

**$\beta$ -Enaminonitrile in the Synthesis of Tetrahydrobenzo[*b*]thiophene Candidates with DFT Simulation, *In vitro* Antiproliferative Assessment, Molecular docking, and Modeling Pharmacokinetics**

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**Supporting information:**

## DFT study

**Table S1.** Energy level distribution of frontier orbitals and global reactivity indices of substances **2-12**.

Compds.	*E	E <sub>HOMO</sub> (eV)	E <sub>LUMO</sub> (eV)	ΔE (eV)	μ (Debye)	η (eV)	ζ (eV <sup>-1</sup> )	μ <sub>o</sub> (eV)	ω (eV)	n (eV <sup>-1</sup> )	I <sub>p</sub> (eV)	EA (eV)	x (eV)
<b>2</b>	11.256	-6.994	0.367	7.361	-1.357	3.680	0.272	-3.313	1.491	0.671	6.994	-0.367	3.313
<b>3</b>	9.888	-8.164	0.366	8.530	-9.302	4.265	0.234	-3.899	1.782	0.561	8.164	-0.366	3.899
<b>4</b>	13.319	-7.055	0.365	7.420	-7.469	3.710	0.269	-3.345	1.508	0.663	7.055	-0.365	3.345
<b>5</b>	29.559	-8.065	-1.975	6.090	-3.633	0.987	1.013	5.020	12.766	0.078	8.065	1.975	5.020
<b>6</b>	11.020	-8.151	0.366	8.517	-8.823	4.258	0.235	-3.892	1.779	0.562	8.151	-0.366	3.892
<b>7</b>	14.159	-7.071	0.365	7.436	-6.829	3.718	0.269	-3.353	1.512	0.661	7.071	-0.365	3.353
<b>8</b>	40.965	-8.120	-3.458	8.486	-14.058	4.243	0.236	-5.789	3.949	0.253	8.120	3.458	5.789
<b>9</b>	23.498	-6.650	0.366	7.016	1.185	3.508	0.285	-3.142	1.407	0.711	6.650	-0.366	3.142
<b>10</b>	18.968	-7.618	0.366	7.984	-3.135	3.992	0.250	-3.626	1.647	0.607	7.618	-0.366	3.626
<b>11</b>	31.245	-7.152	-5.612	1.540	3.458	0.770	1.299	-6.382	26.448	0.038	7.152	5.612	6.382
<b>12</b>	47.800	-7.439	-5.463	1.976	-1.165	0.988	1.012	-6.451	21.060	0.047	7.439	5.463	6.451
<b>Dox.</b>	67.785	-9.189	-7.149	2.040	3.954	1.020	0.98	-8.169	32.72	0.030	9.189	7.149	8.169

\*E: Minimized Energy (kcal/mol)

Dox.: Doxorubicin

μ: Dipole/dipole

η: Global Hardness

ζ: Global Softness

μ<sub>o</sub>: Chemical Potential

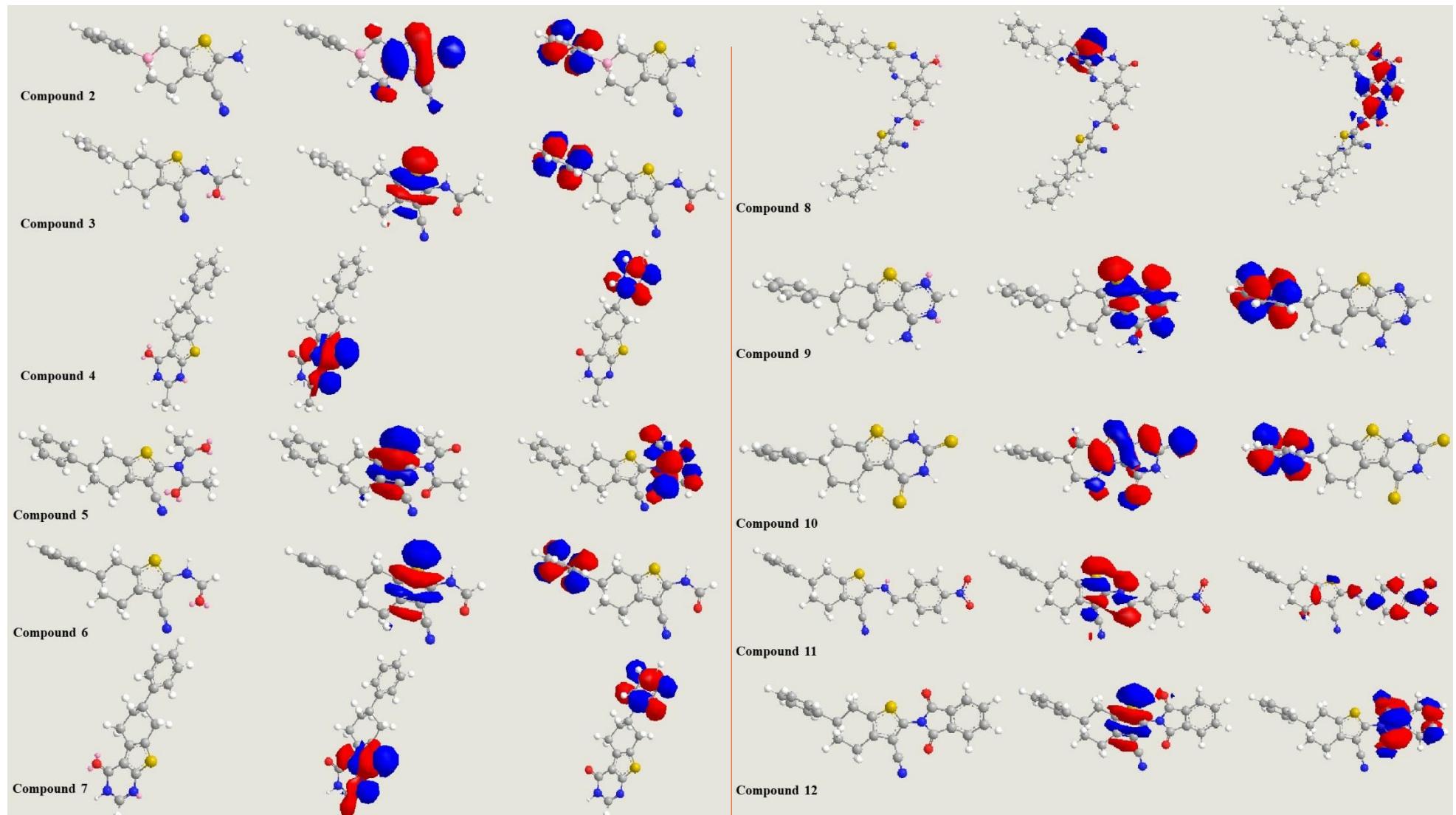
ω: Global Electrophilicity Index

n: Nucleophilicity Index

I<sub>p</sub>: Ionization Potential

EA: Electron Affinity

x: Electronegativity



**Fig. S1.** Optimized configurations (left), HOMO (middle), and LUMO (right) of substances **2-12**.

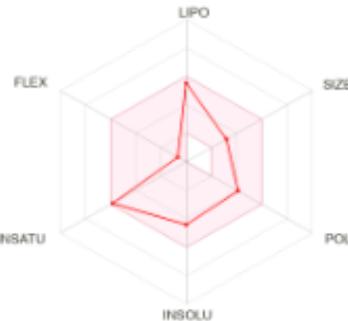
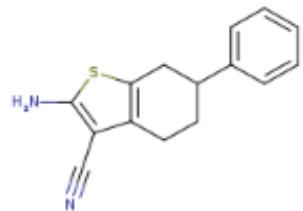
Atom color index: grey C, white H, blue N, red O, yellow S, and green Cl.

**Table S2.** Physicochemical Properties / Lipophilicity / Drug-likeness properties of compounds **2-12**.

Entry	Compounds										
	2	3	4	5	6	7	8	9	10	11	12
Molecular weight (g/mol)	254.35	296.39	296.39	338.42	282.36	282.36	638.80	281.38	330.49	387.45	384.45
Num. heavy atoms	18	21	21	24	20	20	46	20	21	28	28
Num. arom. heavy	11	11	15	11	11	15	28	15	15	17	17
Fraction Csp3	0.27	0.29	0.29	0.32	0.25	0.25	0.21	0.25	0.25	0.18	0.17
Num. rotatable bonds	1	3	1	4	3	1	8	1	1	4	2
Num. H-bond acceptor	1	2	2	3	2	2	4	2	0	4	3
Num. H-bond donors	1	1	1	0	1	1	2	1	2	0	0
Molar Refractivity	75.36	85.27	87.13	95.17	80.85	82.16	183.89	83.74	94.11	113.47	111.47
TPSA (Å <sup>2</sup> )	78.05	81.13	73.99	89.41	81.13	73.99	162.26	80.04	124.00	110.21	89.41
Consensus Log P <sub>o/w</sub>	3.41	3.48	3.71	3.45	3.38	3.42	7.33	3.47	4.74	4.39	4.37
Lipinski's Rule	Yes	Yes	Yes	Yes	Yes	Yes	No	Yes	Yes	Yes	Yes
Bioavailability Score	0.55	0.55	0.55	0.55	0.55	0.55	0.17	0.55	0.55	0.55	0.55
Pharmacokinetics											
GI absorption	High	High	High	High	High	High	Low	High	Low	Low	High
BBB permeant	Yes	No	Yes	No	No	Yes	No	No	No	No	No
P-gp substrate	Yes	No	Yes	No	No	Yes	No	Yes	Yes	No	No
CYP1A2 inhibitor	Yes	Yes	Yes	No	Yes						

CYP2C19 inhibitor	Yes	Yes	Yes	Yes	Yes	Yes	No	Yes	Yes	Yes	Yes
CYP2C9 inhibitor	Yes	Yes	Yes	Yes	Yes	Yes	No	Yes	Yes	Yes	Yes
CYP2D6 inhibitor	No										
CYP3A4 inhibitor	No	Yes	No	Yes	No	No	No	Yes	Yes	Yes	Yes
Log K <sub>p</sub> (Skin permeation) (cm/s)	-4.91	-5.27	-5.74	-5.94	-5.17	-5.65	-3.52	-5.30	-5.28	-4.83	-5.23

(2)



SMILES N#Cc1c(N)sc2c1CCC(C2)c1ccccc1

## Physicochemical Properties

Formula	C15H14N2S
Molecular weight	254.35 g/mol
Num. heavy atoms	18
Num. arom. heavy atoms	11
Fraction Csp3	0.27
Num. rotatable bonds	1
Num. H-bond acceptors	1
Num. H-bond donors	1
Molar Refractivity	75.38
TPSA	78.05 Å <sup>2</sup>

## Lipophilicity

Log $P_{\text{o/w}}$ (iLOGP)	2.52
Log $P_{\text{o/w}}$ (XLOGP3)	4.15
Log $P_{\text{o/w}}$ (WLOGP)	3.48
Log $P_{\text{o/w}}$ (MLOGP)	2.50
Log $P_{\text{o/w}}$ (SILICOS-IT)	4.39
Consensus Log $P_{\text{o/w}}$	3.41

Water Solubility	
Log S (ESOL)	-4.42
Solubility	9.72e-03 mg/ml ; 3.82e-05 mol/l
Class	Moderately soluble
Log S (Ali)	-5.50
Solubility	8.10e-04 mg/ml ; 3.19e-06 mol/l
Class	Moderately soluble
Log S (SILICOS-IT)	-4.79
Solubility	4.09e-03 mg/ml ; 1.61e-05 mol/l
Class	Moderately soluble
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	Yes
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log $K_p$ (skin permeation)	-4.91 cm/s
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55
Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	3.28

Fig. S2. ADME of compound 2.

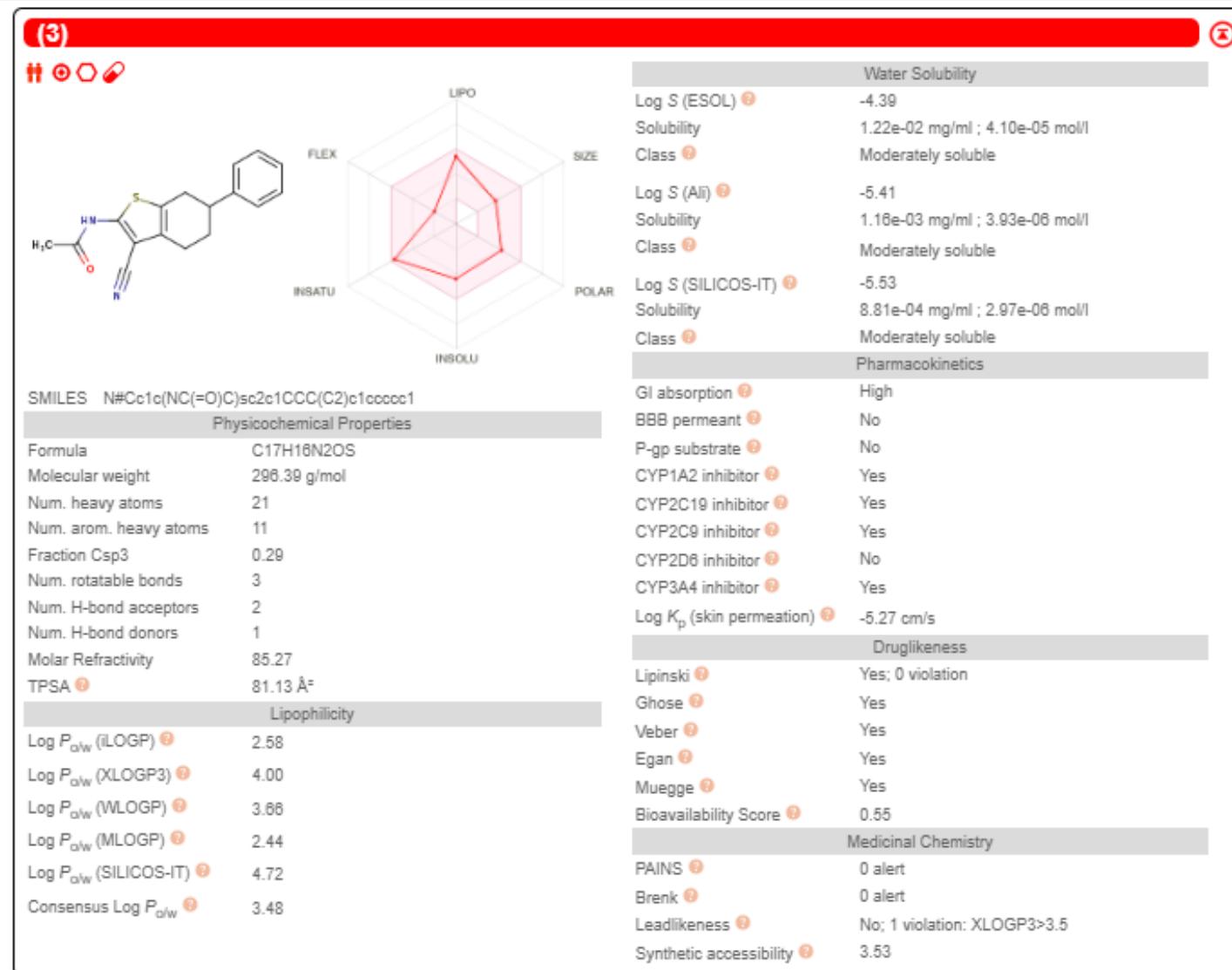
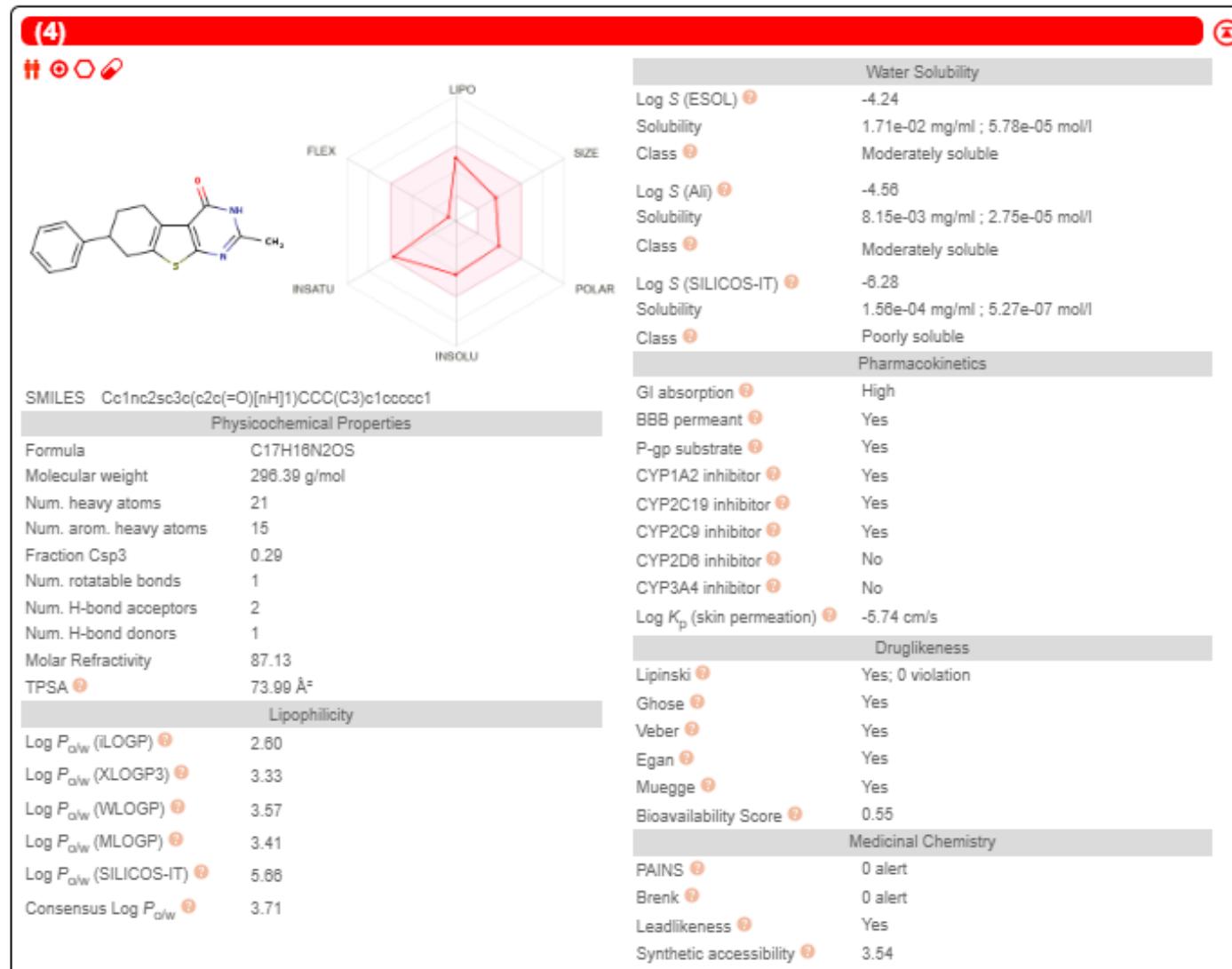


Fig. S3. ADME of compound 3.



**Fig. S4.** ADME of compound 4.

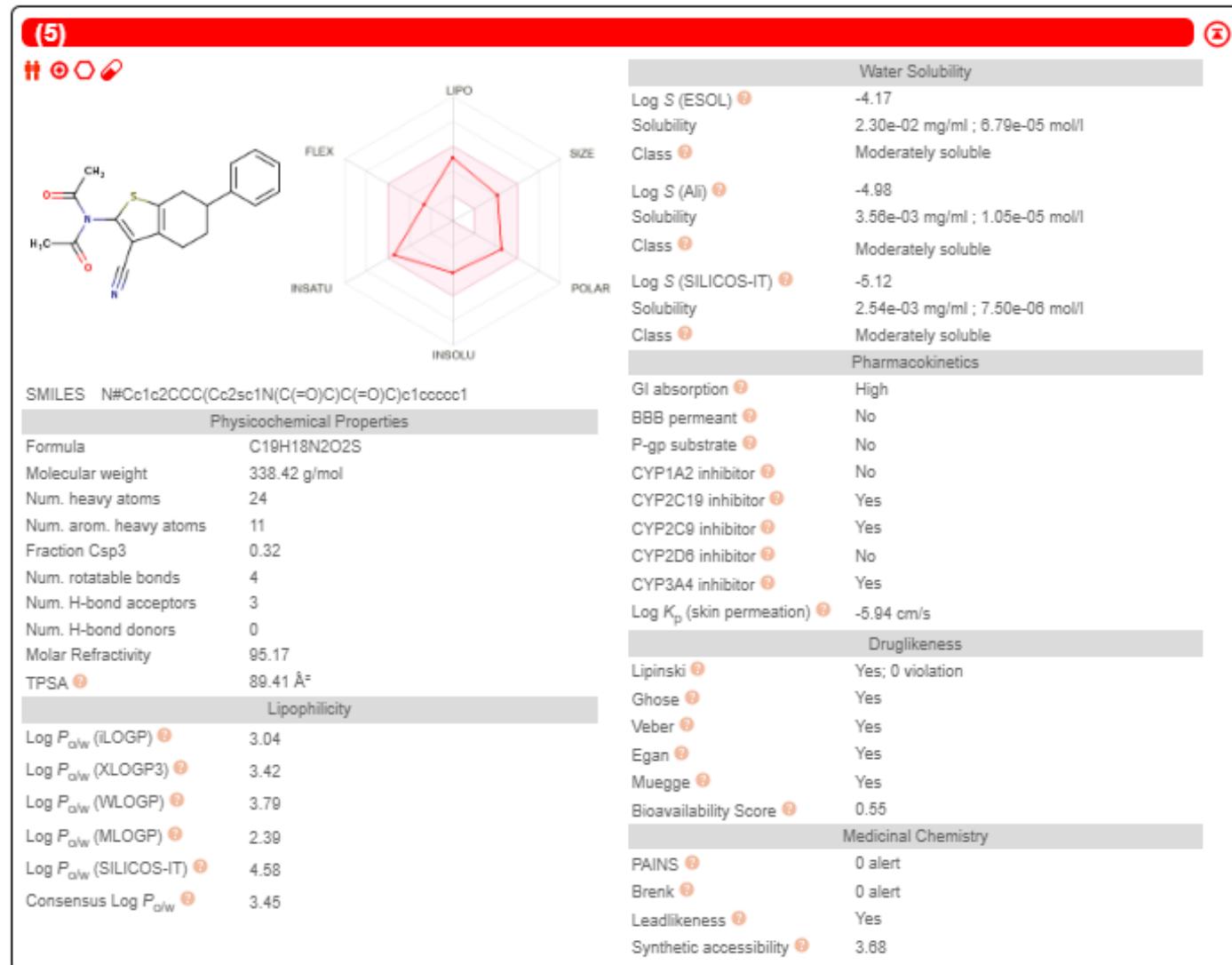
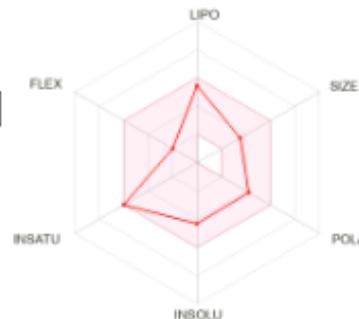
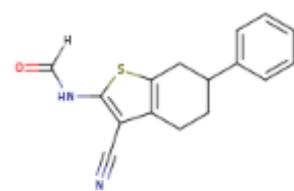


Fig. S5. ADME of compound 5.

(6)



SMILES O=CNC1SC2C(C1C#N)CCC(C2)c1ccccc1

## Physicochemical Properties

Formula	C <sub>18</sub> H <sub>14</sub> N <sub>2</sub> OS
Molecular weight	282.36 g/mol
Num. heavy atoms	20
Num. arom. heavy atoms	11
Fraction Csp <sup>3</sup>	0.25
Num. rotatable bonds	3
Num. H-bond acceptors	2
Num. H-bond donors	1
Molar Refractivity	80.85
TPSA	81.13 Å <sup>2</sup>

## Lipophilicity

Log P <sub>o/w</sub> (iLOGP)	2.48
Log P <sub>o/w</sub> (XLOGP3)	4.02
Log P <sub>o/w</sub> (WLOGP)	3.27
Log P <sub>o/w</sub> (MLOGP)	2.61
Log P <sub>o/w</sub> (SILICOS-IT)	4.50
Consensus Log P <sub>o/w</sub>	3.38

## Water Solubility

Log S (ESOL)	-4.33
Solubility	1.31e-02 mg/ml ; 4.85e-05 mol/l
Class	Moderately soluble
Log S (Ali)	-5.43
Solubility	1.06e-03 mg/ml ; 3.75e-06 mol/l
Class	Moderately soluble
Log S (SILICOS-IT)	-5.14
Solubility	2.02e-03 mg/ml ; 7.16e-06 mol/l
Class	Moderately soluble

## Pharmacokinetics

GI absorption	High
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K <sub>p</sub> (skin permeation)	-5.17 cm/s

## Druglikeness

Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

## Medicinal Chemistry

PAINS	0 alert
Brenk	1 alert: aldehyde
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	3.45

Fig. S6. ADME of compound 6.

