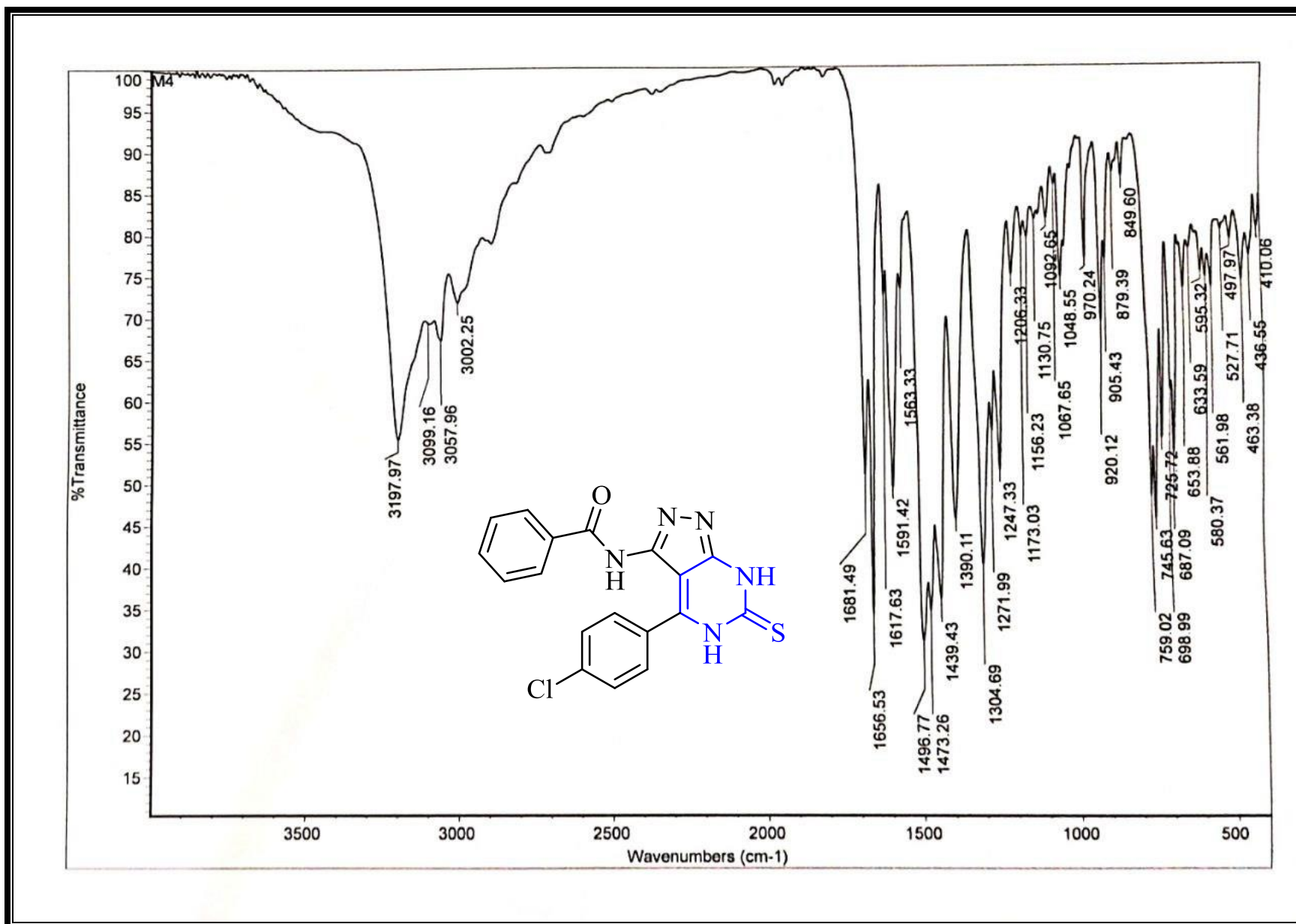


1. Chemistry

Using a Pye Unicam SP1200 spectrophotometer, IR-spectra were recorded using the KBr wafer method (Pye Unicam Ltd., Cambridge, UK). The ^1H -NMR spectra were obtained on a Bruker Avance (III) with a Varian-Gemini 400 MHz and an internal standard of Tetramethyl silane (chemical shifts in scale ppm), while the ^{13}C -NMR spectra were obtained at 100 MHz. TMS was used as an internal standard in deuterated Dimethyl sulfoxide ($\text{DMSO-}d_6$).



IR of *N*-(4-(4-chlorophenyl)-6-thioxo-6,7-dihydro-5H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (2).

Paula Soliman_H_M4

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12.4080
11.8513
11.4613

8.0368
8.0346
7.6941
7.6855
6.7632
6.7592
6.7546
6.7505

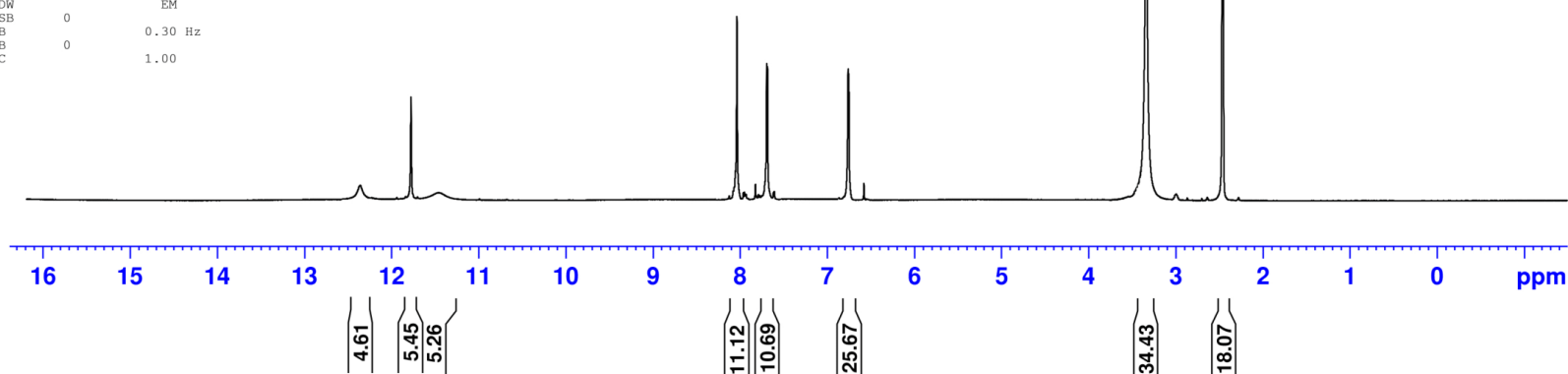
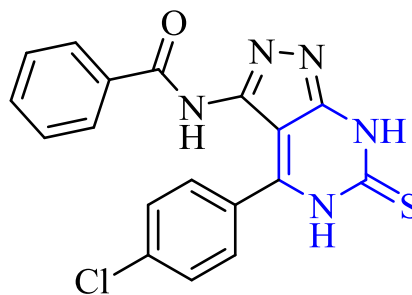
3.3482
2.5087

Current Data Parameters
NAME Paula Soliman_H_M4
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210712
Time 8.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.46
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H-NMR of *N*-(4-(4-chlorophenyl)-6-thioxo-6,7-dihydro-5H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (2).

Paula Soliman_H_M4_D2O

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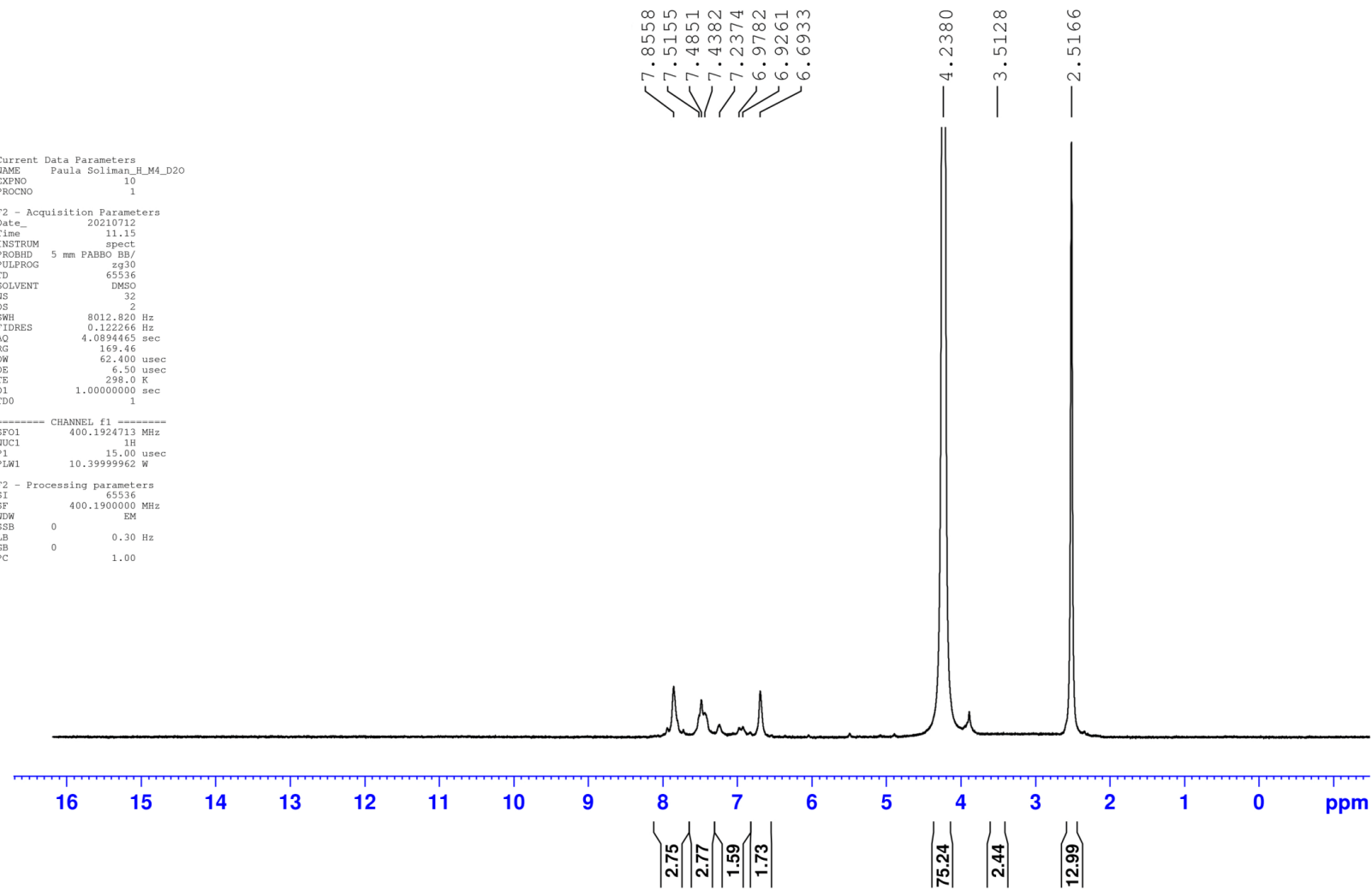


Current Data Parameters
NAME Paula Soliman_H_M4_D2O
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.46
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SF01 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



D₂O of *N*-(4-(4-chlorophenyl)-6-thioxo-6,7-dihydro-5H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (2).

Paula Soliman_C_M4

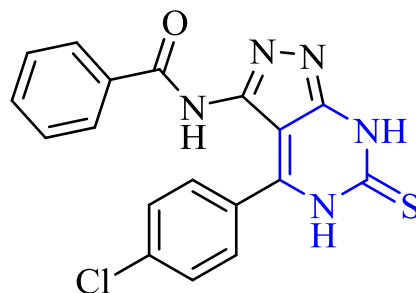
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187.64
173.70
170.94
159.63
156.79
156.08
150.07
148.01
146.48
145.94
124.37
117.58
112.88
90.19
41.16
40.61
40.40
40.19
39.98
39.78
39.57
39.36

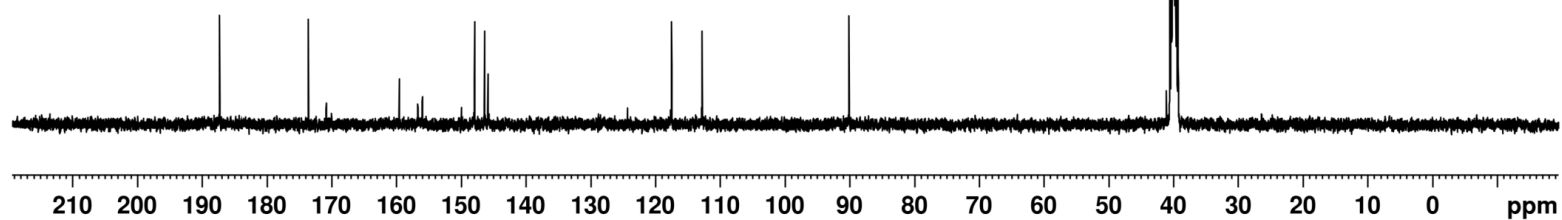
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NAME Paula Soliman_C_M4
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210712
Time 9.30
INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

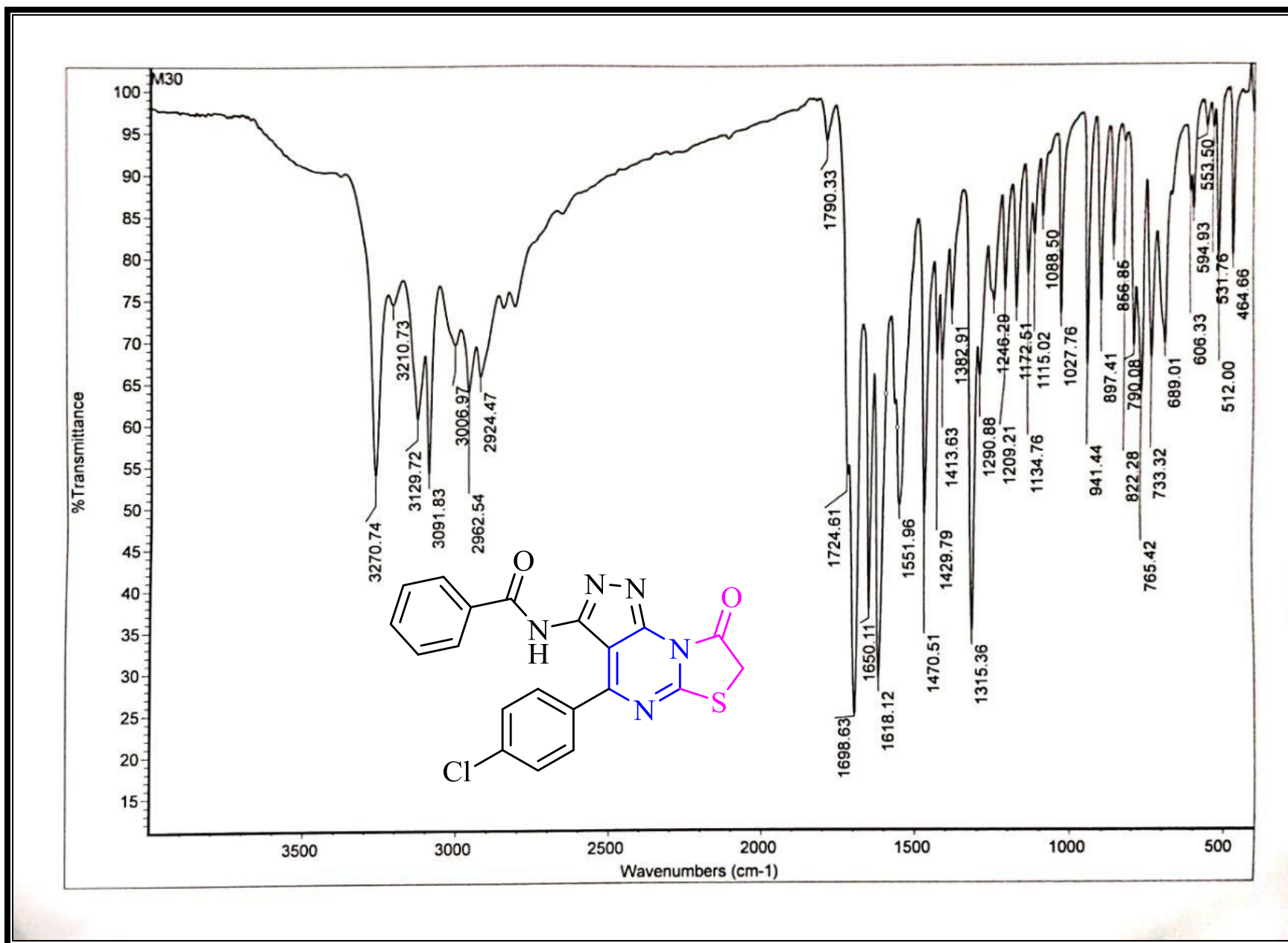


==== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W

==== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2] waltz16



¹³C-NMR of *N*-(4-(4-chlorophenyl)-6-thioxo-6,7-dihydro-5H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (2).



IR of *N*-(4-(4-chlorophenyl)-8-oxo-7,8-dihydropyrazolo[4,3-*e*]thiazolo[3,2-*a*]pyrimidin-3-yl)benzamide (3).

Paula Soliman_H_M30

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12.9243
12.9154

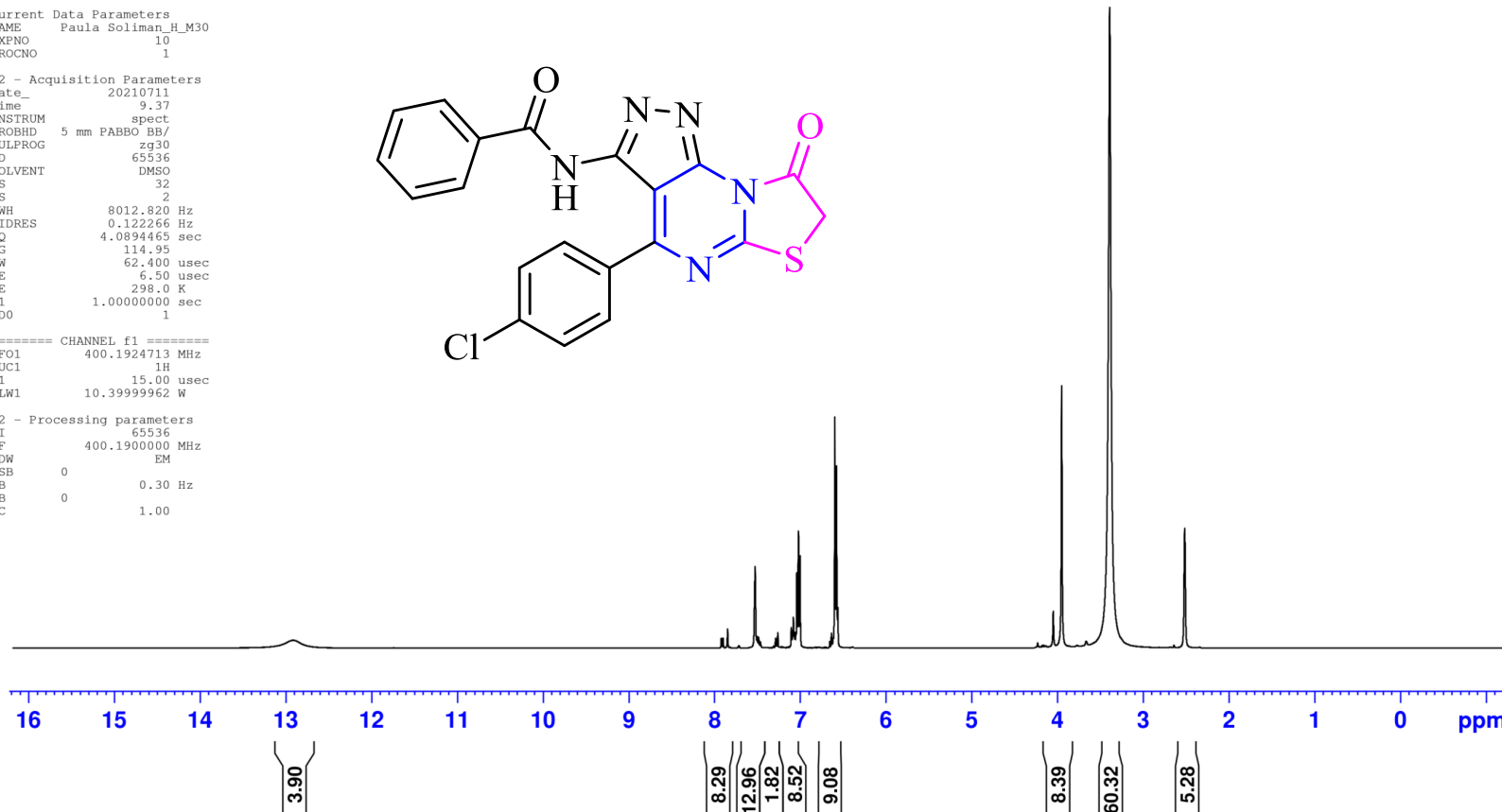
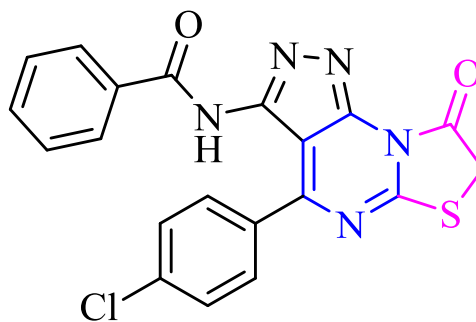
8.0315
8.0280
8.0119
8.0082
7.9571
7.6376
7.4011
7.3948
7.3788
7.3729
7.1948
7.1540
7.1353
7.1147
6.7132
6.6949
6.6935
6.6771
4.0455
3.9469
3.3868
2.5113

Current Data Parameters
NAME Paula Soliman_H_M30
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210711
Time_ 9.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 114.95
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H-NMR of *N*-(4-(4-chlorophenyl)-8-oxo-7,8-dihydropyrazolo[4,3-*e*]thiazolo[3,2-*a*]pyrimidin-3-yl)benzamide (3).

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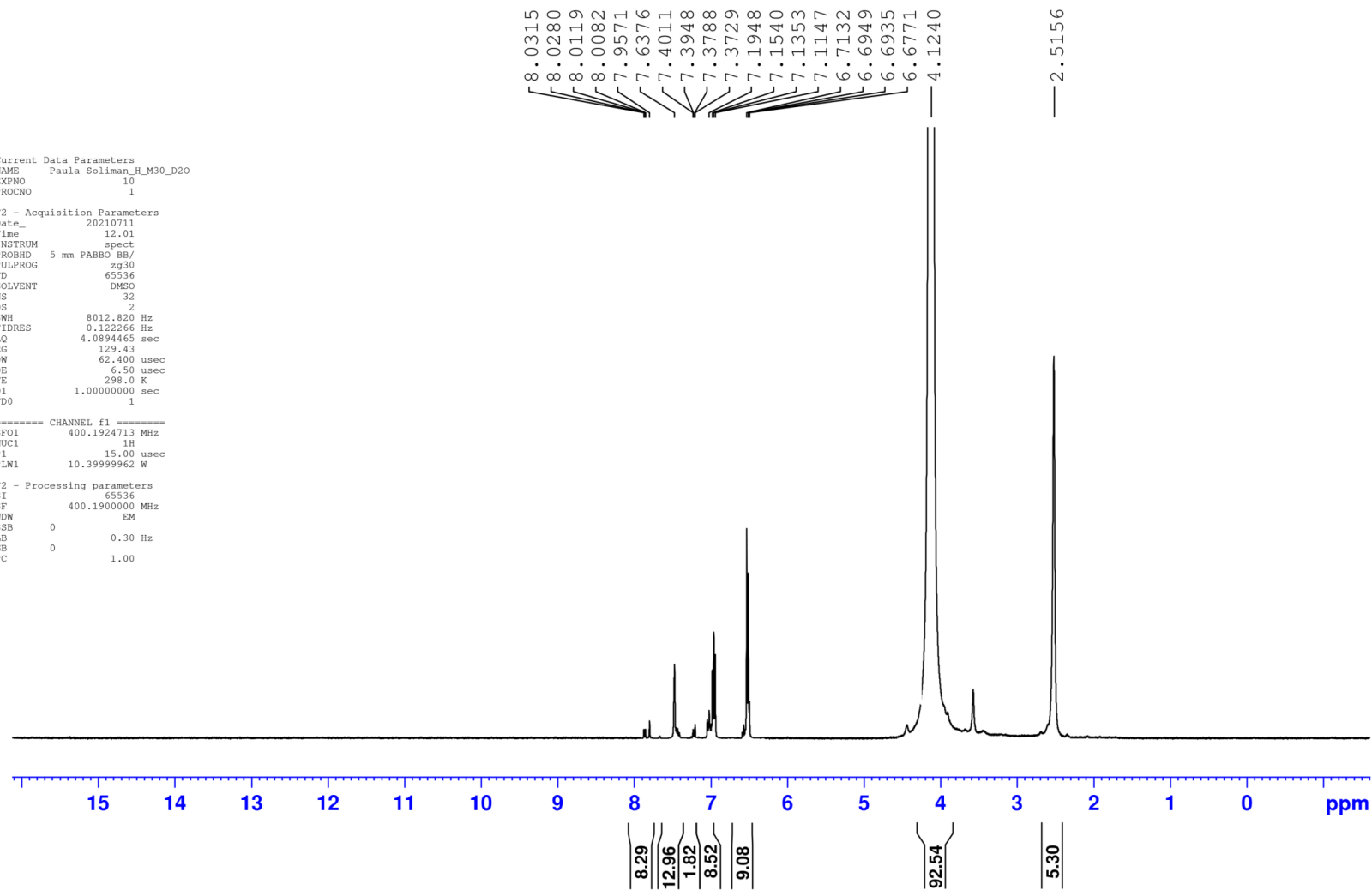


Current Data Parameters
NAME Paula Soliman_H_M30_D2O
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210711
Time 12.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 129.43
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



D₂O of *N*-(4-(4-chlorophenyl)-8-oxo-7,8-dihydropyrazolo[4,3-*e*]thiazolo[3,2-*a*]pyrimidin-3-yl)benzamide (3).

Paula Soliman_C_M30

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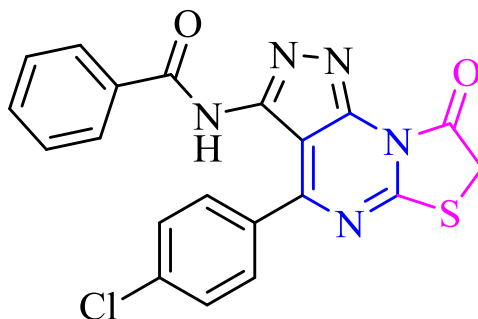


169.66
168.85
166.93
159.51
158.87
152.45
140.38
134.43
131.66
129.98
128.56
126.08
123.69
123.33
120.44
117.41
116.04

40.59
40.38
40.17
39.96
39.75
39.55
39.34
22.83

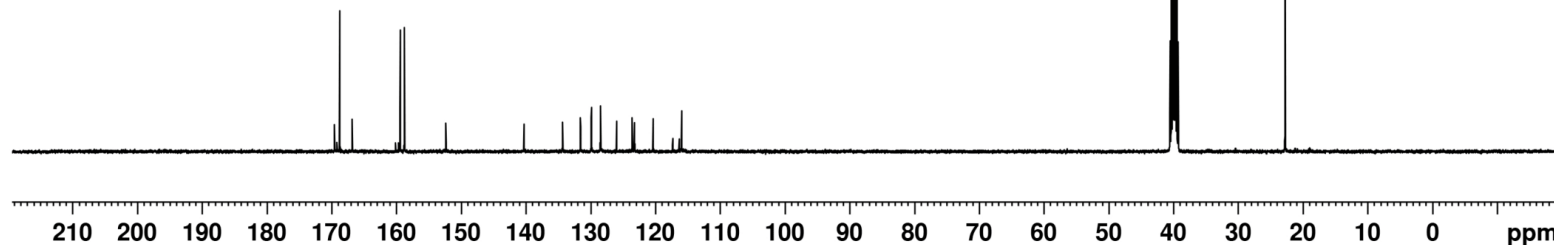
Current Data Parameters
NAME Paula Soliman_C_M30
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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Time 10.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

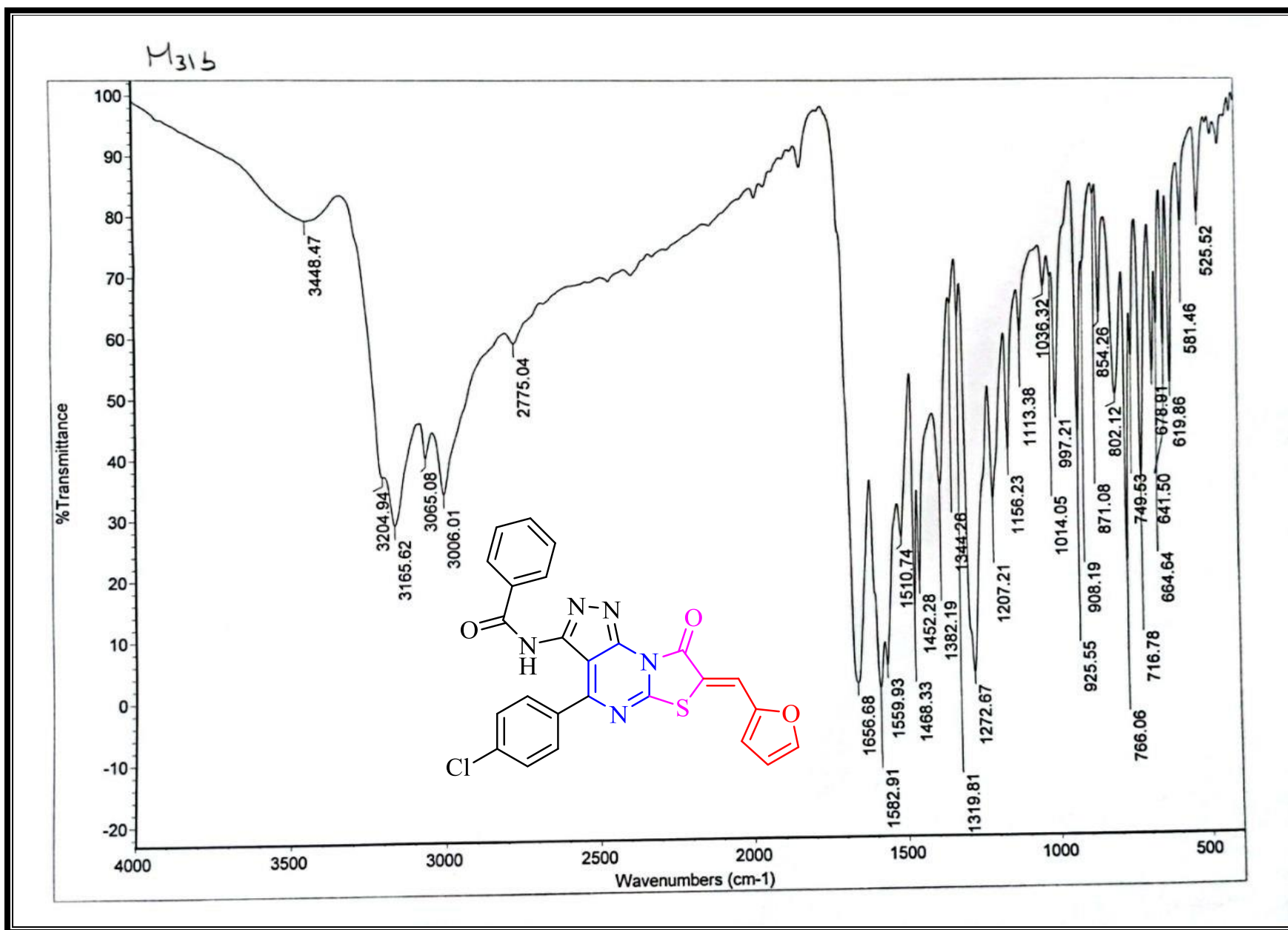


==== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W

==== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG2 waltz16



¹³C-NMR of *N*-(4-(4-chlorophenyl)-8-oxo-7,8-dihydropyrazolo[4,3-*e*]thiazolo[3,2-*a*]pyrimidin-3-yl)benzamide (3).



IR of *(E,Z)*-*N*-(4-(4-chlorophenyl)-7-(furan-2-ylmethylene)-8-oxo-7,8-dihydropyrazolo[4,3-*e*]thiazolo[3,2-*a*]pyrimidin-3-yl)benzamide (4).

