This week in techniques

Approach	Summary	Licensing status	Publication and contact information
Computational models			
Computer-based tool for identifying biologically active chemical scaffolds <i>in silico</i> (Scaffold Hunter)	The cheminformatics tool Scaffold Hunter could be useful for evaluating the bioactivity of chemical scaffolds and helping identify biologically active compounds <i>in silico</i> . In a PubChem database containing 51,415 molecules, Scaffold Hunter identified potential scaffolds for pyruvate kinase inhibitors and activators with about a 10% hit rate, which compares with the 0.34% historical average hit rate for PubChem high throughput screening. Next steps include using Scaffold Hunter to identify new small molecule inhibitors and incorporating additional search features into the software.	Scaffold Hunter is unpatented; available for licensed use under a GNU General Public License, which allows the software to be used for free; software available at http://www.scaffoldhunter.com	Wetzel, S. <i>et al. Nat. Chem. Biol.</i> ; published online June 28, 2009; doi:10.1038/nchembio.187 Contact: Herbert Waldmann, Max Planck Institute, Dortmund, Germany e-mail: herbert.waldmann@mpi-dortmund.mpg.de
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