

Computational Discovery of Selectivity Filters for the Cancer Pharmacokinome

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Synopsis

A molecular-level understanding of cancer is vital to develop much needed diagnostic and therapeutic tools. Progress requires a biophysical dissection of basic events like the inhibition of signal transduction controlling cell growth and cell fate. Combining our expertise in biomolecular structure and bioinformatics, we propose to perform foundational research that will enable the translation of novel biomolecular concepts on drug-susceptible signaling proteins into clinical/therapeutic tools. Target selectivity has been one of the major goals of drug development. We propose that enhanced target selectivity for specific signaling proteins will lead to reduced toxicity and enhanced antitumor activity. We intend to use a novel structure-based indicator of interactivity to rationally redesign protein ligands in order to enhance the specificity of their inhibitory impact across the human kinome.