Paula Soliman_H_M31A

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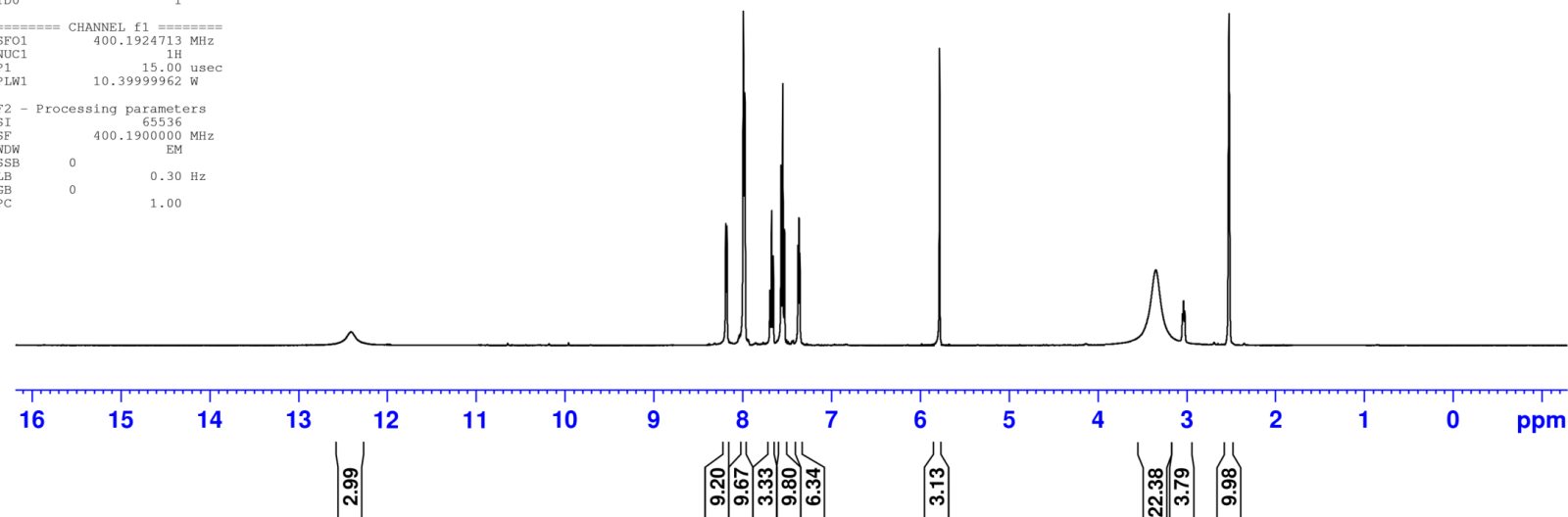
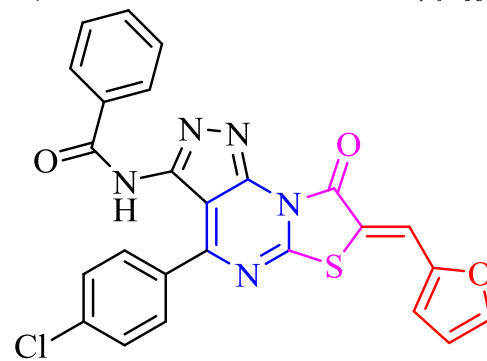
Current Data Parameters
NAME Paula Soliman_H_M31A
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220130
Time_ 0.16
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.46
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

12.4130
8.1902
8.1778
7.9932
7.9756
7.6930
7.6745
7.6559
7.5678
7.5482
7.5293
7.3777
7.3661
7.3558
5.8634
3.3455
3.0417
3.0284
3.0140
2.5103



¹H-NMR of (E,Z)-N-(4-(4-chlorophenyl)-7-(furan-2-ylmethylene)-8-oxo-7,8-dihydropyrazolo[4,3-e]thiazolo[3,2-a]pyrimidin-3-yl)benzamide (4).

Paula Soliman_H_M31A_D2O

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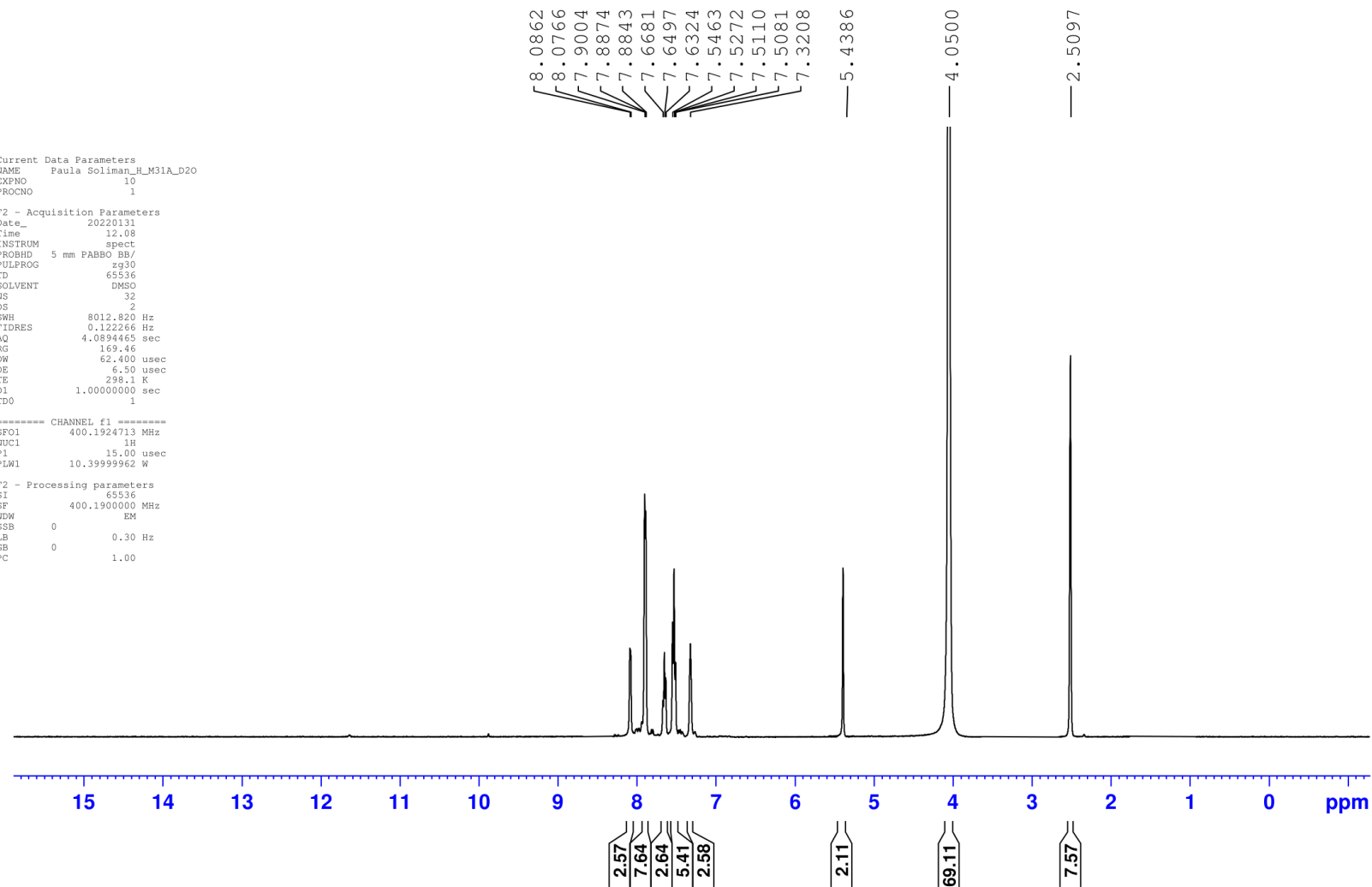


Current Data Parameters
NAME Paula Soliman_H_M31A_D2O
EXPNO 10
PROCNO 1

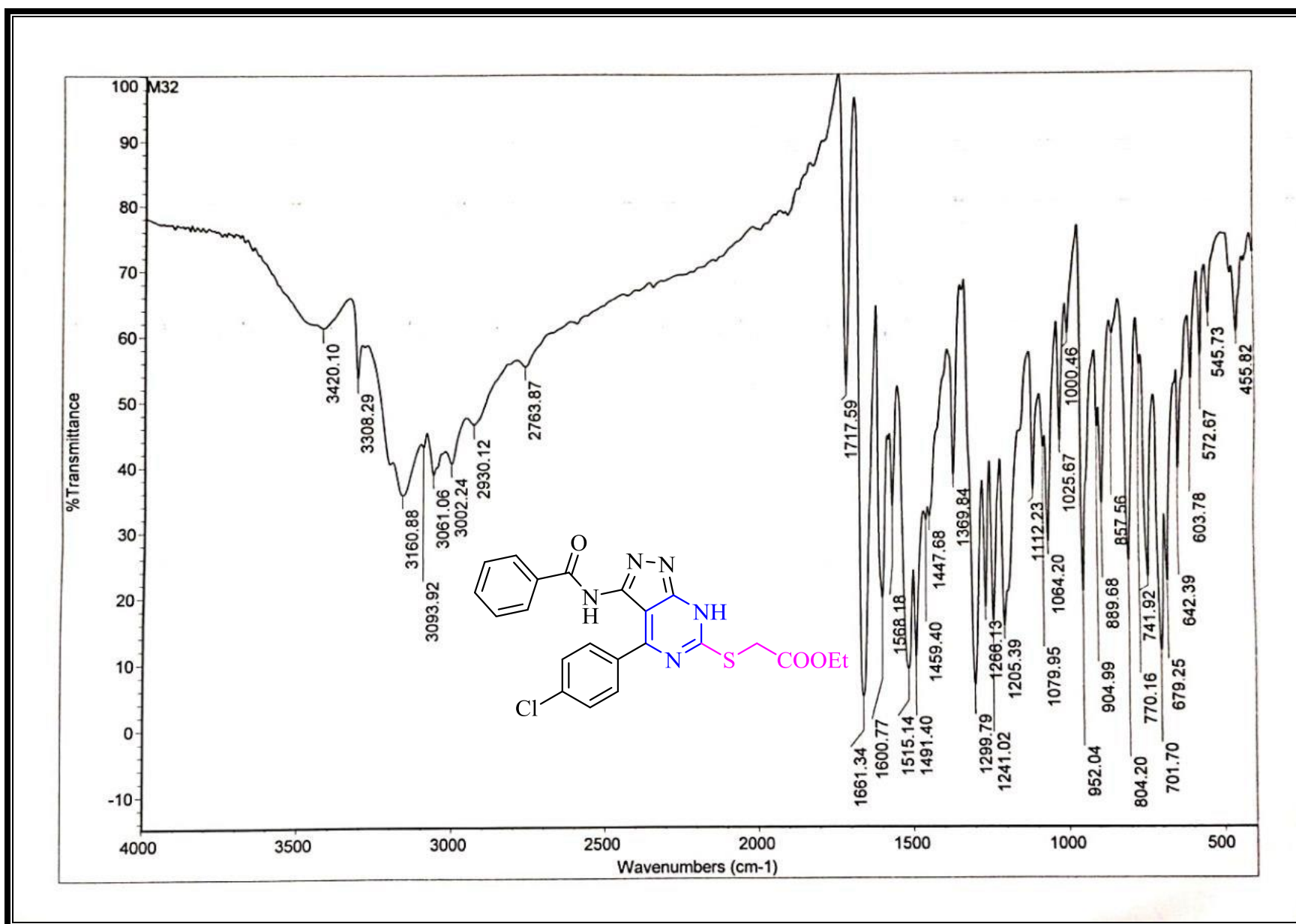
F2 - Acquisition Parameters
Date_ 20220131
Time 12.08
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.46
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SF01 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



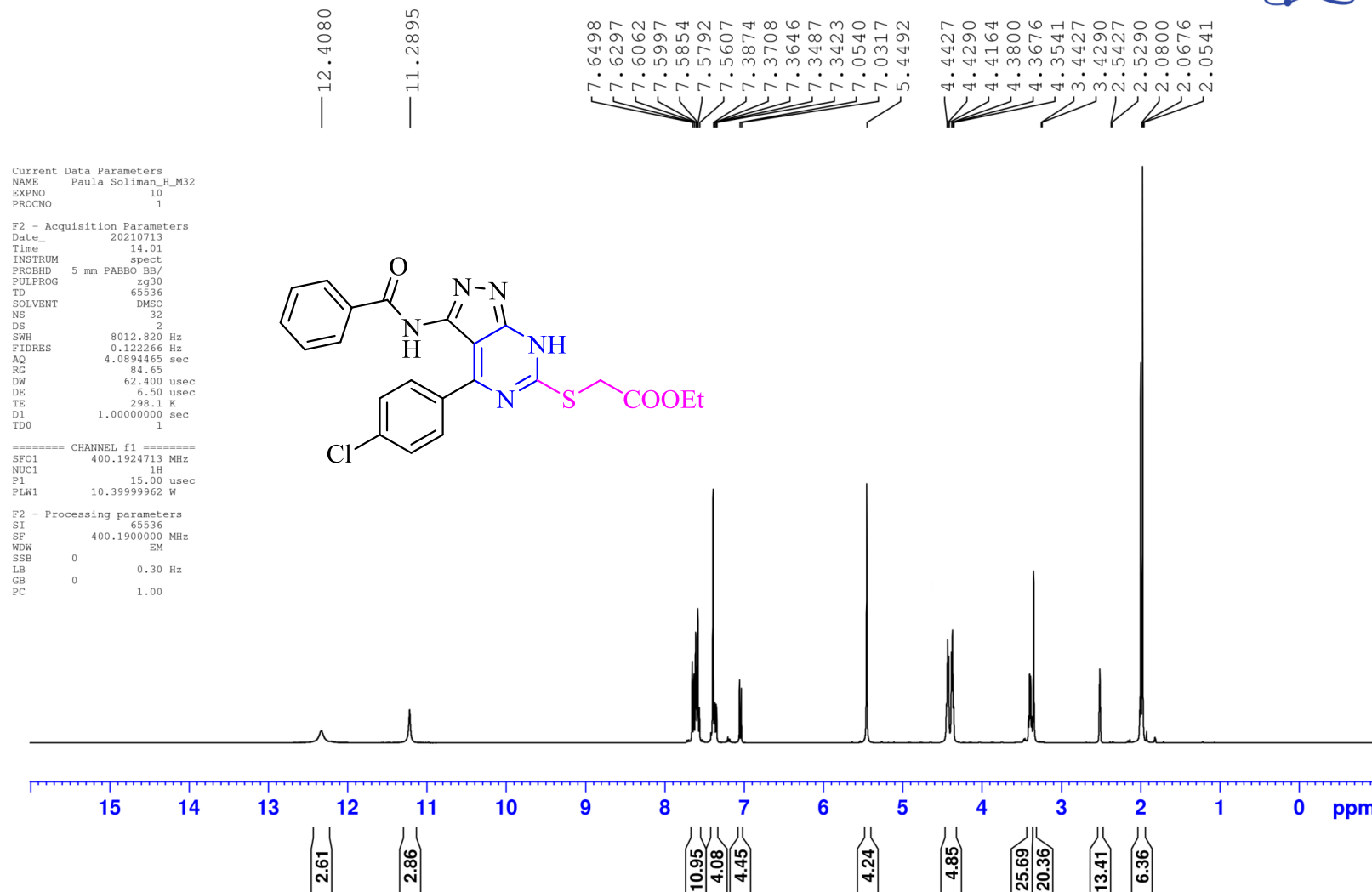
D₂O of (*E,Z*)-*N*-(4-(4-chlorophenyl)-7-(furan-2-ylmethylene)-8-oxo-7,8-dihydropyrazolo[4,3-*e*]thiazolo[3,2-*a*]pyrimidin-3-yl)benzamide (4).



IR of Ethyl 2-((3-benzamido-4-(4-chlorophenyl)-7H-pyrazolo[3,4-d]pyrimidin-6-yl)thio)acetate (5).

Paula Soliman_H_M32

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¹H-NMR of Ethyl 2-((3-benzamido-4-(4-chlorophenyl)-7H-pyrazolo[3,4-d]pyrimidin-6-yl)thio)acetate (5).

Paula Soliman_H_M32_D2O

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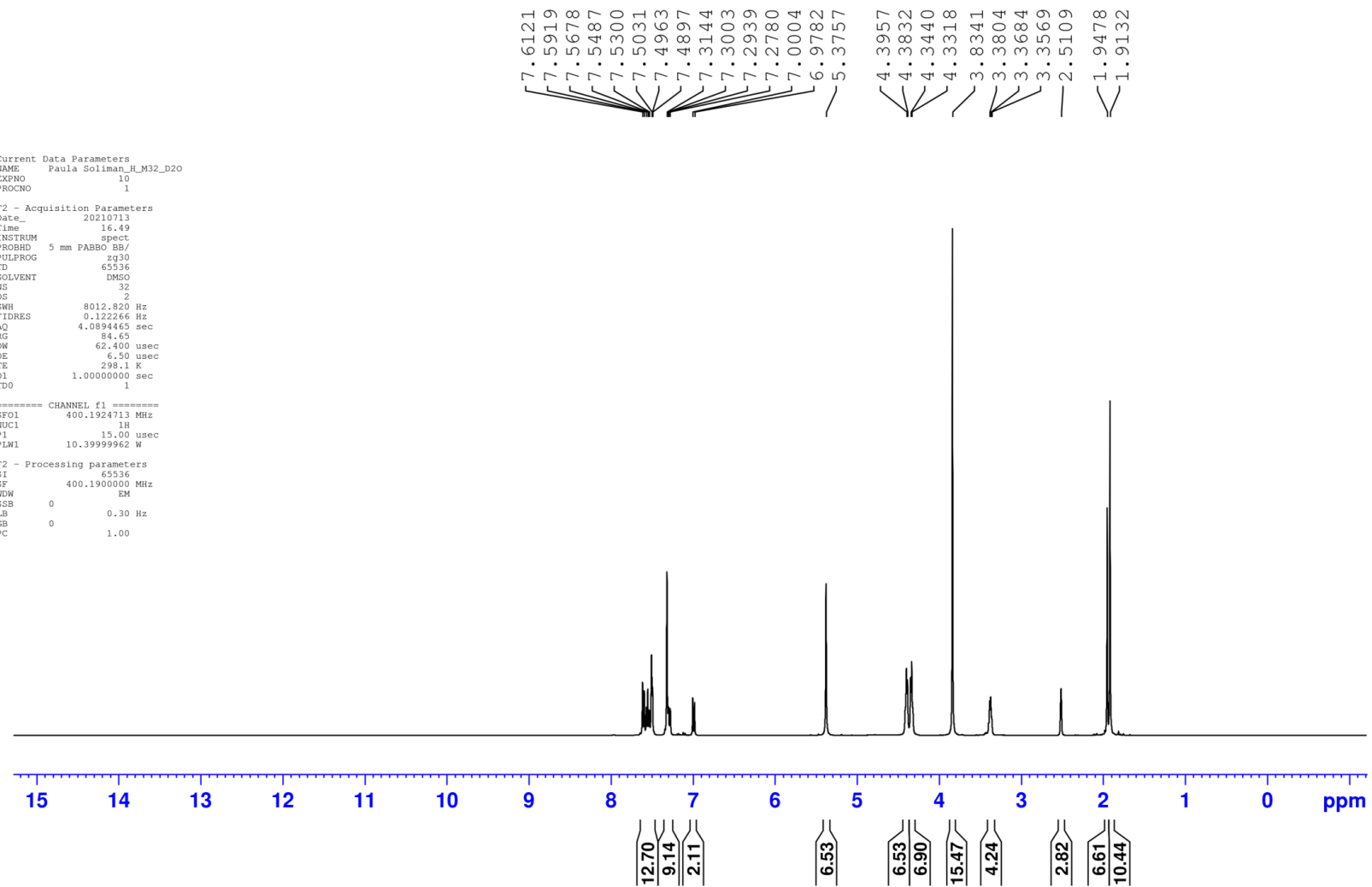


Current Data Parameters
NAME Paula Soliman_H_M32_D2O
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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Time 16.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 84.65
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0 0.30 Hz
GB 0
PC 1.00



D₂O of Ethyl 2-((3-benzamido-4-(4-chlorophenyl)-7H-pyrazolo[3,4-d]pyrimidin-6-yl)thio)acetate (5).

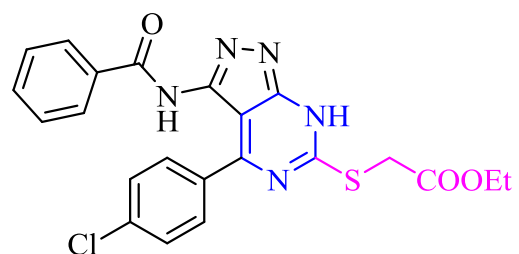
Paula Soliman_C_M32

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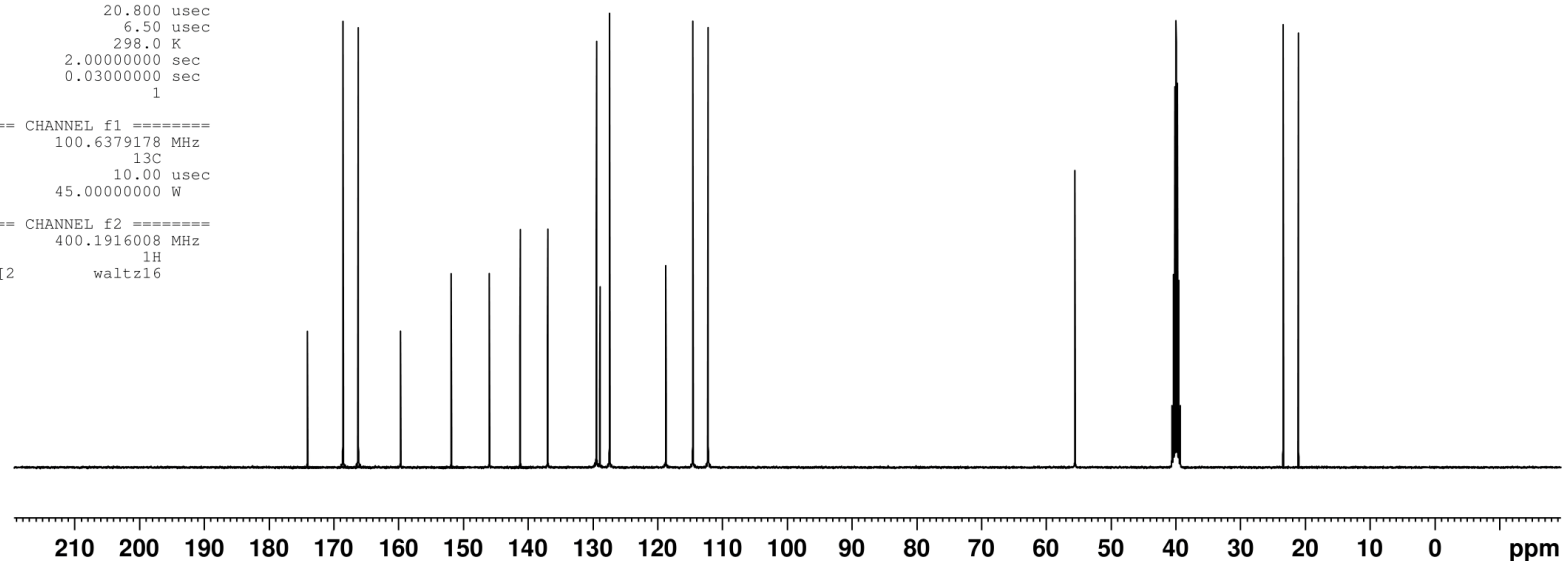


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NAME Paula Soliman_C_M32
EXPNO 10
PROCNO 1

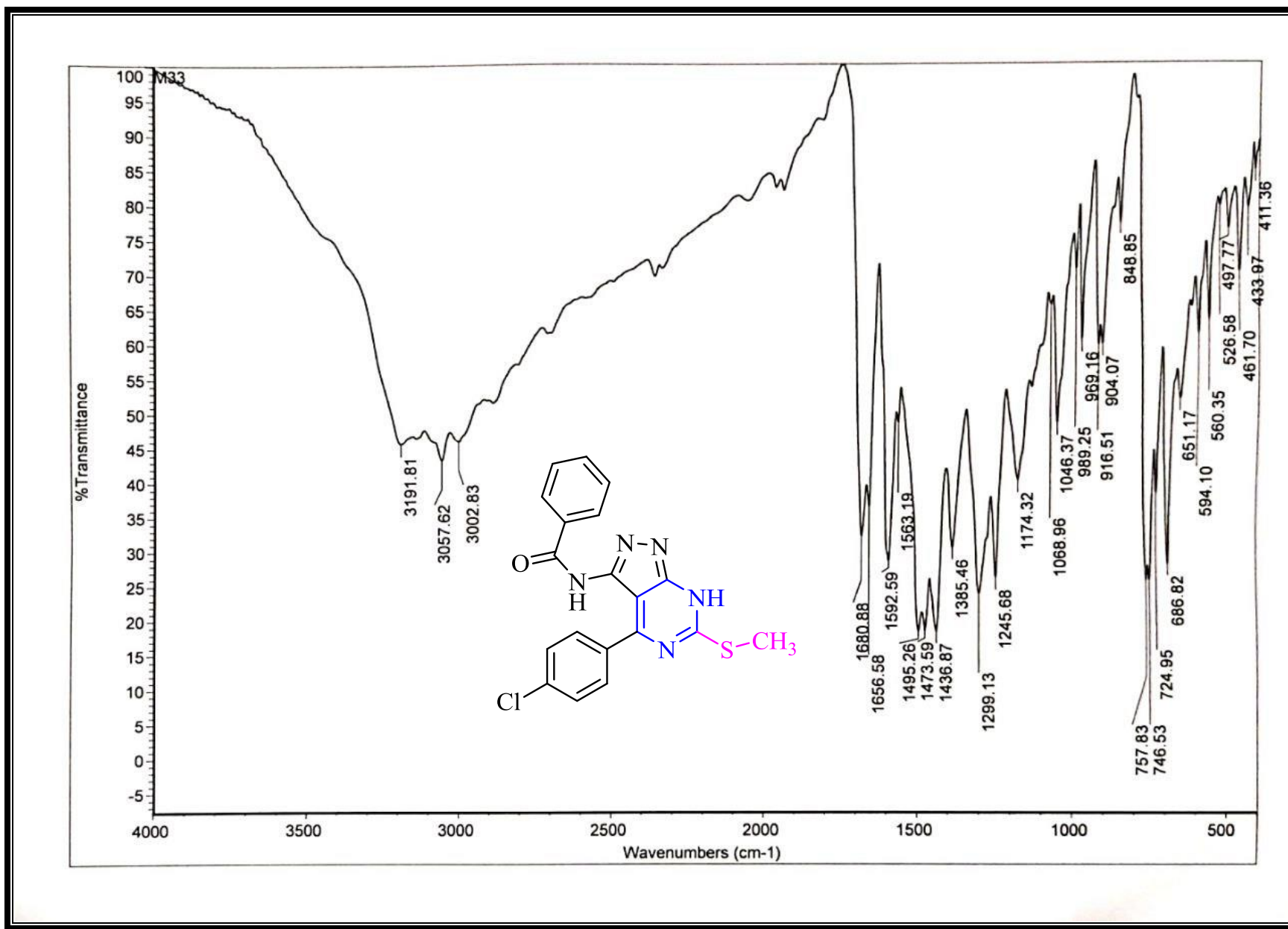
F2 - Acquisition Parameters
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Time 15.00
INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1



==== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W
==== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2] waltz16



¹³C-NMR of Ethyl 2-((3-benzamido-4-(4-chlorophenyl)-7H-pyrazolo[3,4-d]pyrimidin-6-yl)thio)acetate (5).



IR of *N*-(4-(4-chlorophenyl)-6-(methylthio)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (6).

Paula Soliman_H_M33

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—13.6373

—11.7813

8.0511
8.0487
7.8008
7.7923
6.7867
6.7825
6.7778
6.7736

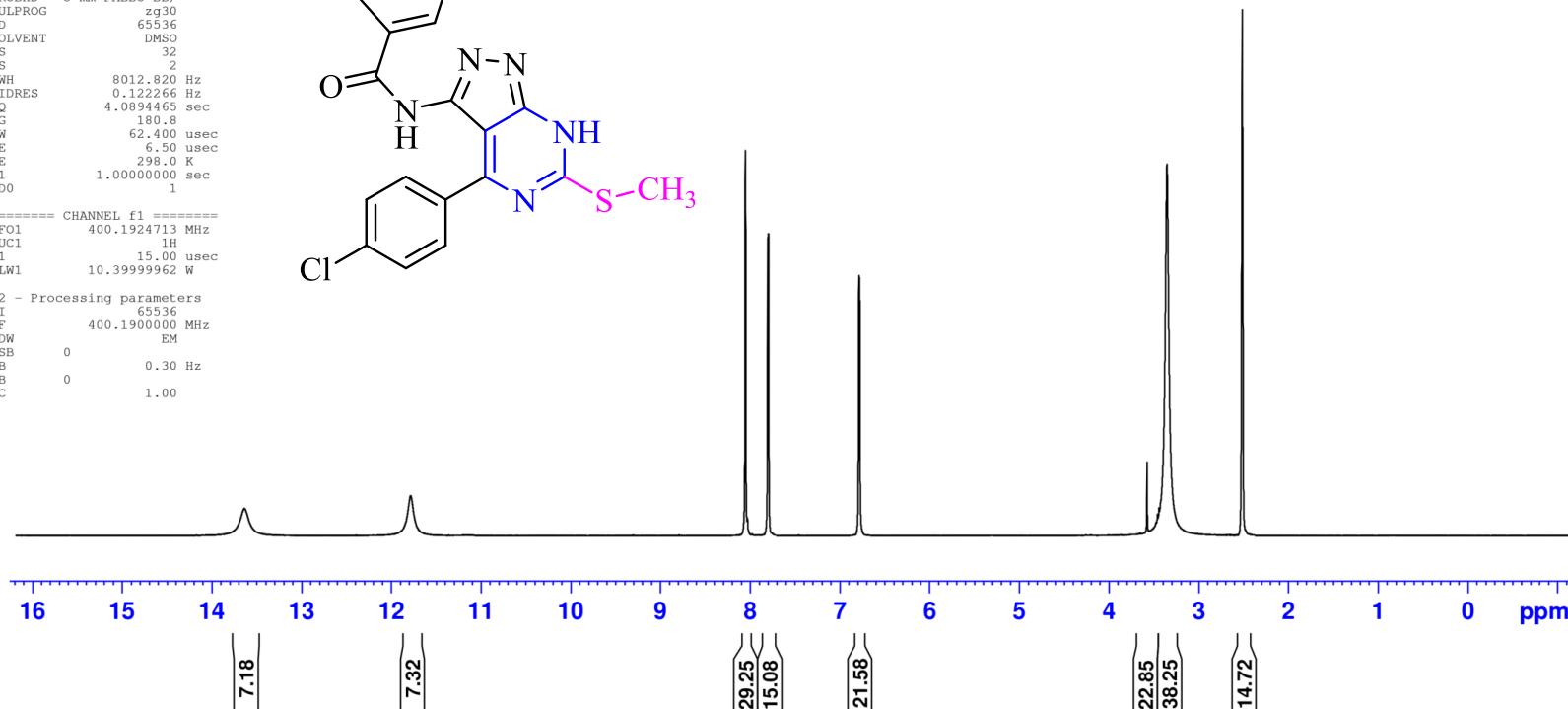
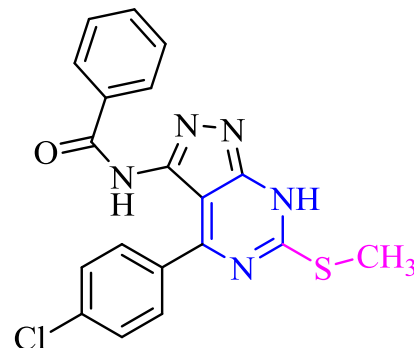
3.5716
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Current Data Parameters
NAME Paula Soliman_H_M33
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210712
Time 2.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 180.8
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H-NMR of *N*-(4-(4-chlorophenyl)-6-(methylthio)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (6).

Paula Soliman_H_M33_D2O

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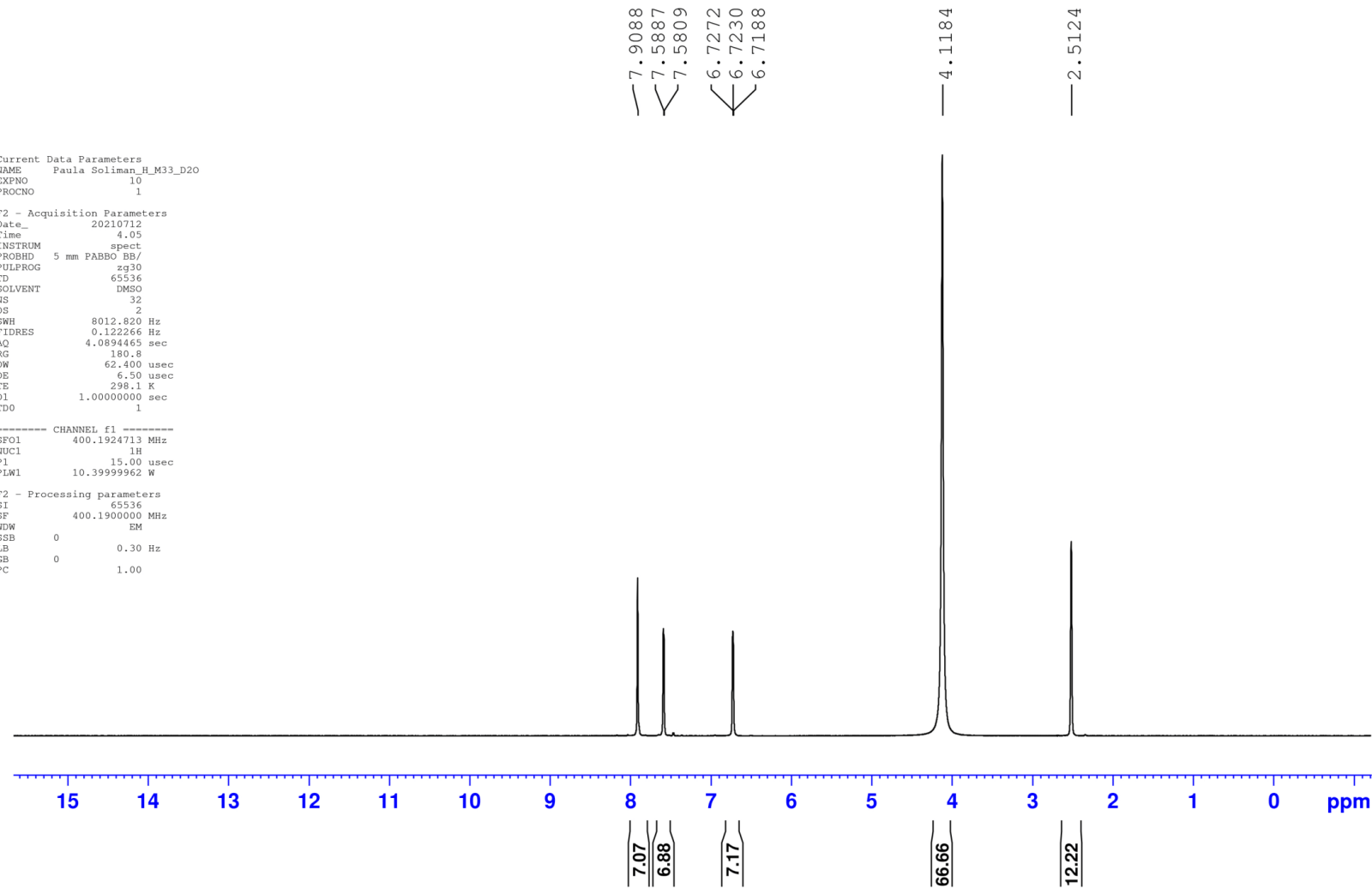


Current Data Parameters
NAME Paula Soliman_H_M33_D2O
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210712
Time 4.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 180.8
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.0000000 sec
TDO 1

----- CHANNEL f1 -----
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



D₂O of *N*-(4-(4-chlorophenyl)-6-(methylthio)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (6).

