ABSORPTION SPECTRA OF PROTOPORPHYRIN IX, PHEOPHORBIDE A, AND ITS 1 HYDROXYETHYL DERIVATIVE: A THEORETICAL ANALYSIS

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Introduction

Electronic absorption spectra of protoporphyrin IX, Pheophorbide a, and its 1 Hydroxyethyl derivatives have been calculated to elucidate their potentialities as active molecules in photodynamic therapy (PDT). PDT is treatment teccnique for cancer and for certain benign conditions which utilizes the combination of visible light and a photosensitizer to produce reactive oxygen species in cells. Photosensitizers with the red-most absorption at as long wavelength as possible and with enhanced absorption in this region are necessary for successful aplication of PDT.

Experimental

All calculations were carried out by using the Gaussian 03W version 6.0. Electronic excitation energies and oscillator stregths were computed as vertical excitations from minima of the ground state structures by using Zindo and TD-DFT approach in vacuo. The simulated spectra was obtained by using the GaussSum 2.2.0 program.

Results & Discussion

The results showed that chlorin compounds, is however more promising candidates to be utilized in PDT as they display the red-most absorption (Qx) at longer wavelengths and the

absorption is stronger compared to the corresponding porphyrin compounds. On the other hand, 1-hydroxyethyl deritative was not able to red-shift the absorption compared with parent compounds.

Conclusion

In the prerent work, we studied the ground state geometries at the density functional level of theory. Electronic absorption spectra of protoporphyrin IX, pheophorbide *a* and its 1-hydroxithyl derivates were computed within Zindo and TD-DFT in vacuo, analized and compared with available experimental data. In conclusion, we hope taht our theoretical investigation will help the experimental applications of protoporphyrin IX, pheophorbide a and its derivates.

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1	Emma S. E. Eriksson, Leif A. Eriksson. "Computational design of chlorin based photosensitizers with enhanced absorption properties", Physical Chemistry Chemical Physics, 2011 Crossref	59 words — 17%
2	Anette Weyergang, Kristian Berg, Olav Kaalhus, Qian Peng, Pål K. Selbo. " Photodynamic Therapy Targets the mTOR Signaling Network and ", Molecular Pharmaceutics, 2008 Crossref	18 words — 5%

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