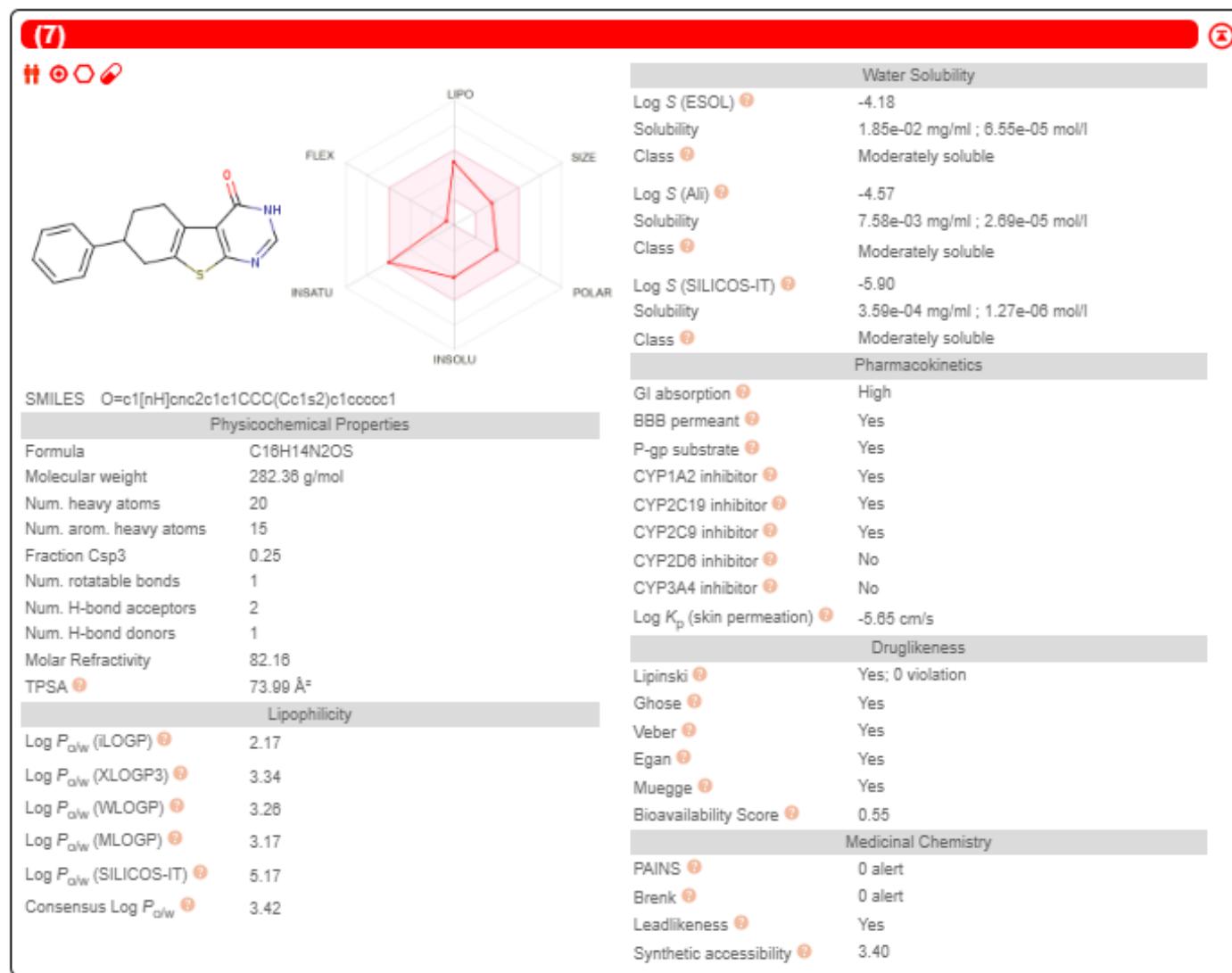
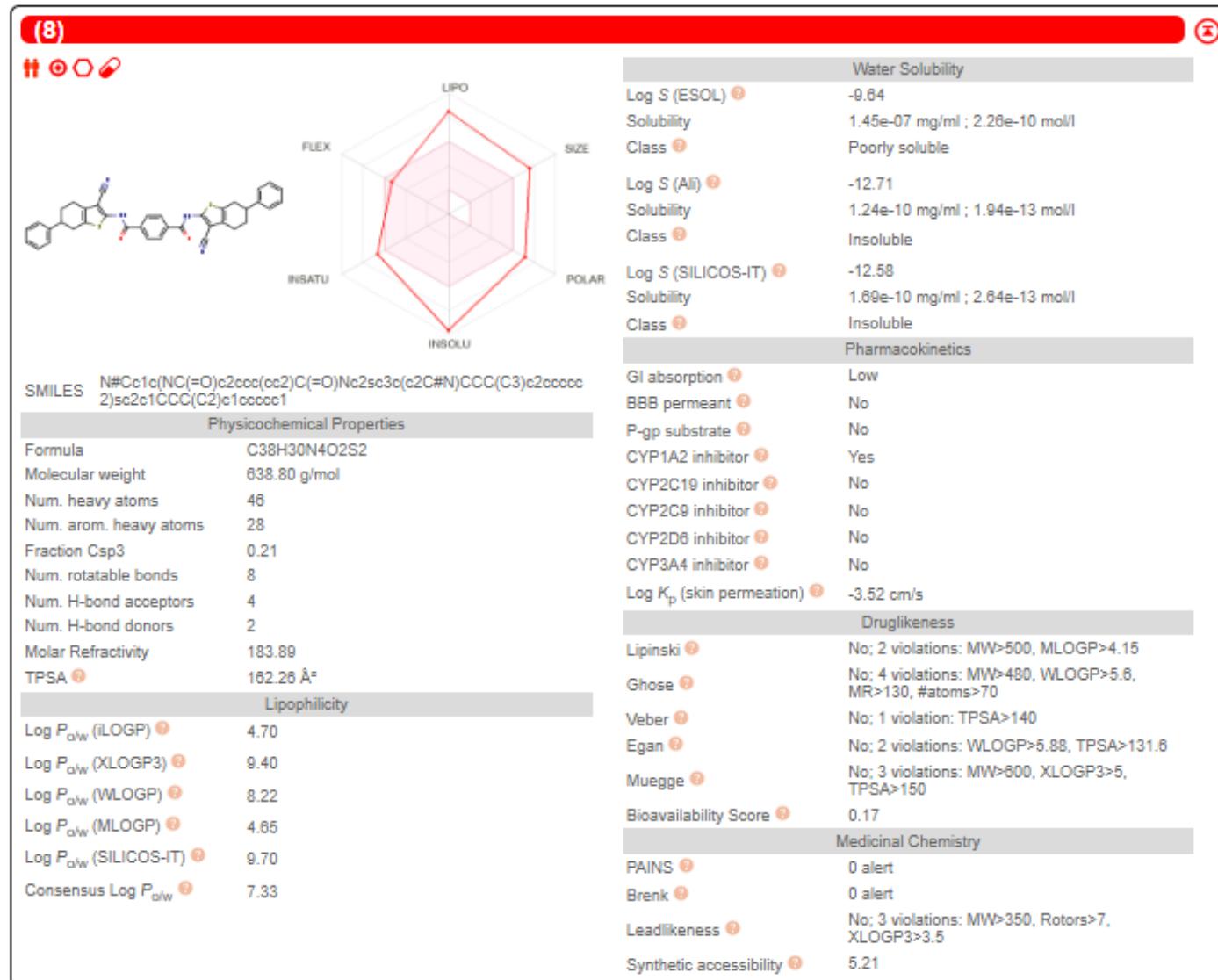


Fig. S7. ADME of compound 7.



**Fig. S8.** ADME of compound 8.

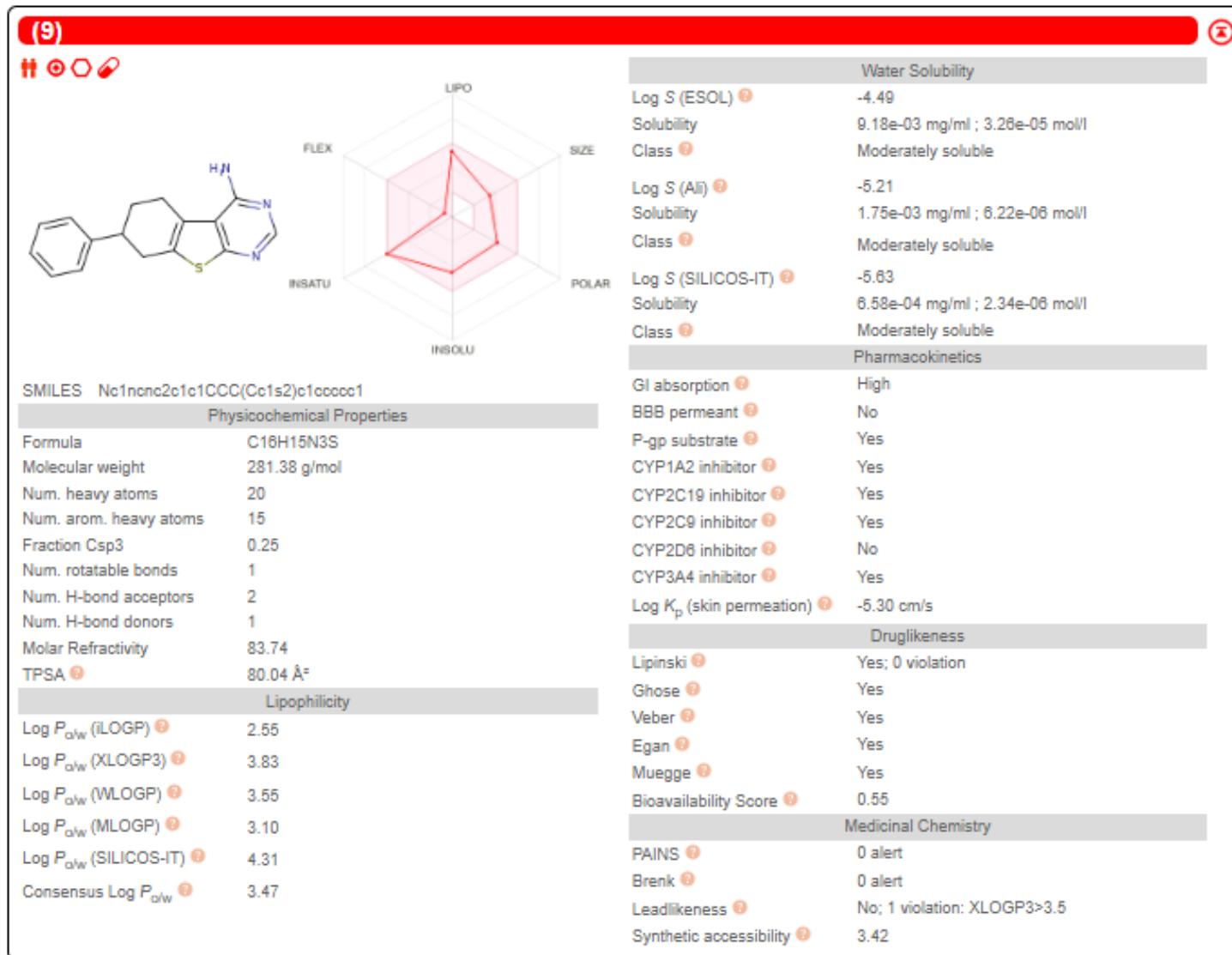
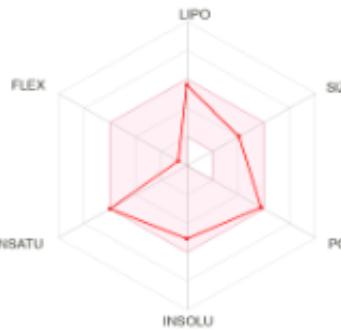
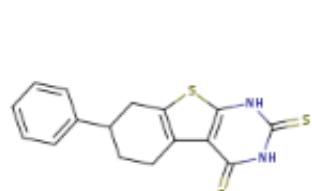


Fig. S9. ADME of compound 9.

**(10)**

SMILES S=c1[nH]c2sc3c(c2c(=S)[nH]1)CCC(C3)c1ccccc1

**Physicochemical Properties**

Formula C16H14N2S3

Molecular weight 330.49 g/mol

Num. heavy atoms 21

Num. arom. heavy atoms 15

Fraction Csp3 0.25

Num. rotatable bonds 1

Num. H-bond acceptors 0

Num. H-bond donors 2

Molar Refractivity 94.11

TPSA 124.00 Å<sup>2</sup>**Lipophilicity**Log P<sub>ow</sub> (iLOGP) 2.76Log P<sub>ow</sub> (XLOGP3) 4.28Log P<sub>ow</sub> (WLOGP) 5.29Log P<sub>ow</sub> (MLOGP) 3.16Log P<sub>ow</sub> (SILICOS-IT) 8.20Consensus Log P<sub>ow</sub> 4.74**Water Solubility**

Log S (ESOL) -5.05

Solubility 2.96e-03 mg/ml ; 8.95e-06 mol/l

Class Moderately soluble

Log S (Ali) -6.60

Solubility 8.37e-05 mg/ml ; 2.53e-07 mol/l

Class Poorly soluble

Log S (SILICOS-IT) -6.19

Solubility 2.15e-04 mg/ml ; 6.50e-07 mol/l

Class Poorly soluble

**Pharmacokinetics**

GI absorption Low

BBB permeant No

P-gp substrate Yes

CYP1A2 inhibitor Yes

CYP2C19 inhibitor Yes

CYP2C9 inhibitor Yes

CYP2D6 inhibitor No

CYP3A4 inhibitor Yes

Log K<sub>p</sub> (skin permeation) -5.28 cm/s**Druglikeness**

Lipinski Yes; 0 violation

Ghose Yes

Veber Yes

Egan Yes

Muegge Yes

Bioavailability Score 0.55

**Medicinal Chemistry**

PAINS 0 alert

Brenk 1 alert: thiocarbonyl\_group

Leadlikeness No; 1 violation: XLOGP3&gt;3.5

Synthetic accessibility 3.62

**Fig. S10.** ADME of compound 10.

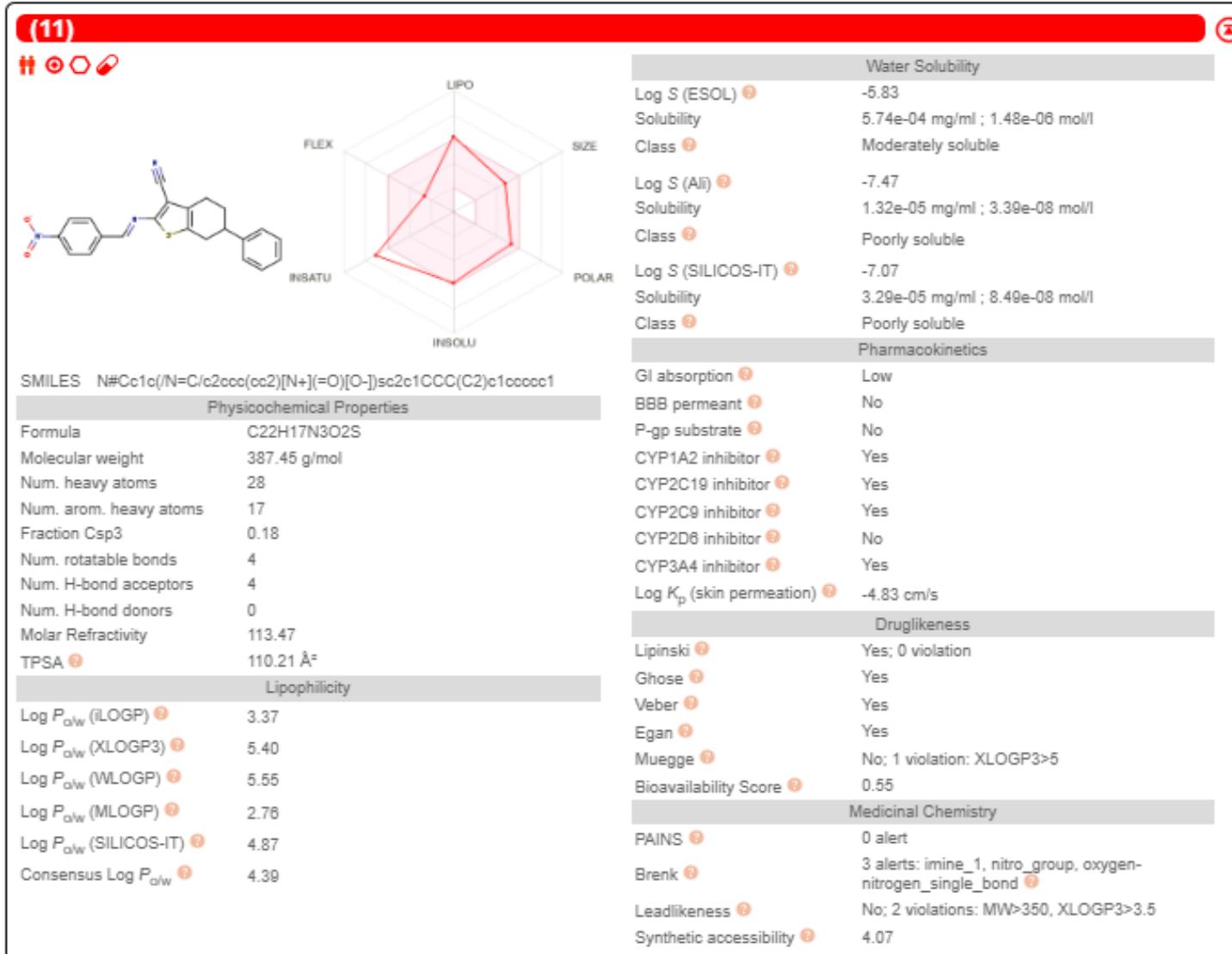
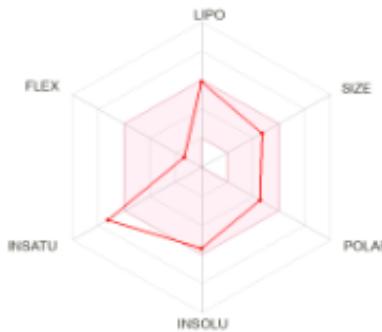
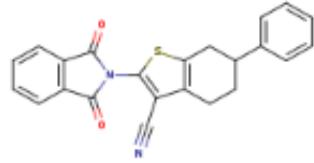


Fig. S11. ADME of compound 11.

**(12)**

Water Solubility	
Log S (ESOL) ⓘ	-5.57
Solubility	1.03e-03 mg/ml ; 2.68e-06 mol/l
Class ⓘ	Moderately soluble
Log S (Ali) ⓘ	-6.42
Solubility	1.46e-04 mg/ml ; 3.80e-07 mol/l
Class ⓘ	Poorly soluble
Log S (SILICOS-IT) ⓘ	-7.26
Solubility	2.09e-05 mg/ml ; 5.43e-08 mol/l
Class ⓘ	Poorly soluble

#### Pharmacokinetics

GI absorption ⓘ	High
BBB permeant ⓘ	No
P-gp substrate ⓘ	No
CYP1A2 inhibitor ⓘ	Yes
CYP2C19 inhibitor ⓘ	Yes
CYP2C9 inhibitor ⓘ	Yes
CYP2D6 inhibitor ⓘ	No
CYP3A4 inhibitor ⓘ	Yes
Log $K_p$ (skin permeation) ⓘ	-5.23 cm/s

#### Druglikeness

Lipinski ⓘ	Yes; 0 violation
Ghose ⓘ	Yes
Veber ⓘ	Yes
Egan ⓘ	Yes
Muegge ⓘ	Yes
Bioavailability Score ⓘ	0.55

#### Medicinal Chemistry

PAINS ⓘ	0 alert
Brenk ⓘ	1 alert: phthalimide ⓘ
Leadlikeness ⓘ	No; 2 violations: MW>350, XLOGP3>3.5
Synthetic accessibility ⓘ	3.70

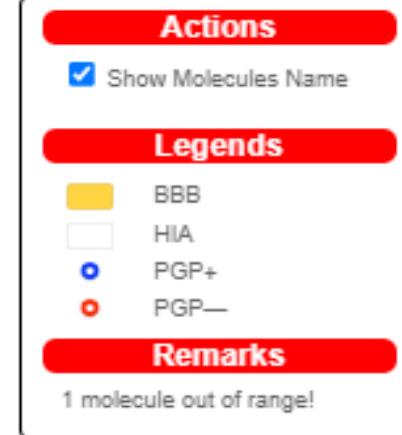
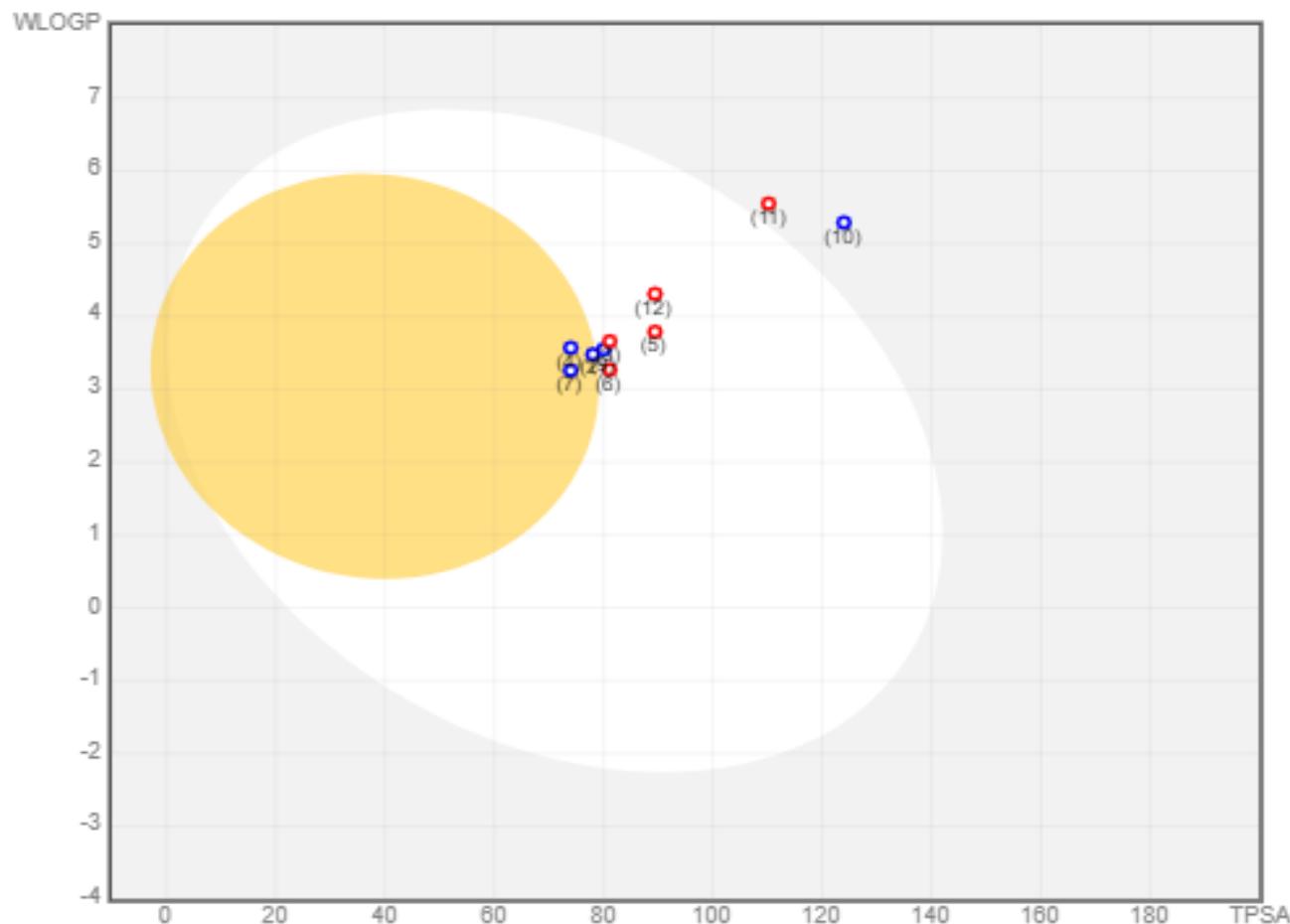
**Fig. S12.** ADME of compound 12.

[Hide BOILED-Egg](#)

Retrieve data:



POWERED BY ChemAxon



**Fig. S13.** BOILED-EGG chart of compounds 2-10.

## **Experimental**

### **Cytotoxicity assay**

#### ***Materials and methods***

##### ***Cell lines***

The cell lines: mammary gland breast cancer (MCF7) and hepatocellular cancer (HePG2) were obtained from ATCC *via* Holding company for biological products and vaccines (VACSERA), Cairo, Egypt. Doxorubicin was used as a reference anticancer agent for comparison.

##### ***Chemical reagents***

The reagents RPMI-1640 medium, MTT, and DMSO (Sigma Co., St. Louis, USA), and Fetal bovine serum (GIBCO, UK).

##### ***MTT assay***

The cell lines mentioned above were used to determine the inhibitory effects of compounds on cell growth using the MTT assay.[41] This colorimetric assay is based on the conversion of the yellow tetrazolium bromide (MTT) to a purple formazan derivative by mitochondrial succinate dehydrogenase in viable cells. Cell lines were cultured in RPMI-1640 medium with 10% fetal bovine serum. Antibiotics added were 100 units/mL penicillin and 100 mg/mL streptomycin at 37 °C in a 5% CO<sub>2</sub> incubator. The cell lines were seeded in a 96-well plate at a density of 1.0 x 10<sup>4</sup> cells/well at 37 °C for 48 h under 5% CO<sub>2</sub>. After incubation, the cells were treated with different concentrations of compounds and incubated for 24 h. After 24 h of drug treatment, 20 µL of MTT solution at 5 mg/mL was added and incubated for 4 h. Dimethyl sulfoxide (DMSO) in volume of 100 µL is added into each well to dissolve the purple formazan formed. The colorimetric assay is measured and recorded at an absorbance of 570 nm using a plate reader (EXL 800, USA). The relative cell viability in percentage was calculated as (A<sub>570</sub> of treated samples/A<sub>570</sub> of untreated samples) x 100.