Paula Soliman_C_M33

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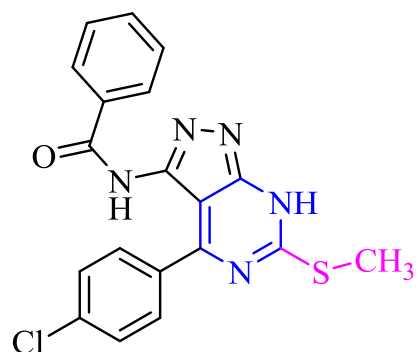
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145.40
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141.45
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121.58
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40.61
40.40
40.20
39.99
39.78
39.57
39.36

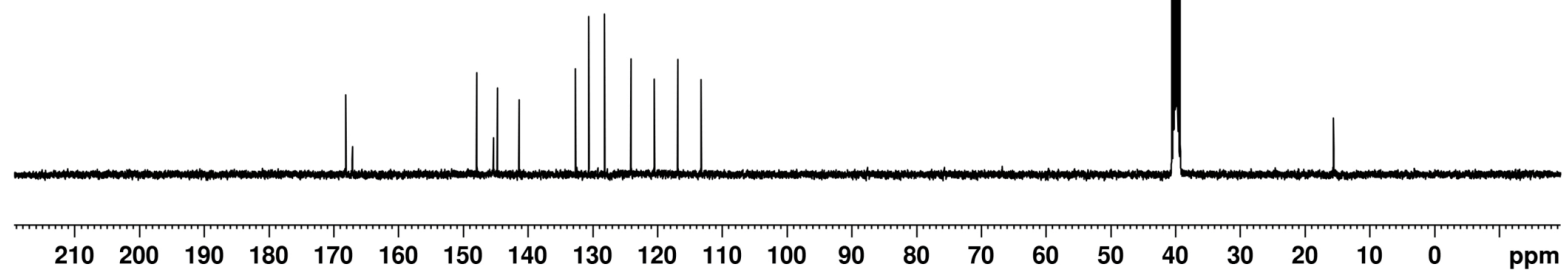
15.65

Current Data Parameters
NAME Paula Soliman_C_M33
EXPNO 10
PROCNO 1

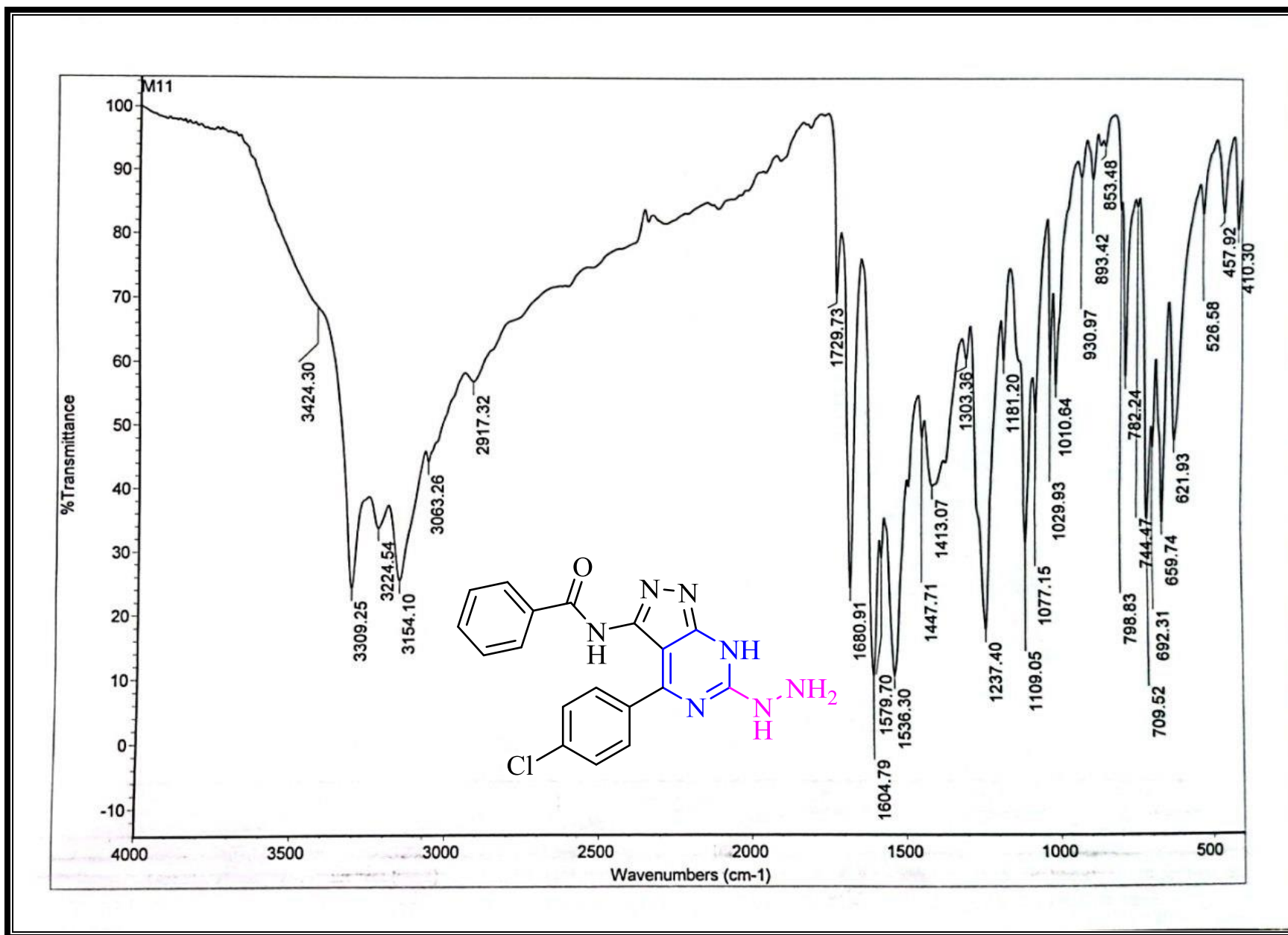
F2 - Acquisition Parameters
Date_ 20210712
Time 3.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1



==== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W
==== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2] waltz16



¹³C-NMR of *N*-(4-(4-chlorophenyl)-6-(methylthio)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (6).



IR of *N*-(4-(4-chlorophenyl)-6-hydrazineyl-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (7).

Paula Soliman_H_M11

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— 13.6932
< 12.8543
12.8481

8.0382
7.7815
7.7075
7.6991
7.2727
6.7639
6.7603
6.7557
6.7519

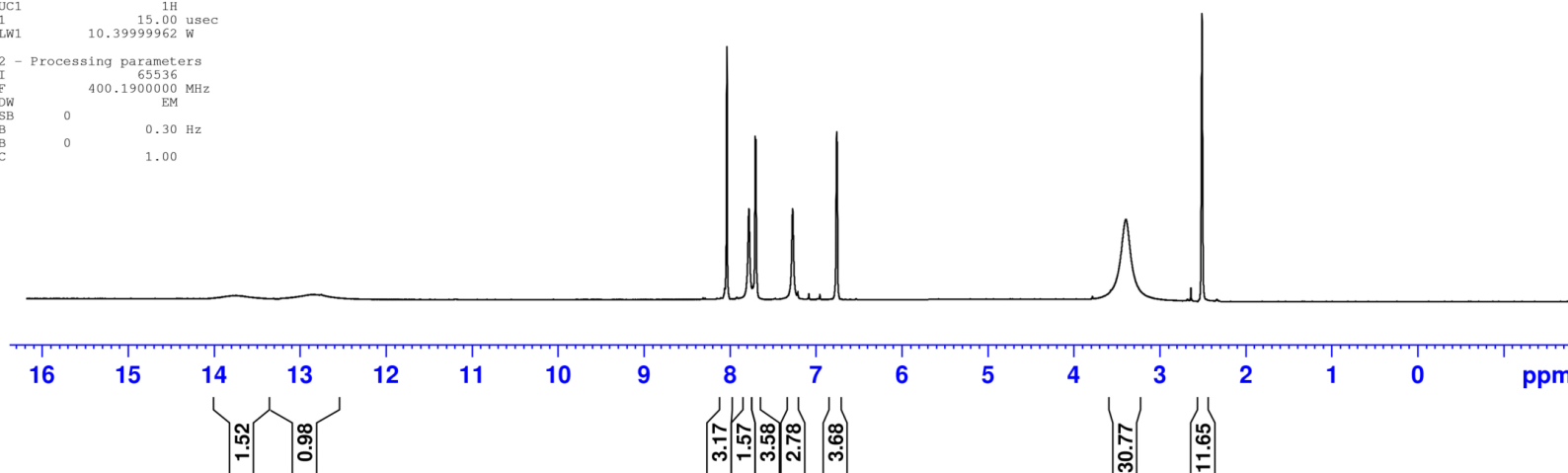
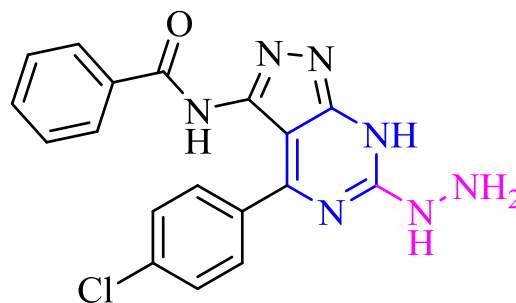
— 3.3959
— 2.5102

Current Data Parameters
NAME Paula Soliman_H_M11
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210712
Time 1.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.46
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H-NMR of N-(4-(4-chlorophenyl)-6-hydrazineyl-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (7).

Paula Soliman_H_M11_D2O

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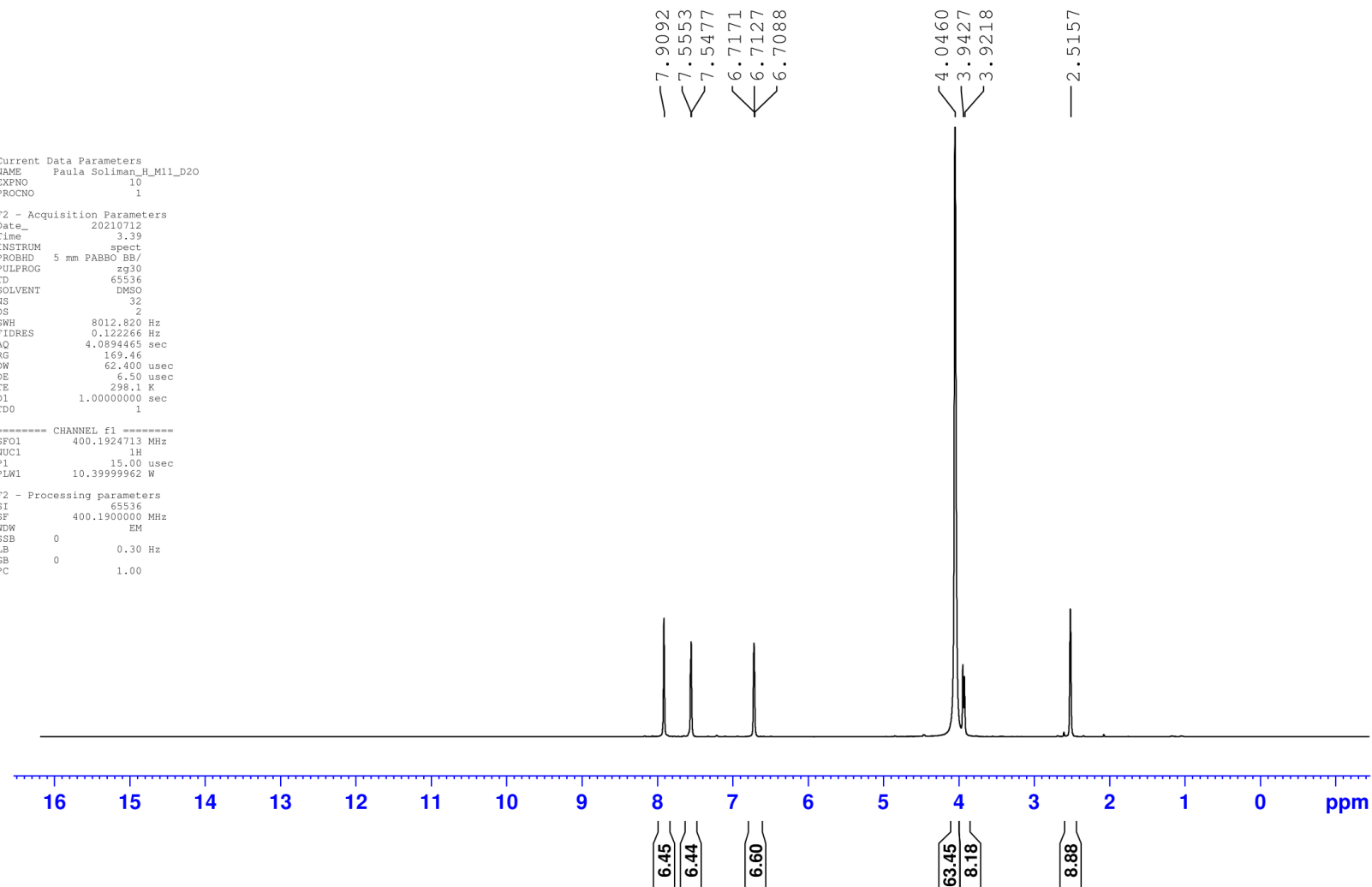


Current Data Parameters
NAME Paula Soliman_H_M11_D2O
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.46
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.0000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



D₂O of N-(4-(4-chlorophenyl)-6-hydrazineyl-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (7).

Paula Soliman_C_M11

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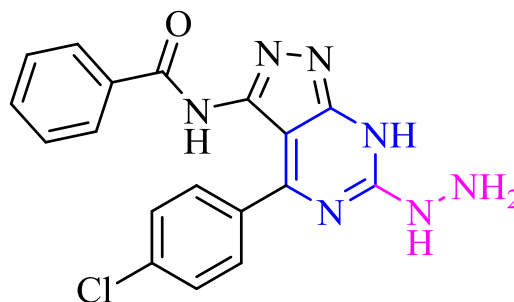


169.81
160.28
159.08
156.27
148.04
140.38
134.43
131.66
129.98
128.56
126.08
123.69
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40.61
40.40
40.19
39.98
39.78
39.57
39.36

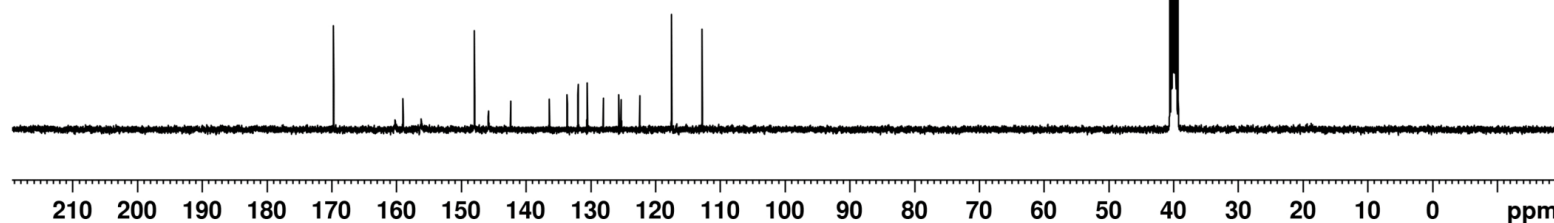
Current Data Parameters
NAME Paula Soliman_C_M11
EXPNO 10
PROCNO 1

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INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
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DW 20.800 usec
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TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

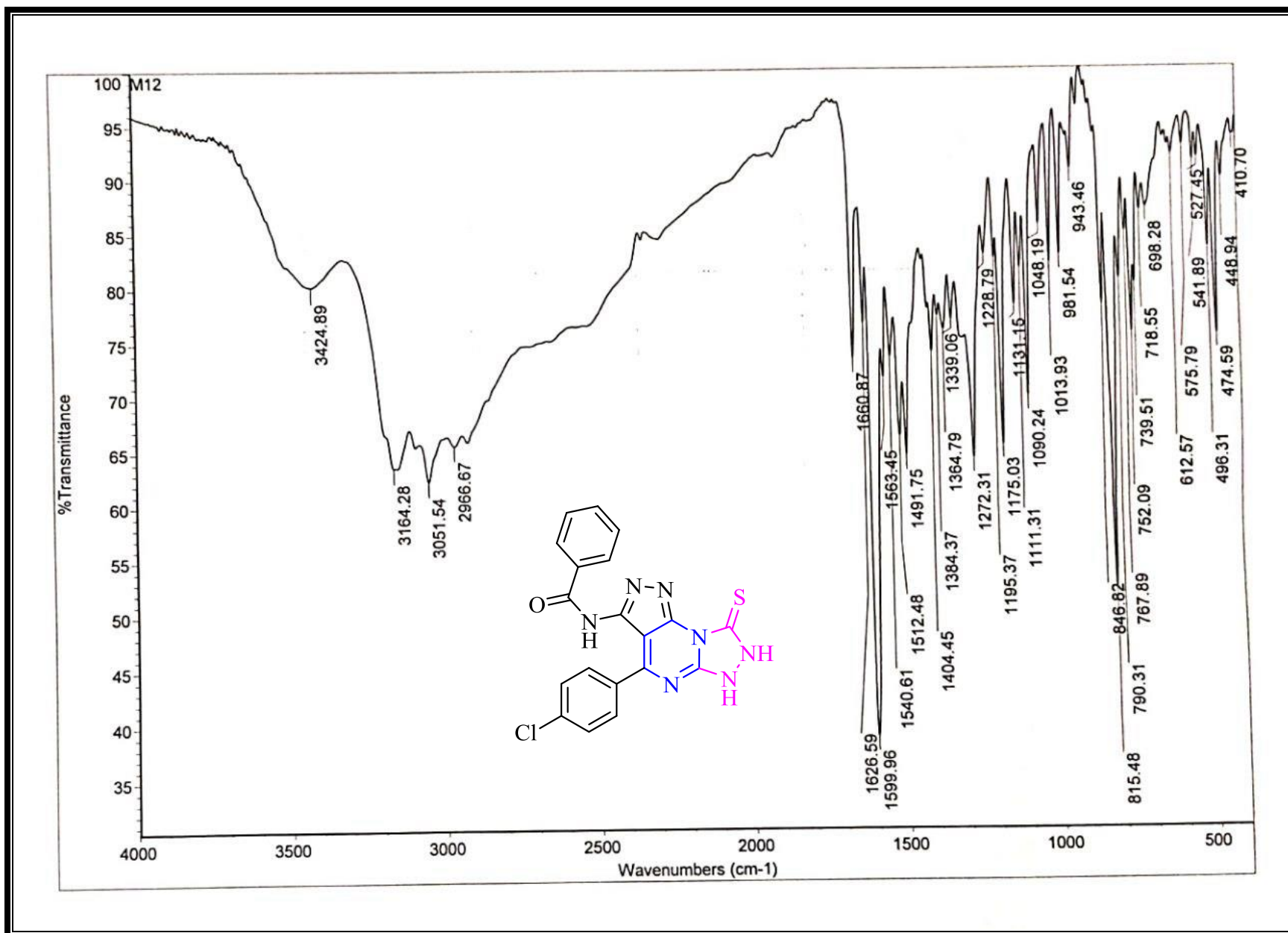


==== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W

==== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2] waltz16



¹³C-NMR of N-(4-(4-chlorophenyl)-6-hydrazineyl-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (7).



IR of *N*-(4-(4-chlorophenyl)-8-thioxo-7,8-dihydro-6H-pyrazolo[4,3-*e*][1,2,4]triazolo[4,3-*a*]pyrimidin-3-yl)benzamide (8).

Paula Soliman_H_M12

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13.3986
13.3549

11.4474

8.2514
8.0630
8.0479
8.0417
7.7193
7.7107
7.6686
7.6472
6.7718
6.7677
6.7631
6.7591

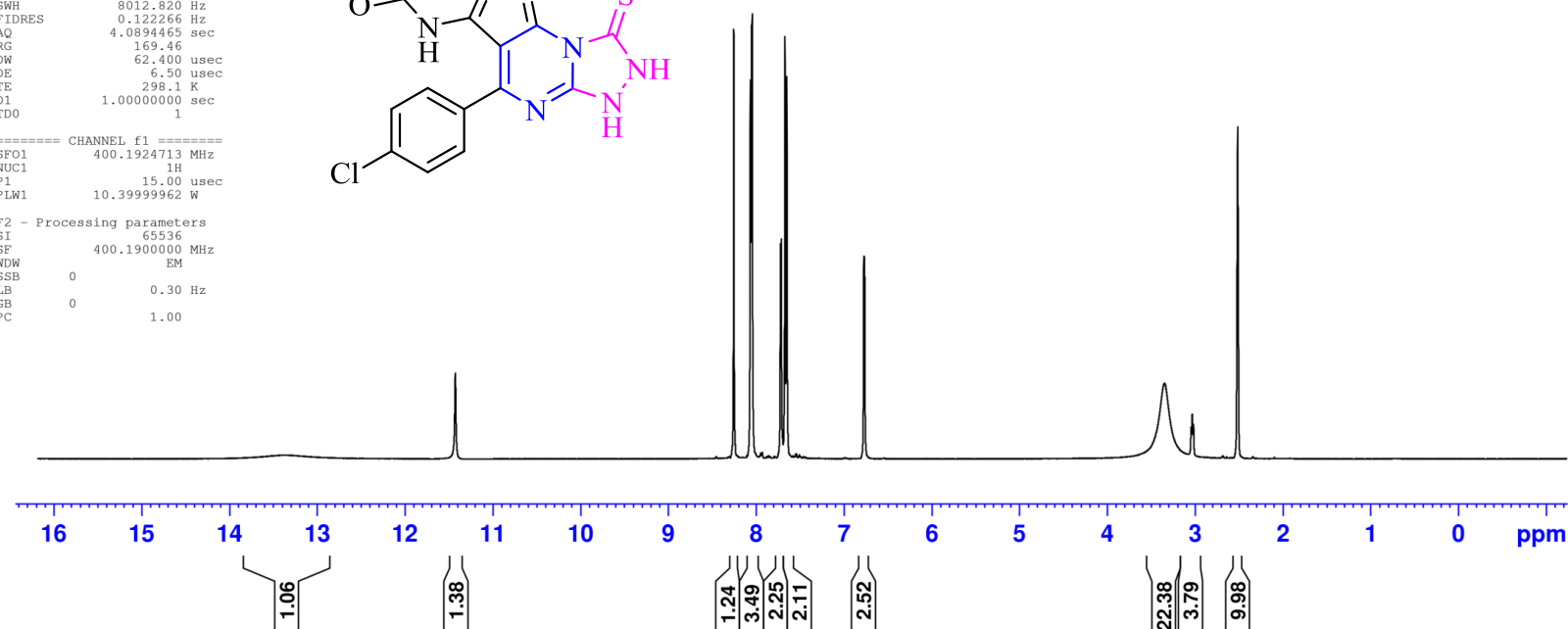
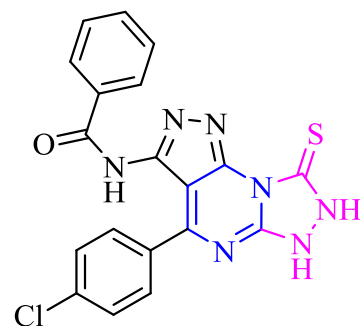
3.3455
3.0417
3.0284
3.0140
2.5103

Current Data Parameters
NAME Paula Soliman_H_M12
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210711
Time 13.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.46
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H-NMR of *N*-(4-(4-chlorophenyl)-8-thioxo-7,8-dihydro-6H-pyrazolo[4,3-e][1,2,4]triazolo[4,3-a]pyrimidin-3-yl)benzamide (8).

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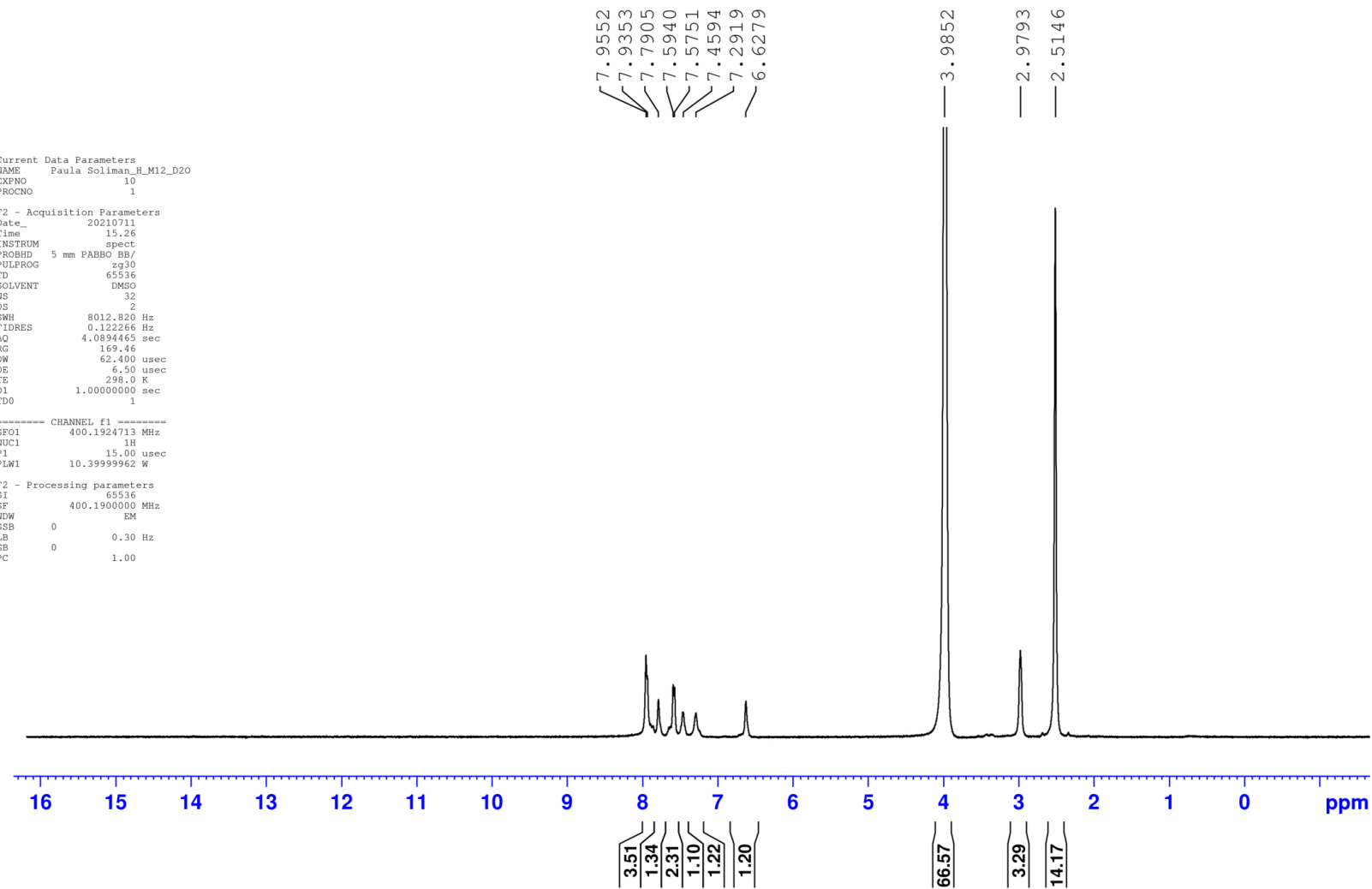


Current Data Parameters
NAME Paula Soliman_H_M12_D2O
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210711
Time 15.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.46
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SF01 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



D₂O of *N*-(4-(4-chlorophenyl)-8-thioxo-7,8-dihydro-6H-pyrazolo[4,3-*e*][1,2,4]triazolo[4,3-*a*]pyrimidin-3-yl)benzamide (8).

Paula Soliman_C_M12

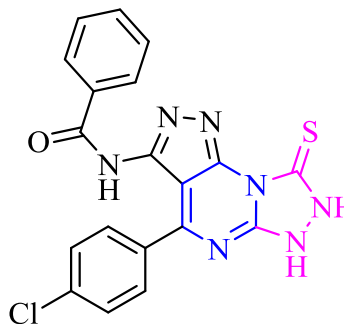
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171.52
160.49
159.10
156.91
148.22
146.39
146.12
136.85
132.04
131.93
129.74
117.93
115.85
112.94
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40.41
40.20
39.99
39.78
39.58
39.37

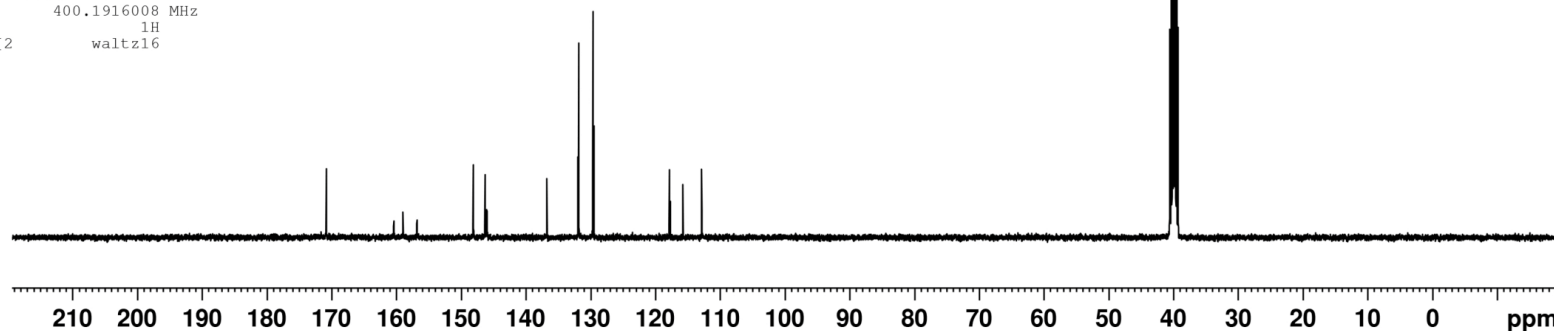
Current Data Parameters
NAME Paula Soliman_C_M12
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210711
Time 2.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

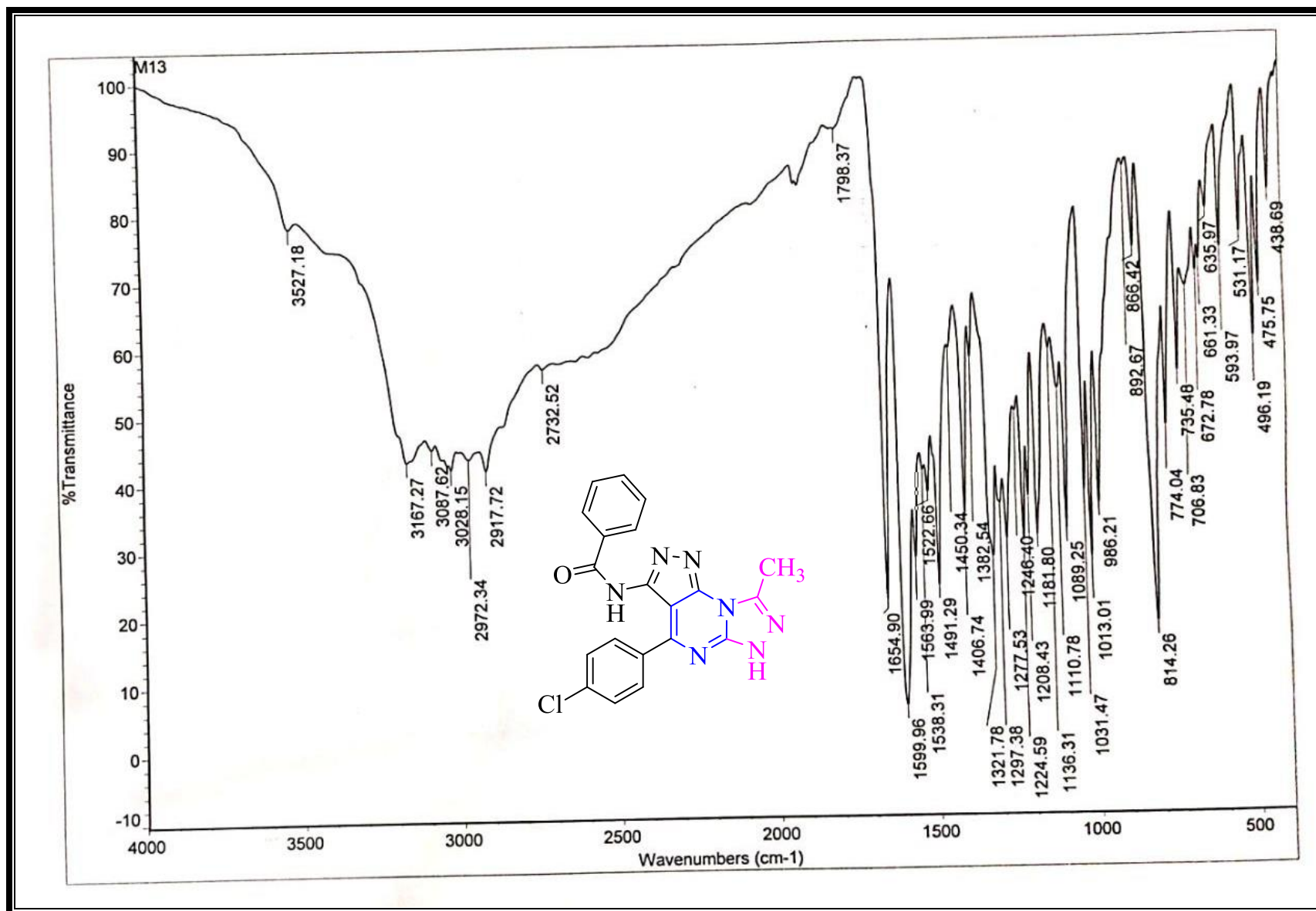


==== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W

==== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2] waltz16



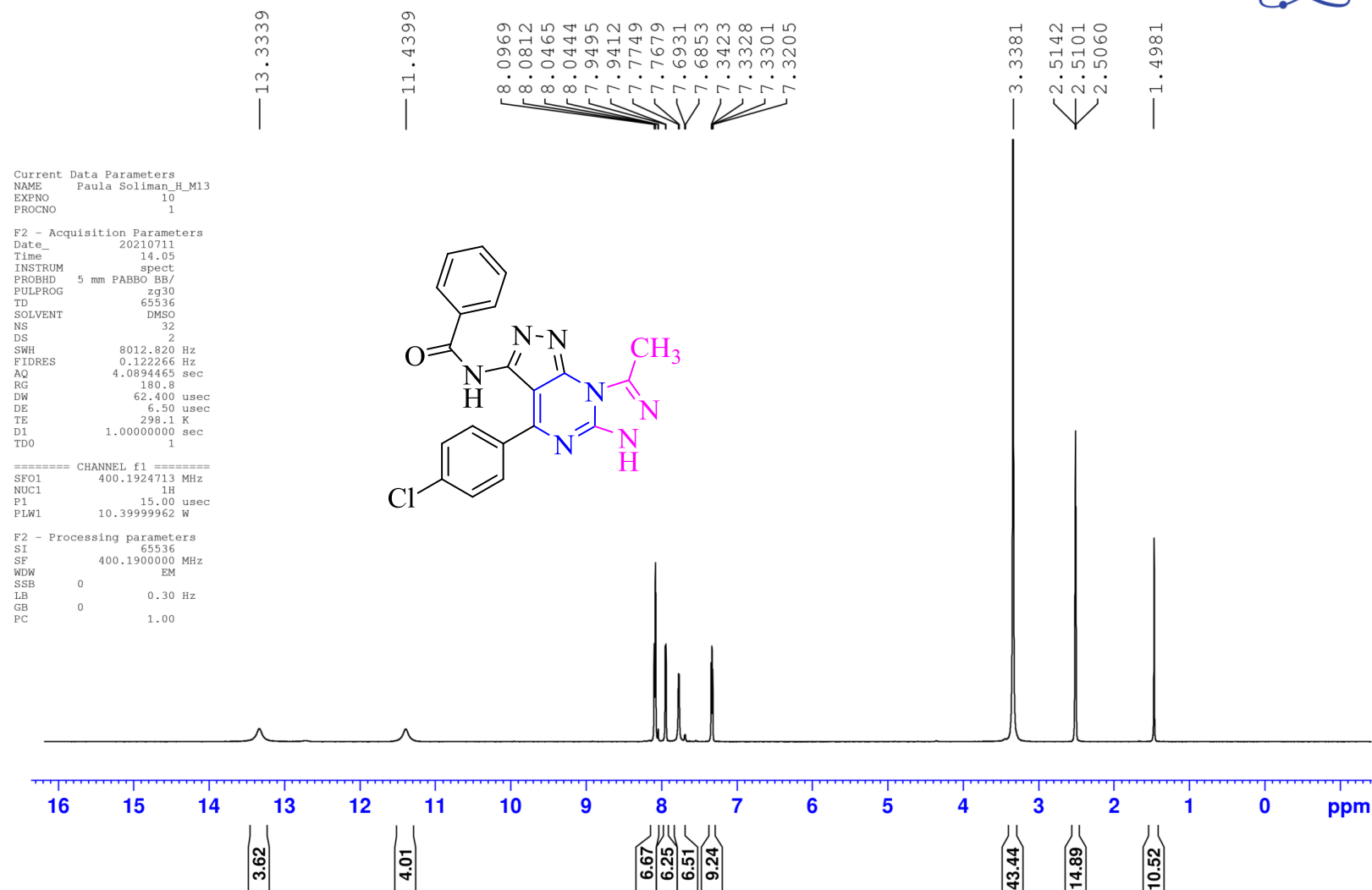
¹³C-NMR of *N*-(4-(4-chlorophenyl)-8-thioxo-7,8-dihydro-6H-pyrazolo[4,3-e][1,2,4]triazolo[4,3-a]pyrimidin-3-yl)benzamide (8).



