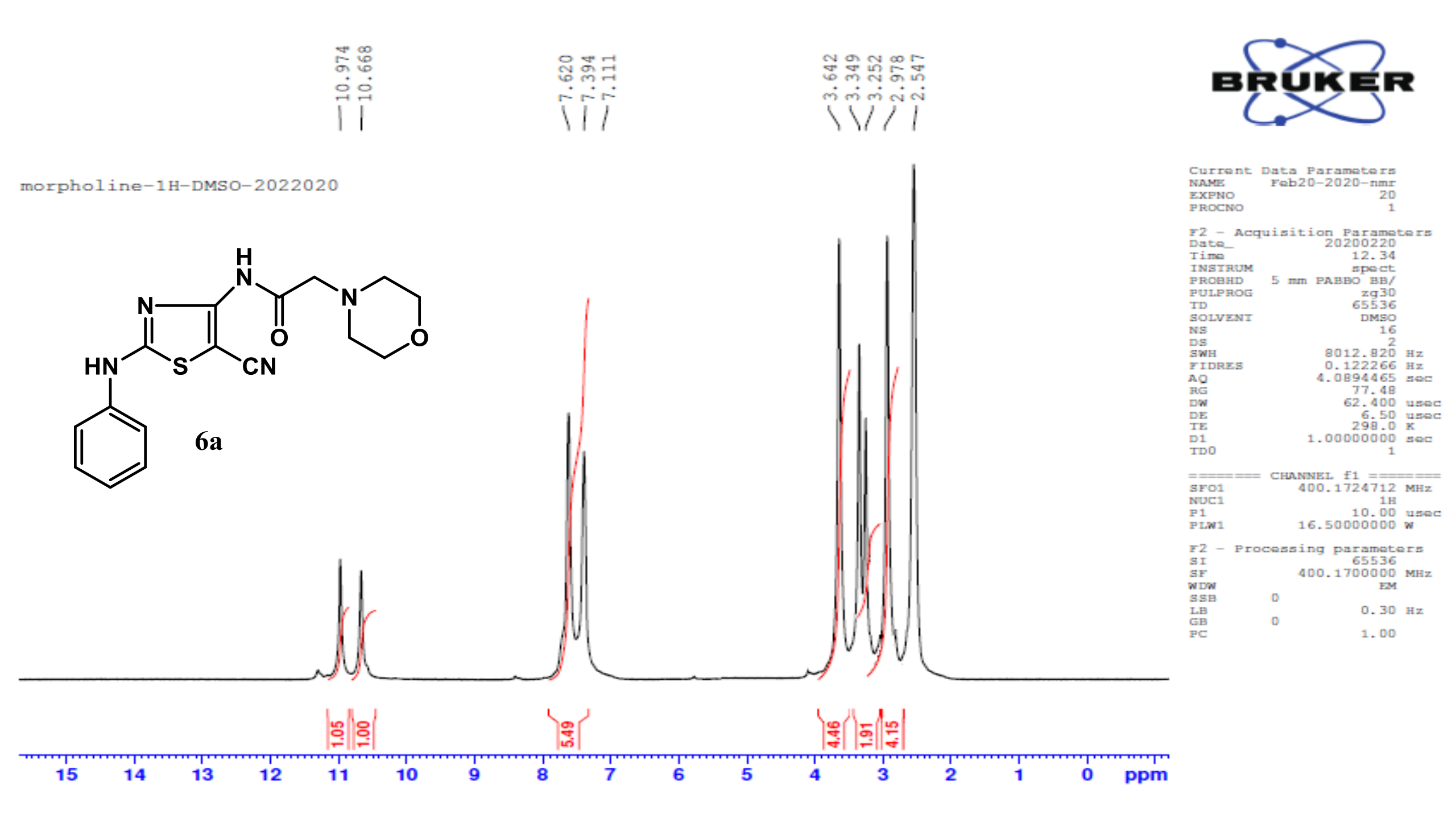
```
Current Data Parameters
NAME      Alaa Abdullah - 11 - C13 - T
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220516
Time              16.32 h
INSTRUM             spect
PROBHD     Z108618_0945 (
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                  2100
DS                     4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                197.77
DW                20.800 usec
DE                 6.50 usec
TE                296.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6404331 MHz
NUC1                 13C
P1                10.00 usec
PLW1          47.00000000 W
SFO2          400.2016008 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          13.00000000 W
PLW12          0.29249999 W
PLW13          0.14713000 W

F2 - Processing parameters
SI                 32768
SF            100.6303700 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


19 a
% Transmittance
Wavenumbers (cm-1)
3404.56
3273.66
3208.05
3009.60
2992.78
2922.48
2854.42
2805.04
2201.73
1681.47
1608.55
1574.99
1635.38
1494.66
1460.57
1446.02
1431.05
1403.48
1350.97
1321.82
1294.51
1264.99
1235.49
1182.73
1076.09
1027.72
900.11
830.75
802.43
752.17
720.07
687.36
663.88
651.19
585.34
569.92
537.83
501.08
475.05
6a

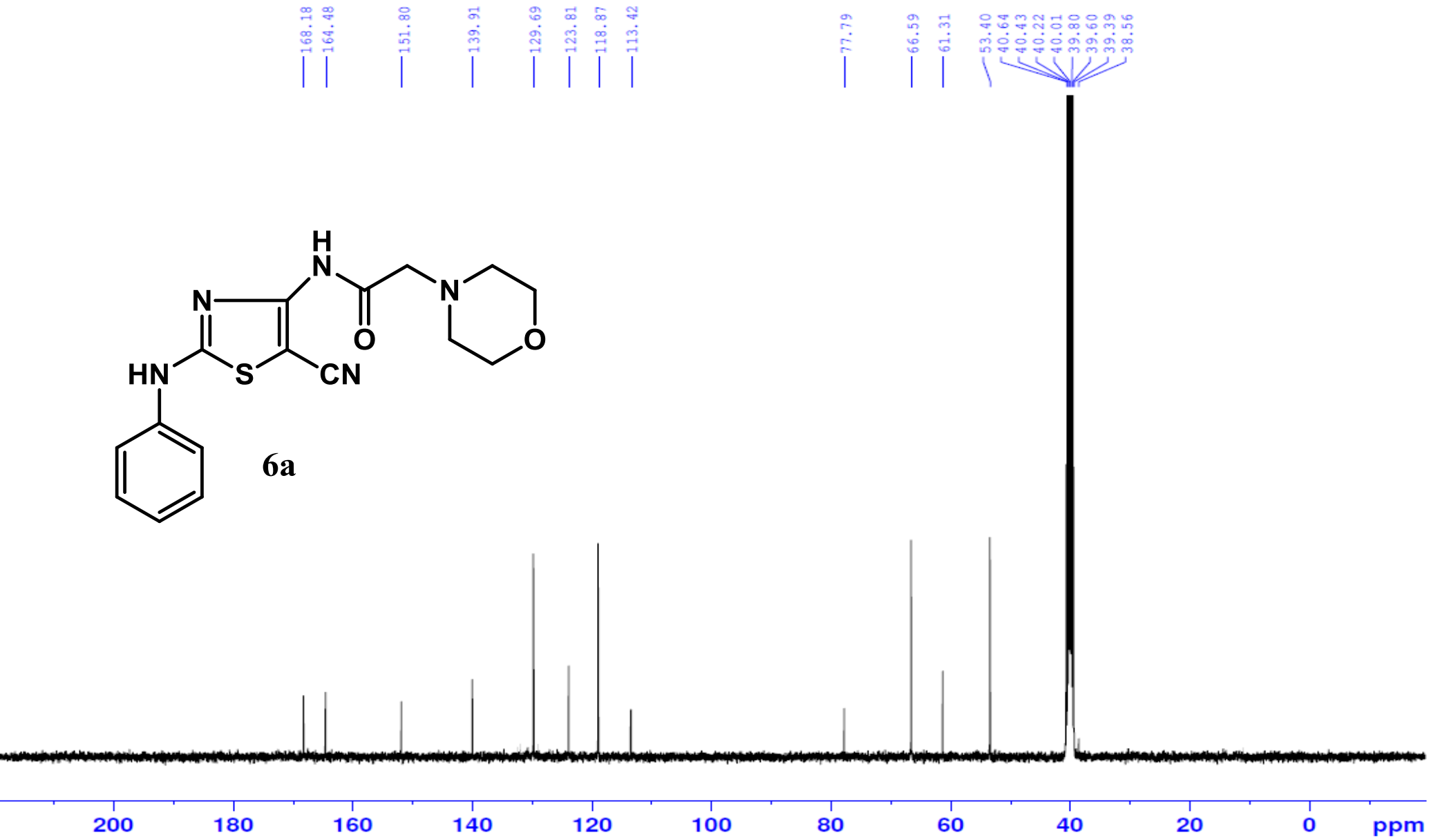
alaa-19a #239-242 RT: 4.02-4.07 AV: 4 SB: 2 2.71 , 2.71 NL: 1.11E2
T: + cEI Full ms [40.00-1000.00]



6a

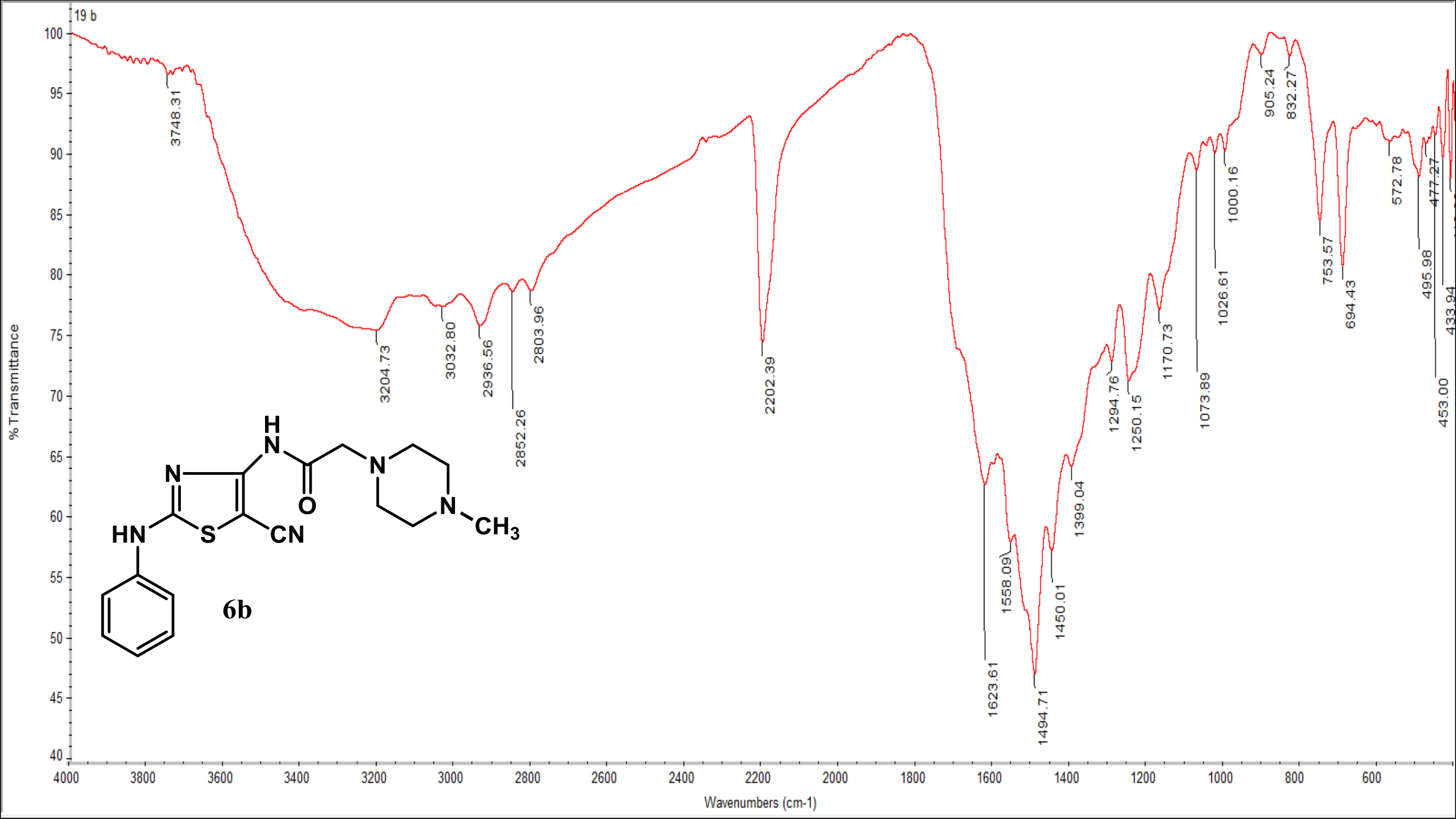

10.974
10.668
7.620
7.394
7.111
3.642
3.349
3.252
2.978
2.547
morpholine-1H-DMSO-2022020
HN
N
S
CN
N
O
O
HN
6a
1.05
1.00
5.49
4.46
1.91
4.15
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
BRUKER
Current Data Parameters
NAME Feb20-2020-nmr
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200220
Time 12.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 77.48
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1724712 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.50000000 W
F2 - Processing parameters
SI 65536
SF 400.1700000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

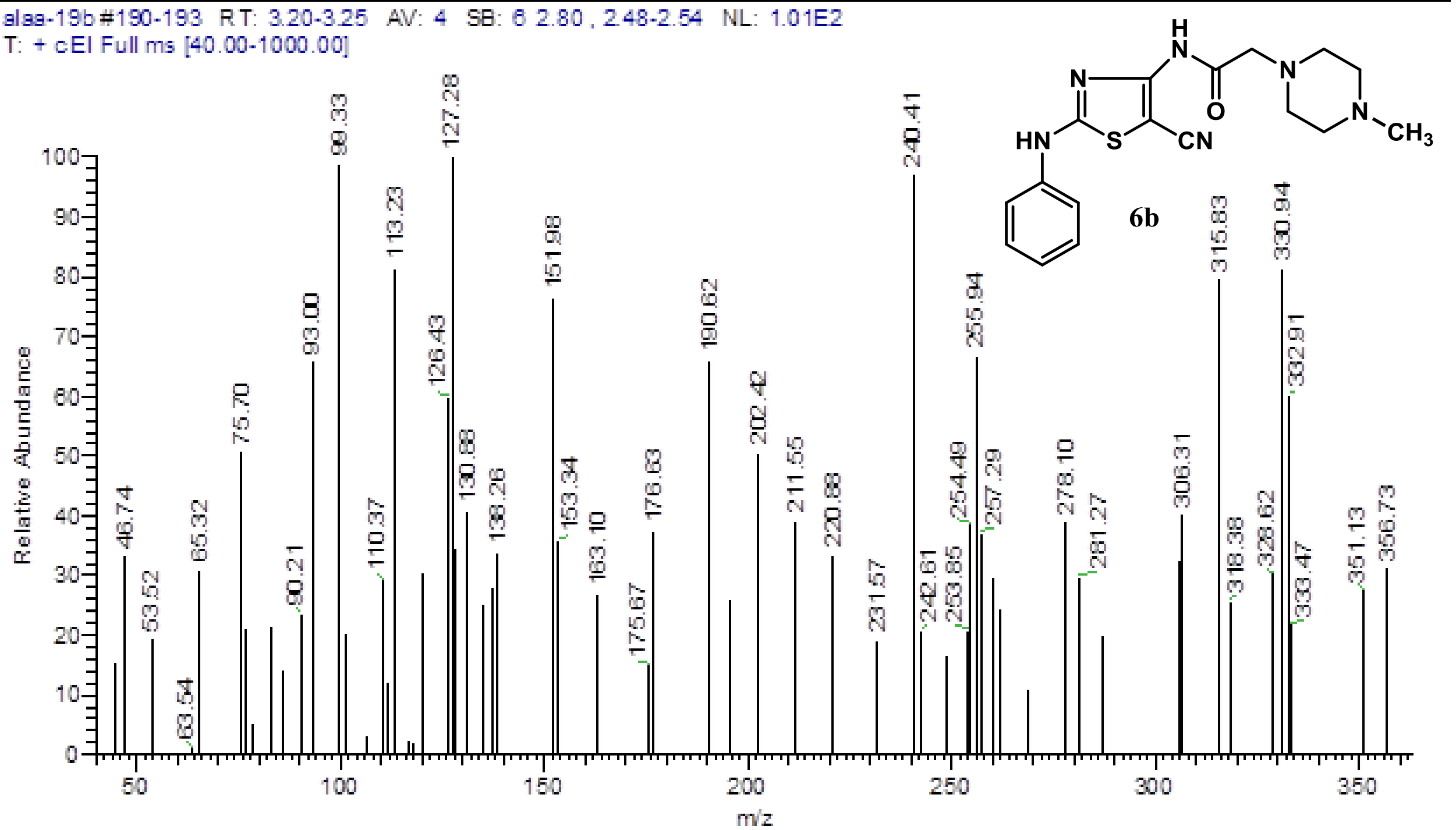
MORPHOLINE-13C-DMSO-132020



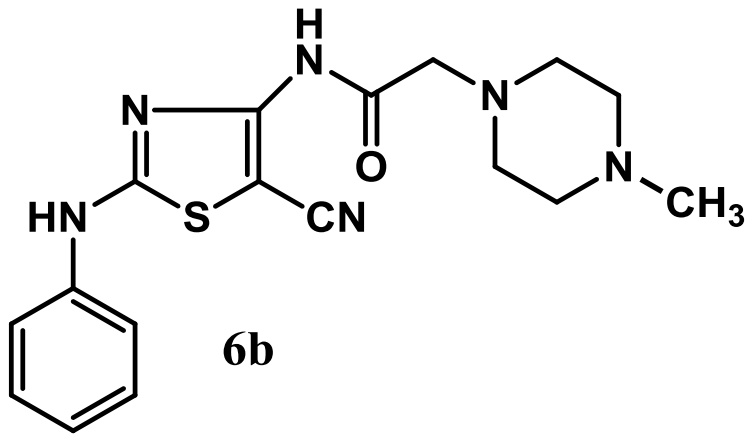
6a

```
Current Data Parameters
NAME      Mar01-2020-nmr
EXPNO                20
PROCNO                1

F2 - Acquisition Parameters
Date_          20200301
Time              13.36
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT             DMSO
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                194.81
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6328883 MHz
NUC1                13C
P1                10.00 usec
PLW1       66.00000000 W

======== CHANNEL f2 ========
SFO2        400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2       16.50000000 W
PLW12       0.20370001 W
PLW13       0.16500001 W

F2 - Processing parameters
SI                32768
SF          100.6228270 MHz
WDW                EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


19 b
% Transmittance
Wavenumbers (cm-1)
3748.31
3204.73
3032.80
2936.56
2852.26
2803.96
2202.39
1623.61
1558.09
1494.71
1450.01
1399.04
1294.76
1250.15
1170.73
1073.89
1026.61
1000.16
905.24
832.27
753.57
694.43
572.78
495.98
477.27
453.00
433.94
HN
N
S
CN
O
N
N
CH3
6b


alaa-19b #190-193 RT: 3.20-3.25 AV: 4 SB: 6 2.80 , 2.48-2.54 NL: 1.01E2
T: + cEI Full ms [40.00-1000.00]
Relative Abundance
m/z
6b
46.74
53.52
63.54
65.32
75.70
90.21
93.00
99.33
110.37
113.23
126.43
127.28
130.88
138.26
151.98
153.34
163.10
175.67
176.63
190.62
202.42
211.55
220.88
231.57
240.41
242.61
253.85
254.49
255.94
257.29
278.10
281.27
306.31
315.83
318.38
326.62
330.94
332.91
333.47
351.13
356.73

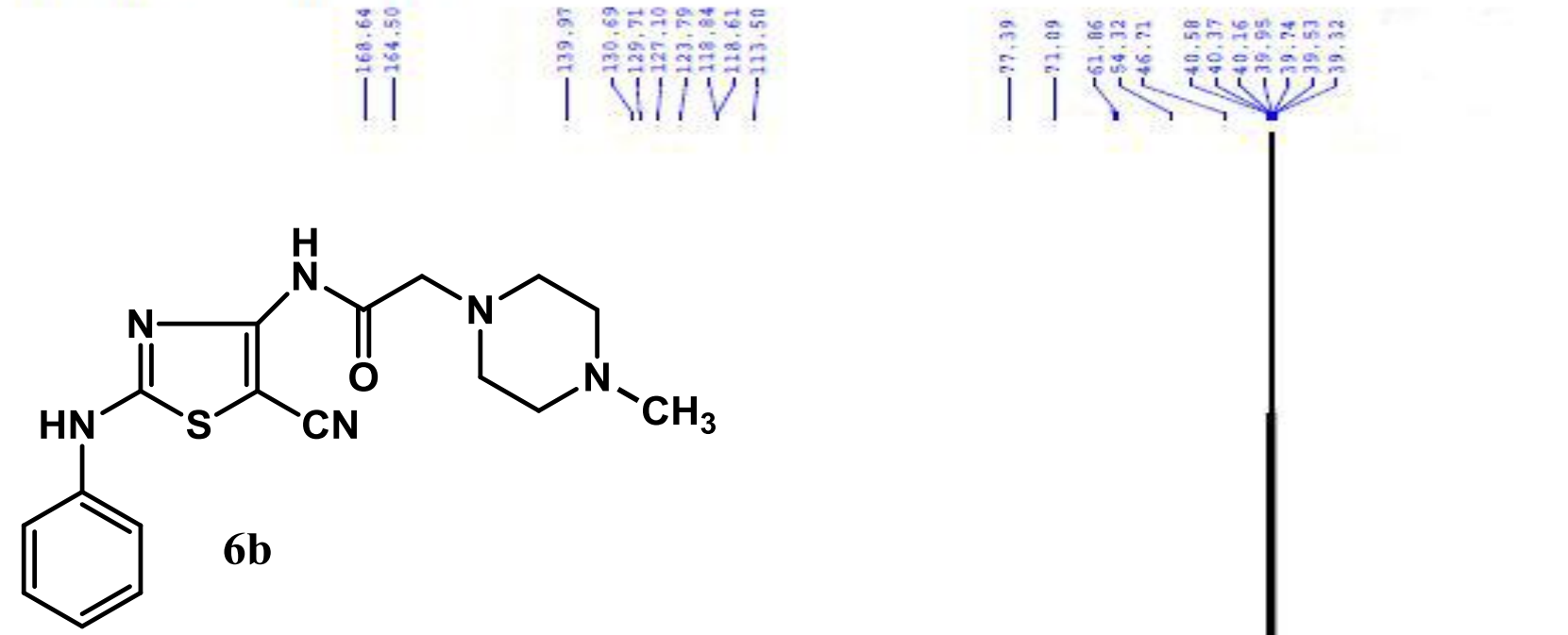
Alaa abdallah-2A-Hnmr-Es



6b

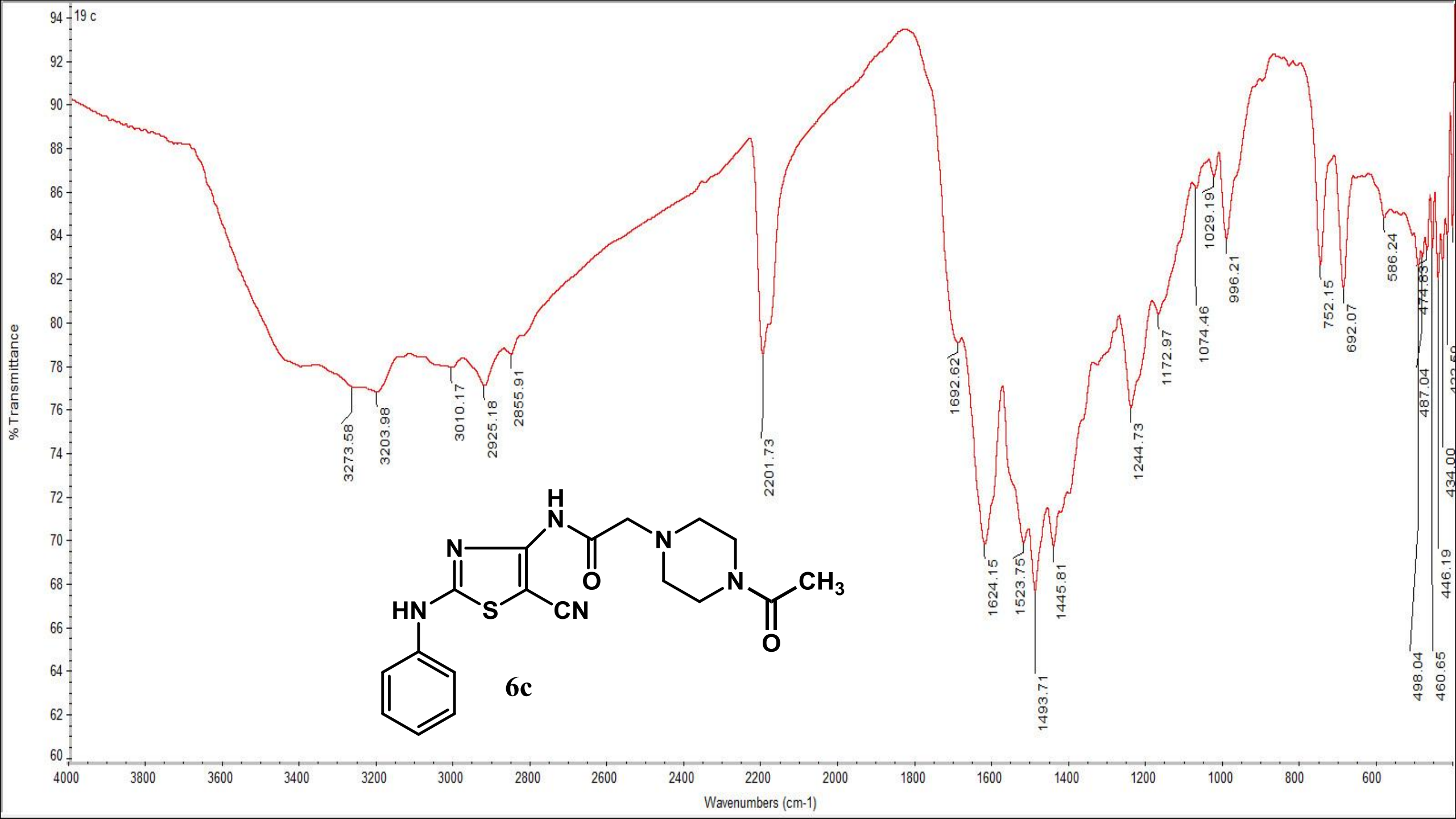

```
Current Data Parameters
NAME      Alaa abdallah-2A-Hn
EXPNO                     10
PROCNO                     1

F2 - Acquisition Parameters
Date_               20210211
Time                  7.55 h
INSTRUM                spect
PROBHD    Z108618_0945 (
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH                8012.820 Hz
FIDRES             0.244532 Hz
AQ                 4.0894465 sec
RG                      99.3
DW                   62.400 usec
DE                    6.50 usec
TE                   293.0 K
D1                1.00000000 sec
TD0                        1
SFO1           400.2024712 MHz
NUC1                      1H
P1                    13.50 usec
PLW1          13.00000000 W

F2 - Processing parameters
SI                    65536
SF             400.2000000 MHz
WDW                       EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

alaa abdallah 6A -M c13

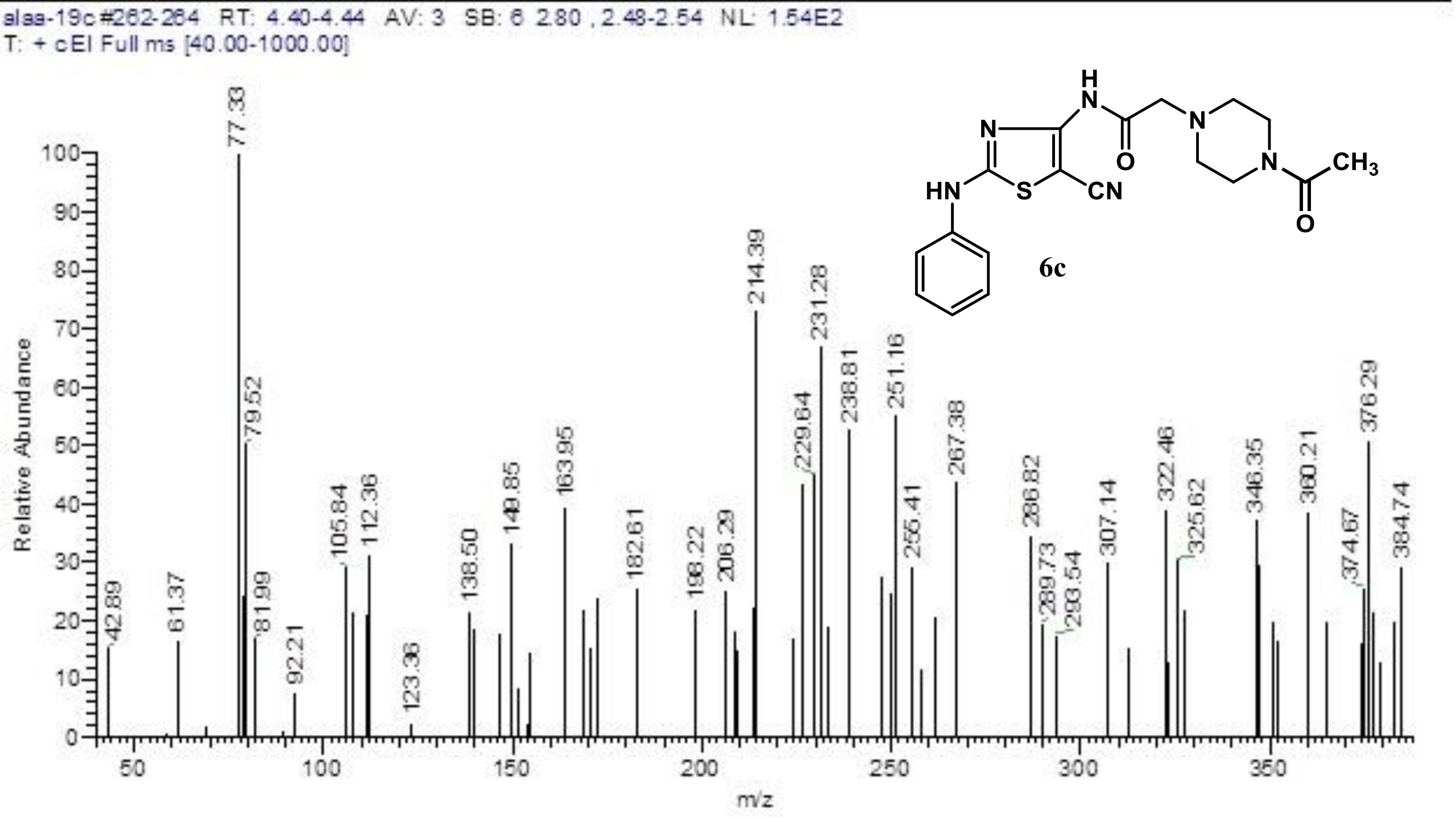


6b

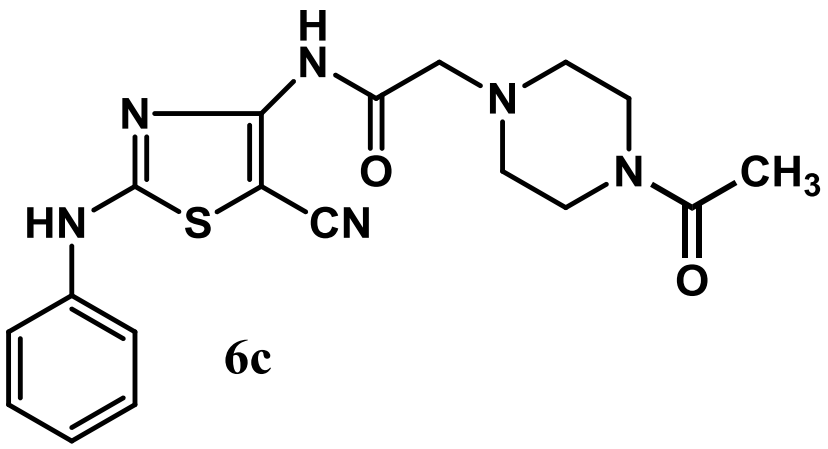

```
Current Data Parameters
NAME      alaa abdallah 6A -M c13
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Data_              20210302
Time                3.27 h
INSTRUM             spect
PROBHD    Z108618_0945 (
PULPROG            zgpg30
TD                 65536
SOLVENT              DMSO
NS                   2100
DS                      4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                 197.77
DW                 20.800 usec
DE                  6.50 usec
TE                 293.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         100.6404331 MHz
NUC1                 13C
P1                 10.00 usec
PLW1         47.00000000 W
SFO2         400.2016008 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         13.00000000 W
PLW12         0.29249999 W
PLW13         0.14713000 W

F2 - Processing parameters
SI                 32768
SF           100.6303700 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


19 c
% Transmittance
Wavenumbers (cm-1)
3273.58
3203.98
3010.17
2925.18
2855.91
2201.73
1692.62
1624.15
1523.75
1493.71
1445.81
1244.73
1172.97
1074.46
1029.19
996.21
752.15
692.07
586.24
498.04
487.04
474.83
460.65
446.19
434.00
HN
N
S
CN
O
N
N
CH3
O

6c


alaa-19c #262-264 RT: 4.40-4.44 AV: 3 SB: 6 2.80 , 2.48-2.54 NL: 1.54E2
T: + cEI Full ms [40.00-1000.00]
Relative Abundance
m/z
6c