### ***Statistical analysis***

All data were presented as mean  $\pm$  SD ( $n = 3$ ) using the SPSS 13.0 program (SPSS Inc. USA).

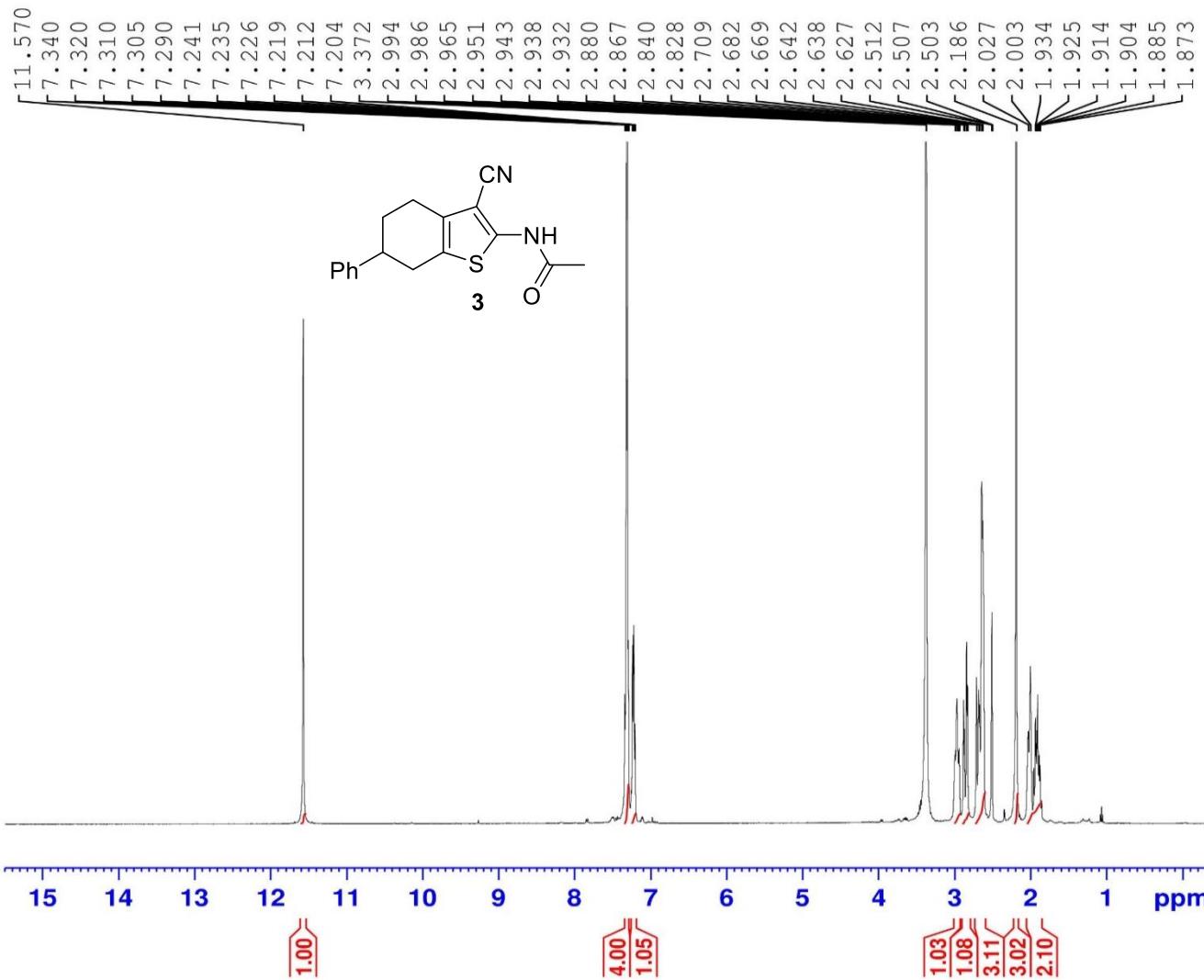
### ***Molecular Docking***

All molecular modeling studies were investigated using Molecular Operating Environment (MOE, 2014.0901) software. All minimizations were performed with MOE until an RMSD gradient of  $0.1 \text{ kcal.mol}^{-1}\text{\AA}^{-1}$  with the MMFF94x force field, and the partial charges were automatically calculated. The X-ray crystallographic structure of tubulin (TUB) domain complexed with colchicine (COL) (PDB ID: 5NM5) was downloaded from the protein data bank (<https://www.rcsb.org/structure/5NM5>). For the co-crystallized enzyme, water molecules and ligands, which are not involved in the binding, were removed, and the protein was prepared for the docking study utilizing the Protonate 3D protocol in MOE with default options. The co-crystallized ligand (COL) was used to define the binding site for docking. The Triangle Matcher placement method and London dG scoring function were used for docking.

### ***ADME Profiling***

The ADME properties of all compounds were studied by the SwissADME free web tool (<http://www.swissadme.ch/index.php>), accessed on 26 Feb. 2024.

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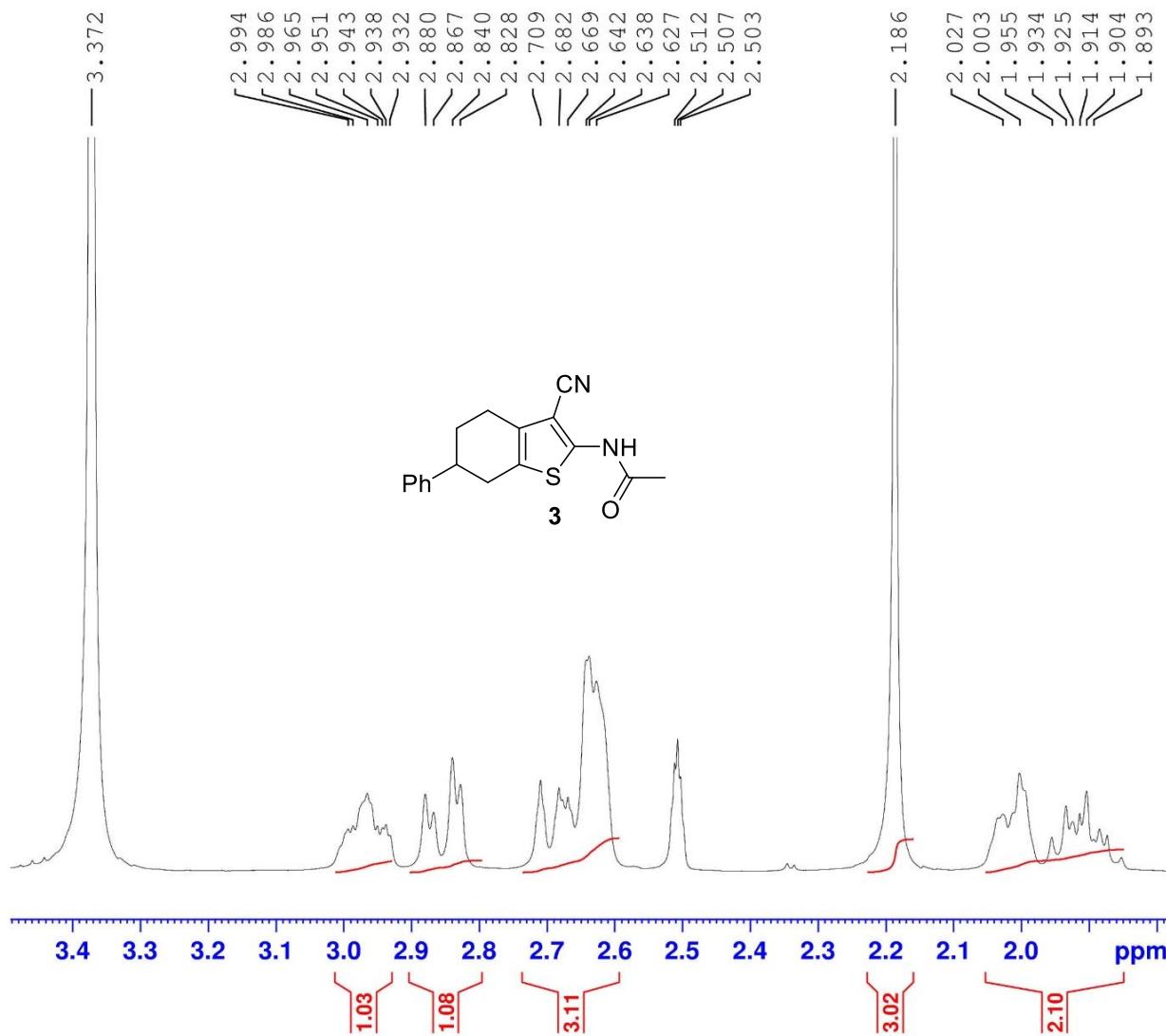


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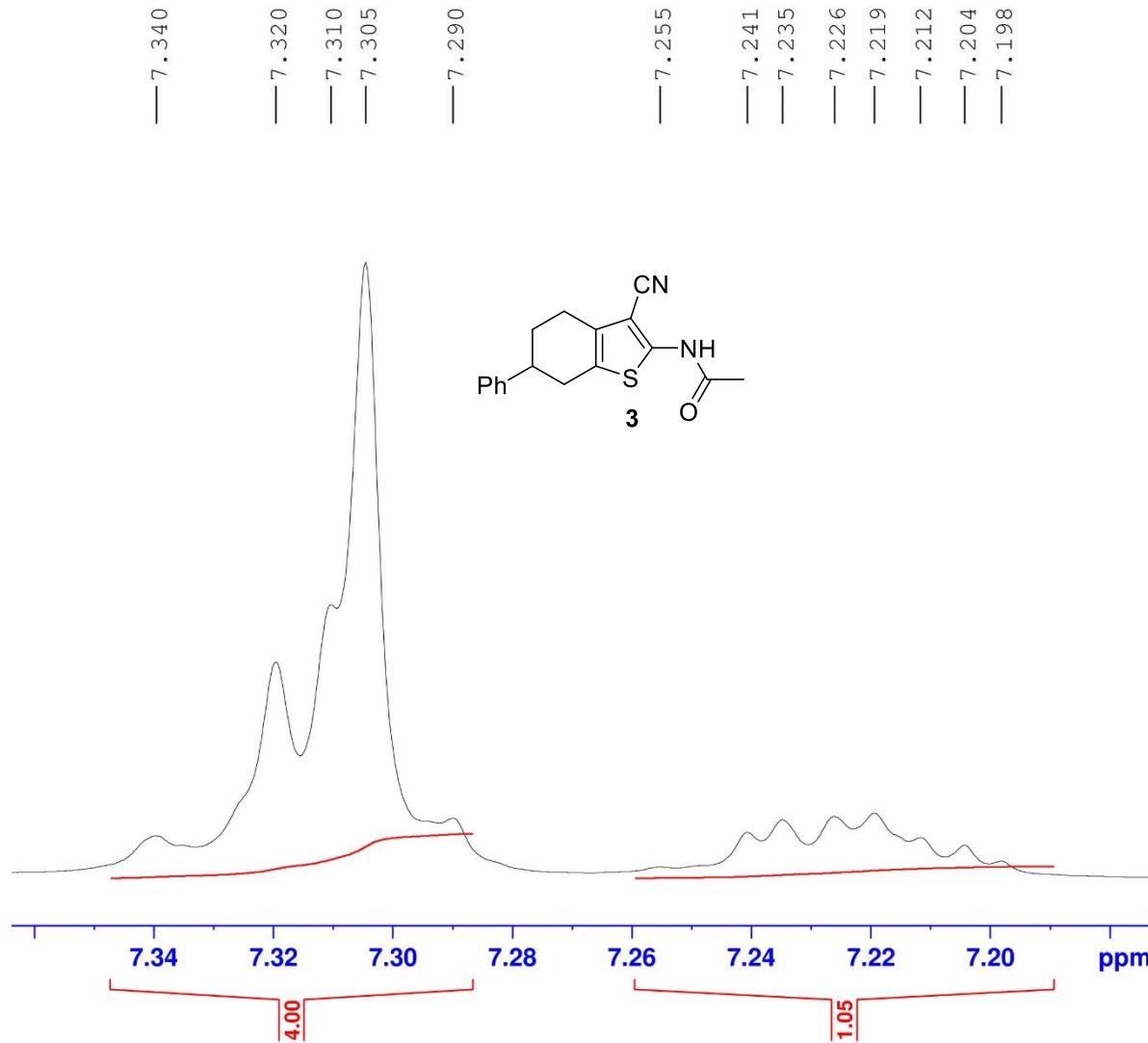


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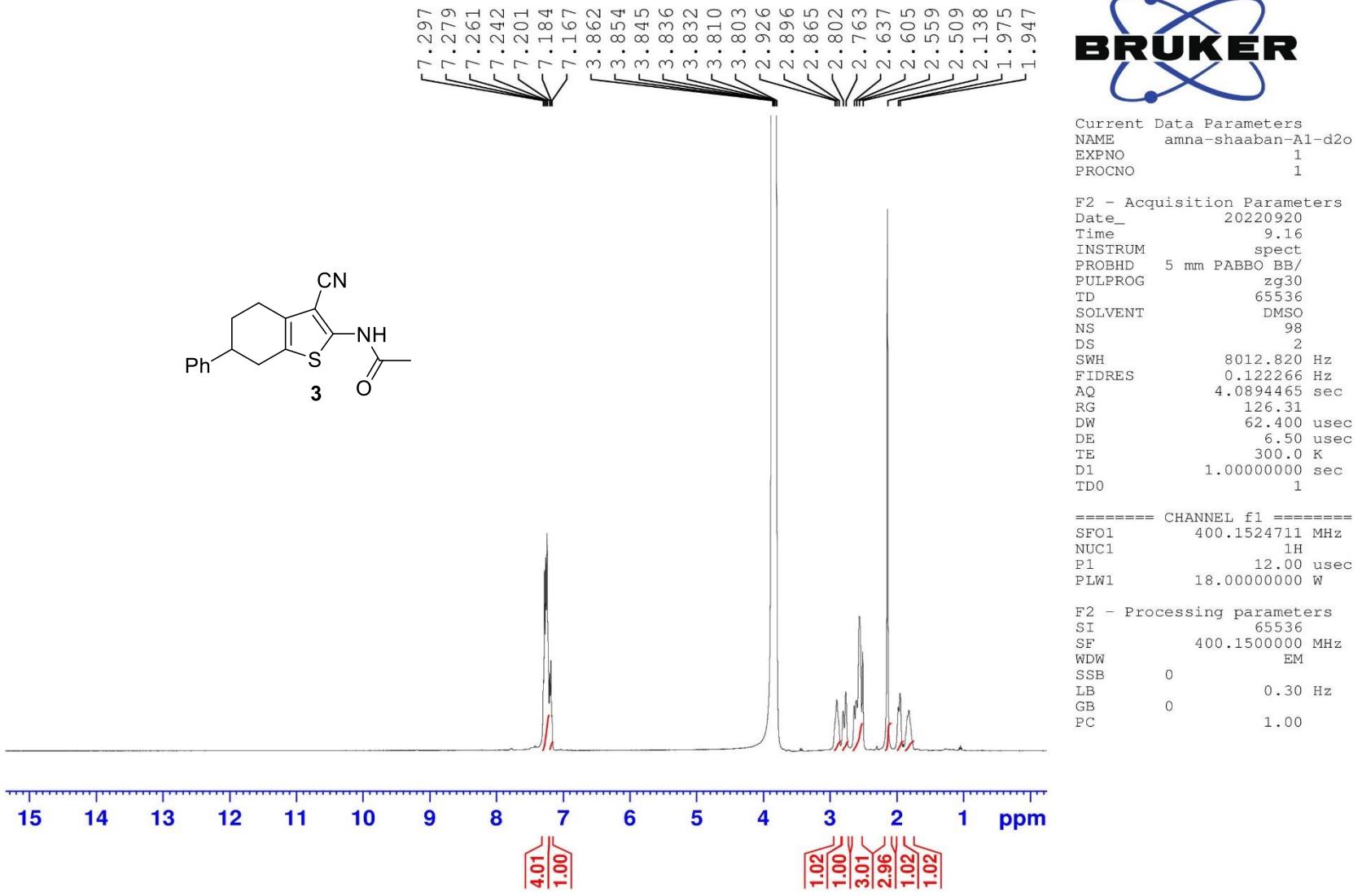


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 EXPNO 1  
 PROCNO 1

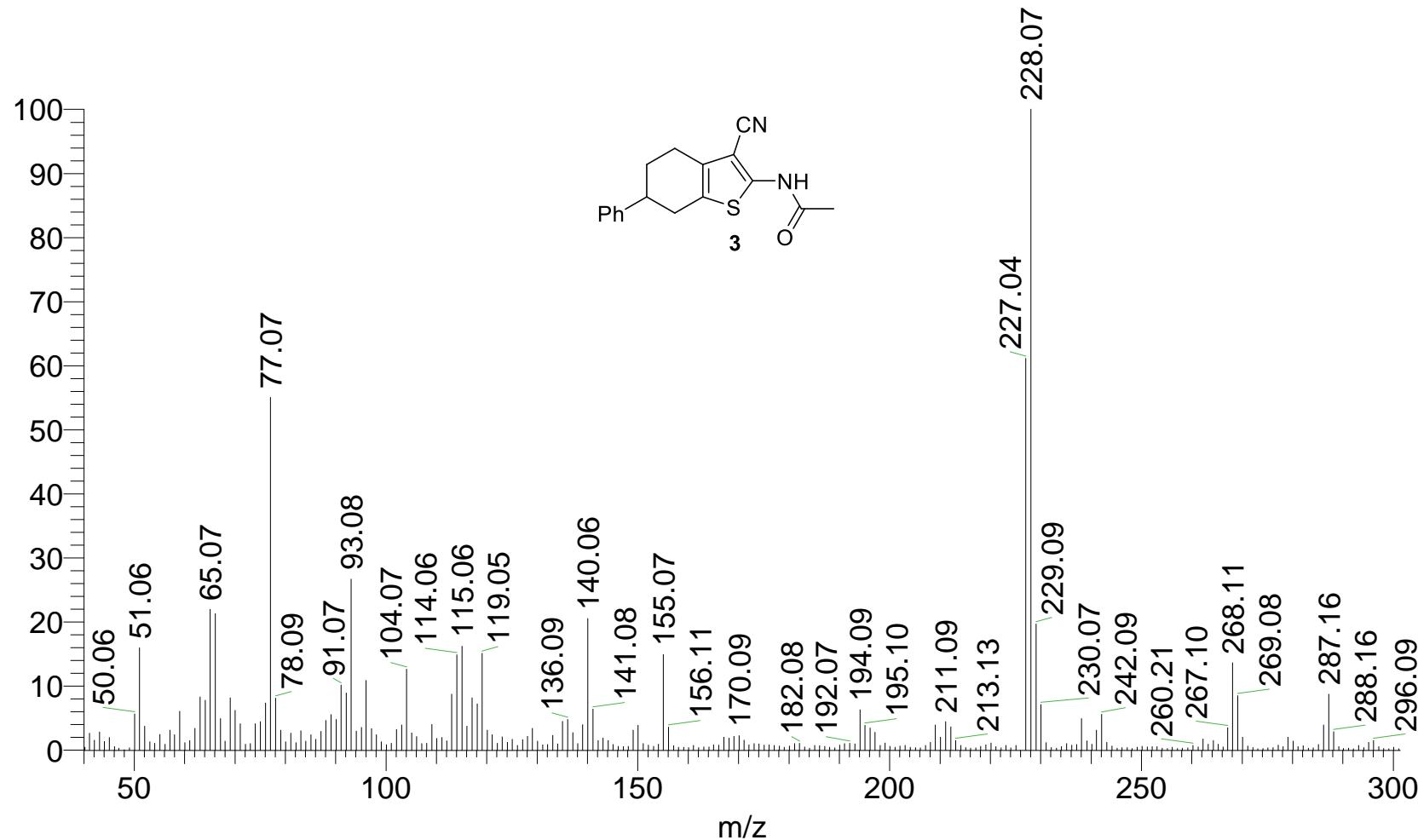
F2 - Acquisition Parameters  
 Date\_ 20220913  
 Time 11.06  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 106  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 205.37  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.0000000 sec  
 TDO 1

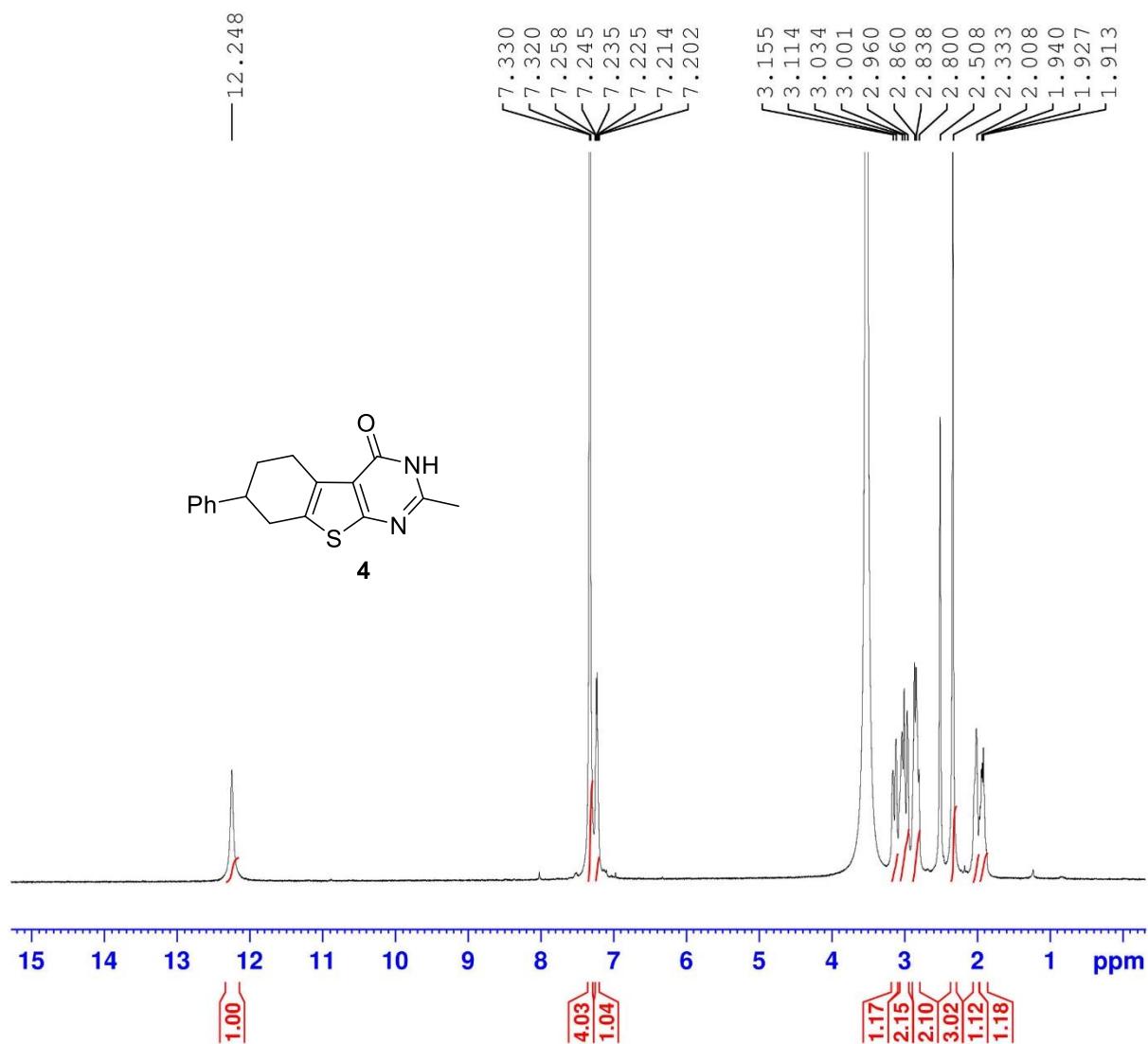
===== CHANNEL f1 =====  
 SFO1 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.0000000 W

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



sayed-karam-A1 #190 RT: 3.20 AV: 1 SB: 26 1.21-1.34 , 0.87-1.14 NL: 4.31E8  
T: {0,0} + c EI Full ms [40.00-1000.00]



