

## Supplementary Materials

# Isolation and Structure Elucidation of Novel Mycosporine-like Amino Acids from the Two Intertidal Red Macroalgae *Bostrychia scorpioides* and *Catenella caespitosa*

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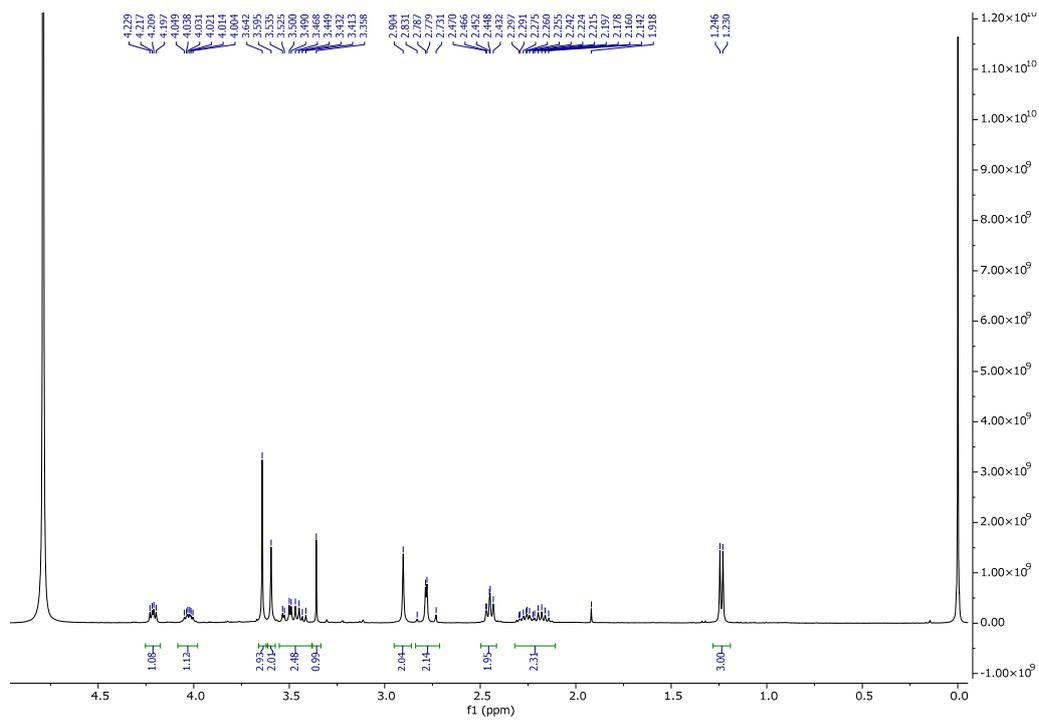


Figure S1.  $^1\text{H}$  NMR spectrum of compound **1** in  $\text{D}_2\text{O}$

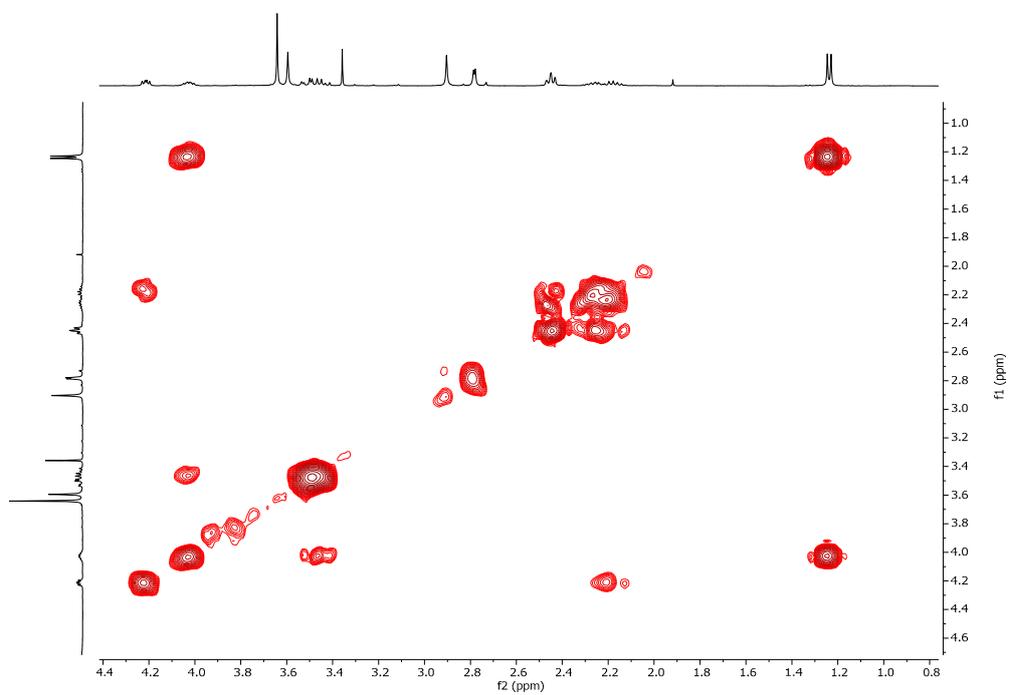


Figure S2. COSY spectrum of compound **1** in  $\text{D}_2\text{O}$

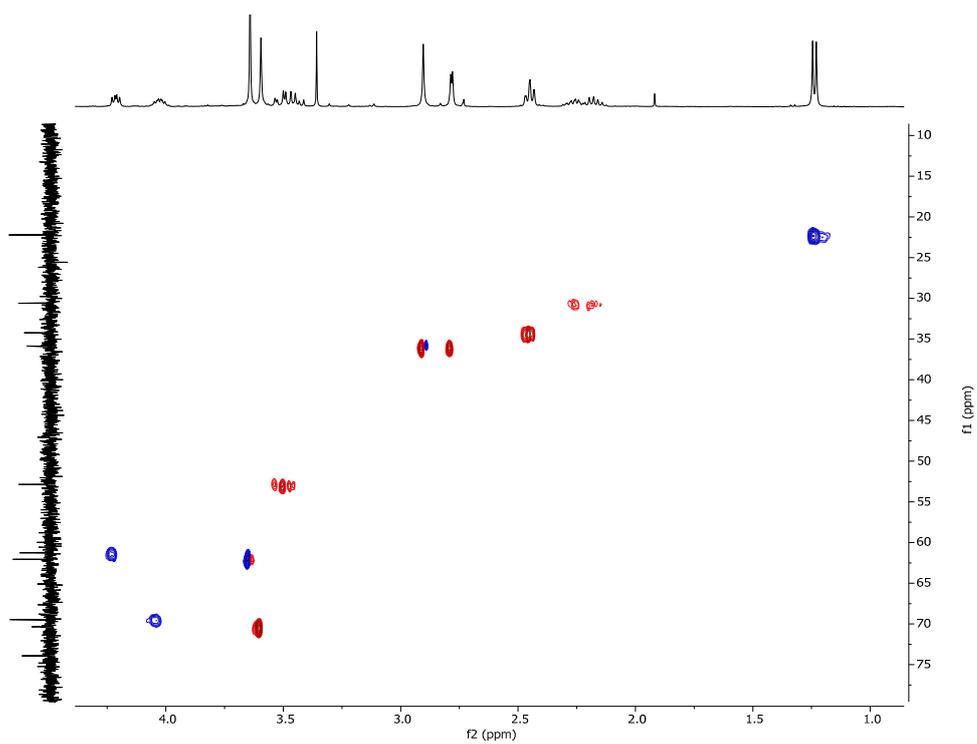


Figure S3. HSQC spectrum of compound **1** in D<sub>2</sub>O

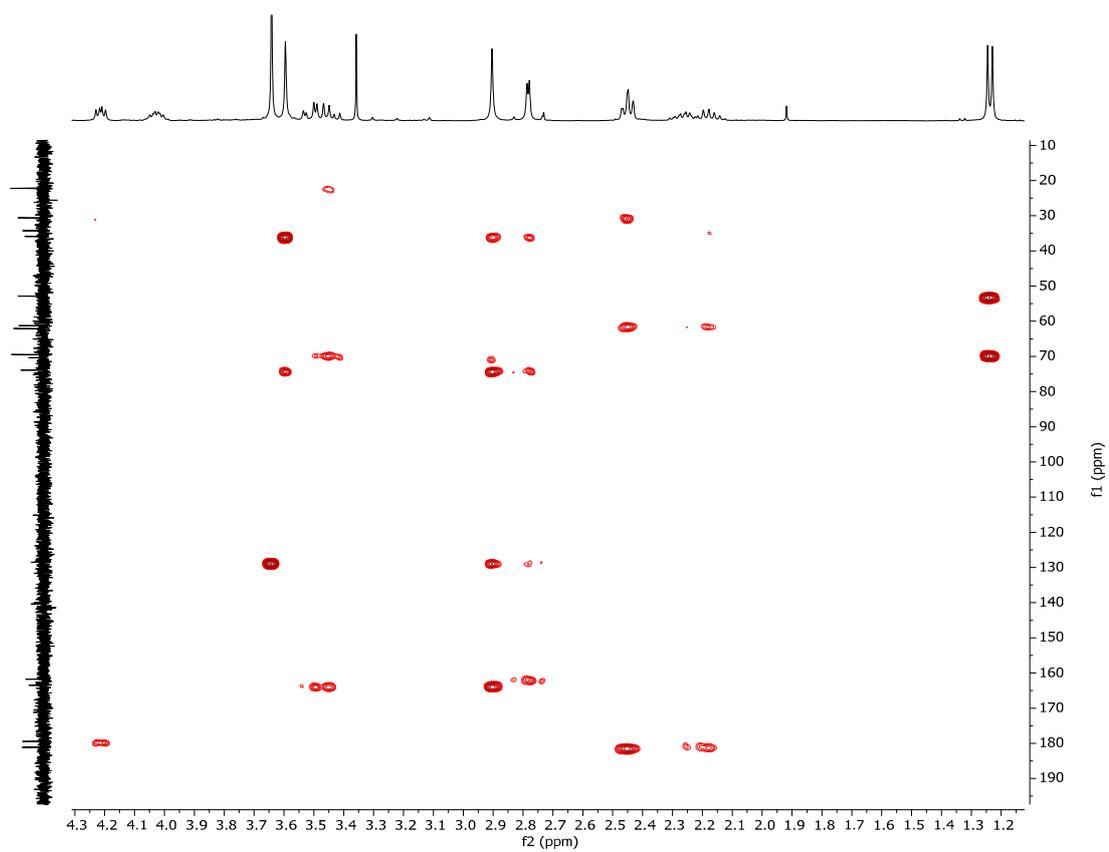
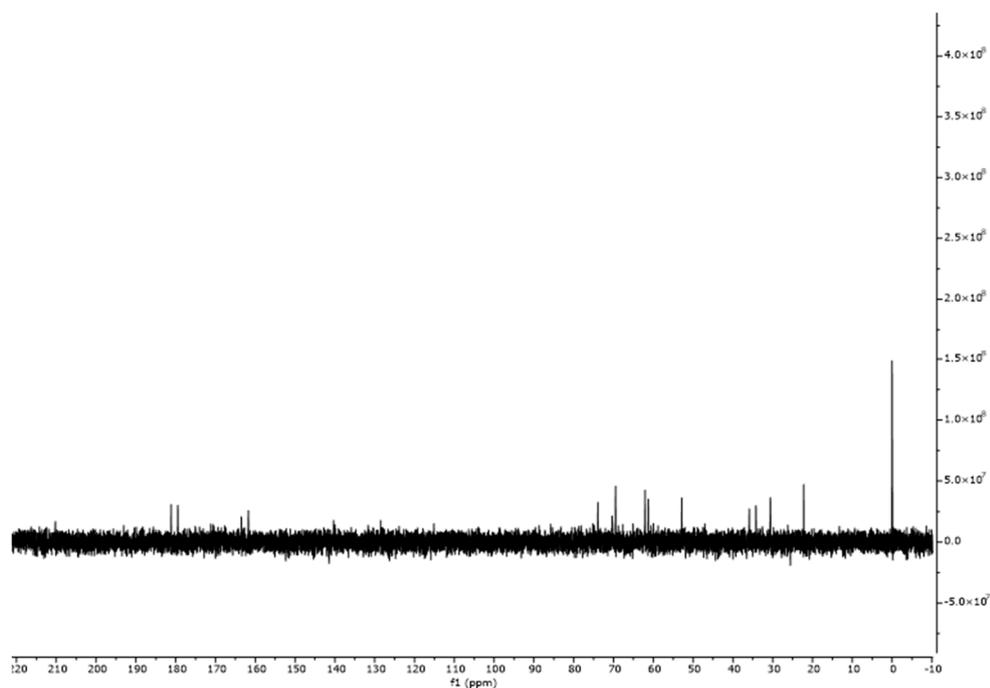
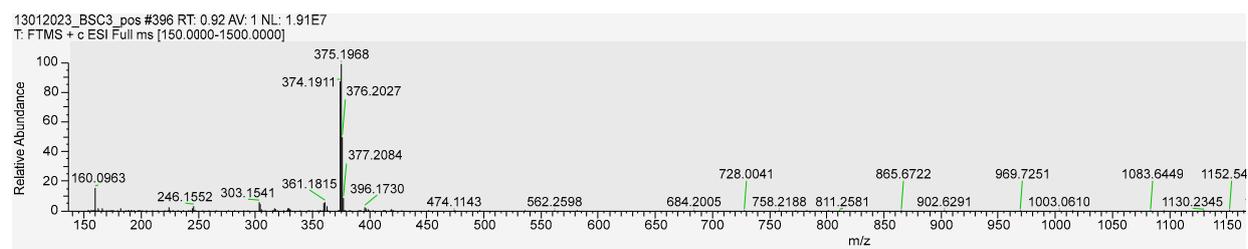


