

## Supporting Information

### **Absolute Configuration of Peyssonoside A using Vibrational Circular Dichroism Spectroscopy: A Day-and-Night Difference Made by f-functions**

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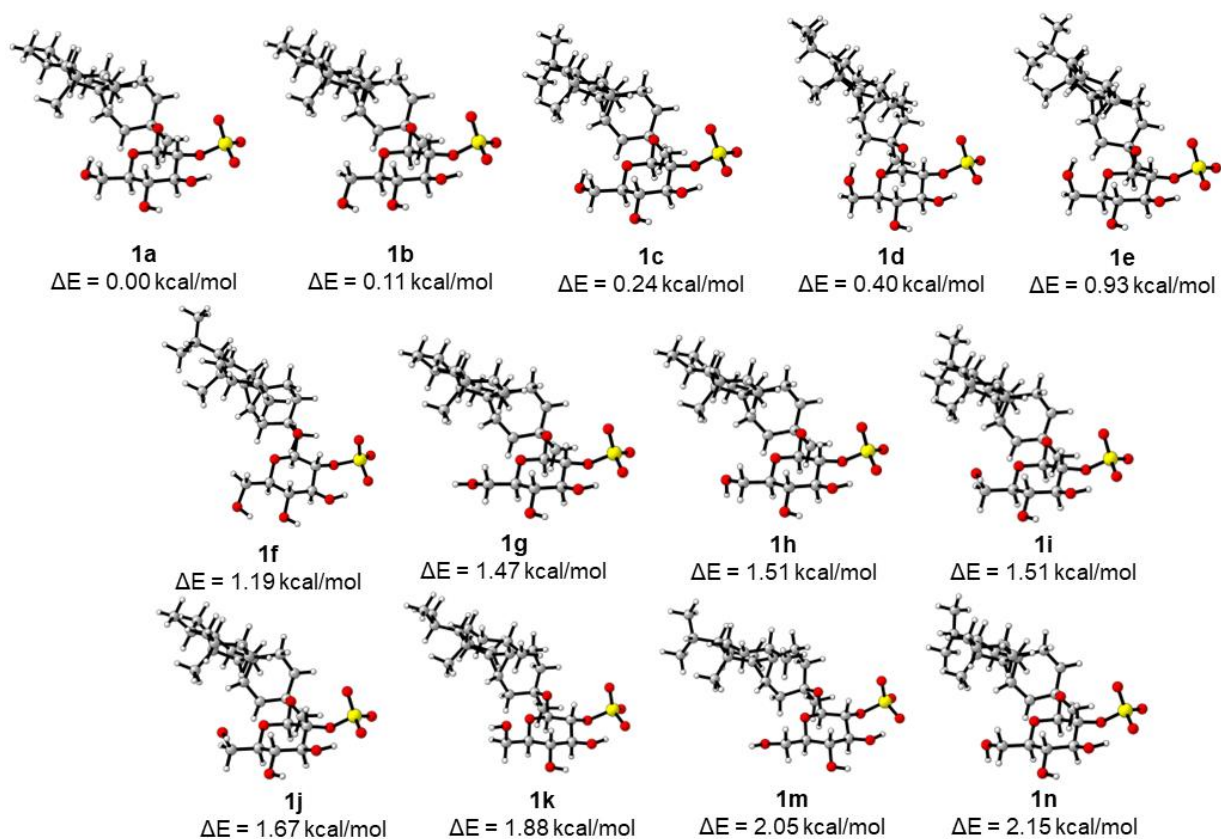
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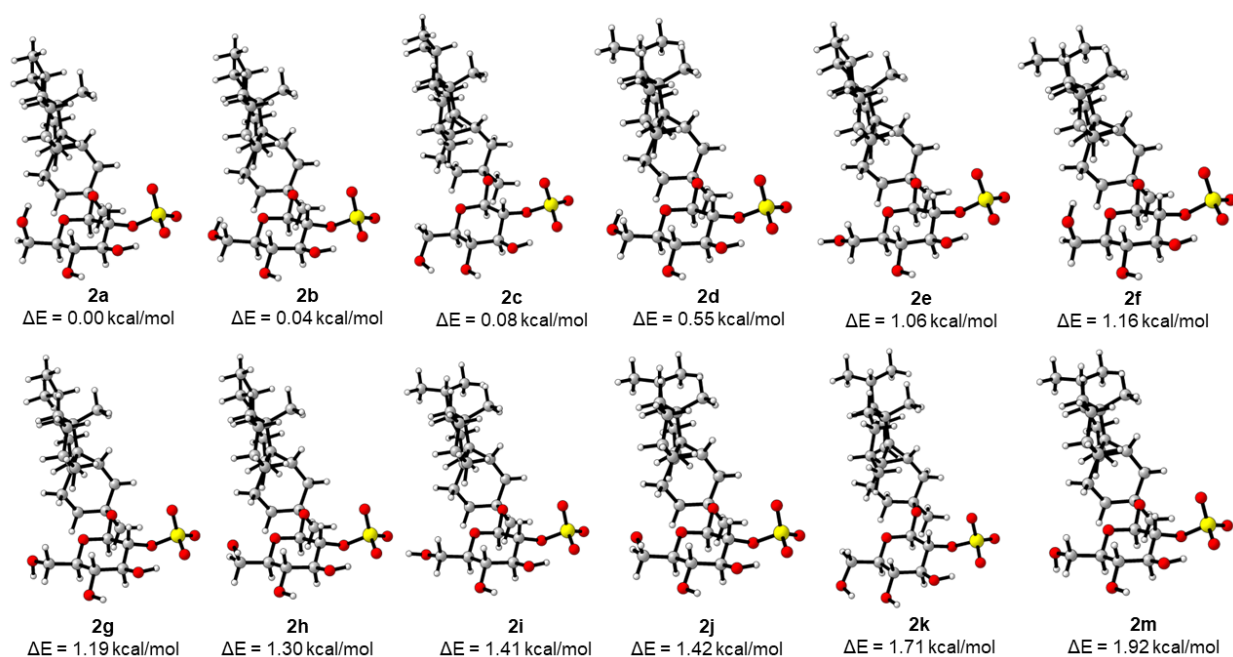
#### **Summary of Supplementary Information**

**Figure S1:** Conformers for diastereomer **1** at the B3PW91/6-311G(3df,2pd)/PCM level

**Figure S2:** Conformers for diastereomer **2** at the B3PW91/6-311G(3df,2pd)/PCM level



**Figure 1.** The 13 unique conformers for diastereomer **1** at the B3PW91/6-311G(3df,2pd)/PCM level.



**Figure 2.** The 12 unique conformers for diastereomer **2** at the B3PW91/6-311G(3df,2pd)/PCM level.