Electronic Supplementary Material (ESI) for RSC Advances.

β-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_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (Debye)	η (eV)	ς (eV^{-1})	μ_o (eV)	ω (eV)	n (eV^{-1})	Ip (eV)	EA (eV)	x (eV)
2	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
3	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
4	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
5	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
6	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
7	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
8	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
9	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
10	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
11	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
12	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
Dox.	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

ς: Global Softness μ_o: Chemical Potential ω: Global Electrophilicity Index

n: Nucleophilicity Index Ip: Ionization Potential EA: Electron Affinity x: Electronegativity

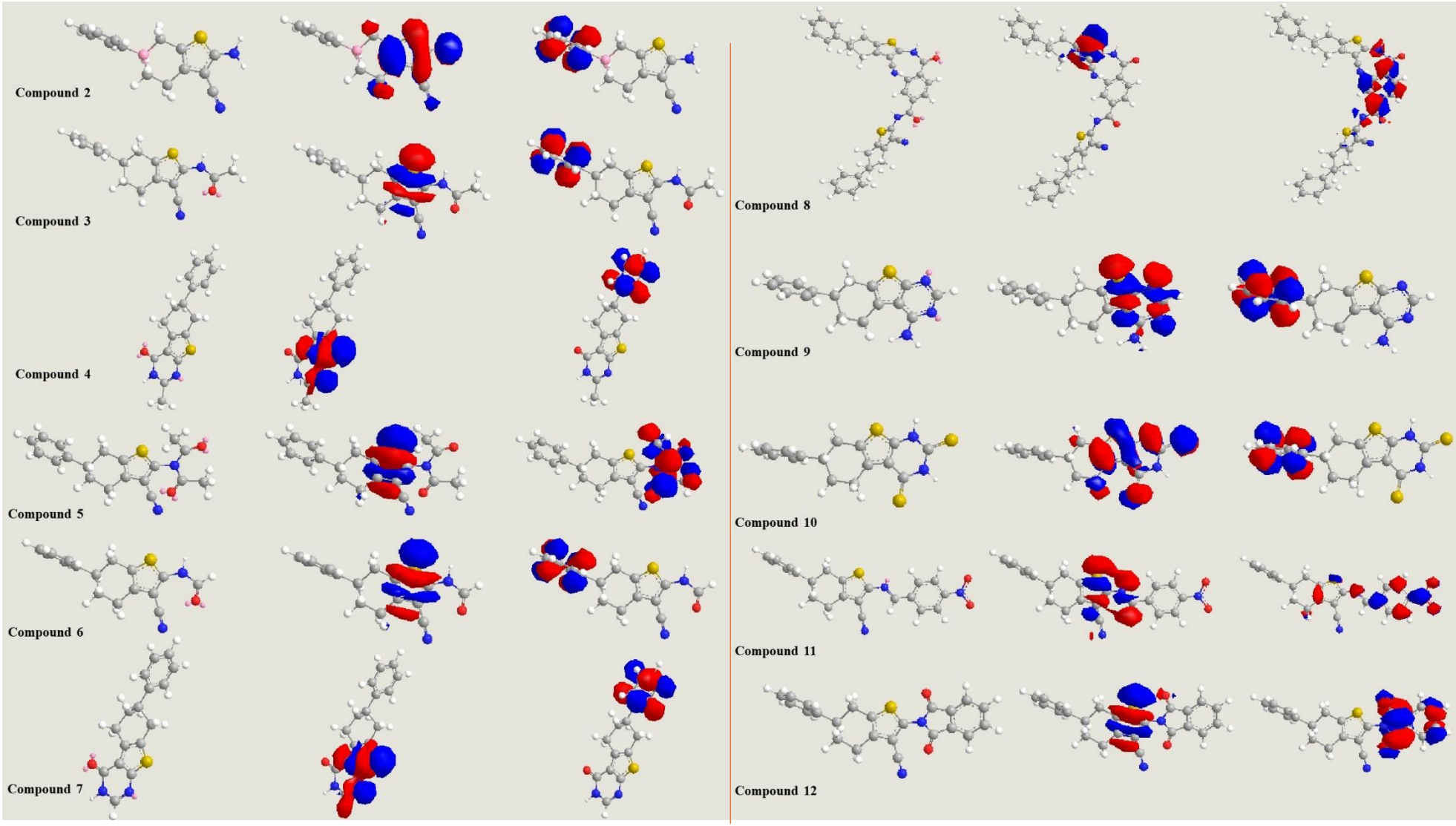


Fig. S1. Optimized configurations (left), HOMO (middle), and LUMO (right) of substances **2-12**.

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 ($Å^2$)	78.05	81.13	73.99	89.41	81.13	73.99	162.26	80.04	124.00	110.21	89.41
Consensus Log $P_{o/w}$	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	Yes	Yes	Yes	Yes	Yes	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	No	No	No	No	No	No	No	No	No	No
CYP3A4 inhibitor	No	Yes	No	Yes	No	No	No	Yes	Yes	Yes	Yes
Log K_p (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

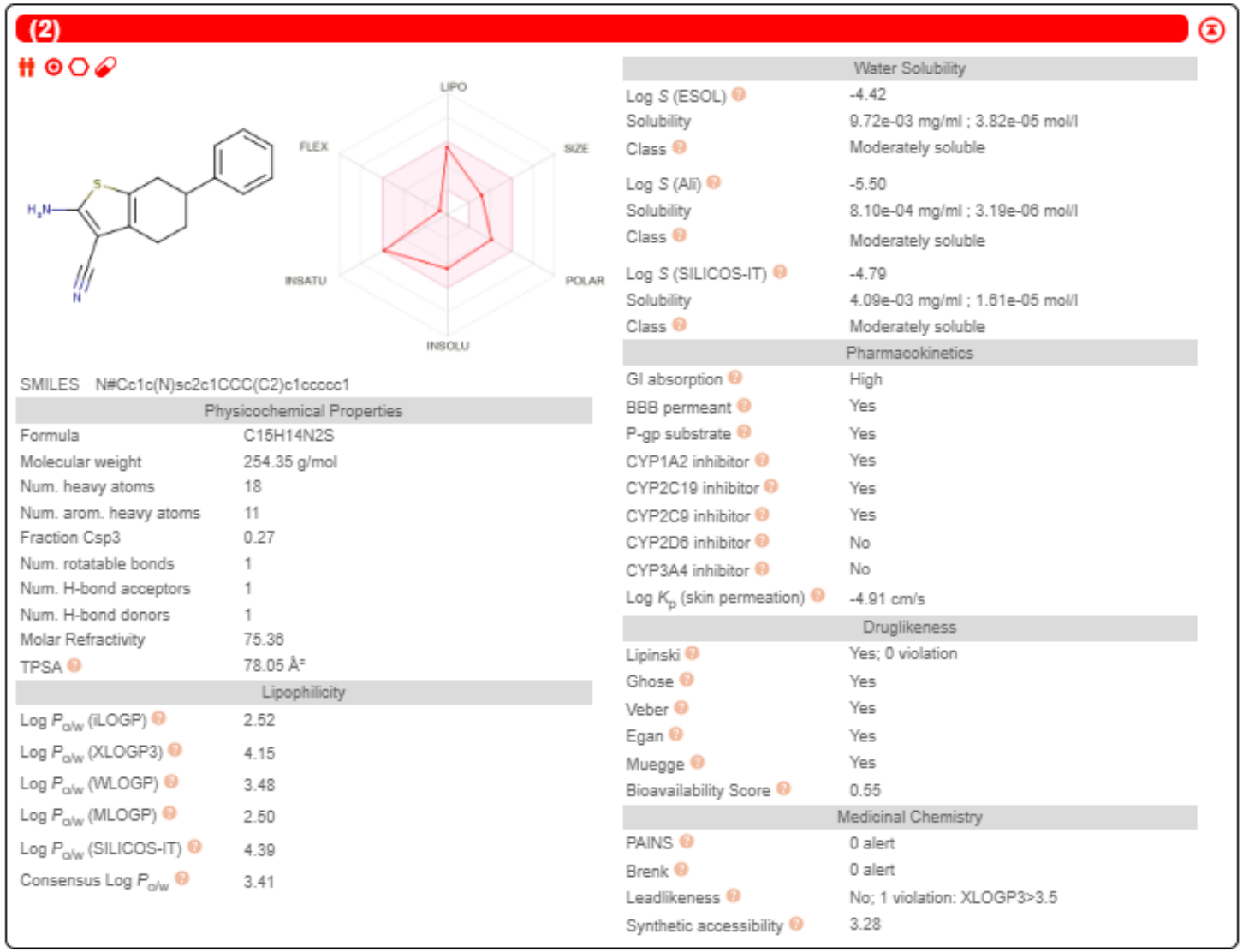


Fig. S2. ADME of compound **2**.

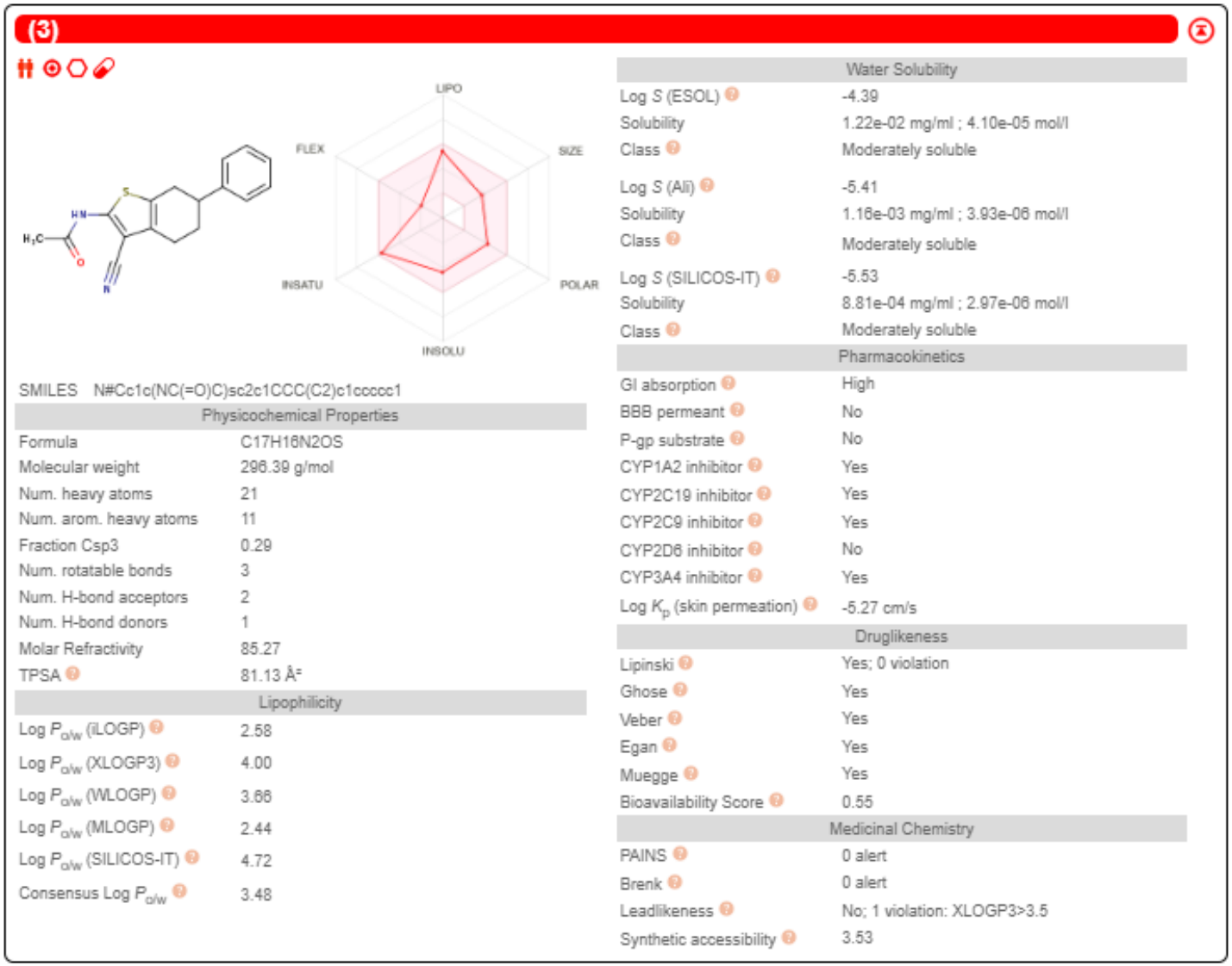
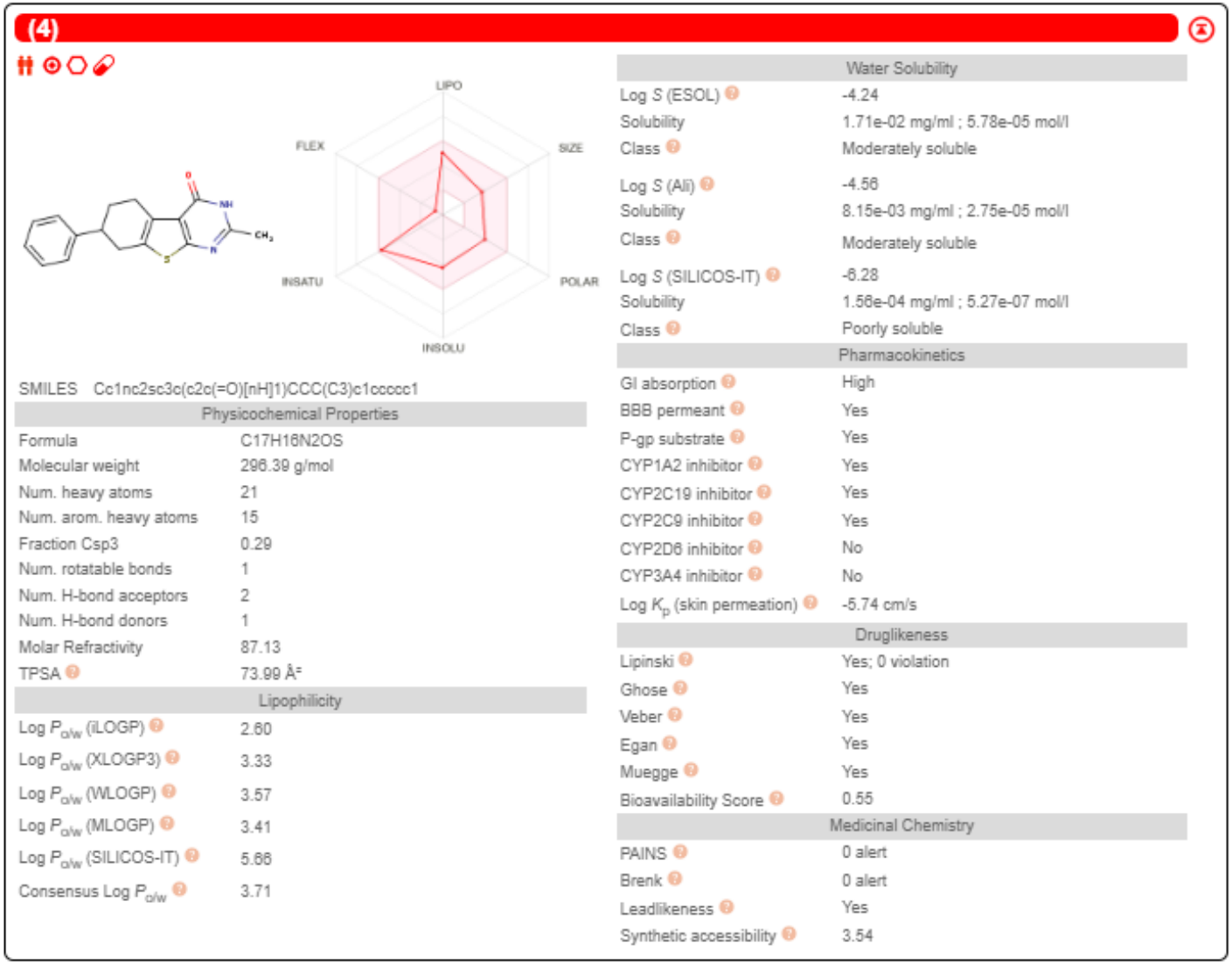


Fig. S3. ADME of compound **3**.



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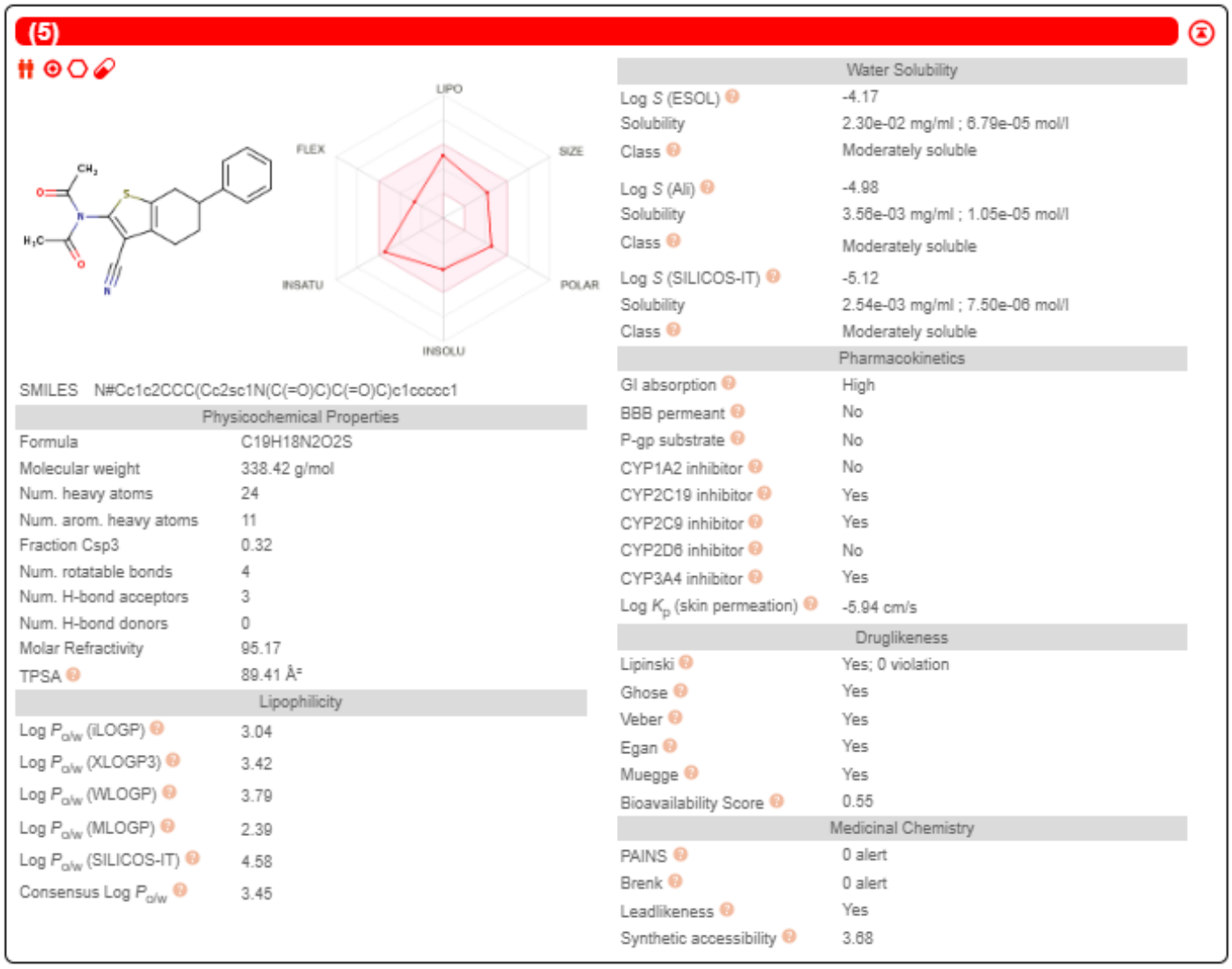

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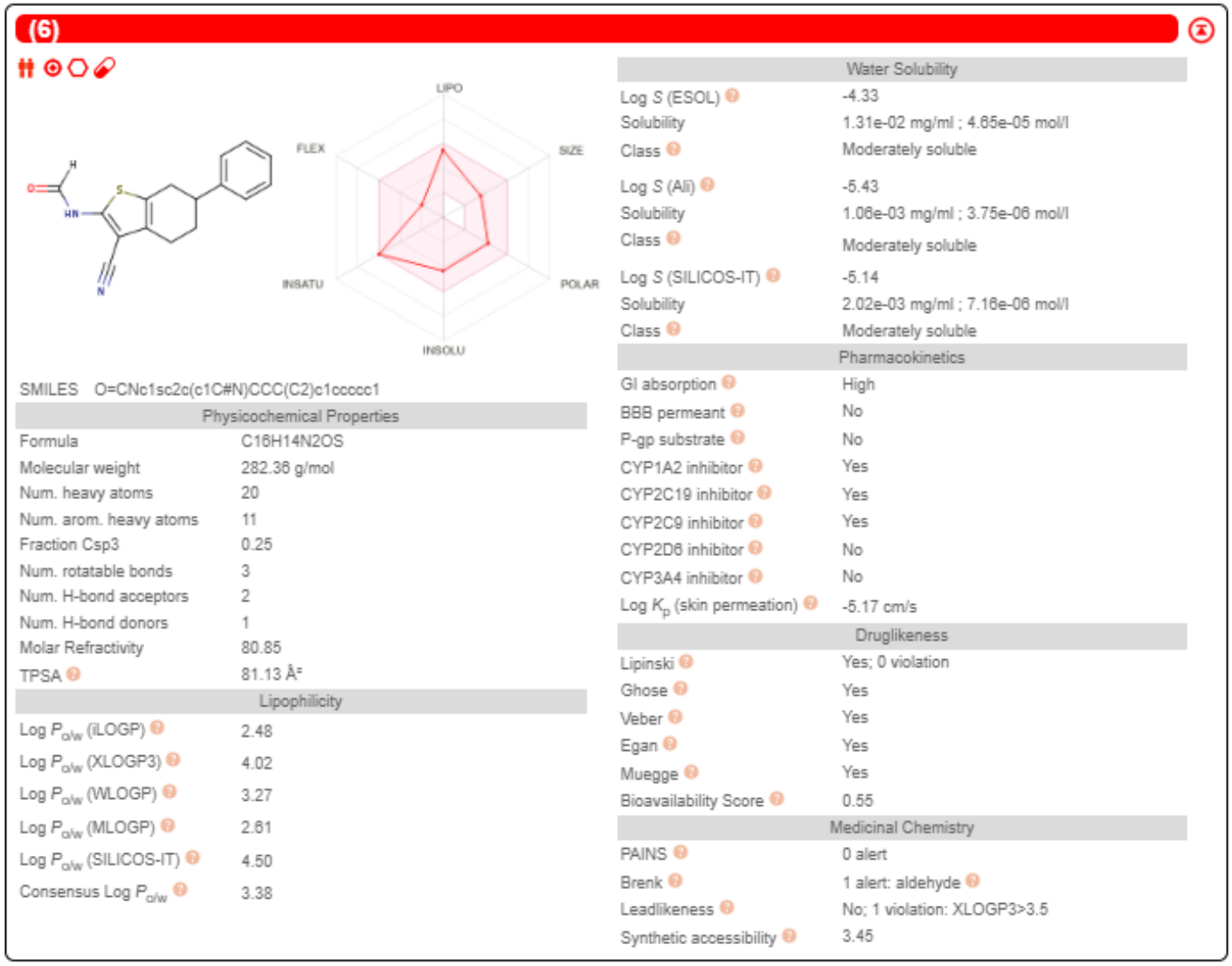
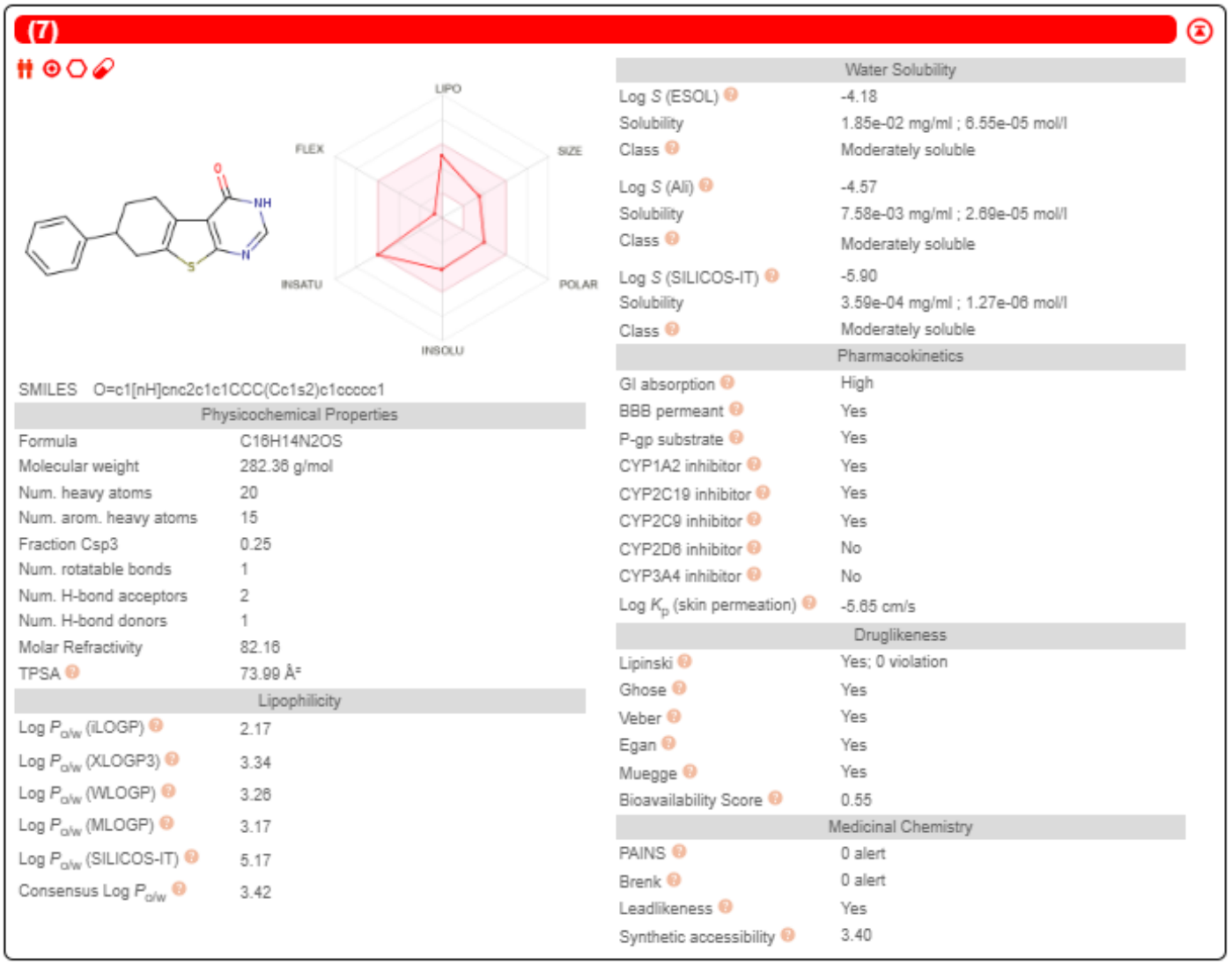


Fig. S6. ADME of compound **6**.



