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Exploring Impacts of Oil and Water Environments on Structural and Electronic Features of Vitamin B3 along with DFT Calculations

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Density functional theory (DFT) calculations were performed to investigate the features of vitamin B3 (Vit-B3) in oil and water environments. Two up and down structural conformations were found based on the orientation of hydrogen atom of attached carboxylic acid group to pyridine scaffold, in which the up-conformation was found more suitable than the down-conformation. The models were stabilized in gas phases and 1-octanol and water solvents environments to explore the partition coefficient (LogP) for each conformation. In addition, the electronic features were investigated based on frontier molecular orbital levels. The results of this work indicated a higher suitability of formation for the up-conformation in all three environments and the highest suitability of formation of both up and down conformations in water medium. Accordingly, the LogP value was found smaller than one indicating watery tendency for the models. As a final remark, the structural and electronic features of Vit-B3 indicated insights into its development for further applications. © 2023 by SPC (Sami Publishing Company).

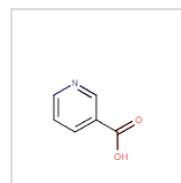
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Density functional theory; LogP ; Niacin; Nicotinic acid; Solvents; Vitamin B3

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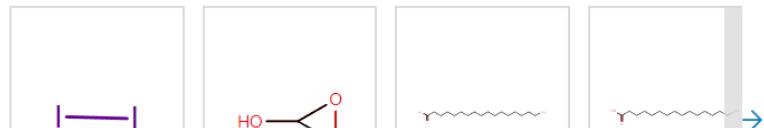
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Author keywords

Epoxidized; Non-epoxidized; Olive oil; Soybean oil; Sunflower oil; UV irradiation

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