Alaa abdallah-3-Hnmr-ES

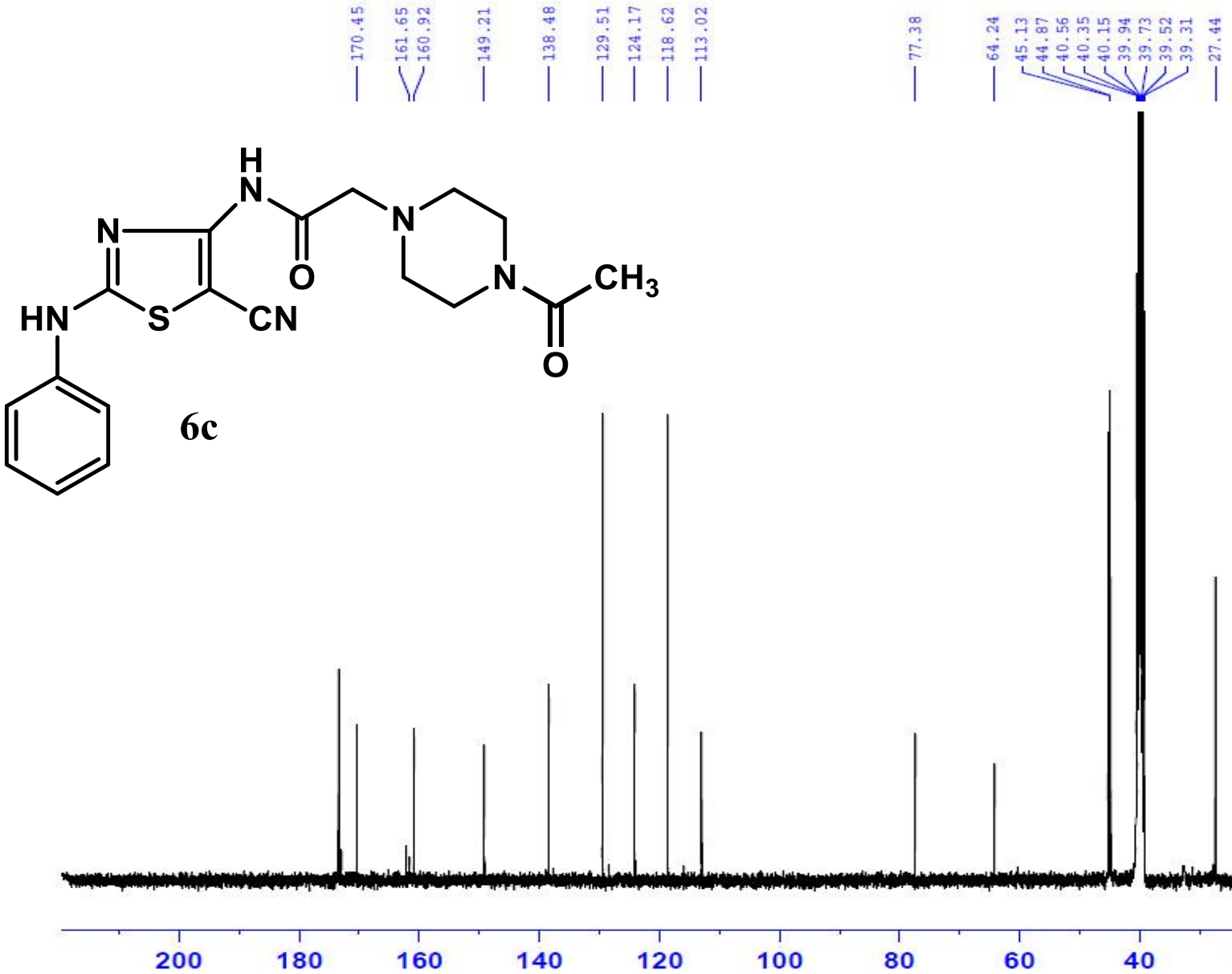


6c

Faculty of Pharmacy

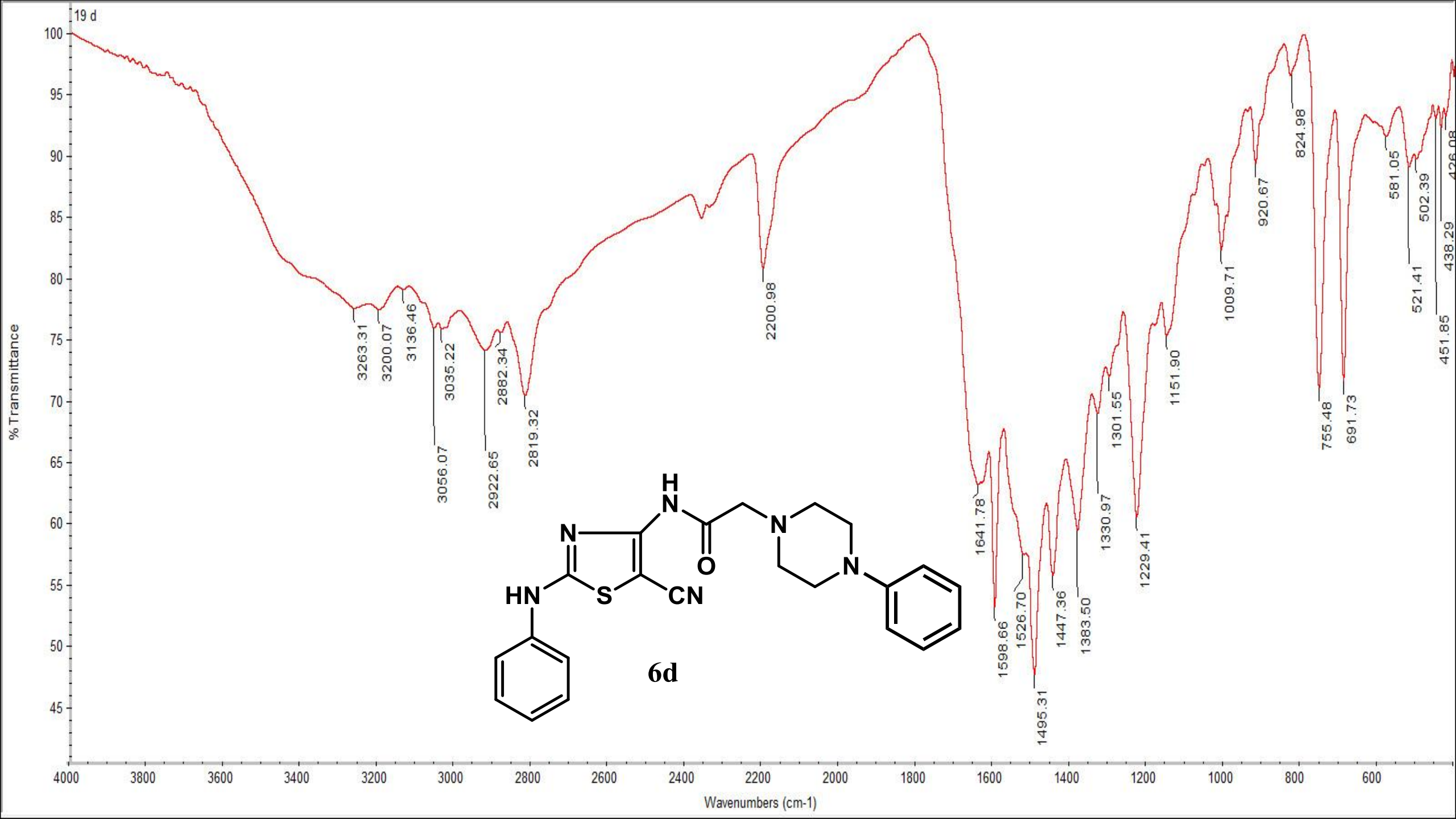
```
Current Data Parameters
NAME      Alaa abdallah-poc
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameter
Date_             20210427
Time                12.06 h
INSTRUM              spect
PROBHD    Z108618_0945 (
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES             0.244532 Hz
AQ                 4.0894465 se
RG                    176.72
DW                    62.400 us
DE                     6.50 us
TE                    298.0 K
D1              1.00000000 se
TD0                       1
SFO1           400.2024712 MH
NUC1                    1H
P1                    13.50 us
PLW1           13.00000000 W

F2 - Processing parameters
SI                    65536
SF             400.2000000 MH
WDW                      EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

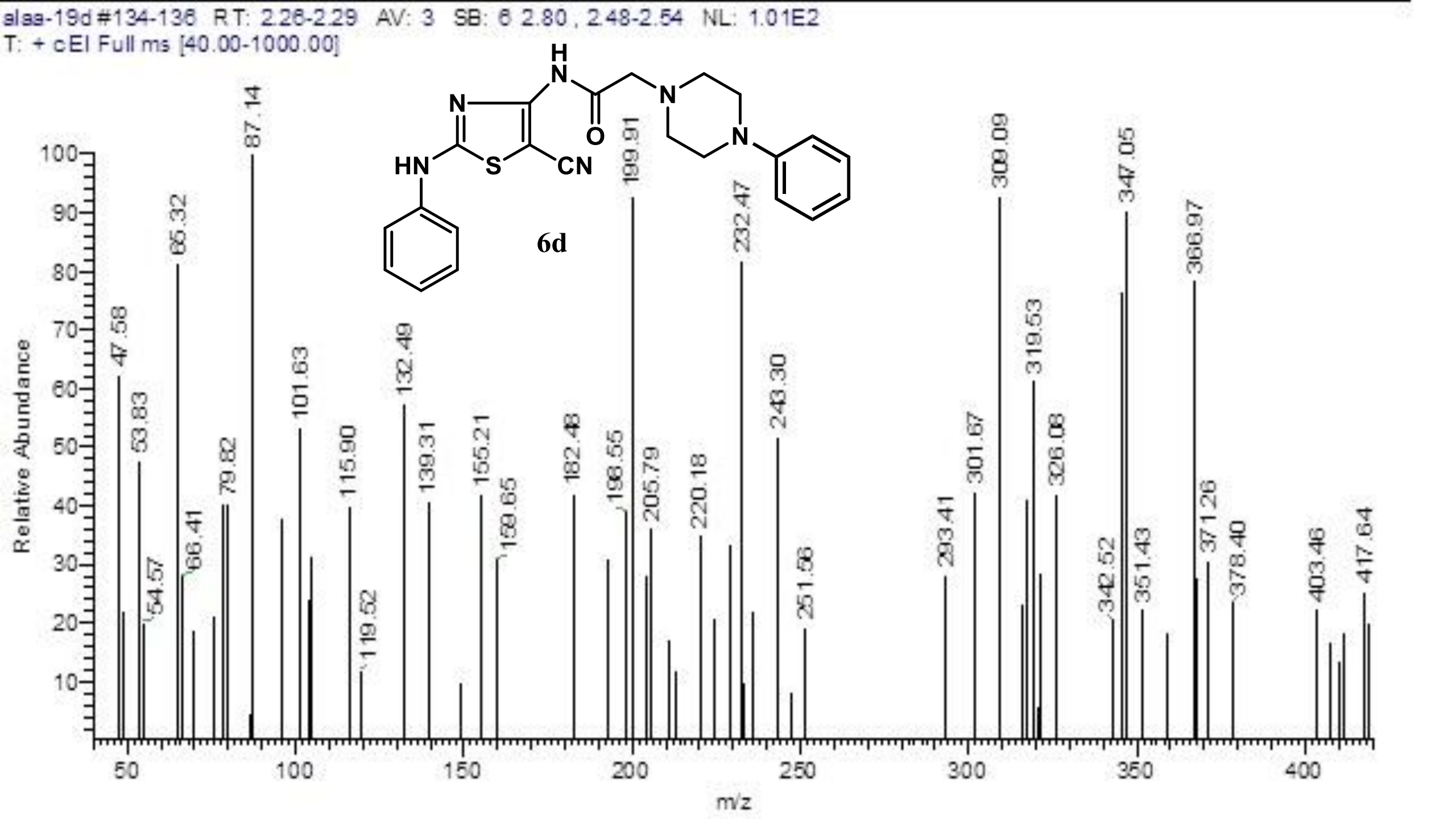
Alaa abdallah-3-M c13



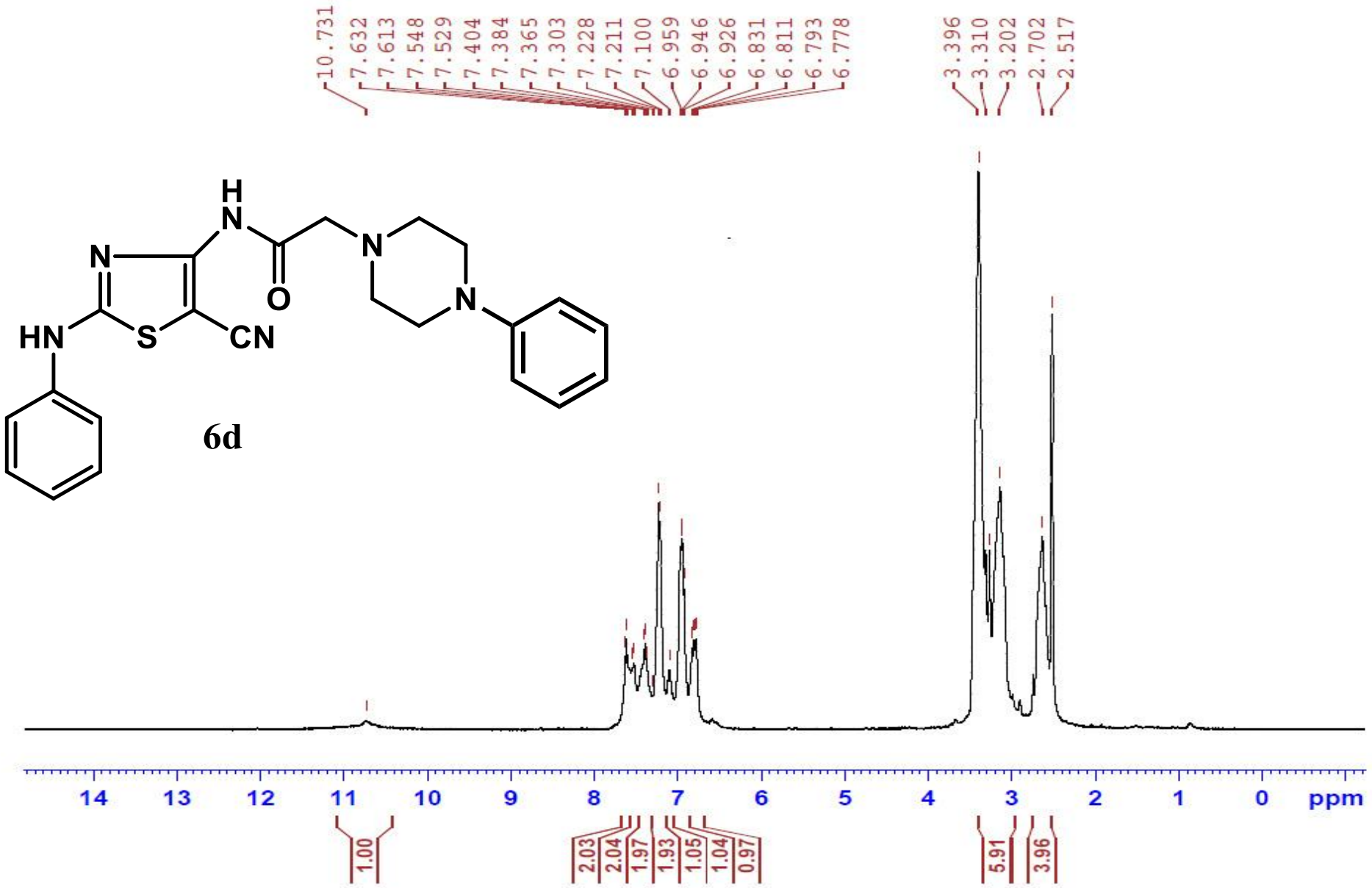
Faculty of Pharmacy

```
Current Data Parameters
NAME      alaa abdallah clbcl -M c13
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210302
Time                9.37 h
INSTRUM            spect
PROBHD    Z108618_0945 (
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                  2100
DS                     4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            1.3631488 sec
RG               197.77
DW               20.800 usec
DE                6.50 usec
TE        0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        100.6404331 MHz
NUC1                13C
P1                10.00 usec
PLW1         47.00000000 W
SFO2        400.2016008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.00000000 W
PLW12         0.29249999 W
PLW13         0.14713000 W

F2 - Processing parameters
SI                 32768
SF          100.6303700 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```


19 d
% Transmittance
Wavenumbers (cm-1)
3263.31
3200.07
3136.46
3056.07
3035.22
2922.65
2882.34
2819.32
2200.98
1641.78
1598.66
1526.70
1495.31
1447.36
1383.50
1330.97
1301.55
1229.41
1151.90
1009.71
920.67
824.98
755.48
691.73
581.05
521.41
502.39
451.85
438.29
426.08
HN
N
S
CN
O
N
N
H
6d


alaa-19d #134-136 RT: 2.26-2.29 AV: 3 SB: 6 2.80 , 2.48-2.54 NL: 1.01E2
T: + c EI Full ms [40.00-1000.00]
6d
Relative Abundance
m/z
47.58
53.83
54.57
65.32
66.41
79.82
87.14
101.63
115.90
119.52
132.49
139.31
155.21
159.65
182.48
196.55
199.91
205.79
220.18
232.47
243.30
251.96
293.41
301.67
309.09
319.53
326.08
342.52
347.05
351.43
366.97
371.26
378.40
403.46
417.64

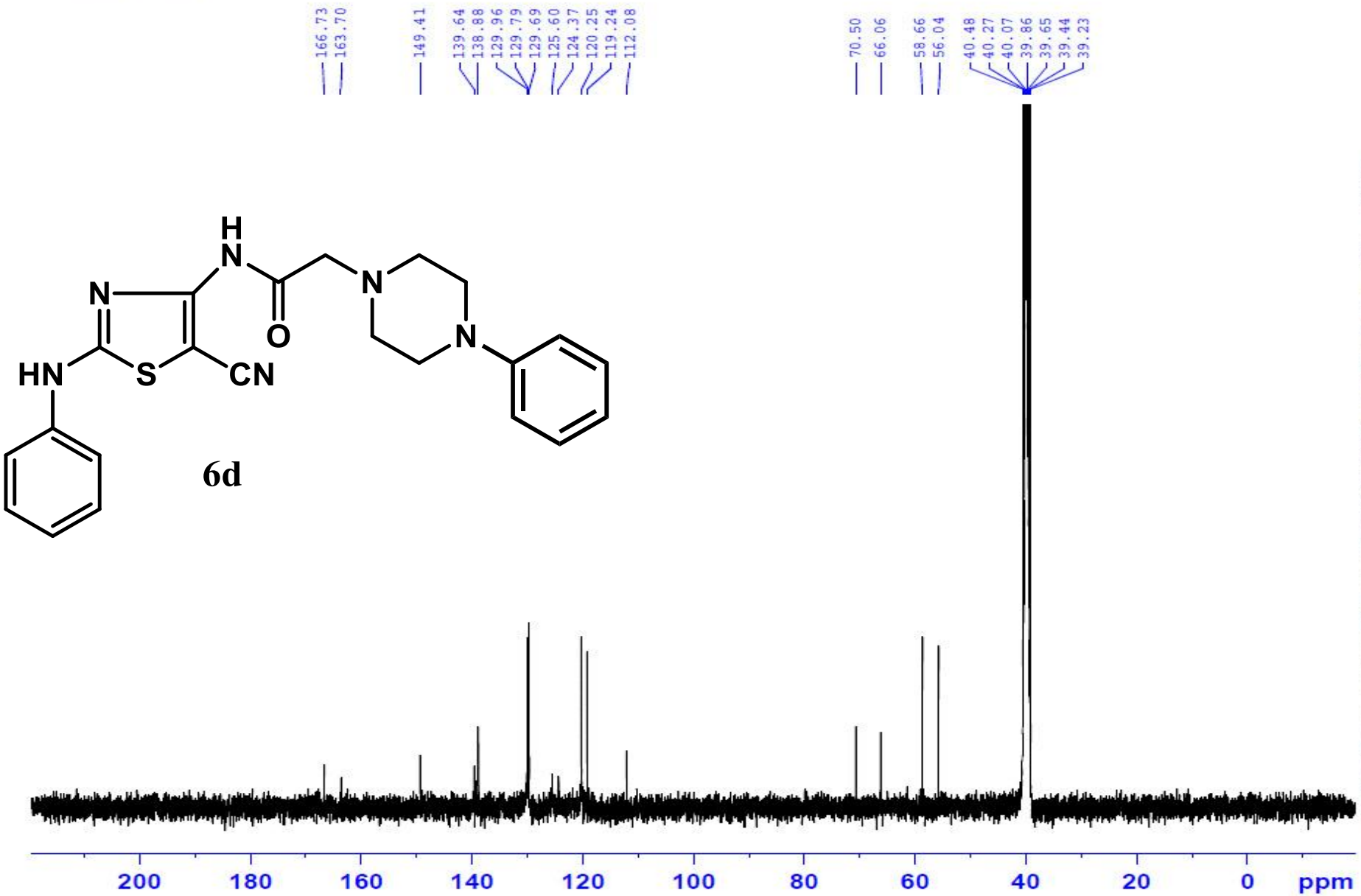
alaa abdallah 4A -M hnmr



Faculty of Pharmacy

```
Current Data Parameters
NAME      alaa abdallah 4A -M
EXPNO                     10
PROCNO                     1

F2 - Acquisition Parameters
Date_               20201130
Time                   13.32 h
INSTRUM                spect
PROBHD    Z108618_0945 (
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                  4.0894465 sec
RG                     112.56
DW                     62.400 usec
DE                      6.50 usec
TE                     292.9 K
D1                1.00000000 sec
TD0                        1
SFO1           400.2024712 MHz
NUC1                      1H
P1                     13.50 usec
PLW1          13.00000000 W

F2 - Processing parameters
SI                    65536
SF             400.2000000 MHz
WDW                      EM
SSB       0
LB                      0.30 Hz
GB        0
PC                      1.00
```

alaa abdallah 6 -M c13



6d

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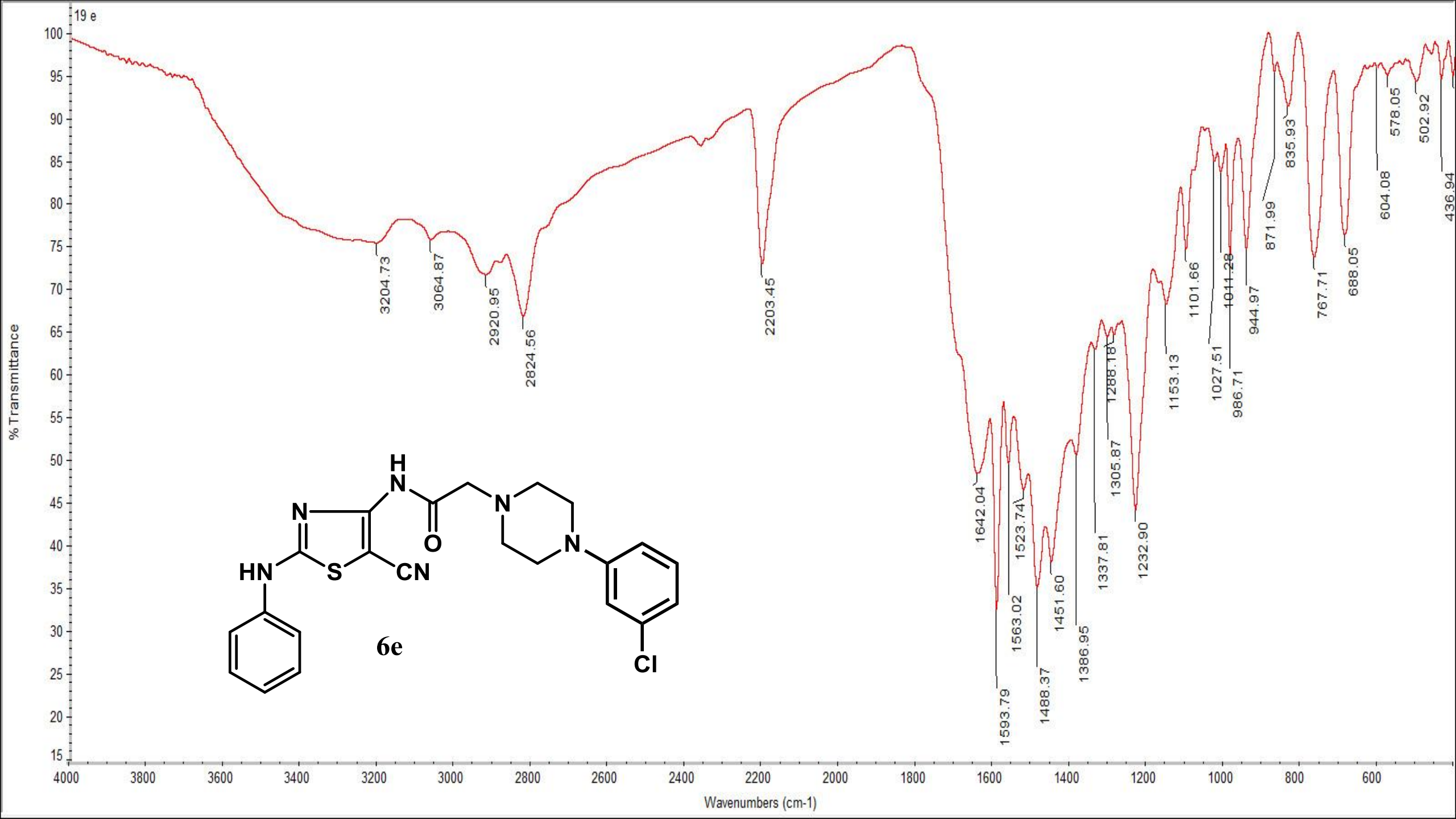
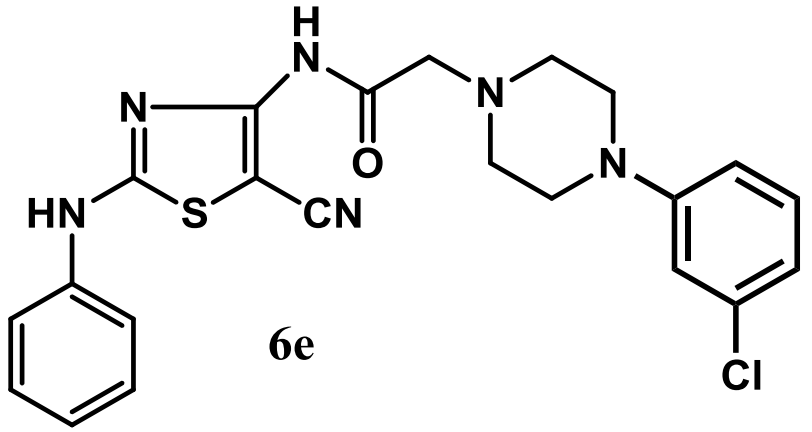
```
Current Data Parameters
NAME      alaa abdallah 6 -M c13
EXPNO                    10
PROCNO                    1

F2 - Acquisition Parameters
Date_              20210302
Time                  1.23 h
INSTRUM              spect
PROBHD    Z108618_0945 (
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                    2100
DS                       4
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ                1.3631488 sec
RG                   197.77
DW                  20.800 usec
DE                   6.50 usec
TE                  293.9 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1
SFO1          100.6404331 MHz
NUC1                   13C
P1                  10.00 usec
PLW1          47.00000000 W
SFO2          400.2016008 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               90.00 usec
PLW2          13.00000000 W
PLW12          0.29249999 W
PLW13          0.14713000 W

F2 - Processing parameters
SI                   32768
SF            100.6303700 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

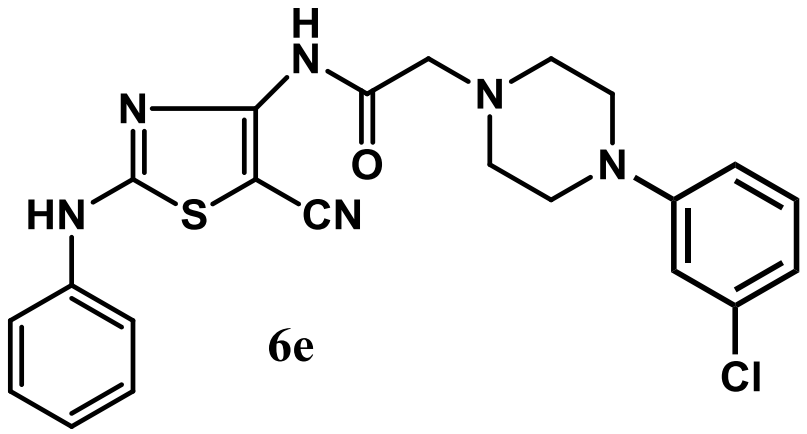

19 e
% Transmittance
Wavenumbers (cm-1)
3204.73
3064.87
2920.95
2824.56
2203.45
1642.04
1593.79
1563.02
1523.74
1488.37
1451.60
1386.95
1337.81
1305.87
1288.18
1232.90
1153.13
1101.66
1027.51
1011.28
986.71
944.97
871.99
835.93
767.71
688.05
604.08
578.05
502.92
436.94
HN
N
S
CN
O
N
N
Cl
6e

alaa-19e #166-167 RT: 2.79-2.81 AV: 2 SB: 2 2.86 , 2.90 NL: 1.11E4
T: {0,0} + c EI Full ms [40.00-1000.00]



6e

Alaa abdallah-7A-Hnmr-Es



6e

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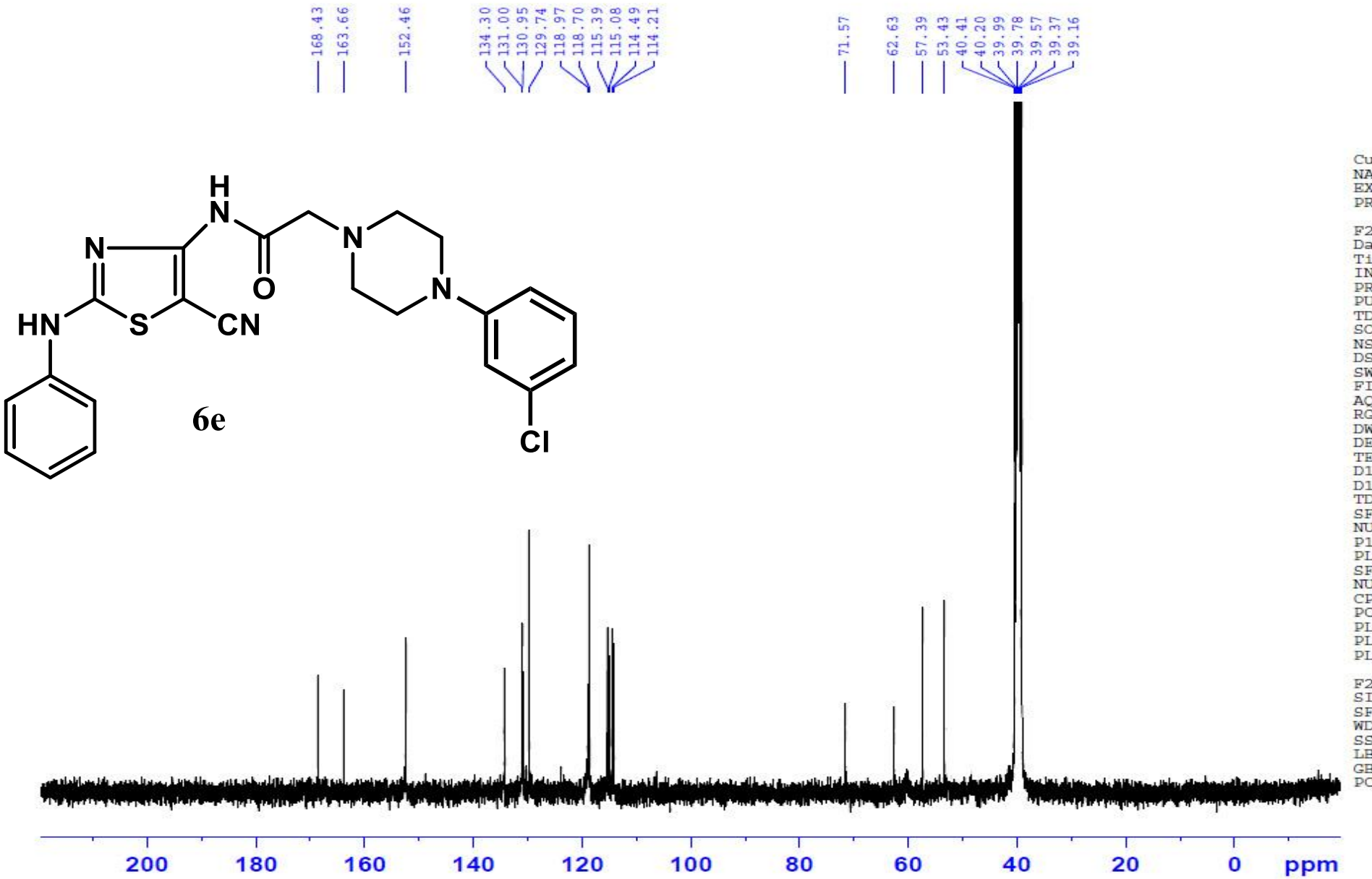
Faculty of Pharmacy

```
Current Data Parameters
NAME      Alaa abdallah-7A-Hr
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_            20210211
Time                 8.00 h
INSTRUM             spect
PROBHD    Z108618_0945 (
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                  120.93
DW                  62.400 usec
DE                   6.50 usec
TE                  292.9 K
D1              1.00000000 sec
TD0                     1
SFO1           400.2024712 MHz
NUC1                   1H
P1                  13.50 usec
PLW1           13.00000000 W

F2 - Processing parameters
SI                  65536
SF             400.2000000 MHz
WDW                    EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