IR of *N*-(4-(4-chlorophenyl)-8-methyl-6H-pyrazolo[4,3-*e*][1,2,4]triazolo[4,3-*a*]pyrimidin-3-yl)benzamide (9).

Paula Soliman_H_M13

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¹H-NMR of N-(4-(4-chlorophenyl)-8-methyl-6H-pyrazolo[4,3-e][1,2,4]triazolo[4,3-a]pyrimidin-3-yl)benzamide (9).

Paula Soliman_H_M13_D2O

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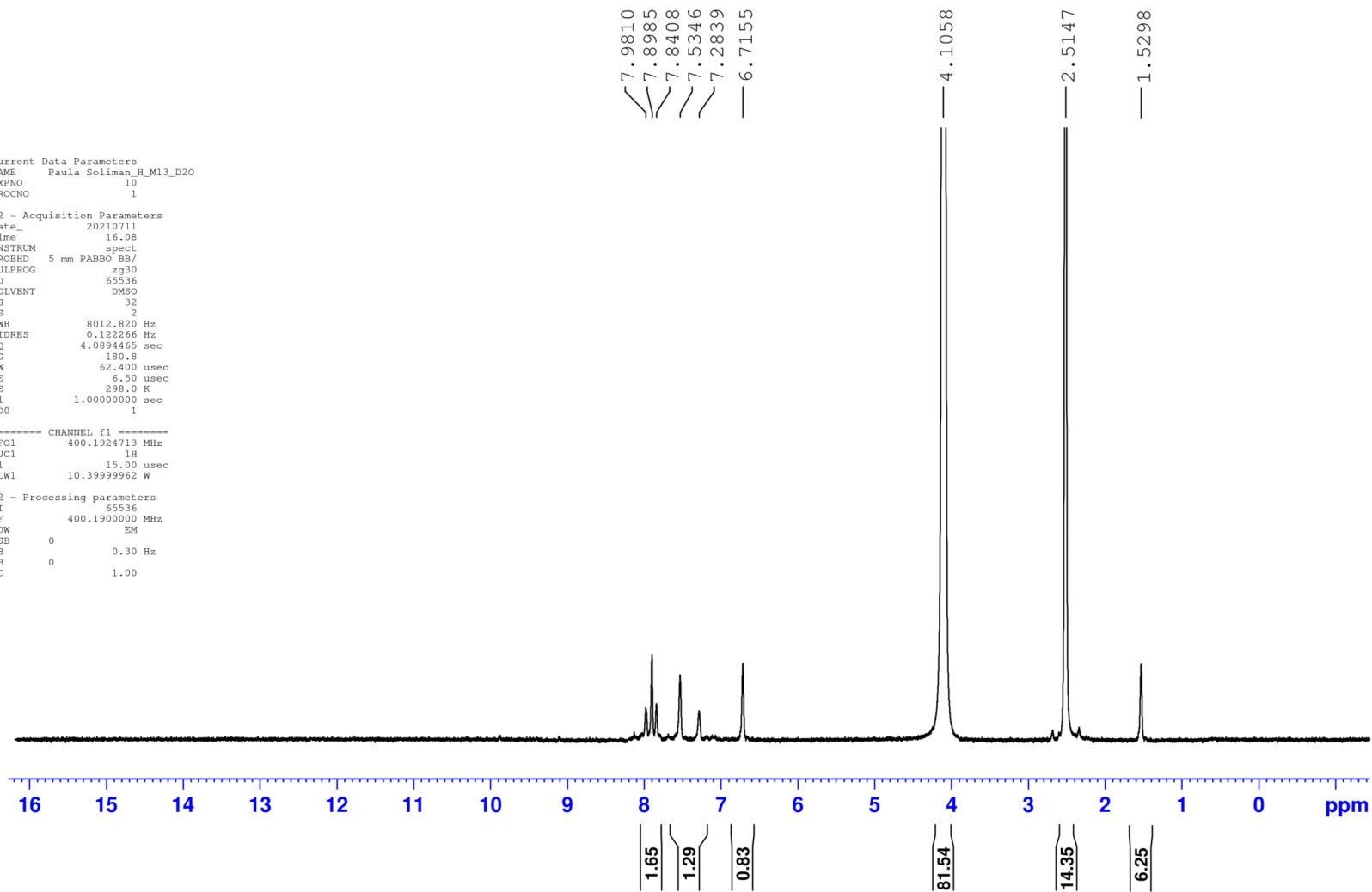


Current Data Parameters
NAME Paula Soliman_H_M13_D2O
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 180.8
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
TDO 1

----- CHANNEL f1 -----
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



D₂O of *N*-(4-(4-chlorophenyl)-8-methyl-6H-pyrazolo[4,3-e][1,2,4]triazolo[4,3-a]pyrimidin-3-yl)benzamide (9).

Paula Soliman_C_M13

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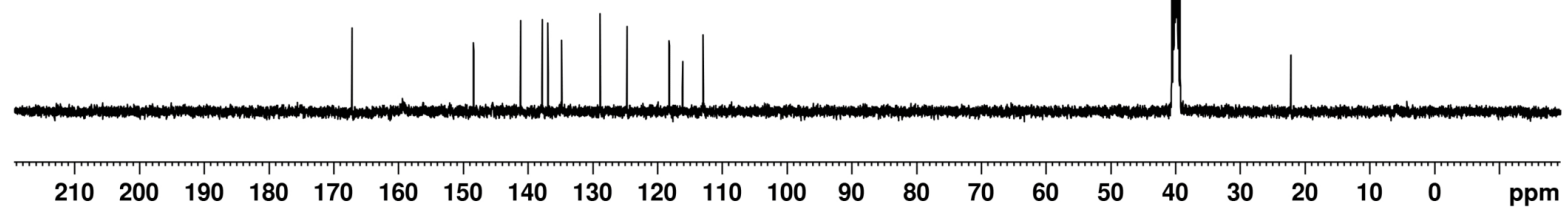
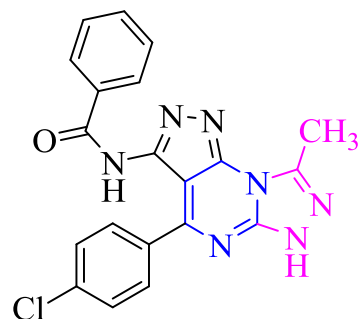
167.95 159.46 148.49 141.22 137.88 136.99 134.88 128.94 125.48 118.26 116.20 113.03 40.62 40.41 40.20 39.99 39.79 39.58 39.37 22.64

Current Data Parameters
NAME Paula Soliman_C_M13
EXPNO 10
PROCNO 1

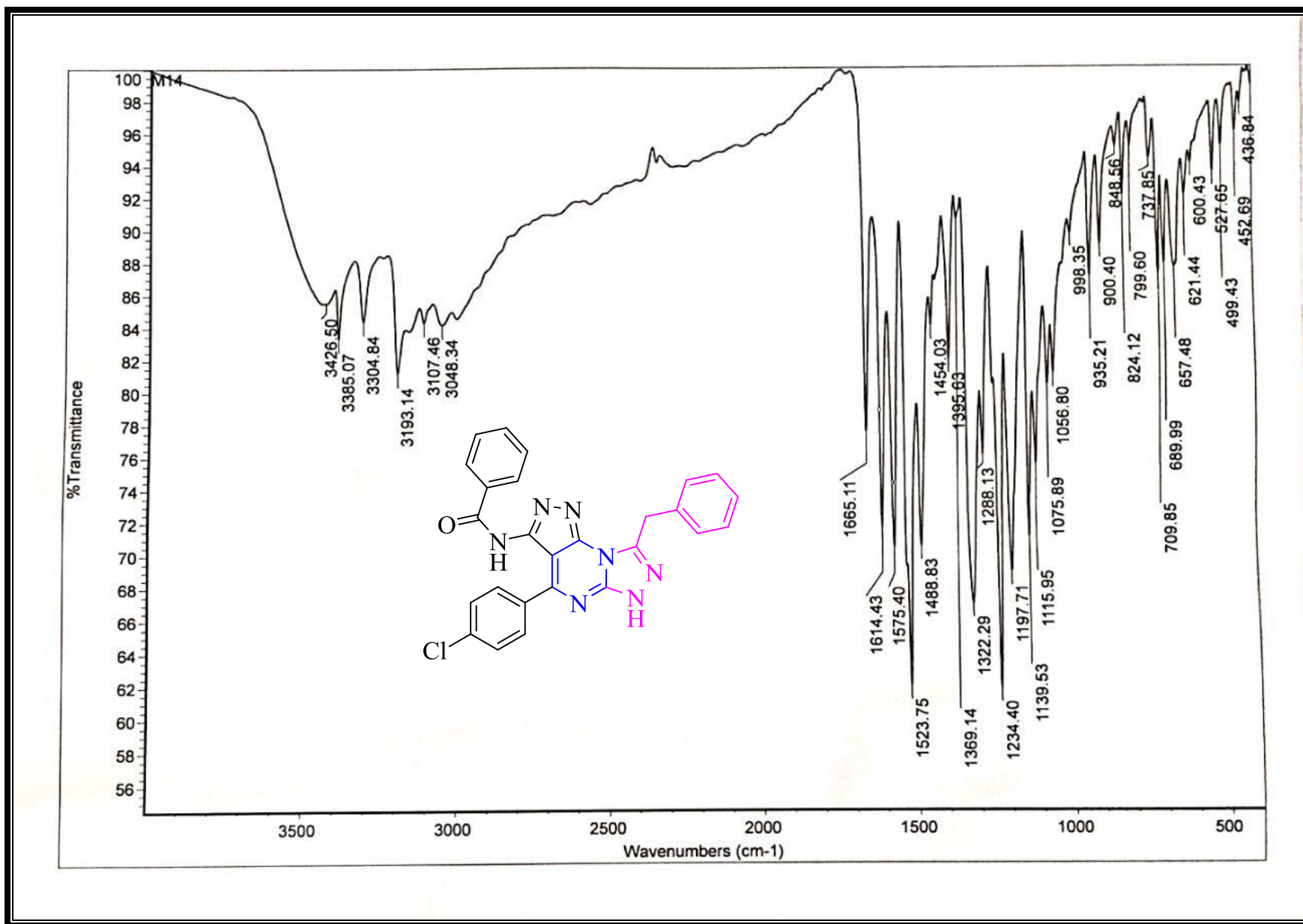
F2 - Acquisition Parameters
Date_ 20210711
Time 15.15
INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W

==== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2] waltz16



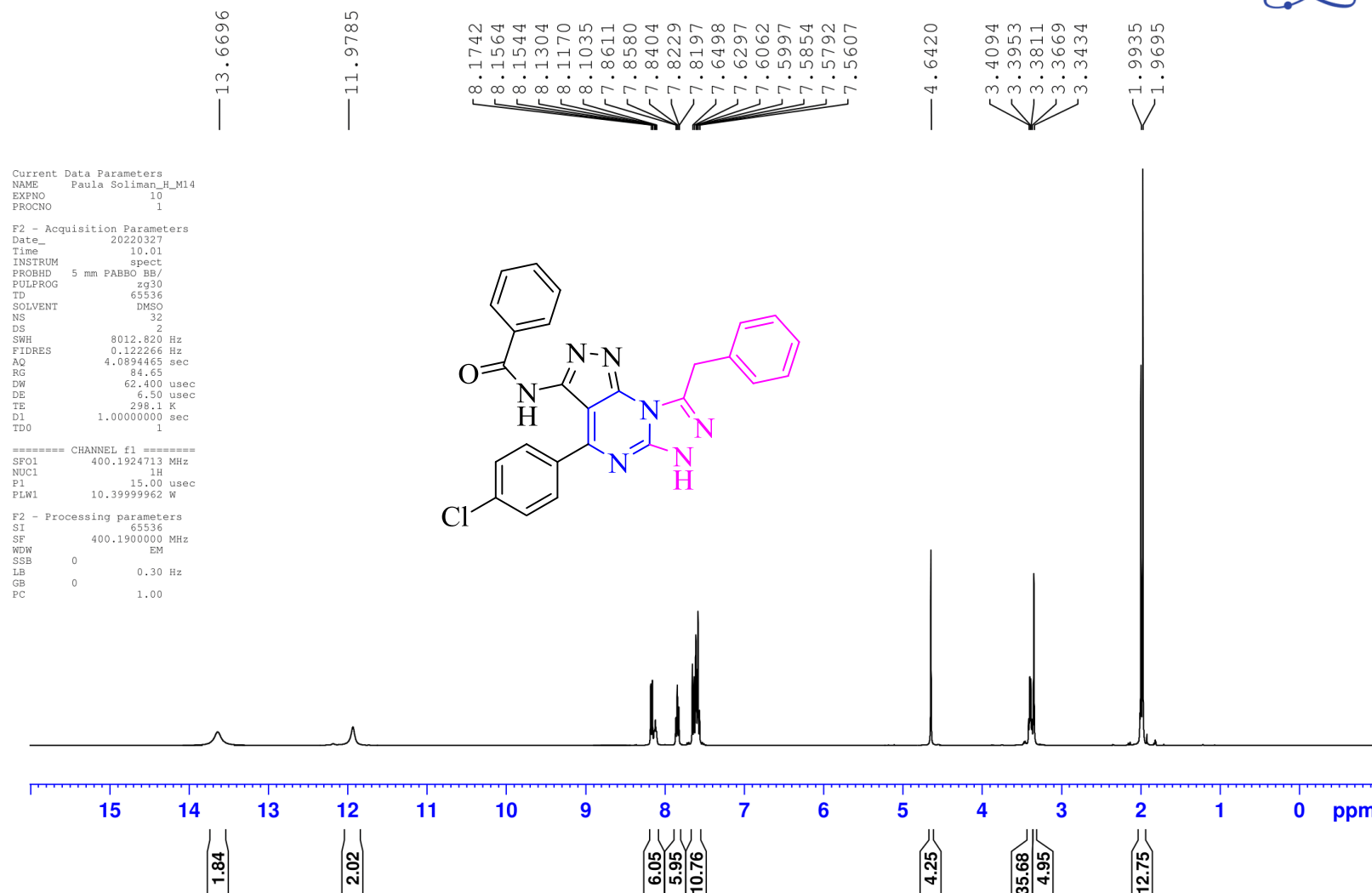
¹³C-NMR of *N*-(4-(4-chlorophenyl)-8-methyl-6H-pyrazolo[4,3-*e*][1,2,4]triazolo[4,3-*a*]pyrimidin-3-yl)benzamide (9).



IR of *N*-(4-(4-chlorophenyl)-8-phenyl-6H-pyrazolo[4,3-*e*][1,2,4]triazolo[4,3-*a*]pyrimidin-3-yl)benzamide (10).

Paula Soliman_H_M14

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¹H-NMR of *N*-(4-(4-chlorophenyl)-8-phenyl-6H-pyrazolo[4,3-*e*][1,2,4]triazolo[4,3-*a*]pyrimidin-3-yl)benzamide (10).

Paula Soliman_H_M14_D2O

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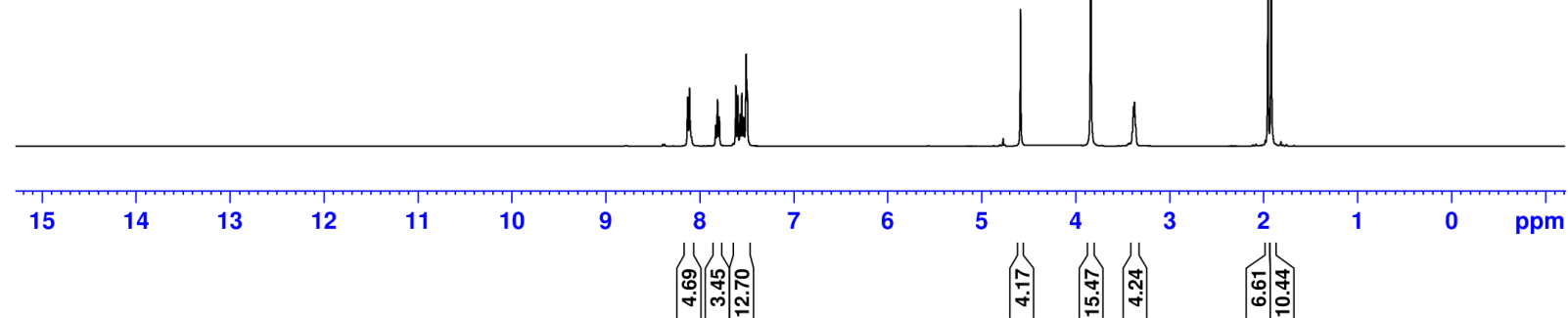
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7.5919
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7.5487
7.5300
7.5031
7.4963
7.4897
4.5821
3.8341
3.3804
3.3684
3.3569
1.9478
1.9132

Current Data Parameters
NAME Paula Soliman_H_M14_D2O
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220327
Time 12.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0884465 sec
RG 84.65
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
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NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

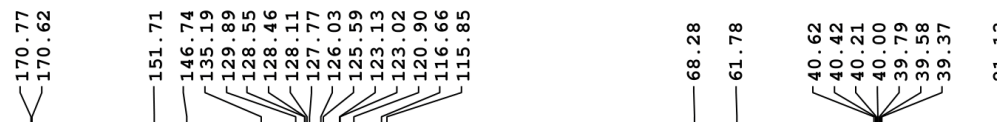
F2 - Processing parameters
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WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



D₂O of *N*-(4-(4-chlorophenyl)-8-phenyl-6H-pyrazolo[4,3-*e*][1,2,4]triazolo[4,3-*a*]pyrimidin-3-yl)benzamide (10).

Paula Soliman_C_M14

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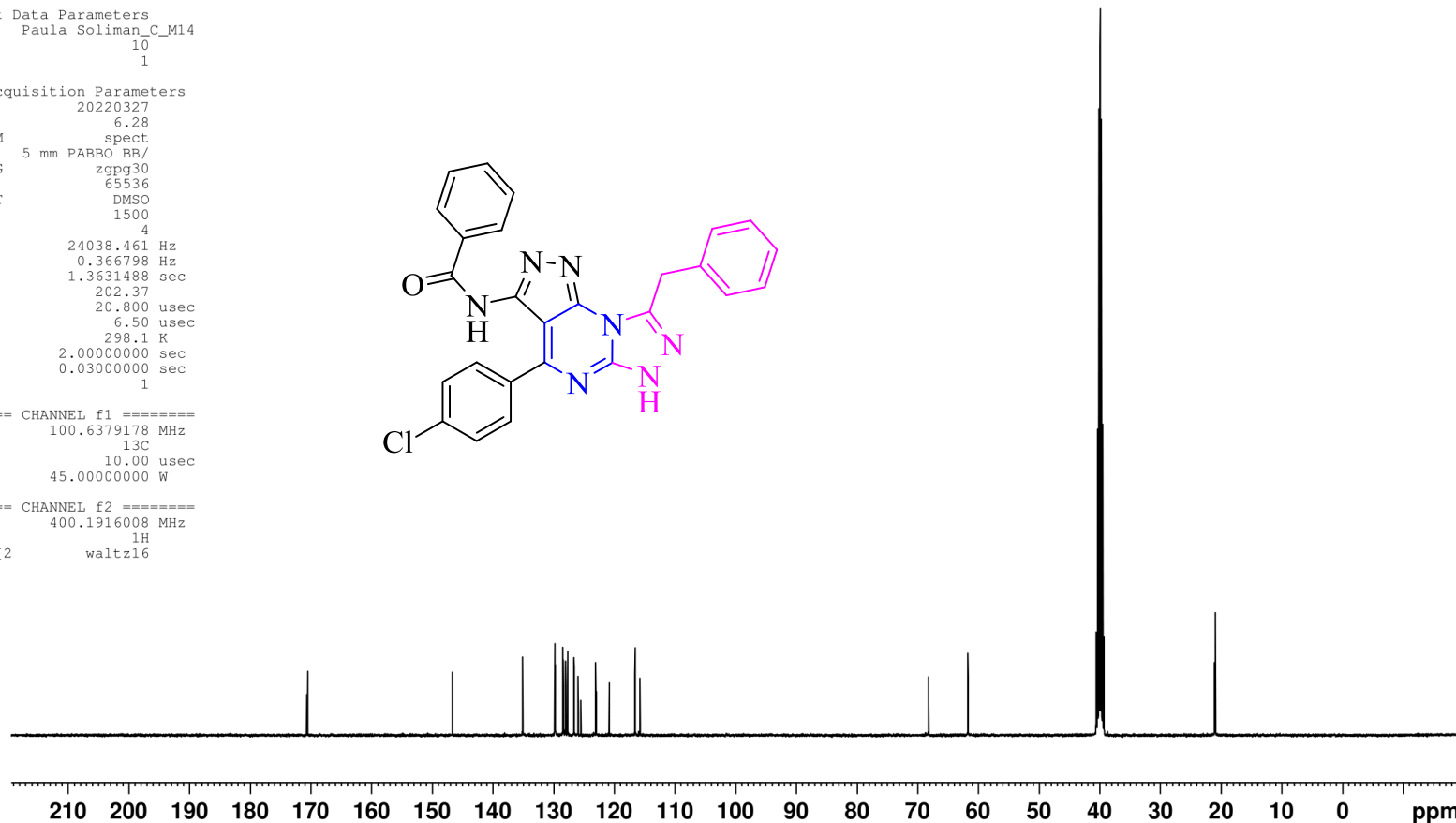
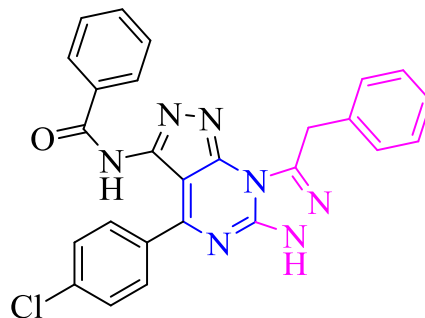


Current Data Parameters
NAME Paula Soliman_C_M14
EXPNO 10
PROCNO 1

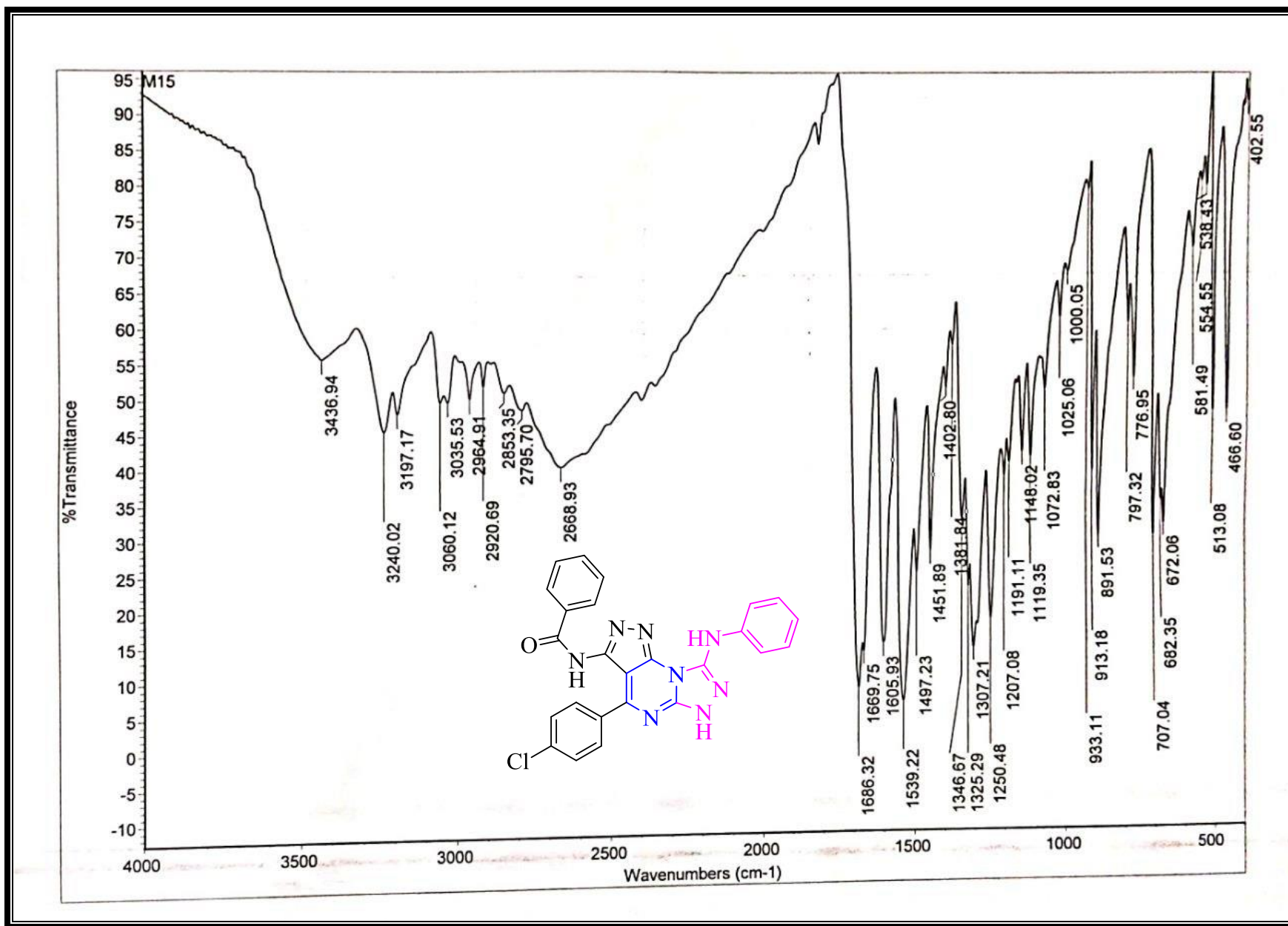
F2 - Acquisition Parameters
Date_ 20220327
Time 6.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W

===== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2] waltz16



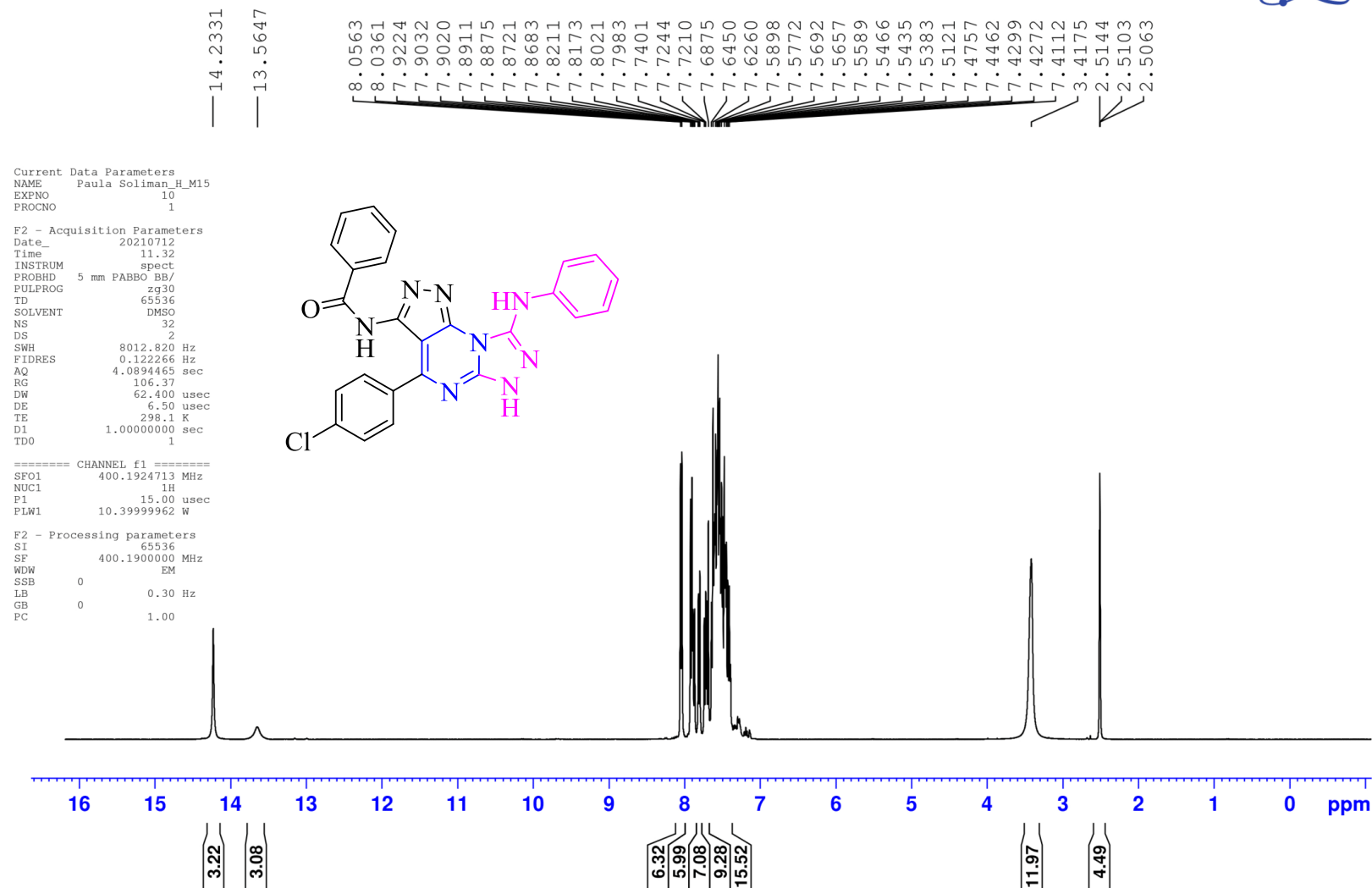
¹³C-NMR of N-(4-(4-chlorophenyl)-8-phenyl-6H-pyrazolo[4,3-e][1,2,4]triazolo[4,3-a]pyrimidin-3-yl)benzamide (10).



IR of *N*-(4-(4-chlorophenyl)-8-(phenylamino)-6H-pyrazolo[4,3-*e*][1,2,4]triazolo[4,3-*a*]pyrimidin-3-yl)benzamide (12).

Paula Soliman_H_M15

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¹H-NMR of *N*-(4-(4-chlorophenyl)-8-(phenylamino)-6H-pyrazolo[4,3-*e*][1,2,4]triazolo[4,3-*a*]pyrimidin-3-yl)benzamide (12).

