

Chemogenomics - knowledge-based approaches to drug discovery

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



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

Two additional studies exemplifying this approach are worth mentioning. The SOSA approach proceeds in two steps.

Chemogenomics : Knowledge

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Along the same line, a biospectra similarity analysis was performed by clustering a set of 1567 drugs for which percent inhibition values determined at single high ligand concentration was available for a set of 92 assays. A good example is the rule-based methods derived from human expertise on the biotransformation of ligands for its application in the prediction of sites labile to drug metabolism.

Chemogenomics: Knowledge

Unfortunately, primarily because of technical difficulties for example, membrane-bound proteins , not all of the therapeutically relevant protein families are at present equally covered by 3D structures.

Chemogenomics : Knowledge

Comparative studies have suggested that information about a target obtained from known bioactive ligands is as valuable as knowledge of the target structures for identifying novel bioactive scaffolds through virtual screening ; For instance, common motifs can be identified within the chemical structures of ligand sets binding to a specific receptor class or to a set of receptors sharing a common sequence motif.

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