

## 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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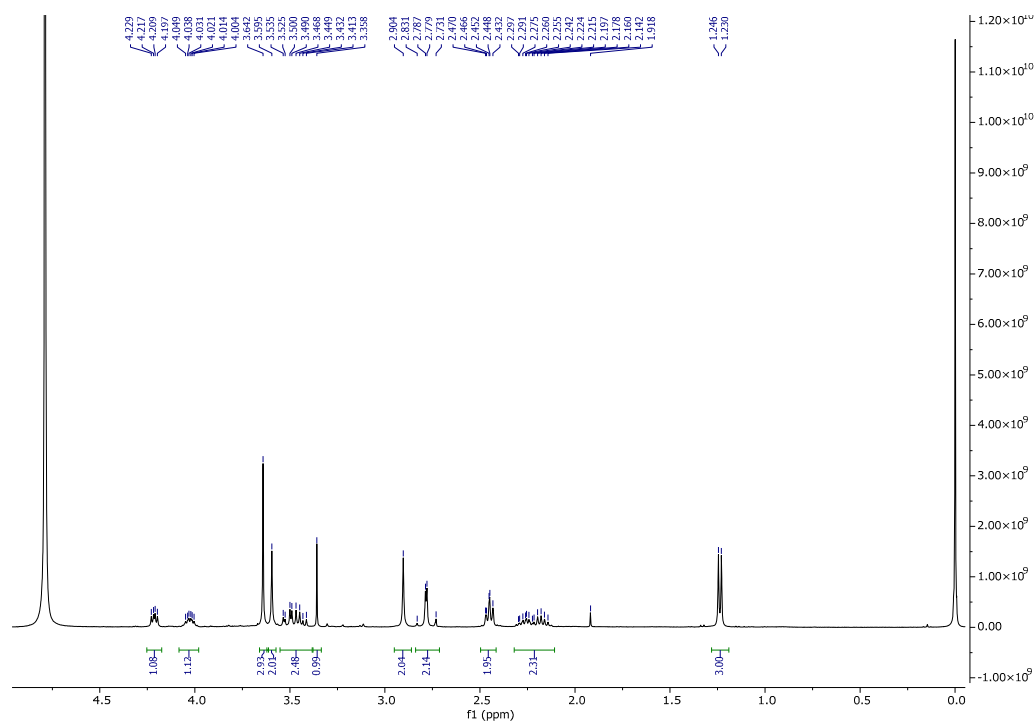
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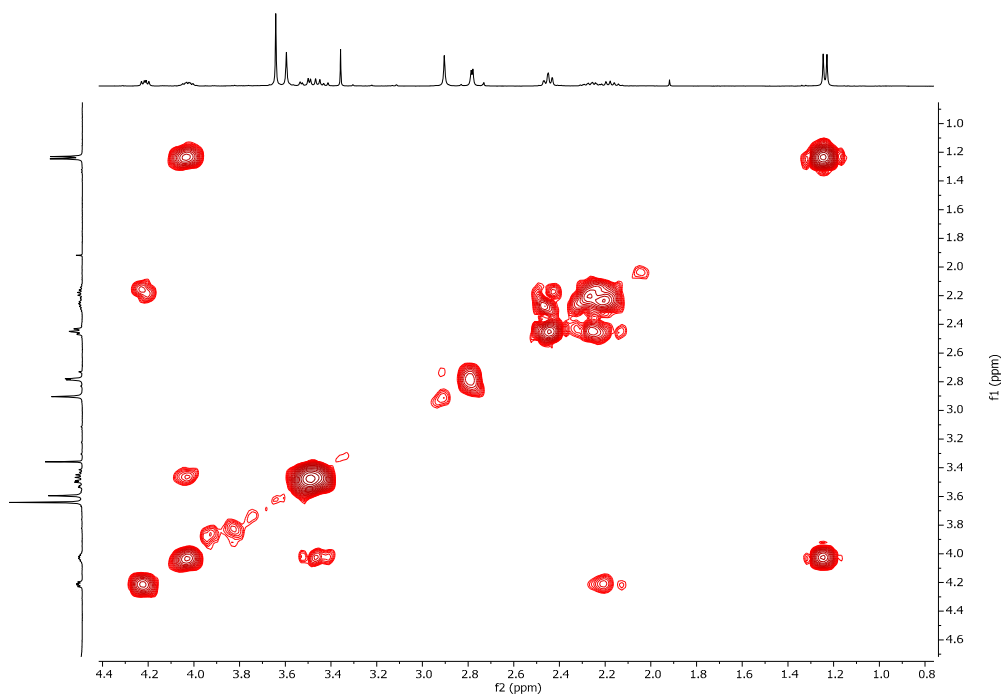
## Contents

Figure S1. $^1\text{H}$ NMR spectrum of compound 1 in $\text{D}_2\text{O}$ .....	4
Figure S2. COSY spectrum of compound 1 in $\text{D}_2\text{O}$ .....	4
Figure S3. HSQC spectrum of compound 1 in $\text{D}_2\text{O}$ .....	5
Figure S4. HMBC spectrum of compound 1 in $\text{D}_2\text{O}$ .....	5
Figure S5. $^{13}\text{C}$ NMR spectrum of compound 1 in $\text{D}_2\text{O}$ .....	6
Figure S6. High-resolution mass spectrum of compound 1 .....	6
Figure S7. Overlayed 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. ....	6
Figure S8. $^1\text{H}$ NMR spectrum of compound 2 in $\text{D}_2\text{O}$ .....	7
Figure S9. COSY spectrum of compound 2 in $\text{D}_2\text{O}$ .....	7
Figure S10. HSQC spectrum of compound 2 in $\text{D}_2\text{O}$ .....	8
Figure S11. HMBC spectrum of compound 2 in $\text{D}_2\text{O}$ .....	8
Figure S12. $^{13}\text{C}$ NMR spectrum of compound 2 in $\text{D}_2\text{O}$ .....	9
Figure S13. High-resolution mass spectrum of compound 2 .....	9
Figure S14. Overlayed 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. ....	10
Figure S15. $^1\text{H}$ NMR spectrum of compounds 3 and 4 in $\text{D}_2\text{O}$ .....	10
Figure S16. COSY spectrum of compounds 3 and 4 in $\text{D}_2\text{O}$ .....	11
Figure S17. HSQC spectrum of compounds 3 and 4 in $\text{D}_2\text{O}$ .....	12
Figure S18. HMBC spectrum of compounds 3 and 4 in $\text{D}_2\text{O}$ .....	12
Figure S19. $^{13}\text{C}$ NMR spectrum of compounds 3 and 4 in $\text{D}_2\text{O}$ .....	13
Figure S20. High-resolution mass spectrum of compounds 3 and 4.....	13
Figure S21. $^1\text{H}$ NMR spectrum of compounds 5 and 6 in $\text{D}_2\text{O}$ .....	14
Figure S22. COSY spectrum of compounds 5 and 6 in $\text{D}_2\text{O}$ .....	14
Figure S23. HSQC spectrum of compounds 5 and 6 in $\text{D}_2\text{O}$ .....	15
Figure S24. HMBC spectrum of compounds 5 and 6 in $\text{D}_2\text{O}$ .....	16
Figure S25. $^{13}\text{C}$ NMR spectrum of compounds 5 and 6 in $\text{D}_2\text{O}$ .....	16
Figure S26. High-resolution mass spectrum of compounds 5 and 6.....	16
Figure S27. $^1\text{H}$ NMR spectrum of compound 7 in $\text{D}_2\text{O}$ .....	17
Figure S28. COSY spectrum of compound 7 in $\text{D}_2\text{O}$ .....	17
Figure S29. HSQC spectrum of compound 7 in $\text{D}_2\text{O}$ .....	18
Figure S30. HMBC spectrum of compound 7 in $\text{D}_2\text{O}$ .....	18

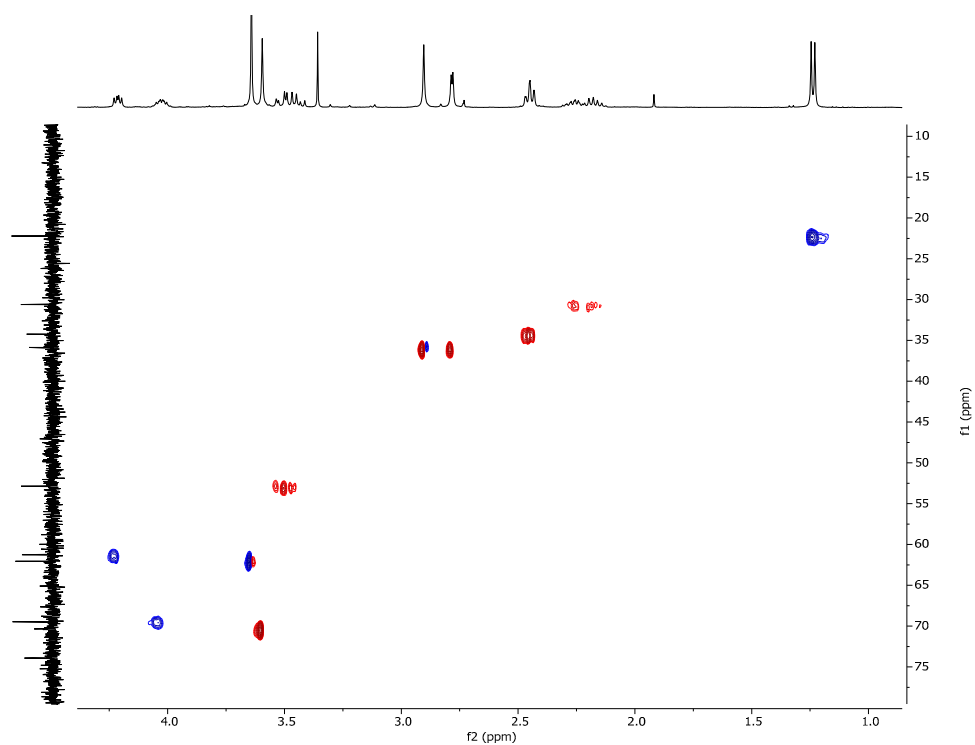
Figure S31. $^{13}\text{C}$ NMR spectrum of compound 7 in $\text{D}_2\text{O}$ .....	19
Figure S32. High-resolution mass spectrum of compound 7 .....	19
Figure S33. Overlayed conformers and population of Boltzmann averaged conformers of compound 7 optimized at the DFT/wb97xd/6-31+g(d,p) level in the gas phase. ....	20
Figure S34. $^1\text{H}$ NMR spectrum of compound 8 in $\text{D}_2\text{O}$ .....	21
Figure S35. COSY spectrum of compound 8 in $\text{D}_2\text{O}$ .....	21
Figure S36. HSQC spectrum of compound 8 in $\text{D}_2\text{O}$ .....	22
Figure S37. HMBC spectrum of compound 8 in $\text{D}_2\text{O}$ .....	22
Figure S38. $^{13}\text{C}$ NMR spectrum of compound 8 in $\text{D}_2\text{O}$ .....	23
Figure S39. High-resolution mass spectrum of compound 8 .....	23
Figure S40. Overlayed 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. ....	23
Figure S41. Absorbance spectra of compounds 1-8 in water. ....	24



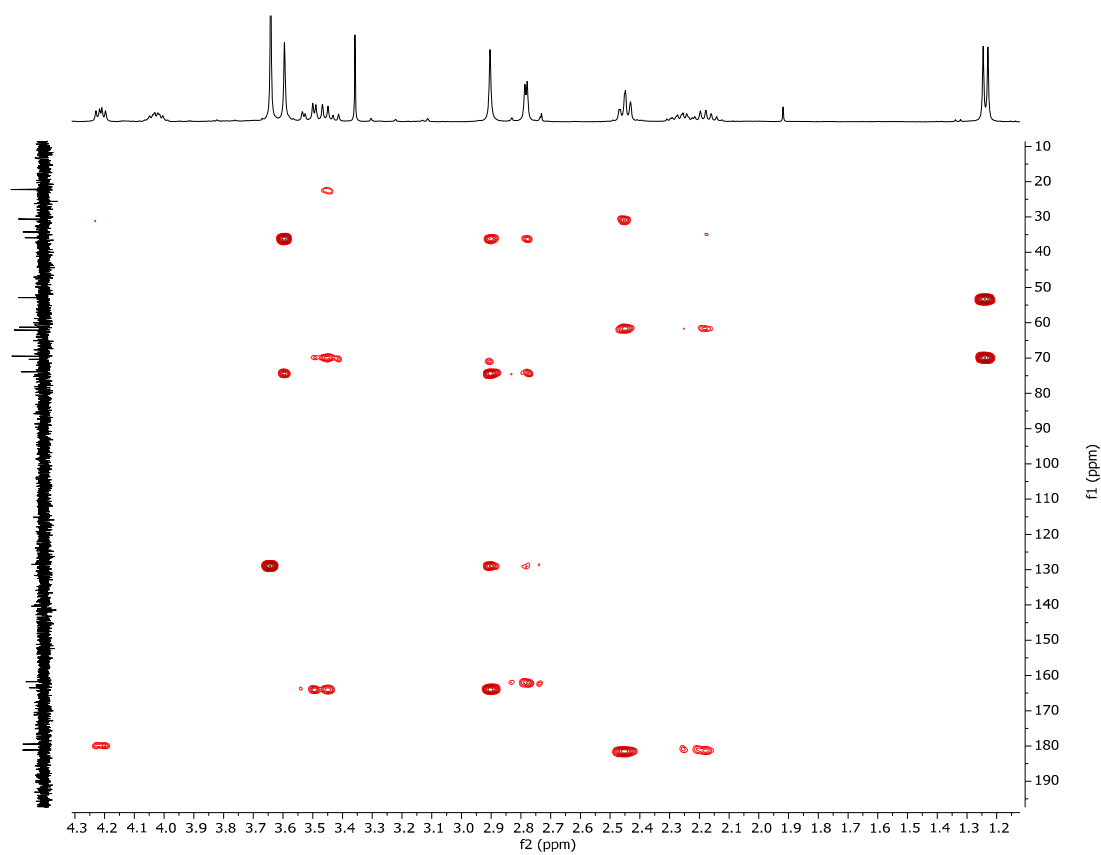
**Figure S1.**  $^1\text{H}$  NMR spectrum of compound **1** in  $\text{D}_2\text{O}$