Paula Soliman_H_M15_D2O

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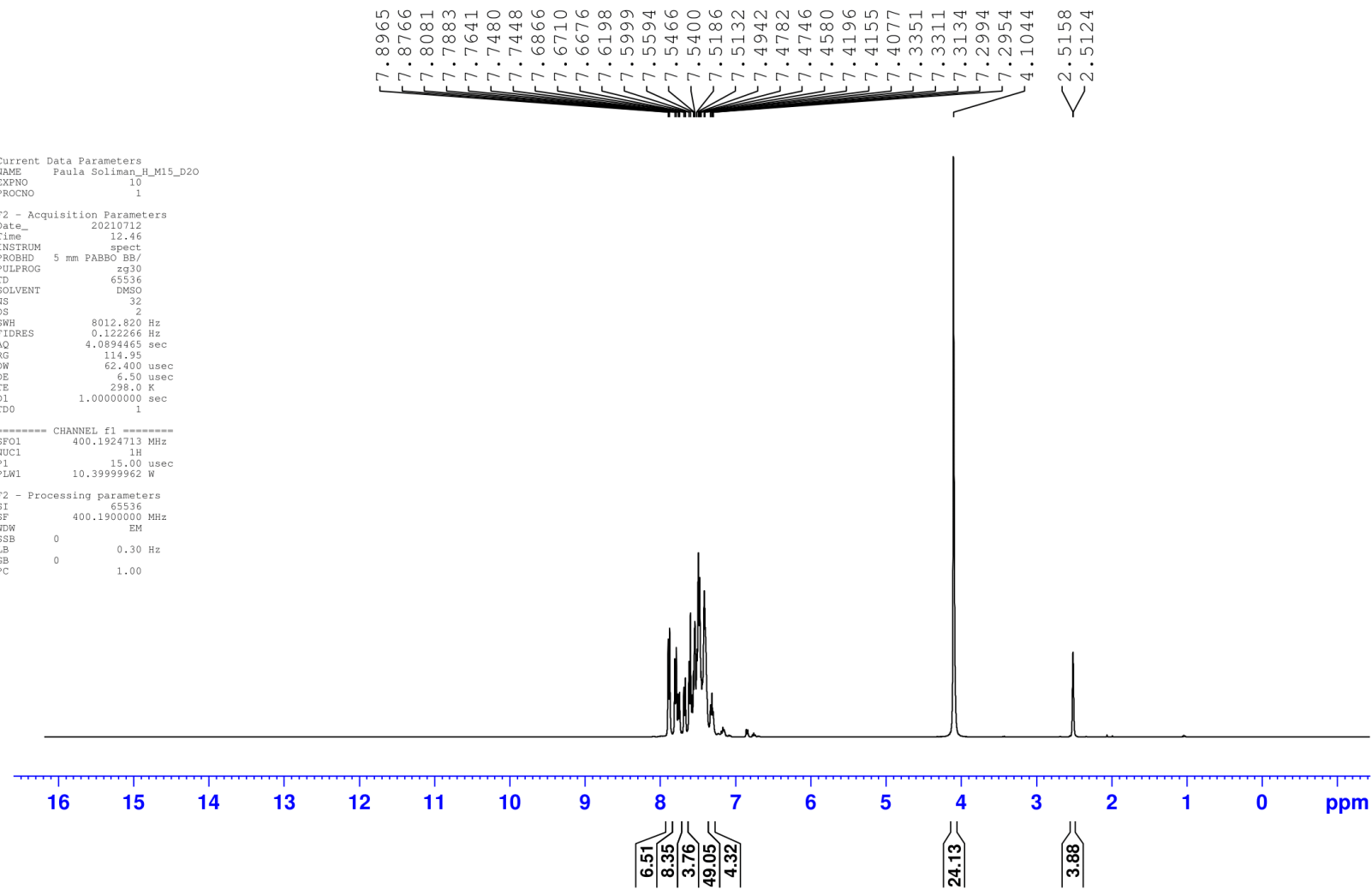


Current Data Parameters
NAME Paula Soliman_H_M15_D2O
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210712
Time 12.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 114.95
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



D₂O of *N*-(4-(4-chlorophenyl)-8-(phenylamino)-6H-pyrazolo[4,3-*e*][1,2,4]triazolo[4,3-*a*]pyrimidin-3-yl)benzamide (12).

Paula Soliman_C_M15

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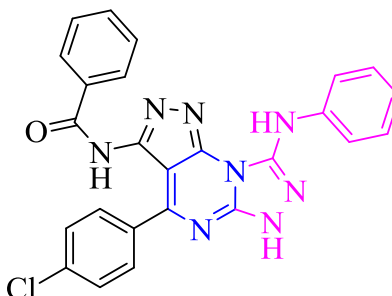


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131.08
130.94
130.44
130.44
129.39
129.21
128.36
128.11
127.82
125.54
124.27

40.62
40.42
40.21
40.00
39.79
39.58
39.37

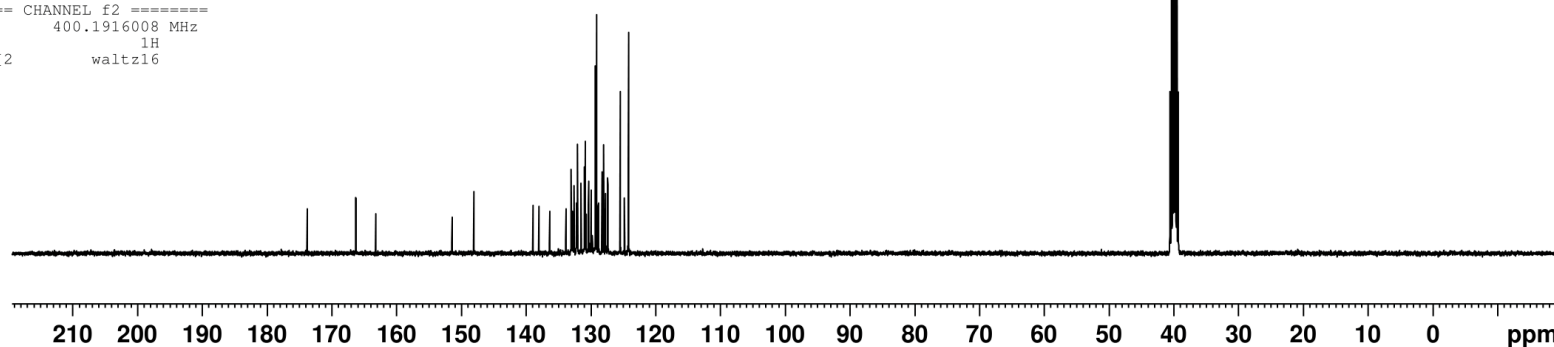
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NAME Paula Soliman_C_M15
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

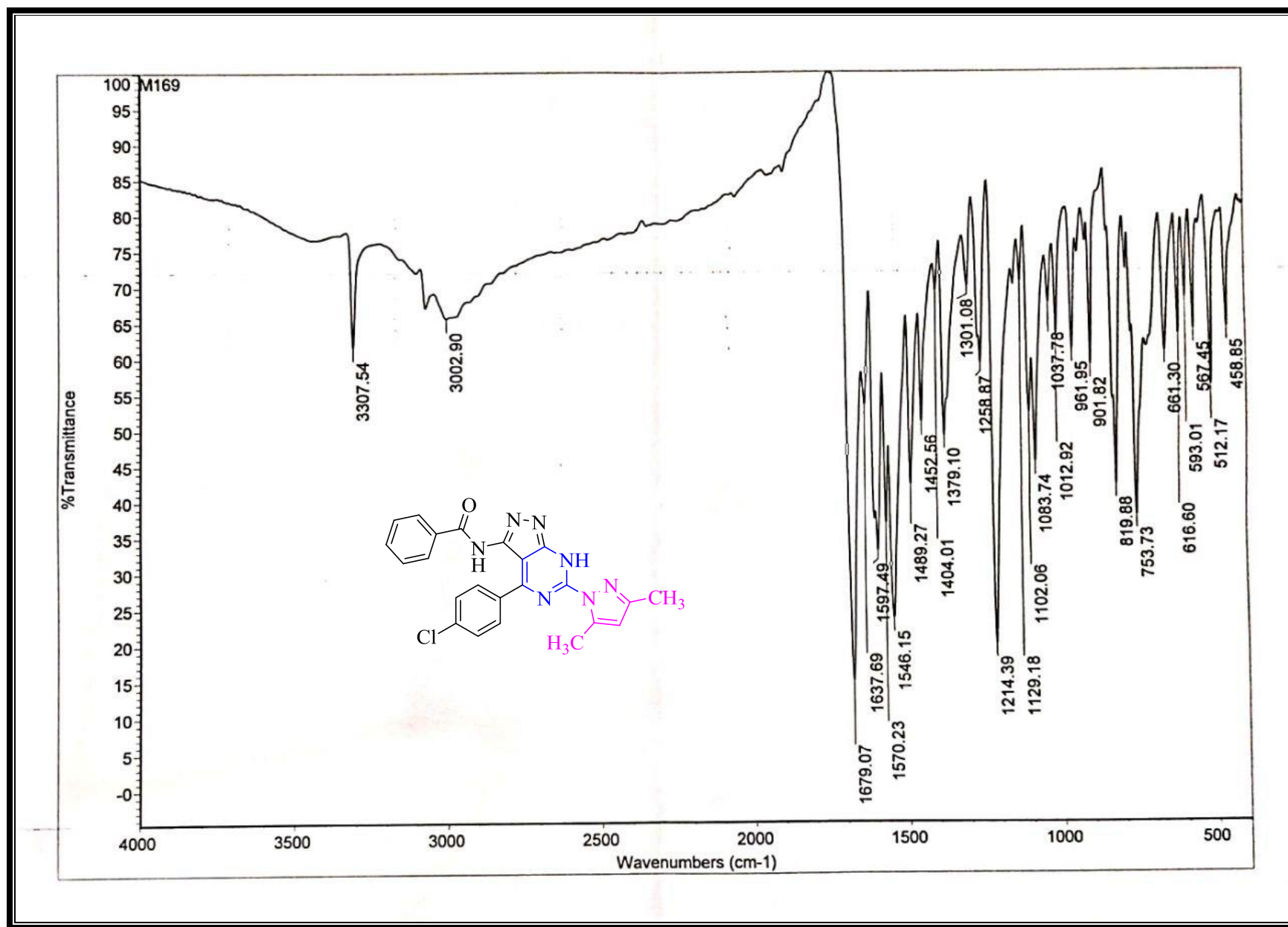


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NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W

==== CHANNEL f2 =====
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NUC2 1H
CPDPRG[2] waltz16



¹³C-NMR of *N*-(4-(4-chlorophenyl)-8-(phenylamino)-6H-pyrazolo[4,3-*e*][1,2,4]triazolo[4,3-*a*]pyrimidin-3-yl)benzamide (12).



IR of *N*-(4-(4-chlorophenyl)-6-(3,5-dimethyl-1H-pyrazol-1-yl)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (13a).

Paula Soliman_H_M16a

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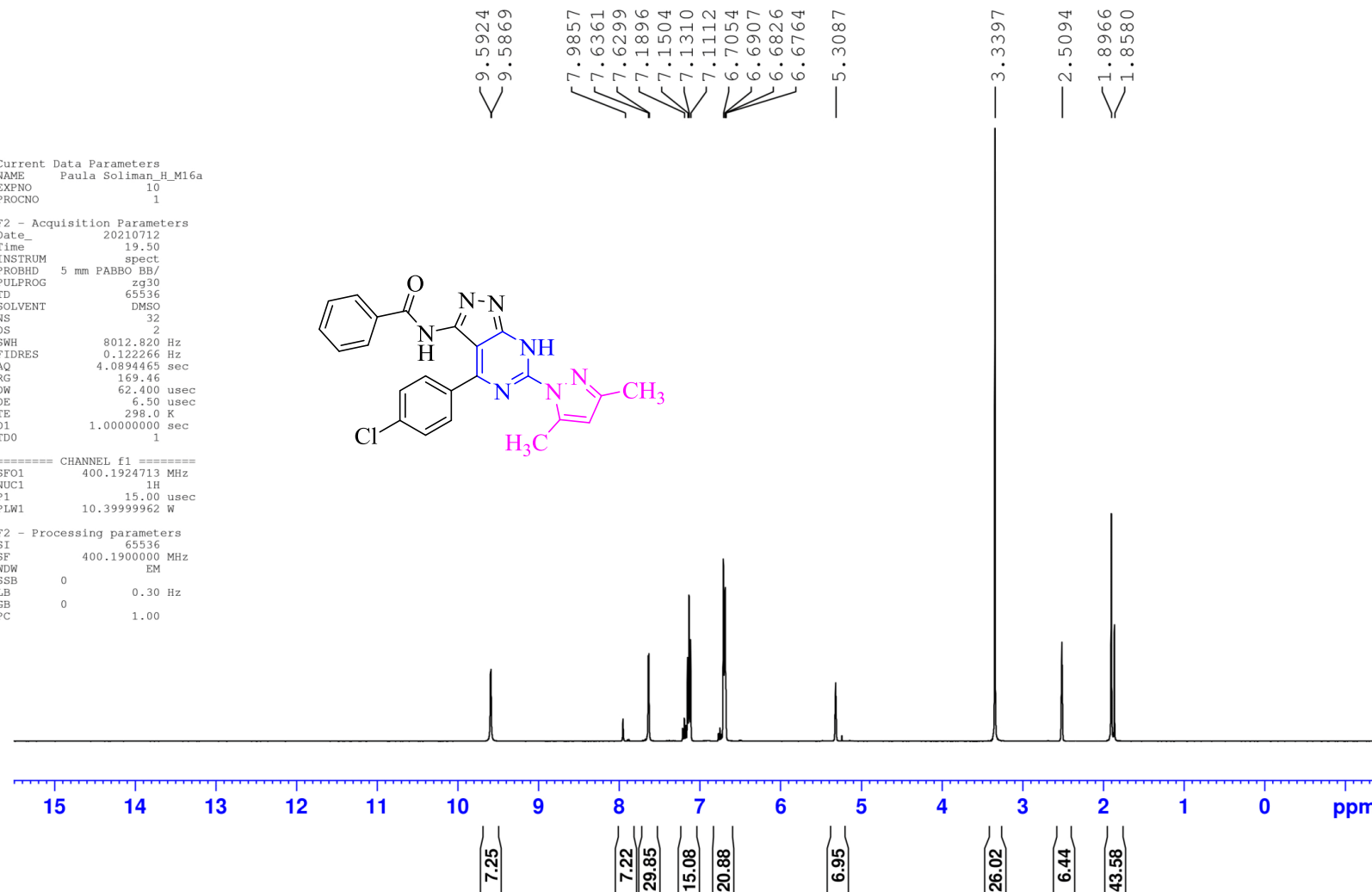
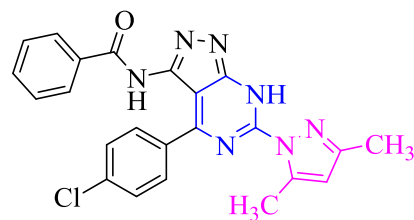


Current Data Parameters
NAME Paula Soliman_H_M16a
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210712
Time 19.50
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.46
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
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NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

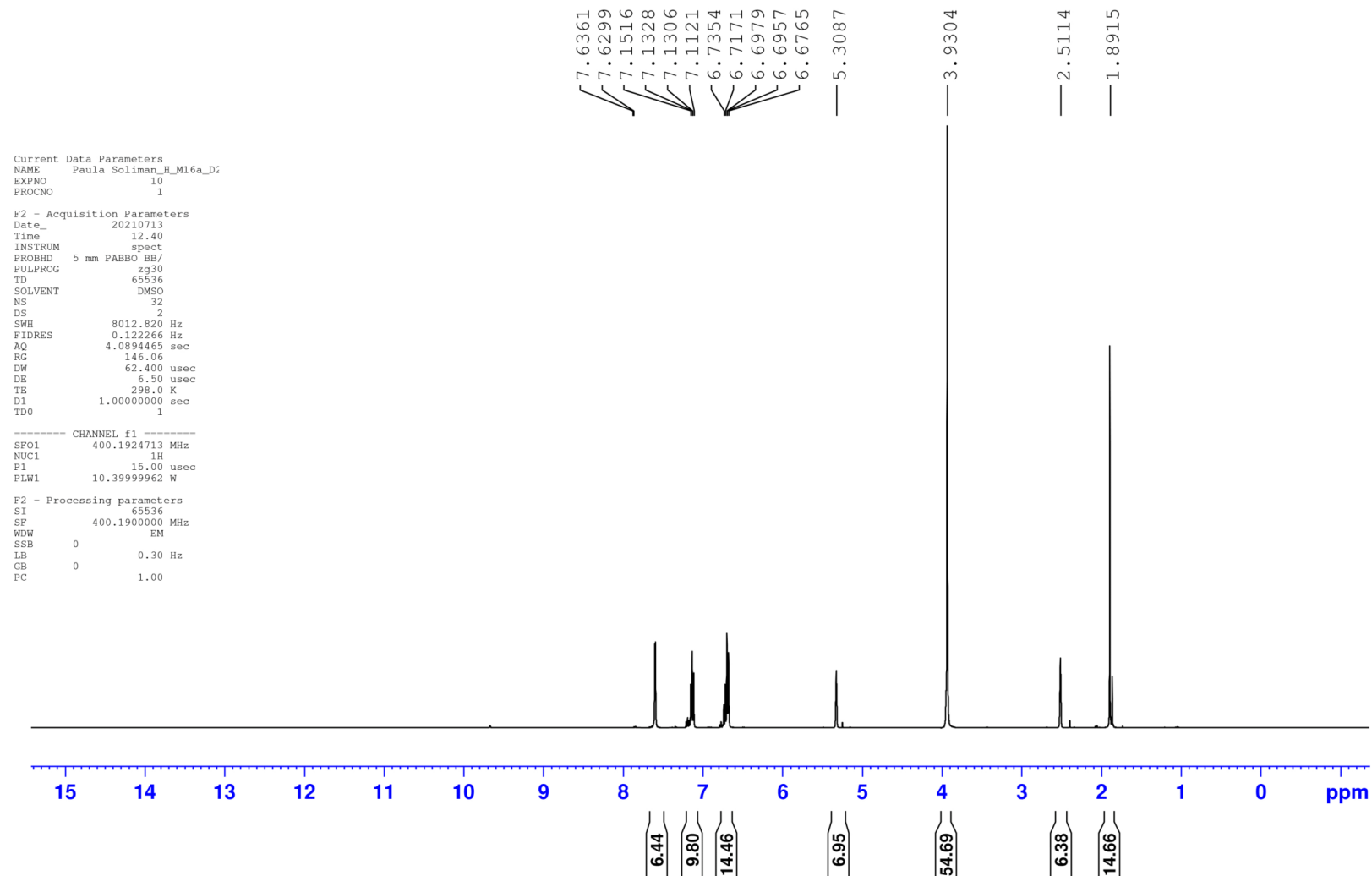
F2 - Processing parameters
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WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



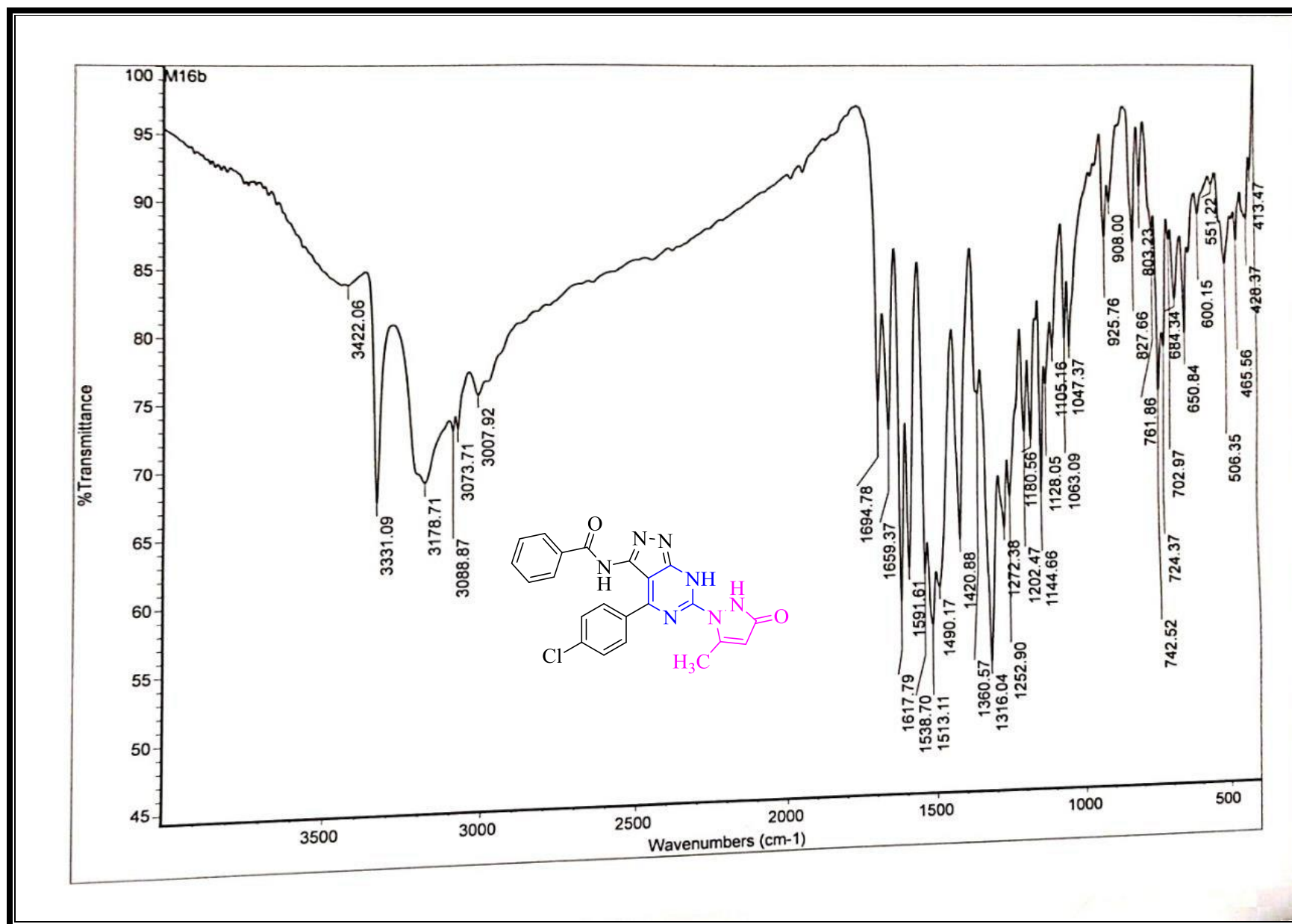
¹H-NMR of *N*-(4-(4-chlorophenyl)-6-(3,5-dimethyl-1H-pyrazol-1-yl)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (13a).

Paula Soliman_H_M16a_D2O

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D₂O of *N*-(4-(4-chlorophenyl)-6-(3,5-dimethyl-1H-pyrazol-1-yl)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (13a).



IR of *N*-(4-(4-chlorophenyl)-6-(5-methyl-3-oxo-2,3-dihydro-1H-pyrazol-1-yl)-7H-pyrazolo[3,4-*d*]pyrimidin-3-yl)benzamide (13b).

Paula Soliman_H_M16b

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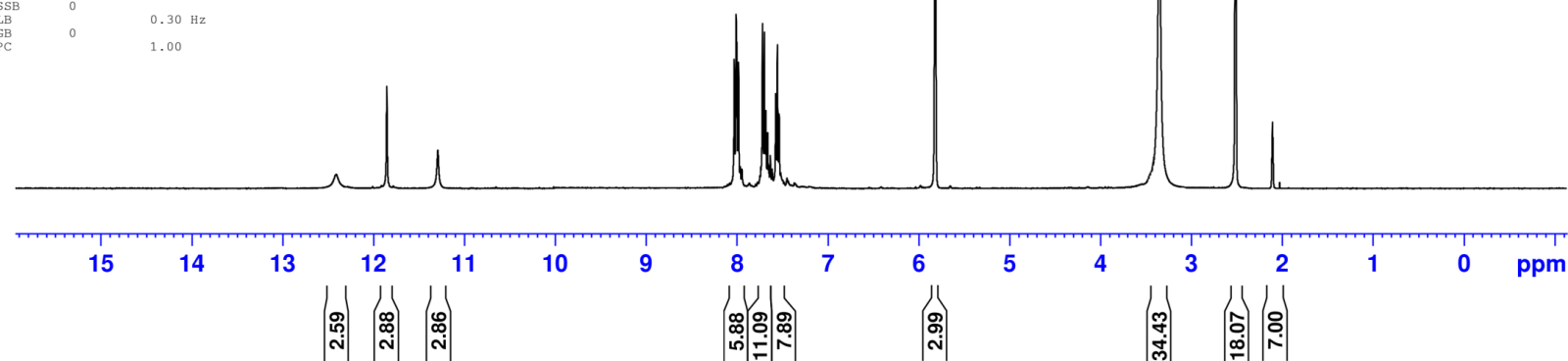
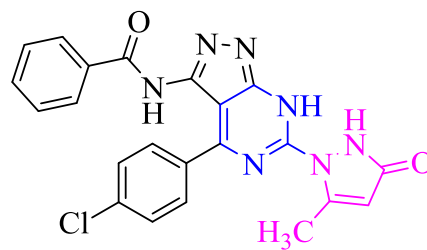
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—11.8513
—11.2895
8.0276
8.0059
8.0001
7.9809
7.7161
7.6949
7.6783
7.6597
7.5710
7.5516
7.5327
—5.8325
—3.3482
—2.5087
—2.1158

Current Data Parameters
NAME Paula Soliman_H_M16b
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210713
Time 10.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 202.37
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H-NMR of *N*-(4-(4-chlorophenyl)-6-(5-methyl-3-oxo-2,3-dihydro-1H-pyrazol-1-yl)-7H-pyrazolo[3,4-*d*]pyrimidin-3-yl)benzamide (13b).

Paula Soliman_H_M16b_D2O

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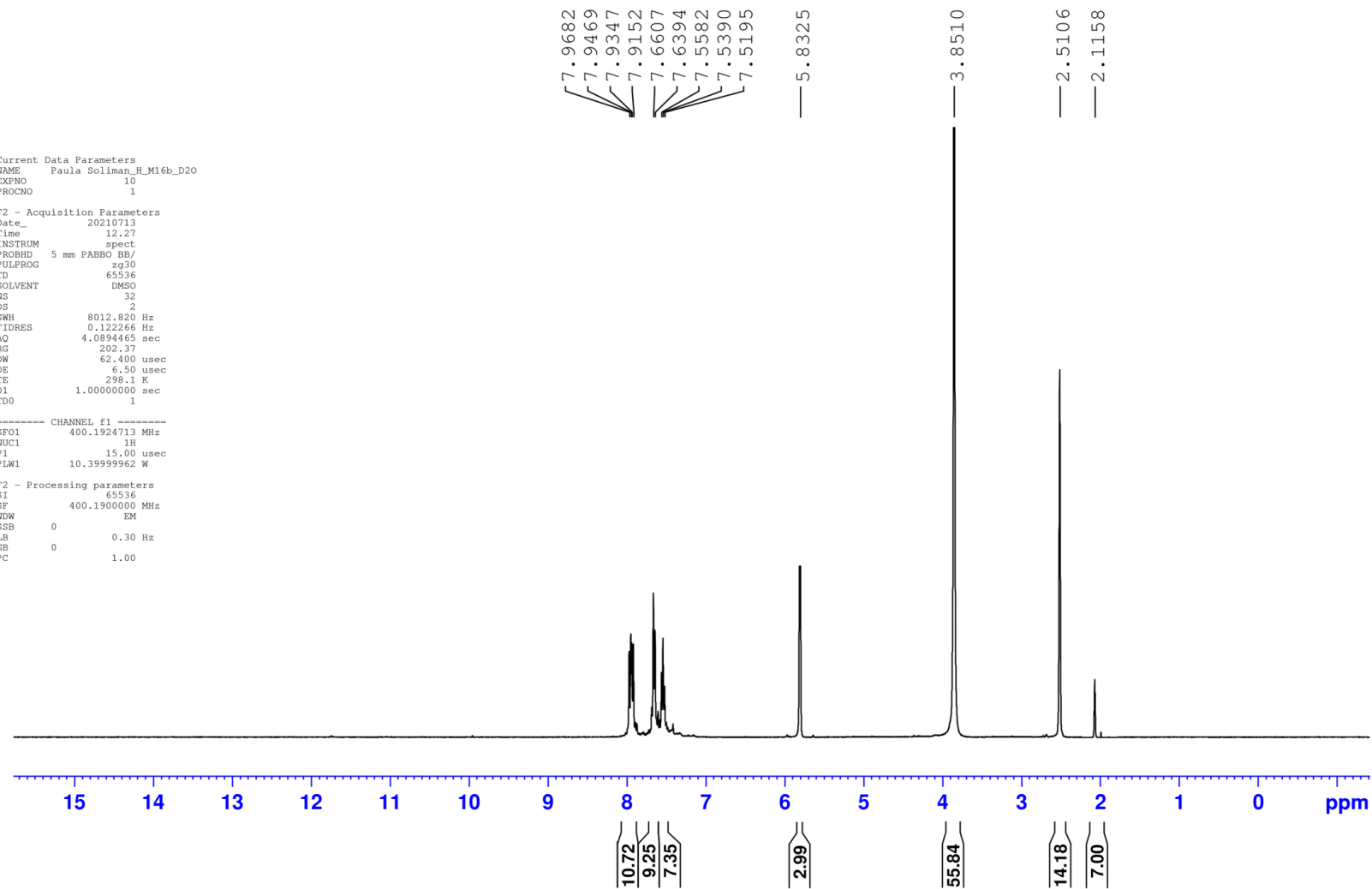


Current Data Parameters
NAME Paula Soliman_H_M16b_D2O
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210713
Time 12.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 202.37
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SF01 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



D₂O of *N*-(4-(4-chlorophenyl)-6-(5-methyl-3-oxo-2,3-dihydro-1H-pyrazol-1-yl)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (13b).

