Accelerating Drug Discovery with Advanced Computational Modeling and Deep Learning

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Achieving highly potent binding, while also maintaining ligand properties required for safety and biological efficacy, is a primary objective of small molecule drug discovery. We will present how machine learning models can be used to rapidly accelerate the identification of property satisfactory matter under realistic drug-discovery project conditions, focusing on the application of deep-learning systems to synthesis-aware compound enumeration and predictive free-energy calculations. We will also discuss the successful application of deep learning and molecular graph convolution to the application of deep learning to QSAR modeling. Finally, we will discuss the state of novel deep-neural-network architectures for recapitulating quantum mechanical calculations, and discuss the potential impact of these new methods on drug discovery projects.