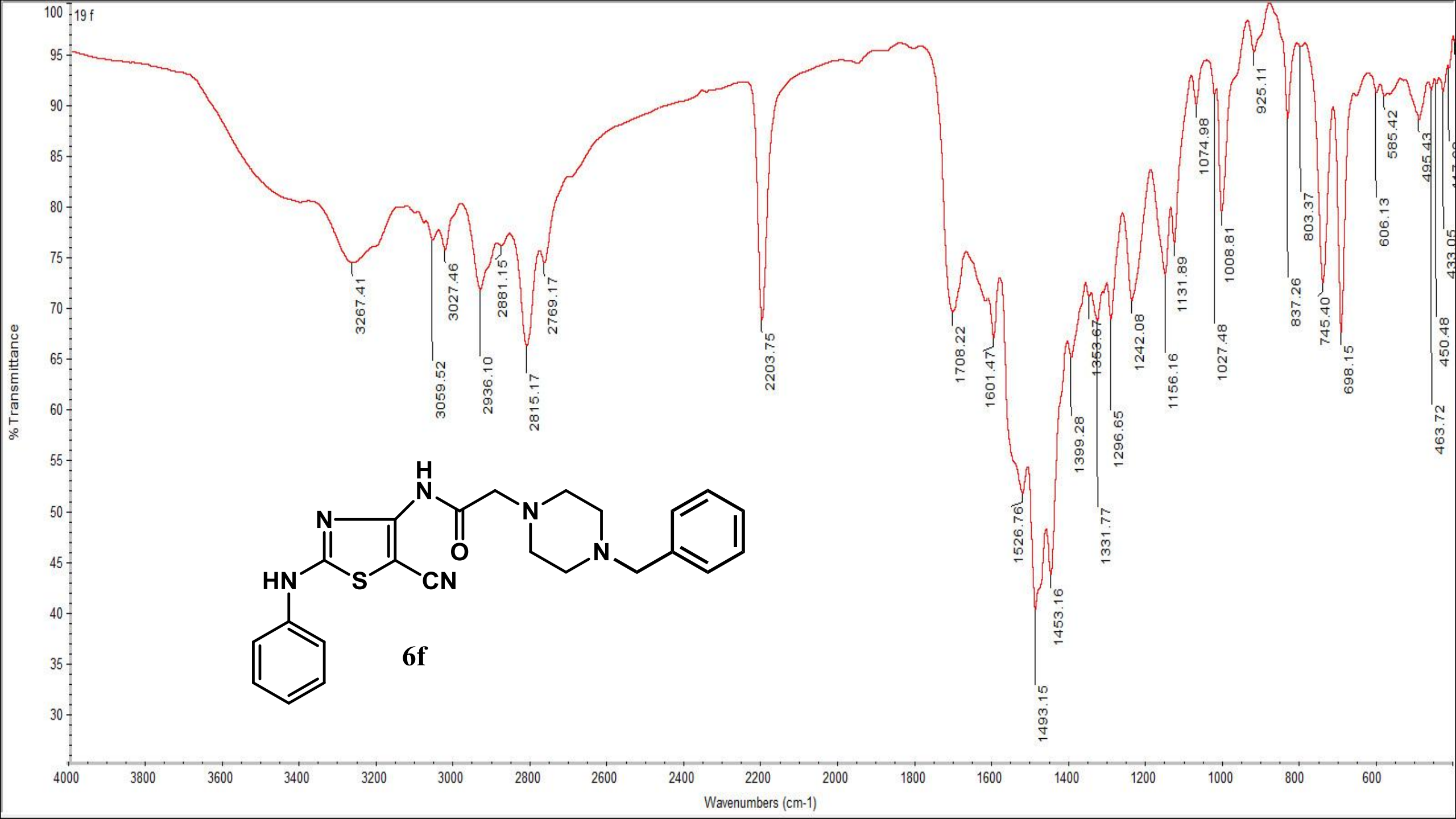
alaa abdallah 7a -M c13



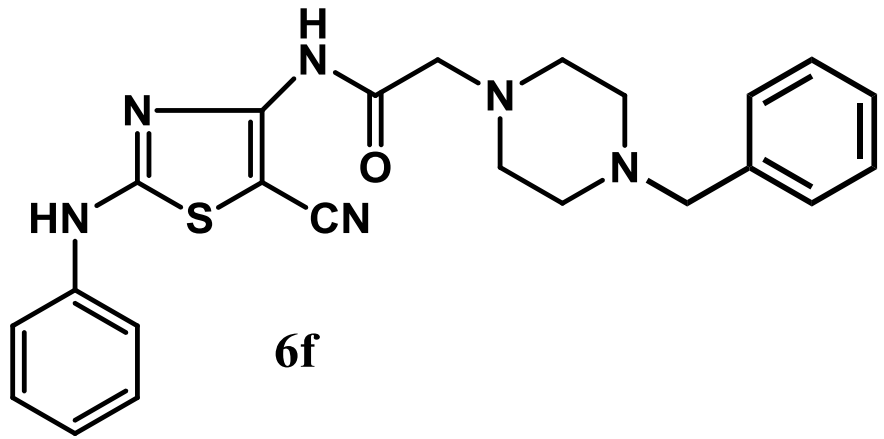
6e

Faculty of Pharmacy

```
Current Data Parameters
NAME      alaa abdallah 7a -M c13
EXPNO                         10
PROCNO                         1

F2 - Acquisition Parameters
Date_               20210302
Time                    5.30 h
INSTRUM                 spect
PROBHD    Z108618_0945 (
PULPROG                 zgpg30
TD                      65536
SOLVENT                 DMSO
NS                      2100
DS                         4
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                  1.3631488 sec
RG                     197.77
DW                     20.800 usec
DE                      6.50 usec
TE                     294.1 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                        1
SFO1              100.6404331 MHz
NUC1                      13C
P1                     10.00 usec
PLW1              47.00000000 W
SFO2              400.2016008 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                  90.00 usec
PLW2              13.00000000 W
PLW12              0.29249999 W
PLW13              0.14713000 W

F2 - Processing parameters
SI                        32768
SF                100.6303700 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

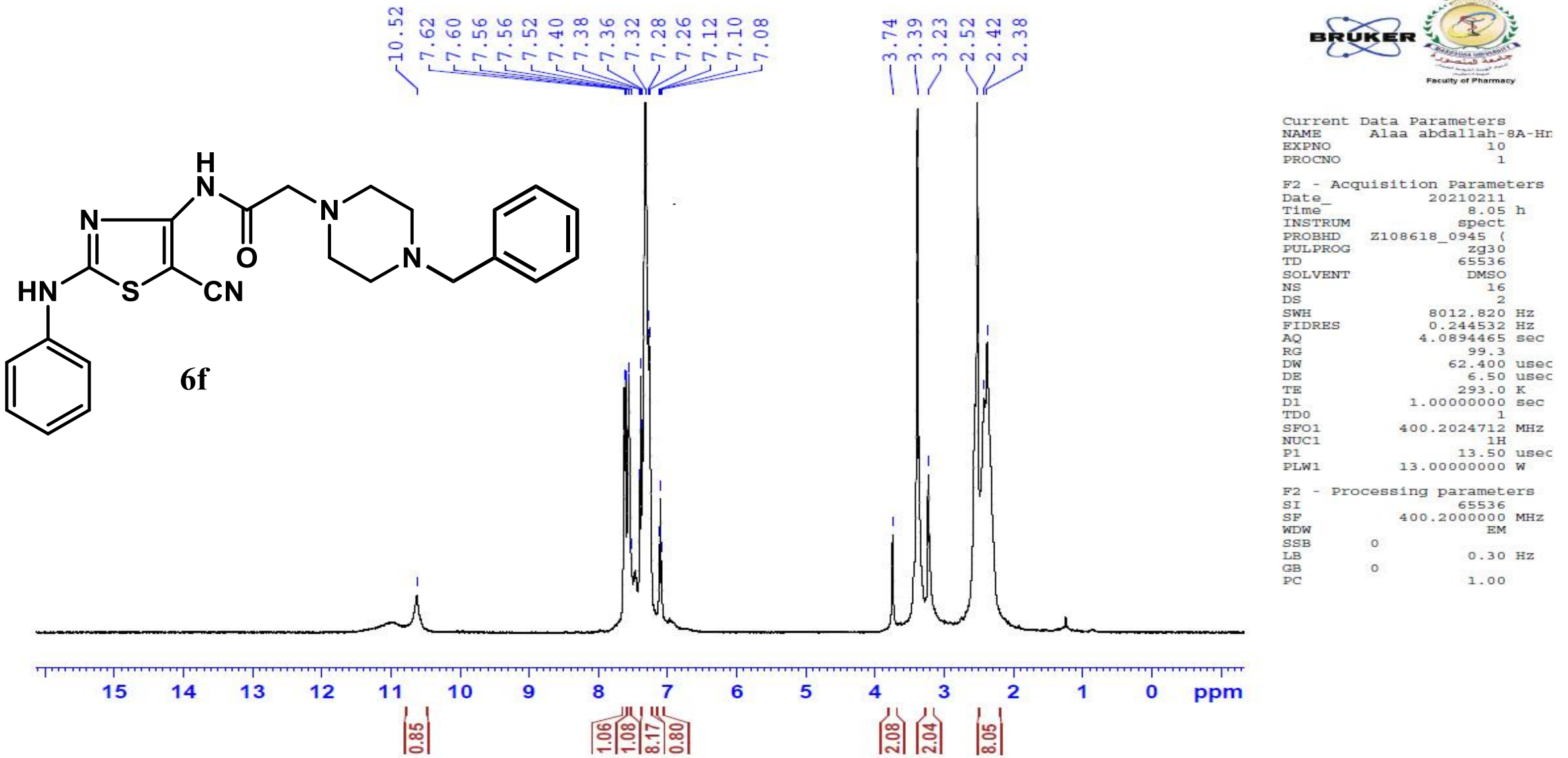

19 f
% Transmittance
Wavenumbers (cm-1)
3267.41
3059.52
3027.46
2936.10
2881.15
2815.17
2769.17
2203.75
1708.22
1601.47
1526.76
1493.15
1453.16
1399.28
1353.67
1331.77
1296.65
1242.08
1156.16
1131.89
1074.98
1027.48
1008.81
925.11
837.26
803.37
745.40
698.15
606.13
585.42
495.43
463.72
450.48
433.05
6f

alaa-19f #133-136 RT: 2.24-2.29 AV: 4 SB: 2 1.74 , 1.67 NL: 1.28E2
T: + cEI Full ms [40.00-1000.00]



6f

Alaa abdallah-8A-Hnmr-Es



6f

BRUKER

Faculty of Pharmacy

Current Data Parameters

NAME	Alaa abdallah-8A-Hr
EXPNO	10
PROCNO	1

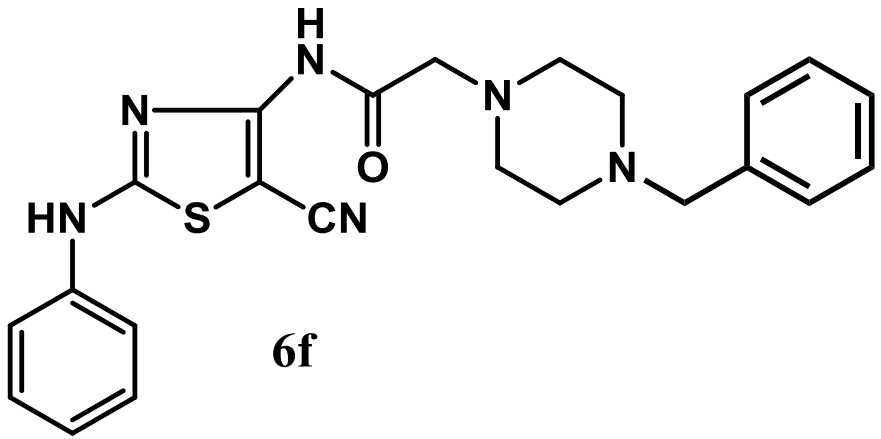
F2 - Acquisition Parameters

Date_	20210211	
Time	8.05	h
INSTRUM	spect	
PROBHD	Z108618_0945 (	
PULPROG	zg30	
TD	65536	
SOLVENT	DMSO	
NS	16	
DS	2	
SWH	8012.820	Hz
FIDRES	0.244532	Hz
AQ	4.0894465	sec
RG	99.3	
DW	62.400	usec
DE	6.50	usec
TE	293.0	K
D1	1.00000000	sec
TD0	1	
SFO1	400.2024712	MHz
NUC1	1H	
P1	13.50	usec
PLW1	13.00000000	W

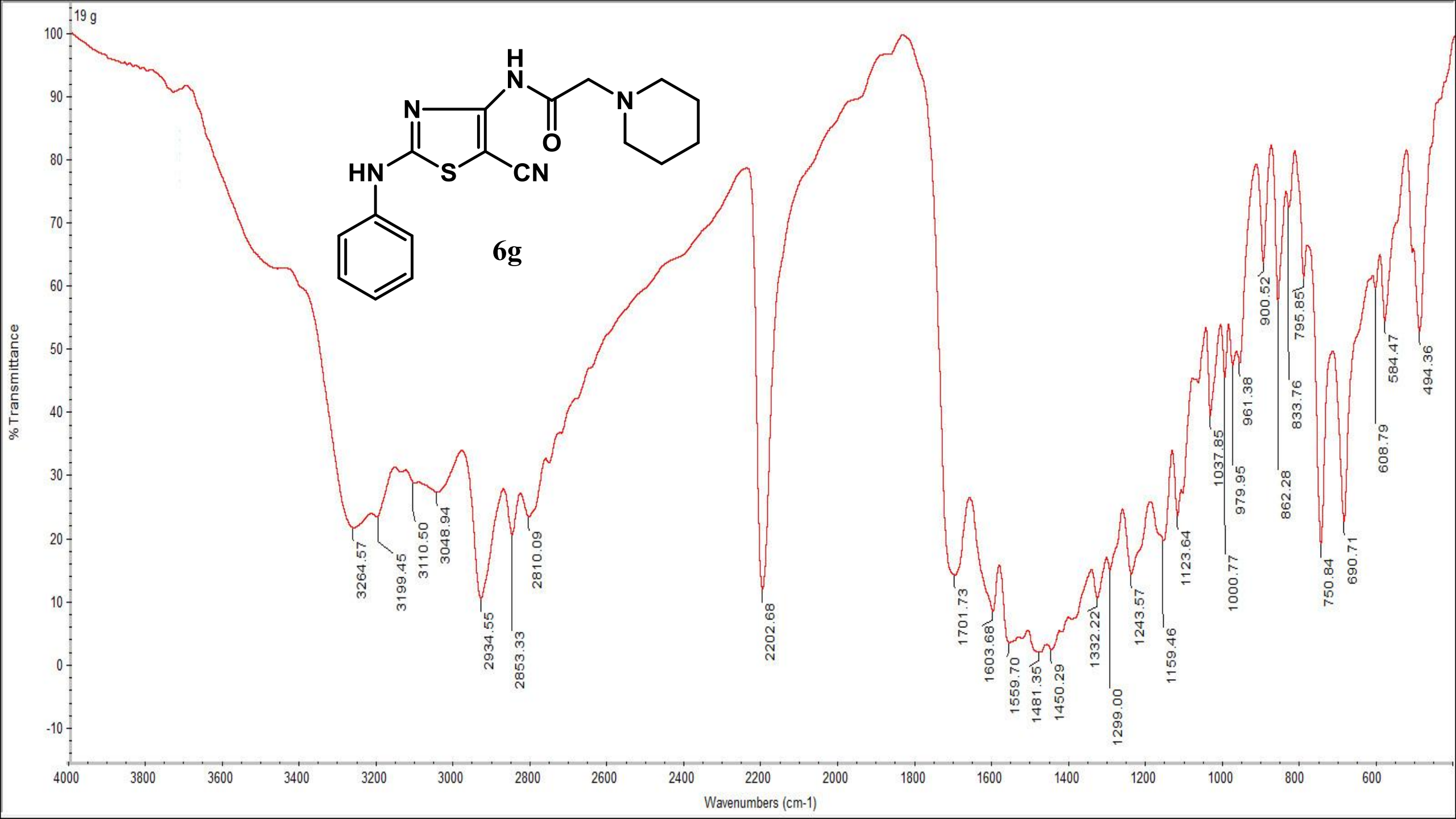
F2 - Processing parameters

SI	65536	
SF	400.2000000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

alaa abdallah 8a -M c13

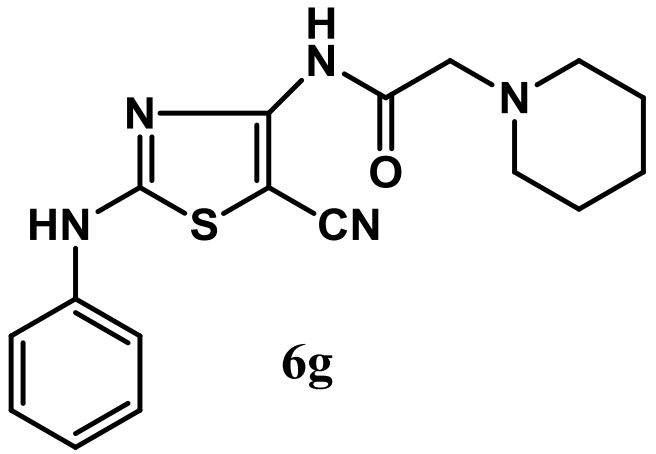


6f


19 g
% Transmittance
Wavenumbers (cm-1)
3264.57
3199.45
3110.50
3048.94
2934.55
2853.33
2810.09
2202.68
1701.73
1603.68
1559.70
1481.35
1450.29
1332.22
1299.00
1243.57
1159.46
1123.64
1037.85
1000.77
979.95
961.38
900.52
862.28
833.76
795.85
750.84
690.71
608.79
584.47
494.36
HN
N
S
CN
O
N
H
N

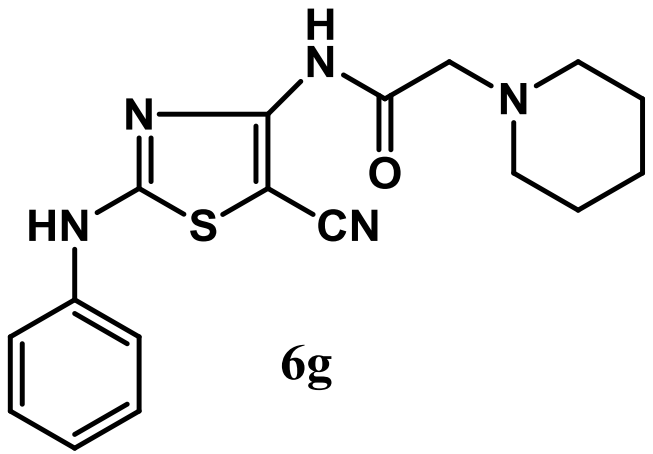
6g

alaa-19g #34 RT: 0.59 AV: 1 SB: 18 0.54-0.74 , 0.50-0.57 NL: 1.89E3
T: {0,0} + c EI Full ms [40.00-1000.00]



6g

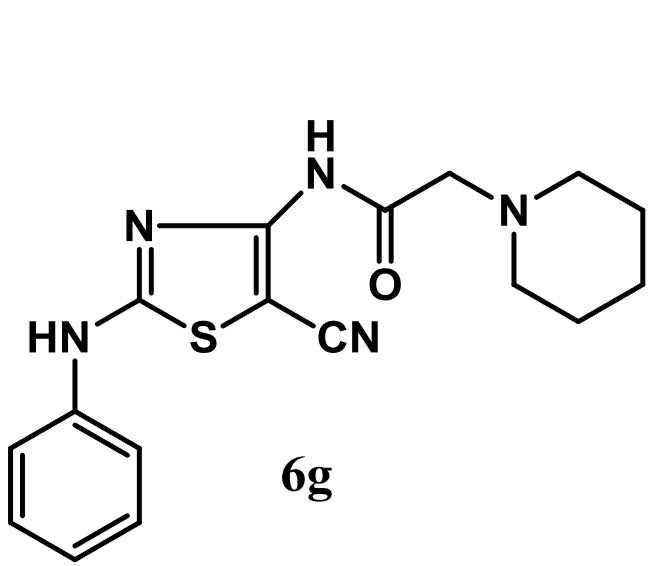
Alaa abdallah-6A-Hnmr-Es



6g

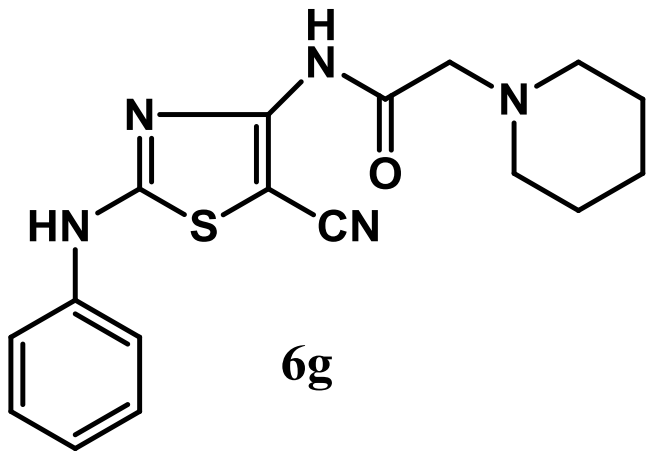

```
Current Data Parameters
NAME      Alaa abdallah-6A-Hr
EXPNO                     10
PROCNO                     1

F2 - Acquisition Parameters
Date_               20210211
Time                    7.55 h
INSTRUM                spect
PROBHD    Z108618_0945 (
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                  4.0894465 sec
RG                       99.3
DW                     62.400 usec
DE                      6.50 usec
TE                     293.0 K
D1                1.00000000 sec
TD0                        1
SFO1            400.2024712 MHz
NUC1                      1H
P1                     13.50 usec
PLW1           13.00000000 W

F2 - Processing parameters
SI                    65536
SF              400.2000000 MHz
WDW                      EM
SSB       0
LB                      0.30 Hz
GB        0
PC                      1.00
```

Alaa abdallah-6A-Hnmr-Es



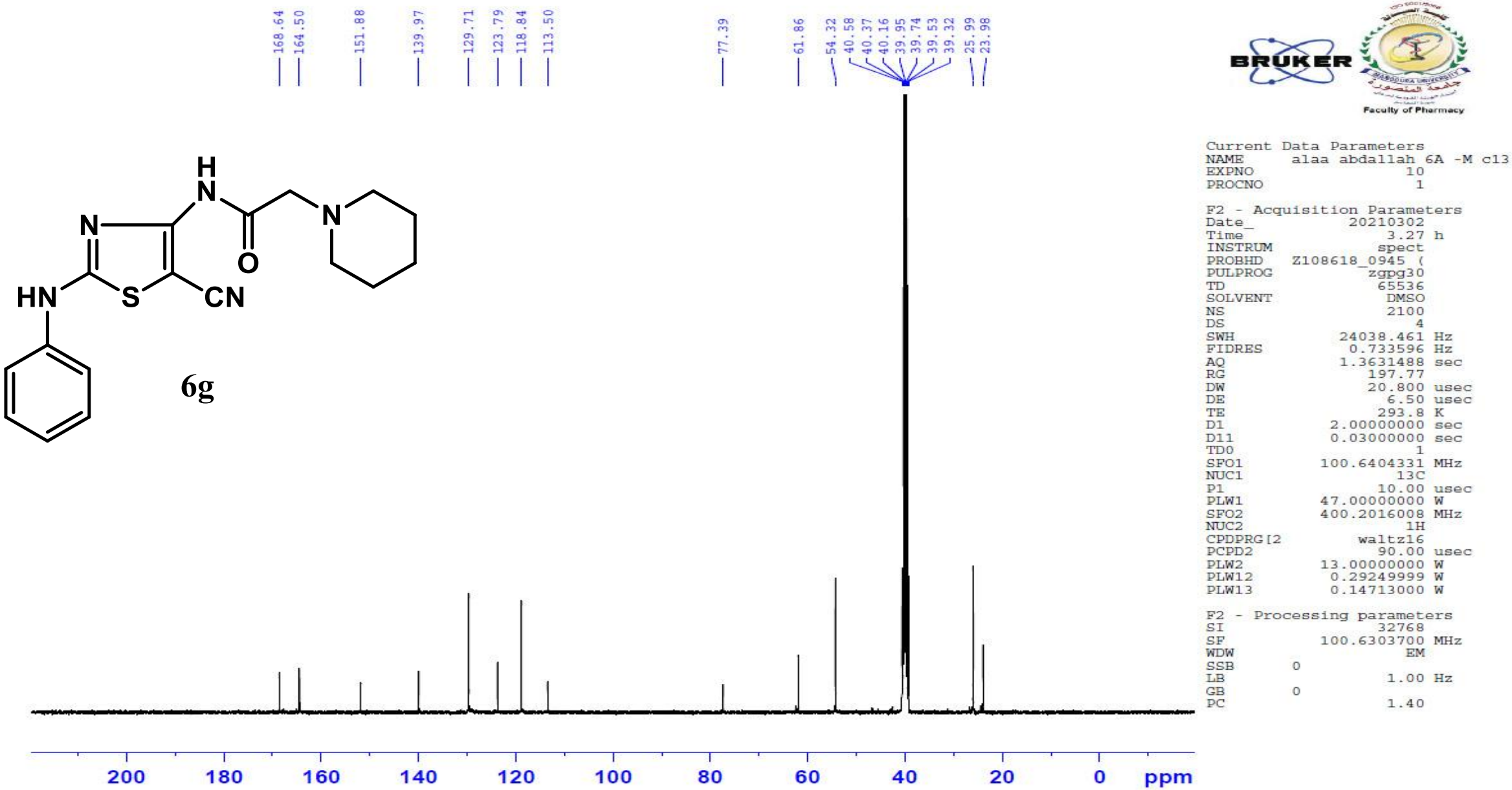
6g

Alaa abdallah-6A-Hnmr-Es



6g

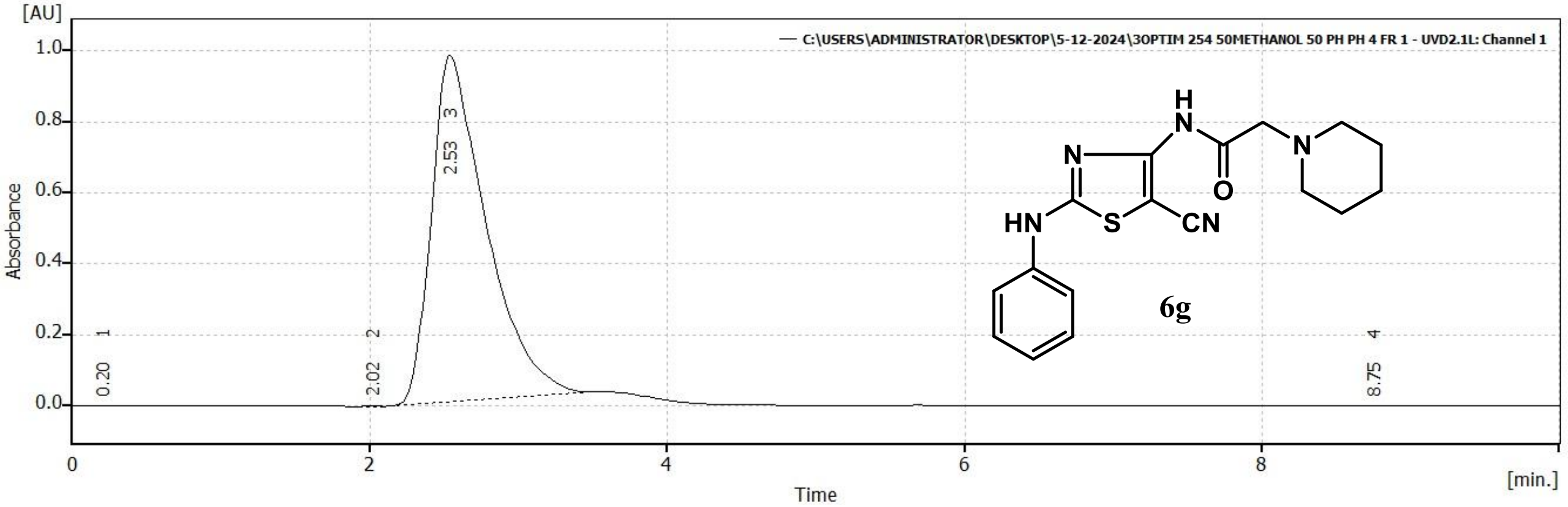
alaa abdallah 6A -M c13



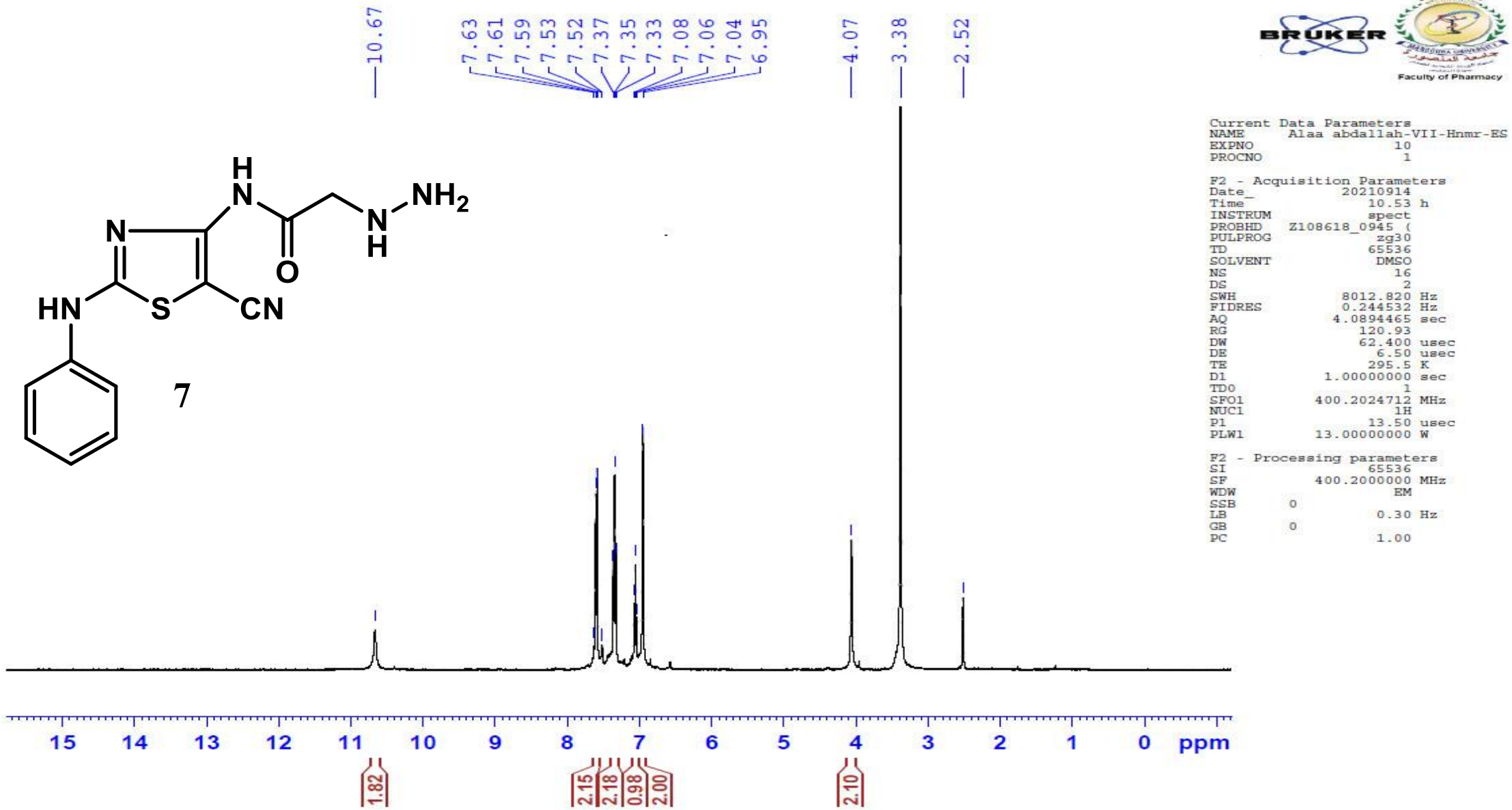
6g

Faculty of Pharmacy

```
Current Data Parameters
NAME      alaa abdallah 6A -M c13
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210302
Time              3.27 h
INSTRUM           spect
PROBHD   Z108618_0945 (
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 2100
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                197.77
DW                20.800 usec
DE                 6.50 usec
TE                293.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1
SFO1         100.6404331 MHz
NUC1                13C
P1                10.00 usec
PLW1         47.00000000 W
SFO2         400.2016008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.00000000 W
PLW12         0.29249999 W
PLW13         0.14713000 W

F2 - Processing parameters
SI                32768
SF           100.6303700 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```


[AU]
1.0
0.8
0.6
0.4
0.2
0.0
Absorbance
— C:\USERS\ADMINISTRATOR\DESKTOP\5-12-2024\3OPTIM 254 50METHANOL 50 PH PH 4 FR 1 - UVD2.1L: Channel 1
1
0.20
2
2.02
3
2.53
4
8.75
0
2
4
6
8
Time
[min.]
H
N
N
N
O
HN
S
CN
6g