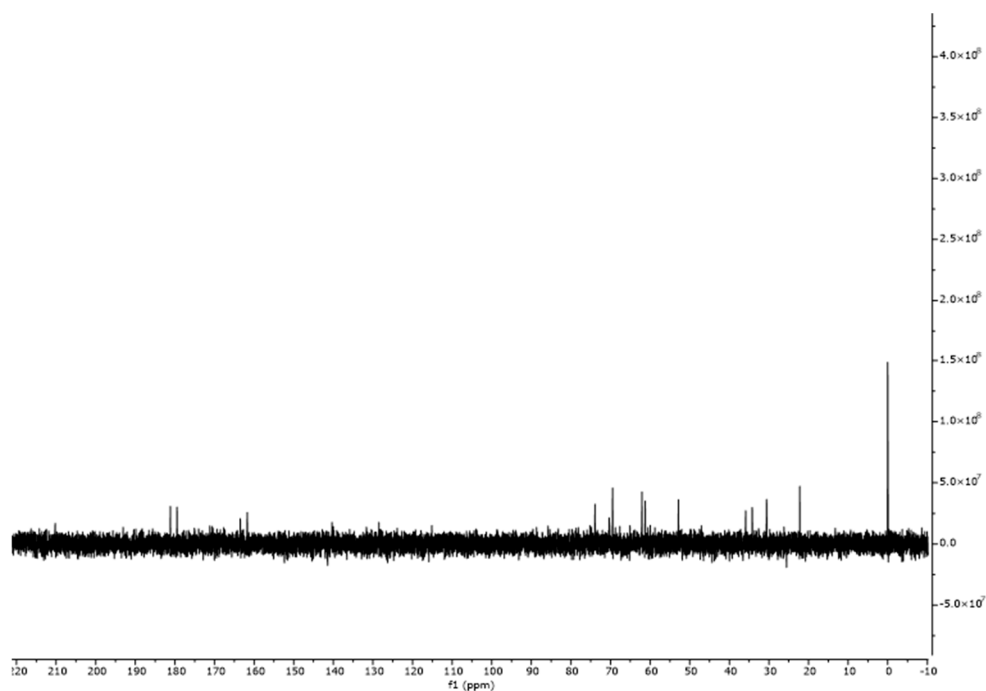
**Figure S2.** COSY spectrum of compound **1** in  $\text{D}_2\text{O}$



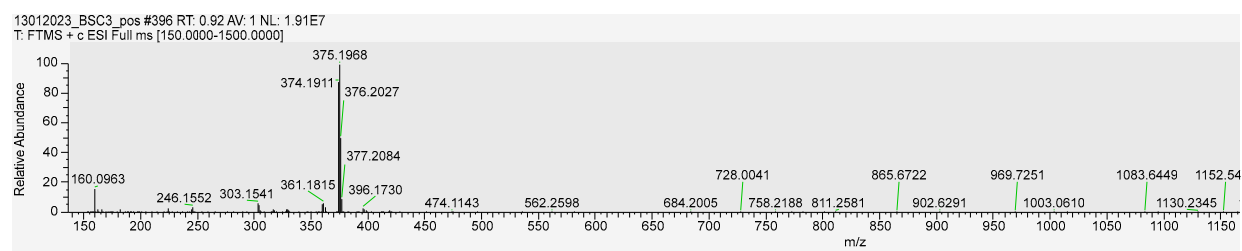
**Figure S3.** HSQC spectrum of compound **1** in D<sub>2</sub>O



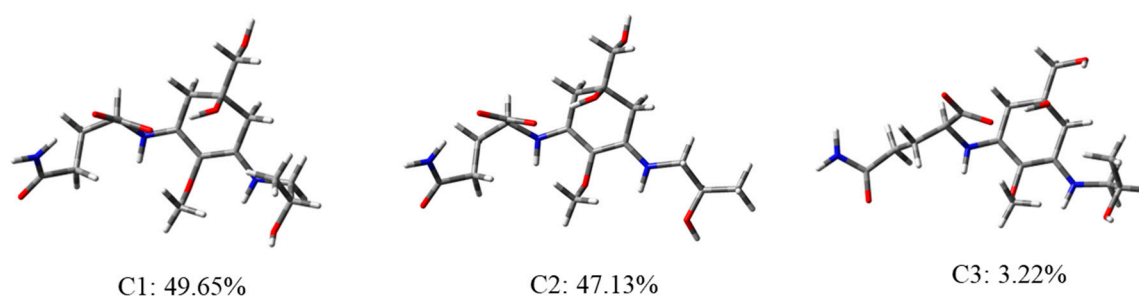
**Figure S4.** HMBC spectrum of compound **1** in D<sub>2</sub>O



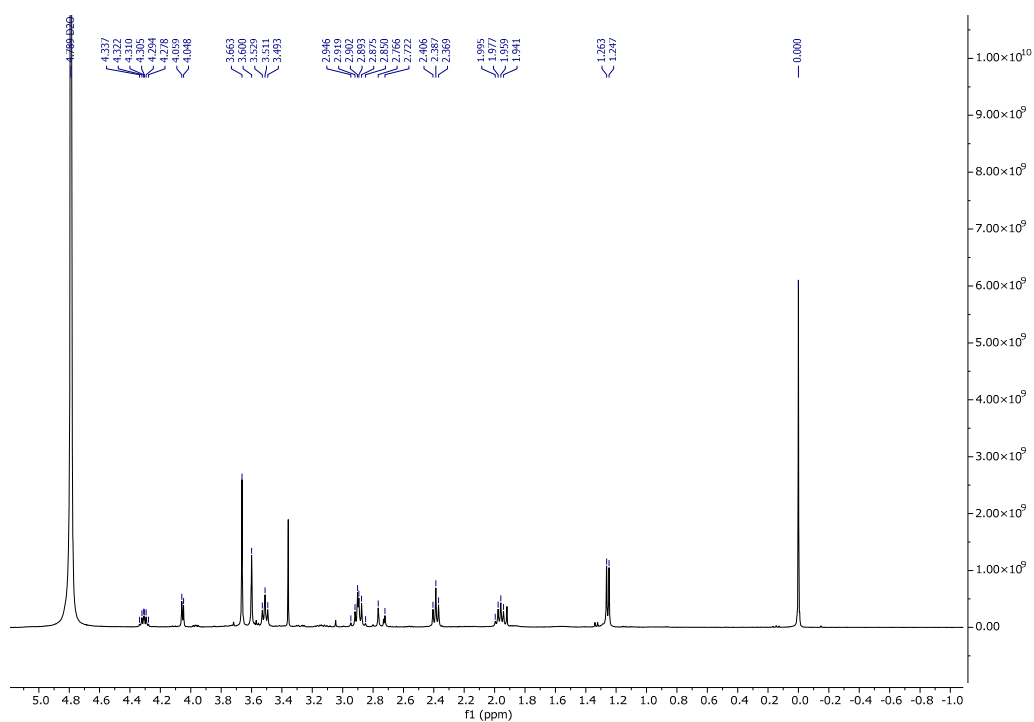
**Figure S5.**  $^{13}\text{C}$  NMR spectrum of compound **1** in  $\text{D}_2\text{O}$



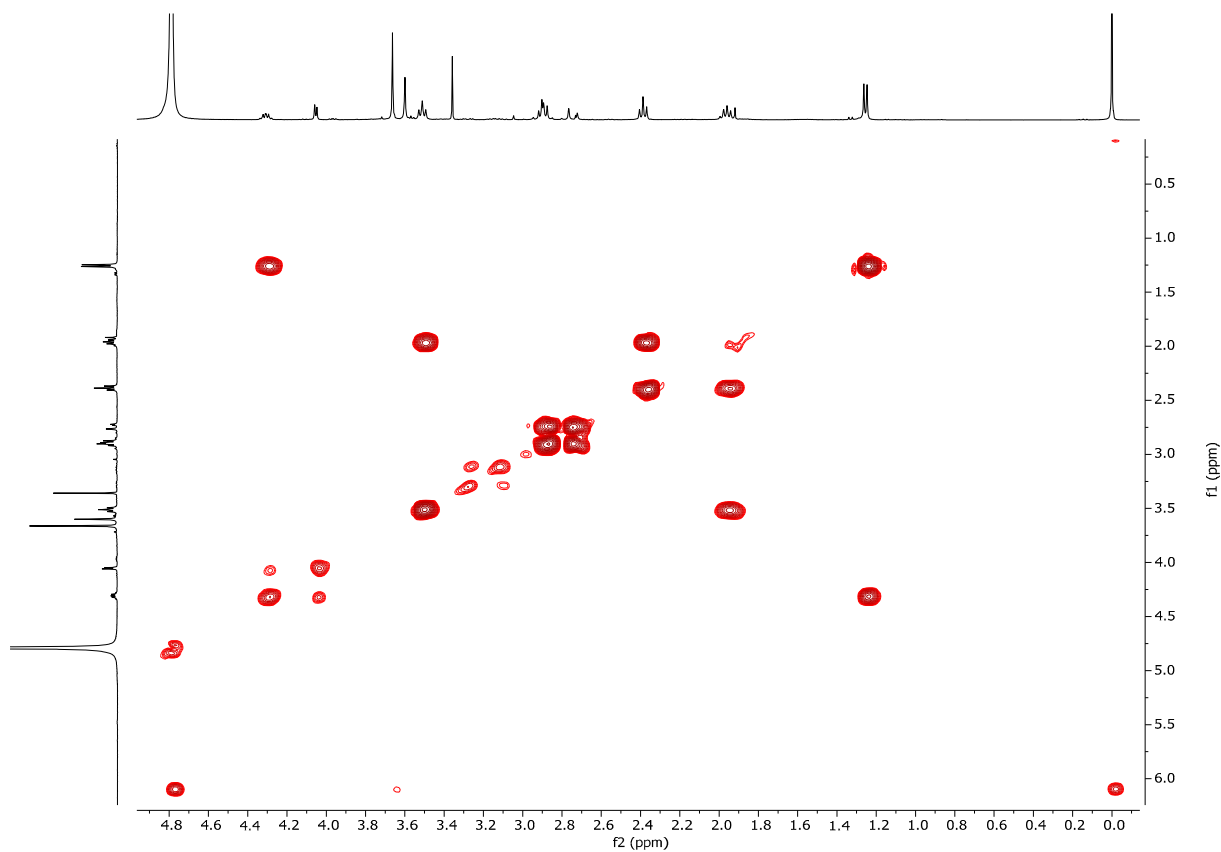
**Figure S6.** High-resolution mass spectrum of compound **1**



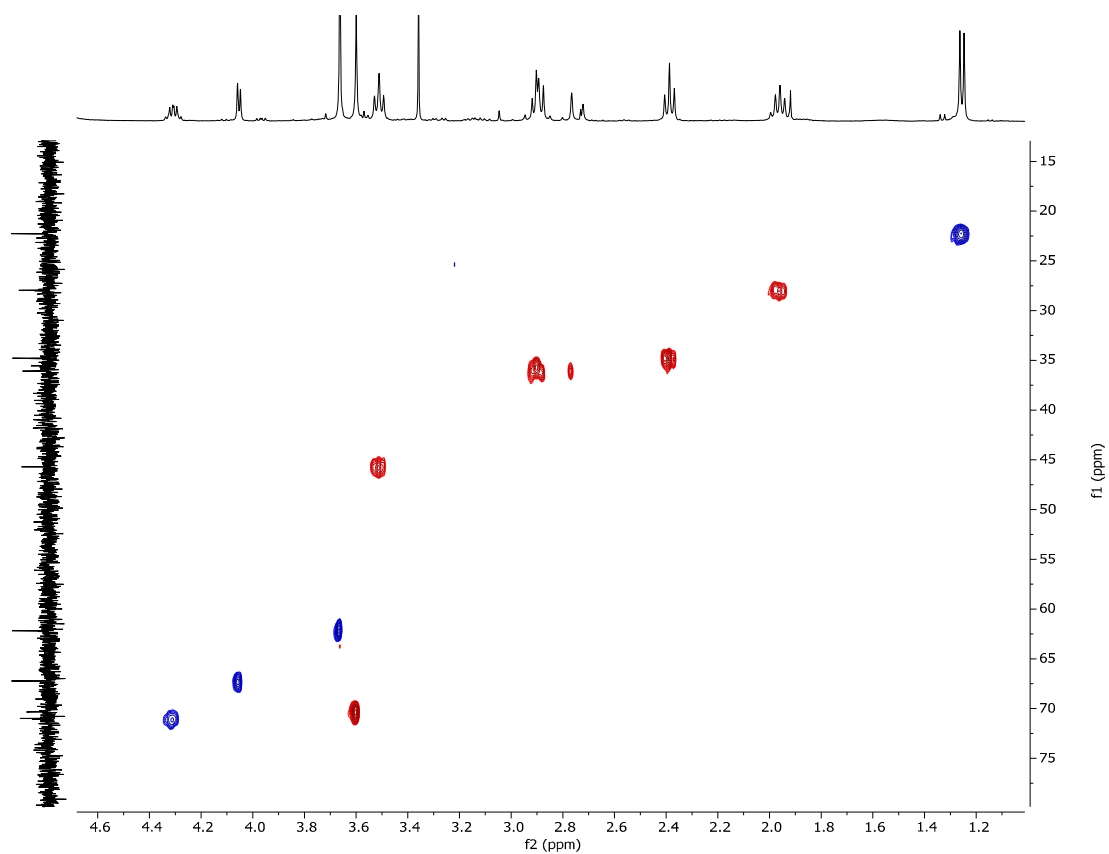
**Figure S7.** Overlayed conformers and population of Boltzmann averaged conformers of compound **1** optimized at the DFT/wb97xd/6-31+g(d,p) level in the gas phase.



