This week in techniques

Approach	Summary	Licensing status	Publication and contact information
Computational methods			
A set of ADMET guidelines derived from multiple assays	Analysis of 15 different ADMET assays carried out at GlaxoSmithKline plc using ~30,000 different molecules from the company's compound collection produced a set of rules that could be useful for supplementing computational drug design to identify leads. Increasing the molecular weight or the log of permeability generally had a negative effect on at least one ADMET parameter, whereas ionization states either positively or negatively influenced a given parameter.	Guidelines not patented; unavailable for licensing	Gleeson, P. *J. Med. Chem.*; published online Jan. 31, 2008; doi:10.1021/jm701122q **Contact:** M. Paul Gleeson, Computational and Structural Chemistry, GlaxoSmithKline, Medicines Research Centre, Stevenage, Hertfordshire, U.K. e-mail: paul.x.gleeson@gsk.com