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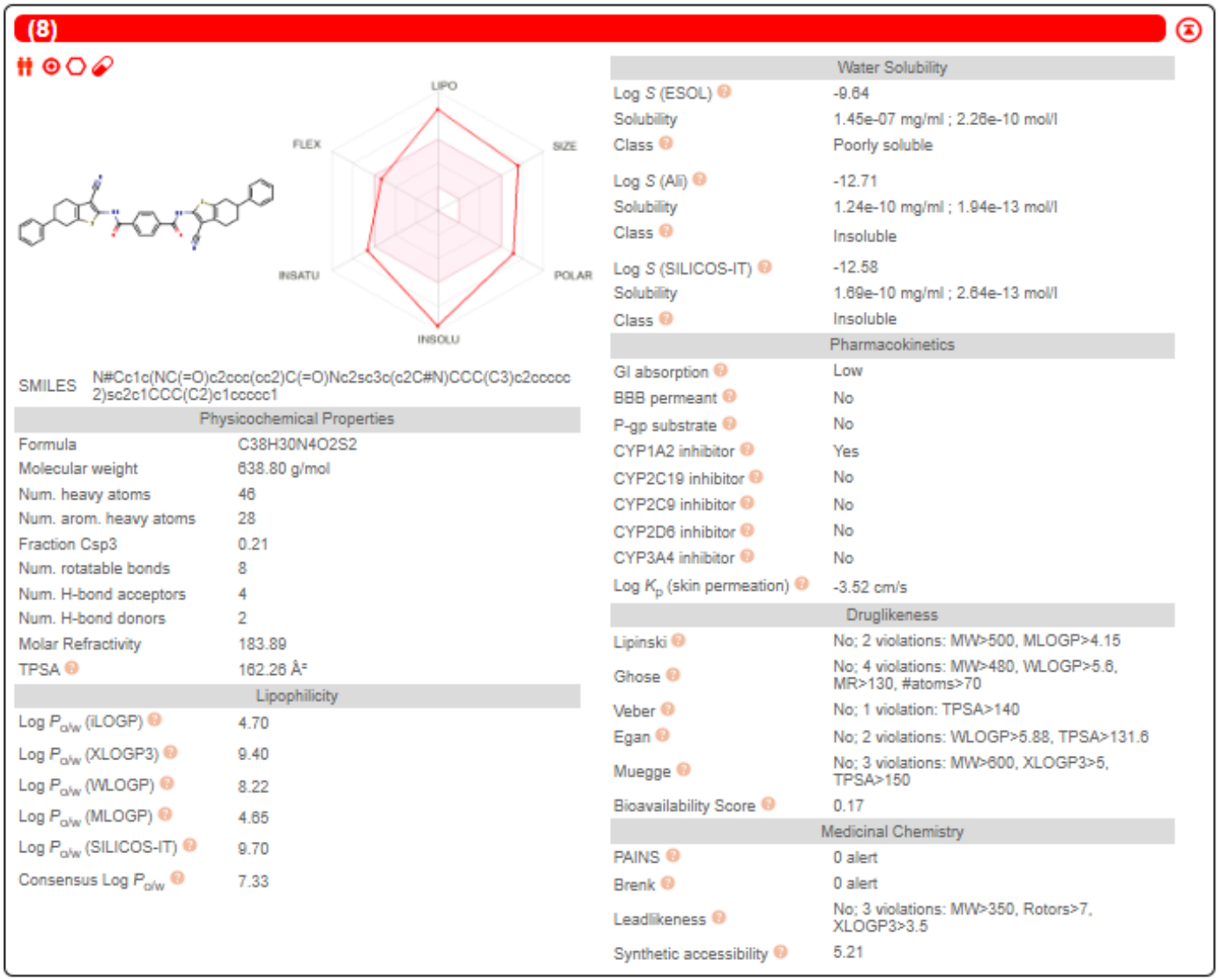

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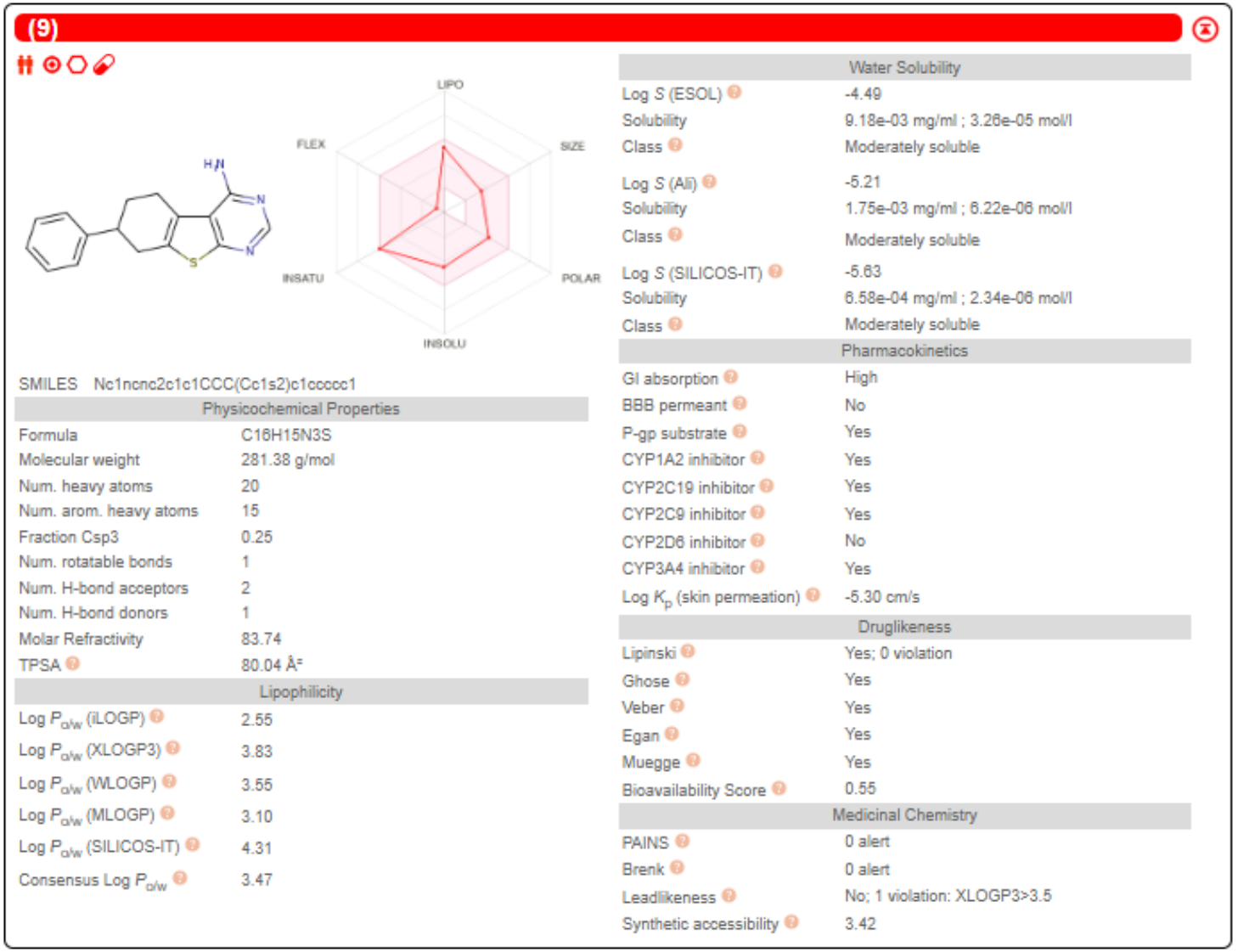

Fig. S9. ADME of compound **9**.

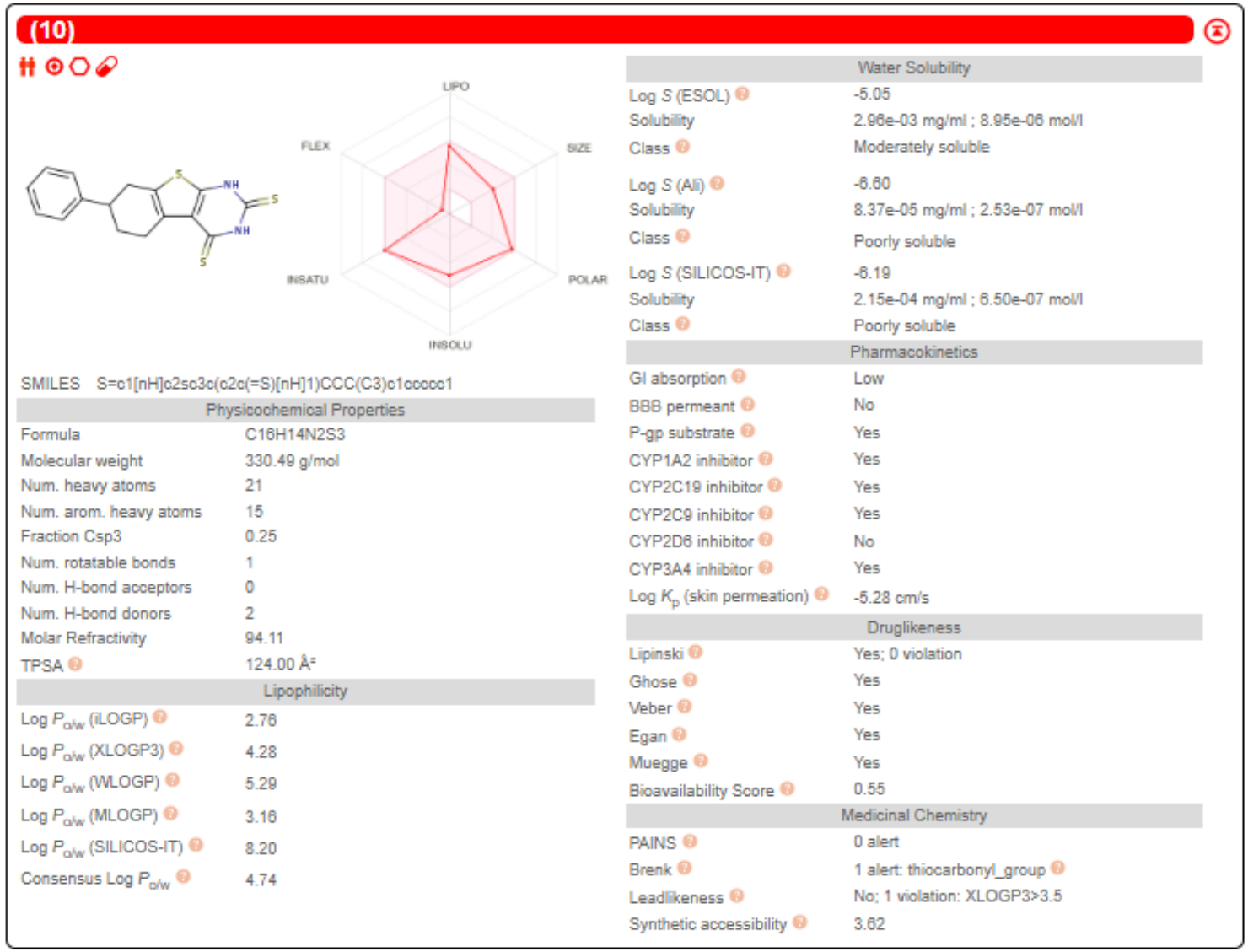

Fig. S10. ADME of compound **10**.

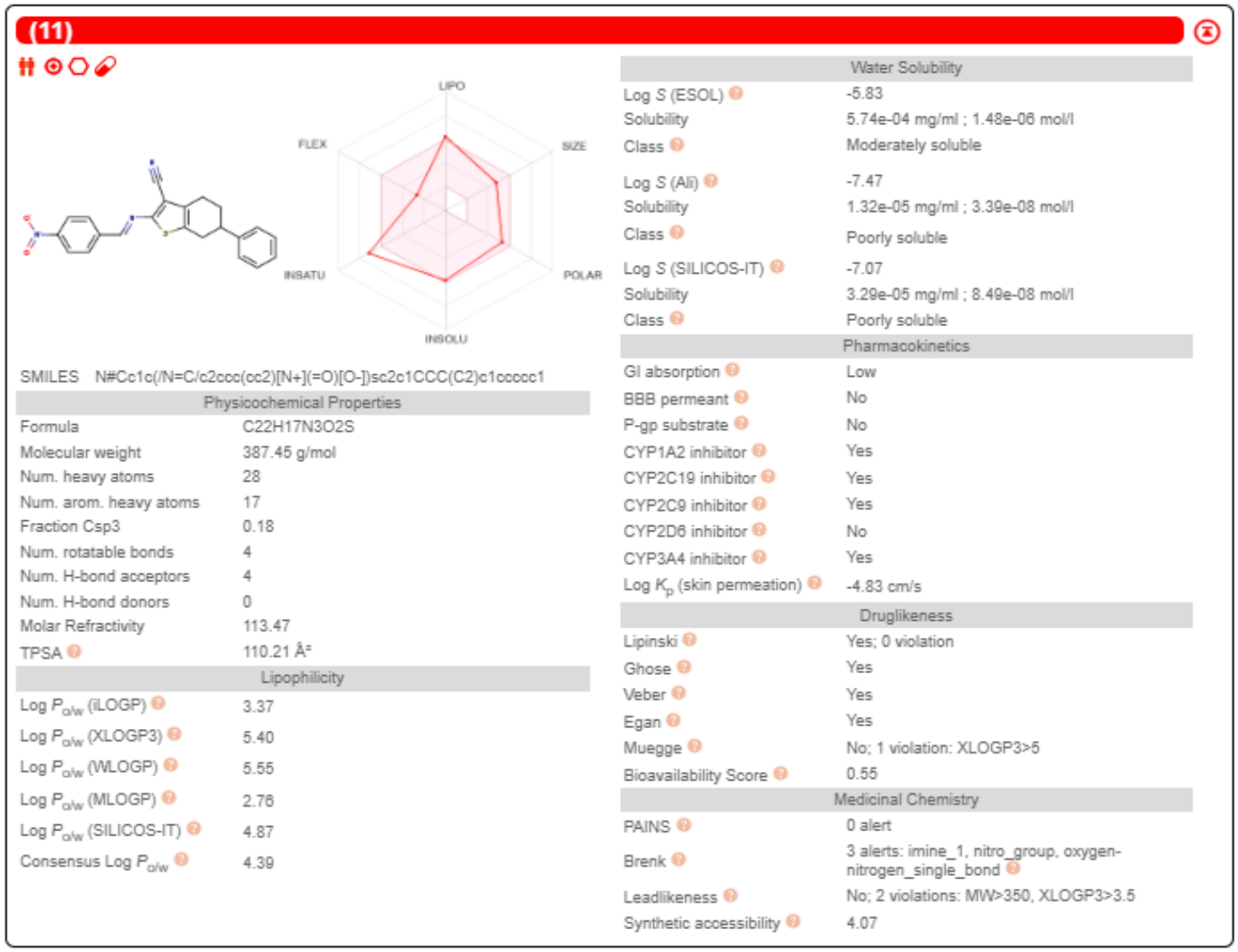

Fig. S11. ADME of compound **11**.

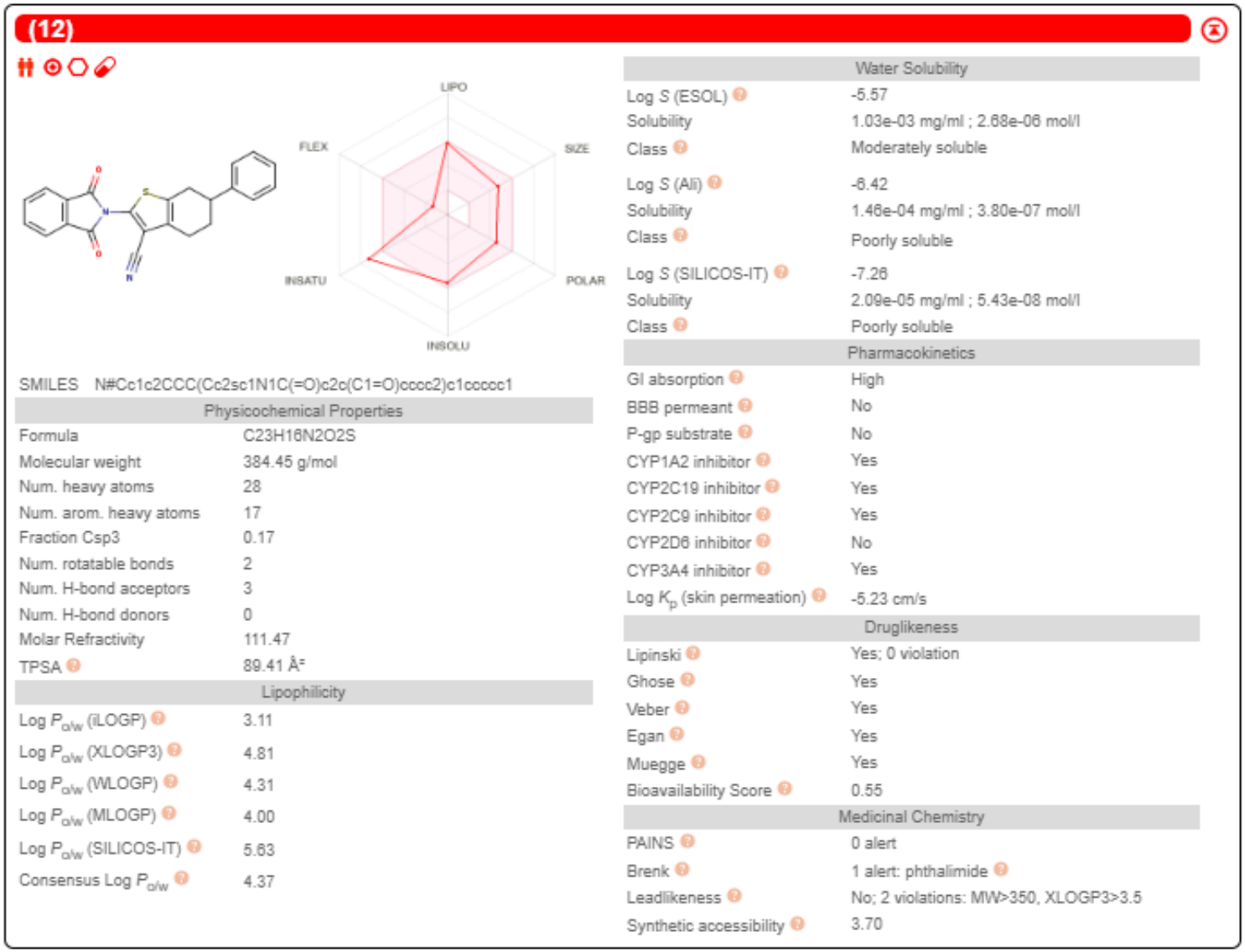

Fig. S12. ADME of compound **12**.

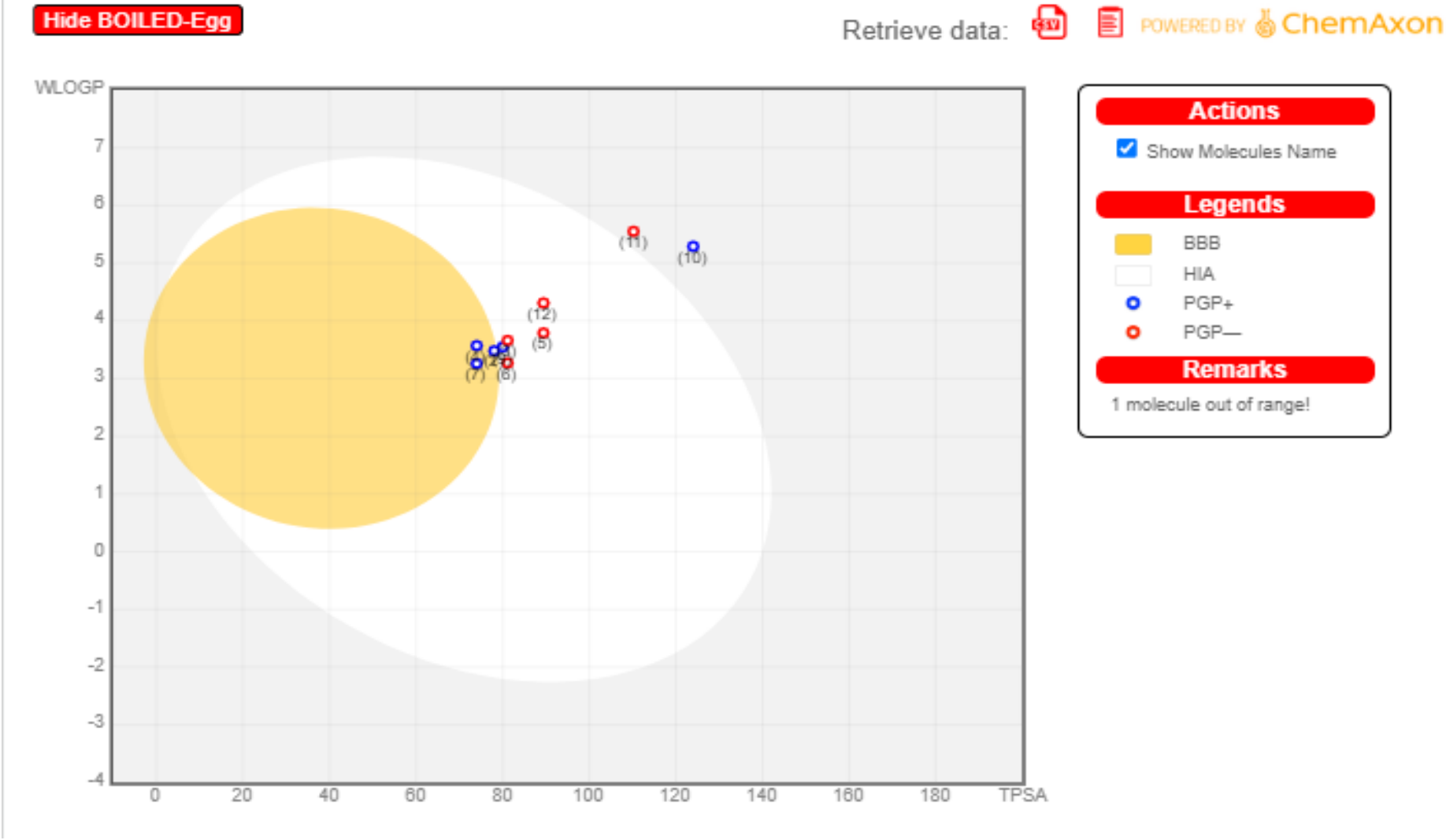

Fig. S13. BOILED-EGG chart of compounds **2-10**.