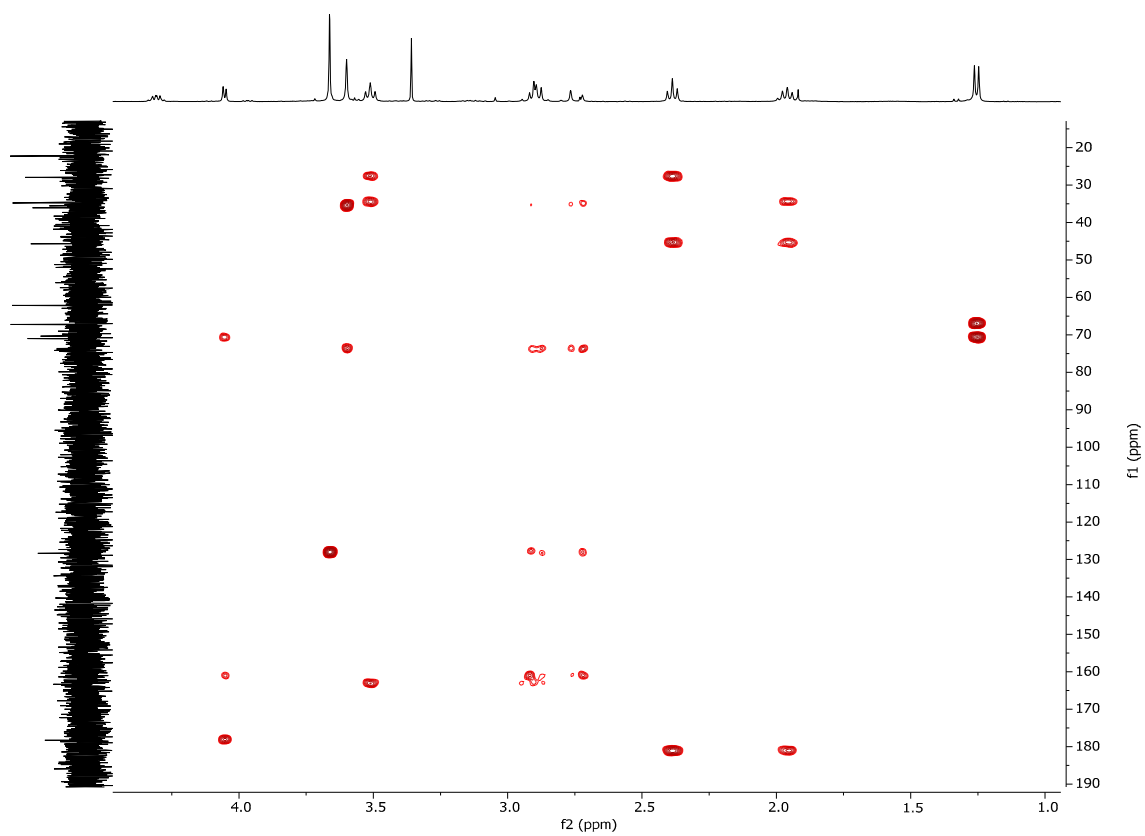
**Figure S8.** <sup>1</sup>H NMR spectrum of compound **2** in D<sub>2</sub>O



**Figure S9.** COSY spectrum of compound **2** in D<sub>2</sub>O

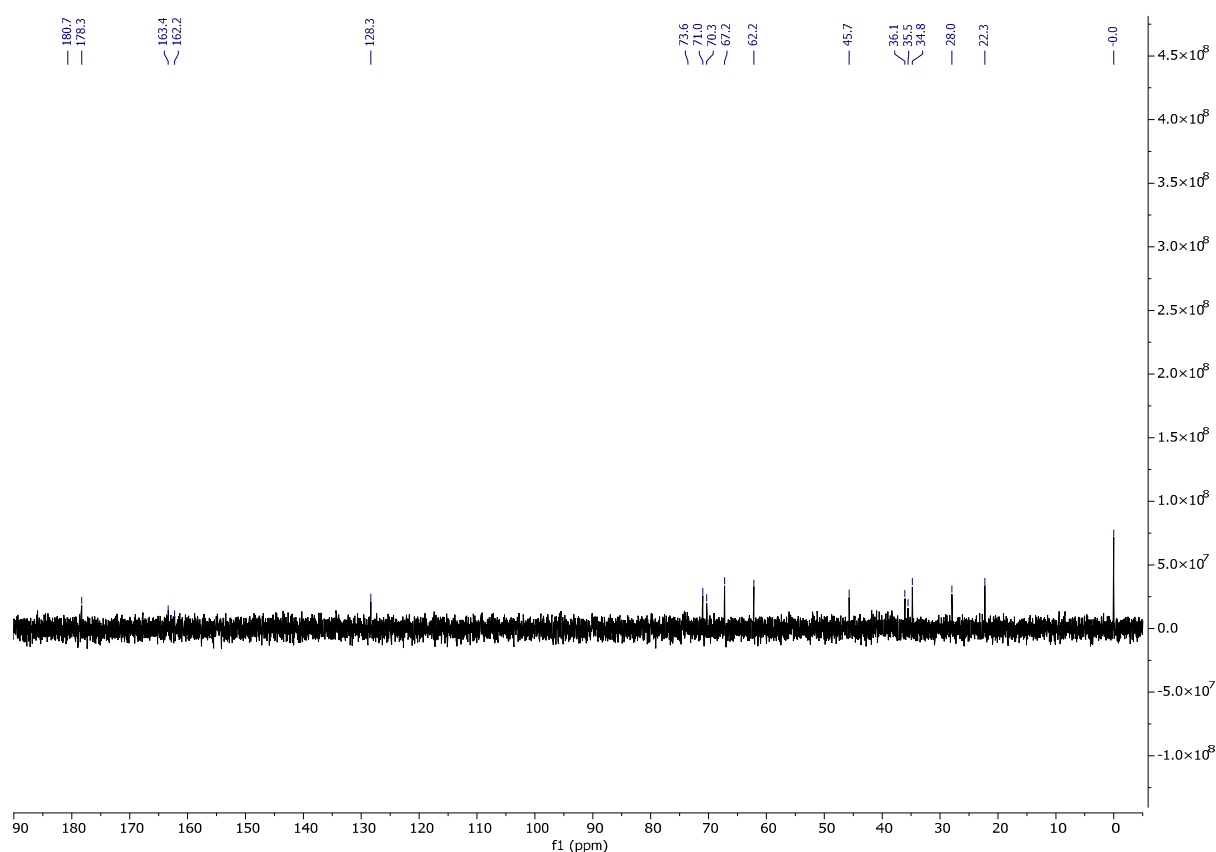


**Figure S10.** HSQC spectrum of compound **2** in D<sub>2</sub>O

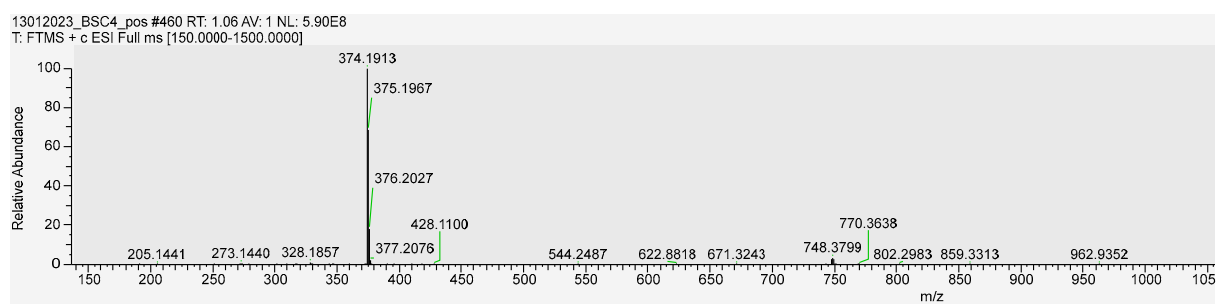


**Figure S11.** HMBC spectrum of compound **2** in D<sub>2</sub>O

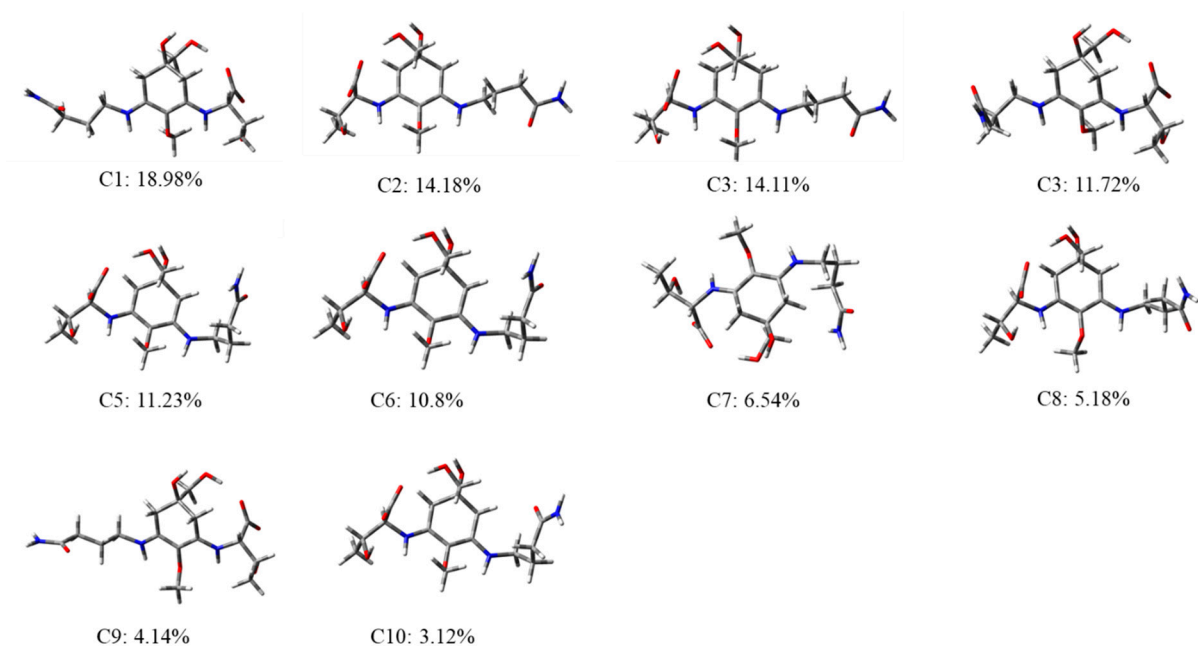




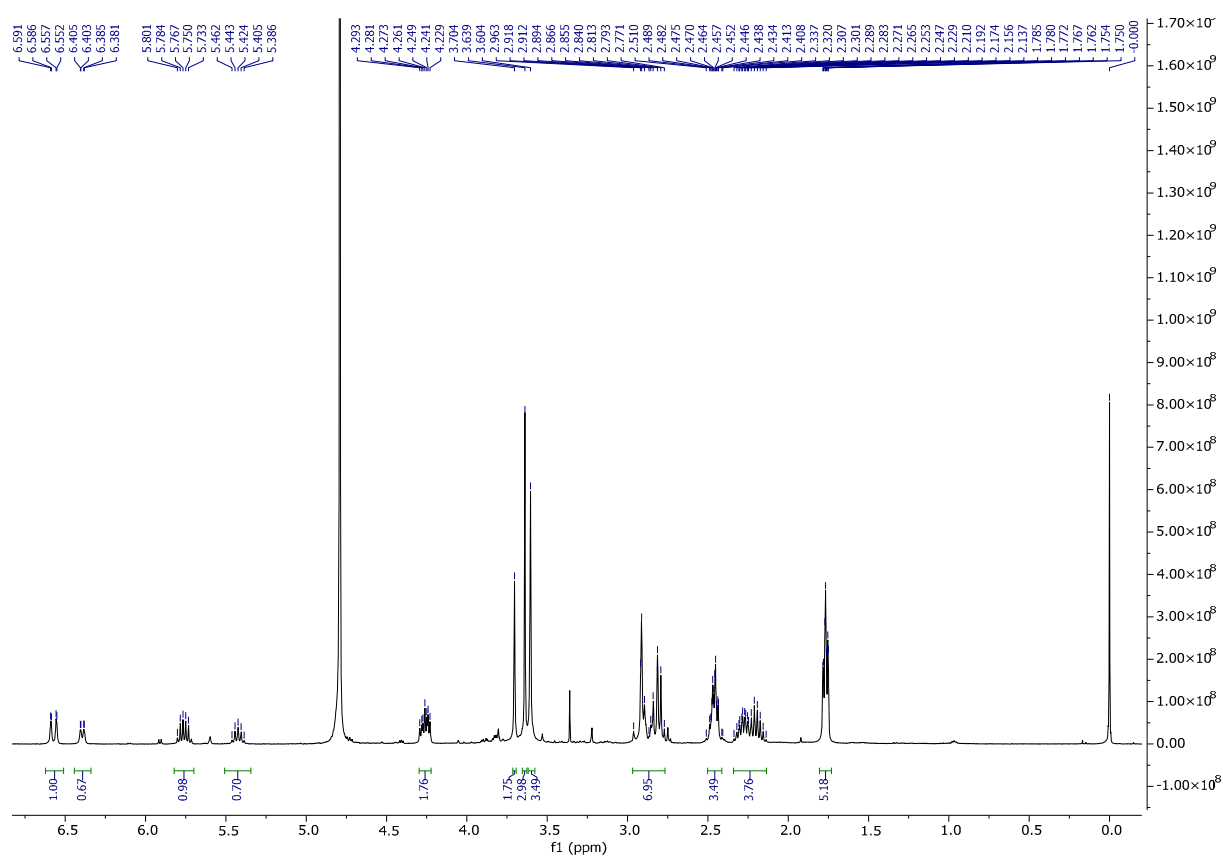
**Figure S12.** <sup>13</sup>C NMR spectrum of compound 2 in D<sub>2</sub>O



