Journal of Medicinal and Chemical Sciences • *Open Access* • Volume 6, Issue 10, Pages 2419 - 2431 • October 2023

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ISSN
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DOI
10.26655/JMCHEMSCI.2023.10.17

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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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Abstract

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).

Author keywords

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

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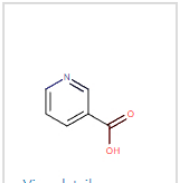

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The degree of photochemical cleavage of epoxidized and non-epoxidized oils of sunflower (Helianthus annuus), soybean (Glycine max), and olive (Olea europaea) exposed to 1000 watts ultraviolet light (UV) at different times were studied using iodine value and infrared spectroscopy. The epoxidation was conducted with a mole ratio of 1:0.5:2 for the oil, hydrogen peroxide and formic acid, respectively, for 6 hours at 50oC. The oxirane oxygen content and their percentages of conversion to epoxides for the oils were: sunflower oil (6.75, 89.52 ± 0.25%), soybean oil (7.10, 95.95 ± 0.33%), and olive oil (4.25, 84.89 ± 0.18%), respectively. The results showed that the difference in oxirane oxygen content between sunflower and soybean oils corroborate the slight increases in iodine value of the irradiated oils. The oxirane oxygen content of epoxidized olive oil established the baseline value for monounsaturated oils. The results for the UV irradiation showed that after twelve hours of irradiation, the iodine value increased for non-epoxidized sunflower oil and non-epoxidized soybean oil, while it decreased for non-epoxidized olive oil. However, the iodine values of epoxidized sunflower oil and epoxidized soybean oil increased, while the epoxidized olive oil decreased. It was suggested that the increases observed in the iodine values for non-epoxidized and epoxidized sunflower and soybean oils were as a result of molecular rearrangement of the alkene functional groups and recyclization of the cleaved epoxides residues after irradiation due largely to multiple bond effect. This effect is more marked in sunflower oil with 63% polyunsaturated fatty acid content, than in soybean oil with 61% polyunsaturated fatty acid content. This result corroborates the C-H deformation vibration at 1379 cm-1 as evidences of cyclized products. The monounsaturated olive oil characterized by a marked reduction in iodine value for both the non-epoxidized and epoxidized oils indicated marked reduction in unsaturation as it has only one double bond per molecular chain. Thus, the possibility of molecular rearrangement or recyclization of epoxidized residues is unlikely as shown by the results. Hence, the monounsaturated olive oil produced more stable cleaved products as evidenced by a marked reduction in the iodine value of the products.

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Comparative Study on Ultraviolet Irradiation of Epoxidized and Non-Epoxidized Sunflower, Soybean, and Olive Oil

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Abstract

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Author keywords

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

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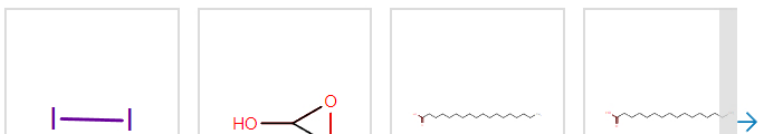

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