

Electronic Supplementary Information for

**Design, synthesis, and biological evaluation with molecular dynamic study of
novel pyrazolo[3, 4-*d*]pyrimidine derivatives as anti-cancer agents**

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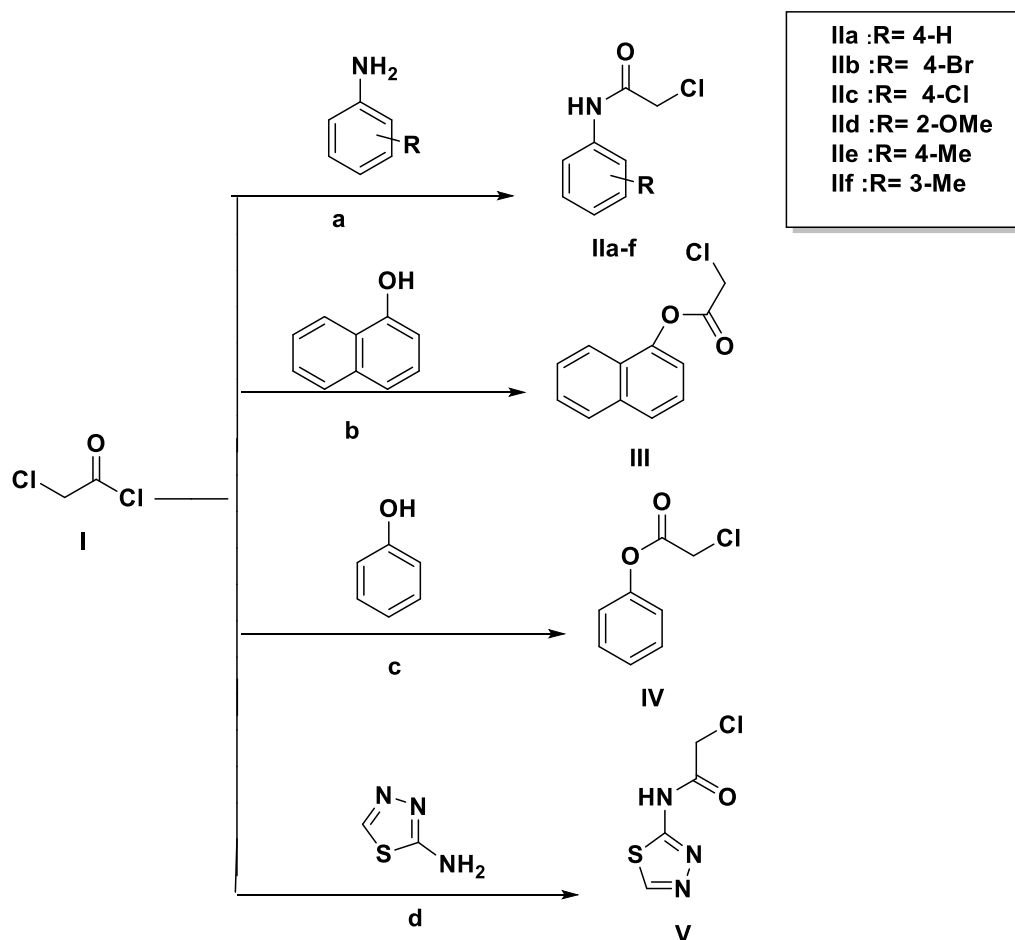
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Results and Discussion

Chemistry

The starting intermediates in **scheme S1** were prepared via the reaction of chloroacetyl chloride (**I**) with aniline derivatives in glacial acetic acid to give **Ila-f** ^[1-3]. Similarly, the precursor **III** was prepared by reacting chloroacetyl chloride with α -naphthol & β -naphthol in presence of triethyl amine. Also, compound **IV** was prepared by reacting chloroacetyl chloride with phenol in presence of pyridine ^[4]. Reacting chloroacetyl chloride with 1,3,4-thiadiazol-2-amine in ethanol yields intermediate **V**



Scheme S1: Synthesis of intermediates, Reagents and conditions: (a) sodium acetate, acetic acid, reflux, 1 h **(b)** TEA, DCM, rt, 1 h **(c)** Pyridine, rt, 2 h **(d)** Ethanol , rt, 12 h

Primary single high dose (10^{-5} M) full NCI 60 cell panel *in vitro* assay

Table S1 the Sixty human tumor cell lines anticancer screening data at single dose assay (10^{-5} M concentration) as percent cell inhibition of compounds XVIIIa-f

Cell line	Compound No					
	XVIIIa	XVIIIb	XVIIIc	XVIIId	XVIIIe	XVIIIf
Leukemia						
CCRF-CEM	37.04	NT	38.83	NT	33.10	37.31
HL-60(TB)	41.31	45.24	42.03	39.41	33.46	39.75
K-562	45.28	54.72	58.76	52.06	41.45	56.17
MOLT-4	64.34	46.03	53.95	59.22	53.98	41.80
RPMI-8226	28.61	27.77	46.21	28.52	39.51	24.25
SR	10.44	32.07	43.10	36.24	38.59	77.28
Non-Small Cell Lung Cancer						
A549/ATCC	14.76	33.64	32.95	2.61	13.30	34.67
EKVX	36.46	50.11	65.02	37.26	41.79	46.29
HOP-62	15.75	39.06	18.30	19.52	7.34	32.59
HOP-92	37.94	53.34	19.18	53.24	24.06	49.40
NCI-H226	36.98	53.83	38.92	23.86	32.48	45.47
NCI-H23	35.62	43.26	NT	44.26	NT	41.59
NCI-H322M	25.50	23.36	28.90	3.89	18.90	30.70
NCI-H460	17.17	41.61	38.45	23.23	13.27	35.00
NCI-H522	39.99	73.62	50.17	30.00	38.95	106.93
Colon Cancer						
COLO 205	0.82	-6.21	14.00	-3.91	4.09	2.65
HCC-2998	-5.28	19.24	18.54	-6.72	2.24	13.63
HCT-116	31.76	48.71	40.84	47.41	24.95	41.35
HCT-15	26.93	35.44	28.21	39.23	20.95	27.06
HT29	17.24	14.47	11.17	5.71	-0.16	16.48
KM12	36.06	63.08	53.33	23.31	27.37	59.40
SW-620	9.81	26.84	37.84	15.17	9.80	18.47
CNS Cancer						
SF-268	20.86	26.90	36.13	21.64	28.18	26.70
SF-295	30.01	60.81	30.05	31.27	-8.80	53.42
SF-539	15.92	39.70	52.89	22.56	10.11	40.11
SNB-19	14.63	16.93	9.53	19.11	8.31	11.10
SNB-75	28.47	64.72	14.00	33.72	9.19	46.50
U251	3.37	16.97	10.42	7.85	6.63	12.86
Melanoma						
LOX IMVI	35.95	47.20	25.76	32.87	22.72	46.18

MALME-3M	31.60	30.70	5.53	32.06	8.08	27.24
M14	24.29	44.22	57.82	25.17	21.65	37.84
MDA-MB-435	30.09	42.94	48.55	29.11	25.09	41.02
SK-MEL-2	52.67	57.89	69.89	56.03	60.01	53.34
SK-MEL-28	13.04	39.02	48.94	10.99	10.55	41.00
SK-MEL-5	78.34	67.48	74.36	83.62	64.82	62.50
UACC-257	24.78	32.45	34.00	25.13	16.94	33.09
UACC-62	49.01	66.54	72.78	35.66	45.81	65.43
Ovarian Cancer						
IGROV1	32.45	38.59	36.98	33.46	34.14	40.59
OVCAR-3	16.18	13.45	33.49	8.87	39.34	6.00
OVCAR-4	43.70	48.72	33.83	49.21	31.39	48.39
OVCAR-5	8.88	15.16	23.23	-0.74	10.31	16.18
OVCAR-8	19.70	38.53	37.01	22.37	18.01	34.76
NCI/ADR-RES	35.34	39.38	27.26	26.01	19.30	39.38
SK-OV-3	21.35	37.67	23.86	23.22	-0.33	32.91
Renal Cancer						
786-0	14.38	22.68	19.44	5.32	19.13	19.21
A498	3.93	-10.34	1.06	-2.92	11.23	-7.50
ACHN	38.35	58.25	59.54	30.65	39.34	54.65
CAKI-1	44.38	52.63	50.17	43.62	40.24	52.25
RXF 393	16.76	24.11	4.64	2.13	5.05	23.66
SN12C	20.83	28.02	42.52	21.91	37.47	23.10
TK-10	-7.06	-7.58	-28.78	-28.83	-26.24	6.15
UO-31	69.29	68.99	68.08	67.93	66.08	65.74
Prostate Cancer						
PC-3	32.54	29.20	41.85	29.85	37.97	29.99
DU-145	15.85	33.73	28.62	13.03	16.64	24.61
Breast Cancer						
MCF7	47.59	59.22	63.37	56.61	48.62	54.43
MDA-MB-231/ATCC	32.07	30.93	30.90	21.92	26.47	35.04
HS 578T	12.13	44.12	36.90	16.05	24.69	39.60
BT-549	31.11	32.27	56.87	53.92	52.53	23.13
T-47D	70.38	72.72	63.26	74.01	62.13	66.43
MDA-MB-468	61.75	67.77	53.75	69.23	42.37	64.22

^a NT, not tested

Table S2 the Sixty human tumor cell lines anticancer screening data at single dose assay (10^{-5} M concentration) as percent cell inhibition of compounds XXIa-f

Cell line	Compound No					
	XXIa	XXIb	XXIc	XXId	XXIe	XXIf
Leukemia						
CCRF-CEM	NT	36.81	18.82	NT	51.56	NT
HL-60(TB)	5.57	35.17	9.21	19.50	39.93	4.48
K-562	8.89	48.67	38.56	37.27	62.12	38.51
MOLT-4	-4.25	54.79	18.45	41.75	66.10	18.38
RPMI-8226	2.35	23.74	16.59	27.38	31.51	30.86
SR	16.19	91.41	85.90	87.74	87.57	86.09
Non-Small Cell Lung Cancer						
A549/ATCC	-3.26	23.83	19.42	41.16	36.94	45.71
EKVX	10.97	13.79	23.62	18.57	30.12	37.29
HOP-62	15.01	29.43	62.57	68.13	24.15	102.01
HOP-92	13.96	32.10	52.79	67.98	44.84	85.26
NCI-H226	16.20	15.08	39.40	90.89	32.68	47.67
NCI-H23	3.88	22.47	35.61	40.03	40.52	44.51
NCI-H322M	-0.24	24.15	24.56	33.15	31.64	33.22
NCI-H460	-1.73	56.18	30.85	44.16	65.47	46.69
NCI-H522	8.01	42.35	39.05	58.83	47.07	62.01
Colon Cancer						
COLO 205	-21.09	9.64	1.34	20.26	11.43	22.56
HCC-2998	-2.68	0.90	9.53	13.04	14.00	17.39
HCT-116	1.00	44.91	39.72	33.37	53.16	58.09
HCT-15	5.21	50.09	41.73	57.28	66.45	47.72
HT29	-7.82	22.02	13.56	19.55	33.18	20.93
KM12	2.45	20.28	7.53	15.60	25.85	12.68
SW-620	2.94	23.38	18.26	19.53	15.98	31.08
CNS Cancer						
SF-268	2.06	19.83	41.49	36.18	38.38	58.84
SF-295	3.14	30.66	51.65	42.22	60.52	65.83
SF-539	4.55	26.23	117.45	67.71	47.68	88.81
SNB-19	6.80	15.14	53.43	89.85	15.95	71.82
SNB-75	20.11	46.26	92.11	68.31	37.96	97.65
U251	1.85	14.09	43.46	44.91	31.30	61.67
Melanoma						

LOX IMVI	11.05	36.62	58.87	37.74	52.33	85.69
MALME-3M	5.96	21.91	46.60	42.23	35.60	43.95
M14	-3.82	13.24	16.85	36.94	27.59	20.09
MDA-MB-435	-2.18	22.81	19.75	15.17	33.34	10.77
SK-MEL-2	-4.29	8.35	12.64	42.43	25.37	11.22
SK-MEL-28	-9.66	14.39	22.87	49.96	27.22	17.53
SK-MEL-5	3.03	44.05	25.02	28.35	70.91	23.66
UACC-257	-8.37	11.02	11.35	45.64	13.88	16.21
UACC-62	10.60	25.76	39.39	59.23	37.74	31.15
Ovarian Cancer						
IGROV1	4.37	20.60	27.95	33.61	47.19	29.12
OVCAR-3	-7.99	-12.67	10.39	16.86	23.43	51.88
OVCAR-4	1.54	54.20	58.13	45.87	47.69	83.49
OVCAR-5	-5.47	7.19	18.20	20.67	7.39	16.17
OVCAR-8	-3.57	32.23	52.56	48.71	26.39	61.71
NCI/ADR-RES	4.96	28.22	46.15	38.26	35.52	71.86
SK-OV-3	8.65	30.89	43.04	92.70	13.85	58.20
Renal Cancer						
786-0	2.16	1.41	27.98	17.17	6.09	72.18
A498	5.64	-24.04	-3.87	-14.66	-1.45	31.61
ACHN	6.89	20.36	30.76	35.65	19.63	75.48
CAKI-1	27.24	15.17	52.22	71.93	32.48	72.33
RXF 393	-4.71	22.99	30.94	50.07	34.23	56.91
SN12C	2.37	35.15	51.60	53.96	33.35	71.70
TK-10	-41.53	-39.82	-26.85	-1.06	-28.90	-8.77
UO-31	25.43	25.60	29.27	31.02	55.63	60.05
Prostate Cancer						
PC-3	9.97	28.10	35.15	41.04	41.04	52.74
DU-145	-10.17	13.60	12.69	20.13	32.78	18.93
Breast Cancer						
MCF7	19.61	47.60	50.15	45.67	59.24	61.12
MDA-MB-231/ATCC	2.81	15.80	24.59	19.84	32.63	42.88
HS 578T	14.05	29.51	46.17	48.98	32.81	67.25
BT-549	4.08	13.81	34.90	11.76	29.90	36.47
T-47D	27.57	33.36	26.89	29.74	67.22	42.76
MDA-MB-468	0.71	33.29	21.99	38.82	62.35	35.39

^a NT, not tested

In vitro 5 dose full NCI 60 cell panel assay

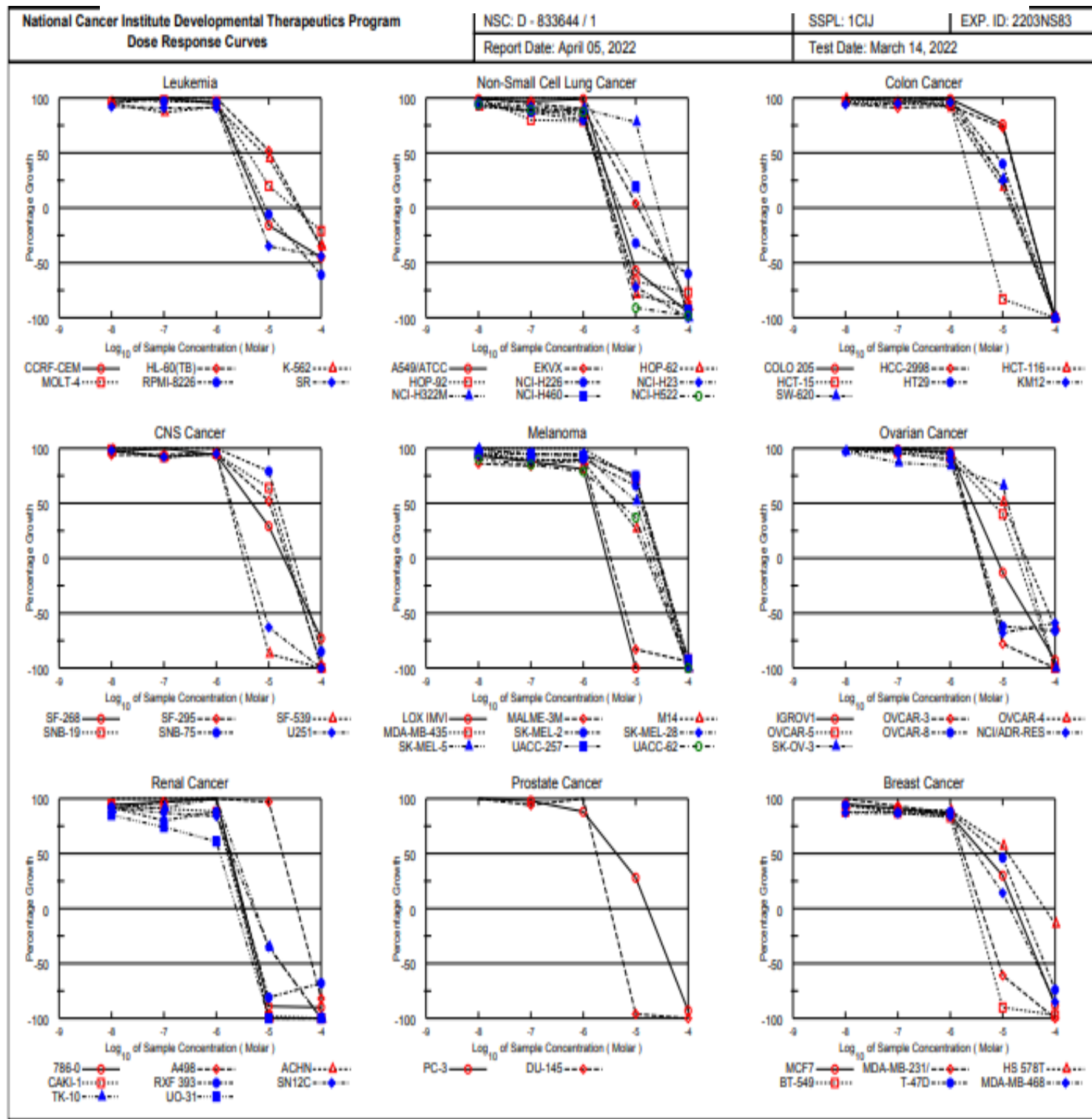


Figure S1 Dose response curve for compound XVI in 9 Cell panels (Leukemia, Melanoma, NSLC, Colon, CNS, Ovarian, renal, prostate and breast cancers).

Biological evaluation

***In vitro* anticancer activity against a panel of sixty human cancer cell lines**

National Cancer Institute (NCI) evaluates different compounds for their anticancer activity. The screening is a two-stage process, beginning with the evaluation of all compounds against the full NCI 60 cell lines panel representing leukemia, Non-Small Cell Lung Cancer, melanoma, colon cancer, CNS cancer, breast cancer, ovarian cancer, renal cancer and prostate cancer at a single dose of 10^{-5} M. The output from the single dose screen is reported as a mean graph. Compounds which exhibit significant growth inhibition are evaluated against the 60 cell panel at five concentration levels.

Assay protocol

The human tumor cell lines of the cancer screening panel are grown in RPMI 1640 medium containing 5% fetal bovine serum and 2 mM L-glutamine. For a typical screening experiment, cells are inoculated into 96 well microtiter plates in 100 μ L at plating densities ranging from 5,000 to 40,000 cells/well depending on the doubling time of individual cell lines. After cell inoculation, the microtiter plates are incubated at 37° C, 5 % CO₂, 95 % air and 100 % relative humidity for 24 h prior to addition of experimental drugs.

After 24 h, two plates of each cell line are fixed *in situ* with TCA, to represent a measurement of the cell population for each cell line at the time of drug addition (T_z). Experimental drugs are solubilized in dimethyl sulfoxide at 400-fold the desired final maximum test concentration and stored frozen prior to use. At the time of drug addition, an aliquot of frozen concentrate is thawed and diluted to twice the desired final maximum test concentration with complete medium containing 50 μ g/ml gentamicin. Additional four, 10-fold or ½ log serial dilutions are made to provide a total of five drug concentrations plus control. Aliquots of 100 μ l of these different drug dilutions are added to the appropriate microtiter wells already containing 100 μ l of medium, resulting in the required final drug concentrations.

Following drug addition, the plates are incubated for an additional 48 h at 37°C, 5 % CO₂, 95 % air, and 100 % relative humidity. For adherent cells, the assay is terminated by the addition of cold TCA. Cells are fixed *in situ* by the gentle addition of 50 μ l of cold 50 % (w/v) TCA (final

concentration, 10 % TCA) and incubated for 60 minutes at 4°C. The supernatant is discarded, and the plates are washed five times with tap water and air dried. Sulforhodamine B (SRB) solution (100 µl) at 0.4 % (w/v) in 1 % acetic acid is added to each well, and plates are incubated for 10 minutes at room temperature. After staining, unbound dye is removed by washing five times with 1 % acetic acid and the plates are air dried. Bound stain is subsequently solubilized with 10 mM trizma base, and the absorbance is read on an automated plate reader at a wavelength of 515 nm. For suspension cells, the methodology is the same except that the assay is terminated by fixing settled cells at the bottom of the wells by gently adding 50 µl of 80 % TCA (final concentration, 16 % TCA).

Data analysis

Using the seven absorbance measurements [time zero, (Tz), control growth, (C), and test growth in the presence of drug at the five concentration levels (Ti)], the percentage growth is calculated at each of the drug concentrations levels. Percentage growth is calculated as:

$[(Ti-Tz)/(C-Tz)] \times 100$ for concentrations for which $Ti \geq Tz$

$[(Ti-Tz)/Tz] \times 100$ for concentrations for which $Ti < Tz$.

Three dose response parameters are calculated for each experimental agent. Growth inhibition of 50 % (GI50) is calculated from $[(Ti-Tz)/(C-Tz)] \times 100 = 50$, which is the drug concentration resulting in a 50% reduction in the net protein increase (as measured by SRB staining) in control cells during the drug incubation. The drug concentration resulting in total growth inhibition (TGI) is calculated from $Ti = Tz$. The LC50 (concentration of drug resulting in a 50% reduction in the measured protein at the end of the drug treatment as compared to that at the beginning) indicating a net loss of cells following treatment is calculated from $[(Ti-Tz)/Tz] \times 100 = -50$. Values are calculated for each of these three parameters if the level of activity is reached; however, if the effect is not reached or is exceeded, the value for that parameter is expressed as greater or less than the maximum or minimum concentration tested. [5, 6]

Results for each compound were reported as a mean graph of the percent growth of the treated cells when compared to the untreated control cells. There after obtaining the results for one dose assay, analysis of historical Development Therapeutics Programme (DTP) was performed and compounds which satisfies predetermined threshold inhibition criteria is selected for NCI full

panel 5 dose assay. The number reported for the One-dose assay is growth relative to the no-drug control, and relative to the time zero number of cells. This allows detection of both growth inhibition (values between 0 and 100) and lethality (values less than 0). This is the same as for the 5-dose assay, described below. For example, a value of 100 means no growth inhibition. A value of 40 would mean 60% growth inhibition. A value of 0 means no net growth over the course of the experiment. A value of -40 would mean 40% lethality. A value of -100 means all cells are dead.

Molecular docking

Molecular modeling was carried out using Molecular Operating Environment (MOE, 2015.10), to evaluate the activity of the newly synthesized compounds, achieve an overview into the SAR of the designed compounds, and to understand the results obtained by the biological evaluation on the basis of the ligand–protein interactions. Crystal structure of FLT3 Kinase domain bound to the selective inhibitor was obtained from protein data bank (<http://www.rcsb.org/>, PDB code: 4RT7, resolution of 3.20 Å). Water molecules and ligands which are not involved in the binding were removed. The partial charges were calculated automatically. Protein Structure preparation protocol including 3D Protonation & structure correction was used with its default MOE options to prepare the protein. Energy minimization was carried out then a validation step was performed for the docking protocol by re-docking of the co-crystallized inhibitor, Quizartinib, and the obtained low RMSD value indicated the valid performance (RMSD = 1.46 Å)

The method used for docking was general docking. The scoring methodology was selected as GBVI/WSA dG for the refinement methodology. On the other hand, the scoring methodology was applied as London dG for the placement methodology, which was selected as a triangle matcher. The applied forcefield was Amber10: EHT. The prepared MDB file was inserted containing all newly synthesized compounds then docking calculations was performed automatically. Only one pose was selected for each compound and the selection was based on the binding scores, rmsd_refine values, and interaction modes.

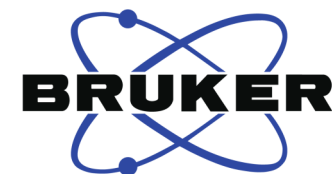
Molecular Dynamics

The FLT3 structure (PDB ID: 4RT7) was subjected to 1 μ s molecular dynamics simulation at NPT ensemble. The simulation system was prepared using OpenMM Setup utility [7]. AMBER14 [8] force field was used for the protein parameters and TIP3P-FB water model [8] was used for water molecules. Hydrogen atoms were added at pH value of 7.0. The protein was immersed in a cubic water box with a padding distance of 1.3 nm along each axis of the protein molecule. NaCl ions were added with ionic strength of 0.1 Molar to neutralize the model. The final simulation system ended up with 88,222 atoms. The FLT3 structure (PDB ID: 4RT7) used for MD simulation with XIIb, XIIc, XVI & Quizratinib was treated by the same parameters. Generalized Amber Force Field (GAFF) [9] parameters were used for the four compounds. Both GAFF parameters and ELF10 charges were generated on the fly by the OpenEye toolkits 2019.4.1 [10]. Particle Mesh Ewald (PME) method [11] was used for the calculation of long-range electrostatic interactions with a 0.0005 error tolerance for truncating the Ewald summation. A 1.2 nm cut off was used for both PME direct space interactions and Lennard-Jones interactions. The length of all bonds that involve a hydrogen atom, and the water molecules, involving their bond length and angles, were constrained. Langevin integrator was utilized for integrating force equations with step size of 2 ns, temperature of 310 K and friction coefficient of 1 ps^{-1} . Monte Carlo barostat [12] was used for pressure coupling with assigning 310 K as constant temperature value, 1 atm as constant pressure value and 25 steps as pressure update frequency. The dynamics simulations were carried out using OpenMM python application layer [7]. We started the simulation with a minimization step with 10 kJ/mol as energy convergence criteria, then, 3,000,000 equilibration steps (6 ns). Finally, the simulation was carried out for 500 million steps (1 μ s). A trajectory snapshot was reported every 35,000 steps (70 ps), resulting in a final trajectory file of 14,285 total frames. The production was run for 25 million steps (50 ns), and trajectory reporting was set to one snapshot per 1,000 steps resulting in a trajectory file of 25,000 snapshots. RMSD, RMSF and radius of gyration was calculated out using ProDy python library.

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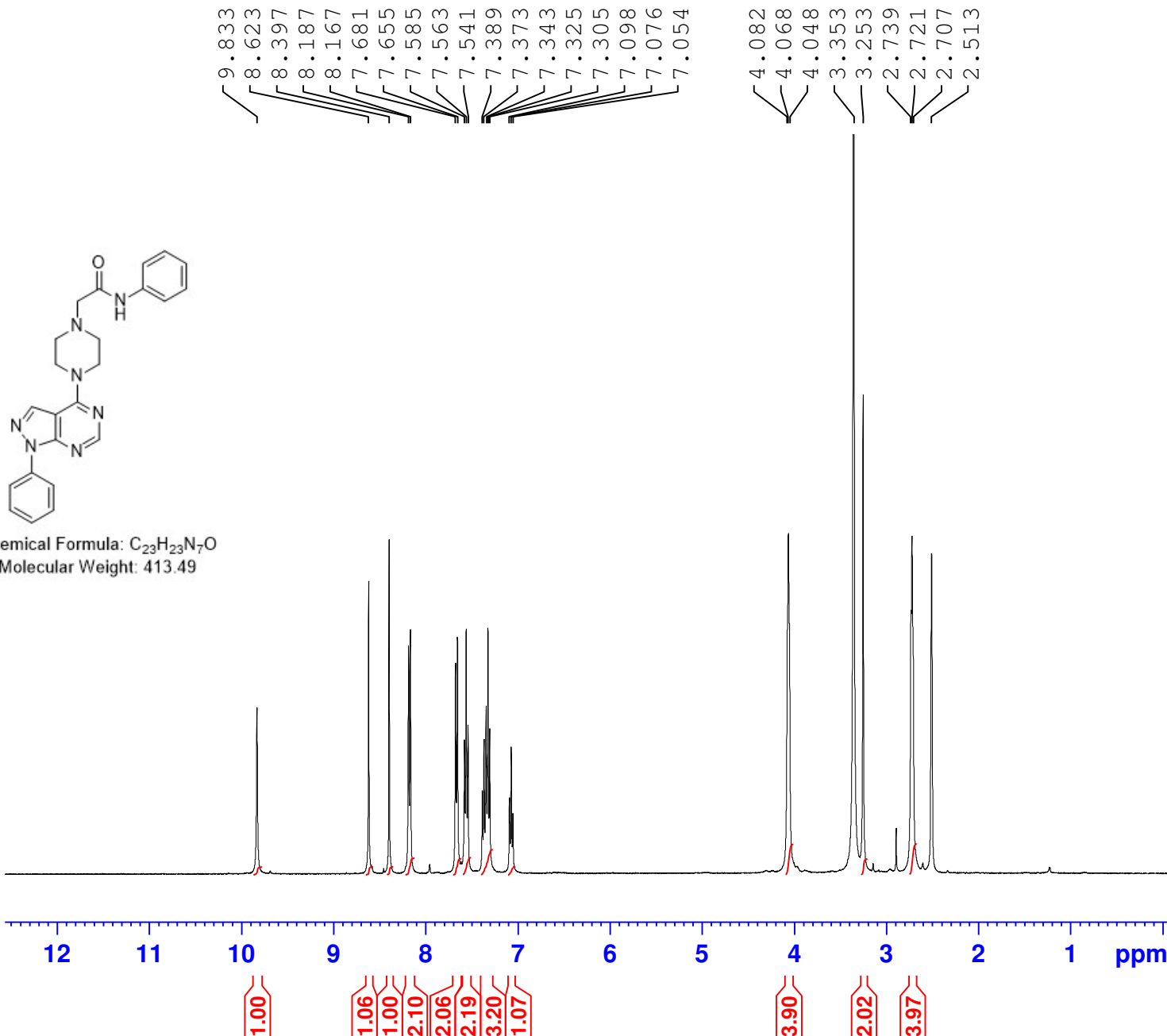


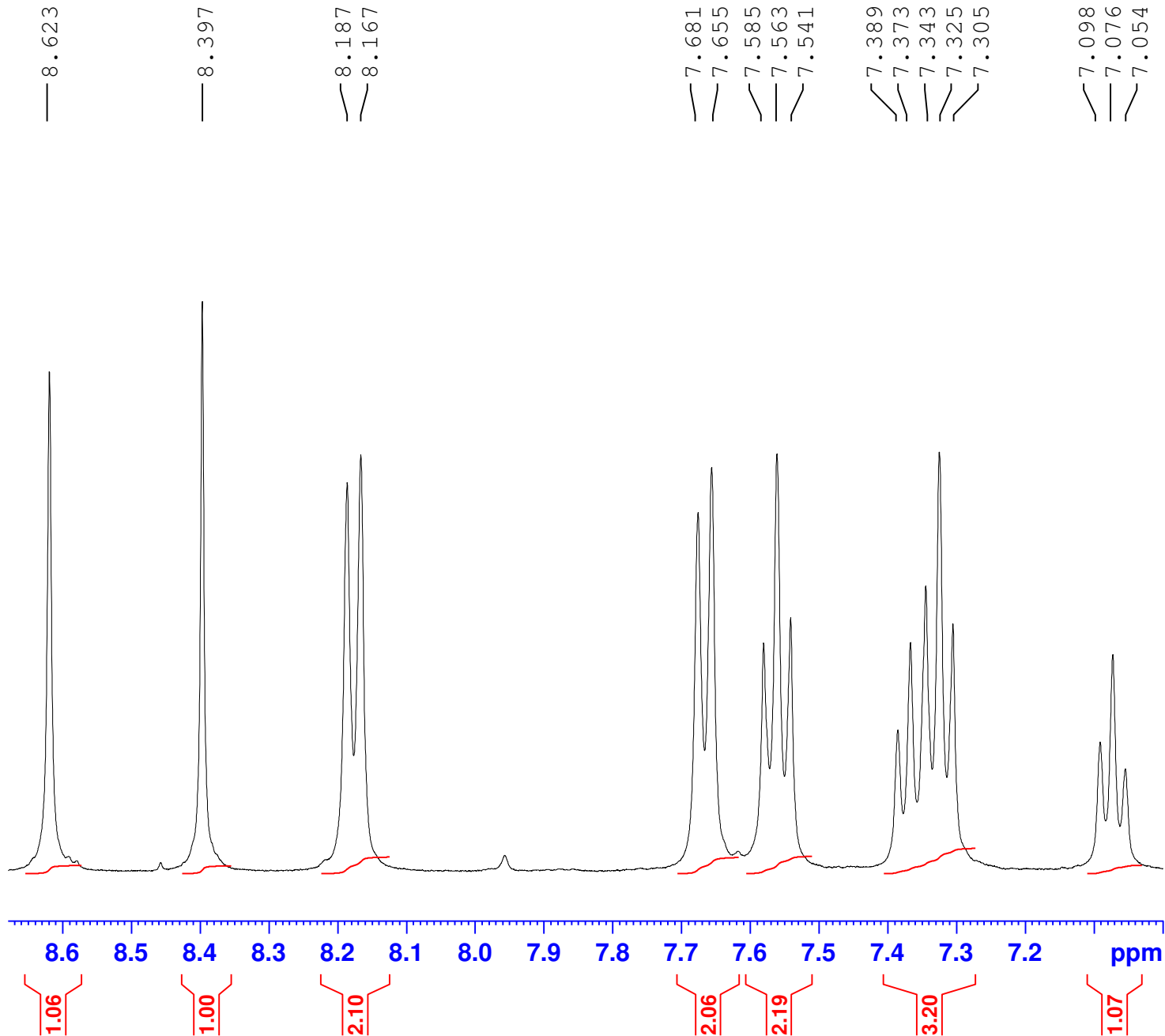
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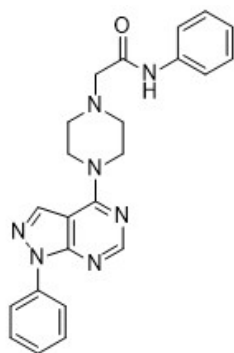
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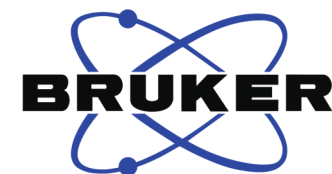
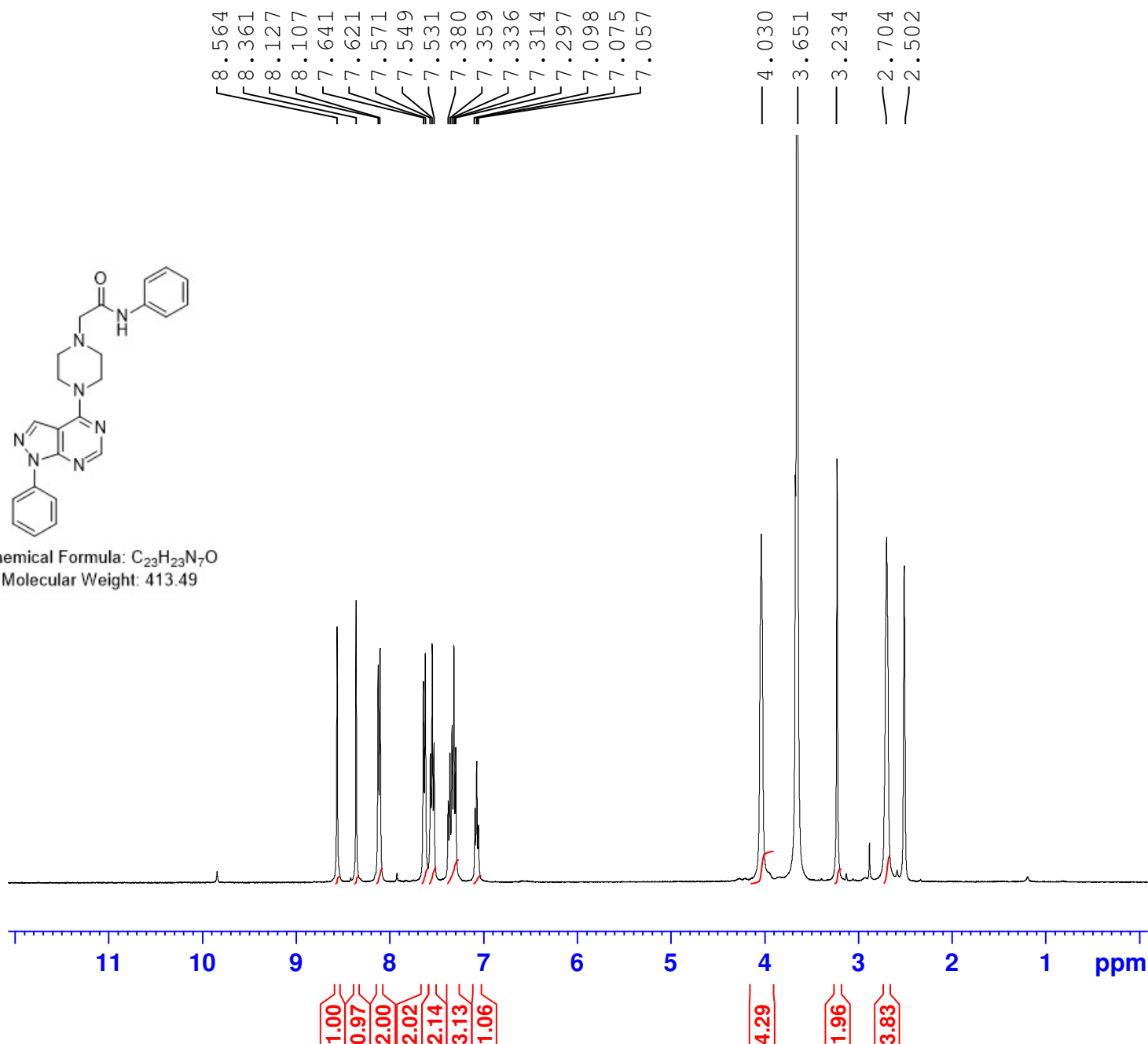
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NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