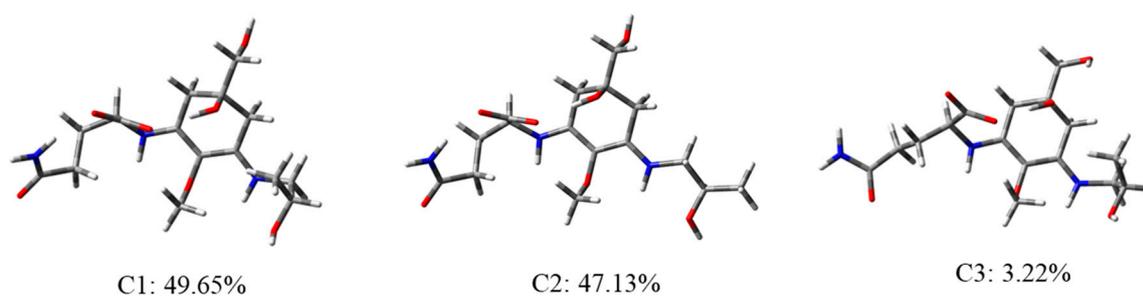
Figure S4. HMBC spectrum of compound **1** in D<sub>2</sub>O



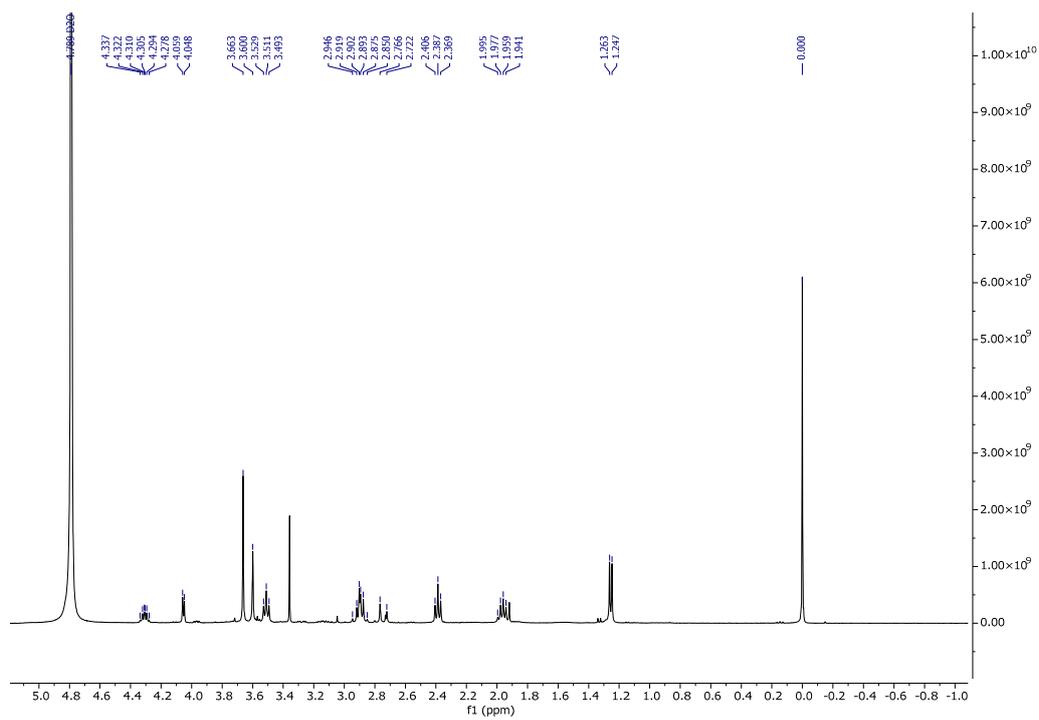
**Figure S5.**  $^{13}\text{C}$  NMR spectrum of compound **1** in  $\text{D}_2\text{O}$



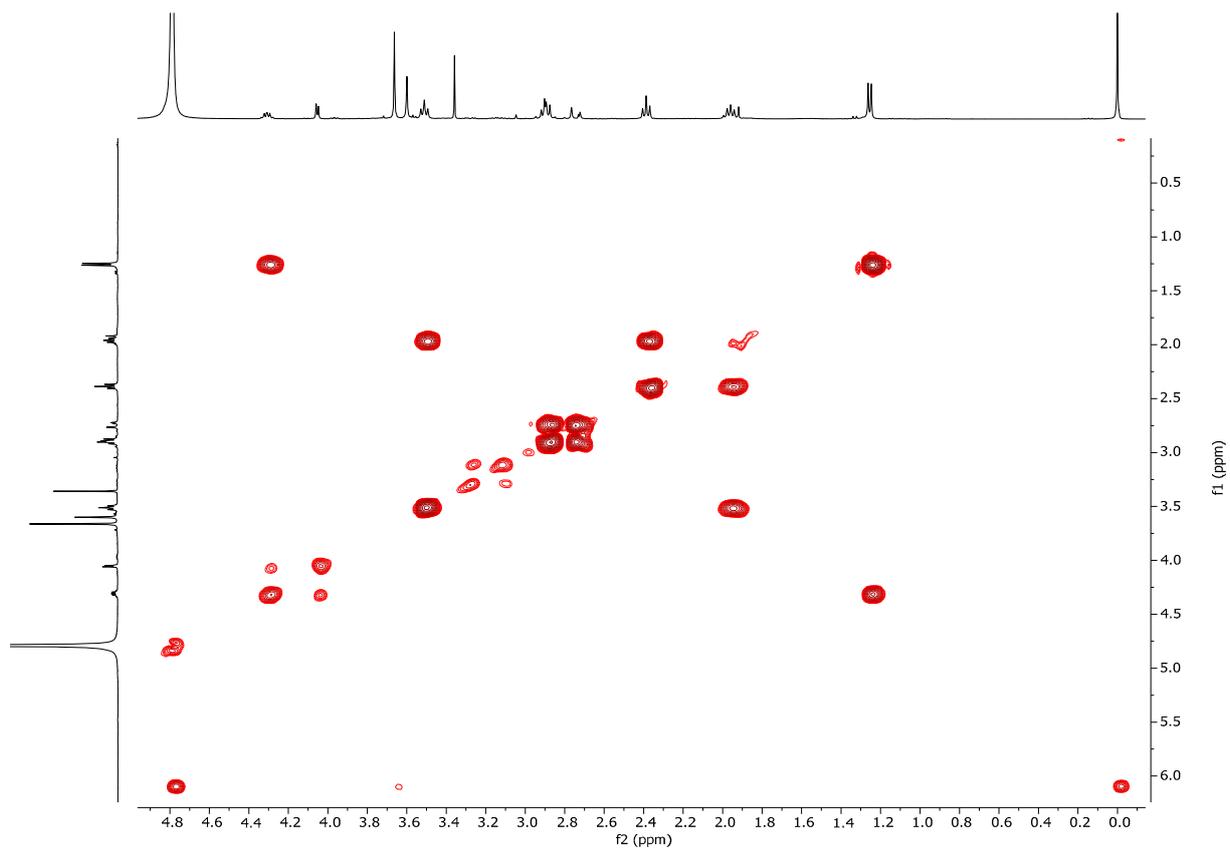
**Figure S6.** High-resolution mass spectrum of compound **1**



**Figure S7.** Overlayered conformers and population of Boltzmann averaged conformers of compound **1** optimized at the DFT/wb97xd/6-31+g(d,p) level in the gas phase.



