

## Supporting information

### Sulfonamide vs. Sulfonimide:

#### Tautomerism and Electronic Structure Analysis of *N*-Heterocyclic Arenesulfonamides

Sumit S. Chourasiya,<sup>a</sup> Dhara Patel,<sup>a</sup> C. M. Nagaraja,<sup>b</sup> Asit K. Chakraborti<sup>a</sup> and Prasad V. Bharatam<sup>a\*</sup>

<sup>a</sup>Department of Medicinal Chemistry  
National Institute of Pharmaceutical Education and Research (NIPER)  
S.A.S. Nagar-160 062, Punjab, India  
Department of Chemistry, Indian Institute of Technology (IIT), Ropar  
Roopnagar – 140 001, Punjab, India  
E-mail: [pybharatam@gmail.com](mailto:pybharatam@gmail.com)

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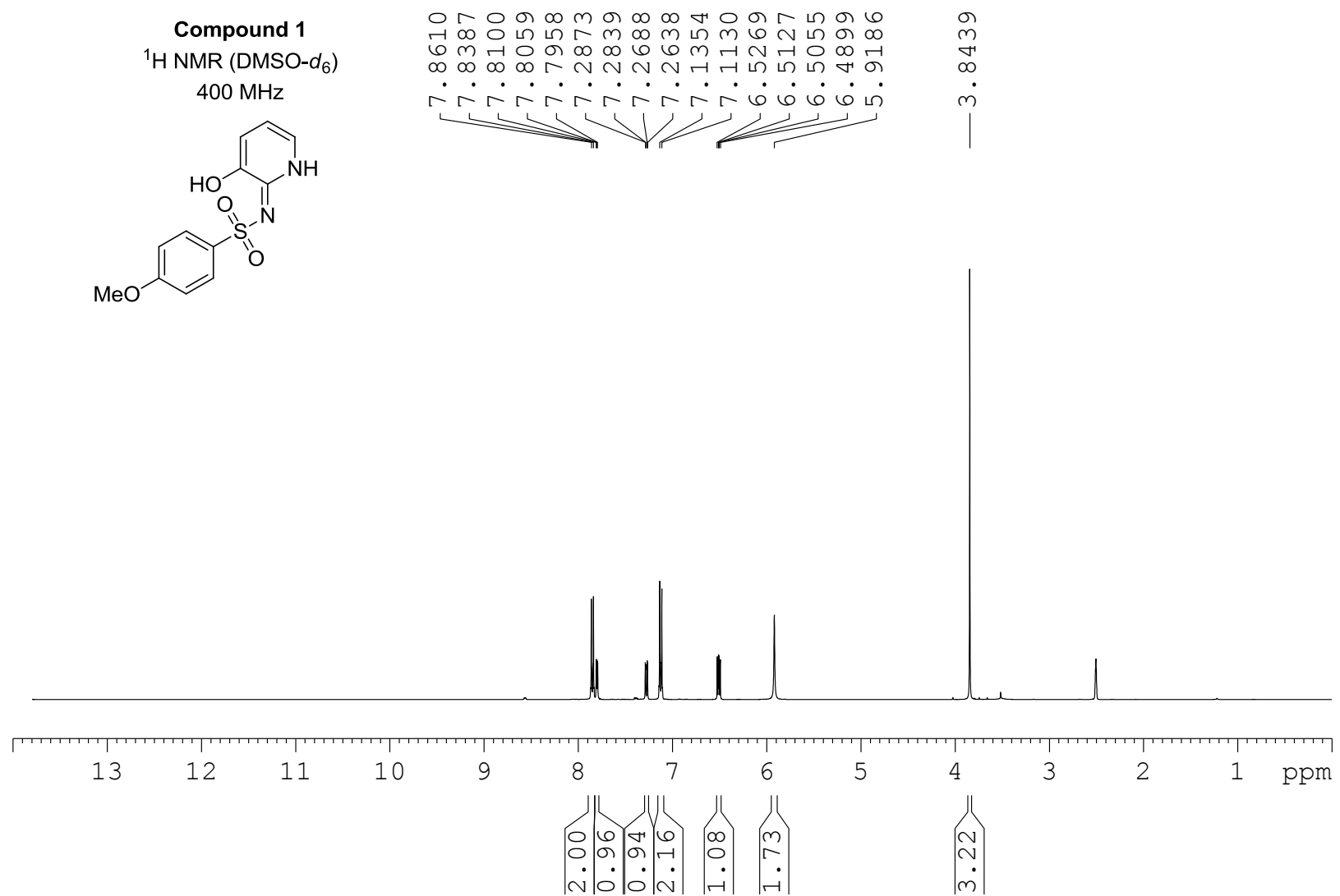
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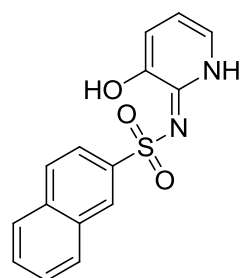
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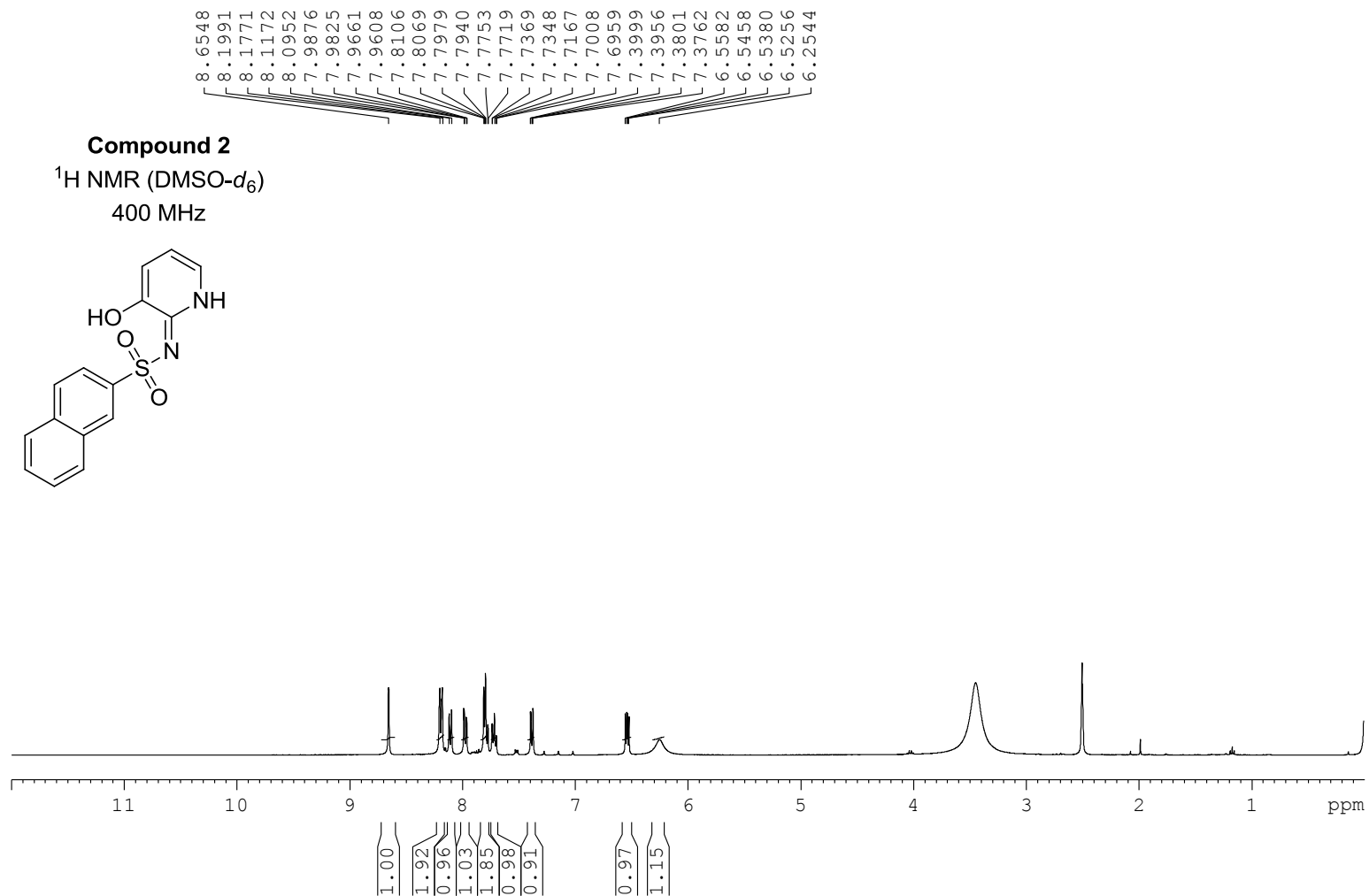
## **Spectral data**

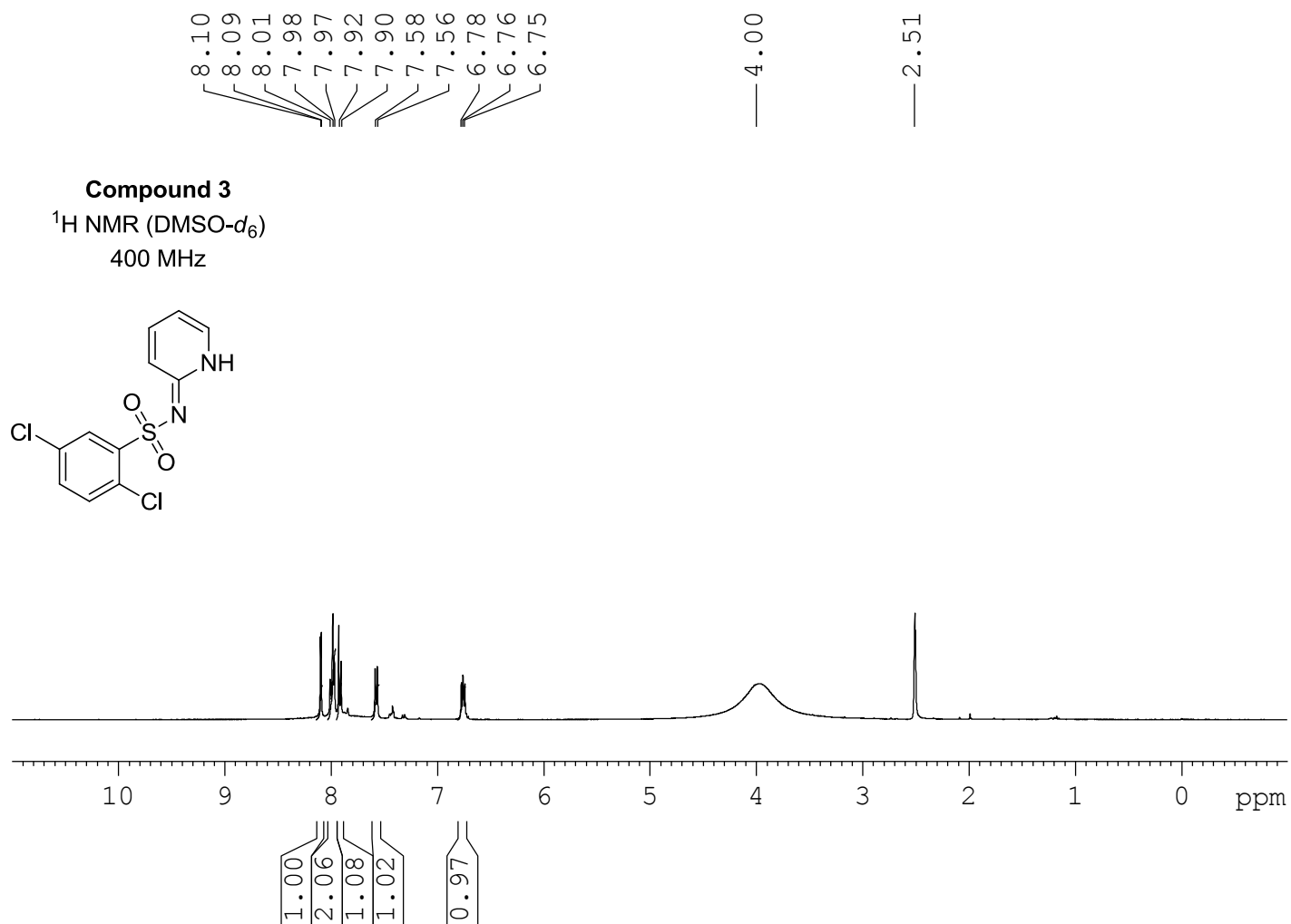
### **$^1\text{H}$ NMR spectra of compounds 1-10**

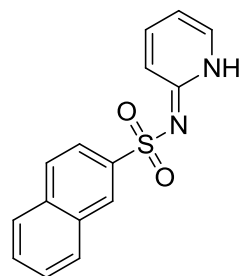




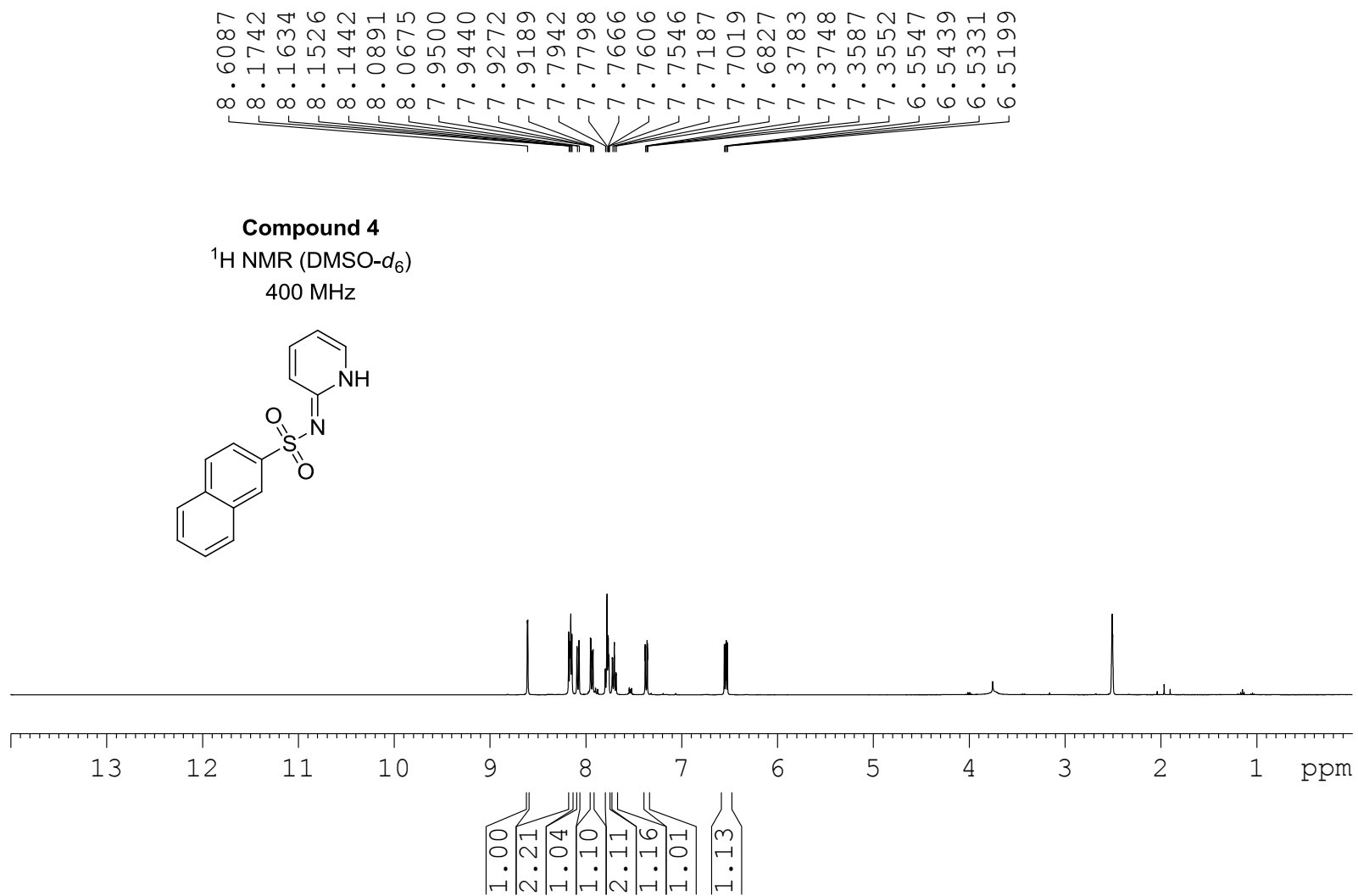
**Compound 2**  
<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>)  
 400 MHz

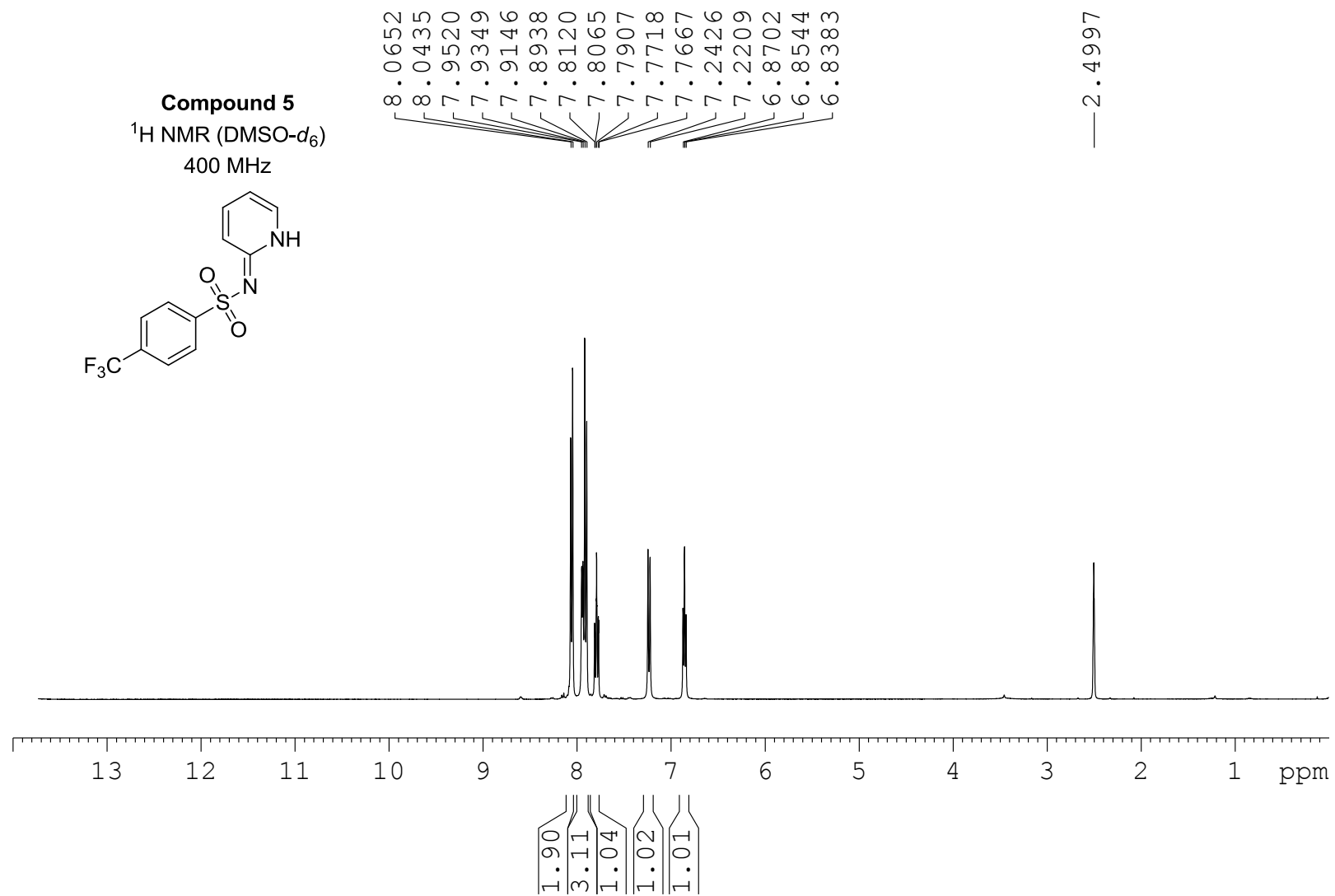


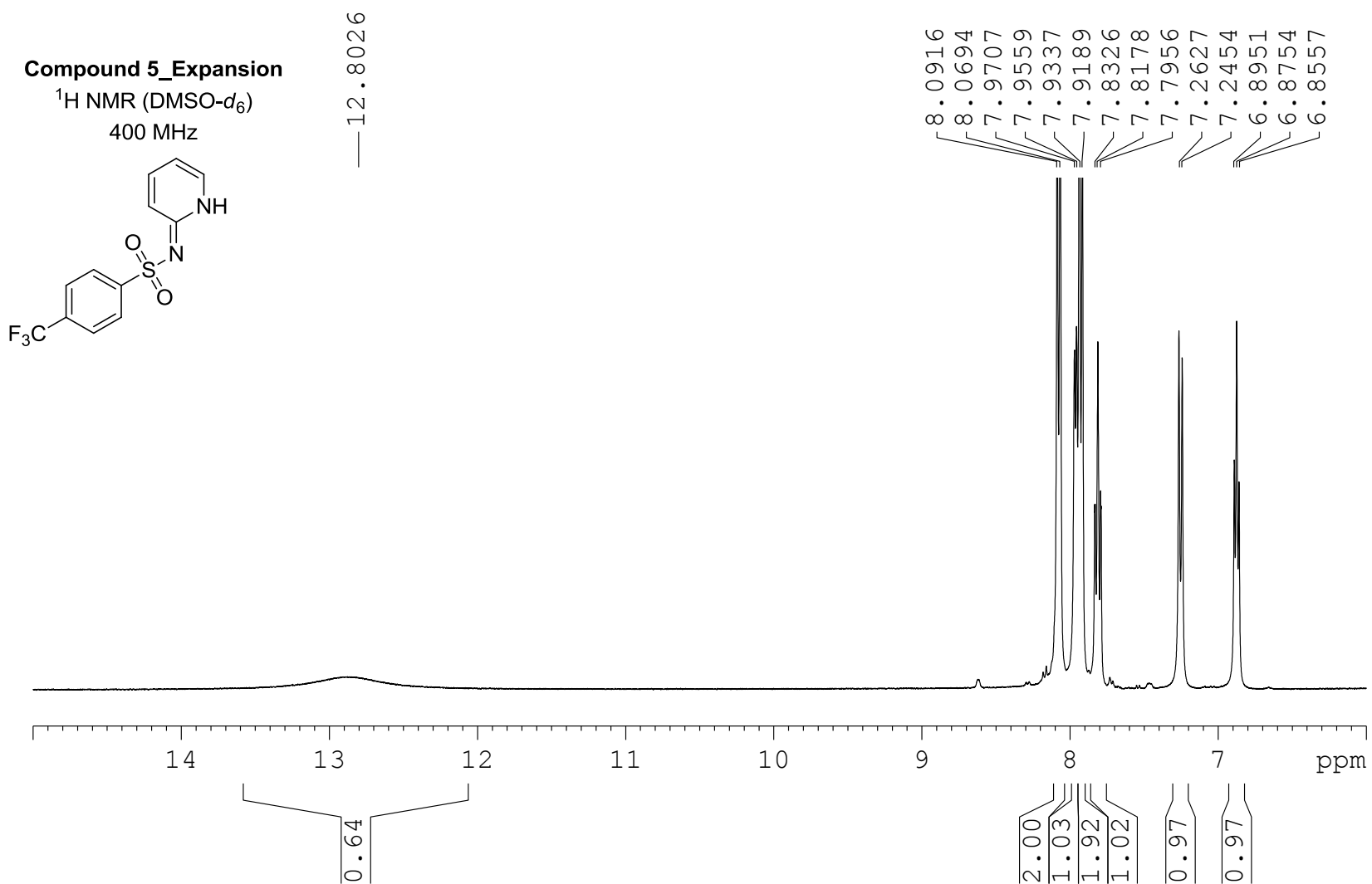




**Compound 4**  
 $^1\text{H}$  NMR (DMSO- $d_6$ )  
 400 MHz

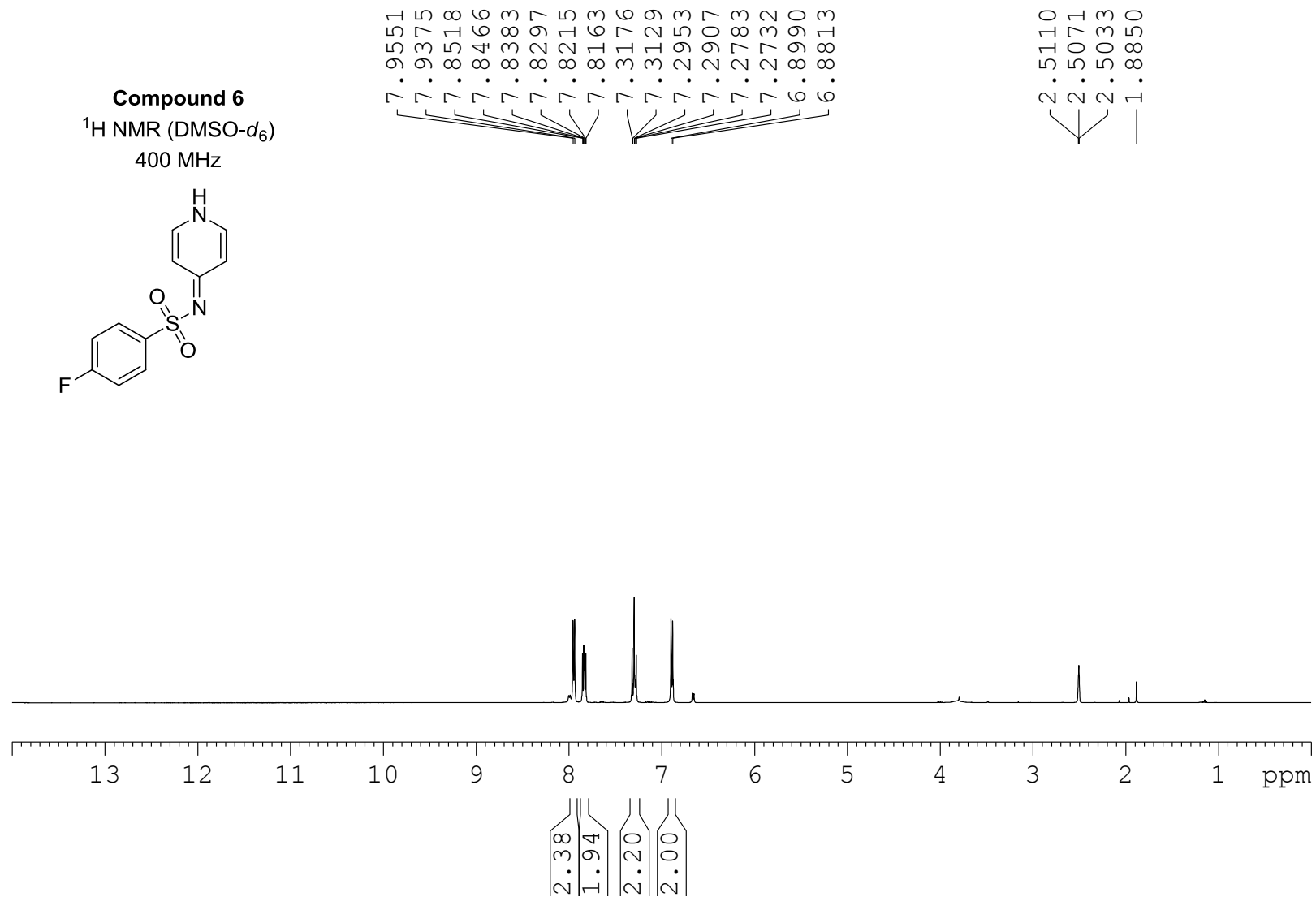
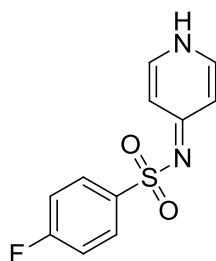




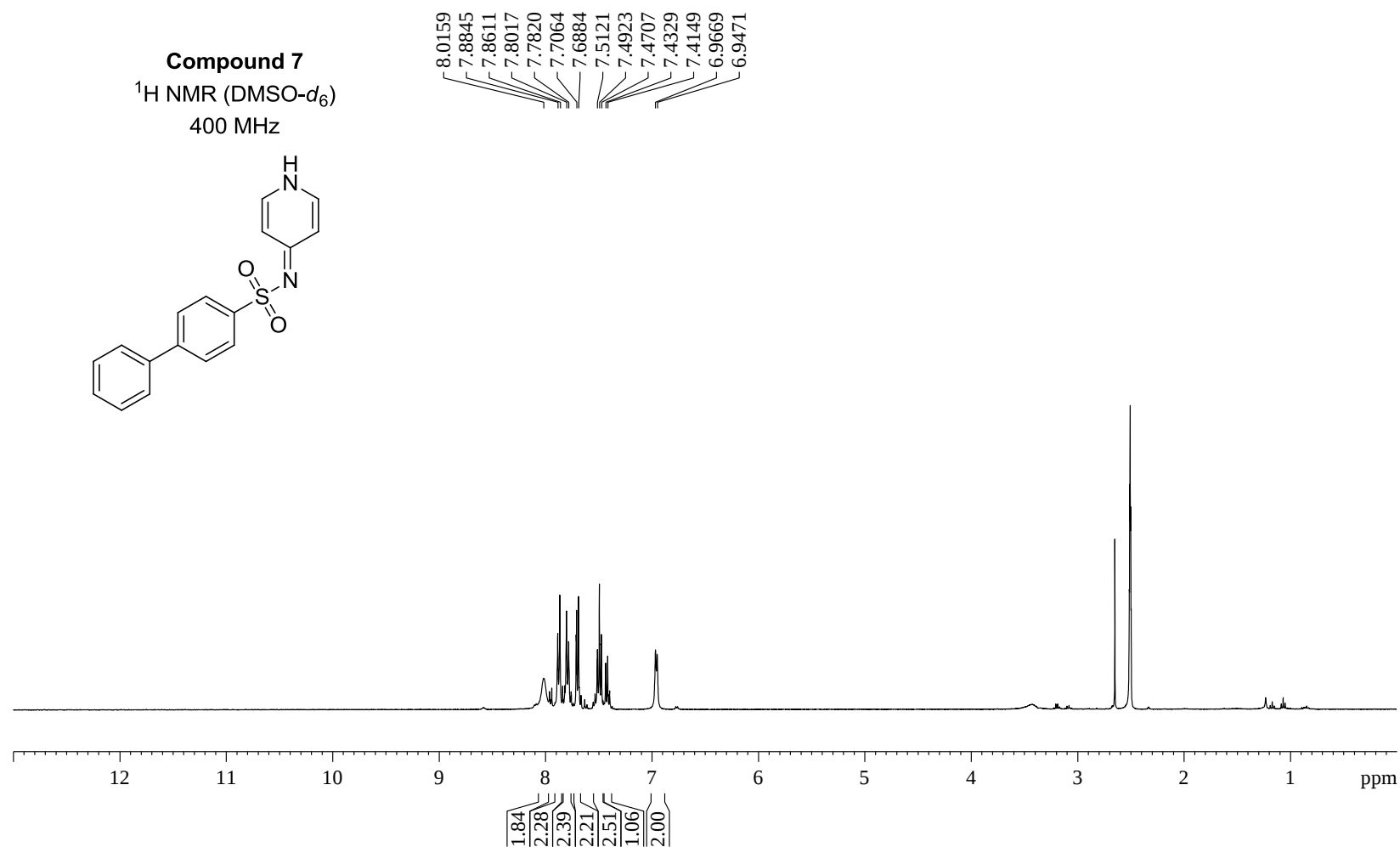
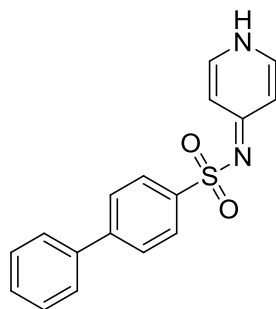


