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This week in techniques

Approach	Summary	Licensing status	Publication and contact information
Drug platforms			
Integrated and iterative screen of drug-like scaffolds	A drug discovery platform combining virtual screening, chemical synthesis and NMR could identify inhibitors of protein-protein interactions faster and more efficiently than high-throughput screening or conventional synthesis alone. A computational docking method screened a virtual library of drug-like scaffolds for molecules that bound X-linked inhibitor of apoptosis (XIAP). Top hits from the screen were synthesized and NMR identified the molecule with the best XIAP binding affinity. A library of virtual derivatives of this compound was subjected to a second round of screening, resulting in a lead with good selectivity and low micromolar binding affinity for XIAP. The researchers are now applying this approach to identify inhibitors of undisclosed proteases.	Unpatented	Huang, J.-W. *et al. J. Med. Chem.*; published online Oct. 29, 2008; doi:10.1021/jm8006992 **Contact:** Maurizio Pellecchia, Burnham Institute for Medical Research, La Jolla, Calif. e-mail: mpellecchia@burnham.org

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