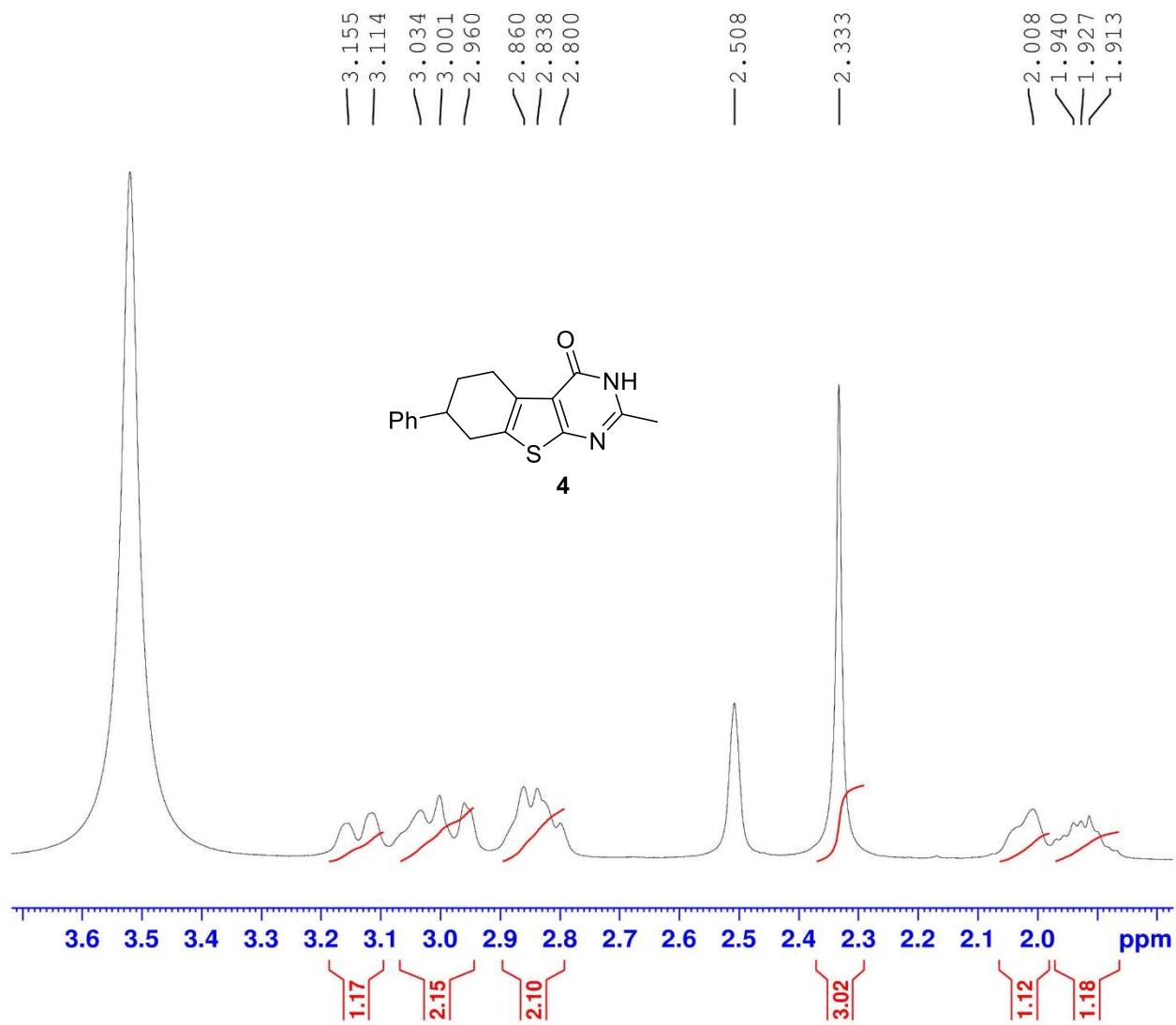


Current Data Parameters  
 NAME amna-shaabani-A2  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220913  
 Time 10.04  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 88  
 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 1.0000000 sec  
 TDO 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

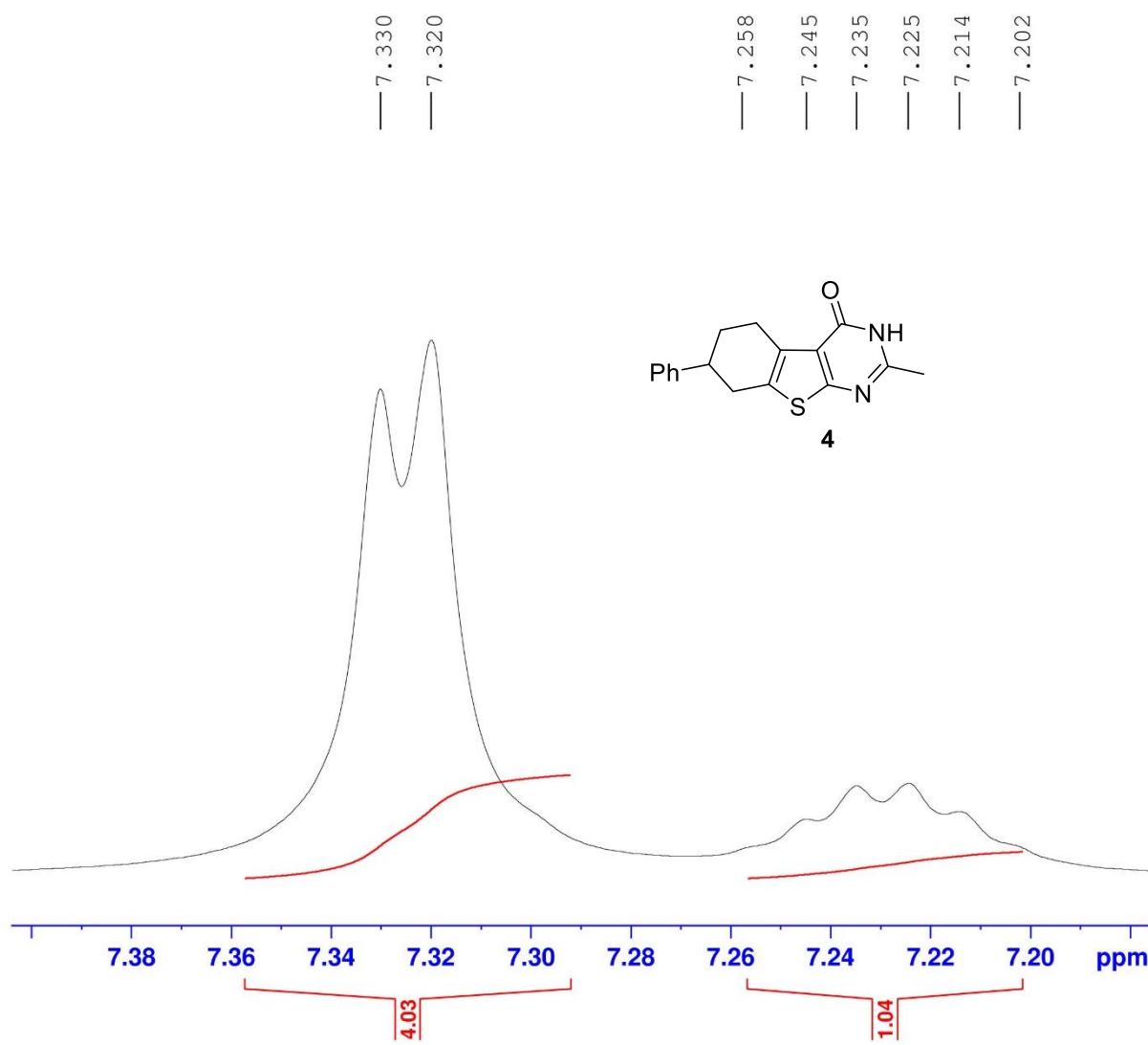


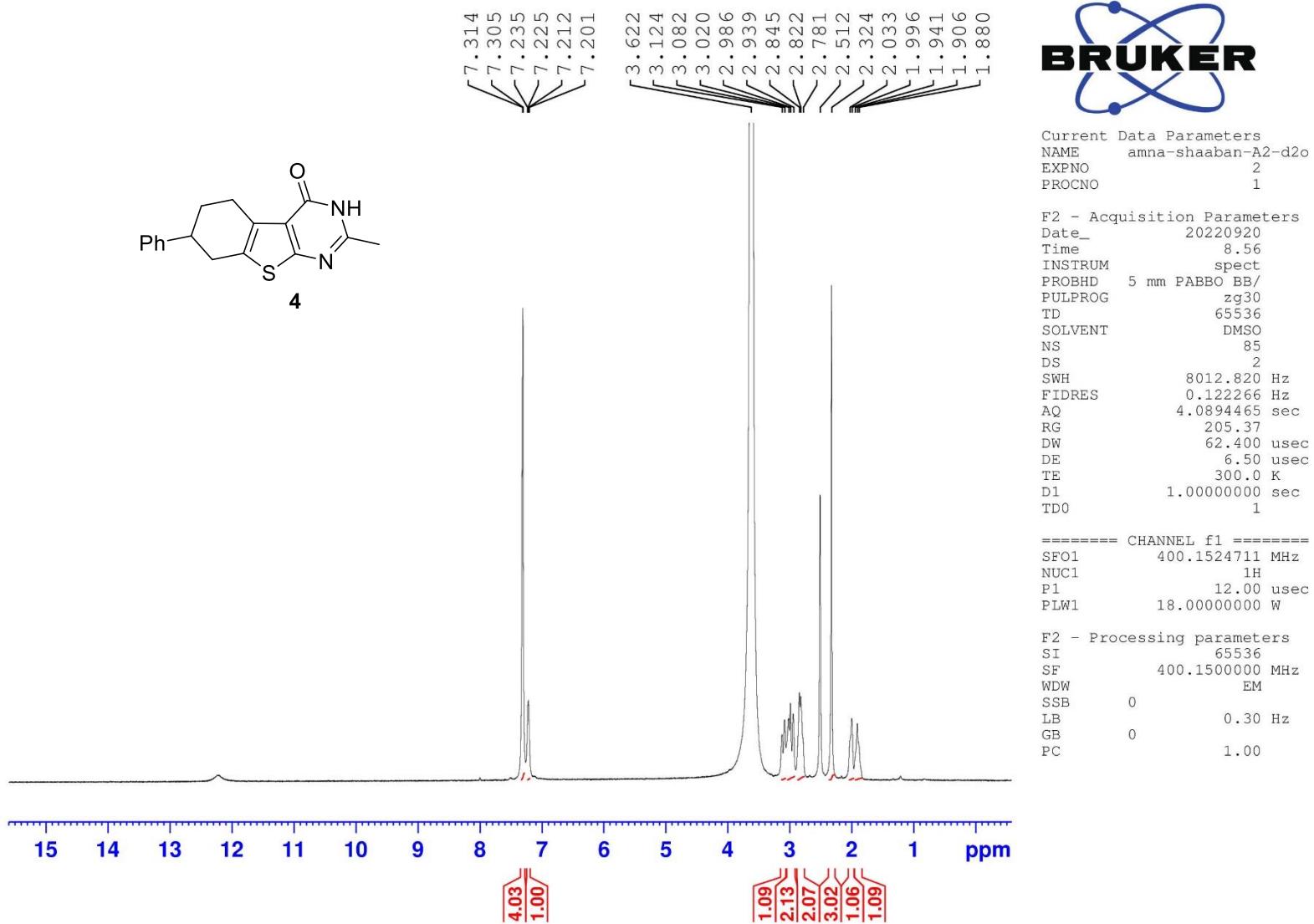
Current Data Parameters  
 NAME amna-shaabani-A2  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220913  
 Time 10.04  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 88  
 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 1.0000000 sec  
 TDO 1

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

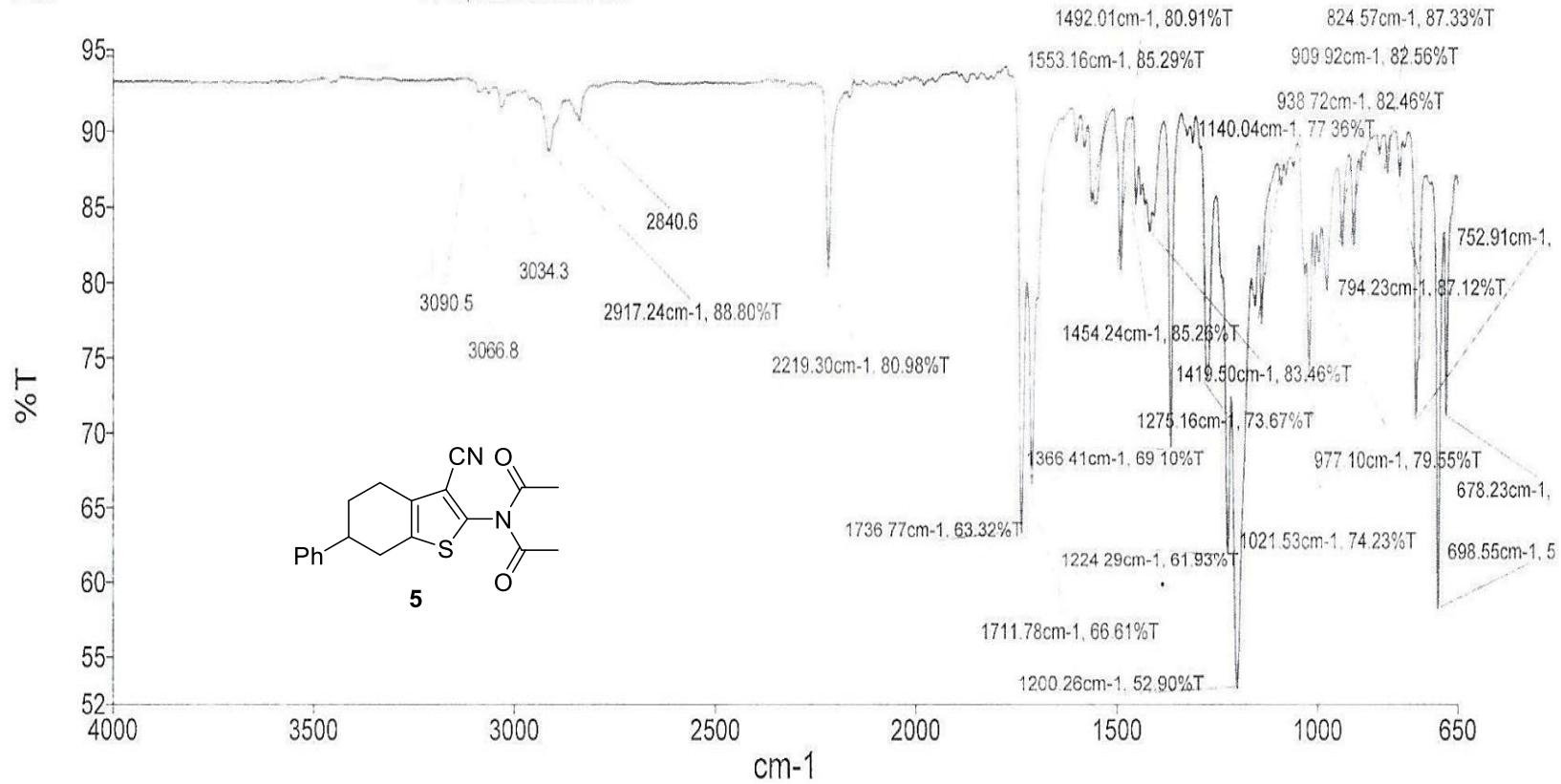
F2 - Processing parameters  
 SI 65536  
 SF 400.1500000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