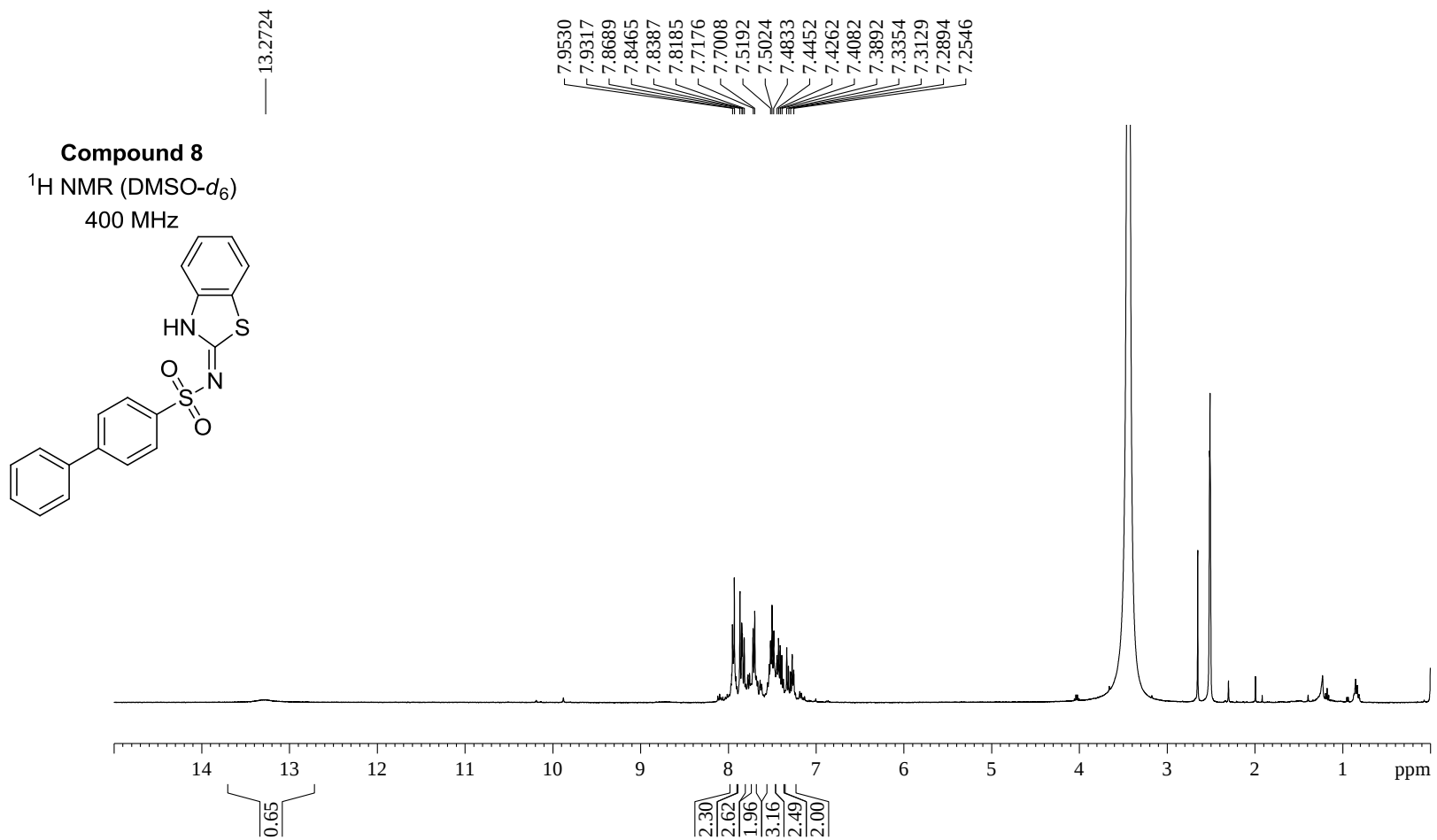
Compound 6

**Compound 6**  
<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>)  
 400 MHz

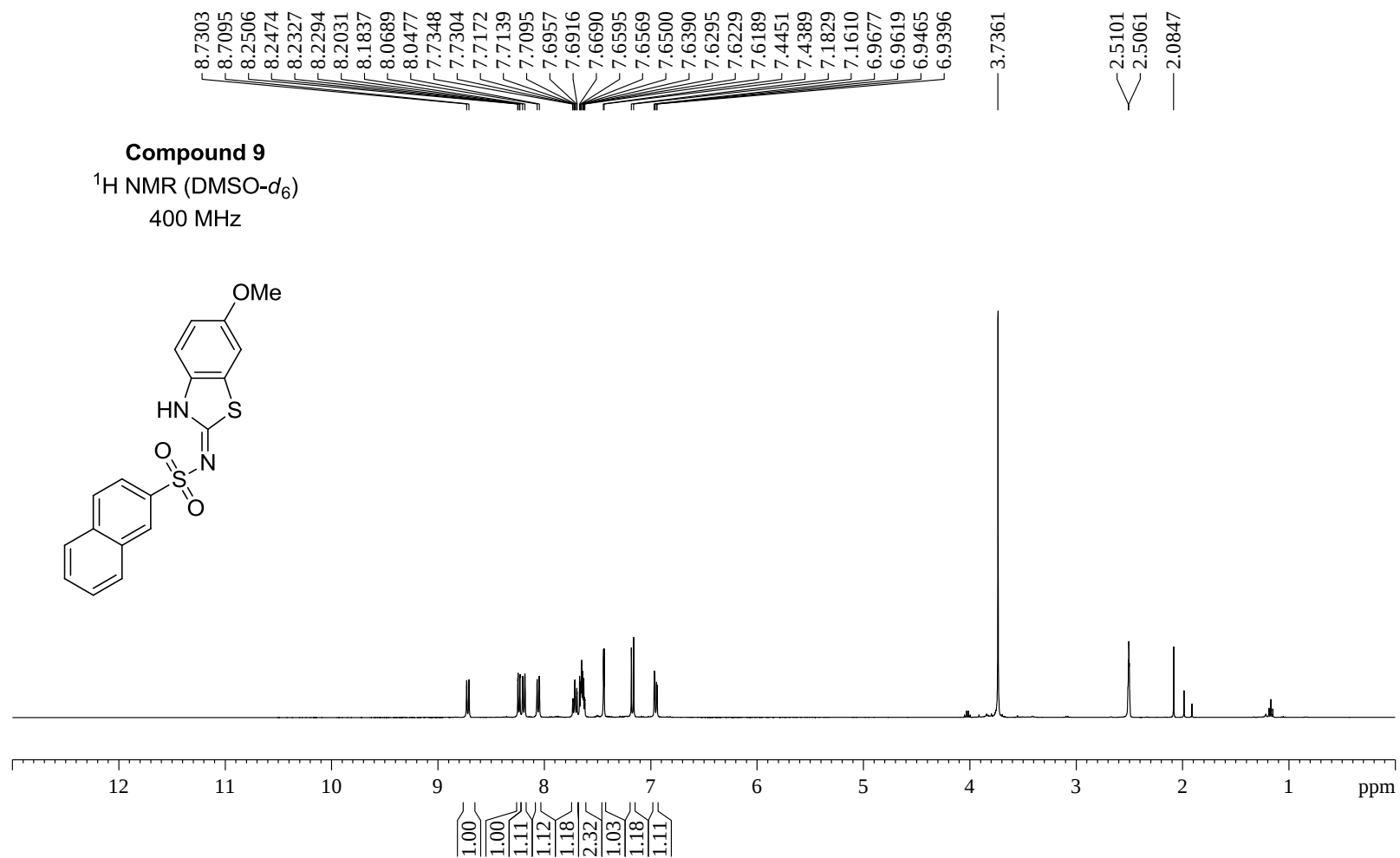


**Compound 7**  
 $^1\text{H}$  NMR (DMSO- $d_6$ )  
400 MHz

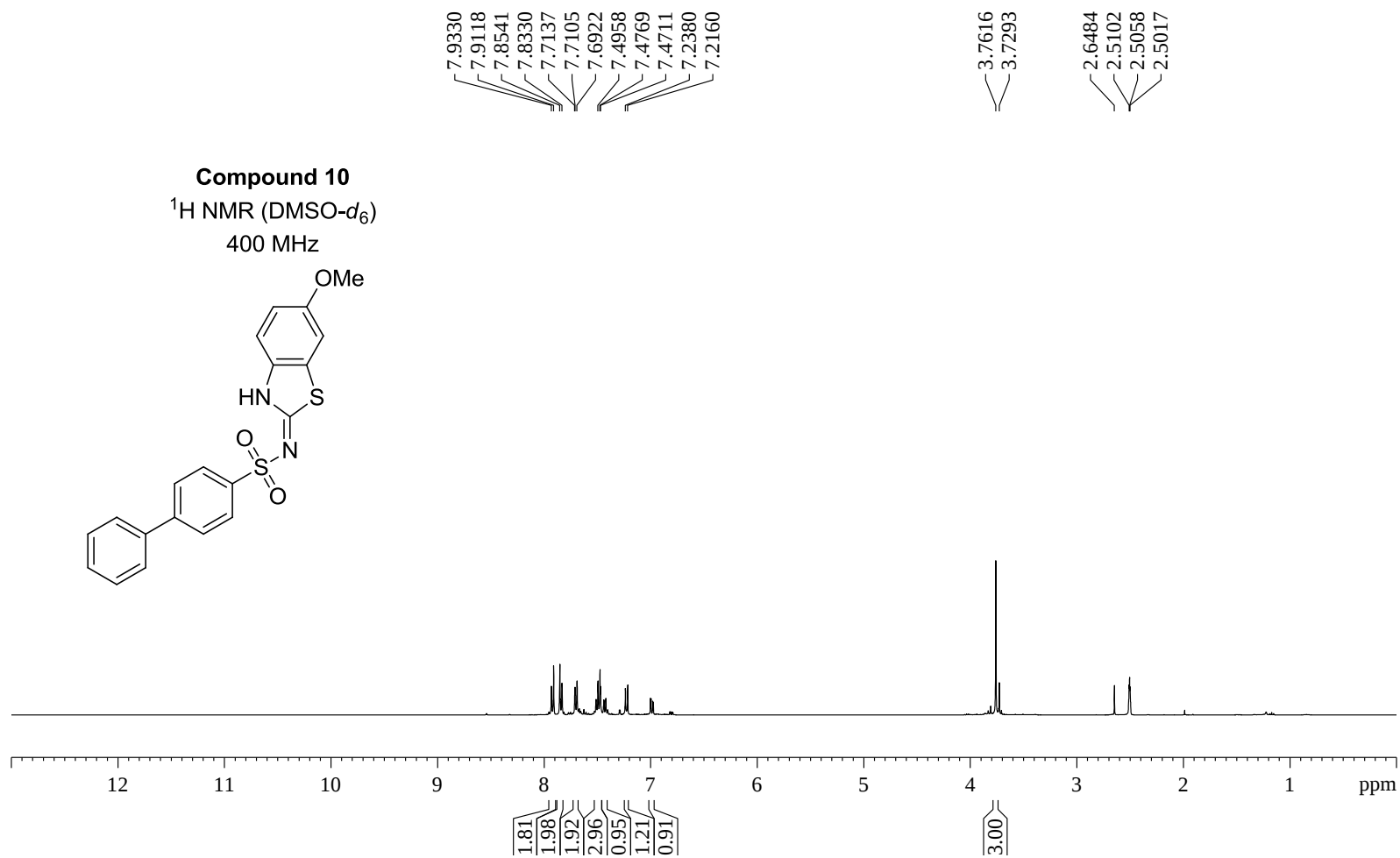




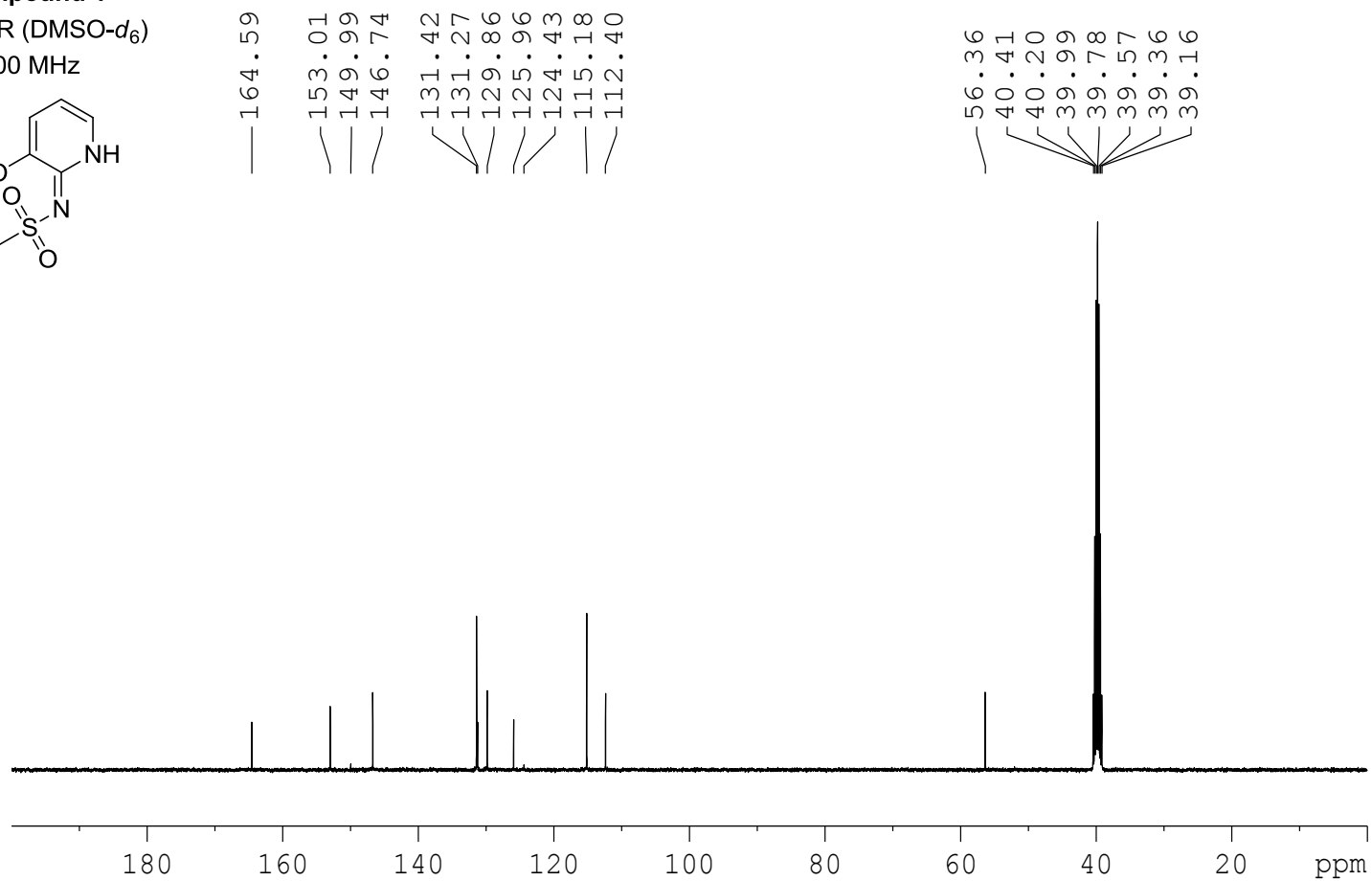
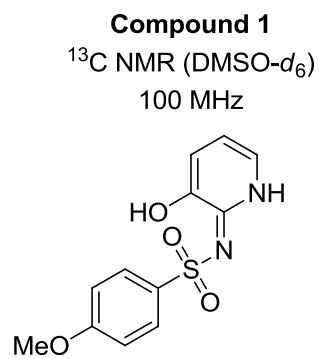
Compound 9

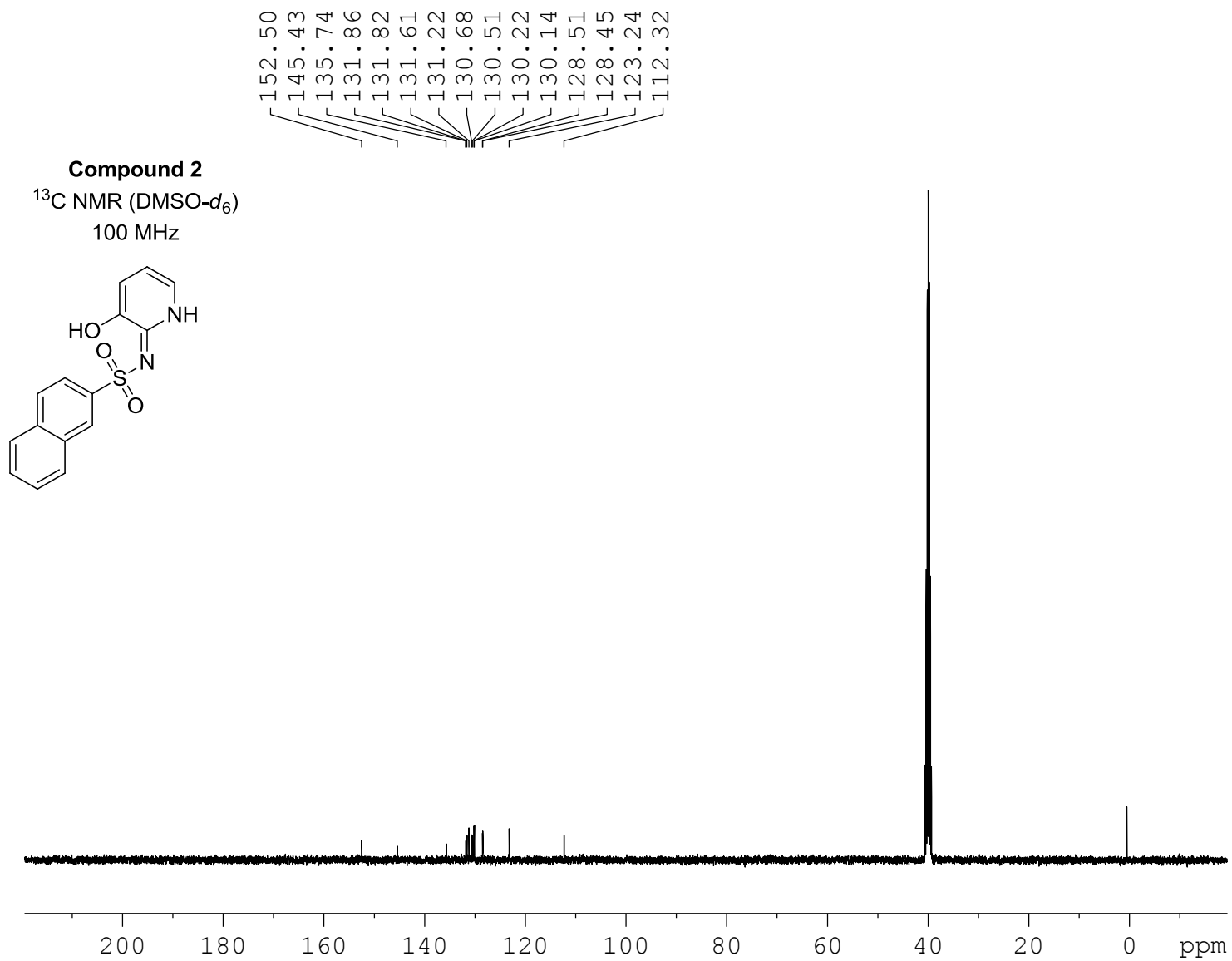


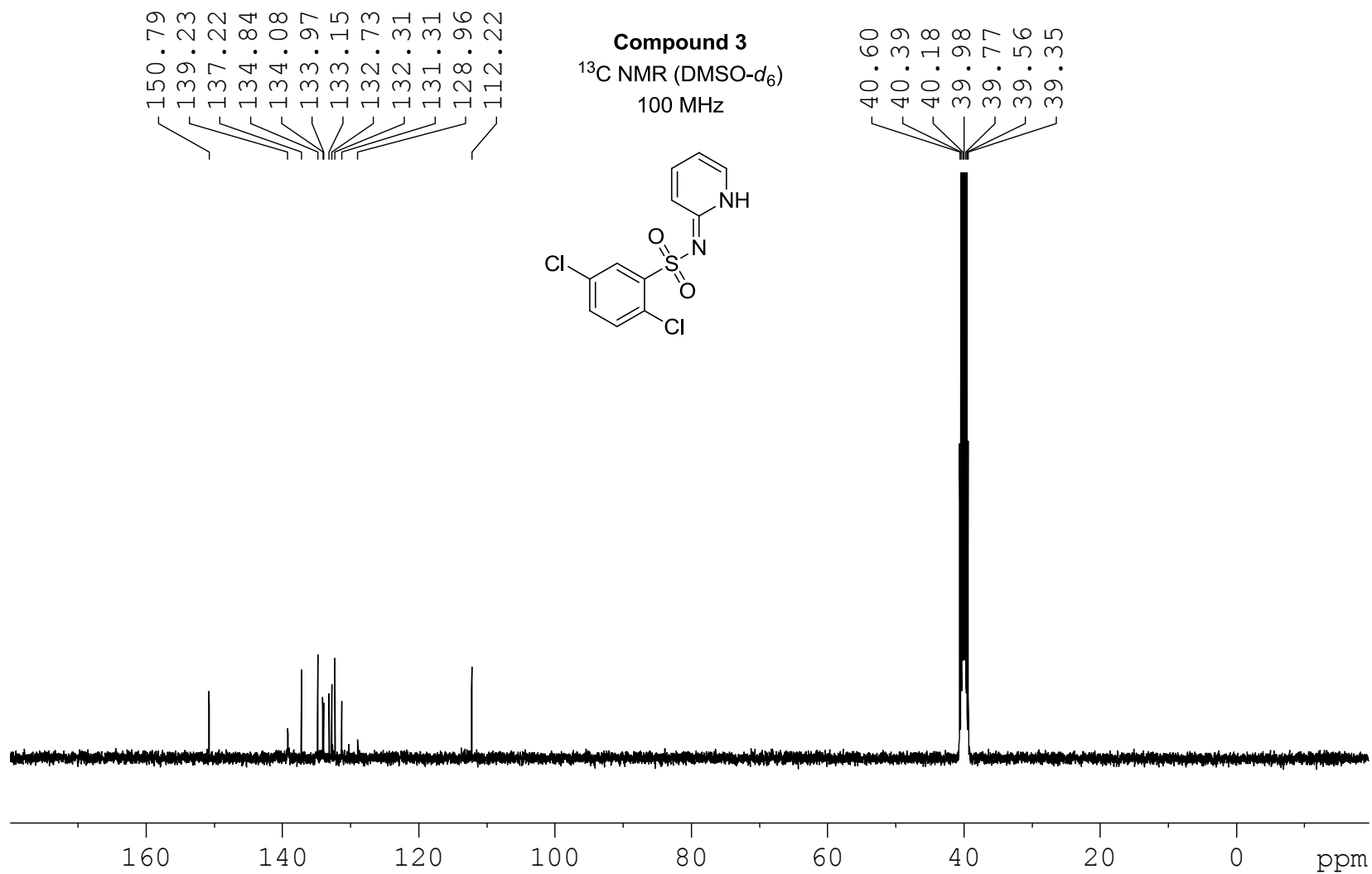
Compound 10

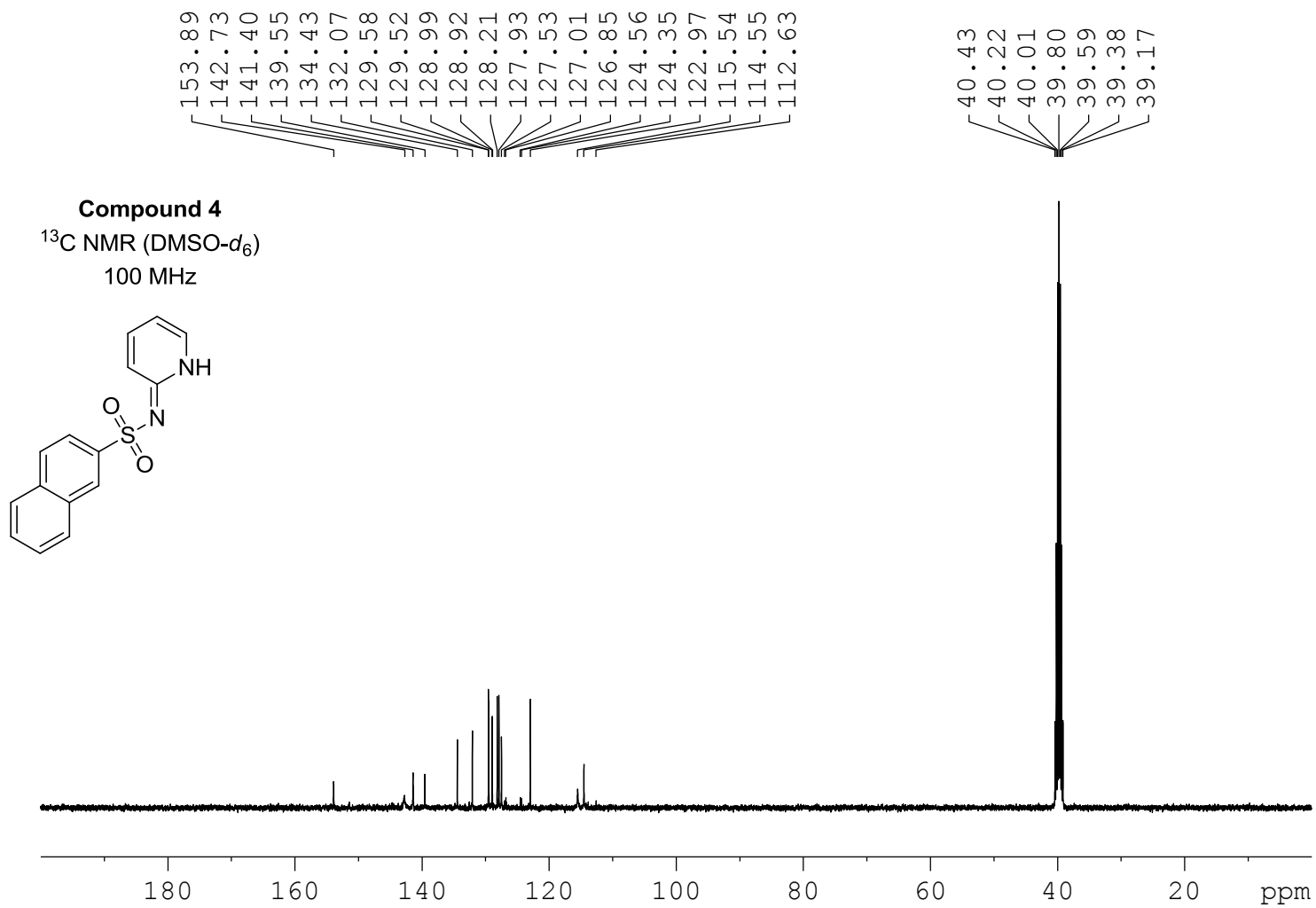


## **$^{13}\text{C}$ NMR spectra of compounds 1-10**

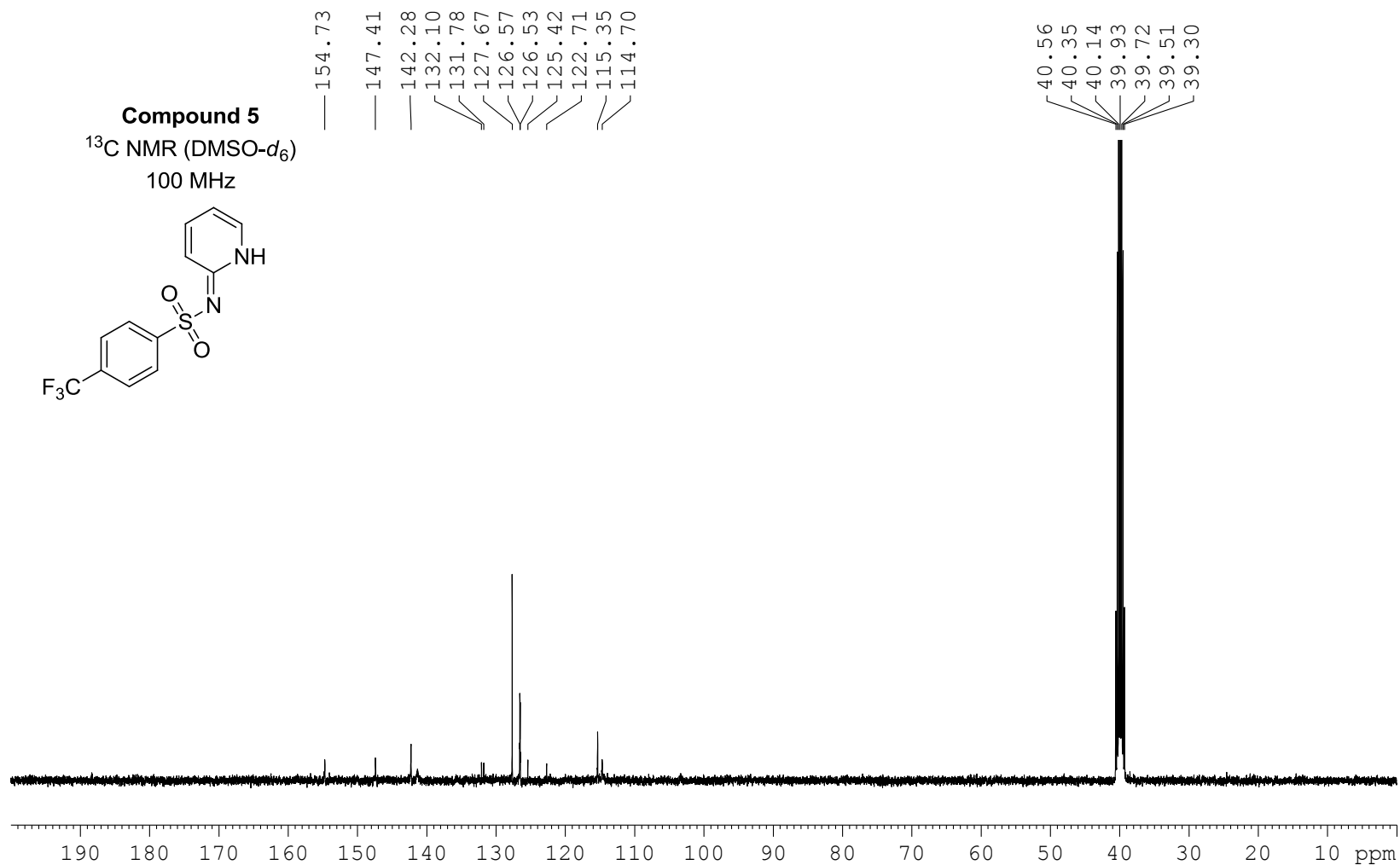
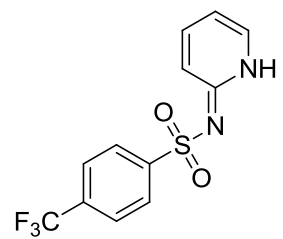