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 ºC in a 5% CO_2 incubator. The cell lines were seeded in a 96-well plate at a density of 1.0 x 10^4 cells/well at 37 ºC for 48 h under 5% CO_2. 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_{570} of treated samples/A_{570} of untreated samples) x 100.

Statistical analysis

All data were presented as mean ± 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 kcal.mol^{-1}Å^{-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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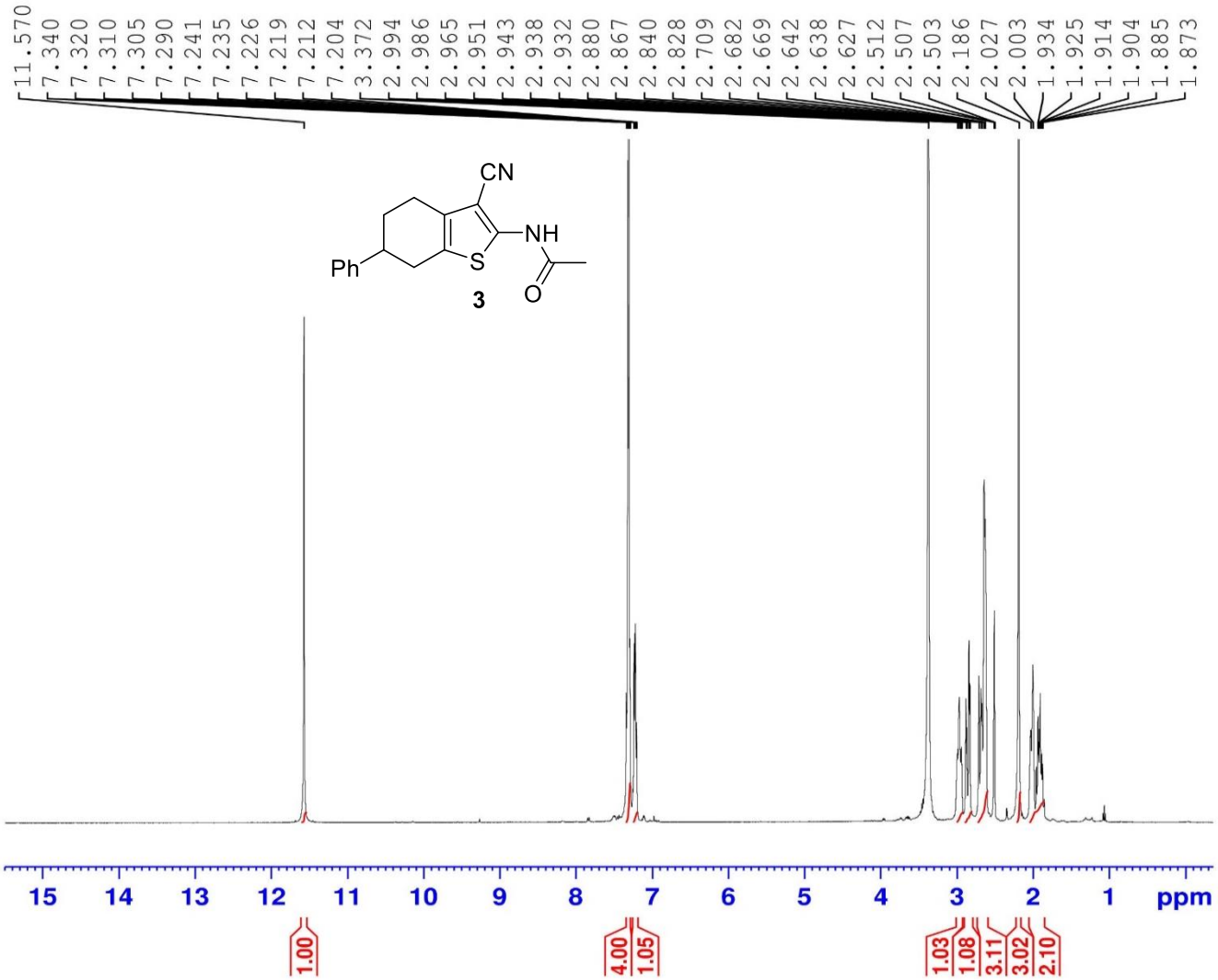

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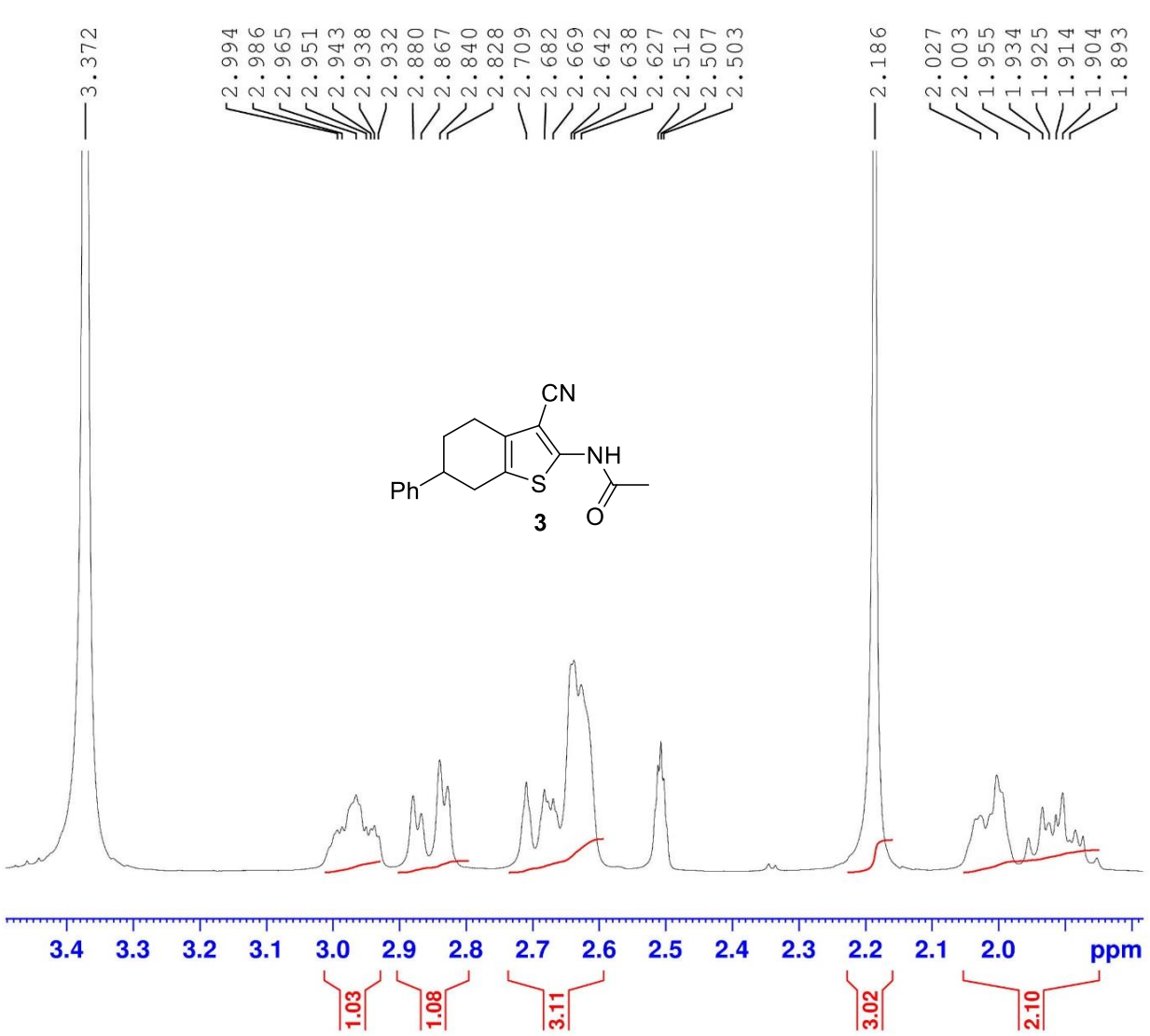

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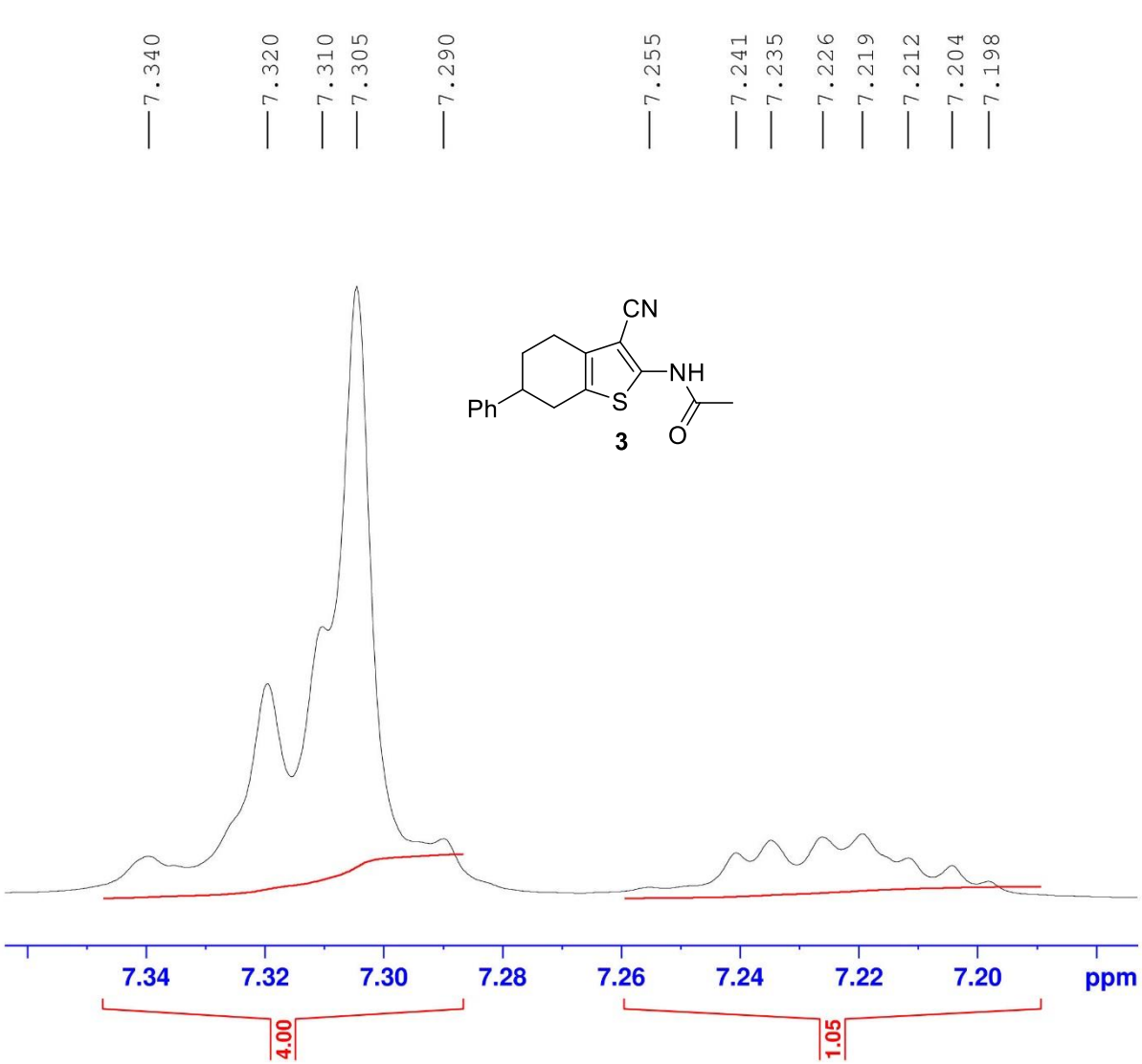

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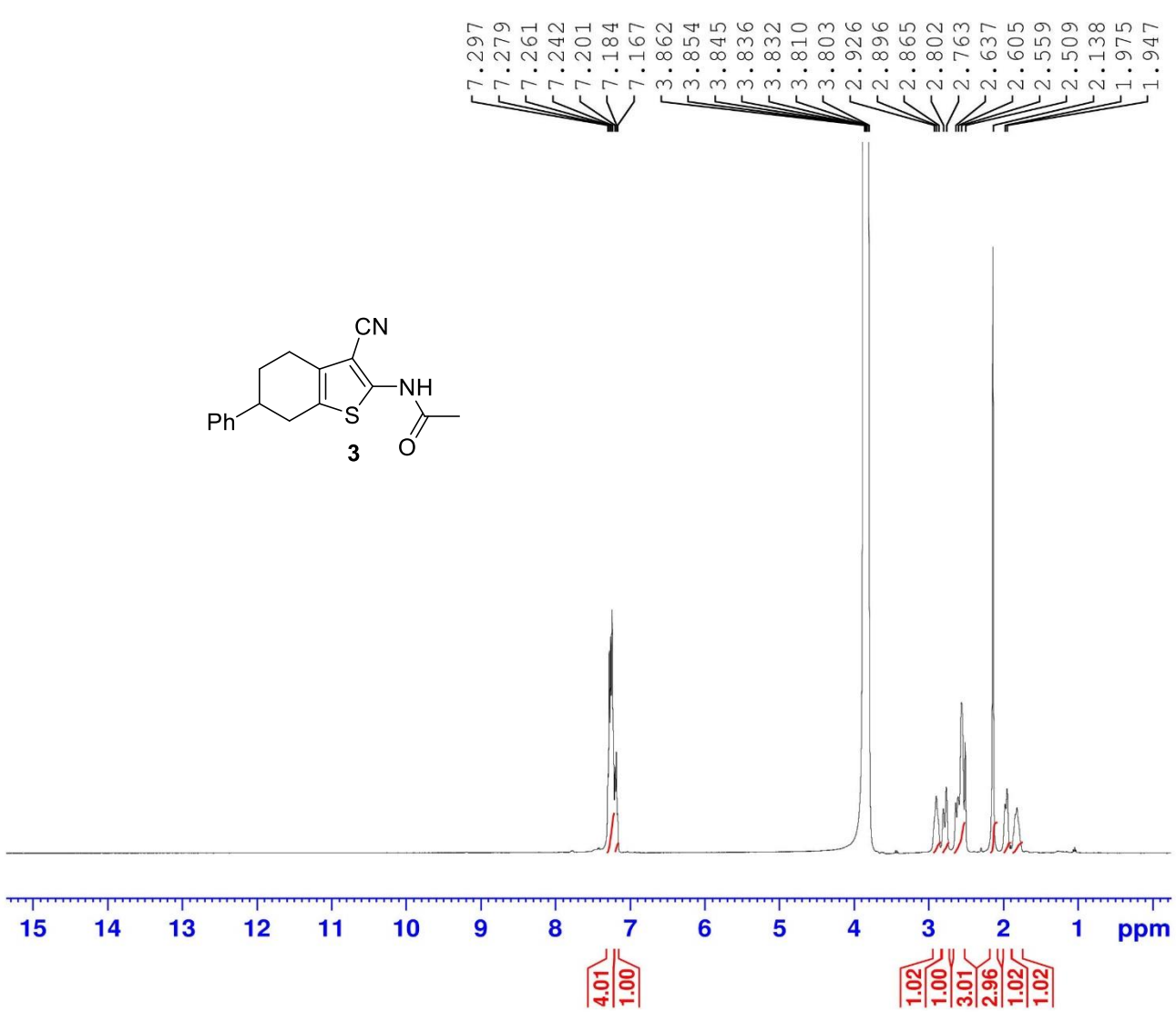

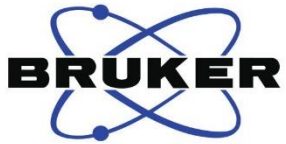

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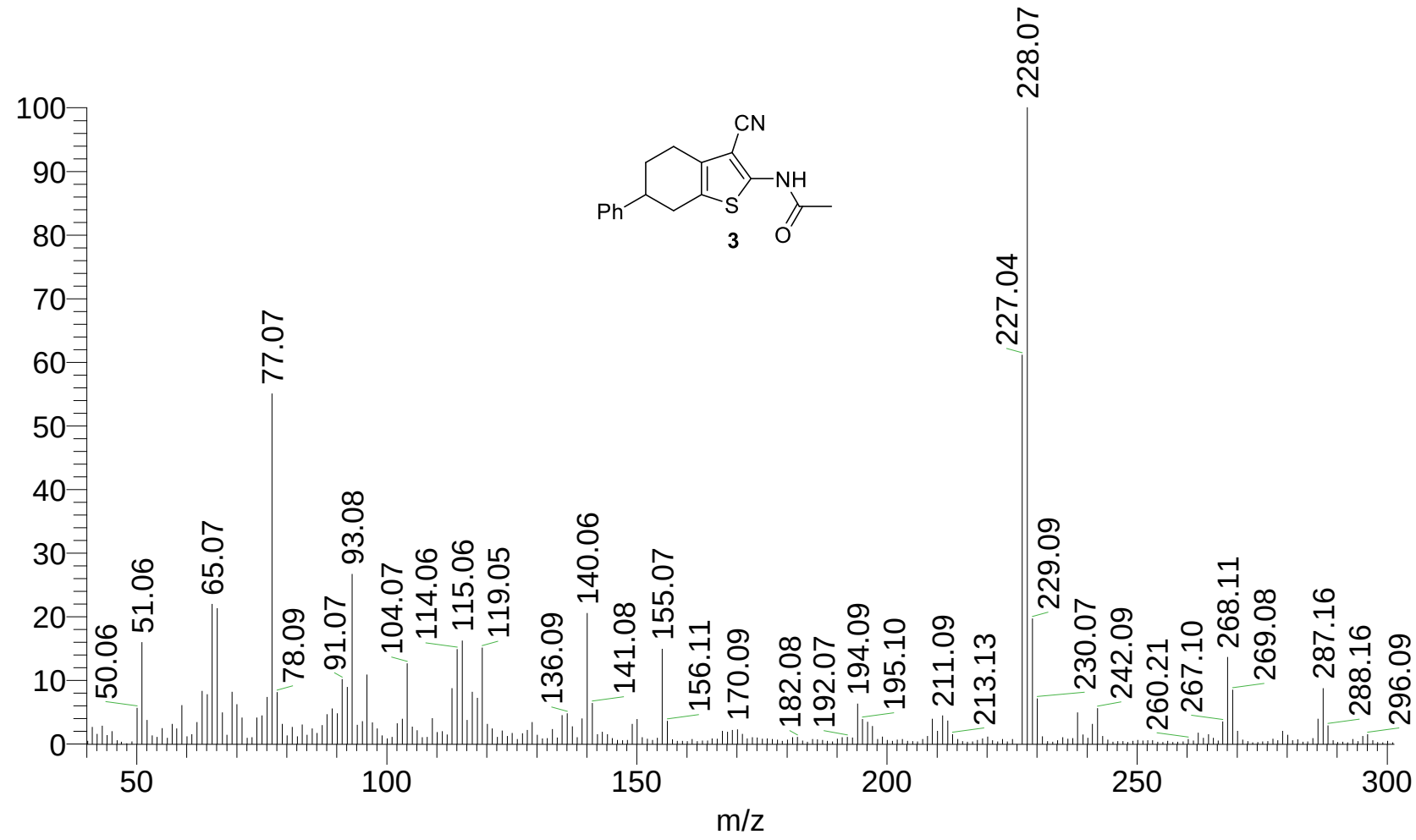

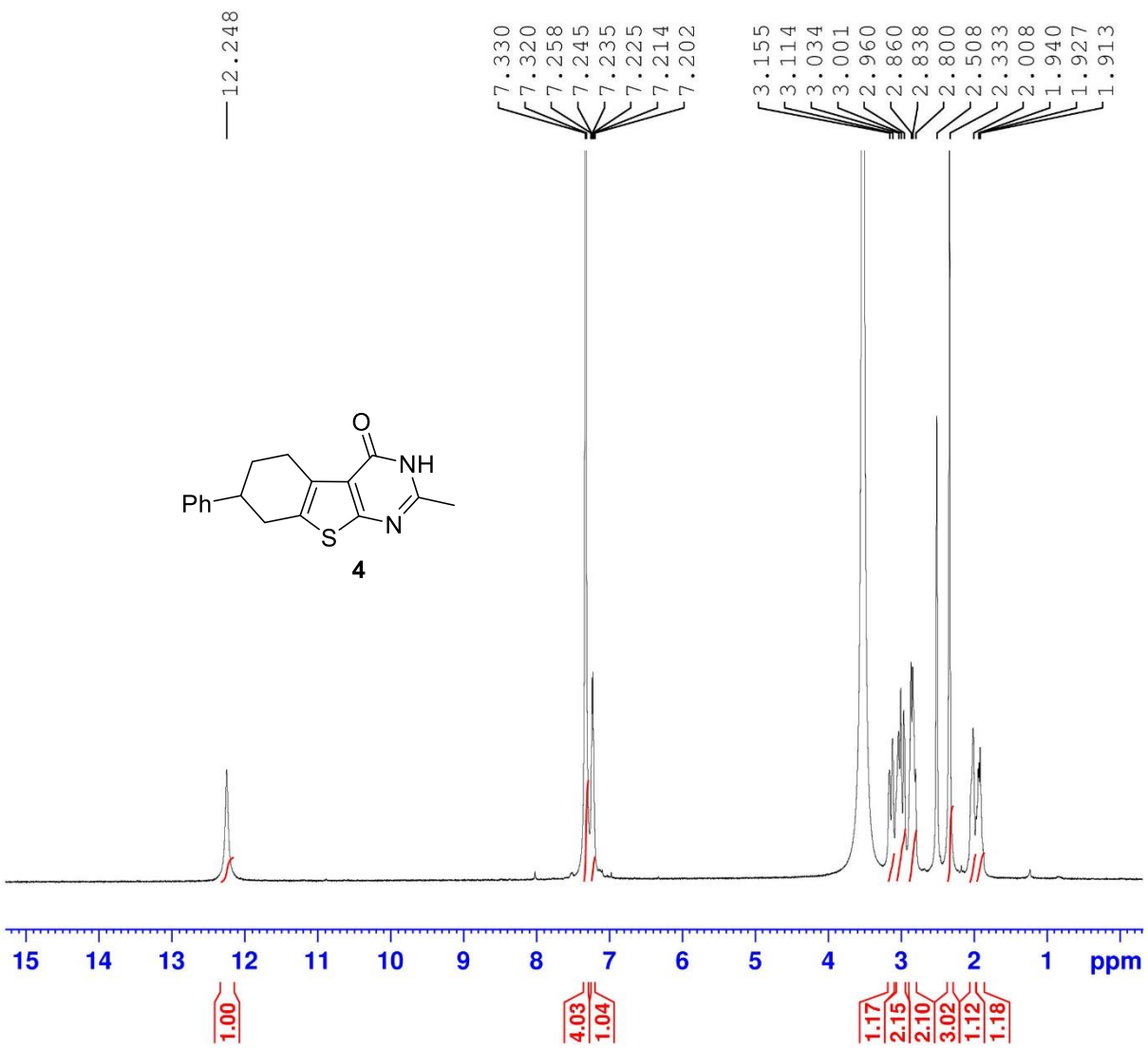

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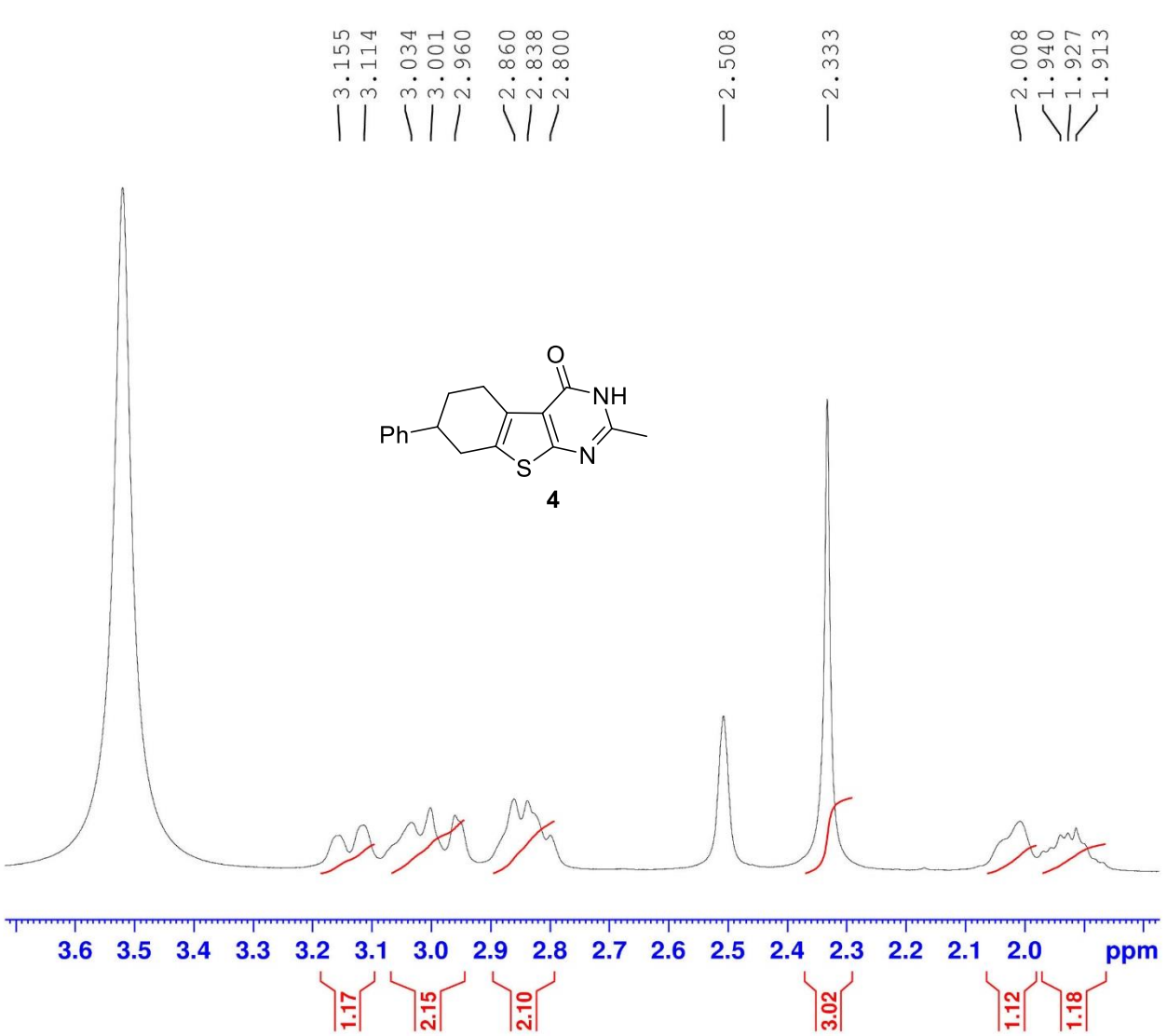