XIIa D2O



Chemical Formula: $C_{23}H_{23}N_7O$
Molecular Weight: 413.49



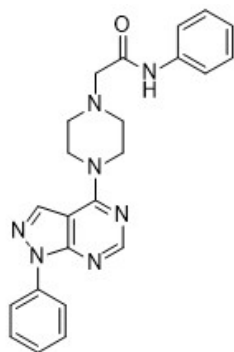
Current Data Parameters
NAME AMA-7a-d2o
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190505
Time 9.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

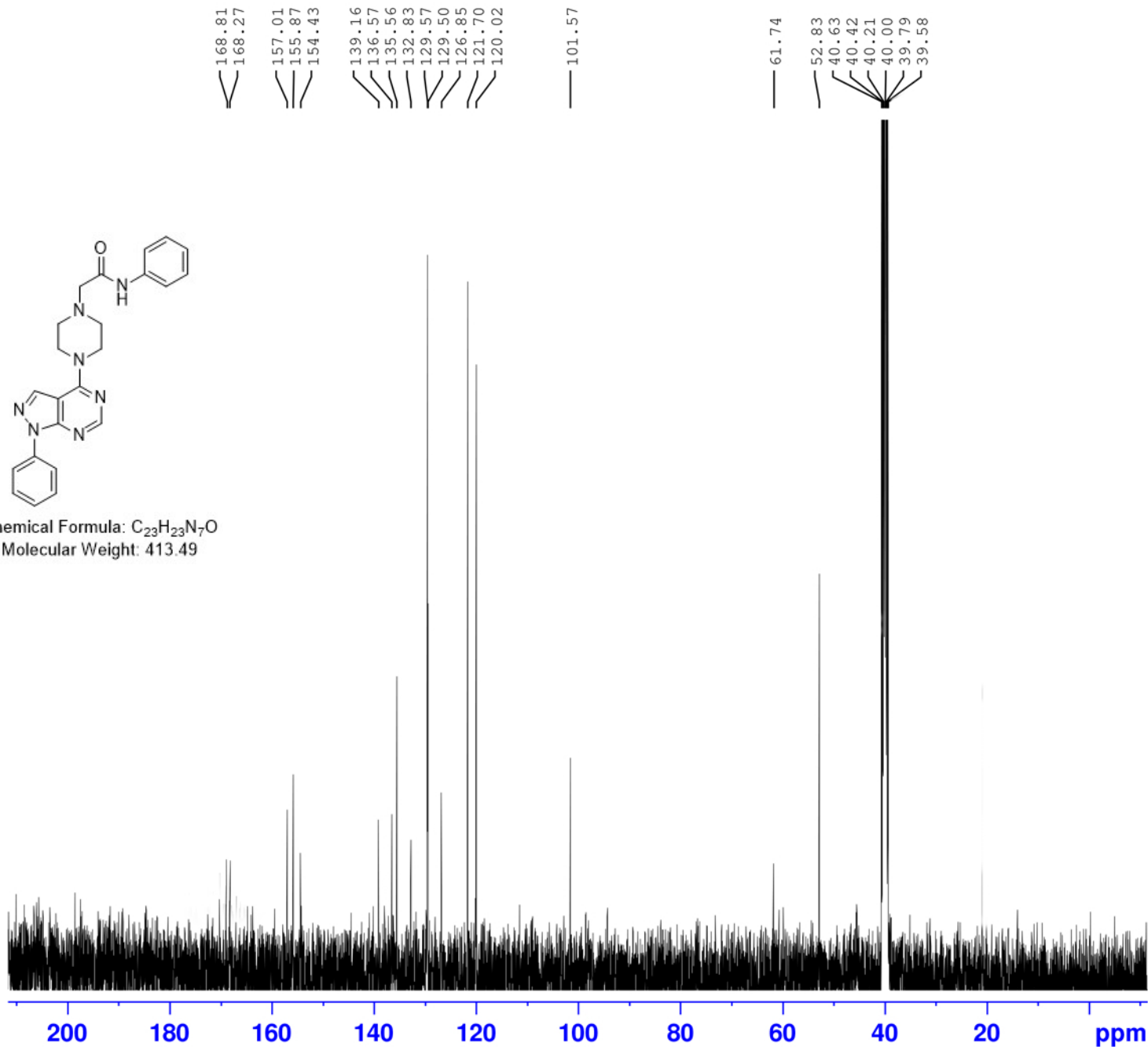
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SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

XIIa 13C NMR



Chemical Formula: C₂₃H₂₃N₇O
Molecular Weight: 413.49



Current Data Parameters
NAME rania-mohamed-7a
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210408
Time 10.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1340
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.37
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 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.34722000 W
PLW13 0.28125000 W

F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N-(4-Bromophenyl)-2-(4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)piperazin-1-yl)acetamide XIIb

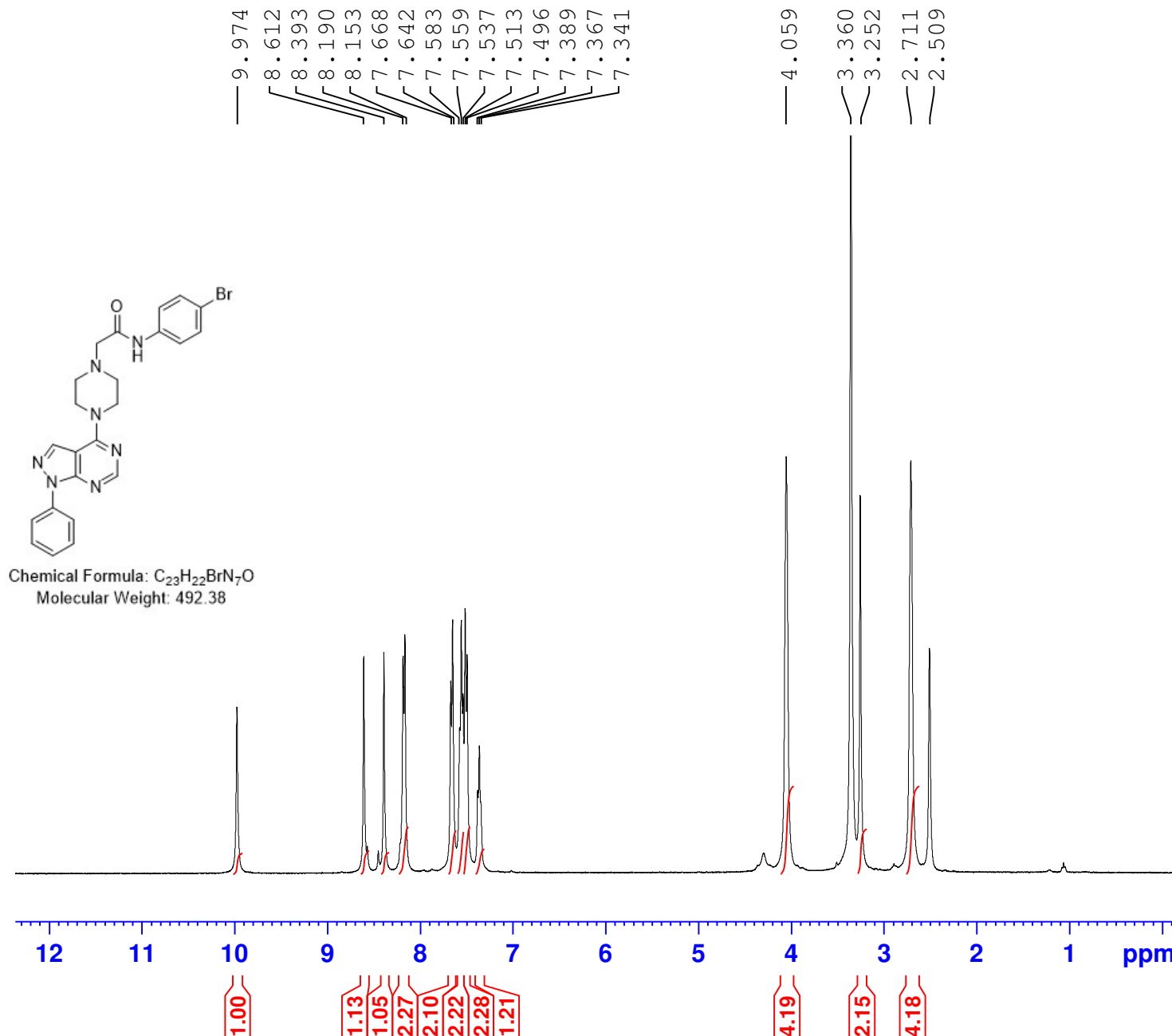


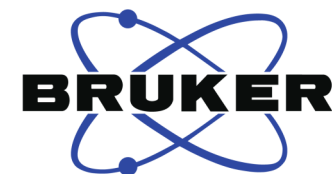
Current Data Parameters
 NAME RM-7e
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190701
 Time 9.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 64
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 205.37
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 18.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



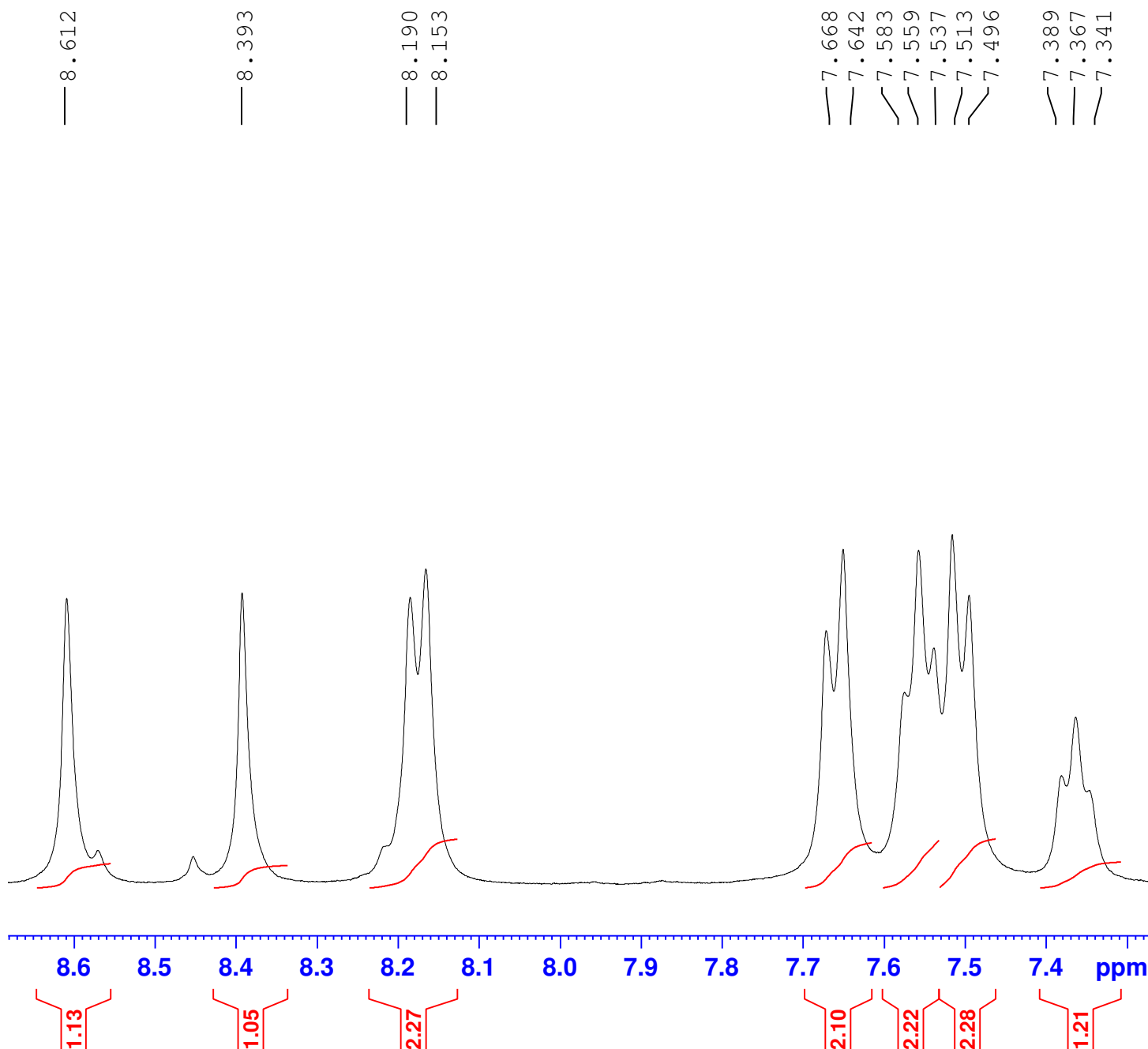


Current Data Parameters
NAME RM-7e
EXPNO 1
PROCNO 1

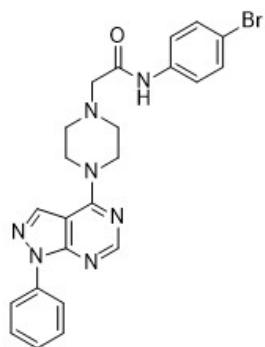
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Date_ 20190701
Time 9.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

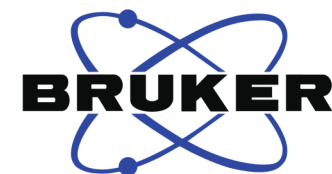
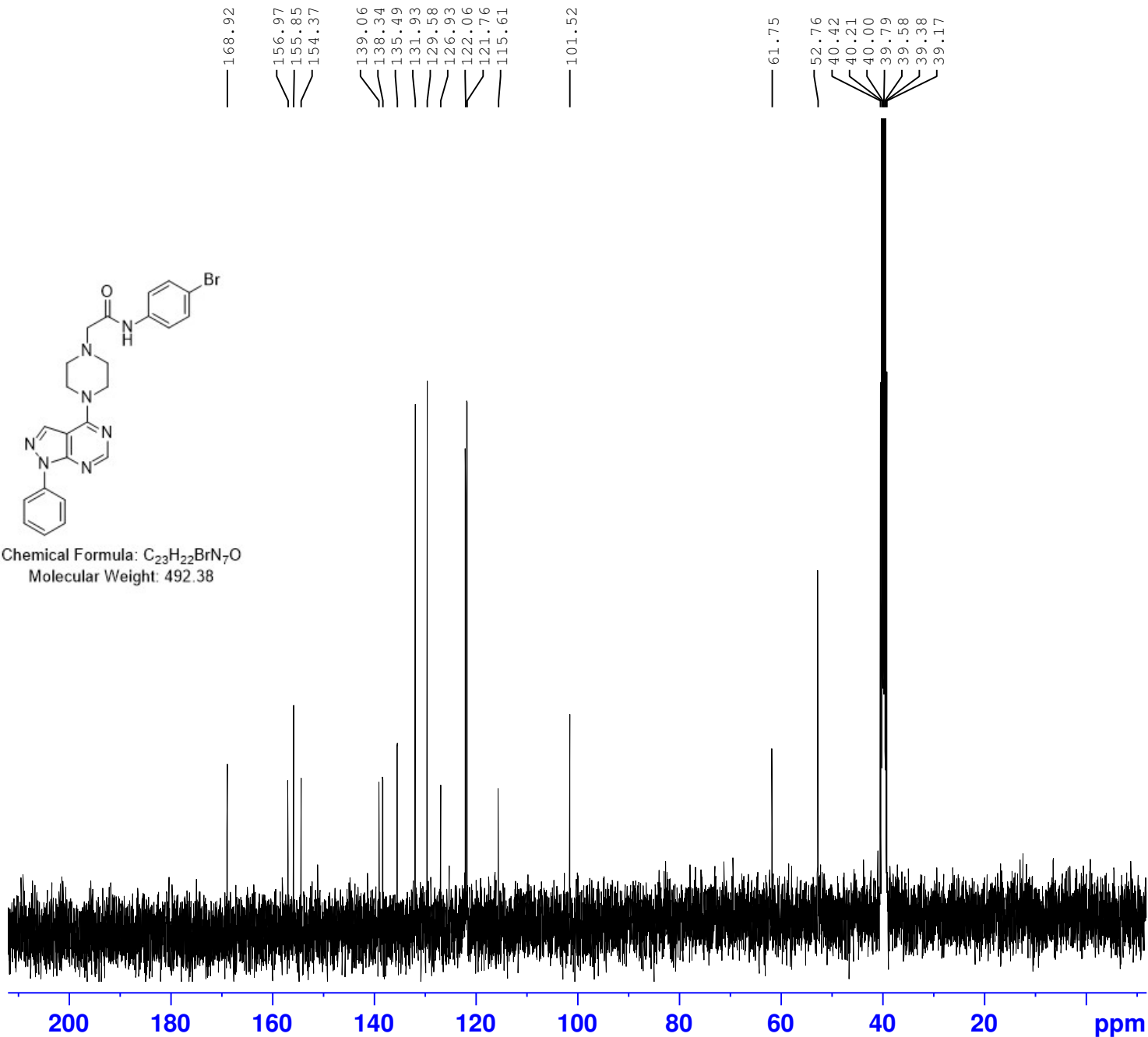
F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



XIib 13C NMR



Chemical Formula: C₂₃H₂₂BrN₇O
Molecular Weight: 492.38



Current Data Parameters
NAME RM-7e
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190711
Time 8.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 780
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.37
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

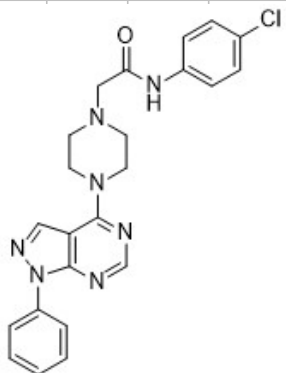
===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.34722000 W
PLW13 0.28125000 W

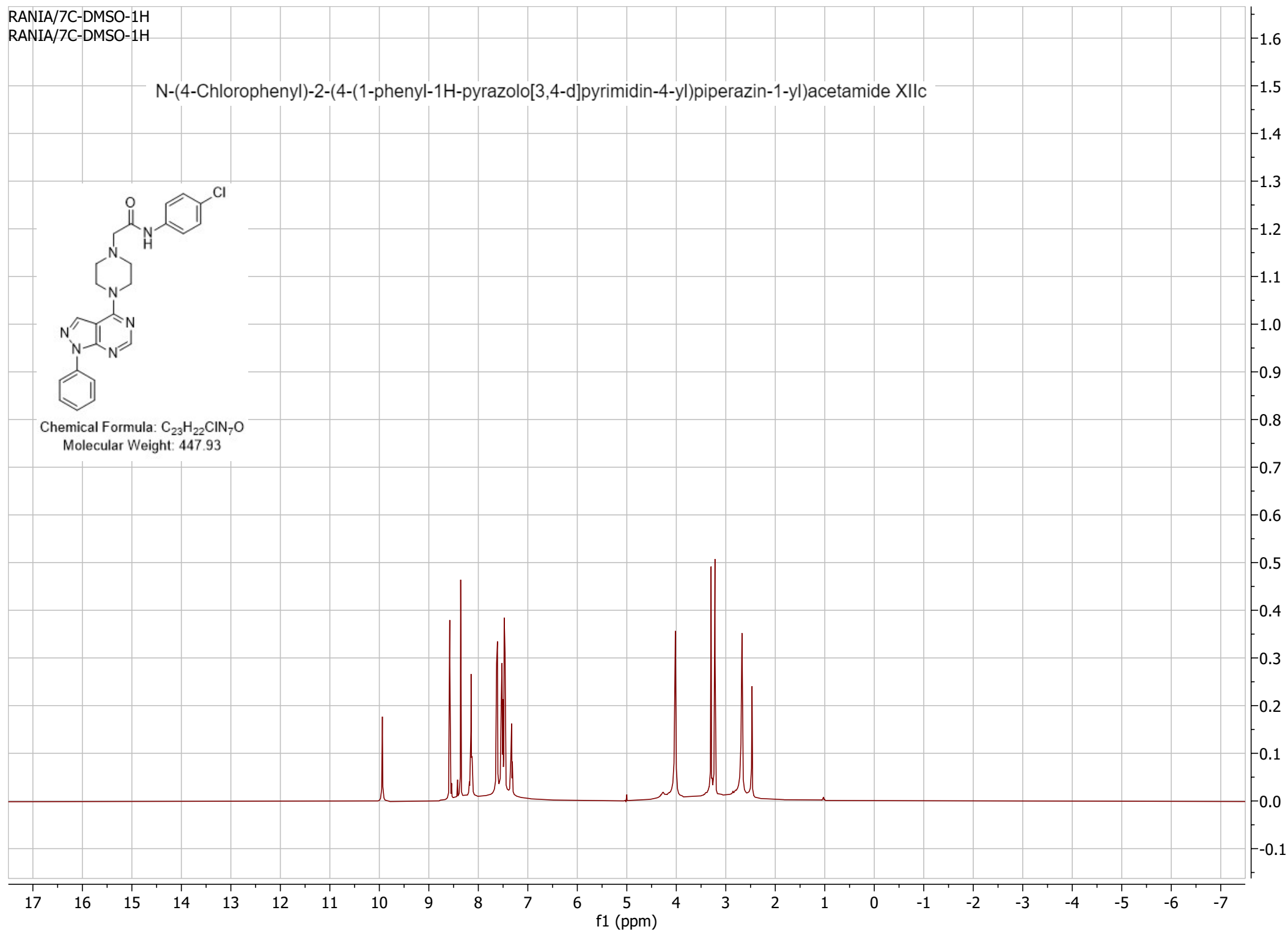
F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

RANIA/7C-DMSO-1H
RANIA/7C-DMSO-1H

N-(4-Chlorophenyl)-2-(4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)piperazin-1-yl)acetamide XIIc

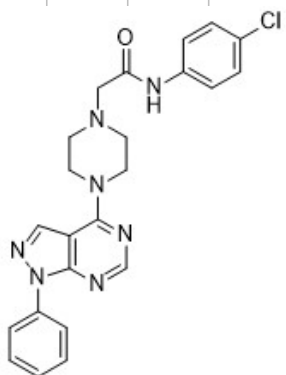


Chemical Formula: C₂₃H₂₂ClN₇O
Molecular Weight: 447.93

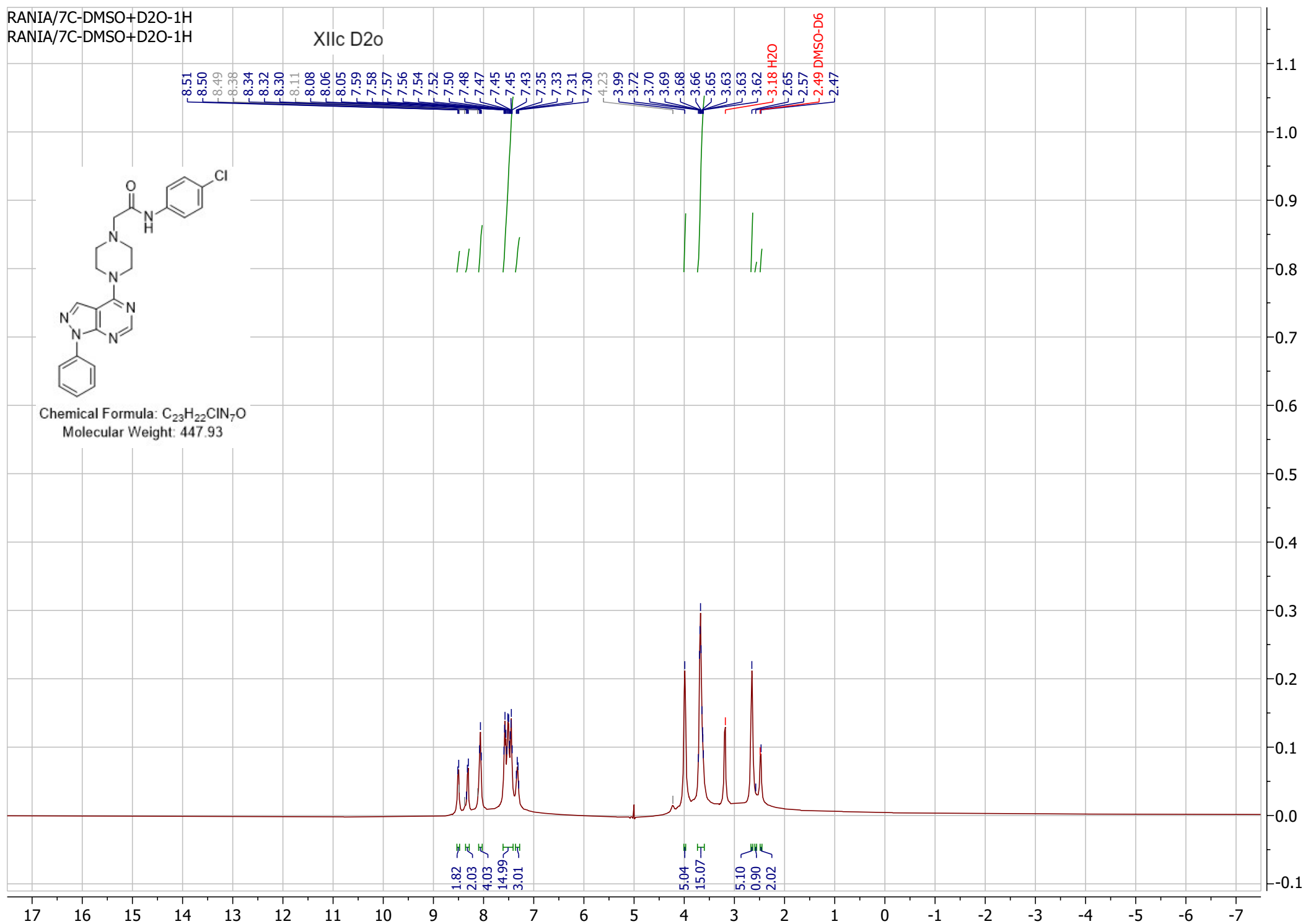


RANIA/7C-DMSO+D2O-1H
RANIA/7C-DMSO+D2O-1H

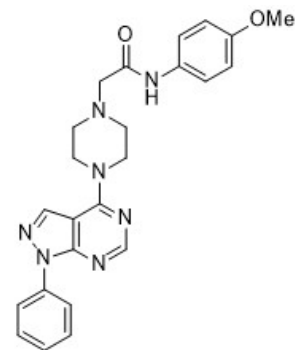
XIIc D2o



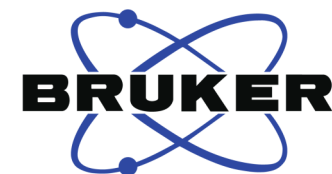
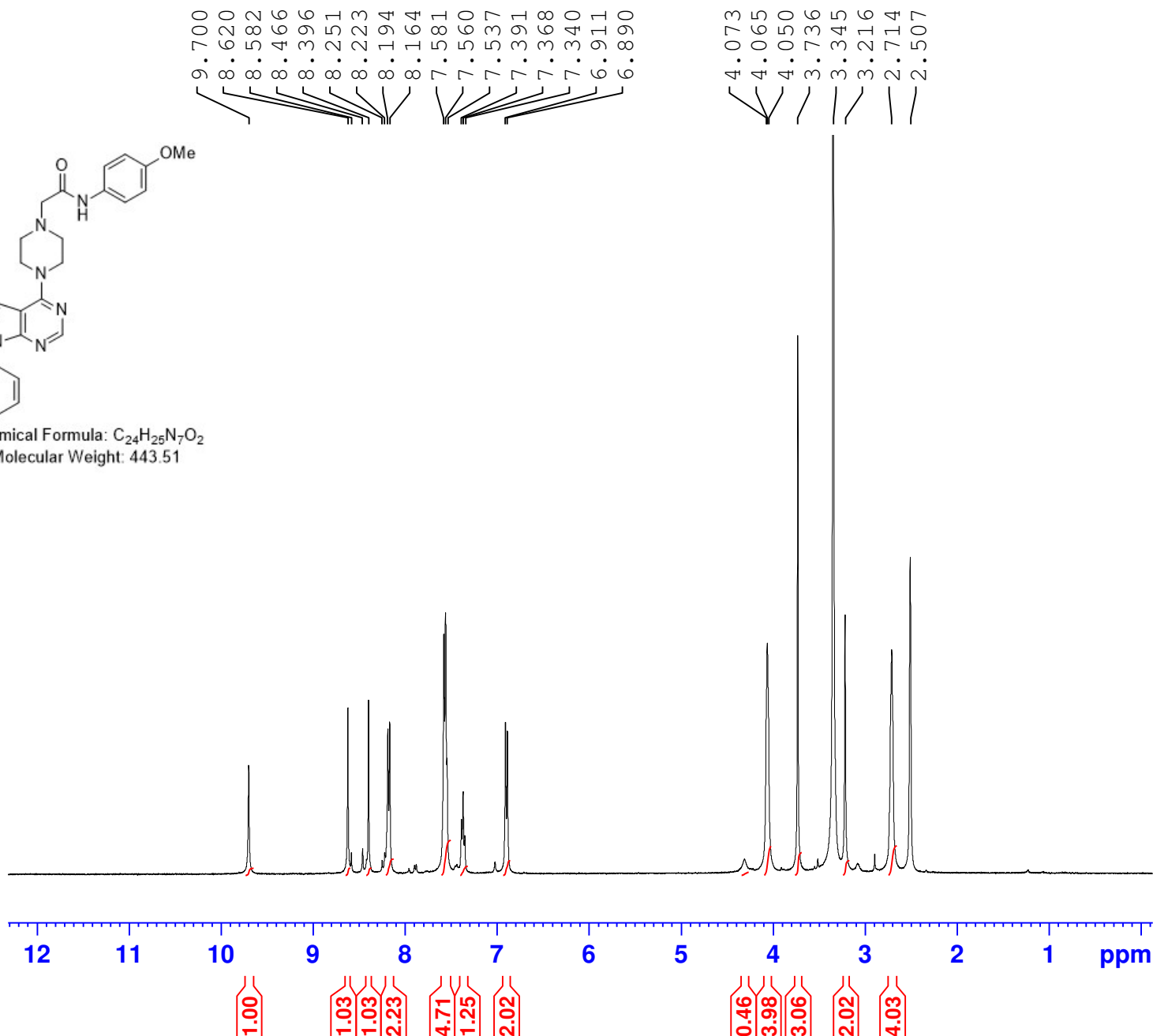
Chemical Formula: C₂₃H₂₂ClN₇O
Molecular Weight: 447.93



N-(4-methoxyphenyl)-2-(4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)piperazin-1-yl)acetamide XIId



Chemical Formula: $C_{24}H_{25}N_7O_2$
Molecular Weight: 443.51



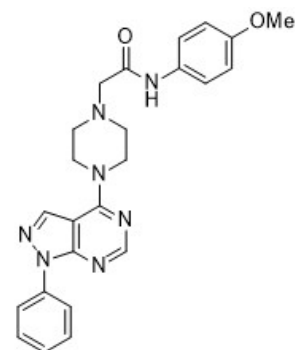
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NAME RM-7d
EXPNO 1
PROCNO 1

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Date_ 20190701
Time 9.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 52
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

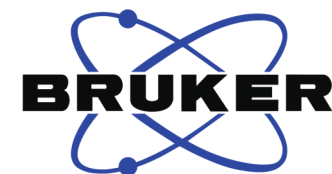
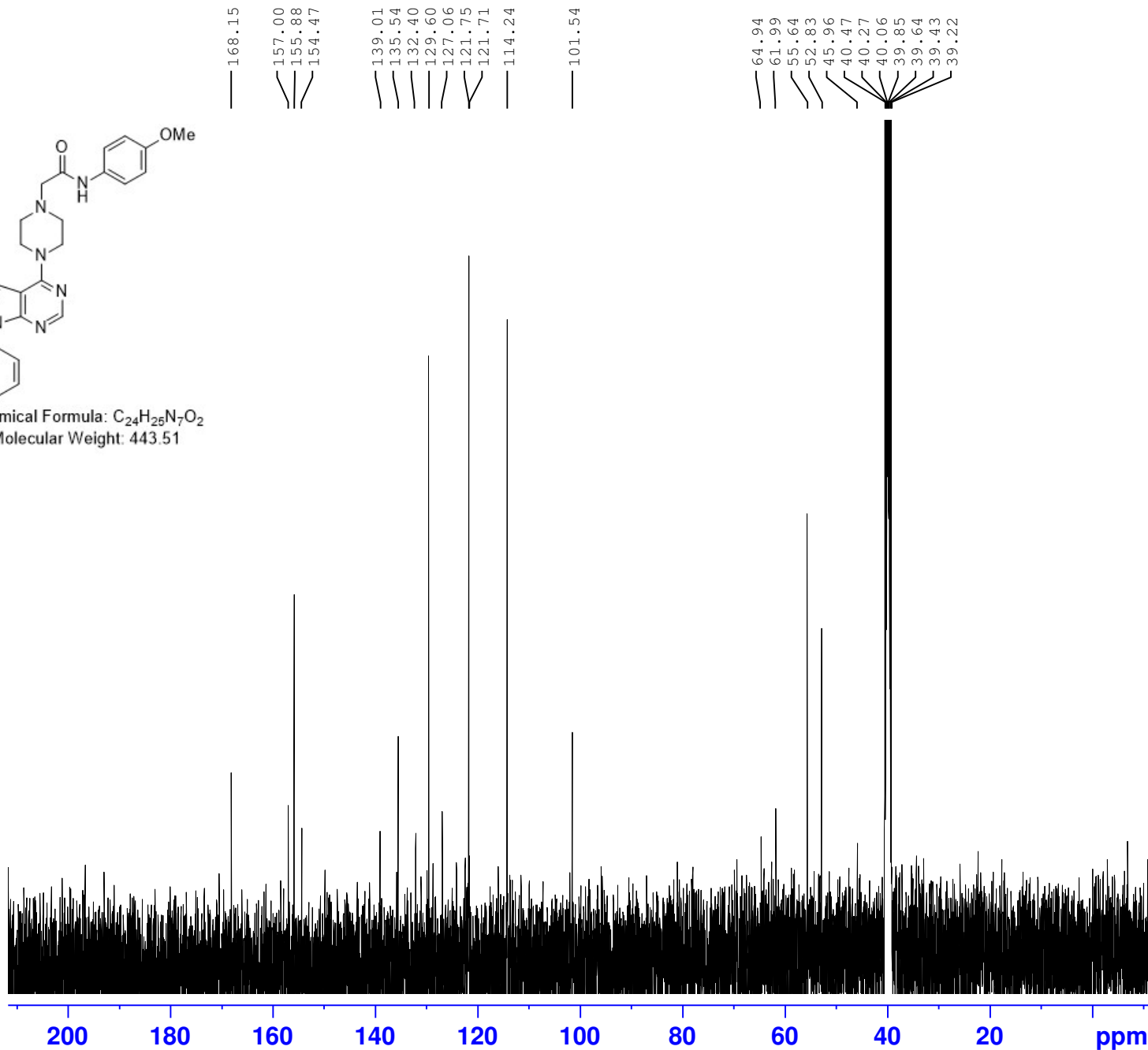
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NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

XIIId 13C NMR



Chemical Formula: $C_{24}H_{25}N_7O_2$
Molecular Weight: 443.51



Current Data Parameters
NAME RM-7d
EXPNO 2
PROCNO 1

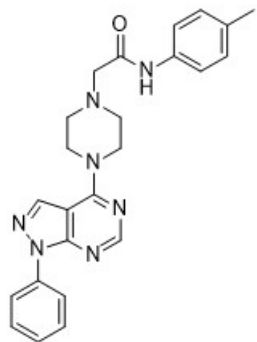
F2 - Acquisition Parameters
Date_ 20190710
Time 12.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 995
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.37
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W

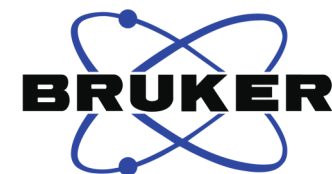
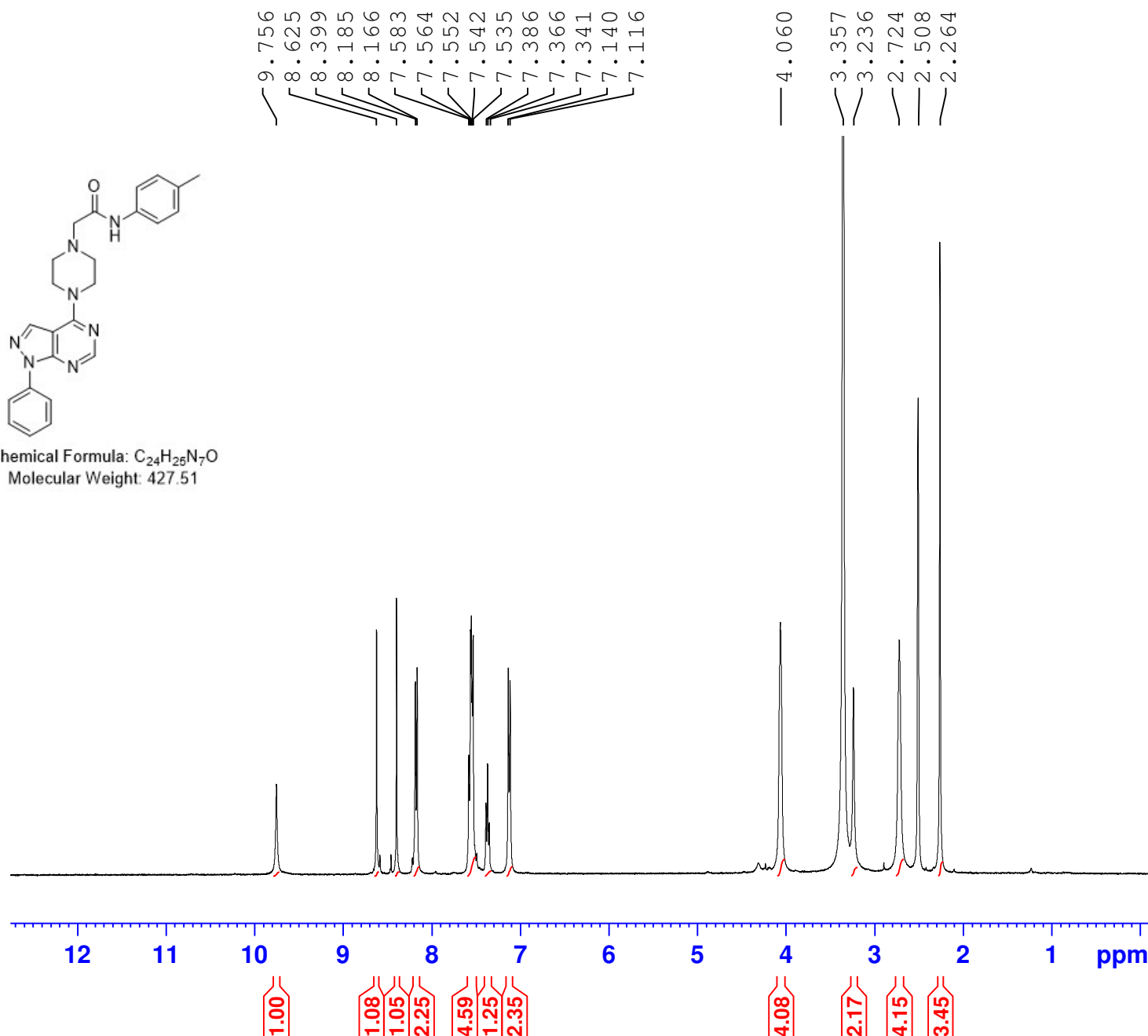
===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.34722000 W
PLW13 0.28125000 W