**Figure S8.**  $^1\text{H}$  NMR spectrum of compound **2** in  $\text{D}_2\text{O}$



**Figure S9.** COSY spectrum of compound **2** in  $\text{D}_2\text{O}$

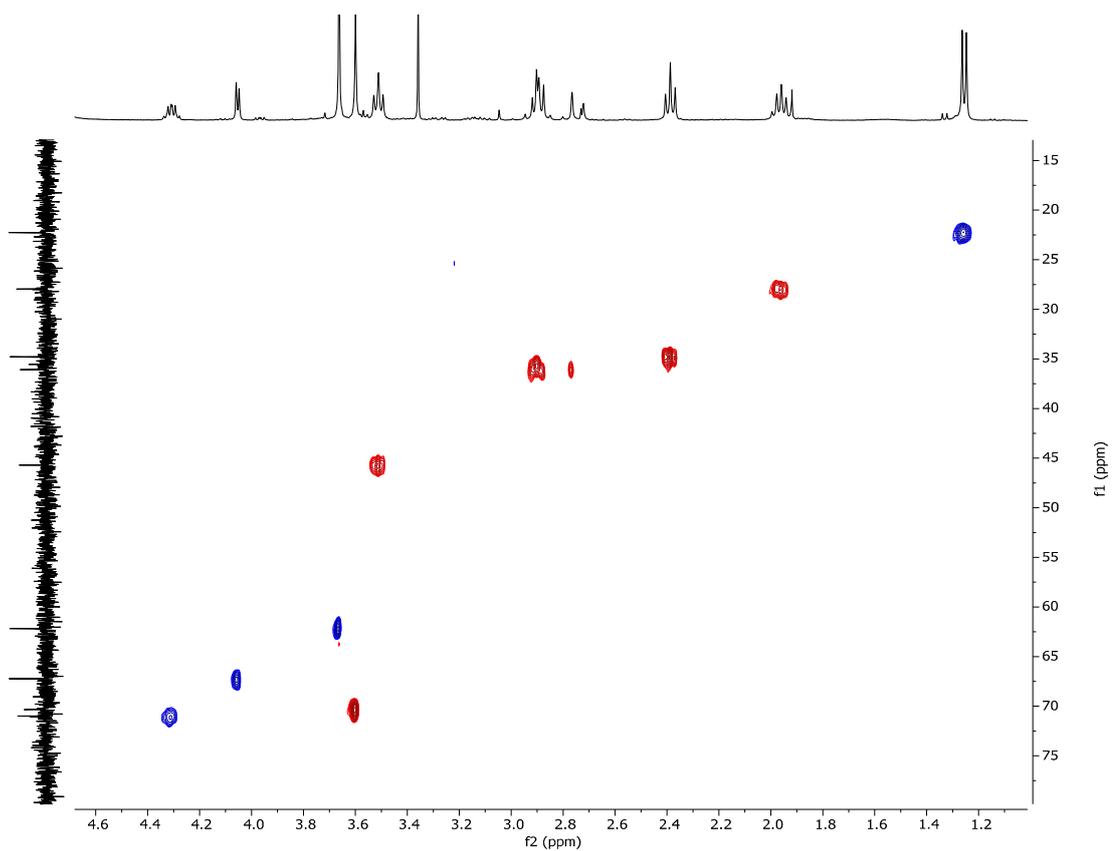


Figure S10. HSQC spectrum of compound **2** in D<sub>2</sub>O

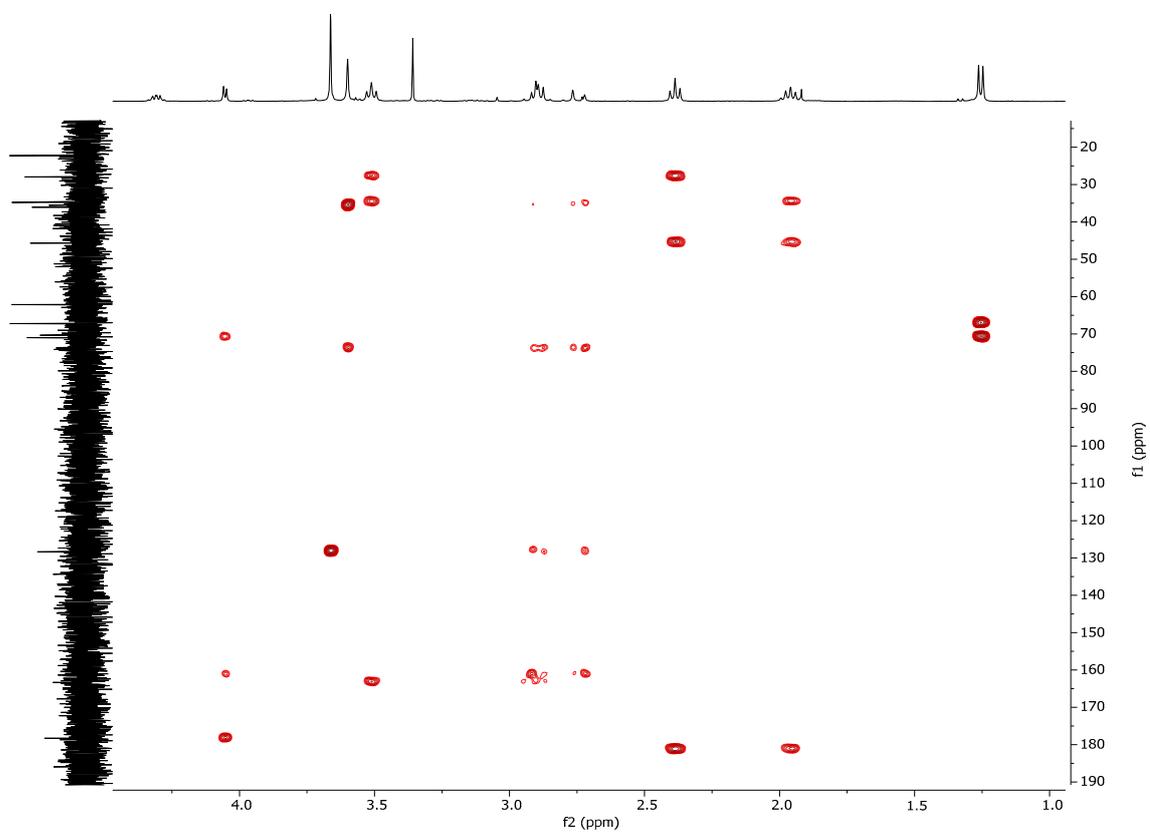
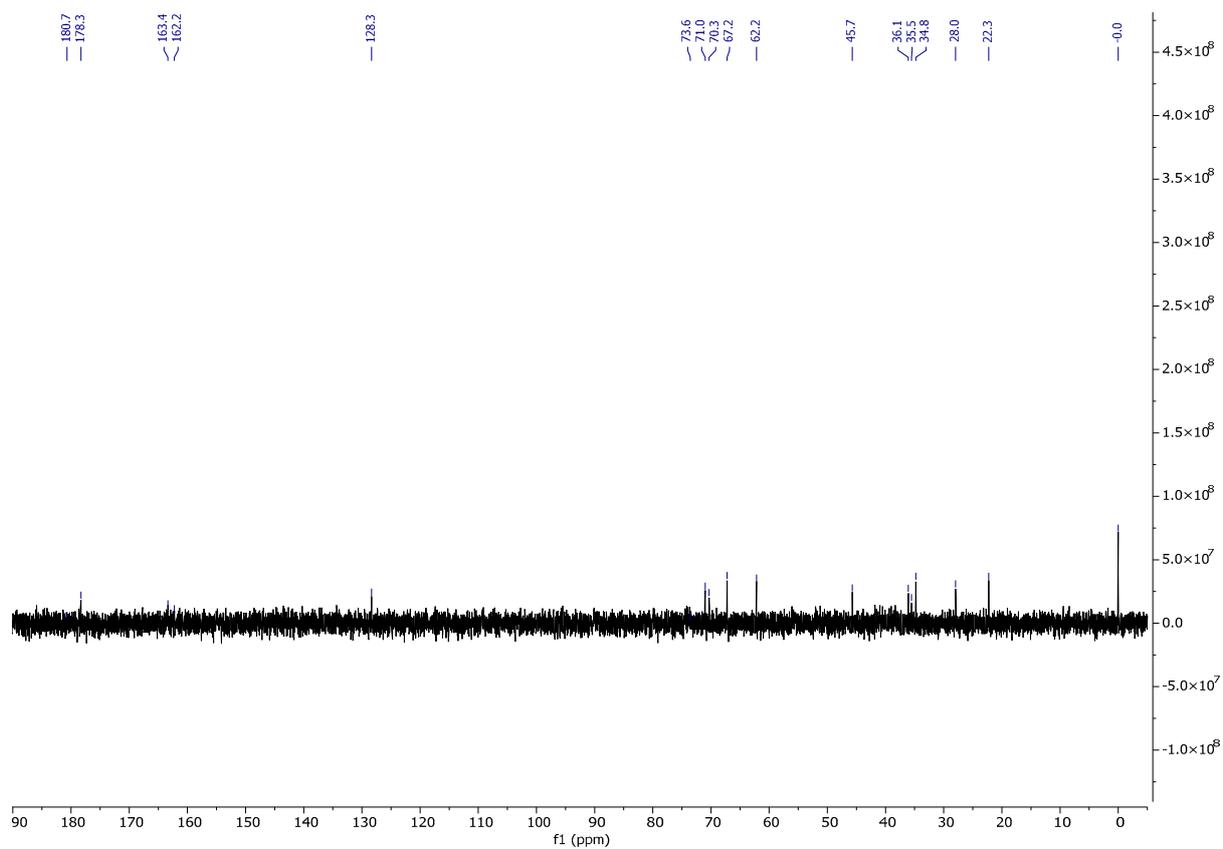
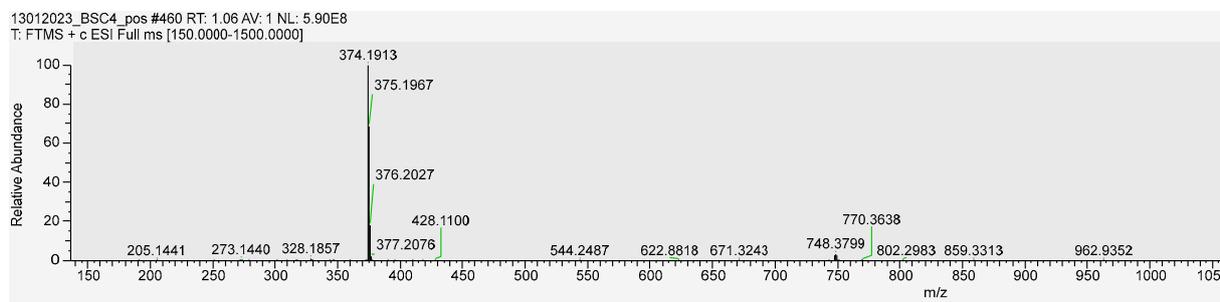


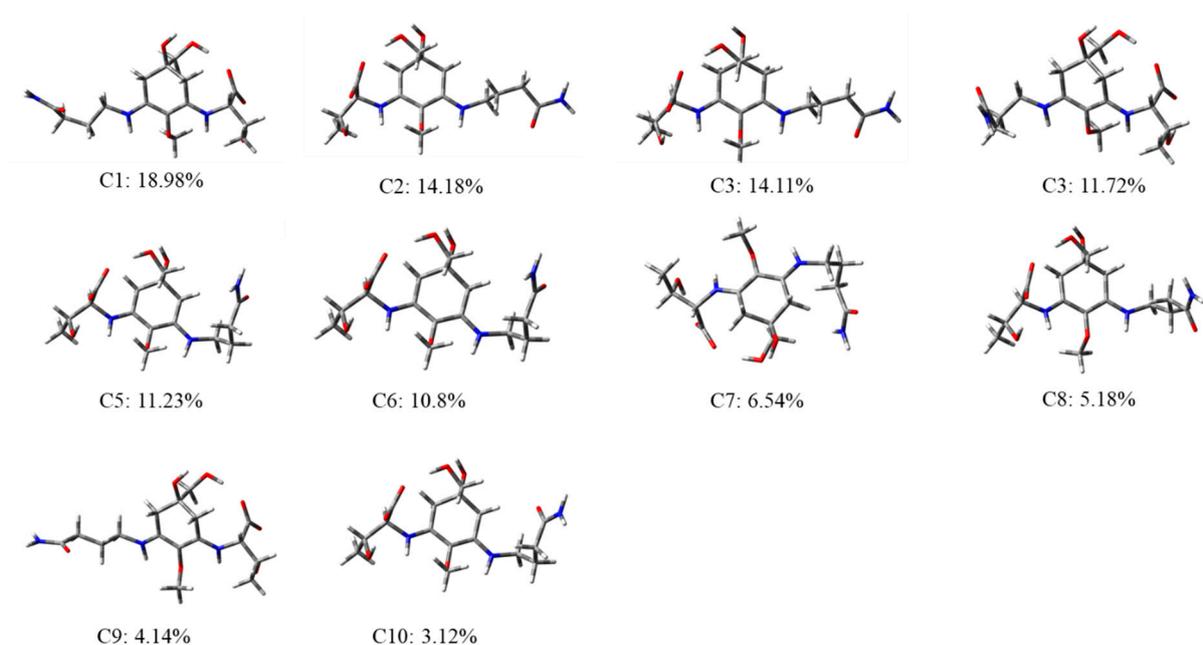
Figure S11. HMBC spectrum of compound **2** in D<sub>2</sub>O



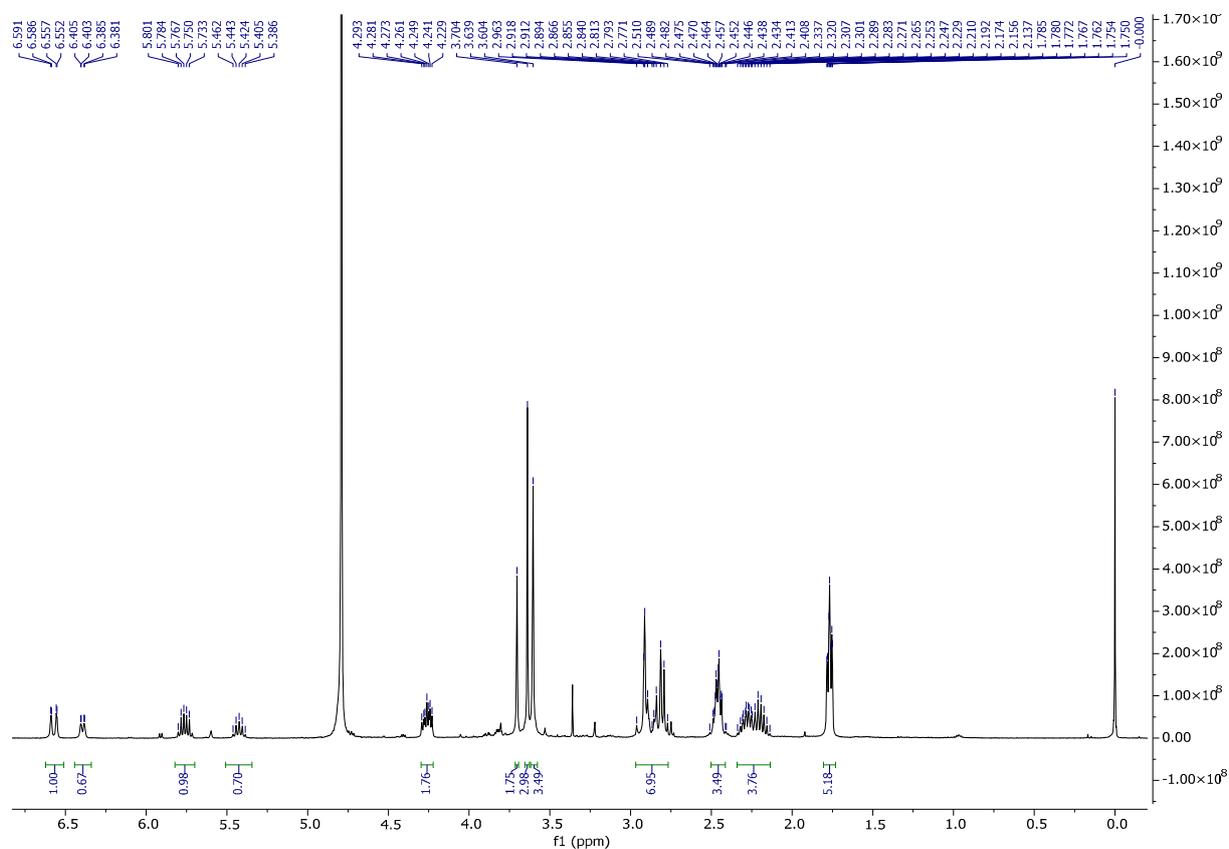
**Figure S12.**  $^{13}\text{C}$  NMR spectrum of compound **2** in  $\text{D}_2\text{O}$



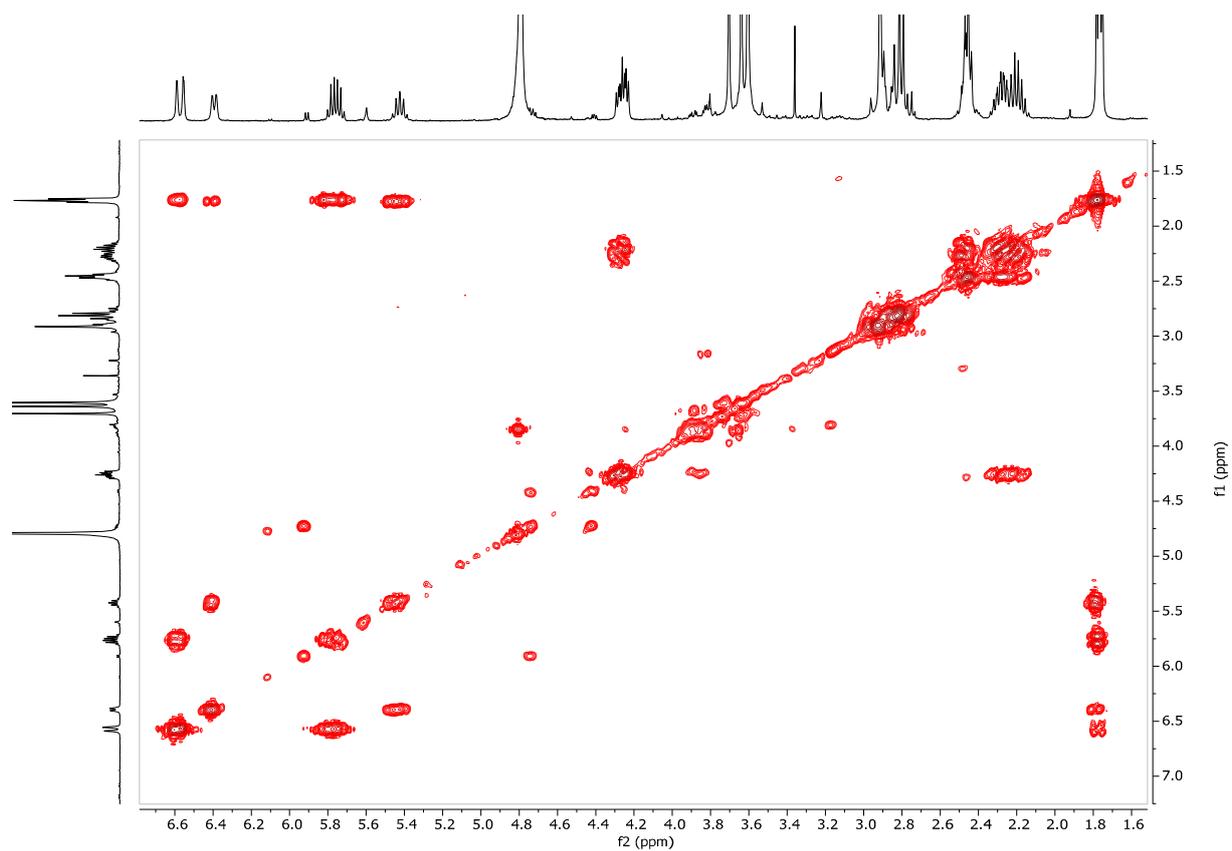
**Figure S13.** High-resolution mass spectrum of compound **2**



**Figure S14.** Overlaid conformers and population of Boltzmann averaged conformers of compound **2** optimized at the DFT/wb97xd/6-31+g(d,p) level in the gas phase.