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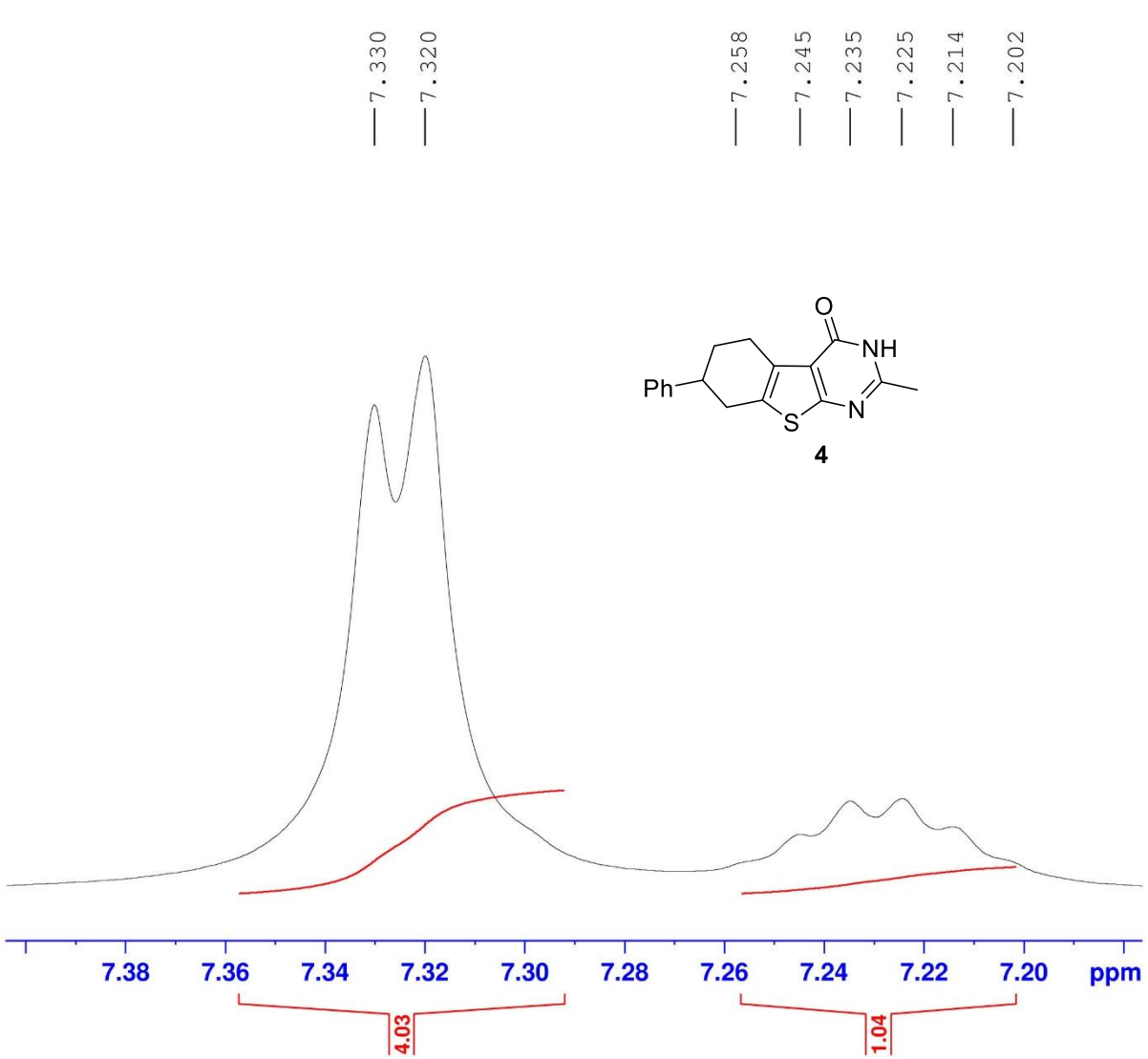


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D1             1.00000000 sec
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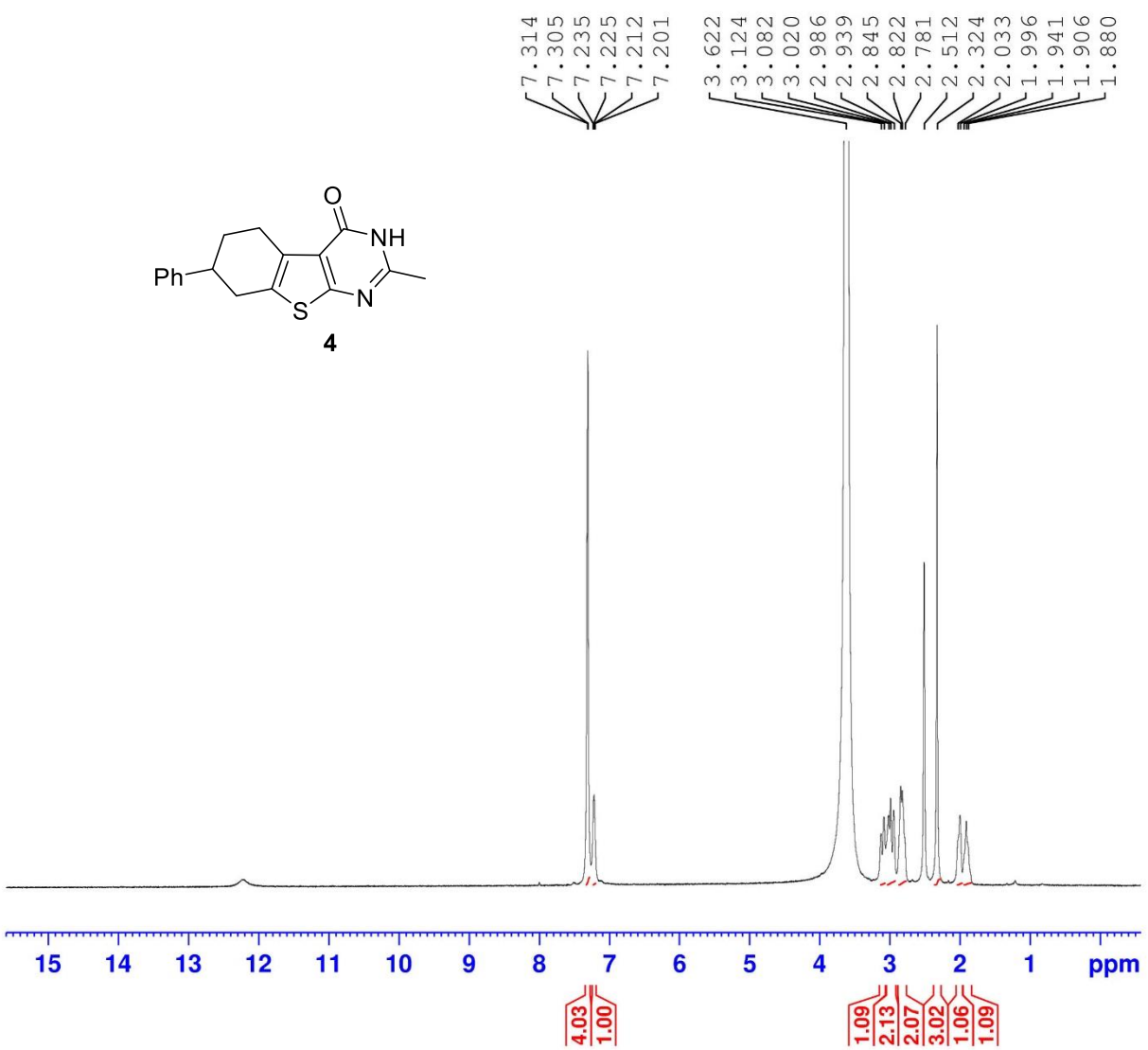

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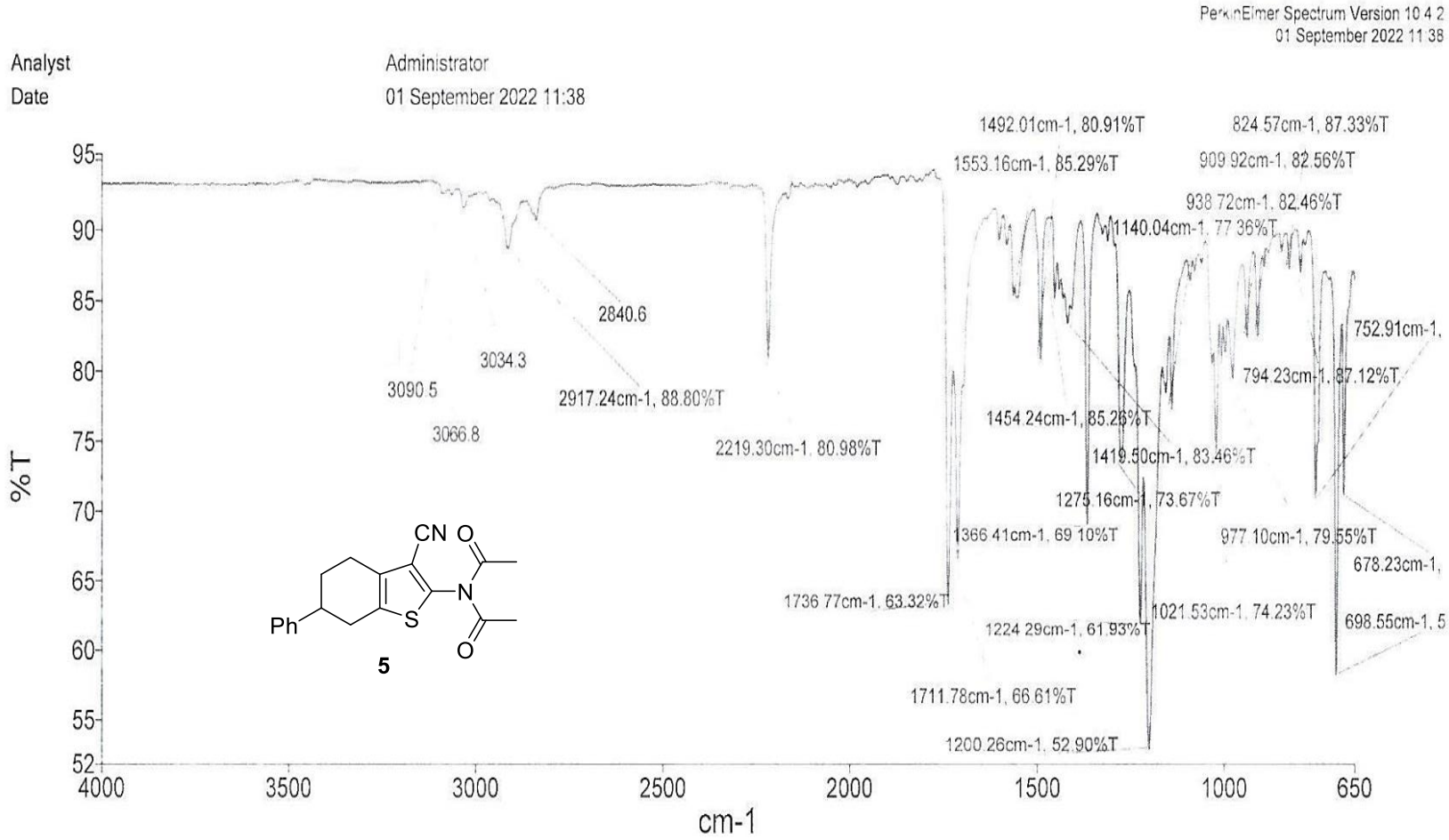
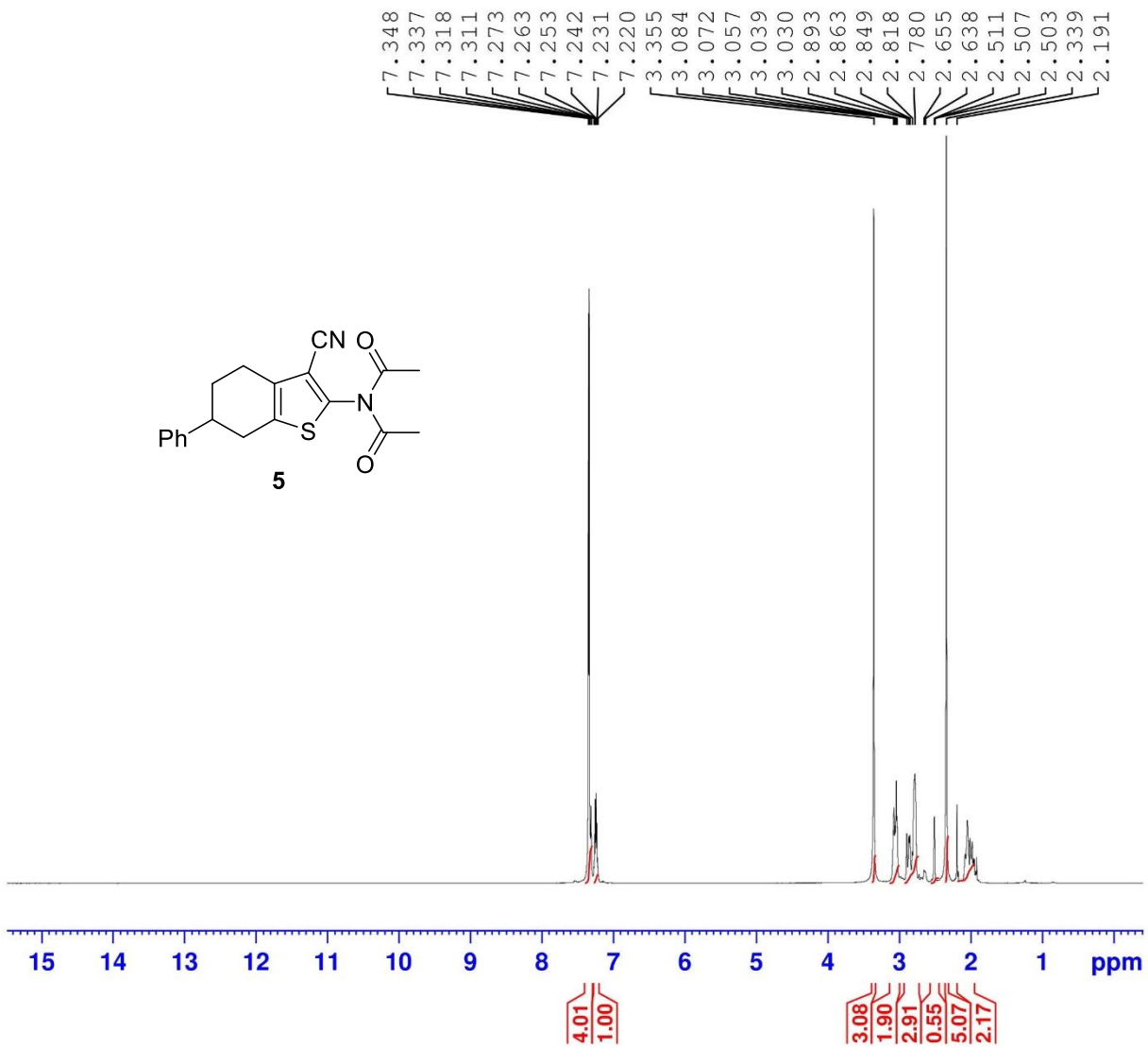
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                 205.37
DW                 62.400 usec
DE                  6.50 usec
TE                 300.0 K
D1              1.00000000 sec
TD0                    1

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

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



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.



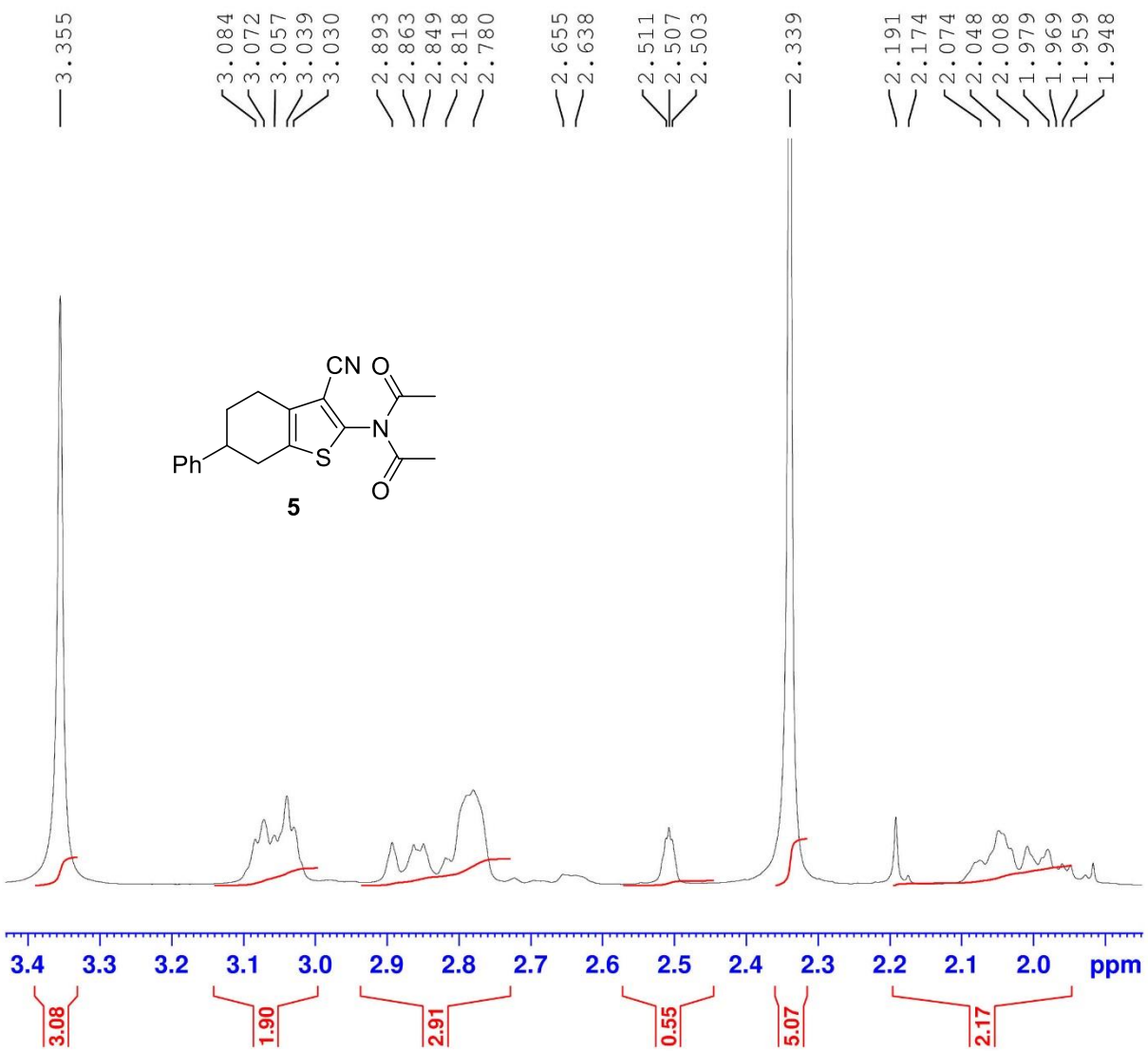
BRUKER

```
Current Data Parameters
NAME      amna-shaaban-A31
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220912
Time                12.55
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                    128
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                 205.37
DW                 62.400 usec
DE                  6.50 usec
TE                 300.0 K
D1              1.00000000 sec
TD0                     1

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

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



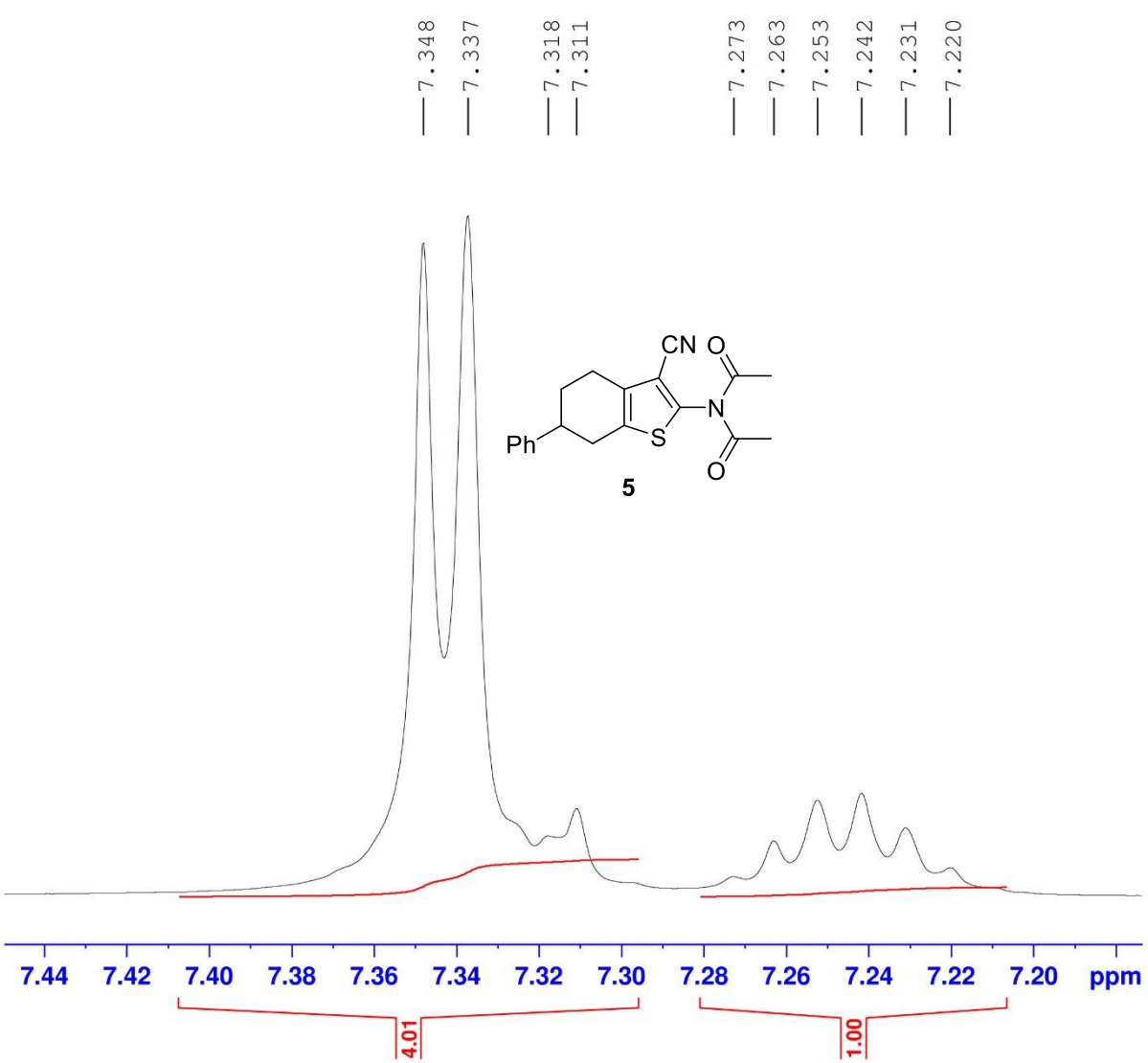
BRUKER