F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2-(4-(1-Phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)piperazin-1-yl)-N-(p-tolyl)acetamide Xlle



Chemical Formula: C₂₄H₂₆N₇O
Molecular Weight: 427.51

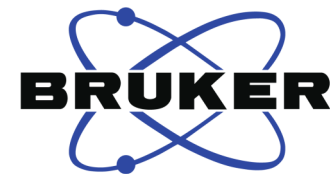
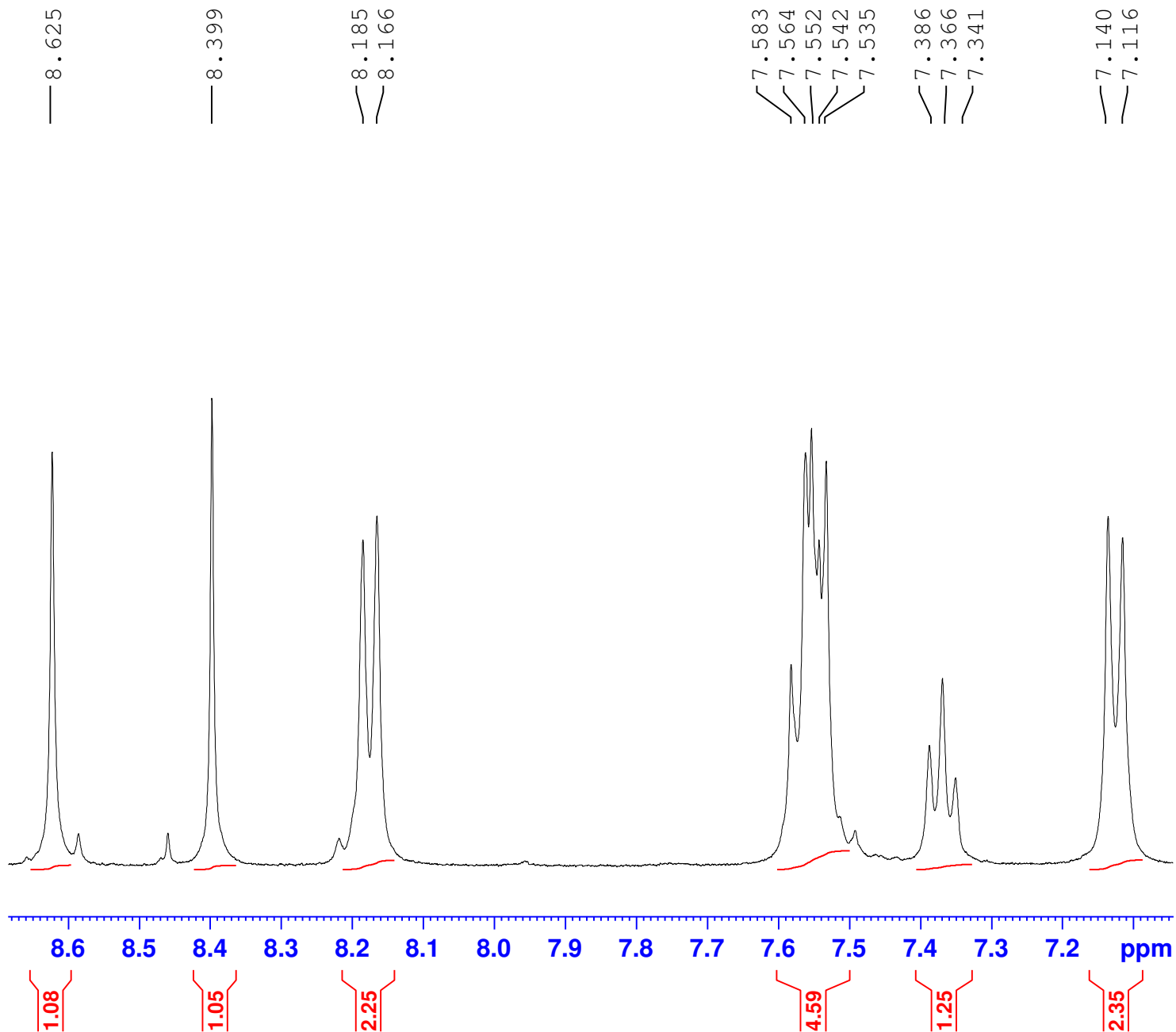


Current Data Parameters
NAME AM-7b
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190521
Time 8.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



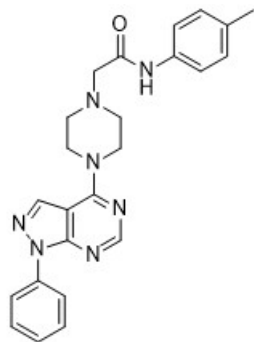
Current Data Parameters
 NAME AM-7b
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190521
 Time 8.44
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 64
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 205.37
 DW 62.400 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 18.00000000 W

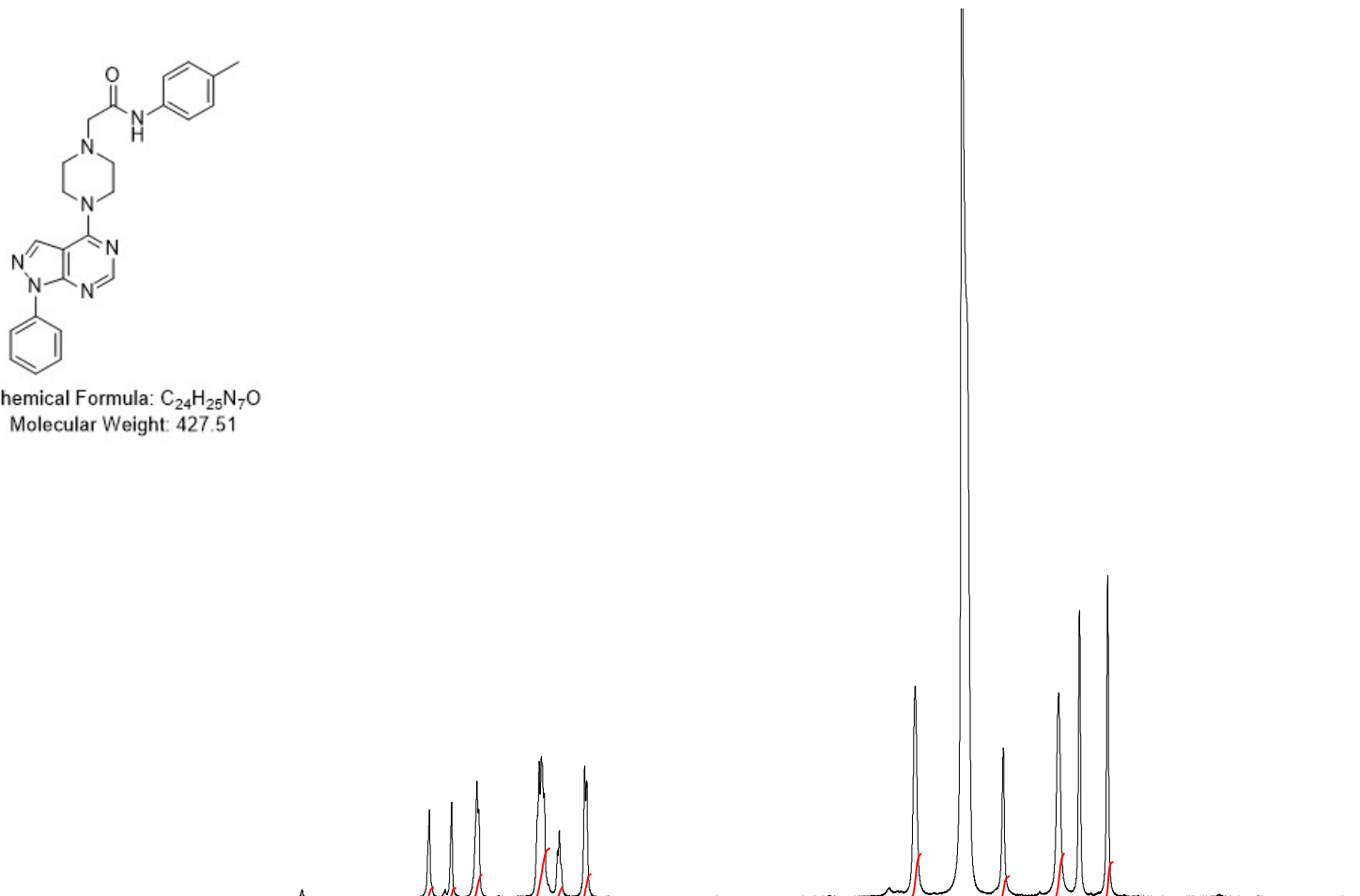
F2 - Processing parameters
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 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

XIIe D2O



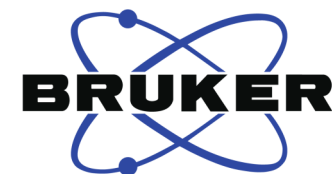
Chemical Formula: C₂₄H₂₆N₇O
Molecular Weight: 427.51

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8.372
8.137
8.117
7.572
7.551
7.532
7.523
7.508
7.379
7.362
7.344
7.129
7.111
4.041
3.610
3.558
3.221
2.707
2.511
2.241



1.00
0.94
2.01
4.10
1.06
2.04

3.67
1.90
3.70
3.01



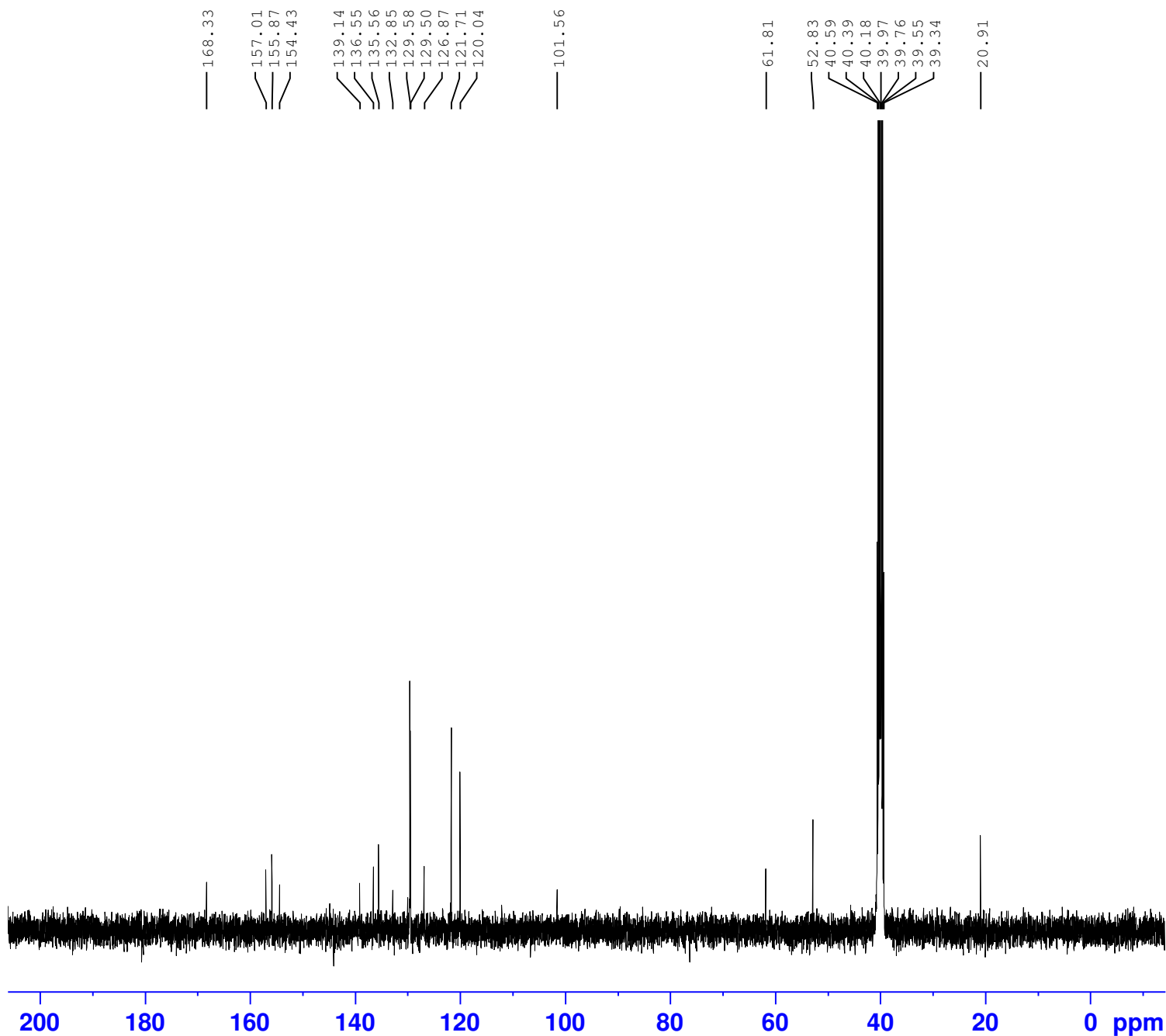
Current Data Parameters
NAME AM-7b-d2o
EXPNO 1
PROCNO 1

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Time 8.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 33
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

XIle 13C NMR



Current Data Parameters
 NAME rania-mohamed-8b
 EXPNO 3
 PROCNO 1

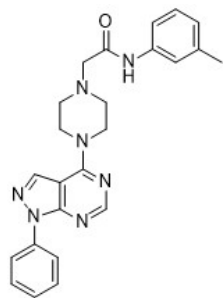
F2 - Acquisition Parameters
 Date_ 20230220
 Time 15.06
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2058
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 205.37
 DW 20.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6278588 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 47.00000000 W

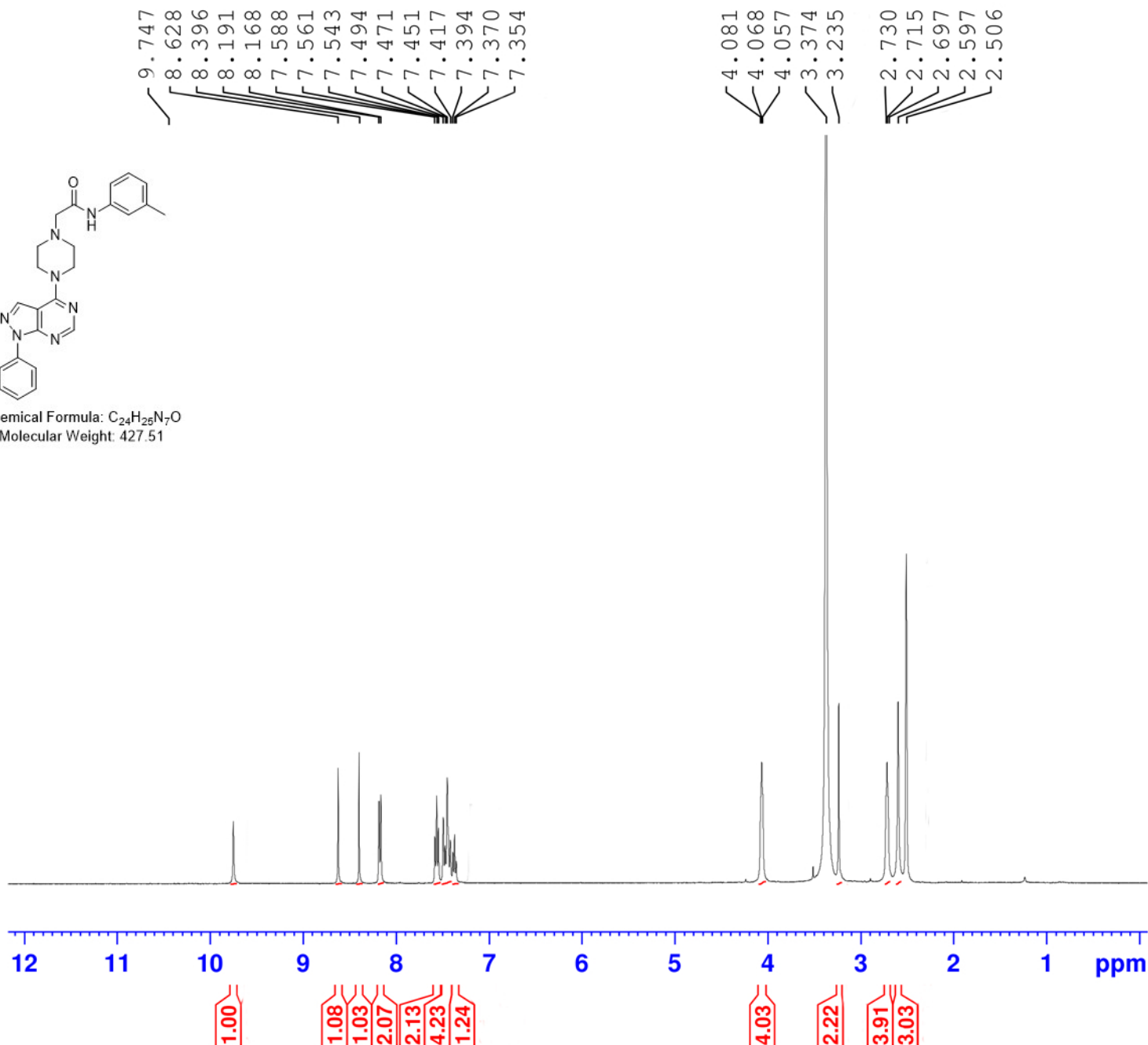
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 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 18.00000000 W
 PLW12 0.34722000 W
 PLW13 0.28125000 W

F2 - Processing parameters
 SI 32768
 SF 100.6177975 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

2-(4-(1-Phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)piperazin-1-yl)-N-(m-tolyl)acetamide XIIIf



Chemical Formula: C₂₄H₂₅N₇O
Molecular Weight: 427.51



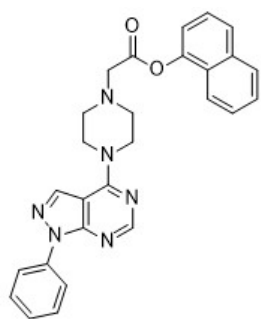
Current Data Parameters
NAME RS-7F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190722
Time 10.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 128
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

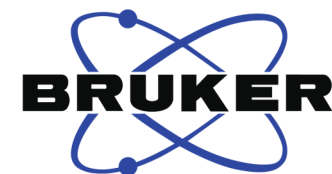
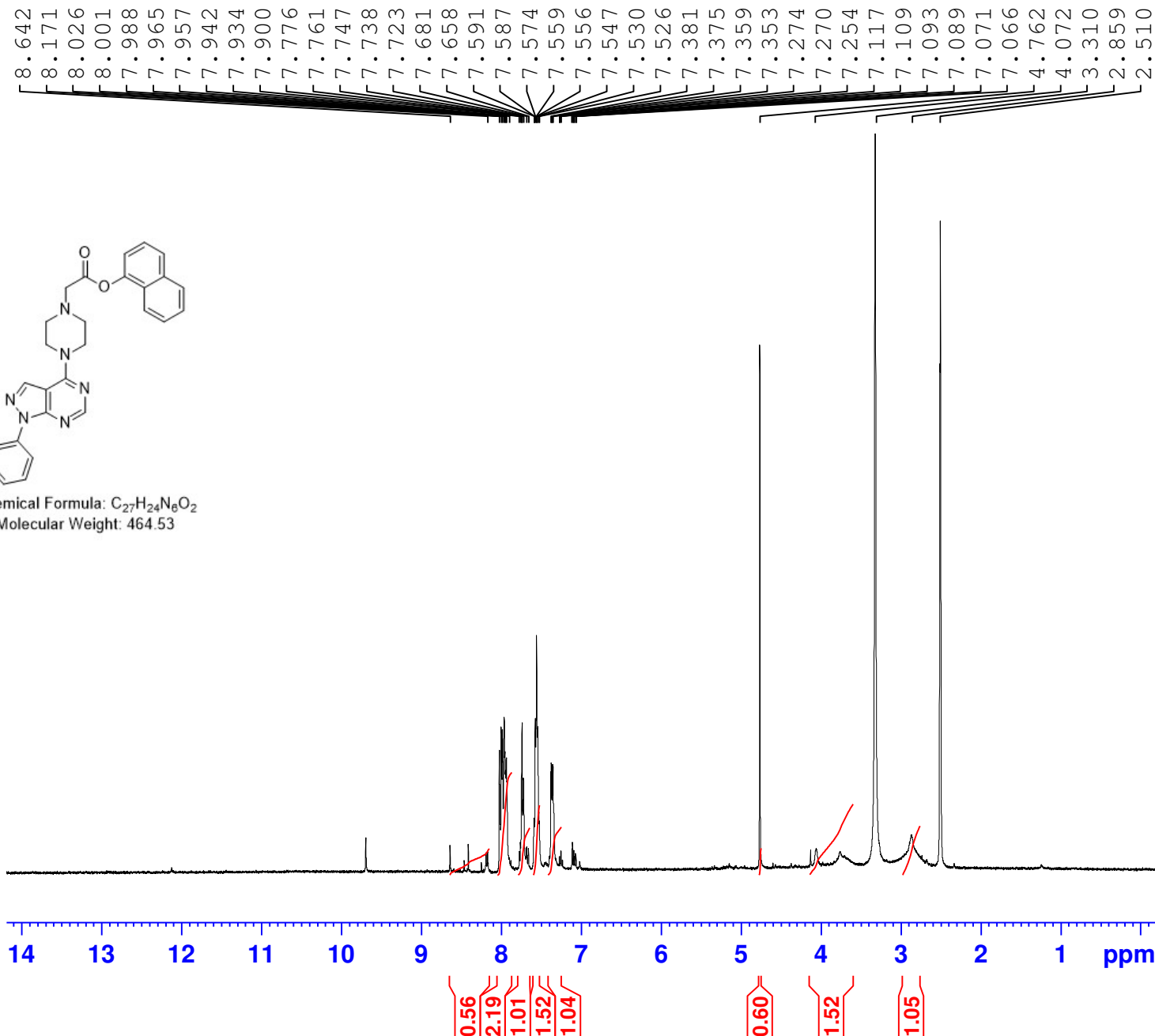
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NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Naphthalen-1-yl 2-(4-(1-phenyl-1H-pyrazolo [3,4-d] pyrimidin-4-yl) piperazin-1-yl)acetate XIII



Chemical Formula: C₂₇H₂₄N₈O₂
Molecular Weight: 464.53

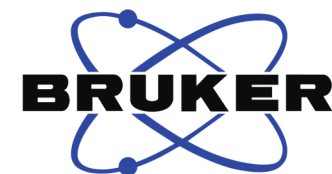


Current Data Parameters
NAME rania-mohammed-9a
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210405
Time 14.06
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 74
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
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PC 1.00

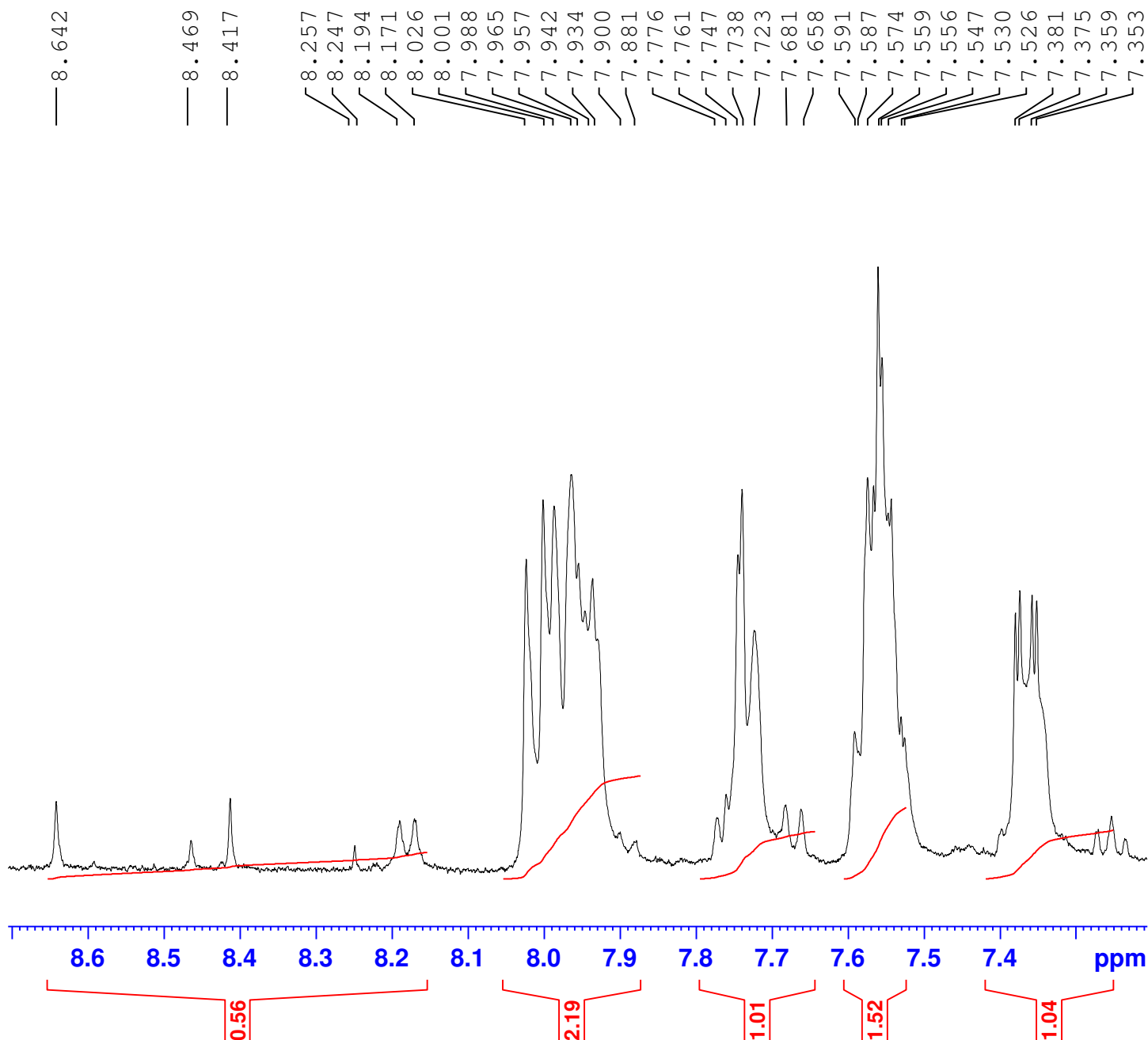


Current Data Parameters
NAME rania-mohammed-9a
EXPNO 1
PROCNO 1

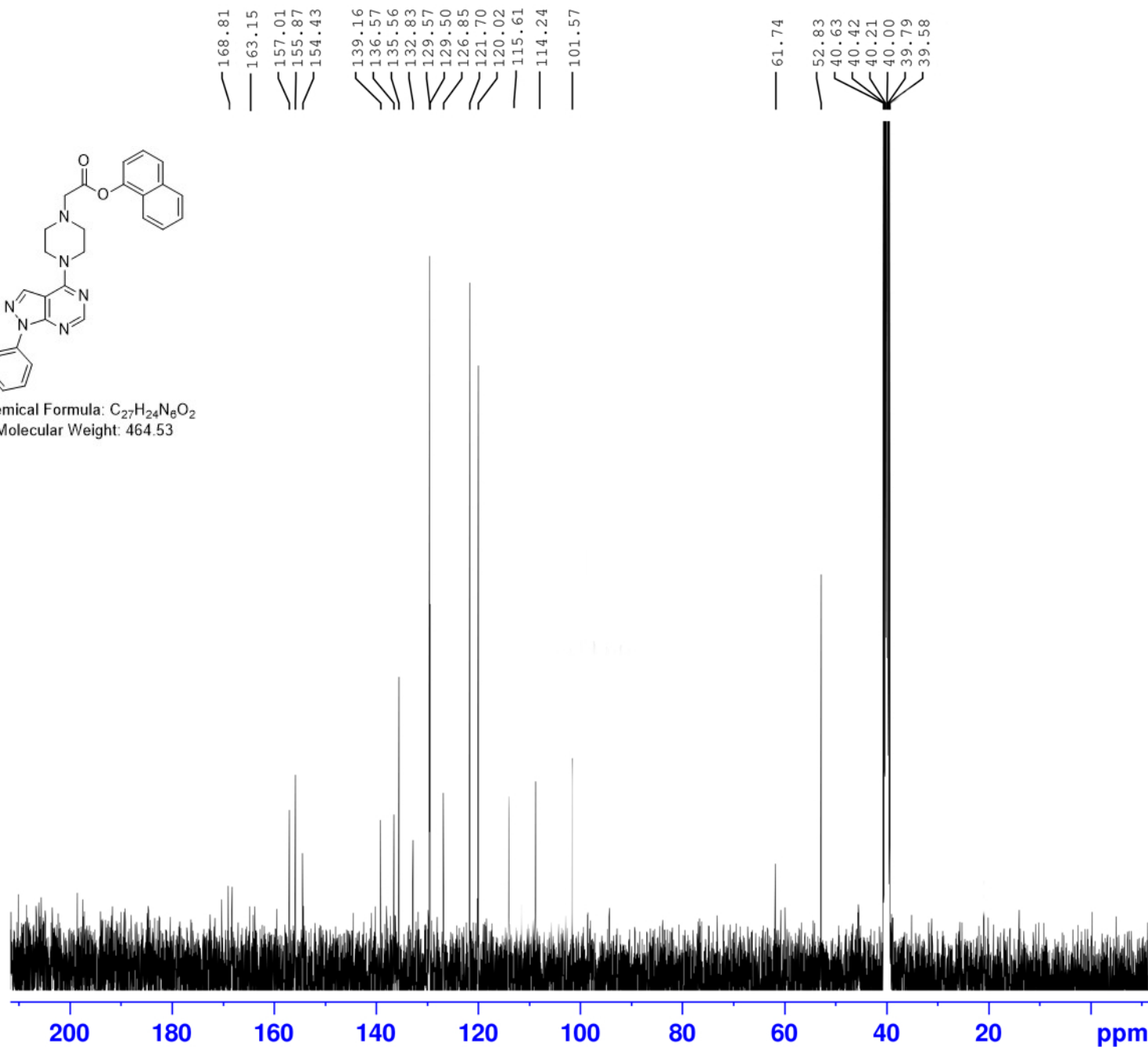
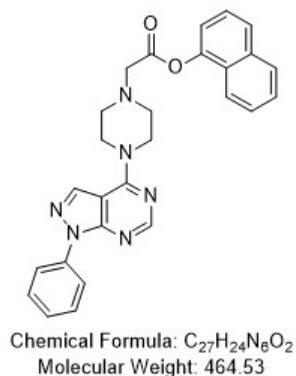
F2 - Acquisition Parameters
Date_ 20210405
Time 14.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 74
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



XIII 13C NMR



Current Data Parameters
NAME rania-mohammed-9a
EXPNO 1
PROCNO 1

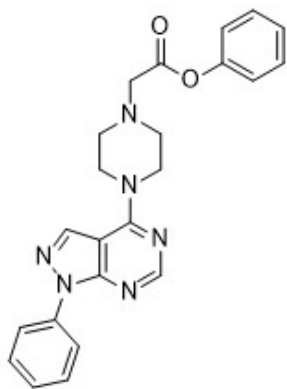
F2 - Acquisition Parameters
Date_ 20210408
Time 10.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1340
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.37
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W

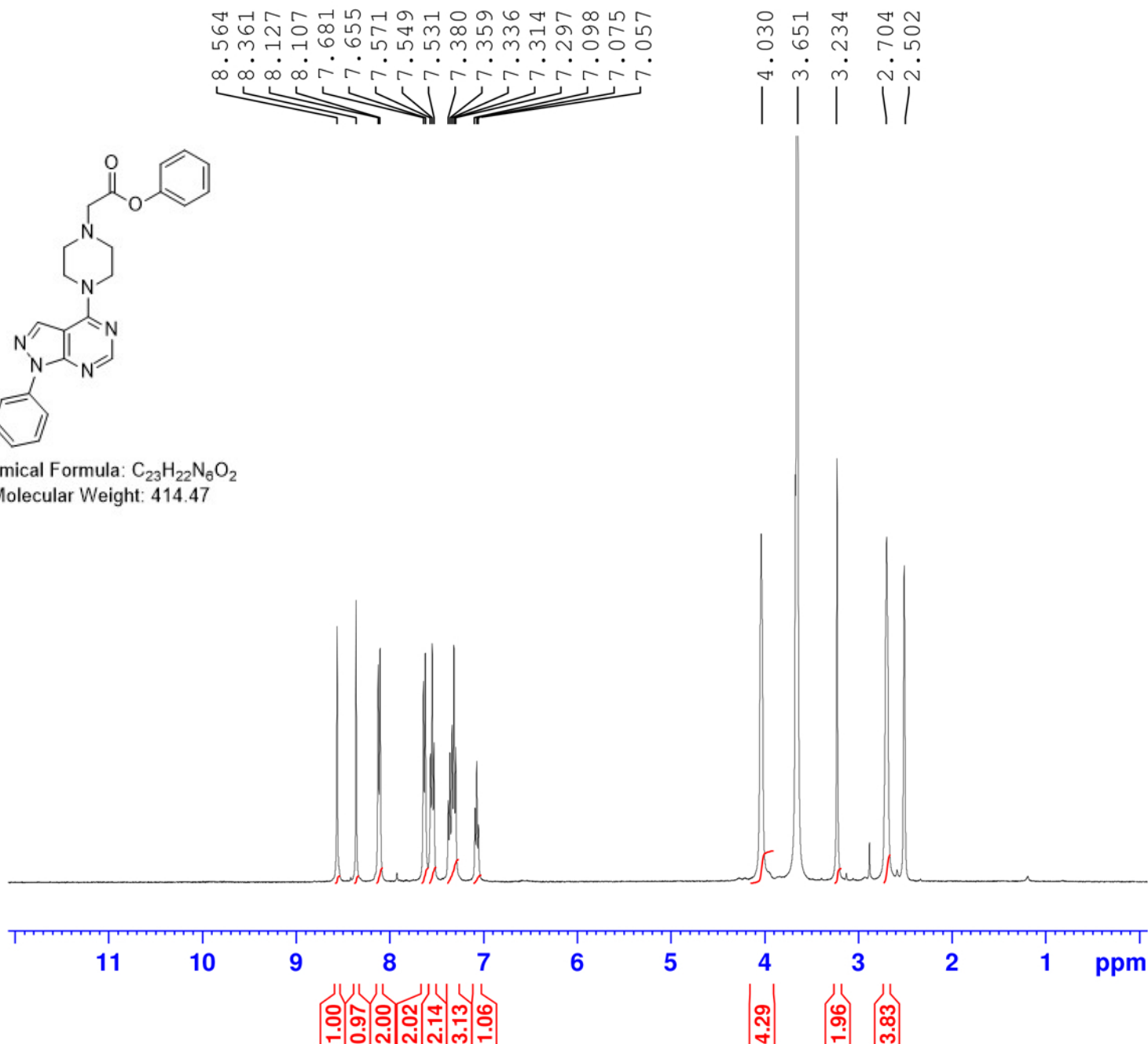
===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.34722000 W
PLW13 0.28125000 W

F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

phenyl 2-(4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)piperazin-1-yl)acetate XIV



Chemical Formula: $C_{23}H_{22}N_6O_2$
Molecular Weight: 414.47



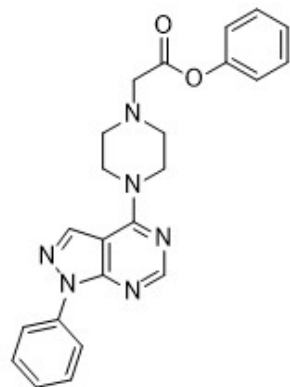
Current Data Parameters
NAME rania-mohammed-9b
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210405
Time 15.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 128
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

