

Artificial Intelligence in Chemistry: Designing Molecules with Desired Properties

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The recent development of artificial intelligence (AI) has profoundly changed the approach to designing novel chemical entities. One of the key applications of AI in chemistry is the prediction and generation of molecular structures with desired biological or physicochemical properties, such as protein-binding affinity, solubility, or metabolic stability [1,2]. This presentation highlights current methods of data-driven molecule generation, with particular attention to biologically active compounds exhibiting cytoprotective activity toward cell membranes. Generative neural models, including encoder–decoder architectures and variational approaches, were employed to propose and prioritize new compounds capable of stabilizing erythrocyte membranes—viewed as dynamic lipid–aqueous phase boundaries [2,3]. Key descriptors such as lipophilicity, polarizability, and hydrogen-bonding capacity were used to identify molecules that improve membrane integrity and reduce susceptibility to osmotic stress. Computationally generated candidates were evaluated using machine learning models trained to predict biochemical effects on model lipid membranes and erythrocyte behavior. Beyond cytoprotection, the talk will briefly discuss AI-assisted prediction of enantioselectivity in asymmetric epoxidation reactions catalyzed by metal complexes [4,5]. Here, deep-learning models combining molecular descriptors with experimental enantiomeric excess data illustrate the growing role of AI not only in drug design but also in physical organic chemistry and phase-boundary phenomena. Finally, we address current limitations—most notably, limited availability of large, high-quality chemical datasets, the need for greater interpretability of predictive models, and the importance of synergistic integration with quantum-chemical computations and experimental data. Altogether, AI emerges as a powerful tool for accelerating molecular discovery in both biomedical and physical chemistry contexts.

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