```
Current Data Parameters
NAME      amna-shaaban-A31
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20220912
Time               12.55
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                   128
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                205.37
DW                62.400 usec
DE                 6.50 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

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

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



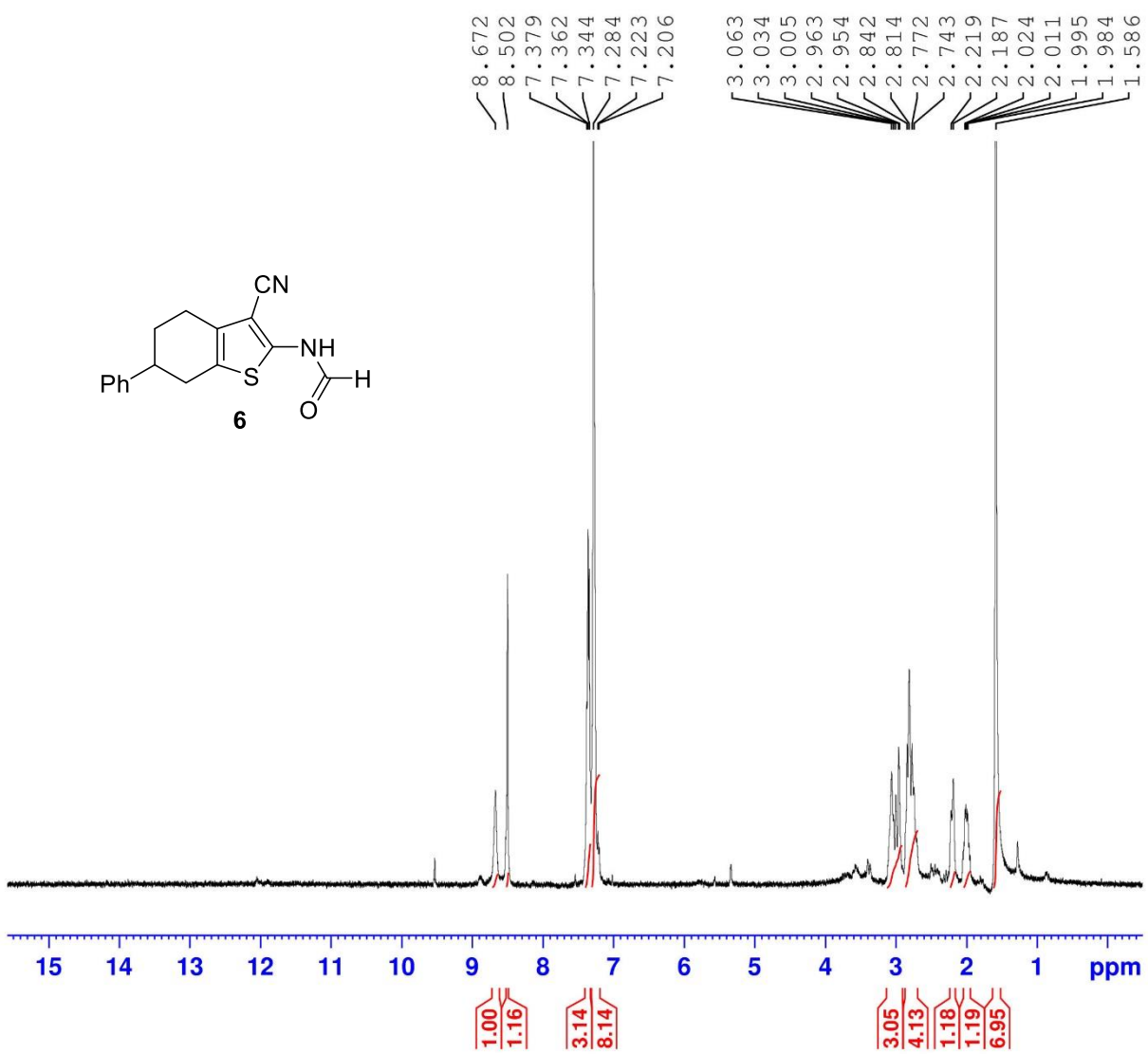
BRUKER

```
Current Data Parameters
NAME      amna-shaaban-A31
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220912
Time                12.55
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                   128
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                205.37
DW                62.400 usec
DE                 6.50 usec
TE                300.0 K
D1            1.00000000 sec
TD0                    1

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

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

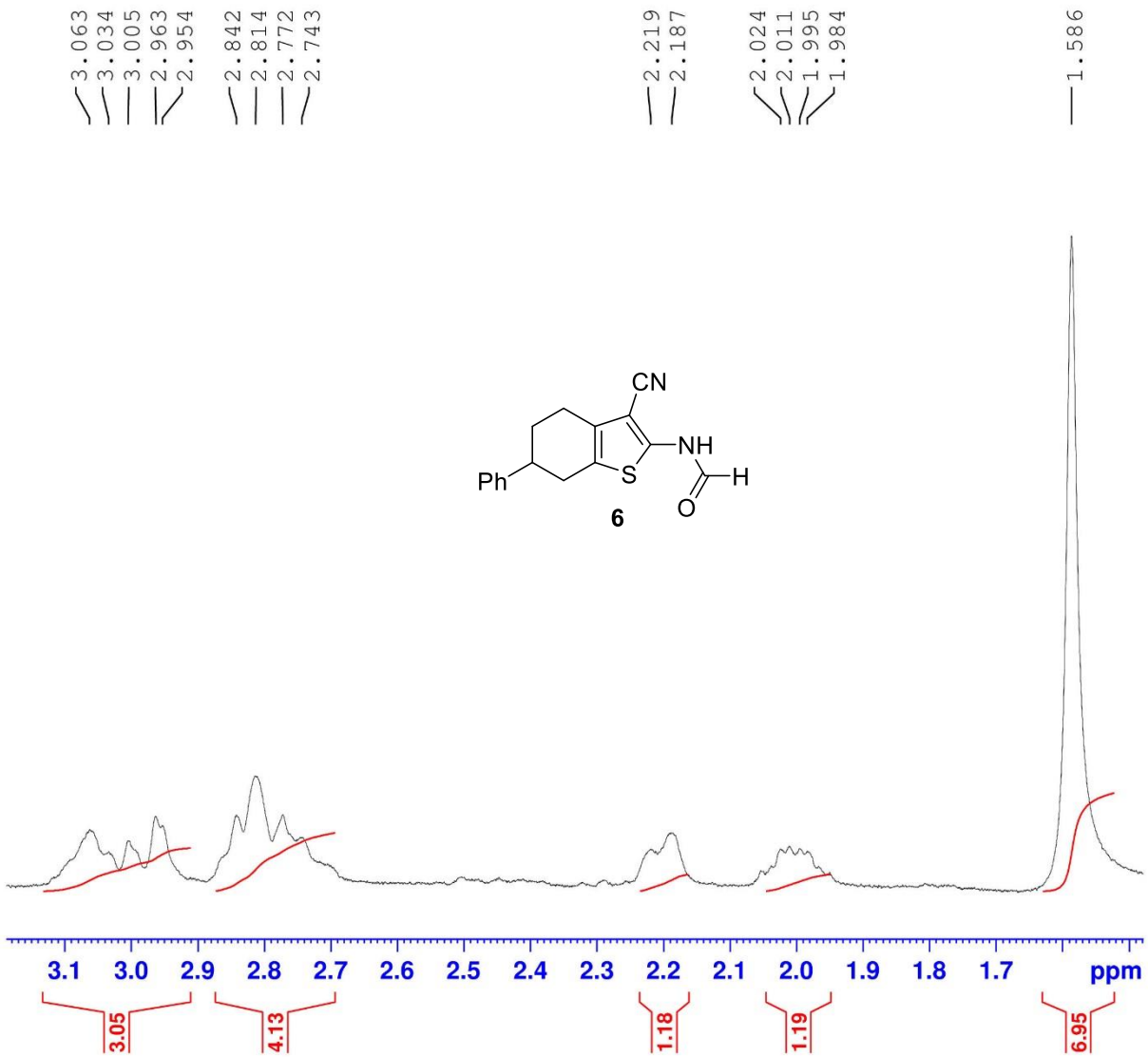



```
Current Data Parameters
NAME      amna-shaaban-A5
EXPNO                  2
PROCNO                 1

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            1.00000000 sec
TD0                    1

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

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



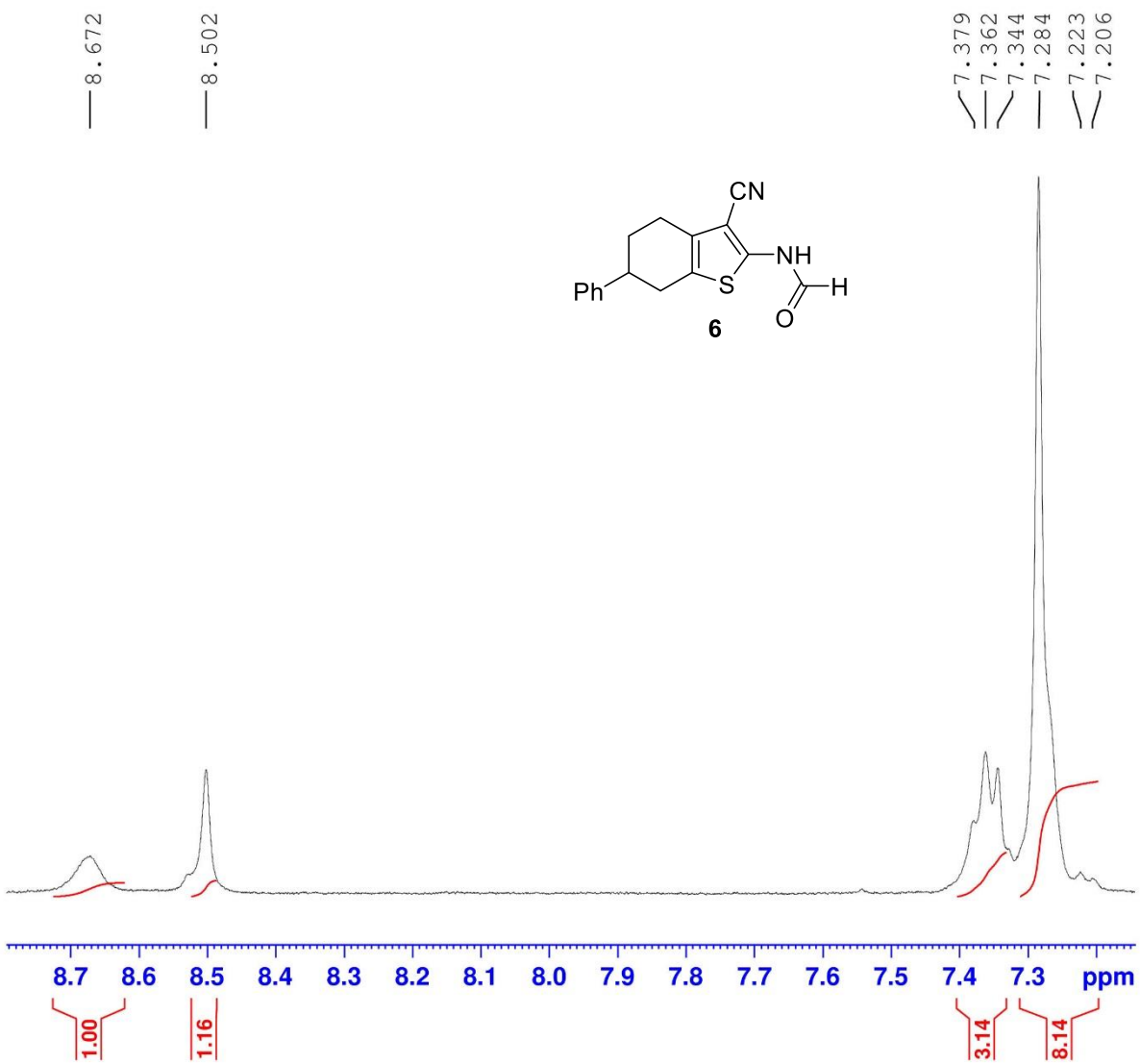
BRUKER

```
Current Data Parameters
NAME      amna-shaaban-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              1.00000000 sec
TD0                    1

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

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



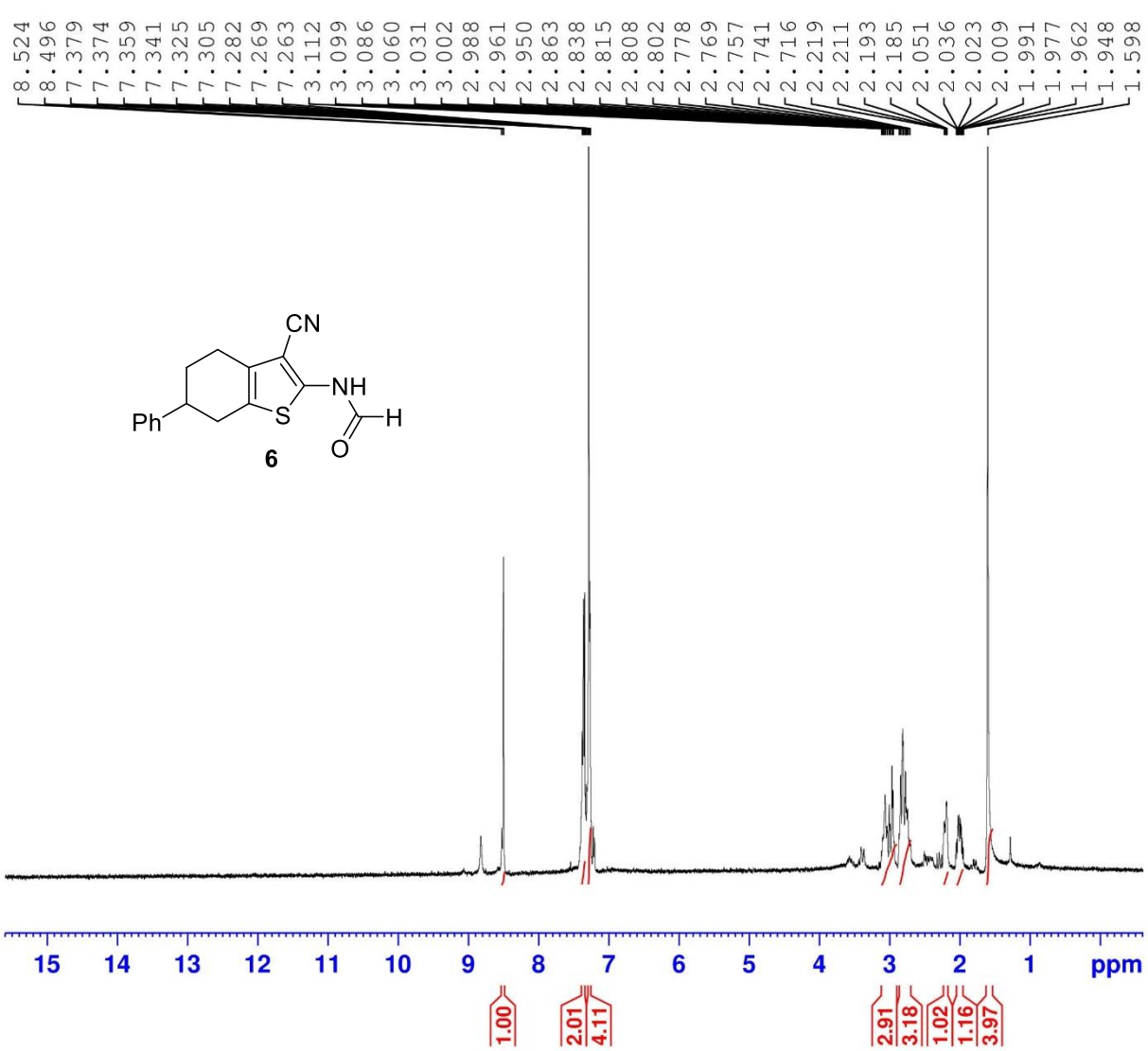
BRUKER

```
Current Data Parameters
NAME      amna-shaaban-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            1.00000000 sec
TD0                   1

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

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

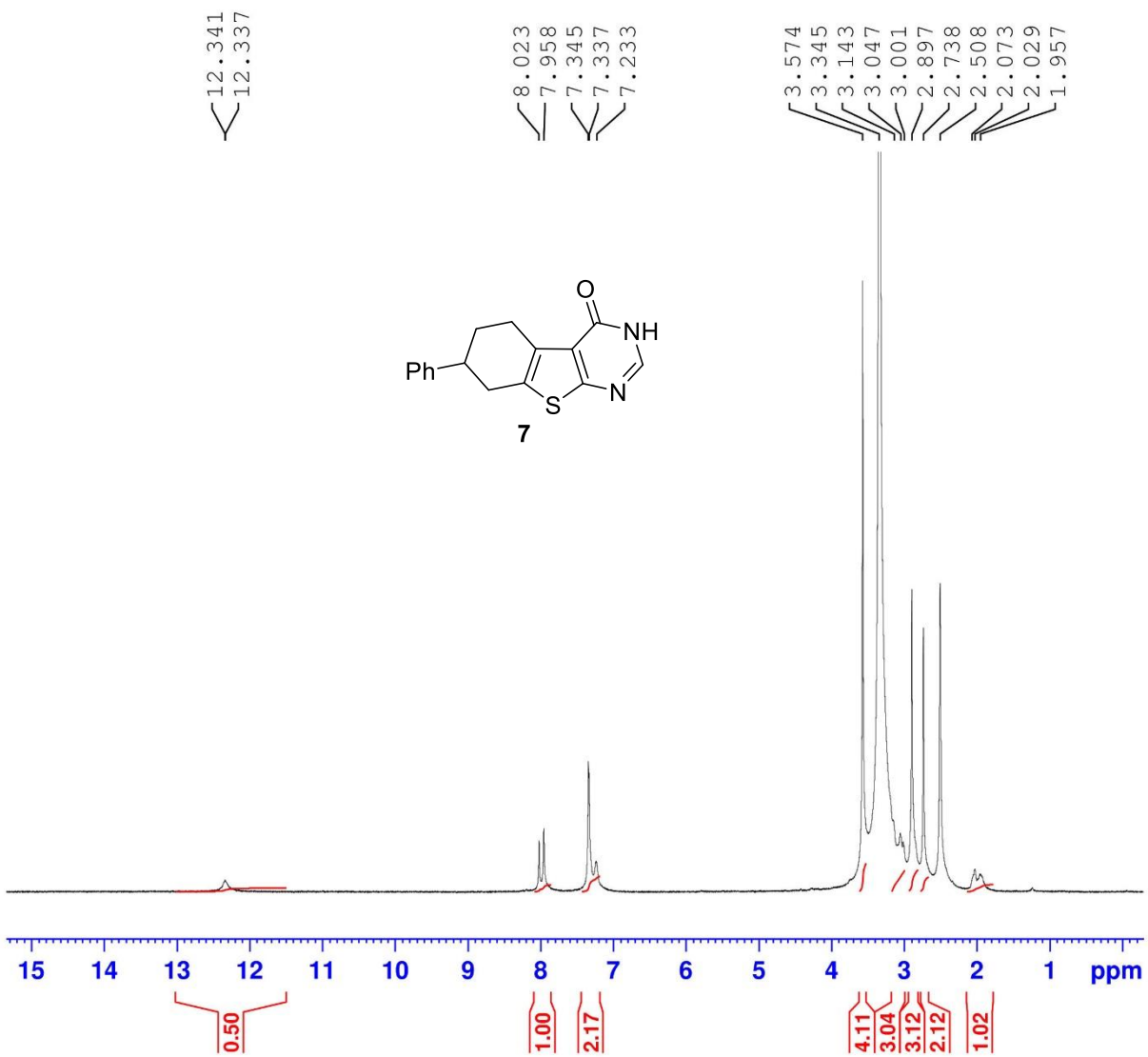



```
Current Data Parameters
NAME      amna-shaaban-A5-d2o
EXPNO                      1
PROCNO                     1

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
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
```

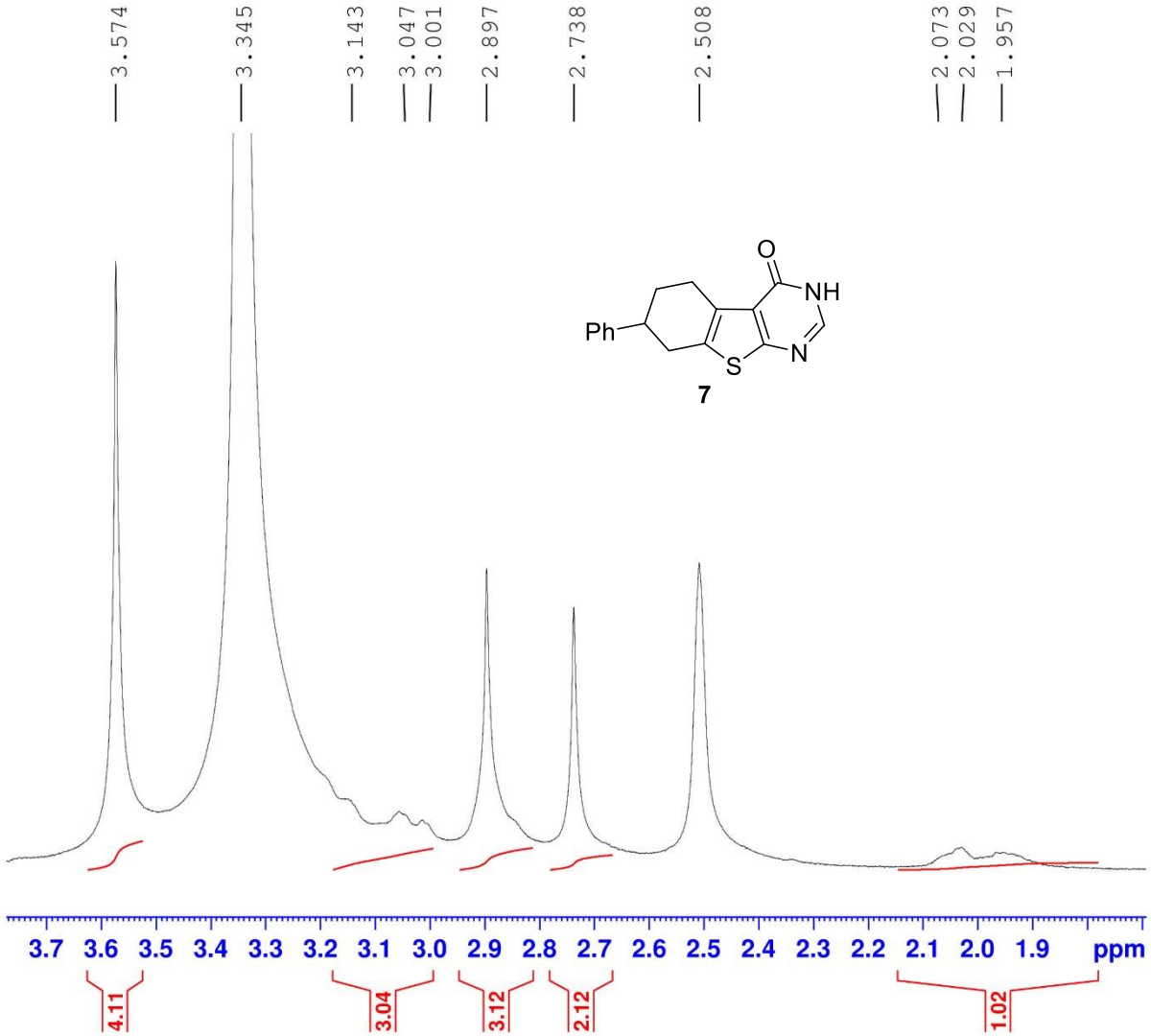


Current Data Parameters
NAME amna-shaaban-A6
EXPNO 1
PROCNO 1

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 1.00000000 sec
TD0 1

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

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



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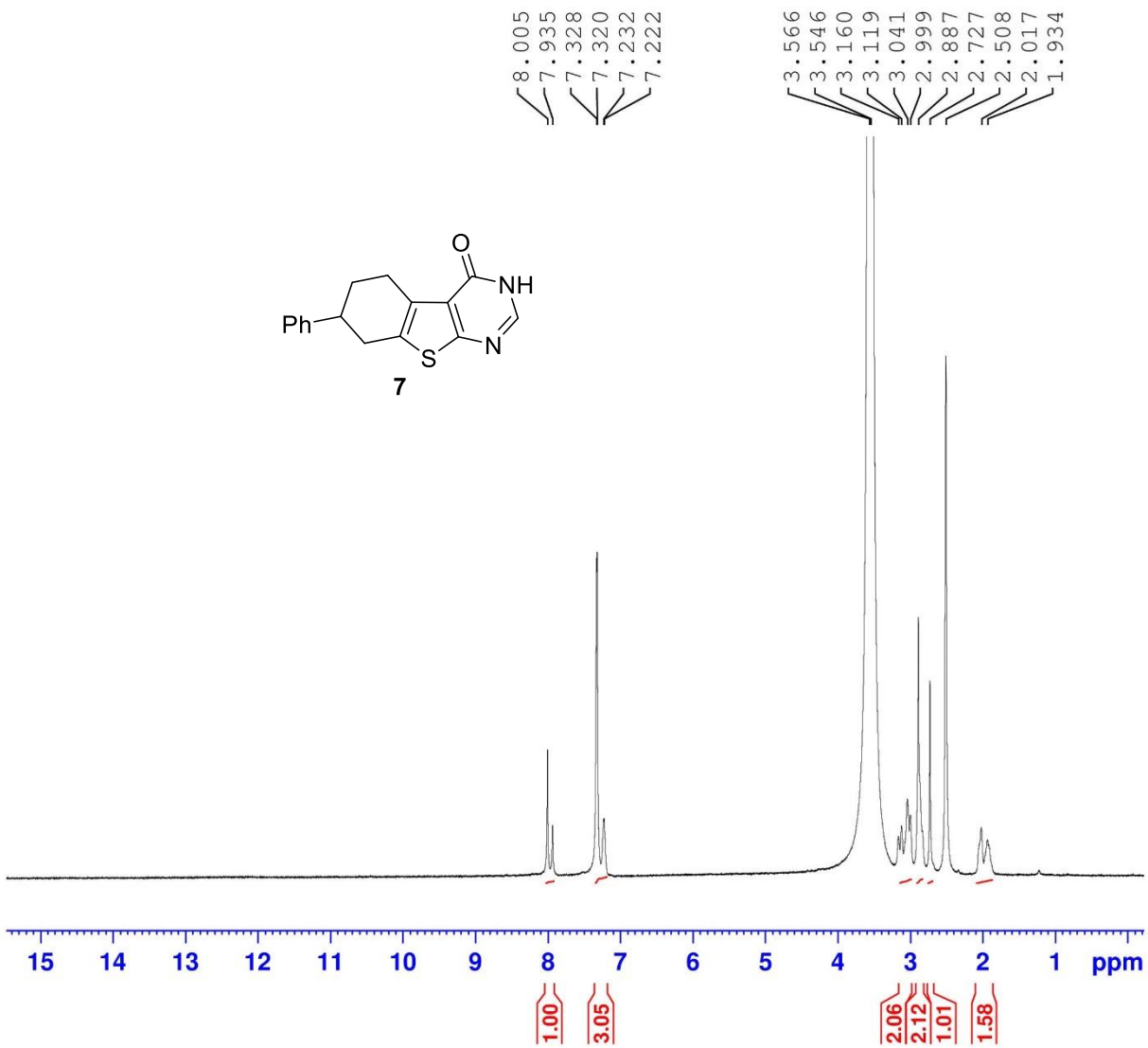
```
Current Data Parameters
NAME      amna-shaaban-A6
EXPNO                  1
PROCNO                 1

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             1.00000000 sec
TD0                    1

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

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



BRUKER