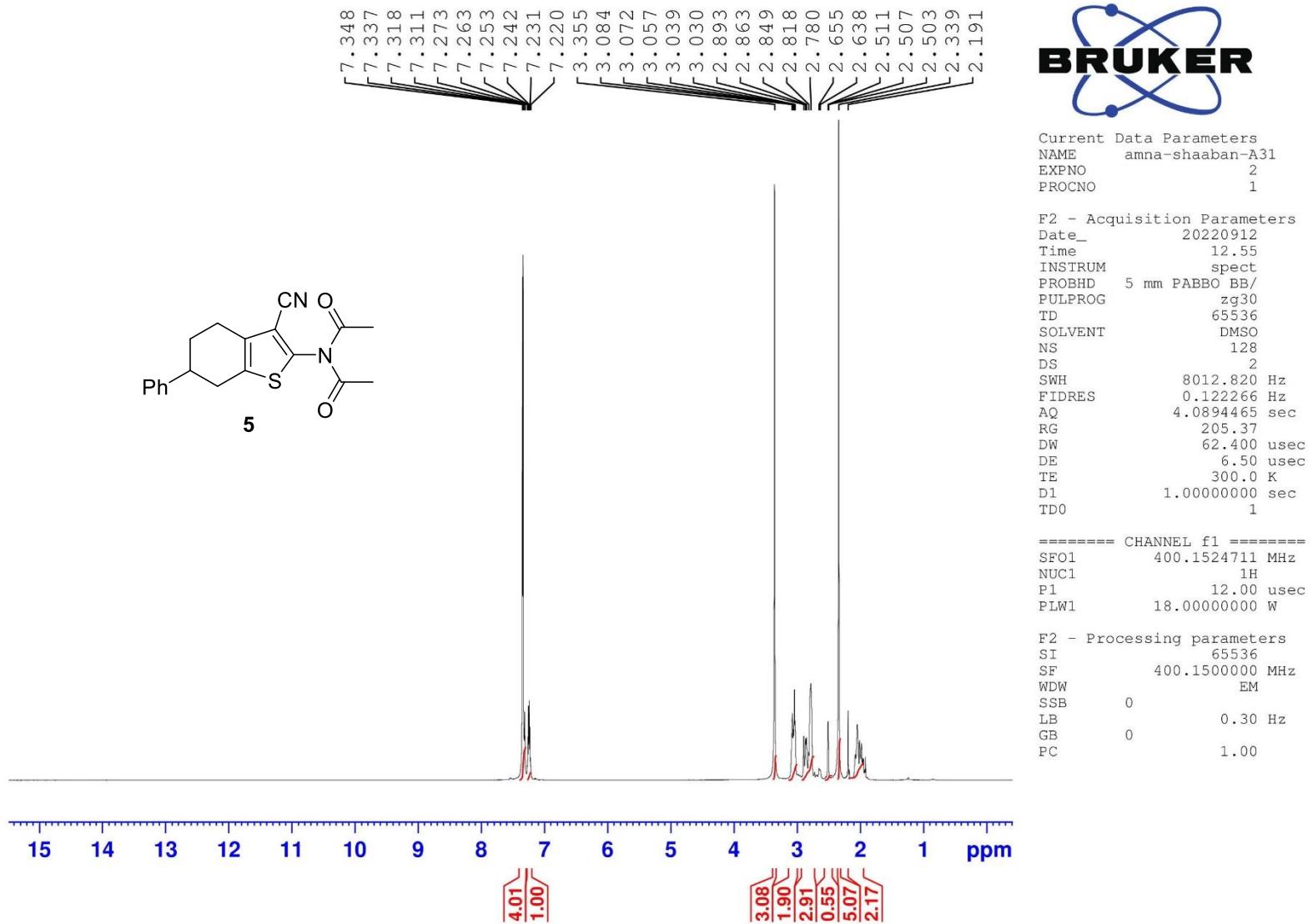


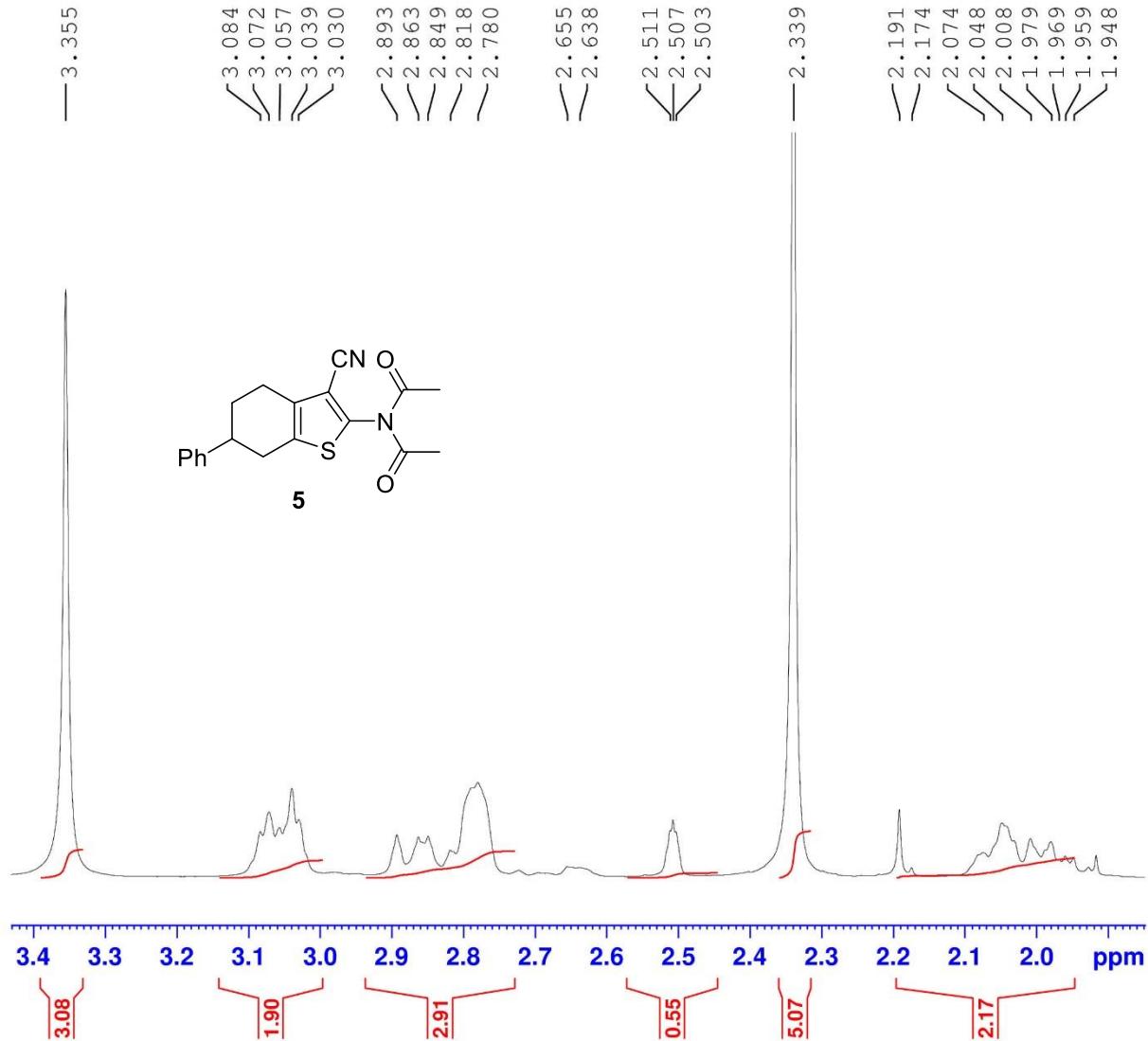
Analyst  
Date

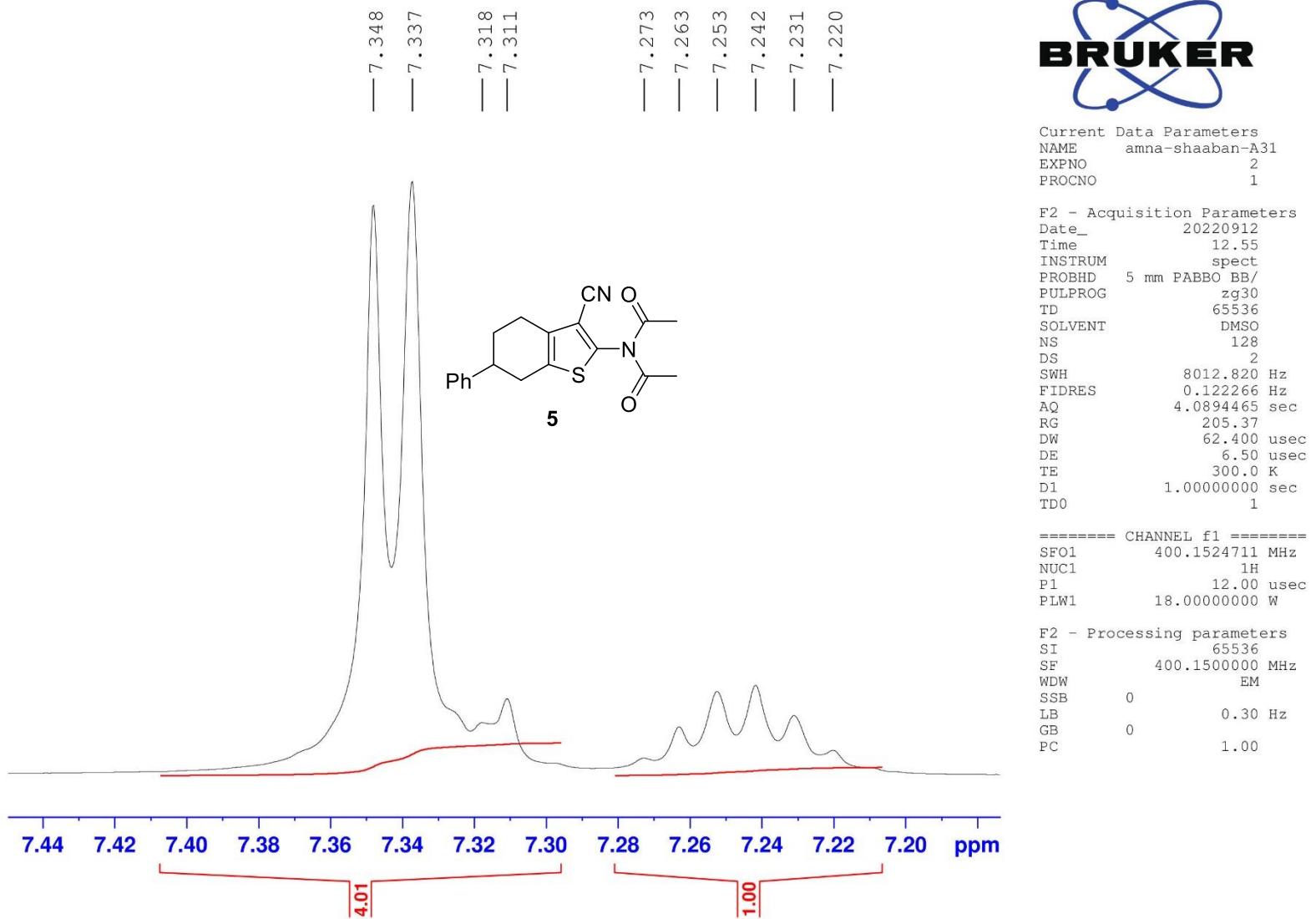
Administrator  
01 September 2022 11:38

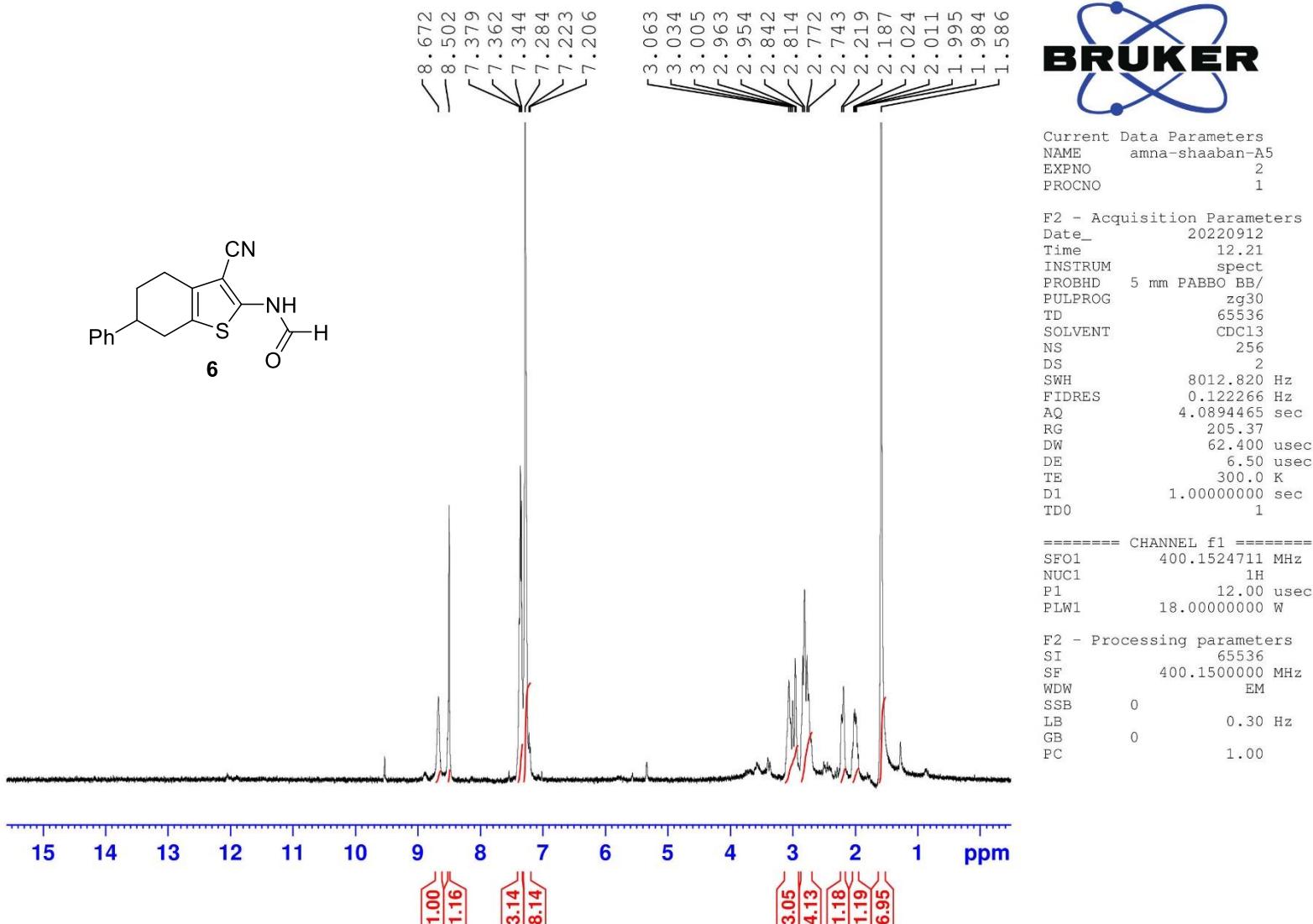


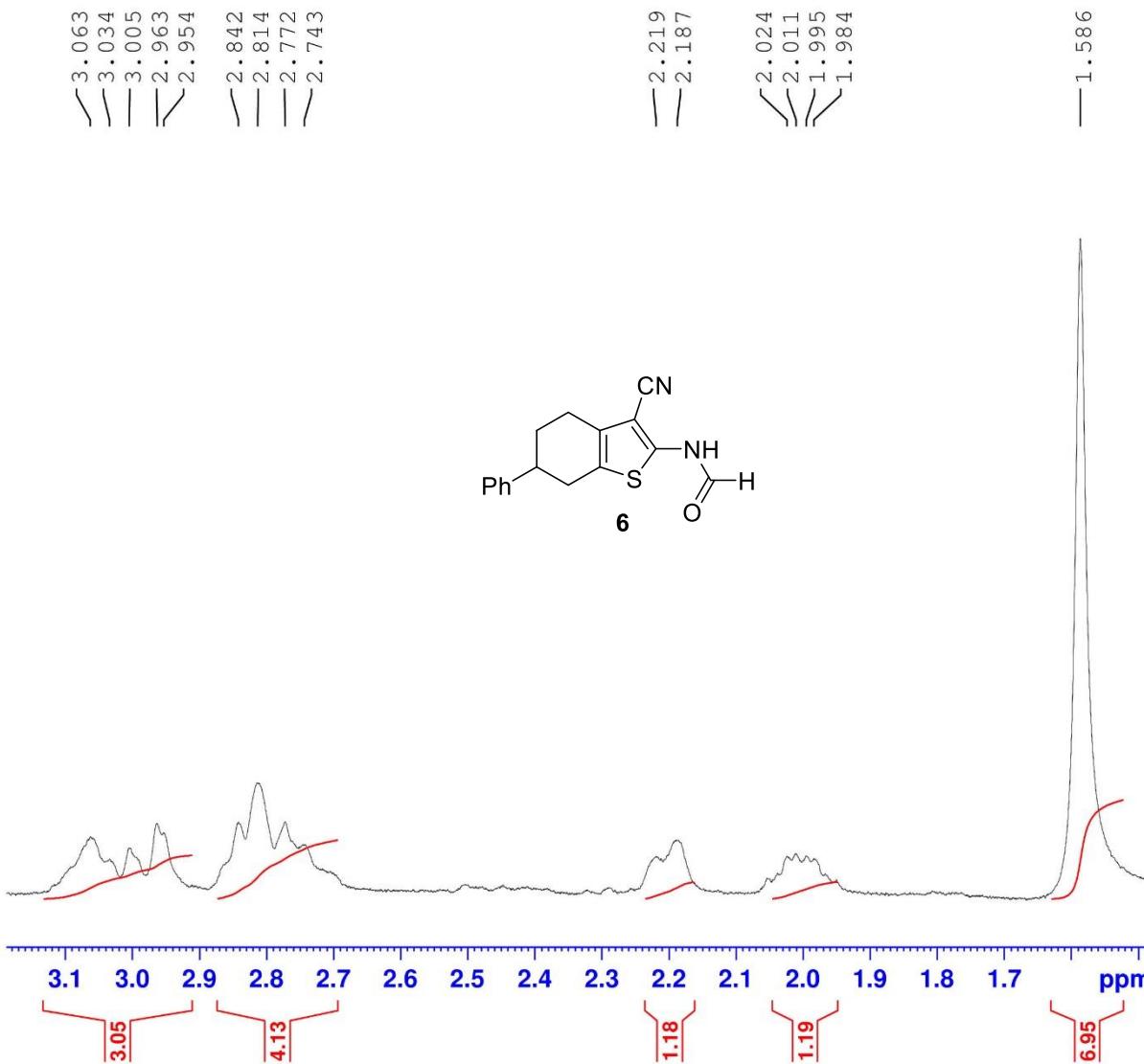
Sample Name	Description	Quality Checks
A31	Sample 001 By Administrator Date Thursday, September 01 2022	The Quality Checks do not report any warnings for the sample.









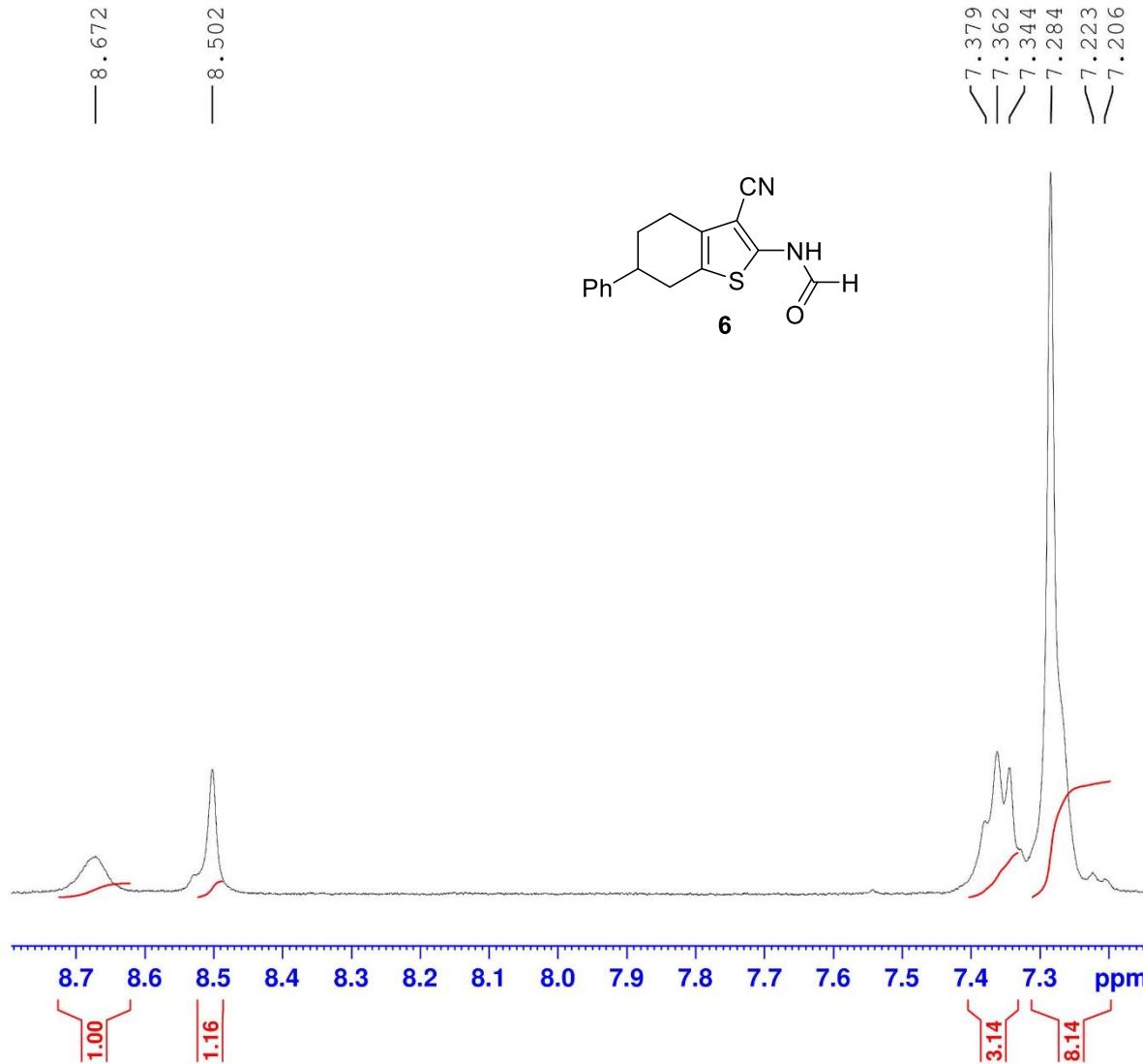


Current Data Parameters  
 NAME amna-shaabani-A5  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220912  
 Time 12.21  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 256  
 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 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SF01 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.0000000 W

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

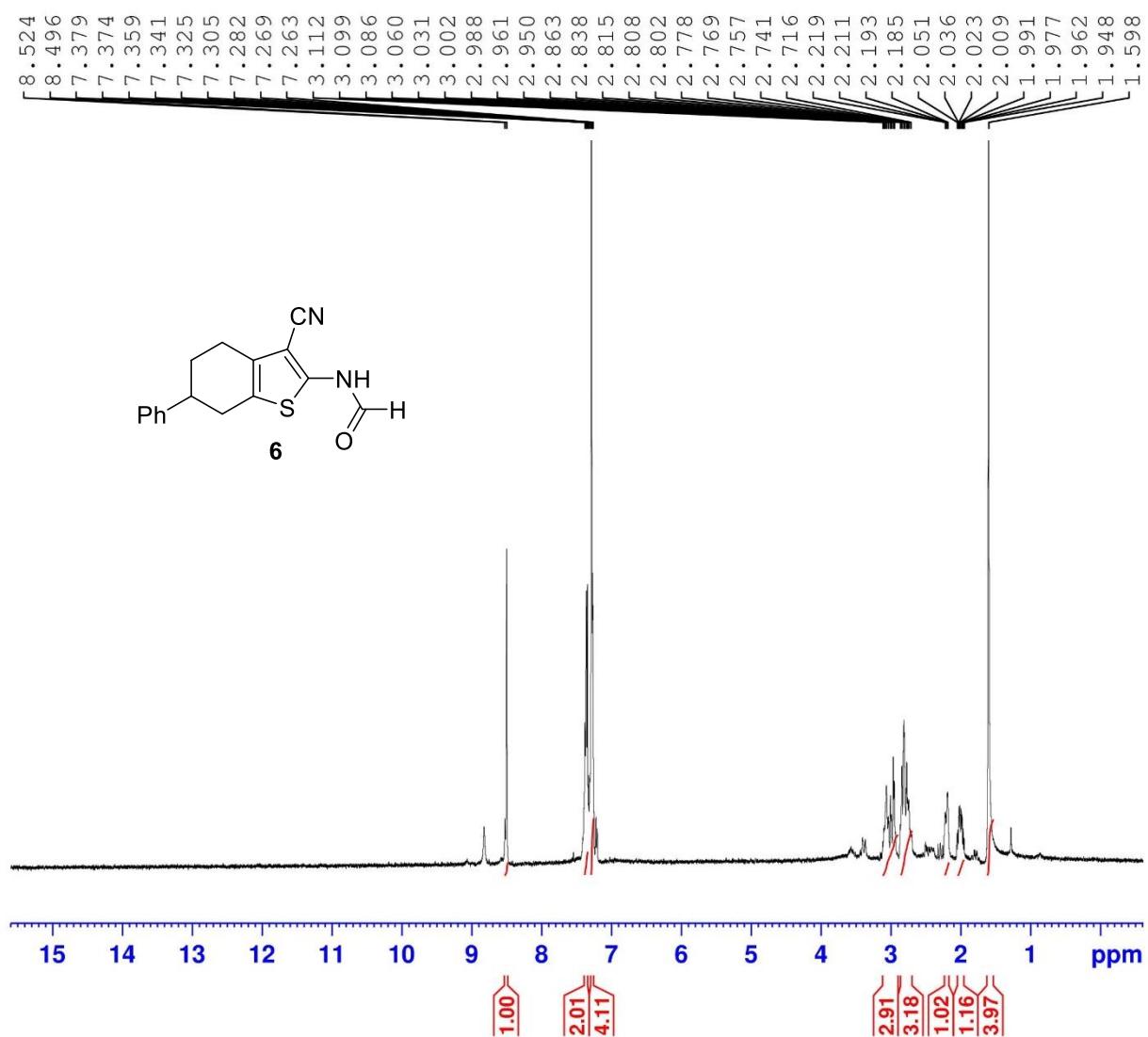


Current Data Parameters  
 NAME amna-shaabani-A5  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220912  
 Time 12.21  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 256  
 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 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SF01 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.0000000 W

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

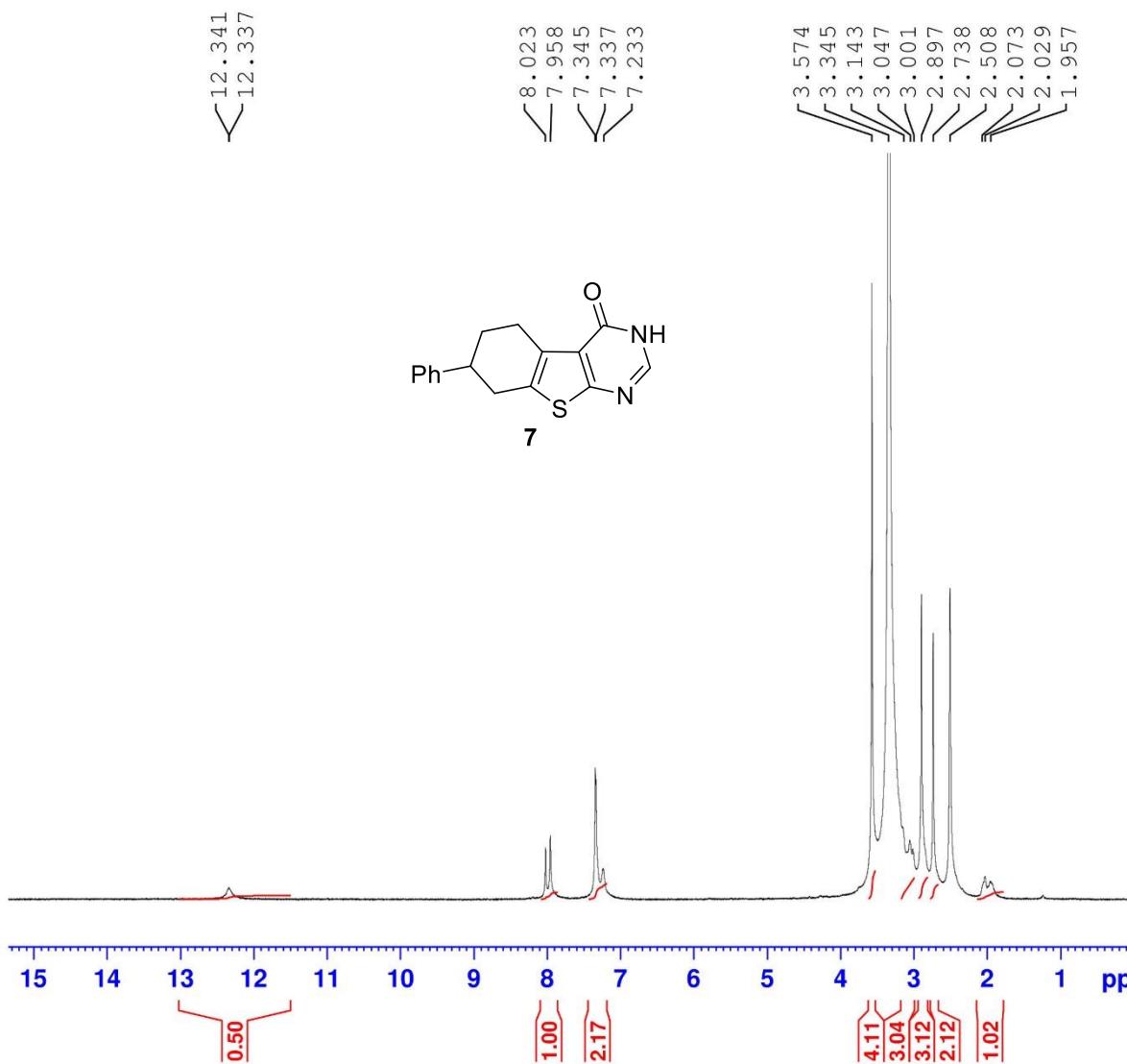


Current Data Parameters  
 NAME amna-shaabani-A5-d2o  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220921  
 Time 9.04  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 127  
 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  
 TDO 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 0.30 Hz  
 LB 0  
 GB 0 1.00  
 PC

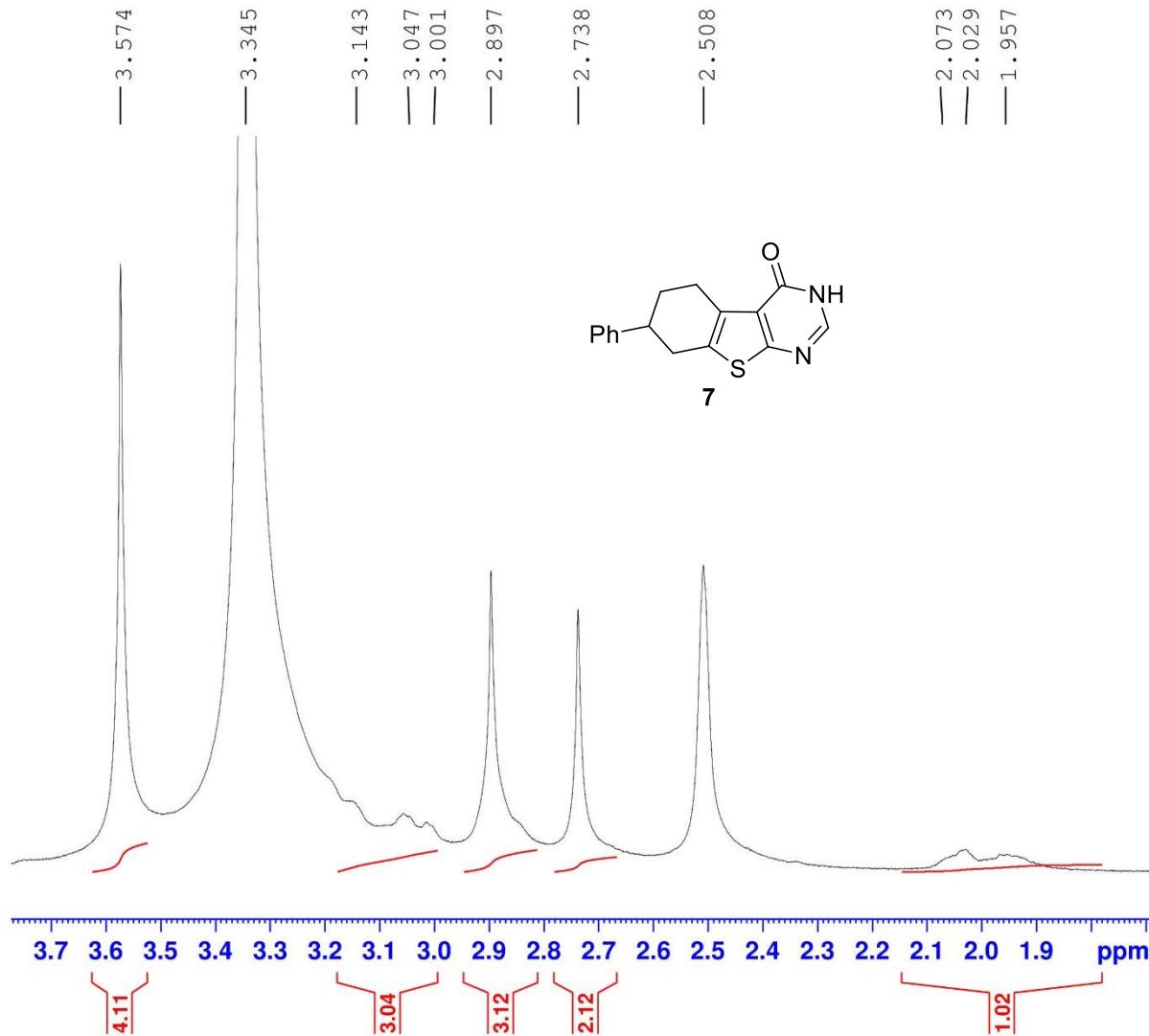


Current Data Parameters  
 NAME amna-shaabani-A6  
 EXPNO 1  
 PROCNNO 1

F2 - Acquisition Parameters  
 Date\_ 20220913  
 Time 12.58  
 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 1.0000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SF01 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.0000000 W

