The Role Played by Vitamin A as a Probe in Milk: A Vibrational and Electronic Study

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Vitamin A has been employed as a naturally spectroscopic marker in milk. M. Brandão *et al.*, in the frame of time-correlated single photon counting (TCSPC), have observed specific shifts in the electronic spectra and fluorescence of this vitamin from skimmed to milk whole [1]. In this present study it will be investigated which molecular action mechanism can be responsible for such behaviors. For thus, the geometries of retinol, retinyl ester, retinol acetate and retinal were fully optimised at $\mathrm{CAM-B3LYP/6-31+G(d,p)}$ level of theory in the gas phase and in solution. The medium effects were included using the polarizable continuum model (PCM) [2]. The vibrational spectra (Infrared and Raman) were obtained at the same level of theory. Time-Dependent DFT approach [3] is used to study the electronically excited states of retinol, retinyl ester, retinol acetate and retinal. To investigate Time-Resolved Fluorescence measures of retinol in milk, lifetime decays were calculated and compared with the experiment. The obtained results provide theoretical support to the experimental counterparts and rationalisations to changes in average decay lifetime. Our findings contribute to understanding its profile in different environments, either to differentiate types of milk or to assess the quality of dairy products. All calculations were performed using GAUSSIAN09 program [4].

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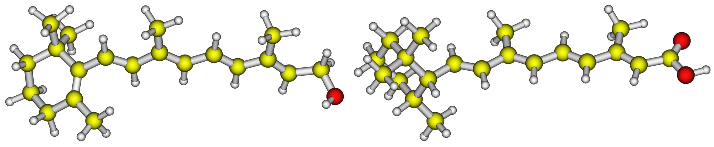
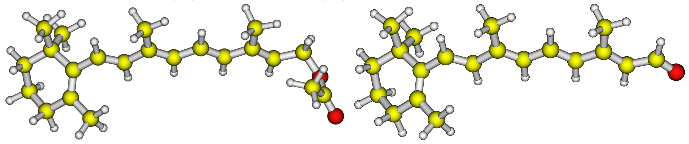


(a) Retinol (b) Retinyl ester



(c) Retinol acetate (d) Retinal

References

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