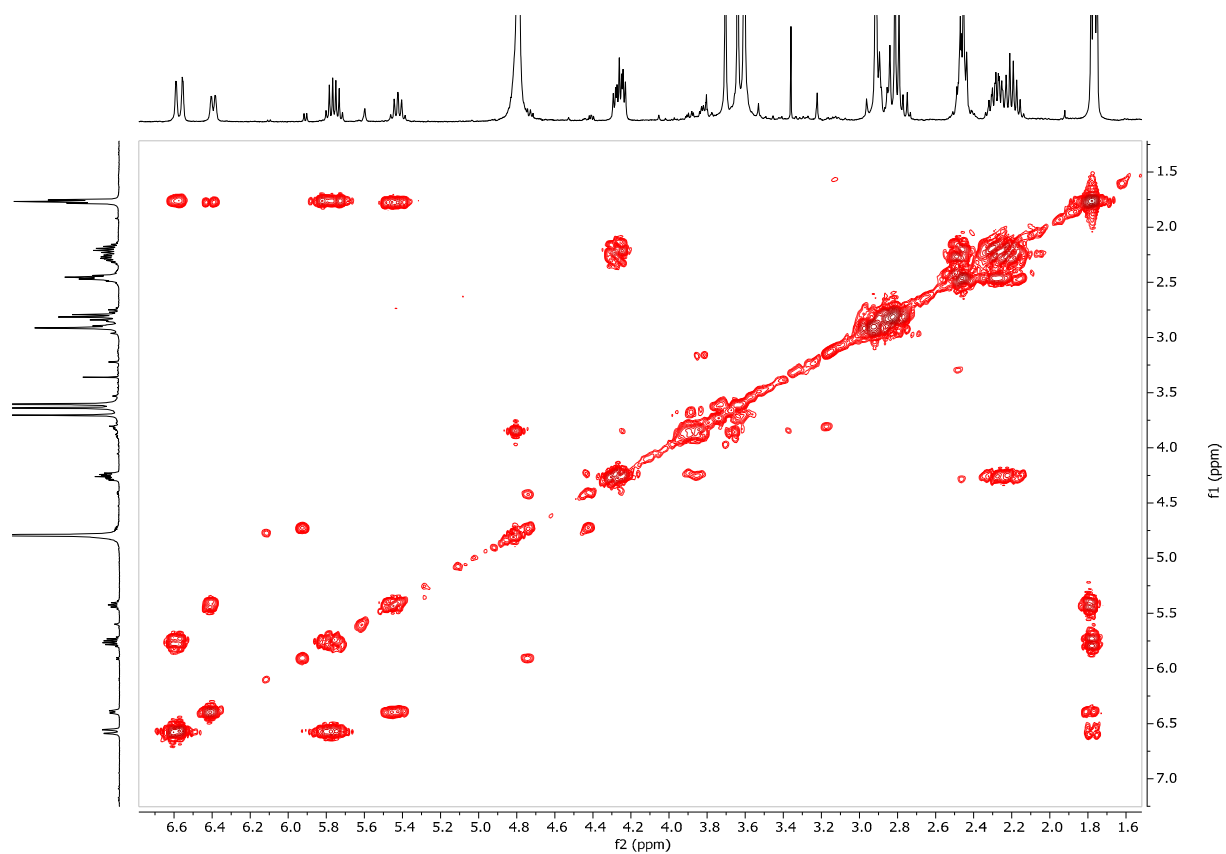
**Figure S13.** High-resolution mass spectrum of compound 2



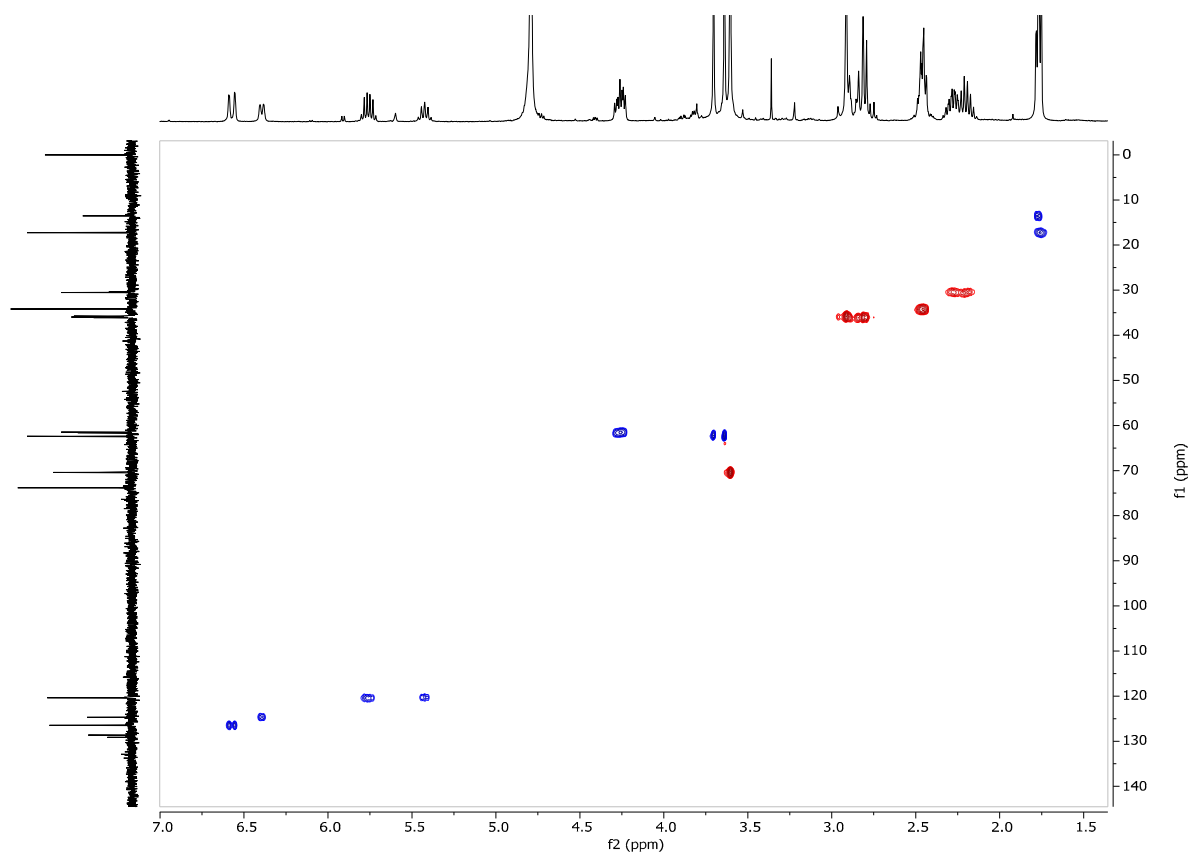
**Figure S14.** Overlayered conformers and population of Boltzmann averaged conformers of compound 2 optimized at the DFT/wb97xd/6-31+g(d,p) level in the gas phase.



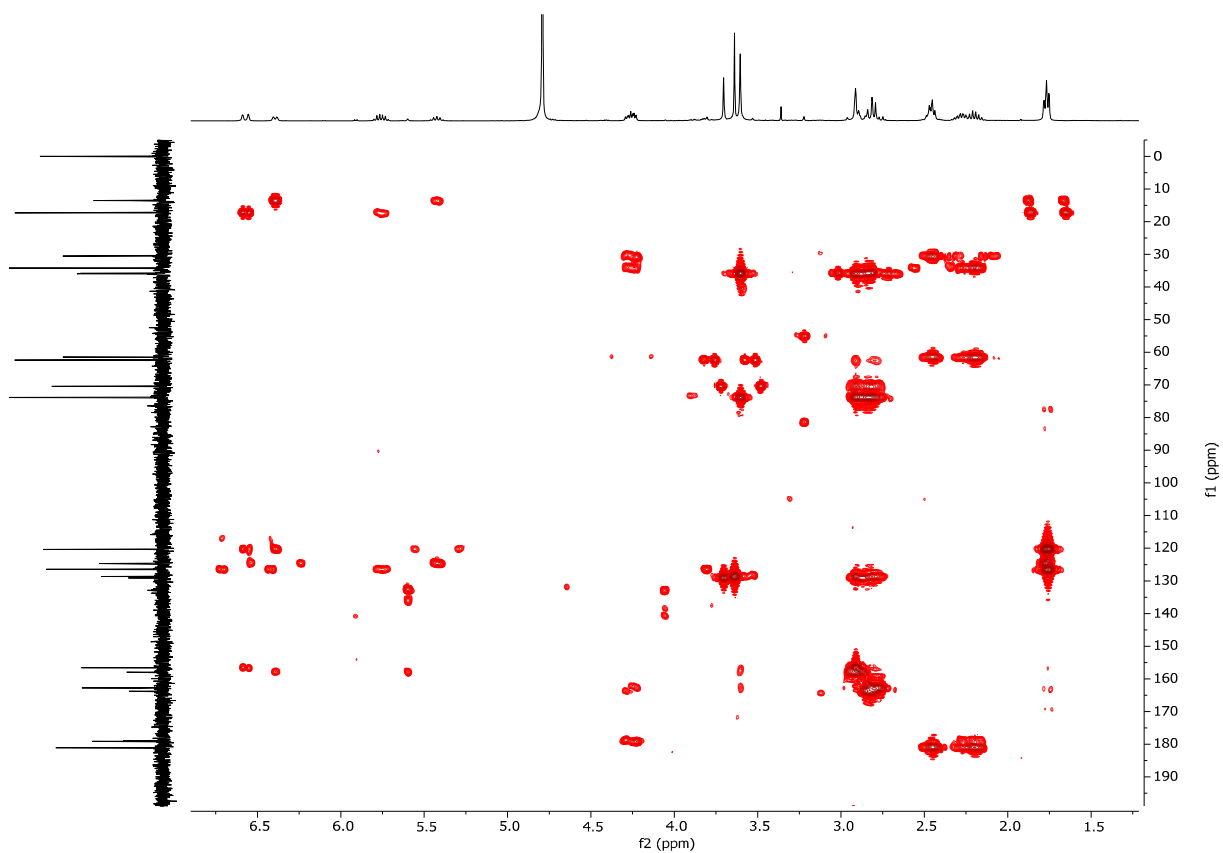
**Figure S15.**  $^1\text{H}$  NMR spectrum of compounds 3 and 4 in  $\text{D}_2\text{O}$



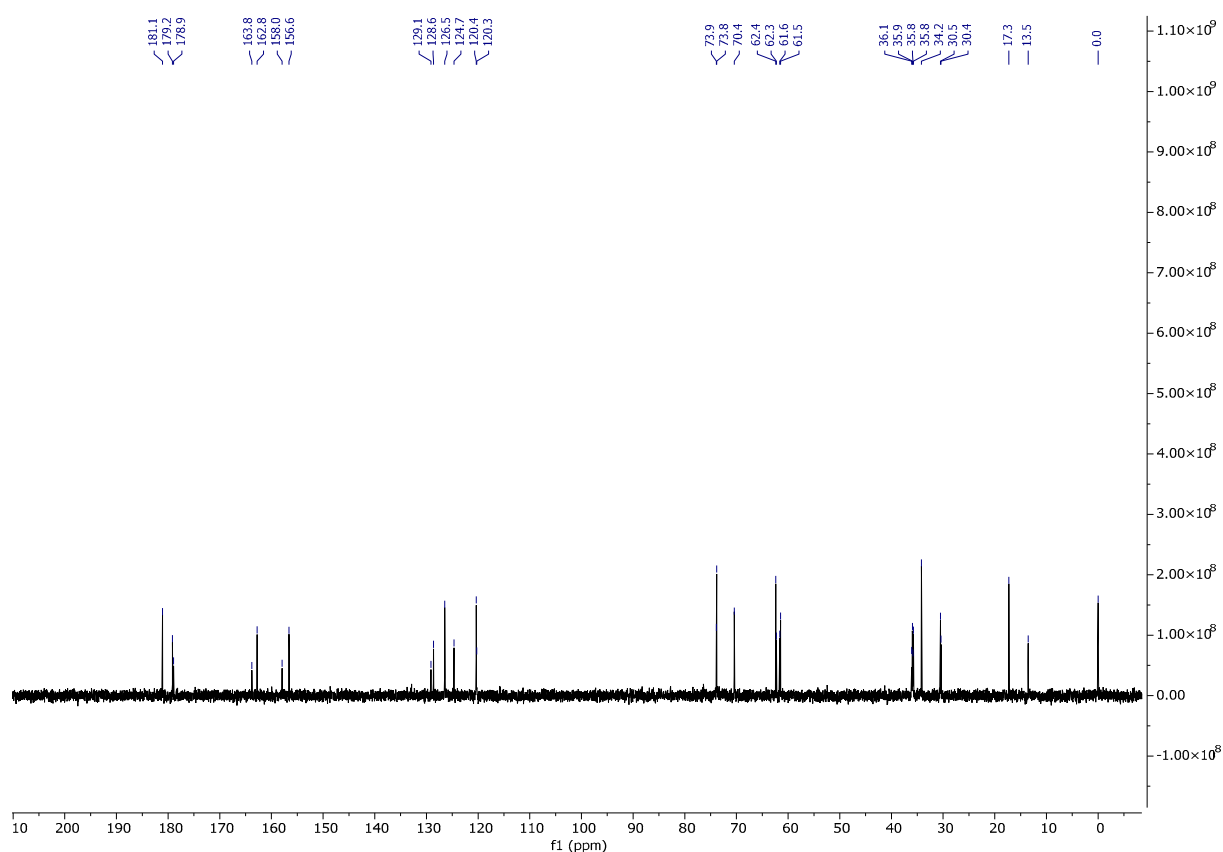
**Figure S16.** COSY spectrum of compounds **3** and **4** in D<sub>2</sub>O



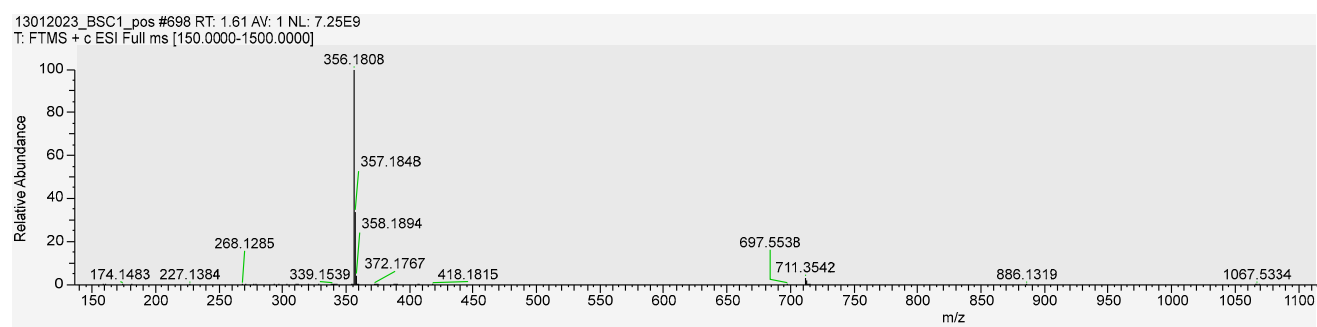
**Figure S17.** HSQC spectrum of compounds **3** and **4** in  $\text{D}_2\text{O}$