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

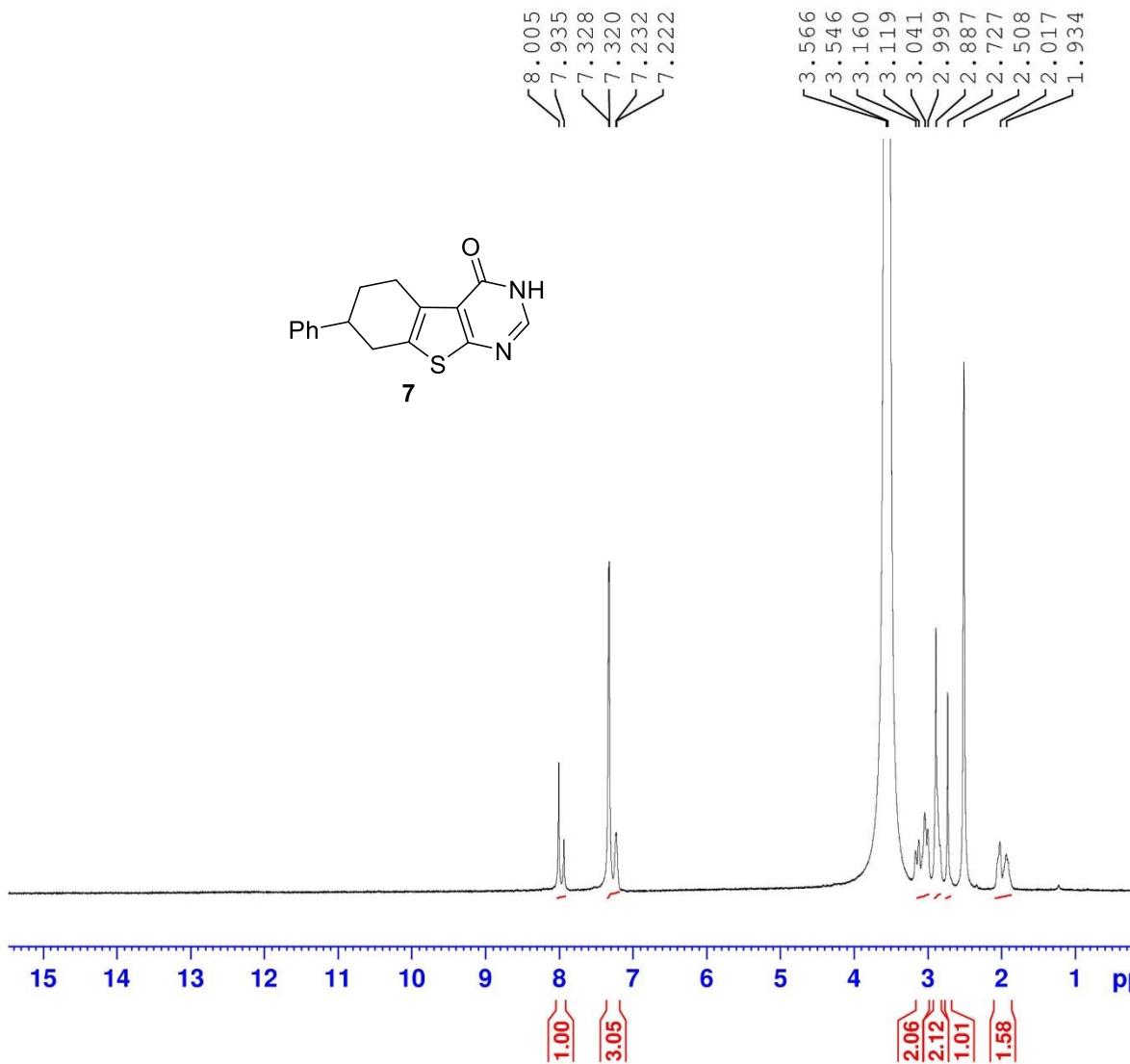


Current Data Parameters  
 NAME amna-shaabani-A6  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220913  
 Time 12.58  
 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 1.0000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SF01 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.0000000 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 amna-shaabani-A6-d2o  
 EXPNO 1  
 PROCNO 1

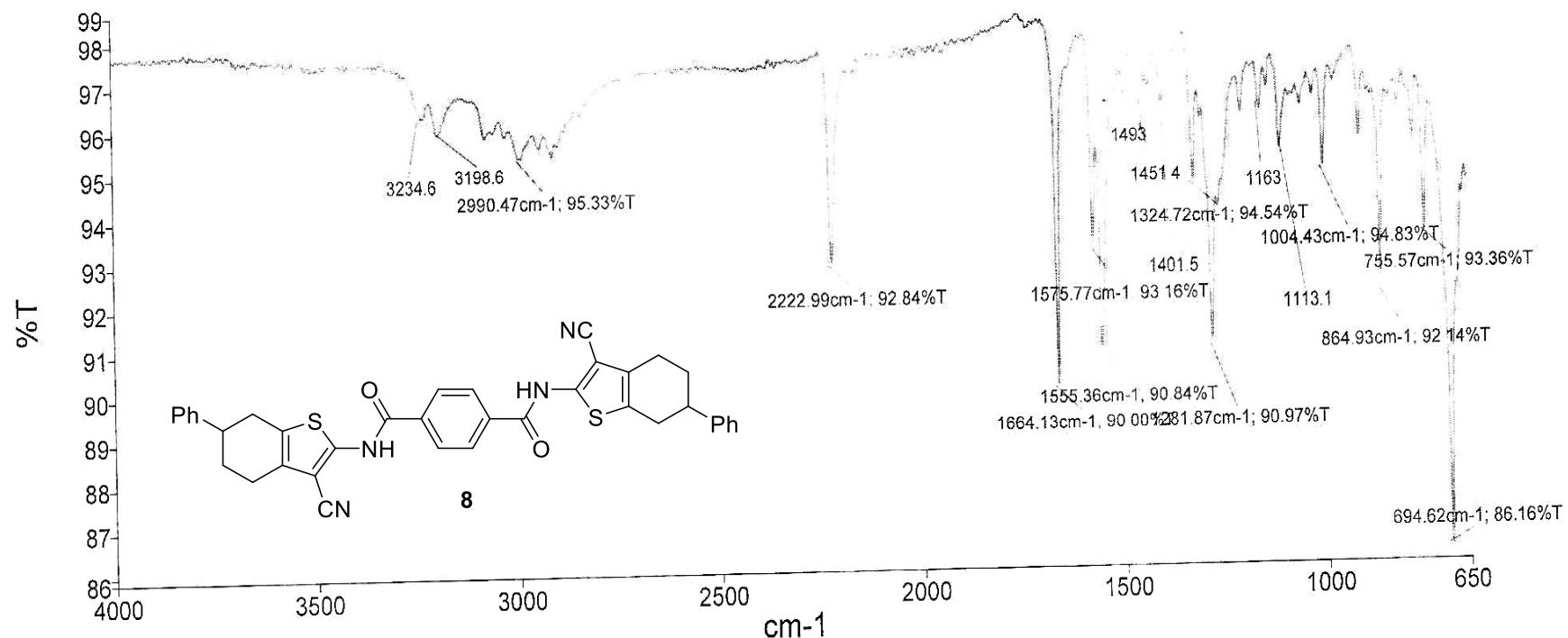
F2 - Acquisition Parameters  
 Date\_ 20220920  
 Time 10.27  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 128  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 205.37  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SF01 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.0000000 W

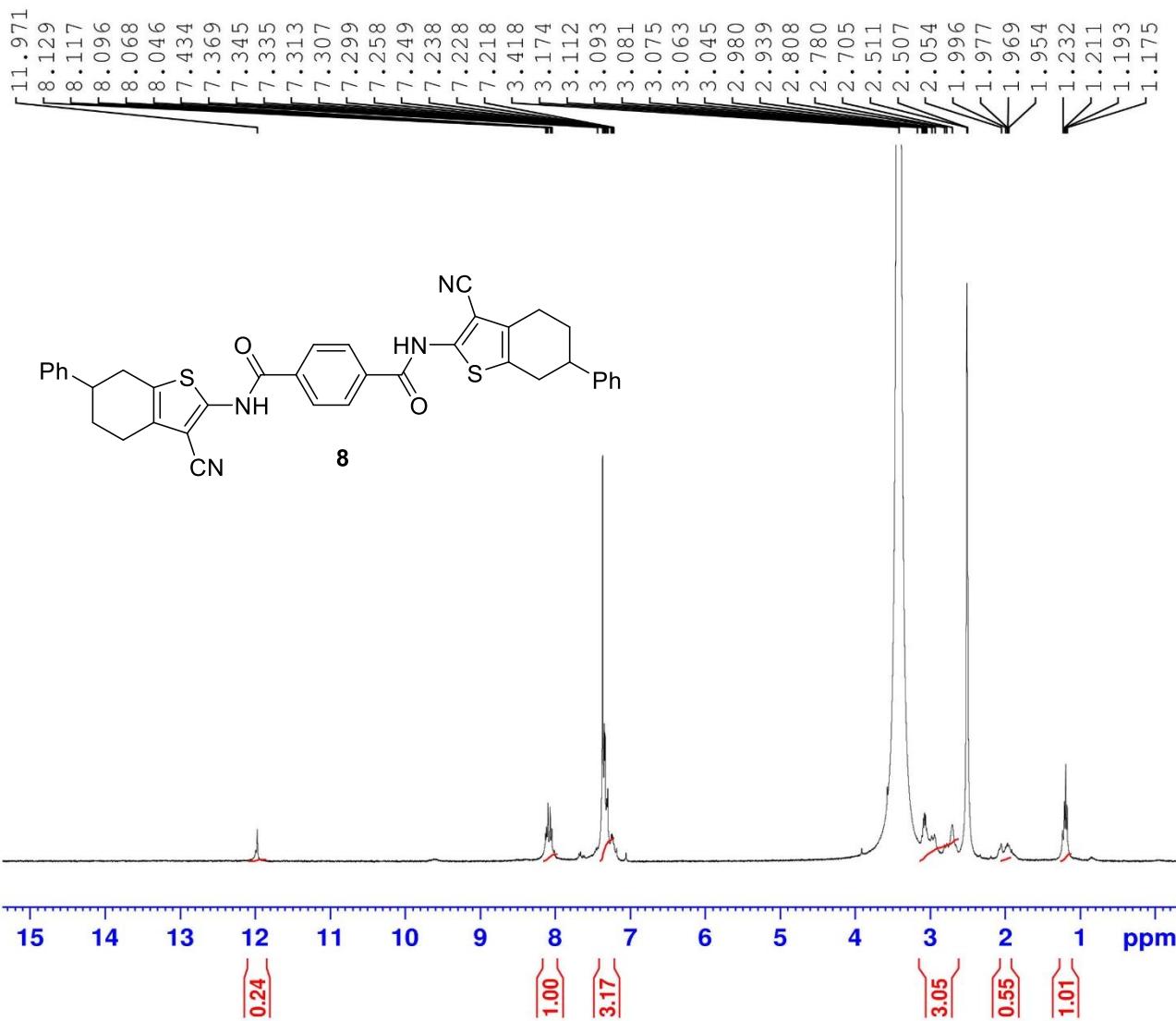
F2 - Processing parameters  
 SI 65536  
 SF 400.1500000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Analyst  
Date

Administrator  
02 , 01:18 2021 دیسمبر



Sample Name	Description	Quality Checks
A70	الخطيب, دیسمبر 02 2021 Sample 1388 By Administrator Date 2021 02	The Quality Checks give rise to a Weak Bands warning for the sample.

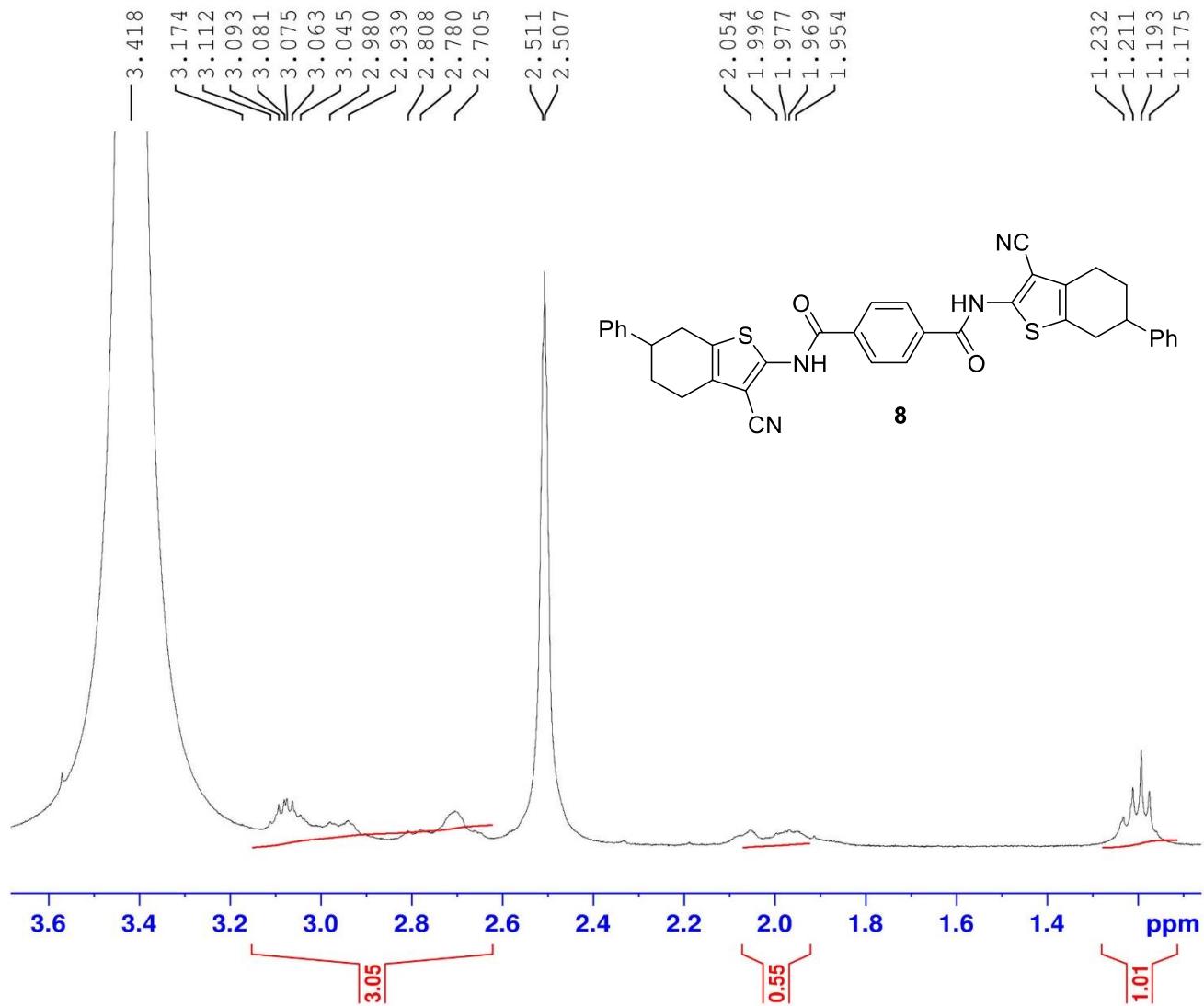


Current Data Parameters  
NAME amna-shaabani-A7  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220913  
Time 12.39  
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 1.0000000 sec  
TD0 1

===== CHANNEL f1 ======  
SF01 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

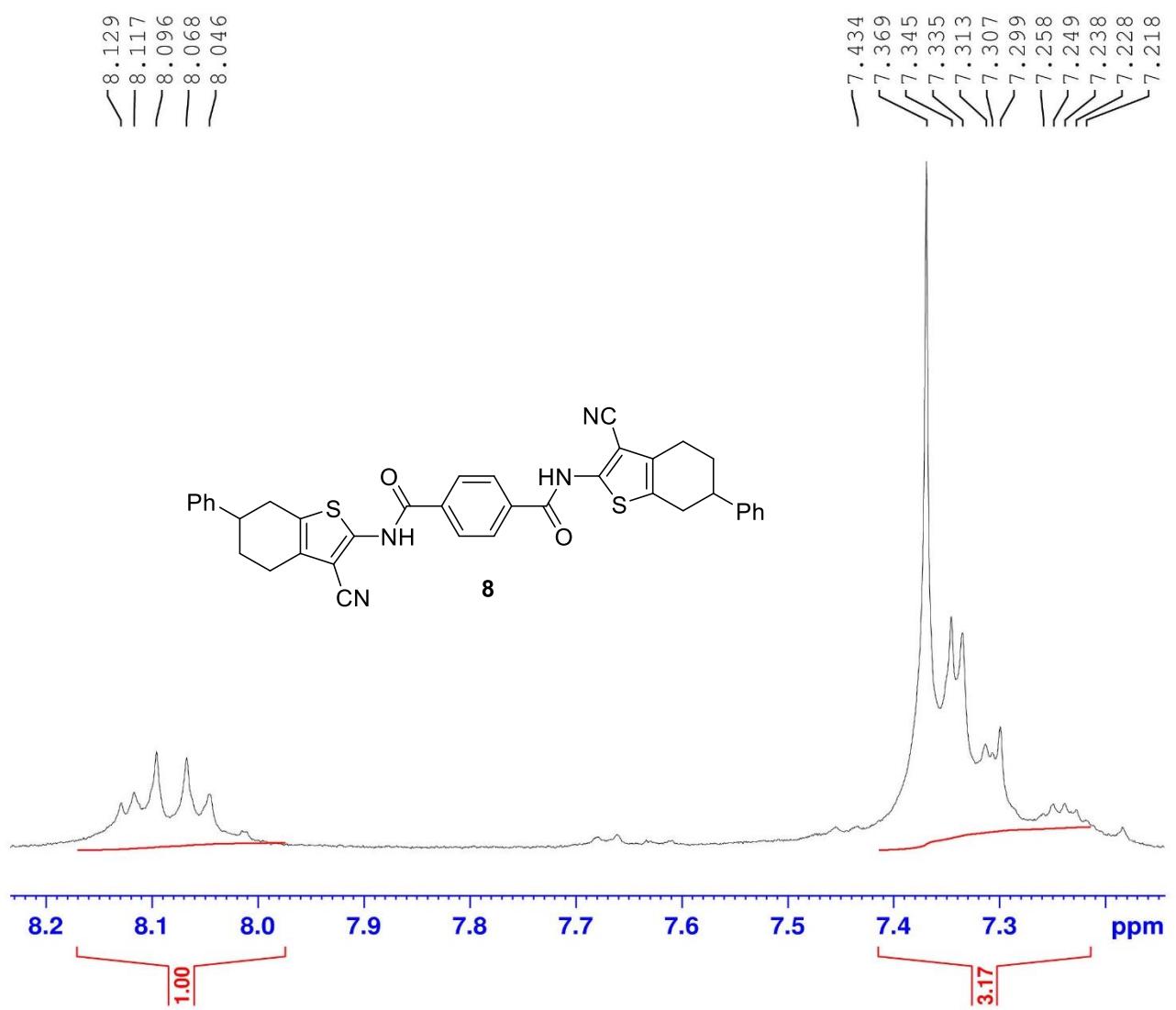


Current Data Parameters  
 NAME amna-shaabani-A7  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220913  
 Time 12.39  
 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  
 TDO 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

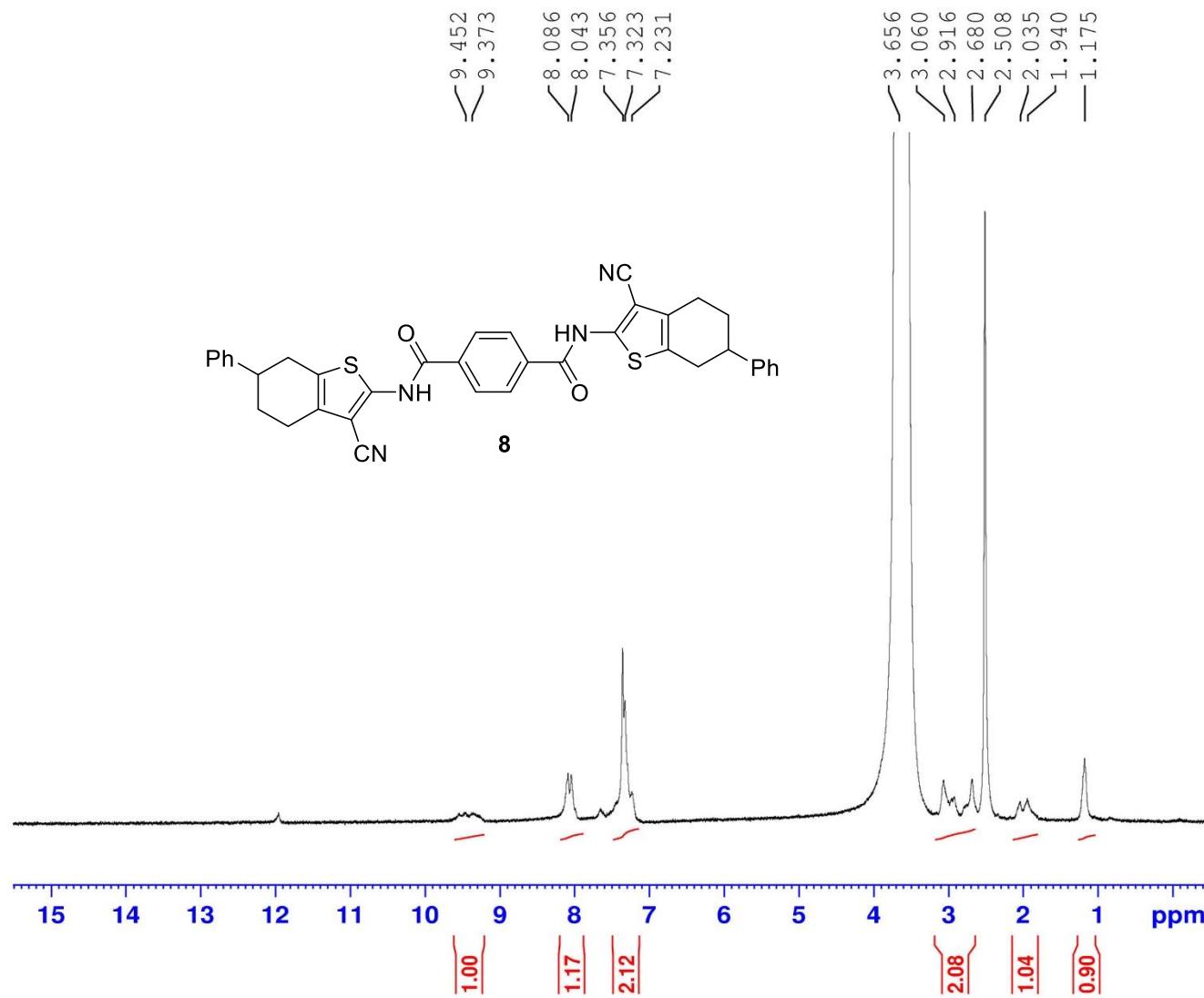


Current Data Parameters  
 NAME amna-shaabani-A7  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220913  
 Time 12.39  
 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 1.0000000 sec  
 T0D 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

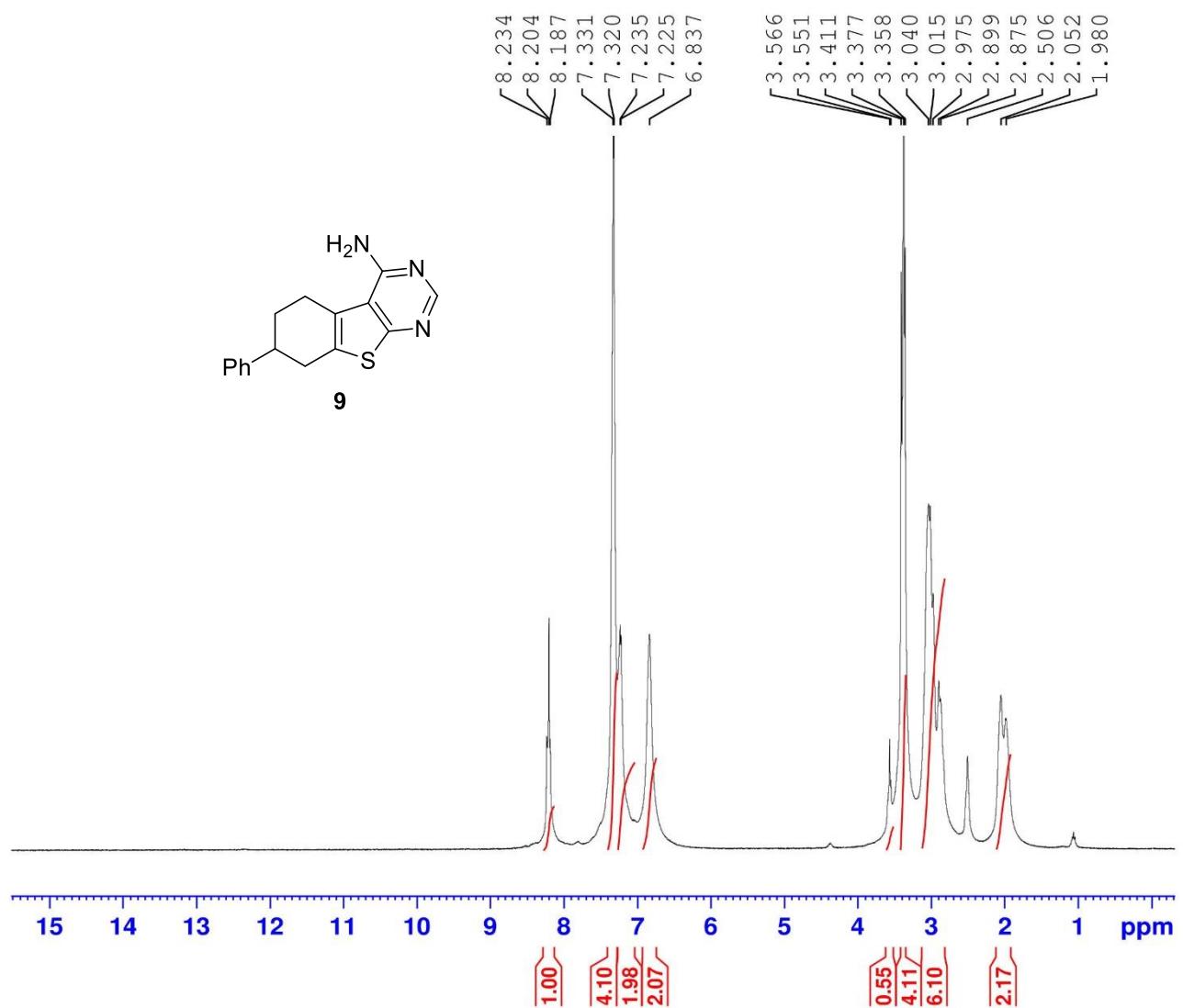


Current Data Parameters  
 NAME amna-shaabani-A7-d2o  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20220920  
 Time 12.25  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 58  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 164.32  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.0000000 W

