This week in techniques

Approach	Summary	Licensing status	Publication and contact information
Computational models			
Identification of chemically feasible molecular fragments to aid in drug discovery	<p>A computational tool that analyzes molecular fragments could aid in drug discovery. The tool identifies molecular fragments important for the properties of a molecule and uses this information to build a fragment database and virtual library of compounds. Researchers used the tool to identify virtual structures for small molecule melanin-concentrating hormone receptor 1 (MCHR1) antagonists that may have less potential for cardiovascular side effects. Synthesis and evaluation of the compounds yielded three candidates that were equipotent to a reference MCHR1 antagonist and had over fivefold lower affinity for a class of potassium channels for which binding is associated with cardiovascular side effects. Next steps include synthesizing additional candidates from the virtual library and evaluating and optimizing their ADME properties in preclinical studies.</p> <p>SciBX 2(13); doi:10.1038/scibx.2009.554 Published online April 2, 2009</p>	Work unpatented; licensing status not applicable	<p>Oyarzabal, J. <i>et al. J. Med. Chem.</i>; published online March 16, 2009; doi:10.1021/jm8016199</p> <p>Contact: Julen Oyarzabal, Johnson & Johnson Pharmaceutical R&D, Toledo, Spain e-mail: joyarzabal@cnio.es</p>