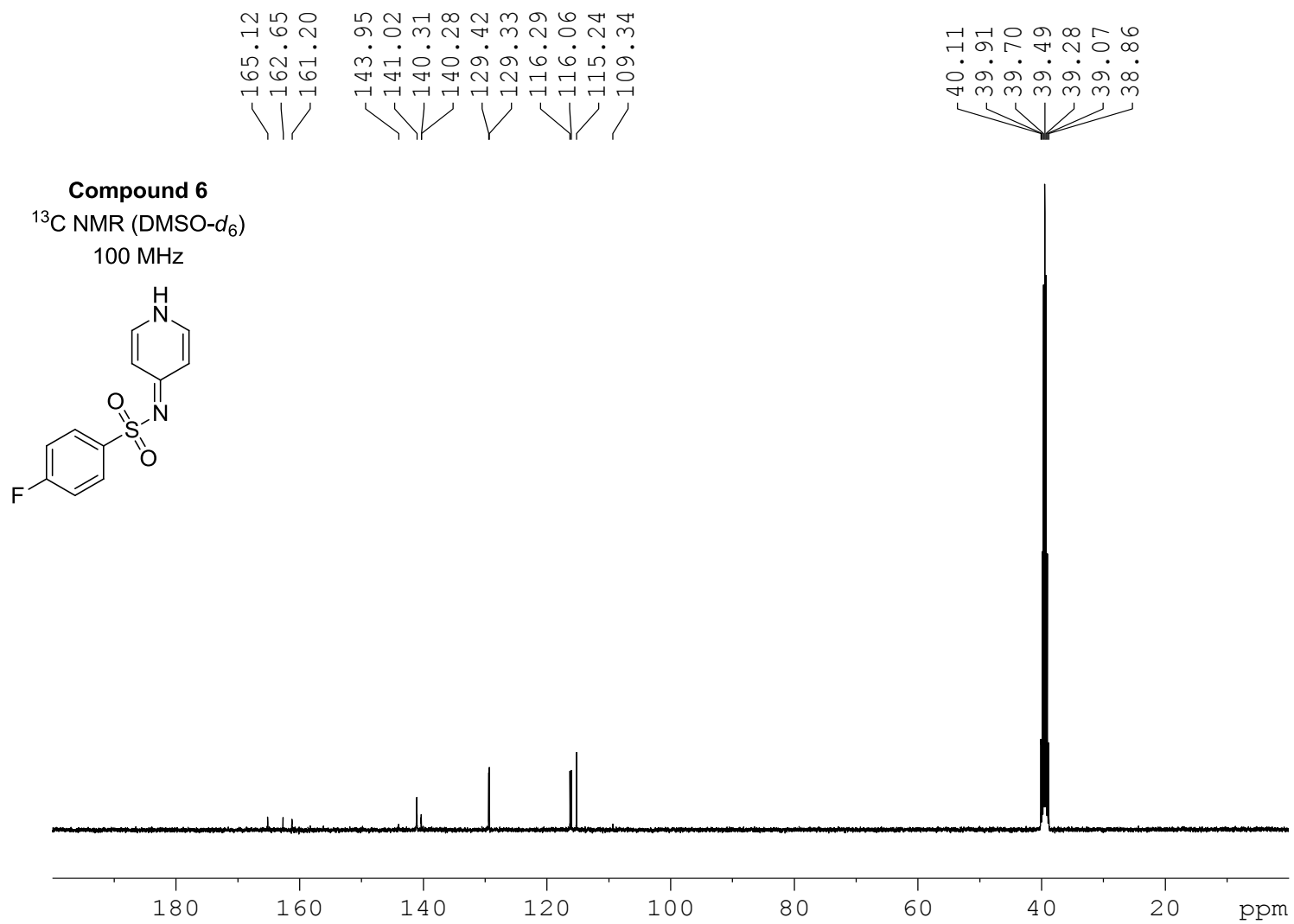


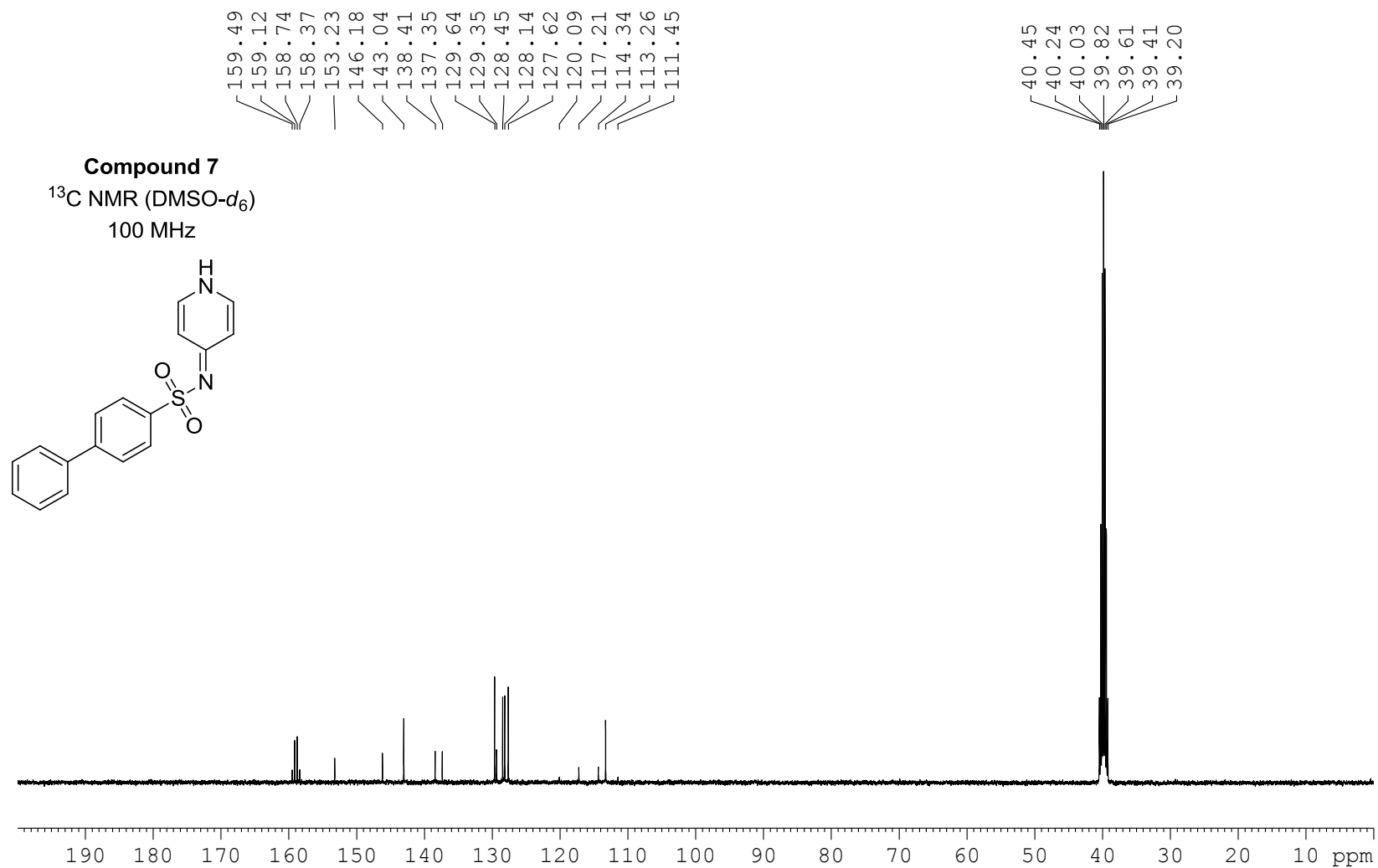


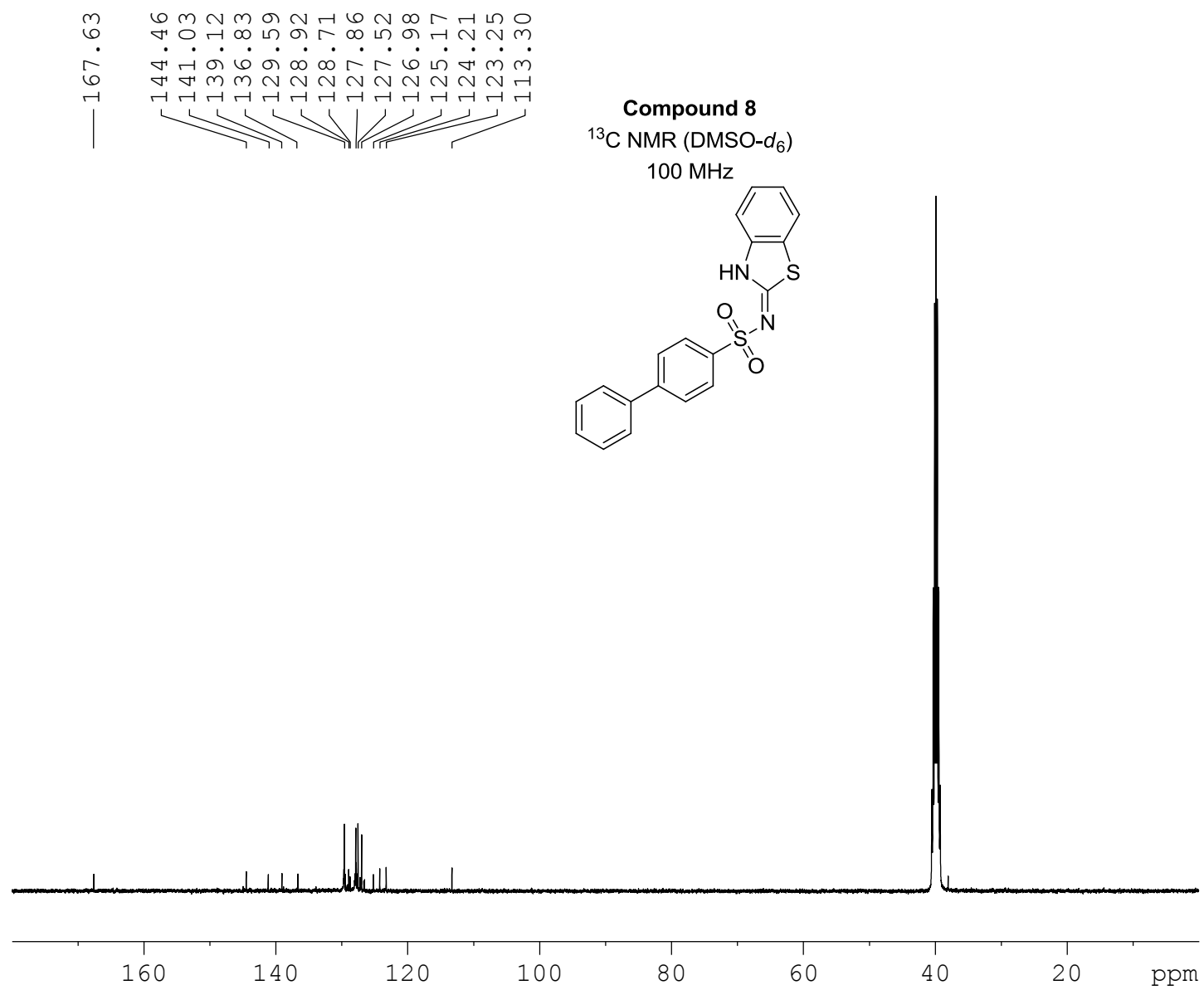


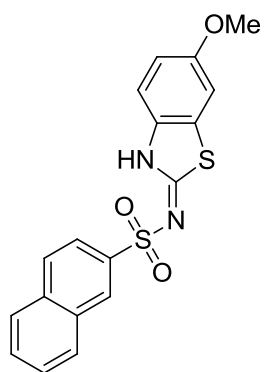
Compound 5



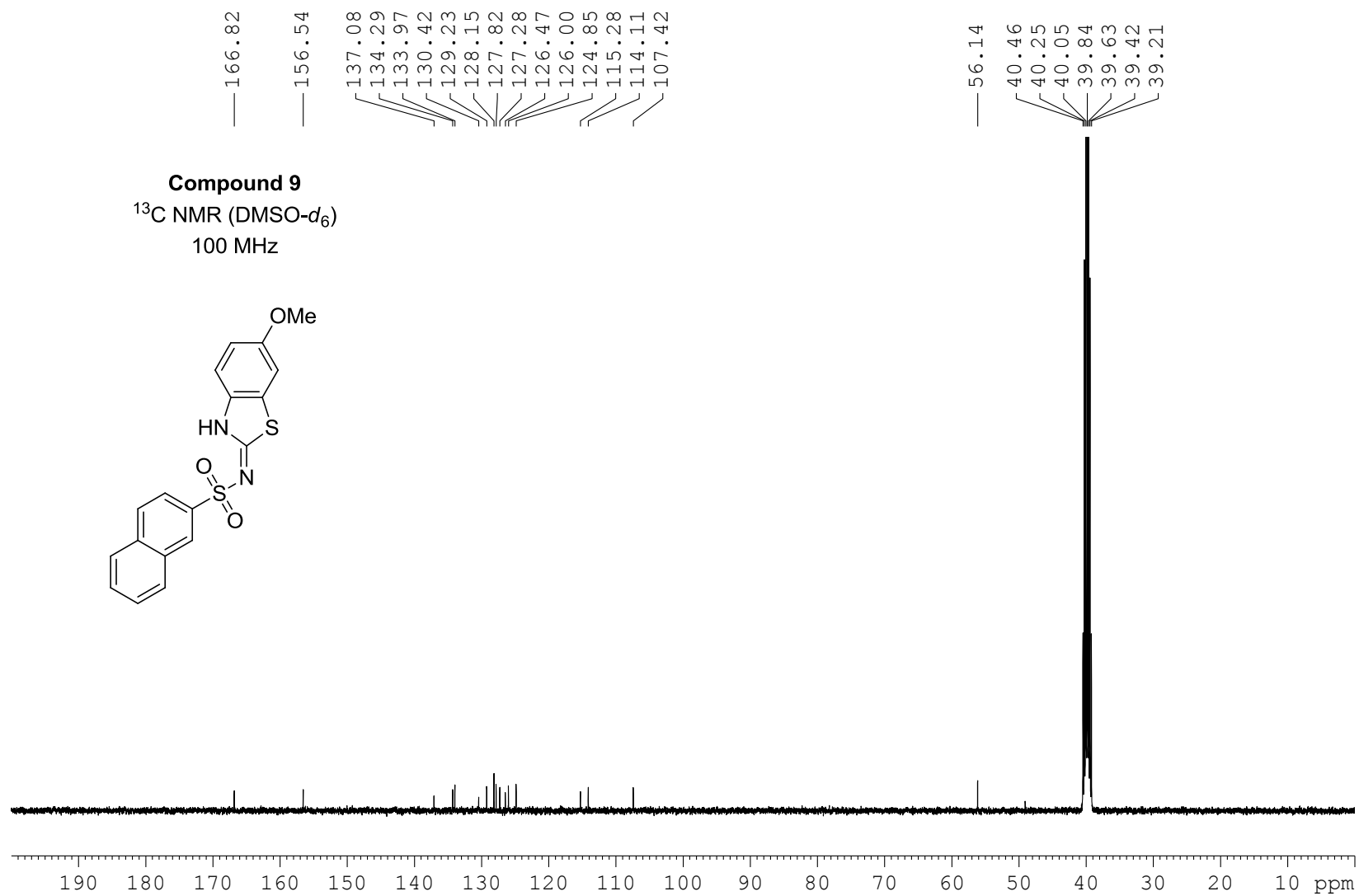


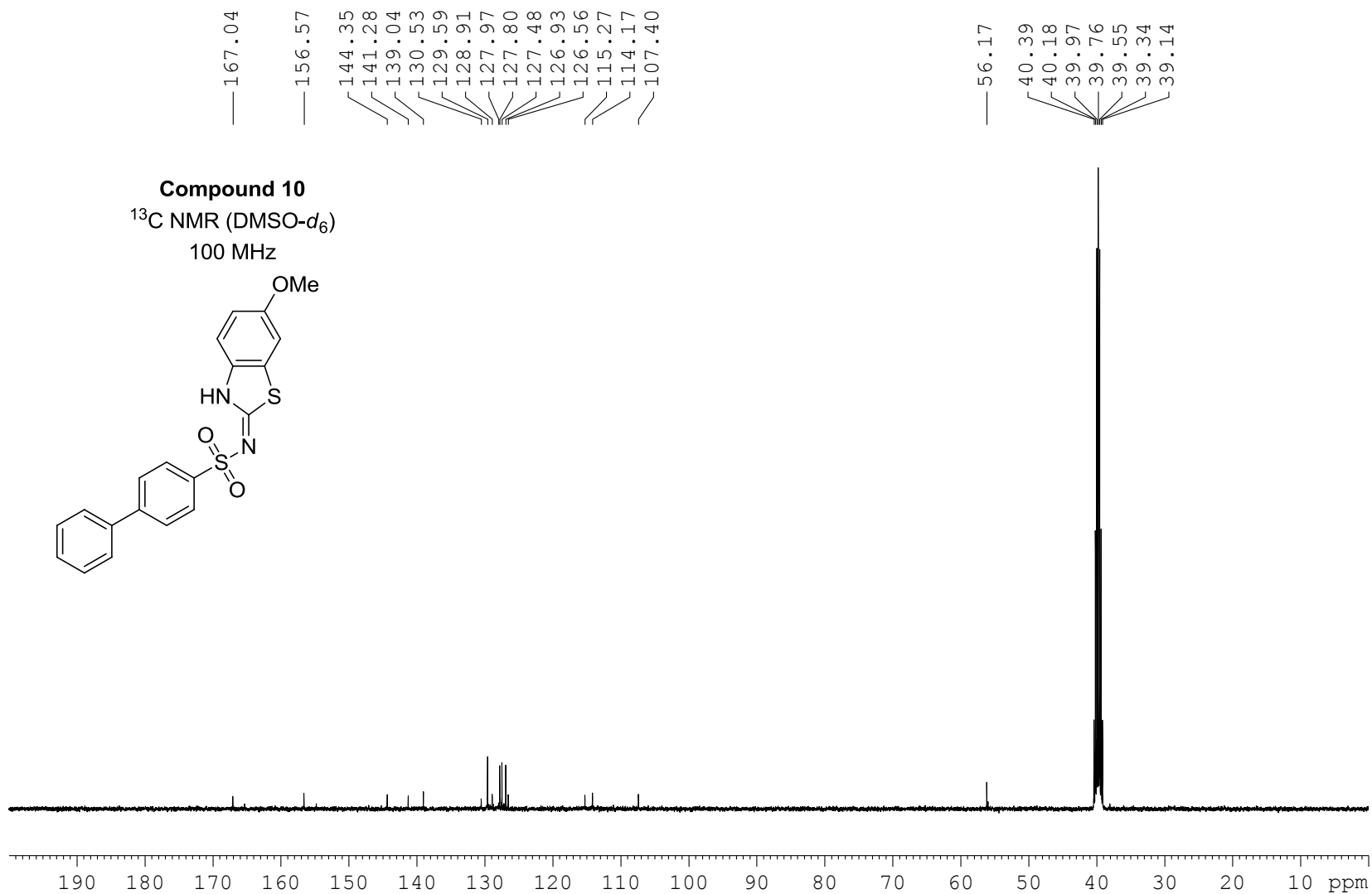




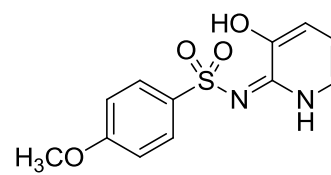


**Compound 9**  
 $^{13}\text{C}$  NMR ( $\text{DMSO-}d_6$ )  
 100 MHz



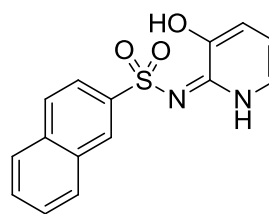


## **IR spectra of compounds 1-10**

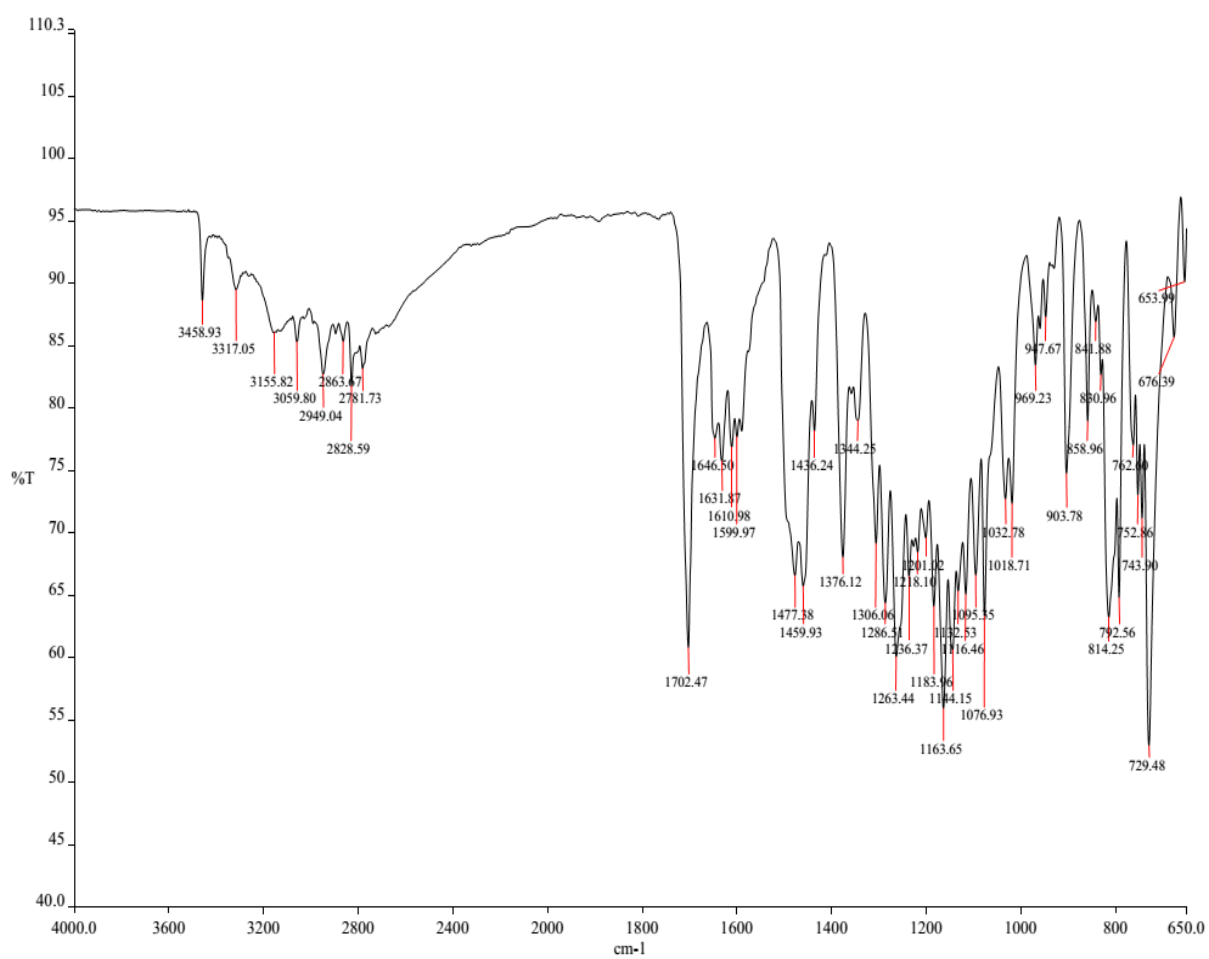


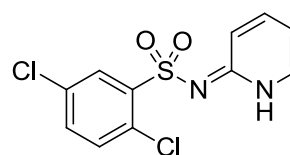
Compound 1



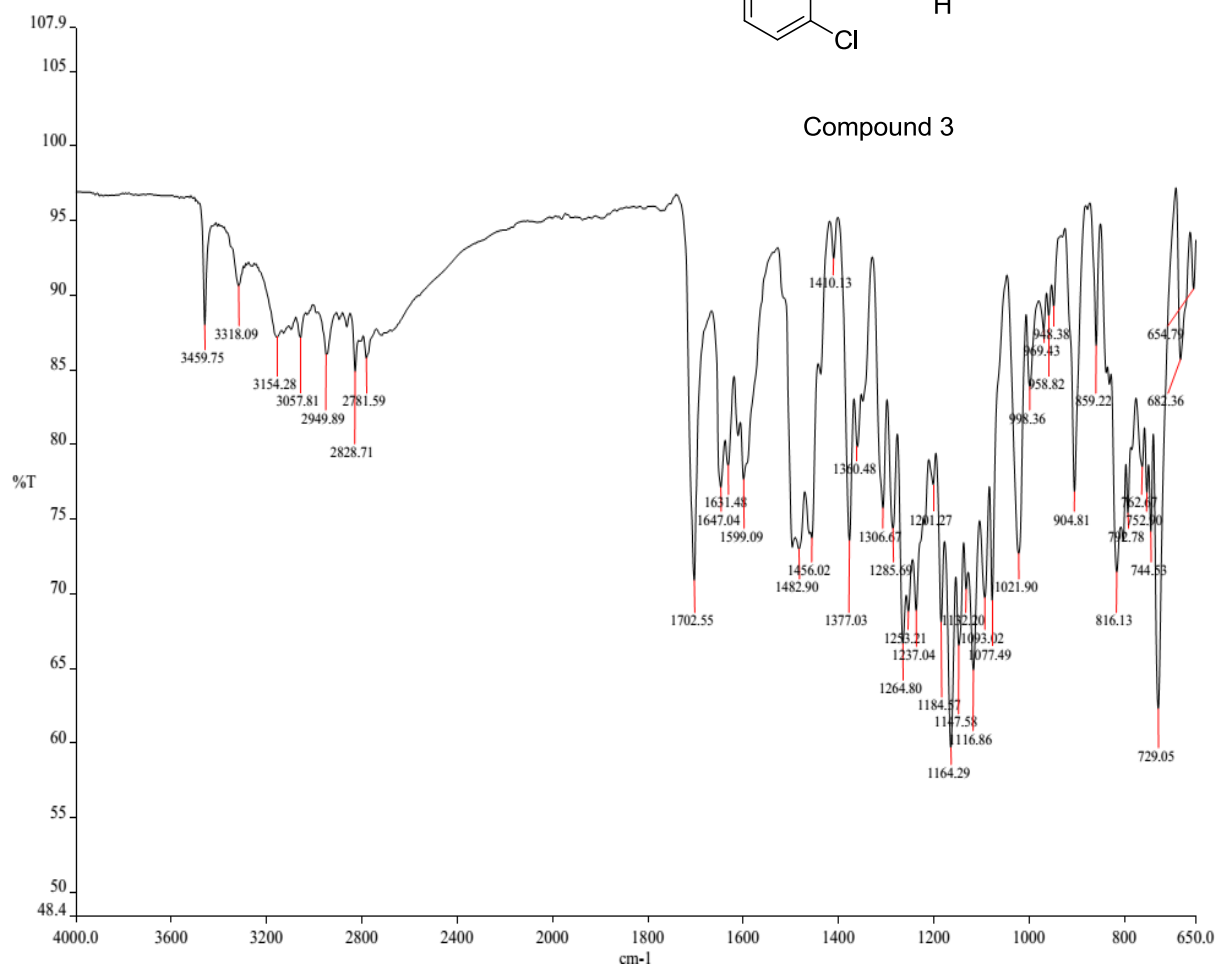


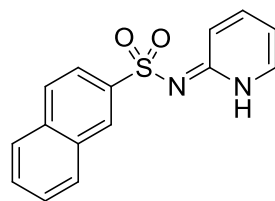
Compound 2



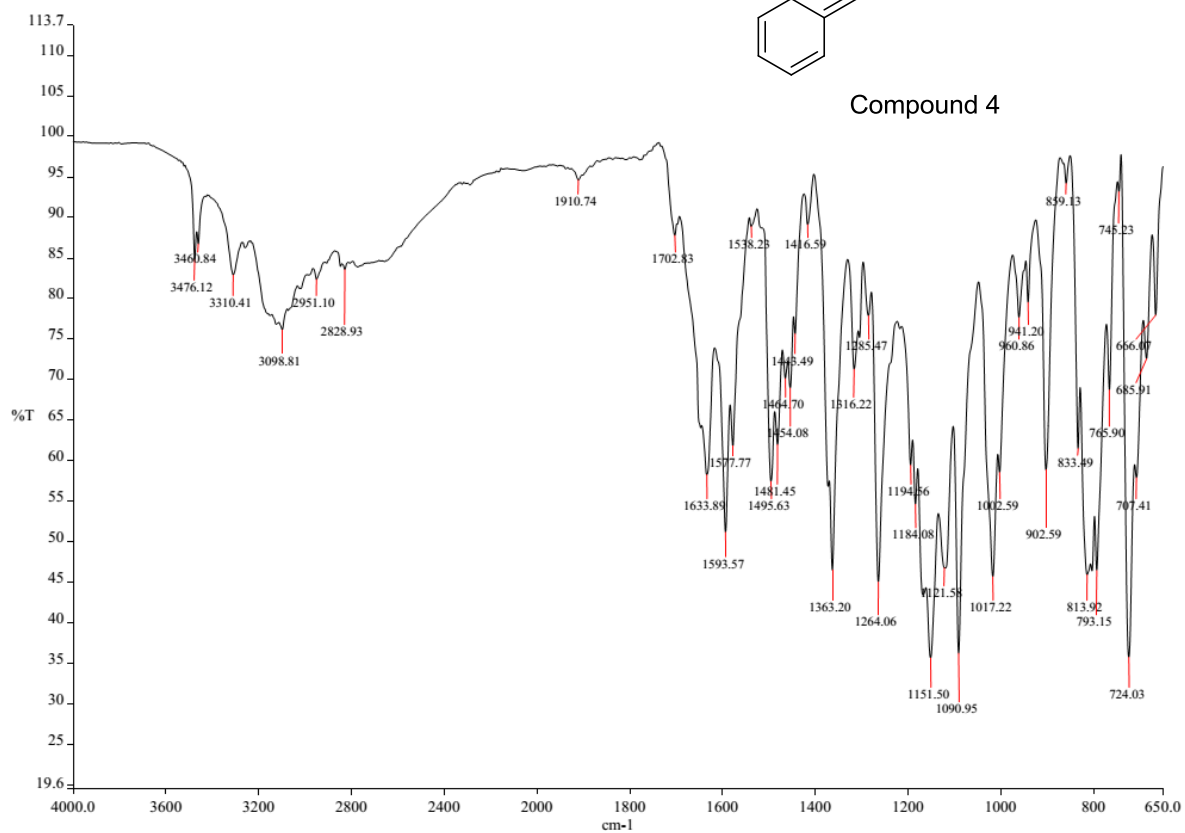


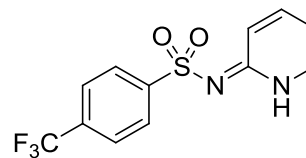
Compound 3



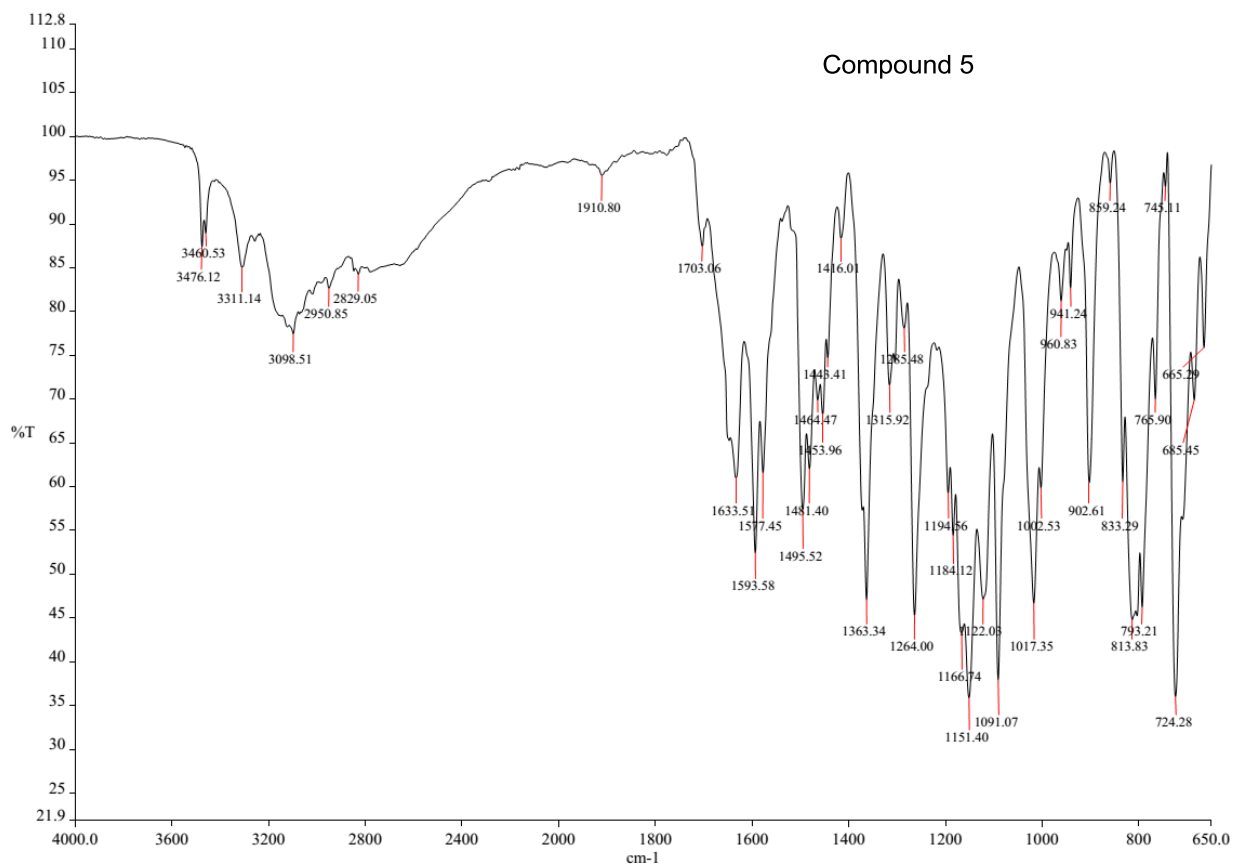


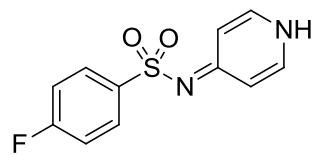
Compound 4



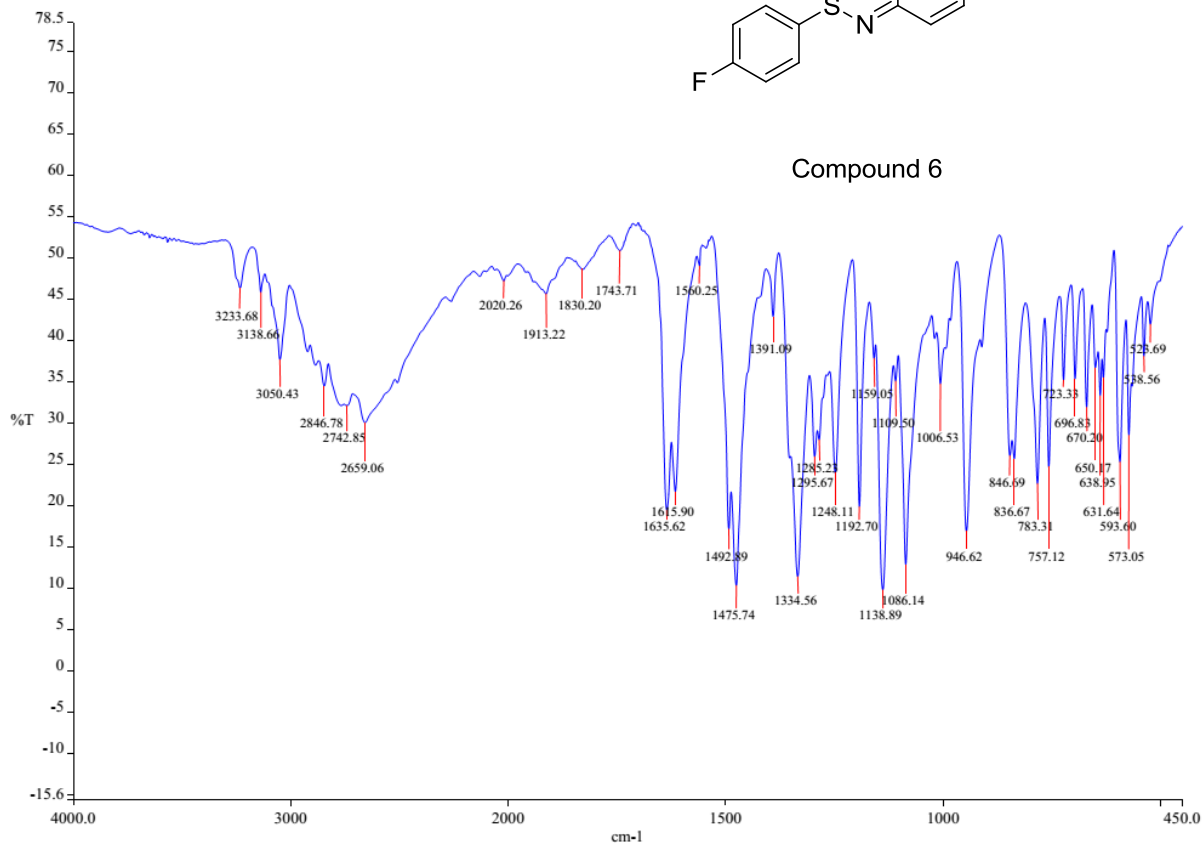


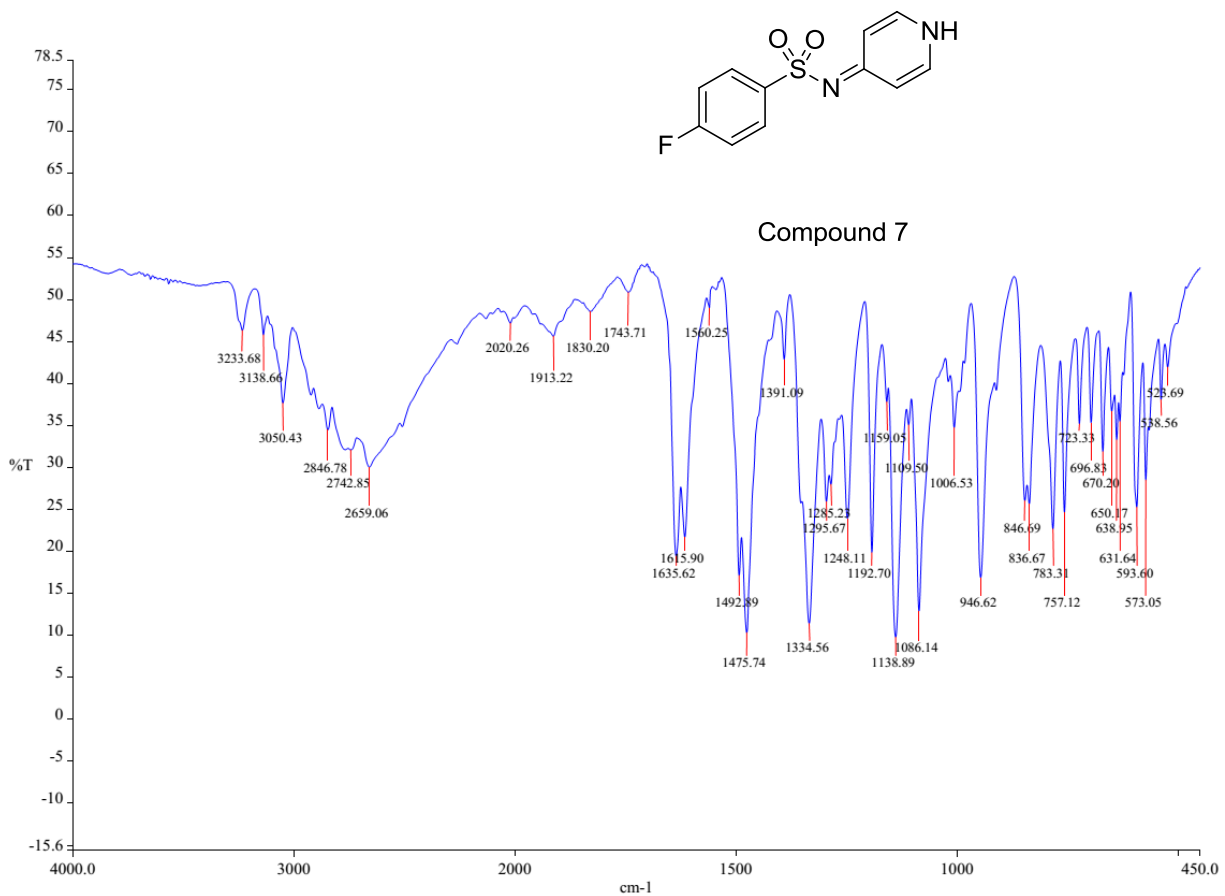
Compound 5

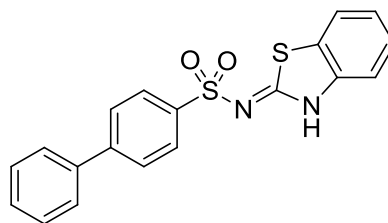




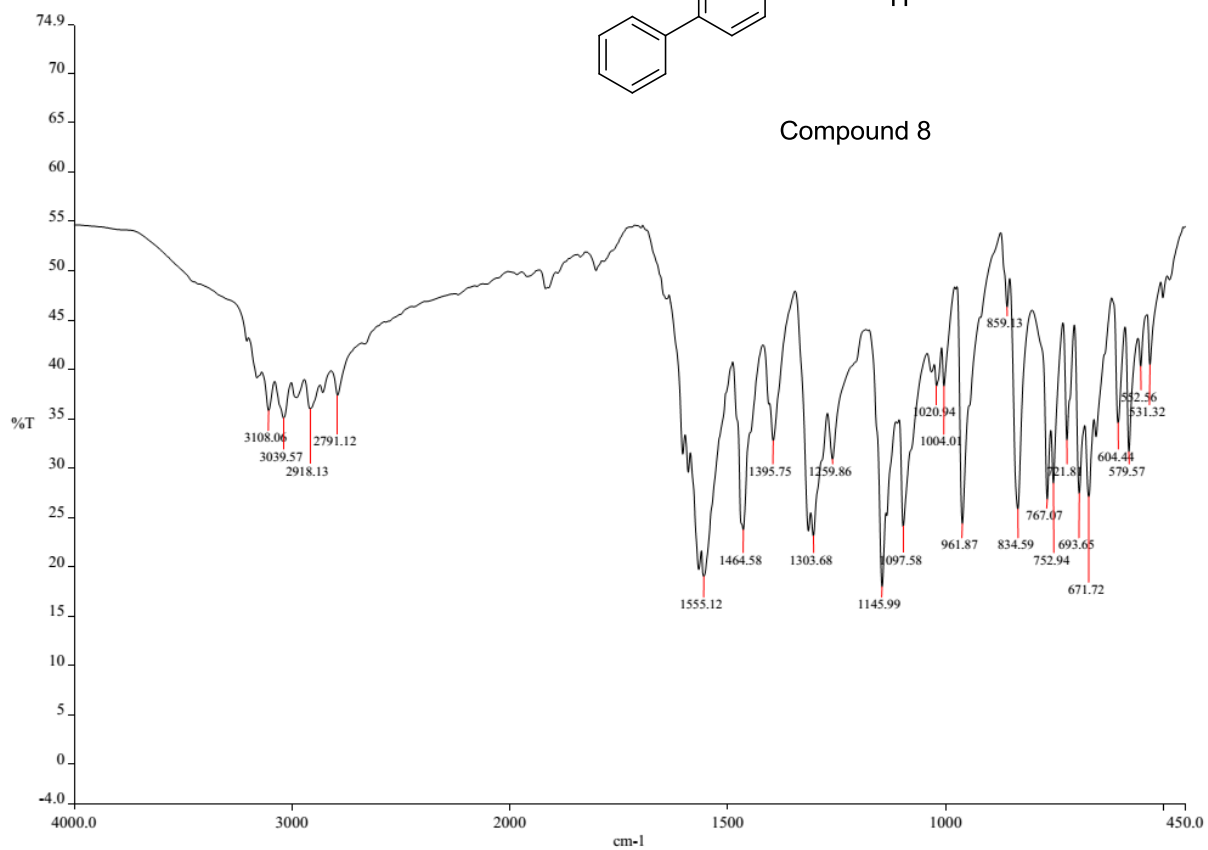
Compound 6

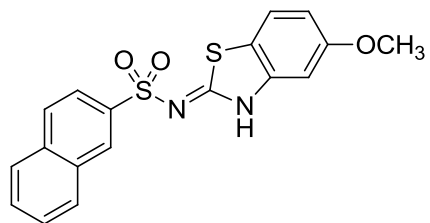




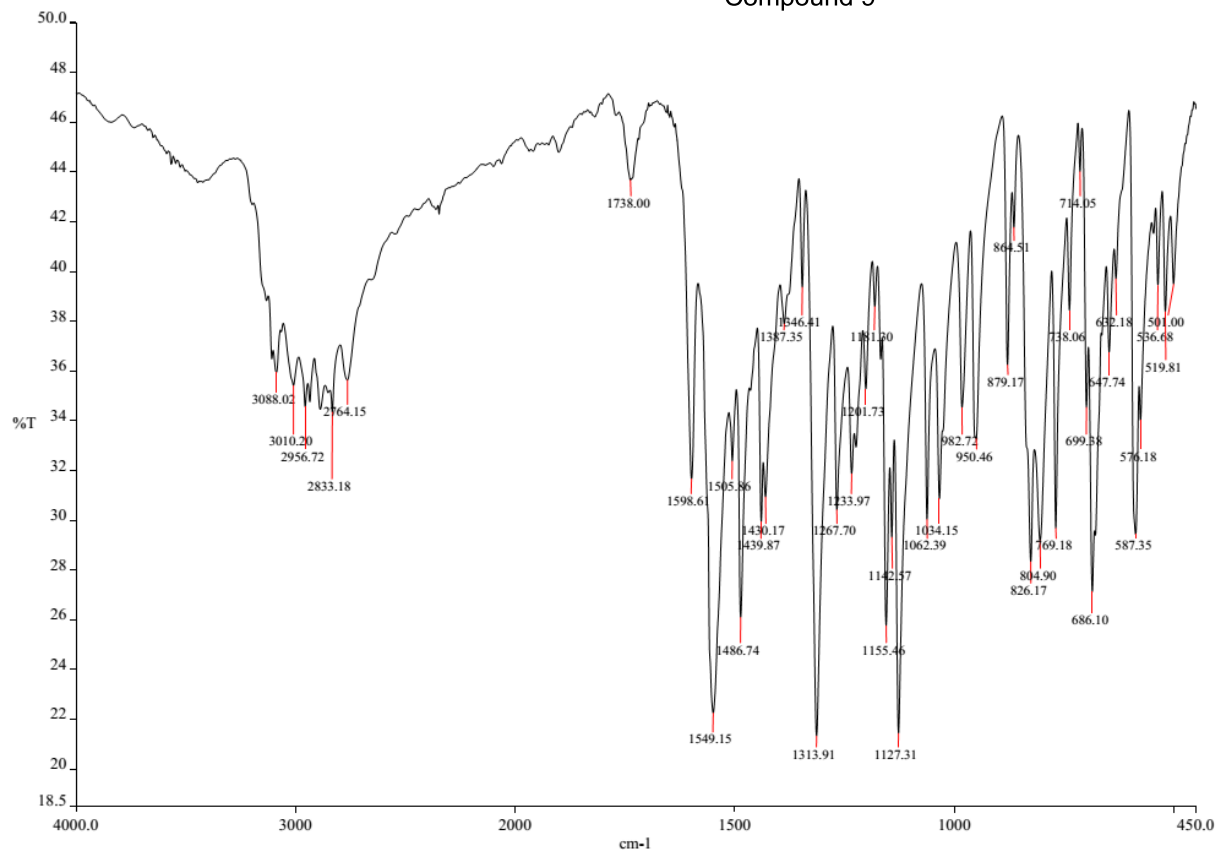


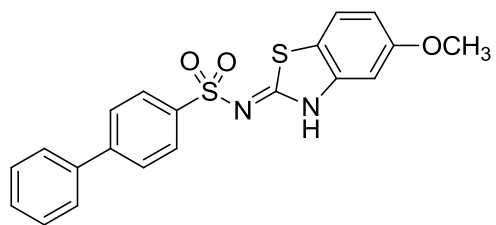
Compound 8



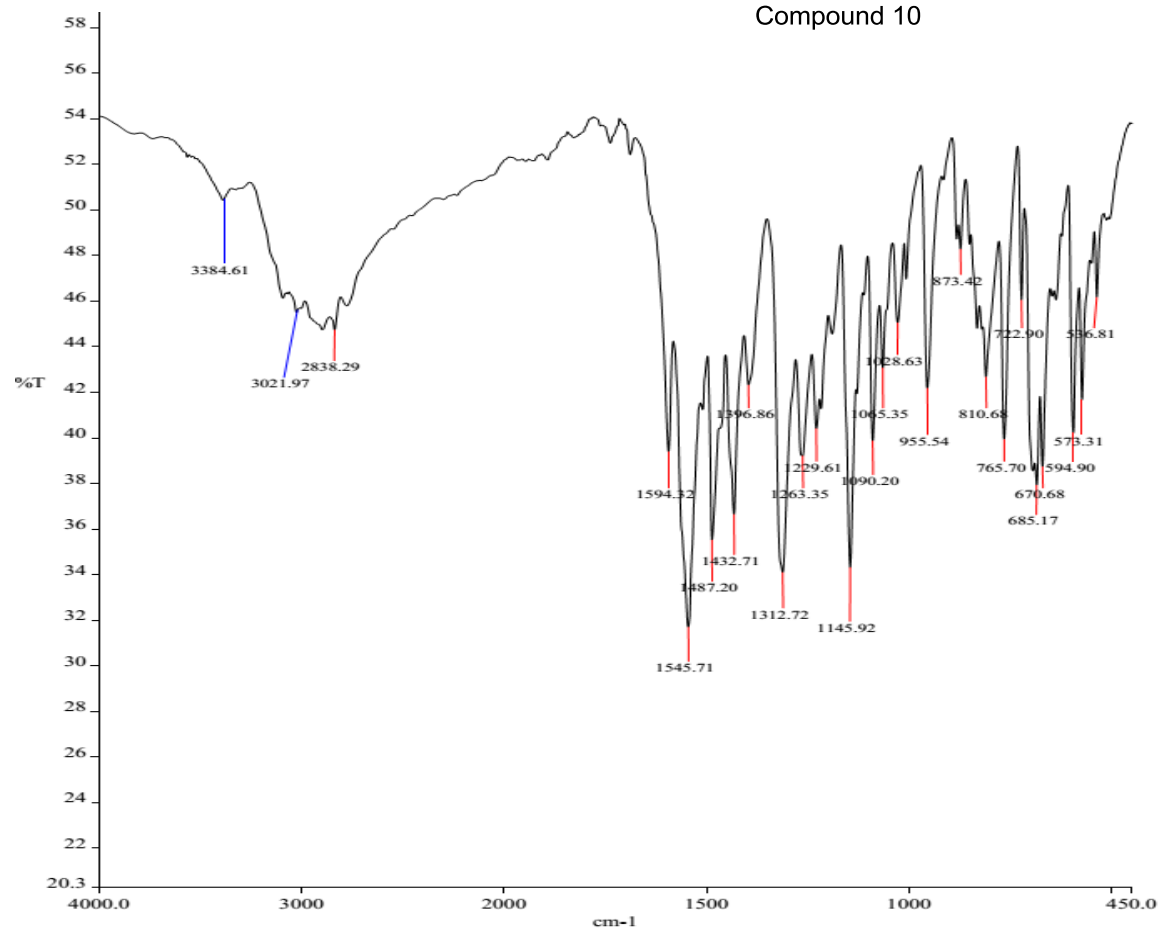


Compound 9

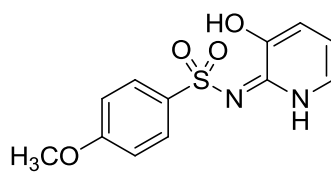




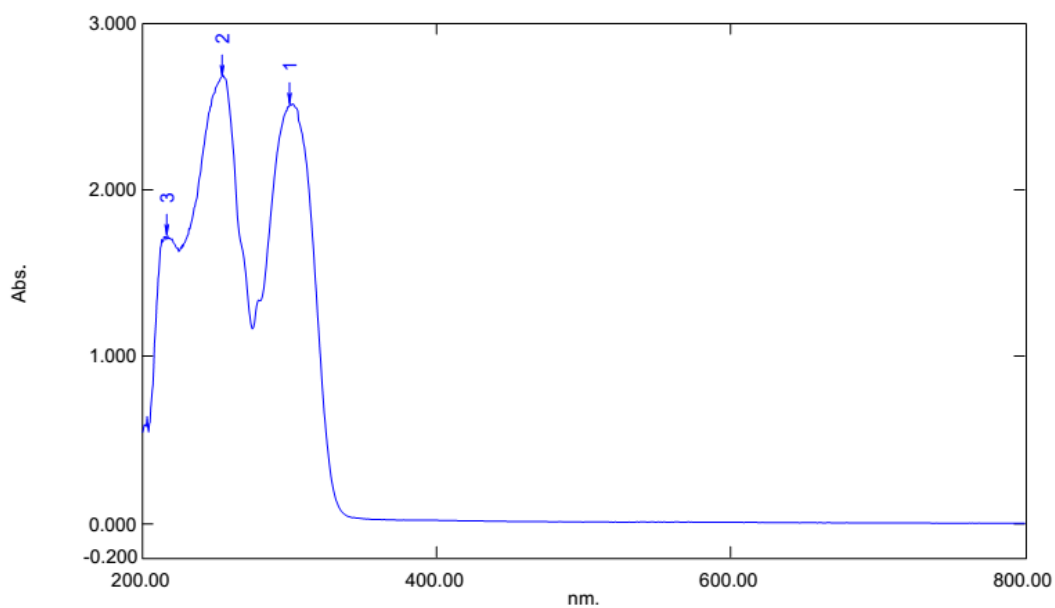
Compound 10



## **UV spectra of compounds 1-10**



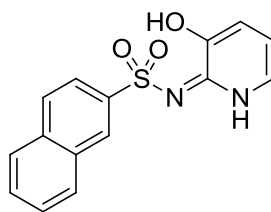
Compound 1



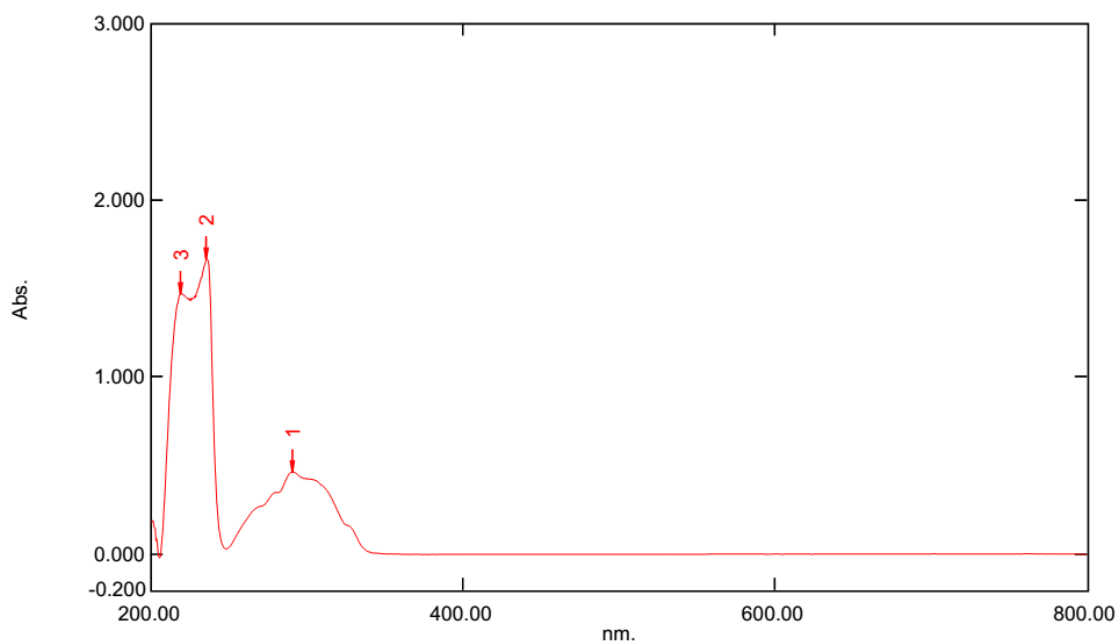
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Wavelength Range (nm.): 200.00 to 800.00  
Scan Speed: Medium  
Sampling Interval: 0.5  
Auto Sampling Interval: Enabled  
Scan Mode: Single

Instrument Properties  
Instrument Type: UV-2400PC Series  
Measuring Mode: Absorbance  
Slit Width: 1.0 nm  
Light Source Change Wavelength: 360.0 nm  
S/R Exchange: Normal

| No. | P/V | Wavelength | Abs.  | Description |
|-----|-----|------------|-------|-------------|
| 1   | 📈   | 300.00     | 2.518 |             |
| 2   | 📈   | 254.50     | 2.690 |             |
| 3   | 📈   | 217.00     | 1.728 |             |



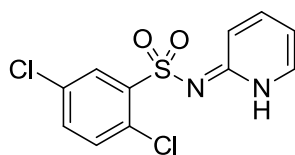
Compound 2



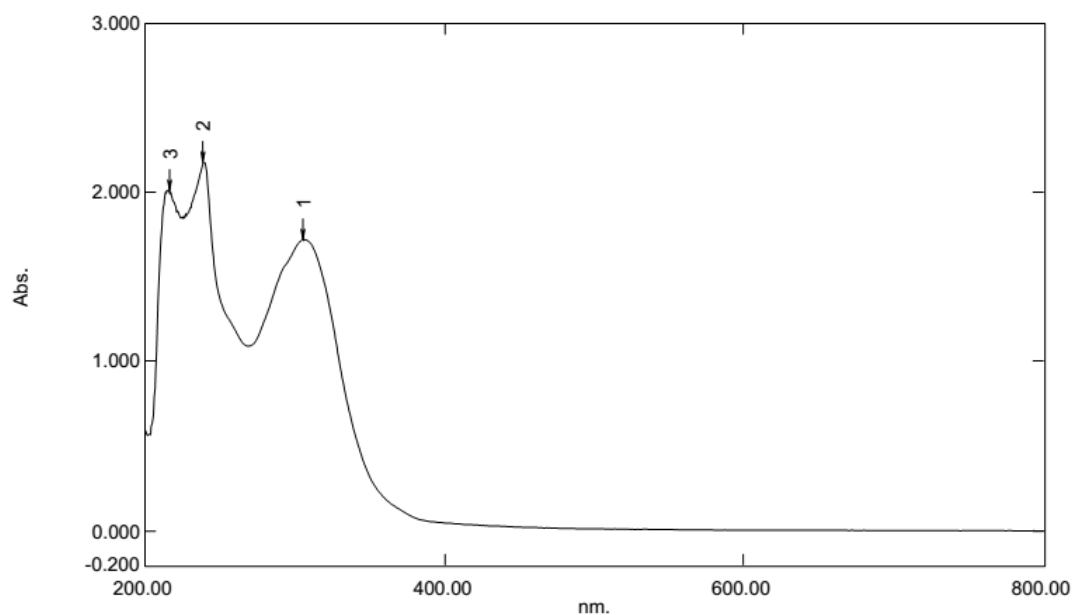
Measurement Properties  
Wavelength Range (nm.): 200.00 to 800.00  
Scan Speed: Medium  
Sampling Interval: 0.5  
Auto Sampling Interval: Enabled  
Scan Mode: Single

| No. | P/V | Wavelength | Abs.  | Description |
|-----|-----|------------|-------|-------------|
| 1   |     | 290.50     | 0.466 |             |
| 2   |     | 235.50     | 1.668 |             |
| 3   |     | 219.00     | 1.475 |             |

Instrument Properties  
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Measuring Mode: Absorbance  
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S/R Exchange: Normal



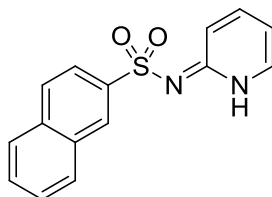
Compound 3



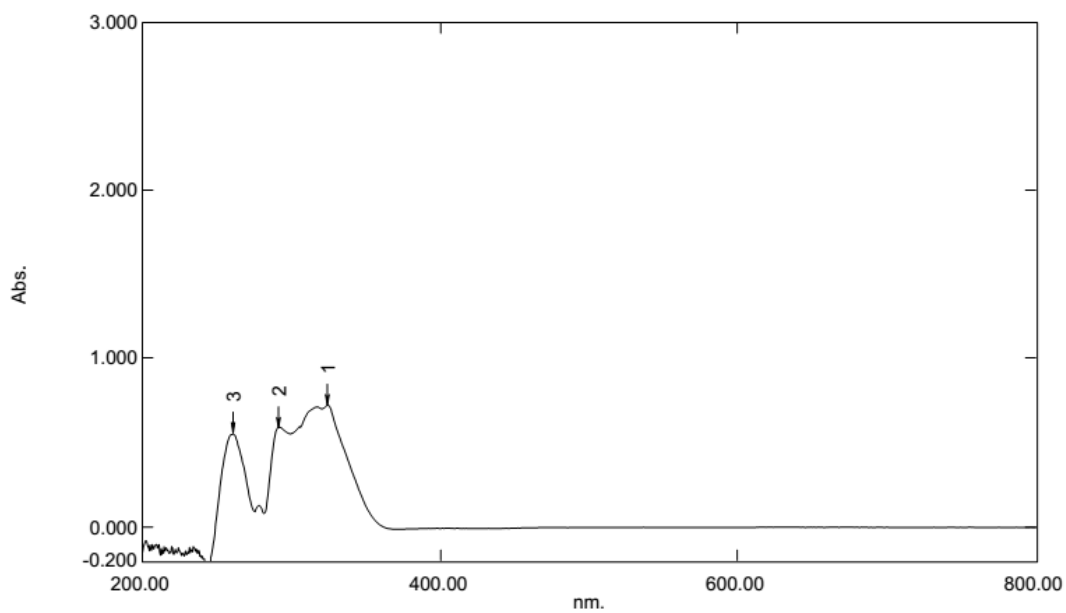
Measurement Properties  
Wavelength Range (nm.): 200.00 to 800.00  
Scan Speed: Medium  
Sampling Interval: 0.5  
Auto Sampling Interval: Enabled  
Scan Mode: Single

| No. | P/V | Wavelength | Abs.  | Description |
|-----|-----|------------|-------|-------------|
| 1   |     | 305.50     | 1.727 |             |
| 2   |     | 239.00     | 2.179 |             |
| 3   |     | 216.00     | 2.017 |             |

Instrument Properties  
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Light Source Change Wavelength: 360.0 nm  
S/R Exchange: Normal



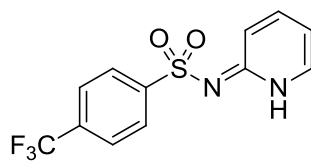
Compound 4



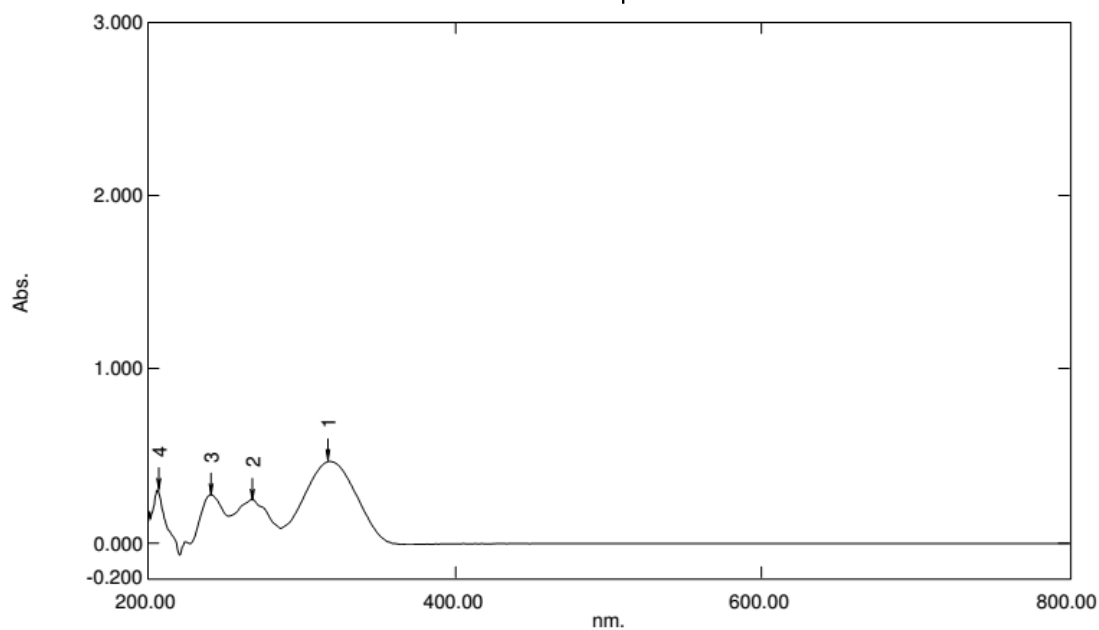
Measurement Properties  
Wavelength Range (nm.): 200.00 to 800.00  
Scan Speed: Medium  
Sampling Interval: 0.5  
Auto Sampling Interval: Enabled  
Scan Mode: Single

| No. | P/V | Wavelength | Abs.  | Description |
|-----|-----|------------|-------|-------------|
| 1   | 📍   | 324.50     | 0.726 |             |
| 2   | 📍   | 291.50     | 0.595 |             |
| 3   | 📍   | 260.50     | 0.554 |             |

Instrument Properties  
Instrument Type: UV-2400PC Series  
Measuring Mode: Absorbance  
Slit Width: 1.0 nm  
Light Source Change Wavelength: 360.0 nm  
S/R Exchange: Normal



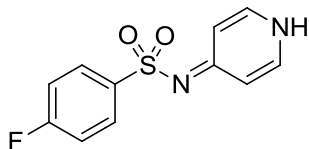
Compound 5



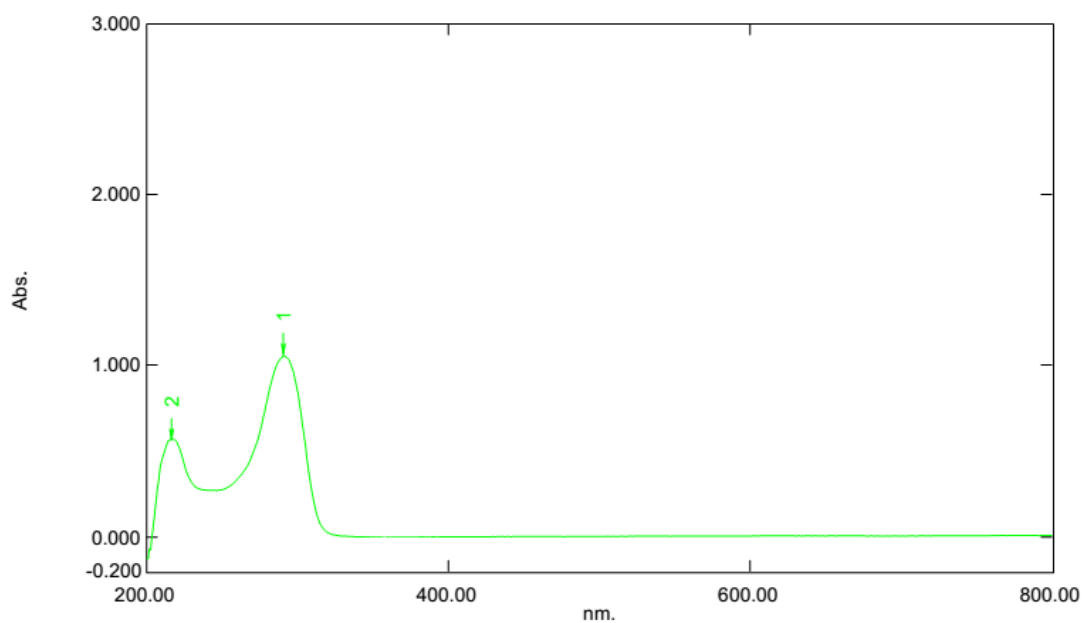
Measurement Properties  
Wavelength Range (nm.): 200.00 to 800.00  
Scan Speed: Medium  
Sampling Interval: 0.5  
Auto Sampling Interval: Enabled  
Scan Mode: Single

| No. | P/V | Wavelength | Abs.  | Description |
|-----|-----|------------|-------|-------------|
| 1   | ⬆   | 317.50     | 0.471 |             |
| 2   | ⬆   | 267.50     | 0.251 |             |
| 3   | ⬆   | 241.50     | 0.278 |             |
| 4   | ⬆   | 206.50     | 0.306 |             |

Instrument Properties  
Instrument Type: UV-2400PC Series  