**Figure S15.**  $^1\text{H}$  NMR spectrum of compounds **3** and **4** in  $\text{D}_2\text{O}$



**Figure S16.** COSY spectrum of compounds **3** and **4** in D<sub>2</sub>O

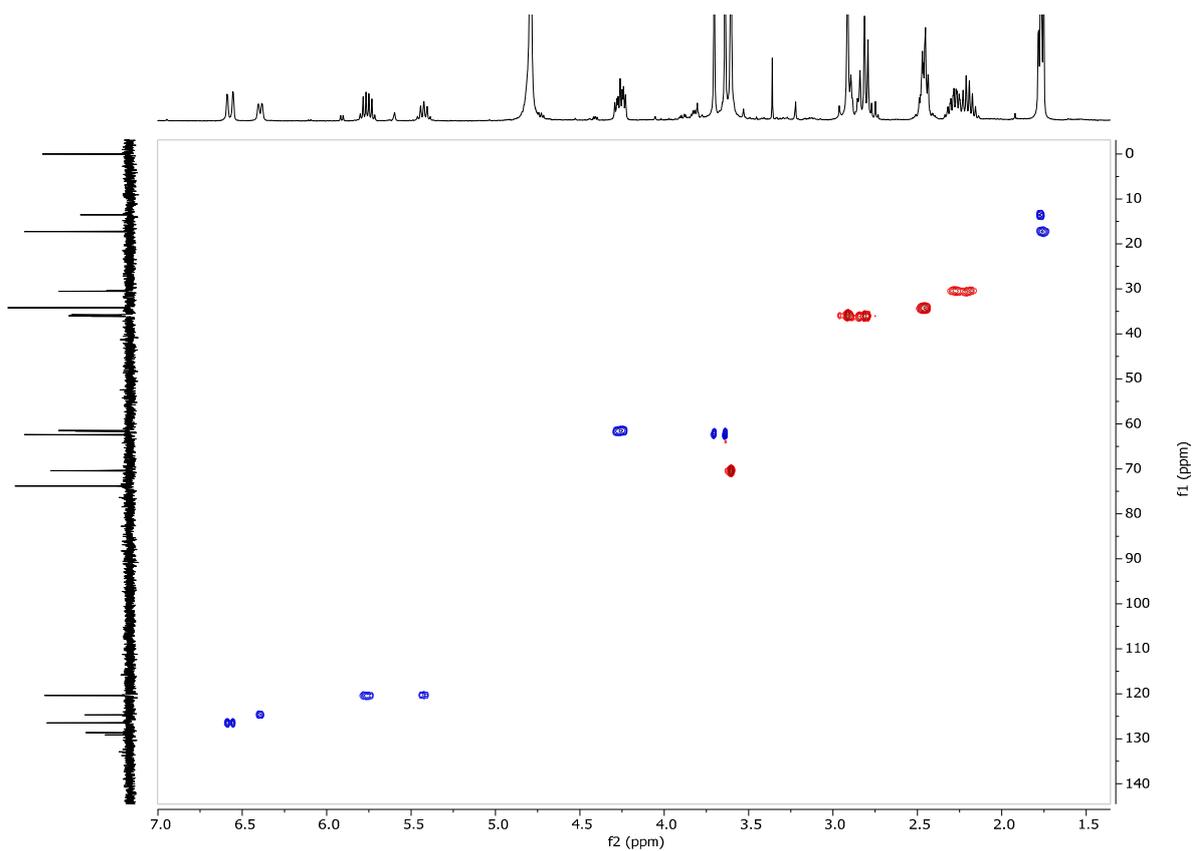


Figure S17. HSQC spectrum of compounds **3** and **4** in D<sub>2</sub>O

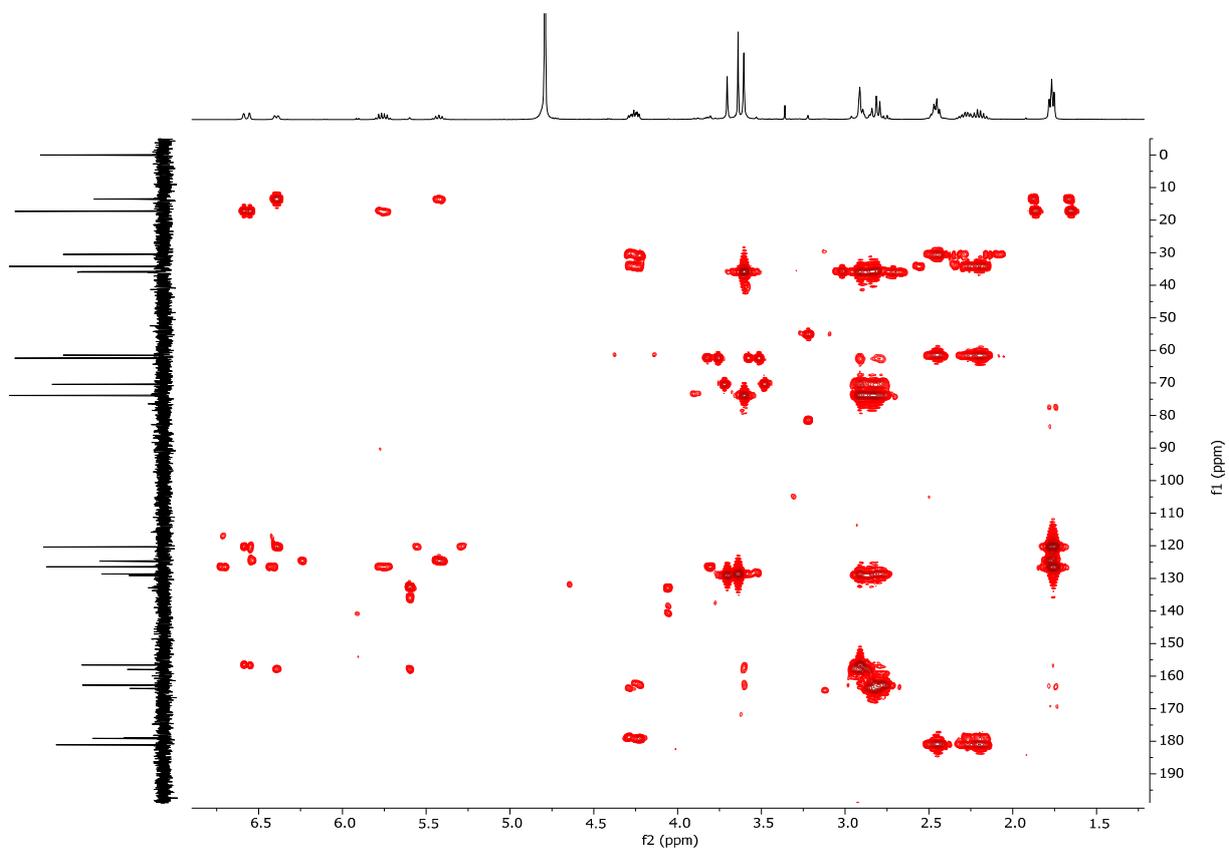
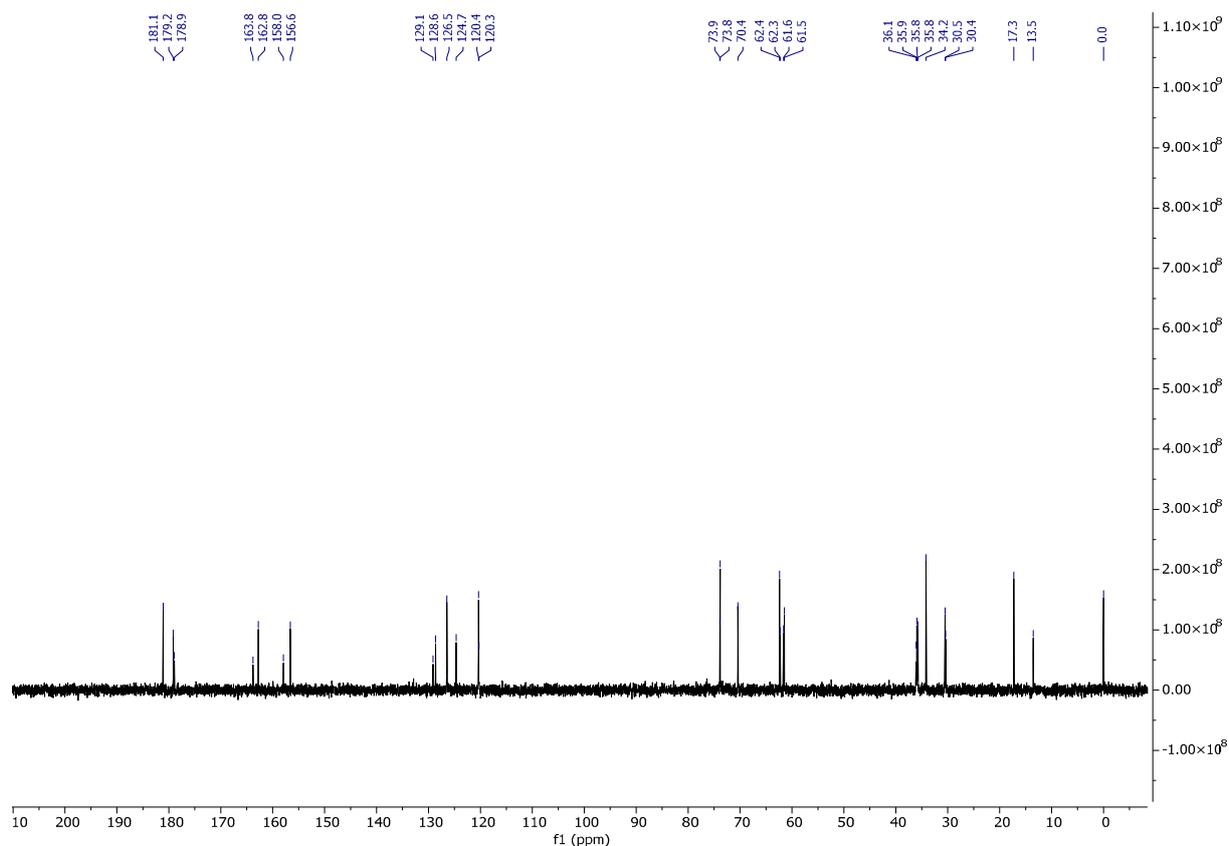
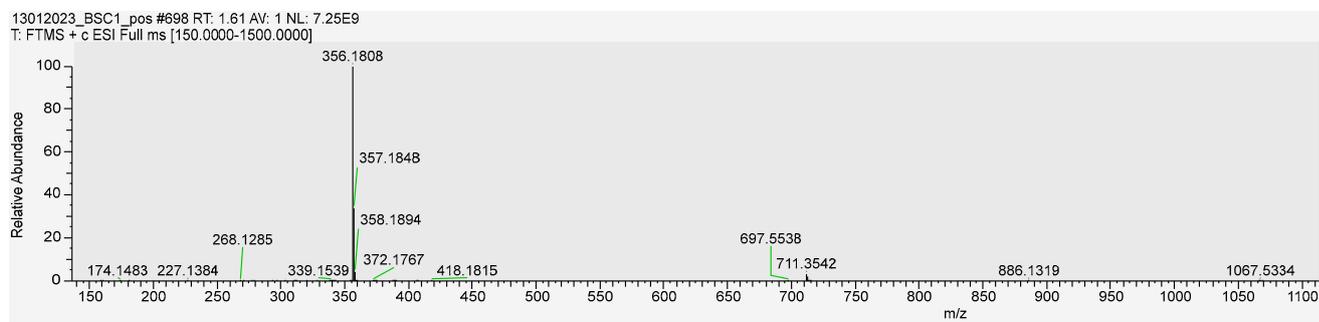


Figure S18. HMBC spectrum of compounds **3** and **4** in D<sub>2</sub>O



**Figure S19.**  $^{13}\text{C}$  NMR spectrum of compounds **3** and **4** in  $\text{D}_2\text{O}$



**Figure S20.** High-resolution mass spectrum of compounds **3** and **4**

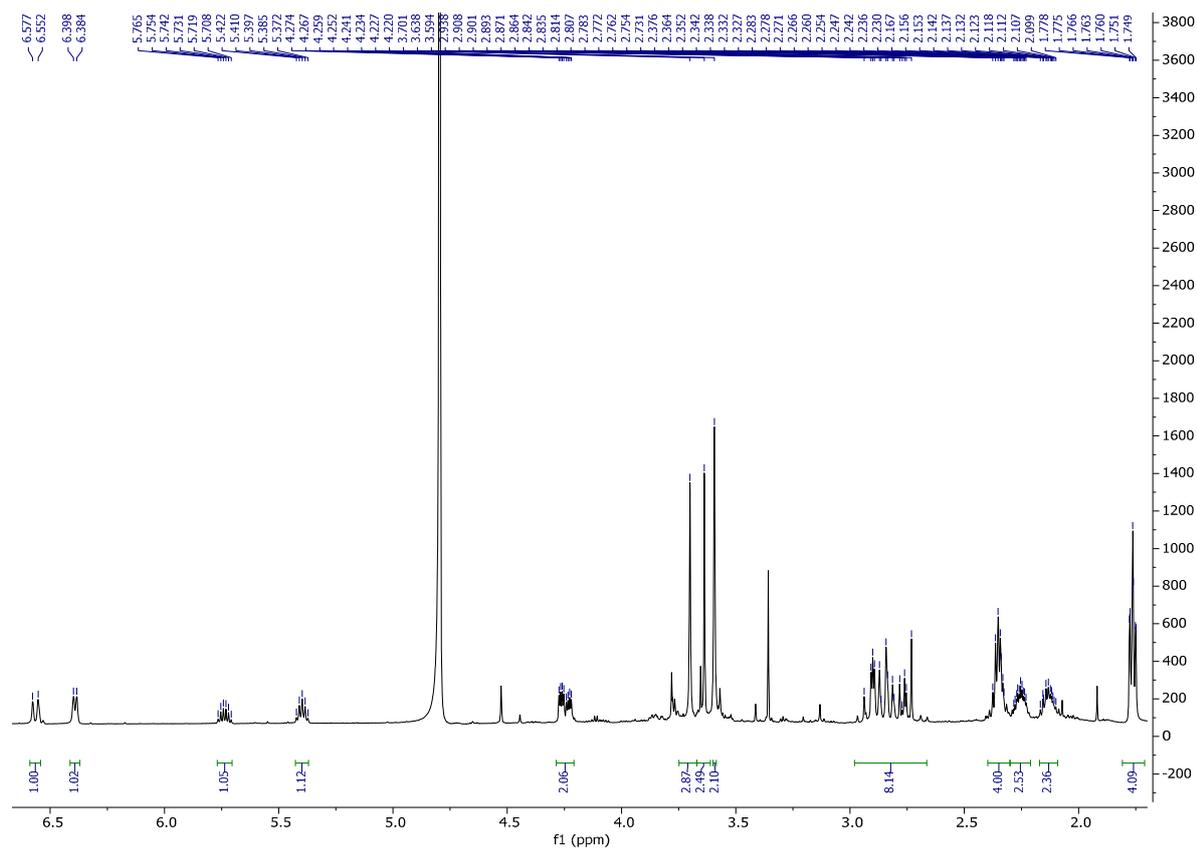


Figure S21.  $^1\text{H}$  NMR spectrum of compounds **5** and **6** in  $\text{D}_2\text{O}$

