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A Scalable Active-Learning and Physics-Based Framework for Virtual Screening of Complex Targets

The evolution of drug discovery is increasingly driven by advancements in AI, physics-based simulation, and multi-modal data integration. To address the challenges in drug discovery, we have developed approaches that integrate AI protein structure prediction, AI binding affinity predictions, and physics-based methodologies to better understand protein flexibility and ligand affinity. The application of these methods to real projects will be highlighted, showcasing the evaluation of novel drug discovery solutions for hit finding applied on a P-type ATPase implicated in Parkinson's Disease. This case study presented a significant challenge due to the protein's complexity, conformational flexibility, and lack of available structures. We report a comprehensive active-learning (AL) guided virtual screening workflow that integrates proprietary co-folding with a multimodal site identification strategy for hit finding. By employing AL-docking and our proprietary free energy calculation method (AL-AQFEP), we efficiently prioritized compounds in a library of >5M compounds based on rigorous free-energy calculations. The approach resulted in the identification of allosteric pockets. This work also provides a scalable framework for virtual screening, demonstrating that combining active learning with physics-based methods can help successfully navigate chemical space for virtual screening.

Curriculum vitae of Dr. Kenneth Goossens

Kenneth Goossens is a computational chemist with expertise spanning physics-based modeling, free energy methods, and machine learning approaches for drug discovery. He received his PhD in Computational Chemistry from the University of Antwerp, after which he started a joint Post Doc between the University of Antwerp and Janssen Pharmaceutica, developing and applying free energy calculation methods to cryo-EM enabled projects. Before joining SandboxAQ, Kenneth spent several years at Galapagos, where he led computational chemistry efforts across multiple drug discovery projects and applied approaches ranging from free energy perturbation and virtual screening to de novo generative design and development of machine learning prediction models for ADME and potency. Today, at SandboxAQ, he works at the interface of applied Computational Chemistry and technology development, with a particular focus on machine learning in ADME and development of virtual screening workflows.

