

ElexoPharm - From Hit To Lead

General procedure

The strategy to develop a hit into a lead compound is dependent on whether the protein structure is available or not. If the protein structure is available reasonable structural modifications can be proposed by docking experiments and Elexopharm's medicinal chemistry experience.

If the protein structure is unknown, ligand based drug design can be approached in three different ways. Structurally complicated hits (natural compounds) can be simplified and at very simple hit compounds additional functional groups can be introduced into the molecule. After identification of a number of hits a pharmacophore model can be constructed which may help to find even more potent hit compounds.

After syntheses of these modifications of the identified hits, structure activity relationships will be analysed using Elexopharm's experience and modern evaluation tools. All synthesised compounds are tested for activity, but only compounds with an activity higher than a given threshold value are examined for selectivity, etc. The screening cascade contains further tests of absorption, protein binding, metabolic stability and toxicity.

