This week in techniques

Approach	Summary	Licensing status	Publication and contact information
Computational methods			
Computational model for designing inhibitors of solute carrier family 22 organic cation transporter member 1 (SLC22A1; OCT1)	A computational model could be useful for identifying OCT1 inhibitors to treat diabetes and cancer. A high throughput OCT1 inhibition screen identified 47 new OCT1 inhibitors out of 191 structurally diverse compounds. The results of the screen then guided the development of a qualitative predictive model of OCT1 inhibition, which correctly predicted 82% of OCT1 inhibitors and 88% of noninhibitors in a proof-of-concept test set. Researchers said they are not planning to commercialize the model but can make it available to interested parties upon request.	Not patented; unlicensed	Ahlin, G. *et al. J. Med. Chem.*; published online Sept. 13, 2008; doi:10.1021/jm8003152 **Contact:** Per Artursson, Uppsala University, Uppsala, Sweden e-mail: Per.Artursson@farmaci.uu.se

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