This week in techniques

Approach	Summary	Licensing status	Publication and contact information
Computational models			
Chemical database of drug-like molecules with 13 or fewer atoms	The GDB-13 virtual database of >970 million drug-like molecules could help guide virtual screening, fragment-based drug design and other computational drug discovery approaches. The molecules in GDB-13, of which the vast majority have molecular weights <200Da, contain a maximum of 13 atoms of C, N, O, S and/or Cl. In addition to meeting the Lipinski rules, the molecules satisfy other criteria related to drug likeness, such as degree of ring strain and ratio of heteroatoms to carbon atoms. GDB-13 does not include predictably unstable or chemically impossible structures. Ongoing work is expanding the virtual database to include molecules with a maximum of 15 atoms, which would encompass up to 10 billion molecules.	Unpatented; unlicensed; database is available for free at: http://www.gdb.unibe.ch	Blum, L. & Reymond, J.-L. <i>J. Am. Chem. Soc.</i> ; published online June 8, 2009; doi:10.1021/ja902302h Contact: Jean-Louis Reymond, University of Berne, Berne, Switzerland e-mail: jean-louis.reymond@ioc.unibe.ch
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