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

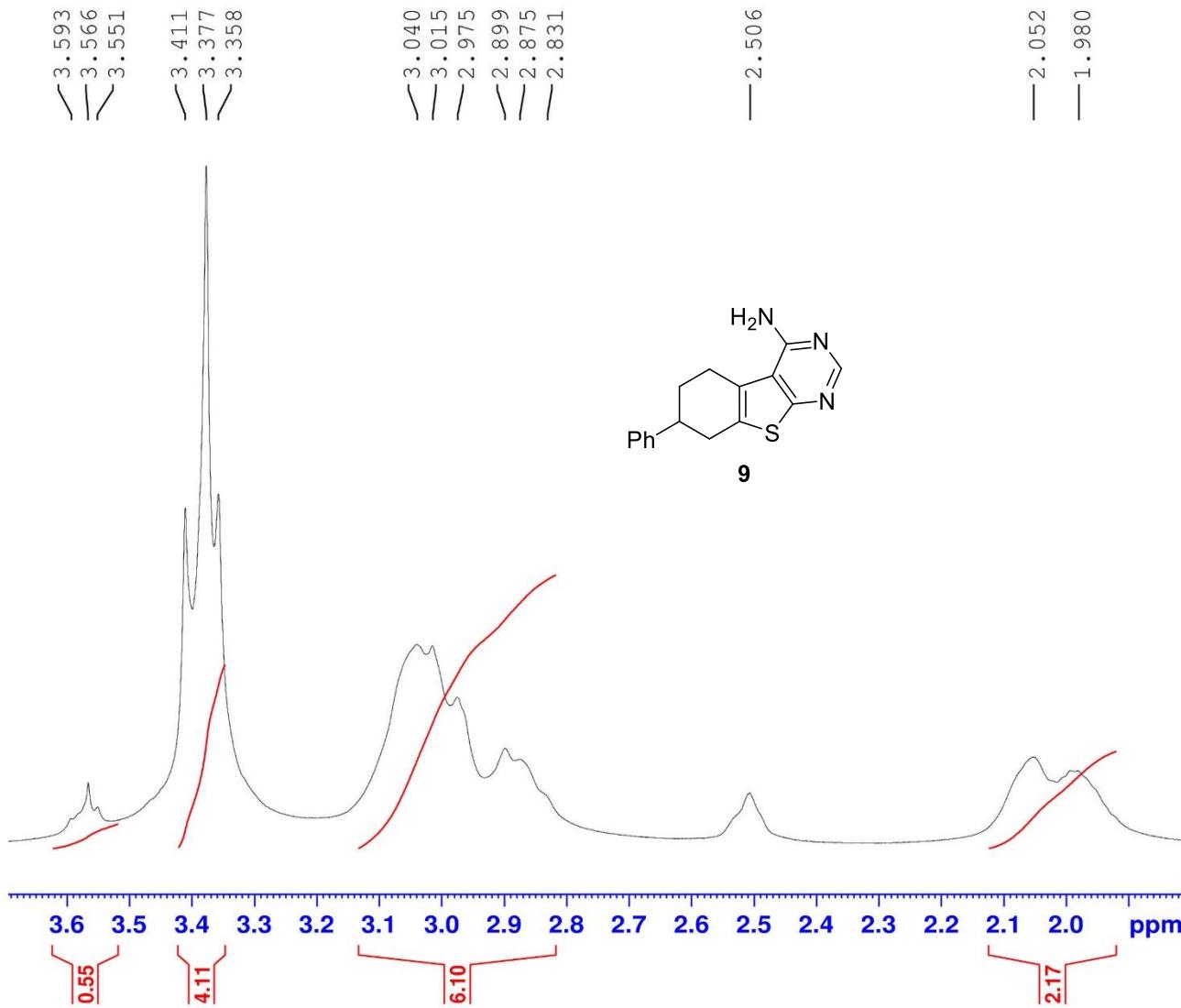


Current Data Parameters  
 NAME amna-shaabani-A3  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220913  
 Time 11.15  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 65  
 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 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.0000000 W

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

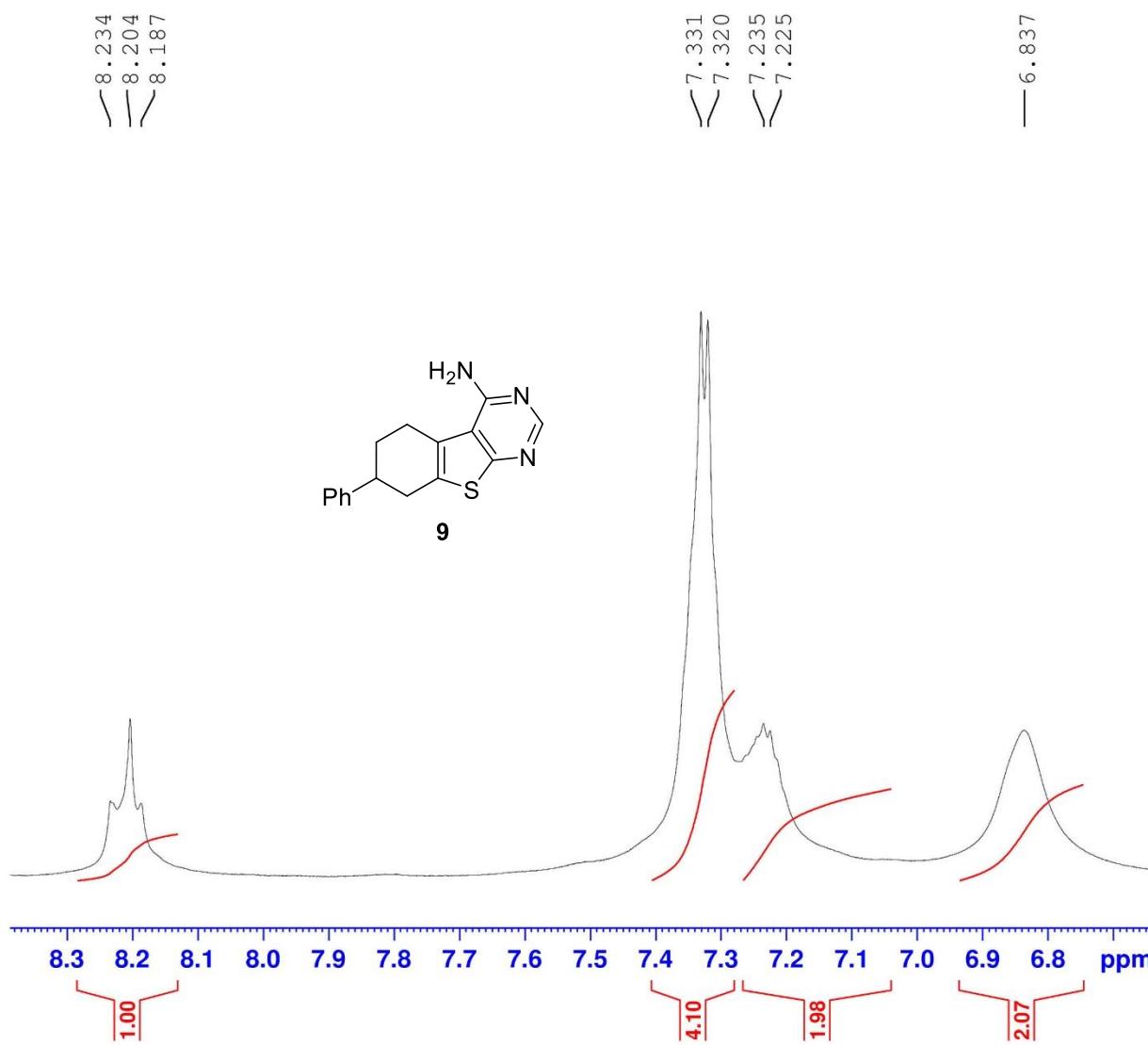


Current Data Parameters  
NAME amna-shaabani-A3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220913  
Time 11.15  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 65  
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 1.0000000 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

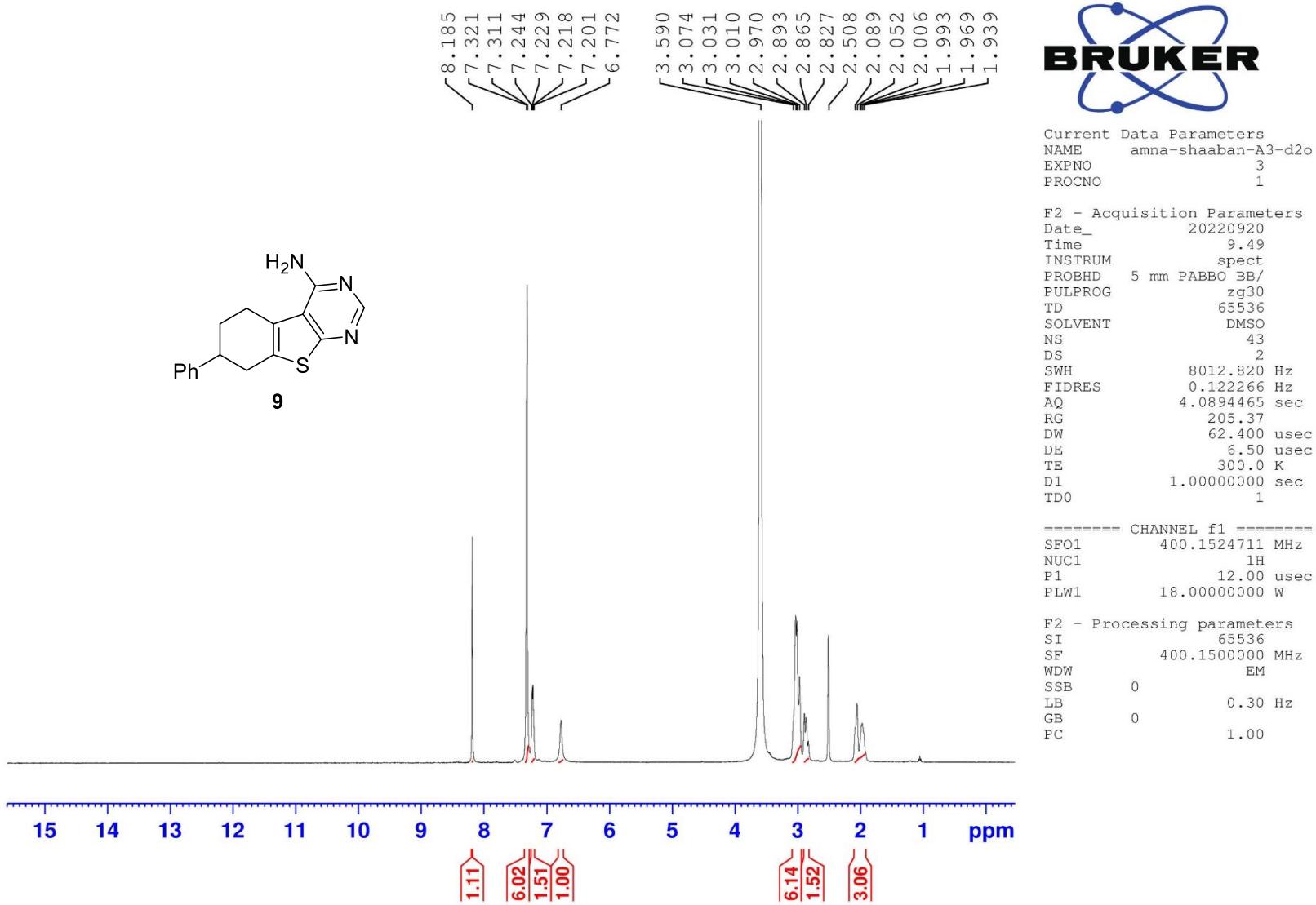


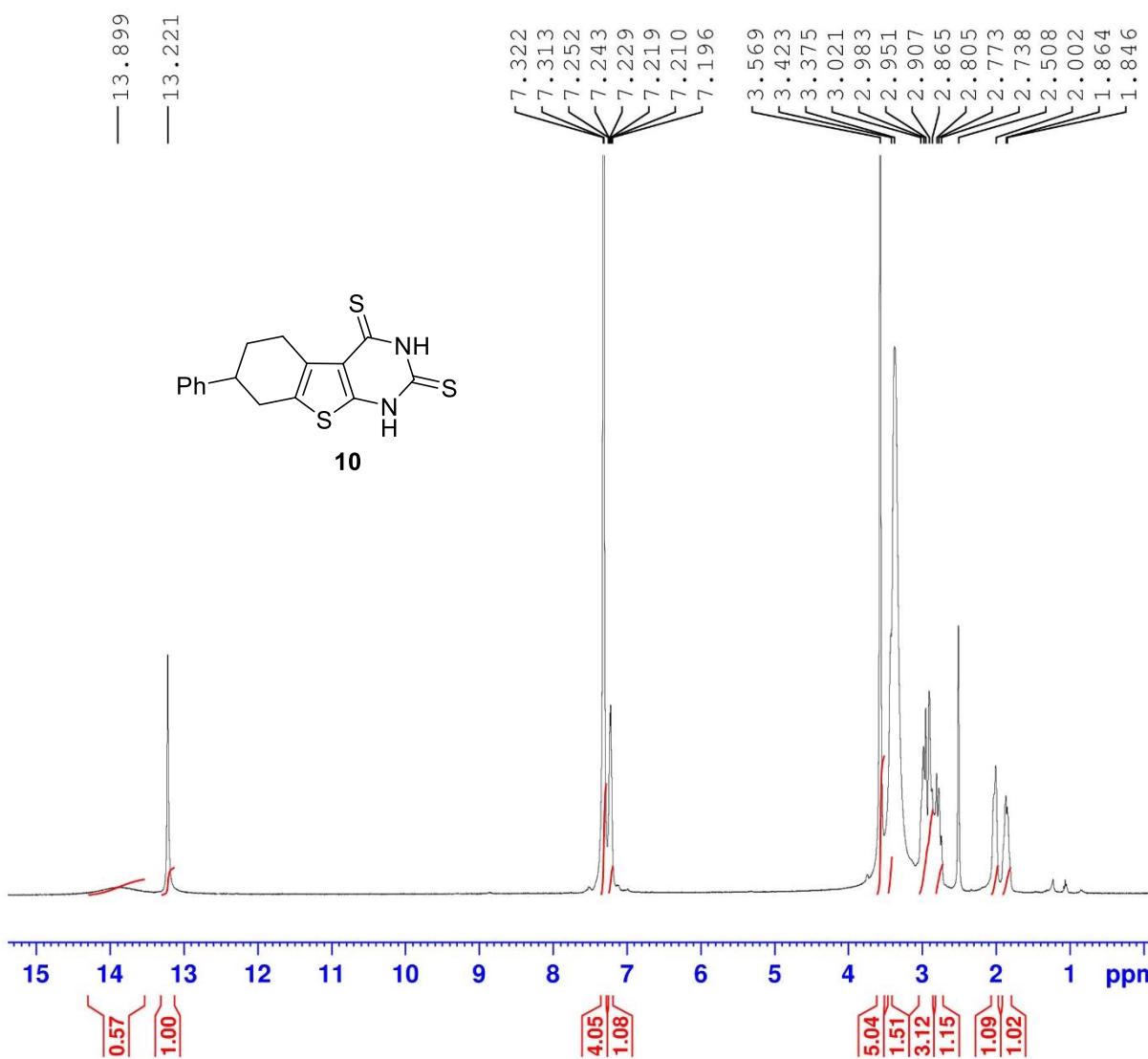
Current Data Parameters  
 NAME amna-shaabani-A3  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220913  
 Time 11.15  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 65  
 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  
 TDO 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



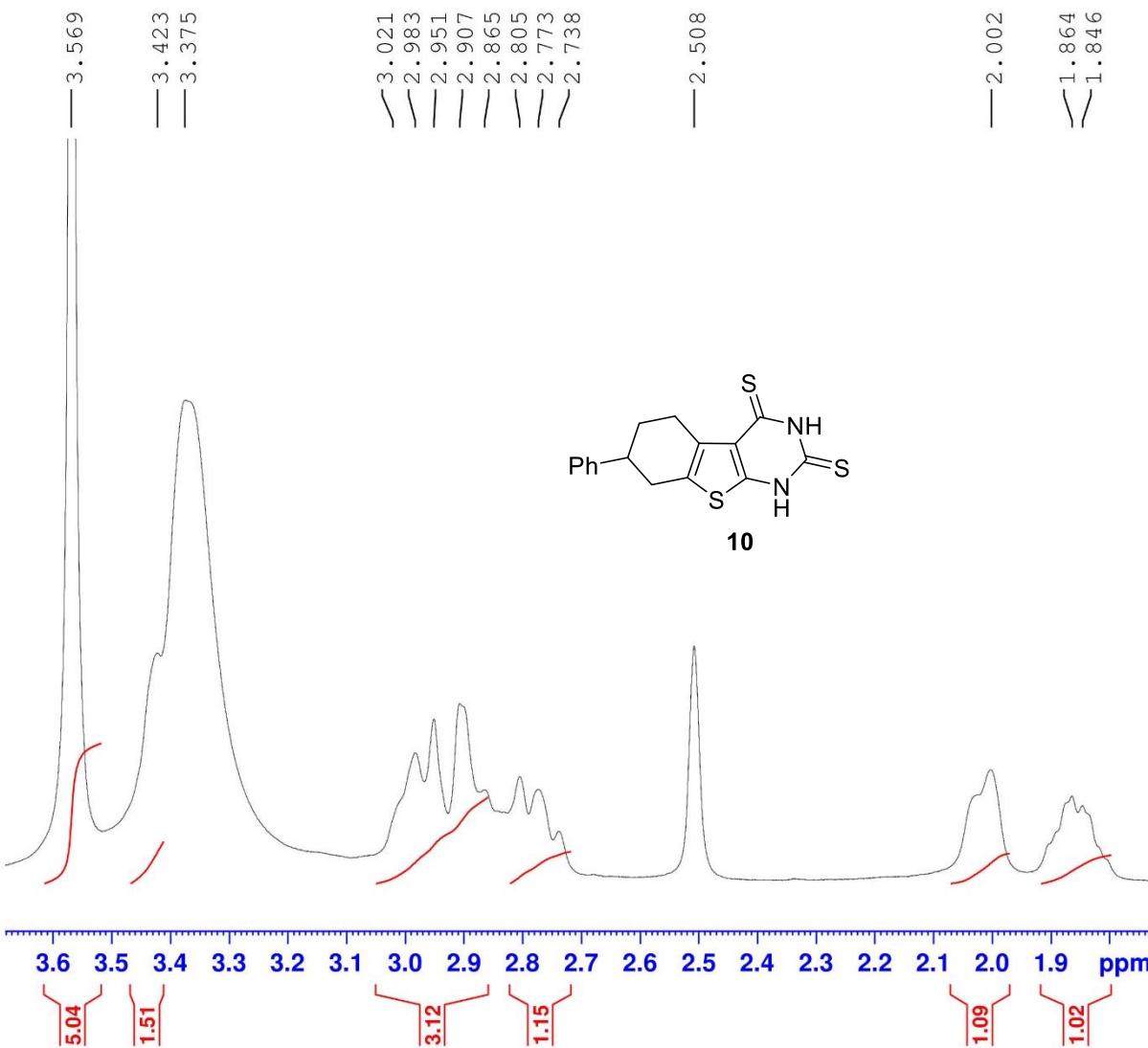


Current Data Parameters  
NAME amna-shaabani-1A13  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220913  
Time 10.45  
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 1.0000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.0000000 W

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

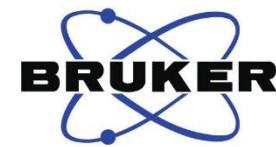
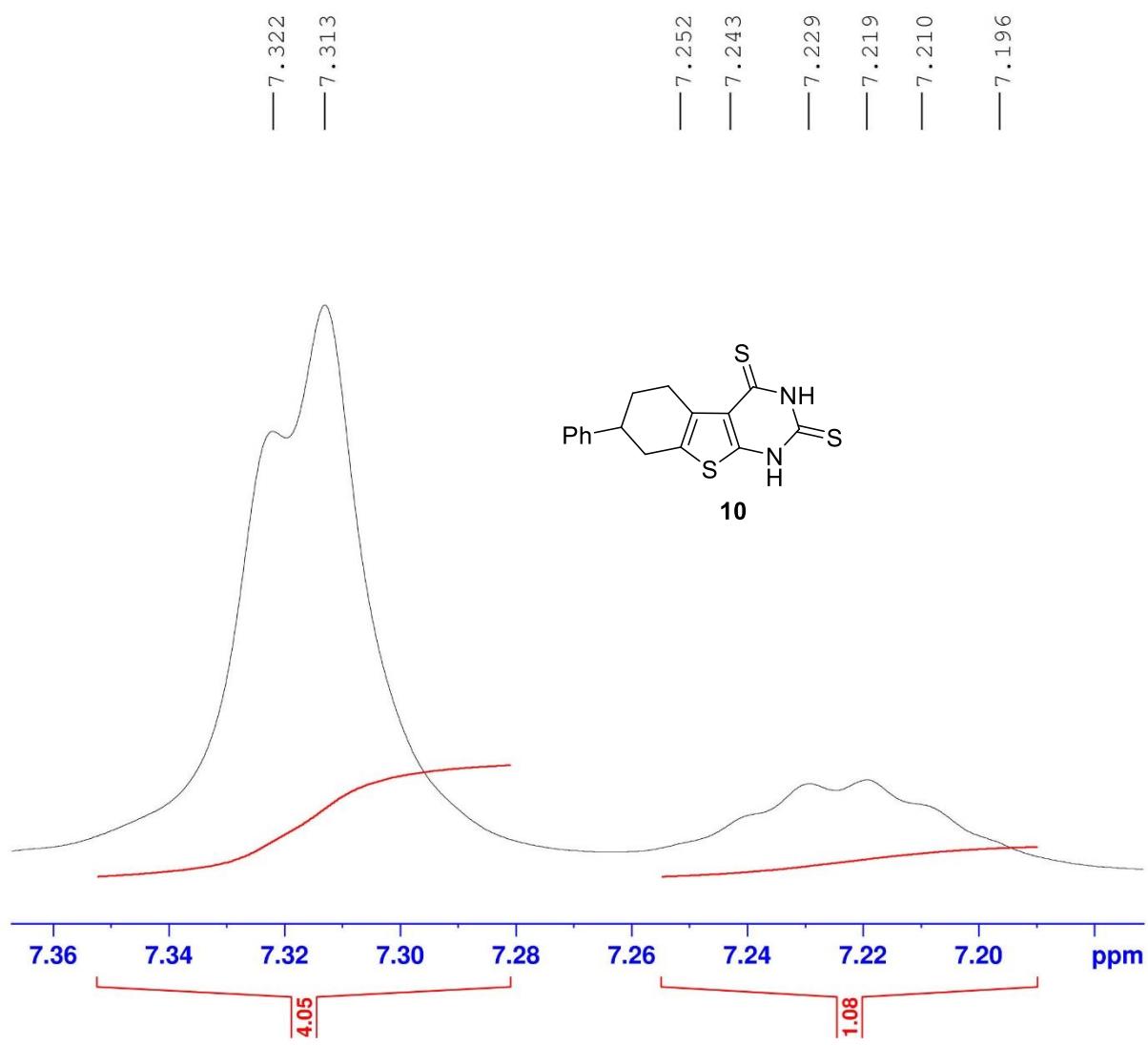


Current Data Parameters  
 NAME amna-shaabani-1A13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220913  
 Time 10.45  
 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 1.0000000 sec  
 TDO 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

