This week in techniques

Approach	Summary	Licensing status	Publication and contact information
Computational models			
Computational strategy for predicting mechanism of action for drugs and probes	<p>A computational strategy could be useful for predicting the mechanism of action and molecular targets of existing drugs and probes. The strategy, called the similarity ensemble approach (SEA), predicted a candidate molecule's affinity for a given target based on the molecule's structural similarity to known ligands of the target. The strategy predicted the molecular target of 59 of 78 drugs in a database. In two additional databases, the strategy plus literature searches predicted the molecular target of 308 of 352 and 340 of 556 drugs, respectively. Next steps include using the computational strategy to help predict the molecular targets for lead candidates emerging from phenotypic screens. SeaChange Pharmaceuticals Inc. is developing software that uses the SEA.</p> <p>SciBX 5(27); doi:10.1038/scibx.2012.713 Published online July 12, 2012</p>	<p>Predicted interactions and SEA unpatented; unlicensed; software developed by SeaChange Pharmaceuticals protected by trademark and copyright; software available for licensing</p>	<p>Gregori-Puigjané, E. <i>et al. Proc. Natl. Acad. Sci. USA</i>; published online June 18, 2012; doi:10.1073/pnas.1204524109 Contact: Brian K. Shoichet, University of California, San Francisco, Calif. e-mail: bshoichet@gmail.com Contact: Bryan L. Roth, The University of North Carolina at Chapel Hill School of Medicine, Chapel Hill, N.C. e-mail: bryan_roth@med.unc.edu</p>