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Title: “*Computational drug discovery: from proteome to drugs*”

Proteomics and computational biology are integrated to accelerate and rationalize the discovery of drug candidates that modulate protein:protein and protein:membrane interactions. We are particularly interested in characterizing the dynamics of proteins to reproduce the conformational selection binding mechanism of drug candidates. This process improves the success rate of hit discovery by an order of magnitude compared to a traditional approach that uses only a single structure for a protein target. Beyond hit discovery, we are describing how this dynamics-based approach can predict the pre-clinical and clinical fate of drug candidates and opens the door to personalized pharmacogenomics discovery. We describe the future of computer-assisted pharmacogenomics in terms of computational developments, genome-wide characterization of protein-ligand interactions, as well as the novel finding, collaborative and business approaches that are re-shaping pharmaceutical research in the post-genomics era.

**REFERENCES:**

Ensemble-based docking: From hit discovery to metabolism and toxicity predictions  
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