Measuring Mode: Absorbance  
Slit Width: 1.0 nm  
Light Source Change Wavelength: 360.0 nm  
S/R Exchange: Normal



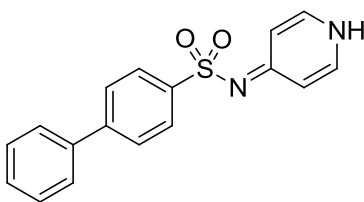
Compound 6



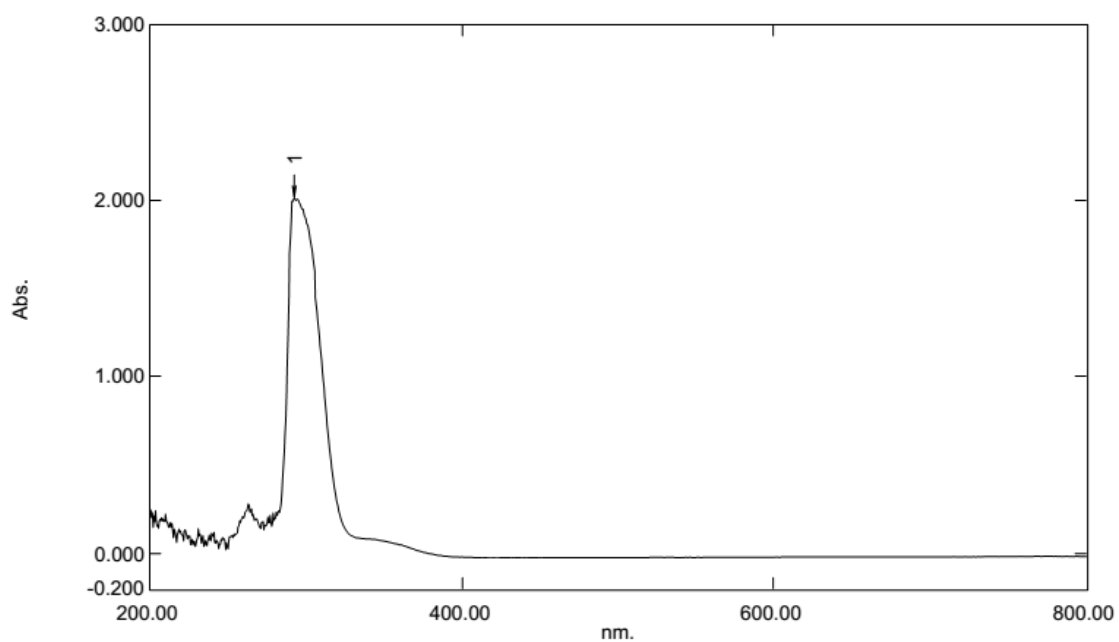
Measurement Properties  
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Scan Speed: Medium  
Sampling Interval: 0.5  
Auto Sampling Interval: Enabled  
Scan Mode: Single

Instrument Properties  
Instrument Type: UV-2400PC Series  
Measuring Mode: Absorbance  
Slit Width: 1.0 nm  
Light Source Change Wavelength: 360.0 nm  
S/R Exchange: Normal

| No. | P/V | Wavelength | Abs.  | Description |
|-----|-----|------------|-------|-------------|
| 1   | ⬆   | 290.50     | 1.063 |             |
| 2   | ⬆   | 216.00     | 0.574 |             |



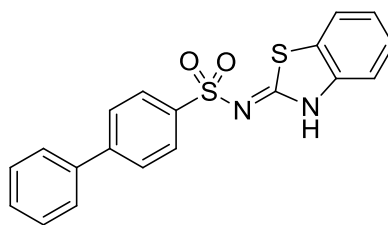
Compound 7



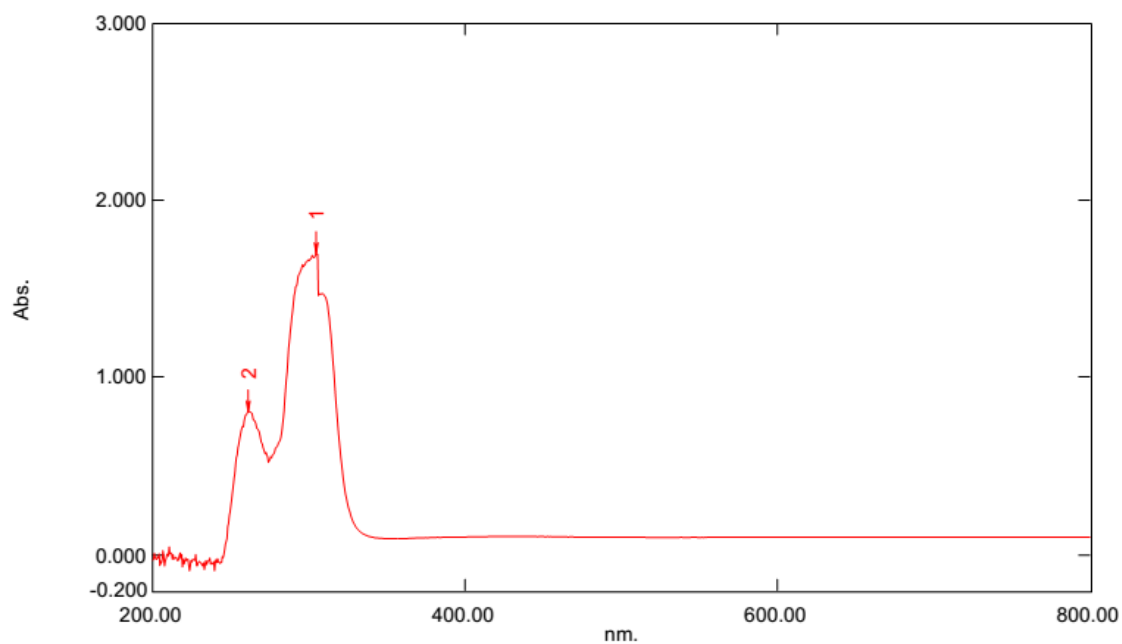
Measurement Properties  
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Scan Speed: Medium  
Sampling Interval: 0.5  
Auto Sampling Interval: Enabled  
Scan Mode: Single

| No. | P/V | Wavelength | Abs.  | Description |
|-----|-----|------------|-------|-------------|
| 1   |     | 292.50     | 2.021 |             |

Instrument Properties  
Instrument Type: UV-2400PC Series  
Measuring Mode: Absorbance  
Slit Width: 1.0 nm  
Light Source Change Wavelength: 360.0 nm  
S/R Exchange: Normal



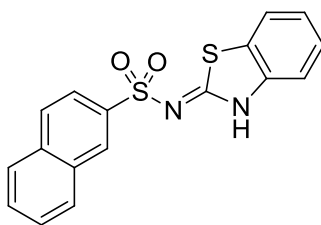
Compound 8



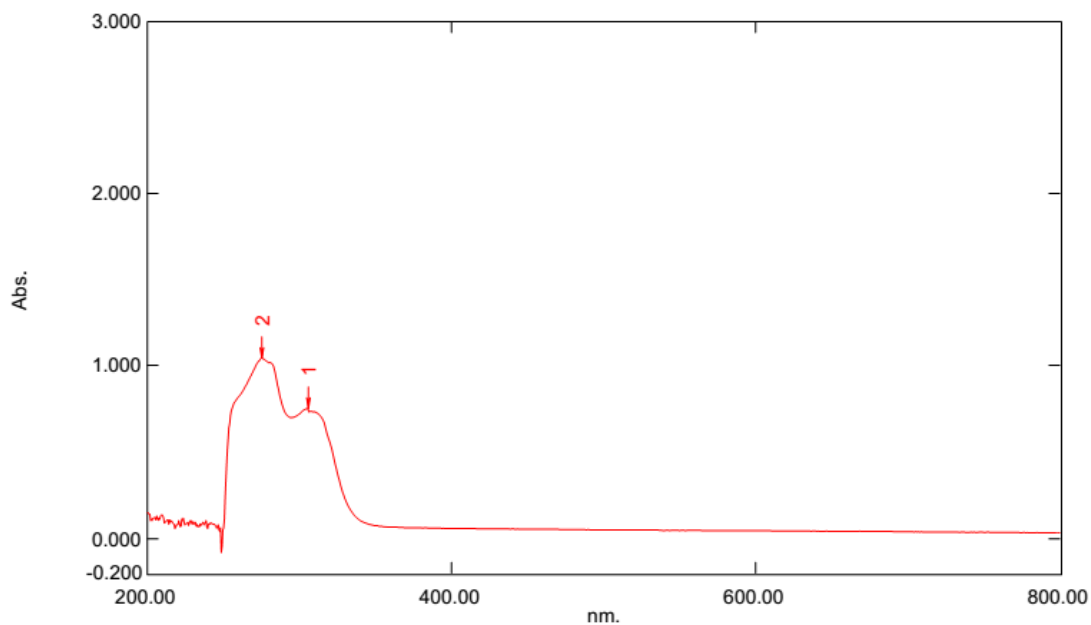
Measurement Properties  
Wavelength Range (nm.): 200.00 to 800.00  
Scan Speed: Medium  
Sampling Interval: 0.5  
Auto Sampling Interval: Enabled  
Scan Mode: Single

| No. | P/V | Wavelength | Abs.  | Description |
|-----|-----|------------|-------|-------------|
| 1   | ⬆   | 304.50     | 1.701 |             |
| 2   | ⬆   | 261.00     | 0.810 |             |

Instrument Properties  
Instrument Type: UV-2400PC Series  
Measuring Mode: Absorbance  
Slit Width: 1.0 nm  
Light Source Change Wavelength: 360.0 nm  
S/R Exchange: Normal



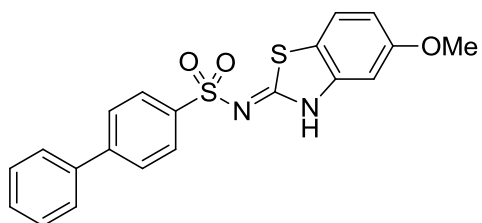
Compound 9



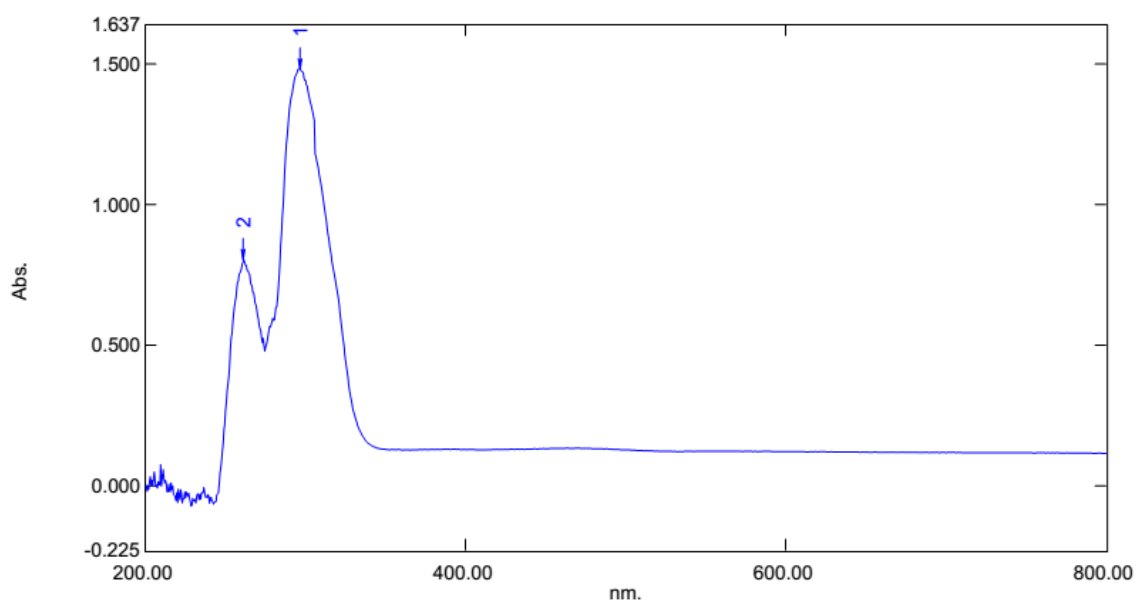
Measurement Properties  
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Scan Speed: Medium  
Sampling Interval: 0.5  
Auto Sampling Interval: Enabled  
Scan Mode: Single

Instrument Properties  
Instrument Type: UV-2400PC Series  
Measuring Mode: Absorbance  
Slit Width: 1.0 nm  
Light Source Change Wavelength: 360.0 nm  
S/R Exchange: Normal

| No. | P/V | Wavelength | Abs.  | Description |
|-----|-----|------------|-------|-------------|
| 1   | 📌   | 305.50     | 0.758 |             |
| 2   | 📌   | 275.00     | 1.049 |             |



Compound 10



Measurement Properties  
Wavelength Range (nm.): 200.00 to 800.00  
Scan Speed: Medium  
Sampling Interval: 0.5  
Auto Sampling Interval: Enabled  
Scan Mode: Single

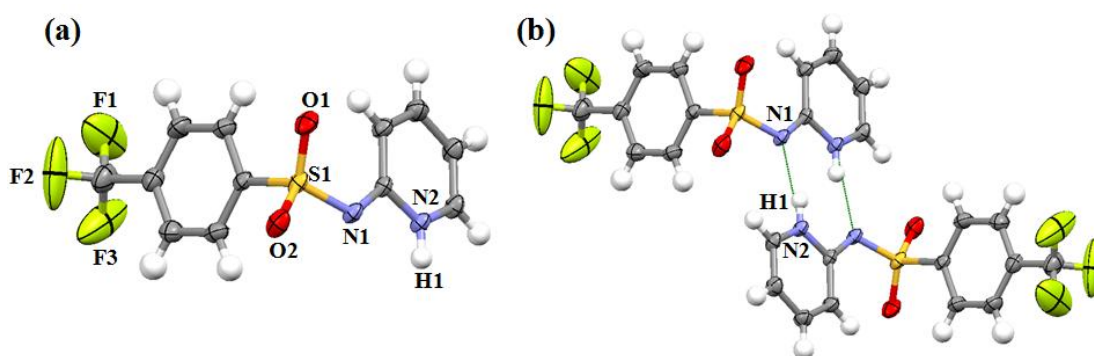
Instrument Properties  
Instrument Type: UV-2400PC Series  
Measuring Mode: Absorbance  
Slit Width: 1.0 nm  
Light Source Change Wavelength: 360.0 nm  
S/R Exchange: Normal

| No. | P/V | Wavelength | Abs.  | Description |
|-----|-----|------------|-------|-------------|
| 1   |     | 296.50     | 1.482 |             |
| 2   |     | 261.50     | 0.805 |             |

## **X-ray crystallography details**

## 2. X-Ray crystallography studies

Single crystals of compound **5** suitable for X-ray structural determination were obtained by slow evaporation of the methanol solution of the compound at room temperature. The X-ray structure of **5** unambiguously confirmed the formation of the compound and reveal the presence of bent structure.\* The sulfur atom (S1) is in a distorted Tetrahedral environment with the Td angles in the range of 105.57(11)- 117.08(14)° (Table S1). Interestingly, the molecule undergoes self-dimerization via N-H...H (2.080Å) hydrogen bonding interactions as shown in Figure (b). In addition the oxygens O1 and O2 are engaged in C-H...O hydrogen bonding interactions with the hydrogens of phenyl rings (Table S2).



**Figure 1.** (a) Crystal structure of compound **5** (b) View of molecular dimer involving the N-H...H hydrogen bonding interactions.

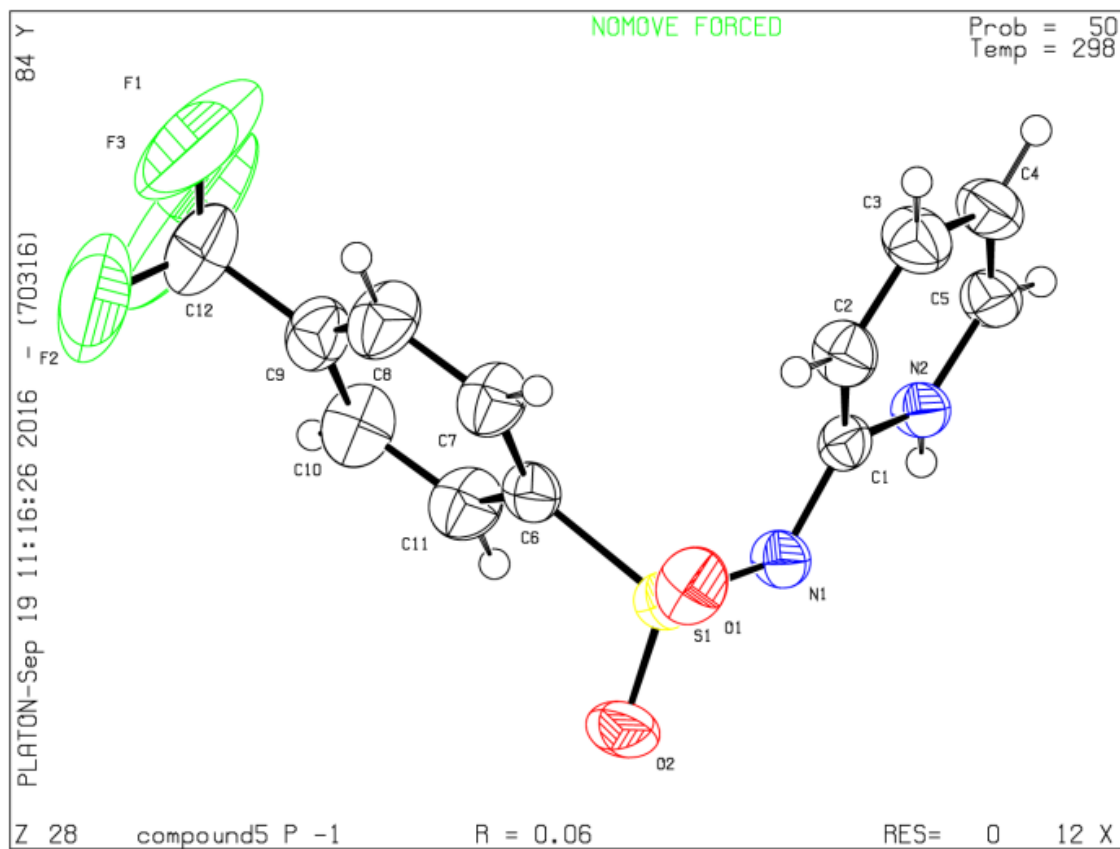
\* **Crystal data for 5:** C<sub>12</sub>H<sub>9</sub>F<sub>3</sub>N<sub>2</sub>O<sub>2</sub>S, M = 302.28, Triclinic, space group P $\bar{1}$ , a = 5.8417(3) Å, b = 8.9060(5) Å, c = 12.8197(7) Å,  $\alpha$  = 86.180(2)°,  $\beta$  = 88.587(2)°,  $\gamma$  = 72.272(2)°, V = 633.87(6) Å<sup>3</sup>, Z = 2, D<sub>c</sub> = 1.584 g/cm<sup>3</sup>,  $\mu$ (Mo-K $\alpha$ ) = 0.295 mm<sup>-1</sup>, T = 298(2) K, 30889 reflections collected. Refinement of 2875 reflections with I > 2 $\sigma$ (I) converged at a final R1 = 0.064, wR2 = 0.1906, GOF = 1.09.