```
Current Data Parameters
NAME      amna-shaaban-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              1.00000000 sec
TD0                      1

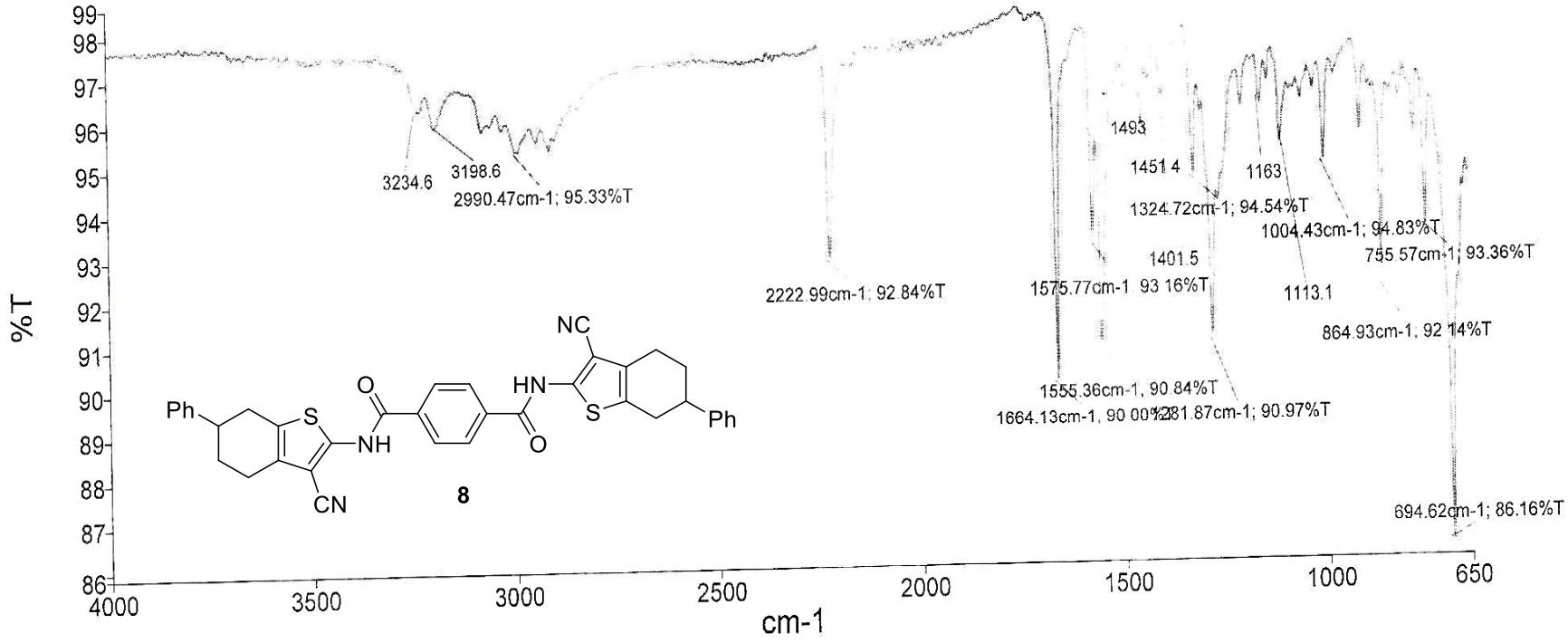
======== CHANNEL f1 ========
SFO1           400.1524711 MHz
NUC1                    1H
P1                   12.00 usec
PLW1           18.00000000 W

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

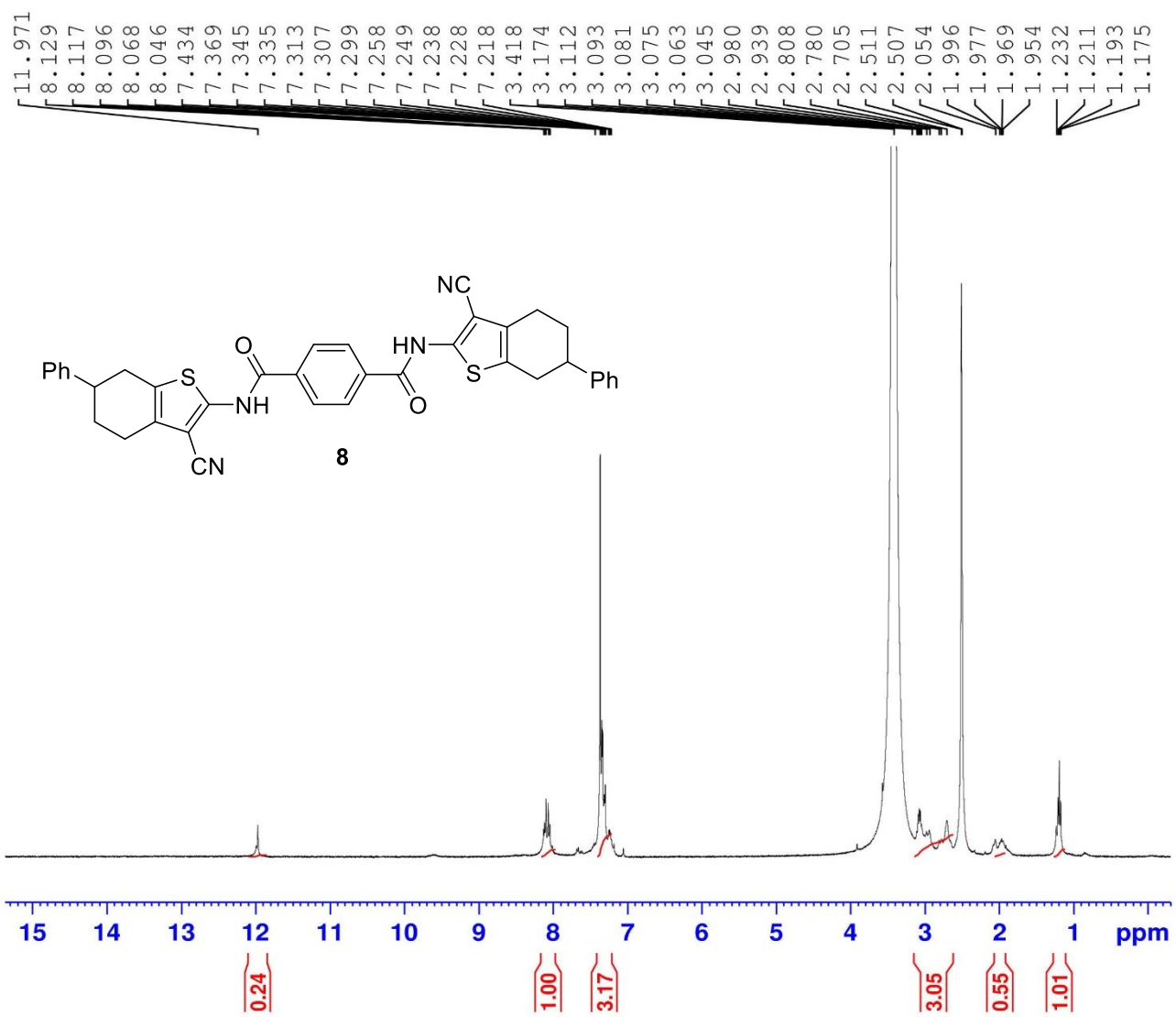
PerkinElmer Spectrum Version 10.4.2
02 م 01:18 2021 ,ديسمبر

Analyst
Date

Administrator
02 م 01:18 2021 ,ديسمبر



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



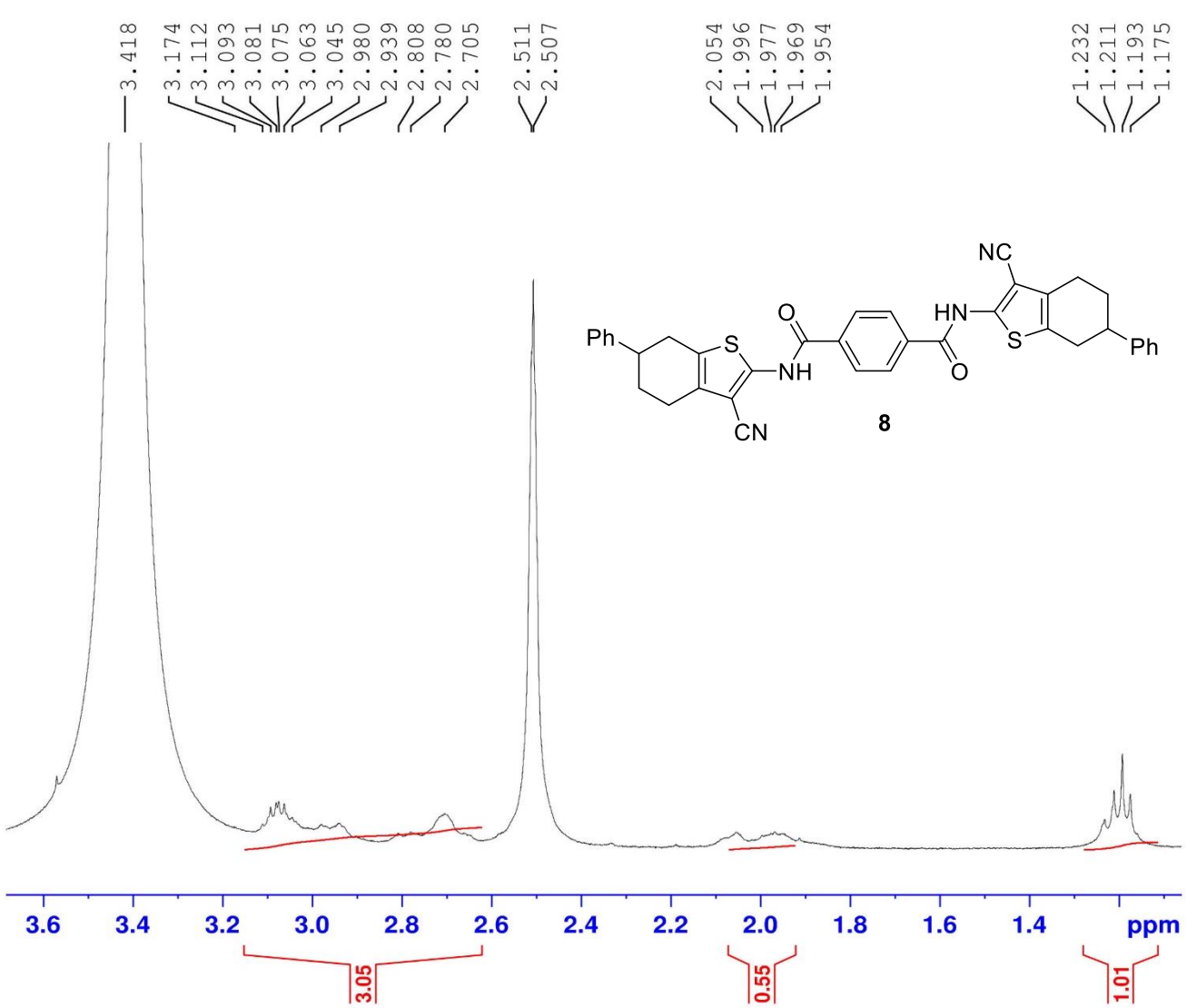
BRUKER

```
Current Data Parameters
NAME      amna-shaaban-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
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
```



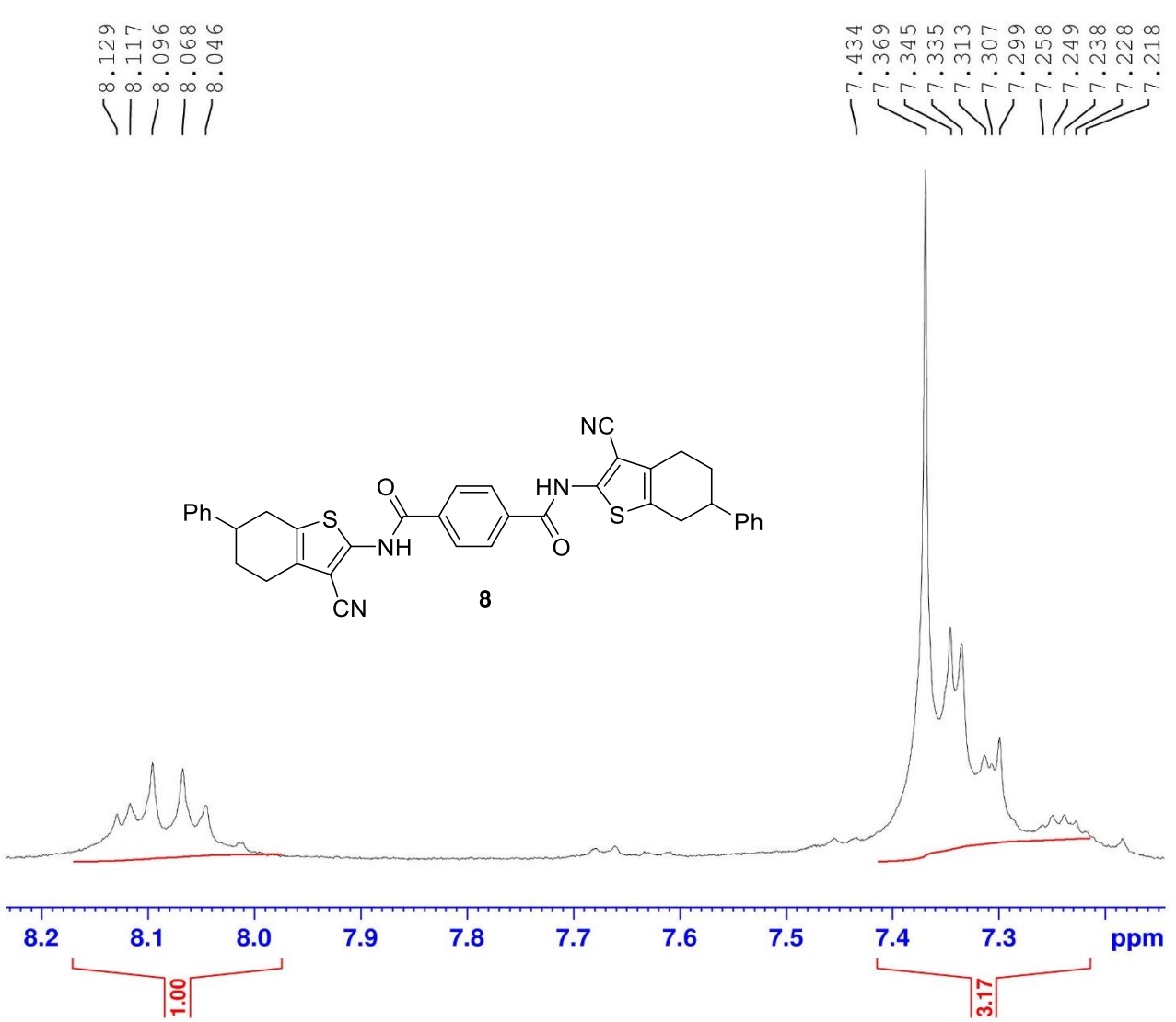
BRUKER

```
Current Data Parameters
NAME      amna-shaaban-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
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
```



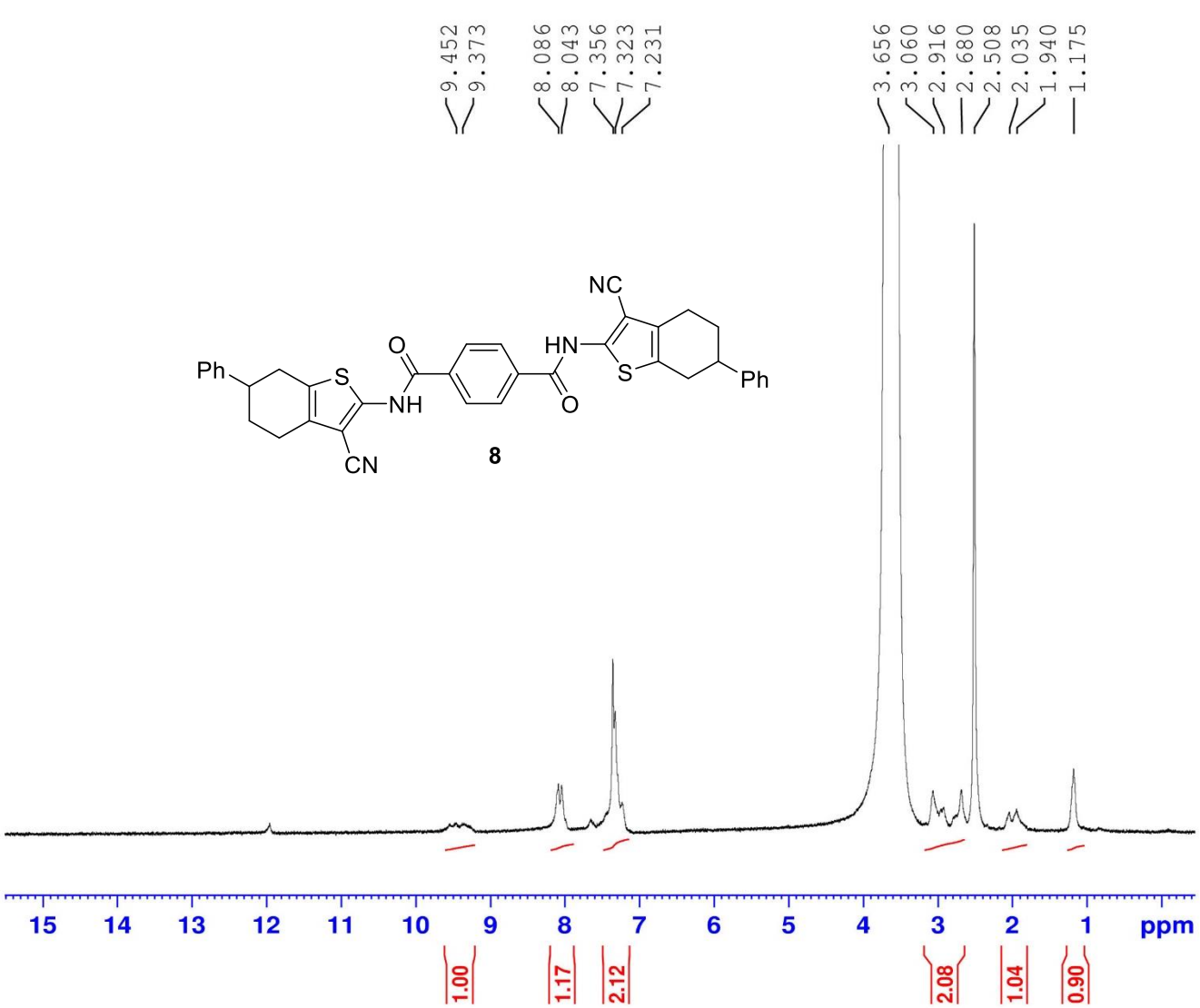
BRUKER

```
Current Data Parameters
NAME      amna-shaaban-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
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
```