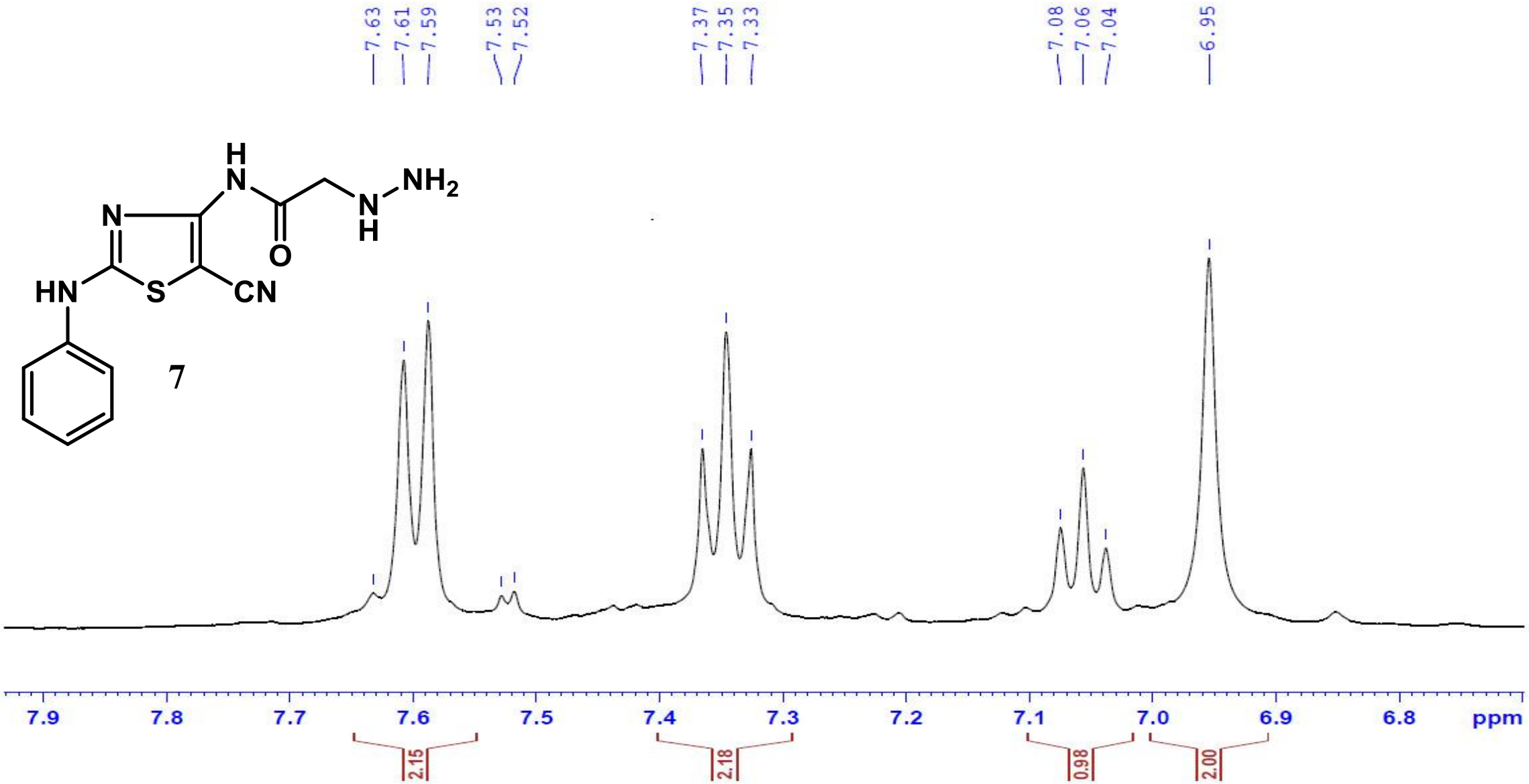
Alaa abdallah-VII-Hnmr-ES



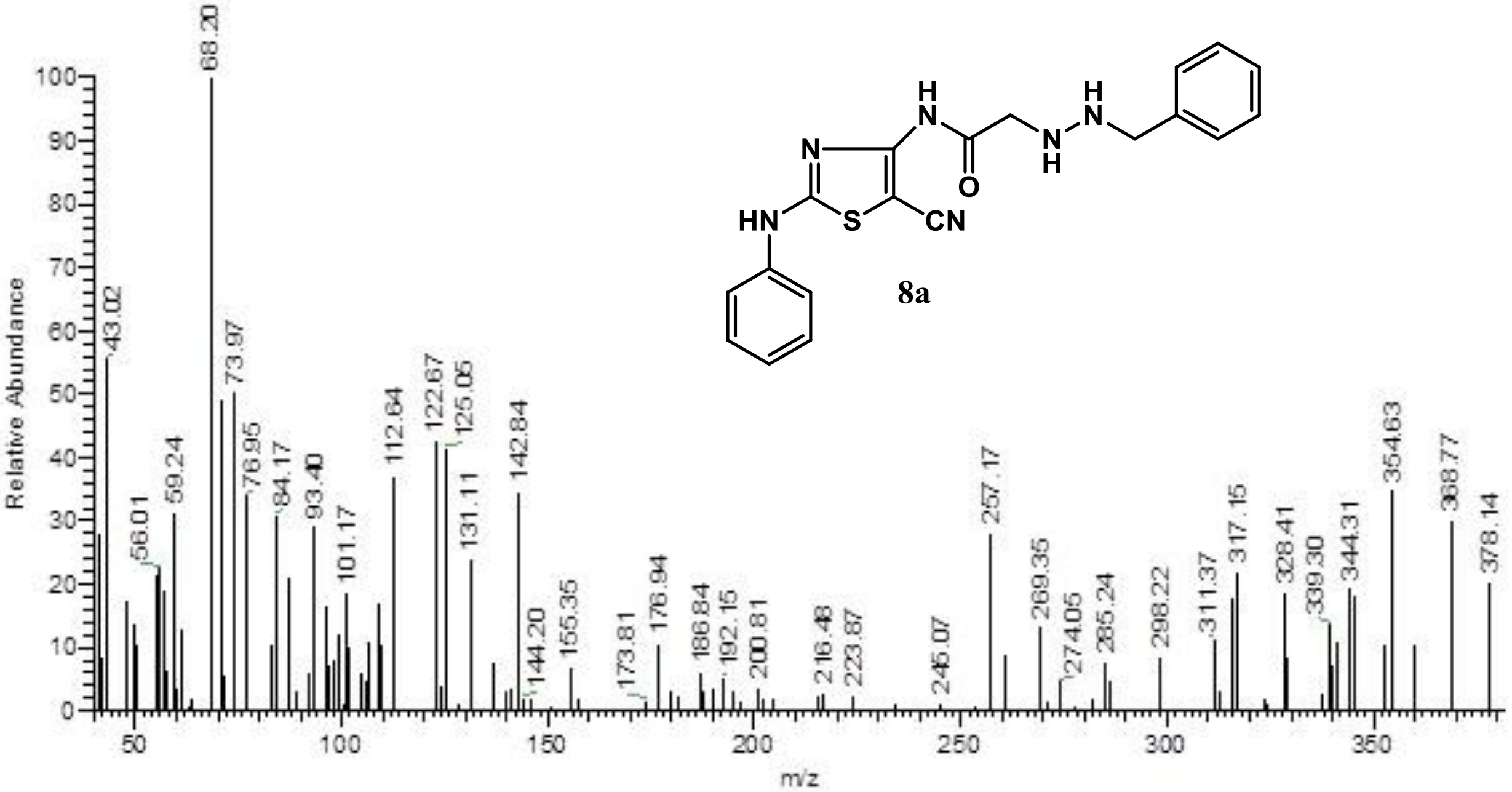
Faculty of Pharmacy

```
Current Data Parameters
NAME      Alaa abdallah-VII-Hnmr-ES
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210914
Time              10.53 h
INSTRUM           spect
PROBHD   Z108618_0945 (
PULPROG           zg30
TD               65536
SOLVENT           DMSO
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG               120.93
DW               62.400 usec
DE                6.50 usec
TE               295.5 K
D1            1.00000000 sec
TD0                   1
SFO1         400.2024712 MHz
NUC1                 1H
P1                13.50 usec
PLW1         13.00000000 W

F2 - Processing parameters
SI               65536
SF           400.2000000 MHz
WDW                  EM
SSB      0
LB               0.30 Hz
GB       0
PC               1.00
```

Alaa abdallah-VII-Hnmr-ES

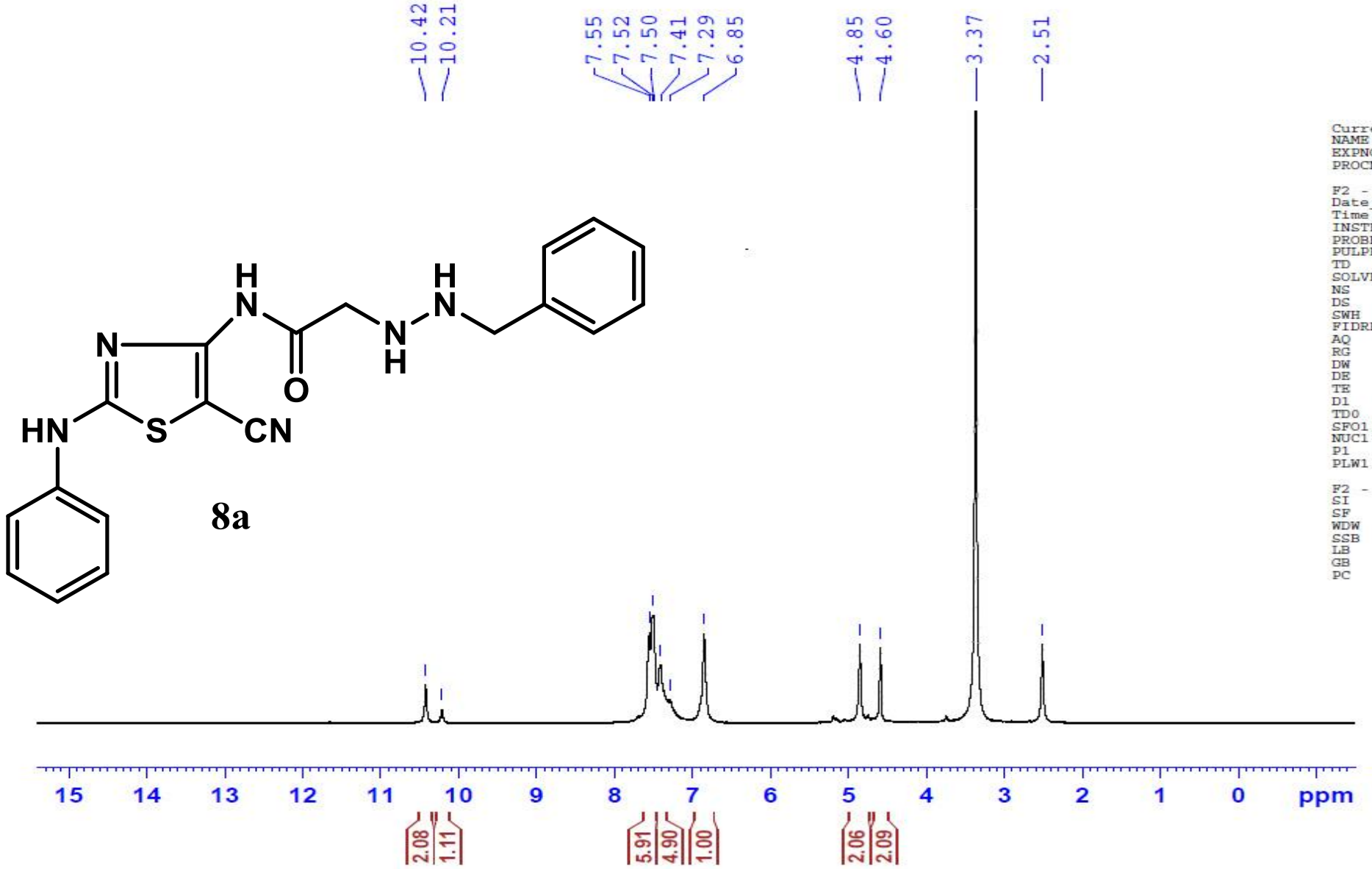


alaa-21a #64 RT: 1.09 AV: 1 SB: 2 0.97 , 1.15 NL: 3.72E3
T: {0,0} + c EI Full ms [40.00-1000.00]



8a

Alaa abdallah-VI-Hnmr-ES

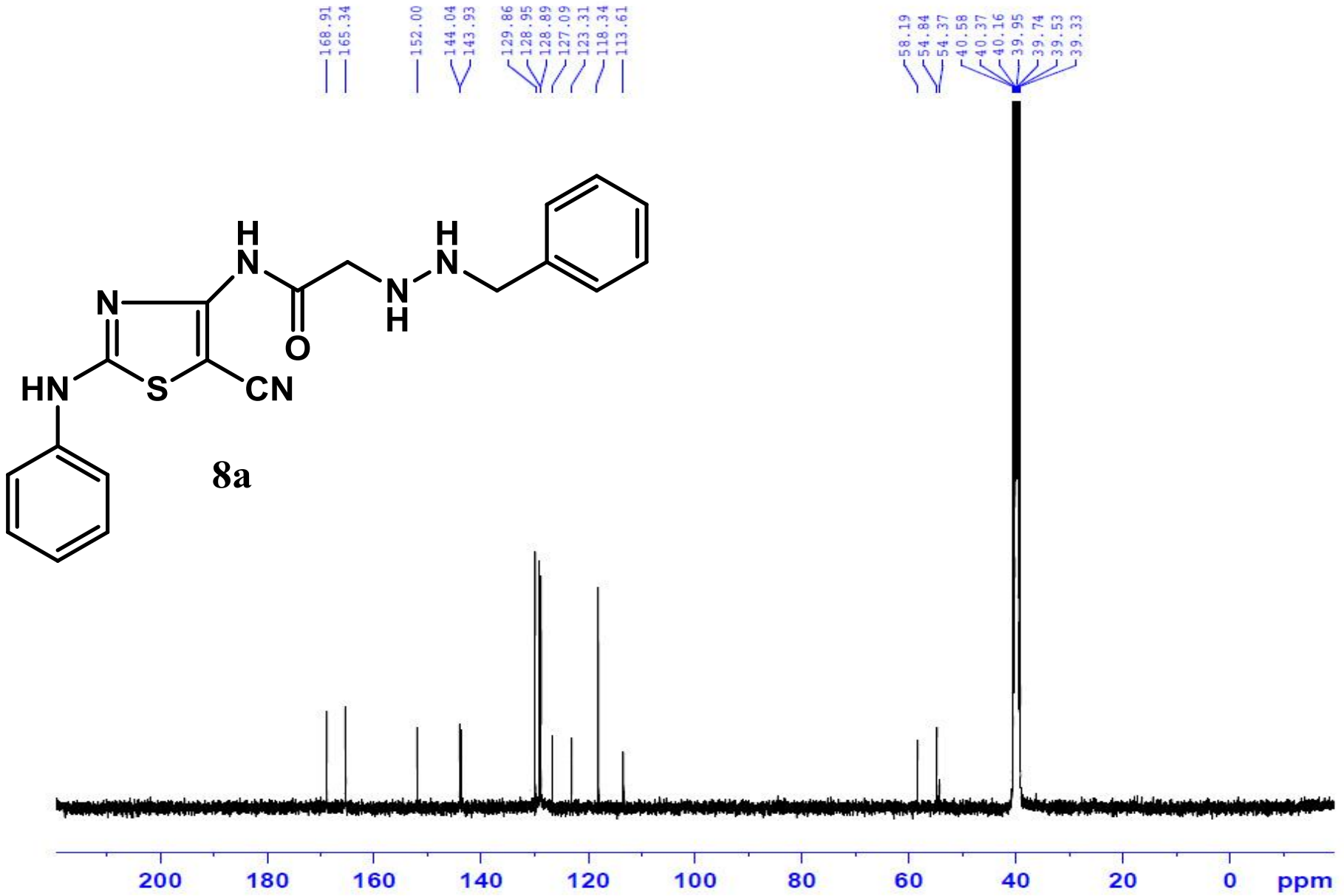


8a

Faculty of Pharmacy

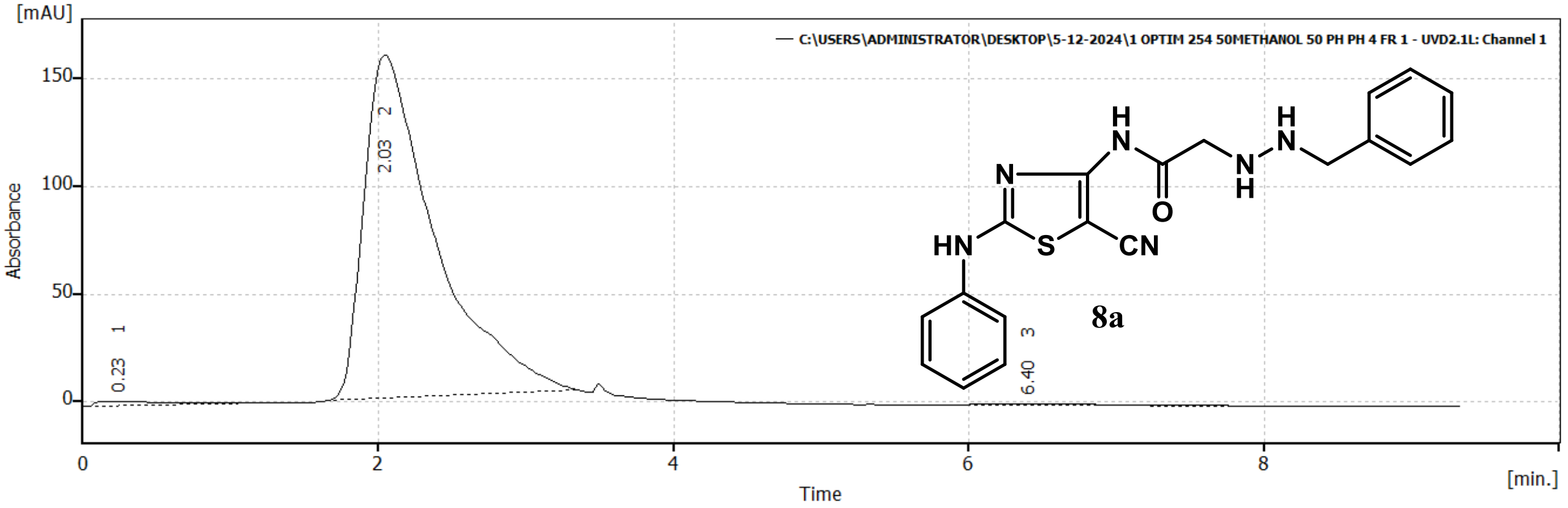
```
Current Data Parameters
NAME      Alaa abdallah-VI-Hnmr-ES
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210914
Time              10.48 h
INSTRUM           spect
PROBHD    Z108618_0945 (
PULPROG             zg30
TD                65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                135.42
DW                62.400 usec
DE                 6.50 usec
TE                295.4 K
D1             1.00000000 sec
TD0                    1
SFO1         400.2024712 MHz
NUC1                  1H
P1                13.50 usec
PLW1         13.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2000000 MHz
WDW                   EM
SSB       0
LB              0.30 Hz
GB        0
PC                1.00
```

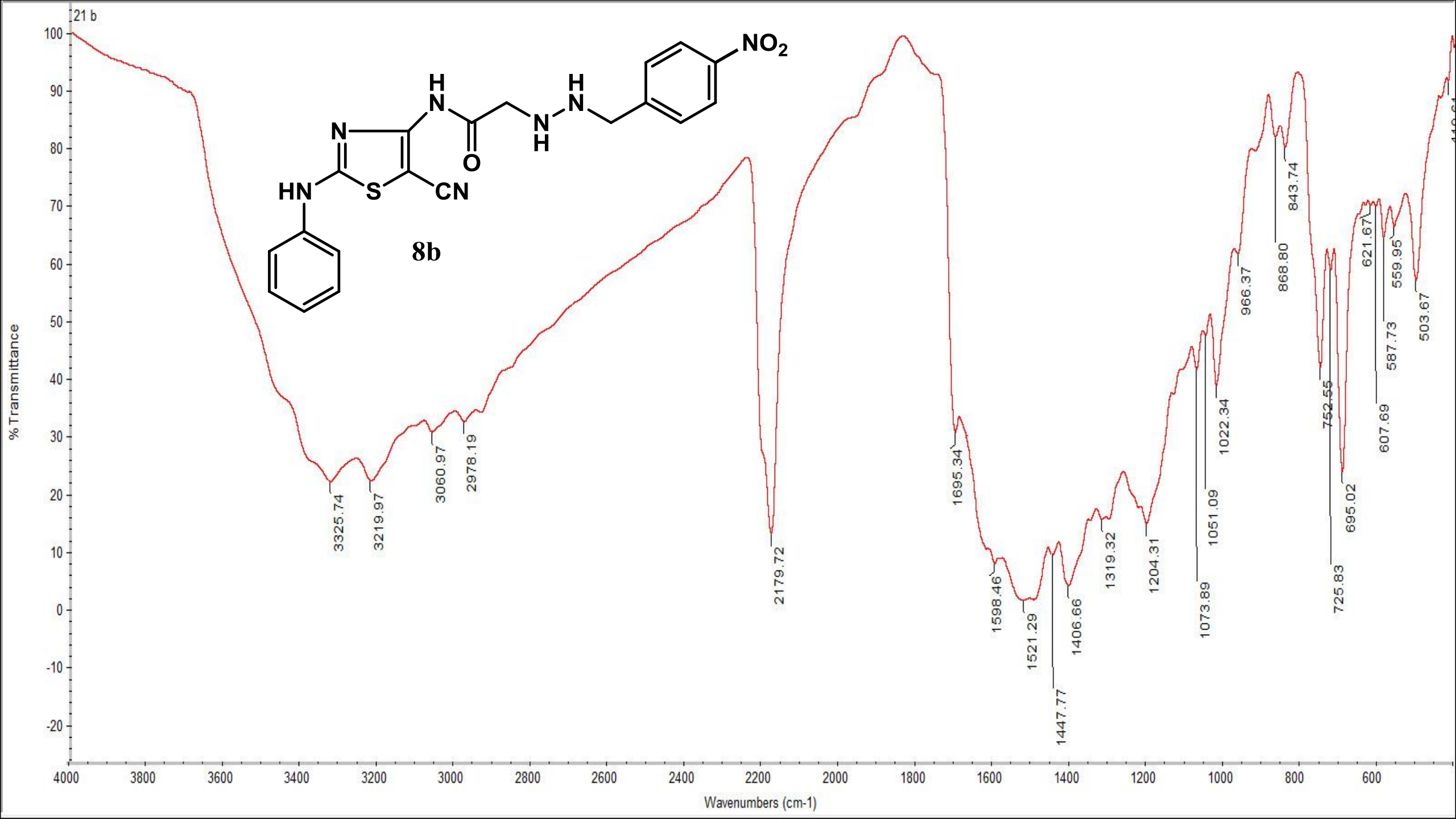
Allaa abdallah-VI-carbon-ES

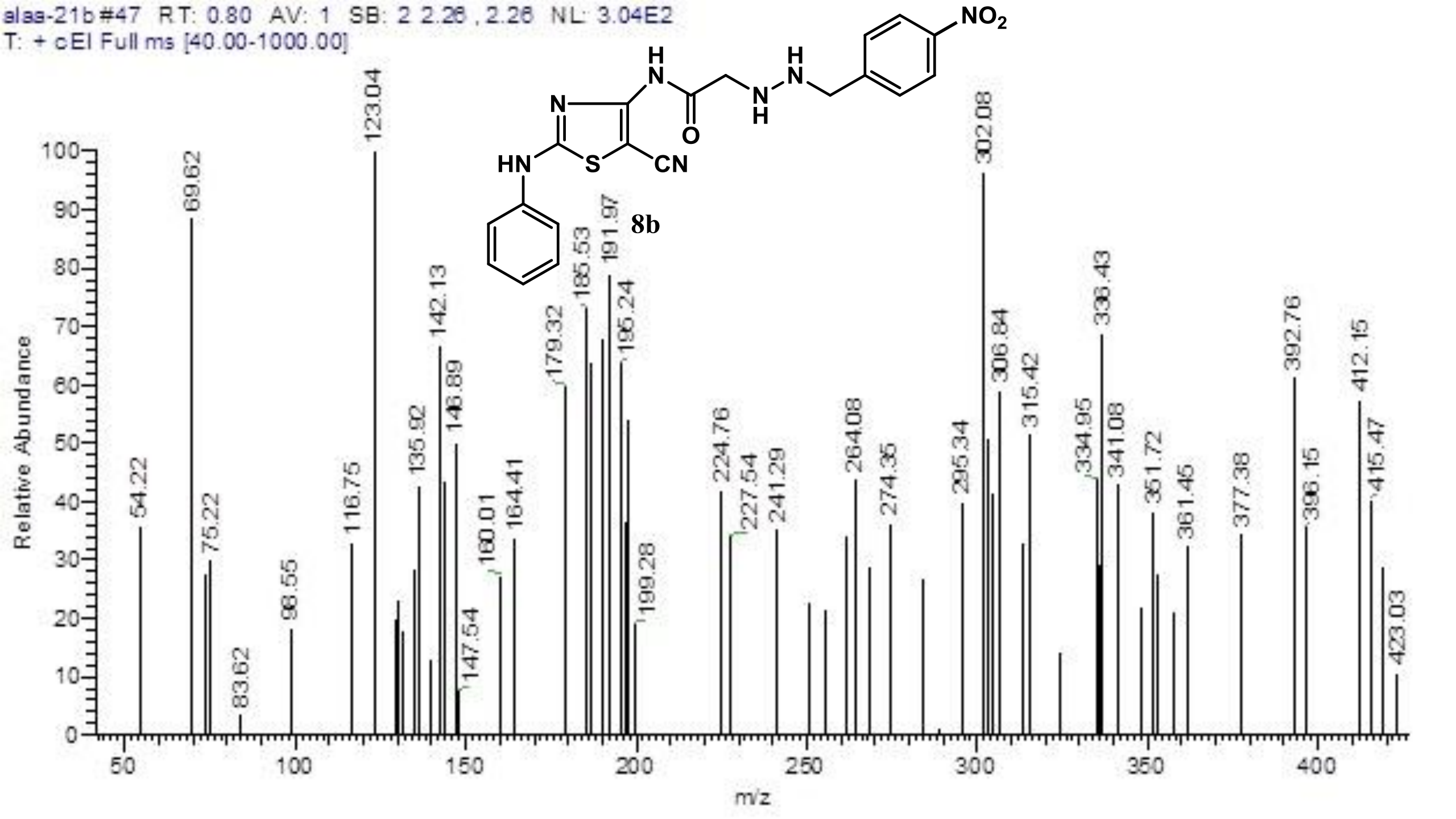


8a

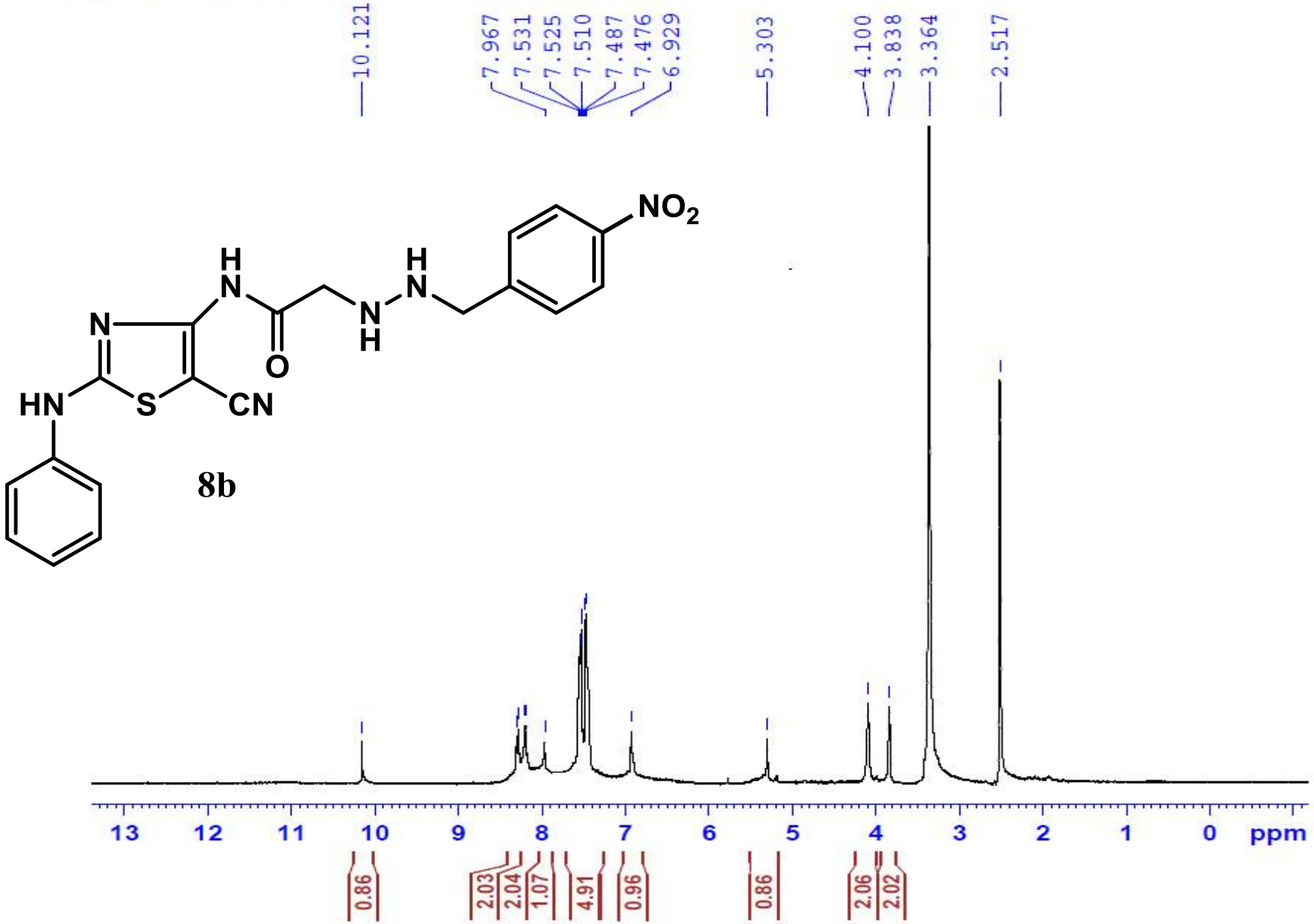
```
Current Data Parameters
NAME      Allaa abdallah-VI-carbon-ES
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211016
Time       0 h
INSTRUM              spect
PROBHD    Z108618_0945 (
PULPROG           zgpg30
TD                65536
SOLVENT             DMSO
NS                  2200
DS                     4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                197.77
DW                20.800 usec
DE                 6.50 usec
TE                295.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6404331 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          47.00000000 W
SFO2          400.2016008 MHz
NUC2                  1H
CPDPRG[2           waltz16
PCPD2              90.00 usec
PLW2          13.00000000 W
PLW12          0.29249999 W
PLW13          0.14713000 W

F2 - Processing parameters
SI                 32768
SF            100.6303700 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


[mAU]
150
100
50
0
Absorbance
— C:\USERS\ADMINISTRATOR\DESKTOP\5-12-2024\1 OPTIM 254 50METHANOL 50 PH PH 4 FR 1 - UVD2.1L: Channel 1
2.03
2
0.23
1
6.40
3
0
2
4
6
8
Time
[min.]
H
N
N
H
N
H
N
O
HN
S
CN
8a


21 b
NO2
H
N
N
H
N
H
O
N
S
HN
CN
8b
% Transmittance
Wavenumbers (cm-1)
3325.74
3219.97
3060.97
2978.19
2179.72
1695.34
1598.46
1521.29
1447.77
1406.66
1319.32
1204.31
1073.89
1051.09
1022.34
966.37
868.80
843.74
752.55
725.83
695.02
621.67
607.69
587.73
559.95
503.67


alaa-21b #47 RT: 0.80 AV: 1 SB: 2 2.28 , 2.26 NL: 3.04E2
T: + cEI Full ms [40.00-1000.00]
8b
Relative Abundance
m/z
54.22
69.62
75.22
83.62
98.55
116.75
123.04
135.92
142.13
146.89
147.54
160.01
164.41
179.32
185.53
191.97
195.24
199.28
224.76
227.54
241.29
264.08
274.35
295.34
302.08
306.84
315.42
334.95
338.43
341.08
351.72
361.45
377.38
392.76
396.15
412.15
415.47
423.03

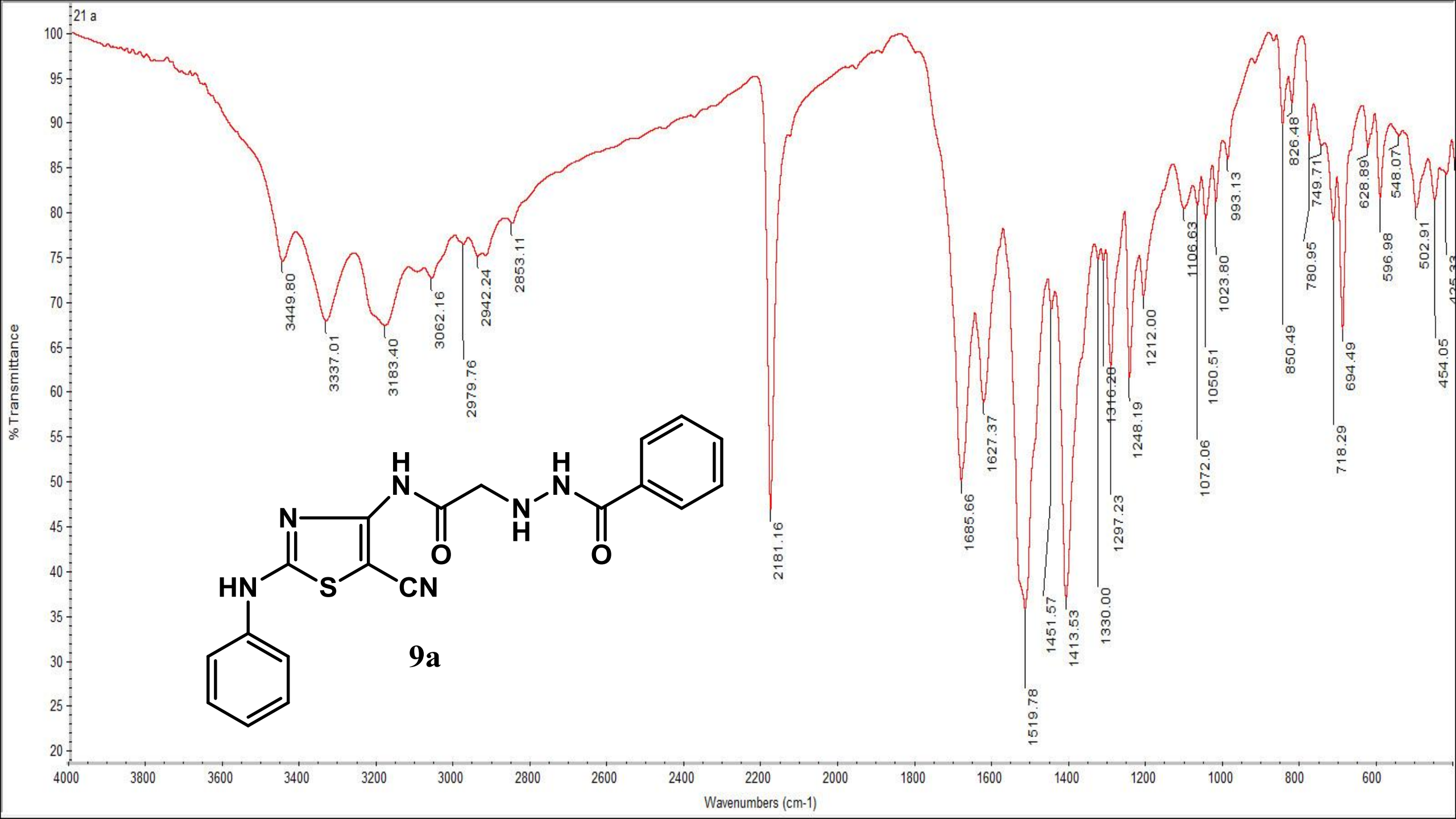
Alaa Abdallah-4-Hnmr-DMSO-A



8b

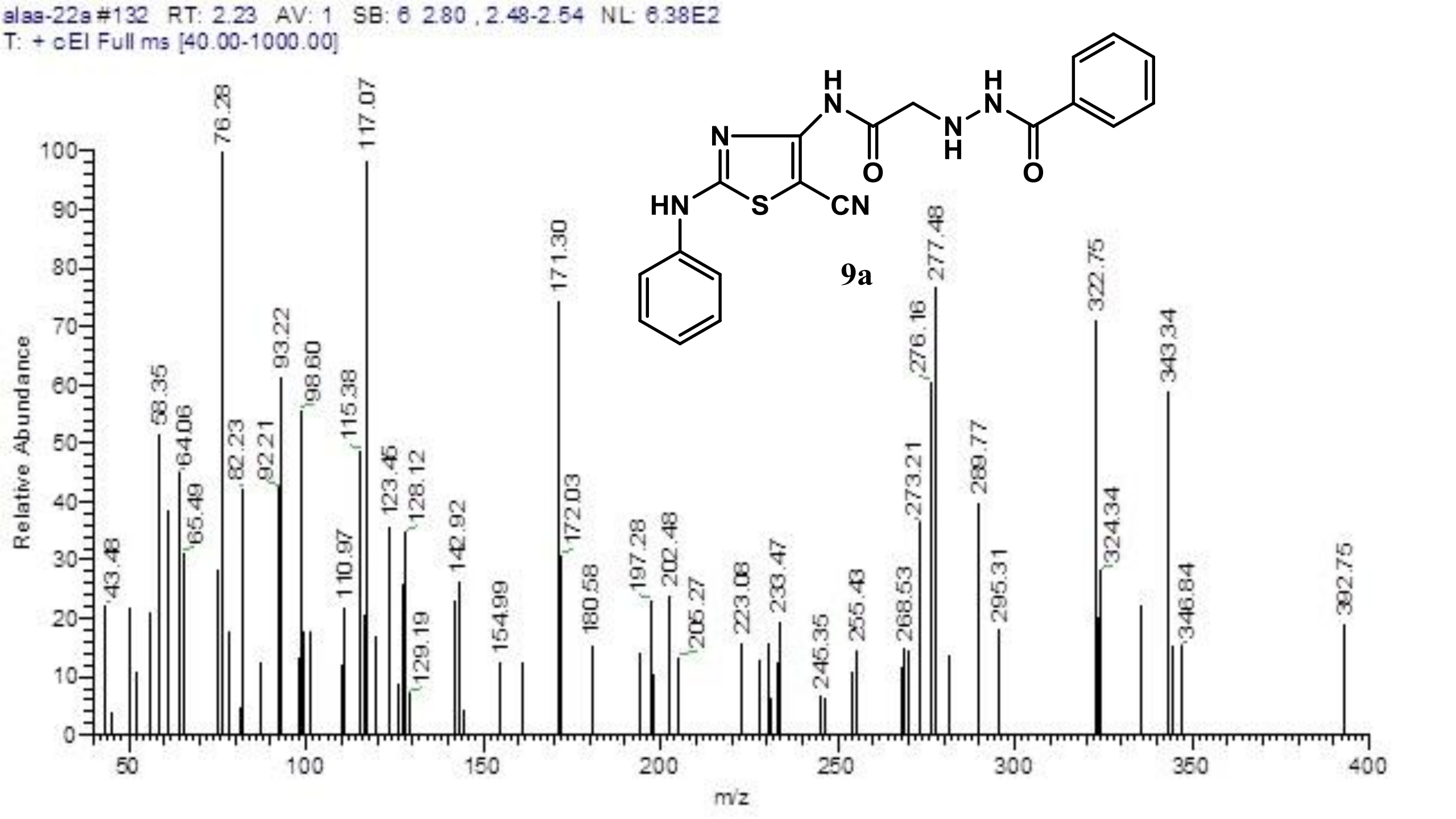
Faculty of Pharmacy