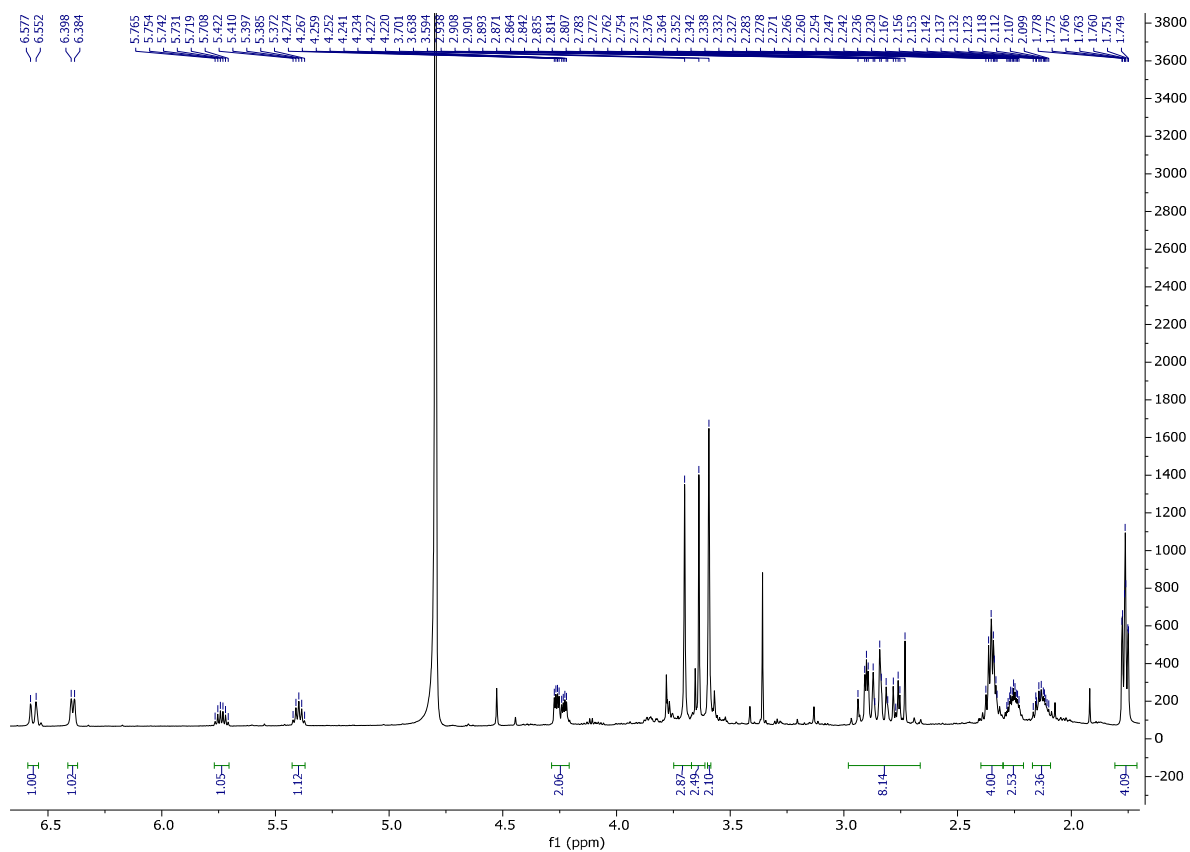
**Figure S18.** HMBC spectrum of compounds **3** and **4** in  $\text{D}_2\text{O}$



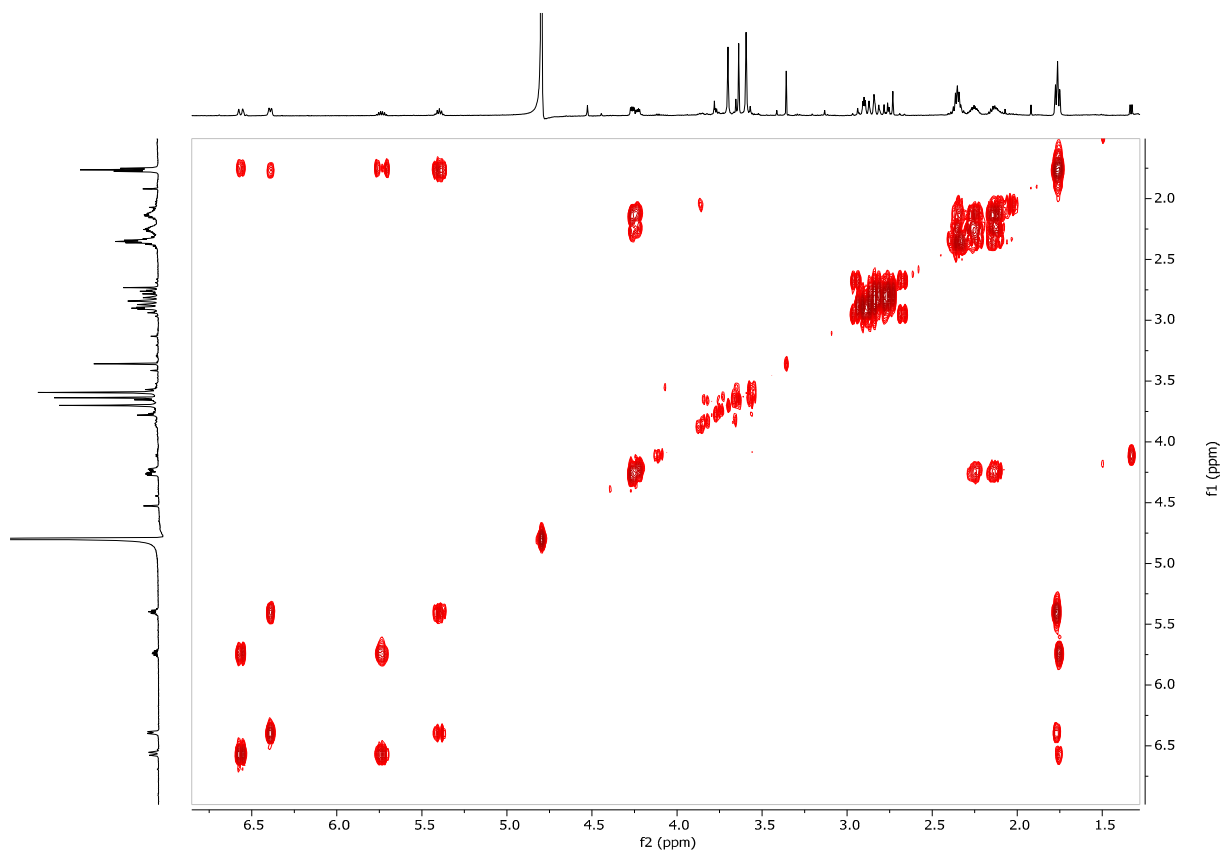
**Figure S19.** <sup>13</sup>C NMR spectrum of compounds **3** and **4** in D<sub>2</sub>O



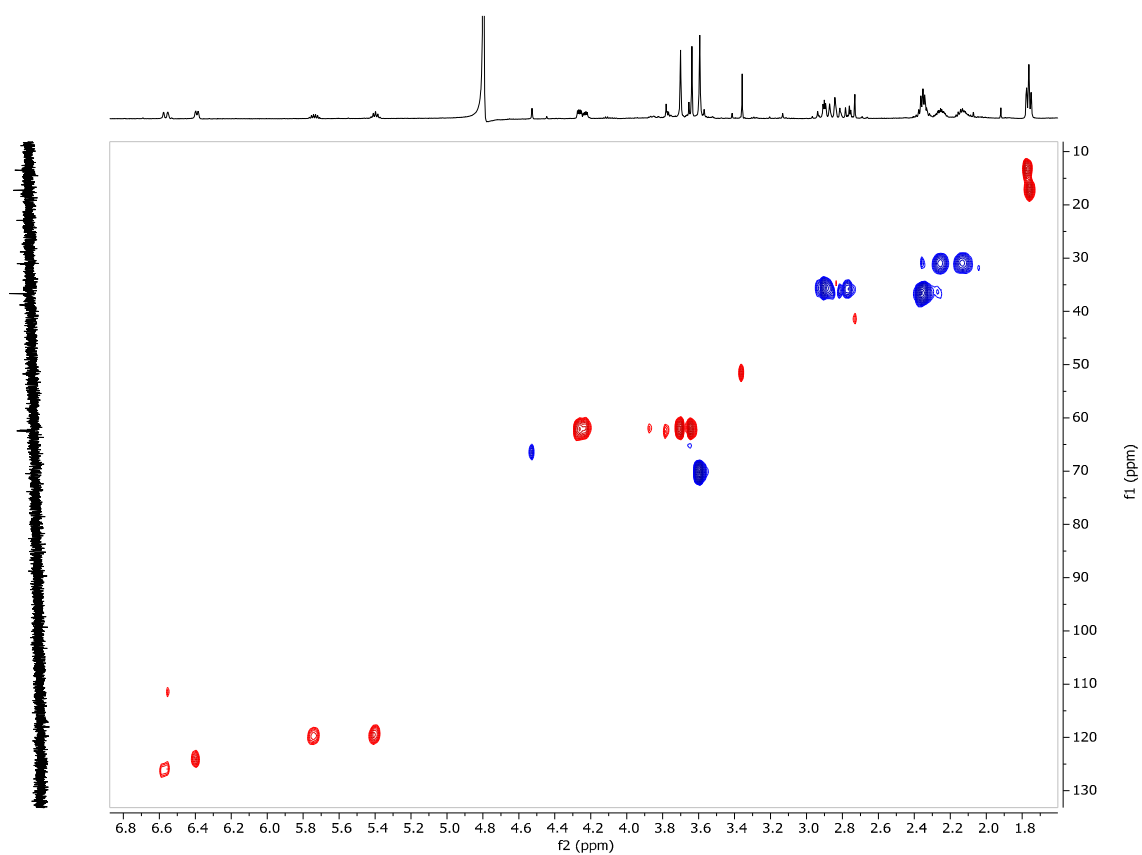
**Figure S20.** High-resolution mass spectrum of compounds **3** and **4**



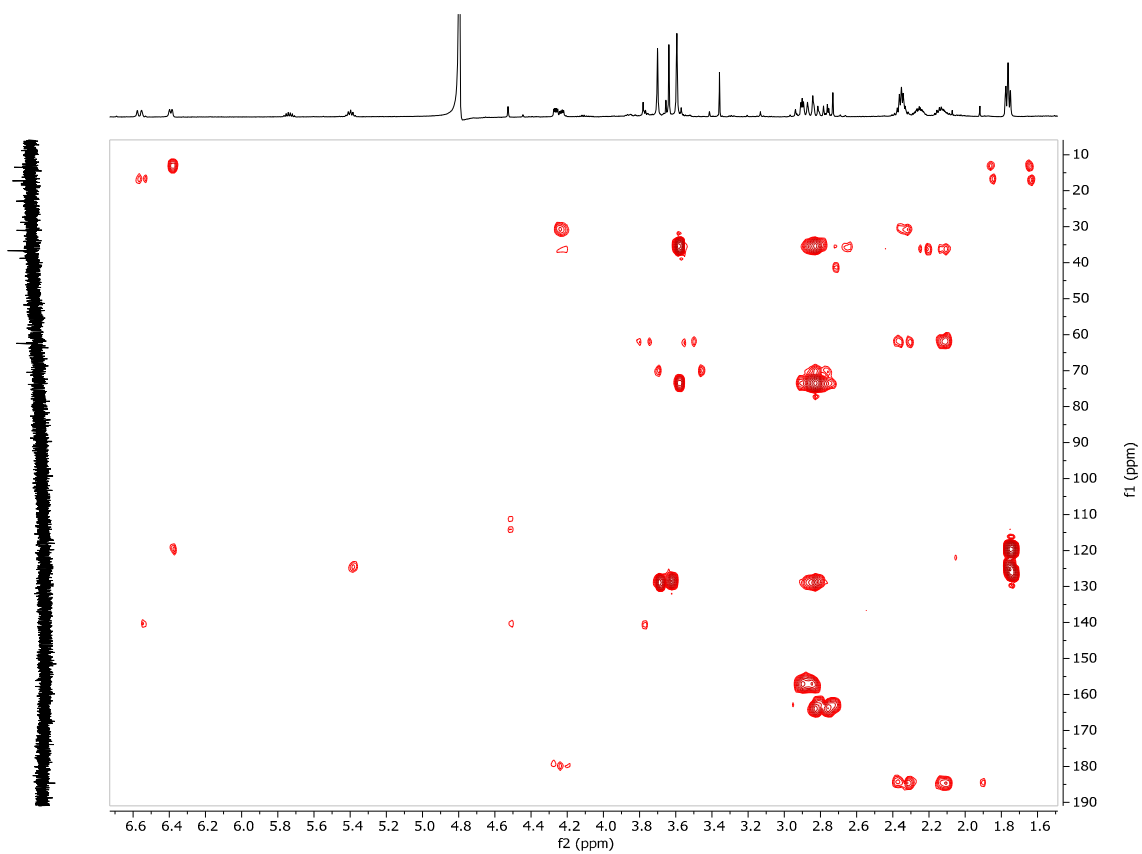
**Figure S21.**  $^1\text{H}$  NMR spectrum of compounds **5** and **6** in  $\text{D}_2\text{O}$