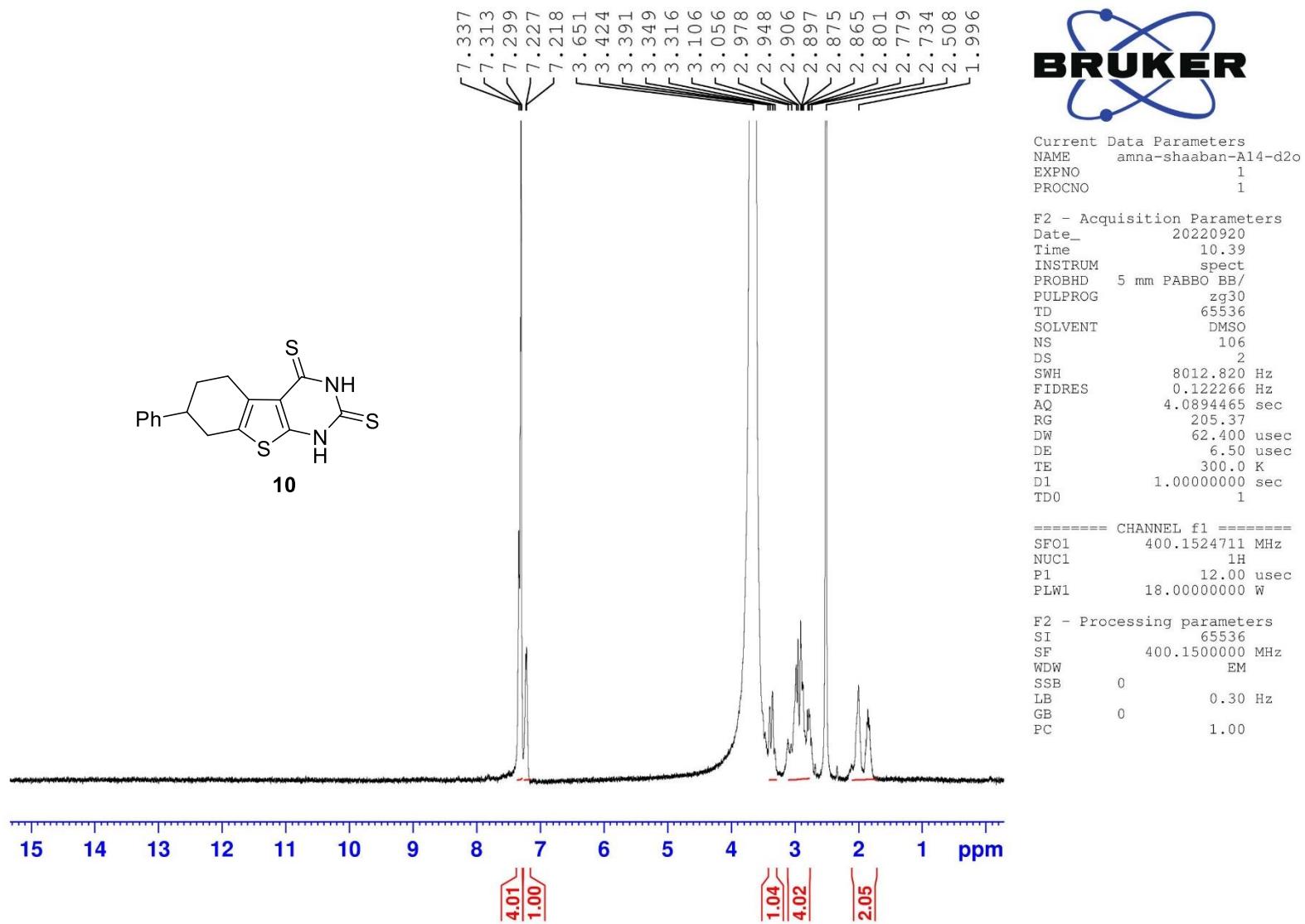


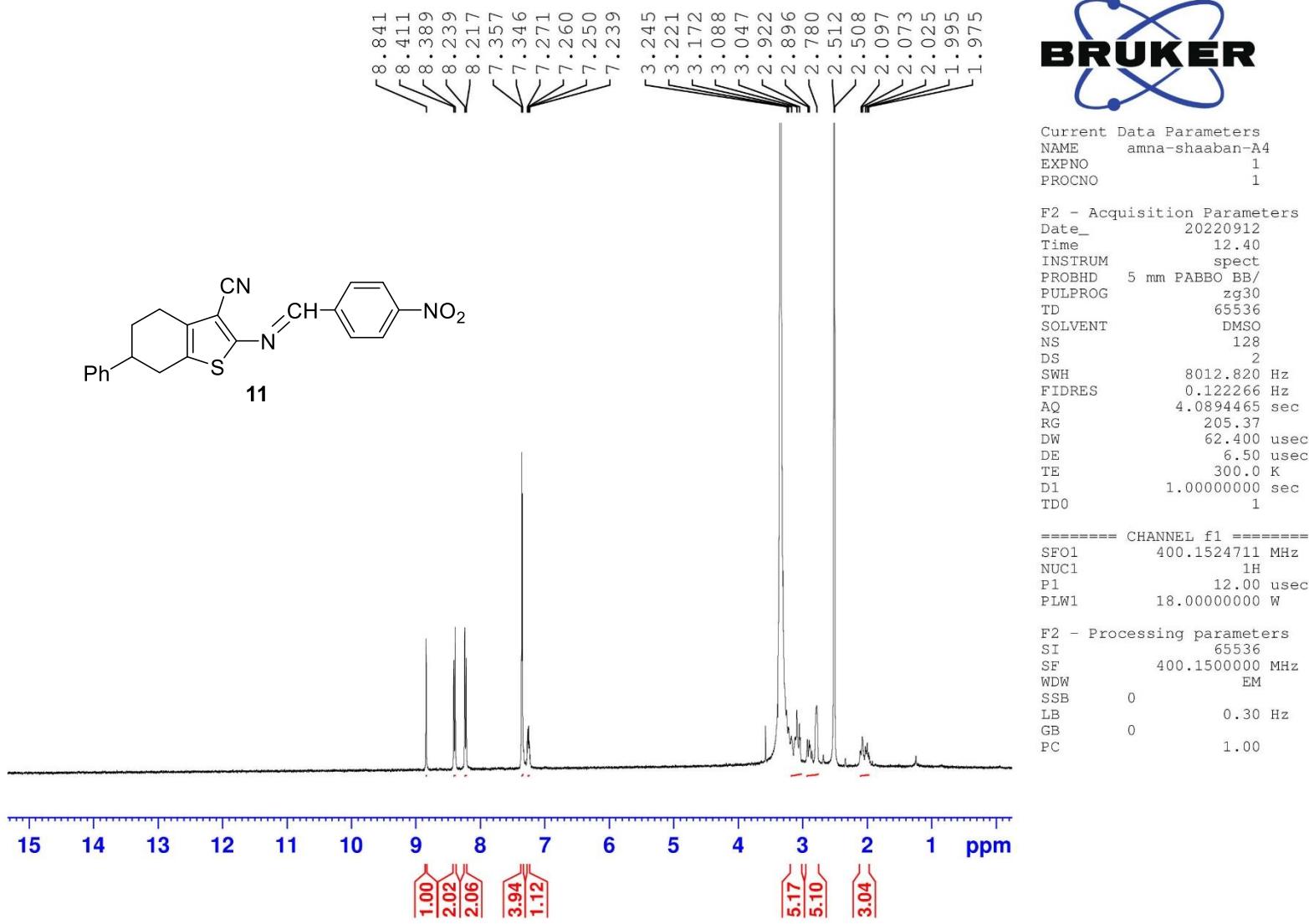
Current Data Parameters  
 NAME amna-shaabani-1A13  
 EXPNO 1  
 PROCNO 1

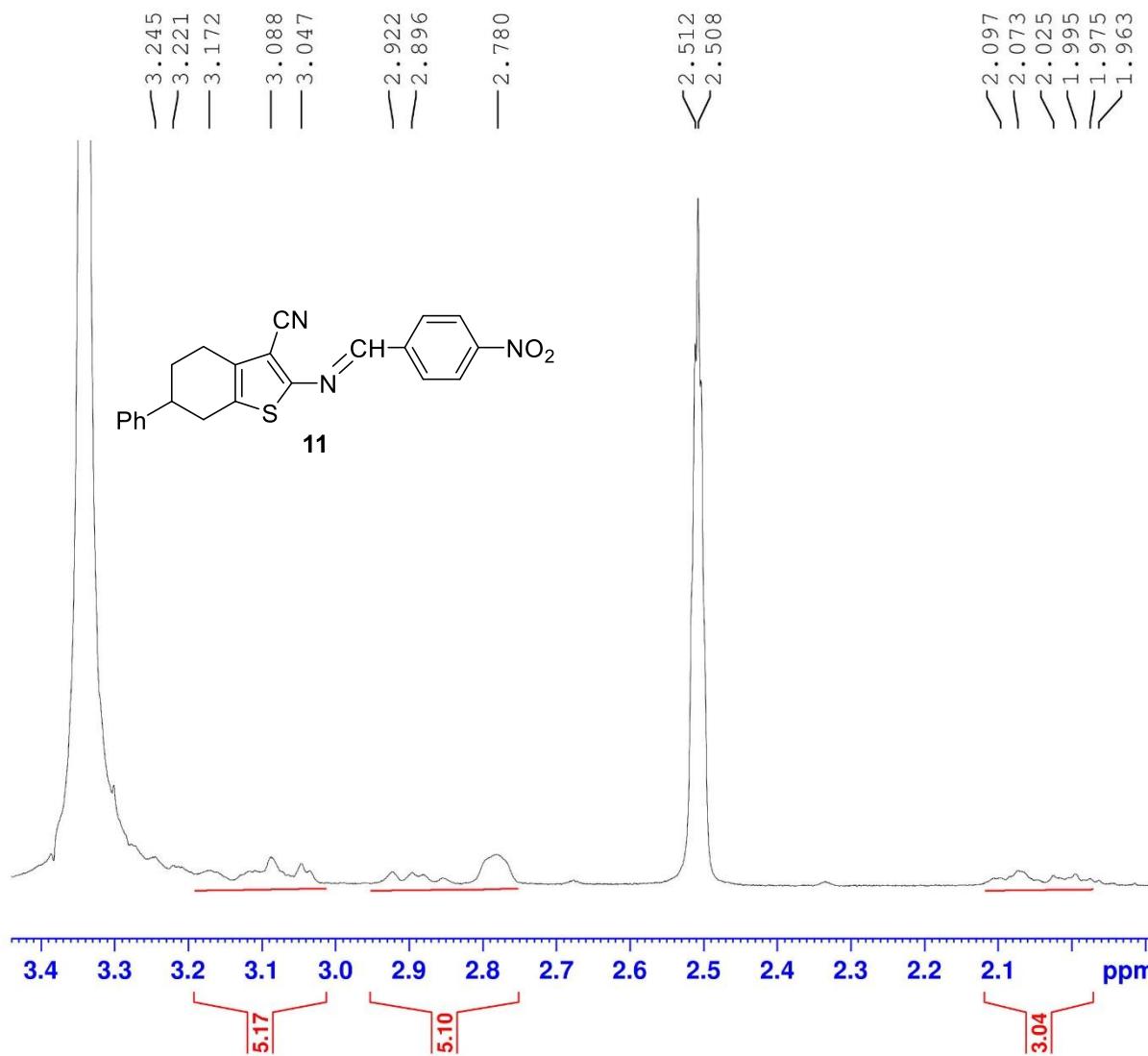
F2 - Acquisition Parameters  
 Date\_ 20220913  
 Time 10.45  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 128  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 205.37  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.0000000 sec  
 TDO 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 0.30 Hz  
 LB 0  
 GB 0 1.00  
 PC







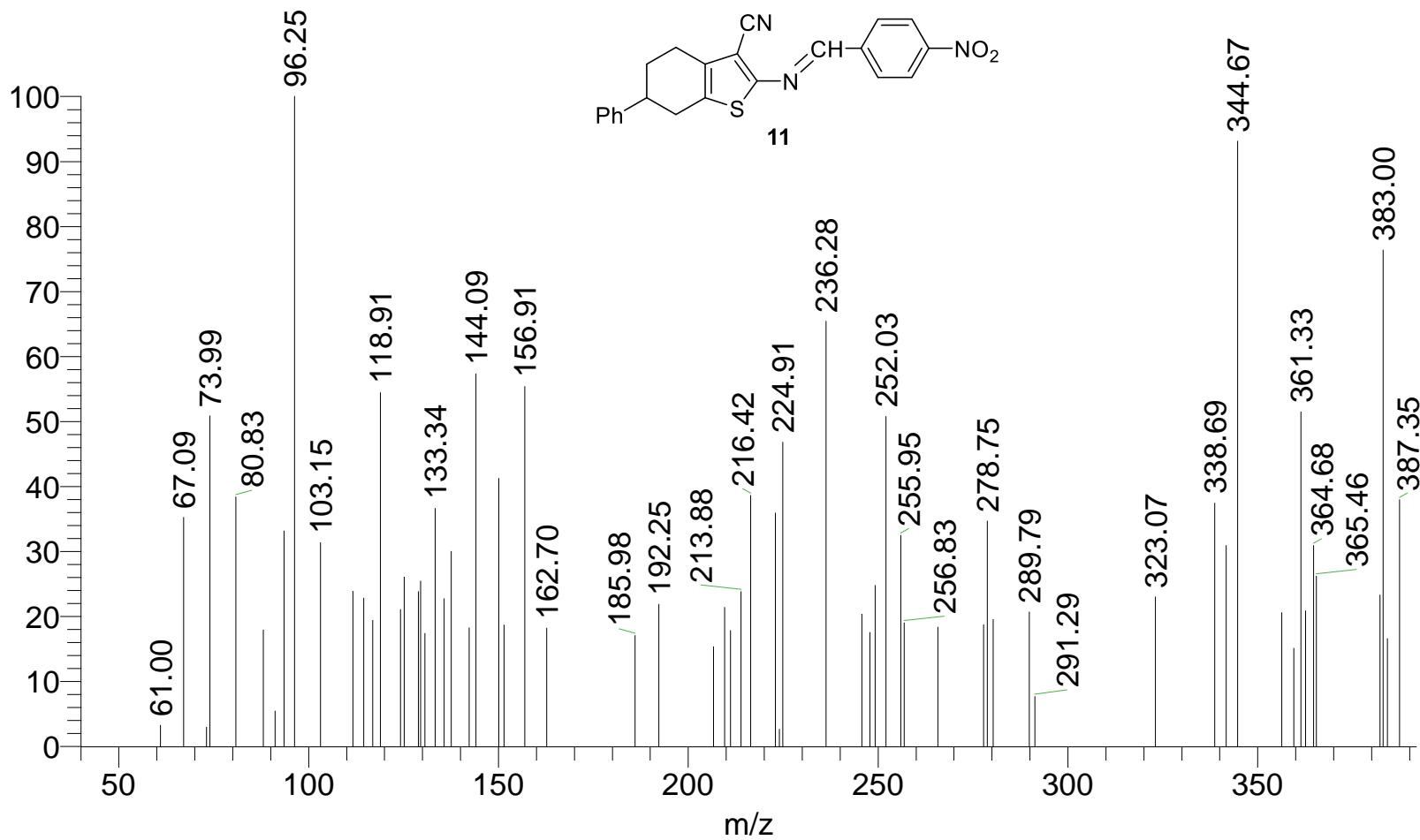
Current Data Parameters  
 NAME amna-shaabani-A4  
 EXPNO 1  
 PROCNO 1

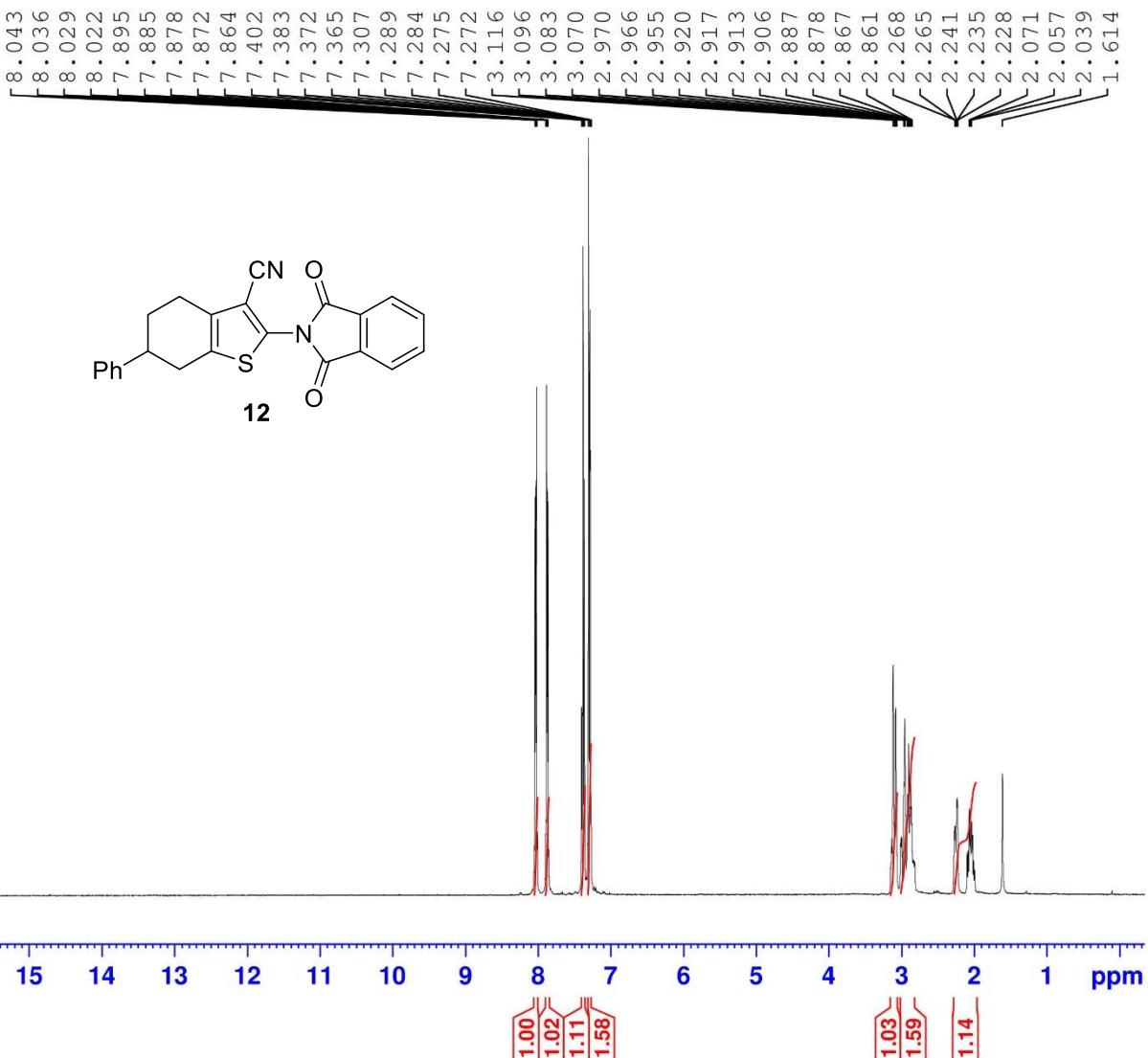
F2 - Acquisition Parameters  
 Date\_ 20220912  
 Time 12.40  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 128  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 205.37  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.0000000 W

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

sayed-karam-A4 #62 RT: 1.05 AV: 1 SB: 26 1.21-1.34 , 0.87-1.14 NL: 3.70E2  
T: {0,0} + c EI Full ms [40.00-1000.00]



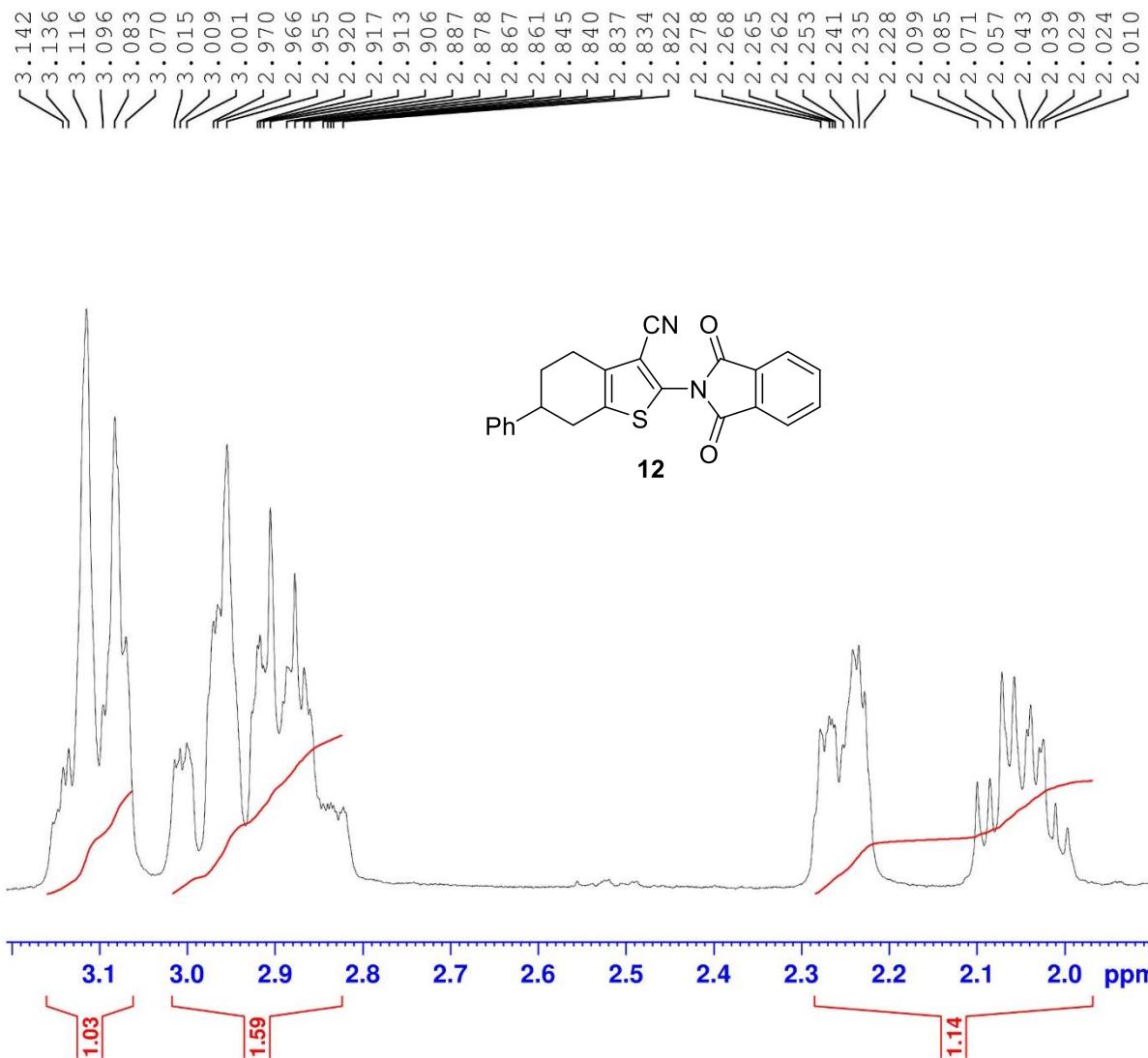


Current Data Parameters  
 NAME amna-shaabani-A21  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220912  
 Time 9.01  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 54  
 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 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SF01 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 0.30 Hz  
 LB 0  
 GB 0 1.00  
 PC

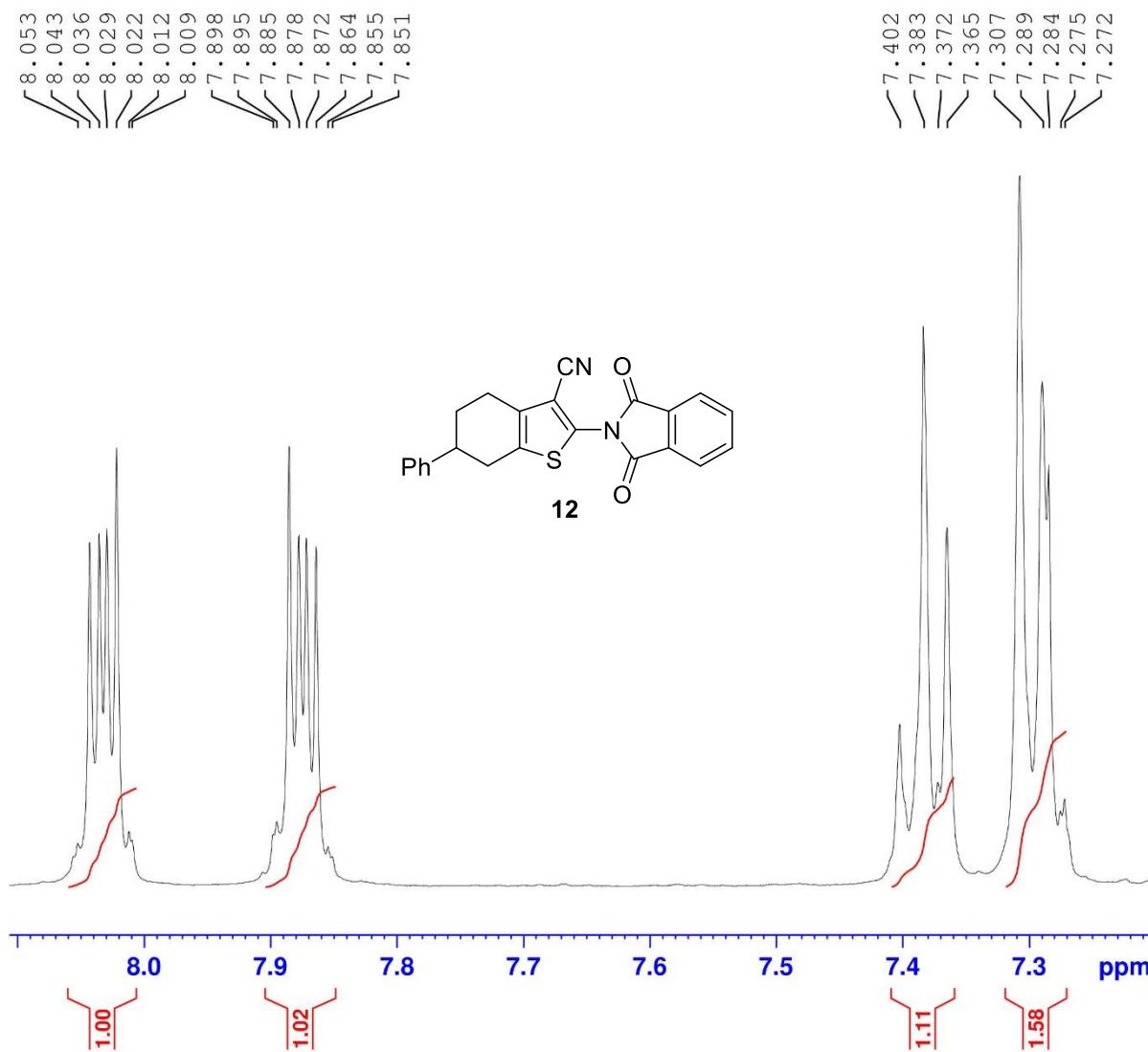


Current Data Parameters  
 NAME amna-shaabani-A21  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20220912  
 Time 9.01  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 54  
 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 1.0000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 400.1524711 MHz  
 NUC1 <sup>1</sup>H  
 P1 12.00 usec  
 PLW1 18.0000000 W

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



Current Data Parameters  
 NAME amna-shaabani-A21  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220912  
 Time 9.01  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 54  
 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 1.0000000 sec  
 TDO 1

===== CHANNEL f1 ======  
 SFO1 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.0000000 W

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

sayed-karam-A21 #292 RT: 4.90 AV: 1 SB: 26 1.21-1.34 , 0.87-1.14 NL: 2.70E6  
T: {0,0} + c EI Full ms [40.00-1000.00]