```
Current Data Parameters
NAME      Alaa Abdallah-4-Hnmr-DMSO-A
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220421
Time              13.30 h
INSTRUM             spect
PROBHD   Z108618_0945 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                135.42
DW                62.400 usec
DE                 6.50 usec
TE                296.7 K
D1             1.00000000 sec
TD0                    1
SFO1         400.2024712 MHz
NUC1                  1H
P1                13.50 usec
PLW1         13.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2000000 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```


21 a
% Transmittance
Wavenumbers (cm-1)
3449.80
3337.01
3183.40
3062.16
2979.76
2942.24
2853.11
2181.16
1685.66
1627.37
1519.78
1451.57
1413.53
1330.00
1316.28
1297.23
1248.19
1212.00
1106.63
1072.06
1050.51
1023.80
993.13
850.49
826.48
780.95
749.71
718.29
694.49
628.89
596.98
548.07
502.91
454.05
HN
S
N
H
N
O
N
H
O
CN

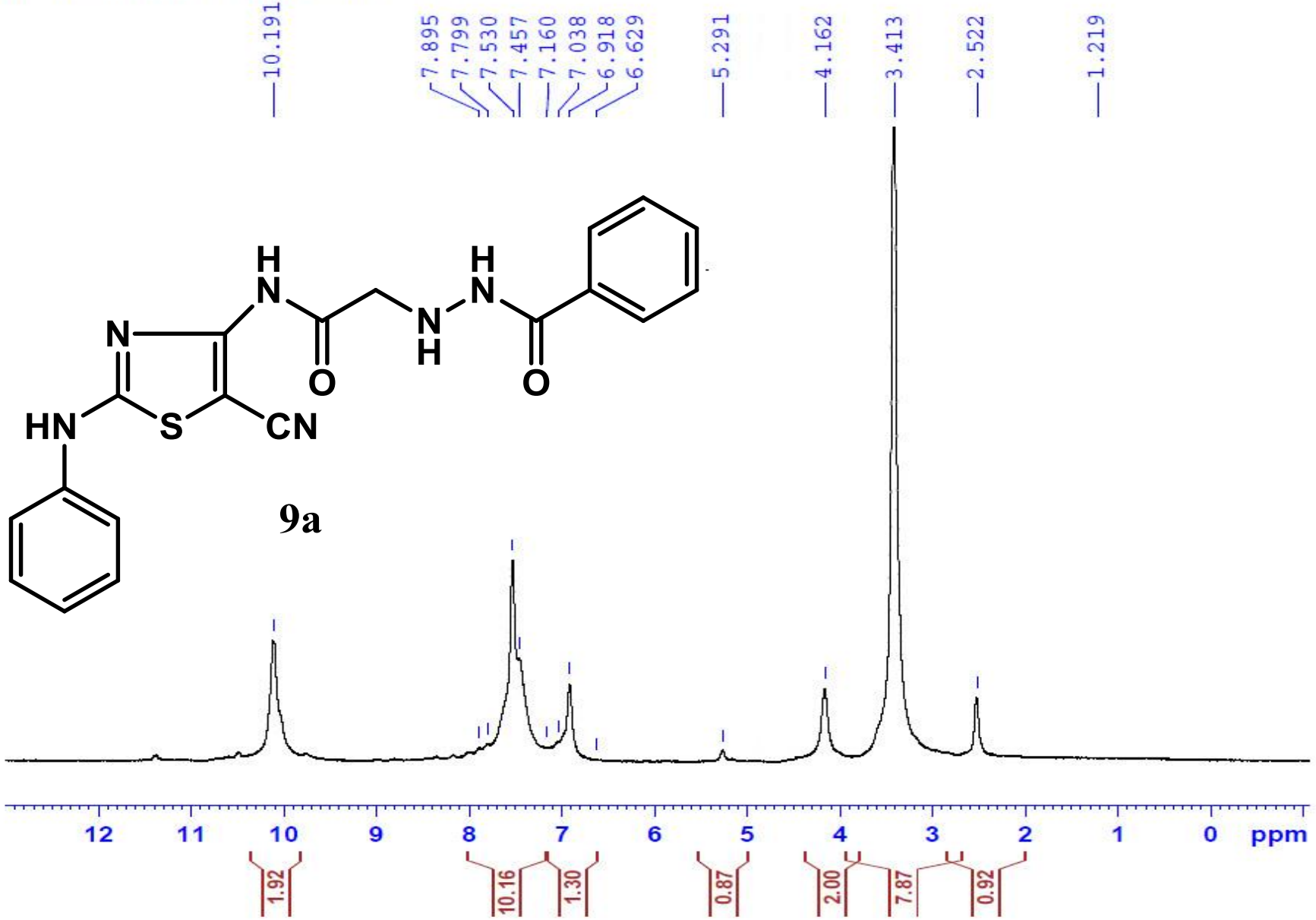
9a

alaa-22a #132 RT: 2.23 AV: 1 SB: 6 2.80 , 2.48-2.54 NL: 6.38E2
T: + cEI Full ms [40.00-1000.00]



9a

Alaa Abdullah-13-HNMR-DMSO-AF



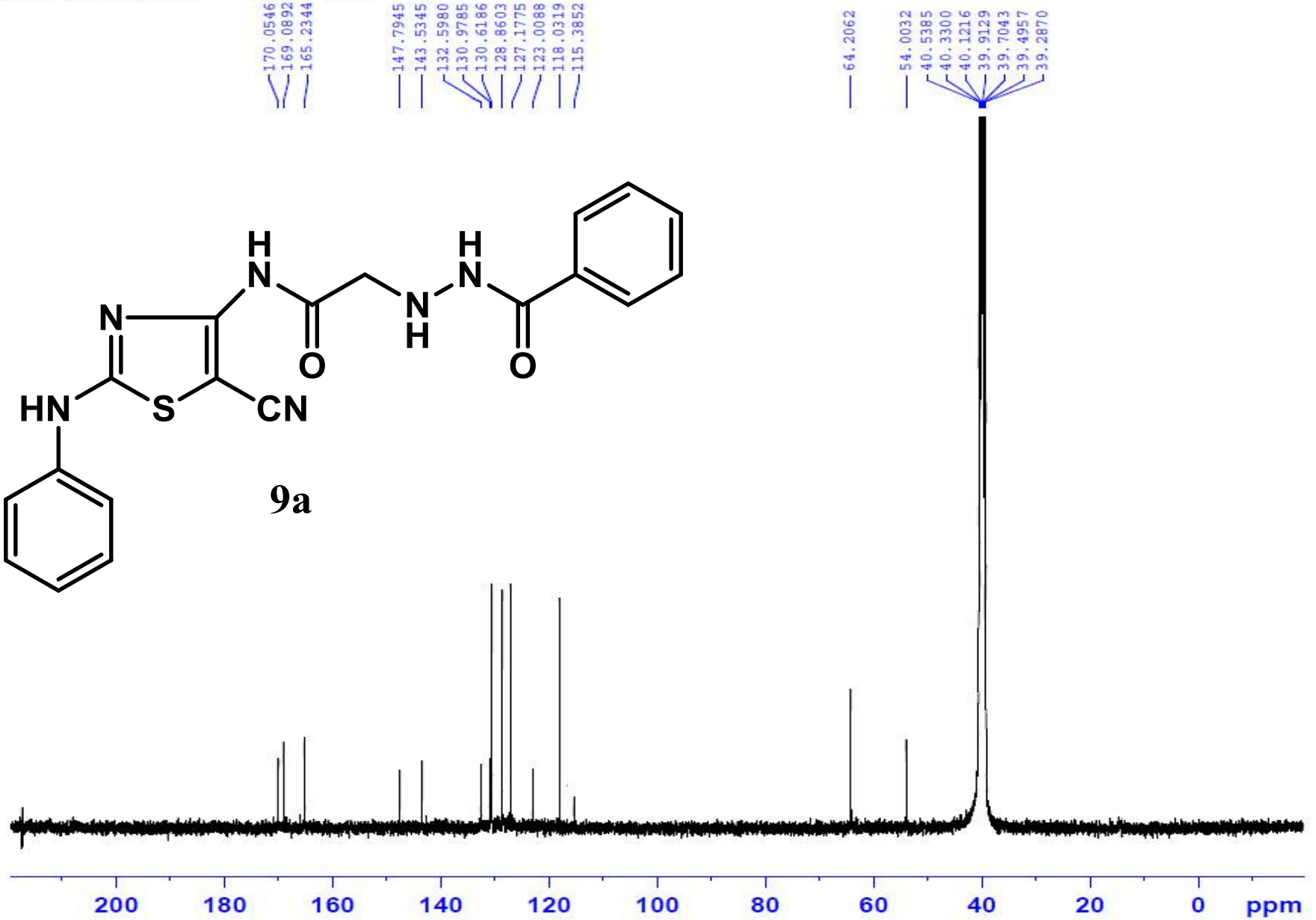
9a

BRUKER

Faculty of Pharmacy

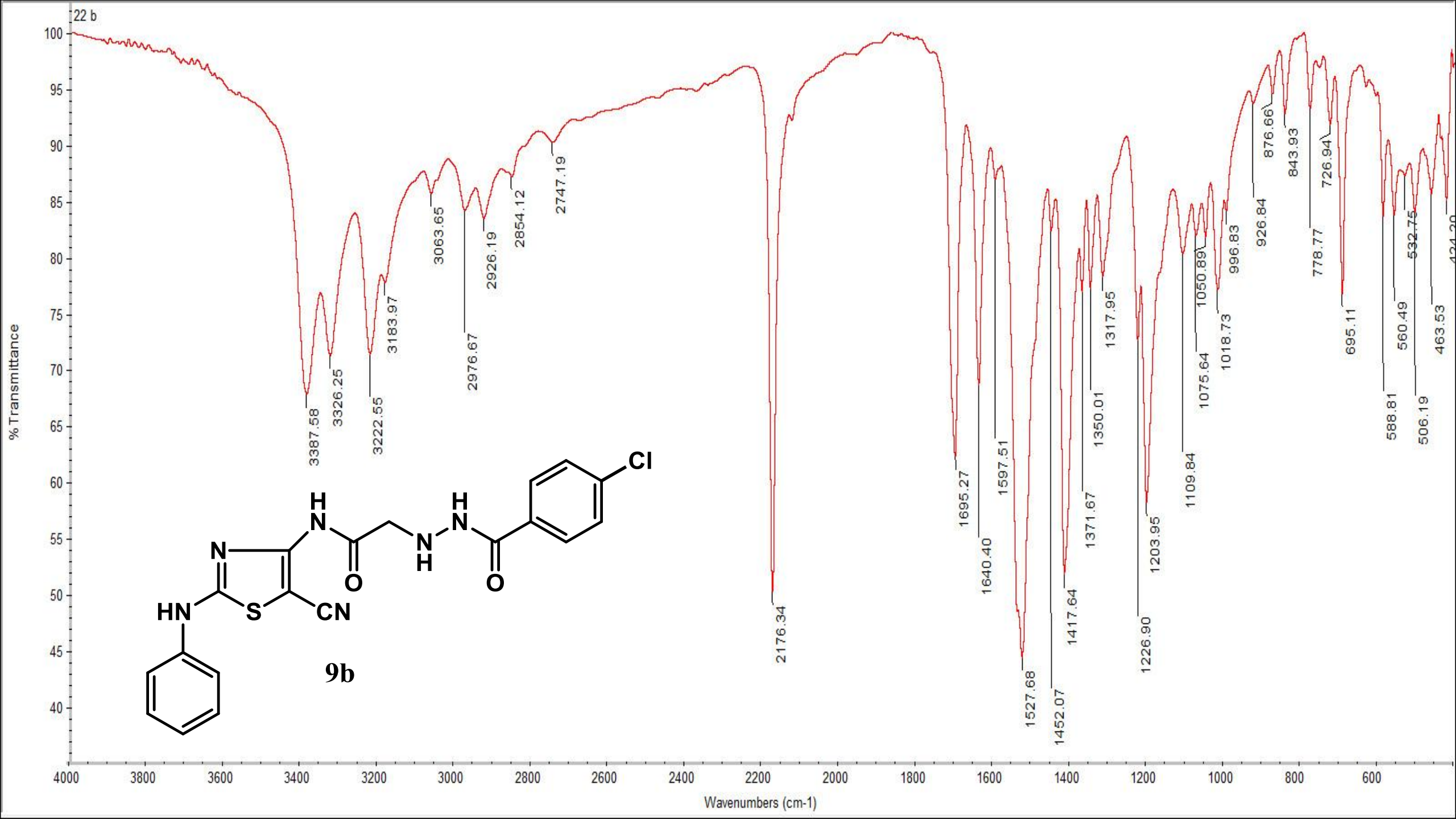
```
Current Data Parameters
NAME      Alaa Abdullah-13-HNMR
EXPNO                       10
PROCNO                       1

F2 - Acquisition Parameters
Date_               20220510
Time                  20.05 h
INSTRUM                spect
PROBHD    Z108618_0945 (
PULPROG                 zg30
TD                     65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                  4.0894465 sec
RG                     88.92
DW                    62.400 usec
DE                     6.50 usec
TE                    295.1 K
D1                  1.00000000 sec
TD0                        1
SFO1              400.2024712 MHz
NUC1                      1H
P1                    13.50 usec
PLW1             13.00000000 W

F2 - Processing parameters
SI                     65536
SF                400.2000000 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

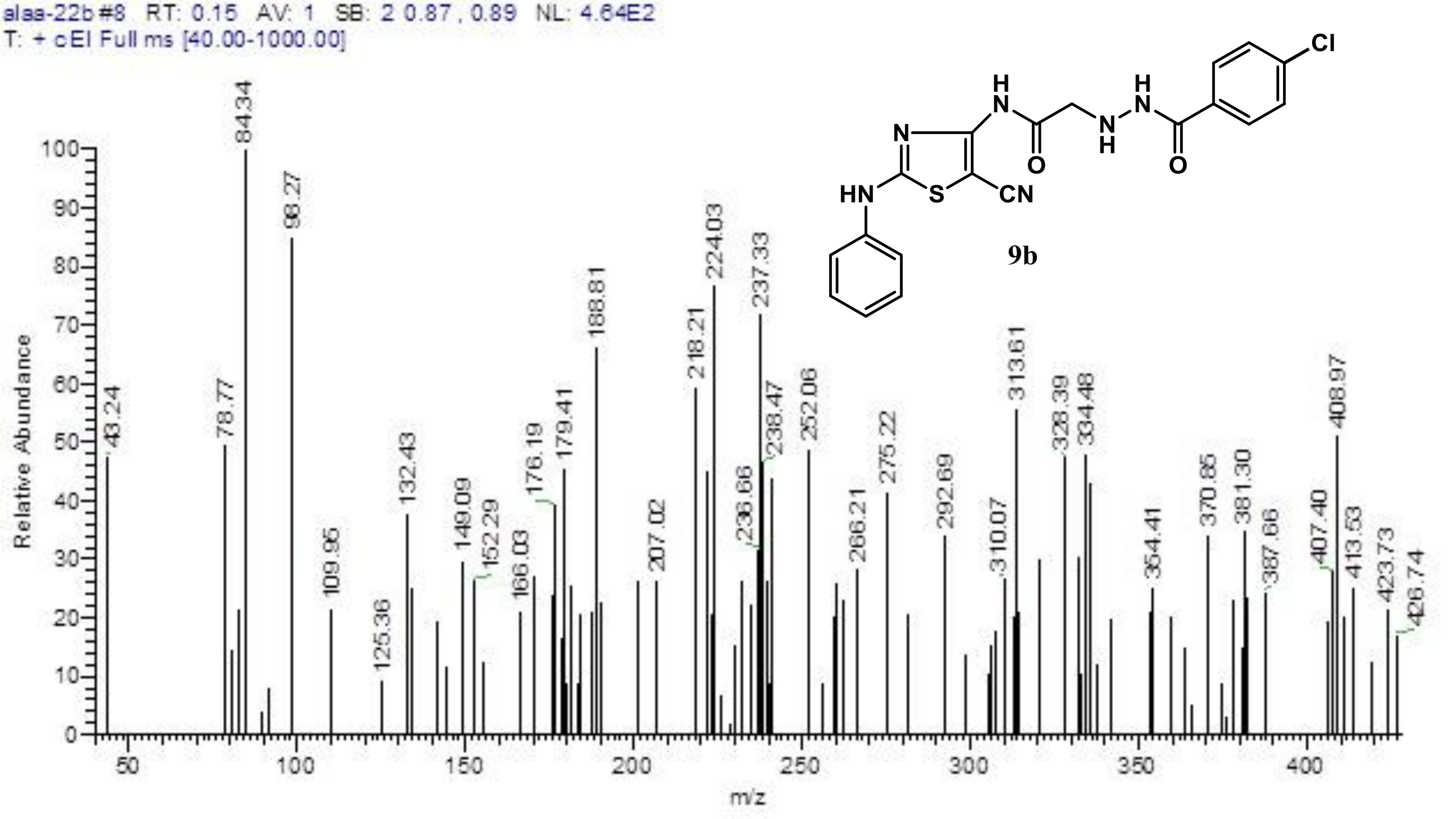
Alaa Abdullah - 13 - C13 - T



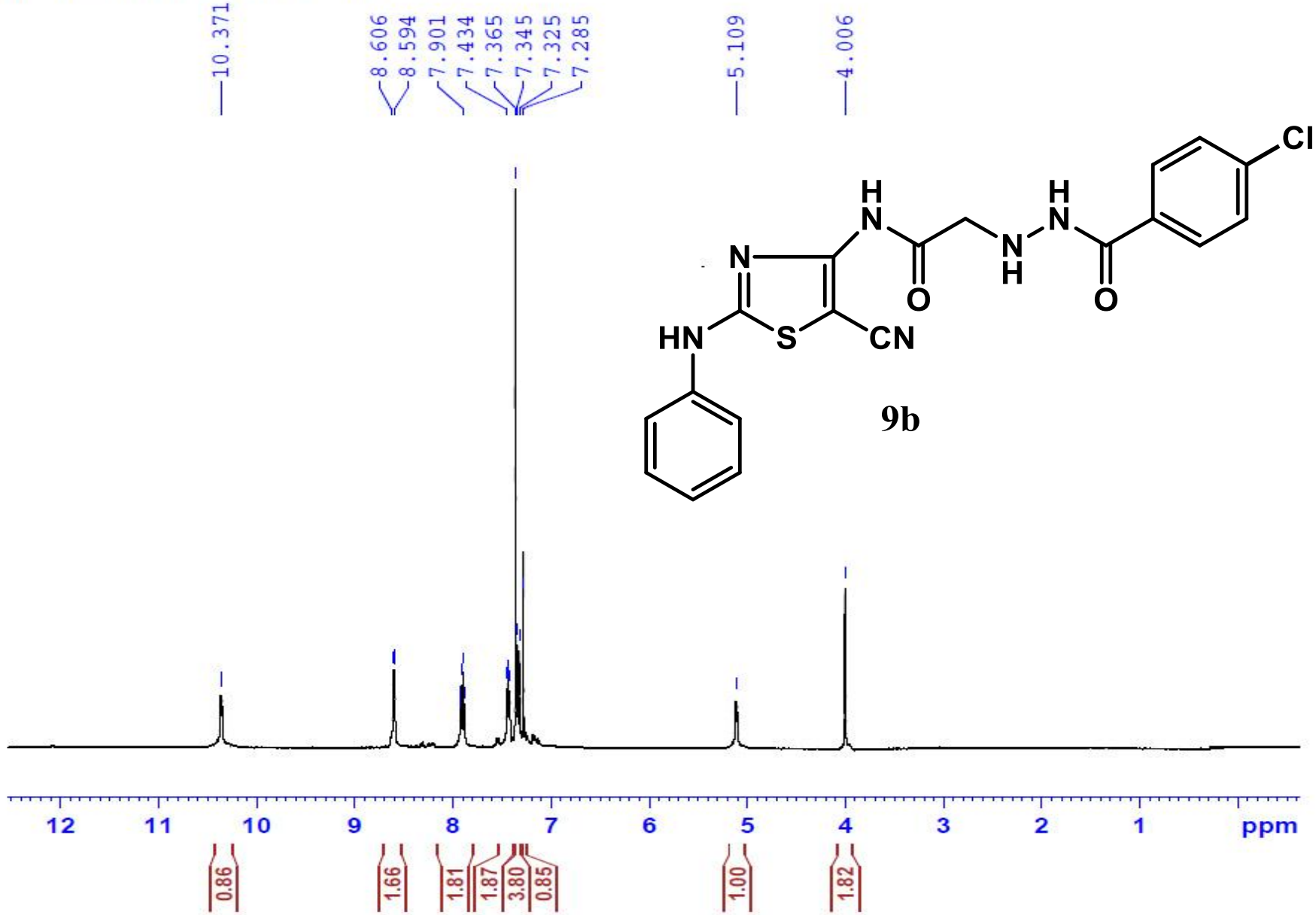
Faculty of Pharmacy

```
Current Data Parameters
NAME      Alaa Abdullah - 13 - C13 - T
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220516
Time              20.41 h
INSTRUM            spect
PROBHD   Z108618_0945 (
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                  2100
DS                     4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                197.77
DW                20.800 usec
DE                 6.50 usec
TE                300.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        100.6404331 MHz
NUC1                13C
P1                10.00 usec
PLW1        47.00000000 W
SFO2        400.2016008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        13.00000000 W
PLW12        0.29249999 W
PLW13        0.14713000 W

F2 - Processing parameters
SI                 32768
SF          100.6303700 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


22 b
% Transmittance
Wavenumbers (cm-1)
3387.58
3326.25
3222.55
3183.97
3063.65
2976.67
2926.19
2854.12
2747.19
2176.34
1695.27
1640.40
1597.51
1527.68
1452.07
1417.64
1371.67
1350.01
1317.95
1226.90
1203.95
1109.84
1075.64
1050.89
1018.73
996.83
926.84
876.66
843.93
778.77
726.94
695.11
588.81
560.49
532.75
506.19
463.53
HN
S
CN
N
H
N
O
N
H
N
H
O
Cl
9b


alaa-22b #8 RT: 0.15 AV: 1 SB: 2 0.87 , 0.89 NL: 4.64E2
T: + cEI Full ms [40.00-1000.00]
Relative Abundance
m/z
43.24
78.77
84.34
98.27
109.95
125.36
132.43
149.09
152.29
166.03
176.19
179.41
188.81
207.02
218.21
224.03
236.66
237.33
238.47
252.06
266.21
275.22
292.69
310.07
313.61
328.39
334.48
354.41
370.85
381.30
387.66
407.40
408.97
413.53
423.73
426.74
9b

Alaa Abdullah-14-HNMR-DMSO-AF

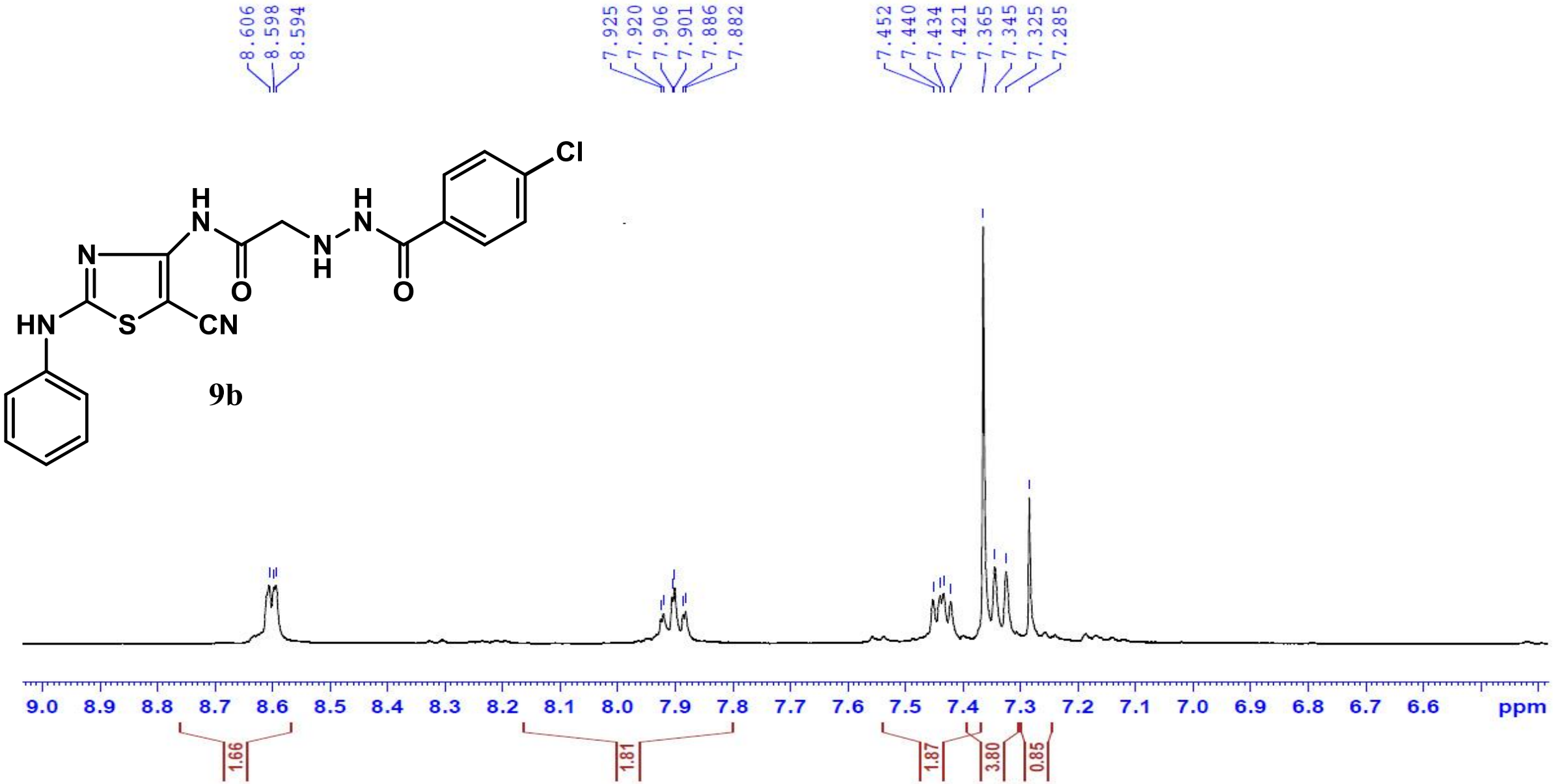


9b

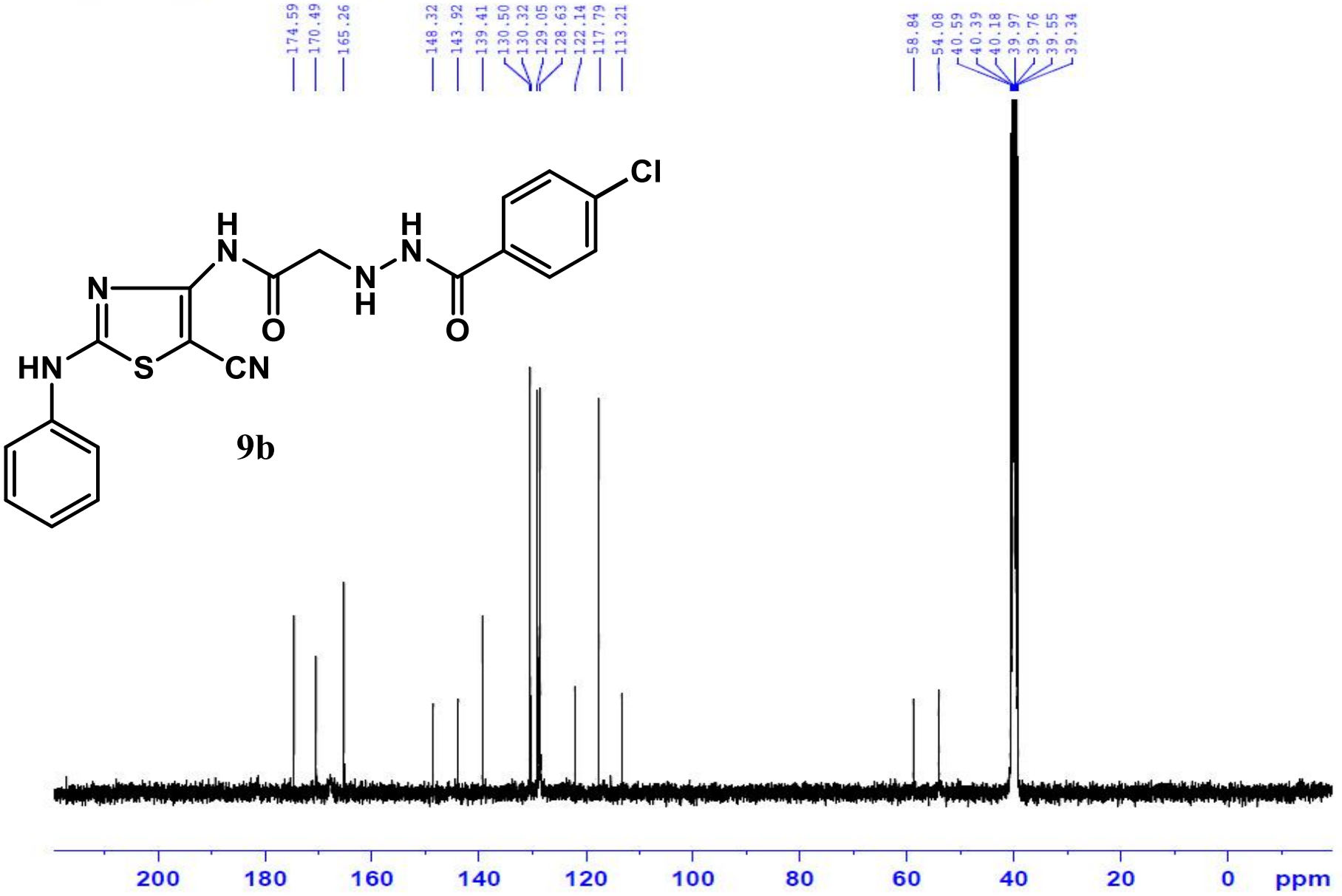
Faculty of Pharmacy

```
Current Data Parameters
NAME      Alaa Abdullah-14-HNMR
EXPNO                       10
PROCNO                       1

F2 - Acquisition Parameters
Date_               20220510
Time                  20.11 h
INSTRUM                 spect
PROBHD    Z108618_0945 (
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                  4.0894465 sec
RG                     88.92
DW                    62.400 usec
DE                     6.50 usec
TE                    295.0 K
D1                 1.00000000 sec
TD0                        1
SFO1           400.2024712 MHz
NUC1                      1H
P1                    13.50 usec
PLW1           13.00000000 W

F2 - Processing parameters
SI                     65536
SF             400.2000000 MHz
WDW                       EM
SSB          0
LB                    0.30 Hz
GB           0
PC                     1.00
```