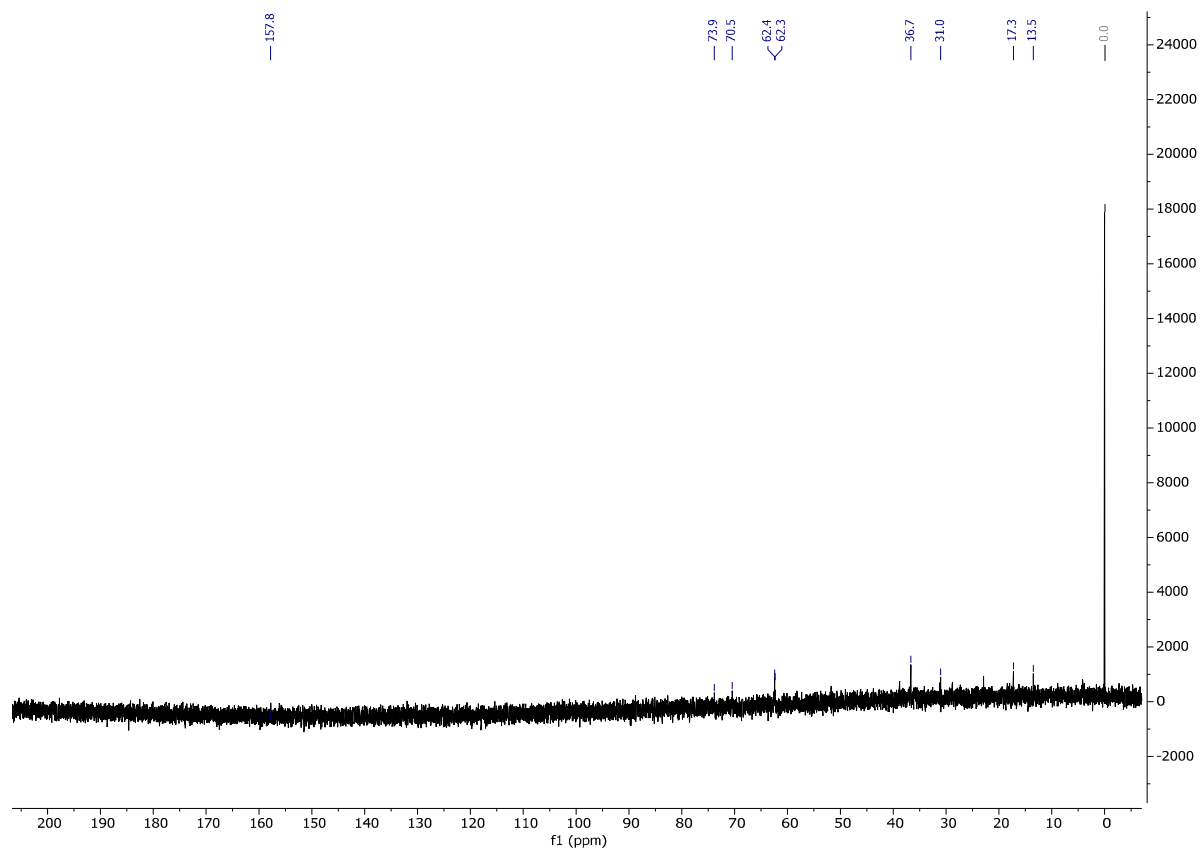
**Figure S22.** COSY spectrum of compounds **5** and **6** in  $\text{D}_2\text{O}$



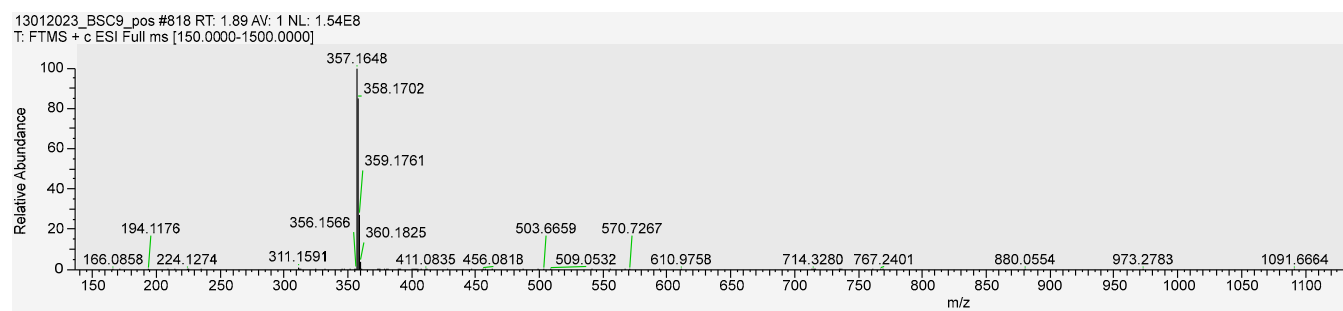
**Figure S23.** HSQC spectrum of compounds **5** and **6** in D<sub>2</sub>O



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

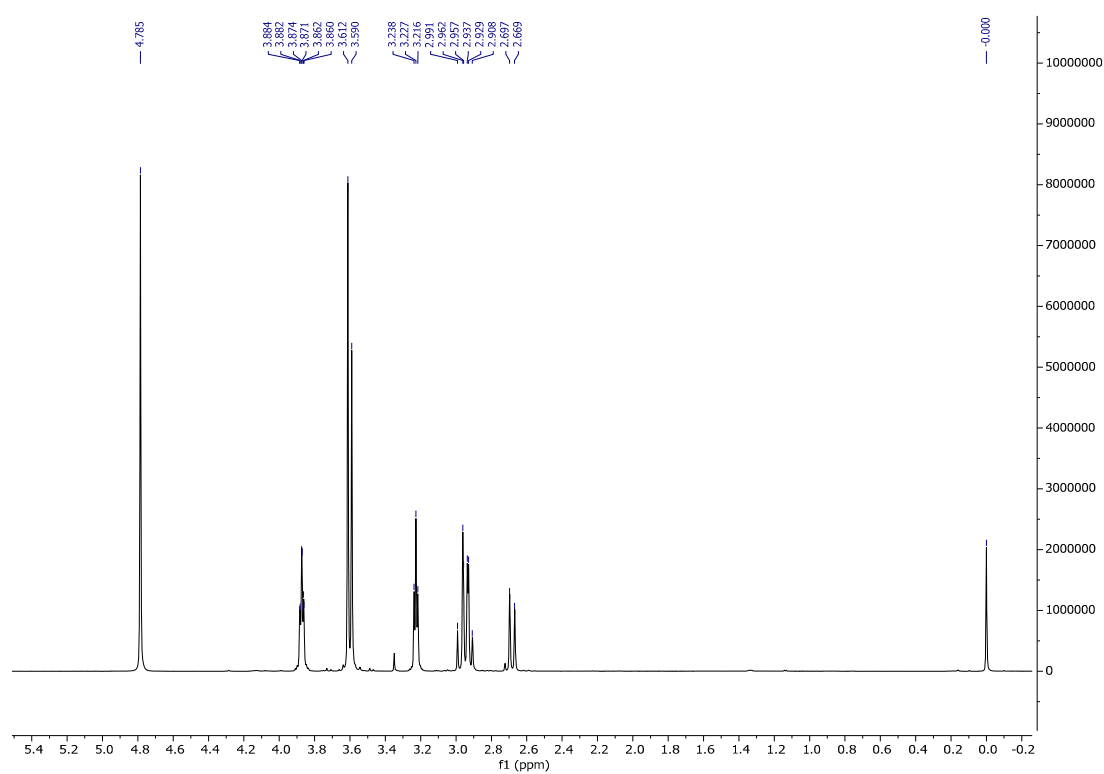


**Figure S25.** <sup>13</sup>C NMR spectrum of compounds **5** and **6** in D<sub>2</sub>O

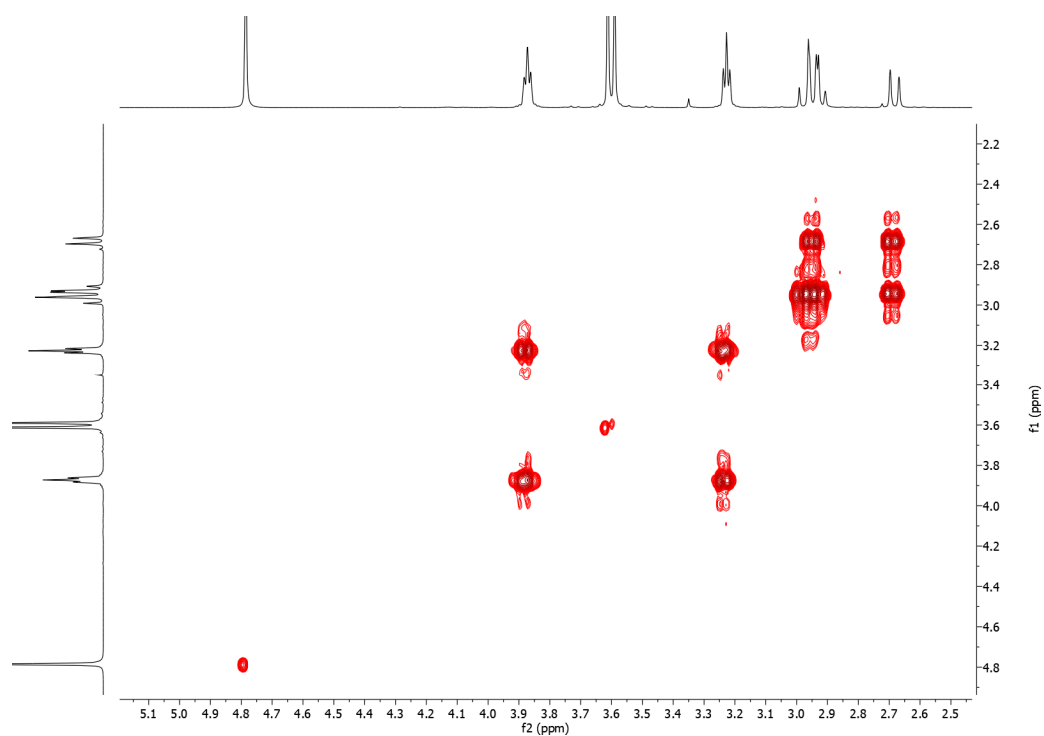


**Figure S26.** High-resolution mass spectrum of compounds **5** and **6**

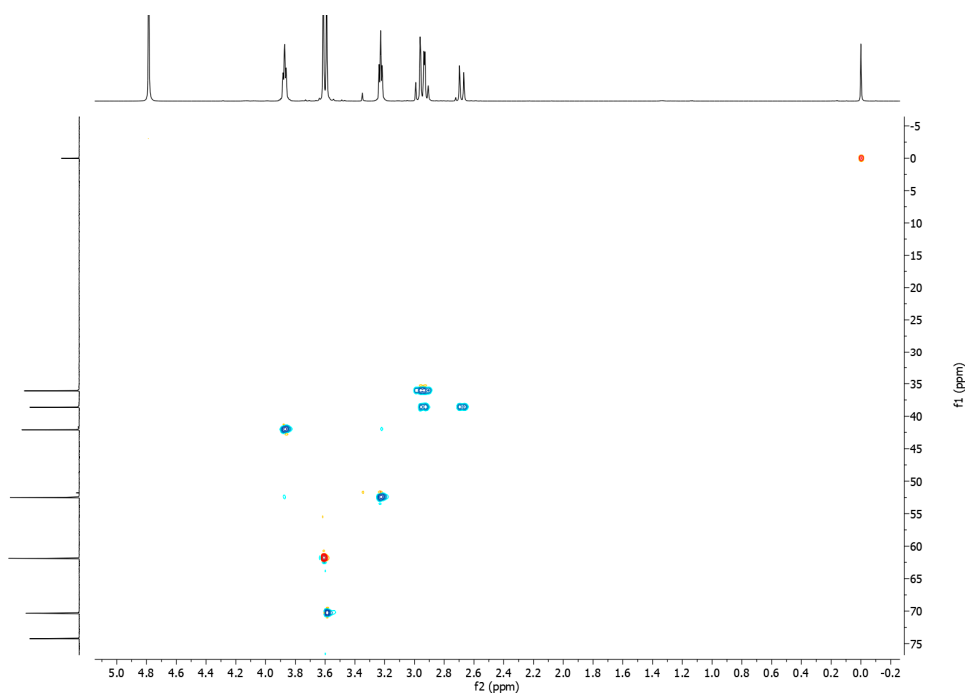




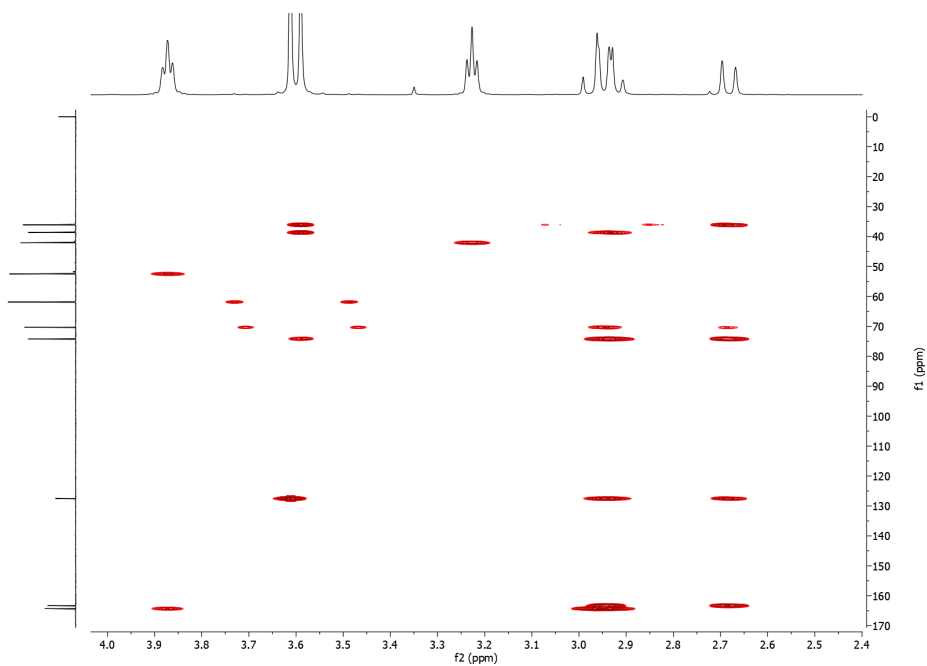
**Figure S27.** <sup>1</sup>H NMR spectrum of compound 7 in D<sub>2</sub>O



