

Section III

Cheminformatics - Advanced: *Applications of Cheminformatics in Drug Research (Chemical Libraries, Virtual Screening, Structure-Activity Relationships, Prediction of Pharmacological Properties)*

For a better understanding of the applications of cheminformatics in drug design, the following papers are recommended to be read it:

1. Chemical Libraries (Databases)

- Tudor I Oprea and Alexander Tropsha Target, chemical and bioactivity databases - integration is key *Drug Discovery Today: Technologies* **2006**, 3, 357-365. [[PDF1](#)]
- Marius M. Olah, Cristian G. Bologa and Tudor I. Oprea Strategies for Compound Selection. *Current Drug Discovery Technologies* **2004**, 1, 211-220. [[PDF2](#)]
- Oprea, Tudor I. Property distribution of drug-related chemical databases. *J. Comput. -Aided Mol. Des.* **2000**, 14, 251-264. [[PDF3](#)]

2. Virtual Screening, SAR, Prediction of Pharmacological Properties

- Dan C Fara, Tudor I Oprea, Eric R Prossnitz, Cristian G Bologa, Bruce S Edwards and Larry A Sklar Integration of virtual and physical screening *Drug Discovery Today: Technologies* **2006**, 2, 377-385. [[PDF4](#)]
- Cristian G Bologa, Chetana M Revankar, Susan M Young, Bruce S Edwards, Jeffrey B Arterburn, Alexander S Kiselyov, Matthew A Parker, Sergey E Tkachenko, Nikolay P Savchuck, Larry A Sklar, Tudor I Oprea and Eric R Prossnitz Virtual and biomolecular screening converge on a selective agonist for GPR30 *Nature Chemical Biology* **2006**, 2, 207-212. [[PDF5](#)]
- Hristozov D, Oprea TI, Gasteiger J. Ligand-Based Virtual Screening by Novelty Detection with Self-Organizing Maps. *J. Chem. Inf. Model.* **2007**, 47, 2044-2062. [[PDF6](#)]
- Tudor I. Oprea Current trends in lead discovery: Are we looking for the appropriate properties? *J. Comput.-Aided Mol. Design* **2002**, 16, 325-334. [[PDF7](#)]

3. Lead-like, Drug-like

- Mike M. Hann and Tudor I. Oprea Pursuing the leadlikeness concept in pharmaceutical research. *Current Opinion in Chemical Biology* **2004**, 8, 255-263. [[PDF8](#)]
- Tudor I. Oprea, Tharun Kumar Allu, Dan C. Fara, Ramona F. Rad, Lili Ostopovici & Cristian G. Bologa Lead-like, Drug-like or "Pub-like": how different are they? *J. Comp. Aid. Mol. Design* **2007**, 21, 113-119. [[PDF9](#)]

4. General

- David G. Lloyd, Georgia Golfis, Andrew J. S. Knox, Darren Fayne, Mary J. Meegan and Tudor I. Oprea Oncology exploration: charting cancer medicinal chemistry space *Drug Discovery Today* **2006**, 11, 149-159. [[PDF10](#)]