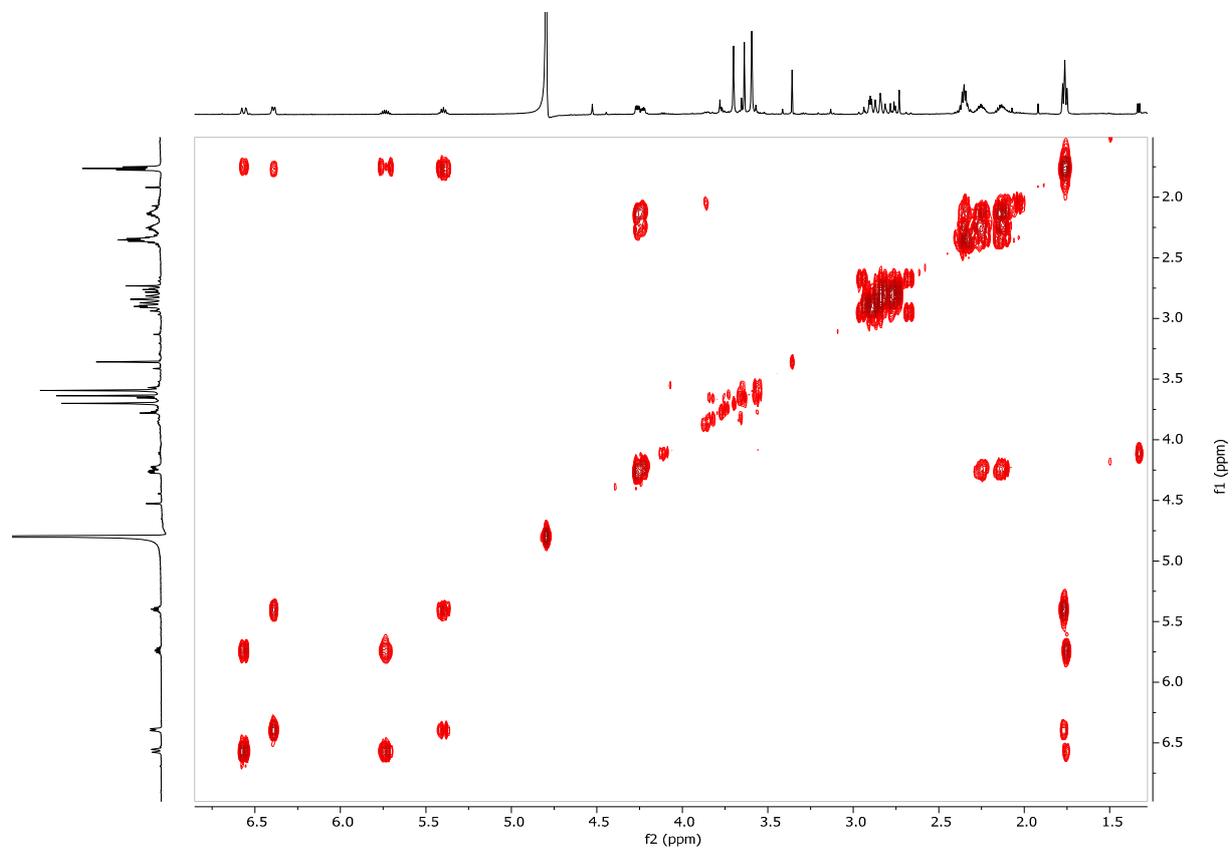


Figure S22. COSY spectrum of compounds **5** and **6** in  $\text{D}_2\text{O}$

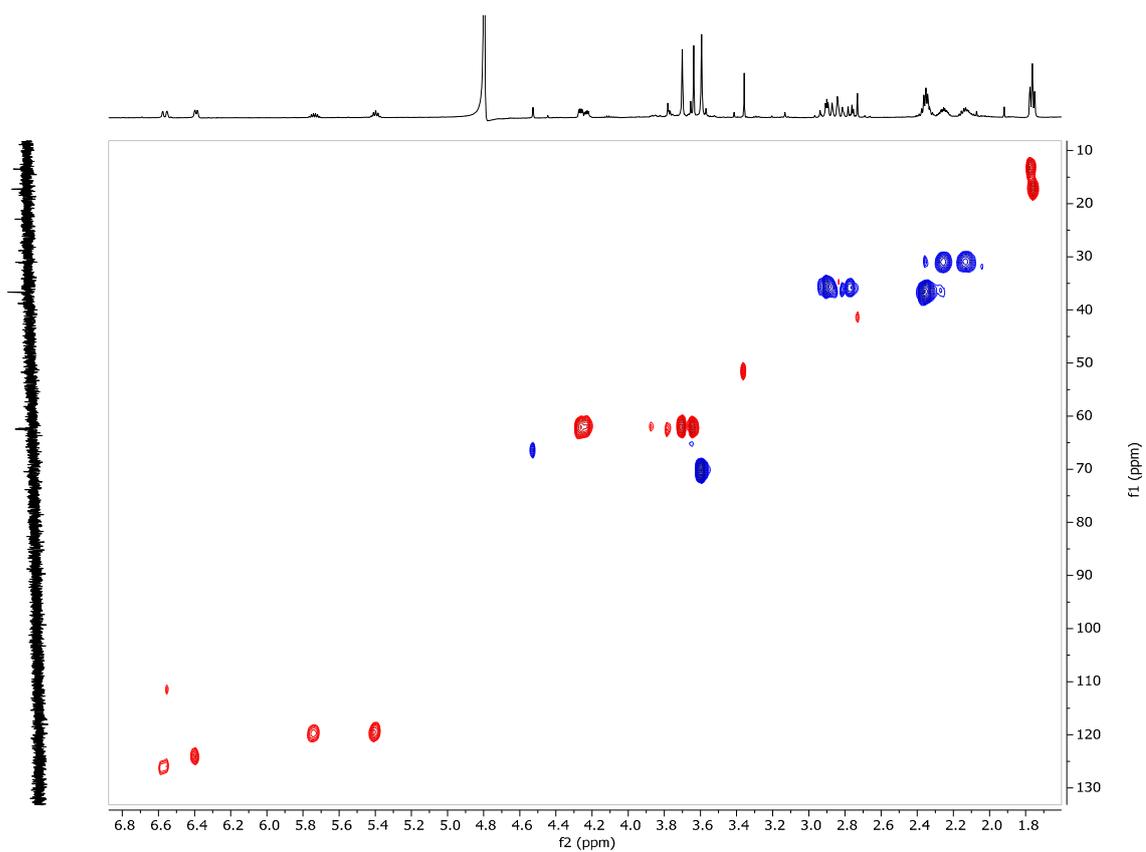
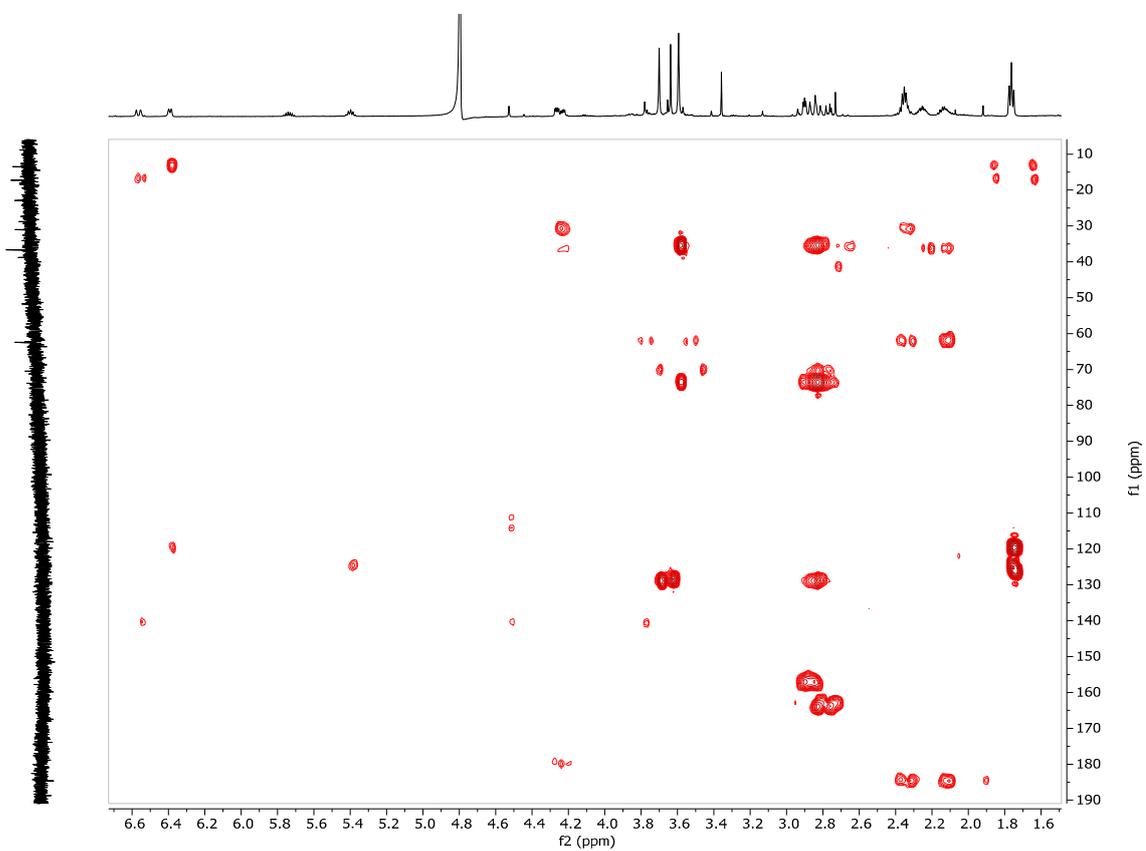
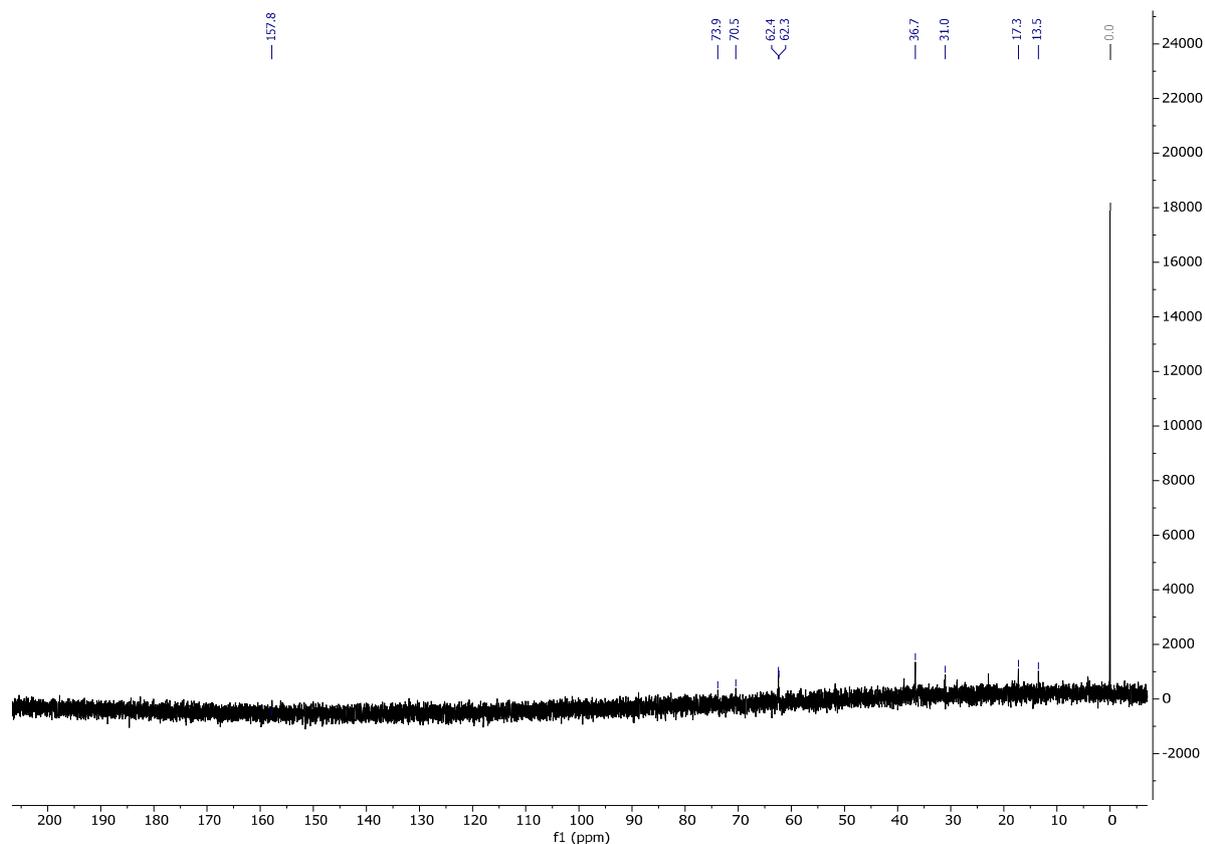


