Malinee Promkatkaew 2014: Experimental and Theoretical Study on the Physical, Photophysical, and Biological Properties of UV Absorbers and Skin Sensitizers. Doctor of Philosophy (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Professor Supa Hannongbua, Dr.rer.nat. 135 pages.

Experimental and theoretical study in this work consists of 3 parts. Firstly, the photophysical properties, photochemistry, and photostablity of various substituted cinnamic acids and cinnamates for UV absorbers were investigated experimentally and theoretically. These series include monohydroxy-, -nitro, and -fluoro derivatives for 18 compounds. Theoretical calculations were performed using both the time-dependent density functional theory (TD-DFT) and symmetry-adapted cluster configuration interaction (SAC-CI) methods. The obtained results showed that *para*-hydroxy derivative was found to be an appropriate UV absorber based on its broad absorption in the UVB/UVA regions, less emission, and higher photostability. Secondly, the photostability of five host-guest inclusion complexes between methoxycinnamic acids (CA) and cyclodextrins (CD) was investigated. All possible conformers were considered and analyzed for their structural and energetic behaviors using quantum chemical calculations. The calculated results revealed that CA and CD can form stable inclusion complexes in both the gas phase and water. Their stability depends on molecular size and shape complementation. Tail orientation showed the most favorable and stable orientation that absorbed in the UVB/UVA regions which is similar to the parent CA. Therefore, the agreement between theoretical results and experimental data can be a potent way to determine the geometry of supramolecular system. Thirdly, a non-animal model for skin sensitization was studied. This work is concerned with the nucleophilic aromatic substitution (S_NAr) domain. A set of 23 halo- and pseudohalobenzenes, 12 of which are reported skin sensitizers and 11 of which are reported nonsensitizers, was investigated using quantum chemical calculations. A model cysteine based nucleoephile was simulated using $–SCH_3$. The reaction coordinate associated with the nucleophilic attack by $–SCH_3$ for the 23 chemicals was evaluated. The barriers and enthalphies were subsequently used to successfully discriminate the sensitizers/reactive molecules from nonsensitizers/unreactive molecules of 23 S_NAr compounds. In these perspectives, the experimental and theoretical investigation provides a useful insight into the physical, photophysical, and biological properties of UV absorbers and skin sensitizers and a useful tool for designing and developing the novel UV compounds and predicting the new compounds for skin sensitizers.

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