

Knowledge-based Small Molecule and Antibody Design Strategies

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Abstract

Some of the most productive design methods of the past 30 years have been knowledge-based. The best known is surely homology modelling, now a standard tool in most pharmaceutical and agrochemical companies.

The rapid increase in DNA, protein sequence and 3D structure data, so called big data, as well as newer initiatives to put small molecule and bio-assay data into the public domain, have opened up a wealth of new predictive opportunities, but complex commercial systems cannot keep pace with these developments.

Based on our translational research approach, we take research software from universities and young biotech and license their technology-advanced software directly customers or work with clients to tailor to their specific research efforts.

The presentation will cover:

- knowledge-based fragments
- evolution-seeded drug design
- applications of the ChEMBL knowledge-base for drug discovery
- antibody humanness score for biomolecule ADME/Tox assessment.

You can download this presentation as a [PDF](#) .