

This week in techniques

Approach	Summary	Licensing status	Publication and contact information
Computational methods			
Virtual screening for GPCR antagonists	<p>A four-step virtual screening method could be superior to current GPCR virtual screens for identifying therapeutic leads to treat multiple diseases. Unlike previous GPCR screens, the new screen includes conformational flexibility and multiple transmembrane interactions of GPCRs. Using a model of the thyrotropin-releasing hormone complexed with its GPCR (TRH-R), a virtual screen of more than 1 million commercially available compounds identified antagonists with specificity for TRH-R1 over the almost identical TRH-R2. Further studies are necessary to optimize the compounds and identify more clinically relevant GPCR ligands.</p> <p>Compugen Ltd. has a virtual ligand discovery technology to identify GPCR agonists.</p>	Neither the method nor the antagonists have been patented; unavailable for licensing	<p>Engel, S. <i>et al.</i> <i>J. Am. Chem. Soc.</i>; published online March 24, 2008; doi:10.1021/ja077620l</p> <p>Contact: Marvin C. Gershengorn, National Institutes of Health, Bethesda, Md. e-mail: marving@intra.niddk.nih.gov</p>