Alaa Abdullah-14-HNMR-DMSO-AF



Alaa Abdallah-14-carbon-WH



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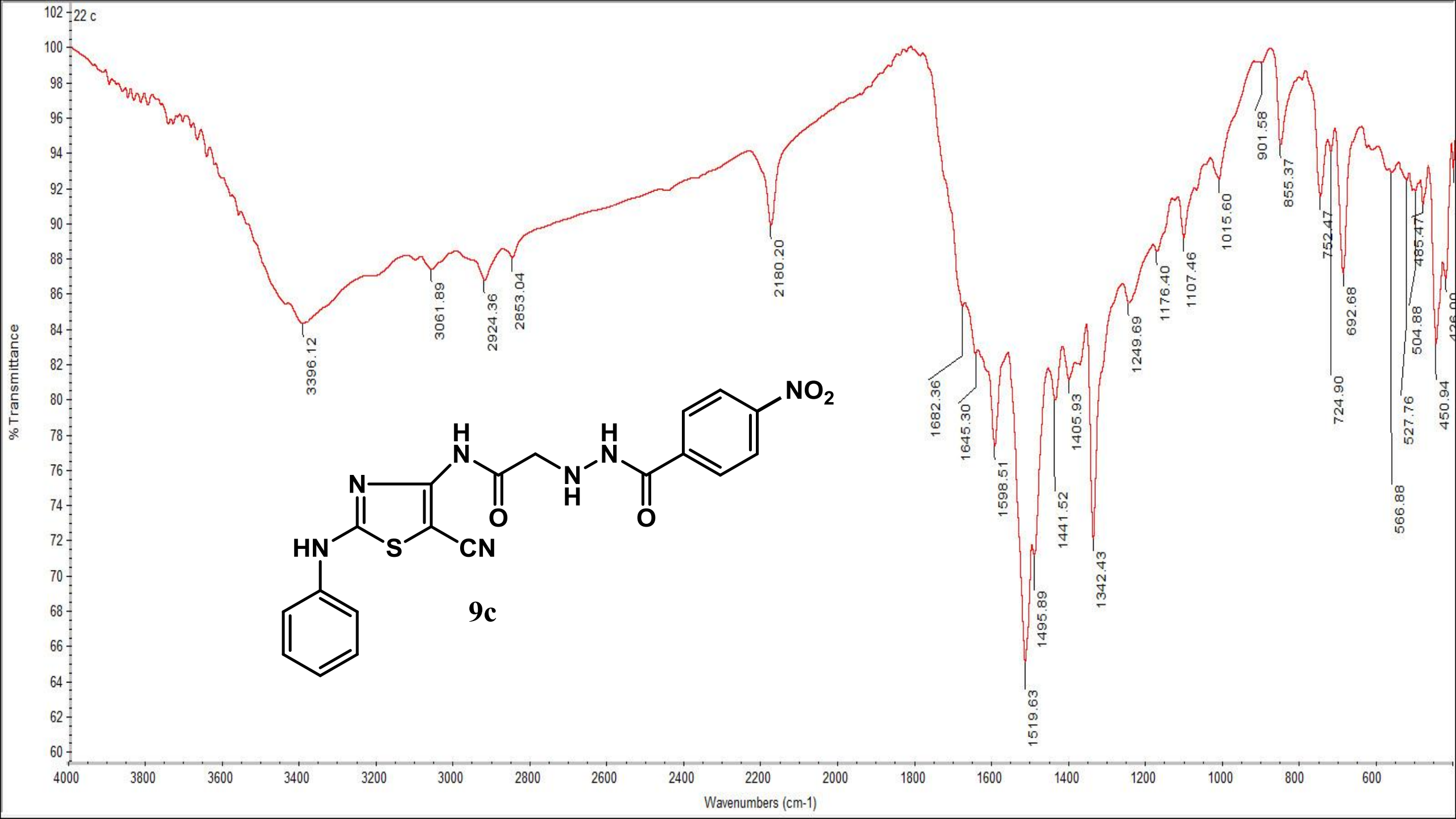
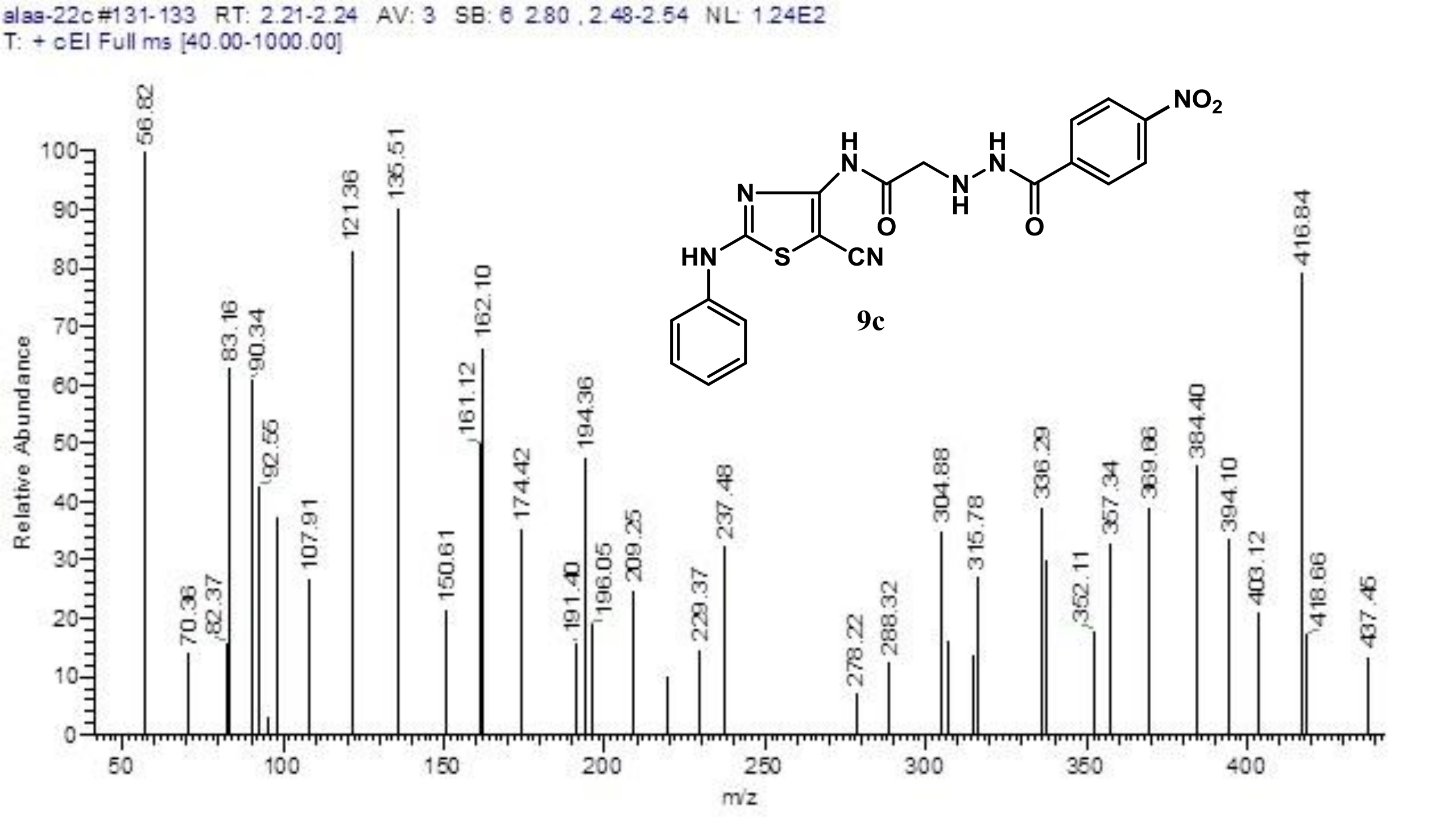
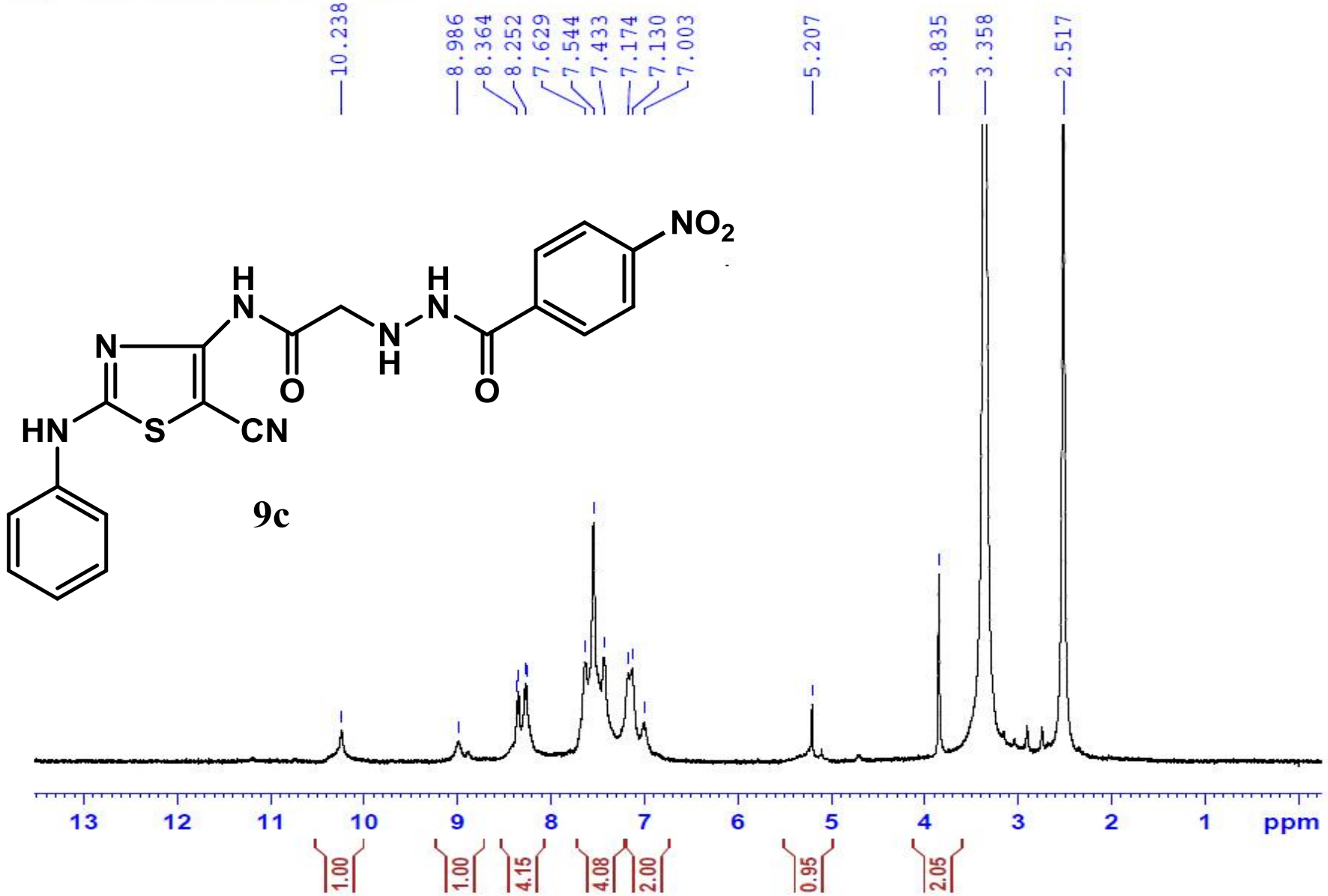
```
Current Data Parameters
NAME      Alaa Abdallah-Et.cl.A+phNCS-carbon-WH
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210903
Time_              2.43 h
INSTRUM           spect
PROBHD   Z108618_0945 (
PULPROG        zgpg30
TD              65536
SOLVENT          DMSO
NS                2220
DS                   4
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            1.3631488 sec
RG               197.77
DW               20.800 usec
DE                6.50 usec
TE              298.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        100.6404331 MHz
NUC1              13C
P1               10.00 usec
PLW1        47.00000000 W
SFO2        400.2016008 MHz
NUC2              1H
CPDPRG[2       waltz16
PCPD2            90.00 usec
PLW2        13.00000000 W
PLW12        0.29249999 W
PLW13        0.14713000 W

F2 - Processing parameters
SI               32768
SF          100.6303700 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```


22 c
% Transmittance
Wavenumbers (cm-1)
3396.12
3061.89
2924.36
2853.04
2180.20
1682.36
1645.30
1598.51
1519.63
1495.89
1441.52
1405.93
1342.43
1249.69
1176.40
1107.46
1015.60
901.58
855.37
752.47
724.90
692.68
566.88
527.76
504.88
485.47
450.94
NO2
H
N
N
H
N
H
O
O
N
S
HN
CN
9c


alaa-22c #131-133 RT: 2.21-2.24 AV: 3 SB: 6 2.80 , 2.48-2.54 NL: 1.24E2
T: + cEI Full ms [40.00-1000.00]
Relative Abundance
m/z
56.82
70.36
82.37
83.16
90.34
92.55
107.91
121.36
135.51
150.61
161.12
162.10
174.42
191.40
194.36
196.05
209.25
229.37
237.48
278.22
288.32
304.88
315.78
336.29
352.11
357.34
369.06
384.40
394.10
403.12
416.84
418.66
437.45
NO2
H
N
N
N
H
N
H
O
O
HN
S
CN
9c

Alaa Abdullah-24-HNMR-DMSO-AF



9c

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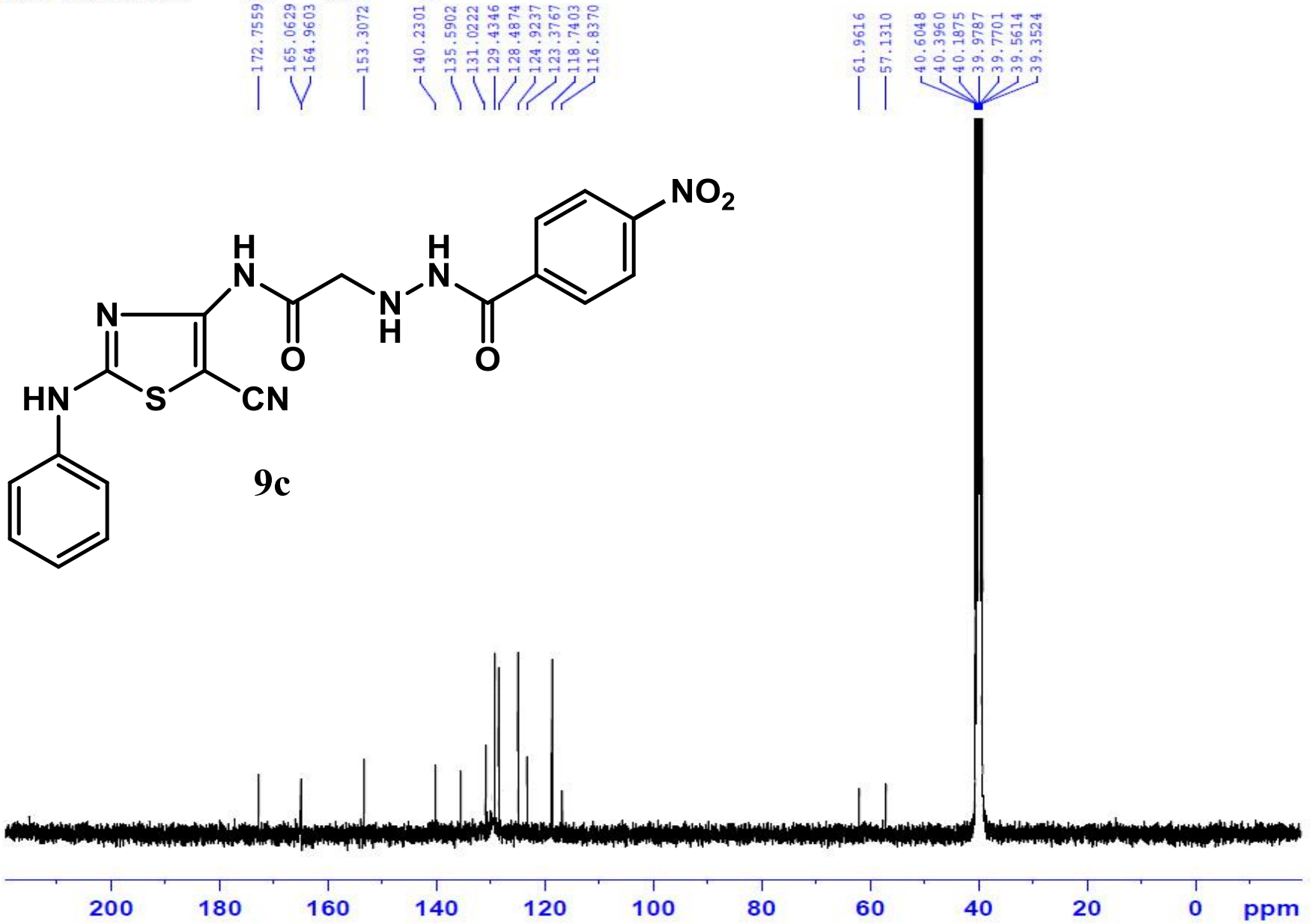
```
Current Data Parameters
NAME      Alaa Abdullah-24-HNMR
EXPNO                       10
PROCNO                       1

F2 - Acquisition Parameters
Date_               20220510
Time                  15.28 h
INSTRUM                spect
PROBHD    Z108618_0945 (
PULPROG                 zg30
TD                     65536
SOLVENT                 DMSO
NS                        16
DS                         2
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                  4.0894465 sec
RG                     197.77
DW                     62.400 usec
DE                      6.50 usec
TE                     295.4 K
D1                  1.00000000 sec
TD0                        1
SFO1             400.2024712 MHz
NUC1                       1H
P1                     13.50 usec
PLW1            13.00000000 W

F2 - Processing parameters
SI                     65536
SF               400.2000000 MHz
WDW                       EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

Alaa Abdullah - 20 - C13 - T



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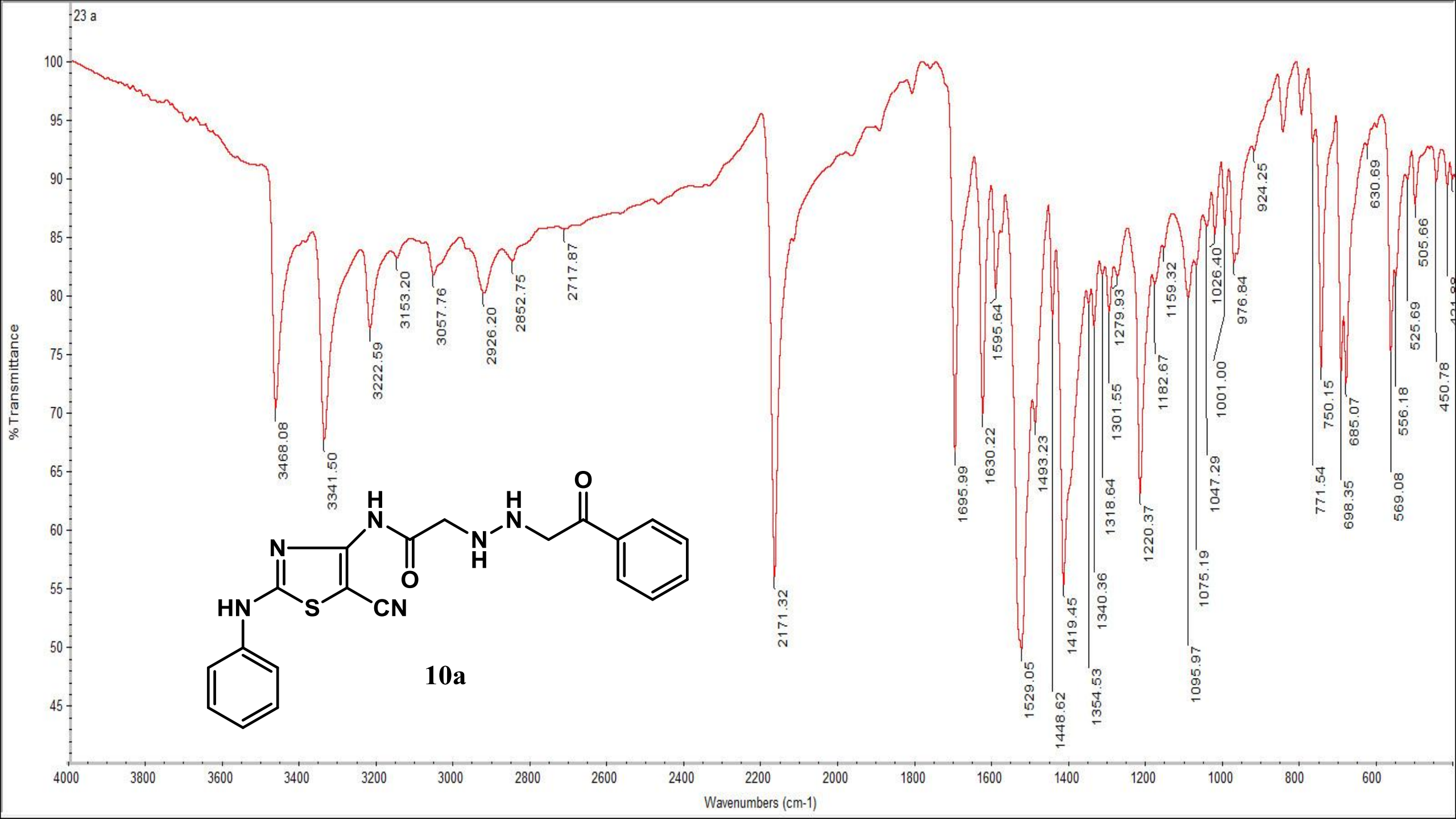
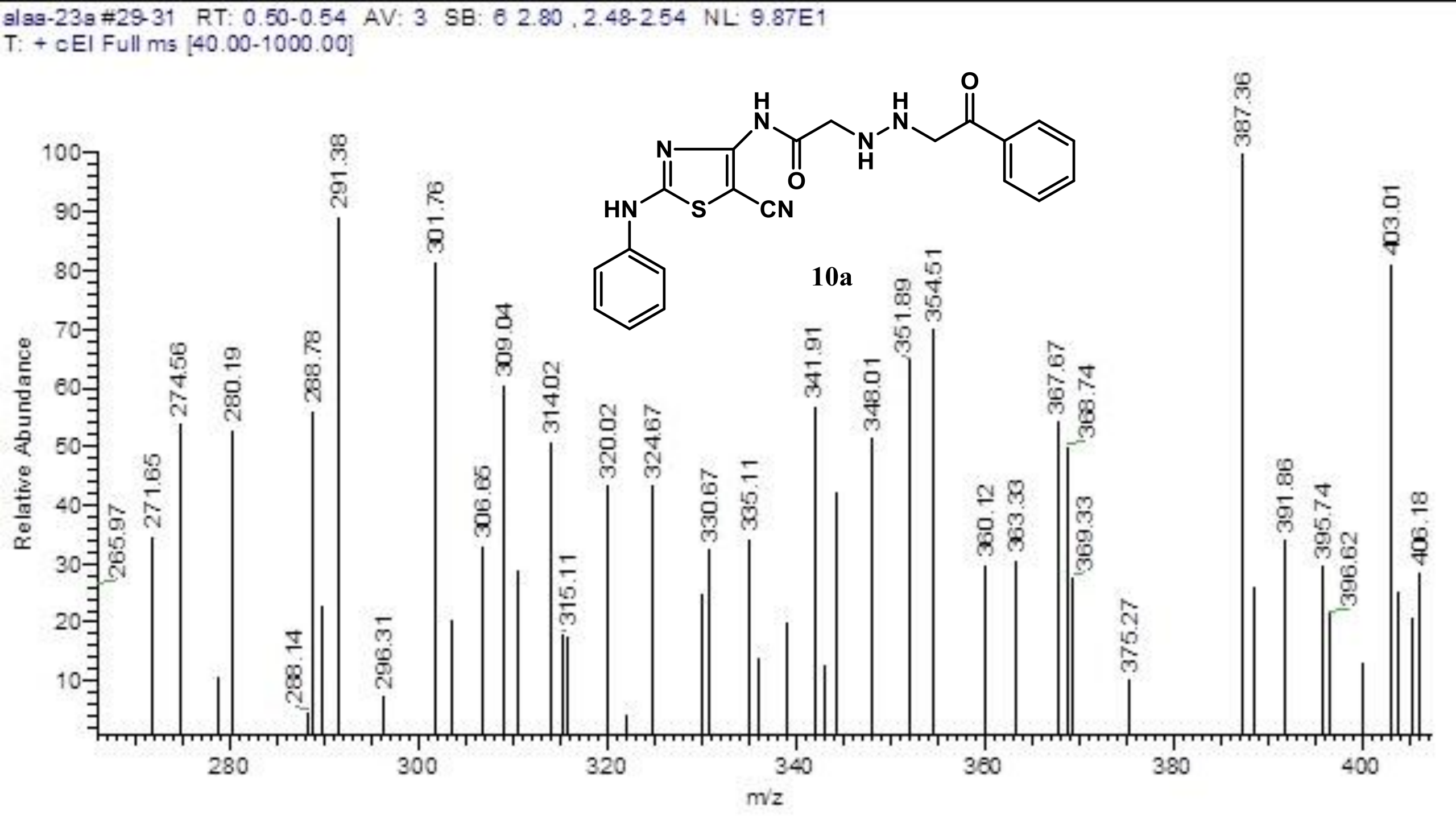
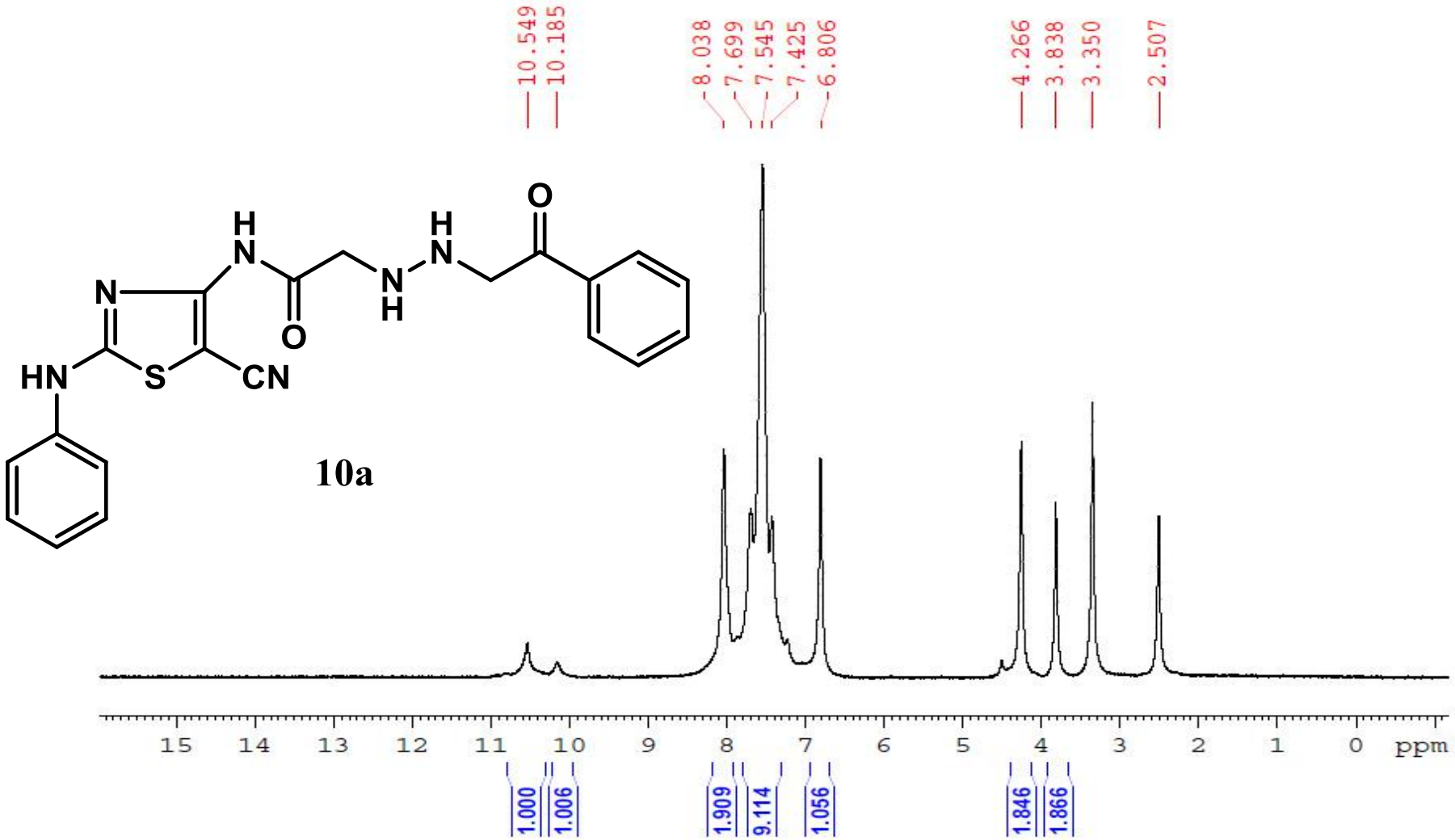
```
Current Data Parameters
NAME      Alaa Abdullah - 20 - C13 - T
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220517
Time               4.54 h
INSTRUM           spect
PROBHD    Z108618_0945 (
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                  2100
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                197.77
DW                20.800 usec
DE                 6.50 usec
TE                296.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        100.6404331 MHz
NUC1                13C
P1                10.00 usec
PLW1        47.00000000 W
SFO2        400.2016008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        13.00000000 W
PLW12        0.29249999 W
PLW13        0.14713000 W

F2 - Processing parameters
SI                 32768
SF          100.6303700 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


23 a
% Transmittance
Wavenumbers (cm-1)
3468.08
3341.50
3222.59
3153.20
3057.76
2926.20
2852.75
2717.87
2171.32
1695.99
1630.22
1595.64
1529.05
1493.23
1448.62
1419.45
1354.53
1340.36
1318.64
1301.55
1279.93
1220.37
1182.67
1159.32
1095.97
1075.19
1047.29
1026.40
1001.00
976.84
924.25
771.54
750.15
698.35
685.07
630.69
569.08
556.18
525.69
505.66
450.78
HN
N
S
CN
H
N
O
N
H
H
N
O

10a


alaa-23a #29-31 RT: 0.50-0.54 AV: 3 SB: 6 2.80 , 2.48-2.54 NL: 9.87E1
T: + cEI Full ms [40.00-1000.00]
10a
Relative Abundance
m/z
265.97
271.65
274.56
280.19
288.14
288.78
291.38
296.31
301.76
306.85
309.04
314.02
315.11
320.02
324.67
330.67
335.11
341.91
348.01
351.89
354.51
360.12
363.33
367.67
368.74
369.33
375.27
387.36
391.86
395.74
396.62
403.01
406.18

Alaa Abdallah-ClAcl+PhCl-AS-proton



10a

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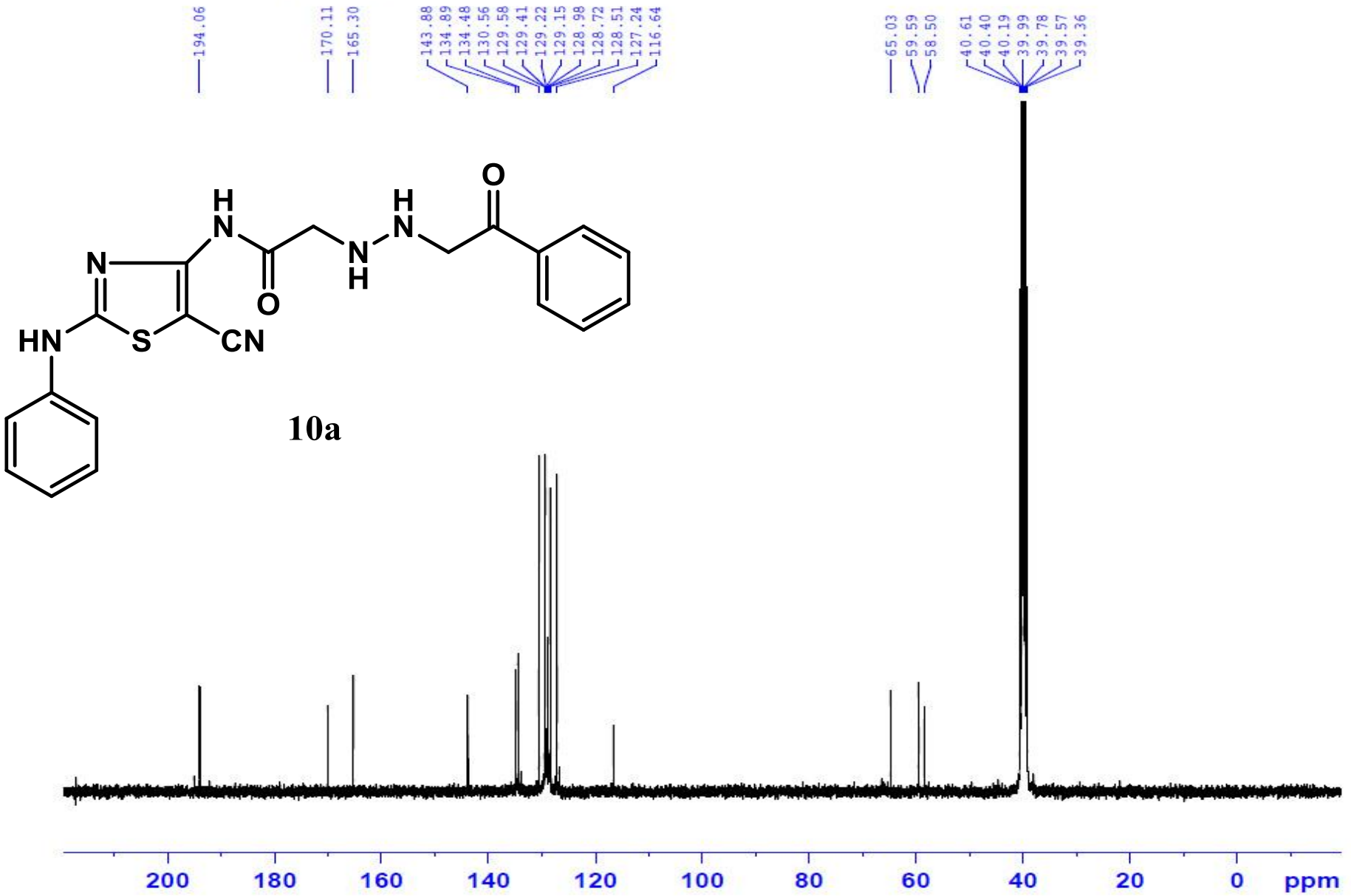
```
Current Data Parameters
NAME      Alaa Abdallah-ClAcl+PhCl-AS-proton
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210815
Time               9.37 h
INSTRUM           spect
PROBHD   Z108618_0945 (
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                158.72
DW                62.400 usec
DE                 6.50 usec
TE                295.5 K
D1             1.00000000 sec
TD0                    1
SFO1          400.2024712 MHz
NUC1                  1H
P1                13.50 usec
PLW1          13.00000000 W

