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 $Exploring\ Impacts\ of\ Oil\ and\ Water\ Environments\ on\ Structural\ and\ Electronic\ Features\ of\ Vitamin\ B3\ along\ with\ DFT\ Calculations$ Saadh M.J., Muhammad F.A., Mahdavi R., Parizi Y.N., Balali E., Cotrina-Aliaga J.C., Adil M., (...), Harismah K. (2023) Journal of Medicinal and Chemical Sciences, 6 (10), pp. 2419-2431.

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Open Access	^	1	Comparative Study on Ultraviolet Irradiation of Epoxidized	Madukwe, C.J., Egharevba, F., Odia,	2024	Asian Journal of	1
All Open Access	(1) >		and Non-Epoxidized Sunflower, Soybean, and Olive Oil	A.E.	Green Chemistry 8(1), pp. 57-67		
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Year	^		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				nax), and
2024	(1) >						
2023	(1) >		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				
Author name	^						
Al Zahrani, S.	(1) >		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. This result corroborates the C-H				
Alhabib, N.A.	(1) >						
Da'i, M.	(1) >						
Egharevba, F.	(1) >		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				
Maaliw, R.R.	(1) >						
Madukwe, C.J.	(1) >		value of the products.				
Mirzaei, M.	(1) >						
Odia, A.E.	(1) >	□ 2	Metal-doped fullerenes as promising drug carriers of Salem-Bekhit, M.M., Al Zahrani, S., 2023 Chemical Physics				3
Salem-Bekhit, M.M.	(1) >		hydroxycarbamide anticancer: Insights from density Alhabib, N.A., (), Da'i, M., Mirzaei, Impact functional theory M. 7,100347 Open Access				
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Chemistry	(2) >						
Materials Science	(2) >		Assessing an idea of metal-doped fullerenes (MF) as promising drug carriers of hydroxycarbamide; also known as hydroxyurea, (Hyd) anticancer was done in this work by performing density functional theory (DFT) calculations. A model of carbon fullerene was doped by each of iron (Fe), nickel (Ni), and zinc (Zn) transition metal atoms to provide enhanced FeF, NiF, and ZnF doped fullerenes for working towards the Hyd anticancer regarding the drug delivery issues. The model were optimized and their evaluated features indicated a possibility of occurrence of MF → Hyd@MF mechanism through the involving OM and HC interactions from the Hyd side to the MF side. The longest recovery time duration was supposed to be found for the Hyd@ZnF complex because of the largest strength and the highest conductance rate variation was supposed to be found for the Hyd@NiF complex because of the smallest energy gap. However, all the complex models were in a reasonable level of formations and electronic variations to be monitored for approaching a sensing or detecting function. In this regard, the enhanced models of FeF, NiF, and ZnF doped fullerenes were found suitable to work as promising carriers of Hyd anticancer regarding the drug delivery issues by the formation of interacting Hyd@FeF, Hyd@NiF, and Hyd@ZnF complexes in meaningful levels of structural and electronic features.				
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