

# Chemogenomics - knowledge-based approaches to drug discovery

**Imperial College Press - Chemogenomic approaches to drug discovery: similar receptors bind similar ligands**



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## Chemogenomic approaches to drug discovery: similar receptors bind similar ligands

These are based on maximally exploiting this information to extract knowledge and derive rules that can then be applied to estimate quantitatively potential biological effects of molecules from structure.

## Chemogenomics: Knowledge

The recent discovery via HTS that key intermediates of the Krebs cycle like succinate and  $\alpha$ -ketoglutarate activate extracellular GPCR systems with key regulatory roles in energy homeostasis provides a relevant example.

## Chemogenomic approaches to drug discovery: similar receptors bind similar ligands

A stepwise approach for defining the applicability domain of SAR and QSAR models. The *in vivo* pharmacodynamic and pharmacokinetic aspects become in the later stages of the discovery chain more and more important and form the essence of the art of medicinal chemistry which is characterized by detail and dynamic complexity.

## In silico pharmacology for drug discovery: methods for virtual ligand screening and profiling

Strict quality standard guidelines ensure the construction of a high quality database of reliable and reproducible data.

## In silico pharmacology for drug discovery: methods for virtual ligand screening and profiling

Studies in the Sciences of Complexity. University International Line: San Diego; 2000. Unfortunately, experience in a large number and diverse range of applications over the last four decades shows this is not always the case ;



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