F2 - Processing parameters
SI                65536
SF            400.2000000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

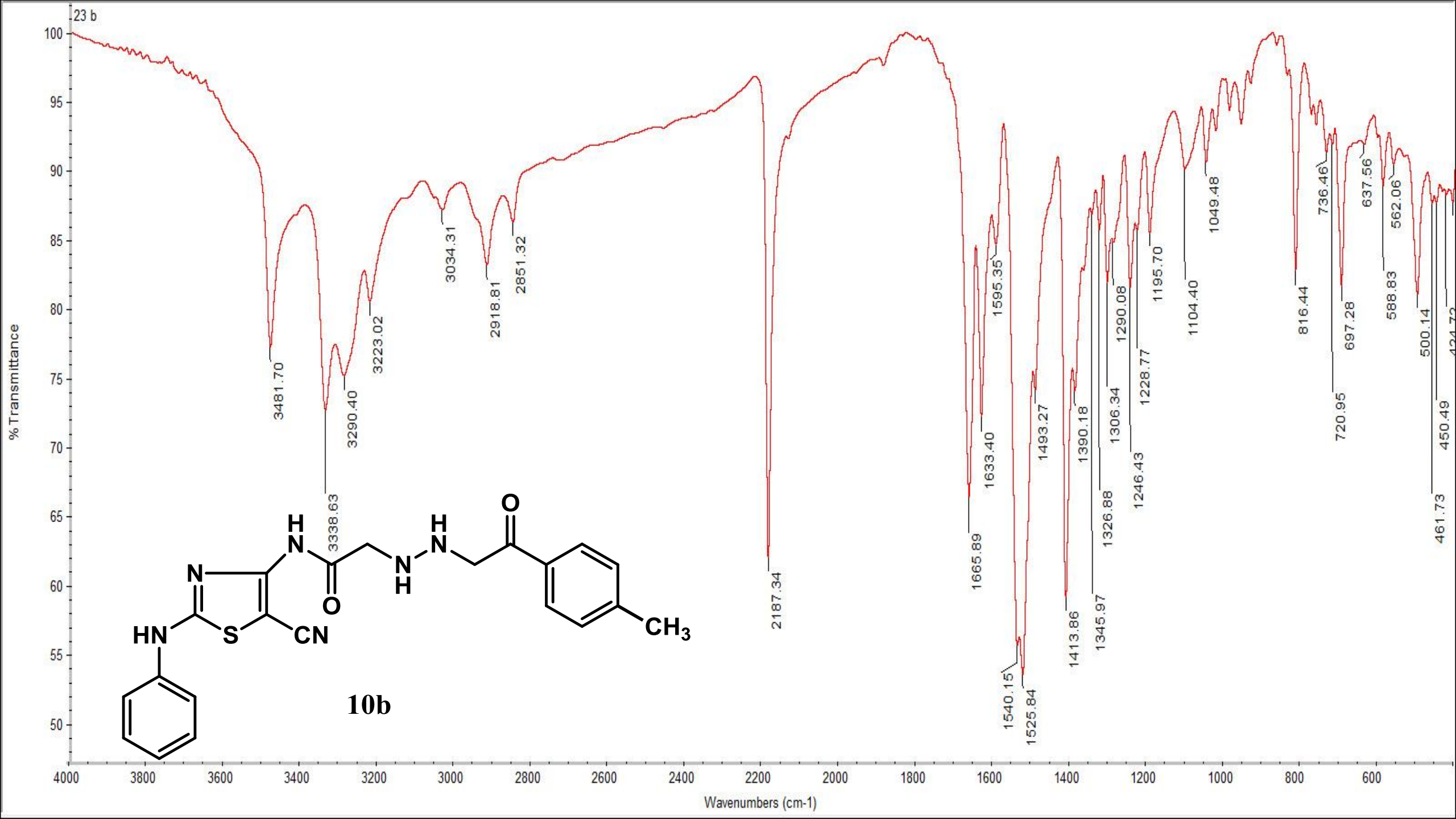
Alaa Abdallah-cl.Acl+ph.cl-carbon-WH



10a

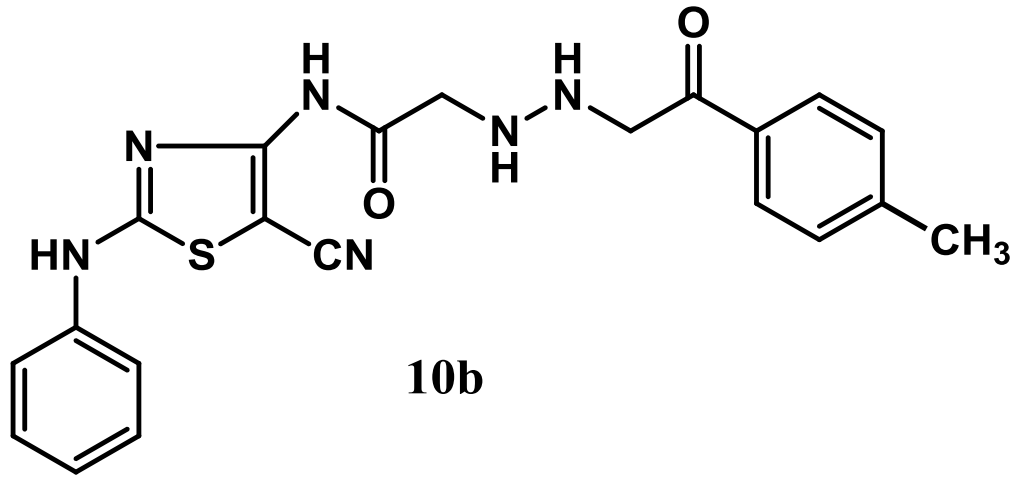
Faculty of Pharmacy

```
Current Data Parameters
NAME      Alaa Abdallah-cl.Acl+ph.cl-carbon-WH
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210902
Time               22.22 h
INSTRUM             spect
PROBHD   Z108618_0945 (
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                  2220
DS                     4
SWH            24038.461 Hz
FIDRES             0.733596 Hz
AQ                 1.3631488 sec
RG                   197.77
DW                  20.800 usec
DE                   6.50 usec
TE                  298.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6404331 MHz
NUC1                  13C
P1                  10.00 usec
PLW1          47.00000000 W
SFO2          400.2016008 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          13.00000000 W
PLW12          0.29249999 W
PLW13          0.14713000 W

F2 - Processing parameters
SI                 32768
SF            100.6303700 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```


23 b
% Transmittance
Wavenumbers (cm-1)
3481.70
3338.63
3290.40
3223.02
3034.31
2918.81
2851.32
2187.34
1665.89
1633.40
1595.35
1540.15
1525.84
1493.27
1413.86
1390.18
1345.97
1326.88
1306.34
1290.08
1246.43
1228.77
1195.70
1104.40
1049.48
816.44
736.46
720.95
697.28
637.56
588.83
562.06
500.14
461.73
450.49
HN
N
S
CN
H
N
O
N
H
H
N
O
CH3

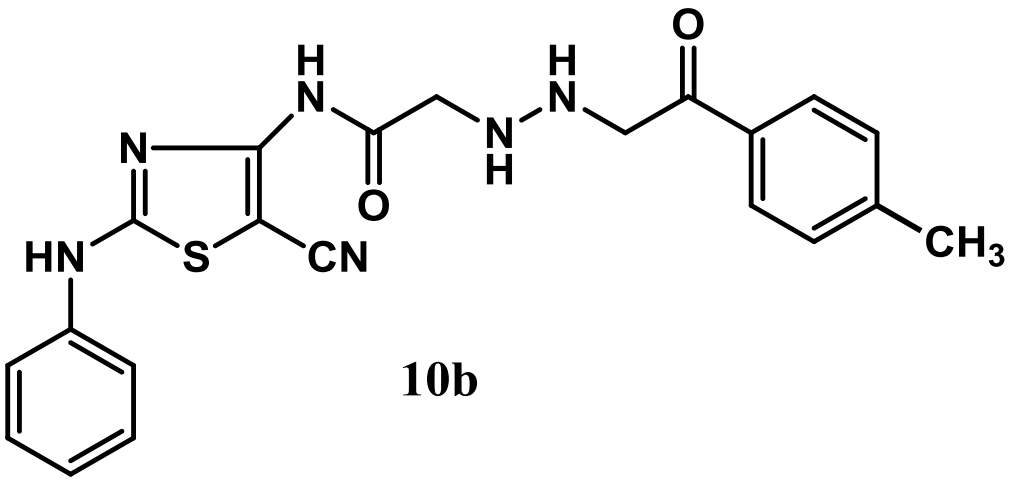
10b

alaa-23b #168-169 RT: 2.83-2.85 AV: 2 SB: 6 2.80 , 2.48-2.54 NL: 2.42E2
T: + cEI Full ms [40.00-1000.00]



10b

Alaa Abdallah - 23(2) - Hnmr - T



10b

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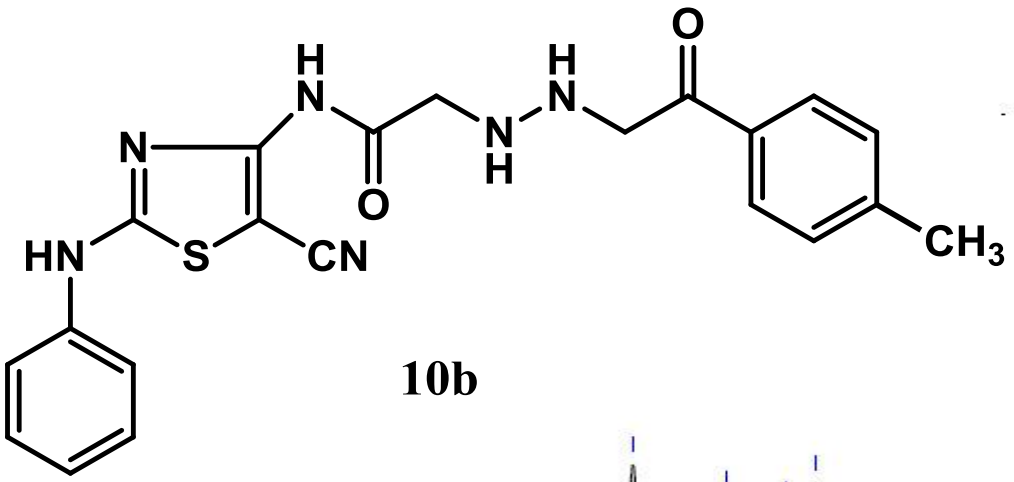
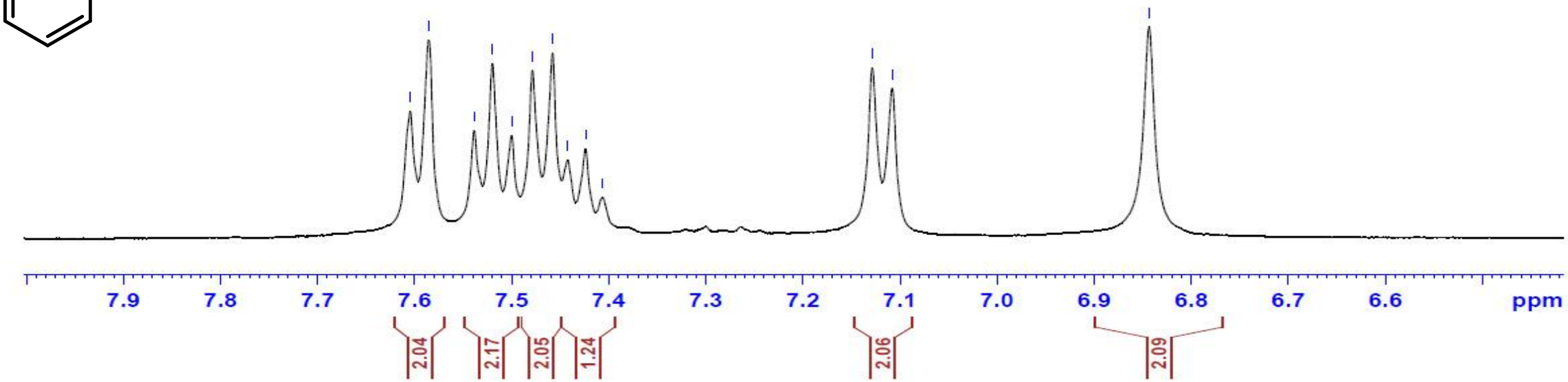
```
Current Data Parameters
NAME      Alaa Abdallah - 23(2) - Hnmr - T
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220528
Time                22.25 h
INSTRUM             spect
PROBHD   Z108618_0945 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                  158.72
DW                  62.400 usec
DE                   6.50 usec
TE                  297.4 K
D1               1.00000000 sec
TD0                    1
SFO1           400.2024712 MHz
NUC1                  1H
P1                  13.50 usec
PLW1            13.00000000 W

F2 - Processing parameters
SI                 65536
SF             400.2000000 MHz
WDW                   EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

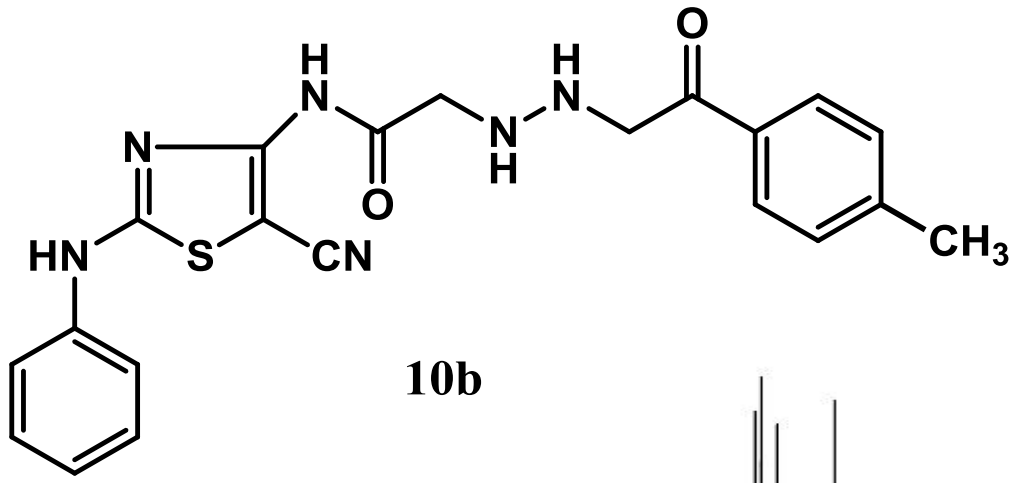
Alaa Abdallah - 23(2) - Hnmr - T



10b



Alaa Abdallah - 23(2) - C13 - T



10b

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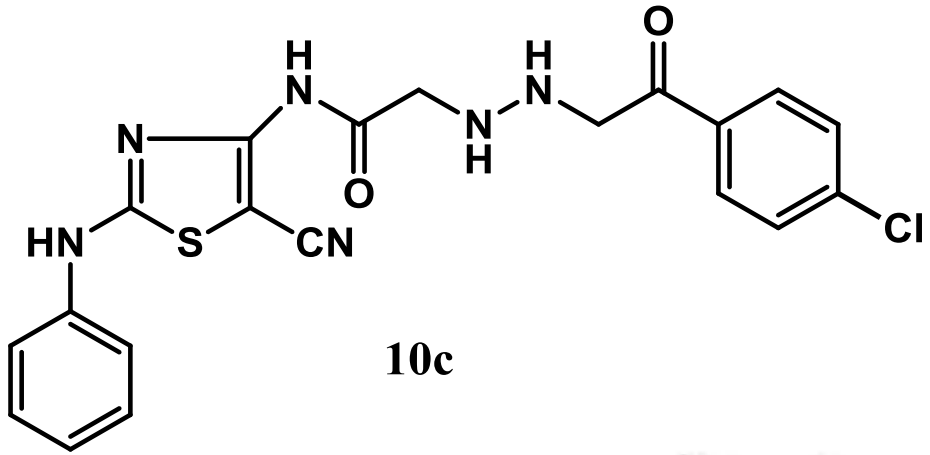
```
Current Data Parameters
NAME      Alaa Abdallah - 23(2) - C13 - T
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220606
Time              14.53 h
INSTRUM             spect
PROBHD    Z108618_0945 (
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                  2100
DS                     4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                197.77
DW                20.800 usec
DE                 6.50 usec
TE                296.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         100.6404331 MHz
NUC1                13C
P1                 10.00 usec
PLW1         47.00000000 W
SFO2         400.2016008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.00000000 W
PLW12         0.29249999 W
PLW13         0.14713000 W

F2 - Processing parameters
SI                 32768
SF           100.6303700 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

alaa-23c #245-246 RT: 4.12-4.13 AV: 2 SB: 6 2.80 , 2.48-2.54 NL: 3.00E2
T: + cEI Full ms [40.00-1000.00]



10c

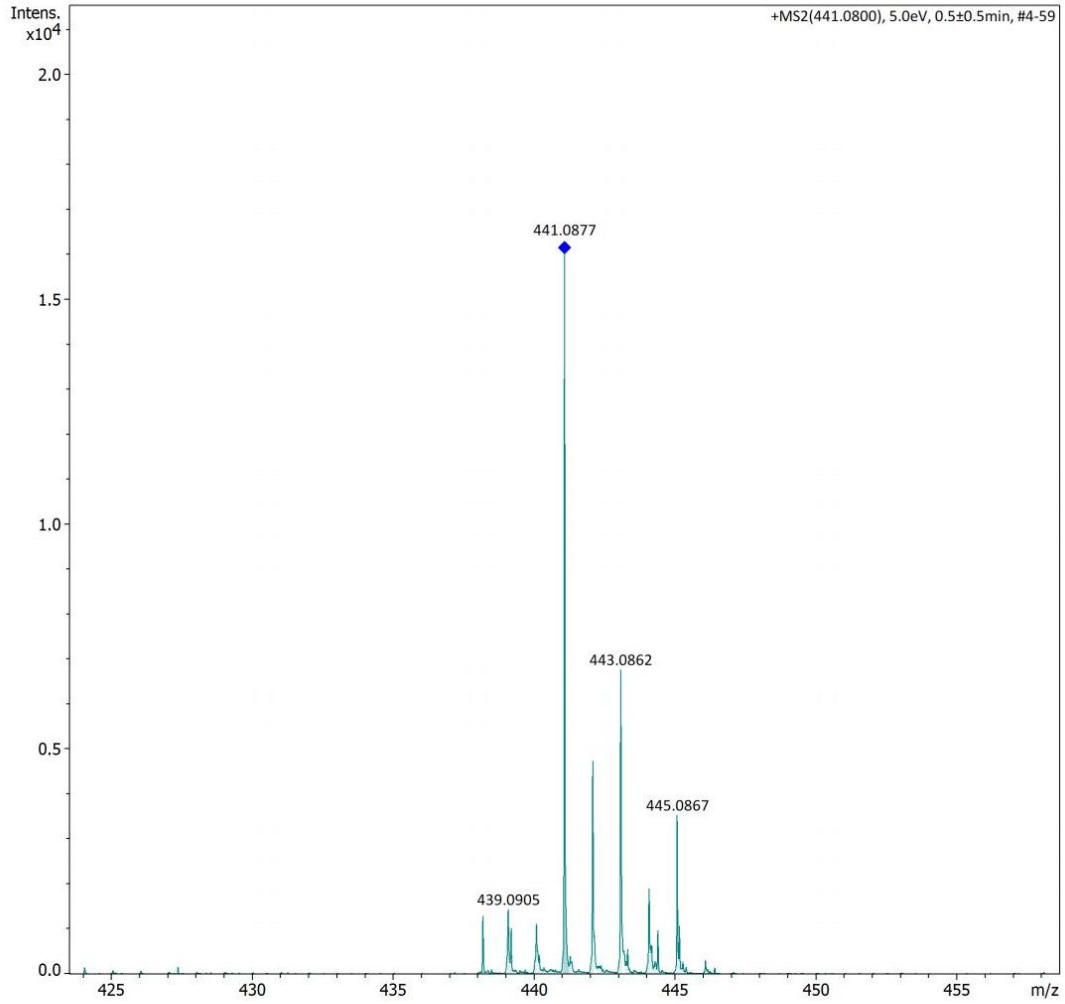
Display Report

Analysis Info

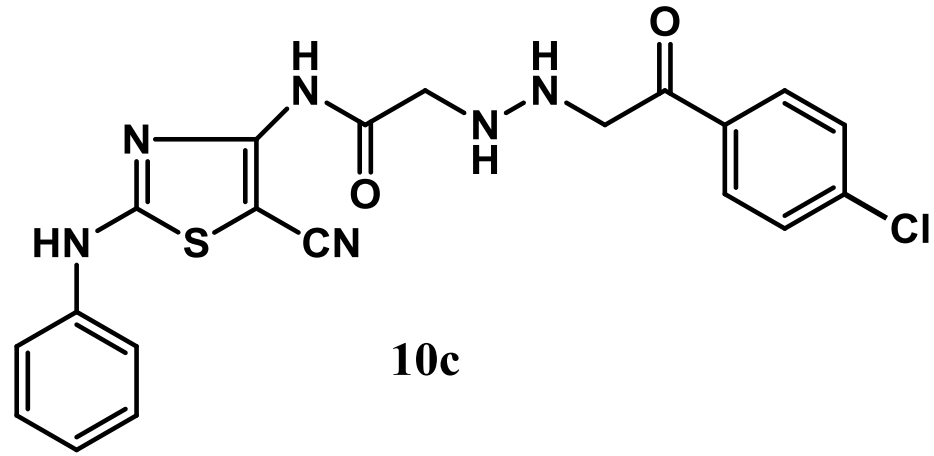
Analysis Name	D:\Data\Training\Alaa Abd Allah\10 c\New folder\10c 10ppm.d	Acquisition Date	2/12/2024 10:13:53 AM
Method	pip1.m	Operator	Demo User
Sample Name	10c	Instrument	compact 8255754.20351
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	400 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

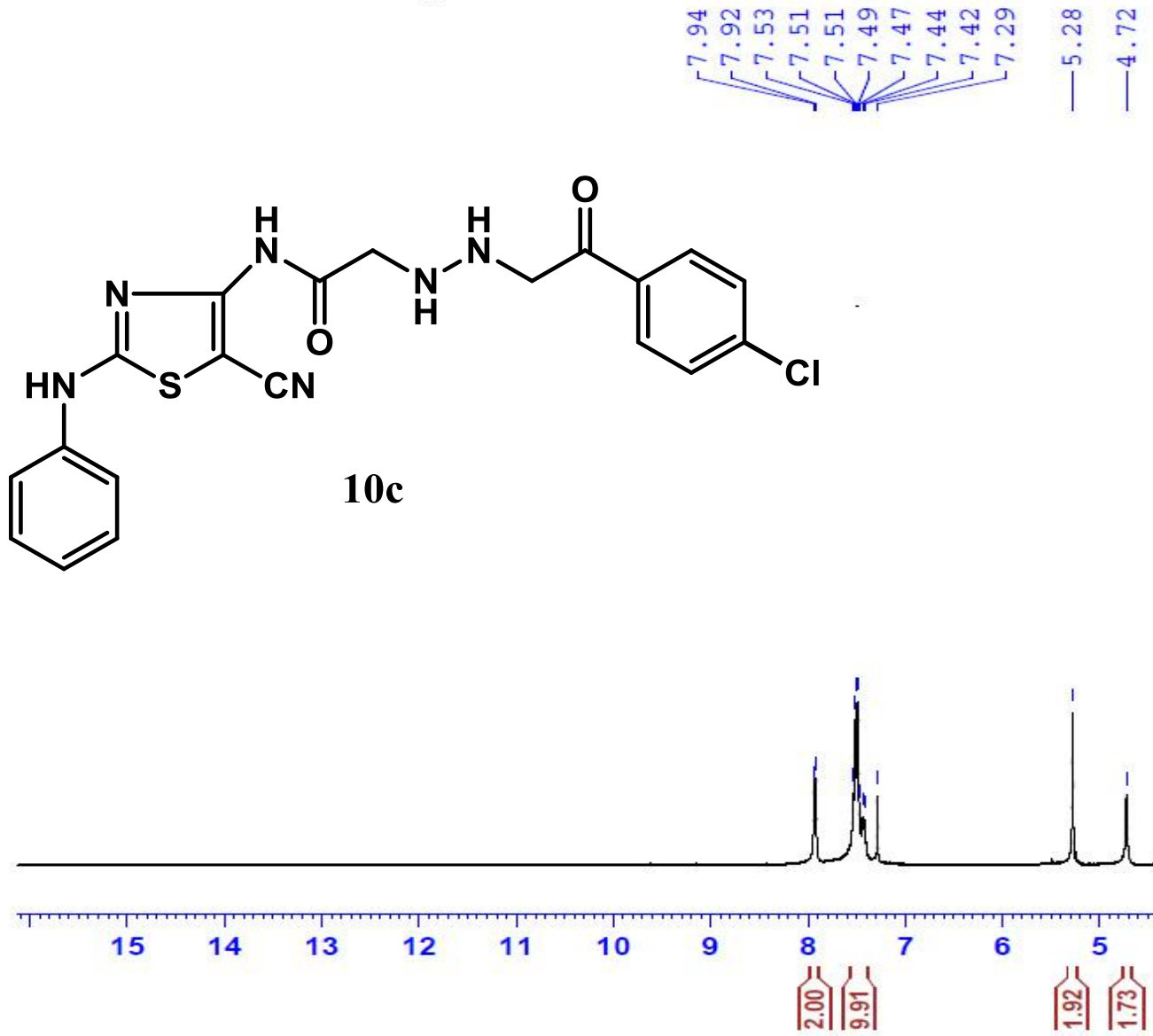


10c 10ppm.d



10c

alaa abdallah-clAcl.clphBr-H-em



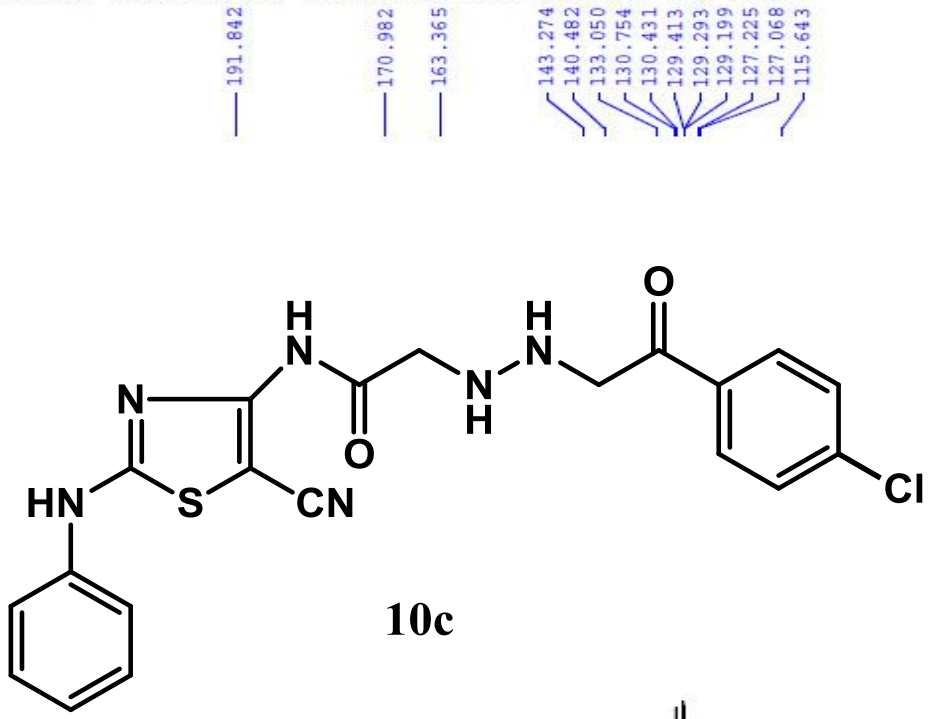
10c

Current Data Parameters
NAME alaa abdallah-clAcl.clphBr-H-em
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211013
Time 13.53 h
INSTRUM spect
PROBHD Z108618_0945 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 176.72
DW 62.400 usec
DE 6.50 usec
TE 293.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2024712 MHz
NUC1 1H
P1 13.50 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Alaa abdallah-Cl.A.Cl+Cl.Ph.Br-RR-C13



10c

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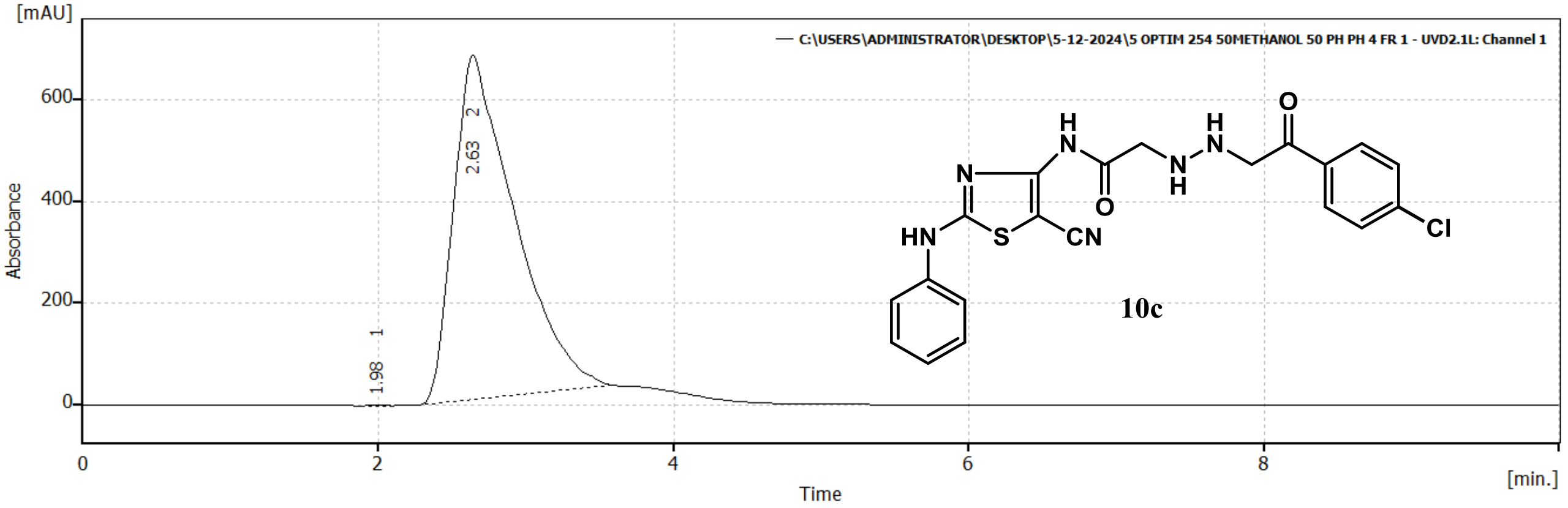
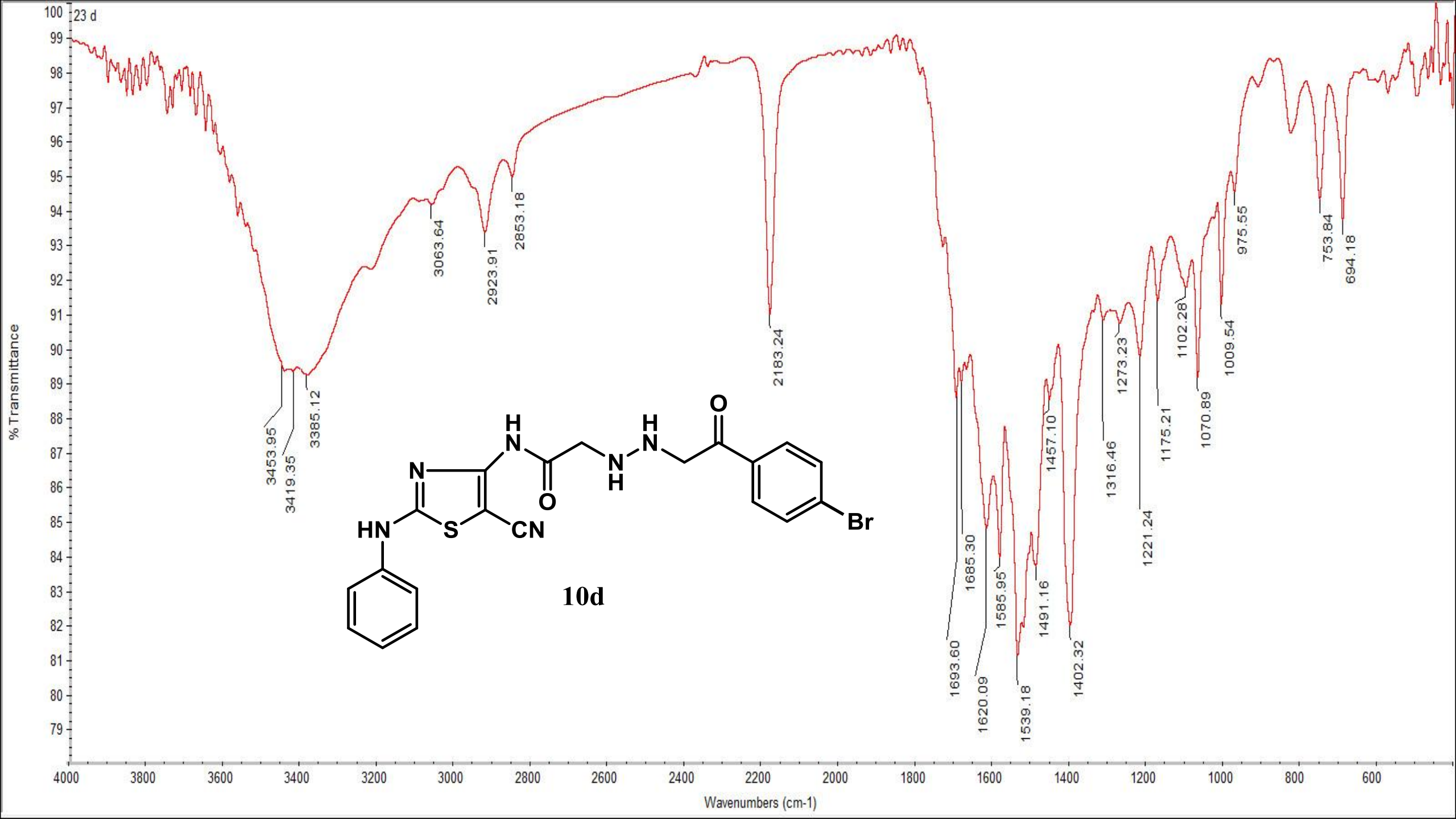
```
Current Data Parameters
NAME      Alaa abdallah-Cl.A.Cl+Cl.Ph.Br-RR-C13
EXPNO                10
PROCNO                1