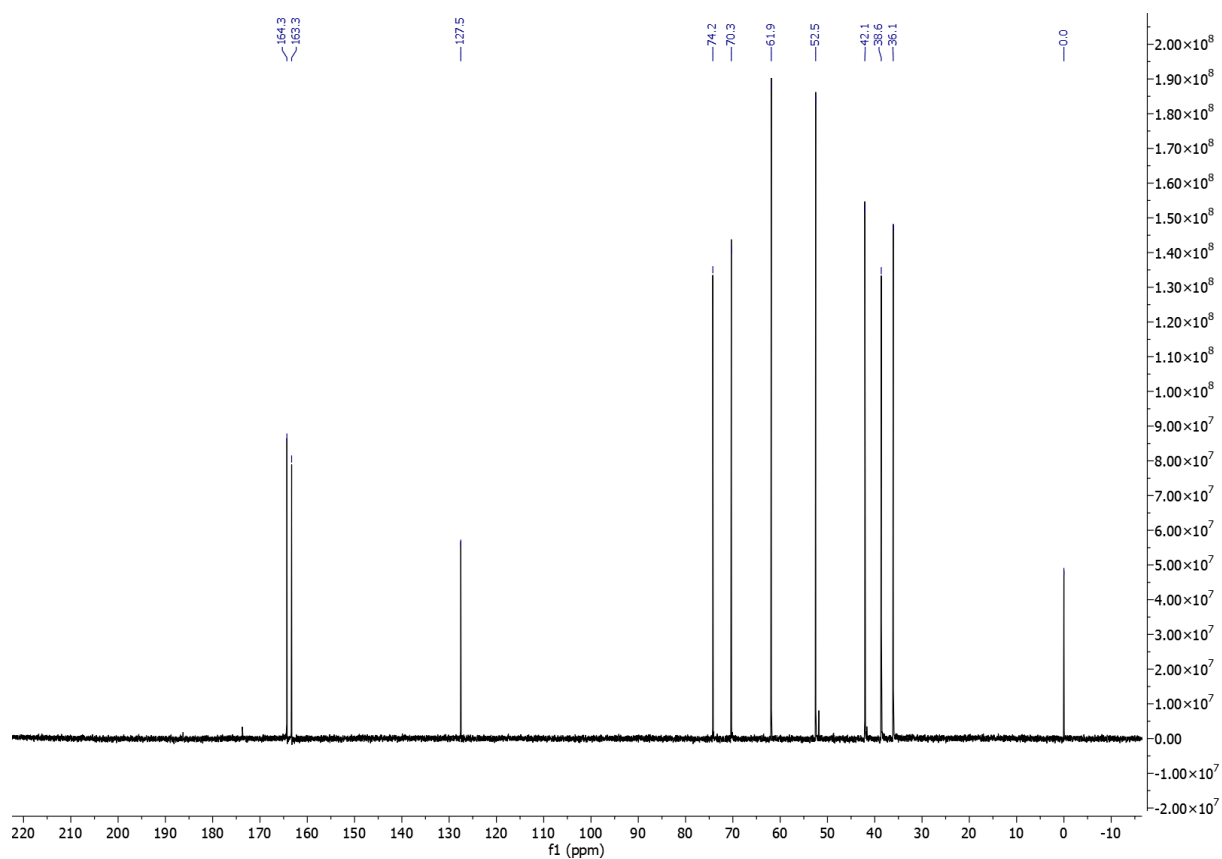
**Figure S28.** COSY spectrum of compound 7 in D<sub>2</sub>O



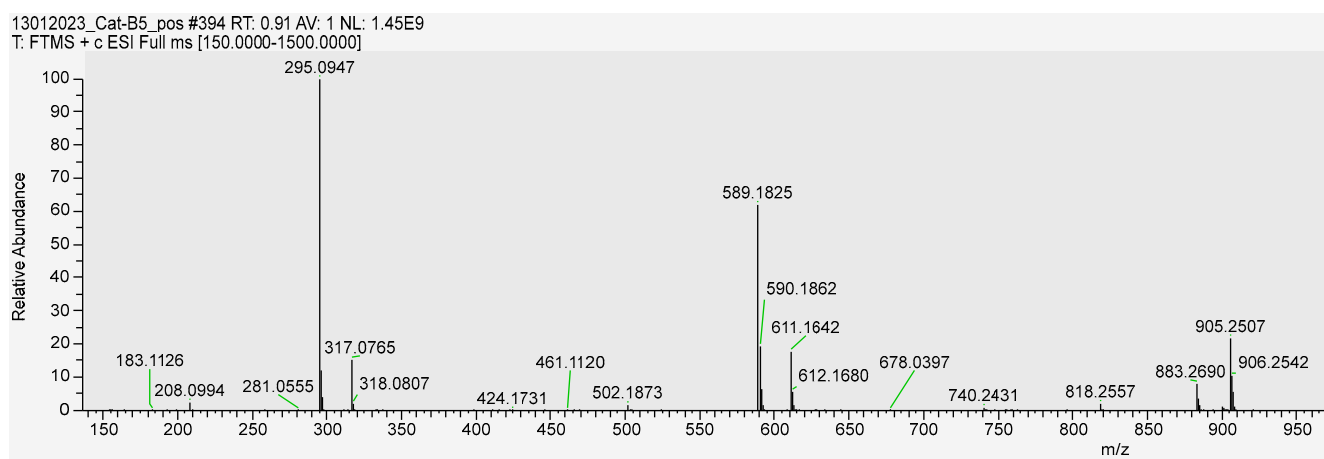
**Figure S29.** HSQC spectrum of compound **7** in D<sub>2</sub>O



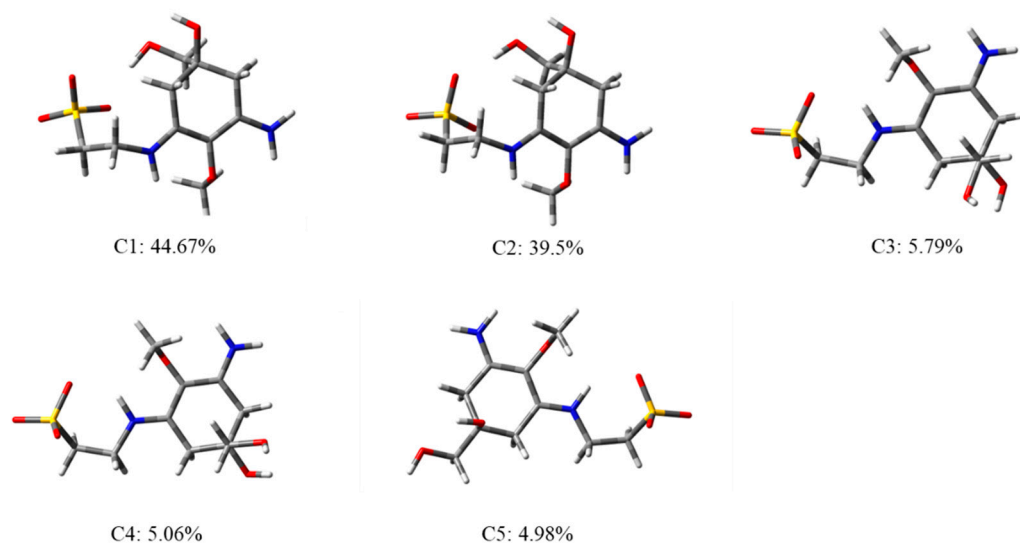
**Figure S30.** HMBC spectrum of compound **7** in D<sub>2</sub>O



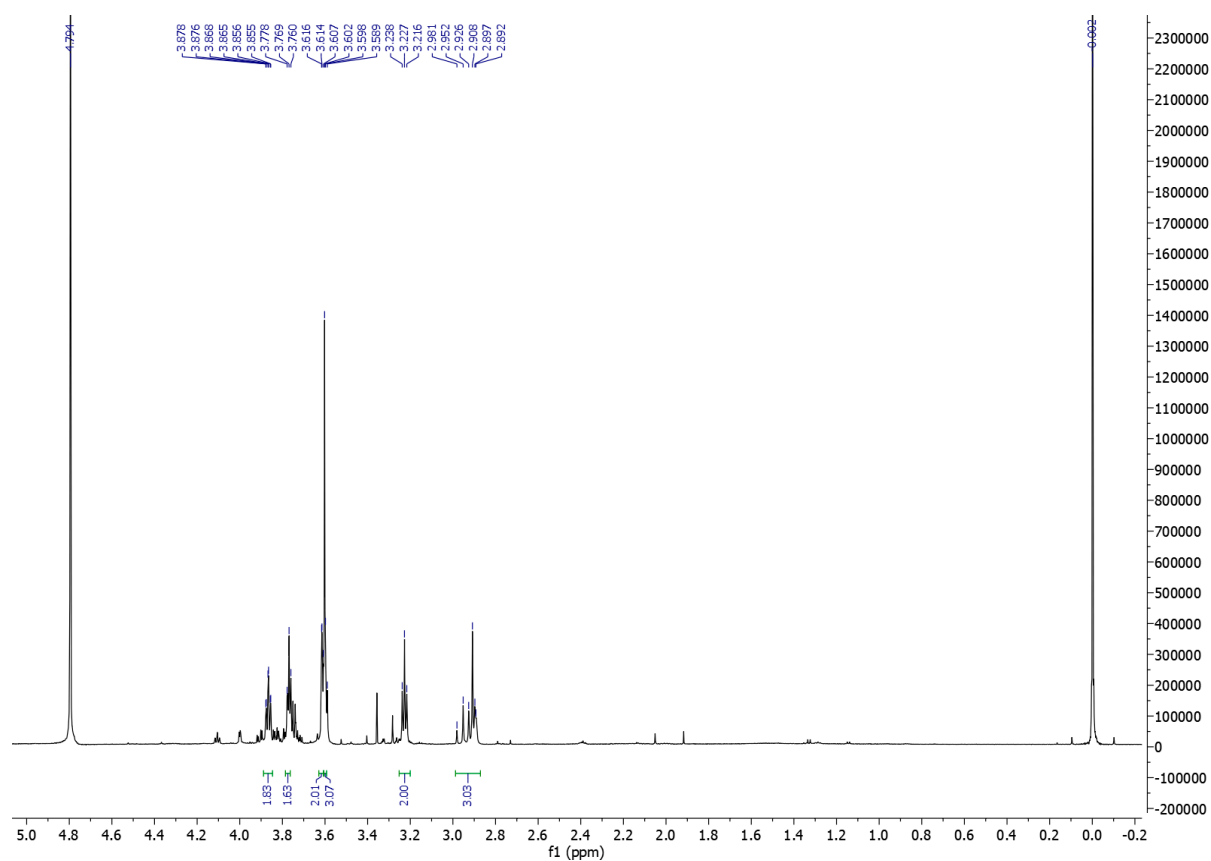
**Figure S31.** <sup>13</sup>C NMR spectrum of compound **7** in D<sub>2</sub>O



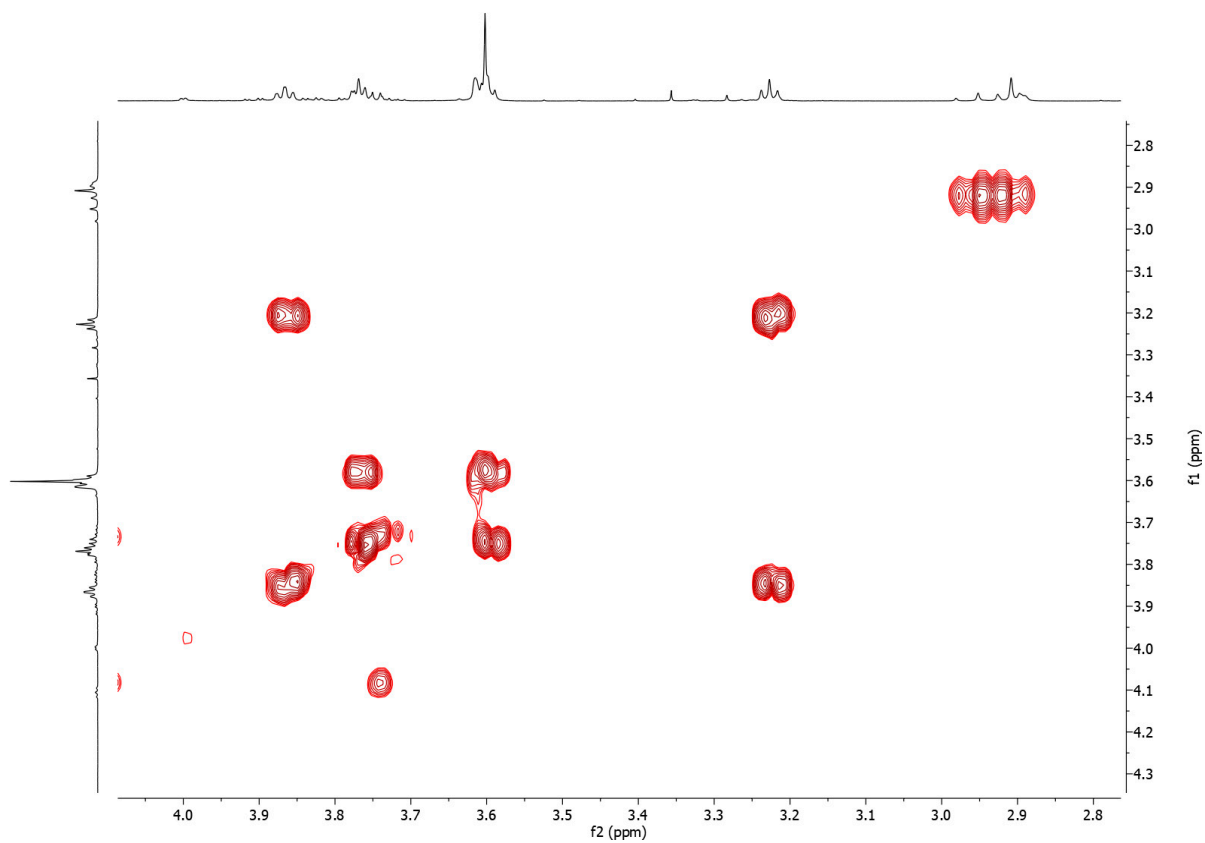
**Figure S32.** High-resolution mass spectrum of compound **7**