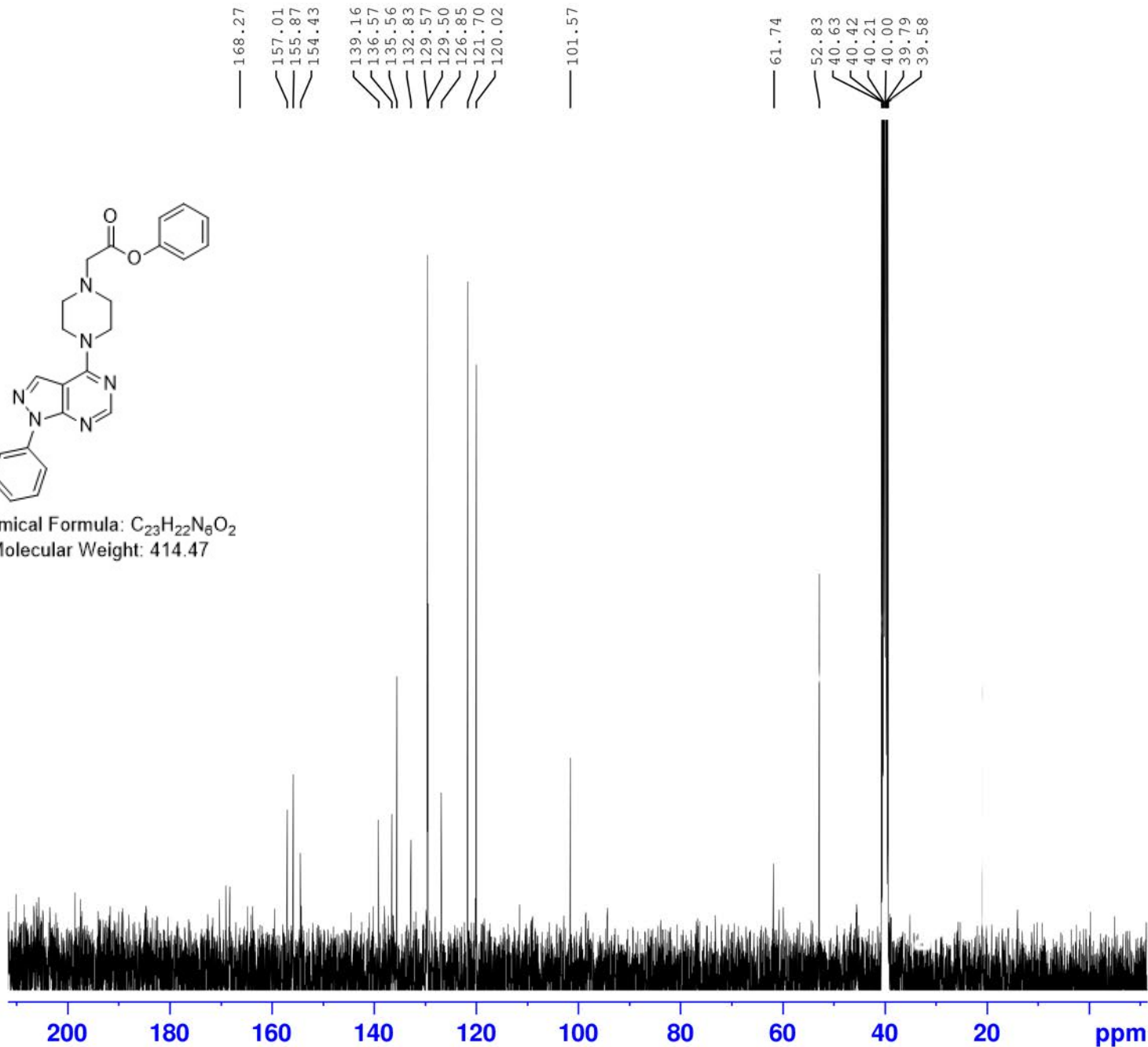
===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

XIV ¹³C NMR



Chemical Formula: C₂₃H₂₂N₄O₂
Molecular Weight: 414.47



Current Data Parameters
NAME rania-mohammed-9b
EXPNO 1
PROCNO 1

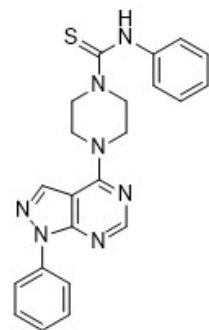
F2 - Acquisition Parameters
Date_ 20210408
Time 10.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1340
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.37
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W

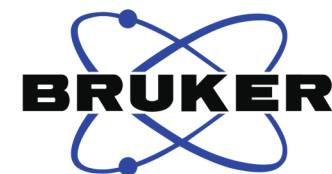
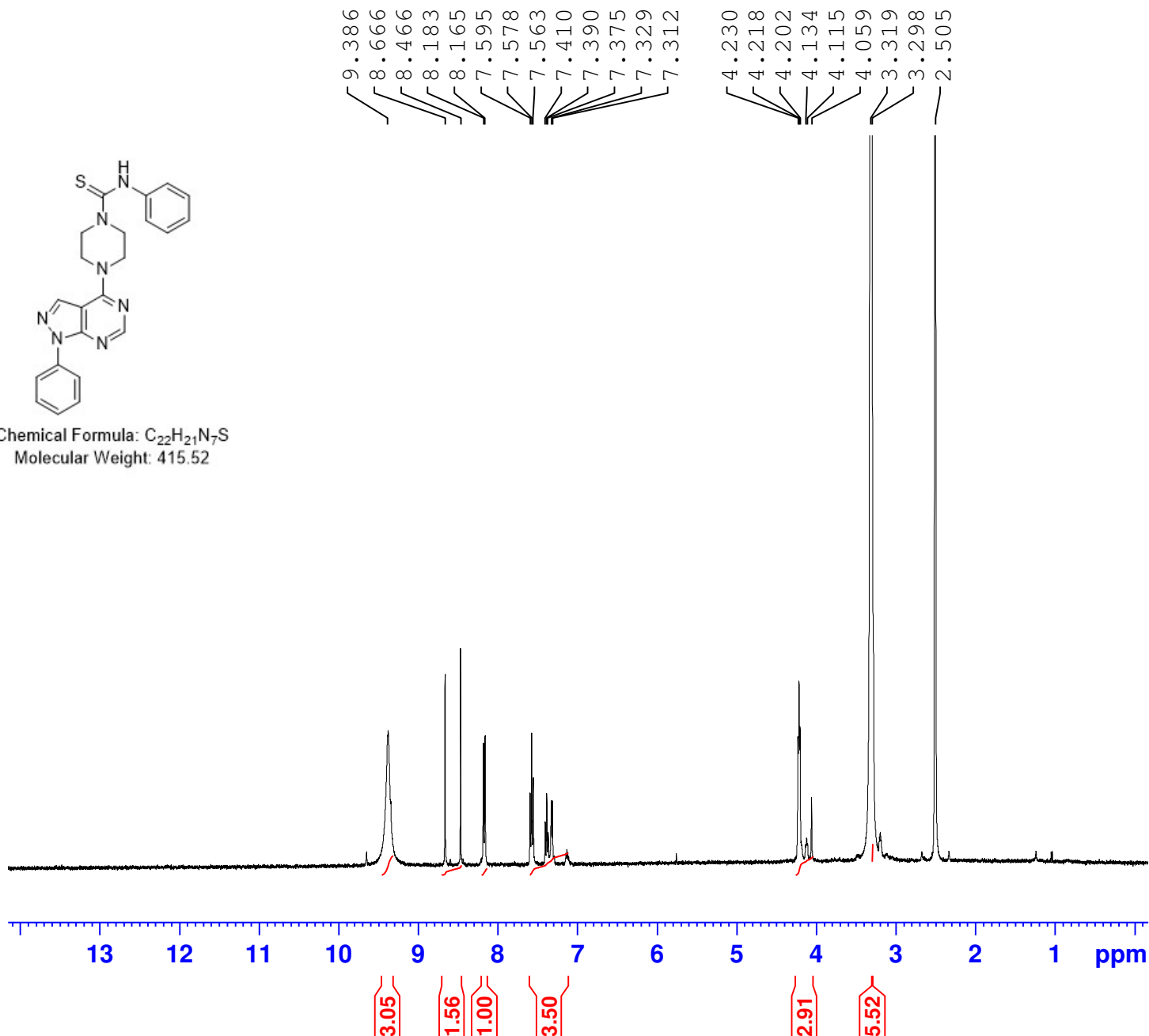
===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.34722000 W
PLW13 0.28125000 W

F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N-phenyl-4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)piperazine-1-carbothioamide XV



Chemical Formula: C₂₂H₂₁N₇S
Molecular Weight: 415.52

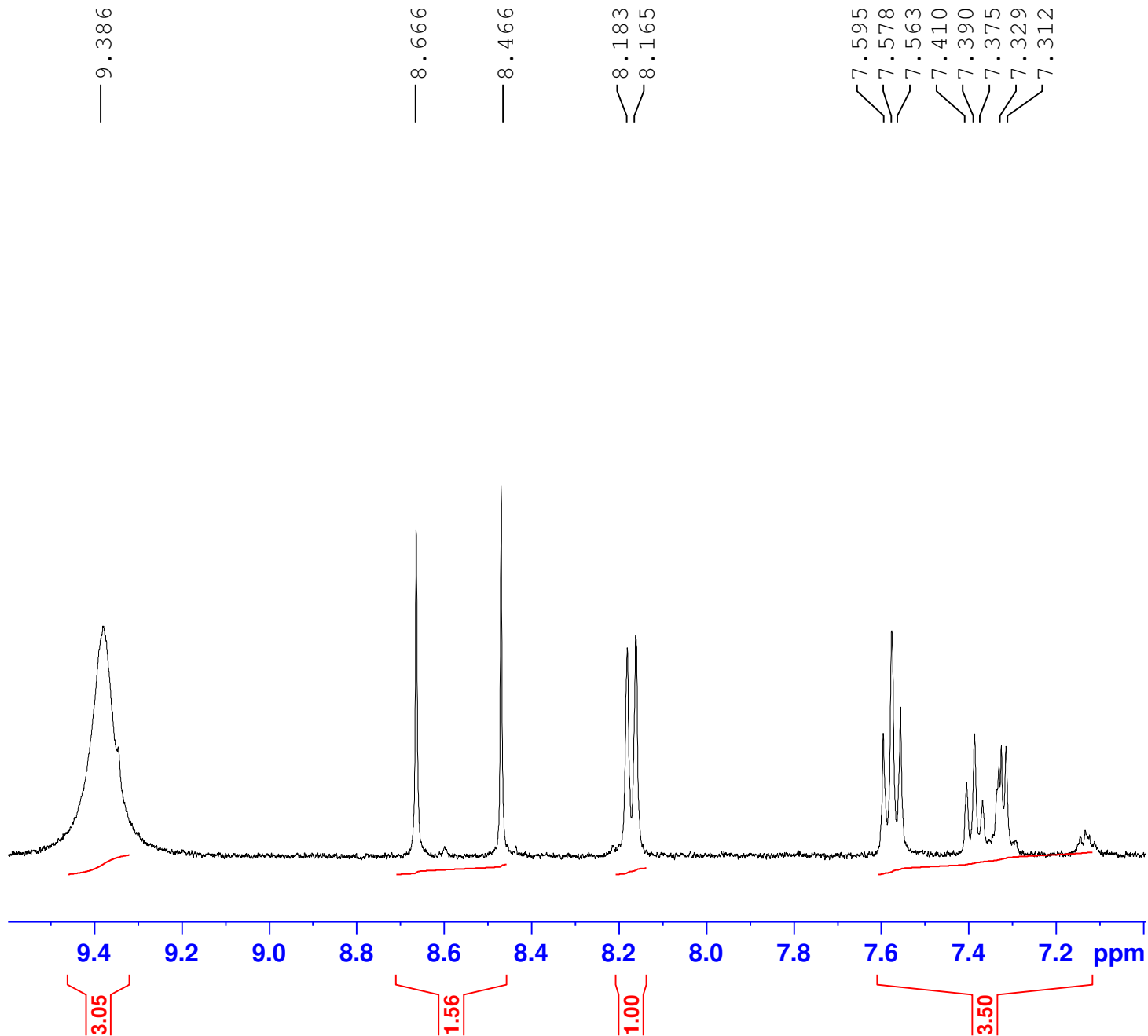


Current Data Parameters
NAME rania-mohammed-10a
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210405
Time 14.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 128
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



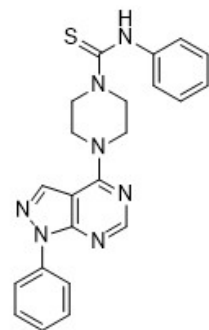
Current Data Parameters
 NAME rania-mohammed-10a
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210405
 Time 14.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 128
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 205.37
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

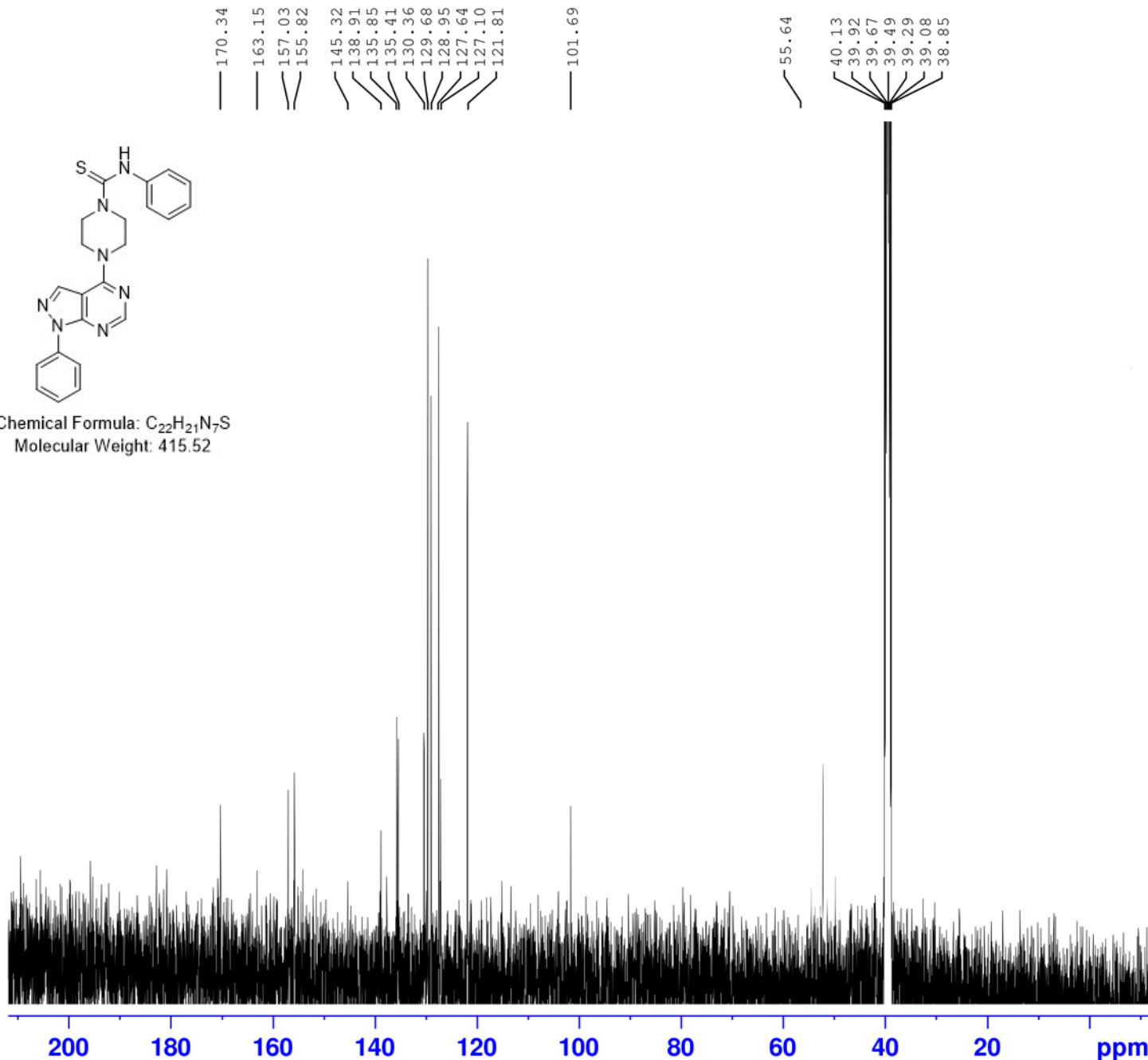
===== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 18.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

XV 13C NMR



Chemical Formula: C₂₂H₂₁N₇S
Molecular Weight: 415.52



Current Data Parameters
NAME rania-mohammed-10a
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210405
Time 13.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1800
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.37
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 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.34722000 W
PLW13 0.28125000 W

F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2-(4-(1-Phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)piperazin-1-yl)-N-(1,3,4-thiadiazol-2-yl)acetamide XVI

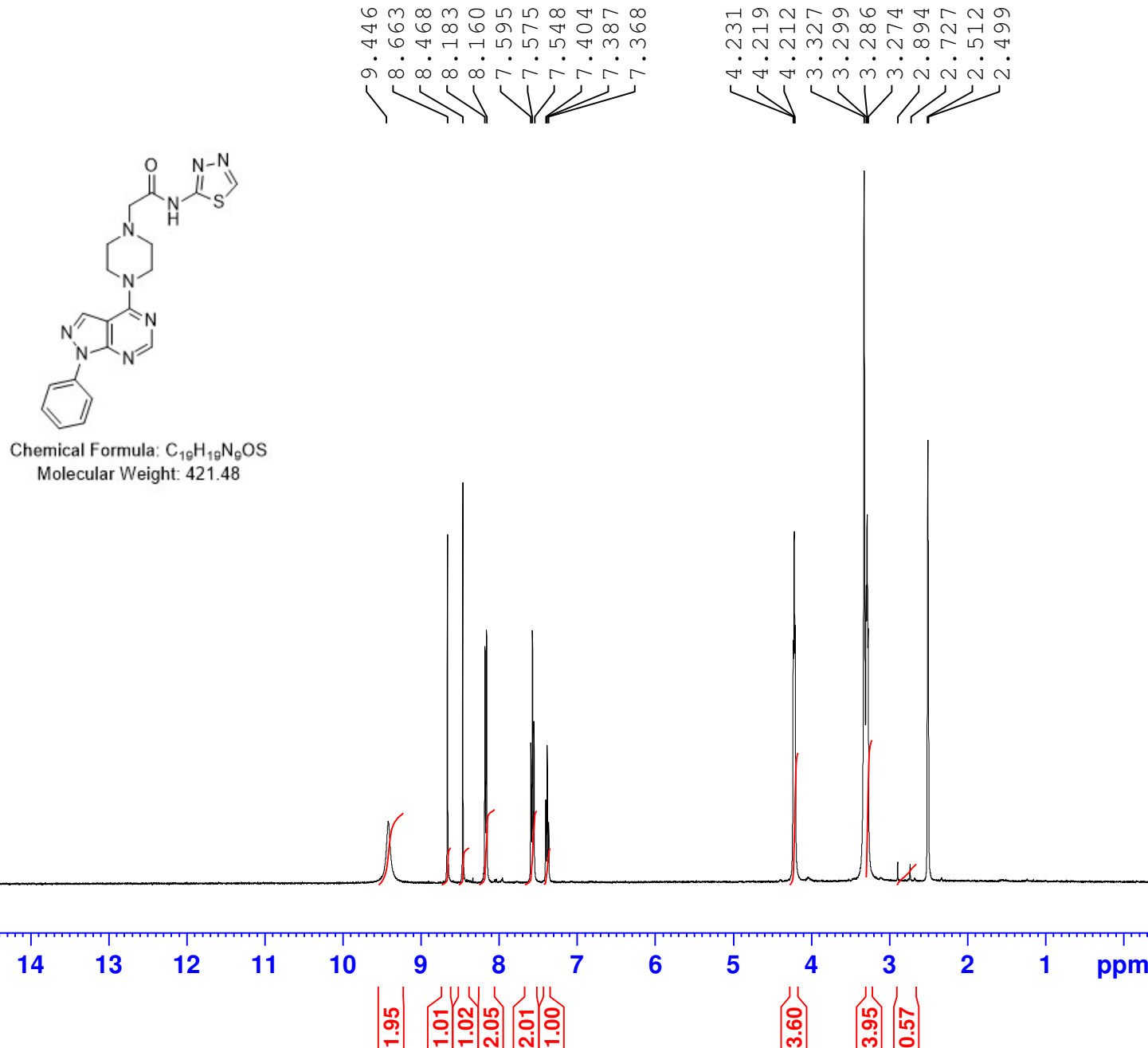


Current Data Parameters
 NAME rania-mohammed-7m
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210405
 Time 14.59
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 72
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 205.37
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 18.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



— 9.446

— 8.663

— 8.468

— 8.183
— 8.160

— 7.595
— 7.575
— 7.548
— 7.404
— 7.387
— 7.368

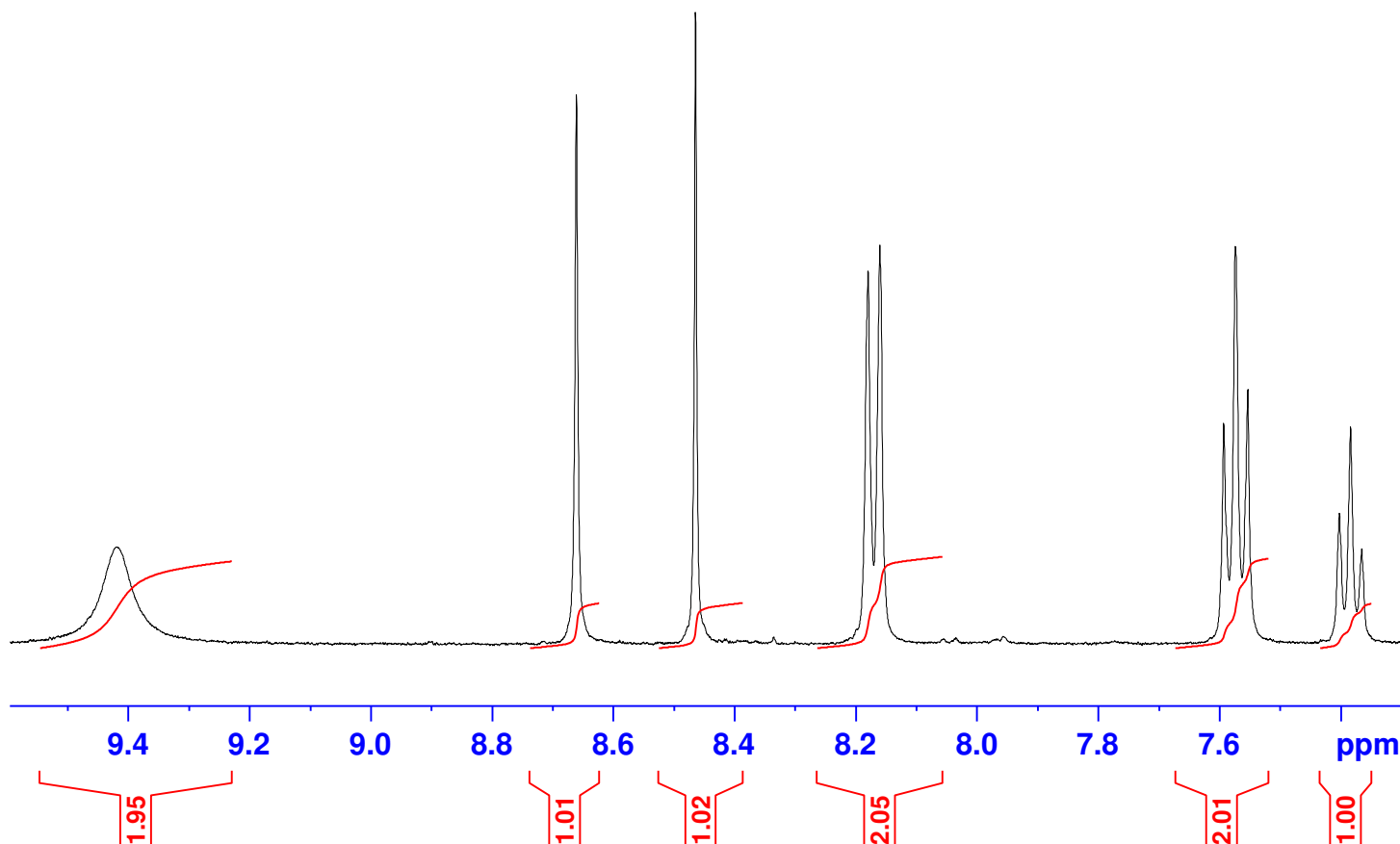


Current Data Parameters
NAME rania-mohammed-7m
EXPNO 1
PROCNO 1

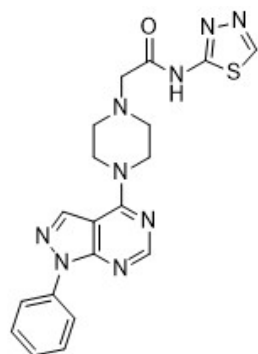
F2 - Acquisition Parameters
Date_ 20210405
Time 14.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 72
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

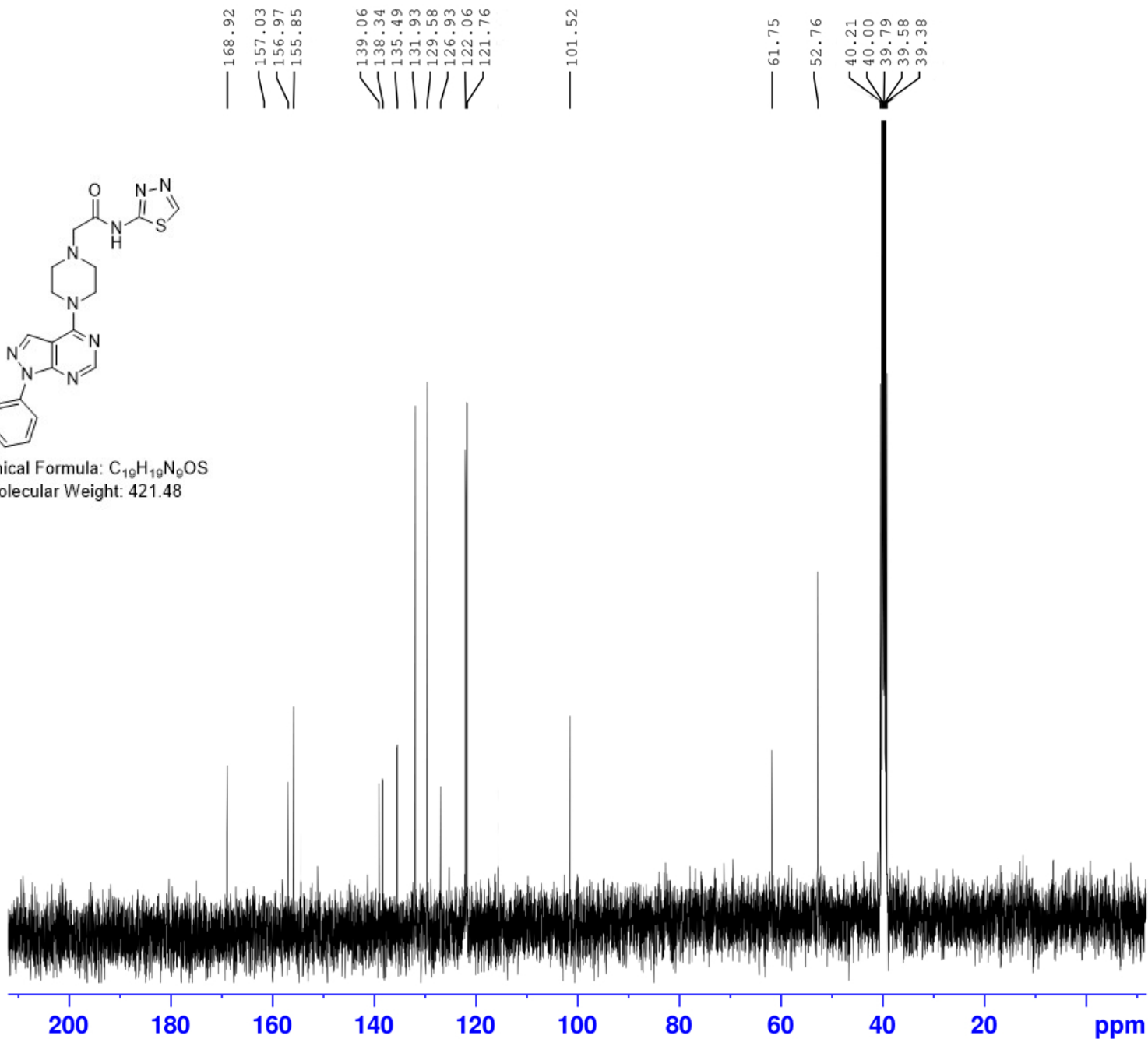
F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



XVI 13C NMR



Chemical Formula: C₁₉H₁₉N₅OS
Molecular Weight: 421.48



Current Data Parameters
NAME RM-7
EXPNO 2
PROCNO 1

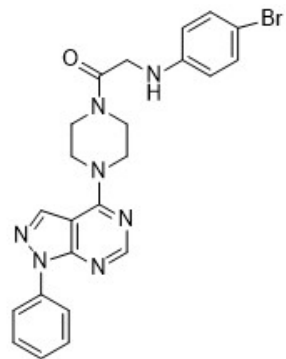
F2 - Acquisition Parameters
Date_ 20190711
Time 8.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 780
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.37
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.34722000 W
PLW13 0.28125000 W

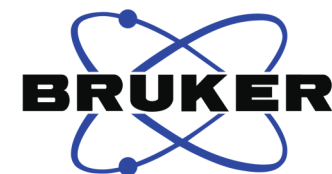
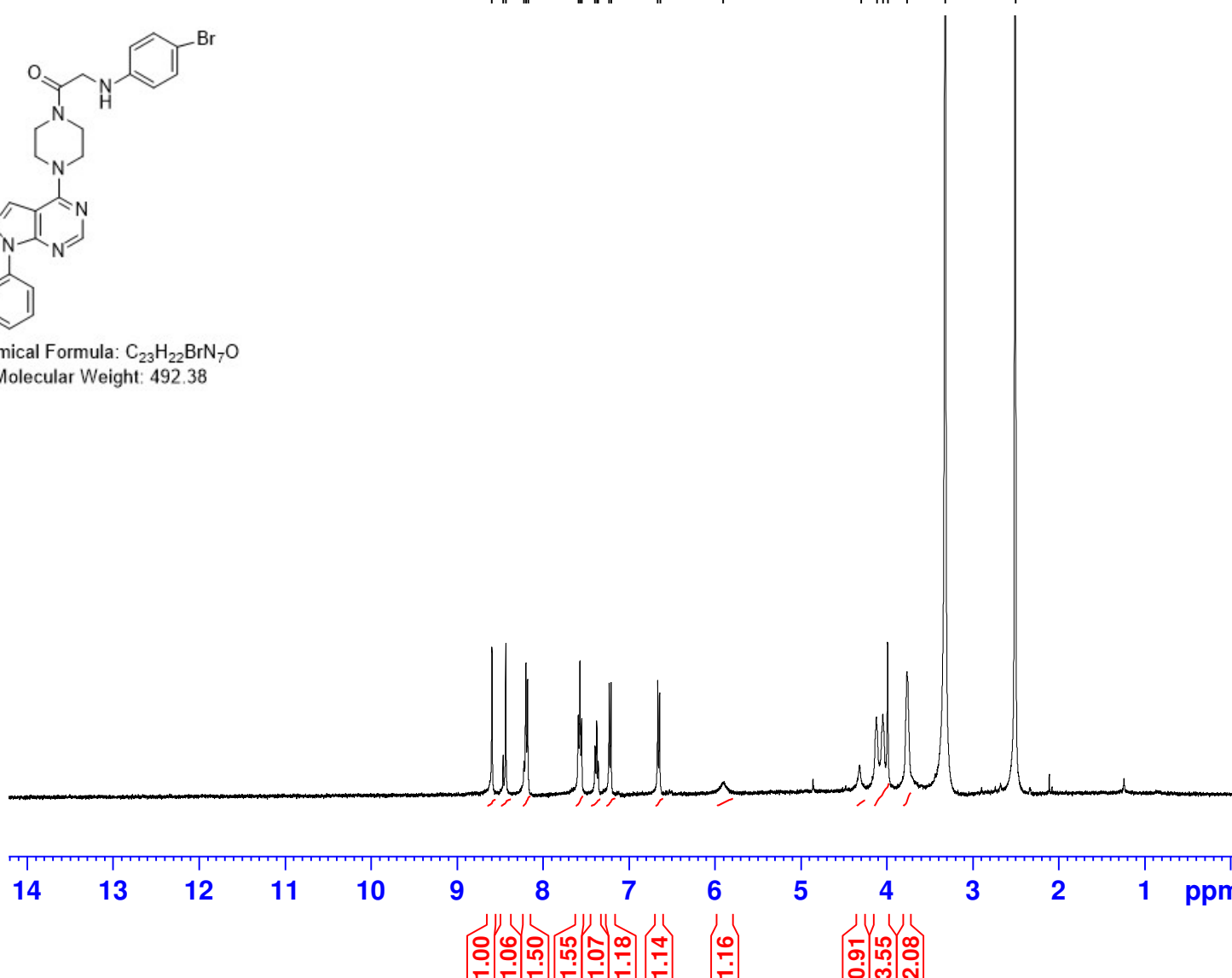
F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2-((4-Bromophenyl)amino)-1-(4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)piperazin-1-yl)ethan-1-one XVIIIb



Chemical Formula: C₂₃H₂₂BrN₇O
Molecular Weight: 492.38

8.595
8.465
8.432
8.224
8.200
8.175
7.589
7.569
7.549
7.395
7.375
7.357
7.232
7.209
6.666
6.637
5.902
4.302
4.118
4.043
3.986
3.766
3.323
2.505



Current Data Parameters
NAME rania-mohammed-8e
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210405
Time 15.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 128
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

— 8.595

— 8.465

— 8.432

— 8.224

— 8.200

— 8.175

— 7.589

— 7.569

— 7.549

— 7.395

— 7.375

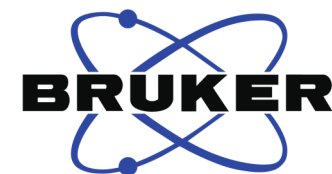
— 7.357

— 7.232

— 7.209

— 6.666

— 6.637

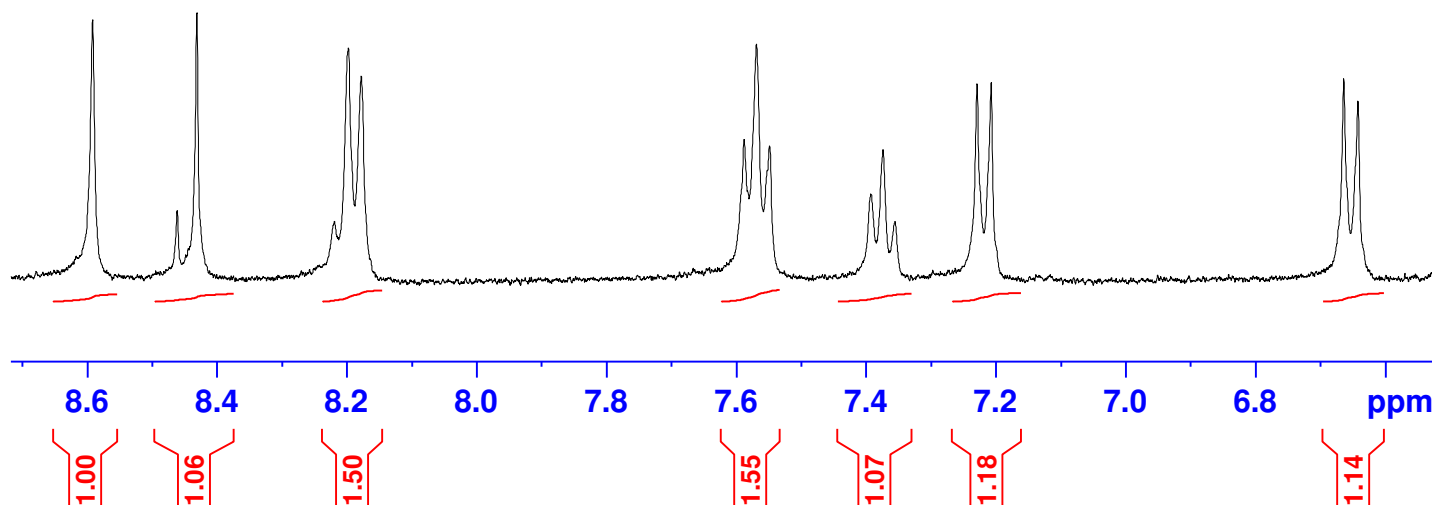


Current Data Parameters
NAME rania-mohammed-8e
EXPNO 1
PROCNO 1

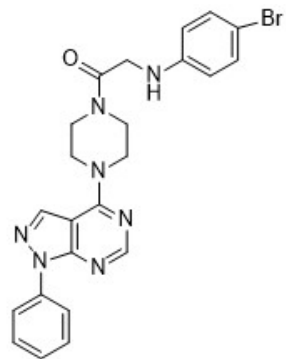
F2 - Acquisition Parameters
Date_ 20210405
Time 15.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 128
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