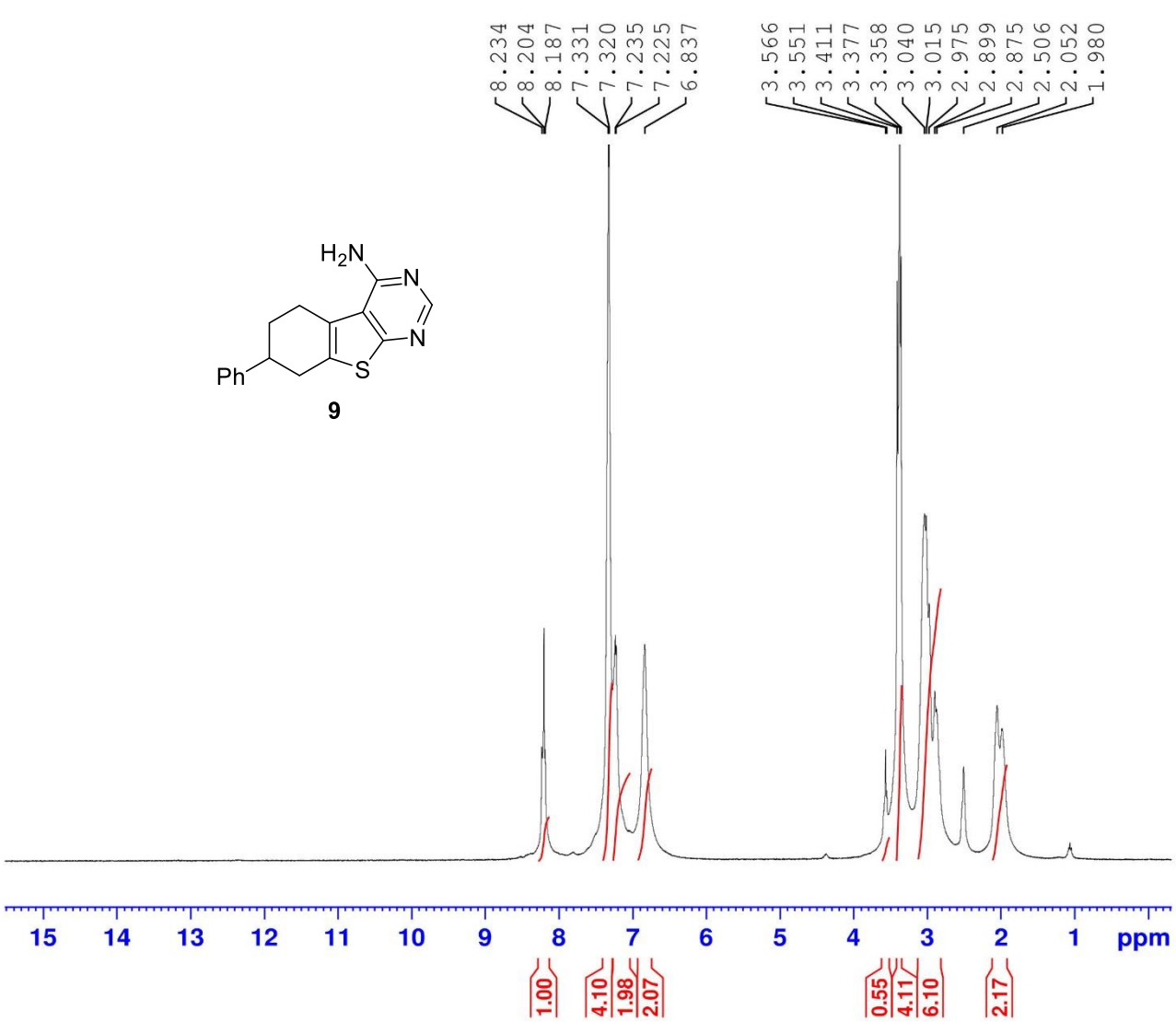
BRUKER

```
Current Data Parameters
NAME      amna-shaaban-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                 1.00000000 sec
TD0                       1

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

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



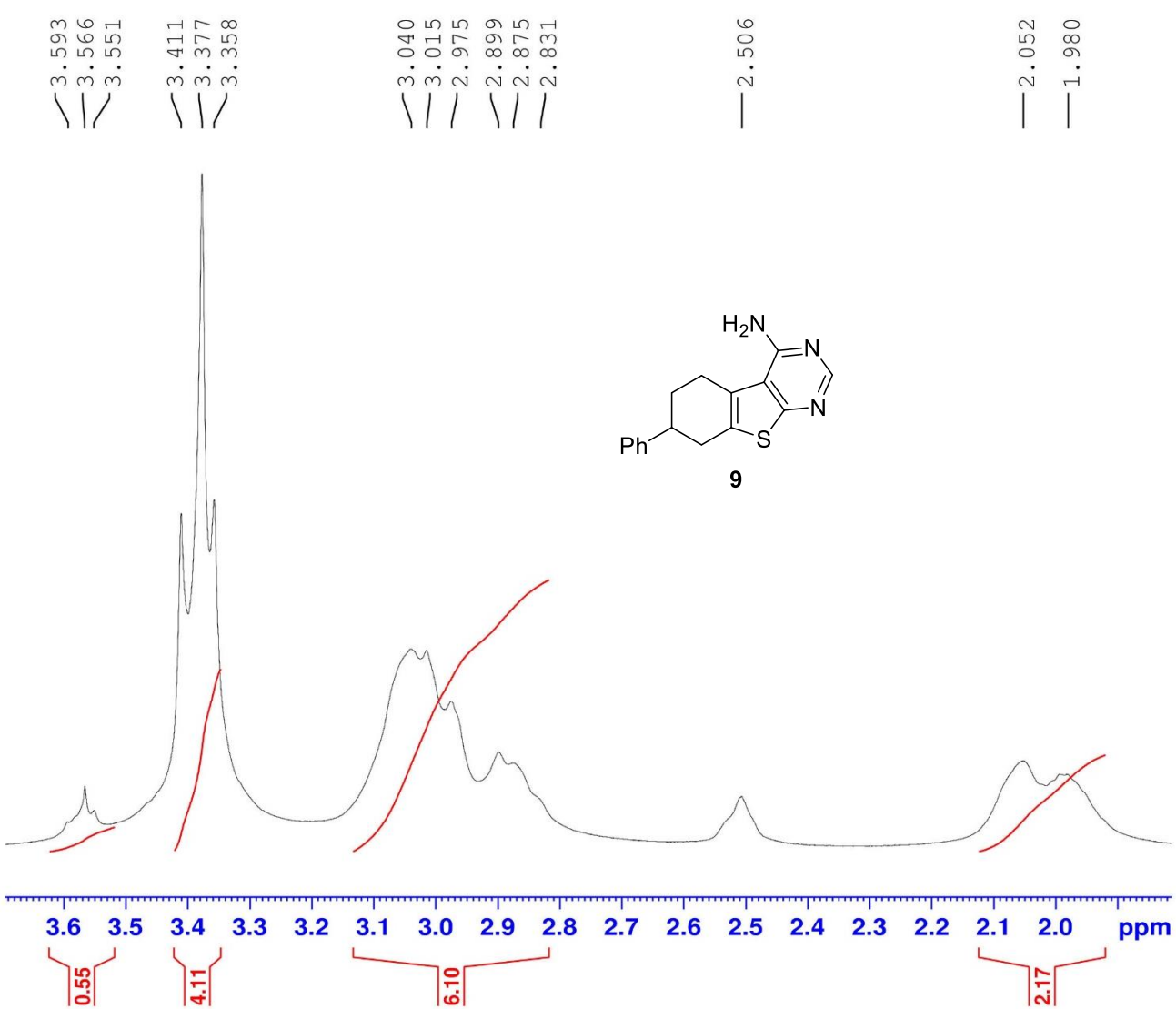
BRUKER

```
Current Data Parameters
NAME      amna-shaaban-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
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
```



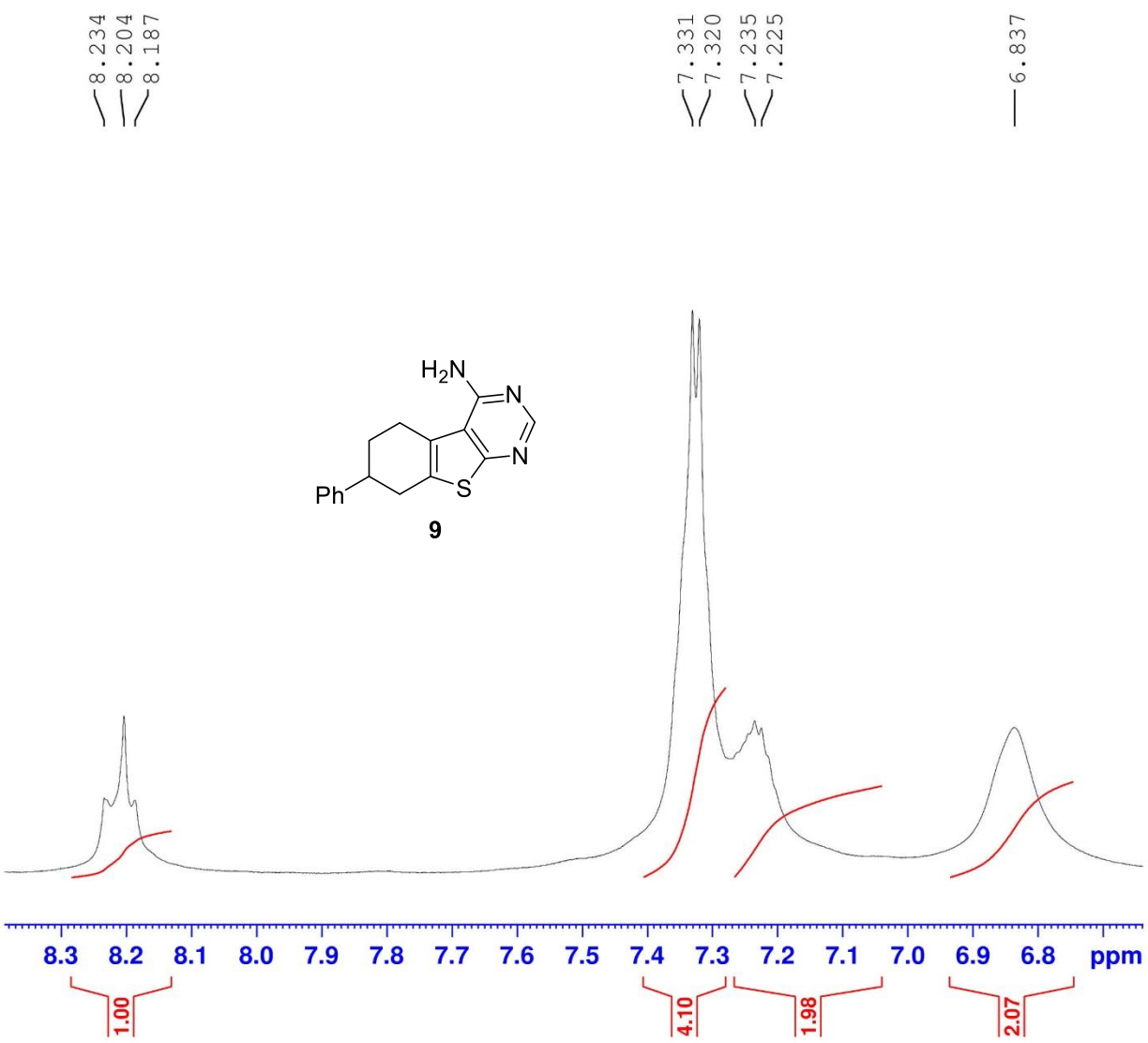
BRUKER

```
Current Data Parameters
NAME      amna-shaaban-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
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
```



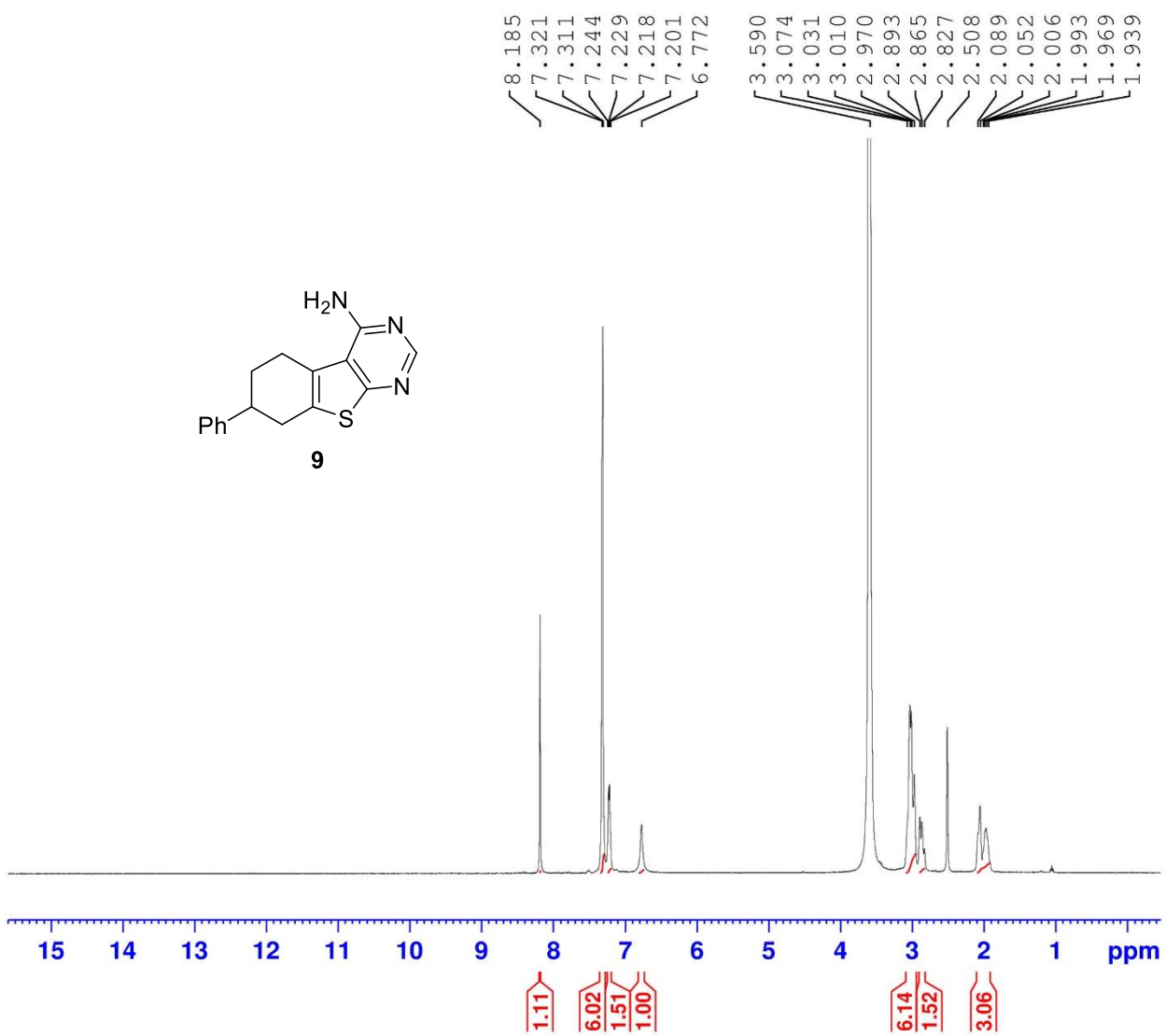
BRUKER

```
Current Data Parameters
NAME      amna-shaaban-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
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
```



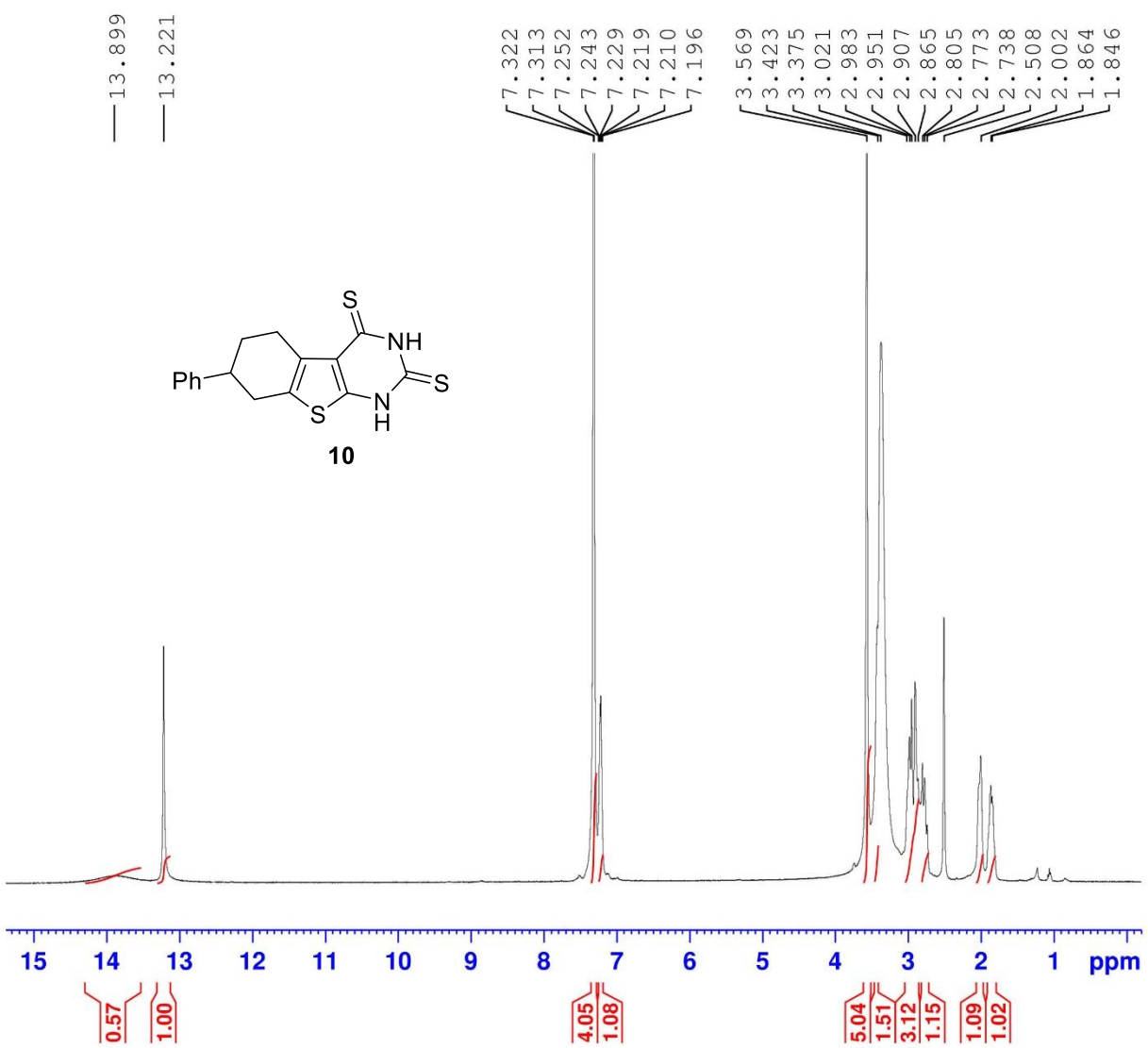
BRUKER

```
Current Data Parameters
NAME      amna-shaaban-A3-d2o
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_            20220920
Time                 9.49
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     43
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                 205.37
DW                 62.400 usec
DE                  6.50 usec
TE                 300.0 K
D1              1.00000000 sec
TD0                    1