## X-ray crystal structure of **5**

Single crystal X-ray structural data of compound **5** was collected on a CMOS based Bruker D8 Venture PHOTON 100 diffractometer equipped with a INCOATEC micro-focus source with graphite monochromated Mo K $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) operating at 50 kV and 30 mA. The SAINT<sup>1</sup> program was used for integration of diffraction profiles and absorption correction was done with SADABS<sup>2</sup> program. The structure was initially solved by SIR 92<sup>3</sup> and refined by full matrix least square method using SHELXL-2013<sup>4</sup> and WinGX system, Ver 2013.3.<sup>5</sup> The non hydrogen atoms were located from the difference Fourier map and refined anisotropically. The hydrogen atoms were fixed by HFIX and placed in ideal positions and included in the refinement process using riding model with isotropic thermal parameters. The crystallographic information file is deposited with the CCDC No. 1504792.

## References

- (1) SMART (V 5.628), SAINT (V 6.45a), XPREP, SHELXTL; Bruker AXS Inc., Madison, Wisconsin, USA, **2004**.
- (2) Sheldrick, G.M.; *Siemens Area Detector Absorption Correction Program*, University of Göttingen, Göttingen, Germany, **2004**.
- (3) Altomare, A.; Cascarano, G.; Giacovazzo, C.; Guagliardi, A. *J. Appl. Crystallogr.* **1993**, 26, 343-350.
- (4) Sheldrick, G. M.; *SHELXL-2014, Program for Crystal Structure Solution and Refinement*; University of Göttingen, Göttingen, Germany, **2014**.
- (5) Farrugia, L. J. *WinGX-A Windows Program for Crystal Structure Analysis* *J. Appl. Crystallogr.* **2012**, 45, 849-854.



**Figure 2:** ORTEP diagram of **5** with 50% thermal probability ellipsoids.

**Table S1-2.** Selected hydrogen bonding geometry (Å,°) for compound **5**

| D–H···A      | D···H    | H···A    | D···A    | D–H···A               |
|--------------|----------|----------|----------|-----------------------|
| N2--H1...N1  | 0.840(3) | 2.080(3) | 2.900(3) | 164.00 <sup>i</sup>   |
| C2--H2...O1  | 0.9300   | 2.4500   | 3.050(4) | 123.00                |
| C5-- H5...O2 | 0.9300   | 2.5000   | 3.207(3) | 132.00 <sup>ii</sup>  |
| C5-- H5...O2 | 0.9300   | 2.4900   | 3.158(4) | 129.00 <sup>iii</sup> |

Symmetry codes: (i) -x,1-y,-z; (ii) -1+x,1+y,z; (iii) -x,1-y,-z

## **Computational details**

Table SI-1: Dipole moments of Amide (**A**) and Imide (**C**) tautomers of NHAS **1-10**

| Synthesized NHBS | Dipole moment (in debye) |               |
|------------------|--------------------------|---------------|
|                  | Amide form (A)           | Imide form(C) |
| 1                | 6.65                     | 7.15          |
| 2                | 6.04                     | 6.82          |
| 3                | 5.25                     | 7.20          |
| 4                | 5.74                     | 6.52          |
| 5                | 4.00                     | 8.33          |
| 6                | 3.33                     | 8.90          |
| 7                | 5.54                     | 7.74          |
| 8                | 5.82                     | 6.42          |
| 9                | 6.43                     | 7.63          |
| 10               | 6.90                     | 7.76          |

**Table SI-3.** Important geometric parameters in compounds with possible  $(L \rightarrow N \leftarrow L')^+$  interaction. The  $L \rightarrow N$  bond lengths vary between 1.313 to 1.358 Å in these systems.

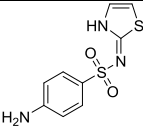
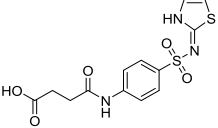
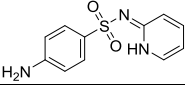
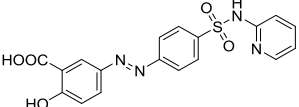
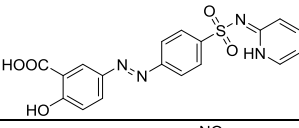
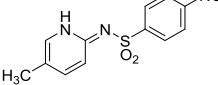
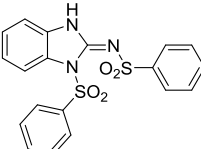
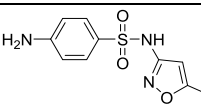
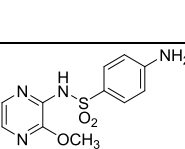
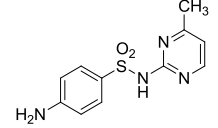
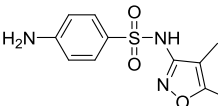
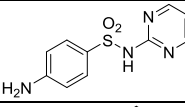
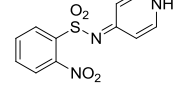
| Sr. No. | Structure in original representation | Structure with possible $(L \rightarrow N \leftarrow L')^+$ representation | Experimental bond lengths (Å) | Bond angle (°)  | CCDC No./DOI No.          | Reference                                              |
|---------|--------------------------------------|----------------------------------------------------------------------------|-------------------------------|-----------------|---------------------------|--------------------------------------------------------|
| 1.      |                                      |                                                                            | N1-C1=1.327<br>N1-C2= 1.332   | C1-N1-C2=122.8  | 10.1107/S0567740877003203 | <i>Acta Cryst.</i> <b>1977</b> , B33, 237.             |
| 2.      |                                      |                                                                            | N1-C1=1.336<br>N1-C2= 1.356   | C1-N1-C2=121.31 | 10.1039/dt9780000989      | <i>J. Chem. Soc., Dalton Trans.</i> <b>1978</b> , 989. |
| 3.      |                                      |                                                                            | N1-C1=1.3367<br>N1-C2= 1.350  | C1-N1-C2=122.17 | 666982                    | <i>J. Mol. Struct.</i> , <b>2010</b> , 966, 23.        |
| 4.      |                                      |                                                                            | N1-C1=1.339<br>N1-C2= 1.342   | C1-N1-C2=123.0  | 205100                    | <i>J. Am. Chem. Soc.</i> <b>2002</b> , 124, 8741.      |
| 5.      |                                      |                                                                            | N1-C1=1.333<br>N1-C2= 1.346   | C1-N1-C2=123.1  | 233144                    | <i>J. Appl. Cryst.</i> <b>2003</b> , 36, 1334.         |
| 6.      |                                      |                                                                            | N1-C1=1.340<br>N1-C2= 1.343   | C1-N1-C2=121.6  | 690394                    | <i>J. Mater. Chem.</i> , <b>2008</b> , 18, 5524.       |

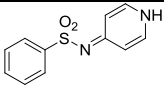
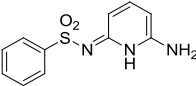
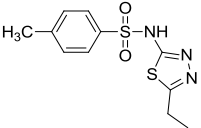
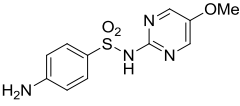
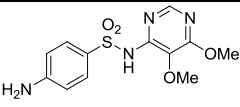
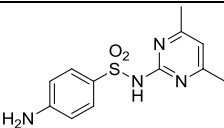
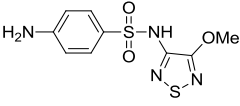
|     |  |  |                               |                  |                                   |                                                                   |
|-----|--|--|-------------------------------|------------------|-----------------------------------|-------------------------------------------------------------------|
| 7.  |  |  | N1-C1=1.332<br>N1-C2= 1.348   | C1-N1-C2=122.2   | 10.1107/S01<br>0827018801<br>4246 | <i>Acta Cryst.</i> <b>1989</b> ,<br>C45, 911.                     |
| 8.  |  |  | N1-C1=1.358<br>N1-C2= 1.333   | C1-N1-C2=121.91  | 745429                            | <i>Crystal Growth &amp;<br/>Design</i> , <b>2004</b> , 4,<br>441. |
| 9.  |  |  | N2-C7=1.335<br>N2-C8= 1.336   | C7-N2-C8=122.1   | 245287                            | <i>Acta Cryst.</i> <b>2004</b> ,<br>E60, o1165.                   |
| 10. |  |  | N7-C13=1.331<br>N7-C14= 1.335 | C13-N7-C14=123.8 | 641812                            | <i>Acta Cryst.</i> <b>2007</b> ,<br>C63, o185.                    |
| 11. |  |  | N2-C7=1.340<br>N2-C8= 1.345   | C7-N2-C8=121.2   | 807381                            | <i>Acta Cryst.</i> <b>2011</b> ,<br>E67, o118-o119.               |
| 12. |  |  | N2-C7=1.324<br>N2-C8= 1.336   | C7-N2-C8=123.37  | 803189                            | <i>Acta Cryst.</i> <b>2010</b> .<br>E66, o3187.                   |

|     |                                        |                                        |                                                                      |                                                |        |                                                   |
|-----|----------------------------------------|----------------------------------------|----------------------------------------------------------------------|------------------------------------------------|--------|---------------------------------------------------|
| 13. | <p>R=CHMe<sub>2</sub></p>              | <p>R=CHMe<sub>2</sub></p>              | N1-C1=1.332<br>N1-C4 1.331                                           | C1-N1-C4=124.9                                 | 729002 | <i>Chem. Eur. J.</i><br><b>2009</b> , 15, 9477.   |
| 14. | <p>R=CH<sub>2</sub>CMe<sub>3</sub></p> | <p>R=CH<sub>2</sub>CMe<sub>3</sub></p> | N1A-C1A=1.333,<br>N1A-C4A= 1.336                                     | C1-N1-C4=126.86                                | 729003 | -do-                                              |
| 15. | <p>R = iPr</p>                         |                                        | N1-C1= 1.332<br>N1-C1= 1.332                                         | C1-N1-C1= 120.47                               | 911773 | <i>Chem. Eur. J.</i><br><b>2013</b> , 19, 3542.   |
| 16. | <p>2 Cl<sup>-</sup></p>                | <p>2 Cl<sup>-</sup></p>                | N10-C12= 1.337<br>N12-C11= 1.341<br>N22-C20= 1.313<br>N22-C21= 1.349 | C10-N12-C11=<br>121.6<br>C21-N22-C20=<br>122.2 | 291494 | <i>Can. J. Chem.</i> ,<br><b>2006</b> , 84, 1426. |
| 17. | <p>2 Cl<sup>-</sup></p>                | <p>2 Cl<sup>-</sup></p>                | N3-C2= 1.320<br>N3-C1= 1.343<br>N8-C10= 1.334<br>N8-C9= 1.340        | C1-N3-C2= 122.4<br>C10-N8-C9= 122.6            | 291495 | -do-                                              |

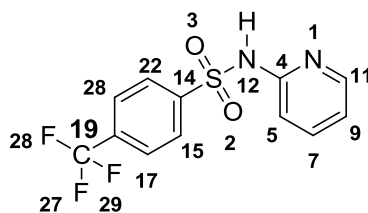
|      |  |  |                                                               |                                     |        |                                                 |
|------|--|--|---------------------------------------------------------------|-------------------------------------|--------|-------------------------------------------------|
| 18.  |  |  | N3-C7= 1.336<br>N3-C8= 1.348<br>N8-C9= 1.336<br>N8-C10= 1.340 | C1-N3-C2= 121.8<br>C10-N8-C9= 123.0 | 291497 | -do-                                            |
| 19.* |  |  | N1-C7=1.384<br>N1-C12= 1.293                                  | C7-N1-C12=<br>119.51                | 979462 | <i>Org. Lett.</i> , <b>2014</b> ,<br>16 , 2790. |

**Table SI-04:** Selected geometrical parameters of 20 examples of NHAS available in literature.

| Sr.No | Structures                                                                          | Tautomeric form | Bond lengths (Å) |             | C-N-S Bond angle (°) | References                                                                     |
|-------|-------------------------------------------------------------------------------------|-----------------|------------------|-------------|----------------------|--------------------------------------------------------------------------------|
|       |                                                                                     |                 | C-N              | S-N         |                      |                                                                                |
| 1.    |    | Imide           | 1.31             | 1.61        | 120.97               | <i>Acta Cryst.</i> <b>1972</b> , B28, 272                                      |
| 2.    |    | Imide           | 1.330            | 1.604       | 120.38               | <i>CrystEngComm</i> , <b>2014</b> , 16, 4706.                                  |
| 3.    |    | Imide           | 1.366            | 1.627       | 124.03               | <i>Acta Cryst.</i> <b>1988</b> , C44, 900.                                     |
| 4.    |    | Amide           | 1.425            | 1.654       | 117.49               | <i>Acta Cryst.</i> <b>2001</b> , C57, 435                                      |
| 5.    |    | Imide           | 1.343            | 1.586       | 120.19               | <i>Acta Cryst.</i> <b>2004</b> , C60, o226.                                    |
| 6.    |   | Imide           | 1.356            | 1.592       | 123.54               | <i>Cryst. Growth Des.</i> , <b>2013</b> , 13, 4002–                            |
| 7.    |  | Imide           | 1.307-1.319      | 1.589-1.599 | 121.6-122.3          | <i>J. Heterocyclic Chem.</i> , <b>1995</b> , 32, 1613.                         |
| 8.    |  | Amide           | 1.388            | 1.653       | 121.06               | <i>Acta Crystallogr., Sec C: Cryst. Struct. Commun.</i> <b>2011</b> , 67, 487. |
| 9.    |  | Amide           | 1.397            | 1.647       | 124.80               | <i>Cryst. Growth Des.</i> , <b>2013</b> , 13, 4002.                            |
| 10.   |  | Amide           | 1.378            | 1.644       | 128.34               | <i>Acta Cryst.</i> <b>2006</b> , E62, o2166.                                   |
| 11.   |  | Amide           | 1.383            | 1.653       | 121.22               | <i>Acta Cryst.</i> <b>1984</b> , C40, 658.                                     |
| 12.   |  | Amide           | 1.380            | 1.650       | 126.04               | <i>Acta Cryst.</i> <b>1995</b> , C51, 333.                                     |
| 13.   |  | Imide           | 1.37             | 1.60        | 122.84               | <i>Acta Cryst.</i> <b>2008</b> , E64, o204.                                    |

|     |                                                                                    |       |      |      |        |                                                      |
|-----|------------------------------------------------------------------------------------|-------|------|------|--------|------------------------------------------------------|
| 14. |   | Imide | 1.33 | 1.57 | 122.21 | <i>Acta Cryst.</i> <b>2007</b> , E63, o3720.         |
| 15. |   | Imide | 1.35 | 1.56 | 120.94 | <i>Angew. Chem. Int. Ed.</i> <b>2003</b> , 42, 1963. |
| 16. |   | Imide | 1.30 | 1.58 | 119.14 | <i>Acta Cryst.</i> <b>2014</b> , C70, 784.           |
| 17. |   | Amide | 1.39 | 1.64 | 126.23 | <i>Supramol. Chem.</i> , <b>1993</b> , 2, 201.       |
| 18. |   | Amide |      |      |        | <i>J. Pharm. Sci.</i> , <b>1972</b> , 61, 872.       |
| 19. |   | Amide | 1.31 | 1.63 | 127.9  | <i>J. Pharm. Sci.</i> , <b>2010</b> , 99, 4042.      |
| 20. |  | Amide | 1.37 | 1.64 | 126.2  | <i>Bull. Korean Chem. Soc.</i> <b>1982</b> , 3, 9.   |

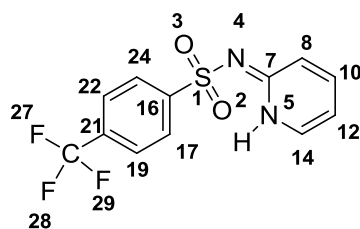
**Table SI-05: NBO charges for sulphonamide 5A**



**5A**

| Atom | Number | NBO charge |
|------|--------|------------|
| N    | 1      | -0.486     |
| N    | 12     | -0.845     |
| S    | 13     | 2.217      |
| O    | 2      | -0.907     |
| O    | 3      | -0.899     |
| C    | 4      | 0.369      |
| C    | 5      | -0.281     |
| C    | 7      | -0.148     |
| C    | 9      | -0.257     |
| C    | 11     | -0.069     |
| C    | 14     | -0.259     |
| C    | 15     | -0.182     |
| C    | 17     | -0.167     |
| C    | 19     | -0.125     |
| C    | 20     | -0.164     |
| C    | 22     | -0.182     |
| C    | 26     | 1.067      |
| F    | 27     | -0.353     |
| F    | 28     | -0.354     |
| F    | 29     | -0.354     |

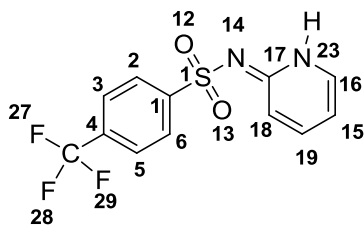
**Table SI-06: NBO charges for sulphonamide 5B**



**5B**

| Atom | Number | NBO charge |
|------|--------|------------|
| N    | 4      | -0.825     |
| N    | 5      | -0.542     |
| S    | 1      | 2.189      |
| O    | 2      | -0.978     |
| O    | 3      | -0.899     |
| C    | 7      | 0.429      |
| C    | 8      | -0.229     |
| C    | 10     | -0.140     |
| C    | 12     | -0.287     |
| C    | 14     | -0.082     |
| C    | 16     | -0.237     |
| C    | 17     | -0.174     |
| C    | 19     | -0.168     |
| C    | 21     | -0.133     |
| C    | 22     | -0.170     |
| C    | 24     | -0.187     |
| C    | 26     | 1.067      |
| F    | 27     | -0.356     |
| F    | 28     | -0.356     |
| F    | 29     | -0.355     |

**Table SI-07: NBO charges for sulphonamide 5C**



**5C**

| Atom | Number | NBO charge |
|------|--------|------------|
| N    | 14     | -0.840     |
| N    | 23     | -0.514     |
| S    | 11     | 2.187      |
| O    | 12     | -0.917     |
| O    | 13     | -0.936     |
| C    | 1      | -0.233     |
| C    | 2      | -0.177     |
| C    | 3      | -0.170     |
| C    | 4      | -0.135     |
| C    | 5      | -0.171     |
| C    | 6      | -0.182     |
| C    | 15     | -0.291     |
| C    | 16     | 0.078      |
| C    | 17     | 0.439      |
| C    | 18     | -0.259     |
| C    | 19     | -0.129     |
| C    | 26     | 1.067      |
| F    | 27     | -0.356     |
| F    | 28     | -0.355     |
| F    | 29     | -0.357     |

## Molecular orbital analysis

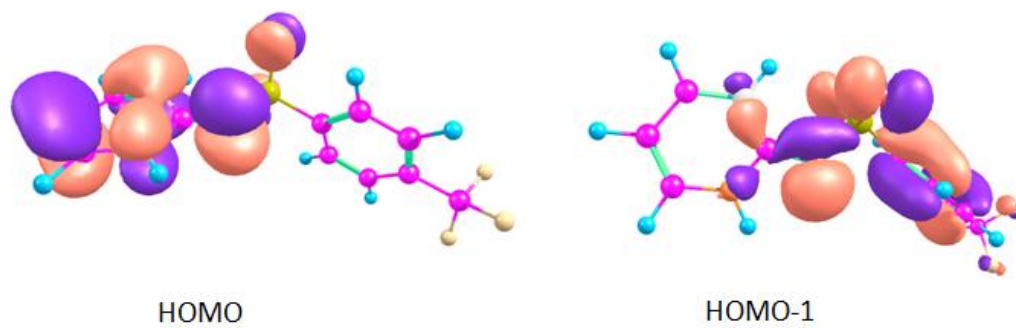


Figure SI-1: Molecular Orbital Analysis of **5B**

**Table SI-8: List of absolute (in Hartrees) and relative Gibbs free energies ( $\Delta G_T$ , in kcal/mol) of 1-10 and their imide tautomers (C) calculated at B3LYP/6- 311++G(d,p) level.**

| Entry | Compound | Absolute Gibbs Free Energy<br>(Gas-Phase) | $\Delta G_T$<br>(Gas) | Absolute Gibbs Free Energy<br>(DMSO, $\epsilon = 46.7$ ) | $\Delta G_T$<br>(DMSO) | $\Delta G_T$<br>(Water) |
|-------|----------|-------------------------------------------|-----------------------|----------------------------------------------------------|------------------------|-------------------------|
| 1.    | 1_Amide  | -1273.101185                              | 6.00                  | -1273.111585                                             | 2.39                   | 2.38                    |
|       | 1_Imide  | -1273.091631                              |                       | -1272.111585                                             |                        |                         |
| 2.    | 2_Amide  | -1312.206374                              | 5.47                  | -1312.215868                                             | 1.26                   | 1.25                    |
|       | 2_Imide  | -1312.197643                              |                       | -1312.213855                                             |                        |                         |
| 3.    | 3_Amide  | -2002.582104                              | 5.26                  | -2002.59543                                              | -0.61                  | -0.74                   |
|       | 3_Imide  | -2002.573711                              |                       | -2002.596406                                             |                        |                         |
| 4.    | 4_Amide  | -1236.958824                              | 4.93                  | -1236.974229                                             | -0.14                  | -0.23                   |
|       | 4_Imide  | -1236.950963                              |                       | -1236.97446                                              |                        |                         |
| 5.    | 5_Amide  | -1420.47305                               | 4.77                  | -1420.487871                                             | -0.87                  | -0.96                   |
|       | 5_Imide  | -1420.465445                              |                       | -1420.489271                                             |                        |                         |
| 6.    | 6_Amide  | -1182.593587                              | 4.19                  | -1182.611112                                             | -0.74                  | -0.81                   |
|       | 6_Imide  | -1182.586897                              |                       | -1182.612304                                             |                        |                         |
| 7.    | 7_Amide  | -1314.355285                              | 5.12                  | -1314.373406                                             | -0.39                  | -3.06                   |
|       | 7_Imide  | -1314.347122                              |                       | -1314.374034                                             |                        |                         |
| 8.    | 8_Amide  | -1788.804803                              | -1.18                 | -1788.820704                                             | -4.59                  | -4.60                   |
|       | 8_Imide  | -1788.806684                              |                       | -1788.828031                                             |                        |                         |
| 9.    | 9_Amide  | -1825.920063                              | -2.24                 | -1825.937171                                             | -5.50                  | -5.58                   |
|       | 9_Imide  | -1825.927316                              |                       | -1825.94594                                              |                        |                         |
| 10.   | 10_Amide | -1903.330734                              | -0.89                 | -1903.349025                                             | -4.31                  | -4.37                   |
|       | 10_Imide | -1903.332163                              |                       | -1903.3559                                               |                        |                         |

**Table SI-9: List of absolute (in Hartrees) and relative Gibbs free energies ( $\Delta G_T$ , in kcal/mol) of Sulfonamides (given in Table 2) and their imide tautomers calculated at B3LYP/6- 311+G(d,p) level.**

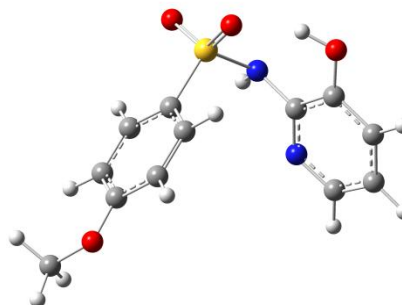
| Entry | Sulfonamides              | Absolute Gibbs Free Energy | $\Delta G_T$ |
|-------|---------------------------|----------------------------|--------------|
| 1.    | Sulfathiazole_Amide       | -1459.484256               | -0.33        |
|       | Sulfathiazole_Imide       | -1459.484256               |              |
| 2.    | Sulfapyridine_Amide       | -1138.68962                | 6.83         |
|       | Sulfapyridine_Imide       | -1138.678722               |              |
| 3.    | Molecule VI_Amide         | -1138.696077               | 9.38         |
|       | Molecule VI_Imide         | -1138.681115               |              |
| 4.    | TMBS_Amide                | -1538.063786               | -4.22        |
|       | TMBS_Imide                | -1538.063786               |              |
| 5.    | Sulfadiazine_Amide        | -1154.74716                | 12.66        |
|       | Sulfadiazine_Imide        | -1154.72697                |              |
| 6.    | Sulfamethoxazole_Amide    | -1154.72697                | 10.59        |
|       | Sulfamethoxazole_Imide    | -1175.758925               |              |
| 7.    | Sulfamethoxydiazine_Amide | -1269.270288               | 15.16        |
|       | Sulfamethoxydiazine_Imide | -1269.246117               |              |
| 8.    | Sulfadoxine_Amide         | -1383.8007                 | 17.71        |
|       | Sulfadoxine_Imide         | -1383.783864               |              |
| 9.    | Sulfamethazine_Amide      | -1233.363341               | 12.0         |
|       | Sulfamethazine_Imide      | -1233.34421                |              |
| 10.   | Sulfametrole_Amide        | -1574.003623               | 15.67        |
|       | Sulfametrole_Imide        | -1574.003623               |              |
| 11.   | Sulfalene_Amide           | -1269.236993               | 14.28        |
|       | Sulfalene_Imide           | -1269.251428               |              |
| 12.   | Sulfamethiazole_Amide     | -1514.829121               | -3.15        |
|       | Sulfamethiazole_Imide     | -1514.834155               |              |

**Cartesian coordinates of all the optimized structures of all the possible isomers (tautomers)  
of NHAS 1-10 at B3LYP/6-311++G(d,p) level of theory**

**Compound\_1A\_AMIDE**

0 1

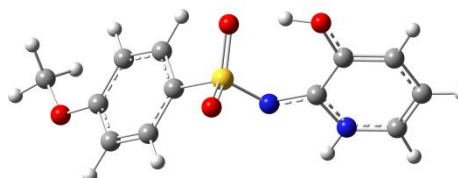
|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -1.77406700 | 1.30419400  | -1.47103000 |
| O | -1.17730400 | -2.07635900 | 1.19920300  |
| O | -0.26725200 | -3.03527300 | -0.98746700 |
| C | -2.10293600 | 0.33863500  | -0.61595800 |
| C | -2.90602800 | 0.56059600  | 0.52390800  |
| C | -3.36036800 | 1.86454600  | 0.73102100  |
| H | -3.98748500 | 2.05659900  | 1.59350000  |
| C | -3.02237000 | 2.86725300  | -0.16765000 |
| H | -3.37202500 | 3.88251300  | -0.02427100 |
| C | -2.22720400 | 2.54117900  | -1.26307100 |
| N | -1.69054200 | -0.97344500 | -1.00420400 |
| S | -0.56544100 | -1.90009500 | -0.12616900 |
| C | 0.92135300  | -0.93931300 | 0.10219400  |
| C | 1.06988000  | -0.13953300 | 1.24011400  |
| H | 0.30278600  | -0.13220400 | 2.00350500  |
| C | 2.21705900  | 0.61919400  | 1.39040700  |
| H | 2.36440300  | 1.24360000  | 2.26271800  |
| C | 3.22200500  | 0.58371600  | 0.41158600  |
| C | 3.07011700  | -0.22813700 | -0.71973300 |
| H | 3.83964800  | -0.28137400 | -1.47712700 |
| C | 1.91578800  | -0.99081200 | -0.86981900 |
| H | 1.79897500  | -1.63561700 | -1.73196100 |
| H | -1.41971800 | -0.97243800 | -1.98441700 |
| H | -1.94564700 | 3.28727800  | -1.99857600 |
| O | -3.30052600 | -0.39230200 | 1.39298000  |
| H | -2.72141200 | -1.17743800 | 1.34289700  |
| O | 4.30333500  | 1.36312700  | 0.65422400  |
| C | 5.37133900  | 1.37996100  | -0.29009800 |
| H | 5.03172500  | 1.74118800  | -1.26585200 |
| H | 6.10990500  | 2.06923600  | 0.11409600  |
| H | 5.82033900  | 0.38766000  | -0.39810100 |



**Compound\_1C\_IMIDE**

0 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| S | -0.29402600 | -1.09592700 | 0.37976300  |
| O | -0.43854800 | -1.82982800 | 1.63890800  |
| O | -0.57105400 | -1.84590800 | -0.88133900 |
| N | -1.12418000 | 0.31022500  | 0.42808900  |
| C | 1.38444800  | -0.49852300 | 0.25777400  |
| C | 1.98042100  | -0.36030700 | -0.98858800 |
| C | 3.28969200  | 0.10941700  | -1.08302900 |
| C | 3.99199500  | 0.43913200  | 0.08114600  |
| C | 3.38115400  | 0.28883500  | 1.33524200  |
| C | 2.08223900  | -0.18068600 | 1.42525200  |
| C | -2.39964100 | 0.49979900  | 0.12561700  |
| N | -2.84729400 | 1.75921400  | 0.46764200  |
| C | -4.10050000 | 2.26297900  | 0.28333100  |

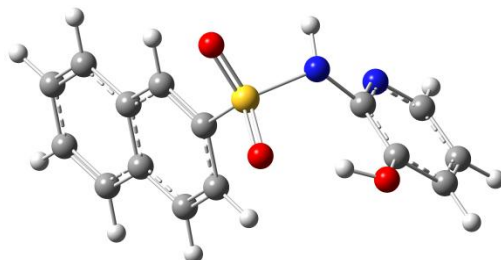


|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -5.04604700 | 1.47381500  | -0.29639800 |
| C | -4.67802400 | 0.17045000  | -0.69377100 |
| C | -3.40653900 | -0.33412000 | -0.51390400 |
| H | 1.43100800  | -0.63287900 | -1.88066000 |
| H | 3.94992600  | 0.53781100  | 2.22262400  |
| H | 1.61046600  | -0.31737400 | 2.39015200  |
| H | -2.13658500 | 2.32502800  | 0.91504200  |
| H | -4.26222400 | 3.27640100  | 0.62115100  |
| H | -6.04945900 | 1.84304800  | -0.45359700 |
| H | -5.39981500 | -0.48259500 | -1.16974400 |
| O | -3.17141200 | -1.58889900 | -0.91678100 |
| H | -2.20454800 | -1.80174800 | -0.98268500 |
| H | 3.74645000  | 0.20423200  | -2.05846000 |
| O | 5.26910300  | 0.90397300  | 0.10208700  |
| C | 5.96151000  | 1.06772200  | -1.13088100 |
| H | 5.45788200  | 1.79432200  | -1.77686800 |
| H | 6.94890500  | 1.44227900  | -0.86743500 |
| H | 6.06377200  | 0.11445100  | -1.65958000 |

# Compound\_2A\_AMIDE

0 1

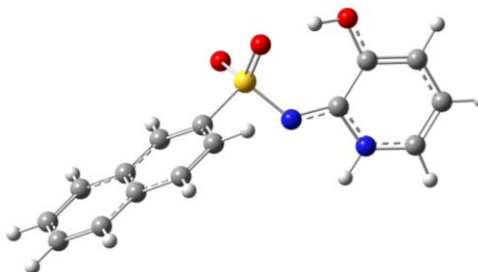
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|---|-------------|-------------|-------------|
| N | -2.03734500 | 1.25991800  | -1.50930100 |
| O | -1.52328400 | -2.00165900 | 1.27046000  |
| O | -0.41564800 | -3.02676200 | -0.79142000 |
| C | -2.40896900 | 0.28353900  | -0.68514100 |
| C | -3.34791500 | 0.46704700  | 0.35309300  |
| C | -3.89254300 | 1.74535900  | 0.49142500  |
| H | -4.62339100 | 1.90780600  | 1.27467300  |
| C | -3.50772800 | 2.75994100  | -0.37446800 |
| H | -3.92513700 | 3.75548900  | -0.28356100 |
| C | -2.57642000 | 2.47166900  | -1.36870400 |
| N | -1.88742900 | -1.00825400 | -1.00972900 |
| S | -0.81504900 | -1.86584300 | -0.01028400 |
| C | 0.63059300  | -0.84805500 | 0.29208900  |
| C | 0.59784700  | 0.10959700  | 1.33361600  |
| H | -0.27975900 | 0.19627800  | 1.96027500  |
| C | 1.70198700  | 0.89552500  | 1.54715600  |
| H | 1.69568700  | 1.63018500  | 2.34495200  |
| C | 2.86956500  | 0.75717300  | 0.75026000  |
| C | 2.88811900  | -0.22443200 | -0.29134500 |
| C | 1.73735600  | -1.02378000 | -0.50312100 |
| H | 1.73961700  | -1.78211600 | -1.27709500 |
| H | -1.52464400 | -1.00586200 | -1.95993500 |
| H | -2.25297600 | 3.22787500  | -2.07604300 |
| C | 4.05981100  | -0.37637500 | -1.07866100 |
| H | 4.06971200  | -1.12381500 | -1.86452300 |
| C | 5.16185600  | 0.41113300  | -0.85019000 |
| H | 6.05186600  | 0.28994100  | -1.45680200 |
| C | 5.14385300  | 1.38349200  | 0.17795900  |
| H | 6.02124000  | 1.99712700  | 0.34778600  |
| C | 4.02589300  | 1.55193000  | 0.95959800  |
| H | 4.01481000  | 2.29556000  | 1.74919300  |
| O | -3.78825500 | -0.50107400 | 1.18261700  |
| H | -3.15514800 | -1.24325100 | 1.22418000  |



## Compound\_2C\_IMIDE

O 1

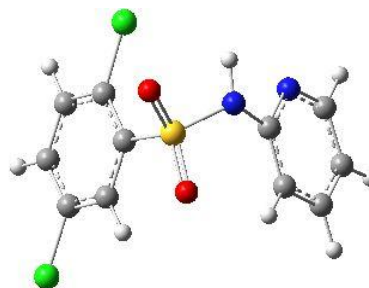
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| S | -0.60671700 | -1.05746200 | -0.23544500 |
| O | -1.04959900 | -1.91429200 | 0.90381800  |
| O | -0.55625700 | -1.68753300 | -1.55679200 |
| N | -1.43005200 | 0.34894400  | -0.27188300 |
| C | 1.03462100  | -0.46518600 | 0.17593000  |
| C | 1.99567000  | -0.46722700 | -0.80111900 |
| C | 3.30673000  | -0.01422000 | -0.50045800 |
| C | 3.59850100  | 0.43637300  | 0.82546800  |
| C | 2.56682400  | 0.41243100  | 1.80369700  |
| C | 1.30680800  | -0.03128900 | 1.49464100  |
| C | -2.74225600 | 0.51195700  | -0.16830500 |
| N | -3.14829700 | 1.78806300  | -0.49461300 |
| C | -4.42168100 | 2.27360000  | -0.47487100 |
| C | -5.43432200 | 1.44238700  | -0.10359800 |
| C | -5.11411300 | 0.11756400  | 0.26017600  |
| C | -3.82189500 | -0.36792600 | 0.24929500  |
| H | 1.75410400  | -0.82023500 | -1.79660500 |
| H | 2.79259700  | 0.74459800  | 2.81138000  |
| H | 0.52692700  | -0.06700800 | 2.24440000  |
| H | -2.38448500 | 2.38496500  | -0.78805200 |
| H | -4.54388200 | 3.30665200  | -0.76651400 |
| H | -6.45532200 | 1.79590600  | -0.08155600 |
| H | -5.89137300 | -0.56837000 | 0.57533000  |
| C | 4.33604400  | 0.00136800  | -1.47724500 |
| H | 4.11052600  | -0.34421500 | -2.48038100 |
| C | 5.59757300  | 0.44452300  | -1.15896300 |
| H | 6.37737200  | 0.45201900  | -1.91194400 |
| C | 5.88680800  | 0.89121100  | 0.15159500  |
| H | 6.88621700  | 1.23719700  | 0.39021700  |
| C | 4.91094100  | 0.88629600  | 1.12038500  |
| H | 5.13445900  | 1.22692900  | 2.12588400  |
| O | -3.63253500 | -1.64287000 | 0.60794000  |
| H | -2.68161800 | -1.86172700 | 0.79092600  |



## Compound\_3A\_AMIDE

O 1

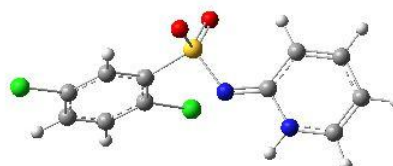
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|----|-------------|-------------|-------------|
| N  | -2.91769100 | -0.01784400 | -1.08772200 |
| O  | -0.33977700 | -0.03168300 | 2.52668500  |
| O  | -0.14699400 | -2.46310800 | 1.81486900  |
| C  | -2.35497700 | 0.19344900  | 0.10174300  |
| C  | -2.35861700 | 1.43304800  | 0.75146800  |
| H  | -1.91600400 | 1.54067000  | 1.73132200  |
| C  | -2.96235200 | 2.49801300  | 0.09593900  |
| H  | -2.98255200 | 3.47562000  | 0.56403400  |
| C  | -3.55755800 | 2.29505800  | -1.14854100 |
| H  | -4.04562600 | 3.10151900  | -1.68128000 |
| C  | -3.51717300 | 1.01454000  | -1.68871300 |
| N  | -1.80709700 | -0.97684300 | 0.68718500  |
| S  | -0.33146600 | -1.05906300 | 1.49378200  |
| C  | 0.94481700  | -0.55117000 | 0.30039100  |
| C  | 1.69676000  | 0.57404700  | 0.63871500  |
| H  | 1.48334100  | 1.09602600  | 1.56136300  |
| C  | 2.71163300  | 0.99866500  | -0.20947300 |
| C  | 2.98541300  | 0.31851100  | -1.39148200 |
| C  | 2.23136200  | -0.80070100 | -1.72591500 |
| H  | 2.43211900  | -1.33835200 | -2.64359000 |
| C  | 1.21143600  | -1.24203000 | -0.88674300 |
| H  | -1.94690600 | -1.79145000 | 0.09594800  |
| H  | -3.97733700 | 0.80007000  | -2.64850400 |
| H  | 3.77814800  | 0.65723800  | -2.04592700 |
| Cl | 0.30170900  | -2.65115900 | -1.38093200 |
| Cl | 3.65485000  | 2.41211400  | 0.21699800  |



