

ElexoPharm - Hit Identification

Hit identification using virtual screening

For hit identification some information about either the target protein or an active (natural) compound (or endogenous ligand) is necessary. In the case of a known structure of the protein a virtual screening of compound libraries leads to virtual hits which will be synthesised and tested afterwards or tested immediately (if commercially available).

If the structure of the natural substrate is known, a ligand based approach will be accomplished. The computer searches for similar compounds and the resulting hits are checked for drug like properties.

At least one structure should be known

(A) : target protein

(B) : active (natural) compound or endogenous ligand

(A) : virtual screening of compound libraries (ACD etc.)

(B) : computer search for similar compounds

Hits A, B are checked for drug like properties

