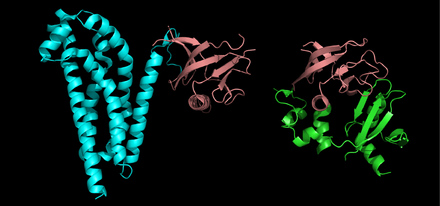


Source: [Biochemical Society Transactions | Portland Press](https://portlandpress.com/biochemsoctrans/issue/46/5)

**Business use case:** non-redundant representative subsets of protein sequence using UD-MIS

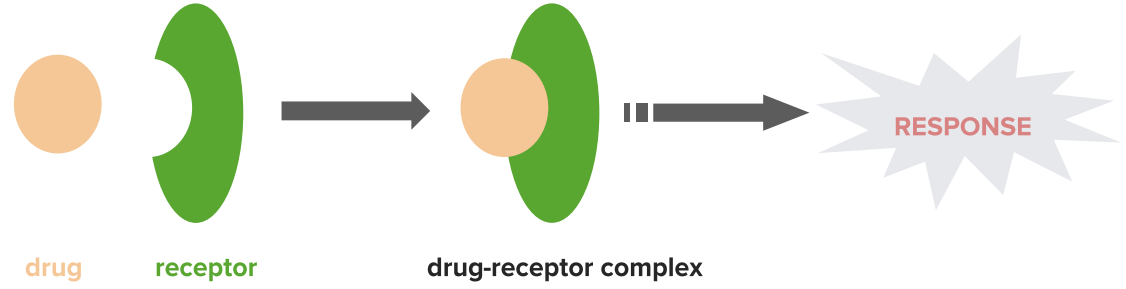
The application of UD-MIS for choosing non redundant representative sets of protein from sequence data sets can be served in a variety of applications. For instance, selecting representative sets of protein structure which is one of the biology problems in the world.



Two protein structure

Source: https://www.wikiwand.com/en/Protein\_structure

Protein structure is the three-dimensional arrangement of atoms in an amino acid-chain molecule. It enables us to understand ligand protein binding and develop binding affinity techniques [1]. Binding affinity is the strength of the binding interaction between a single biomolecule (e.g. protein or DNA) to its ligand/binding partner (e.g. drug or inhibitor) [2].



Drug receptor

Source: <https://www.lecturio.com/magazine/biological-interaction/>

**Business pitch.**

**Are you thinking how to increase your market share? Do you want to make more effective medicine with less side effects to the human body? Here is our reliable solution:**

It becomes possible to firstly predict how and where a particular small molecule might interact with a protein and then to identify putative ligands for a specific protein site [1].

Targeting specific chosen protein to evaluate ligand affinity can be done by selecting and analyzing representative sets of protein structure. Target-oriented drug design aims to find a high affinity ligand that would bind the target protein in order to block its disease-associated function catalytic activity or interaction with other molecules.

Structural knowledge on the exact interactions of drugs with their target protein has been applied mainly to predict potency changes of chemically modified lead compounds in protein structure-based drug design industry [3][4].

**Drug design industry overview**:

Drug discovery has traditionally been a linear, empirical process. The process begins with identifying and validating a target, followed by generating a lead molecule, optimizing its properties and assessing its effectiveness through clinical trials.

In recent years, the drug discovery technologies industry has seen remarkable developments and rapid progress. Biology, chemistry and computation provide an amalgamation that is reflective of the industry’s future.

According to the market research reports, the global market for drug discovery should grow from $69.8 billion in 2020 to $110.4 billion by 2025 with a compound annual growth rate (CAGR) of 9.6% for the period of 2020-2025[5].

**Potential customer**:

Company name: Pfizer

Country: USA

Profit: $ 41.9 billion – 2020

Company name: AstraZeneca

Country: United Kingdom

Profit: $ 26.6 billion – 2020

Company name: Regeneron pharmaceuticals:

Country: USA

Profit: $ 8.497 billion – 2020

Company name: Sygnature Discovery

Country: United Kingdom

Profit: $ 68.9 million – 2020

[1] <https://portlandpress.com/biochemsoctrans/article-abstract/46/5/1367/67796/Protein-structure-and-computational-drug-discovery?redirectedFrom=fulltext>

[2] [Binding Affinity | Dissociation Constant | Malvern Panalytical](https://www.malvernpanalytical.com/en/products/measurement-type/binding-affinity)

[3] <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4236214/>

[4] [Frontiers | Bridging Molecular Docking to Molecular Dynamics in Exploring Ligand-Protein Recognition Process: An Overview | Pharmacology (frontiersin.org)](https://www.frontiersin.org/articles/10.3389/fphar.2018.00923/full)

Video: https://www.youtube.com/watch?v=WORIhbaRABg