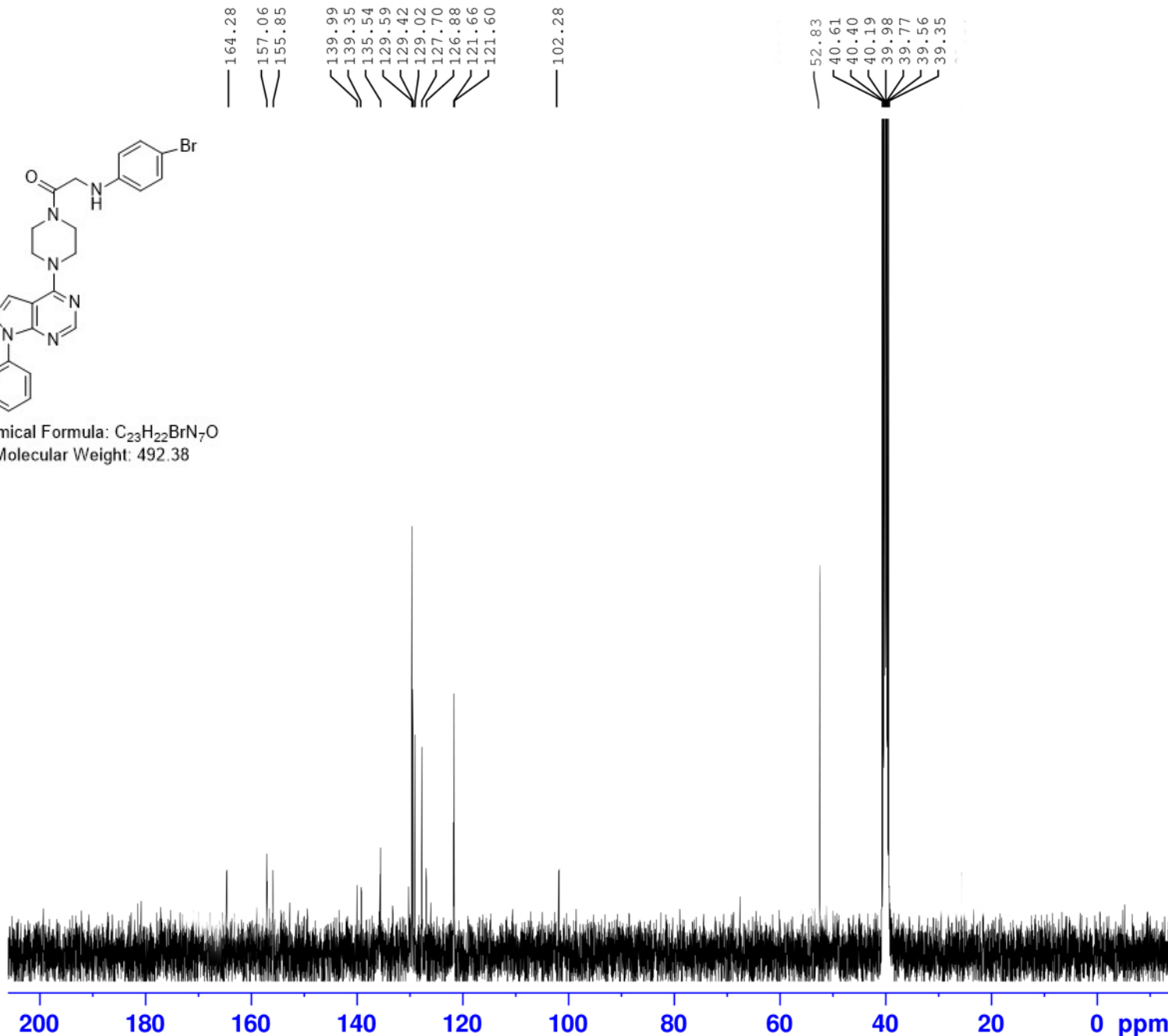
F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



XVIIIb ¹³C NMR



Chemical Formula: C₂₃H₂₂BrN₇O
Molecular Weight: 492.38



Current Data Parameters
NAME rania-mohammed-d
EXPNO 2
PROCNO 1

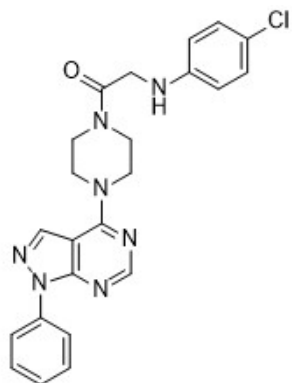
F2 - Acquisition Parameters
Date_ 20230223
Time 17.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2203
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.37
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.34722000 W
PLW13 0.28125000 W

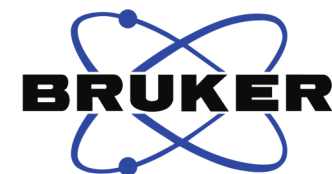
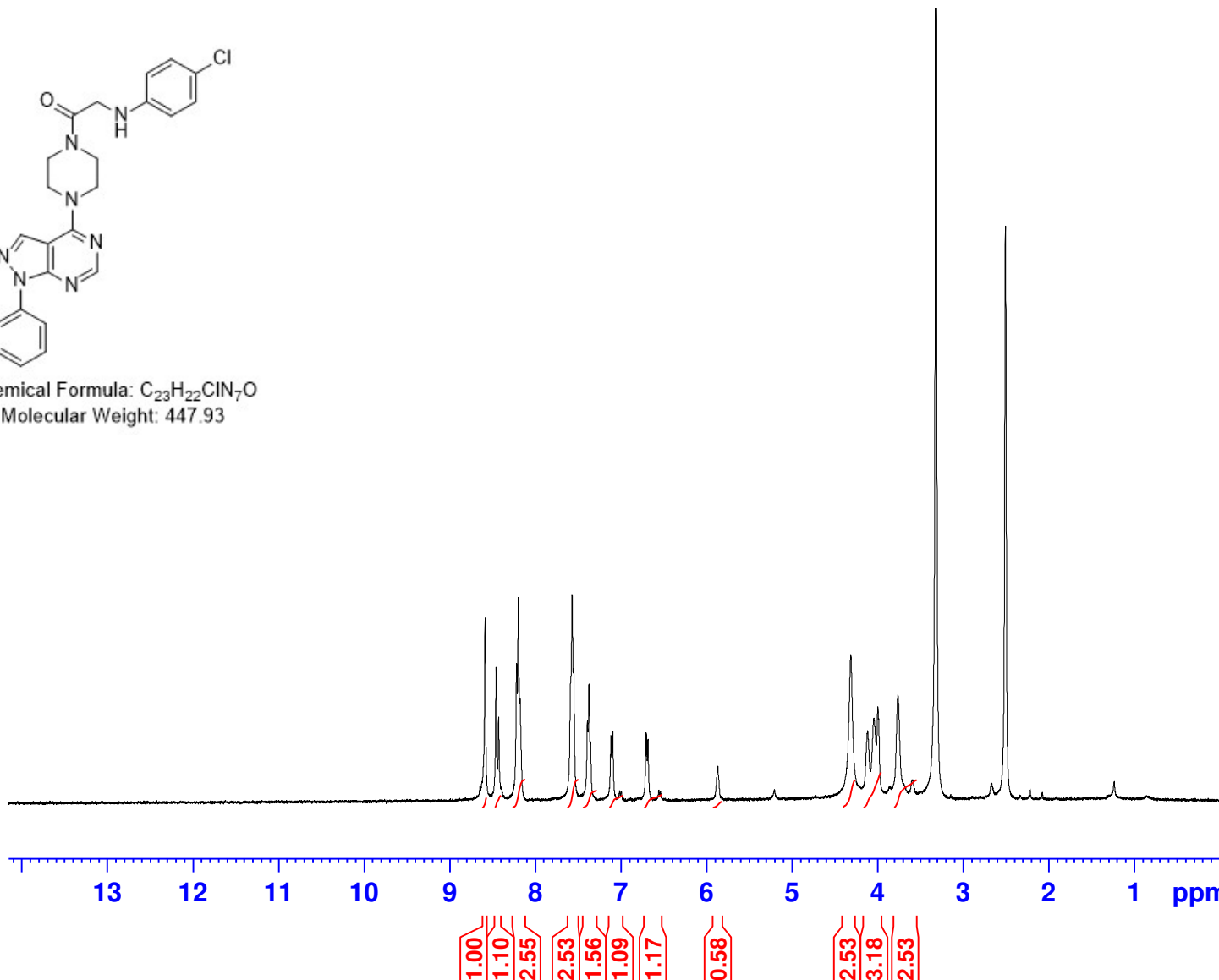
F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2-((4-Chlorophenyl)amino)-1-(4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)piperazin-1-yl)ethan-1-one XVIIIc



Chemical Formula: $C_{23}H_{22}ClN_7O$
Molecular Weight: 447.93

8.587
8.463
8.430
8.219
8.196
8.179
7.587
7.570
7.553
7.393
7.372
7.358
7.116
7.095
6.704
6.679
6.559
6.531
5.878
4.316
4.116
4.047
4.002
3.985
3.964
3.760
3.598
3.311
2.499

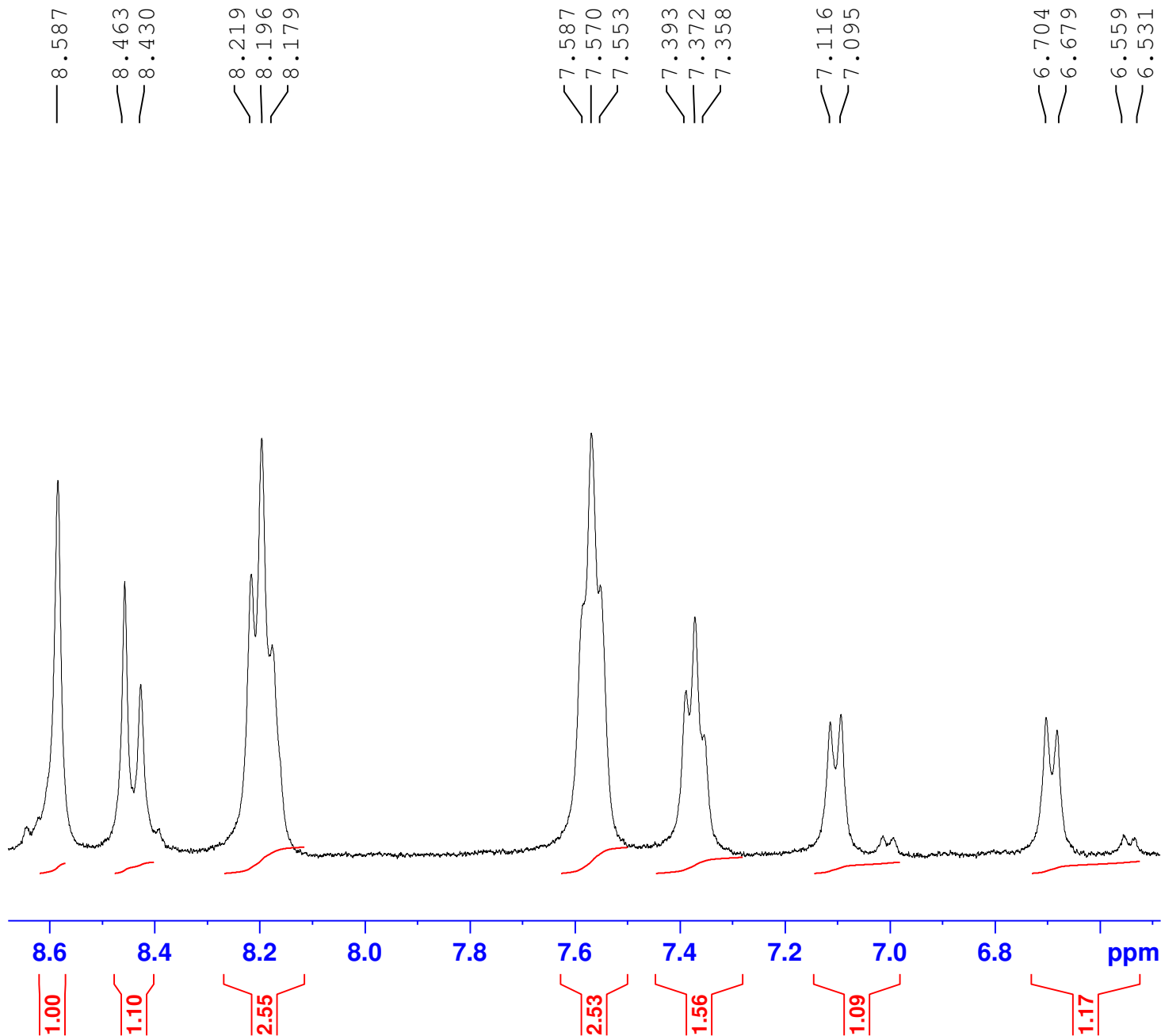


Current Data Parameters
NAME rania-mohammed-8c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210405
Time 13.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 128
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



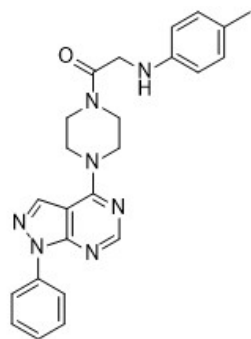
Current Data Parameters
 NAME rania-mohammed-8c
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210405
 Time 13.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 128
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 205.37
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

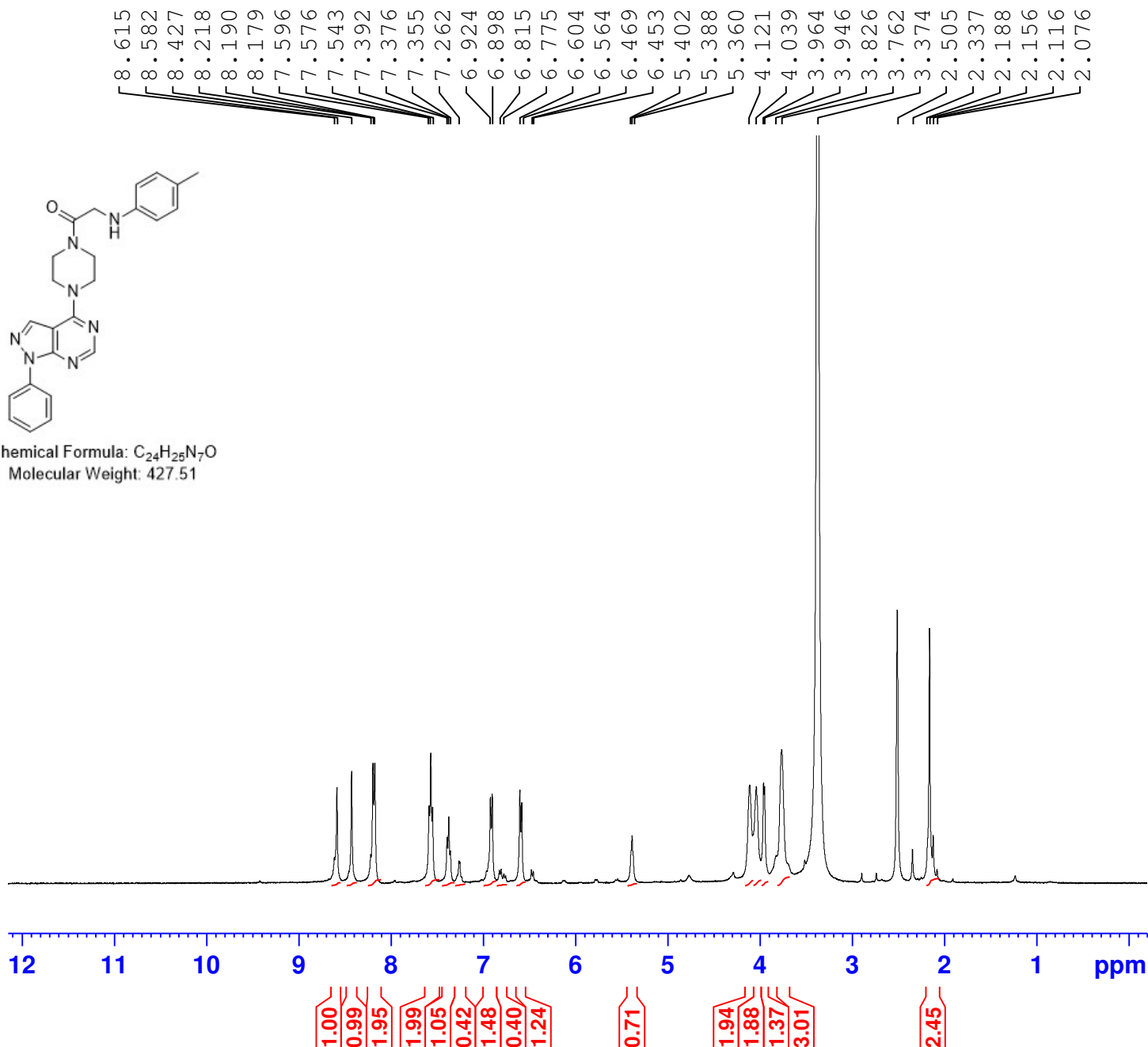
===== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 18.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1-(4-(1-Phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)piperazin-1-yl)-2-(p-tolylamino)ethan-1-one XVIIIe



Chemical Formula: C₂₄H₂₅N₇O
Molecular Weight: 427.51



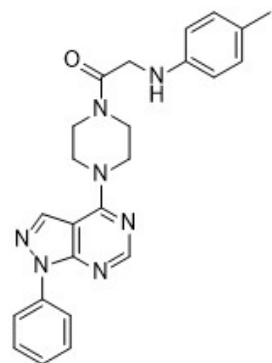
Current Data Parameters
NAME RS-8b
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190722
Time 10.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

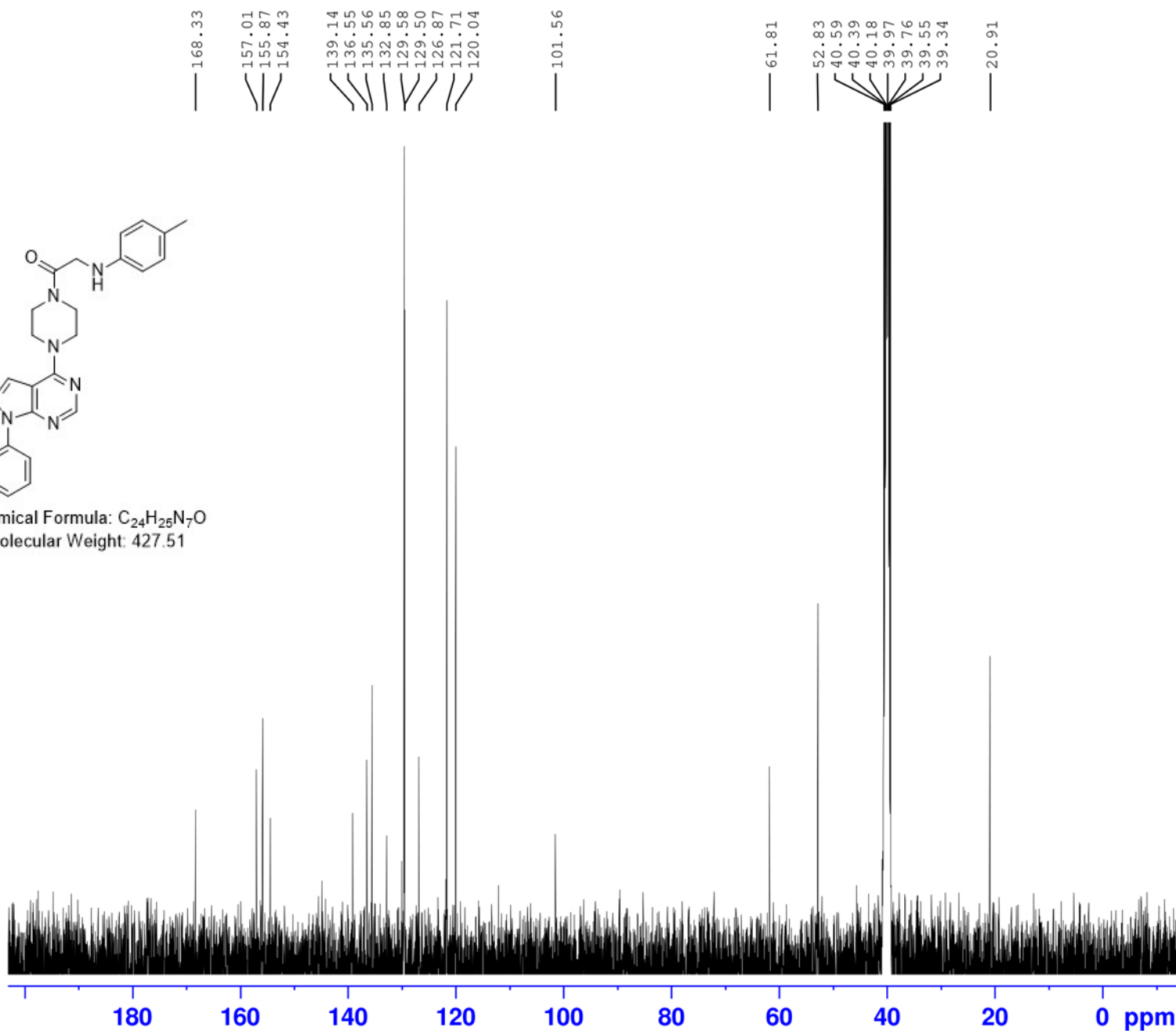
===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

XVIIIe 13C NMR



Chemical Formula: $C_{24}H_{25}N_7O$
Molecular Weight: 427.51



Current Data Parameters
NAME rania-mohamed-
EXPNO 3
PROCNO 1

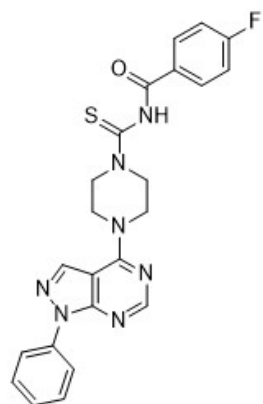
F2 - Acquisition Parameters
Date_ 20230220
Time 15.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2058
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.37
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W

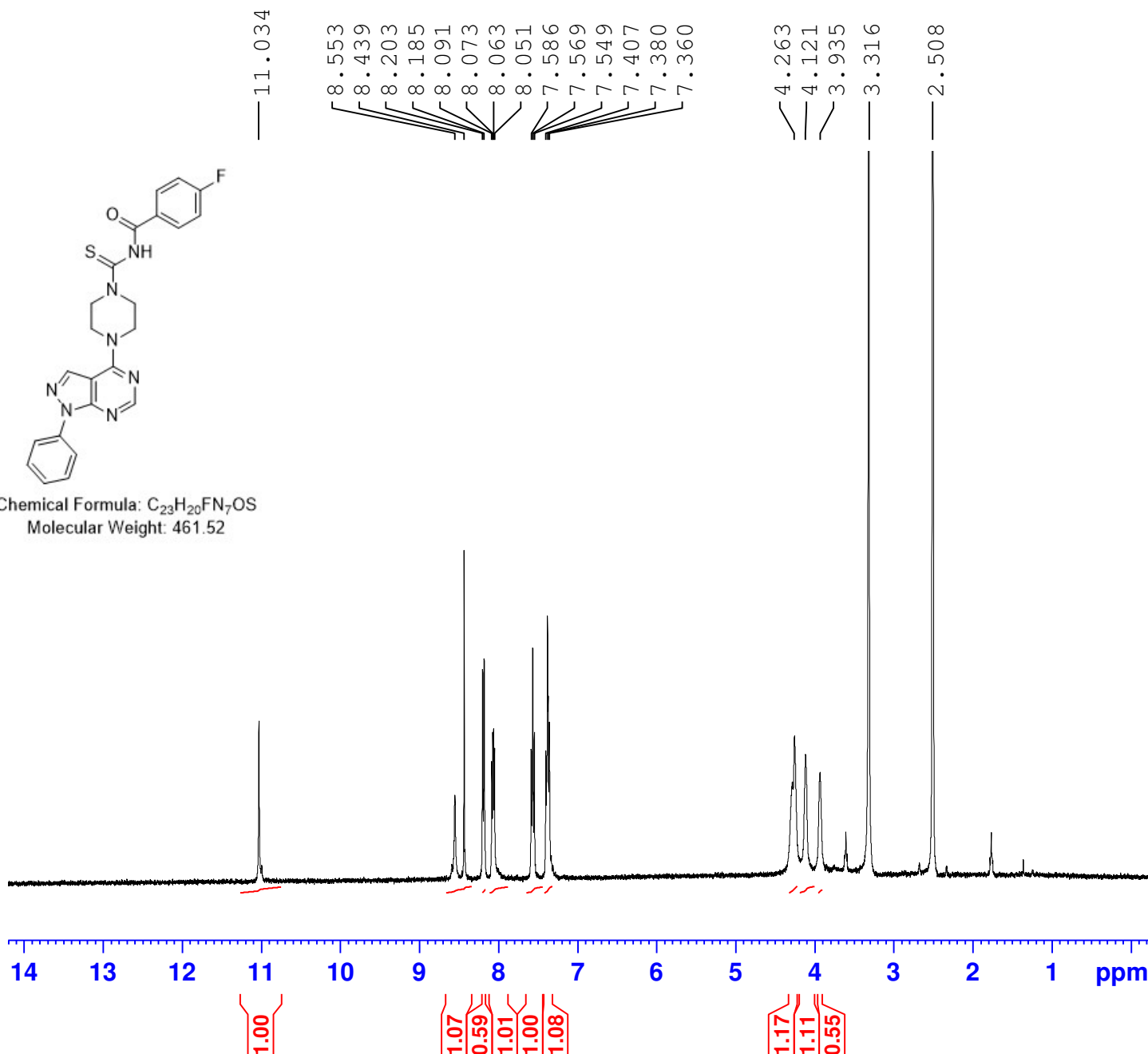
===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.34722000 W
PLW13 0.28125000 W

F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4-Fluoro-N-(4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)piperazine-1-carbonothioyl) benzamide XXIb



Chemical Formula: $C_{23}H_{20}FN_7OS$
Molecular Weight: 461.52

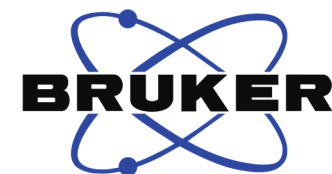


Current Data Parameters
NAME rania-mohammed-ds3f
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210405
Time 15.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 114
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

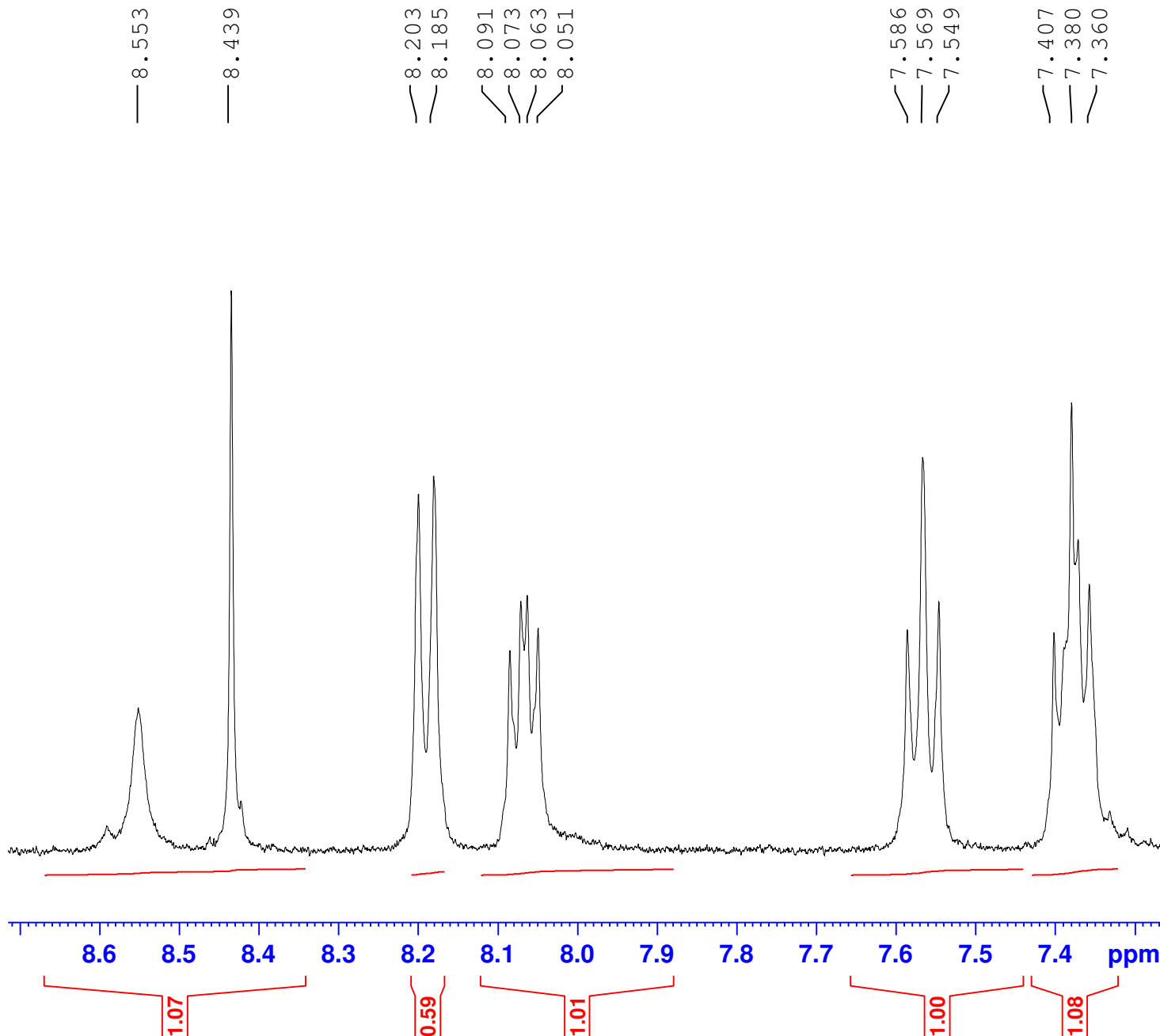


Current Data Parameters
NAME rania-mohammed-ds3f
EXPNO 1
PROCNO 1

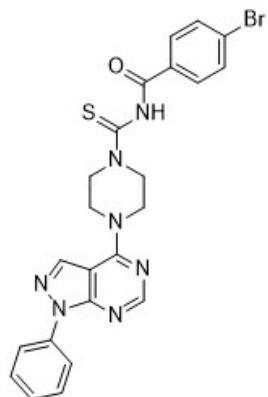
F2 - Acquisition Parameters
Date_ 20210405
Time 15.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 114
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

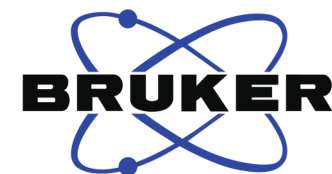
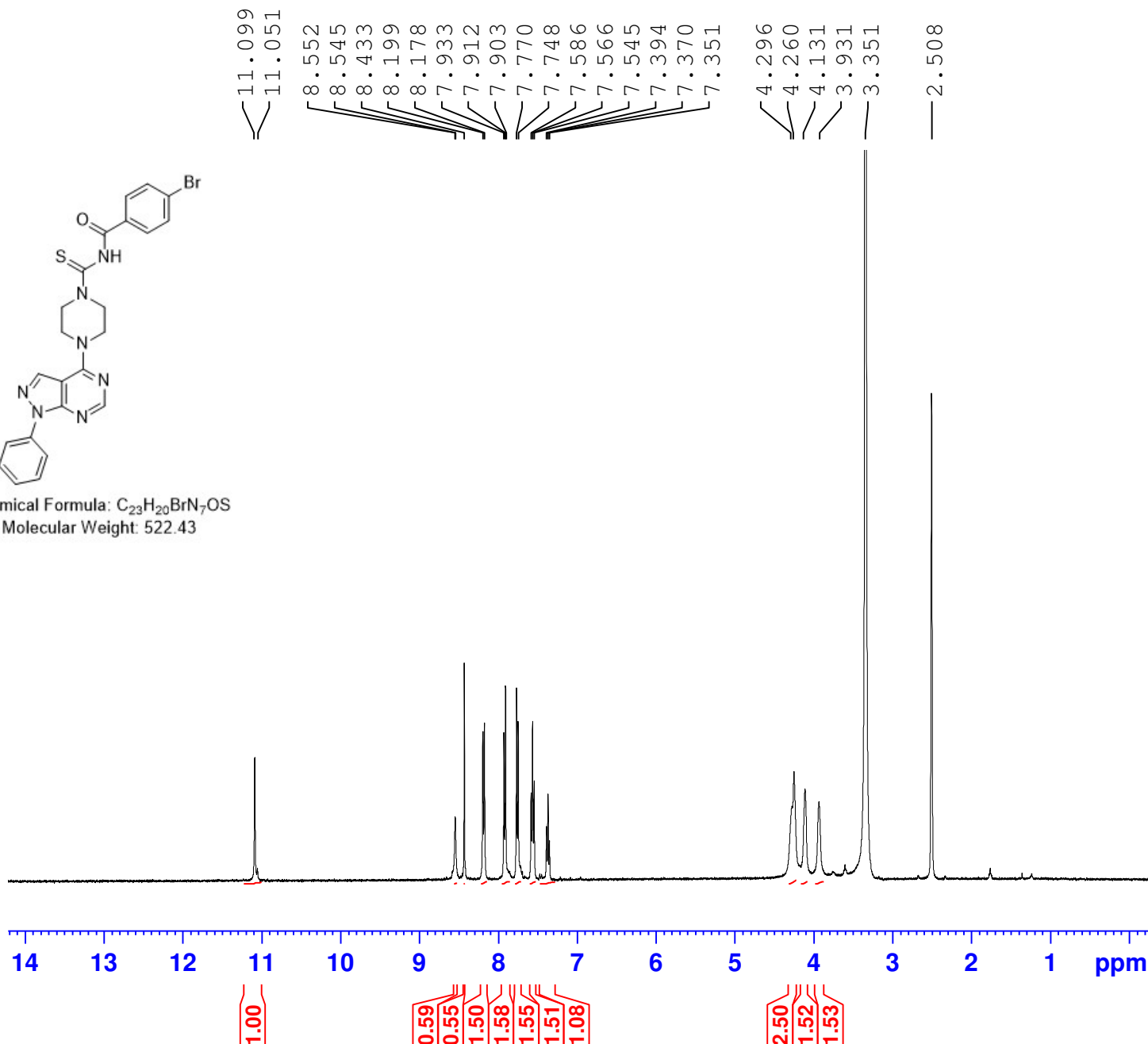
F2 - Processing parameters
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SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



4-Bromo-N-(4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)piperazine-1-carbonothioyl) benzamide XXIc



Chemical Formula: $C_{23}H_{20}BrN_7OS$
Molecular Weight: 522.43

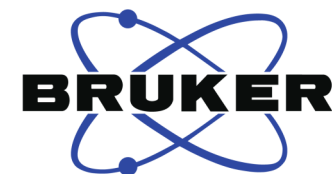


Current Data Parameters
NAME rania-mohamed-DS3e
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210318
Time 13.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

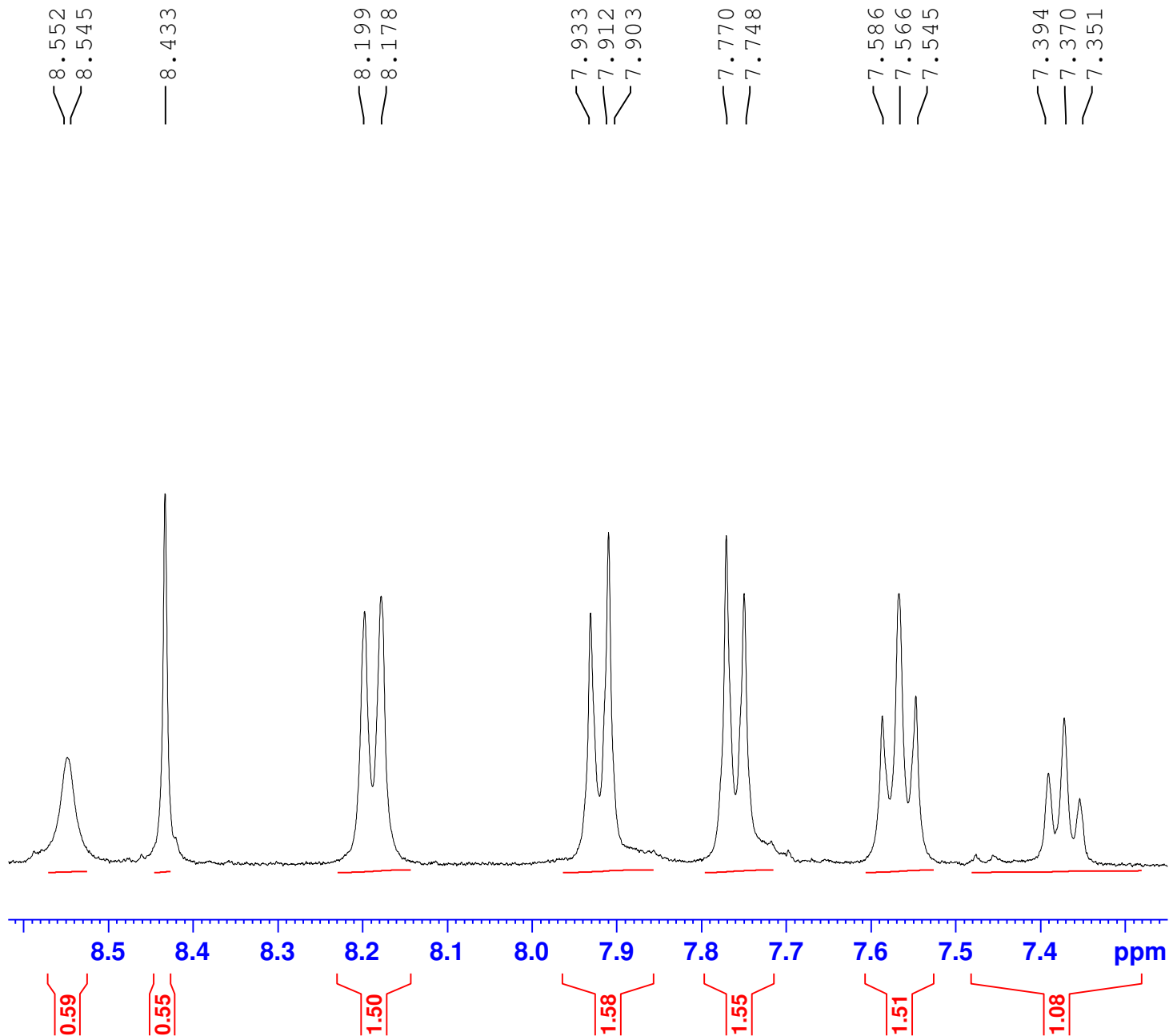


Current Data Parameters
NAME rania-mohamed-DS3e
EXPNO 1
PROCNO 1

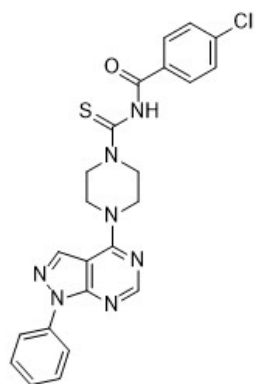
F2 - Acquisition Parameters
Date_ 20210318
Time 13.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

