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Quantum chemical (QM) calculations for life science applications have traditionally been constrained to small model systems, or computationally inexpensive but lower-accuracy methods, due to computational limitations. Most biomolecular modeling approaches rely on empirical parametrization and thus, at least indirectly, on some sort of training, which introduces biases and restricts their applicability. In particular, crucial drug targets such as RNA and metalloproteins often fall outside the scope of conventional methods, requiring extensive parametrization efforts. Recent advances in quantum chemistry, alongside improvements in computing hardware, have enabled the application of high-accuracy QM methods – such as hybrid density functional theory (DFT) and coupled cluster (CCSD(T)) – to biomolecular systems.[1, 2, 3] These developments now allow for the accurate simulation of ligands in solution as well as in complex biological environments, including their chemical stability, potential degradation pathways, and photochemical reactivity. Moreover, the integration of QM calculations with machine learning models further enhances their predictive power, opening new avenues for drug discovery. In this talk, we illustrate how state-of-the-art QM approaches are applied across various stages of drug development, from predicting photochemical degradation to elucidating binding mechanisms in metal-containing proteins.

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