MOLECULOMICS
working molecular knowledge across genomes

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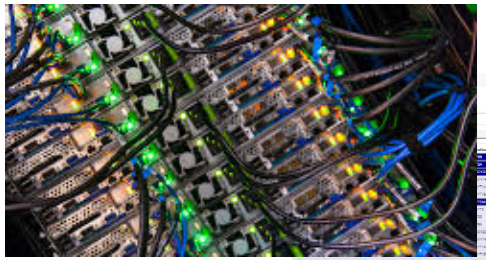

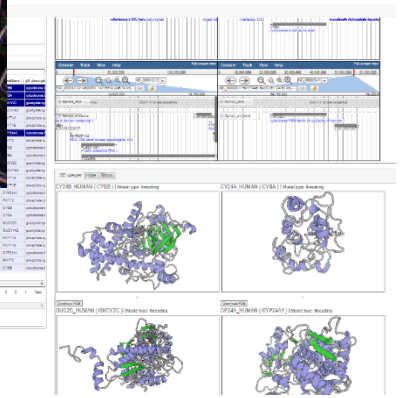

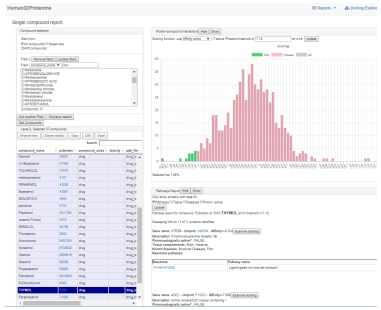

Moleculomics

Working Molecular Knowledge Across Genomes

Tuesday, 29 May 18

Swansea University Prifysgol Abertawe
Medical School Ysgol Feddygaeth

MOLECULOMICS
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Human3DProteome

Whole system drug discovery, drug repurposing and toxicity screening

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Moleculomics *in silico* technologies

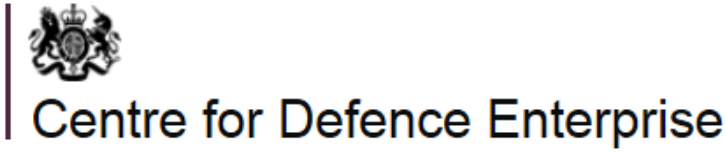
MOLECULOMICS
working molecular knowledge across genomes

Based on:

- 20 years of research, algorithm development in structural bioinformatics - at Swansea University since 2003, company founded 2012
- > 60 journal publications
- Validated technologies in partnership with big industry – Pharma, Biotech, Chemical, Defence, Government, Health
- Validated with relevant *in vitro* and (available) *in vivo* data – e.g. ChEMBL, DrugBank, ToxCast, CTD etc. → *in vitro* knowledgebase
- Molecular interaction → MIE → Metabolic / Signalling Pathway

Dow AgroSciences

Swansea University
Prifysgol Abertawe



Human3DProteome

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- Breakthrough technology for rapid discovery of better and safer drug compounds
- *in silico* platform of the **entire human proteome**
- Unique molecular level structural database including detailed characterisation of tens of thousands of active sites and millions of protein-compound interactions
- Linkage to metabolic / signalling pathways and therapeutic areas
- Automated reports per compound or per target

"Comprehensive mechanistic framework for the optimisation of drug discovery"

Human3DProteome – Options

MOLECULOMICS
working molecular knowledge across genomes

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

Human3D Drug Discovery Pipeline

- machine learning (AI) similarity searching / clustering approaches, widening discovery in both biological and chemical space

Human3D Drug Discovery Database

- continually updated, thousands of pre-run "clean leads" screened for interaction with more than 1,600 known drug targets, 750 with known pharmacological action (1800 CPU years used in the past 3 years)

Drug-target hits linked by in vitro knowledgebase to downstream metabolic and signalling pathways and to specific therapeutic areas