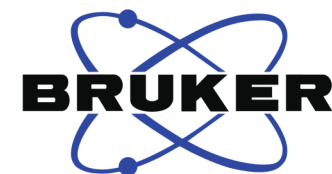
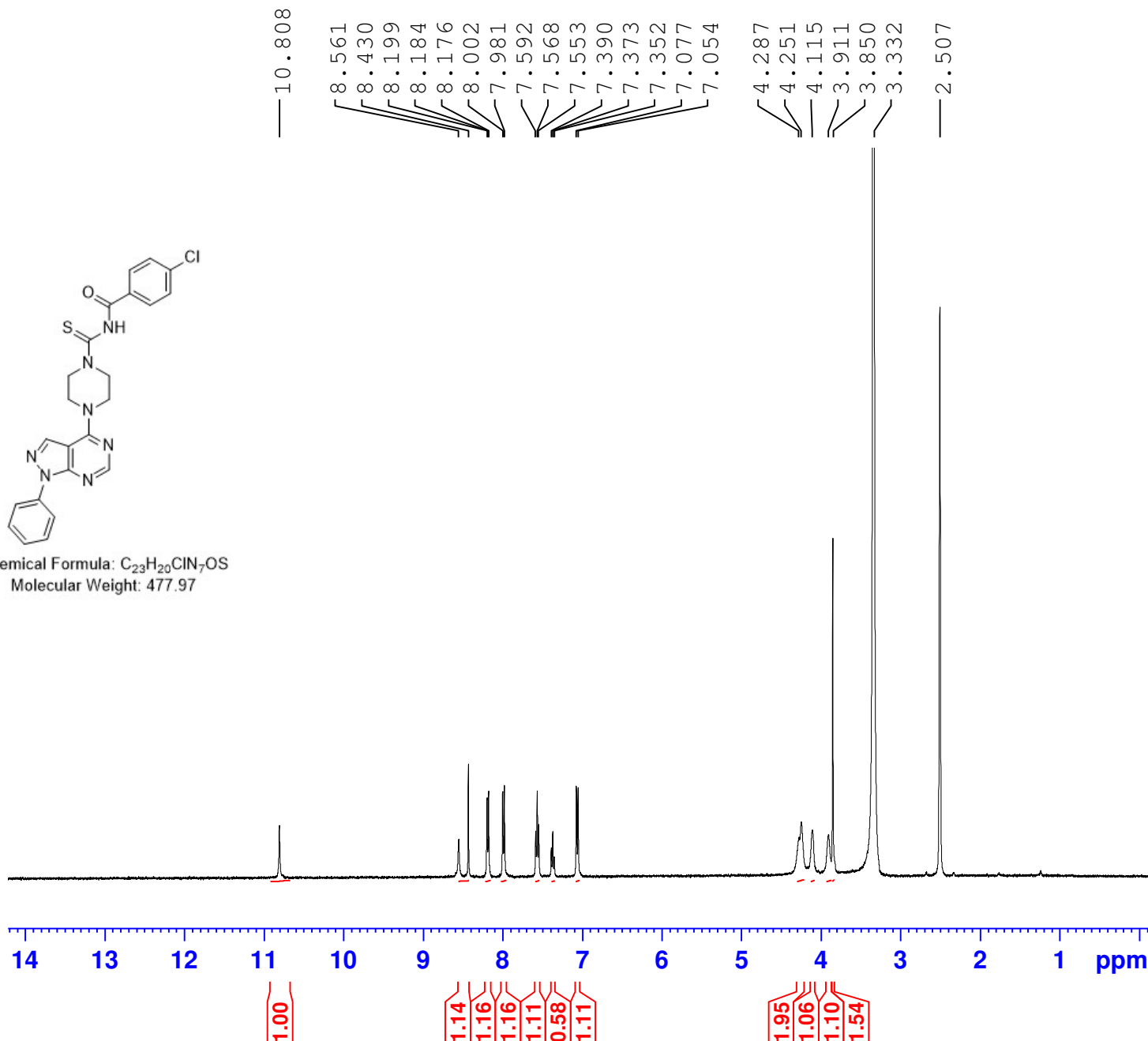
F2 - Processing parameters
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SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



4-Chloro-n-(4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)piperazine-1-carbonothioyl) benzamide XXIId



Chemical Formula: C₂₃H₂₀ClN₇OS
Molecular Weight: 477.97

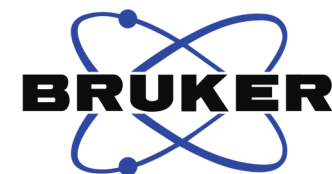


Current Data Parameters
NAME rania-mohammed-DS3C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210318
Time 13.42
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

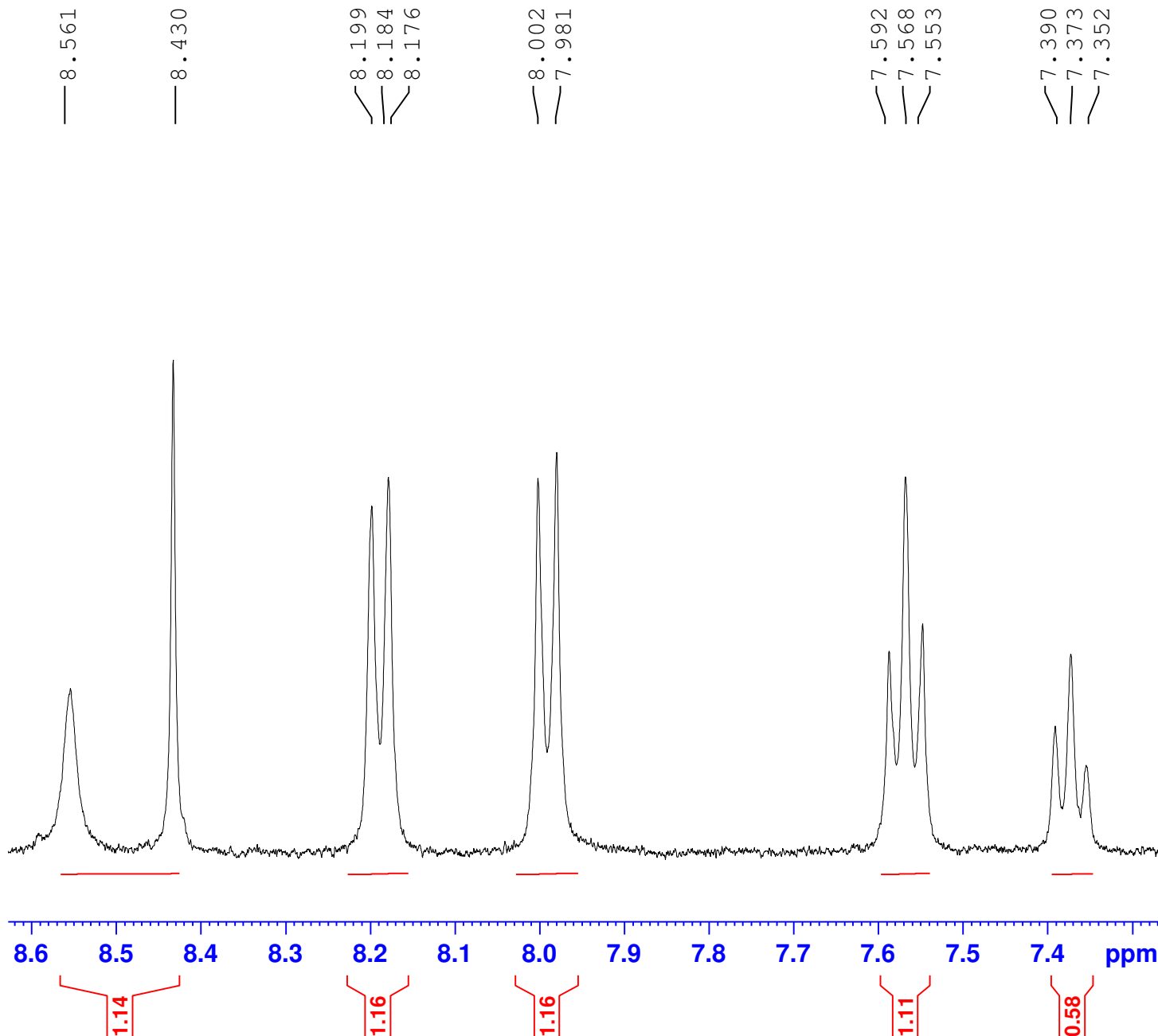


Current Data Parameters
NAME rania-mohamed-DS3C
EXPNO 1
PROCNO 1

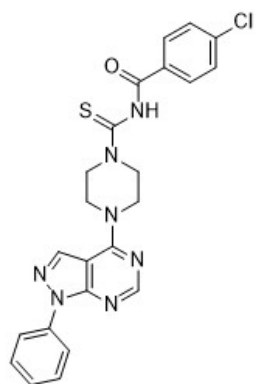
F2 - Acquisition Parameters
Date_ 20210318
Time 13.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

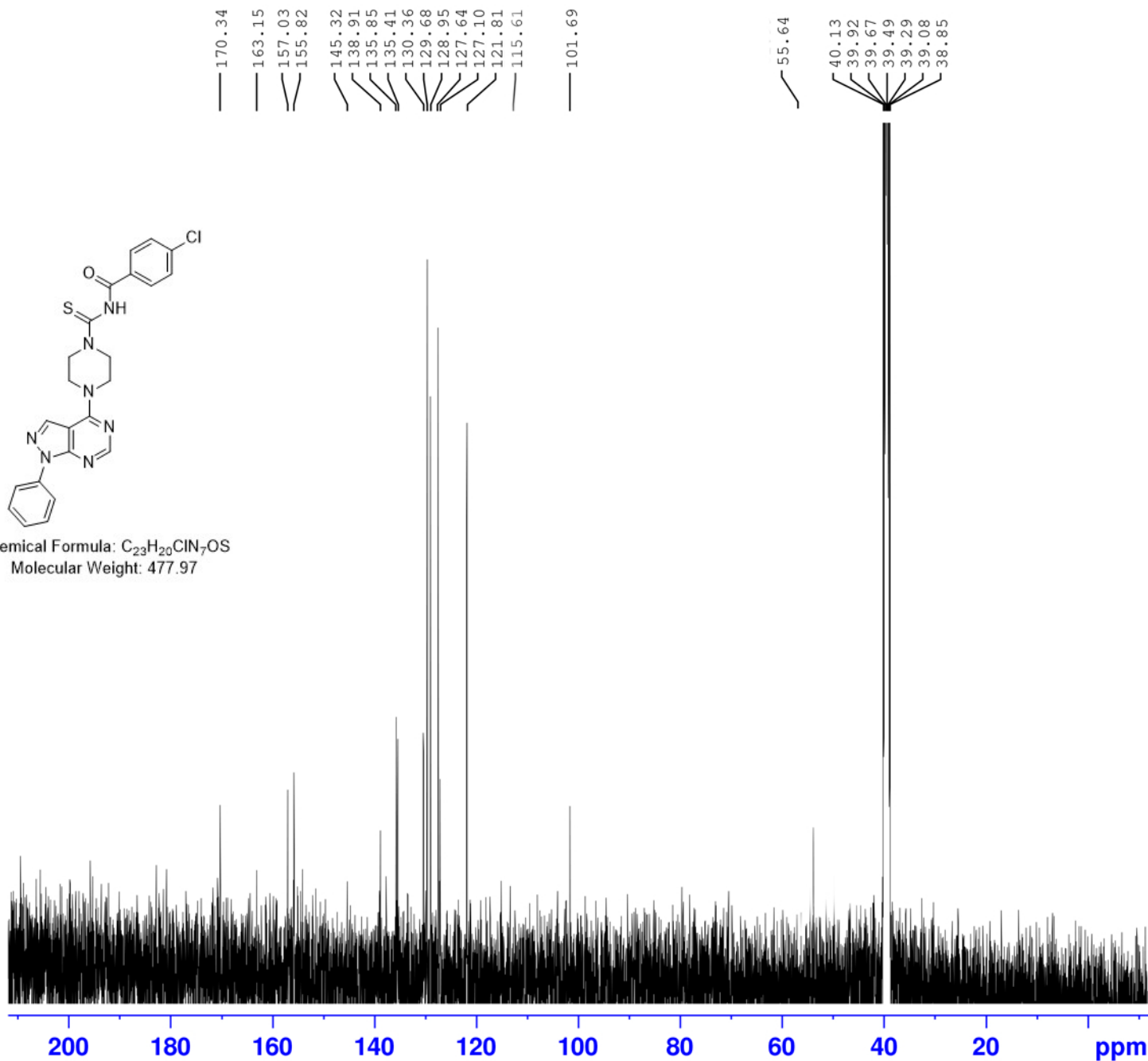
F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



XXId 13C NMR



Chemical Formula: $C_{23}H_{20}ClN_7OS$
Molecular Weight: 477.97



Current Data Parameters
NAME rania-mohamed-DS3b
EXPNO 3
PROCNO 1

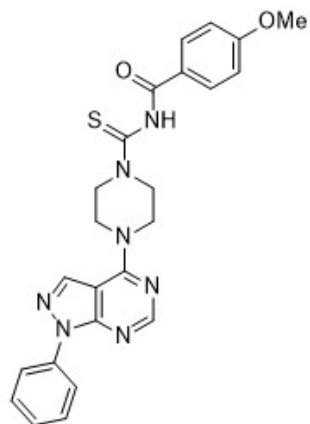
F2 - Acquisition Parameters
Date_ 20210321
Time 13.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1800
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.37
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W

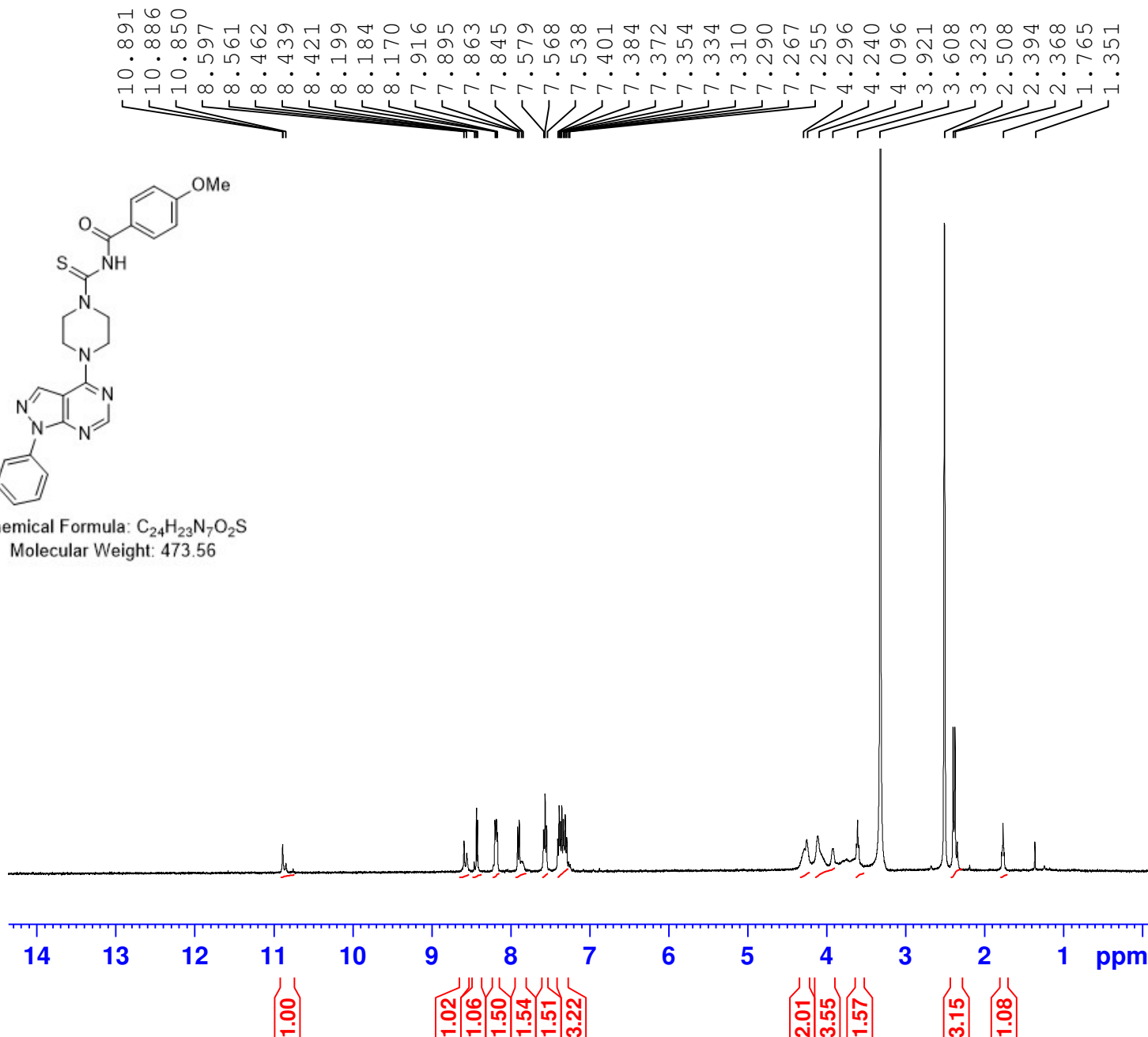
===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.34722000 W
PLW13 0.28125000 W

F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4-Methoxy-n-(4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)piperazine-1-carbonothioyl) benzamide XXIe



Chemical Formula: C₂₄H₂₃N₇O₂S
Molecular Weight: 473.56



Current Data Parameters
NAME rania-mohammed-ds3d
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210405
Time 14.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 128
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

— 8.597
— 8.561

— 8.462
— 8.439
— 8.421

— 8.199
— 8.184
— 8.170

— 7.916
— 7.895
— 7.863
— 7.845

— 7.579
— 7.568
— 7.538

— 7.401
— 7.384
— 7.372
— 7.354
— 7.334
— 7.310
— 7.290

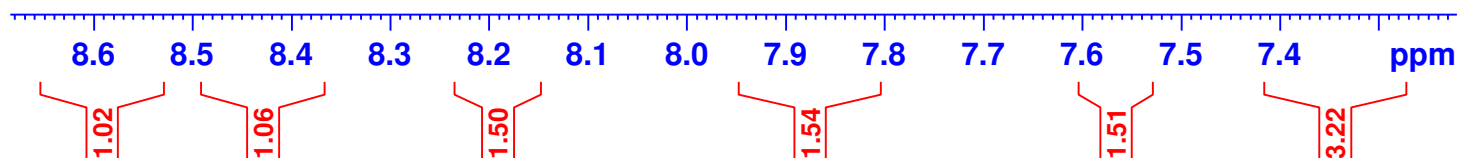
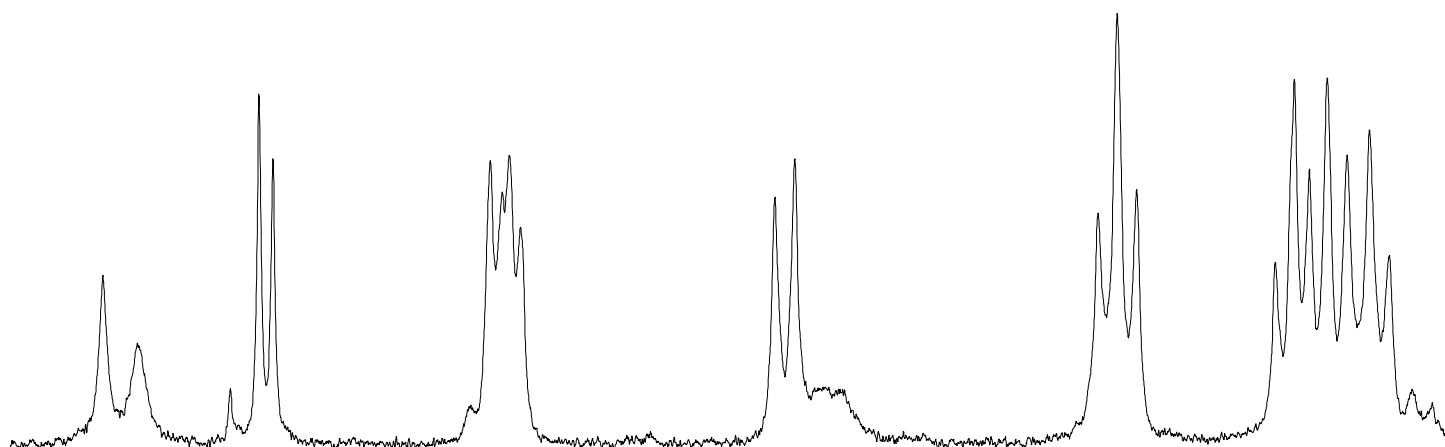


Current Data Parameters
NAME rania-mohammed-ds3d
EXPNO 1
PROCNO 1

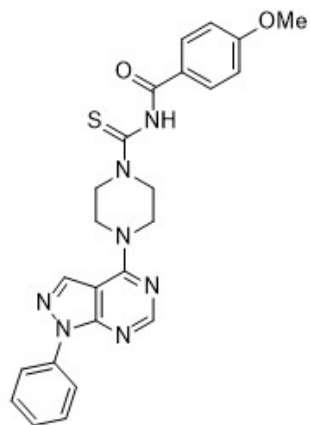
F2 - Acquisition Parameters
Date_ 20210405
Time 14.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 128
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

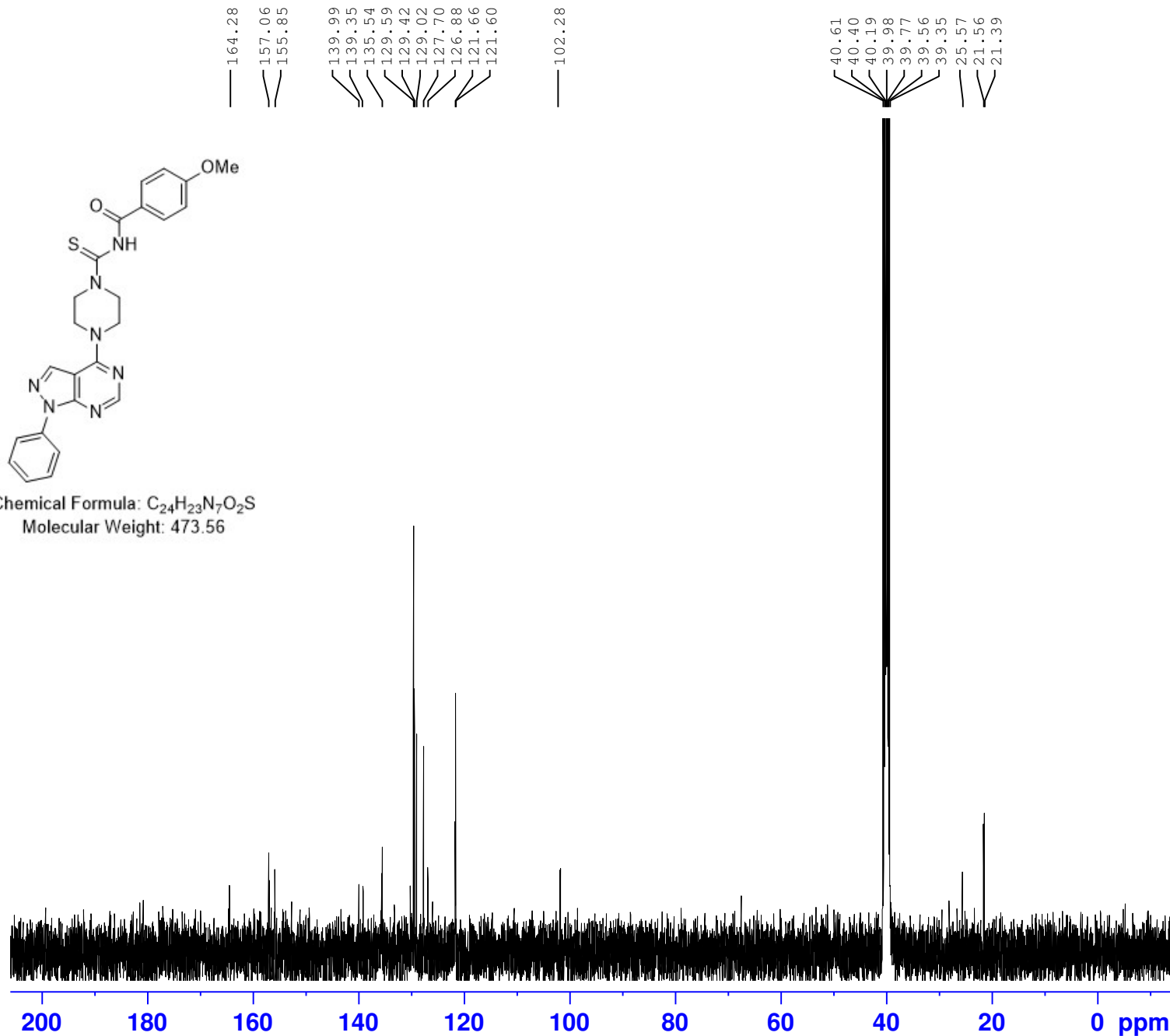
F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



XXIe 13C NMR



Chemical Formula: C₂₄H₂₃N₇O₂S
Molecular Weight: 473.56



Current Data Parameters
NAME rania-mohammed-ds3d
EXPNO 2
PROCNO 1

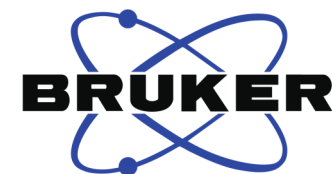
F2 - Acquisition Parameters
Date_ 20230223
Time 17.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2203
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.37
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.34722000 W
PLW13 0.28125000 W

F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4-Methyl-n-(4-(1-phenyl-1H-pyrazolo[3,4-d]pyrimidin-4-yl)piperazine-1-carbonothioyl) benzamide XXIf

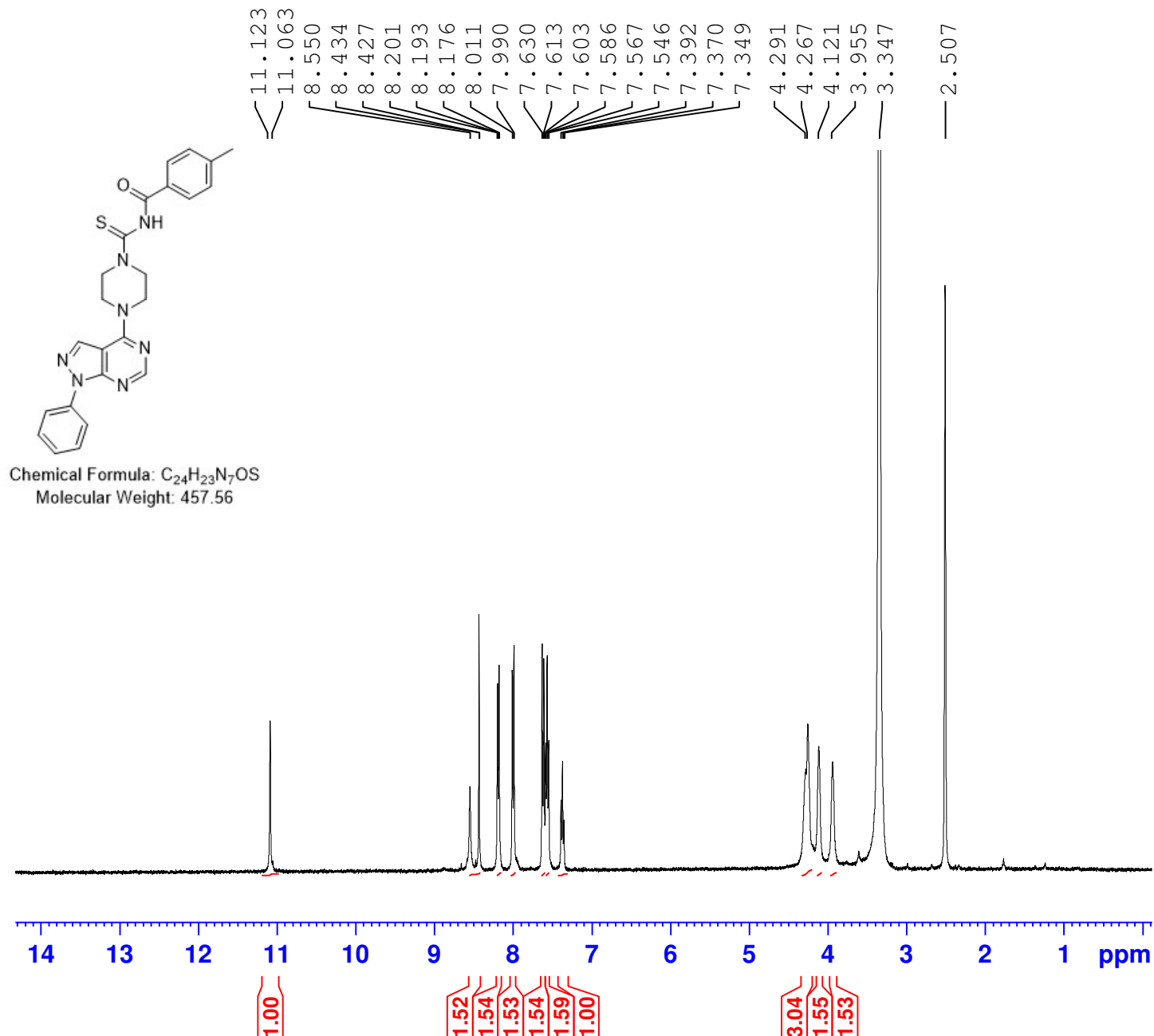


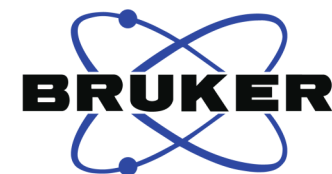
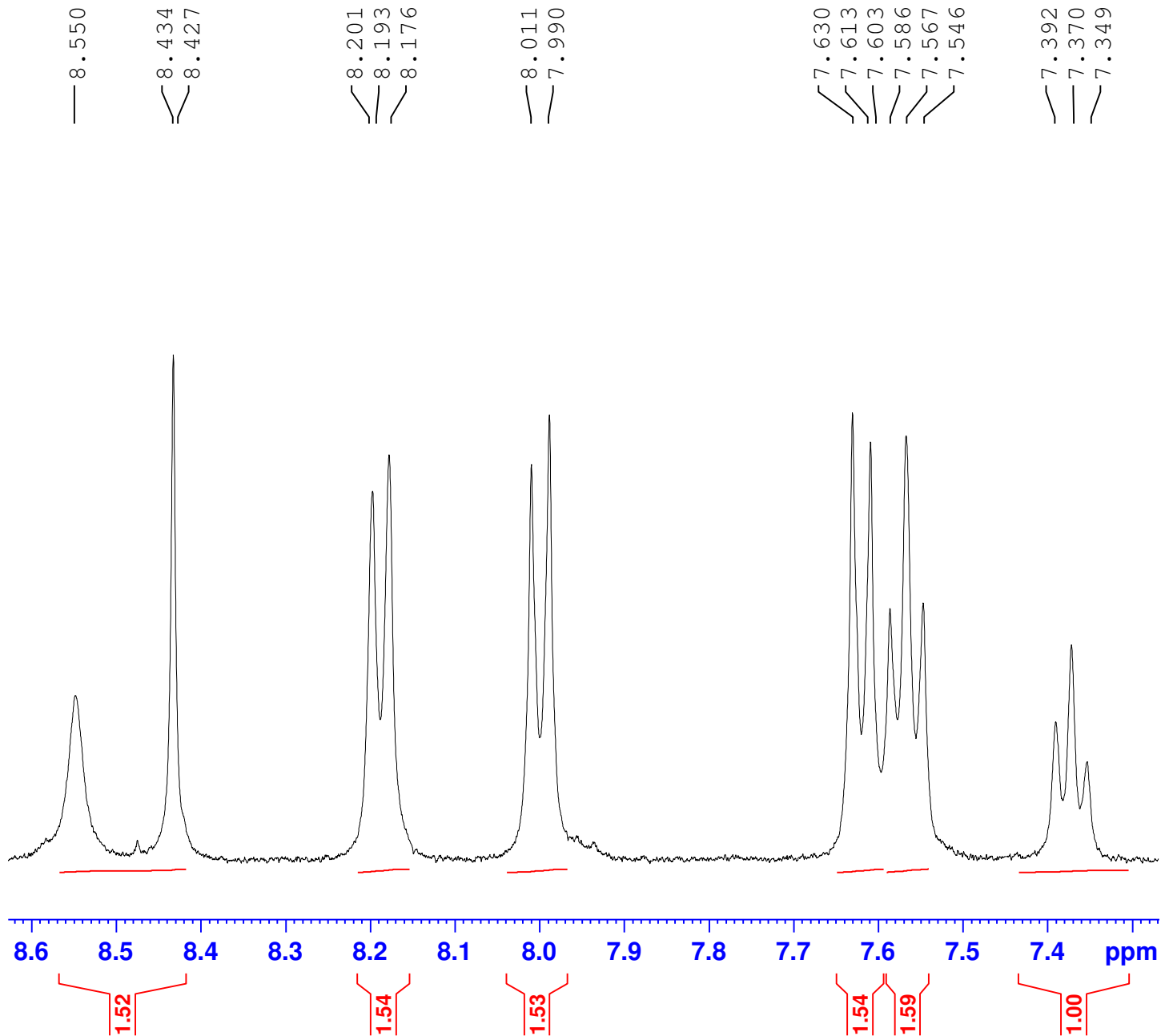
Current Data Parameters
 NAME rania-mohamed-DS3b
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210318
 Time 13.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 43
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 205.37
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 18.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





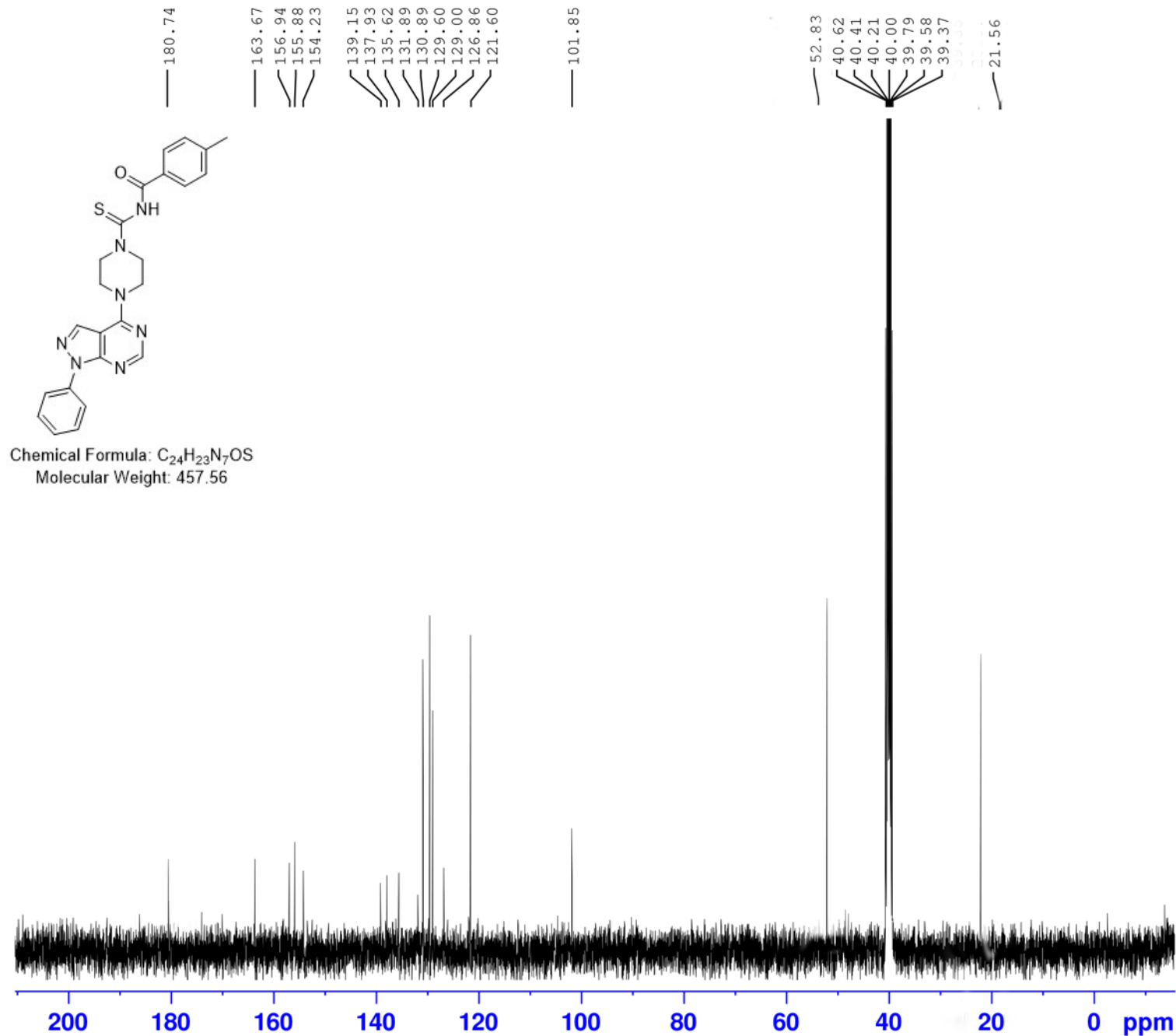
Current Data Parameters
 NAME rania-mohamed-DS3b
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210318
 Time 13.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 43
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 205.37
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 18.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

XXIf 13C NMR



Current Data Parameters
NAME rania-mohamed-DS3b
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230219
Time 17.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.37
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 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.34722000 W
PLW13 0.28125000 W

F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Al-Azhar University

The Regional Center for Mycology and Biotechnology



Requester Data:

Name: Dr. Rania Shaban El-Maghraby
Authority: Faculty of Pharmacy,
 MSA University

Sample Data:

Twenty samples had been submitted for elemental analysis.

