AI-DRIVEN DESIGN OF NOVEL NORBORNADIENE SYSTEMS FOR MOLECULAR SOLAR THERMAL APPLICATION

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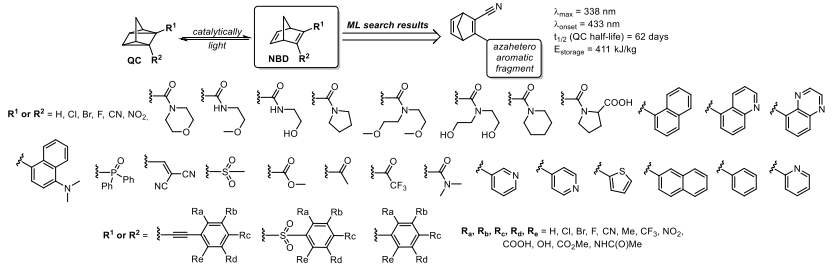
Certain molecular photoswitches can undergo isomerization to a metastable, high-energy state upon exposure to sunlight. These photoisomers can then revert to their ground state either thermally or under catalytic conditions, releasing the stored energy as heat. This reversible photochemical cycle forms the basis for molecular solar thermal (MOST) energy storage systems. Among the various photoswitchable scaffolds investigated, the norbornadiene (NBD)-quadricyclane (QC) isomeric pair stands out as particularly promising. For practical and efficient MOST performance, several key criteria must be met: absorption characteristics well matched to the solar spectrum (including appropriate λ_{max} and λ_{onset} values), minimal spectral overlap between the two isomers, a high photoisomerization quantum yield, an extended lifetime of the metastable QC isomer, and a substantial energy difference (ΔH) between the NBD and QC forms. Additionally, the compounds should be readily accessible and amenable to straightforward preparative scalability. To address these requirements systematically, we compiled an experimental dataset comprising approximately 250 literature-reported norbornadiene derivatives, each characterized with respect to relevant physicochemical and photochemical properties.

To identify molecular switches with optimal photophysical properties, we employed a computational pipeline that combines machine-learning-guided property prediction with Monte Carlo Tree Search (MCTS) and reinforcement learning (RL) for chemical space exploration. ML models were trained on our curated datasets. These surrogate models served as reward functions within an AlphaZero-style neural MCTS framework, which iteratively assembled candidate molecules from a fragment library while optimizing a multi-objective reward combining predicted photophysical properties and synthetic accessibility. Fragment-based construction ensured structural validity and retention of the norbornadiene core throughout the generative process. High-throughput molecular generation enabled the identification of the most promising structural class: nitrile-functionalized norbornadienes bearing an azahetero-aromatic moiety as the electron-donating component in a push-pull conjugation system.



Currently, a synthesis of the most promising candidates identified by machine learning algorithms is underway. The results of their experimental evaluation including photochemical characterization and assessment of suitability for molecular solar thermal energy storage applications will be presented in due course.

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