This week in techniques

Approach	Summary	Licensing status	Publication and contact information
Assays & screens			
Design of Genuine Structures (DOGS) software for <i>de novo</i> computer-assisted drug design	<p>A computational software package called DOGS could be useful for discovering new therapeutic leads to treat cancer and other diseases. The software uses a library of 25,000 molecular building blocks and a set of 83 chemical reactions to design chemotypes with scaffolds that are distinct from a template molecule but still mimic its pharmacophore features. The software was used to design an inhibitor of the cancer-associated polo-like kinase 1 (PLK1; STPK13). In a human cervical cancer cell line, the designed compound inhibited proliferation with an EC₅₀ value of 4 μM. Next steps include evaluating the DOGS software in ongoing drug discovery projects in collaboration with industry partners.</p> <p>SciBX 5(48); doi:10.1038/scibx.2012.1268 Published online Dec. 13, 2012</p>	Patent and licensing status undisclosed	<p>Spänkuch, B. <i>et al. Angew. Chem. Int. Ed.</i>; published online Nov. 20, 2012; doi:10.1002/anie.201206897</p> <p>Contact: Gisbert Schneider, Swiss Federal Institute of Technology Zurich (ETHZ), Zurich, Switzerland e-mail: gisbert.schneider@pharma.ethz.ch</p>