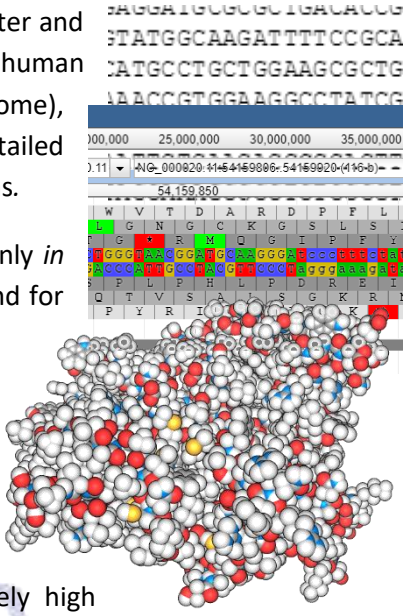
MOLECULOMICS
working molecular knowledge across genomes

Human3DProteome

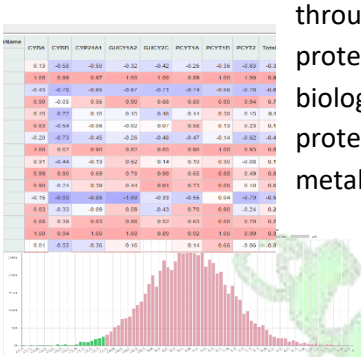
Human3DProteome – whole system drug discovery, drug repurposing and toxicity screening



Human3DProteome is a breakthrough technology for rapid discovery of better and safer drug compounds - a comprehensive in silico platform of the entire human proteome (all the receptors, enzymes etc., encoded by the human genome), providing a unique molecular level structural database including detailed characterisation of active sites and millions of protein-compound interactions.

It is a powerful open-ended, virtual lead discovery environment, and the only *in silico* platform that allows for screening against all receptor drug targets and for off-target interactions of a compound against the whole proteome.

Human3DProteome is available as a licensed web or installed platform service and offers the following product options, either individually or together:



Human3D Drug Discovery Pipeline – the molecular docking pipeline is applied to user-specified query compounds from small scale to extremely high throughput and employs machine learning approaches for widening discovery of protein-compound interactions involving comprehensive similarity searching of biological and chemical space, considering high chemical diversity across the entire proteome. Drug-target hits are linked by our *in vitro* knowledgebase to downstream metabolic and signalling pathways and to specific therapeutic areas.

Human3D Drug Discovery Database –The continually updated structure-function database provides thousands of pre-run "clean lead" compounds, pharmacophores and their conformers screened for interaction with more than 1,600 known drug targets, including 750 with known pharmacological action. Drug-target hits are linked by our *in vitro* knowledgebase to downstream metabolic and signalling pathways and to specific therapeutic areas. Compounds of interest may be run through the Human3D Drug Discovery Pipeline.

Human3D Drug Repurposing Platform - specialised capability for drug repurposing with validated multi-method dockings of all 1,600 FDA approved drugs to known targets, and tens of thousands of new repurposing leads, continually updated.

Human3D Toxicity Screen – providing early indication of potential toxicity of compounds by in silico molecular docking with a selection of specialist panels or every protein in the human body. This approach is fully complementary with SAR approaches but provides greater coverage of biological space.

Visit Human3DProteome.com