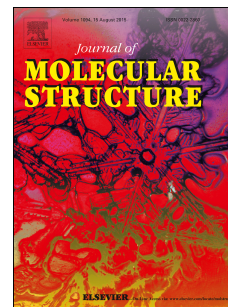


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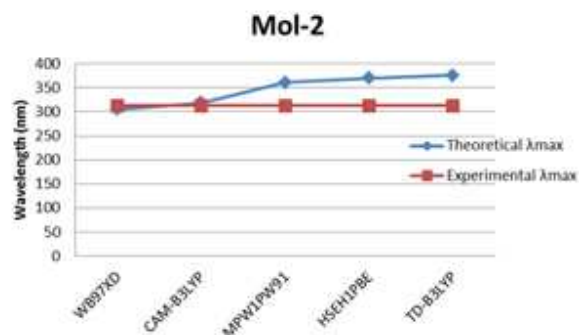
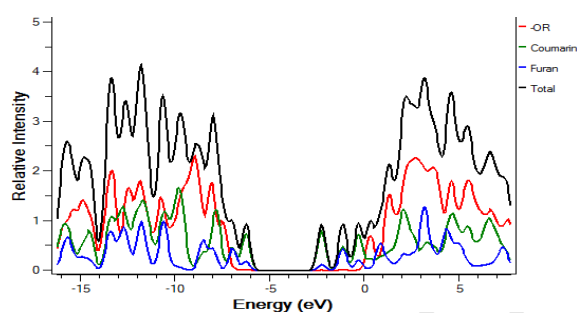
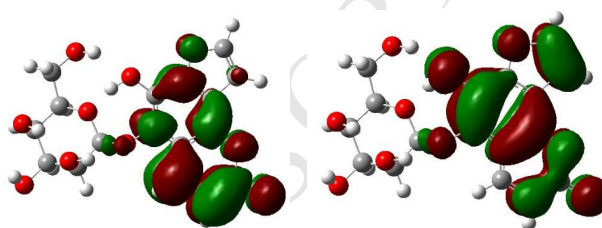
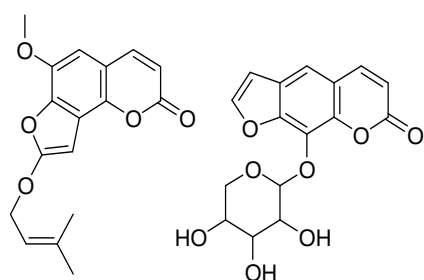
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Benchmark study of UV/Visible spectra of coumarin derivatives by computational approach.

Muhammad Irfan¹, Javed Iqbal^{1,2*}, Bertil Eliason³, Khurshid Ayub⁴, Usman Ali Rana⁵, Salah Ud-Din Khan⁵



Abstract

A benchmark study of UV/Visible spectra of Coumarin derivatives was conducted by employing the Density Functional Theory (DFT) and Time Dependent Density Functional Theory (TD-DFT) approaches. This study provided an effective insight about the electronic characteristics of the selected compounds and provided an effective tool for developing and designing the better UV absorber compounds.

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