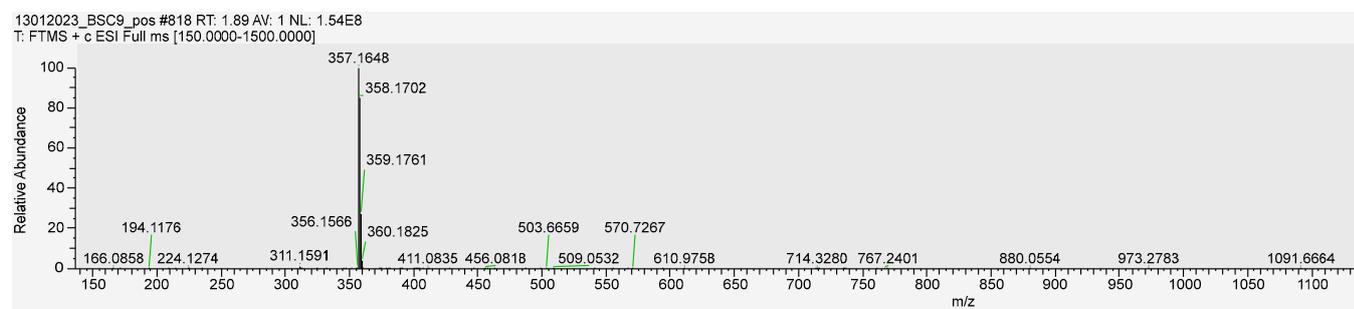
Figure S23. HSQC spectrum of compounds **5** and **6** in  $\text{D}_2\text{O}$



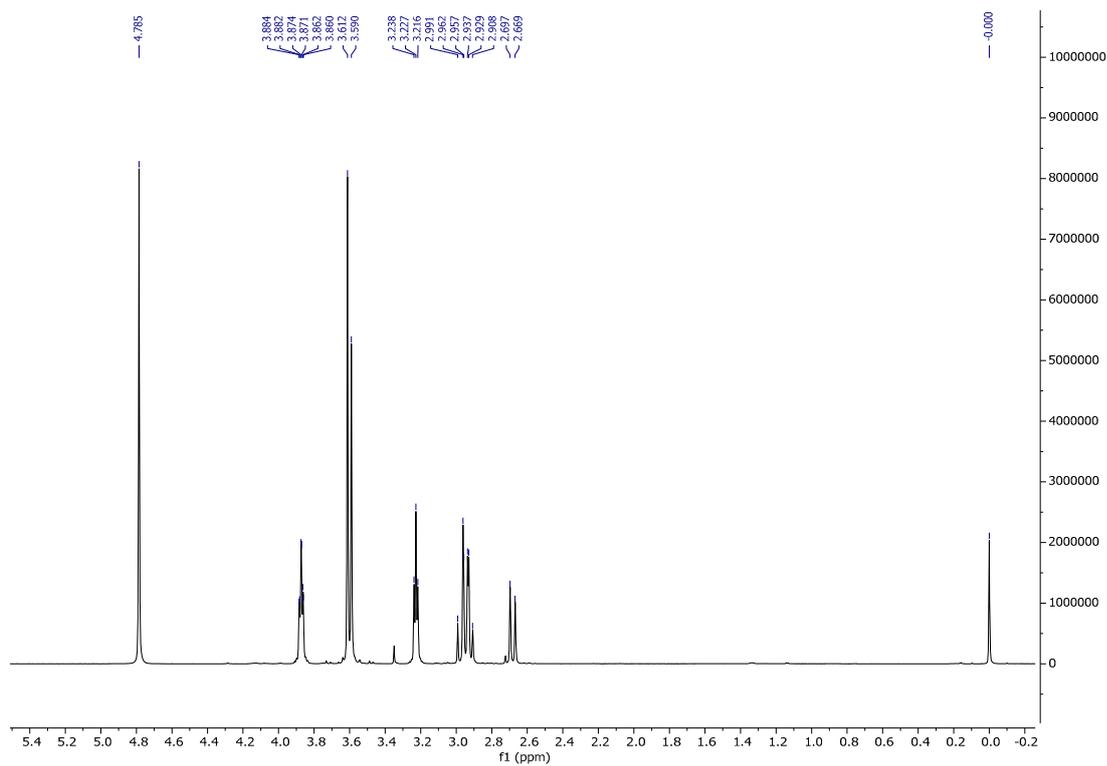
**Figure S24.** HMBC spectrum of compounds **5** and **6** in D<sub>2</sub>O



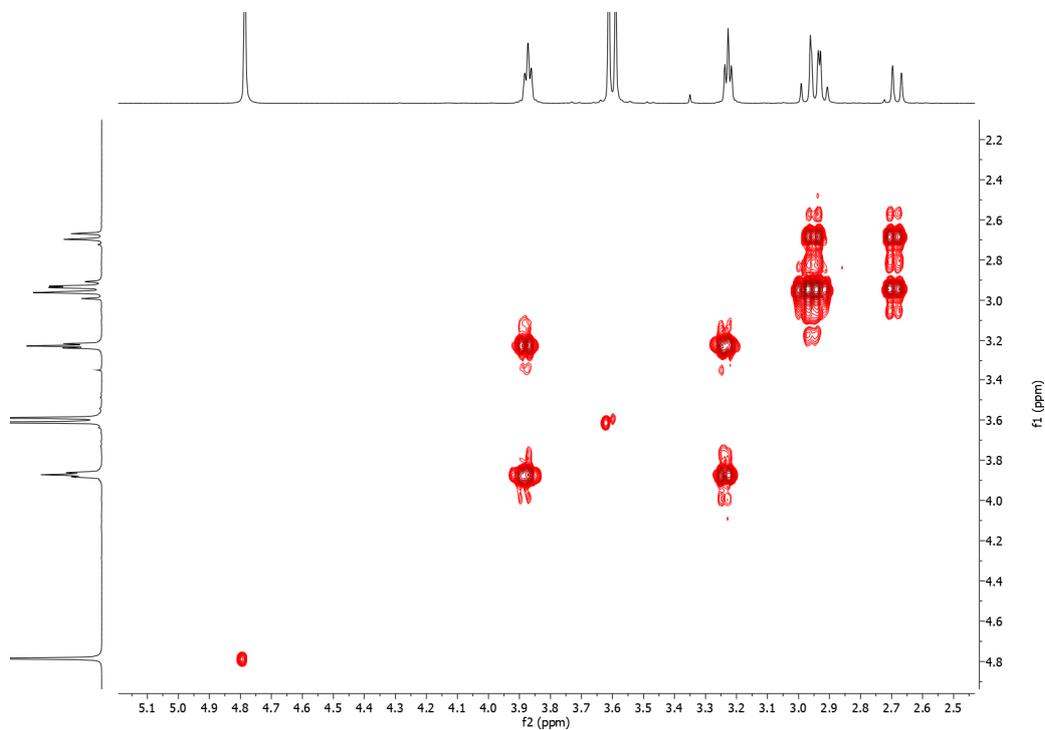
**Figure S25.** <sup>13</sup>C NMR spectrum of compounds **5** and **6** in D<sub>2</sub>O



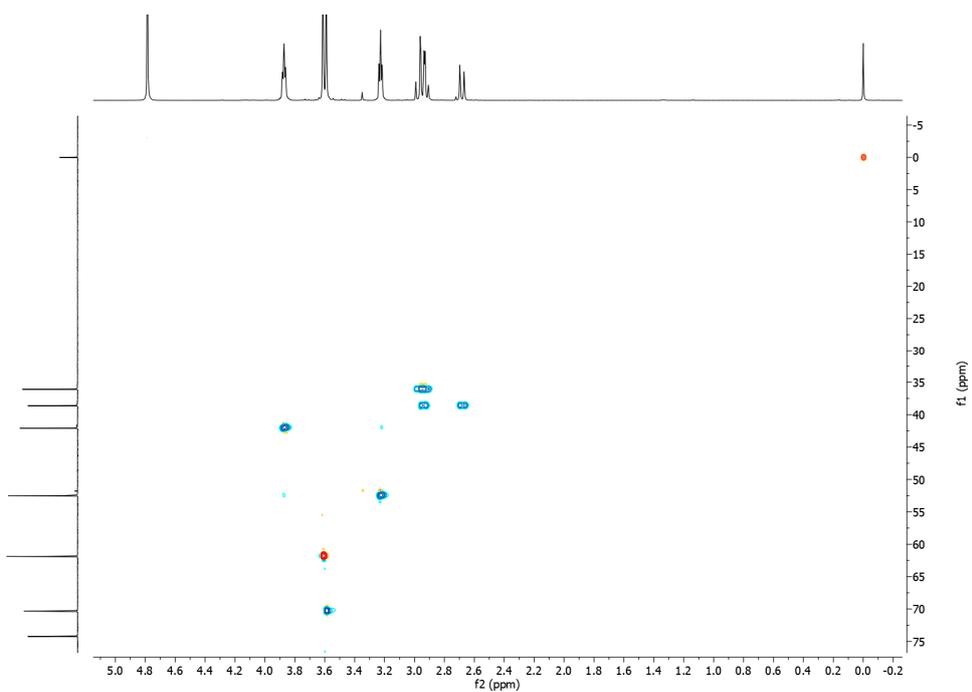
**Figure S26.** High-resolution mass spectrum of compounds **5** and **6**



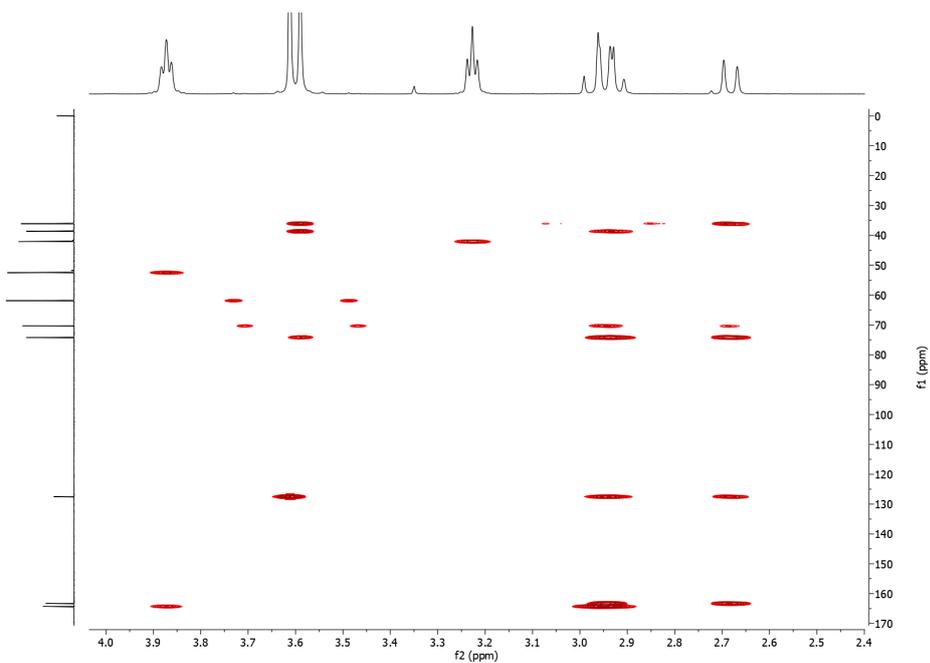
**Figure S27.**  $^1\text{H}$  NMR spectrum of compound **7** in  $\text{D}_2\text{O}$



