

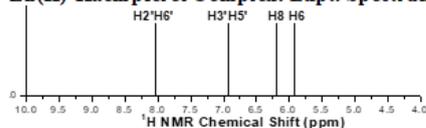
## DFT Calculations of Spectroscopic Properties for Zn (II) -Kaempferol Complexes

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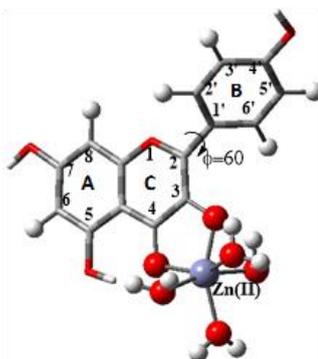
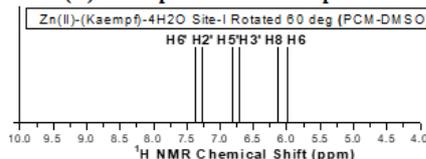
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**Abstract:** The coordination of Zn(II) ion with the flavonoid kaempferol were found to improve the anticancer effects compared to the free kaempferol and, therefore, a theoretical study of structural and spectroscopic properties of Zn(II)-kaempferol complex can be relevant as a starting point for the investigation of the mechanism of action at a molecular level [1,2]. Recently, our group [3] through DFT calculations studied the  $^1\text{H}$  NMR chemical shifts for three polyphenols in order to assess the conformation adopted by these molecules in solution. We showed that a rotation of the B ring (Figure 1) through the inter-ring dihedral angles, causing a deviation from the planar configuration predicted by theoretical gas phase full geometry optimization, is essential to reach a good agreement with experimental  $^1\text{H}$  NMR spectra measured in solution (DMSO solvent). Here, we report DFT calculations of spectroscopic properties ( $^1\text{H}$  NMR, IR and UV-Vis spectra) of distinct Zn(II)-kaempferol complexes. We compared our theoretical results with experimental data in solution just published. As  $^1\text{H}$  NMR chemical shifts of the kaempferol molecule are very sensitive to the molecular chemical environment due to the presence of the metal (Figure 1), the best match between experimental and theoretical  $^1\text{H}$  NMR profile can lead to information on the Zn(II)-Kaempferol complex molecular structure in solution, which is difficult to achieve on experimental basis only. This is valuable information for futures studies involving structure-activity relationship and interaction mechanism with DNA.

### Zn(II)-Kaempferol Complex: Expt. Spectrum



### Zn(II)-Kaemp.4H2O: Theor. Spectrum



**Figure 1.** B3LYP/6-31G(d,p)-LANL2DZ optimized Zn(II)-kaempferol complex structures leading to the best agreement with experimental  $^1\text{H}$  NMR spectra in DMSO, with the B ring rotated  $60^\circ$ .

**Key-words:** Flavonoids, Anticancer Drugs, DFT calculations,  $^1\text{H}$  NMR spectra.

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### References:

- [1] L. -V. Tu, J. Pi, H. Jin, J. -Y. Cai, S. -P. Deng, *Bioorg. Med. Chem. Lett.*, 26, 2730 (2016).
- [2] Y. Wei, M. Guo, *Biol. Trace Elem. Res.*, 161, 223 (2014).
- [3] L. A. De Souza, W. M. G. Tavares, A. P. M. Lopes, M. M. Soeiro, W. B. De Almeida, *Chem. Phys. Lett.* 676, 46 (2017).