This week in techniques

Approach	Summary	Licensing status	Publication and contact information
Assays & screens			
Computational strategy for predicting drug activity on side-effect targets	A computational strategy for predicting a compound's activity against targets associated with side effects could aid the design of drugs with reduced adverse effects. The strategy uses a computational methodology called the similarity ensemble approach, which predicts where a molecule will bind its target based on how similar that molecule's chemical features are to features of known ligands of the target. The strategy was used to predict the ability of 656 drugs to bind to 73 targets associated with drug adverse reactions. In the study, 48% of the predicted drug-target associations were confirmed using a chemical database or follow-up experimental assays. Next steps include using the computational strategy to help identify new therapeutic indications for existing drugs and to predict adverse effects. SciBX 5(26); doi:10.1038/scibx.2012.686 Published online June 28, 2012	Algorithmic methods underlying approach unpatented; software using the method protected by trademark and copyright; software available for licensing from SeaChange Pharmaceuticals Inc.	Lounkine, E. <i>et al. Nature</i> ; published online June 10, 2012; doi:10.1038/nature11159 Contact: Brian K. Shoichet, University of California, San Francisco, Calif. e-mail: bshoichet@gmail.com Contact: Laszlo Urban, Novartis Institutes for BioMedical Research, Boston, Mass. e-mail: laszlo.urban@novartis.com