SciBX
Science-Business eXchange

THE DISTILLERY

This week in techniques

Approach	Summary	Licensing status	Publication and contact information
Computational models			
Computational filters for removing poor drug development candidates from chemical libraries	A computational system for removing poor drug development candidates from chemical libraries could help reduce costs associated with evaluating hits from high throughput screens. The method is designed to remove compounds that bind nonspecifically to proteins across many different screening assays. In a library of commercially available research tool molecules, the computational three-filter system removed 9% of compounds that could be unsuitable for drug development. Next steps include identifying and better defining the features of unsuitable drug development candidates and using this information to refine the filtering criteria. *SciBX* 3(8); doi:10.1038/scibx.2010.260 Published online Feb. 25, 2010	Work unpatented; filter algorithms freely available in the article's supplementary information section	Baell, J.B. & Holloway, G.A. *J. Med. Chem.*; published online Feb. 4, 2010; doi:10.1021/jm901137j **Contact:** Lindsay B. Hough, Albany Medical College, Albany, N.Y. e-mail: houghl@mail.amc.edu **Contact:** Xinxin Ding, Wadsworth Center, New York State Department of Health, Albany, N.Y. e-mail: xxd01@health.state.ny.us