

Covalent hydration of nitrobenzofurazans compounds from the perspective of the HSAB principle and reactivity–selectivity descriptor

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Abstract :

Global and local DFT-based reactivity descriptors are used to characterize covalent hydration reactions of series of nitrobenzofurazans compounds. The conceptual framework to rationalize the trends observed in reaction rate constants and to explain the main reaction product encountered experimentally is provided by the Pearson's HSAB principle. Molecular hardness of the reactant molecules indicates that the reactions are favored when hard–hard interactions are present. The reactivity–selectivity and the Fukui function are found to be the most efficient descriptors to characterize the regio-selectivity that might be driving the covalent hydration reactions.

Keywords : Conceptual-DFT, Nitrobenzofurazans, HSAB principle, Dual descriptors

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