## Compound\_3C\_IMIDE

O 1

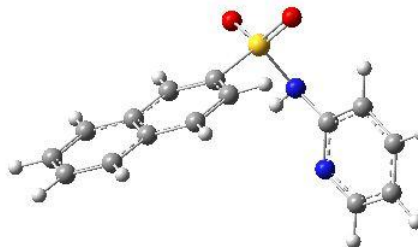
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|---|-------------|-------------|-------------|
| S | -0.24712500 | -0.86371300 | -0.71392000 |
| O | 0.04922200  | -2.29416500 | -0.59723600 |
| O | -0.68480200 | -0.36109900 | -2.02247700 |
| N | -1.22103700 | -0.39275600 | 0.52895700  |
| C | 1.27582600  | 0.00951300  | -0.24600400 |
| C | 1.40014200  | 1.40149100  | -0.20801900 |
| C | 2.62733200  | 1.97687200  | 0.11322600  |
| C | 3.72950900  | 1.17731600  | 0.39588800  |
| C | 3.59405000  | -0.20585600 | 0.35582400  |
| C | 2.37702300  | -0.79556900 | 0.03895500  |
| C | -2.52740700 | -0.32552300 | 0.40739300  |
| N | -3.18564500 | 0.04503900  | 1.57002300  |
| C | -4.53393800 | 0.17347500  | 1.70070200  |
| C | -5.35134300 | -0.06135100 | 0.63732000  |
| C | -4.74515900 | -0.43512600 | -0.59202700 |
| C | -3.39004200 | -0.56552900 | -0.71773100 |
| H | 2.71605900  | 3.05535800  | 0.14056000  |
| H | 2.26248300  | -1.87087500 | 0.00610600  |
| H | -2.57853600 | 0.21326500  | 2.36267300  |
| H | -4.88753000 | 0.46437700  | 2.68079600  |
| H | -6.42251600 | 0.03829800  | 0.73684100  |
| H | -5.37285700 | -0.62194100 | -1.45630300 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -2.93309000 | -0.83308900 | -1.65853300 |
| H  | 4.68226500  | 1.62753500  | 0.64302800  |
| Cl | 0.06160400  | 2.47714500  | -0.54280500 |
| Cl | 4.97858300  | -1.22277200 | 0.71452400  |

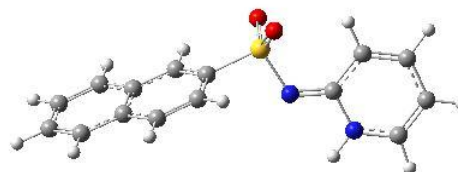
#### Compound\_4A\_AMIDE

|   |             |             |             |
|---|-------------|-------------|-------------|
| 0 | 1           |             |             |
| N | 2.61517000  | -1.04103500 | -1.55171500 |
| O | 1.60939300  | 2.00416700  | 1.47526600  |
| O | 0.55287200  | 3.06964500  | -0.59339500 |
| C | 2.65319200  | -0.15563600 | -0.55500800 |
| C | 3.32003800  | -0.38320100 | 0.65574000  |
| H | 3.34485500  | 0.38348800  | 1.41706500  |
| C | 3.94762100  | -1.60972600 | 0.82328800  |
| H | 4.47275300  | -1.82393000 | 1.74737200  |
| C | 3.91768000  | -2.54716500 | -0.20935500 |
| H | 4.40589900  | -3.50911100 | -0.11558100 |
| C | 3.24863300  | -2.20575600 | -1.37913600 |
| N | 2.02370400  | 1.07667700  | -0.85124800 |
| S | 0.95168000  | 1.90036600  | 0.17833700  |
| C | -0.48981700 | 0.84342300  | 0.37845300  |
| C | -0.48354100 | -0.14964700 | 1.38690500  |
| H | 0.36797900  | -0.23839300 | 2.04817700  |
| C | -1.57658800 | -0.96817400 | 1.52286100  |
| H | -1.58845300 | -1.73071200 | 2.29417100  |
| C | -2.70977000 | -0.82893600 | 0.67819100  |
| C | -2.70410900 | 0.18805100  | -0.32892100 |
| C | -1.56567900 | 1.02274300  | -0.45731900 |
| H | -1.55176400 | 1.80868300  | -1.20327700 |
| H | 1.68260800  | 1.09476500  | -1.80825000 |
| H | 3.20826600  | -2.89417400 | -2.21794200 |
| C | -3.84132900 | 0.33868600  | -1.16536400 |
| H | -3.83373000 | 1.11304200  | -1.92483300 |
| C | -4.93235300 | -0.48294900 | -1.01707000 |
| H | -5.79563600 | -0.36172600 | -1.66116500 |
| C | -4.93772300 | -1.49067900 | -0.02342400 |
| H | -5.80578800 | -2.13126300 | 0.08275300  |
| C | -3.85362000 | -1.65878200 | 0.80454400  |
| H | -3.85991900 | -2.43001100 | 1.56758000  |



#### Compound\_4C\_IMIDE

|   |             |             |             |
|---|-------------|-------------|-------------|
| 0 | 1           |             |             |
| S | -0.80288300 | -1.03462000 | 0.26158900  |
| O | -1.21707200 | -1.52303200 | 1.58630400  |
| O | -0.84434700 | -1.97447900 | -0.86701800 |
| N | -1.59885100 | 0.37441900  | -0.12384300 |
| C | 0.87280200  | -0.39985400 | 0.39879200  |
| C | 1.76015100  | -0.64759900 | -0.61577200 |
| C | 3.09183400  | -0.16532300 | -0.52244100 |
| C | 3.48157500  | 0.57643300  | 0.63708500  |
| C | 2.52475700  | 0.80128400  | 1.66425600  |
| C | 1.24398300  | 0.32245800  | 1.55682500  |
| C | -2.90920500 | 0.39039900  | -0.17422200 |

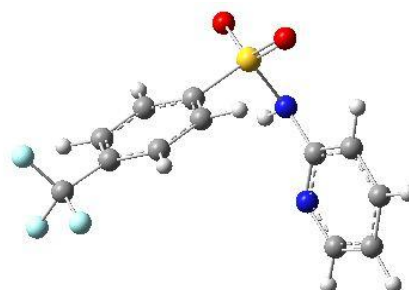


|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -3.46012600 | 1.61020500  | -0.54205800 |
| C | -4.79188800 | 1.86220200  | -0.66815600 |
| C | -5.70290800 | 0.88063300  | -0.42426600 |
| C | -5.21215200 | -0.39666900 | -0.03638000 |
| C | -3.87481400 | -0.64437500 | 0.08865200  |
| H | 1.44389300  | -1.21689000 | -1.48182800 |
| H | 2.82537500  | 1.35431100  | 2.54789300  |
| H | 0.51977400  | 0.47604200  | 2.34673800  |
| H | -2.78324900 | 2.33868700  | -0.73145700 |
| H | -5.05547500 | 2.86784700  | -0.96750900 |
| H | -6.76054300 | 1.07754700  | -0.52368400 |
| H | -5.91692100 | -1.19508600 | 0.16763700  |
| H | -3.51137400 | -1.61403700 | 0.39582100  |
| C | 4.04755000  | -0.39936700 | -1.54516200 |
| H | 3.74785000  | -0.96532900 | -2.42071700 |
| C | 5.33008700  | 0.08144300  | -1.43039800 |
| H | 6.05249000  | -0.10262000 | -2.21749500 |
| C | 5.71576800  | 0.81676900  | -0.28509700 |
| H | 6.73082500  | 1.18953100  | -0.20555700 |
| C | 4.81354400  | 1.05707300  | 0.72429600  |
| H | 5.11116200  | 1.61859500  | 1.60368500  |

# Compound\_5A\_AMIDE

O 1

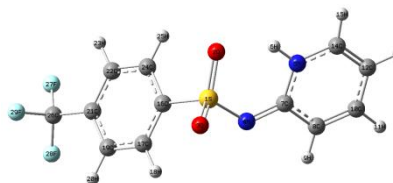
|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -2.76360300 | 1.23907100  | -1.42795300 |
| O | -1.91451100 | -1.93799300 | 1.52421900  |
| O | -1.35885000 | -3.16282500 | -0.65019300 |
| C | -2.81790000 | 0.38968200  | -0.40215300 |
| C | -3.22946400 | 0.75421200  | 0.88516000  |
| H | -3.28567300 | 0.01495600  | 1.67167700  |
| C | -3.57346600 | 2.08278700  | 1.09632600  |
| H | -3.89595300 | 2.40586500  | 2.07967800  |
| C | -3.52466100 | 2.98493800  | 0.03403600  |
| H | -3.79665000 | 4.02513300  | 0.16184700  |
| C | -3.12490300 | 2.50758300  | -1.20925600 |
| N | -2.48825700 | -0.94659800 | -0.74145600 |
| S | -1.44884600 | -1.94661300 | 0.14424900  |
| C | 0.17013500  | -1.14904400 | 0.11721600  |
| C | 0.53189100  | -0.30188000 | 1.16054600  |
| H | -0.13810100 | -0.15323800 | 1.99681300  |
| C | 1.77328900  | 0.32815800  | 1.12047700  |
| H | 2.07073500  | 0.99052900  | 1.92289400  |
| C | 2.62972000  | 0.10330500  | 0.04442100  |
| C | 2.26164300  | -0.75868600 | -0.99135300 |
| H | 2.93732100  | -0.93516000 | -1.81897800 |
| C | 1.02520700  | -1.39146700 | -0.95722200 |
| H | 0.73191800  | -2.07672900 | -1.74241500 |
| H | -2.32102600 | -1.04528600 | -1.73890800 |
| H | -3.08287700 | 3.16630800  | -2.07129400 |
| C | 3.99316700  | 0.74634000  | 0.01168100  |
| F | 4.96070700  | -0.12069600 | 0.39795600  |
| F | 4.32167400  | 1.16413100  | -1.23130100 |
| F | 4.07581700  | 1.81624300  | 0.82946500  |



## Compound\_5B\_IMIDE

O 1

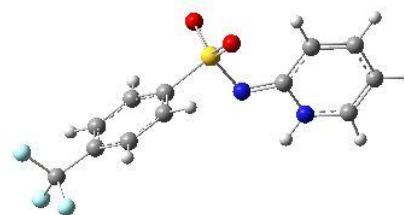
|   |             |             |             |
|---|-------------|-------------|-------------|
| S | -1.15298200 | 1.39797600  | -0.07467700 |
| O | -1.60600500 | 1.52543400  | 1.33828900  |
| O | -1.14857300 | 2.59997400  | -0.90339400 |
| N | -1.93508700 | 0.18655300  | -0.86455800 |
| N | -3.71422600 | -0.00943300 | 0.73926800  |
| H | -3.23073400 | 0.68012100  | 1.32218300  |
| C | -3.06514700 | -0.34735800 | -0.43272800 |
| C | -3.70346200 | -1.36905200 | -1.21054200 |
| H | -3.21483700 | -1.65540200 | -2.13148900 |
| C | -4.87579400 | -1.93647900 | -0.80017100 |
| H | -5.34012500 | -2.70341600 | -1.40984900 |
| C | -5.49662700 | -1.53753400 | 0.41436900  |
| H | -6.42567600 | -1.97632100 | 0.74892700  |
| C | -4.88124600 | -0.57545400 | 1.15592800  |
| H | -5.26771100 | -0.20515700 | 2.09630300  |
| C | 0.53207200  | 0.76158800  | -0.02485900 |
| C | 1.29399500  | 0.77834800  | -1.19149900 |
| H | 0.87741300  | 1.17864200  | -2.10684000 |
| C | 2.59148700  | 0.28277200  | -1.15759600 |
| H | 3.19508700  | 0.28275100  | -2.05649400 |
| C | 3.11367500  | -0.21660900 | 0.03822200  |
| C | 2.34679800  | -0.21636100 | 1.20224600  |
| H | 2.76131300  | -0.59948100 | 2.12583600  |
| C | 1.04390500  | 0.27450400  | 1.17265300  |
| H | 0.43324500  | 0.29172700  | 2.06597900  |
| C | 4.53943700  | -0.70010500 | 0.07845400  |
| F | 4.75232500  | -1.58703800 | 1.07554500  |
| F | 4.90579100  | -1.30125400 | -1.07593200 |
| F | 5.40932800  | 0.32232200  | 0.27497300  |



## Compound\_5C\_IMIDE

O 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| S | -1.12299900 | -1.18938500 | -0.17050600 |
| O | -1.44700500 | -1.83195000 | 1.11275900  |
| O | -1.28741000 | -1.96721000 | -1.40292200 |
| N | -1.85727500 | 0.28780500  | -0.32844400 |
| C | 0.59594800  | -0.64891600 | -0.08598100 |
| C | 1.28819300  | -0.39294100 | -1.26637300 |
| C | 2.61322500  | 0.02185500  | -1.19667800 |
| C | 3.22948700  | 0.17033000  | 0.04783500  |
| C | 2.53061500  | -0.10218500 | 1.22338500  |
| C | 1.20258100  | -0.51504500 | 1.15779100  |
| C | -3.14256800 | 0.42808400  | -0.09592400 |
| N | -3.62928400 | 1.70811600  | -0.31478700 |
| C | -4.92348800 | 2.09380400  | -0.14470600 |
| C | -5.85804800 | 1.19606800  | 0.27280500  |
| C | -5.43085800 | -0.13643900 | 0.52101000  |
| C | -4.13011600 | -0.51857800 | 0.34821100  |
| H | 0.79685200  | -0.52712100 | -2.22156000 |

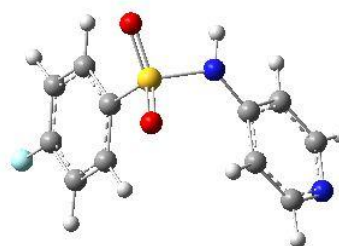


|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.16534900  | 0.22962500  | -2.10472700 |
| H | 3.01763500  | 0.00920200  | 2.18360800  |
| H | 0.64283600  | -0.74206000 | 2.05607800  |
| H | -2.93704900 | 2.37503000  | -0.63256900 |
| H | -5.13903000 | 3.13136500  | -0.36212500 |
| H | -6.88636000 | 1.49860300  | 0.40787100  |
| H | -6.15447400 | -0.87060200 | 0.85733600  |
| H | -3.80998200 | -1.52910500 | 0.55450700  |
| C | 4.67967900  | 0.57065400  | 0.11056100  |
| F | 5.00360700  | 1.14600000  | 1.28958200  |
| F | 5.00768500  | 1.44897700  | -0.86489700 |
| F | 5.50265600  | -0.49754200 | -0.04002000 |

#### Compound\_6A\_AMIDE

O 1

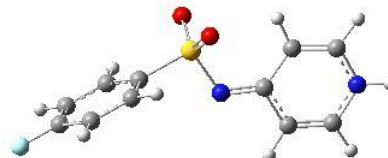
|   |             |             |             |
|---|-------------|-------------|-------------|
| S | -0.02170700 | 1.85778600  | 0.16470200  |
| O | -0.49093800 | 2.98582800  | -0.62863300 |
| O | 0.42383900  | 1.99285800  | 1.54364100  |
| N | 1.29456900  | 1.26349700  | -0.73369400 |
| N | 3.64810700  | -2.13978900 | 0.11046700  |
| C | 3.21156000  | -1.86517900 | -1.12197200 |
| H | 3.50611000  | -2.56066000 | -1.90277200 |
| C | 2.41265200  | -0.77151400 | -1.43742100 |
| H | 2.08038300  | -0.61414400 | -2.45790500 |
| C | 2.05215500  | 0.11546700  | -0.41758900 |
| C | 2.51585900  | -0.14743700 | 0.87499300  |
| H | 2.29022100  | 0.52217100  | 1.69302200  |
| C | 3.29288100  | -1.28460200 | 1.07486800  |
| H | 3.66178900  | -1.50980600 | 2.07146900  |
| C | -1.28579900 | 0.58215200  | 0.12201300  |
| C | -2.21586100 | 0.58694000  | -0.91825700 |
| H | -2.19196300 | 1.37168400  | -1.66389700 |
| C | -3.18666800 | -0.40724100 | -0.96960900 |
| H | -3.93147600 | -0.43285400 | -1.75473300 |
| C | -3.19816100 | -1.37481600 | 0.02617100  |
| C | -2.28728900 | -1.38651500 | 1.07260600  |
| H | -2.34783900 | -2.15565100 | 1.83188200  |
| C | -1.31775700 | -0.38964600 | 1.12219500  |
| H | -0.60690000 | -0.35555200 | 1.93692000  |
| F | -4.14075100 | -2.33823500 | -0.02134700 |
| H | 1.13037700  | 1.41323800  | -1.72256900 |



#### Compound\_6C\_IMIDE

O 1

|   |            |             |             |
|---|------------|-------------|-------------|
| S | 0.02932700 | -0.98708500 | 0.12888400  |
| O | 0.17530000 | -1.68448200 | 1.41477400  |
| O | 0.28411100 | -1.74318500 | -1.10922300 |
| N | 0.87845000 | 0.45079000  | 0.15477400  |
| N | 4.98642600 | 0.69046700  | -0.15043400 |
| H | 5.98815200 | 0.77735400  | -0.21496700 |
| C | 4.21302300 | 1.81079200  | 0.00788600  |
| H | 4.74229800 | 2.75326800  | 0.05151700  |
| C | 2.86504300 | 1.71636600  | 0.10211100  |

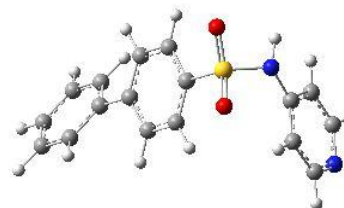


|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.26506200  | 2.60723400  | 0.22786200  |
| C | 2.18912400  | 0.43824600  | 0.04396700  |
| C | 3.06209300  | -0.70674600 | -0.13008400 |
| H | 2.64897400  | -1.70216300 | -0.20076200 |
| C | 4.40635000  | -0.54660200 | -0.21761900 |
| H | 5.08331700  | -1.38103600 | -0.34550200 |
| C | -1.64646900 | -0.34403100 | 0.03693600  |
| C | -2.30959900 | 0.00119400  | 1.21185600  |
| H | -1.81880300 | -0.13310600 | 2.16735700  |
| C | -3.60651800 | 0.50119900  | 1.14359000  |
| H | -4.15694300 | 0.77718500  | 2.03410400  |
| C | -4.19815200 | 0.63698800  | -0.10407500 |
| C | -3.55458300 | 0.28942100  | -1.28222800 |
| H | -4.06526100 | 0.40394200  | -2.22996900 |
| C | -2.25659200 | -0.20907000 | -1.20684900 |
| H | -1.72329200 | -0.50522400 | -2.10115600 |
| F | -5.46049800 | 1.12243200  | -0.17315000 |

# Compound\_7A\_AMIDE

0 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| S | -2.15757400 | -1.86442100 | 0.10032600  |
| O | -2.24742700 | -3.05052900 | -0.74147200 |
| O | -2.63530300 | -1.83749400 | 1.47545900  |
| N | -3.05423000 | -0.70167700 | -0.76510500 |
| N | -3.61561000 | 3.36580000  | 0.22222800  |
| C | -3.34082300 | 2.96739500  | -1.02308900 |
| H | -3.28350600 | 3.74813800  | -1.77635700 |
| C | -3.12075200 | 1.64291400  | -1.38453000 |
| H | -2.88848700 | 1.38899100  | -2.41320500 |
| C | -3.20769100 | 0.65199500  | -0.40067800 |
| C | -3.50941400 | 1.05062000  | 0.90534500  |
| H | -3.61386900 | 0.32237100  | 1.69734000  |
| C | -3.69082500 | 2.40802700  | 1.15237000  |
| H | -3.92454700 | 2.73984000  | 2.16004300  |
| C | -0.45482100 | -1.29683900 | 0.09497300  |
| C | 0.37889200  | -1.65808300 | -0.96290700 |
| H | 0.01276600  | -2.31528400 | -1.74203000 |
| C | 1.68976800  | -1.19842600 | -0.97853600 |
| H | 2.34843300  | -1.50533700 | -1.78220100 |
| C | 2.18494700  | -0.37985100 | 0.04963300  |
| C | 1.32421600  | -0.04295900 | 1.10532000  |
| H | 1.68075300  | 0.59706800  | 1.90355300  |
| C | 0.01045300  | -0.49712200 | 1.13698500  |
| H | -0.64321400 | -0.24296000 | 1.96098300  |
| H | -2.95863500 | -0.87021600 | -1.75993200 |
| C | 3.58574000  | 0.10980900  | 0.02374100  |
| C | 4.35252100  | 0.15771100  | 1.19728300  |
| C | 4.17434200  | 0.53788800  | -1.17539200 |
| C | 5.66589700  | 0.61825800  | 1.17221600  |
| H | 3.92617700  | -0.19255000 | 2.13045600  |
| C | 5.48641600  | 1.00218300  | -1.19931600 |
| H | 3.59249300  | 0.53267700  | -2.09015100 |
| C | 6.23752200  | 1.04361100  | -0.02582900 |
| H | 6.24560200  | 0.63756000  | 2.08816500  |

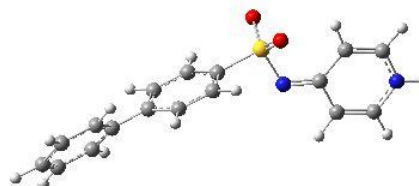


|   |            |            |             |
|---|------------|------------|-------------|
| H | 5.91991900 | 1.33915200 | -2.13420100 |
| H | 7.25971000 | 1.40382500 | -0.04496700 |

# Compound\_7C\_IMIDE

O 1

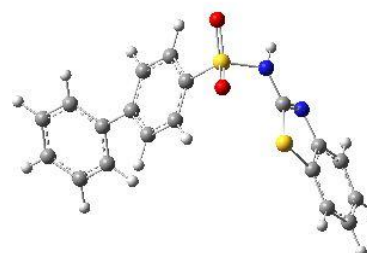
|   |             |             |             |
|---|-------------|-------------|-------------|
| S | 1.68010500  | -1.08177300 | 0.36183700  |
| O | 1.94517800  | -1.51853700 | 1.74042800  |
| O | 2.01681500  | -2.00161900 | -0.73883100 |
| N | 2.33020200  | 0.43734400  | 0.11074900  |
| N | 6.35230500  | 1.14741400  | -0.47739100 |
| H | 7.32946200  | 1.35010400  | -0.61533500 |
| C | 5.44052400  | 2.17046000  | -0.44607500 |
| H | 5.83827800  | 3.16766400  | -0.57932900 |
| C | 4.12280300  | 1.92072900  | -0.25755900 |
| H | 3.41274300  | 2.73603300  | -0.23357400 |
| C | 3.62410900  | 0.57359100  | -0.07758300 |
| C | 4.63753000  | -0.46372100 | -0.12822800 |
| H | 4.36014100  | -1.50214700 | -0.02281300 |
| C | 5.94276700  | -0.14868900 | -0.32022300 |
| H | 6.72118100  | -0.89932400 | -0.36031200 |
| C | -0.06931400 | -0.69150200 | 0.23023300  |
| C | -0.75809600 | -0.24604100 | 1.35452400  |
| H | -0.24174200 | -0.15504700 | 2.30193500  |
| C | -2.11258900 | 0.04858000  | 1.24811500  |
| H | -2.65638300 | 0.36903900  | 2.12917700  |
| C | -2.79307700 | -0.10031800 | 0.02948700  |
| C | -2.07278600 | -0.55848600 | -1.08378400 |
| H | -2.57401800 | -0.66562200 | -2.03872000 |
| C | -0.71688900 | -0.85465000 | -0.99004000 |
| H | -0.16289200 | -1.21390100 | -1.84819000 |
| C | -4.24116200 | 0.21107600  | -0.07590000 |
| C | -5.10087700 | -0.60535400 | -0.82570700 |
| C | -4.78636700 | 1.32878300  | 0.57332600  |
| C | -6.45923900 | -0.31510600 | -0.92180500 |
| H | -4.70642500 | -1.48828600 | -1.31575600 |
| C | -6.14426800 | 1.62053300  | 0.47562100  |
| H | -4.13669600 | 1.98703300  | 1.13905800  |
| C | -6.98699400 | 0.79944800  | -0.27188200 |
| H | -7.10761500 | -0.96571400 | -1.49819900 |
| H | -6.54305300 | 2.49489200  | 0.97803400  |
| H | -8.04460700 | 1.02560200  | -0.34677700 |



# Compound\_8A\_AMIDE

O 1

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 3.69108300 | 1.21467000  | -0.48347800 |
| C | 3.39698800 | 1.30762900  | 0.89431600  |
| C | 3.76007700 | 2.45983300  | 1.60064000  |
| C | 4.40072300 | 3.48927800  | 0.92371300  |
| C | 4.68250900 | 3.38686200  | -0.44676400 |
| C | 4.32792600 | 2.24962600  | -1.16597100 |
| C | 2.53722300 | -0.68993300 | 0.53089700  |
| H | 3.53435600 | 2.52945300  | 2.65782100  |
| H | 4.68774400 | 4.38579700  | 1.46096300  |

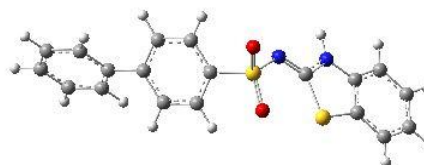


|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.54931800  | 2.17209700  | -2.22372500 |
| S | 3.13646500  | -0.33539000 | -1.10212300 |
| N | 2.73238800  | 0.21594000  | 1.43074100  |
| N | 1.98494400  | -1.92589400 | 0.85494600  |
| S | 0.82581800  | -2.76126400 | -0.08811300 |
| O | 1.36384300  | -2.78305500 | -1.44051600 |
| O | 0.56610300  | -3.96638500 | 0.68478100  |
| C | -0.65727500 | -1.75467400 | -0.08898300 |
| C | -0.84663200 | -0.81282000 | -1.09868600 |
| C | -1.59828900 | -1.92600900 | 0.92530600  |
| C | -1.99083600 | -0.02392200 | -1.07806500 |
| H | -0.12287100 | -0.72046400 | -1.89796600 |
| C | -2.73648200 | -1.12961600 | 0.93075100  |
| H | -1.44322200 | -2.67712700 | 1.68983500  |
| C | -2.95222500 | -0.16328100 | -0.06510800 |
| H | -2.15429000 | 0.68877900  | -1.87756100 |
| H | -3.45989800 | -1.24783800 | 1.72862800  |
| H | 1.79713100  | -2.01233300 | 1.84950700  |
| C | -4.17056400 | 0.68382400  | -0.05193300 |
| C | -4.10002100 | 2.04618700  | -0.37828100 |
| C | -5.41950100 | 0.14249700  | 0.28661400  |
| C | -5.24190900 | 2.84222900  | -0.36425500 |
| H | -3.14086400 | 2.49071300  | -0.61837400 |
| C | -6.56178700 | 0.93807200  | 0.29630100  |
| H | -5.50163400 | -0.91357000 | 0.51729200  |
| C | -6.47725900 | 2.29113100  | -0.02781700 |
| H | -5.16510700 | 3.89556400  | -0.60923500 |
| H | -7.51993600 | 0.49866000  | 0.54983900  |
| H | -7.36663100 | 2.91078000  | -0.01840100 |
| H | 5.18599400  | 4.20163900  | -0.95395400 |

Compound\_8C\_IMIDE

0 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.61400400 | -0.60921500 | -0.50011700 |
| C | -4.38646200 | -0.98264000 | 0.82913900  |
| C | -5.26221700 | -1.83505400 | 1.49619300  |
| C | -6.37572900 | -2.30764100 | 0.80413400  |
| C | -6.60756400 | -1.93666200 | -0.52323900 |
| C | -5.72664500 | -1.08269900 | -1.18675200 |
| C | -2.51781900 | 0.41018700  | 0.49382800  |
| H | -5.08221900 | -2.12213900 | 2.52587700  |
| H | -7.06968900 | -2.97124900 | 1.30606900  |
| H | -5.90618300 | -0.79335300 | -2.21534700 |
| S | -3.34992500 | 0.48281300  | -1.09549500 |
| N | -3.22856500 | -0.40252100 | 1.33326000  |
| N | -1.42995800 | 0.96845100  | 0.91055800  |
| S | -0.55082700 | 2.00820400  | -0.05786100 |
| O | -1.06410400 | 1.97026000  | -1.43741800 |
| O | -0.44577300 | 3.28174000  | 0.64543900  |
| C | 1.06534500  | 1.22890300  | -0.04817100 |
| C | 1.43295800  | 0.40207000  | -1.10619800 |
| C | 1.93228600  | 1.46598100  | 1.01596500  |
| C | 2.68617200  | -0.20065400 | -1.09021400 |
| H | 0.75511900  | 0.25686400  | -1.93797400 |

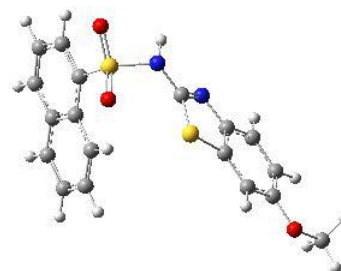


|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.18072900  | 0.85538600  | 1.01989100  |
| H | 1.63137600  | 2.12271100  | 1.82255600  |
| C | 3.57929700  | 0.01151200  | -0.02902500 |
| H | 2.98762800  | -0.81917900 | -1.92737100 |
| H | 3.84914700  | 1.02174200  | 1.85648800  |
| H | -2.89590900 | -0.53067700 | 2.27820900  |
| C | 4.91646200  | -0.63358000 | -0.02076500 |
| C | 5.07540700  | -1.96378300 | -0.43679700 |
| C | 6.05313700  | 0.07205500  | 0.40064600  |
| C | 6.32935600  | -2.56861000 | -0.43021800 |
| H | 4.20692500  | -2.53522100 | -0.74450100 |
| C | 7.30757200  | -0.53179300 | 0.40407100  |
| H | 5.95764700  | 1.10895700  | 0.70219200  |
| C | 7.45076500  | -1.85493400 | -0.01048700 |
| H | 6.42939200  | -3.60091200 | -0.74659000 |
| H | 8.17526200  | 0.03477900  | 0.72308300  |
| H | 8.42738200  | -2.32543100 | -0.00712000 |
| H | -7.47945100 | -2.31364000 | -1.04405700 |

Compound\_9A\_AMIDE

0 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.55819200  | -0.72692000 | -0.29343100 |
| C | 2.22224600  | -0.49903800 | 1.06144000  |
| C | 3.14911700  | 0.13574300  | 1.88819800  |
| C | 4.37667600  | 0.53556000  | 1.37086000  |
| C | 4.68994900  | 0.30659300  | 0.01909600  |
| C | 3.77499100  | -0.32574400 | -0.82719700 |
| C | 0.34023000  | -1.46639200 | 0.44452500  |
| H | 2.90232000  | 0.31547200  | 2.92755900  |
| H | 5.08607100  | 1.02607500  | 2.02286700  |
| H | 4.04219000  | -0.49418300 | -1.86264000 |
| S | 1.22745600  | -1.54684100 | -1.09587600 |
| N | 0.95742400  | -0.92262300 | 1.43837900  |
| N | -0.88983400 | -2.10448000 | 0.60113600  |
| S | -2.27749400 | -1.86462300 | -0.37759200 |
| O | -1.78828200 | -1.79830600 | -1.74757700 |
| O | -3.18733100 | -2.91130200 | 0.06346300  |
| H | -1.14446300 | -2.19652800 | 1.58036200  |
| O | 5.87187900  | 0.66534800  | -0.56345400 |
| C | 6.86732300  | 1.29270500  | 0.23389300  |
| H | 6.51466800  | 2.24810400  | 0.63721000  |
| H | 7.18881300  | 0.64443600  | 1.05611300  |
| C | -2.99887700 | -0.28066600 | 0.12820900  |
| C | -2.50938000 | 0.98959800  | -0.31946300 |
| C | -4.04278600 | -0.38439700 | 1.02256800  |
| C | -1.47248600 | 1.18245300  | -1.27110500 |
| C | -3.13725900 | 2.15522400  | 0.23978700  |
| C | -4.65263500 | 0.77391000  | 1.54481700  |
| H | -4.39583000 | -1.36426100 | 1.31569000  |
| C | -1.06808400 | 2.44811900  | -1.62639100 |
| H | -1.01200800 | 0.32715100  | -1.74047500 |
| C | -2.69077200 | 3.44349700  | -0.15379100 |
| C | -4.20153000 | 2.01271400  | 1.16624400  |
| H | -5.47499300 | 0.67292500  | 2.24280500  |

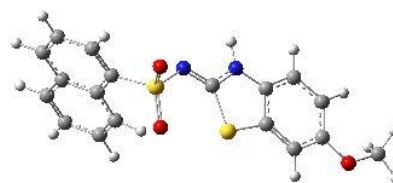


|   |             |            |             |
|---|-------------|------------|-------------|
| C | -1.67330000 | 3.59148800 | -1.06263400 |
| H | -0.27541900 | 2.56605200 | -2.35634800 |
| H | -3.17403800 | 4.31236000 | 0.28008300  |
| H | -4.65907300 | 2.90959800 | 1.57018800  |
| H | -1.33989400 | 4.58040500 | -1.35542500 |
| H | 7.70932000  | 1.47295000 | -0.43231300 |

# Compound\_9C\_IMIDE

0 1

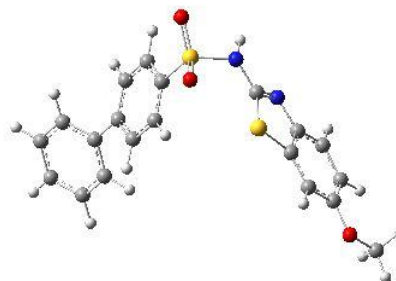
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.95852200  | -0.22166900 | -0.33447100 |
| C | 2.79580600  | -0.19808500 | 1.05685700  |
| C | 3.85765800  | 0.14034700  | 1.88167900  |
| C | 5.09113700  | 0.45481100  | 1.30491900  |
| C | 5.25151000  | 0.42874500  | -0.08601400 |
| C | 4.17573700  | 0.08831600  | -0.91687200 |
| C | 0.62220800  | -0.84790900 | 0.43001100  |
| H | 3.74165100  | 0.16212900  | 2.95920300  |
| H | 5.91629400  | 0.71701200  | 1.95193000  |
| H | 4.32127000  | 0.07288000  | -1.98959600 |
| S | 1.45566300  | -0.68380900 | -1.15475700 |
| N | 1.49886700  | -0.54618300 | 1.43014200  |
| N | -0.59705000 | -1.17228900 | 0.71233700  |
| S | -1.66665900 | -1.65568900 | -0.47235400 |
| O | -1.20510200 | -1.19523900 | -1.79329700 |
| O | -1.94631900 | -3.07719600 | -0.28721000 |
| H | 1.18362900  | -0.61618400 | 2.38688400  |
| O | 6.41766900  | 0.71846100  | -0.73305400 |
| C | 7.56023000  | 1.06286800  | 0.03942100  |
| H | 7.38829500  | 1.97304700  | 0.62427600  |
| H | 7.85102200  | 0.24608300  | 0.70891000  |
| C | -3.14720100 | -0.74046500 | 0.01126700  |
| C | -3.25204100 | 0.67843900  | -0.13271700 |
| C | -4.16437300 | -1.49383700 | 0.54723400  |
| C | -2.25095400 | 1.51298200  | -0.69804200 |
| C | -4.46427900 | 1.29158600  | 0.32888600  |
| C | -5.35609600 | -0.87361300 | 0.98072900  |
| H | -4.03739200 | -2.56509100 | 0.63400300  |
| C | -2.43389100 | 2.87322100  | -0.78410200 |
| H | -1.34952000 | 1.07056700  | -1.09601300 |
| C | -4.61558500 | 2.69882000  | 0.22228800  |
| C | -5.49618500 | 0.48689200  | 0.87910300  |
| H | -6.15073300 | -1.48107800 | 1.39745700  |
| C | -3.62223400 | 3.47715300  | -0.31803900 |
| H | -1.65798300 | 3.48849700  | -1.22562800 |
| H | -5.53741800 | 3.14872900  | 0.57574400  |
| H | -6.40558900 | 0.97188300  | 1.21827000  |
| H | -3.74937200 | 4.55091300  | -0.39558400 |
| H | 8.35925700  | 1.24204100  | -0.67776600 |



# Compound\_10A\_AMIDE

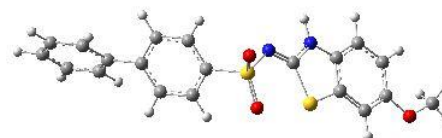
0 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.35105900  | 0.03658800  | -0.32251100 |
| C | 3.03367200  | 0.13837900  | 1.05120400  |
| C | 3.62067800  | 1.15393900  | 1.80508100  |
| C | 4.49853500  | 2.04638100  | 1.19771300  |
| C | 4.79725500  | 1.93286200  | -0.17132600 |
| C | 4.21923000  | 0.92225500  | -0.94504000 |
| C | 1.76669500  | -1.60209700 | 0.57794900  |
| H | 3.38504200  | 1.24129500  | 2.85880900  |
| H | 4.94697700  | 2.82895400  | 1.79392600  |
| H | 4.46923900  | 0.85329300  | -1.99607800 |
| S | 2.49101500  | -1.32790800 | -1.02435500 |
| N | 2.12379200  | -0.79752100 | 1.52032800  |
| N | 0.94342000  | -2.69923800 | 0.82603000  |
| S | -0.36277400 | -3.18042100 | -0.16996700 |
| O | 0.18375600  | -3.27831600 | -1.51570900 |
| O | -0.93047600 | -4.31598600 | 0.54190600  |
| C | -1.55298500 | -1.83990900 | -0.14656000 |
| C | -1.48742100 | -0.84730400 | -1.12274300 |
| C | -2.52546200 | -1.80774800 | 0.85212400  |
| C | -2.40432900 | 0.19685400  | -1.08482800 |
| H | -0.74827000 | -0.90861000 | -1.91087900 |
| C | -3.43343800 | -0.75671000 | 0.87613200  |
| H | -2.57389900 | -2.59880000 | 1.59011300  |
| C | -3.38856300 | 0.26462600  | -0.08671100 |
| H | -2.37444900 | 0.95386100  | -1.85927300 |
| H | -4.17752900 | -0.71910900 | 1.66269200  |
| H | 0.71330000  | -2.78628700 | 1.81164400  |
| C | -4.36319400 | 1.38338100  | -0.05464000 |
| C | -3.95997200 | 2.69493500  | -0.34625800 |
| C | -5.70965700 | 1.15569000  | 0.26610800  |
| C | -4.87355600 | 3.74483200  | -0.31653000 |
| H | -2.91930900 | 2.89790500  | -0.57239200 |
| C | -6.62360600 | 2.20537800  | 0.29219900  |
| H | -6.04939600 | 0.14659200  | 0.46977000  |
| C | -6.20912700 | 3.50415600  | 0.00182300  |
| H | -4.53997000 | 4.75300000  | -0.53514900 |
| H | -7.66220300 | 2.00692500  | 0.53178000  |
| H | -6.92074000 | 4.32157300  | 0.02336200  |
| O | 5.64793900  | 2.76559000  | -0.84097800 |
| C | 6.29472200  | 3.80741600  | -0.12228800 |
| H | 5.57059400  | 4.51407400  | 0.29750300  |
| H | 6.92465400  | 3.40895800  | 0.68024900  |
| H | 6.92063700  | 4.32322400  | -0.84855300 |