Human3DProteome - Discovery Database

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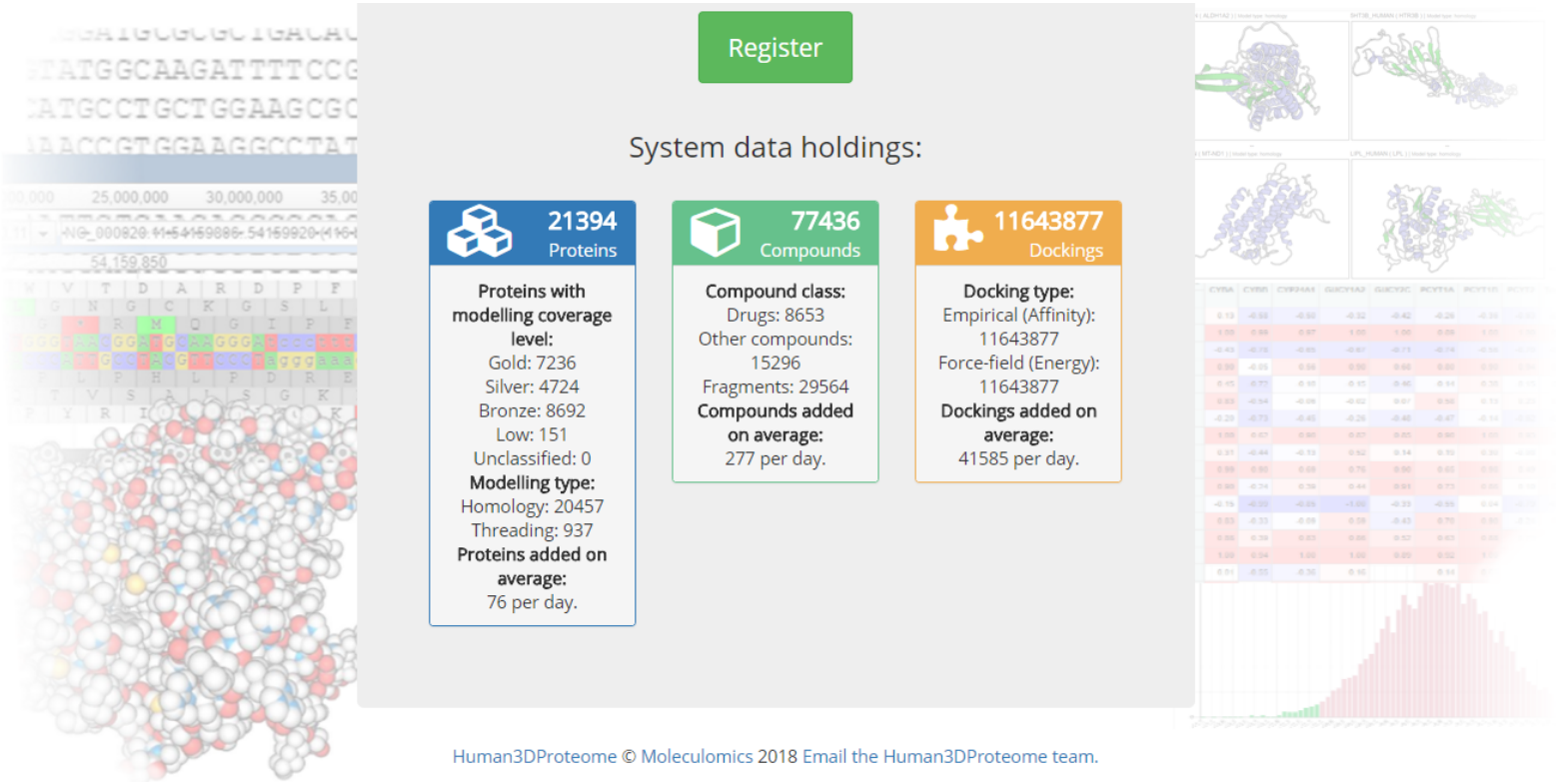

Large compound and fragment libraries, integrated with powerful AI-based tools for similarity searching and clustering widening discovery in both biological and chemical space

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Human3DProteome – Options

MOLECULOMICS
working molecular knowledge across genomes

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

Human3D Drug Repurposing Platform

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

Human3D Toxicity Screen

- early indication of potential toxicity of compounds by molecular docking with a selection of specialist panels or whole proteome.
- fully complementary with QSAR approaches but provides greater coverage of biological space.

Human3DProteome Web Interface

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Search panels

Genome browser

Proteome-wide drug discovery all in one place

3D viewer

Statistical analysis of hits

Heat maps

Register for free demo at
www.Human3DProteome.com

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What we have

MOLECULOMICS
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- Powerful open-ended, virtual lead discovery environment
- The only *in silico* platform that enables screening against all receptor drug targets and for off-target interactions of a compound against the whole human proteome
- Game changing technology

What we want

- Long term partnerships with Pharma / Biotech companies
- Purchases of platform licenses, bespoke implementations

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Diolch yn fawr

Thank You

www.moleculomics.com
www.human3dproteome.com
www.proteomestructure.com

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