Analysis Report:

Sample Code	C%	H%	N%
7b	67.59	6.11	23.16
7c	61.85	5.12	21.72
7d	64.93	5.86	21.97
7e	56.38	4.72	20.04
7f	67.54	6.13	22.75
7k	67.43	6.15	23.04
7m	54.31	4.68	30.15
8b	67.59	6.05	23.78
8c	61.88	5.11	21.75
8d	64.79	5.79	21.98
8e	56.34	4.73	20.15
9a	70.04	5.39	18.35
9b	66.73	5.19	20.37
10a	63.45	5.17	23.84
Ds3a	62.41	4.89	21.97
Ds3b	58.04	4.36	20.78
Ds3c	60.61	5.12	20.87
Ds3d	62.78	5.31	21.29
Ds3e	52.67	3.98	19.03
Ds3f	60.04	4.46	21.45

INVESTIGATOR

M. Elmass

DIRECTOR



[Signature]

Al-Azhar University Campus - Nasr City, Cairo, Egypt.

Tel: 0202 22620373

Fax : 0202 22620373

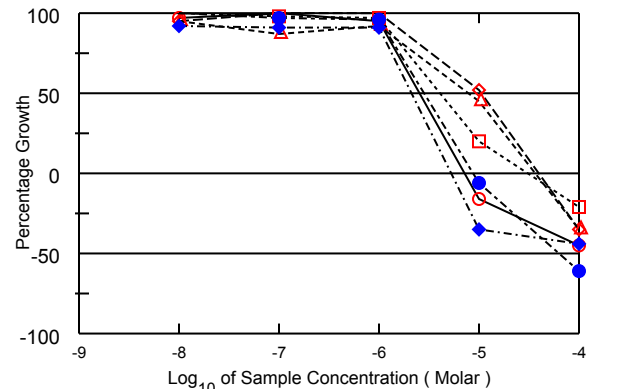
E.mail: rcmb@azhar.edu.eg

Website: <http://www.azhar.edu.eg.htm> * http://www.azhar.edu.eg/pages/fungi_center.htm

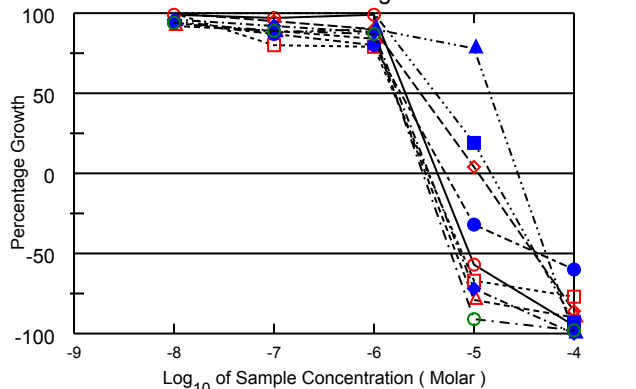
Facebook : RCMB AZHAR

P.O. box mail : 11751 Nasr City Cairo, Egypt.

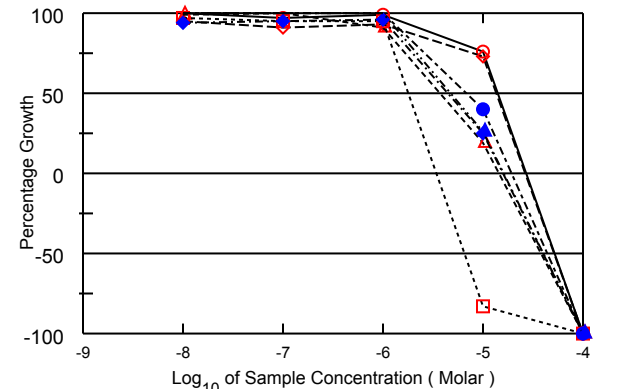
Leukemia



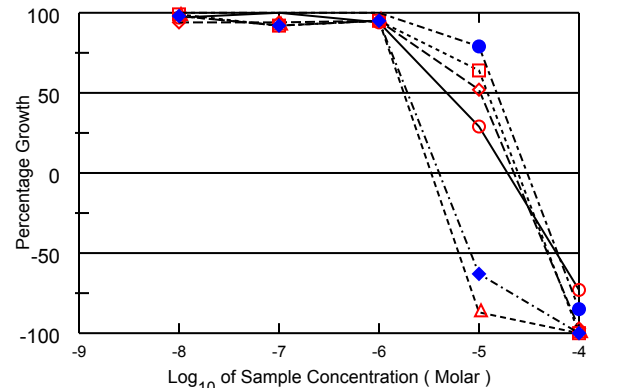
Non-Small Cell Lung Cancer



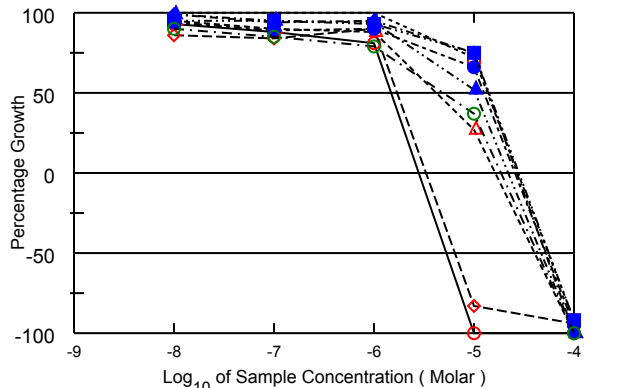
Colon Cancer



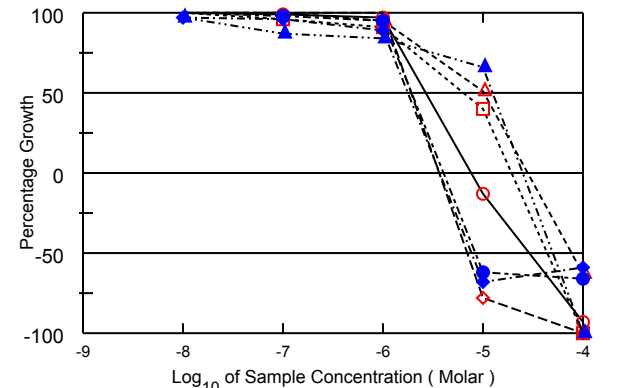
CNS Cancer



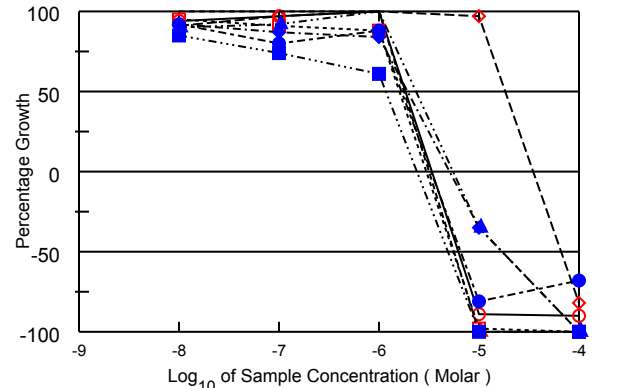
Melanoma



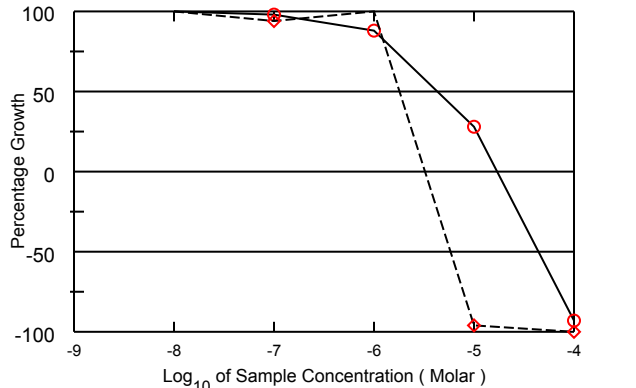
Ovarian Cancer



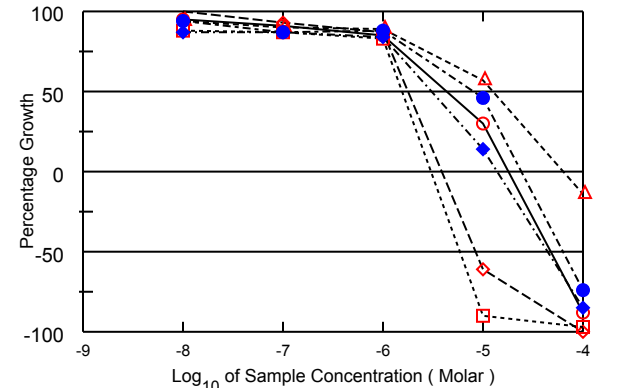
Renal Cancer



Prostate Cancer



Breast Cancer



National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : D - 833644 / 1			Experiment ID : 2203NS83										Test Type : 08		Units : Molar	
Report Date : April 05, 2022			Test Date : March 14, 2022										QNS :		MC :	
COMI : 7m			Stain Reagent : SRB Dual-Pass Related										SSPL : 1CIJ			
Log10 Concentration																
Panel/Cell Line	Time		Mean Optical Densities						Percent Growth				GI50	TGI	LC50	
	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0				
Leukemia																
CCRF-CEM	0.586	2.912	2.849	2.914	2.805	0.492	0.323	97	100	95	-16	-45	2.55E-6	7.17E-6	> 1.00E-4	
HL-60(TB)	0.608	2.988	2.867	3.033	3.020	1.837	0.396	95	102	101	52	-35	1.04E-5	3.95E-5	> 1.00E-4	
K-562	0.117	1.371	1.310	1.204	1.272	0.684	0.076	95	87	92	45	-35	7.91E-6	3.66E-5	> 1.00E-4	
MOLT-4	0.499	2.630	2.635	2.592	2.557	0.932	0.396	100	98	97	20	-21	4.08E-6	3.13E-5	> 1.00E-4	
RPMI-8226	0.691	2.368	2.384	2.314	2.308	0.647	0.269	101	97	96	-6	-61	2.83E-6	8.67E-6	6.28E-5	
SR	0.331	1.900	1.781	1.753	1.759	0.215	0.185	92	91	91	-35	-44	2.11E-6	5.26E-6	> 1.00E-4	
Non-Small Cell Lung Cancer																
A549/ATCC	0.430	1.936	1.922	1.888	1.926	0.185	0.022	99	97	99	-57	-95	2.07E-6	4.31E-6	9.01E-6	
EKVX	0.655	1.990	2.001	1.930	1.851	0.709	0.092	101	95	90	4	-86	2.90E-6	1.11E-5	3.99E-5	
HOP-62	1.026	2.589	2.457	2.420	2.337	0.221	0.101	92	89	84	-79	-90	1.62E-6	3.29E-6	6.68E-6	
HOP-92	1.057	1.455	1.459	1.375	1.370	0.347	0.244	101	80	79	-67	-77	1.57E-6	3.46E-6	7.62E-6	
NCI-H226	0.727	2.033	1.954	1.868	1.768	0.491	0.293	94	87	80	-32	-60	1.84E-6	5.14E-6	4.39E-5	
NCI-H23	0.551	1.829	1.776	1.727	1.682	0.157	-0.015	96	92	88	-72	-100	1.74E-6	3.57E-6	7.33E-6	
NCI-H322M	0.715	2.081	2.016	1.919	1.941	1.786	-0.090	95	88	90	78	-100	1.44E-5	2.75E-5	5.24E-5	
NCI-H460	0.274	2.426	2.537	2.693	2.483	0.680	0.020	105	112	103	19	-93	4.25E-6	1.47E-5	4.13E-5	
NCI-H522	0.758	1.953	1.878	1.823	1.801	0.070	0.015	94	89	87	-91	-98	1.62E-6	3.09E-6	5.90E-6	
Colon Cancer																
COLO 205	0.694	2.324	2.430	2.280	2.304	1.932	-0.003	106	97	99	76	-100	1.40E-5	2.70E-5	5.20E-5	
HCC-2998	0.696	2.070	1.995	1.941	1.970	1.697	-0.030	95	91	93	73	-100	1.36E-5	2.64E-5	5.14E-5	
HCT-116	0.290	2.113	2.095	2.202	1.956	0.643	-0.037	99	105	91	19	-100	3.75E-6	1.45E-5	3.81E-5	
HCT-15	0.378	2.402	2.339	2.303	2.298	0.066	-0.022	97	95	95	-83	-100	1.79E-6	3.42E-6	6.55E-6	
HT29	0.330	1.647	1.764	1.663	1.685	0.855	-0.045	109	101	103	40	-100	6.91E-6	1.93E-5	4.39E-5	
KM12	0.491	2.389	2.280	2.294	2.308	0.972	-0.032	94	95	96	25	-100	4.46E-6	1.59E-5	3.99E-5	
SW-620	0.212	1.529	1.661	1.682	1.598	0.556	-0.015	110	112	105	26	-100	4.99E-6	1.61E-5	4.01E-5	
CNS Cancer																
SF-268	0.731	2.286	2.235	2.321	2.199	1.184	0.198	97	102	94	29	-73	4.79E-6	1.93E-5	5.96E-5	
SF-295	0.697	2.893	2.758	2.750	2.783	1.840	0.018	94	94	95	52	-97	1.03E-5	2.23E-5	4.82E-5	
SF-539	0.540	1.810	1.786	1.714	1.744	0.071	-0.071	98	92	95	-87	-100	1.76E-6	3.32E-6	6.26E-6	
SNB-19	0.668	2.020	2.008	1.913	1.947	1.535	-0.075	99	92	95	64	-100	1.22E-5	2.46E-5	4.96E-5	
SNB-75	1.955	3.049	3.139	3.045	3.072	2.822	0.303	108	100	102	79	-85	1.51E-5	3.05E-5	6.15E-5	
U251	0.352	1.687	1.662	1.575	1.618	0.130	-0.030	98	92	95	-63	-100	1.92E-6	3.99E-6	8.27E-6	
Melanoma																
LOX IMVI	0.212	1.530	1.439	1.369	1.286	-0.003	-0.061	93	88	81	-100	-100	1.49E-6	2.81E-6	5.30E-6	
MALME-3M	0.694	1.217	1.144	1.133	1.163	0.115	0.045	86	84	90	-83	-94	1.69E-6	3.30E-6	6.41E-6	
M14	0.426	1.597	1.533	1.486	1.460	0.737	-0.026	95	90	88	27	-100	4.17E-6	1.62E-5	4.03E-5	
MDA-MB-435	0.649	2.480	2.519	2.479	2.473	1.972	0.050	102	100	100	72	-92	1.36E-5	2.75E-5	5.53E-5	
SK-MEL-2	1.296	2.581	2.509	2.445	2.457	2.146	0.071	94	89	90	66	-95	1.26E-5	2.58E-5	5.28E-5	
SK-MEL-28	0.640	1.769	1.753	1.701	1.715	1.490	-0.076	99	94	95	75	-100	1.39E-5	2.69E-5	5.19E-5	
SK-MEL-5	0.942	2.909	2.893	2.807	2.787	1.956	-0.077	99	95	94	52	-100	1.02E-5	2.19E-5	4.68E-5	
UACC-257	1.216	2.670	2.595	2.597	2.565	2.301	0.103	95	95	93	75	-92	1.41E-5	2.81E-5	5.62E-5	
UACC-62	0.897	2.588	2.411	2.339	2.231	1.530	-0.073	90	85	79	37	-100	4.97E-6	1.87E-5	4.33E-5	
Ovarian Cancer																
IGROV1	0.640	2.289	2.301	2.279	2.238	0.559	0.046	101	99	97	-13	-93	2.68E-6	7.65E-6	2.92E-5	
OVCAR-3	0.443	1.547	1.569	1.578	1.557	0.098	-0.020	102	103	101	-78	-100	1.93E-6	3.67E-6	6.98E-6	
OVCAR-4	0.701	1.807	1.876	1.855	1.757	1.270	0.258	106	104	95	51	-63	1.03E-5	2.81E-5	7.67E-5	
OVCAR-5	0.515	1.462	1.458	1.424	1.377	0.896	-0.073	100	96	91	40	-100	6.41E-6	1.93E-5	4.40E-5	
OVCAR-8	0.456	1.927	1.926	1.899	1.849	0.173	0.154	100	98	95	-62	-66	1.93E-6	4.02E-6	8.38E-6	
NCI/ADR-RES	0.532	1.715	1.680	1.672	1.581	0.173	0.220	97	96	89	-68	-59	1.77E-6	3.69E-6	7.72E-6	
SK-OV-3	1.062	2.053	2.024	1.929	1.896	1.718	-0.082	97	87	84	66	-100	1.25E-5	2.50E-5	5.00E-5	
Renal Cancer																
786-0	0.505	2.041	1.957	2.002	2.185	0.057	0.049	94	97	109	-89	-90	1.99E-6	3.56E-6	6.37E-6	
A498	1.236	1.952	1.890	1.929	2.042	1.933	0.229	91	97	113	97	-82	1.84E-5	3.50E-5	6.67E-5	
ACHN	0.374	1.686	1.732	1.752	1.696	-0.007	-0.077	103	105	101	-100	-100	1.79E-6	3.18E-6	5.64E-6	
CAKI-1	0.551	2.892	2.785	2.689	2.603	0.014	-0.078	95	91	88	-98	-100	1.60E-6	2.97E-6	5.54E-6	
RXF 393	0.678	1.250	1.203	1.135	1.182	0.127	0.215	92	80	88	-81	-68	1.68E-6	3.31E-6	6.53E-6	
SN12C	0.554	1.903	1.794	1.723	1.692	0.358	-0.075	92	87	84	-35	-100	1.94E-6	5.06E-6	1.68E-5	
TK-10	1.015	1.795	1.719	1.736	2.045	0.656	-0.018	90	92	132	-35	-100	3.09E-6	6.14E-6	1.68E-5	
UO-31	0.955	2.310	2.103	1.956	1.781	-0.011	-0.088	85	74	61	-100	-100	1.17E-6	2.39E-6	4.89E-6	
Prostate Cancer																
PC-3	0.573	2.065	2.121	2.038	1.889	0.993	0.043	104	98	88	28	-93	4.33E-6	1.71E-5	4.44E-5	
DU-145	0.356	1.480	1.493	1.415	1.481	0.014	-0.082	101	94	100	-96	-100	1.80E-6	3.24E-6	5.82E-6	
Breast Cancer																
MCF7	0.562	2.526	2.428	2.345	2.225	1.154	0.068	95	91	85	30	-88	4.32E-6	1.80E-5	4.77E-5	
MDA-MB-231/ATCC	0.624	1.313	1.335	1.268	1.224	0.243	-0.032	103	93	87	-61	-100	1.78E-6	3.87E-6	8.41E-6	
HS 578T	1.704	2.891	2.825	2.771	2.755	2.377	1.462	94	90	89	57	-14	1.24E-5	6.30E-5	> 1.00E-4	
BT-549	1.182	1.964	1.869	1.862	1.832	0.120	0.036	88	87	83	-90	-97	1.55E-6	3.02E-6	5.88E-6	
T-47D	1.231	2.602	2.526	2.422	2.432	1.859	0.318	94	87	88	46	-74	7.93E-6	2.41E-5	6.28E-5	
MDA-MB-468	0.850	1.388	1.318	1.317	1.303	0.924	0.127	87	87	84	14	-85	3.05E-6	1.38E-5	4.41E-5	

National Cancer Institute Developmental Therapeutics Program		NSC : D - 833644/1	Units :Molar	SSPL :1CIJ	EXP. ID :2203NS83	
Mean Graphs		Report Date :April 05, 2022		Test Date :March 14, 2022		
Panel/Cell Line	Log ₁₀ GI50	GI50	Log ₁₀ TGI	TGI	Log ₁₀ LC50	LC50
Leukemia						
CCRF-CEM	-5.59		-5.14		> -4.00	
HL-60(TB)	-4.98		-4.40		> -4.00	
K-562	-5.10		-4.44		> -4.00	
MOLT-4	-5.39		-4.50		> -4.00	
RPMI-8226	-5.55		-5.06		> -4.20	
SR	-5.68		-5.28		> -4.00	
Non-Small Cell Lung Cancer						
A549/ATCC	-5.68		-5.37		-5.05	
EKVX	-5.54		-4.96		-4.40	
HOP-62	-5.79		-5.48		-5.18	
HOP-92	-5.80		-5.46		-5.12	
NCI-H226	-5.73		-5.29		-4.36	
NCI-H23	-5.76		-5.45		-5.13	
NCI-H322M	-4.84		-4.56		-4.28	
NCI-H460	-5.37		-4.83		-4.38	
NCI-H522	-5.79		-5.51		-5.23	
Colon Cancer						
COLO 205	-4.85		-4.57		-4.28	
HCC-2998	-4.87		-4.58		-4.29	
HCT-116	-5.43		-4.84		-4.42	
HCT-15	-5.75		-5.47		-5.18	
HT29	-5.16		-4.71		-4.36	
KM12	-5.35		-4.80		-4.40	
SW-620	-5.30		-4.79		-4.40	
CNS Cancer						
SF-268	-5.32		-4.71		-4.23	
SF-295	-4.99		-4.65		-4.32	
SF-539	-5.75		-5.48		-5.20	
SNB-19	-4.91		-4.61		-4.30	
SNB-75	-4.82		-4.52		-4.21	
U251	-5.72		-5.40		-5.08	
Melanoma						
LOX IMVI	-5.83		-5.55		-5.28	
MALME-3M	-5.77		-5.48		-5.19	
M14	-5.38		-4.79		-4.40	
MDA-MB-435	-4.86		-4.56		-4.26	
SK-MEL-2	-4.90		-4.59		-4.28	
SK-MEL-28	-4.86		-4.57		-4.29	
SK-MEL-5	-4.99		-4.66		-4.33	
UACC-257	-4.85		-4.55		-4.25	
UACC-62	-5.30		-4.73		-4.36	
Ovarian Cancer						
IGROV1	-5.57		-5.12		-4.53	
OVCAR-3	-5.72		-5.44		-5.16	
OVCAR-4	-4.99		-4.55		-4.12	
OVCAR-5	-5.19		-4.71		-4.36	
OVCAR-8	-5.71		-5.40		-5.08	
NCI/ADR-RES	-5.75		-5.43		-5.11	
SK-OV-3	-4.90		-4.60		-4.30	
Renal Cancer						
786-0	-5.70		-5.45		-5.20	
A498	-4.74		-4.46		-4.18	
ACHN	-5.75		-5.50		-5.25	
CAKI-1	-5.80		-5.53		-5.26	
RXF 393	-5.78		-5.48		-5.19	
SN12C	-5.71		-5.30		-4.77	
TK-10	-5.51		-5.21		-4.77	
UO-31	-5.93		-5.62		-5.31	
Prostate Cancer						
PC-3	-5.36		-4.77		-4.35	
DU-145	-5.74		-5.49		-5.23	
Breast Cancer						
MCF7	-5.36		-4.74		-4.32	
MDA-MB-231/ATCC	-5.75		-5.41		-5.08	
HS 578T	-4.91		-4.20		> -4.00	
BT-549	-5.81		-5.52		-5.23	
T-47D	-5.10		-4.62		-4.20	
MDA-MB-468	-5.52		-4.86		-4.36	

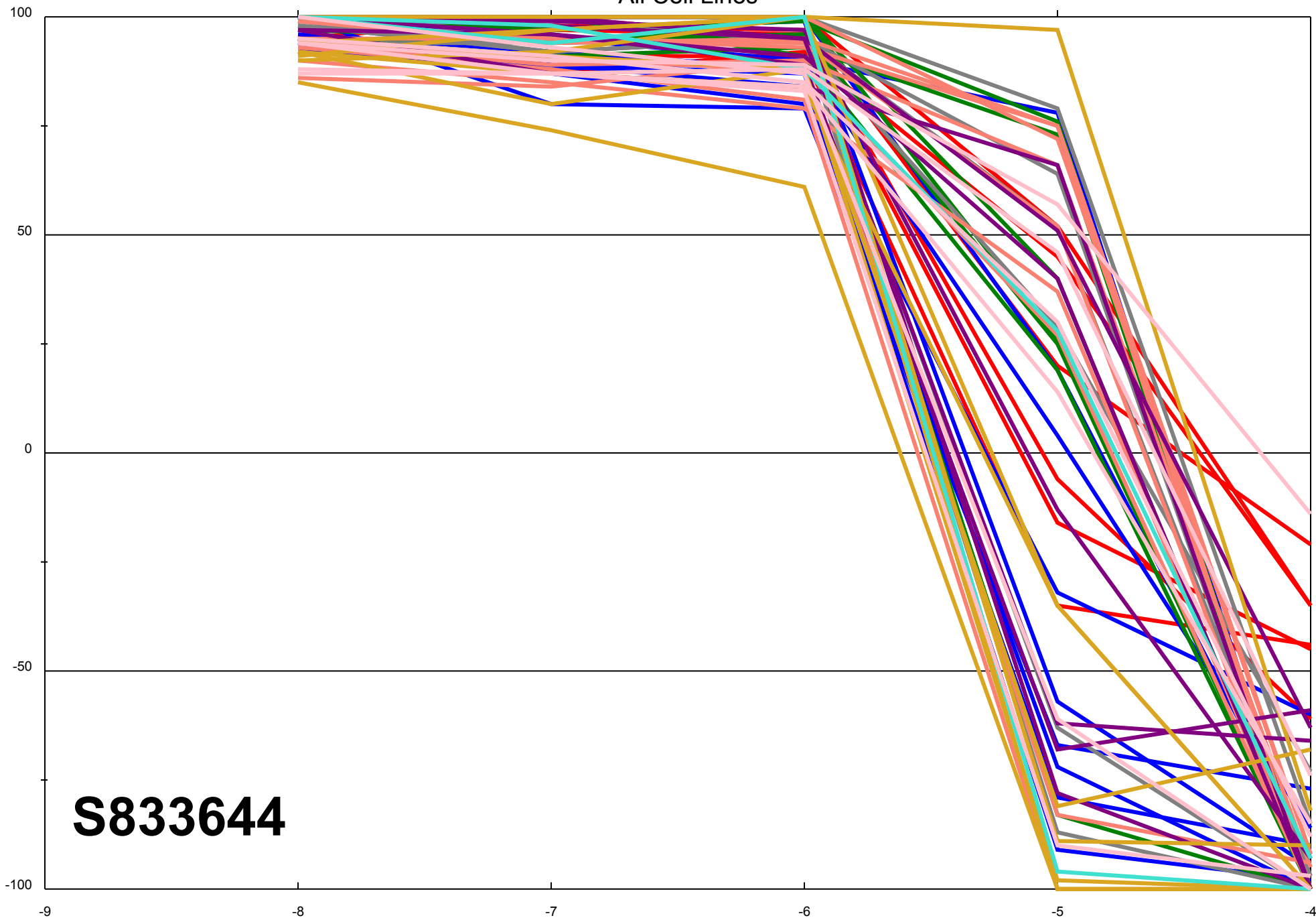
Dose Response Curves

Report Date:April 05, 2022

Test Date:March 14, 2022

All Cell Lines

Percentage Growth



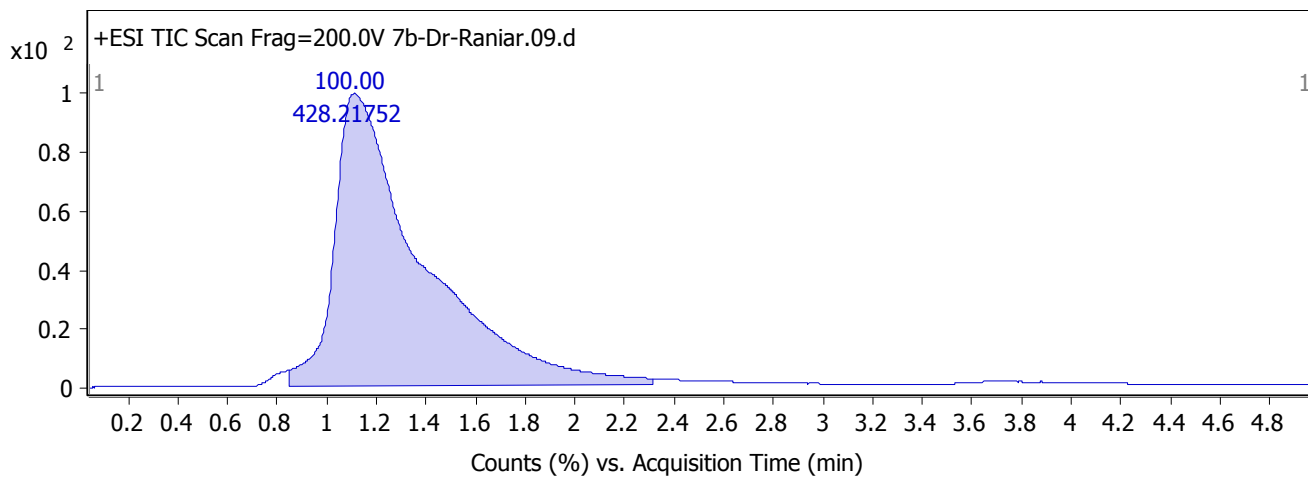
S833644

Log₁₀ of Sample Concentration (Molar)

Data File	7b-Dr-Ranar.09.d	Sample Name	7b
Sample Type	Sample	Position	62
Instrument Name	Instrument 1	User Name	
Acq Method	HRMS-RES.m	Acquired Time	5/18/2023 9:31:48 PM (UTC+02:00)
IRM Calibration Status	Success	DA Method	khalid focused lc-ms.m
Comment	7b-Dr-Rania		
Method part to run:	Acquisition Only	Sample Group	
Info.		Stream Name	LC 1
Acquisition Time (Local)	5/18/2023 10:31:48 PM (UTC+03:00)	Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)
QTOF Driver Version	8.00.00	QTOF Firmware Version	26.723
Tune Mass Range Max.	3200		

Chromatograms

Fragmentor Voltage 200 Collision Energy 0 Ionization Mode ESI



Integration Peak List

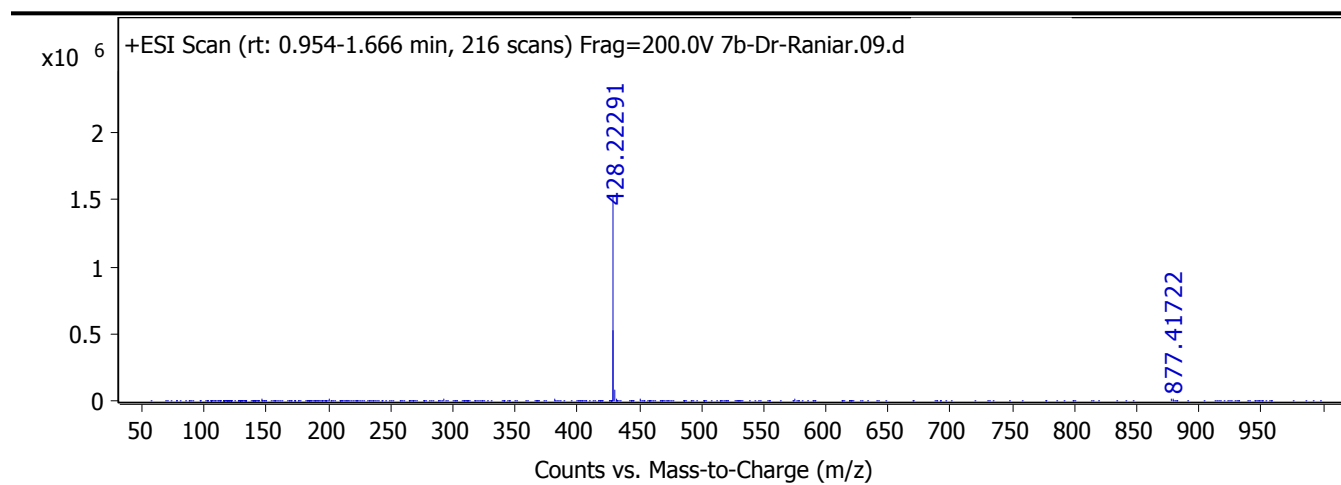
Peak	Start	RT	End	Height	Area	Area %
1	0.851	1.115	2.312	24556427.01	606427026.76	100

Spectra

Fragmentor Voltage 200 Collision Energy 0 Ionization Mode ESI



Qualitative Analysis Report



Peak List

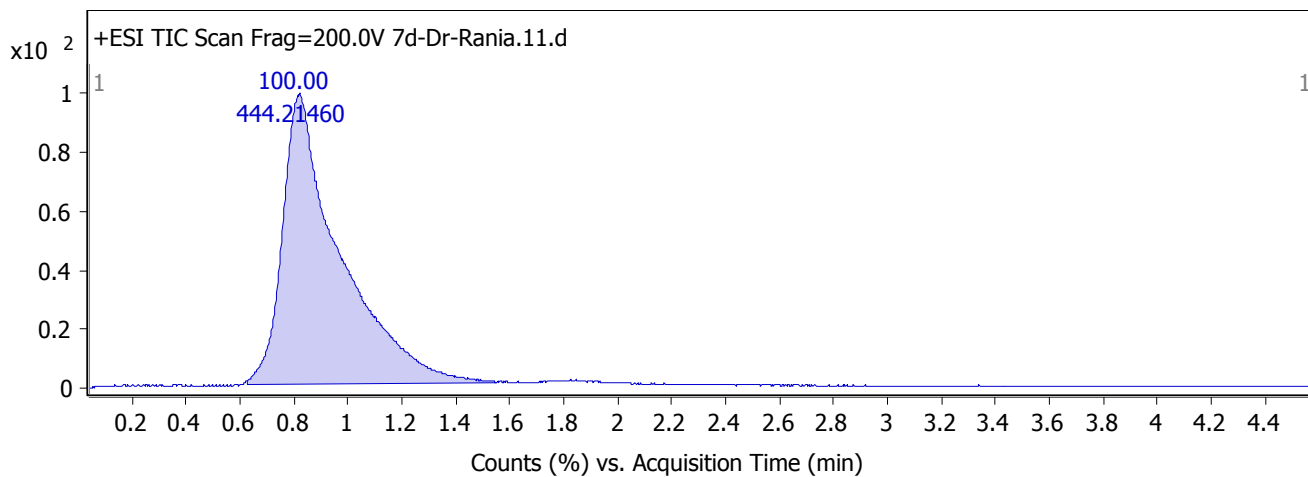
m/z	z	Abund
428.22291	1	1514377.5
429.22566	1	524893.25
430.22842	1	81957.73
877.41722		17515.18

--- End Of Report ---

Data File	7d-Dr-Rania.11.d	Sample Name	7d
Sample Type	Sample	Position	Vial 1
Instrument Name	Instrument 1	User Name	
Acq Method	HRMS-RES.m	Acquired Time	5/20/2023 7:26:01 PM (UTC+02:00)
IRM Calibration Status	Success	DA Method	khalid focused lc-ms.m
Comment	7d-Dr-Rania		
Method part to run:	Acquisition Only	Sample Group	
Info.		Stream Name	LC 1
Acquisition Time (Local)	5/20/2023 8:26:01 PM (UTC+03:00)	Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)
QTOF Driver Version	8.00.00	QTOF Firmware Version	26.723
Tune Mass Range Max.	3200		

Chromatograms

Fragmentor Voltage 200 Collision Energy 0 Ionization Mode ESI



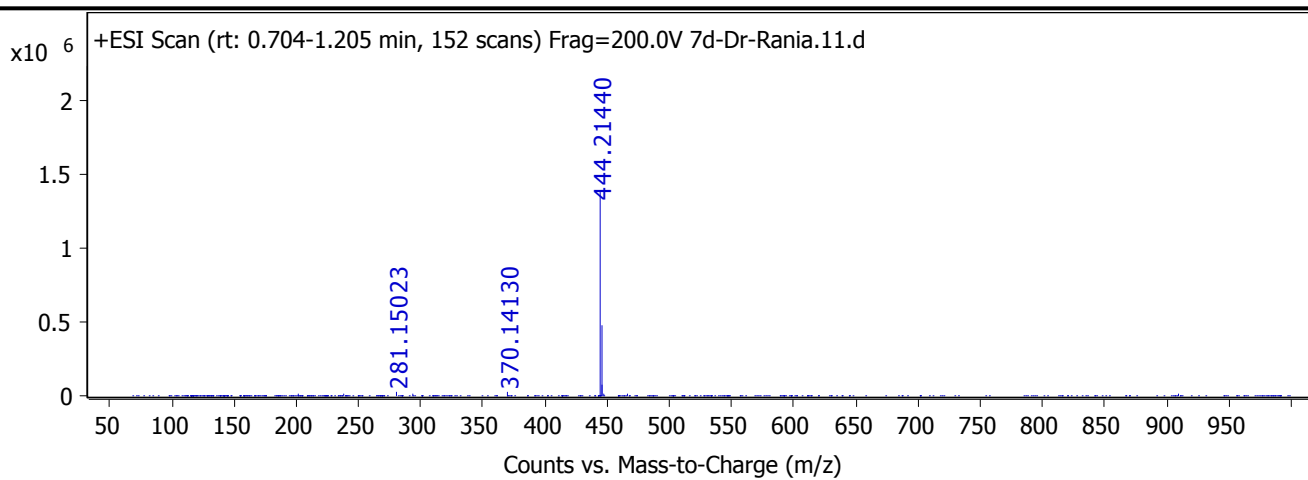
Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	0.625	0.82	1.553	23406481.88	346368601.67	100

