This week in techniques

Approach	Summary	Licensing status	Publication and contact information
Computational models			
Algorithm for chemical space exploration with stochastic search (ACSESS) to develop structurally diverse chemical compound libraries for drug screening	ACSESS could help create diverse chemical libraries for drug screening. ACSESS can be used to design libraries with specific chemical diversity or decrease library size by selecting a representative set of the library's diversity. As proof of concept, ACSESS identified a library representative of the full small molecule universe using filters for size, reactivity, stability and drug-like properties that was more structurally complete than existing libraries. ACSESS also was used to design a reduced library of compounds that have 13 or fewer heavy atoms that had comparable diversity to the complete library. Next steps include designing libraries for general screening and specific targets. SciBX 6(17); doi:10.1038/scibx.2013.423 Published online May 2, 2013	Unpatented; software available for licensing from OpenEye Scientific Software Inc. and Duke University for commercial use; free licenses available for noncommercial use	Virshup, A.M. <i>et al.</i> <i>J. Am. Chem. Soc.</i> ; published online April 2, 2013; doi:10.1021/ja401184g Contact: David N. Beratan, Duke University, Durham, N.C. e-mail: david.beratan@duke.edu Contact: Weitao Yang, same affiliation as above e-mail: weitao.yang@duke.edu