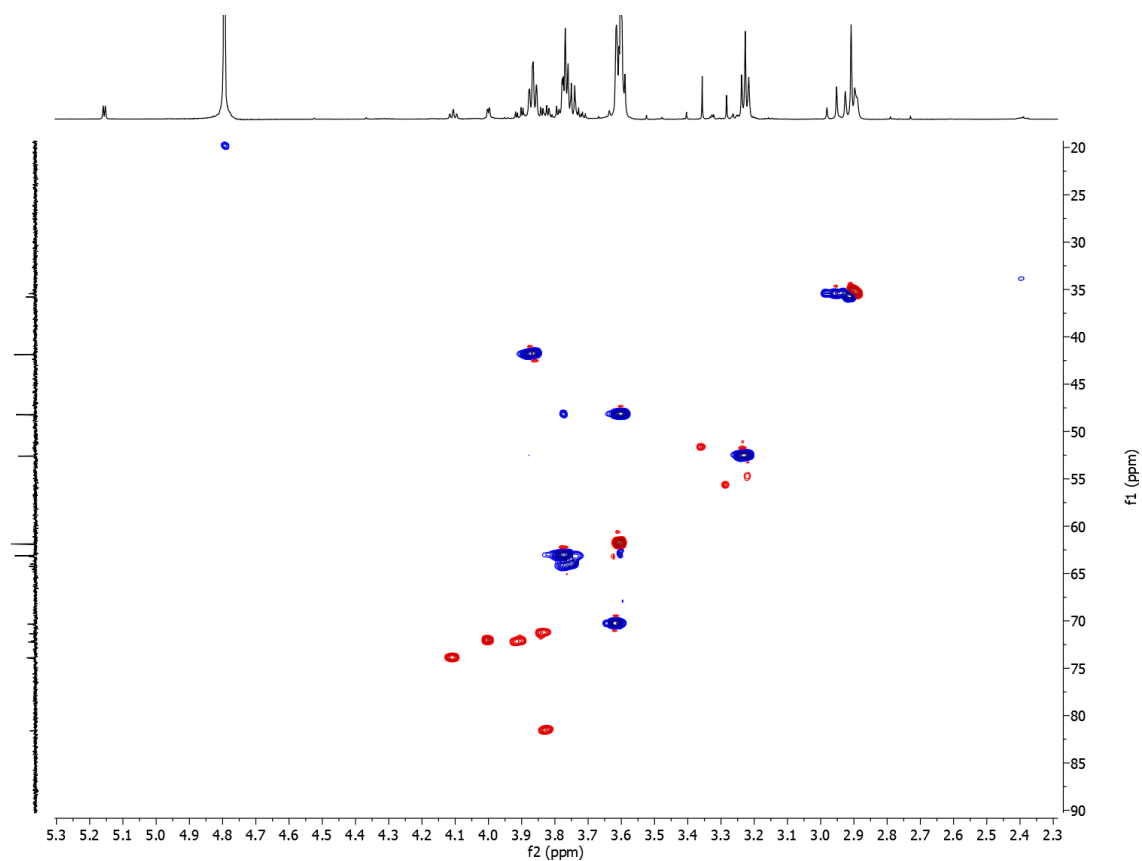
**Figure S33.** Overlayed conformers and population of Boltzmann averaged conformers of compound **7** optimized at the DFT/wb97xd/6-31+g(d,p) level in the gas phase.



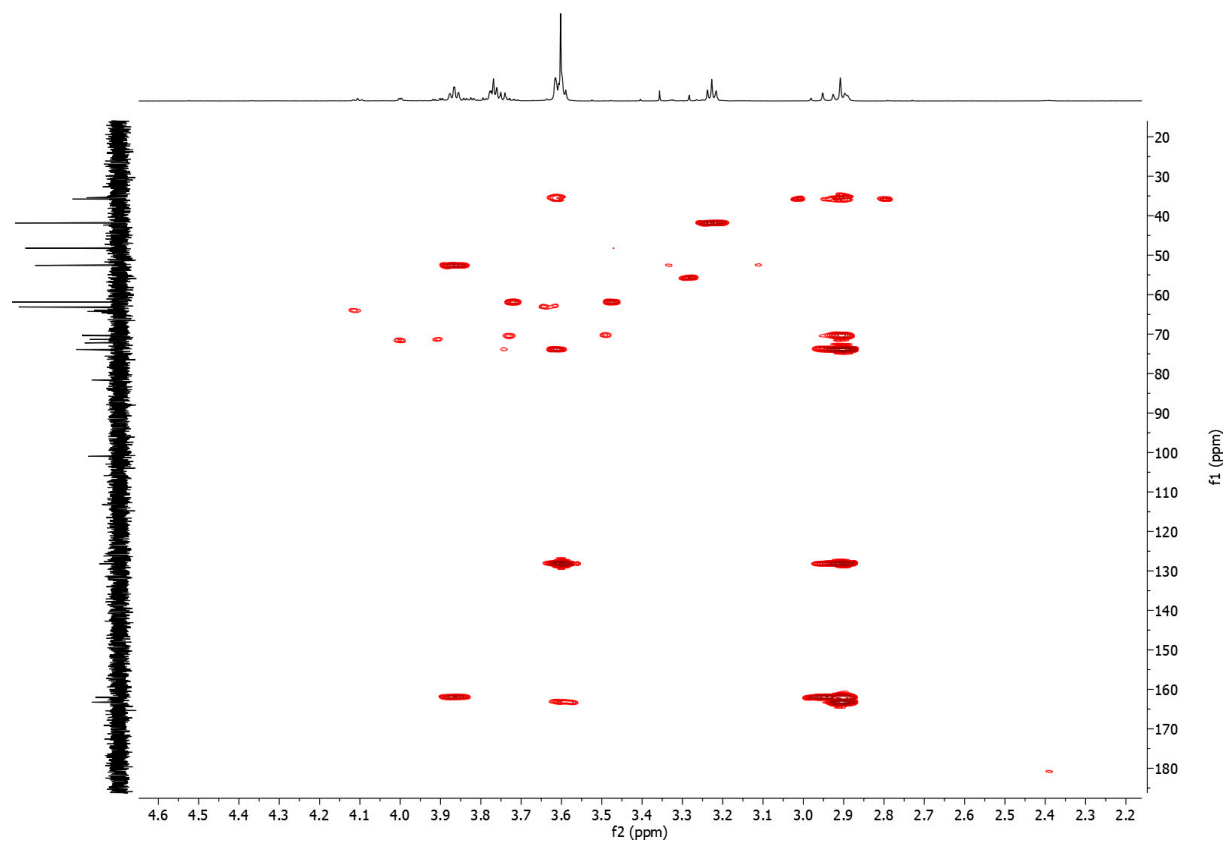
**Figure S34.**  $^1\text{H}$  NMR spectrum of compound **8** in  $\text{D}_2\text{O}$



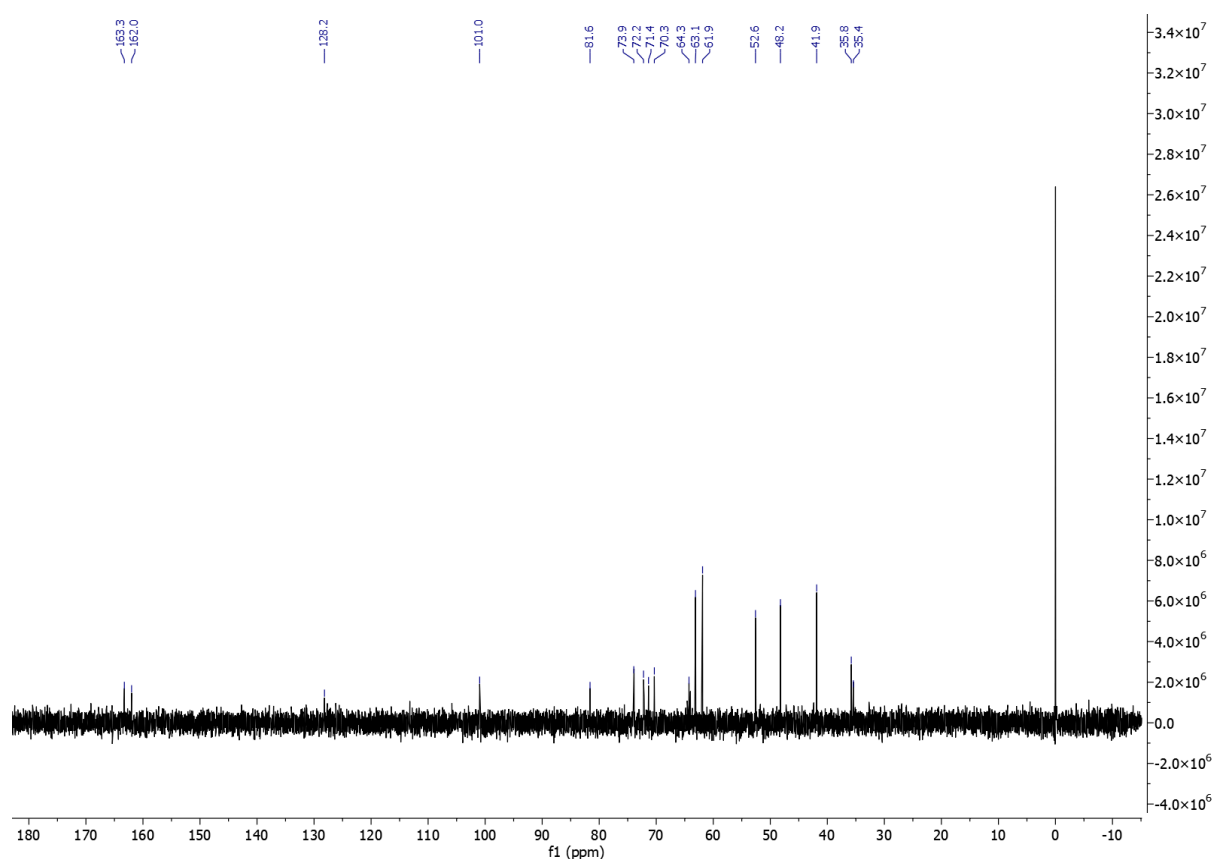
**Figure S35.** COSY spectrum of compound **8** in  $\text{D}_2\text{O}$



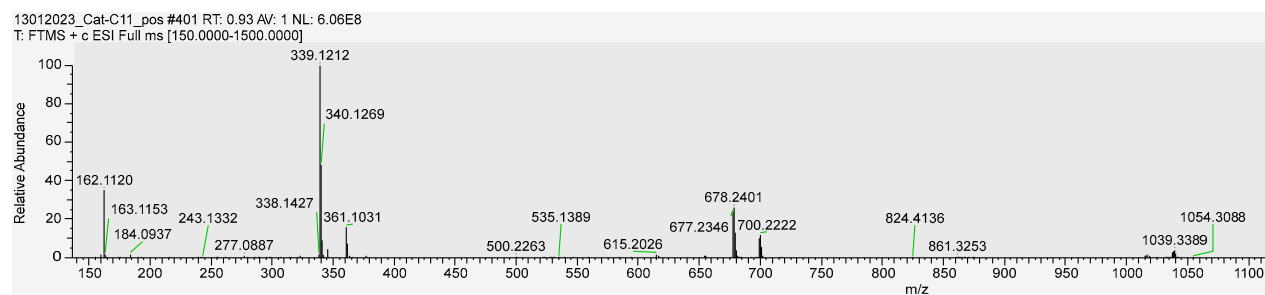
**Figure S36.** HSQC spectrum of compound **8** in D<sub>2</sub>O



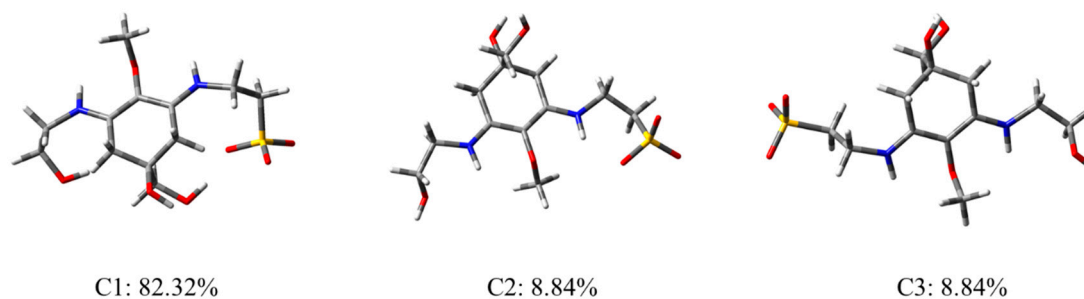
**Figure S37.** HMBC spectrum of compound **8** in D<sub>2</sub>O



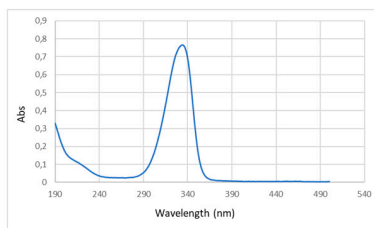
**Figure S38.**  $^{13}\text{C}$  NMR spectrum of compound **8** in  $\text{D}_2\text{O}$



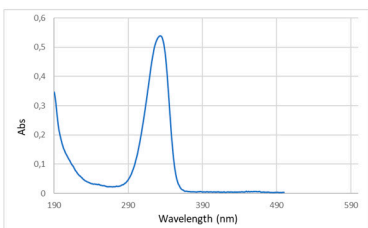
**Figure S39.** High-resolution mass spectrum of compound **8**



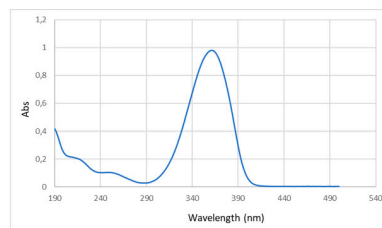
**Figure S40.** Overlayered conformers and population of Boltzmann averaged conformers of compound **8** optimized at the DFT/wb97xd/6-31+g(d,p) level in the gas phase.



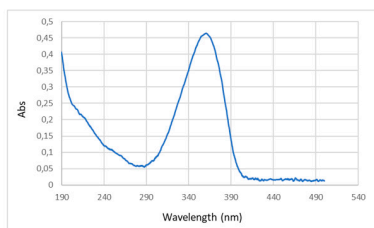
Compound 1



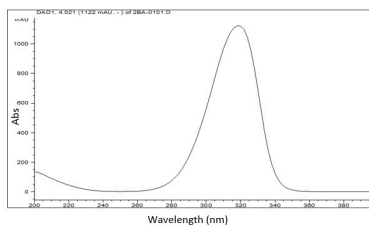
Compound 2



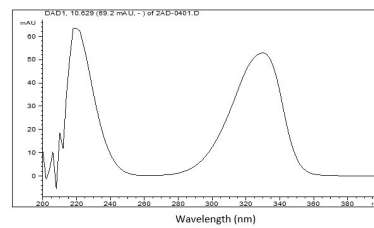
Compounds 3 and 4



Compounds 5 and 6



Compound 7



Compound 8

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