#### Compound\_10C\_IMIDE

|     |             |             |             |
|-----|-------------|-------------|-------------|
| O 1 |             |             |             |
| C   | -4.00012900 | -0.06127500 | -0.31669800 |
| C   | -3.77370500 | -0.34359500 | 1.03663800  |
| C   | -4.71202300 | -1.05031900 | 1.77313400  |
| C   | -5.88640500 | -1.47516900 | 1.14582000  |
| C   | -6.11091700 | -1.19127000 | -0.20694100 |
| C   | -5.15996300 | -0.47740100 | -0.94824700 |
| C   | -1.79549000 | 0.83917700  | 0.55597300  |
| H   | -4.54568900 | -1.27402600 | 2.82066700  |

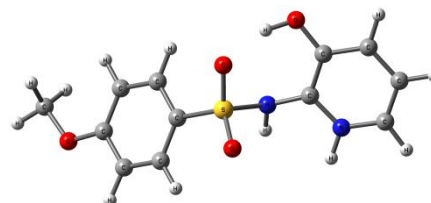


|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -6.61550400 | -2.02527700 | 1.72372000  |
| H | -5.35388700 | -0.26694800 | -1.99243000 |
| S | -2.65715900 | 0.85668300  | -1.02233900 |
| N | -2.55206300 | 0.16726200  | 1.47102600  |
| N | -0.65062900 | 1.33057700  | 0.90174500  |
| S | 0.28851600  | 2.20495500  | -0.16467600 |
| O | -0.26116000 | 2.10567700  | -1.52723700 |
| O | 0.52651200  | 3.51602700  | 0.42933700  |
| C | 1.82911700  | 1.28533300  | -0.12400100 |
| C | 2.12559800  | 0.40012500  | -1.15638900 |
| C | 2.71166800  | 1.47596600  | 0.93694300  |
| C | 3.32225900  | -0.30813500 | -1.11840900 |
| H | 1.43814100  | 0.29033900  | -1.98570000 |
| C | 3.90123500  | 0.75871000  | 0.96423800  |
| H | 2.46812700  | 2.17878400  | 1.72384100  |
| C | 4.22785000  | -0.14561300 | -0.05933900 |
| H | 3.56983300  | -0.97330800 | -1.93731900 |
| H | 4.57904200  | 0.88920600  | 1.79964200  |
| H | -2.21003300 | 0.09047900  | 2.41789000  |
| C | 5.50384900  | -0.90375700 | -0.02497000 |
| C | 5.55141800  | -2.25098000 | -0.41291000 |
| C | 6.69352700  | -0.29110900 | 0.39609100  |
| C | 6.74785800  | -2.96210100 | -0.37968500 |
| H | 4.63989300  | -2.75158900 | -0.71934500 |
| C | 7.89044200  | -1.00144800 | 0.42676500  |
| H | 6.68602400  | 0.75608300  | 0.67643800  |
| C | 7.92271400  | -2.34022400 | 0.03989700  |
| H | 6.76069800  | -4.00538400 | -0.67492600 |
| H | 8.80065000  | -0.50574900 | 0.74537900  |
| H | 8.85468400  | -2.89338500 | 0.06454200  |
| O | -7.22656600 | -1.56586400 | -0.89835400 |
| C | -8.24205900 | -2.28981500 | -0.21607500 |
| H | -7.86663000 | -3.24840800 | 0.15841200  |
| H | -8.65776900 | -1.70901700 | 0.61444100  |
| H | -9.02181200 | -2.47219300 | -0.95339300 |

Cartesian coordinates of optimized structures of protonated form of imide tautomer (C) of NHBS **1-10** calculated at B3LYP/6-311++G(d,p) level of theory

Compound 1\_H

|   |             |             |             |
|---|-------------|-------------|-------------|
| 1 | 1           |             |             |
| S | -0.25475700 | -1.22548100 | 0.25983600  |
| O | -0.86923000 | -1.06566700 | 1.56736000  |
| O | -0.26683300 | -2.46834800 | -0.47595500 |
| N | -1.14245000 | 0.00795400  | -0.79041200 |
| C | 1.35791100  | -0.50860900 | 0.21900500  |
| C | 2.27429700  | -0.95251500 | -0.73601300 |
| C | 3.55214800  | -0.40856500 | -0.76035700 |
| C | 3.91115900  | 0.57381200  | 0.17776400  |
| C | 2.97586400  | 1.00302900  | 1.14151700  |
| C | 1.70592900  | 0.46521400  | 1.16851400  |

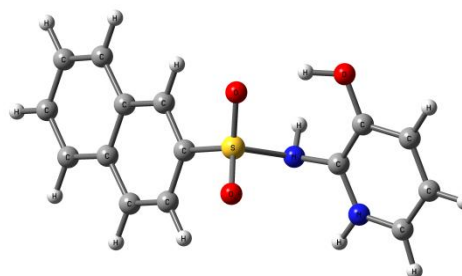


|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.37470100 | 0.48189700  | -0.48194000 |
| N | -2.62710900 | 1.81629800  | -0.52548800 |
| C | -3.84256400 | 2.38878000  | -0.28779000 |
| C | -4.89286700 | 1.58793600  | 0.06493300  |
| C | -4.69993800 | 0.19872200  | 0.13577600  |
| C | -3.46786100 | -0.36562800 | -0.14331400 |
| H | 1.99765900  | -1.72851600 | -1.43890800 |
| H | 3.28694100  | 1.74257000  | 1.86849200  |
| H | 0.99749000  | 0.76536500  | 1.93080200  |
| H | -1.85299700 | 2.43190000  | -0.74837100 |
| H | -3.89452400 | 3.46283000  | -0.39007000 |
| H | -5.86041800 | 2.02461800  | 0.26889600  |
| H | -5.53558600 | -0.44834000 | 0.38016800  |
| O | -3.19813700 | -1.67561200 | -0.17843500 |
| H | -2.28777142 | -1.86128329 | -0.43993893 |
| H | 4.26164800  | -0.76368600 | -1.49429500 |
| O | 5.11562000  | 1.15580700  | 0.24582700  |
| C | 6.15515400  | 0.75547000  | -0.65829200 |
| H | 5.87317700  | 0.96376900  | -1.69374100 |
| H | 7.01977000  | 1.35589700  | -0.38739200 |
| H | 6.39013200  | -0.30465100 | -0.53416000 |
| H | -0.48330400 | 0.66250900  | -1.19630400 |

# Compound\_2\_H

1 1

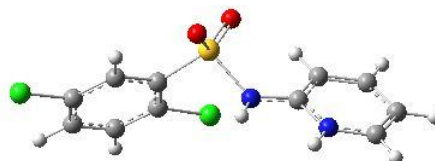
|   |             |             |             |
|---|-------------|-------------|-------------|
| S | 0.50736200  | -1.04325100 | 0.76705700  |
| O | 1.13570600  | -2.14017500 | 0.02331100  |
| O | 0.44906900  | -1.05271300 | 2.21378000  |
| N | 1.50854900  | 0.33610100  | 0.29969800  |
| C | -1.05929900 | -0.61359800 | 0.07890900  |
| C | -2.04961500 | -0.19625600 | 0.94265400  |
| C | -3.32221700 | 0.13969600  | 0.42392500  |
| C | -3.54576700 | 0.03815000  | -0.98839000 |
| C | -2.48771400 | -0.40476200 | -1.83020700 |
| C | -1.25936200 | -0.73263600 | -1.31989300 |
| C | 2.83209400  | 0.29547800  | -0.02208900 |
| N | 3.44065500  | -0.84146800 | -0.41707300 |
| C | 4.75318000  | -0.91191000 | -0.77431700 |
| C | 5.52294700  | 0.21777500  | -0.74701400 |
| C | 4.93974700  | 1.43348400  | -0.34411400 |
| C | 3.61077600  | 1.48358600  | 0.01718300  |
| H | -1.86529400 | -0.13993700 | 2.00873300  |
| H | -2.66865300 | -0.49409500 | -2.89534500 |
| H | -0.46618100 | -1.09377400 | -1.96124700 |
| H | 2.85227000  | -1.68335900 | -0.42380500 |
| H | 5.11163900  | -1.88940500 | -1.06249400 |
| H | 6.56520700  | 0.17089100  | -1.02906100 |
| H | 5.54014300  | 2.33656100  | -0.31184400 |
| C | -4.37990500 | 0.56684300  | 1.26870500  |
| H | -4.20725900 | 0.63618500  | 2.33686200  |
| C | -5.60560600 | 0.88510600  | 0.73668100  |
| H | -6.41122000 | 1.21007500  | 1.38407500  |
| C | -5.82659900 | 0.78776800  | -0.65709800 |
| H | -6.80032200 | 1.04044100  | -1.06008800 |



|   |             |            |             |
|---|-------------|------------|-------------|
| C | -4.82234500 | 0.37338500 | -1.50113800 |
| H | -4.99905000 | 0.29679200 | -2.56799900 |
| O | 2.92802100  | 2.57737500 | 0.42346100  |
| H | 3.48491600  | 3.36444800 | 0.46548700  |
| H | 1.19731600  | 1.22621700 | 0.67823500  |

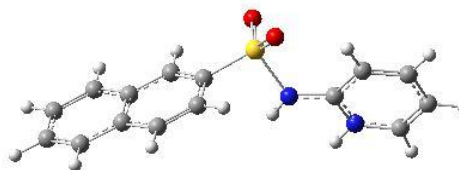
#### Compound\_3\_H

|     |             |             |             |
|-----|-------------|-------------|-------------|
| 1 1 |             |             |             |
| S   | 0.08468000  | -0.96665200 | 0.82518800  |
| O   | -0.27494000 | -2.36851000 | 0.76678100  |
| O   | 0.69467200  | -0.36886200 | 1.99298000  |
| N   | 1.26158700  | -0.78184500 | -0.49325400 |
| C   | -1.31017300 | -0.01237700 | 0.22653600  |
| C   | -1.27261600 | 1.37186900  | 0.00997900  |
| C   | -2.43824600 | 2.02578000  | -0.37617900 |
| C   | -3.62479500 | 1.31863400  | -0.53787200 |
| C   | -3.65094400 | -0.05724400 | -0.31931900 |
| C   | -2.49694800 | -0.73218100 | 0.06310600  |
| C   | 2.58025800  | -0.44366200 | -0.38226100 |
| N   | 3.41646600  | -0.90189800 | -1.35720200 |
| C   | 4.74805700  | -0.61091300 | -1.41996800 |
| C   | 5.31888900  | 0.16676000  | -0.45341500 |
| C   | 4.49448700  | 0.65062300  | 0.57967500  |
| C   | 3.14588100  | 0.36245500  | 0.62200300  |
| H   | -2.41401100 | 3.09415000  | -0.54859000 |
| H   | -2.51368100 | -1.79883900 | 0.24063200  |
| H   | 3.03626500  | -1.49627400 | -2.08564300 |
| H   | 5.28319800  | -1.03478400 | -2.25851600 |
| H   | 6.37436700  | 0.39598400  | -0.49454300 |
| H   | 4.92097100  | 1.27087900  | 1.35920700  |
| H   | 2.51393800  | 0.73313600  | 1.41267400  |
| H   | -4.52757900 | 1.83755400  | -0.83378000 |
| Cl  | 0.18590000  | 2.31534200  | 0.17551900  |
| Cl  | -5.13300000 | -0.94428700 | -0.52456800 |
| H   | 1.00500700  | -1.39659100 | -1.25922100 |



#### Compound\_4\_H

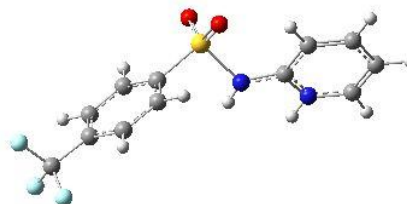
|     |             |             |             |
|-----|-------------|-------------|-------------|
| 1 1 |             |             |             |
| S   | 0.69750600  | -0.98837900 | 0.65924900  |
| O   | 1.26328600  | -2.15087700 | -0.00057400 |
| O   | 0.76035400  | -0.81499200 | 2.09817600  |
| N   | 1.61993500  | 0.40291500  | -0.03773700 |
| C   | -0.91516800 | -0.60175400 | 0.04653300  |
| C   | -1.82737000 | -0.05030900 | 0.92102700  |
| C   | -3.13272800 | 0.24569200  | 0.46190700  |
| C   | -3.46894000 | -0.03542300 | -0.90337900 |
| C   | -2.48764800 | -0.61091200 | -1.75753900 |
| C   | -1.22698700 | -0.89974700 | -1.30420800 |
| C   | 2.97518300  | 0.46244600  | -0.13531400 |
| N   | 3.55721400  | 1.69642000  | -0.15060200 |
| C   | 4.89840900  | 1.90641800  | -0.29845000 |
| C   | 5.74364800  | 0.84177900  | -0.41689000 |
| C   | 5.18769000  | -0.45309700 | -0.39169900 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.83063700  | -0.65149000 | -0.25867300 |
| H | -1.55922800 | 0.13668100  | 1.95413100  |
| H | -2.75429600 | -0.83677100 | -2.78380100 |
| H | -0.49097700 | -1.36368600 | -1.94774700 |
| H | 2.96542800  | 2.51357800  | -0.05246600 |
| H | 5.21425600  | 2.94050100  | -0.30622900 |
| H | 6.80658000  | 1.00261800  | -0.52832600 |
| H | 5.83637600  | -1.31593800 | -0.48641400 |
| H | 3.39814900  | -1.64085300 | -0.25818200 |
| C | -4.11544900 | 0.80346200  | 1.32111600  |
| H | -3.85898600 | 1.00687800  | 2.35483600  |
| C | -5.37551800 | 1.07640300  | 0.84761300  |
| H | -6.12365200 | 1.50045500  | 1.50657600  |
| C | -5.70758100 | 0.80204900  | -0.49999100 |
| H | -6.70727300 | 1.02064500  | -0.85664900 |
| C | -4.77840200 | 0.25820500  | -1.35609200 |
| H | -5.04017900 | 0.04472000  | -2.38624800 |
| H | 1.12590200  | 1.27450300  | 0.12432200  |

# Compound\_5\_H

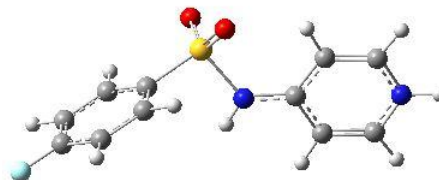
|   |             |             |             |
|---|-------------|-------------|-------------|
| 1 | 1           |             |             |
| S | -1.02152000 | 1.28650700  | 0.11258100  |
| O | -1.46556600 | 1.73966000  | -1.19128800 |
| O | -1.23121200 | 2.05839000  | 1.32081600  |
| N | -1.88345400 | -0.27084000 | 0.36669400  |
| C | 0.65650300  | 0.69149500  | 0.05231200  |
| C | 1.44219800  | 0.80094100  | 1.19962800  |
| C | 2.75768900  | 0.35159900  | 1.14458200  |
| C | 3.25768500  | -0.18771500 | -0.04081000 |
| C | 2.46076700  | -0.27493000 | -1.18411800 |
| C | 1.14440800  | 0.16846700  | -1.14533800 |
| C | -3.21289200 | -0.46879900 | 0.12055300  |
| N | -3.86040800 | -1.39946500 | 0.87821400  |
| C | -5.16825000 | -1.74833500 | 0.70464700  |
| C | -5.91371700 | -1.13089400 | -0.25871000 |
| C | -5.28971500 | -0.15093900 | -1.05378800 |
| C | -3.96136800 | 0.17897100  | -0.87985400 |
| H | 1.04338700  | 1.24409000  | 2.10330900  |
| H | 3.39012500  | 0.42464200  | 2.02006000  |
| H | 2.86659700  | -0.68594100 | -2.09939200 |
| H | 0.51944000  | 0.12364500  | -2.02804000 |
| H | -3.34737300 | -1.87068600 | 1.61511100  |
| H | -5.54331900 | -2.51428300 | 1.36943200  |
| H | -6.95158000 | -1.39958200 | -0.39641200 |
| H | -5.85742800 | 0.35284200  | -1.82722900 |
| H | -3.47549200 | 0.91878500  | -1.49761100 |
| C | 4.70607200  | -0.63069000 | -0.10248600 |
| F | 4.89216400  | -1.58574500 | -1.03189000 |
| F | 5.12102400  | -1.12045100 | 1.08081500  |
| F | 5.50851400  | 0.40588400  | -0.41720200 |
| H | -1.49038100 | -0.76210100 | 1.16367800  |



## Compound\_6\_H

1 1

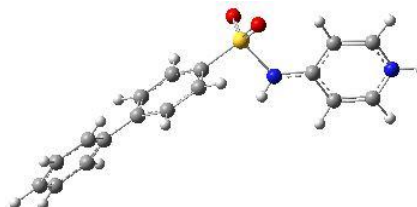
|   |             |             |             |
|---|-------------|-------------|-------------|
| S | -0.08768500 | 1.14169300  | -0.15418000 |
| O | 0.00536100  | 1.89842100  | -1.38733800 |
| O | 0.34371700  | 1.68745800  | 1.12135300  |
| N | 0.92954700  | -0.30387200 | -0.38641700 |
| N | 4.97916800  | -0.74815800 | 0.24885600  |
| H | 5.97383000  | -0.86642800 | 0.39864600  |
| C | 4.30411000  | -1.66828000 | -0.48360300 |
| H | 4.87821500  | -2.49668900 | -0.87571100 |
| C | 2.96366200  | -1.52541000 | -0.70345200 |
| H | 2.44677200  | -2.27072200 | -1.29430300 |
| C | 2.26391100  | -0.41068500 | -0.16513400 |
| C | 3.01000000  | 0.52521100  | 0.60076600  |
| H | 2.53304100  | 1.38441400  | 1.04776800  |
| C | 4.35073900  | 0.32850700  | 0.78336100  |
| H | 4.96403200  | 1.01195700  | 1.35492500  |
| C | -1.68359100 | 0.38308700  | -0.02246900 |
| C | -2.49602100 | 0.32801700  | -1.15843000 |
| H | -2.15864100 | 0.75013300  | -2.09667500 |
| C | -3.75402200 | -0.25180800 | -1.05406500 |
| H | -4.42299700 | -0.31002300 | -1.90296600 |
| C | -4.15765400 | -0.74844300 | 0.18026500  |
| C | -3.35987500 | -0.68450500 | 1.31912300  |
| H | -3.73305300 | -1.07015100 | 2.25912800  |
| C | -2.10214500 | -0.10770300 | 1.21809900  |
| H | -1.46502100 | -0.02166600 | 2.08911300  |
| F | -5.36871700 | -1.30474400 | 0.28061700  |
| H | 0.51690900  | -0.96596000 | -1.03455000 |



## Compound\_7\_H

1 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| S | 1.59589000  | -1.28266300 | 0.36690000  |
| O | 1.87112400  | -1.82147200 | 1.68525500  |
| O | 2.07352000  | -1.93219500 | -0.84283400 |
| N | 2.37110600  | 0.33088700  | 0.33497900  |
| N | 6.27455900  | 1.30589800  | -0.55893000 |
| H | 7.23214900  | 1.55438900  | -0.77424300 |
| C | 5.47274200  | 2.21507600  | 0.04986900  |
| H | 5.91126100  | 3.17722300  | 0.27688800  |
| C | 4.17964500  | 1.90016400  | 0.35435500  |
| H | 3.56025500  | 2.64085900  | 0.84368100  |
| C | 3.65989300  | 0.61422300  | 0.03568500  |
| C | 4.53472300  | -0.30487900 | -0.60678300 |
| H | 4.19465500  | -1.29031500 | -0.88789700 |
| C | 5.81943000  | 0.06926000  | -0.88375600 |
| H | 6.52396200  | -0.59275900 | -1.36872100 |
| C | -0.10240900 | -0.81676600 | 0.22834300  |
| C | -0.86978000 | -0.70164600 | 1.39054400  |
| H | -0.43580100 | -0.91641900 | 2.35920900  |
| C | -2.20777700 | -0.35315500 | 1.27154200  |
| H | -2.81727100 | -0.29807800 | 2.16474400  |
| C | -2.79438900 | -0.12052500 | 0.01435400  |

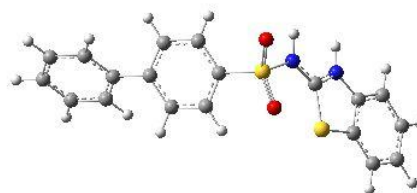


|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.98978600 | -0.25516100 | -1.13320500 |
| H | -2.41744900 | -0.07024300 | -2.11060700 |
| C | -0.65117500 | -0.60300200 | -1.03910500 |
| H | -0.04501800 | -0.71696400 | -1.92909100 |
| C | -4.22414800 | 0.24410300  | -0.09948200 |
| C | -5.00739500 | -0.24640500 | -1.15592700 |
| C | -4.82665000 | 1.08459000  | 0.84968100  |
| C | -6.35348300 | 0.09008000  | -1.25610600 |
| H | -4.57269500 | -0.92151700 | -1.88412500 |
| C | -6.17034400 | 1.42785400  | 0.74194000  |
| H | -4.23610300 | 1.49626200  | 1.66025300  |
| C | -6.93835400 | 0.92991500  | -0.30953100 |
| H | -6.94799000 | -0.30992100 | -2.06906800 |
| H | -6.61712800 | 2.08783700  | 1.47628400  |
| H | -7.98630700 | 1.19370700  | -0.39008300 |
| H | 1.85800000  | 1.01802100  | 0.87616500  |

# Compound\_8\_H

1 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.33879100 | -0.87427000 | -0.50131200 |
| C | -4.34599100 | -0.89424900 | 0.89355700  |
| C | -5.26011400 | -1.66203500 | 1.60796400  |
| C | -6.17263100 | -2.41480600 | 0.87636400  |
| C | -6.16993100 | -2.39756500 | -0.52419300 |
| C | -5.25369500 | -1.62609600 | -1.23282900 |
| C | -2.58328700 | 0.57284100  | 0.50861100  |
| H | -5.26374000 | -1.67429500 | 2.69140900  |
| H | -6.89780100 | -3.02356100 | 1.40174400  |
| H | -5.25686600 | -1.61176600 | -2.31551000 |
| S | -3.08205400 | 0.21203400  | -1.12173100 |
| N | -3.33645100 | -0.06932000 | 1.41505600  |
| N | -1.58239400 | 1.38936200  | 0.85845200  |
| S | -0.46429800 | 2.30214800  | -0.22709800 |
| O | -1.09523700 | 2.13822900  | -1.52382200 |
| O | -0.34278300 | 3.56123100  | 0.47252400  |
| C | 1.04774600  | 1.39875600  | -0.14452900 |
| C | 1.28417700  | 0.37272600  | -1.06453300 |
| C | 1.99466400  | 1.75151300  | 0.82184200  |
| C | 2.48656800  | -0.31391000 | -0.99897600 |
| H | 0.56086900  | 0.14588400  | -1.83736700 |
| C | 3.18810200  | 1.04771000  | 0.87033700  |
| H | 1.80555300  | 2.56743200  | 1.50808500  |
| C | 3.46012300  | 0.00248600  | -0.03222900 |
| H | 2.69352300  | -1.08227700 | -1.73312300 |
| H | 3.91789900  | 1.30425400  | 1.62779400  |
| H | -3.17774900 | 0.02208300  | 2.41096800  |
| C | 4.74121200  | -0.73447800 | 0.02320200  |
| C | 4.78830900  | -2.11138800 | -0.24698600 |
| C | 5.93623600  | -0.07085000 | 0.34343400  |
| C | 5.99323900  | -2.80393400 | -0.19193000 |
| H | 3.87500100  | -2.65058600 | -0.47151600 |
| C | 7.14156900  | -0.76351600 | 0.38739900  |
| H | 5.93110000  | 0.99780900  | 0.52452100  |

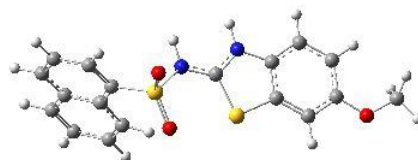


|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 7.17351500  | -2.13190200 | 0.12288100  |
| H | 6.01076400  | -3.86923200 | -0.38994500 |
| H | 8.05750200  | -0.23345000 | 0.62047400  |
| H | 8.11270100  | -2.67112400 | 0.16045400  |
| H | -6.89386500 | -2.99197700 | -1.06745700 |
| H | -1.46328500 | 1.62572900  | 1.83811800  |

#### Compound\_9\_H

1 1

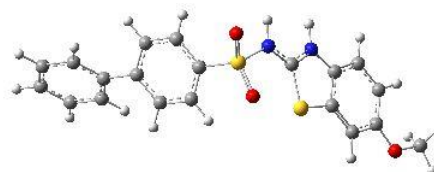
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.07766300  | -0.04271400 | -0.32288500 |
| C | 2.97757200  | -0.26371300 | 1.05336900  |
| C | 4.08727900  | -0.13537100 | 1.87727000  |
| C | 5.30181000  | 0.21638400  | 1.29759500  |
| C | 5.40602800  | 0.43537600  | -0.09018500 |
| C | 4.27845900  | 0.30400000  | -0.91533700 |
| C | 0.78064300  | -0.66383400 | 0.41366200  |
| H | 4.02133900  | -0.30423500 | 2.94563600  |
| H | 6.17016800  | 0.31805000  | 1.93265400  |
| H | 4.37836700  | 0.47542500  | -1.97926100 |
| S | 1.51164800  | -0.27858300 | -1.12250800 |
| N | 1.66665700  | -0.61811400 | 1.41514800  |
| N | -0.52391900 | -0.92971800 | 0.61518500  |
| S | -1.66192500 | -1.49808600 | -0.66363100 |
| O | -1.13275900 | -0.84883100 | -1.85142800 |
| O | -1.69623200 | -2.94071500 | -0.53764000 |
| H | 1.40976400  | -0.82108900 | 2.37324200  |
| O | 6.54389700  | 0.77523700  | -0.72371600 |
| C | 7.75595100  | 0.92610200  | 0.02463100  |
| H | 7.66393300  | 1.72852600  | 0.76185600  |
| H | 8.03211900  | -0.01111800 | 0.51562800  |
| C | -3.18438000 | -0.79568500 | -0.07942200 |
| C | -3.43365000 | 0.61612400  | -0.09927600 |
| C | -4.10797000 | -1.71525400 | 0.38369500  |
| C | -2.54380000 | 1.60721100  | -0.58454700 |
| C | -4.70415300 | 1.03701900  | 0.42112000  |
| C | -5.35106100 | -1.27156200 | 0.86880500  |
| H | -3.87595900 | -2.77205700 | 0.36428300  |
| C | -2.88855700 | 2.93938800  | -0.54214100 |
| H | -1.60108200 | 1.32108900  | -1.02690800 |
| C | -5.02097000 | 2.41965600  | 0.44693200  |
| C | -5.63280200 | 0.07321000  | 0.89066300  |
| H | -6.07437900 | -1.99627300 | 1.22033700  |
| C | -4.13166000 | 3.35496800  | -0.02022700 |
| H | -2.19785800 | 3.67991000  | -0.92843000 |
| H | -5.98476100 | 2.72307900  | 0.83987900  |
| H | -6.58790800 | 0.42070200  | 1.26920000  |
| H | -4.38374600 | 4.40827100  | -0.00032800 |
| H | 8.51539800  | 1.19043800  | -0.70694000 |
| H | -0.79780600 | -1.23253600 | 1.54497600  |



#### Compound\_10\_H

1 1

|   |            |            |             |
|---|------------|------------|-------------|
| C | 3.71877100 | 0.16792700 | -0.30959000 |
|---|------------|------------|-------------|

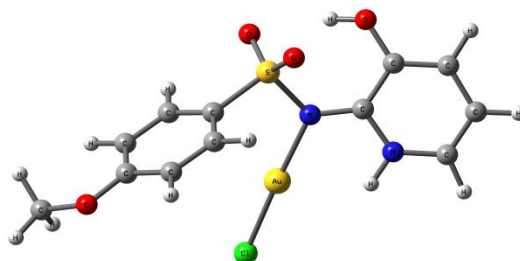


|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.70776300  | 0.05945900  | 1.08370900  |
| C | 4.67763200  | 0.68610000  | 1.85342700  |
| C | 5.65950200  | 1.42703100  | 1.20330600  |
| C | 5.67129000  | 1.53936200  | -0.20058100 |
| C | 4.68782500  | 0.89996100  | -0.97134300 |
| C | 1.84052100  | -1.22048600 | 0.56008900  |
| H | 4.68005400  | 0.60722000  | 2.93418700  |
| H | 6.41766600  | 1.91783200  | 1.79659700  |
| H | 4.71755500  | 0.99261300  | -2.04920900 |
| S | 2.38799800  | -0.75818900 | -1.03114300 |
| N | 2.62620300  | -0.72350500 | 1.52311900  |
| N | 0.77545700  | -1.99126500 | 0.82370900  |
| S | -0.43510400 | -2.63947200 | -0.33656100 |
| O | 0.24229800  | -2.49592300 | -1.61197000 |
| O | -0.76910000 | -3.90465200 | 0.27878100  |
| C | -1.79567100 | -1.51945200 | -0.22405600 |
| C | -1.86646900 | -0.43594200 | -1.10407600 |
| C | -2.79205700 | -1.75918500 | 0.72662600  |
| C | -2.95005600 | 0.42465800  | -1.01272800 |
| H | -1.11230900 | -0.29508000 | -1.86774400 |
| C | -3.86325100 | -0.88233400 | 0.80261900  |
| H | -2.73527800 | -2.62072300 | 1.38009600  |
| C | -3.96585100 | 0.22583700  | -0.05899100 |
| H | -3.03131600 | 1.24237600  | -1.71779900 |
| H | -4.62884700 | -1.05287600 | 1.54906900  |
| H | 2.44508500  | -0.88866300 | 2.50544300  |
| C | -5.11910500 | 1.14847300  | 0.02541000  |
| C | -4.95093800 | 2.52669000  | -0.18151600 |
| C | -6.40514600 | 0.66374000  | 0.31137600  |
| C | -6.03530200 | 3.39386100  | -0.09803500 |
| H | -3.96334600 | 2.92775700  | -0.37904500 |
| C | -7.48983900 | 1.53151300  | 0.38401000  |
| H | -6.56604400 | -0.40000200 | 0.44340500  |
| C | -7.30806200 | 2.89891400  | 0.18254800  |
| H | -5.88638700 | 4.45690900  | -0.24698400 |
| H | -8.47863400 | 1.13910500  | 0.59035200  |
| H | -8.15318900 | 3.57448900  | 0.24267700  |
| O | 6.58575700  | 2.23583500  | -0.90113100 |
| C | 7.64387600  | 2.91191600  | -0.21209800 |
| H | 7.24720800  | 3.67762700  | 0.46039000  |
| H | 8.26474200  | 2.20351500  | 0.34329500  |
| H | 8.23882300  | 3.38444600  | -0.98963800 |
| H | 0.62203400  | -2.31089700 | 1.77430600  |

Cartesian coordinates of optimized structures of imide tautomer (C) of **1-10** complexed with BH<sub>3</sub> and AuCl calculated at B3LYP/6-311++G(d,p) level of theory

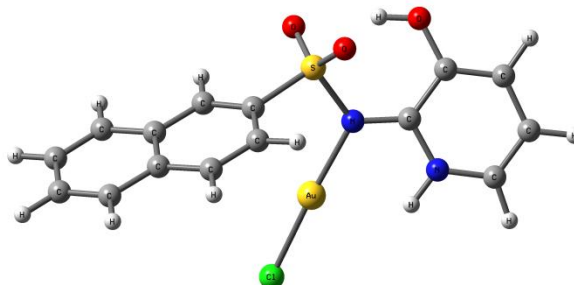
Compound\_1\_AuCl

|     |             |             |             |
|-----|-------------|-------------|-------------|
| 0 1 |             |             |             |
| S   | -0.47626200 | -1.96516800 | -0.42541600 |
| O   | -1.02595500 | -2.85807800 | 0.59726200  |
| O   | -0.50314700 | -2.32369800 | -1.83771300 |
| N   | -1.22151800 | -0.40069800 | -0.19973300 |
| C   | 1.21539400  | -1.59602200 | 0.01226000  |
| C   | 2.13855300  | -1.33042400 | -0.99368200 |
| C   | 3.46443800  | -1.06871200 | -0.66148600 |
| C   | 3.85850300  | -1.08257100 | 0.68142600  |
| C   | 2.92242300  | -1.37832300 | 1.68562900  |
| C   | 1.60523700  | -1.63525300 | 1.35485700  |
| C   | -2.50816200 | -0.29222900 | 0.15272200  |
| N   | -2.87372800 | 0.85937500  | 0.79966300  |
| C   | -4.11672900 | 1.15949500  | 1.26511800  |
| C   | -5.12544600 | 0.25718300  | 1.10703300  |
| C   | -4.85022700 | -0.93194700 | 0.39684500  |
| C   | -3.59633500 | -1.20392500 | -0.09943900 |
| H   | 1.82293100  | -1.32978700 | -2.02905200 |
| H   | 3.25593000  | -1.39728400 | 2.71564300  |
| H   | 0.88049500  | -1.87230700 | 2.12320700  |
| H   | -2.10847100 | 1.52889200  | 0.91405100  |
| H   | -4.22224500 | 2.12150800  | 1.74545500  |
| H   | -6.11691000 | 0.46859600  | 1.48069400  |
| H   | -5.65484700 | -1.62981500 | 0.18863100  |
| O   | -3.31413700 | -2.24721900 | -0.90358400 |
| H   | -3.95573100 | -2.95846500 | -0.80267700 |
| H   | 4.17119300  | -0.85297900 | -1.45025000 |
| O   | 5.11872200  | -0.83390500 | 1.11150900  |
| C   | 6.11104300  | -0.45803700 | 0.15901500  |
| H   | 5.82361800  | 0.45634800  | -0.36862700 |
| H   | 7.01658500  | -0.27649900 | 0.73452700  |
| H   | 6.29361300  | -1.26137200 | -0.56185200 |
| Au  | -0.00611400 | 1.31522300  | -0.24417400 |
| Cl  | 1.21457500  | 3.22354400  | -0.28790900 |



Compound\_2\_AuCl

|     |             |             |             |
|-----|-------------|-------------|-------------|
| 0 1 |             |             |             |
| S   | -0.54978600 | -1.94960900 | -0.35002100 |
| O   | -1.10274800 | -2.86802800 | 0.64793700  |
| O   | -0.46120100 | -2.32716200 | -1.75440000 |
| N   | -1.39298200 | -0.43497000 | -0.18995600 |
| C   | 1.09326500  | -1.47272800 | 0.19685200  |
| C   | 2.07712300  | -1.29794500 | -0.74463900 |
| C   | 3.39542300  | -0.98126100 | -0.33042800 |
| C   | 3.67334800  | -0.85696500 | 1.06743000  |
| C   | 2.62182100  | -1.06341200 | 2.00122100  |
| C   | 1.35297100  | -1.37168000 | 1.58453100  |

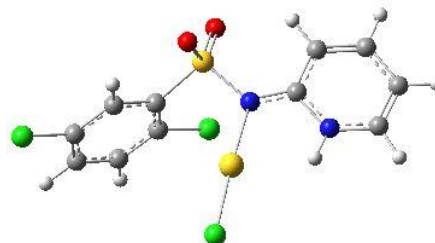


|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.69986800 | -0.39977000 | 0.10210500  |
| N  | -3.16188000 | 0.73232000  | 0.71976300  |
| C  | -4.44138000 | 0.96180300  | 1.12134800  |
| C  | -5.38662100 | -0.00001300 | 0.92335800  |
| C  | -5.00880300 | -1.17458700 | 0.23751700  |
| C  | -3.71802500 | -1.37489800 | -0.19527600 |
| H  | 1.84650500  | -1.40308600 | -1.79771000 |
| H  | 2.83820800  | -0.97979000 | 3.06071000  |
| H  | 0.55673700  | -1.54905400 | 2.29562100  |
| H  | -2.44402800 | 1.44761400  | 0.86171500  |
| H  | -4.62682800 | 1.91930900  | 1.58622000  |
| H  | -6.40578800 | 0.15540200  | 1.24661400  |
| H  | -5.76027600 | -1.91935900 | -0.00407000 |
| C  | 4.44456100  | -0.78357500 | -1.26516400 |
| H  | 4.22702800  | -0.87506800 | -2.32367600 |
| C  | 5.71262600  | -0.47344300 | -0.83679100 |
| H  | 6.50734000  | -0.31893200 | -1.55750100 |
| C  | 5.98833700  | -0.34922200 | 0.54502600  |
| H  | 6.99286800  | -0.10174400 | 0.86907600  |
| C  | 4.99323200  | -0.53718200 | 1.47484700  |
| H  | 5.20593100  | -0.43989800 | 2.53403300  |
| O  | -3.33596800 | -2.40246900 | -0.97808000 |
| H  | -3.93527100 | -3.15246000 | -0.89995100 |
| Au | -0.29104200 | 1.35697600  | -0.22857800 |
| Cl | 0.78127900  | 3.35051600  | -0.26688400 |

