HELIX BIOSTRUCTURES
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Drug modeling + design services

COMPUTATIONAL DRUG MODELING AND DESIGN

Computational drug modeling and design can accelerate drug discovery and preclinical R&D. Helix's computational expertise works with validated (druggable) and novel/non-traditional (undruggable) biological targets. 3-D models are created and examined through individualized computer simulations of selected commercial and/or carefully enumerated virtual compound libraries. This leads to the identification of promising new drug candidates for purchasing/synthesis and screening in biological assays. Helix can elucidate the mode of action of these active compounds against their biological target and design proprietary scaffolds from this information.

EXPEREIENCE INCLUDING THE FOLLOWING

- Kinases
- GPCRs
- DNA–RNA
- Nuclear receptors
- Docking
- Virtual libraries
- Fragment–based
- New active sites
- Peptidases
- Phosphatases
- Small molecules
- De-novo projects

COMPUTATIONAL DESIGN TO TARGET MOLECULE

1 3-D target molecule

- Analysis and creation of 3-D model from target crystal
- Creation of homology model if needed (no human target crystal)
- 3-D model of target alone or in complex (homodimer, heterocomplex) to match true biological active entity

2 3-D de-novo & docking

- High-throughput docking
- Virtual discovery/targeted compound libraries (thousands to millions of compounds)
- De-novo molecule design
- Active site docking
- Allosteric site docking
- Target surface mapping

3 Results & deliverables

- Identification of active commercially available compounds
- Confirmation of target affinity of designed scaffold (proprietary patentable compounds)
- Identification and confirmation of novel biologically active sites (new modes of action)

PREVIOUS WORK

DNA replication target

A 3-D model based on the crystal structure of a target involved in DNA replication was created. Analysis of the model's surface identified a promising site for ligand binding which could inhibit the activity of the cellular target. Helix performed a computer simulation to identify possible compounds with a high probability of binding the target. Cell-based assays confirmed activity of compounds enabling the client to raise capital to continue R&D efforts.

Bispecific cancer targets

This project required the design of a small molecule to inhibit 2 cancer targets. The active sites for each target were analyzed. Key binding features led to the creation of a molecule expected to fit and bind in both active sites. Helix provided a list of compound candidates which were synthesized, tested, and confirmed the desired bispecific activity/cancer inhibition. These results enabled the client to obtain additional grant funding to further develop the target candidate pipeline.

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