This week in techniques

Approach	Summary	Licensing status	Publication and contact information
Computational models			
Computational model for predicting P glycoprotein (MDR1; ABCB1; P-gp; CD243) substrates	A computational model to predict whether a compound may be exported by P-gp could help identify cancer therapeutics that avoid P-gp-mediated resistance. Cytotoxicity data from about 13,000 compounds screened against a panel of 60 human cancer cell lines was used to predict 448 compounds as P-gp substrates and 486 compounds as nonsubstrates. An analysis of these compounds led to the development of a computational model that classified compounds as P-gp substrates or nonsubstrates with 86% accuracy and 82% precision in an independent test set. Next steps include using the model to predict P-gp substrate status for therapeutic candidates and members of chemical libraries.	Unpatented; use of predictive model freely available at http://pgp.biozyne.com ; advanced features available for licensing	Levatić, J. <i>et al. J. Med. Chem.</i> ; published online June 17, 2013; doi:10.1021/jm400328s Contact: Fran Supek, BioZyne Ltd., Zagreb, Croatia e-mail: fran.supek@irb.hr
	SciBX 6(29); doi:10.1038/scibx.2013.769 Published online Aug. 1, 2013		