Compound\_3\_AuCl

0 1

|    |             |             |             |
|----|-------------|-------------|-------------|
| S  | 0.04376900  | -1.51830100 | -1.18383500 |
| O  | -0.30988400 | -1.00934600 | -2.50180900 |
| O  | 0.53623000  | -2.88889800 | -1.05899200 |
| N  | 1.12692400  | -0.41227800 | -0.46527300 |
| C  | -1.41136300 | -1.31875400 | -0.12646900 |
| C  | -1.44453000 | -1.68498300 | 1.22444100  |
| C  | -2.63545000 | -1.55333200 | 1.93499100  |
| C  | -3.78275400 | -1.07718800 | 1.31125200  |
| C  | -3.73960200 | -0.72600800 | -0.03527900 |
| C  | -2.55880700 | -0.84126200 | -0.75895800 |
| C  | 2.43093600  | -0.68670400 | -0.28924700 |
| N  | 3.16247400  | 0.32142600  | 0.28863500  |
| C  | 4.49415600  | 0.26946300  | 0.55088800  |
| C  | 5.20967300  | -0.84988400 | 0.24309800  |
| C  | 4.51326800  | -1.92589800 | -0.35315300 |
| C  | 3.16840000  | -1.86246400 | -0.61986400 |
| H  | -2.65790300 | -1.82616600 | 2.98218100  |
| H  | -2.51292100 | -0.56217700 | -1.80290700 |
| H  | 2.62806000  | 1.16639100  | 0.50930000  |
| H  | 4.91603700  | 1.15635900  | 1.00368800  |
| H  | 6.26935100  | -0.89797900 | 0.44832500  |
| H  | 5.05221300  | -2.82937500 | -0.61467000 |
| H  | 2.64838100  | -2.69155700 | -1.07026200 |
| H  | -4.70467000 | -0.97815000 | 1.86960300  |
| Cl | -0.05088600 | -2.28239000 | 2.07044200  |
| Cl | -5.17289400 | -0.13388200 | -0.82134900 |

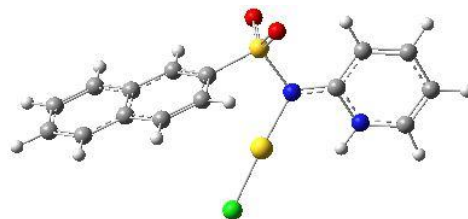


|    |             |            |             |
|----|-------------|------------|-------------|
| Au | 0.33391500  | 1.49043100 | -0.03318700 |
| Cl | -0.42435400 | 3.55600300 | 0.48446800  |

Compound\_4\_ AuCl

O 1

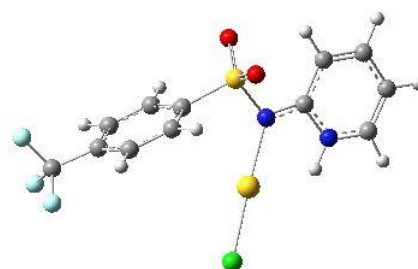
|    |             |             |             |
|----|-------------|-------------|-------------|
| S  | -0.52367000 | -2.01683800 | -0.37416400 |
| O  | -0.97589800 | -3.08233700 | 0.52520100  |
| O  | -0.53272900 | -2.24888700 | -1.81653300 |
| N  | -1.44678400 | -0.59489400 | -0.04499200 |
| C  | 1.11441700  | -1.50164200 | 0.12707000  |
| C  | 2.03424700  | -1.20400200 | -0.84812800 |
| C  | 3.35338300  | -0.84259400 | -0.47732200 |
| C  | 3.69768200  | -0.80110000 | 0.91083500  |
| C  | 2.71030300  | -1.13219400 | 1.87842200  |
| C  | 1.43942400  | -1.48425300 | 1.50470000  |
| C  | -2.78084900 | -0.68921400 | 0.04330100  |
| N  | -3.45407300 | 0.49607000  | 0.21520800  |
| C  | -4.80296700 | 0.61772700  | 0.32783200  |
| C  | -5.59881400 | -0.48737600 | 0.26955300  |
| C  | -4.96656600 | -1.74081400 | 0.08915200  |
| C  | -3.60487100 | -1.85486000 | -0.02010700 |
| H  | 1.75260000  | -1.24546800 | -1.89327300 |
| H  | 2.97764300  | -1.10841000 | 2.92915000  |
| H  | 0.69215500  | -1.75296800 | 2.23992500  |
| H  | -2.85797100 | 1.32771900  | 0.24083500  |
| H  | -5.17151700 | 1.62611800  | 0.45805800  |
| H  | -6.67190200 | -0.39624100 | 0.35604200  |
| H  | -5.57065200 | -2.63931800 | 0.03617100  |
| H  | -3.13707200 | -2.81904000 | -0.13905000 |
| C  | 4.33840700  | -0.51840900 | -1.44585700 |
| H  | 4.07025800  | -0.54798900 | -2.49621100 |
| C  | 5.60824700  | -0.16522800 | -1.05851500 |
| H  | 6.35392200  | 0.08588700  | -1.80393600 |
| C  | 5.94971300  | -0.12266700 | 0.31353700  |
| H  | 6.95489000  | 0.16013900  | 0.60491400  |
| C  | 5.01775300  | -0.43383200 | 1.27518900  |
| H  | 5.28093500  | -0.39879700 | 2.32681600  |
| Au | -0.48666400 | 1.27483000  | -0.05528300 |
| Cl | 0.43940400  | 3.33944400  | -0.04143000 |



Compound\_5\_ AuCl

O 1

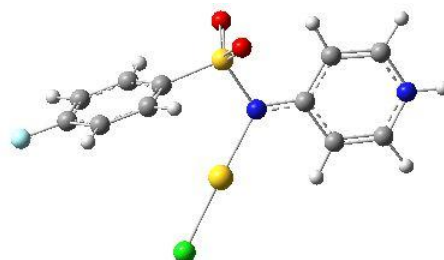
|   |             |             |             |
|---|-------------|-------------|-------------|
| S | -0.69545100 | -1.99653400 | 0.53087000  |
| O | -0.87604400 | -2.20233100 | 1.96490100  |
| O | -0.98277800 | -3.09316100 | -0.39655000 |
| N | -1.59898600 | -0.61417200 | 0.04946700  |
| C | 0.98933800  | -1.43909000 | 0.24309300  |
| C | 1.51524900  | -1.50863100 | -1.04511100 |
| C | 2.83482900  | -1.12555800 | -1.25006500 |
| C | 3.60737200  | -0.69206700 | -0.17097700 |
| C | 3.07363000  | -0.64446100 | 1.11605100  |
| C | 1.75198800  | -1.02268800 | 1.33026700  |
| C | -2.91123700 | -0.75125000 | -0.19938900 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | -3.58601700 | 0.40638700  | -0.49749200 |
| C  | -4.91351400 | 0.48439400  | -0.77799100 |
| C  | -5.68228300 | -0.64158500 | -0.77522700 |
| C  | -5.04612900 | -1.86822600 | -0.47216200 |
| C  | -3.70513900 | -1.93738800 | -0.19291400 |
| H  | 0.90612600  | -1.86040900 | -1.86763700 |
| H  | 3.26153500  | -1.16126600 | -2.24410900 |
| H  | 3.68077300  | -0.30688500 | 1.94586100  |
| H  | 1.31698500  | -0.99857600 | 2.32082700  |
| H  | -3.01342500 | 1.25445800  | -0.48198700 |
| H  | -5.28851900 | 1.47632400  | -0.99010800 |
| H  | -6.73844500 | -0.58535200 | -0.99574100 |
| H  | -5.62906900 | -2.78195400 | -0.45884400 |
| H  | -3.23277400 | -2.88305800 | 0.01993200  |
| C  | 5.05612900  | -0.33501800 | -0.39395800 |
| F  | 5.50540200  | 0.56143000  | 0.50697800  |
| F  | 5.26741600  | 0.18352700  | -1.62213800 |
| F  | 5.85263300  | -1.42900800 | -0.28981100 |
| Au | -0.69679200 | 1.28374000  | 0.12728800  |
| Cl | 0.17798500  | 3.36706300  | 0.17450200  |

Compound\_6\_ AuCl

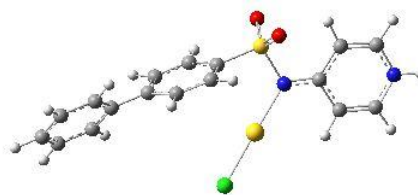
|     |             |             |             |
|-----|-------------|-------------|-------------|
| O 1 |             |             |             |
| S   | -0.31110200 | -2.02880100 | 0.00019600  |
| O   | -0.63163300 | -2.69759200 | -1.26306200 |
| O   | -0.63150000 | -2.69720700 | 1.26368700  |
| N   | -1.08857500 | -0.47469400 | 0.00000500  |
| N   | -5.22380100 | -0.24842900 | -0.00026700 |
| H   | -6.22992000 | -0.17525900 | -0.00032100 |
| C   | -4.46018100 | 0.88315500  | -0.00027400 |
| H   | -4.99292300 | 1.82430900  | -0.00034600 |
| C   | -3.10464400 | 0.80907400  | -0.00019000 |
| H   | -2.51585000 | 1.71740400  | -0.00019400 |
| C   | -2.42492400 | -0.45822600 | -0.00008800 |
| C   | -3.28192700 | -1.61689400 | -0.00009100 |
| H   | -2.87340500 | -2.61506500 | -0.00004100 |
| C   | -4.63416300 | -1.47777000 | -0.00017700 |
| H   | -5.30165500 | -2.32881200 | -0.00018000 |
| C   | 1.42471900  | -1.60259100 | 0.00003200  |
| C   | 2.08999000  | -1.47544700 | -1.21884400 |
| H   | 1.55011200  | -1.60115300 | -2.14822400 |
| C   | 3.45027200  | -1.19182200 | -1.21956700 |
| H   | 4.00535000  | -1.07812700 | -2.14164100 |
| C   | 4.09877900  | -1.05214100 | -0.00021200 |
| C   | 3.45046000  | -1.19164500 | 1.21926200  |
| H   | 4.00567600  | -1.07781400 | 2.14123500  |
| C   | 2.09017500  | -1.47526800 | 1.21878800  |
| H   | 1.55043500  | -1.60083300 | 2.14826600  |
| F   | 5.41897900  | -0.77999800 | -0.00033400 |
| Au  | 0.08841700  | 1.26250400  | 0.00006400  |
| Cl  | 1.30143800  | 3.17623700  | 0.00007400  |



## Compound\_7\_ AuCl

O 1

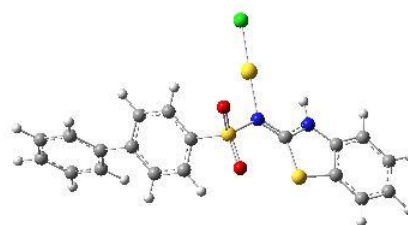
|    |             |             |             |
|----|-------------|-------------|-------------|
| S  | 1.19973300  | -2.01510700 | 0.26380100  |
| O  | 1.50516700  | -2.47012800 | 1.62173600  |
| O  | 1.52117900  | -2.88680300 | -0.87019300 |
| N  | 2.00486700  | -0.49164200 | 0.01488500  |
| N  | 6.13389000  | -0.36126600 | -0.27997700 |
| H  | 7.13887200  | -0.31102700 | -0.34950200 |
| C  | 5.38827400  | 0.77911200  | -0.36875600 |
| H  | 5.93366500  | 1.70131000  | -0.51604600 |
| C  | 4.03497800  | 0.73612300  | -0.27368000 |
| H  | 3.46120800  | 1.65129800  | -0.34436500 |
| C  | 3.33710400  | -0.50661000 | -0.07717900 |
| C  | 4.17584000  | -1.67636900 | 0.00691700  |
| H  | 3.75227400  | -2.65801200 | 0.14845100  |
| C  | 5.52694600  | -1.56821900 | -0.09385000 |
| H  | 6.18050500  | -2.42775000 | -0.03124700 |
| C  | -0.52652300 | -1.56473800 | 0.17296600  |
| C  | -1.20762800 | -1.23780300 | 1.34386800  |
| H  | -0.68963400 | -1.24584300 | 2.29423300  |
| C  | -2.55572900 | -0.91460000 | 1.26587900  |
| H  | -3.09521700 | -0.67030100 | 2.17287900  |
| C  | -3.23357100 | -0.92271000 | 0.03693500  |
| C  | -2.52333900 | -1.28195100 | -1.11894100 |
| H  | -3.02676900 | -1.28099600 | -2.07820200 |
| C  | -1.17396500 | -1.60507200 | -1.06012100 |
| H  | -0.62663000 | -1.87889500 | -1.95292500 |
| C  | -4.67042000 | -0.55978800 | -0.03679000 |
| C  | -5.55987000 | -1.29928600 | -0.82956200 |
| C  | -5.16733800 | 0.53562800  | 0.68428900  |
| C  | -6.90794000 | -0.95751300 | -0.89445900 |
| H  | -5.19810300 | -2.16156800 | -1.37849000 |
| C  | -6.51433100 | 0.87999500  | 0.61402600  |
| H  | -4.48785400 | 1.13974300  | 1.27449500  |
| C  | -7.38988100 | 0.13381000  | -0.17333900 |
| H  | -7.58315200 | -1.54748300 | -1.50415200 |
| H  | -6.87785400 | 1.73856200  | 1.16736900  |
| H  | -8.43895100 | 0.40198600  | -0.22638500 |
| Au | 0.86420900  | 1.26896200  | -0.01781500 |
| Cl | -0.31107700 | 3.20873300  | -0.04914500 |



## Compound\_8\_ AuCl

O 1

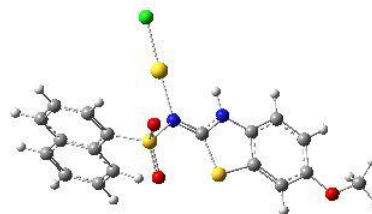
|   |            |             |             |
|---|------------|-------------|-------------|
| C | 4.12282700 | -2.19359000 | -0.25796200 |
| C | 4.06963100 | -1.03424000 | -1.03472500 |
| C | 4.99635600 | -0.79844200 | -2.04675000 |
| C | 5.98290600 | -1.75719800 | -2.26095600 |
| C | 6.04116800 | -2.91945300 | -1.48426200 |
| C | 5.11025100 | -3.14958900 | -0.47316200 |
| C | 2.23447100 | -0.65322200 | 0.36601300  |
| H | 4.94956300 | 0.10307300  | -2.64602300 |
| H | 6.71629700 | -1.59680300 | -3.04190200 |
| H | 5.15645600 | -4.04865800 | 0.12944000  |



|    |             |             |             |
|----|-------------|-------------|-------------|
| S  | 2.82913800  | -2.21746400 | 0.95514700  |
| N  | 3.01048100  | -0.21495600 | -0.65348500 |
| N  | 1.20758100  | 0.06778700  | 0.77640700  |
| S  | 0.21208000  | -0.45263500 | 2.09011800  |
| O  | 0.69792200  | -1.77693700 | 2.48999800  |
| O  | 0.16280500  | 0.64766600  | 3.03645300  |
| C  | -1.39252500 | -0.63702100 | 1.32711400  |
| C  | -1.75570700 | -1.87507500 | 0.79980200  |
| C  | -2.25896400 | 0.45343600  | 1.28620700  |
| C  | -3.00685400 | -2.01356200 | 0.21258000  |
| H  | -1.08110400 | -2.71858400 | 0.87429100  |
| C  | -3.50483900 | 0.29798400  | 0.69110400  |
| H  | -1.96122300 | 1.40412400  | 1.70932900  |
| C  | -3.90082500 | -0.93245200 | 0.14375600  |
| H  | -3.30674000 | -2.98160400 | -0.17033300 |
| H  | -4.16912400 | 1.15138700  | 0.63097600  |
| H  | 2.78874200  | 0.68015900  | -1.08238100 |
| C  | -5.23444900 | -1.09084000 | -0.48697900 |
| C  | -5.39045700 | -1.85318600 | -1.65403100 |
| C  | -6.36933700 | -0.48268200 | 0.06953000  |
| C  | -6.64117400 | -2.00090800 | -2.24677400 |
| H  | -4.52257500 | -2.30981200 | -2.11611800 |
| C  | -7.62060200 | -0.63454100 | -0.52108100 |
| H  | -6.27596500 | 0.09186100  | 0.98405300  |
| C  | -7.76131800 | -1.39343400 | -1.68173900 |
| H  | -6.73936200 | -2.58416500 | -3.15539900 |
| H  | -8.48748200 | -0.16481300 | -0.07027100 |
| H  | -8.73550100 | -1.50939000 | -2.14274900 |
| H  | 6.81901500  | -3.65043300 | -1.66847900 |
| Au | 0.77493900  | 1.92959300  | -0.09802800 |
| Cl | 0.36669000  | 3.91116500  | -1.10427400 |

Compound\_9\_ AuCl

|     |             |             |             |
|-----|-------------|-------------|-------------|
| 0 1 |             |             |             |
| C   | 3.59837800  | -0.77908700 | 0.41729400  |
| C   | 3.27619600  | 0.39822800  | -0.26481700 |
| C   | 4.25153200  | 1.10528300  | -0.95228500 |
| C   | 5.55939300  | 0.61959800  | -0.94811900 |
| C   | 5.88144200  | -0.56152500 | -0.26296700 |
| C   | 4.89207600  | -1.27257200 | 0.42877600  |
| C   | 1.16727200  | -0.14628600 | 0.58492600  |
| H   | 4.00950500  | 2.01787800  | -1.48393600 |
| H   | 6.31967600  | 1.17096300  | -1.48285900 |
| H   | 5.16135500  | -2.18118500 | 0.95203800  |
| S   | 2.16785300  | -1.48009000 | 1.19818600  |
| N   | 1.92068400  | 0.70708300  | -0.14093000 |
| N   | -0.12742000 | 0.06763900  | 0.74215200  |
| S   | -1.05326000 | -0.92527800 | 1.80614700  |
| O   | -0.32564300 | -2.19101100 | 1.95163100  |
| O   | -1.36337000 | -0.13951000 | 2.99053600  |
| H   | 1.47591200  | 1.53012100  | -0.53895000 |
| O   | 7.12948900  | -1.10190500 | -0.20924800 |
| C   | 8.19572800  | -0.44084000 | -0.88235000 |

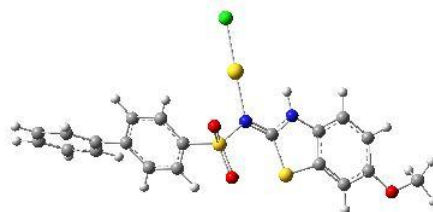


|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 8.01192000  | -0.38443900 | -1.96032200 |
| H  | 8.35668600  | 0.56540800  | -0.48177600 |
| C  | -2.56469900 | -1.16408700 | 0.86429600  |
| C  | -2.60359200 | -1.94659500 | -0.33249100 |
| C  | -3.68256200 | -0.54518600 | 1.37674500  |
| C  | -1.49530900 | -2.62638700 | -0.90201200 |
| C  | -3.87046100 | -2.03637900 | -0.99943200 |
| C  | -4.92079600 | -0.66442700 | 0.71357900  |
| H  | -3.59988800 | 0.03886900  | 2.28380300  |
| C  | -1.63141300 | -3.33733700 | -2.07149700 |
| H  | -0.53948600 | -2.61138900 | -0.39954000 |
| C  | -3.97069100 | -2.78089700 | -2.20304800 |
| C  | -5.00590200 | -1.38676700 | -0.44926700 |
| H  | -5.79278300 | -0.17037000 | 1.12398100  |
| C  | -2.87542400 | -3.41536900 | -2.73396800 |
| H  | -0.77153700 | -3.85158900 | -2.48557600 |
| H  | -4.93432100 | -2.83726800 | -2.69768600 |
| H  | -5.95245000 | -1.47011800 | -0.97255700 |
| H  | -2.96271300 | -3.98000100 | -3.65492800 |
| H  | 9.08034700  | -1.04751300 | -0.69885900 |
| Au | -1.05534500 | 1.75557800  | -0.10026600 |
| Cl | -1.97688800 | 3.58388300  | -1.06019100 |

Compound\_10\_ AuCl

O 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.90731200  | -1.45115800 | 0.36415900  |
| C | 3.76766200  | -0.44309800 | -0.59434600 |
| C | 4.72484200  | -0.27057200 | -1.58319000 |
| C | 5.82887500  | -1.12309200 | -1.60248800 |
| C | 5.96836500  | -2.13457400 | -0.64034500 |
| C | 4.99880400  | -2.30349400 | 0.35683600  |
| C | 1.81877500  | -0.07248100 | 0.64464700  |
| H | 4.62375900  | 0.50873400  | -2.32923400 |
| H | 6.57518300  | -0.98835700 | -2.37243400 |
| H | 5.12669100  | -3.08787100 | 1.09192500  |
| S | 2.55371900  | -1.43880700 | 1.51107200  |
| N | 2.59727000  | 0.29077500  | -0.39733700 |
| N | 0.69002200  | 0.57075300  | 0.88937700  |
| S | -0.32277200 | 0.13941800  | 2.21681300  |
| O | 0.31604400  | -0.99682400 | 2.88801000  |
| O | -0.61431600 | 1.36920900  | 2.93192400  |
| C | -1.81447000 | -0.43387700 | 1.41636000  |
| C | -1.94594900 | -1.78790300 | 1.11271100  |
| C | -2.82584500 | 0.47821900  | 1.12148600  |
| C | -3.10783200 | -2.22727600 | 0.49084500  |
| H | -1.16515800 | -2.48652700 | 1.38549100  |
| C | -3.97949900 | 0.02189300  | 0.49578900  |
| H | -2.71019800 | 1.52390900  | 1.37584700  |
| C | -4.14137900 | -1.33308000 | 0.16732500  |
| H | -3.22838100 | -3.28333700 | 0.28114500  |
| H | -4.75488700 | 0.73324700  | 0.23891400  |
| H | 2.29899300  | 1.07036000  | -0.97786200 |
| C | -5.37800100 | -1.81183900 | -0.49851100 |
| C | -5.31909700 | -2.78013000 | -1.51172000 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -6.63390500 | -1.30795400 | -0.12932100 |
| C  | -6.47904000 | -3.22855000 | -2.13707100 |
| H  | -4.35679600 | -3.16393900 | -1.83102500 |
| C  | -7.79393300 | -1.76012800 | -0.75174900 |
| H  | -6.70519000 | -0.57653500 | 0.66757900  |
| C  | -7.72102800 | -2.72142700 | -1.75851000 |
| H  | -6.41187100 | -3.96846200 | -2.92668900 |
| H  | -8.75614000 | -1.36548900 | -0.44551500 |
| H  | -8.62432900 | -3.07139100 | -2.24491800 |
| O  | 7.01325300  | -3.00530800 | -0.58881200 |
| C  | 8.04945700  | -2.89481500 | -1.55902200 |
| H  | 7.66510200  | -3.05244100 | -2.57214500 |
| H  | 8.54773400  | -1.92160200 | -1.50026400 |
| H  | 8.76302200  | -3.68030500 | -1.31797600 |
| Cl | -0.48843900 | 3.91548700  | -1.65025900 |
| Au | 0.09424300  | 2.19723600  | -0.30166000 |

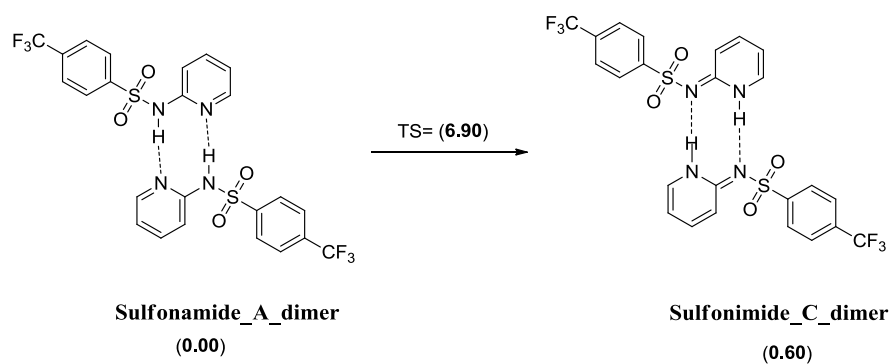
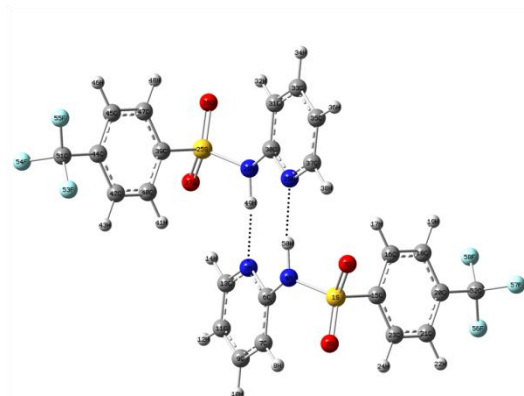


Figure SI-2: Hydrogen transfer in sulfonamide\_A\_dimer by intermolecular mechanism. The values in parentheses represent the relative energy in kcal/mol.

### Cartesian coordinates of Sulfonamide\_5A\_dimer, Transition state, and Sulfonamide\_5C\_dimer

#### Sulfonamide\_5A\_dimer

|     |             |             |             |
|-----|-------------|-------------|-------------|
| 0 1 |             |             |             |
| S   | -2.25719000 | -1.47946000 | -2.05092000 |
| O   | -2.58639300 | -2.87951900 | -2.28905800 |
| O   | -1.87718000 | -0.58980600 | -3.14238100 |
| N   | -0.96664300 | -1.39615900 | -0.97791100 |
| N   | -0.30787300 | -1.30292700 | 1.23608900  |
| C   | -0.93229900 | -2.01370500 | 0.28764800  |
| C   | -1.46301200 | -3.28903700 | 0.52558000  |
| H   | -1.91950000 | -3.84669200 | -0.27932500 |
| C   | -1.36180200 | -3.80778000 | 1.80835800  |
| H   | -1.76580500 | -4.79087300 | 2.02263700  |
| C   | -0.72456200 | -3.07082700 | 2.80579500  |
| H   | -0.62430300 | -3.44803800 | 3.81538700  |
| C   | -0.20244400 | -1.83027700 | 2.46600800  |



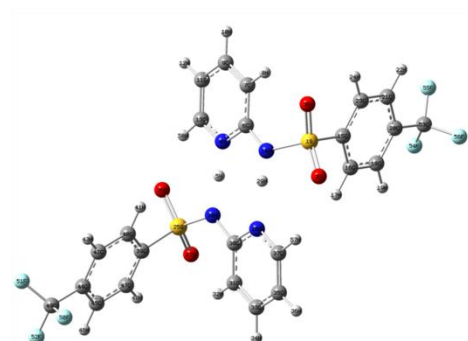
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.32325300  | -1.21750200 | 3.19006200  |
| C | -3.66796700 | -0.74411300 | -1.19224500 |
| C | -3.64414500 | 0.61548800  | -0.88318300 |
| H | -2.79029400 | 1.22609600  | -1.14916100 |
| C | -4.73270800 | 1.17833100  | -0.22959300 |
| H | -4.72749400 | 2.23071700  | 0.02455800  |
| C | -5.83064800 | 0.38104800  | 0.10448700  |
| C | -5.84722800 | -0.97479500 | -0.21495600 |
| H | -6.70230100 | -1.58478900 | 0.04618500  |
| C | -4.75616500 | -1.54635400 | -0.86610800 |
| H | -4.74978800 | -2.59586000 | -1.12895800 |
| S | 2.25722000  | 1.47946200  | 2.05094000  |
| O | 2.58643800  | 2.87951700  | 2.28908000  |
| O | 1.87721600  | 0.58980600  | 3.14240300  |
| N | 0.96665900  | 1.39617600  | 0.97794800  |
| N | 0.30787700  | 1.30295400  | -1.23605000 |
| C | 0.93230400  | 2.01372900  | -0.28760800 |
| C | 1.46301100  | 3.28906500  | -0.52553600 |
| H | 1.91950100  | 3.84671700  | 0.27937000  |
| C | 1.36179200  | 3.80781400  | -1.80831100 |
| H | 1.76579000  | 4.79091100  | -2.02258600 |
| C | 0.72455100  | 3.07086500  | -2.80574800 |
| H | 0.62428600  | 3.44808000  | -3.81533800 |
| C | 0.20244000  | 1.83031100  | -2.46596600 |
| H | -0.32325800 | 1.21753600  | -3.19002000 |
| C | 3.66798000  | 0.74410700  | 1.19224500  |
| C | 3.64415000  | -0.61549700 | 0.88319200  |
| H | 2.79030300  | -1.22610100 | 1.14919100  |
| C | 4.73269900  | -1.17834600 | 0.22958400  |
| H | 4.72747800  | -2.23073300 | -0.02456100 |
| C | 5.83063300  | -0.38106700 | -0.10452300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 5.84722300  | 0.97477800  | 0.21491200  |
| H | 6.70229200  | 1.58476900  | -0.04625100 |
| C | 4.75617300  | 1.54634300  | 0.86608100  |
| H | 4.74980400  | 2.59585100  | 1.12892500  |
| H | 0.49765500  | 0.47272600  | 1.02187200  |
| H | -0.49764200 | -0.47270700 | -1.02183500 |
| C | 7.02906300  | -1.01361900 | -0.76537100 |
| C | -7.02909200 | 1.01359300  | 0.76531500  |
| F | 6.67505000  | -2.00075200 | -1.61690800 |
| F | 7.86341800  | -1.56797800 | 0.14836500  |
| F | 7.75700900  | -0.11909100 | -1.46696800 |
| F | -7.75704400 | 0.11906100  | 1.46690200  |
| F | -7.86343700 | 1.56794500  | -0.14843600 |
| F | -6.67510000 | 2.00073100  | 1.61685500  |

# Sulfonamide\_5A\_H\_transfer\_TS

0 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| S | 2.73189800  | 1.10986100  | 2.28460700  |
| O | 2.32233300  | 0.12205700  | 3.27179300  |
| O | 3.23322800  | 2.41958500  | 2.68404700  |
| N | 0.42672300  | 1.78900000  | -0.75786000 |
| H | -0.26223100 | 0.79287700  | -0.69954700 |
| C | 1.29064400  | 2.15274000  | 0.21778900  |
| C | 2.01376200  | 3.35078200  | 0.09517800  |
| H | 2.66533500  | 3.65894700  | 0.89851300  |
| C | 1.85076100  | 4.12195500  | -1.04219800 |
| H | 2.40765000  | 5.04692900  | -1.14021700 |
| C | 0.96416200  | 3.72246400  | -2.04492100 |
| H | 0.81326100  | 4.30759000  | -2.94168900 |
| C | 0.25823800  | 2.55248600  | -1.85778900 |
| N | 1.37036600  | 1.30175400  | 1.30618200  |
| C | 3.97846500  | 0.36334600  | 1.21216900  |
| C | 3.75282800  | -0.91030100 | 0.69045400  |
| H | 2.83804400  | -1.44548600 | 0.91344300  |
| C | 4.72066700  | -1.48623100 | -0.12239400 |
| H | 4.55781400  | -2.47076100 | -0.54235600 |
| C | 5.89979700  | -0.78948400 | -0.40002900 |
| C | 6.11831400  | 0.47843500  | 0.13391700  |
| H | 7.03528200  | 1.01037500  | -0.08419500 |

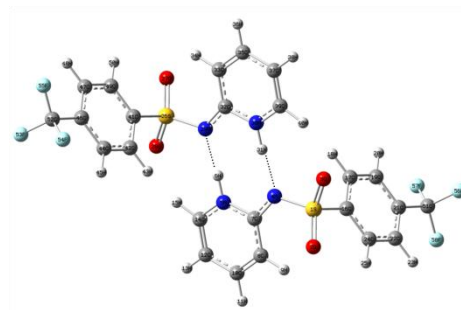


|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 5.14941000  | 1.06484000  | 0.94547000  |
| H | 5.30202000  | 2.04611000  | 1.37511600  |
| S | -2.19170400 | -0.42757100 | -1.94140100 |
| O | -1.99605400 | 0.79789800  | -2.73106800 |
| O | -2.18096200 | -1.71581800 | -2.64278300 |
| N | -0.20730900 | -0.97750500 | 1.29750900  |
| H | 0.73767300  | 0.43621000  | 1.30737900  |
| C | -1.00752300 | -1.31164000 | 0.26129500  |
| C | -1.66480500 | -2.56223100 | 0.24427500  |
| H | -2.24818000 | -2.85745800 | -0.61440500 |
| C | -1.52049600 | -3.41364400 | 1.32555500  |
| H | -2.02786900 | -4.37230000 | 1.31980700  |
| C | -0.71853400 | -3.04426500 | 2.40711200  |
| H | -0.58793700 | -3.68469200 | 3.26952500  |
| C | -0.07421200 | -1.82061200 | 2.33418100  |
| N | -1.10261800 | -0.33122400 | -0.71749500 |
| C | -3.82555300 | -0.29002000 | -1.16179400 |
| C | -4.07603700 | 0.74550100  | -0.26153000 |
| H | -3.28862400 | 1.43863500  | 0.00671300  |
| C | -5.34182300 | 0.87392700  | 0.29280000  |
| H | -5.54793500 | 1.67283500  | 0.99483400  |
| C | -6.35054300 | -0.02798200 | -0.06105900 |
| C | -6.09491400 | -1.05579800 | -0.96420600 |
| H | -6.88022700 | -1.74876600 | -1.23619600 |
| C | -4.82252400 | -1.18929400 | -1.51935900 |
| H | -4.60215300 | -1.98102500 | -2.22379600 |
| C | -7.70953100 | 0.12504600  | 0.56972800  |
| F | -7.66723400 | -0.09522700 | 1.90739000  |
| F | -8.20152000 | 1.37644000  | 0.40425500  |
| F | -8.61909900 | -0.72991100 | 0.05880100  |
| C | 6.96639700  | -1.44645000 | -1.24037600 |
| F | 6.43743200  | -2.21736400 | -2.21434900 |
| F | 7.77433700  | -0.54341000 | -1.83529300 |
| F | 7.75938600  | -2.25057200 | -0.49162600 |
| H | 0.58335000  | -1.47907500 | 3.12583600  |
| H | -0.46829300 | 2.16745400  | -2.56255100 |

# **Sulfonimide\_5C\_imide\_dimer**

0 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| S | -2.56314100 | -0.08815500 | -2.04466300 |
| O | -2.77235100 | -1.11721600 | -3.07046500 |
| O | -2.21300400 | 1.27430700  | -2.46788100 |
| N | -1.41864600 | -0.47952100 | -0.93370800 |
| N | -0.33908300 | -1.83475800 | 0.54867500  |
| H | 0.24459500  | -0.99627000 | 0.73625000  |
| C | -1.31478500 | -1.71115700 | -0.40728200 |
| C | -2.06387800 | -2.88832300 | -0.68678800 |
| H | -2.80686600 | -2.85772100 | -1.46860500 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.80904300 | -4.04805400 | 0.00850200  |
| H | -2.39120700 | -4.93469100 | -0.21778800 |
| C | -0.80518300 | -4.10780900 | 0.99486300  |
| H | -0.59865600 | -5.01467300 | 1.54506400  |
| C | -0.07677500 | -2.97213300 | 1.23402200  |
| H | 0.72865700  | -2.88824100 | 1.95164600  |
| C | -4.11658700 | 0.03113900  | -1.11439400 |
| C | -4.17733700 | 0.82136100  | 0.03278000  |
| H | -3.29498000 | 1.33736100  | 0.38961900  |
| C | -5.38017100 | 0.93394800  | 0.71873600  |
| H | -5.43875800 | 1.53613900  | 1.61664900  |
| C | -6.51227700 | 0.26219900  | 0.25021700  |
| C | -6.44597100 | -0.51847700 | -0.90198300 |
| H | -7.32676100 | -1.03645100 | -1.25960900 |
| C | -5.23954200 | -0.63845000 | -1.58884700 |
| H | -5.16547900 | -1.24068500 | -2.48525800 |
| S | 2.56299900  | 0.08890800  | 2.04485900  |
| O | 2.77246000  | 1.11819000  | 3.07038600  |
| O | 2.21254900  | -1.27335400 | 2.46845900  |
| N | 1.41859700  | 0.48022900  | 0.93379700  |
| N | 0.33936800  | 1.83529500  | -0.54898900 |
| H | -0.24452000 | 0.99689900  | -0.73632300 |
| C | 1.31502000  | 1.71174100  | 0.40702400  |
| C | 2.06437100  | 2.88881600  | 0.68622300  |
| H | 2.80731700  | 2.85827000  | 1.46808200  |
| C | 1.80983200  | 4.04840300  | -0.00941700 |
| H | 2.39219100  | 4.93497200  | 0.21663700  |
| C | 0.80603000  | 4.10810000  | -0.99584000 |
| H | 0.59973900  | 5.01484800  | -1.54632000 |
| C | 0.07735800  | 2.97252700  | -1.23468500 |
| H | -0.72807400 | 2.88861500  | -1.95230700 |
| C | 4.11641600  | -0.03096600 | 1.11460300  |
| C | 4.17694000  | -0.82129800 | -0.03250600 |
| H | 3.29442800  | -1.33705100 | -0.38932100 |
| C | 5.37974700  | -0.93430500 | -0.71844300 |
| H | 5.43815700  | -1.53658100 | -1.61631000 |
| C | 6.51205200  | -0.26286500 | -0.24996600 |
| C | 6.44597100  | 0.51792100  | 0.90217300  |
| H | 7.32691400  | 1.03565800  | 1.25976500  |
| C | 5.23957200  | 0.63831700  | 1.58901400  |
| H | 5.16567900  | 1.24066100  | 2.48536500  |
| C | -7.82578800 | 0.43314100  | 0.96791300  |
| C | 7.82551500  | -0.43425900 | -0.96764100 |
| F | 8.49451800  | -1.52894200 | -0.52734500 |
| F | 7.66022500  | -0.59198400 | -2.29985600 |
| F | 8.64849800  | 0.62191800  | -0.78874000 |
| F | -8.49515200 | 1.52762000  | 0.52766000  |
| F | -7.66053700 | 0.59087200  | 2.30013200  |
| F | -8.64842900 | -0.62329900 | 0.78898300  |

