Predictive Modeling and Experimental Validation of Azo-photo switches in Diverse Solvents Descriptors

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Photoswitches are molecules that can alter their structure and properties when exposed to light. The resulting photoisomers are less stable and can be reversibly transformed back to their stable form by light or heat. Traditionally, the design of photoswitches was performed experimentally, following the chemical intuition. Quantum chemical calculations were helpful, but often expensive and time-consuming. Now, machine learning has been introduced to facilitate the discovery of photoswitches. We present a machine learning model to predict two key properties: maximum absorption wavelength (λ max) and the thermal half-life of the metastable isomer (t1/2), based solely on structural features. The structural features were encoded as 2D descriptors (CircuS, Linear, Morgan, RDKit fingerprints, Avalon, Layered, Atom pairs, and Torsion). Two separate models were developed for λ max and t1/2, using data from both literature and experiments. Additionally, solvent-dependent data were collected, and related physicochemical descriptors were employed to analyse solvatochromic shifts in these systems. Validation involved synthesizing new azo photoswitches, measuring their λ max and t1/2, and comparing these results with model predictions to confirm the model's applicability.