Spectra

Fragmentor Voltage 200 Collision Energy 0 Ionization Mode ESI

Qualitative Analysis Report



Peak List

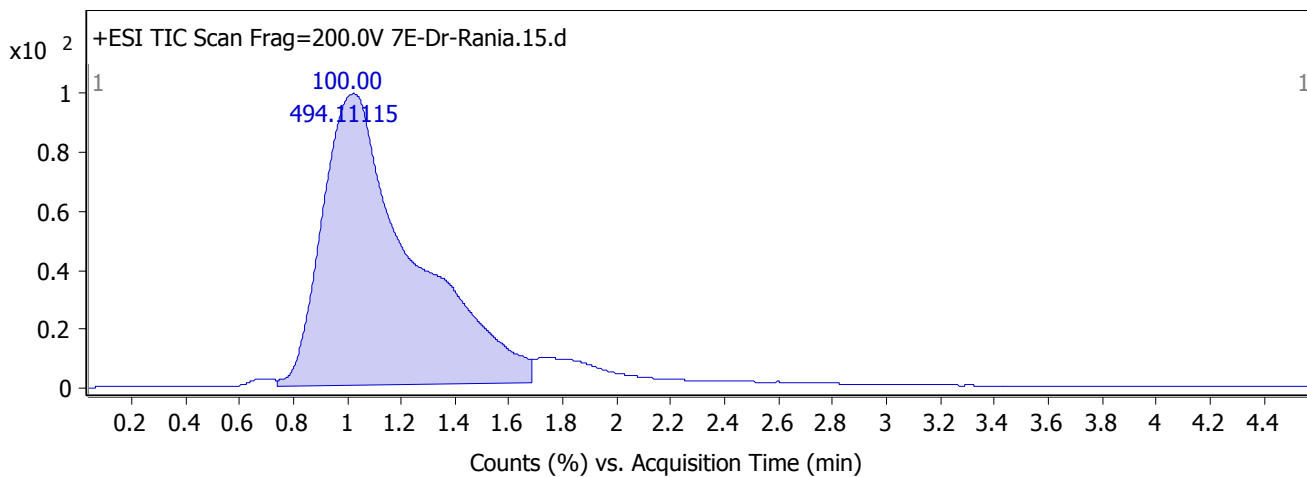
m/z	z	Abund
281.15023		19988.18
370.1413		20526.42
444.2144	1	1376010.88
445.21719	1	476271.06
446.22	1	76895.11

--- End Of Report ---

Data File	7E-Dr-Rania.15.d	Sample Name	7E
Sample Type	Sample	Position	41
Instrument Name	Instrument 1	User Name	
Acq Method	HRMS-RES.m	Acquired Time	5/20/2023 7:55:46 PM (UTC+02:00)
IRM Calibration Status	Success	DA Method	khalid focused lc-ms.m
Comment	7E-Dr-Rania		
Method part to run:	Acquisition Only	Sample Group	
Info.		Stream Name	LC 1
Acquisition Time (Local)	5/20/2023 8:55:46 PM (UTC+03:00)	Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)
QTOF Driver Version	8.00.00	QTOF Firmware Version	26.723
Tune Mass Range Max.	3200		

Chromatograms

Fragmentor Voltage 200 Collision Energy 0 Ionization Mode ESI



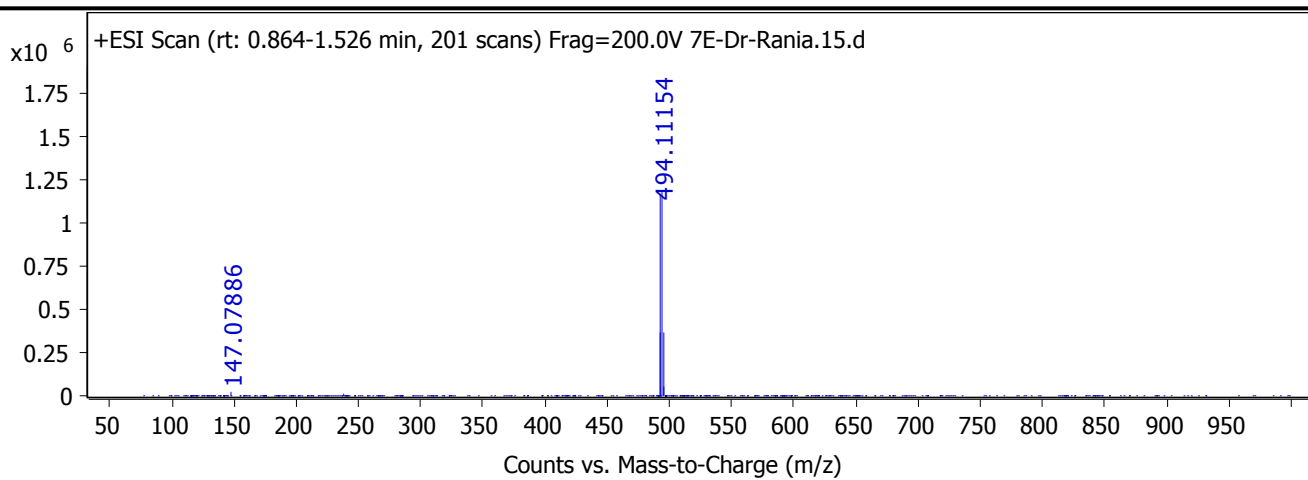
Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	0.741	1.023	1.685	31748532.73	736750333.54	100

Spectra

Fragmentor Voltage 200 Collision Energy 0 Ionization Mode ESI

Qualitative Analysis Report



Peak List

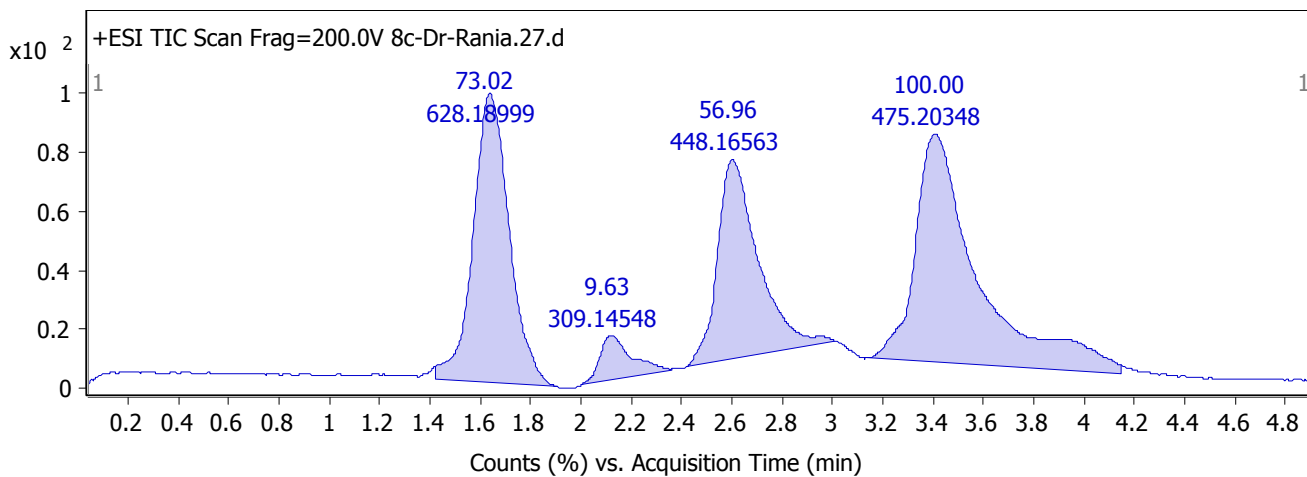
m/z	z	Abund
147.07886		21858.84
492.11328	1	1166414.25
493.11619	1	367688.94
494.11154	1	1175293.38
495.11423	1	364533.09
496.11665	1	53335.01

--- End Of Report ---

Data File	8c-Dr-Rania.27.d	Sample Name	8c
Sample Type	Sample	Position	Vial 21
Instrument Name	Instrument 1	User Name	
Acq Method	HRMS-RES.m	Acquired Time	5/22/2023 3:38:34 PM (UTC+02:00)
IRM Calibration Status	Success	DA Method	khalid focused lc-ms.m
Comment	8c-Dr-Rania		
Method part to run:	Acquisition Only	Sample Group	
Info.		Stream Name	LC 1
Acquisition Time (Local)	5/22/2023 4:38:34 PM (UTC+03:00)	Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)
QTOF Driver Version	8.00.00	QTOF Firmware Version	26.723
Tune Mass Range Max.	3200		

Chromatograms

Fragmentor Voltage 200 Collision Energy 0 Ionization Mode ESI



Integration Peak List

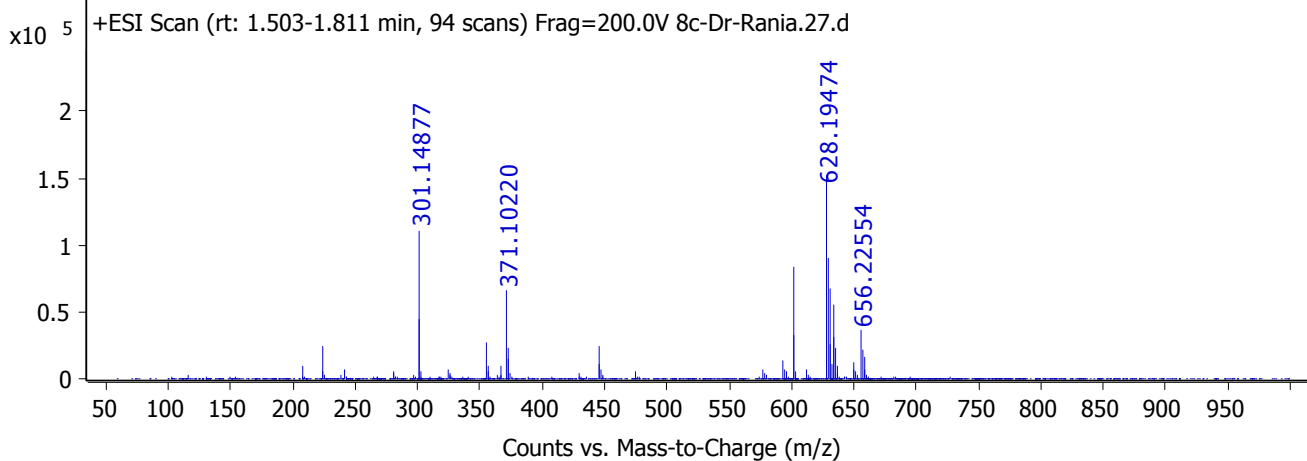
Peak	Start	RT	End	Height	Area	Area %
1	1.423	1.638	1.903	11065998.47	110639290.24	73.02
2	2.003	2.122	2.358	1704730.57	14598089.73	9.63
3	2.421	2.603	3.007	7618926.6	86311964.41	56.96
4	3.137	3.405	4.144	8751927.77	151520436.34	100

Spectra

Fragmentor Voltage 200 Collision Energy 0 Ionization Mode ESI



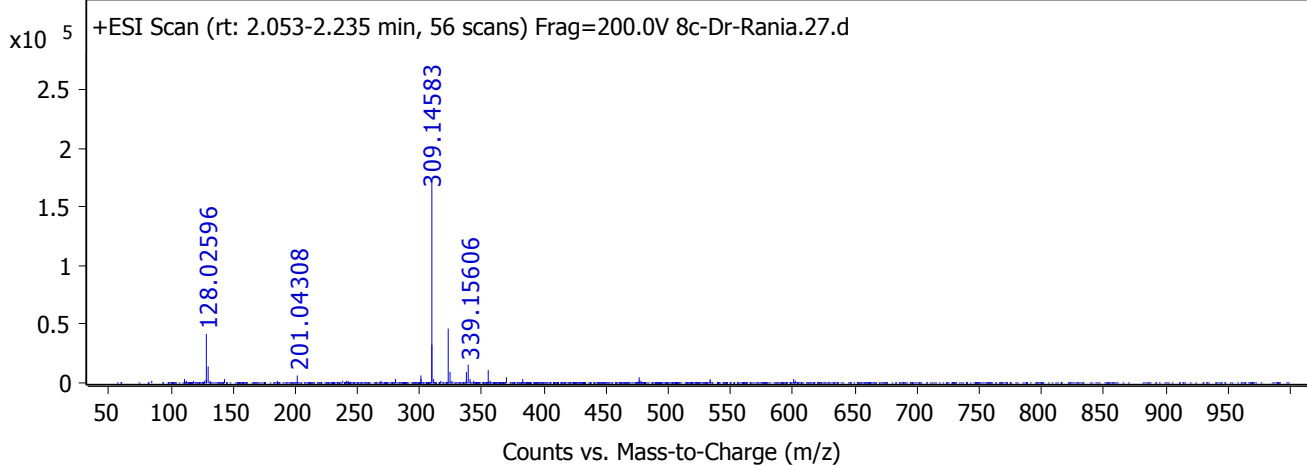
Qualitative Analysis Report



Peak List

m/z	z	Abund
301.14877	2	111043.35
301.64997	2	44084.66
371.1022		65528.15
601.2894	1	83867.04
602.29181	1	31954.3
628.19474	1	151933.89
629.19563	1	89842.7
630.19345	1	67938.5
633.15126	1	54793.11
656.22554		35854.49

Fragmentor Voltage Collision Energy Ionization Mode
200 0 ESI



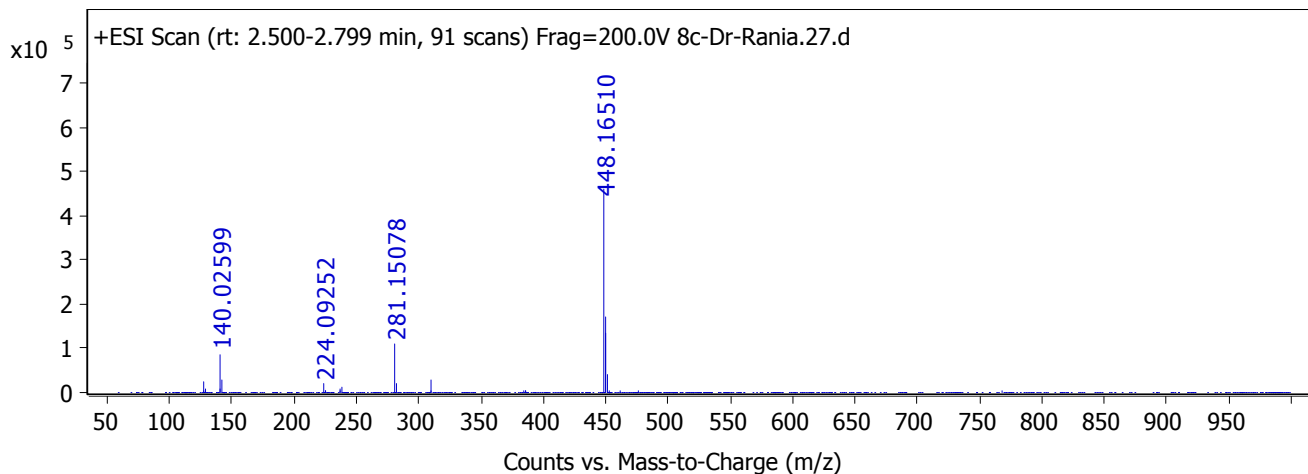
Peak List

m/z	z	Abund
128.02596		41615.01
130.02298		13567.36
201.04308		6271.68
309.14583	1	173092.88

Qualitative Analysis Report

310.14821	1	32461.76
323.16119	1	46535.29
324.1637	1	9252.45
337.14044		9207.94
339.15606		16168.66
355.15071		11590.24

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI

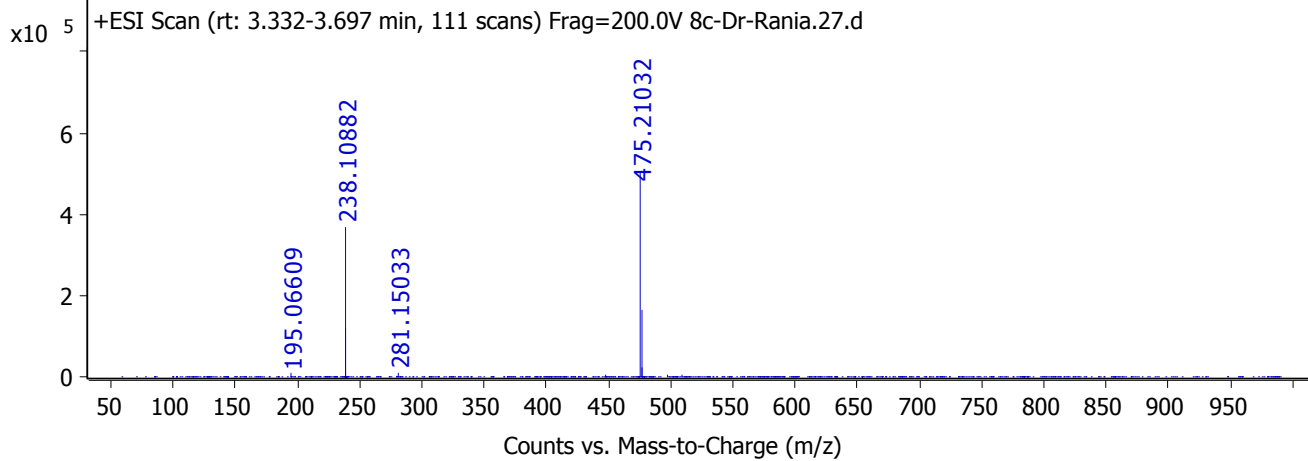


Peak List

<i>m/z</i>	<i>z</i>	Abund
127.01815		23862.56
140.02599		87312.77
142.02301		27247.09
281.15078	1	109109.73
282.15322	1	18973.31
309.14528		27138.03
448.1651	1	459846.06
449.16838	1	133855.31
450.16301	1	170938.72
451.16614	1	41948.74

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI

Qualitative Analysis Report



Peak List

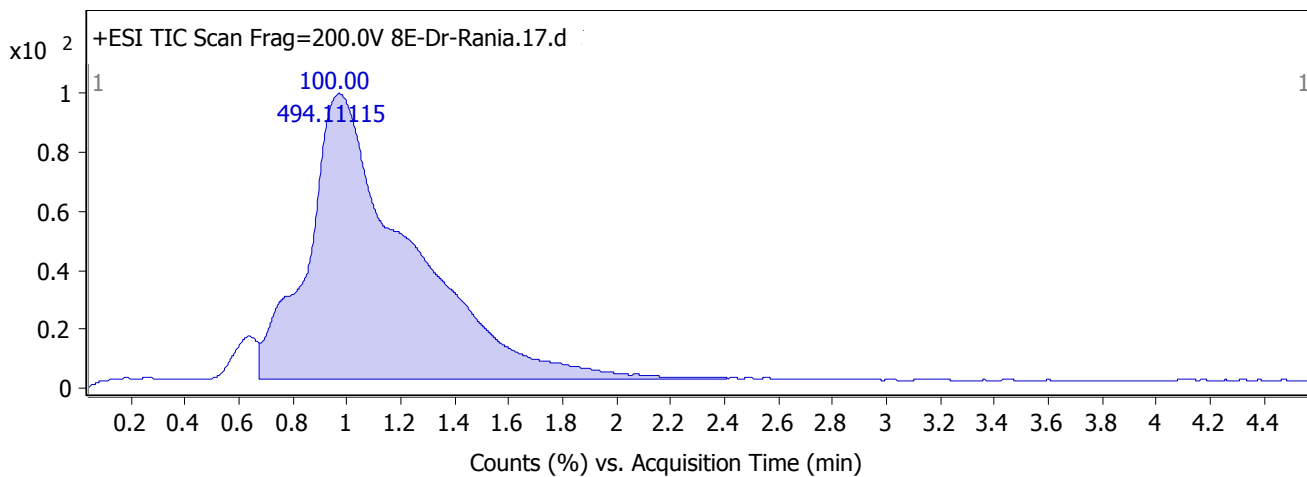
m/z	z	Abund
195.06609		7040.82
238.10882	2	369691.78
238.61019	2	121546.25
239.11138	2	19088.69
281.15033		8980.55
475.21032	1	499582.81
476.21317	1	166287.27
477.21542	1	24352.12

--- End Of Report ---

Data File	8E-Dr-Rania.17.d	Sample Name	8E
Sample Type	Sample	Position	Vial 42
Instrument Name	Instrument 1	User Name	
Acq Method	HRMS-RES.m	Acquired Time	5/20/2023 8:13:00 PM (UTC+02:00)
IRM Calibration Status	Success	DA Method	khalid focused lc-ms.m
Comment	8E-Dr-Rania		
Method part to run:	Acquisition Only	Sample Group	
Info.		Stream Name	LC 1
Acquisition Time (Local)	5/20/2023 9:13:00 PM (UTC+03:00)	Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)
QTOF Driver Version	8.00.00	QTOF Firmware Version	26.723
Tune Mass Range Max.	3200		

Chromatograms

Fragmentor Voltage 200 Collision Energy 0 Ionization Mode ESI



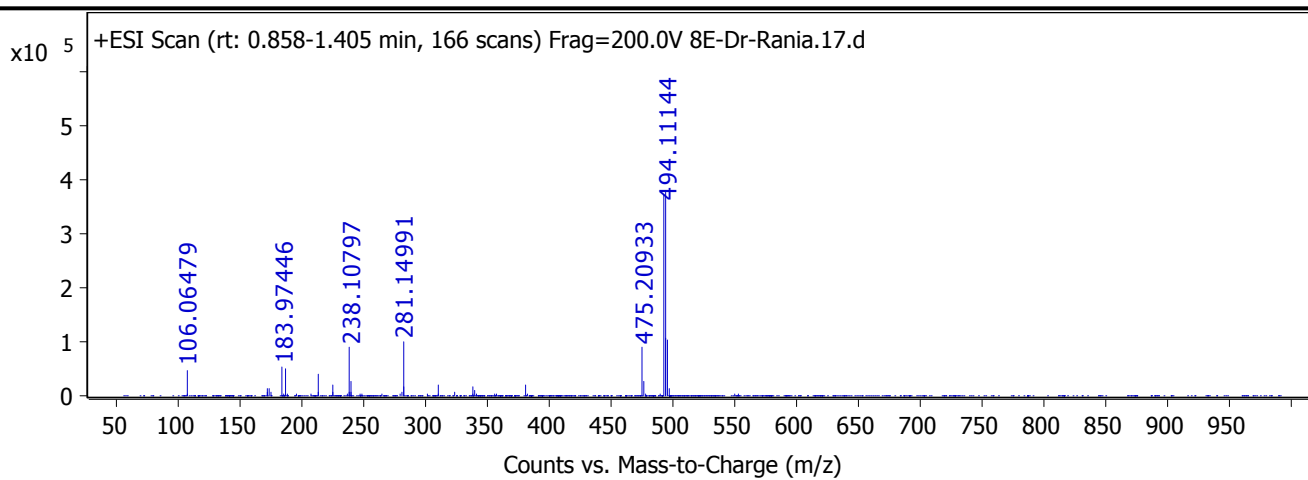
Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	0.676	0.971	2.406	12784931.19	335881713.92	100

Spectra

Fragmentor Voltage 200 Collision Energy 0 Ionization Mode ESI

Qualitative Analysis Report



Peak List

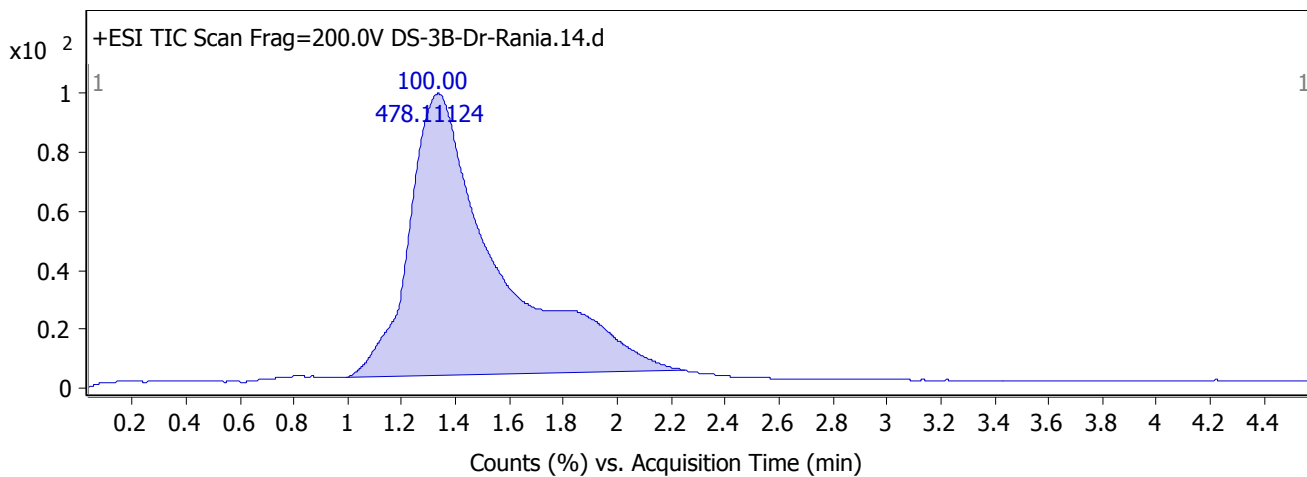
m/z	z	Abund
106.06479		46981.14
183.97446		53126.62
185.97242		51596.07
238.10797		90192.61
281.14991		99395.39
475.20933		90311.39
492.11297	1	374523.78
493.11588	1	107981.57
494.11144	1	377058.16
495.11414	1	105459.79

--- End Of Report ---

Data File	DS-3B-Dr-Rania.14.d	Sample Name	DS-3B
Sample Type	Sample	Position	31
Instrument Name	Instrument 1	User Name	
Acq Method	HRMS-RES.m	Acquired Time	5/20/2023 7:48:46 PM (UTC+02:00)
IRM Calibration Status	Success	DA Method	khalid focused lc-ms.m
Comment	DS-3B-Dr-Rania		
Method part to run:	Acquisition Only	Sample Group	
Info.		Stream Name	LC 1
Acquisition Time (Local)	5/20/2023 8:48:46 PM (UTC+03:00)	Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)
QTOF Driver Version	8.00.00	QTOF Firmware Version	26.723
Tune Mass Range Max.	3200		

Chromatograms

Fragmentor Voltage 200 Collision Energy 0 Ionization Mode ESI



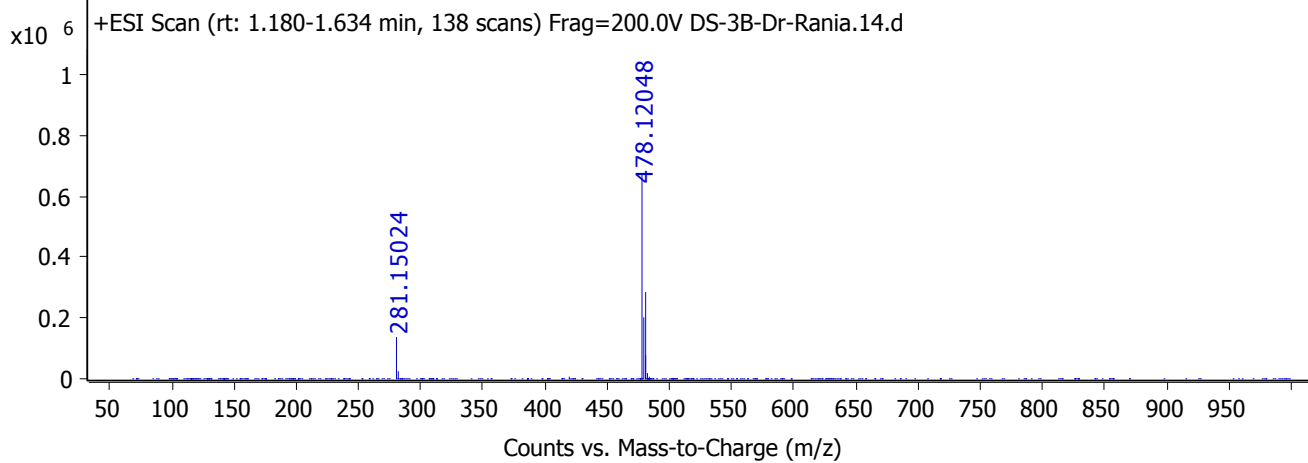
Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	0.991	1.334	2.246	11005857.53	250687066.67	100

Spectra

Fragmentor Voltage 200 Collision Energy 0 Ionization Mode ESI

Qualitative Analysis Report



Peak List

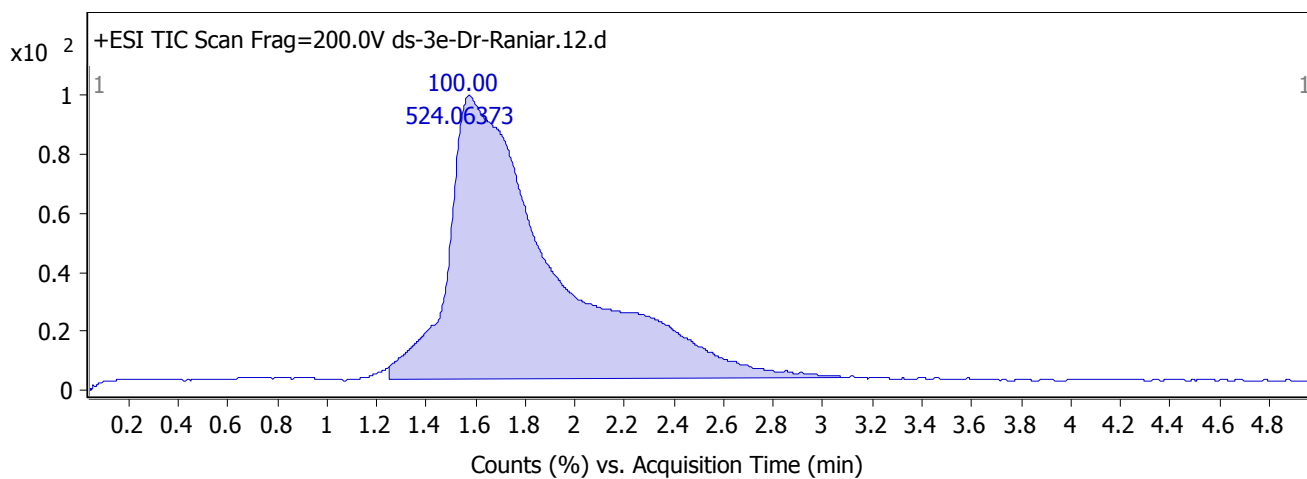
m/z	z	Abund
281.15024	1	135515.03
282.15253	1	24396.43
478.12048	1	667194.13
479.12345	1	200750.36
480.1184	1	281347.44
481.12032	1	76983.36
482.11797	1	19320.46

--- End Of Report ---

Data File	ds-3e-Dr-Raniar.12.d	Sample Name	ds-3e
Sample Type	Sample	Position	Vial 72
Instrument Name	Instrument 1	User Name	
Acq Method	HRMS-RES.m	Acquired Time	5/18/2023 9:56:32 PM (UTC+02:00)
IRM Calibration Status	Success	DA Method	khalid focused lc-ms.m
Comment	ds-3e-Dr-Rania		
Method part to run:	Acquisition Only	Sample Group	
Info.		Stream Name	LC 1
Acquisition Time (Local)	5/18/2023 10:56:32 PM (UTC+03:00)	Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)
QTOF Driver Version	8.00.00	QTOF Firmware Version	26.723
Tune Mass Range Max.	3200		

Chromatograms

Fragmentor Voltage 200 Collision Energy 0 Ionization Mode ESI



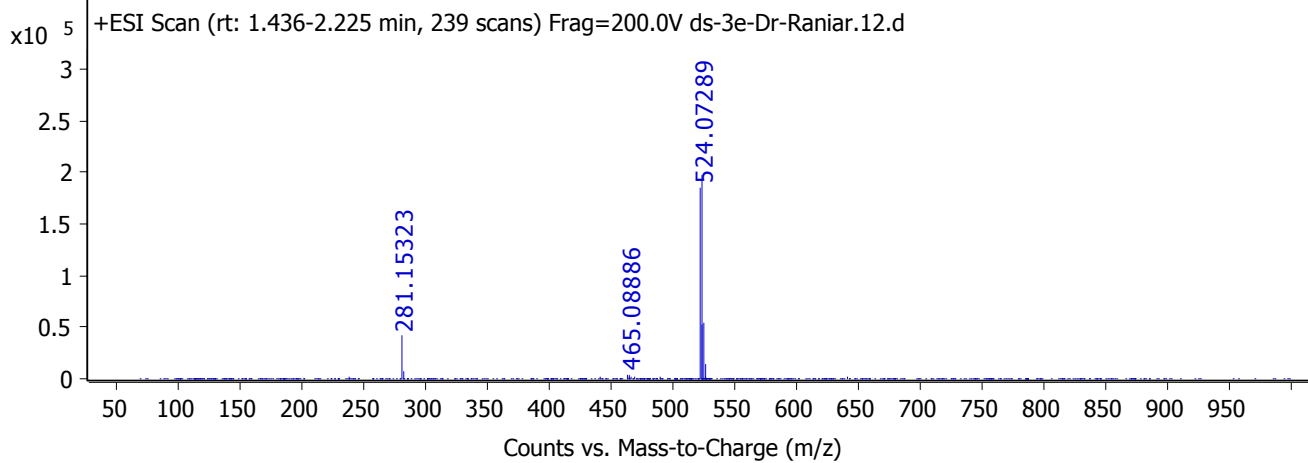
Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	1.254	1.572	3.075	5060699.29	151757689.59	100

Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI

Qualitative Analysis Report



Peak List

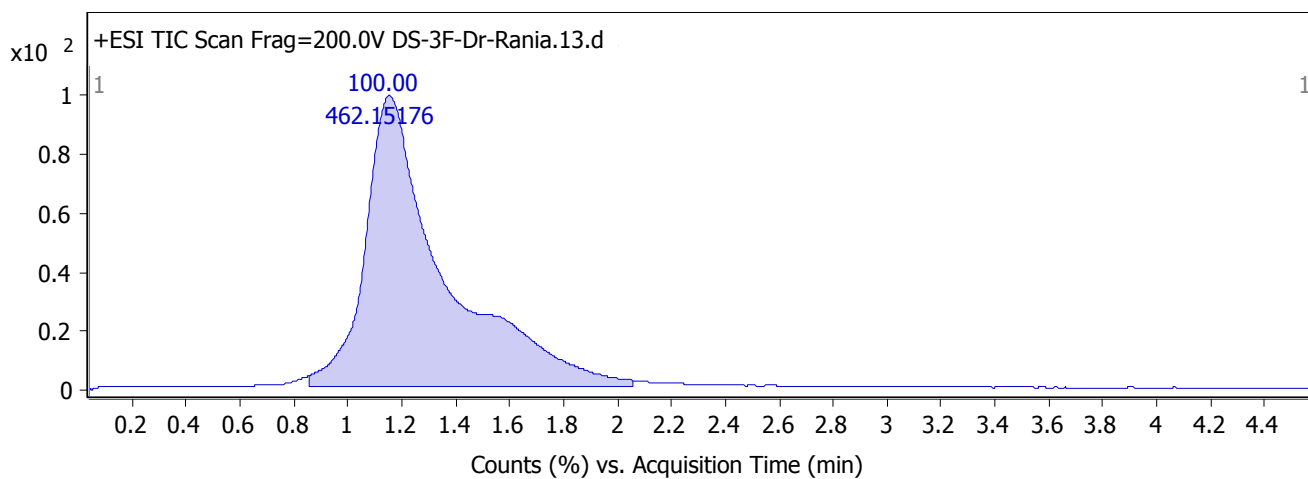
m/z	z	Abund
281.15323	1	41805.18
282.15582	1	7470.37
463.09079		4152.98
465.08886		4169.18
522.0747	1	185651.11
523.07715	1	52852.66
524.07289	1	196952.55
525.07513	1	54468.52
526.07274	1	14549.15
527.0729	1	2662.8

--- End Of Report ---

Data File	DS-3F-Dr-Rania.13.d	Sample Name	DS-3F
Sample Type	Sample	Position	21
Instrument Name	Instrument 1	User Name	
Acq Method	HRMS-RES.m	Acquired Time	5/20/2023 7:41:33 PM (UTC+02:00)
IRM Calibration Status	Success	DA Method	khalid focused lc-ms.m
Comment	DS-3F-Dr-Rania		
Method part to run:	Acquisition Only	Sample Group	
Info.		Stream Name	LC 1
Acquisition Time (Local)	5/20/2023 8:41:33 PM (UTC+03:00)	Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)
QTOF Driver Version	8.00.00	QTOF Firmware Version	26.723
Tune Mass Range Max.	3200		

Chromatograms

Fragmentor Voltage 200 Collision Energy 0 Ionization Mode ESI



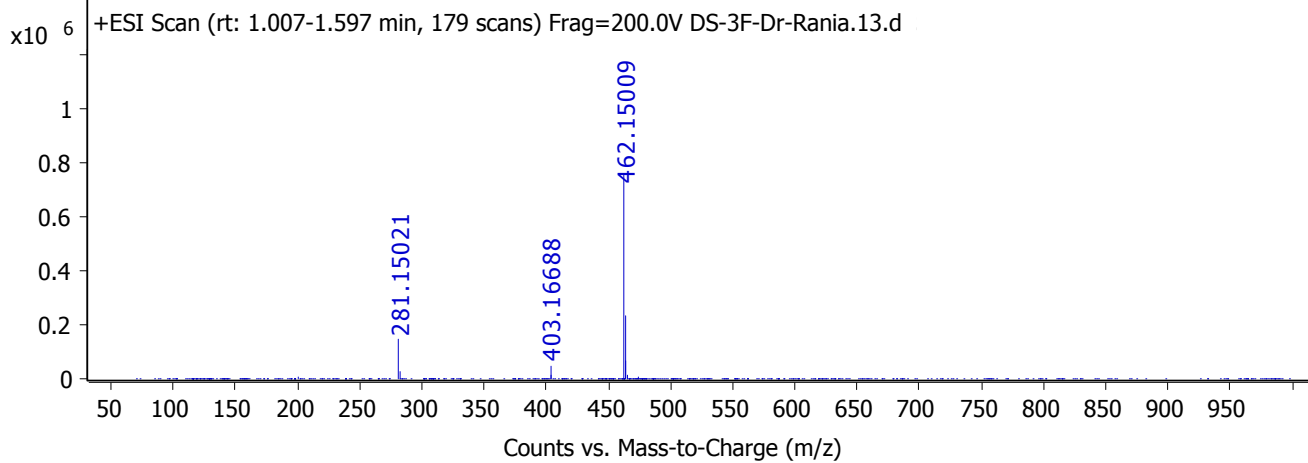
Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	0.858	1.15	2.058	13500367.09	276961649.98	100

Spectra

Fragmentor Voltage 200 Collision Energy 0 Ionization Mode ESI

Qualitative Analysis Report



Peak List

m/z	z	Abund
281.15021	1	146241.2
282.1526	1	26396.88
403.16688	1	49583.14
404.16949	1	12294.46
462.15009	1	753632.44
463.15295	1	231146.73
464.15066	1	69451.95
465.15064	1	12132.56

--- End Of Report ---