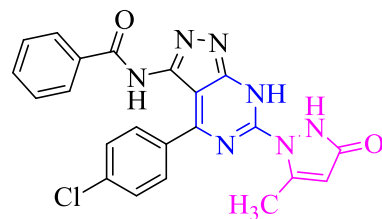
Paula Soliman_C_M16b

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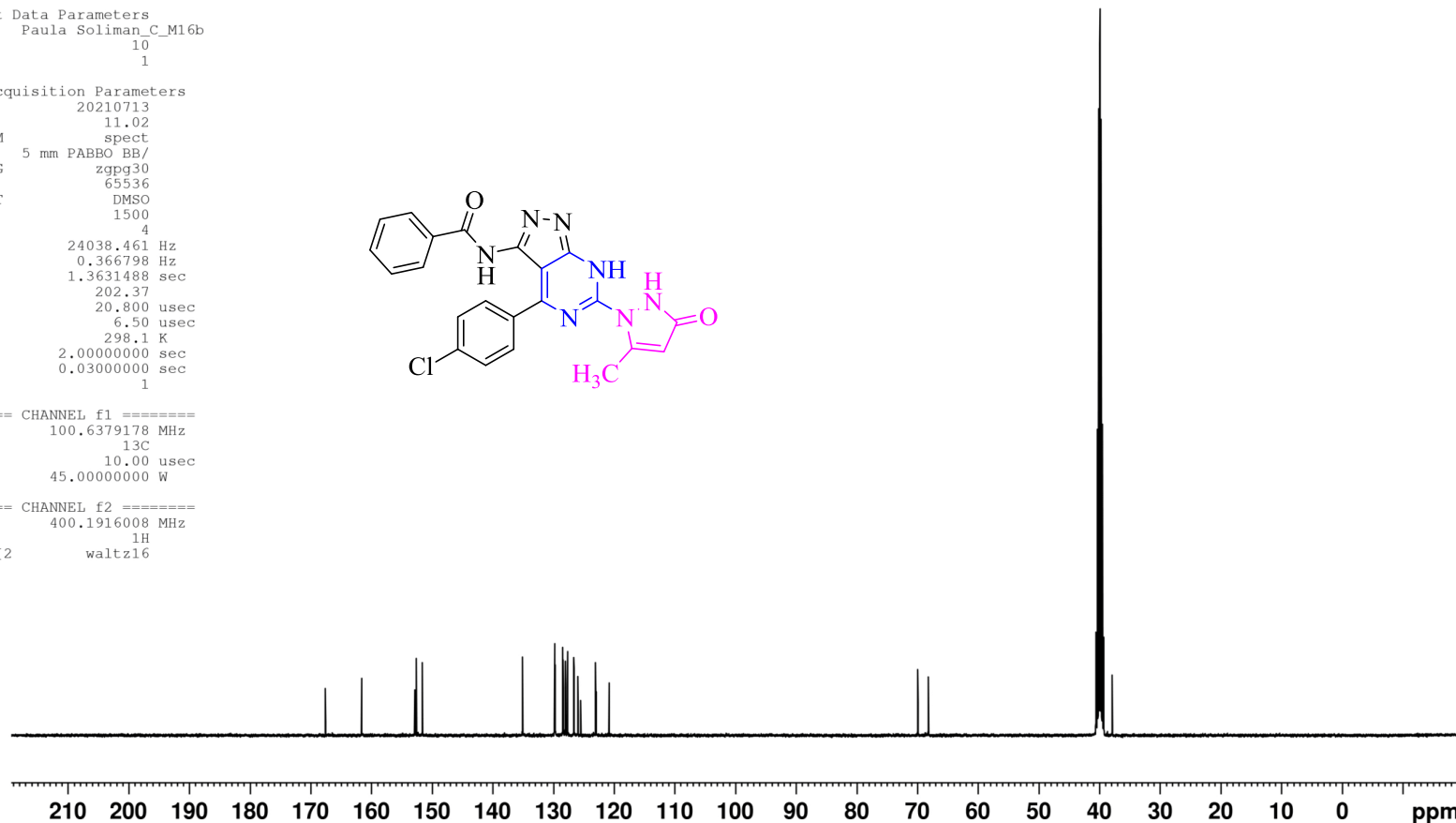


Current Data Parameters
NAME Paula Soliman_C_M16b
EXPNO 10
PROCNO 1

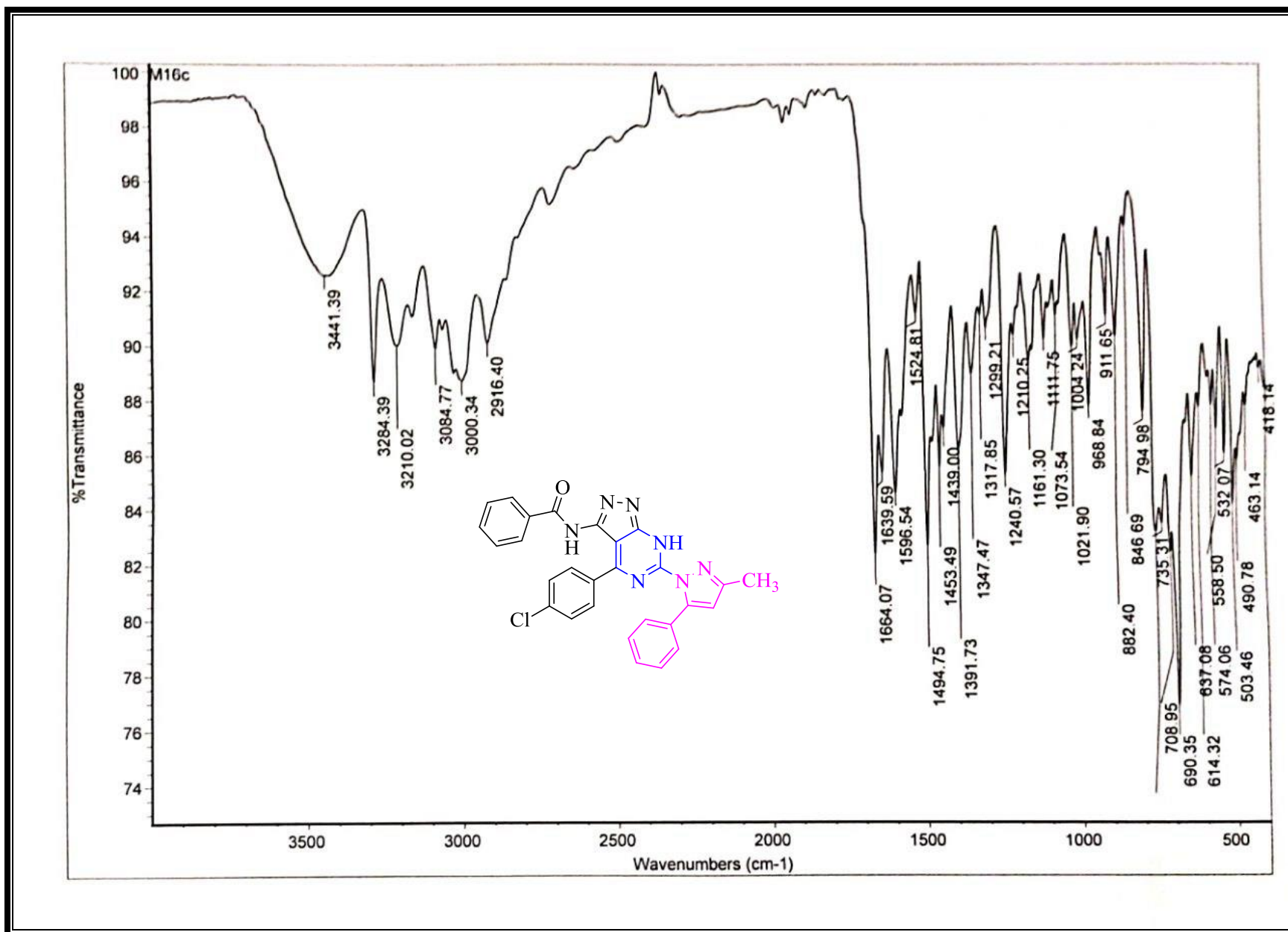
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PULPROG zgpg30
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SOLVENT DMSO
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DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1



==== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W
==== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2] waltz16



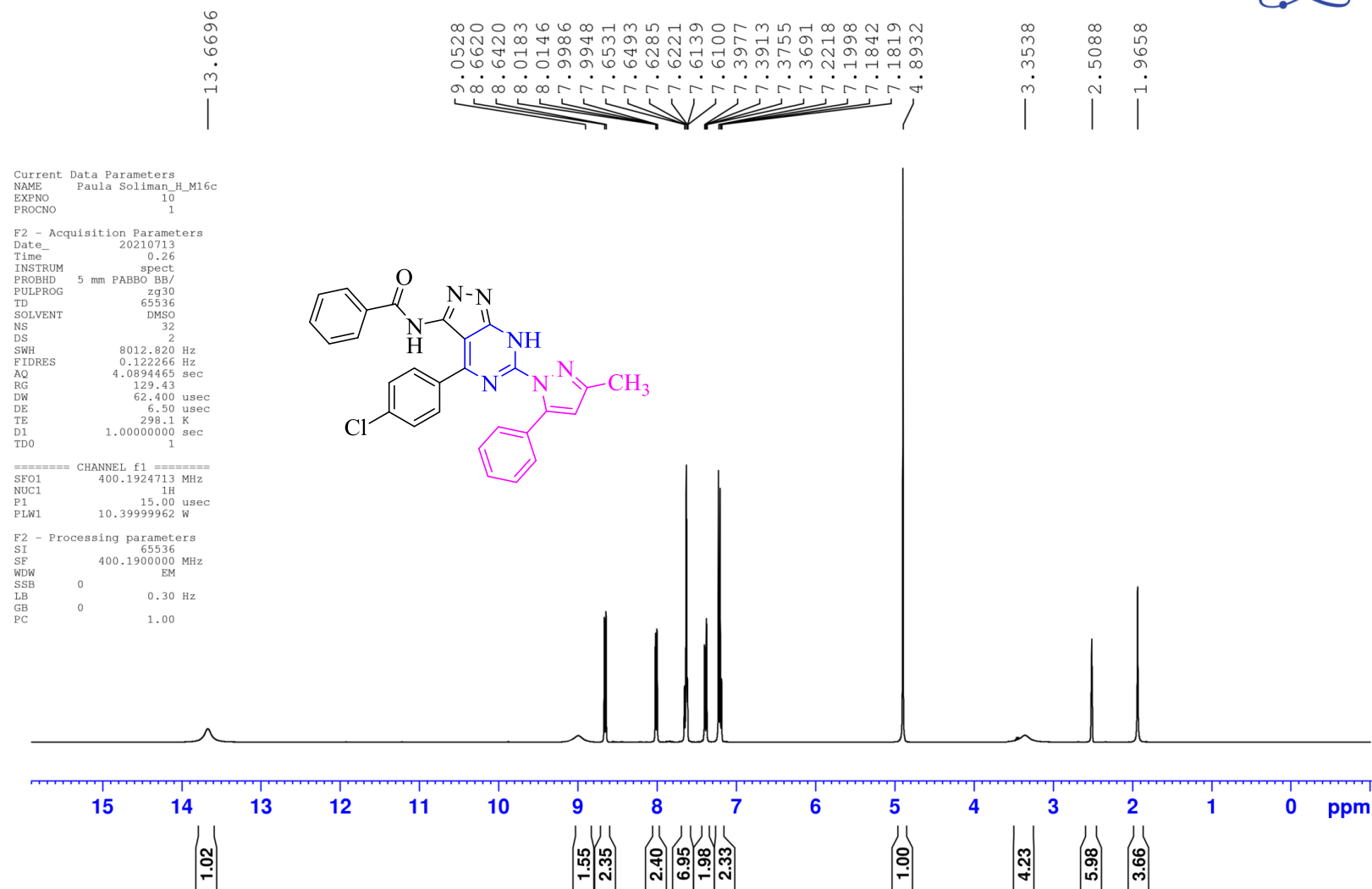
¹³C-NMR of *N*-(4-(4-chlorophenyl)-6-(5-methyl-3-oxo-2,3-dihydro-1H-pyrazol-1-yl)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (13b).



IR of *N*-(4-(4-chlorophenyl)-6-(3-methyl-5-phenyl-1H-pyrazol-1-yl)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (13c).

Paula Soliman_H_M16c

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¹H-NMR of *N*-(4-(4-chlorophenyl)-6-(3-methyl-5-phenyl-1H-pyrazol-1-yl)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (13c).

Paula Soliman_H_M16c_D2O

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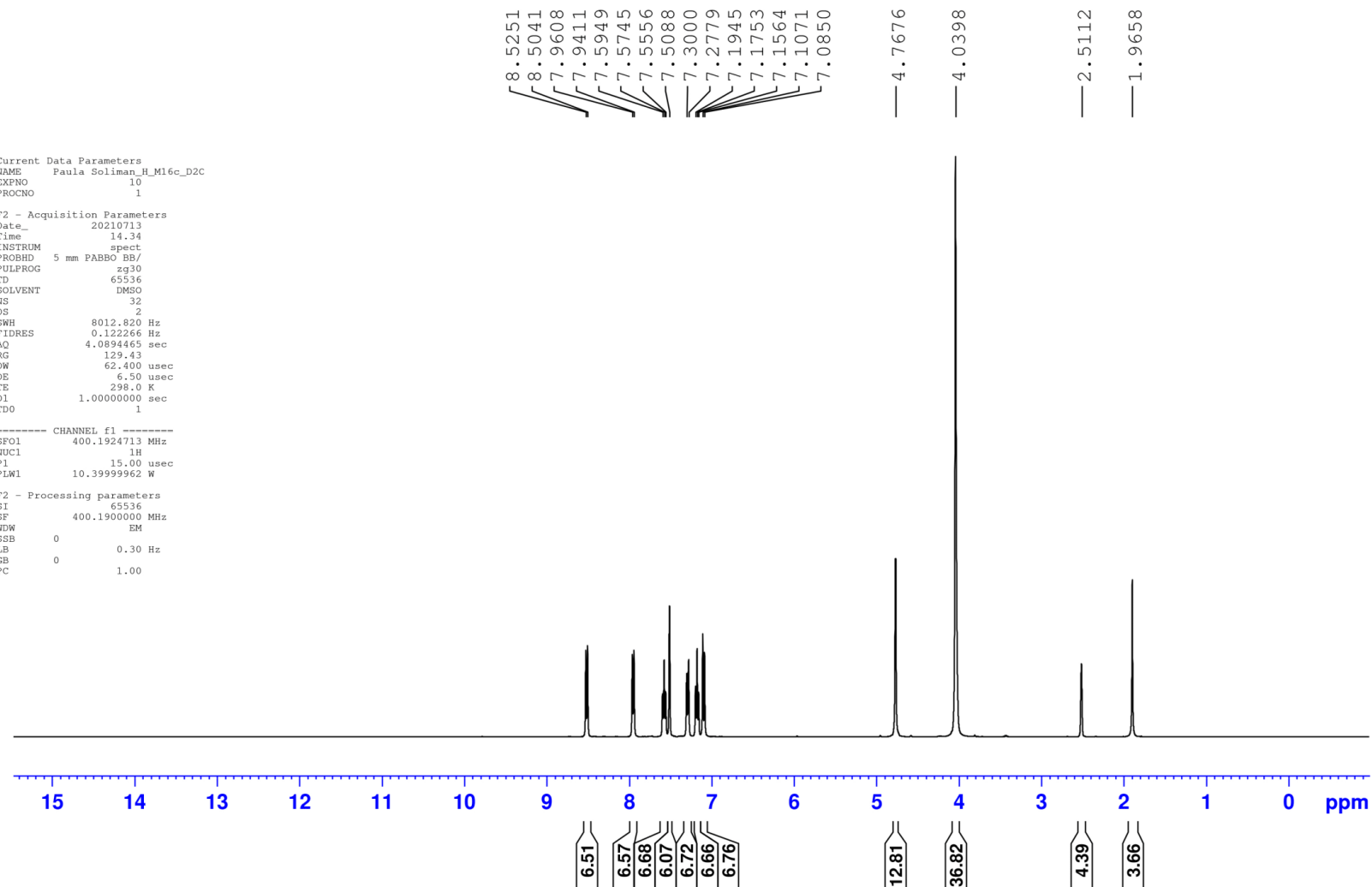


Current Data Parameters
NAME Paula Soliman_H_M16c_D2c
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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Time 14.34
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 129.43
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
TDO 1

----- CHANNEL f1 -----
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NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

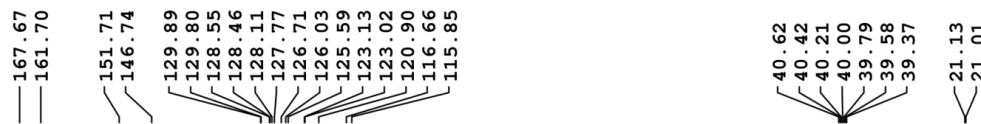
F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



D₂O of *N*-(4-(4-chlorophenyl)-6-(3-methyl-5-phenyl-1H-pyrazol-1-yl)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (13c).

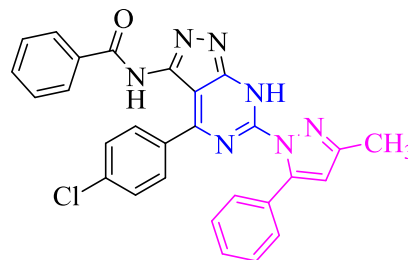
Paula Soliman_C_M16c

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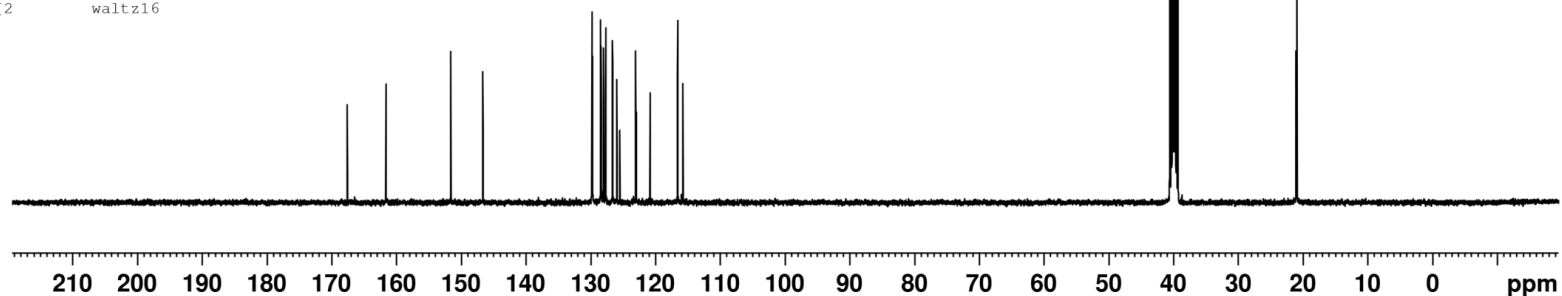


Current Data Parameters
NAME Paula Soliman_C_M16c
EXPNO 10
PROCNO 1

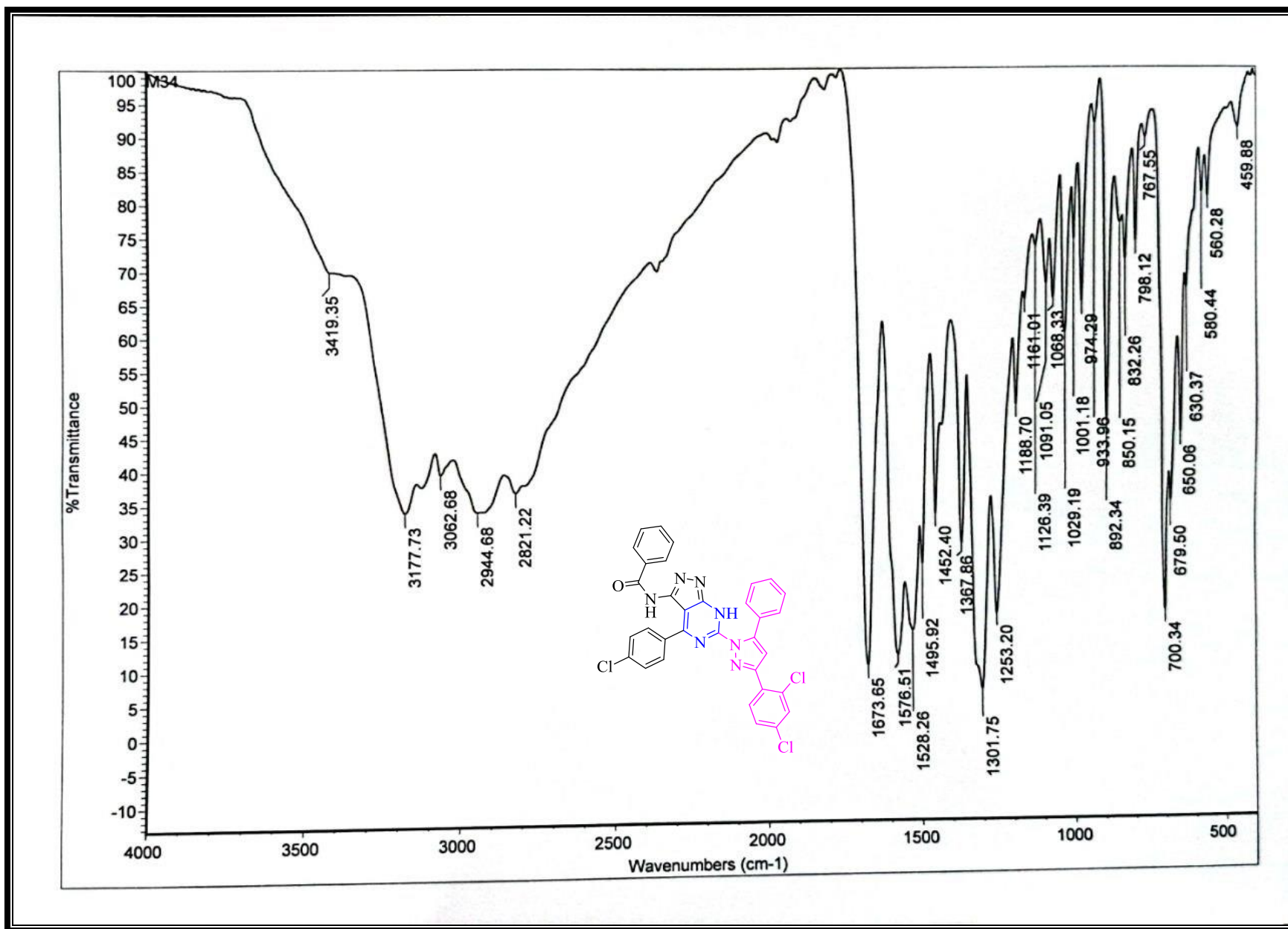
F2 - Acquisition Parameters
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Time 13.20
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1



==== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W
==== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2] waltz16



¹³C-NMR of *N*-(4-(4-chlorophenyl)-6-(3-methyl-5-phenyl-1H-pyrazol-1-yl)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (13c).



IR of *N*-(4-(4-chlorophenyl)-6-(5-(2,4-dichlorophenyl)-3-phenyl-1H-pyrazol-1-yl)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (14).

Paula Soliman_H_M34

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14.1417

8.9593
8.1893
8.1806
8.1607
8.1503
8.1391
8.1351
8.0817
8.0601
8.0416
8.0220
7.9997
7.9785
7.8317
7.7927
7.7220
7.7188
7.7048
7.7018
7.6822
7.6627
7.6602
7.6458
7.6428
7.5746
7.5534
5.3548

3.3417

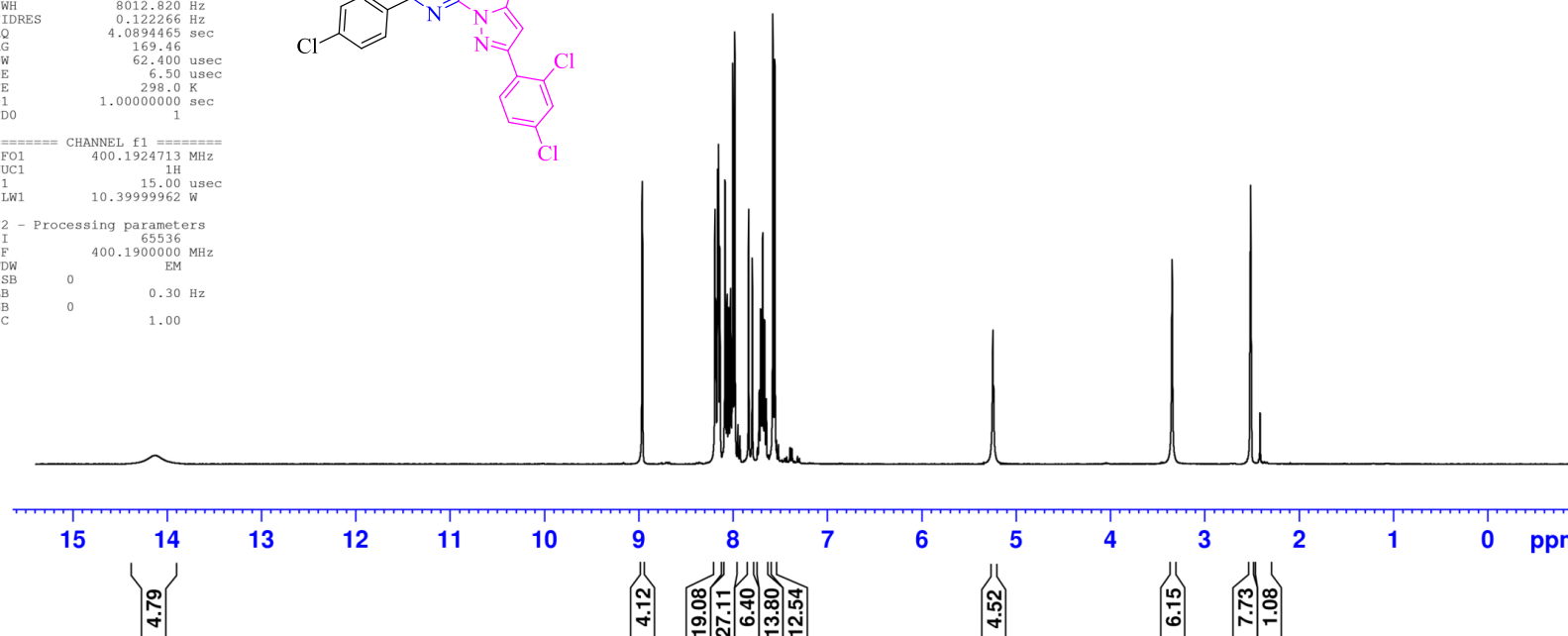
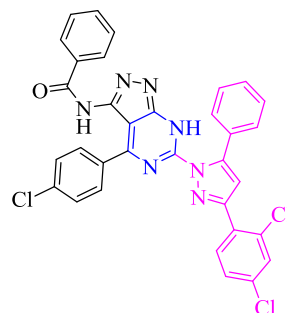
2.5081
2.4082

Current Data Parameters
NAME Paula Soliman_H_M34
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.46
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
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NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

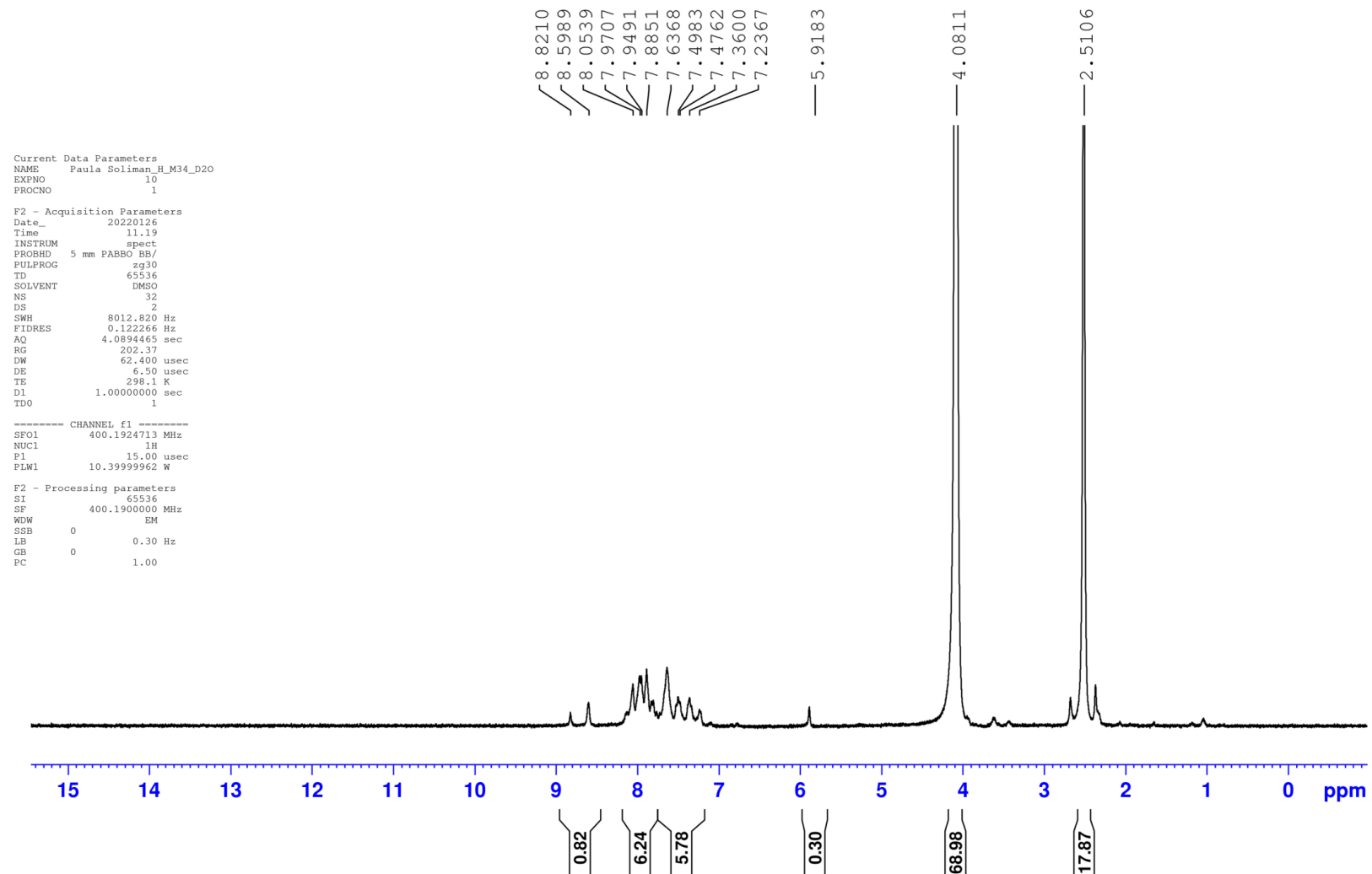
F2 - Processing parameters
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SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



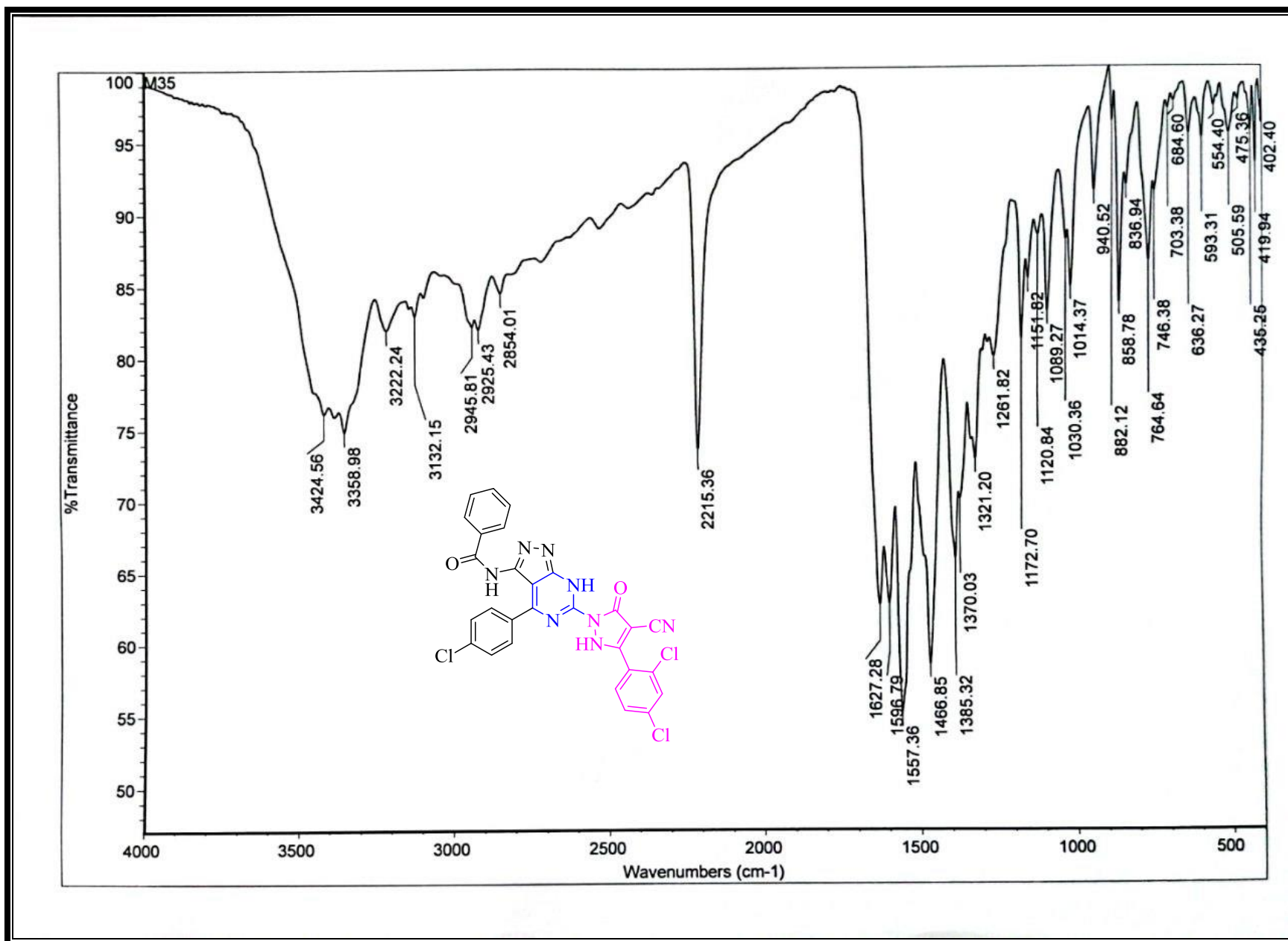
¹H-NMR of *N*-(4-(4-chlorophenyl)-6-(5-(2,4-dichlorophenyl)-3-phenyl-1H-pyrazol-1-yl)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (14).

Paula Soliman_H_M34_D2O

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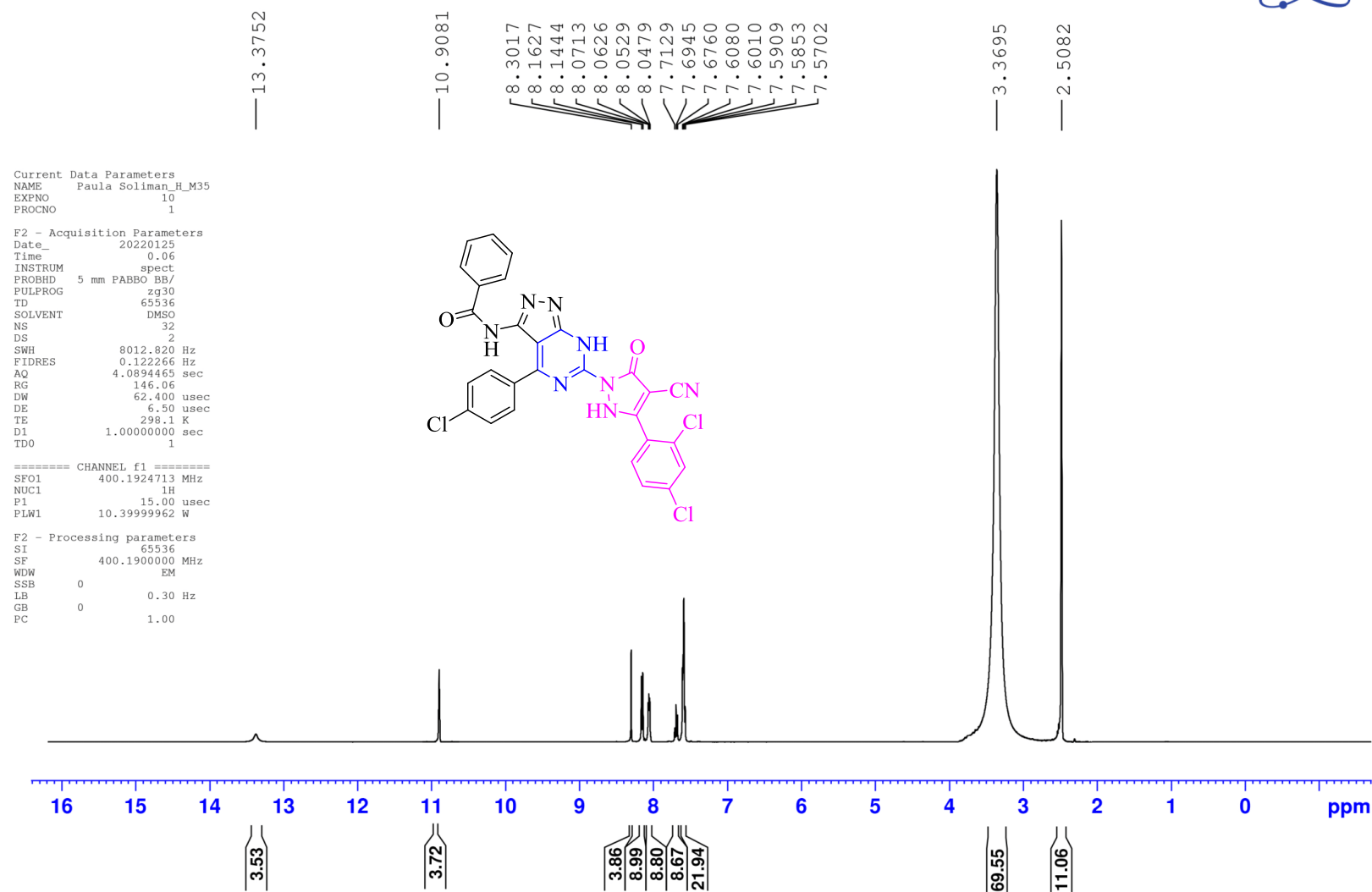
D₂O of *N*-(4-(4-chlorophenyl)-6-(5-(2,4-dichlorophenyl)-3-phenyl-1*H*-pyrazol-1-yl)-7*H*-pyrazolo[3,4-*d*]pyrimidin-3-yl)benzamide (14).



