This week in techniques

Approach	Summary	Licensing status	Publication and contact information
Chemistry			
Guidelines for the design of orally available macrocycles	<p>A set of guidelines derived from an analysis of structures of macrocycles bound to proteins could be used to aid the design of orally bioavailable macrocycles that disrupt protein-protein interactions. The analysis honed in on high-quality structures with relevance to drug discovery, focusing on 22 distinct macrocycle-protein complexes encompassing 19 macrocycles and 13 proteins. The resulting structural guidelines for macrocycles suggest a range of ring sizes from 14–38 constituents and note desirable features including a substantial degree of unsaturation in the ring. Next steps include synthesizing libraries of macrocycles guided by these insights and experimentally testing their properties such as cell permeability.</p> <p>SciBX 7(32); doi:10.1038/scibx.2014.964 Published online Aug. 21, 2014</p>	Unpatented; licensing status not applicable	<p>Villar, E.A. <i>et al. Nat. Chem. Biol.</i>; published online July 20, 2014; doi:10.1038/nchembio.1584 Contact: Adrian Whitty, Boston University, Boston, Mass. e-mail: whitty@bu.edu Contact: Sandor Vajda, same affiliation as above e-mail: vajda@bu.edu Contact: Dima Kozakov, same affiliation as above e-mail: midas@bu.edu</p>