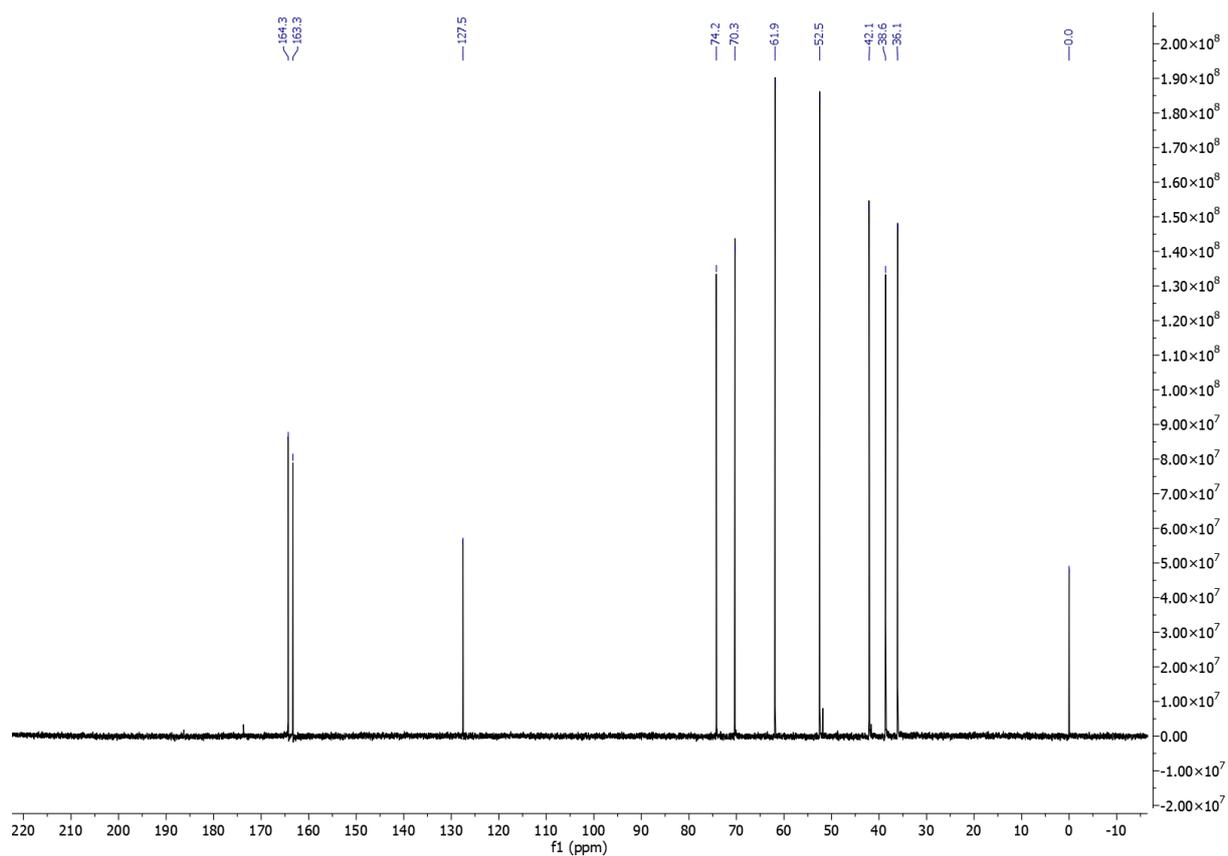
**Figure S28.** COSY spectrum of compound **7** in  $\text{D}_2\text{O}$



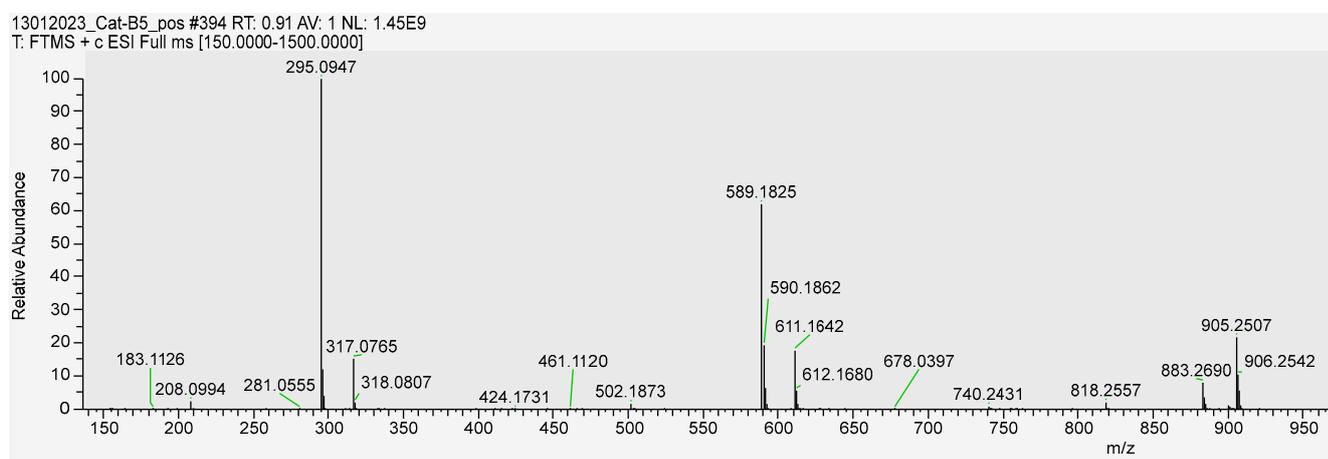
**Figure S29.** HSQC spectrum of compound **7** in D<sub>2</sub>O



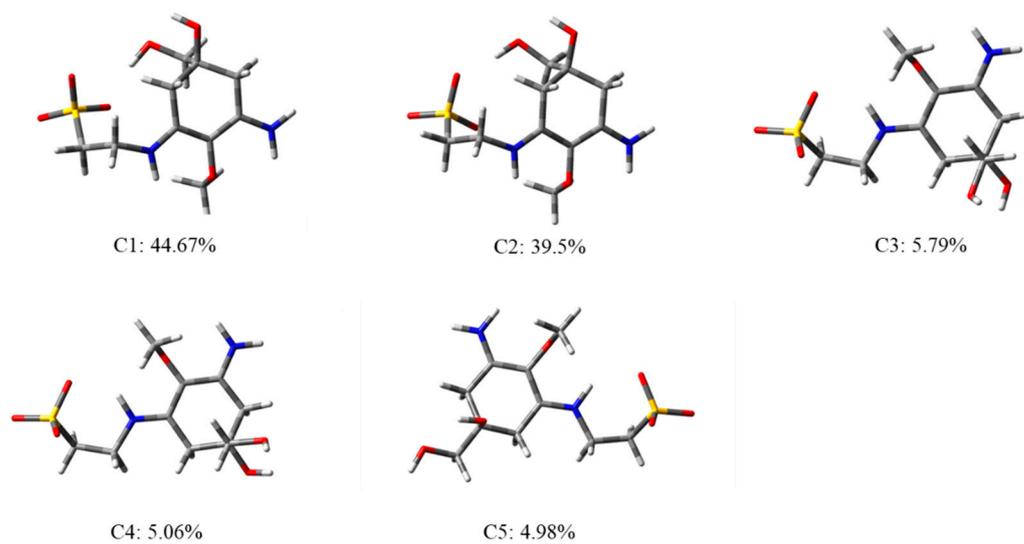
**Figure S30.** HMBC spectrum of compound **7** in D<sub>2</sub>O



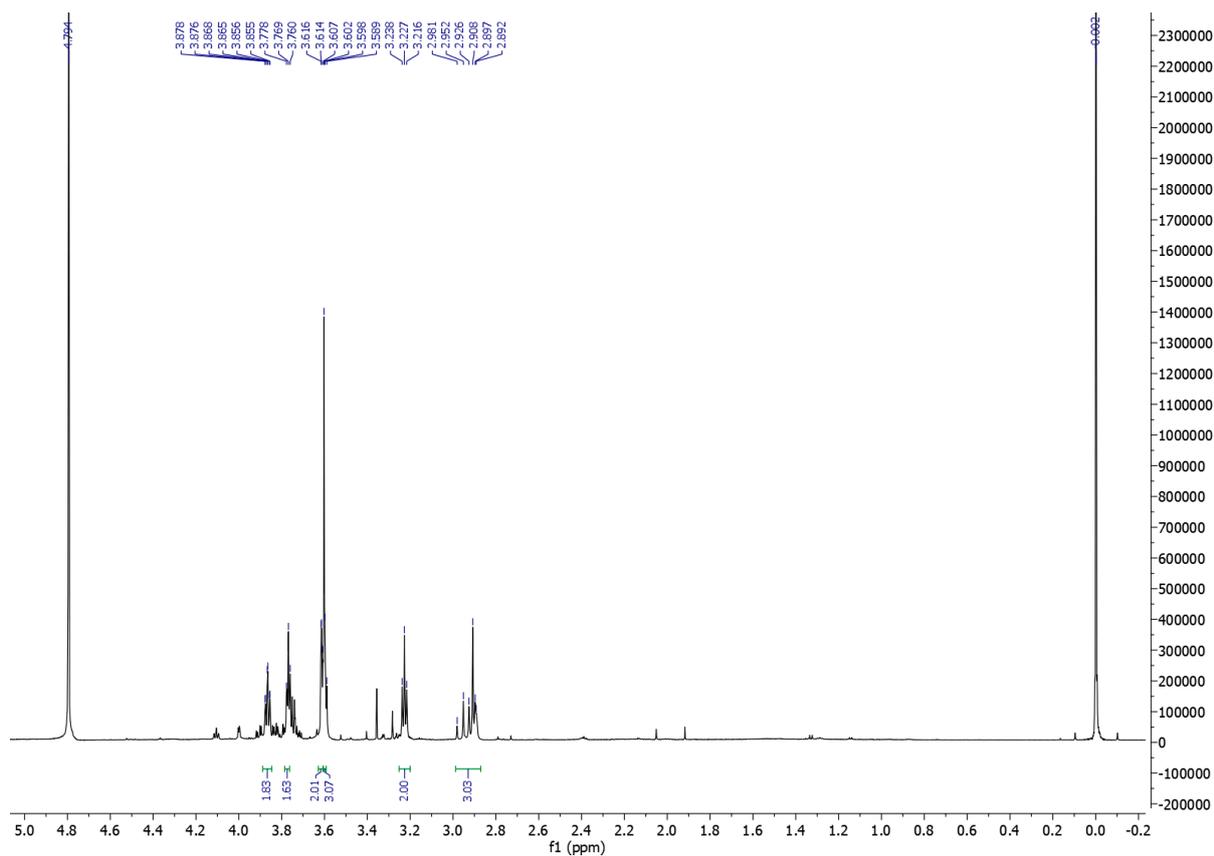
**Figure S31.**  $^{13}\text{C}$  NMR spectrum of compound 7 in  $\text{D}_2\text{O}$



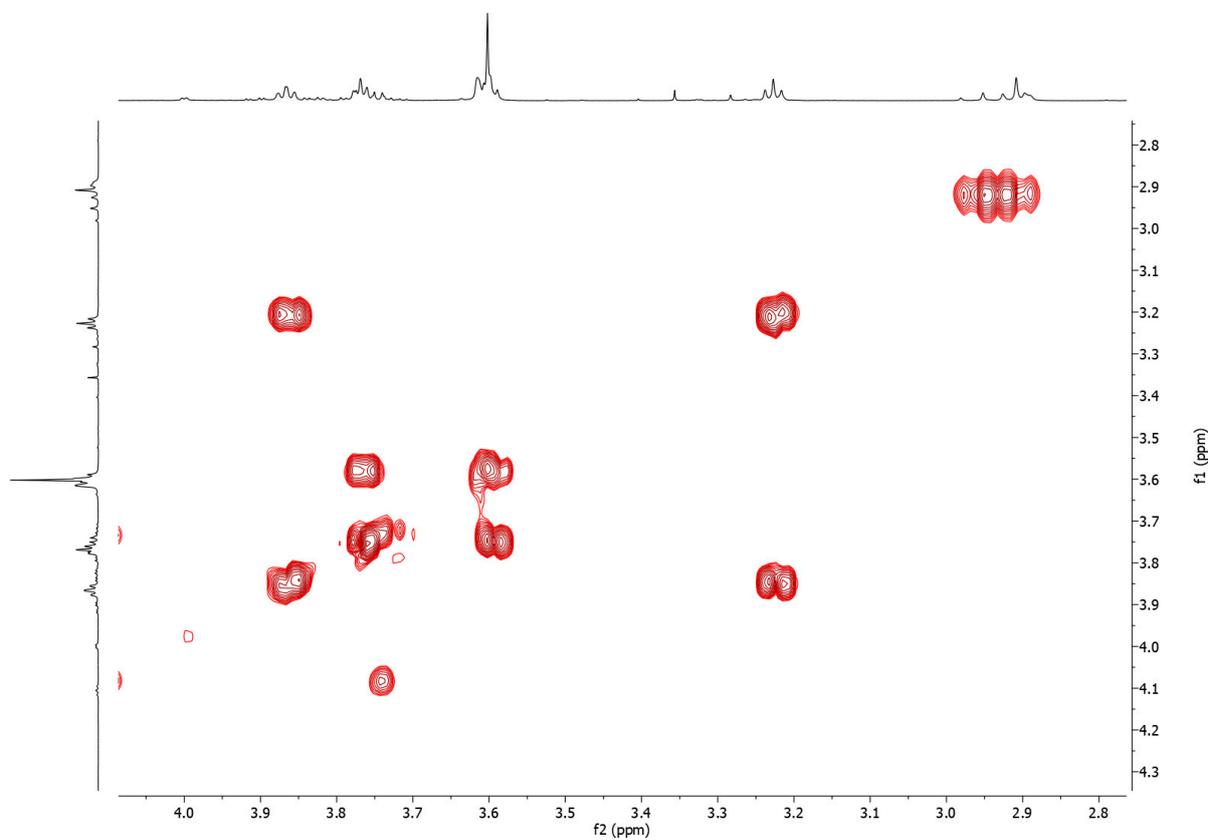
**Figure S32.** High-resolution mass spectrum of compound 7



**Figure S33.** Overlayered conformers and population of Boltzmann averaged conformers of compound 7 optimized at the DFT/wb97xd/6-31+g(d,p) level in the gas phase.



