SciBX
Science-Business eXchange

THE DISTILLERY

This week in techniques

Approach	Summary	Licensing status	Publication and contact information
Computational models			
Computational model to predict compound binding to serotonin (5-HT_{2B}) receptor	A structure-activity relationship model could help identify compounds with predicted cardiovascular side effects due to 5-HT_{2B} receptor–targeting activity. Off-target activation of 5-HT_{2B} has been implicated in valvular heart disease in patients treated with antipsychotics. From a database of 59,000 compounds, the model predicted 122 potential 5-HT_{2B}-binding hits with up to 90% accuracy. Next steps include constructing a computational model that identifies compounds with 5-HT_{2B} receptor–binding activity. *SciBX* **3**(43); doi:10.1038/scibx.2010.1304 Published online Nov. 4, 2010	Unpatented; licensing status unavailable	Hajjo, R. *et al. J. Med. Chem.*; published online Oct. 19, 2010; doi:10.1021/jm100600y **Contact:** Alexander Tropsha, The University of North Carolina at Chapel Hill, Chapel Hill, N.C. e-mail: alex_tropsha@unc.edu