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

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

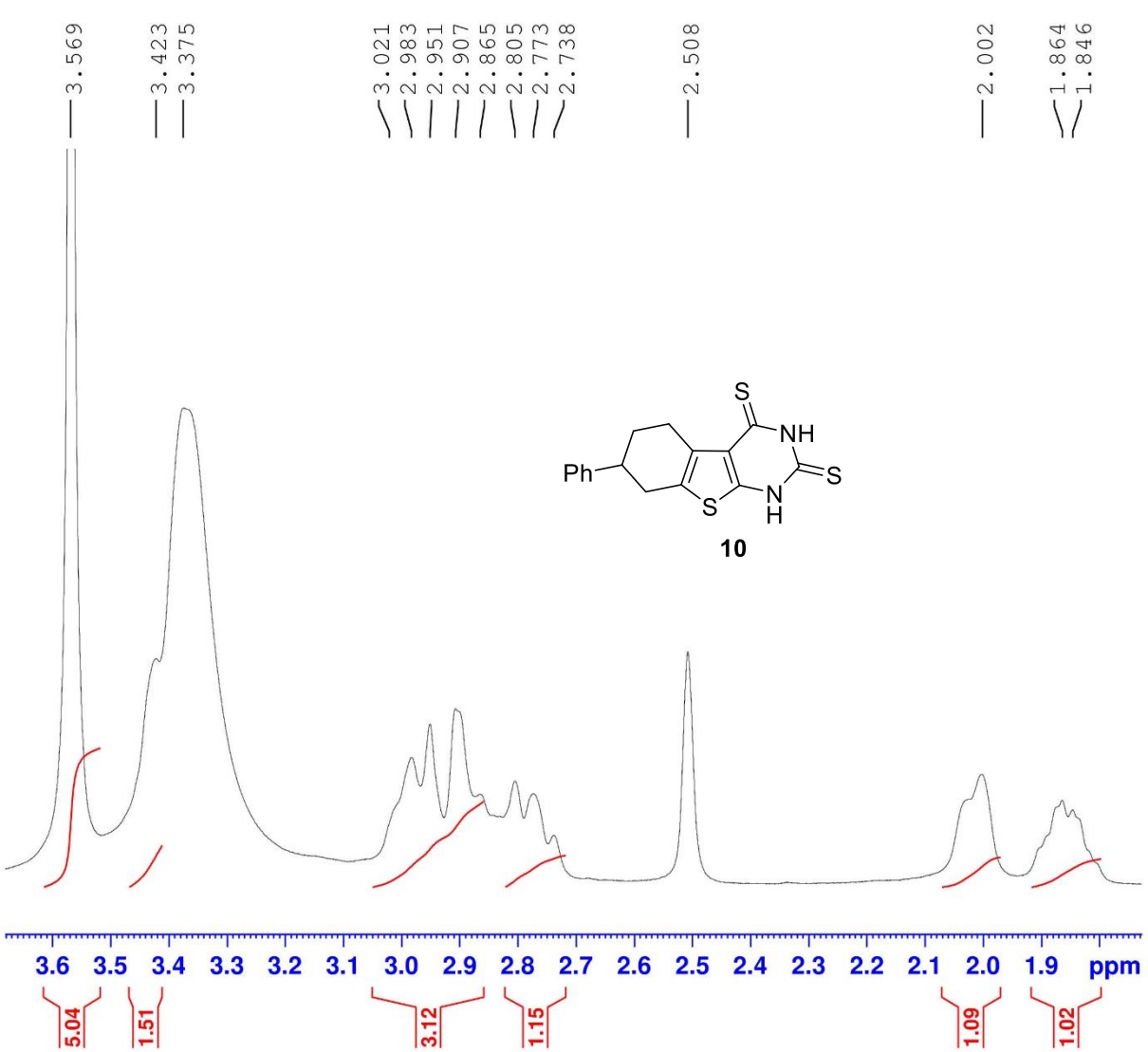


Current Data Parameters
NAME amna-shaaban-1A13
EXPNO 1
PROCNO 1

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 1.00000000 sec
TD0 1

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

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

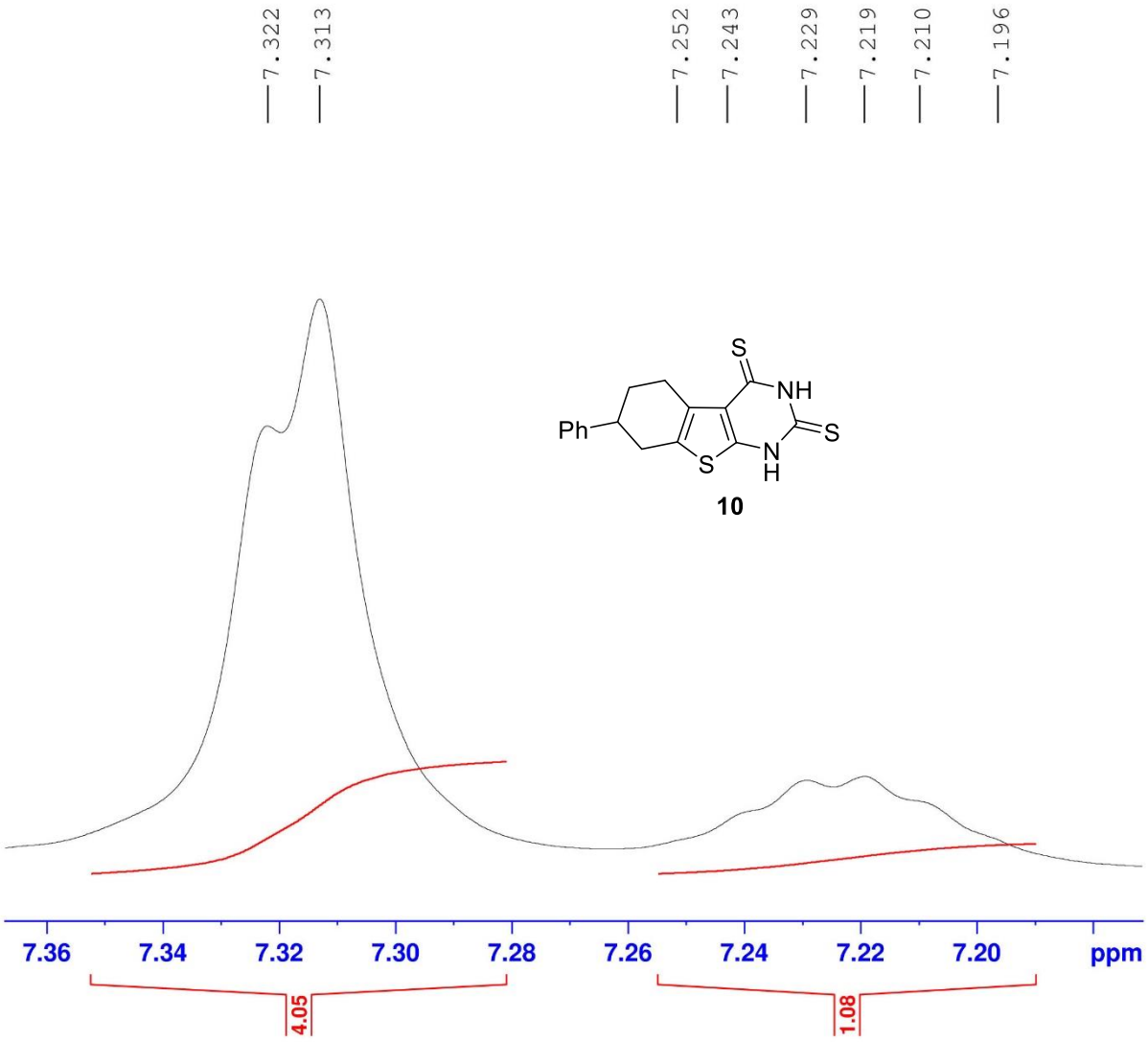



```
Current Data Parameters
NAME      amna-shaaban-1A13
EXPNO                    1
PROCNO                   1

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            1.00000000 sec
TD0                  1

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

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

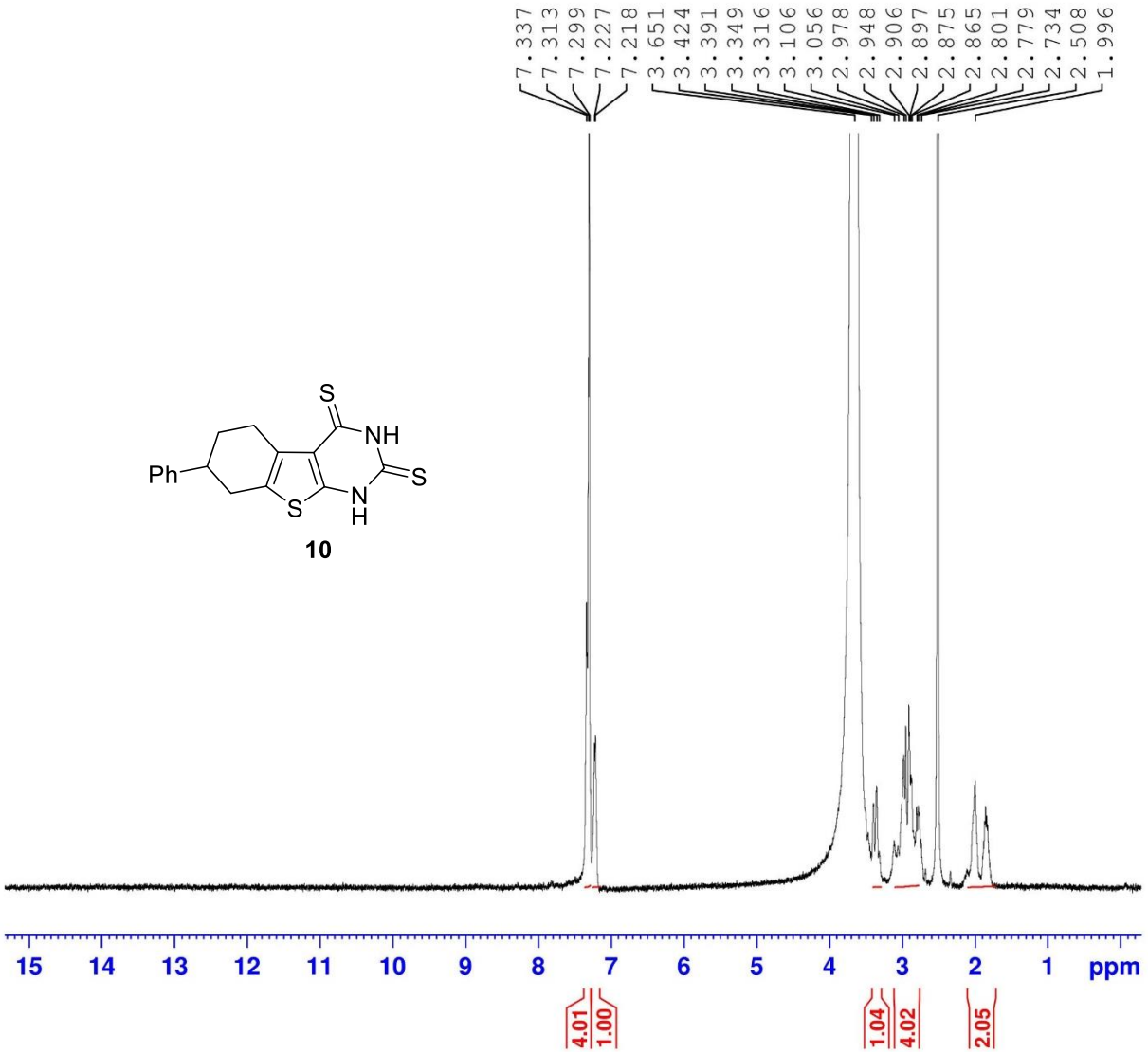


Current Data Parameters
NAME amna-shaaban-1A13
EXPNO 1
PROCNO 1

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 1.00000000 sec
TD0 1

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

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

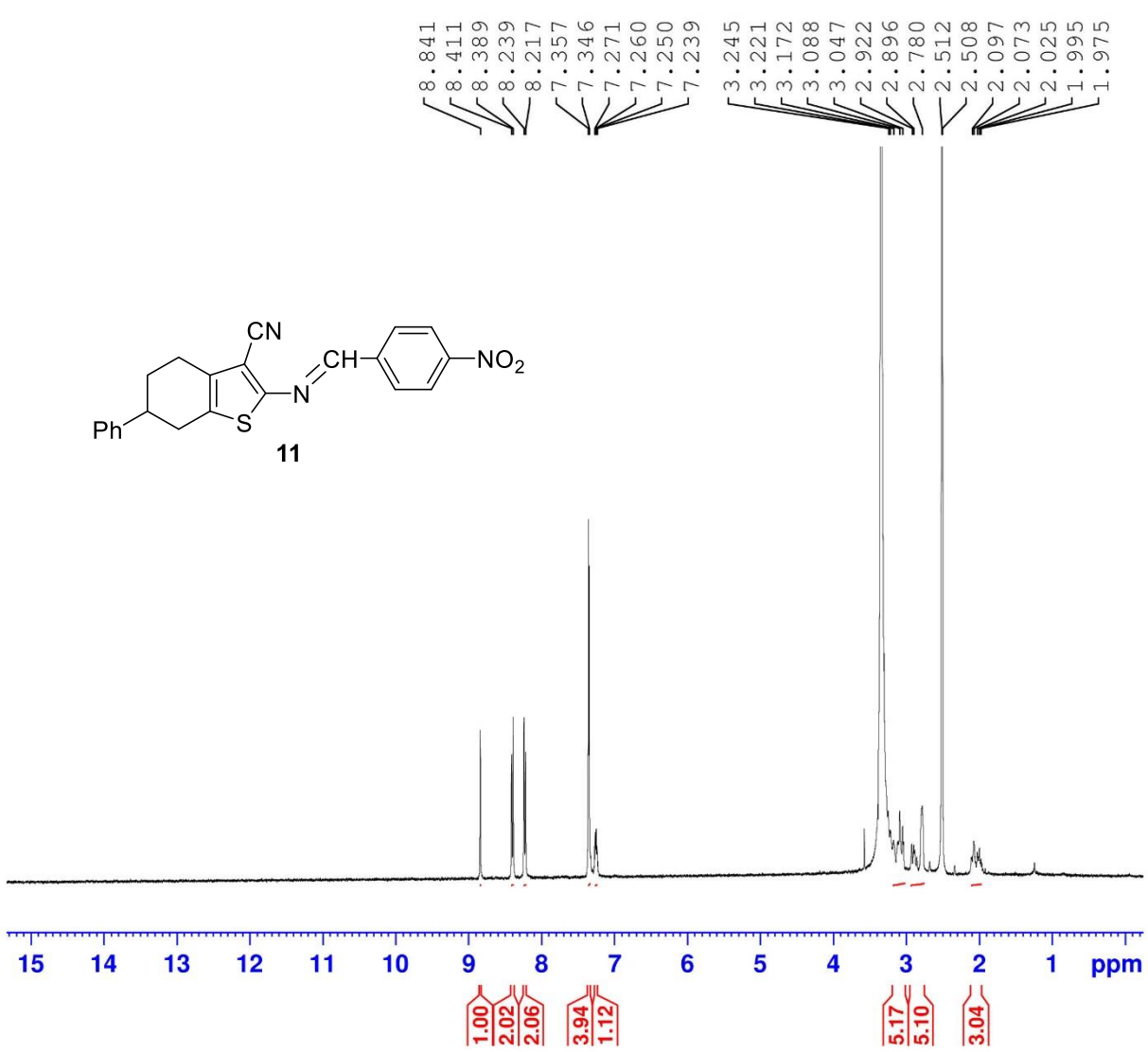



```
Current Data Parameters
NAME      amna-shaaban-A14-d2o
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20220920
Time                  10.39
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              1.00000000 sec
TD0                        1

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

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



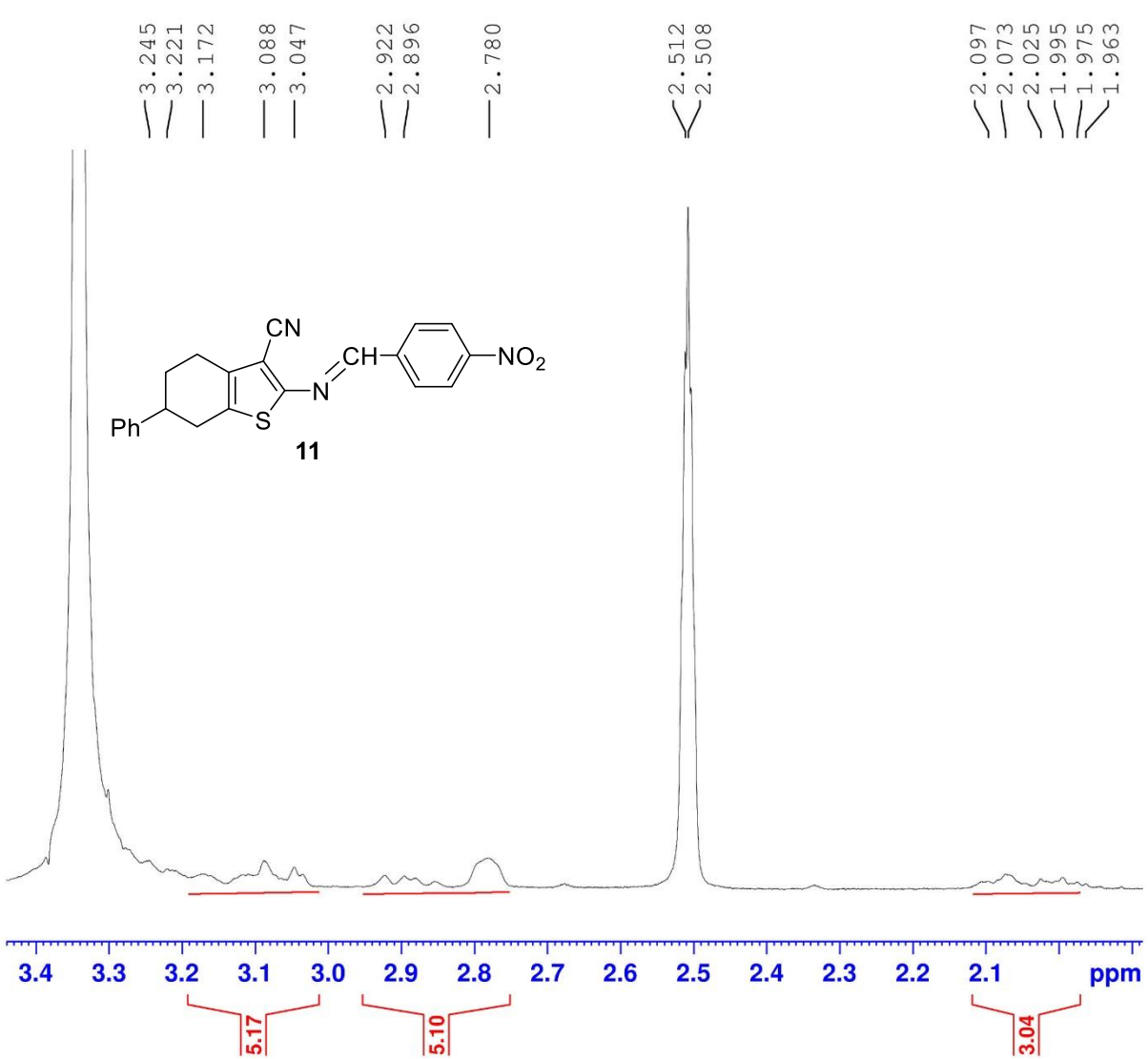
BRUKER

```
Current Data Parameters
NAME      amna-shaaban-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            1.00000000 sec
TD0                    1

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

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



BRUKER

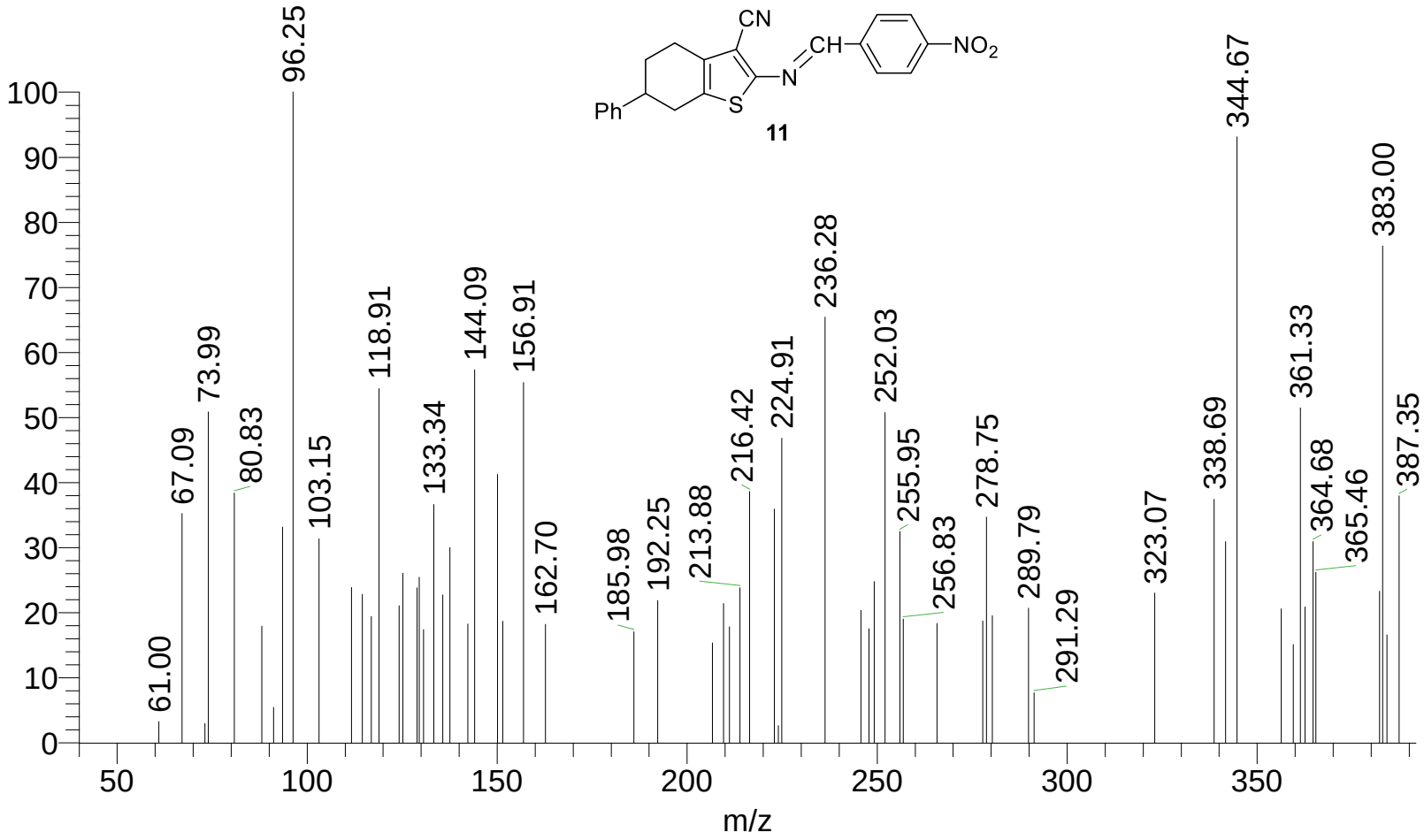
```
Current Data Parameters
NAME      amna-shaaban-A4
EXPNO                    1
PROCNO                   1

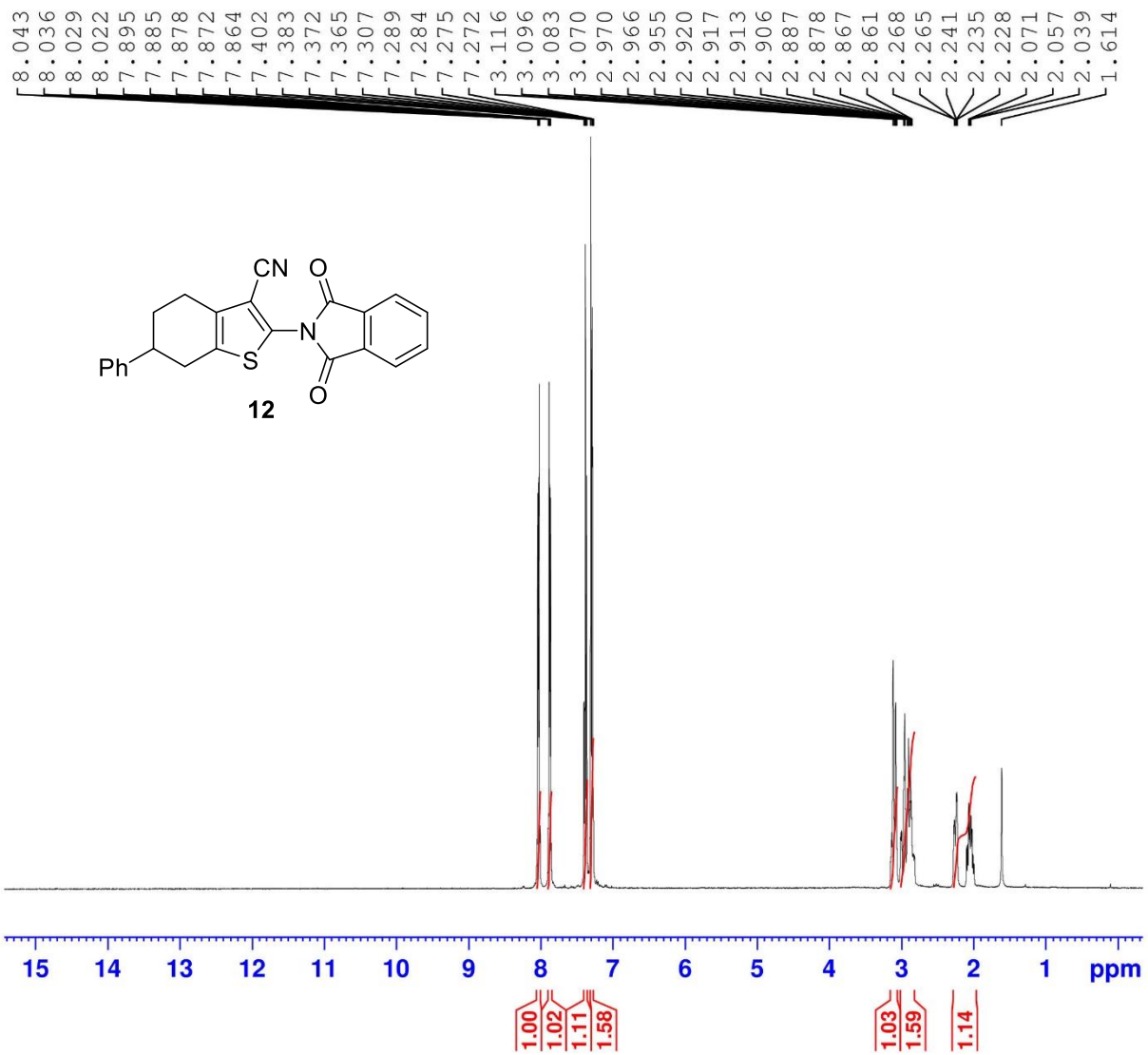
F2 - Acquisition Parameters
Date_             20220912
Time                 12.40
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     128
DS                       2
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                   205.37
DW                   62.400 usec
DE                    6.50 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                      1

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

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

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]



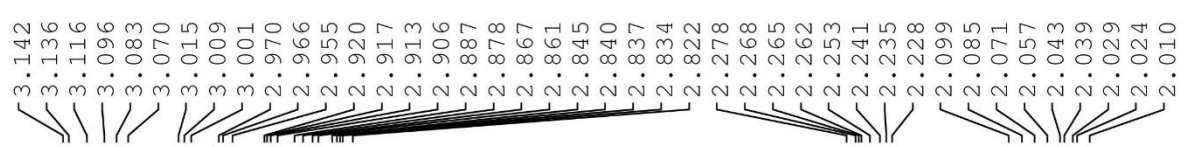


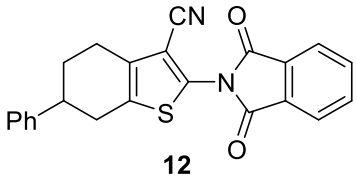

```
Current Data Parameters
NAME      amna-shaaban-A21
EXPNO                    1
PROCNO                   1

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             1.00000000 sec
TD0                   1

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

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





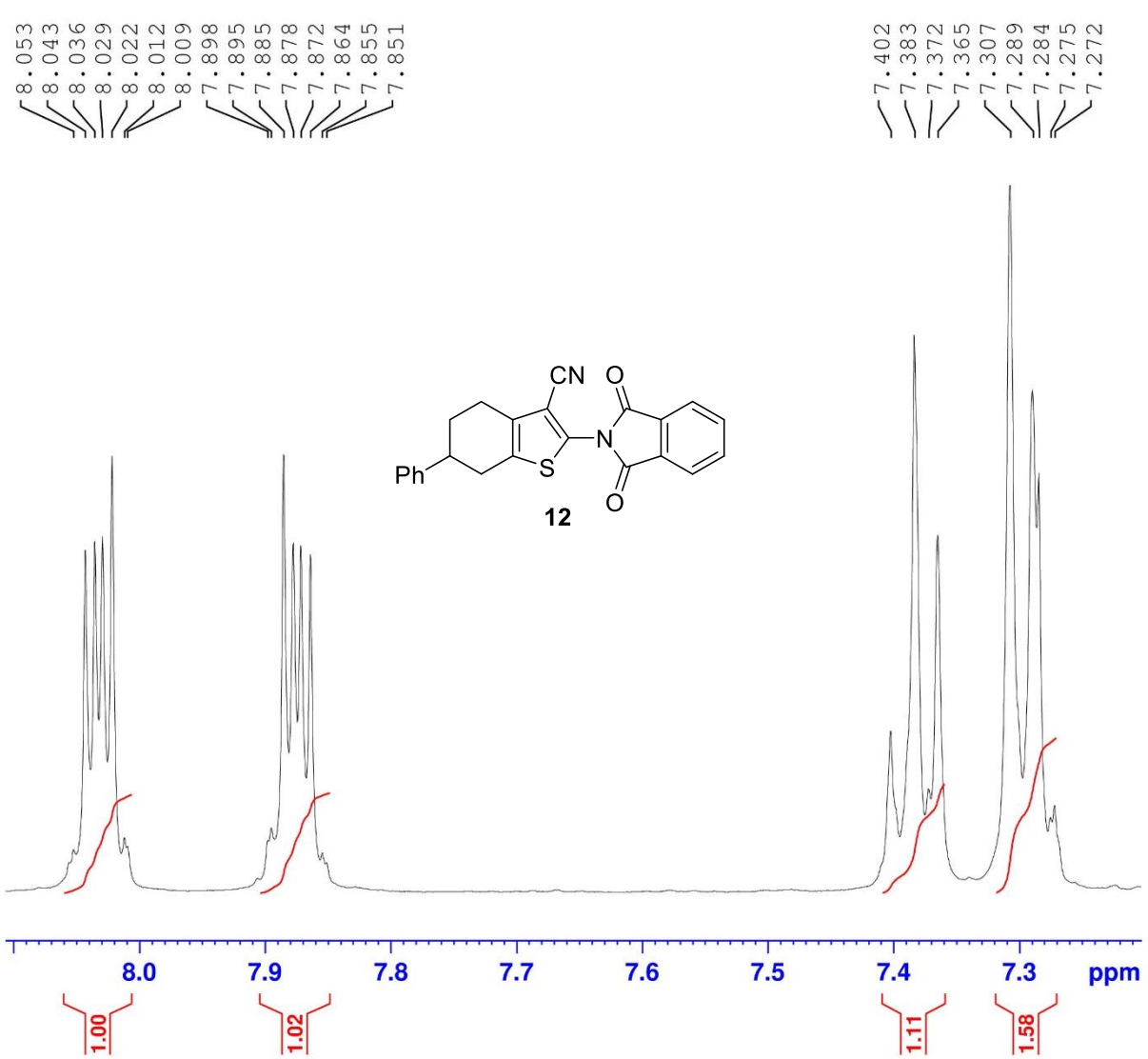
12


```
Current Data Parameters
NAME      amna-shaaban-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            1.00000000 sec
TD0                    1

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

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



BRUKER

```
Current Data Parameters
NAME      amna-shaaban-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             1.00000000 sec
TD0                     1

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

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

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]