**Figure S34.**  $^1\text{H}$  NMR spectrum of compound **8** in  $\text{D}_2\text{O}$



**Figure S35.** COSY spectrum of compound **8** in  $\text{D}_2\text{O}$

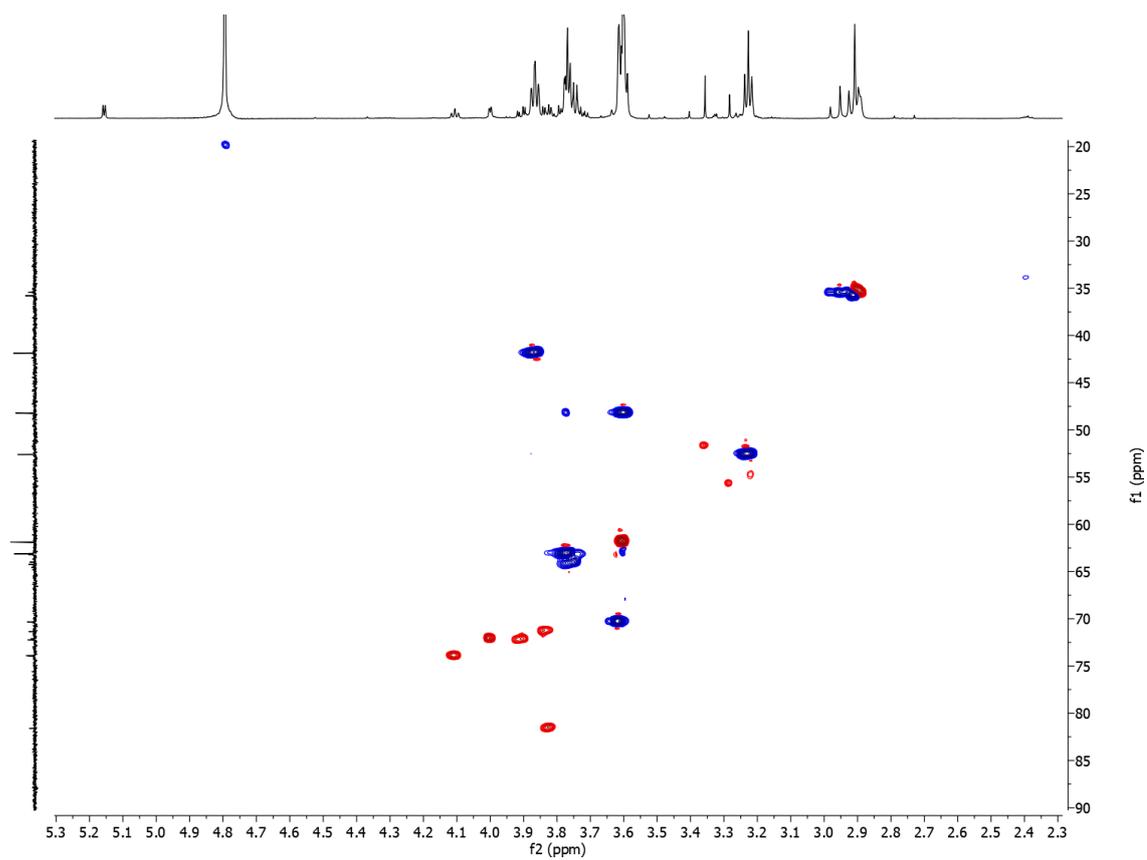


Figure S36. HSQC spectrum of compound **8** in D<sub>2</sub>O

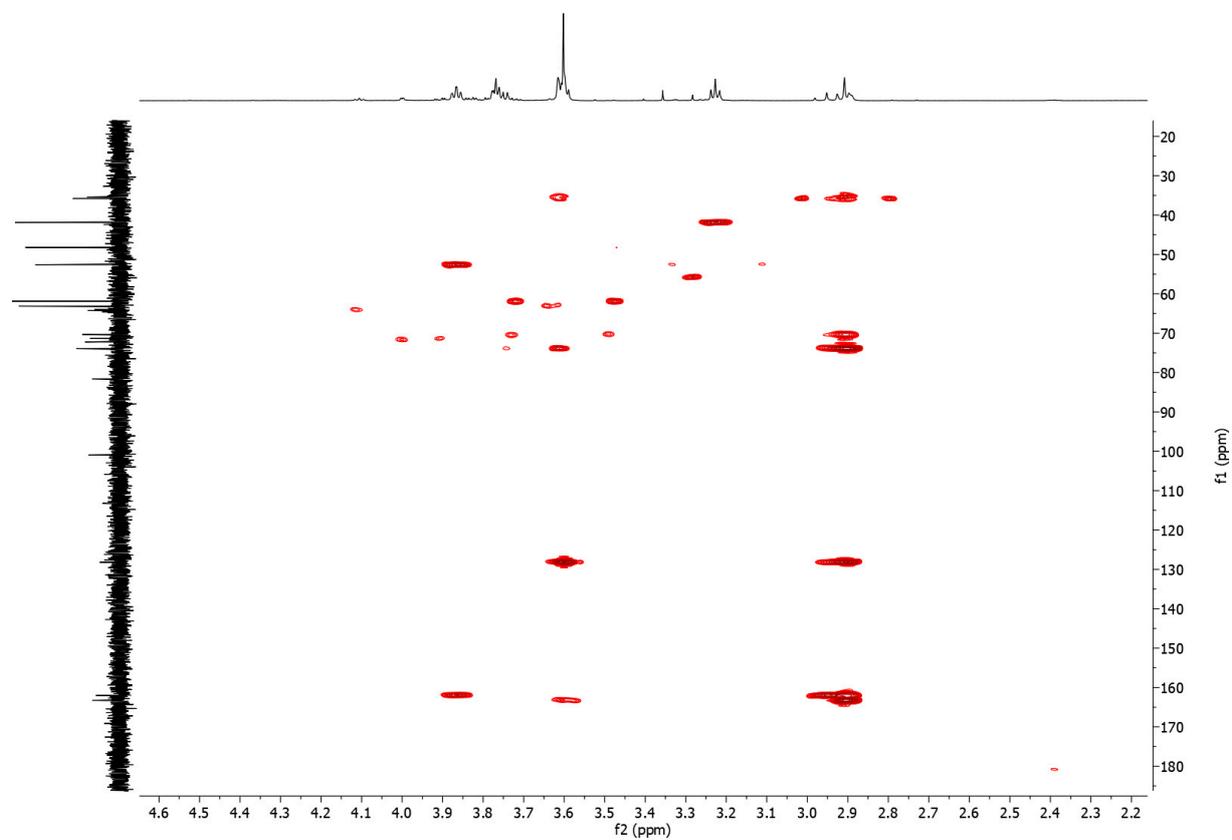
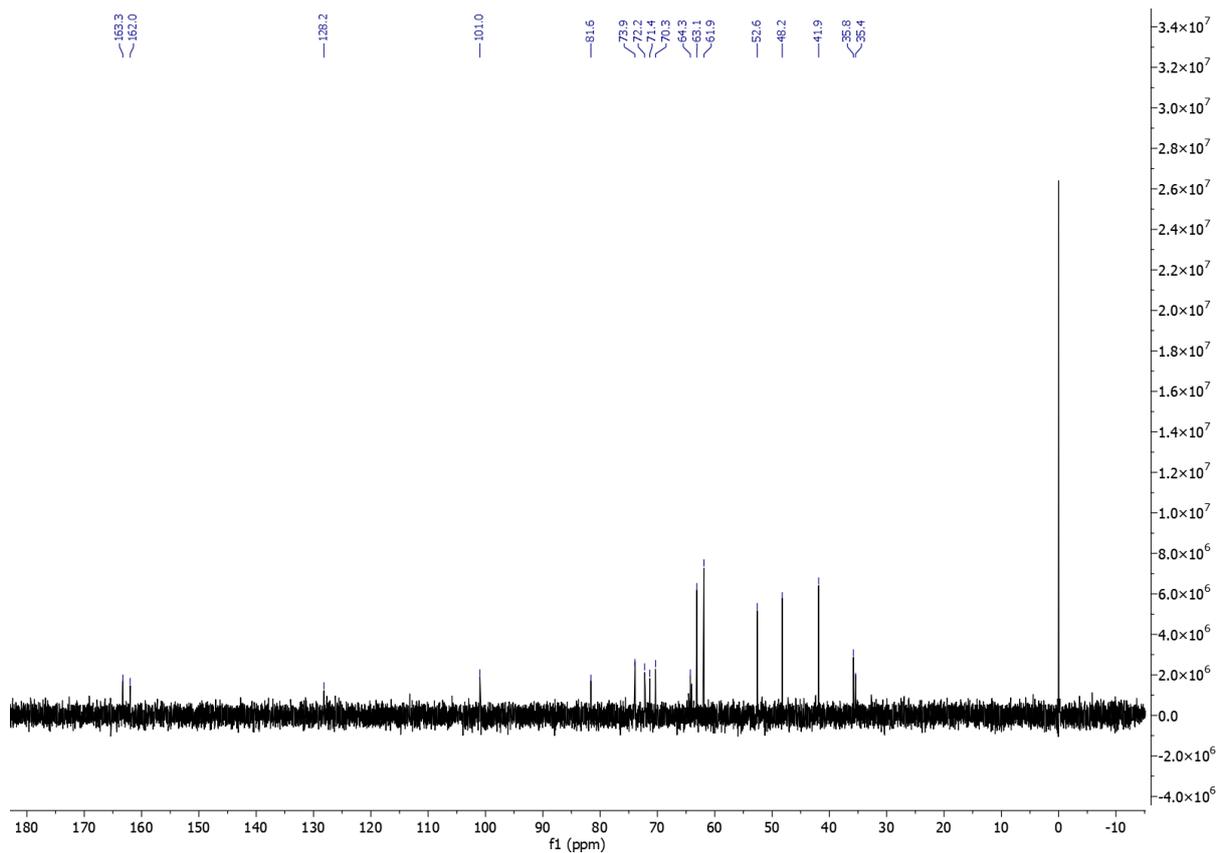
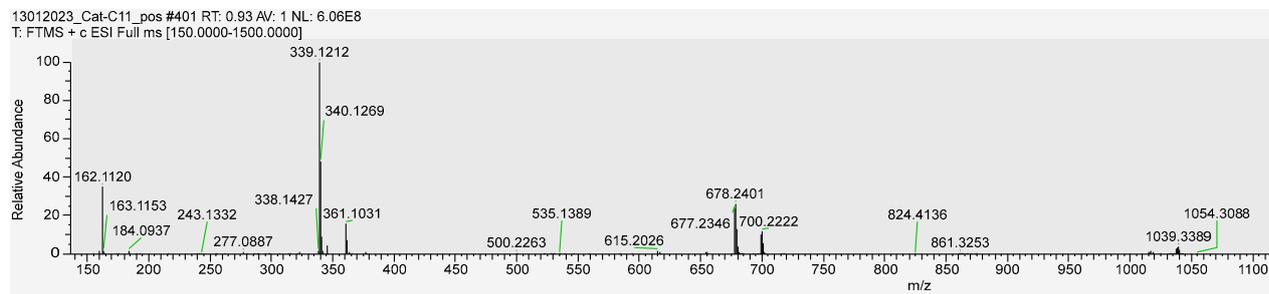


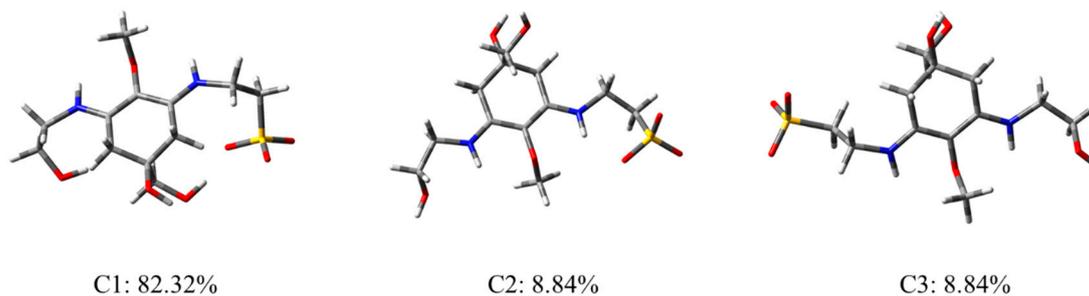
Figure S37. HMBC spectrum of compound **8** in D<sub>2</sub>O



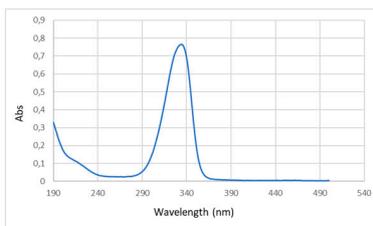
**Figure S38.**  $^{13}\text{C}$  NMR spectrum of compound **8** in  $\text{D}_2\text{O}$



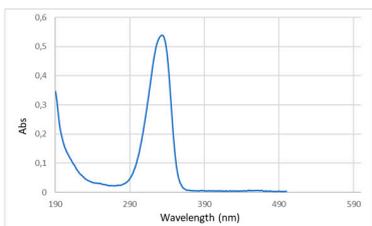
**Figure S39.** High-resolution mass spectrum of compound **8**



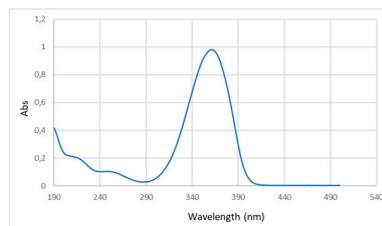
**Figure S40.** Overlayered conformers and population of Boltzmann averaged conformers of compound **8** optimized at the DFT/wb97xd/6-31+g(d,p) level in the gas phase.



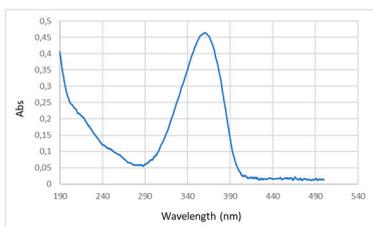
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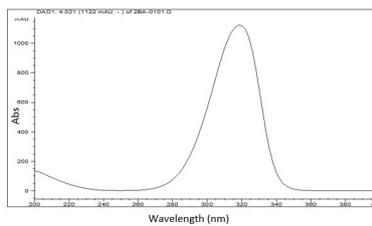
Compound 2



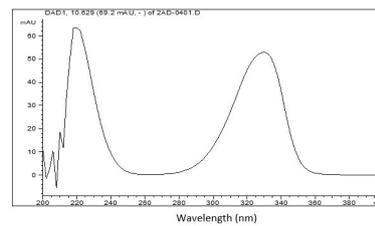
Compounds 3 and 4



Compounds 5 and 6



Compound 7



Compound 8

**Figure S41.** Absorbance spectra of compounds 1-8 in water.