F2 - Acquisition Parameters
Date_              20220319
Time                 22.11 h
INSTRUM                spect
PROBHD     Z108618_0945 (
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    2200
DS                       4
SWH              24038.461 Hz
FIDRES               0.733596 Hz
AQ                1.3631488 sec
RG                   197.77
DW                  20.800 usec
DE                   6.50 usec
TE                  294.2 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1
SFO1            100.6404331 MHz
NUC1                    13C
P1                   10.00 usec
PLW1             47.00000000 W
SFO2             400.2016008 MHz
NUC2                    1H
CPDPRG[2              waltz16
PCPD2                80.00 usec
PLW2             13.00000000 W
PLW12             0.29249999 W
PLW13             0.14713000 W

F2 - Processing parameters
SI                   32768
SF              100.6303700 MHz
WDW                     EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

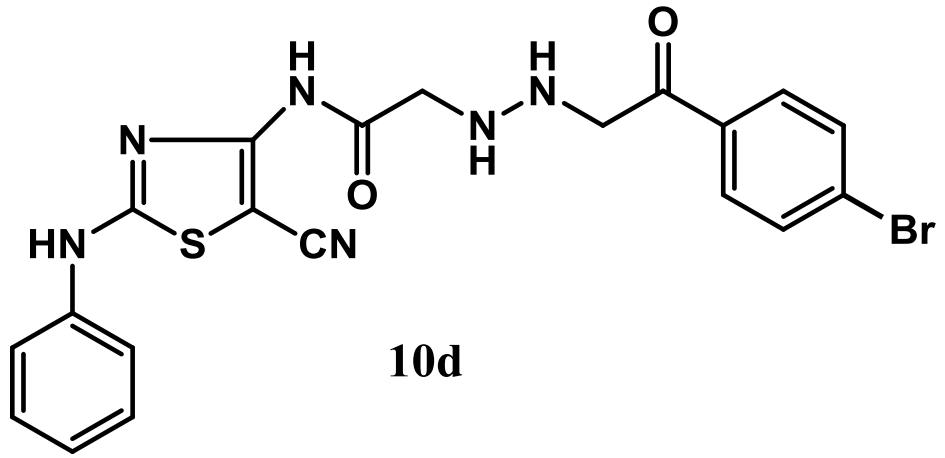

[mAU]
600
400
200
0
Absorbance
C:\USERS\ADMINISTRATOR\DESKTOP\5-12-2024\5 OPTIM 254 50METHANOL 50 PH PH 4 FR 1 - UVD2.1L: Channel 1
1
1.98
2
2.63
0
2
4
6
8
Time
[min.]
H
N
N
H
N
H
O
O
HN
S
CN
Cl

10c


23 d
% Transmittance
Wavenumbers (cm-1)
3453.95
3419.35
3385.12
3063.64
2923.91
2853.18
2183.24
1693.60
1685.30
1620.09
1585.95
1539.18
1491.16
1457.10
1402.32
1316.46
1273.23
1221.24
1175.21
1102.28
1070.89
1009.54
975.55
753.84
694.18
HN
N
S
CN
H
N
O
N
H
H
N
O
Br

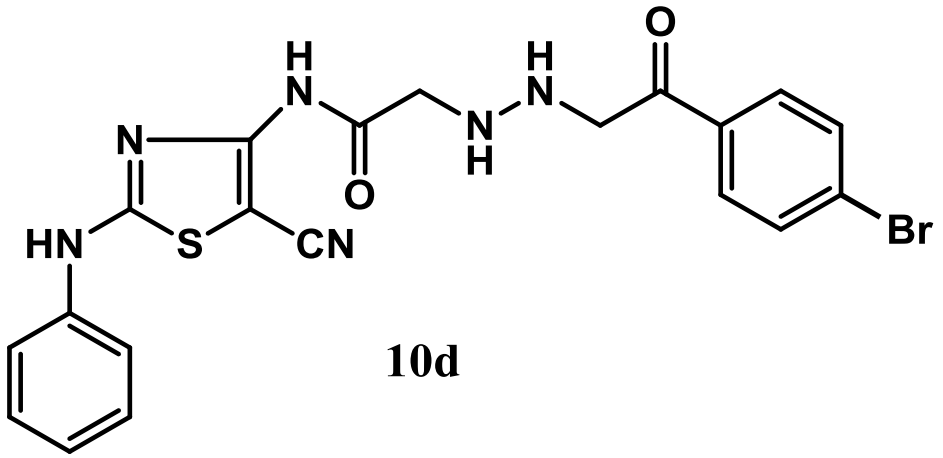
10d

alaa-23d #235-238 RT: 3.95-4.00 AV: 4 SB: 2 3.93 , 3.62 NL: 3.57E2
T: + cEI Full ms [40.00-1000.00]



10d

Alaa Abdullah-18-HNMR-DMSO-AF

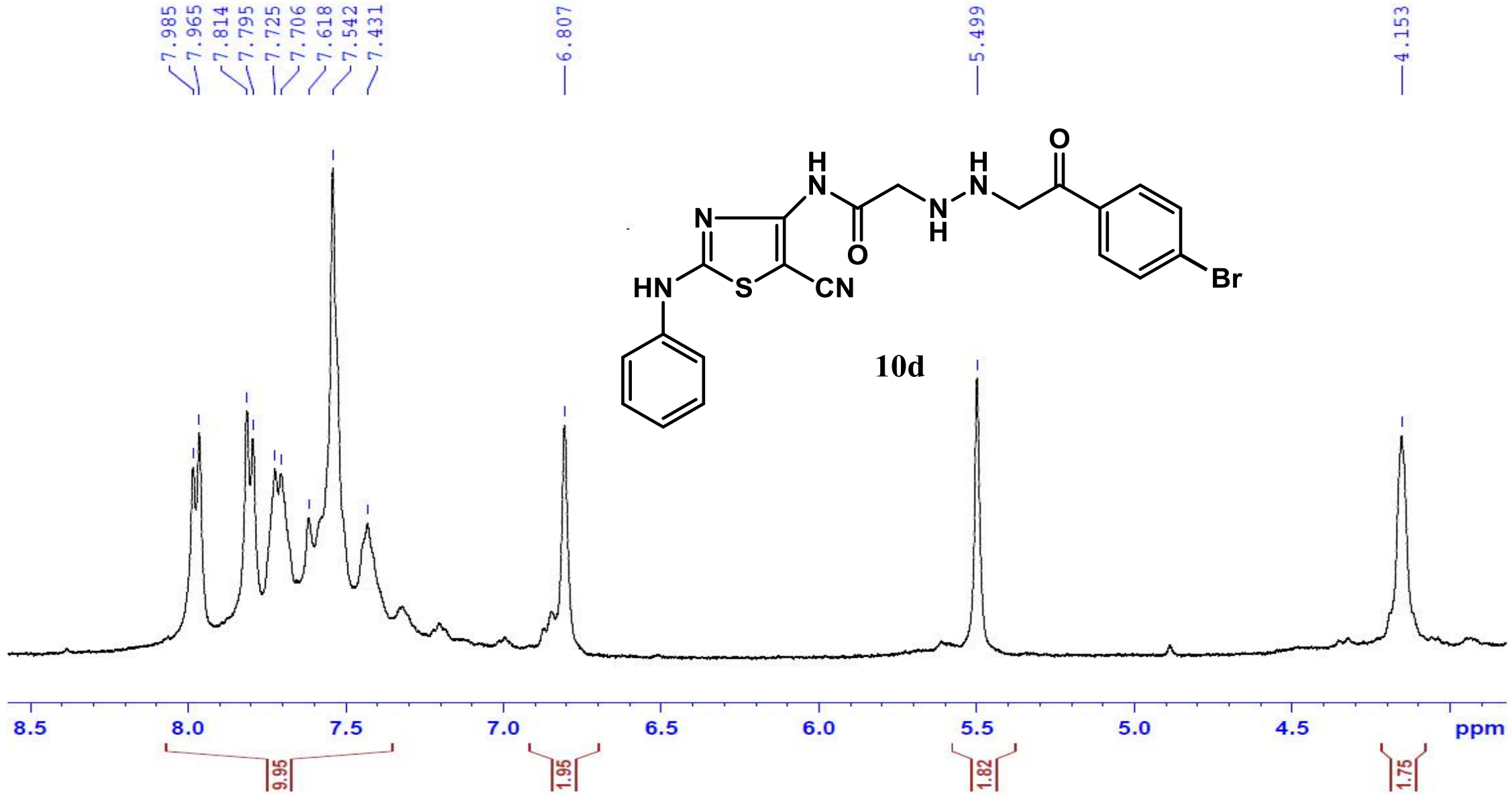


10d

Faculty of Pharmacy

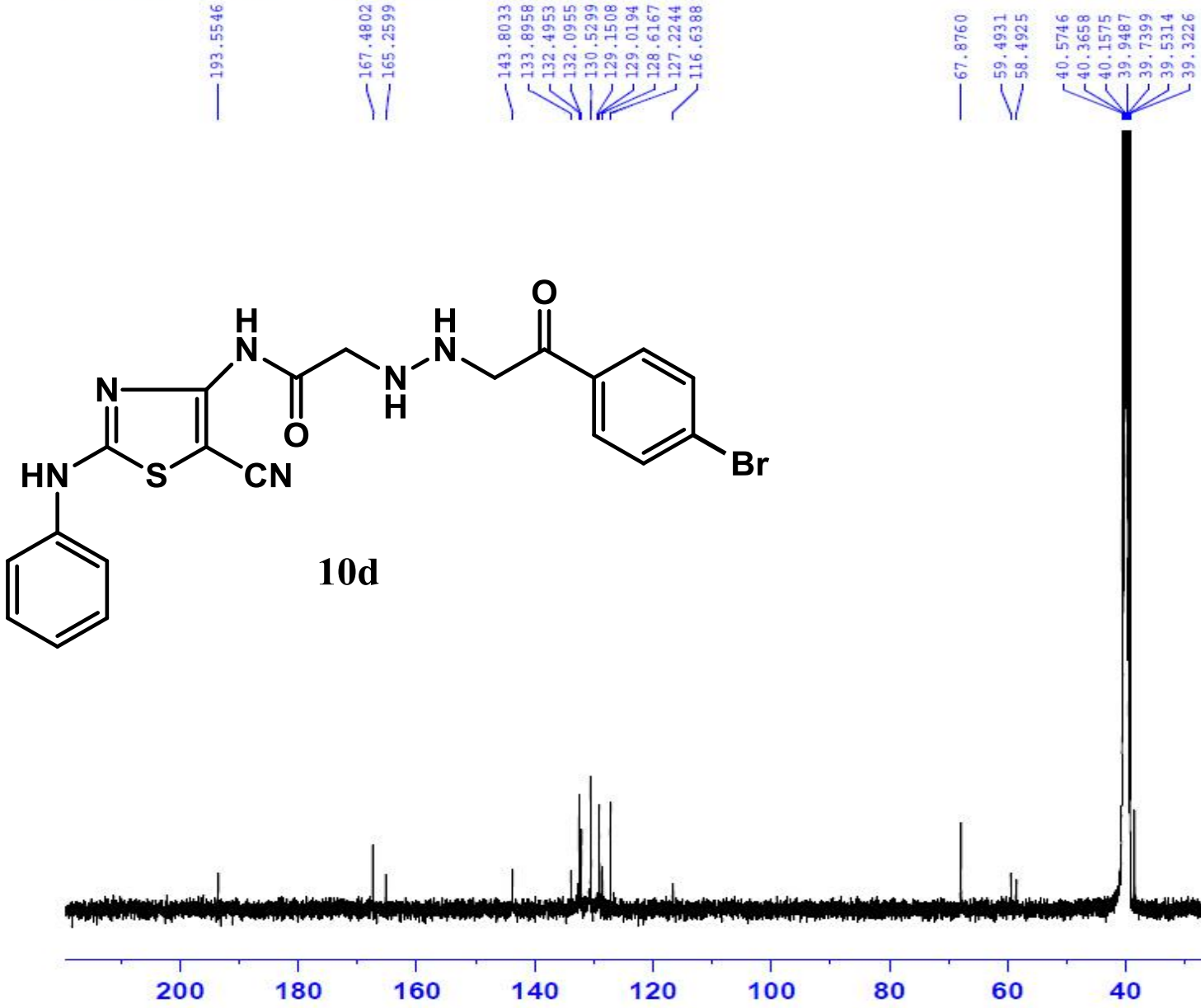
```
Current Data Parameters
NAME      Alaa Abdullah-18-HNMR
EXPNO                       10
PROCNO                       1

F2 - Acquisition Parameters
Date_               20220510
Time                  15.02 h
INSTRUM                spect
PROBHD    Z108618_0945 (
PULPROG                 zg30
TD                     65536
SOLVENT                 DMSO
NS                        16
DS                         2
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                  4.0894465 sec
RG                     135.42
DW                     62.400 usec
DE                      6.50 usec
TE                     295.4 K
D1                  1.00000000 sec
TD0                        1
SFO1             400.2024712 MHz
NUC1                       1H
P1                     13.50 usec
PLW1            13.00000000 W

F2 - Processing parameters
SI                     65536
SF               400.2000000 MHz
WDW                       EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

Alaa Abdullah-18-HNMR-DMSO-AF



10d

Alaa Abdallah - 18 - C13 - T



10d

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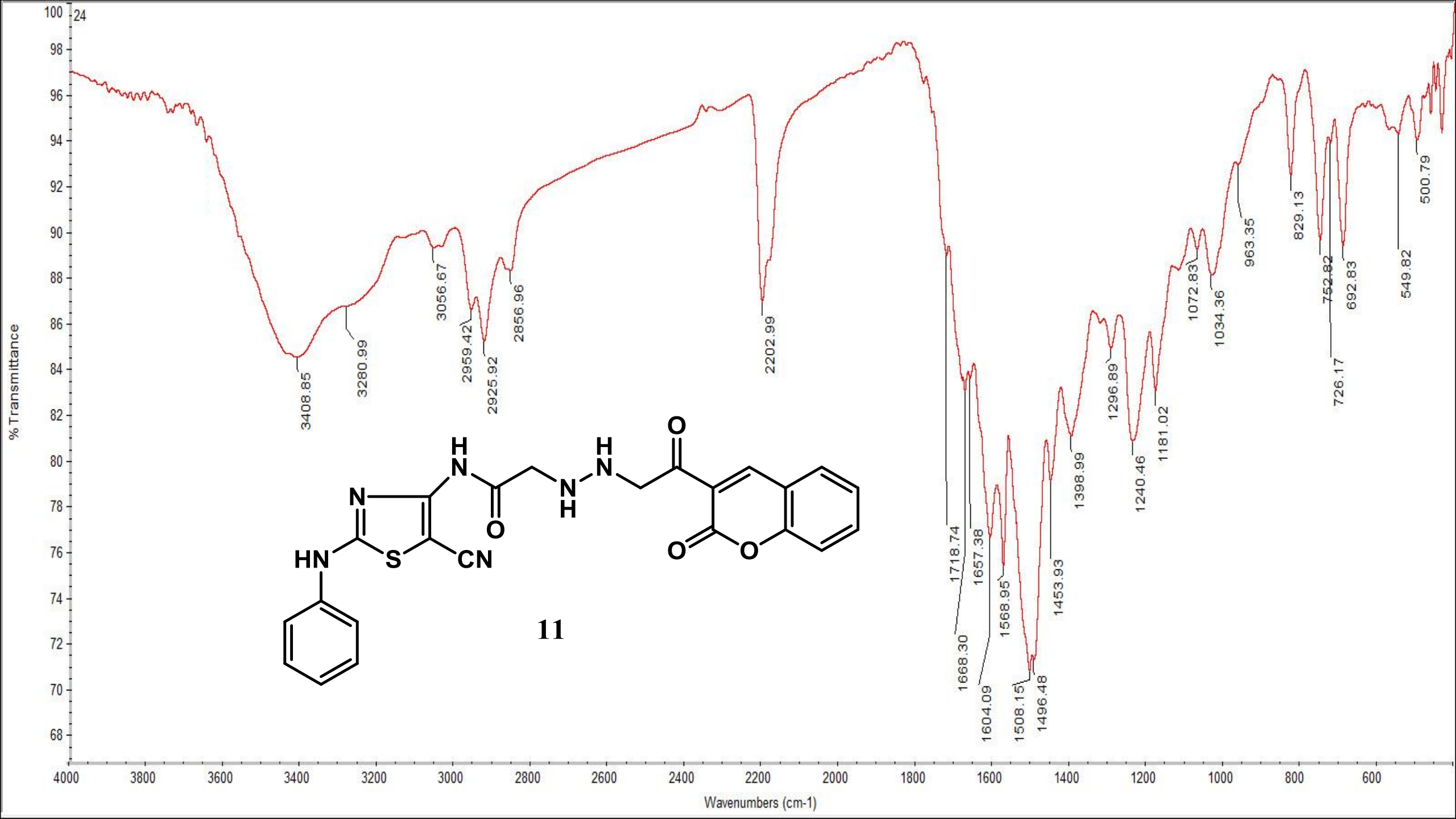
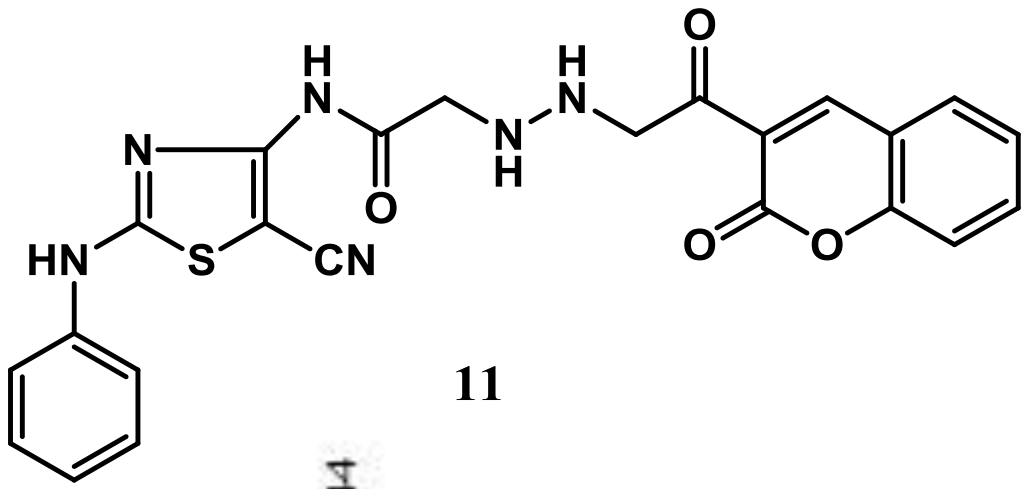
```
Current Data Parameters
NAME      Alaa Abdallah - 18 - C13 - T
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220528
Time                20.02 h
INSTRUM             spect
PROBHD    Z108618_0945 (
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  2100
DS                     4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                197.77
DW                20.800 usec
DE                 6.50 usec
TE                294.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6404331 MHz
NUC1                  13C
P1                10.00 usec
PLW1          47.00000000 W
SFO2          400.2016008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          13.00000000 W
PLW12          0.29249999 W
PLW13          0.14713000 W

F2 - Processing parameters
SI                 32768
SF            100.6303700 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


24
% Transmittance
Wavenumbers (cm-1)
3408.85
3280.99
3056.67
2959.42
2925.92
2856.96
2202.99
1718.74
1668.30
1657.38
1604.09
1568.95
1508.15
1496.48
1453.93
1398.99
1296.89
1240.46
1181.02
1072.83
1034.36
963.35
829.13
752.82
726.17
692.83
549.82
500.79
HN
N
S
CN
H
N
O
N
H
H
N
O
O
O

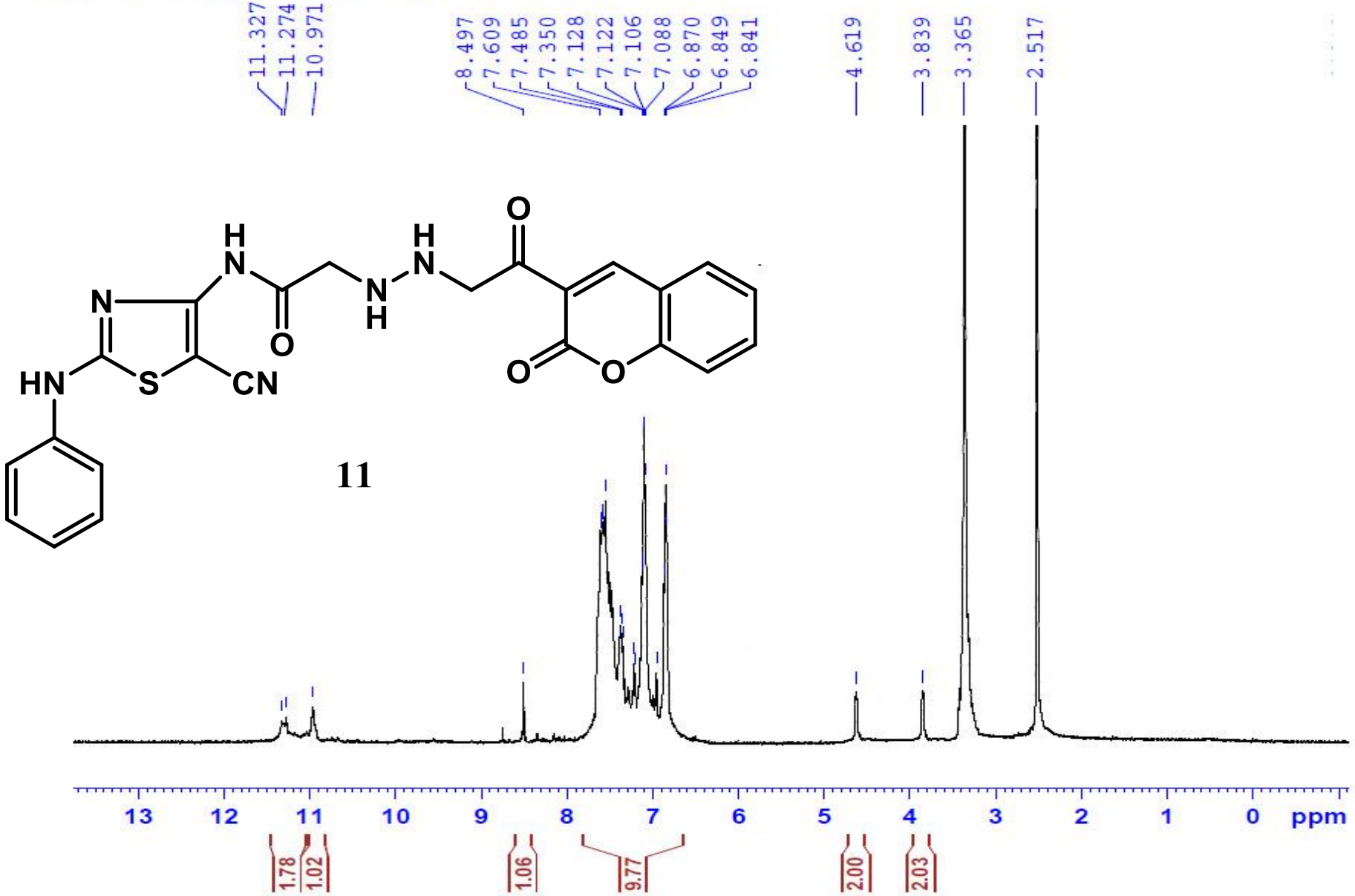
11

alaa-24 #185-187 RT: 3.11-3.15 AV: 3 SB: 6 2.80 , 2.48-2.54 NL: 2.07E2
T: + cEI Full ms [40.00-1000.00]



11

Alaa Abdullah-22-HNMR-DMSO-AF



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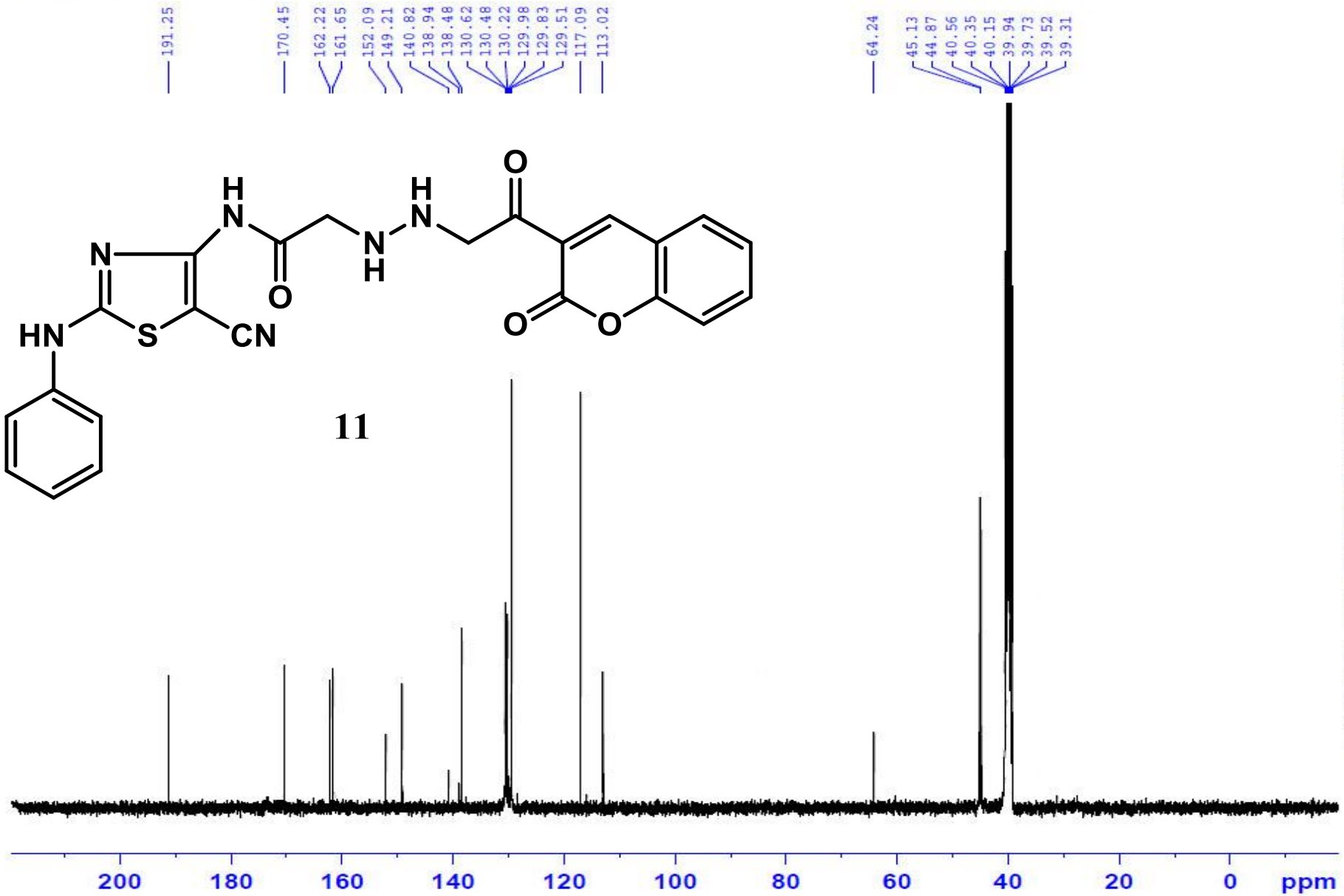
Faculty of Pharmacy

```
Current Data Parameters
NAME      Alaa Abdullah-22-HNMR
EXPNO                       10
PROCNO                       1

F2 - Acquisition Parameters
Date_               20220510
Time                  15.19 h
INSTRUM                spect
PROBHD    Z108618_0945 (
PULPROG                 zg30
TD                     65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                  4.0894465 sec
RG                     135.42
DW                     62.400 usec
DE                      6.50 usec
TE                     295.5 K
D1                  1.00000000 sec
TD0                        1
SFO1             400.2024712 MHz
NUC1                      1H
P1                     13.50 usec
PLW1            13.00000000 W

F2 - Processing parameters
SI                     65536
SF               400.2000000 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

alaa abdallah 22 -M c13



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BRUKER

Faculty of Pharmacy

```
Current Data Parameters
NAME      alaa abdallah clbcl -M c13
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210302
Time               9.37 h
INSTRUM            spect
PROBHD   Z108618_0945 (
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                 2100
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                197.77
DW                20.800 usec
DE                 6.50 usec
TE         0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1
SFO1         100.6404331 MHz
NUC1                13C
P1                10.00 usec
PLW1         47.00000000 W
SFO2         400.2016008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.00000000 W
PLW12         0.29249999 W
PLW13         0.14713000 W

F2 - Processing parameters
SI                 32768
SF           100.6303700 MHz
WDW                  EM
SSB        0
LB                 1.00 Hz
GB         0
PC                 1.40
```