IR of *N*-(4-(4-chlorophenyl)-6-(4-cyano-5-(2,4-dichlorophenyl)-3-oxo-2,3-dihydro-1H-pyrazol-1-yl)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (15).

Paula Soliman_H_M35

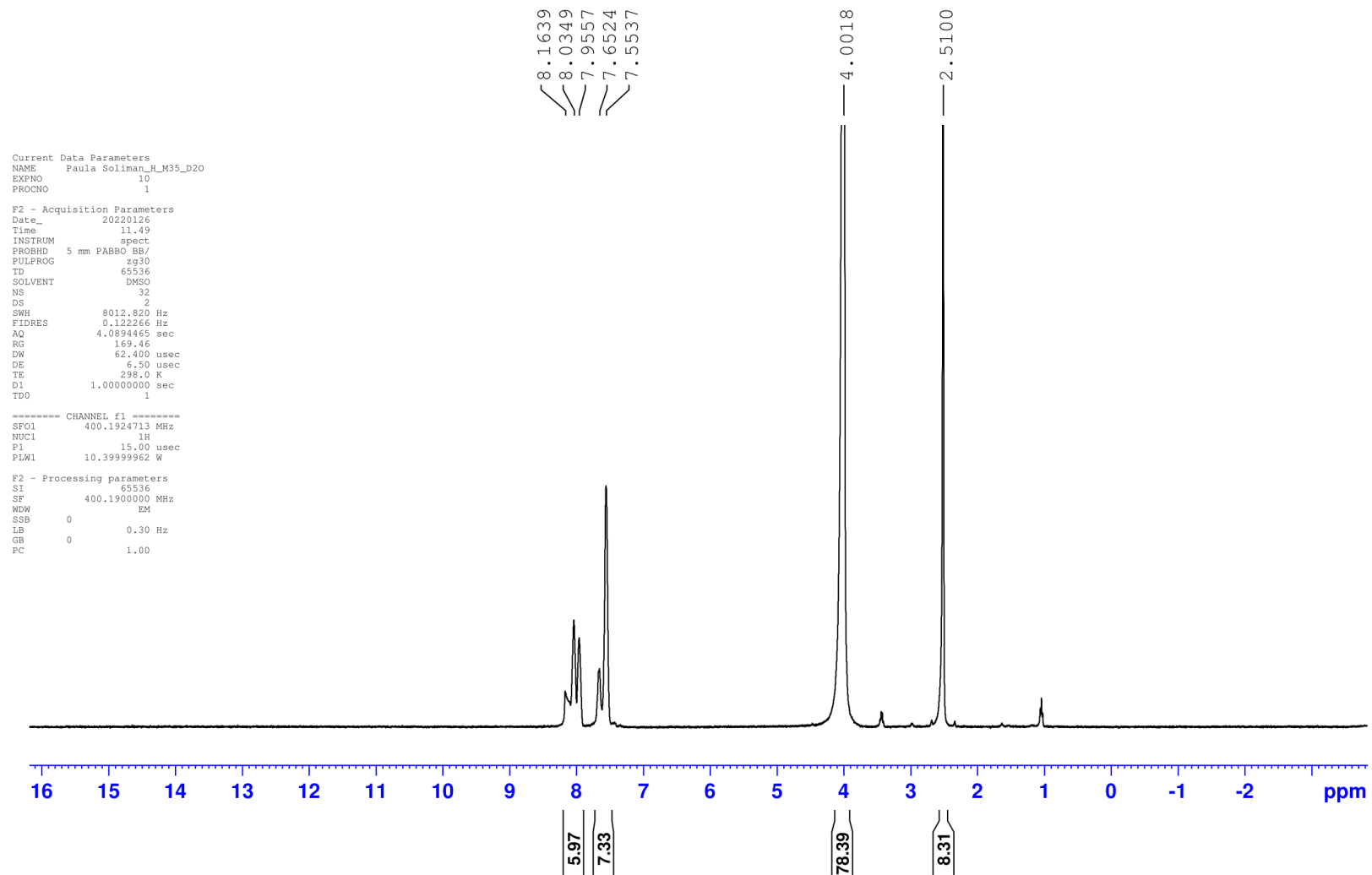
Microanalytical Unit - FOPCU - NMR laboratory
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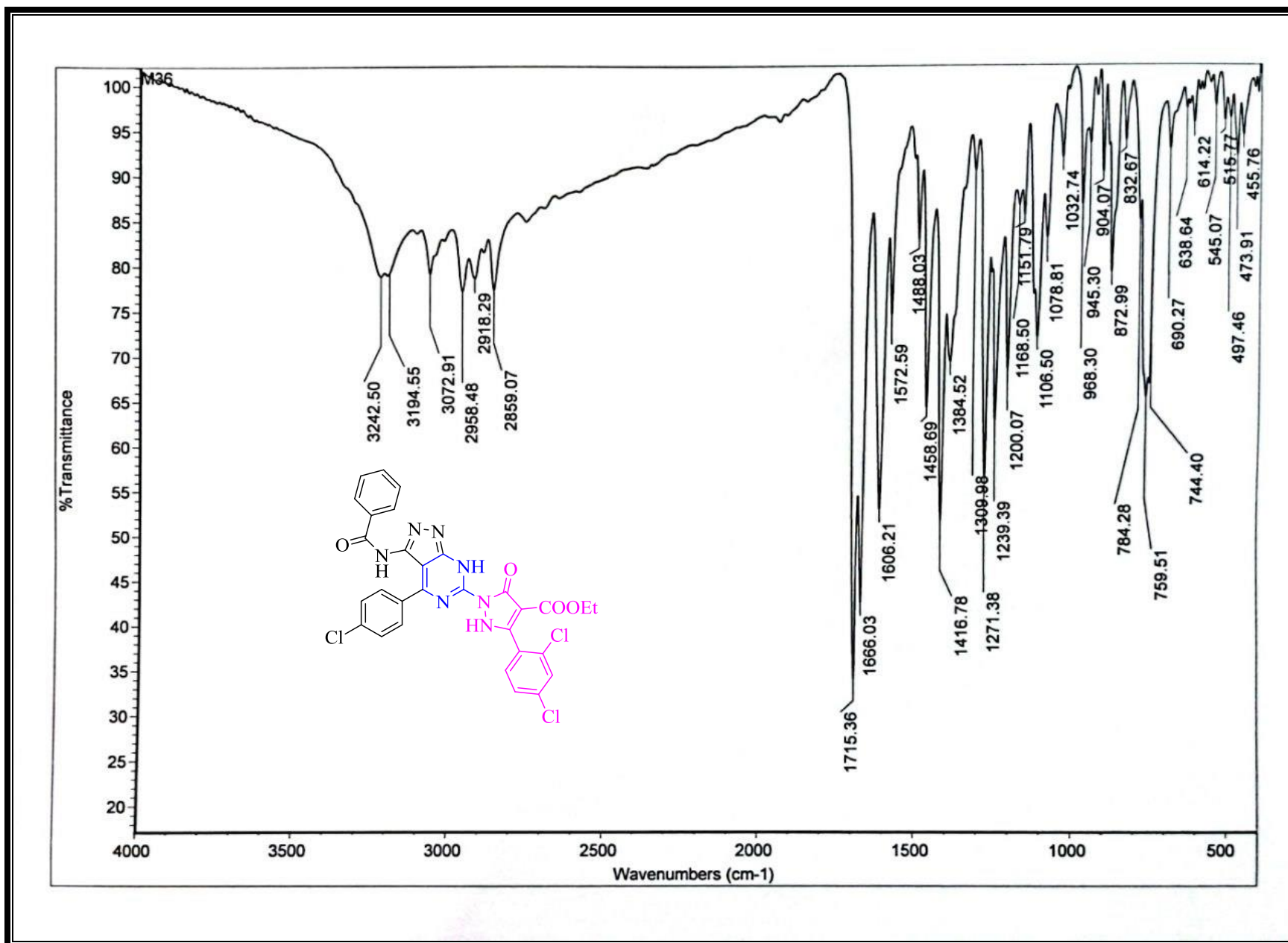
¹H-NMR of *N*-(4-(4-chlorophenyl)-6-(4-cyano-5-(2,4-dichlorophenyl)-3-oxo-2,3-dihydro-1H-pyrazol-1-yl)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (15).

Paula Soliman_H_M35_D2O

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D₂O of *N*-(4-(4-chlorophenyl)-6-(4-cyano-5-(2,4-dichlorophenyl)-3-oxo-2,3-dihydro-1H-pyrazol-1-yl)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (15).



IR of Ethyl 1-(3-benzamido-4-(4-chlorophenyl)-7H-pyrazolo[3,4-d]pyrimidin-6-yl)-5-(2,4-dichlorophenyl)-3-oxo-2,3-dihydro-1H-pyrazole-4-carboxylate (16).

Paula Soliman_H_M36

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14.1866
14.1684

12.8926

10.6528

8.1228
8.0929
8.0744
7.7007
7.6823
7.6639
7.5918
7.5724
7.5536

4.2056
4.1879
4.1702
4.1526
3.5148
3.4539
3.4363
2.5676
2.5079

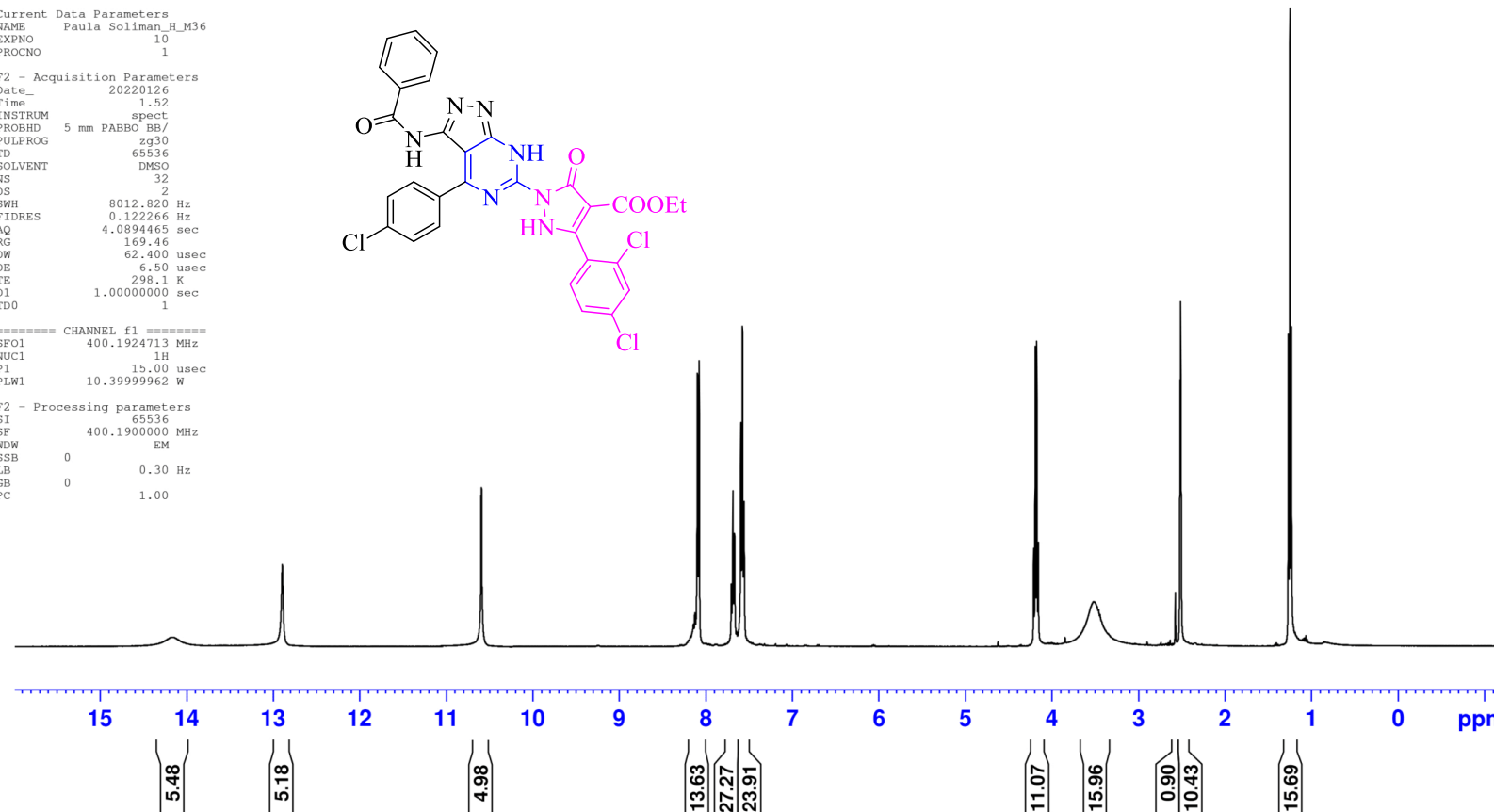
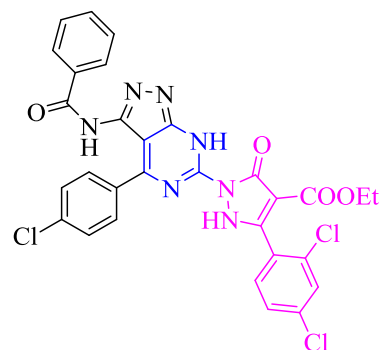
1.2614
1.2437
1.2260

Current Data Parameters
NAME Paula Soliman_H_M36
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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Time 1.52
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.089465 sec
RG 189.46
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H-NMR of Ethyl 1-(3-benzamido-4-(4-chlorophenyl)-7H-pyrazolo[3,4-d]pyrimidin-6-yl)-5-(2,4-dichlorophenyl)-3-oxo-2,3-dihydro-1H-pyrazole-4-carboxylate (16).

Paula Soliman_H_M36_D2O

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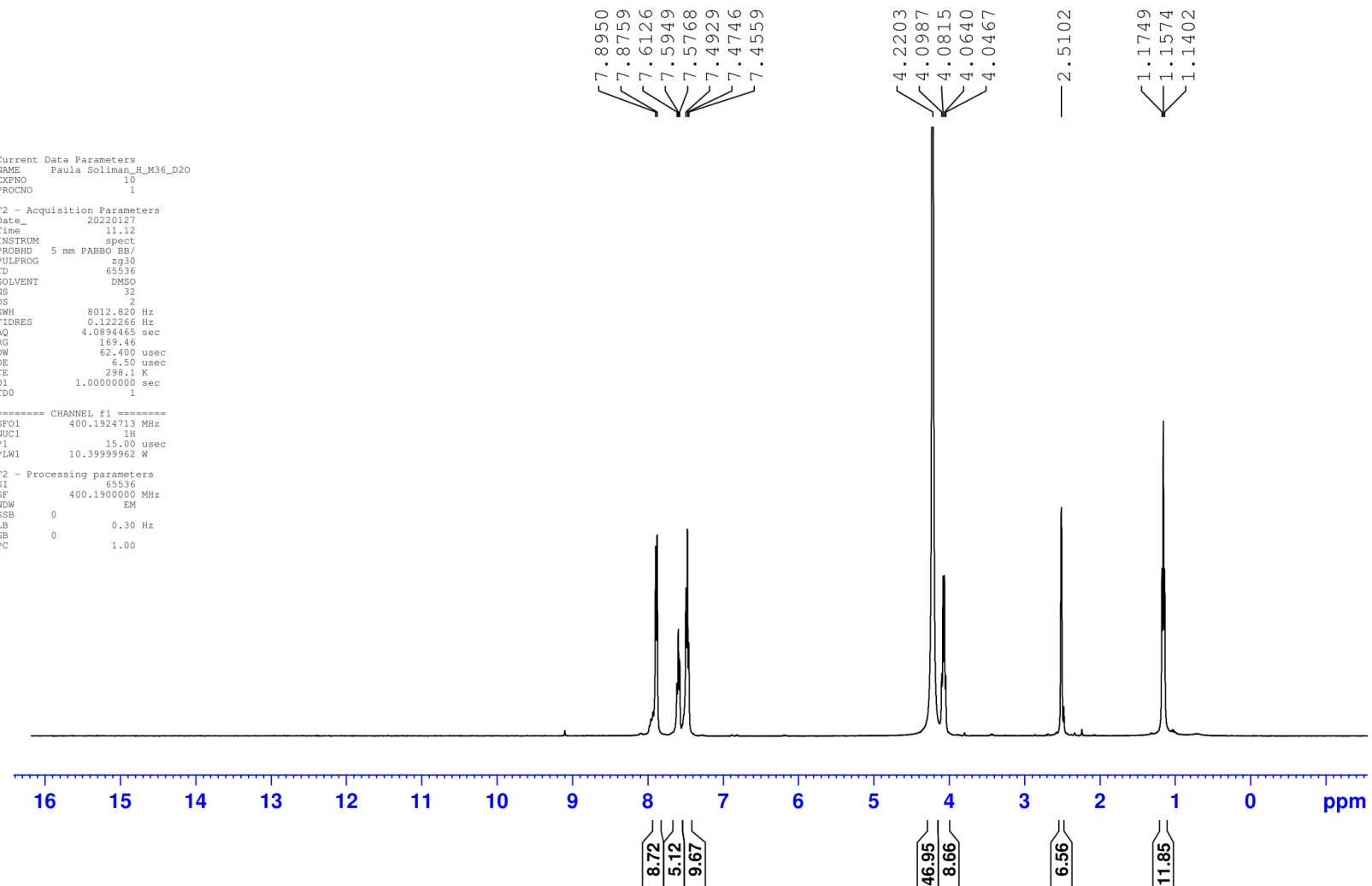


Current Data Parameters
NAME Paula Soliman_H_M36_D2O
EXPNO 10
PROCNO 1

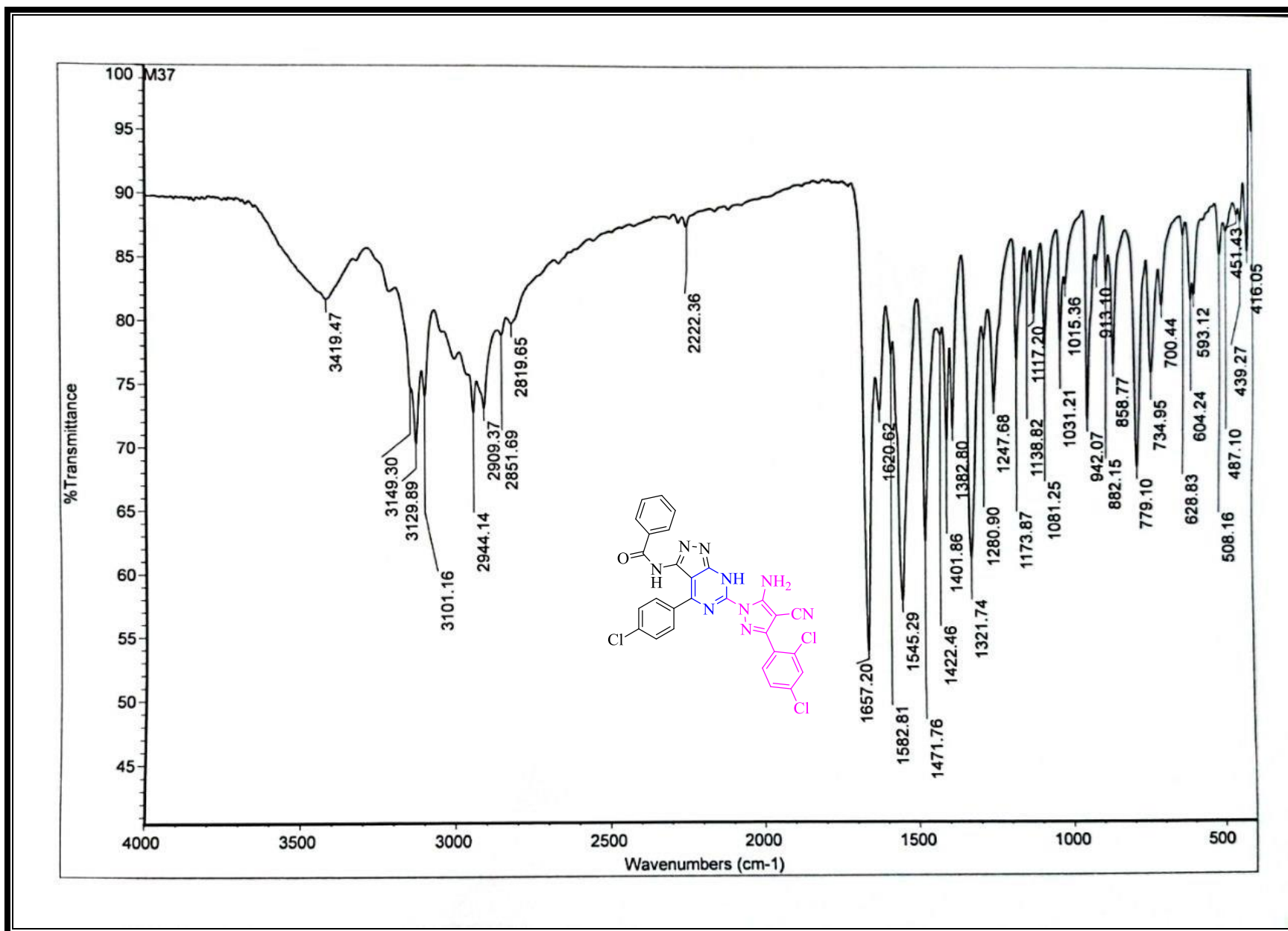
F2 - Acquisition Parameters
Date_ 20220127
Time 11:12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.466
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SF01 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



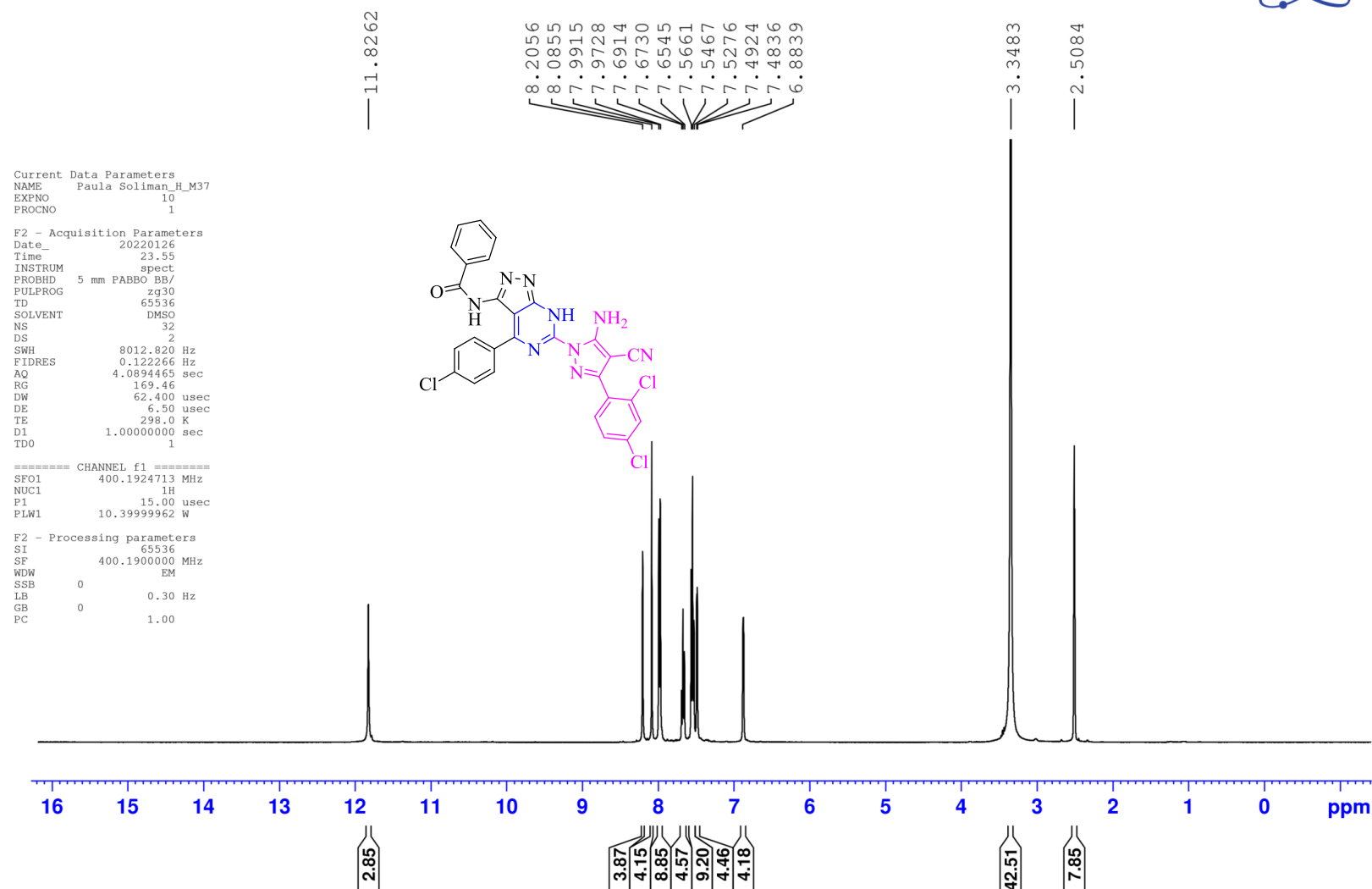
D₂O of Ethyl 1-(3-benzamido-4-(4-chlorophenyl)-7H-pyrazolo[3,4-d]pyrimidin-6-yl)-5-(2,4-dichlorophenyl)-3-oxo-2,3-dihydro-1H-pyrazole-4-carboxylate (16).



IR of *N*-(6-(3-amino-4-cyano-5-(2,4-dichlorophenyl)-1*H*-pyrazol-1-yl)-4-(4-chlorophenyl)-7*H*-pyrazolo[3,4-*d*]pyrimidin-3-yl)benzamide (17).

Paula Soliman_H_M37

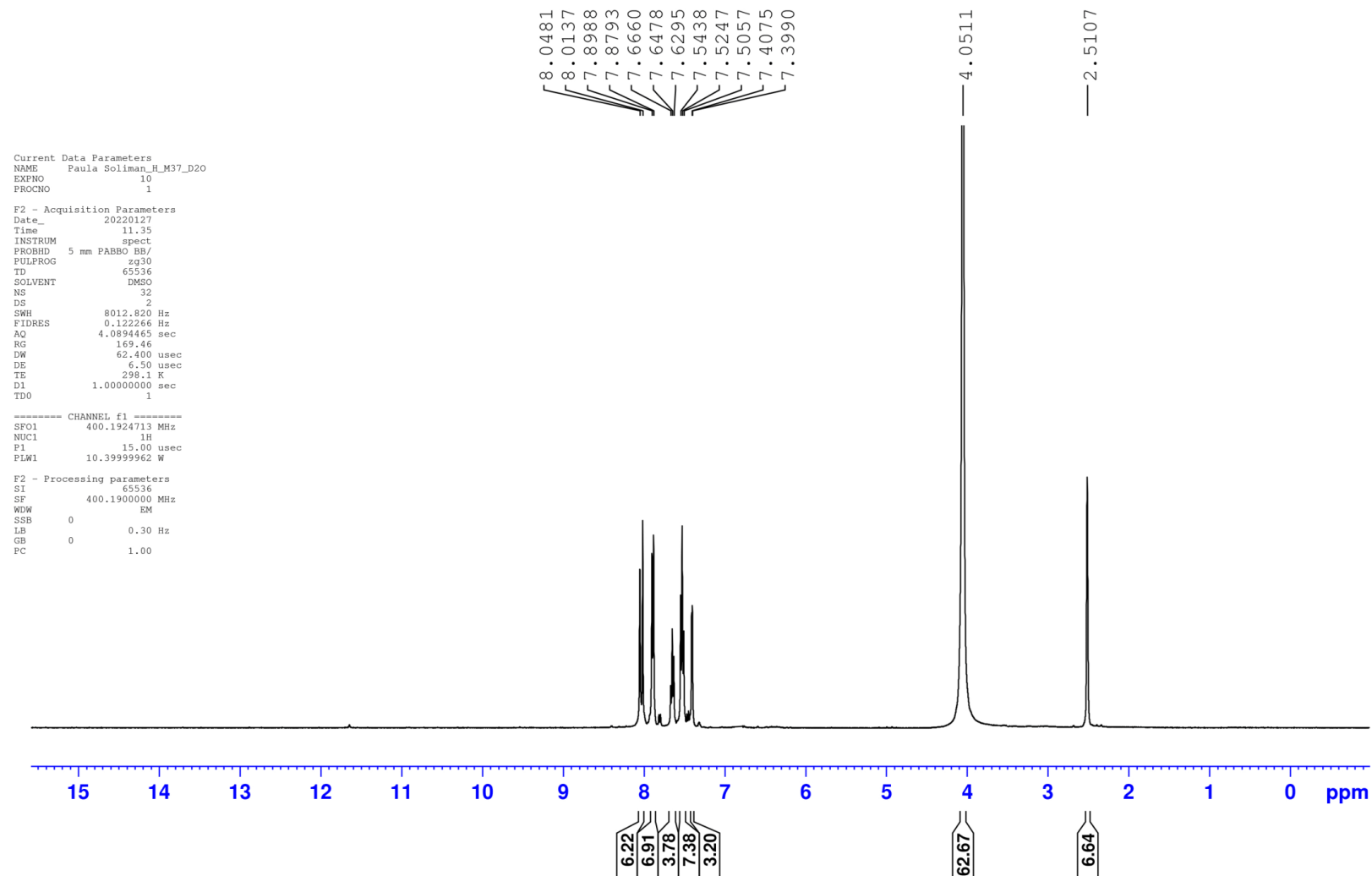
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg



D₂O of *N*-(6-(3-amino-4-cyano-5-(2,4-dichlorophenyl)-1H-pyrazol-1-yl)-4-(4-chlorophenyl)-7H-pyrazolo[3,4-*d*]pyrimidin-3-yl)benzamide (17).

Paula Soliman_H_M37_D2O

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg



D₂O of *N*-(6-(3-amino-4-cyano-5-(2,4-dichlorophenyl)-1*H*-pyrazol-1-yl)-4-(4-chlorophenyl)-7*H*-pyrazolo[3,4-*d*]pyrimidin-3-yl)benzamide (17).

Paula Soliman_C_M37

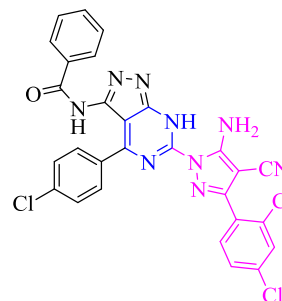
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg



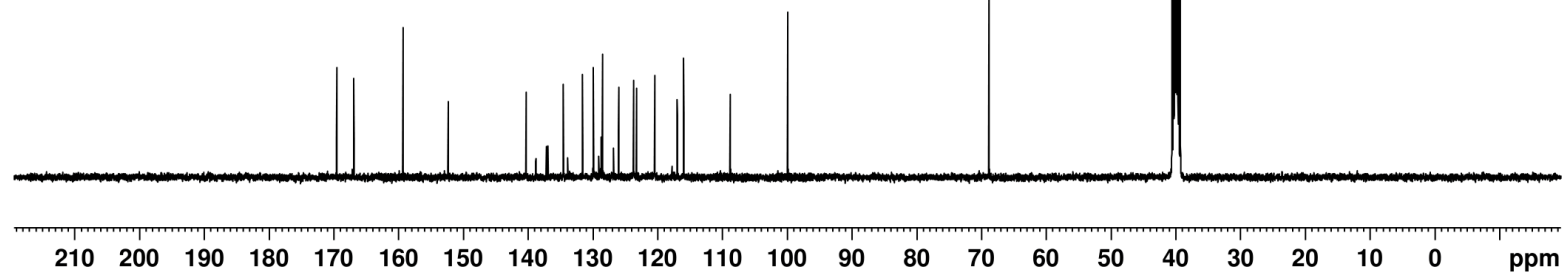
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116.06
109.42
100.05
68.90
40.62
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Current Data Parameters
NAME Paula Soliman_C_M37
EXPNO 10
PROCNO 1

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D1 2.00000000 sec
D11 0.03000000 sec
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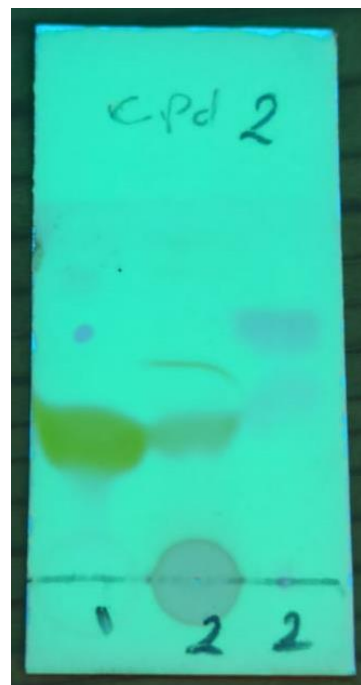


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P1 10.00 usec
PLW1 45.00000000 W
==== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2] waltz16



¹³C-NMR of *N*-(6-(3-amino-4-cyano-5-(2,4-dichlorophenyl)-1H-pyrazol-1-yl)-4-(4-chlorophenyl)-7H-pyrazolo[3,4-d]pyrimidin-3-yl)benzamide (17).

1.2. Impurity Profile



TLC following up for synthesizing compound 2.

TLC (Thin Layer Chromatography) monitoring process for the synthesis of Compound 2.

TLC is a common technique used in organic chemistry to monitor the progress of a reaction and to check the purity of reaction mixtures.

Spot (1): Compound 1 reactant.

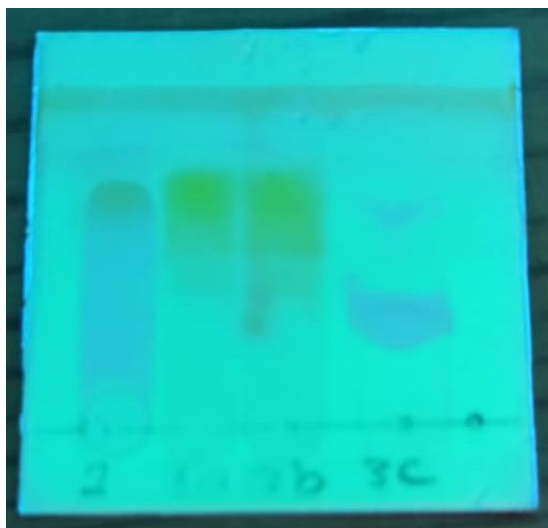
This is the starting material, Compound 1, before any reaction has taken place. It serves as a reference point to compare with subsequent spots.

Spot (2): After 1hr.

After 1 hour, we have a new spot on the TLC plate. This indicates the presence of a new compound formed during the reaction or a change in the starting material.

Spot (3): After reaction completion 3hr.

After 3 hours, we have another spot. This could indicate the formation of the desired Compound 2 or possibly other by-products. The movement of this spot on the TLC plate was provide information about the progress of the reaction and the purity of the final product.



TLC following up for synthesizing compound 3.

TLC (Thin Layer Chromatography) monitoring process for the synthesis of Compound 3.

Spot (1): Compound 2 reactant.

This is the starting material, Compound 2, before any reaction has taken place. It serves as a reference point to compare with subsequent spots.

Spot (2): After 1hr.

After 1hr, there is no changing in reaction, but the color was changed.

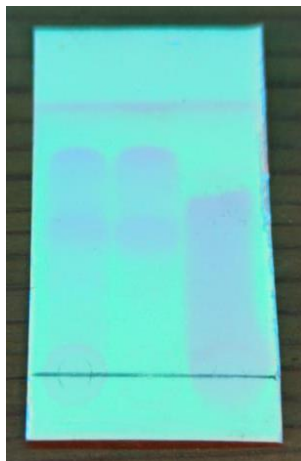
it suggested that there might be a transformation or reaction occurring in the mixture. The change in color could indicate the formation of an intermediate or a by-product that is not separated well on the TLC plate.

Spot (3): After 2.5hr.

After 2.5 hour, we have a new spot on the TLC plate. This indicates the presence of a new compound formed during the reaction or a change in the starting material.

Spot (4): After reaction completion 5hr.

After 5 hours, we have another spot. This could indicate the formation of the desired Compound 3 or possibly other by-products. The movement of this spot on the TLC plate was provide information about the progress of the reaction and the purity of the final product.



TLC following up for synthesizing compound 10.

TLC (Thin Layer Chromatography) monitoring process for the synthesis of Compound 10.

Spot (1): Compound 7 reactant.

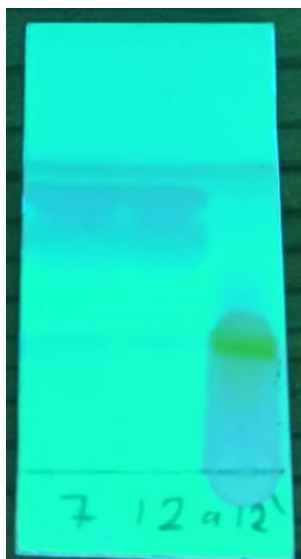
This is the starting material, Compound 7, before any reaction has taken place. It serves as a reference point to compare with subsequent spots.

Spot (2): After 30 min.

After 0.5 hour, we have not any new spot on the TLC plate.

Spot (3): After reaction completion 1.5hr.

After 3 hours, we have another spot. This could indicate the formation of the desired Compound 10 or possibly other by-products. The movement of this spot on the TLC plate was provide information about the progress of the reaction and the purity of the final product.



TLC following up for synthesizing compound 12.

TLC (Thin Layer Chromatography) monitoring process for the synthesis of Compound 12.

Spot (1): Compound 7 reactant.

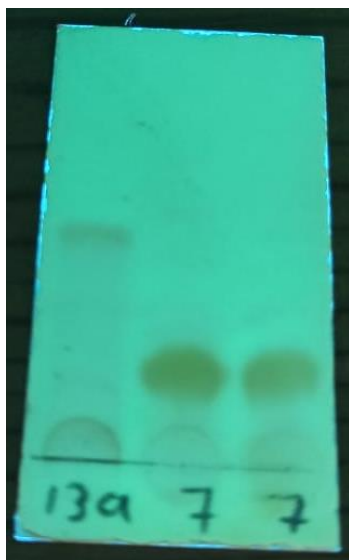
This is the starting material, Compound 7, before any reaction has taken place. It serves as a reference point to compare with subsequent spots.

Spot (2): After 4hr.

After 4 hours, we have not any new spot on the TLC plate.

Spot (3): After reaction completion 15hr.

After 15 hours, we have another spot and changing in color. This could indicate the formation of the desired Compound 12 or possibly other by-products. The movement of this spot on the TLC plate was provide information about the progress of the reaction and the purity of the final product.



TLC following up for synthesizing compound 13a.

TLC (Thin Layer Chromatography) monitoring process for the synthesis of Compound 13a.

Spot (1): Compound 7 reactant.

This is the starting material, Compound 7, before any reaction has taken place. It serves as a reference point to compare with subsequent spots.

Spot (2): After 1hr.

After 1hr, there is no changing in reaction, but the color was changed.

it suggested that there might be a transformation or reaction occurring in the mixture. The change in color could indicate the formation of an intermediate or a by-product that is not separated well on the TLC plate.

Spot (3): After reaction completion 3hr.

After 3 hours, we have another spot and changing in color. This could indicate the formation of the desired Compound 13a or possibly other by-products. The movement of this spot on the TLC plate was provide information about the progress of the reaction and the purity of the final product.

2. Biological Evaluation

2.1. Results of in-vitro primary single dose (10 μ M) full NCI 60 cell panel assay

Table S1: *In vitro* NCI 60 cell line anticancer screening results of compounds (2-17) at single dose of 10 μ M presented as percent cell growth promotion.

Panel/Cell Line	2	3	4	5	6	7	8	9	10	12	13a	13b	13c	14	15	16	17
Leukemia																	
CCRF-CEM	94.83	98.69	23.29	98.53	93.09	92.90	91.31	90.33	96.13	101.27	97.83	87.17	96.28	88.09	30.10	22.60	106.80
HL-60(TB)	96.07	100.71	31.92	93.69	94.10	92.51	93.19	101.91	98.02	116.88	101.08	101.67	111.51	86.24	7.37	5.63	124.44
K-562	97.62	99.49	26.48	82.62	87.33	98.76	87.44	90.78	100.26	100.16	104.53	89.52	93.99	96.74	12.36	11.14	95.51
MOLT-4	99.99	105.81	32.81	99.48	99.11	106.99	100.82	105.01	107.09	103.25	107.67	94.76	97.39	95.53	20.53	2.13	102.78
RPMI-8226	96.30	93.31	44.42	82.25	91.81	96.54	92.04	84.29	93.25	102.22	95.01	89.10	96.03	89.71	33.50	18.74	89.84
SR	91.60	86.05	18.16	84.90	83.15	90.92	75.24	87.02	89.30	101.38	67.82	85.36	94.11	88.85	25.67	7.20	85.43
Non-Small Cell Lung Cancer																	
A549/ATCC	96.74	107.60	57.21	105.81	103.64	102.29	96.48	109.95	102.91	100.71	104.21	103.13	93.11	82.97	24.58	7.56	96.54
EKVX	92.70	88.97	53.79	100.14	93.30	104.04	98.39	101.98	94.95	97.94	93.87	98.49	95.31	84.89	33.37	10.76	95.23
HOP-62	94.66	85.55	31.12	89.52	81.17	95.54	64.56	101.37	97.03	101.85	96.74	85.54	98.05	100.72	3.58	18.76	102.92
HOP-92	90.41	85.52	57.19	109.22	-95.03	94.90	86.33	119.49	98.20	101.99	75.56	106.45	93.70	91.32	56.77	32.34	131.97
NCI-H226	85.25	79.08	23.77	91.05	100.46	108.85	105.79	106.79	94.00	93.67	91.42	94.47	93.79	88.56	19.84	32.16	100.40
NCI-H23	96.86	97.22	58.58	94.27	97.18	99.99	88.54	100.09	94.95	102.42	94.01	101.05	102.17	90.23	1.50	-7.61	100.05
NCI-H322M	101.11	98.93	40.04	96.60	98.84	98.93	98.62	108.20	100.81	95.94	106.85	91.73	80.29	89.01	29.53	24.98	90.32
NCI-H460	99.15	99.35	15.80	97.54	114.75	99.95	111.61	110.25	107.98	104.77	83.25	91.98	98.32	93.32	6.93	4.04	93.04
NCI-H522	104.48	92.01	13.23	73.34	92.57	95.30	94.71	47.89	105.75	90.58	76.48	93.50	88.74	82.72	-9.93	-30.52	99.02
Colon Cancer																	
COLO 205	122.30	126.57	115.51	99.18	N/A	N/A	N/A	N/A	N/A	11.12	N/A	119.94	124.17	103.43	-36.06	-62.28	126.27
HCC-2998	98.77	87.10	54.12	94.24	107.34	107.13	109.22	115.43	108.45	102.64	92.99	112.81	102.70	96.22	3.16	-5.78	108.53
HCT-116	99.08	98.77	38.32	99.26	97.35	98.83	92.71	101.24	94.82	98.26	84.77	88.28	100.11	100.33	9.09	-19.42	114.28
HT29	97.81	100.90	31.74	89.18	99.99	101.83	95.72	90.85	101.89	100.02	96.02	81.15	89.80	69.26	16.72	-29.73	87.90
KM12	104.66	99.79	49.25	109.24	112.25	105.22	117.20	118.60	110.67	101.75	75.73	108.21	113.56	86.65	13.25	0.19	104.59
	98.46	99.34	39.89	100.26	100.10	100.33	97.87	104.51	99.12	105.35	96.53	99.97	101.77	82.91	27.56	-6.67	91.89
	102.58	100.91	48.91	96.40	105.09	106.80	106.16	105.66	101.45	101.55	95.15	96.99	101.44	96.95	22.91	4.14	115.86

SW-620																	
<u>CNS Cancer</u>																	
SF-268	92.78	92.82	42.17	97.39	101.14	109.39	102.95	115.73	100.95	95.36	98.10	92.69	93.17	89.88	38.66	23.77	95.90
SF-295	101.73	91.93	50.97	94.77	96.18	102.91	79.18	102.28	101.57	92.09	77.21	94.46	91.01	86.43	-13.87	16.19	98.58
SF-539	94.69	96.21	46.40	93.99	91.46	96.38	85.37	101.85	96.76	92.70	87.68	92.91	94.70	93.28	-63.68	-4.38	92.81
SNB-19	95.31	94.30	32.65	91.18	85.25	93.80	75.64	89.33	92.11	94.16	86.94	91.59	90.49	93.83	31.06	N/A	93.68
SNB-75	68.54	63.79	50.42	84.72	95.26	92.24	89.00	110.12	82.92	N/A	48.37	N/A	N/A	N/A	N/A	29.18	N/A
U251	106.76	108.54	48.70	102.25	96.68	96.84	72.78	103.09	101.00	98.14	87.92	81.65	93.06	92.89	6.80	2.68	98.32
<u>Prostate Cancer</u>																	
PC-3	92.80	100.67	64.50	104.19	76.29	91.66	94.23	101.31	100.60	96.44	93.79	104.03	96.90	88.28	6.40	-11.29	110.58
DU-145	100.21	101.08	57.23	99.76	106.08	103.18	100.37	105.62	102.59	110.21	106.16	103.32	102.74	88.08	7.01	25.71	102.24
<u>Melanoma</u>																	
LOX IMVI	103.64	109.00	42.53	86.93	104.68	113.53	111.35	118.10	120.02	102.68	102.28	86.82	99.19	64.62	5.24	-98.48	100.58
MALME-3M	89.06	92.15	77.76	85.07	92.71	98.52	98.52	96.01	93.51	99.02	77.76	90.10	97.01	78.85	13.66	-26.04	101.81
M14	100.84	104.34	58.48	98.30	96.79	101.63	106.98	101.24	99.56	106.99	68.24	91.77	103.38	99.11	-3.96	-43.66	110.64
MDA-MB-435	100.22	101.16	56.43	98.75	102.63	103.18	103.14	103.52	100.51	99.74	60.00	99.03	97.31	91.58	-44.38	-19.82	98.92
SK-MEL-2	107.90	104.91	68.94	106.88	107.49	114.78	107.52	114.65	112.83	N/A	86.36	N/A	N/A	N/A	N/A	N/A	N/A
SK-MEL-28	104.18	109.73	48.12	101.54	105.62	105.67	117.02	110.59	111.47	108.39	104.33	92.56	96.21	101.18	53.82	14.35	111.46
SK-MEL-5	96.17	96.28	45.80	97.12	98.91	101.48	97.35	100.14	97.72	98.29	87.86	97.39	78.50	85.74	0.62	-98.61	99.78
UACC-257	106.34	104.22	92.43	105.68	98.82	103.24	104.92	106.74	101.95	101.90	85.19	98.17	98.83	95.90	69.66	20.20	101.52
UACC-62	101.15	99.07	34.05	92.36	94.17	102.03	93.48	105.00	102.19	92.41	76.79	81.08	77.80	66.26	30.11	14.34	82.10
<u>Ovarian Cancer</u>																	
IGROV1	107.22	94.63	40.42	92.51	103.69	100.11	97.46	108.76	118.34	107.33	114.60	109.70	98.36	105.25	26.52	21.89	79.48
OVCAR-3	103.53	104.06	43.93	100.18	112.27	116.73	118.44	117.20	109.37	99.52	119.45	88.82	83.64	92.11	13.52	22.67	86.29
OVCAR-4	100.29	99.72	50.29	94.24	94.57	99.87	96.78	95.36	96.94	95.85	107.35	105.40	103.92	110.87	24.85	11.33	124.63
OVCAR-5	108.44	101.17	66.28	101.03	108.97	103.51	116.32	124.46	121.99	107.66	119.50	98.34	99.65	95.47	11.08	16.48	104.56
OVCAR-8	103.71	99.82	44.43	101.87	98.76	106.16	91.58	105.53	107.40	106.60	102.37	77.28	102.05	89.60	-23.25	-29.69	109.59
SK-OV-3	105.38	94.69	53.65	94.55	82.59	108.44	99.27	108.33	103.02	98.01	110.38	108.15	97.84	100.62	-5.94	19.95	122.91
<u>Renal Cancer</u>																	
786-0	99.74	98.38	53.59	100.76	95.31	98.47	72.41	103.37	96.85	103.31	96.19	101.95	97.92	9187	2.33	7.00	108.46
A498	97.35	107.99	78.80	108.37	117.20	114.49	100.97	106.14	110.45	107.21	119.30	114.54	92.09	90.13	79.21	72.50	121.58
ACHN	96.67	98.73	40.45	100.60	95.15	108.39	78.81	107.17	104.39	100.49	99.37	98.74	91.99	86.67	30.39	12.53	103.15
CAKI-1	91.05	83.81	42.20	90.47	73.15	93.81	74.07	89.09	89.14	90.66	73.94	90.95	97.65	67.05	23.90	13.72	92.68
RXF 393	90.88	99.21	60.61	119.24	101.47	99.66	87.59	105.02	97.16	101.35	102.77	99.76	84.07	96.81	-35.47	-13.52	101.96
SN12C	100.19	96.56	41.15	97.91	92.38	92.59	97.13	103.53	104.12	95.28	92.42	91.64	87.09	85.07	32.54	-17.37	95.19
TK-10	111.70	153.37	51.69	125.43	117.29	138.75	119.03	111.54	120.34	103.45	115.33	108.56	101.92	106.30	56.23	64.00	115.88
UO-31	90.47	89.92	29.60	83.88	64.68	87.99	91.27	82.24	88.29	94.00	75.46	87.58	80.19	76.65	24.46	17.31	95.86

Breast Cancer																	
MCF7	91.49	76.58	52.11	92.64	96.19	96.76	84.28	89.01	91.37	91.32	88.21	88.85	58.32	82.43	16.66	0.67	16.51
MDA-MB 231/ATCC	91.26	86.07	53.75	93.92	80.10	77.04	67.92	94.26	96.33	101.89	74.22	106.69	94.23	72.00	-20.77	-4.05	86.28
HS 578T	96.37	89.15	58.21	92.60	86.73	95.88	74.01	101.05	97.55	93.77	79.95	93.59	70.46	90.47	-0.63	17.55	90.40
BT-549	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	104.29	N/A	99.47	100.35	118.95.	33.47	27.07	120.88
T-47D	98.15	76.23	48.83	89.21	82.52	97.21	89.56	97.61	100.40	95.87	82.28	102.42	84.32	79.14	24.07	7.66	74.02
MDA-MBA-468	91.65	97.02	46.12	96.77	100.38	118.11	106.25	120.31	100.53	96.49	101.68	92.87	72.00	99.03	-36.27	-21.38	-12.76
Mean	98.21	97.40	47.92	96.62	93.18	101.29	94.86	102.81	101.25	100.27	92.06	96.21	93.96	90.12	13.44	2.30	98.35

* Results are presented as percent cell growth promotion.

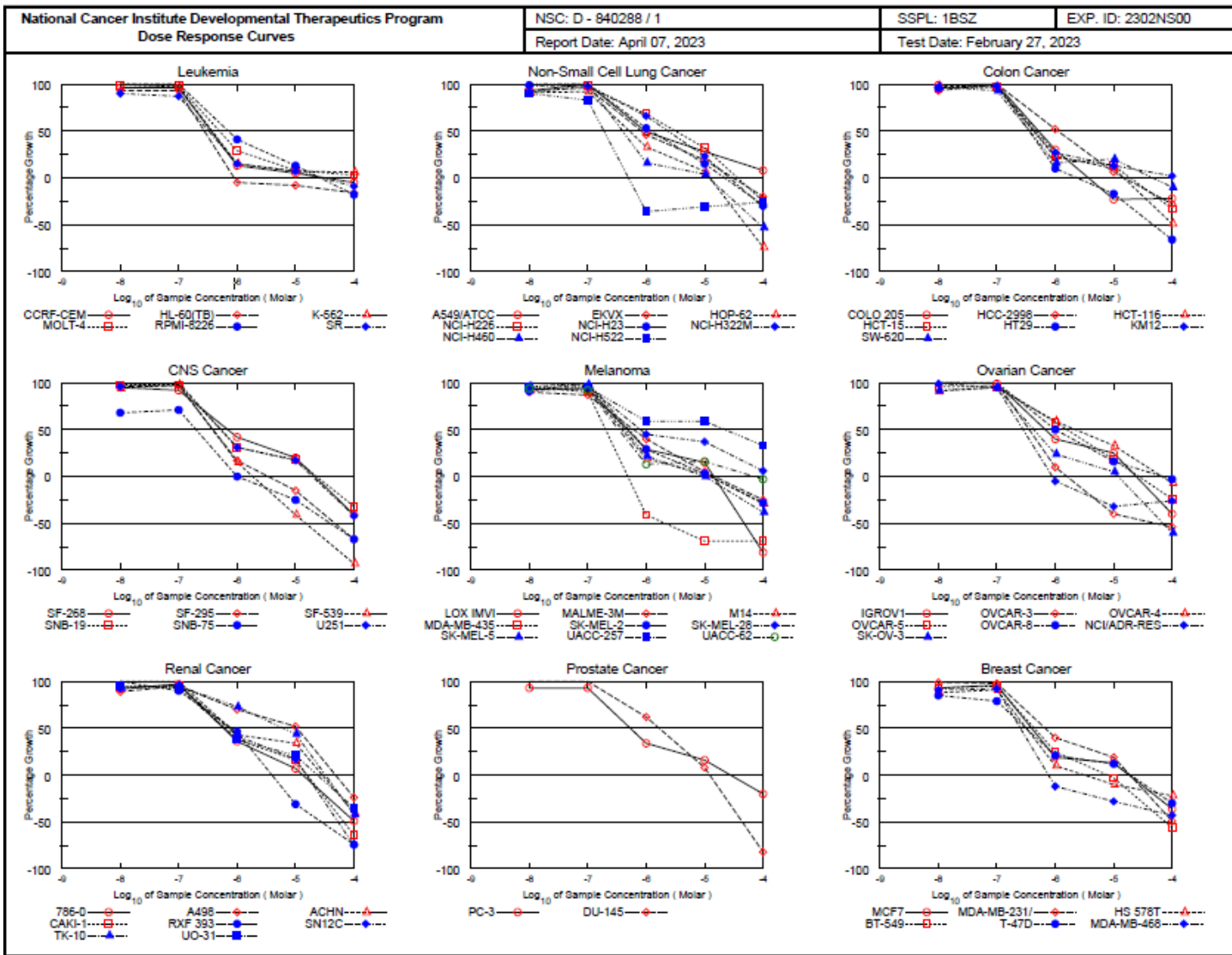
* Values less than 10% growth promotion are presented in bold.

2.2. Five Doses

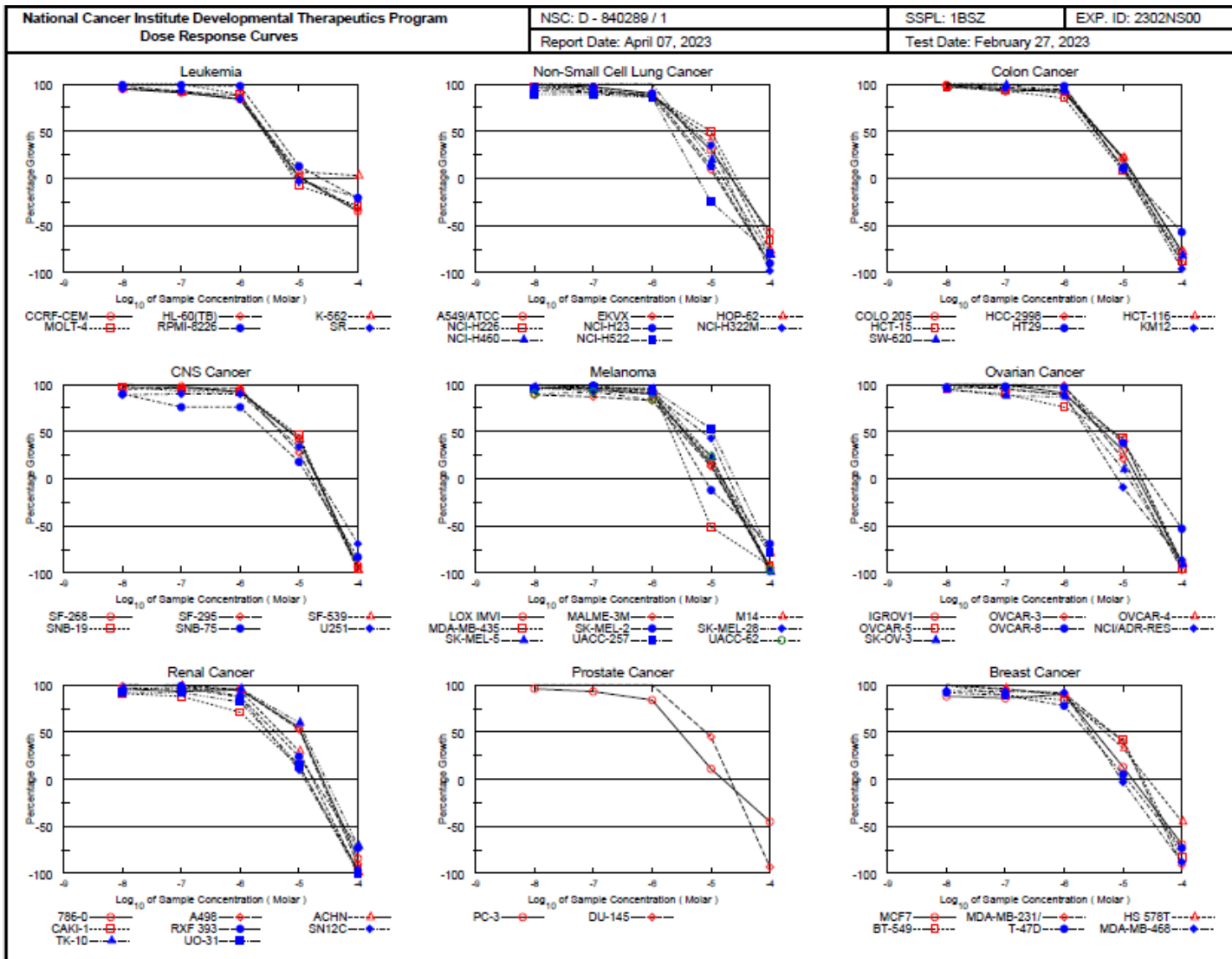
Table S2: *In vitro* NCI 5 log dose results for compounds (15 and 16) in μ M against 60 cell panel.

Panel	Cell Line	Compound 15			Compound 16		
		GI ₅₀	TGI	LC ₅₀	GI ₅₀	TGI	LC ₅₀
Leukemia	CCRF-CEM	3.58	3.28	>100	2.60	1.09	>100
	HL-60(TB)	2.74	8.88	>100	2.76	1.12	>100
	K-562	3.79	>100	>100	2.76	>100	>100
	MOLT-4	5.03	>100	>100	2.54	8.36	>100
	RPMI-8226	7.20	2.69	>100	3.65	2.40	>100
	SR	3.26	2.80	>100	2.47	9.23	>100
Non-Small Cell Lung Cancer	A549/ATCC	9.63	>100	>100	4.62	2.20	8.29
	EKVX	8.44	3.06	>1005.	3.01	1.24	3.97
	HOP-62	5.14	1.21	00	6.99	2.29	5.96
	HOP-92	ND	ND	ND	ND	ND	ND
	NCI-H226	3.17	3.58	>100	9.98	2.71	7.36
	NCI-H23	1.18	2.18	>100	3.27	1.33	4.10
	NCI-H322M	2.40	2.71	>100	5.30	1.83	4.35
	NCI-H460	3.92	1.16	8.76	4.54	1.59	4.91
	NCI-H522	1.89	4.97	>100	2.12	5.99	2.88
Colon Cancer	COLO 205	5.251.	3.69	>100	4.02	1.67	5.25
	HCC-2998	11	1.53	>100	3.97	1.52	4.33
	HCT-116	4.30	1.50	>100	3.92	1.68	5.30
	HCT-15	4.18	1.95	>100	2.86	1.21	4.09
	HT29	3.83	2.38	4.75	3.48	1.40	7.79
	KM12	4.72	>100	>100	3.40	1.29	3.73
	SW-620	3.63	4.62	>100	3.33	1.31	4.50
CNS Cancer	SF-268	6.95	2.16	>100	6.98	2.07	4.88
	SF-295	3.88	3.43	4.80	4.77	1.70	4.37
	SF-539	3.82	1.86	1.47	6.85	2.00	4.60
	SNB-19	5.19	2.27	>100	8.31	2.12	4.79
	SNB-75	2.00	1.01	3.85	2.77	1.50	4.68
	U251	5.38	1.97	>100	5.20	2.15	6.60

Melanoma	LOX IMVI	4.79	1.42	4.70	3.43	1.39	4.03
	MALME-3M	6.06	1.50	>100	2.93	1.31	3.81
	M14	3.88	1.26	>100	3.61	1.53	5.03
	MDA-MB-435	2.03	4.88	2.13	2.06	4.52	9.91
	SK-MEL-2	5.05	1.26	>100	2.58	7.75	4.69
	SK-MEL-28	7.99	>100	>100	7.01	2.02	4.58
	SK-MEL-5	4.24	9.51	>100	4.21	1.54	3.97
	UACC-257	2.18	>100	>100	1.05	2.53	6.10
	UACC-62	3.39	7.29	>100	3.72	1.59	4.13
Ovarian Cancer	IGROV1	6.87	2.44	>100	4.77	1.79	4.69
	OVCAR-3	3.94	1.57	4.91	4.25	1.51	4.01
	OVCAR-4	2.28	6.79	>100	6.67	2.09	5.05
	OVCAR-5	1.59	2.68	>100	6.52	2.06	4.68
	OVCAR-8	1.03	7.13	>100	6.34	2.62	9.19
	NCI/ADR-RES	2.82	8.87	>100	2.52	8.13	3.42
	SK-OV-3	4.30	1.19	7.10	3.00	1.25	3.91
Renal Cancer	786-0	5.90	1.32	>100	1.08	2.48	5.70
	A498	1.07	4.83	>100	1.05	2.35	5.25
	ACHN	7.68	2.88	>100	4.86	1.71	4.15
	CAKI-1	6.27	1.58	6.68	2.33	1.35	3.89
	RXF 393	8.10	3.93	2.71	3.96	1.78	5.84
	SN12C	7.20	1.53	5.31	3.05	1.25	3.69
	TK-10	6.32	3.24	>100	1.20	2.88	6.90
	UO-31	6.11	2.39	>100	2.98	1.35	3.68
Prostate Cancer	PC-3	5.36	2.80	>100	2.92	1.58	>100
	DU-145	1.65	1.22	4.39	8.09	2.11	4.88





Dose response curve for compound 15.


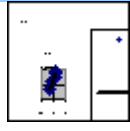


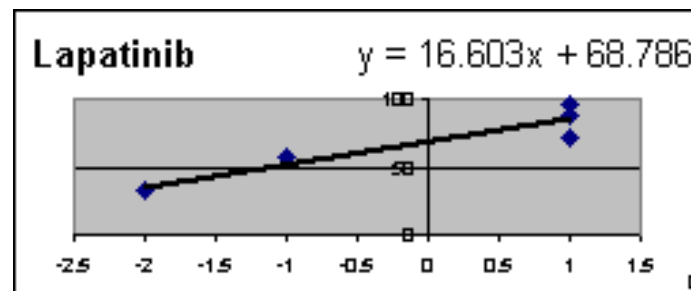
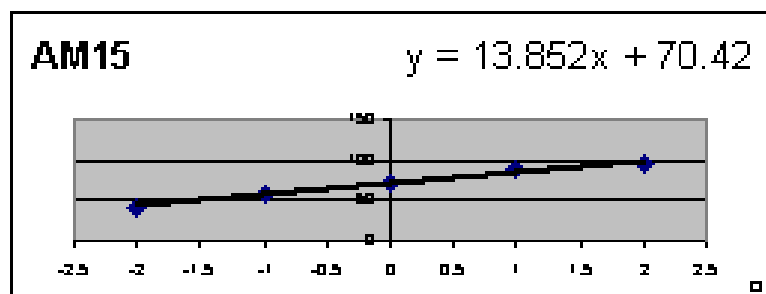
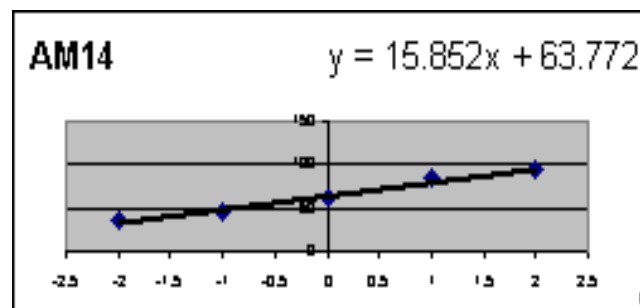
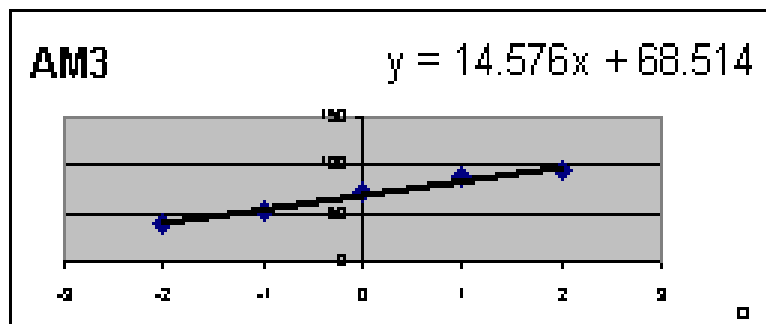
Dose response curve for compound 16.

2.3. In vitro EGFR tyrosine kinase inhibitory activity

Table 3S: Epidermal growth factor receptor biological activity of compounds (4, 15 and 16).

EGFR											
code	IC50	conc	log	%inh	T2	T1	ΔT	RFU2	RFU1	slope	K.Activity
4		100	2	94	30	0	30	6.18	0	3.33333	7.416007
		10	1	87	30	0	30	13.44	0	3.33333	16.12802
		1	0	71	30	0	30	28.57	0	3.33333	34.28403
		0.1	-1	53	30	0	30	46.92	0	3.33333	56.30406
		0.01	-2	38	30	0	30	62.32	0	3.33333	74.78407
	EC				0	30	0	30	100	0	3.33333
code	IC50	conc	log	%inh	T2	T1	ΔT	RFU2	RFU1	slope	K.Activity
15		100	2	94	30	0	30	6.22	0	3.33333	7.464007
		10	1	85	30	0	30	15.28	0	3.33333	18.33602
		1	0	61	30	0	30	39.11	0	3.33333	46.93205
		0.1	-1	45	30	0	30	54.82	0	3.33333	65.78407
		0.01	-2	34	30	0	30	65.71	0	3.33333	78.85208

EC				0	30	0	30	100	0	3.33333	120
code	IC50	conc	log	%inh	T2	T1	ΔT	RFU2	RFU1	slope	K.Activity
16		100	2	94	30	0	30	5.59	0	3.33333	6.708007
		10	1	88	30	0	30	12.03	0	3.33333	14.43601
		1	0	72	30	0	30	27.66	0	3.33333	33.19203
		0.1	-1	56	30	0	30	43.51	0	3.33333	52.21205
		0.01	-2	41	30	0	30	59.11	0	3.33333	70.93207
EC				0	30	0	30	100	0	3.33333	120
code	IC50	conc	log	%inh	T2	T1	ΔT	RFU2	RFU1	slope	K.Activity
Lapatinib		10	1	95	30	0	30	5.07	0	3.33333	6.084006
		10	1	88	30	0	30	11.61	0	3.33333	13.93201
		10	1	71	30	0	30	28.91	0	3.33333	34.69203
		0.1	-1	57	30	0	30	42.55	0	3.33333	51.06005
		0.01	-2	32	30	0	30	67.93	0	3.33333	81.51608
EC				0	30	0	30	100	0	3.33333	120



Curves for compounds **4**, **15**, **16**, and **Lapatinib**