

Human3DProteome

**Whole system drug discovery, drug repurposing
and toxicity screening**



Moleculomics *in silico* technologies

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



BIOCATALYSTS
exceeding enzyme expectations



Dow AgroSciences



Paraza
Pharma, Inc.



Swansea University
Prifysgol Abertawe



MOLECULOMICS
working molecular knowledge across genomes



Centre for Defence Enterprise



Innovate UK



Llywodraeth Cymru
Welsh Government



Human3DProteome

- 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

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

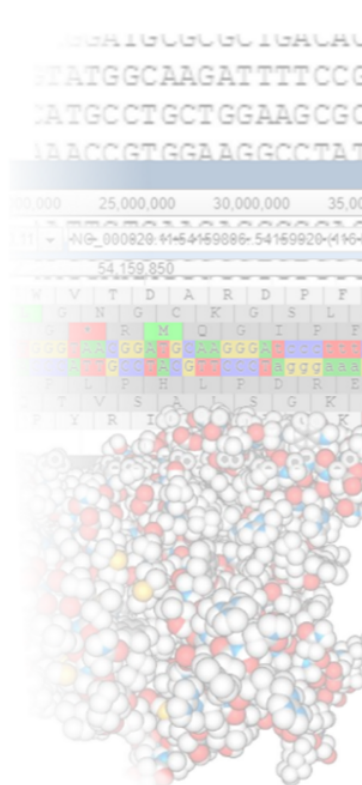
Human3D Drug Discovery Pipeline

- 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



[Register](#)

System data holdings:

- 21394** Proteins
Proteins with modelling coverage level:
Gold: 7236
Silver: 4724
Bronze: 8692
Low: 151
Unclassified: 0
Modelling type:
Homology: 20457
Threading: 937
Proteins added on average: 76 per day.
- 77436** Compounds
Compound class:
Drugs: 8653
Other compounds: 15296
Fragments: 29564
Compounds added on average: 277 per day.
- 11643877** Dockings
Docking type:
Empirical (Affinity): 11643877
Force-field (Energy): 11643877
Dockings added on average: 41585 per day.



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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

Human3DProteome – Options

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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

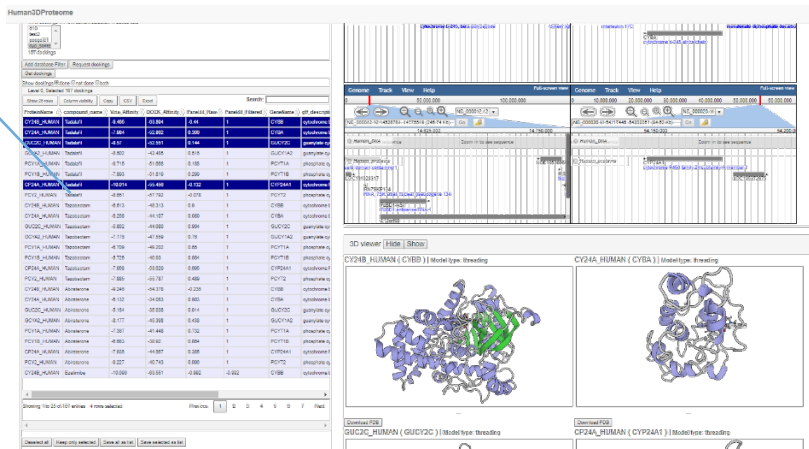
- early indication of potential toxicity of compounds by molecular docking with a selection of specialist panels or whole proteome.
- fully complementary with QSAR approaches but provides greater coverage of biological space.



Human3DProteome Web Interface

*Proteome-wide
drug discovery
all in one place*

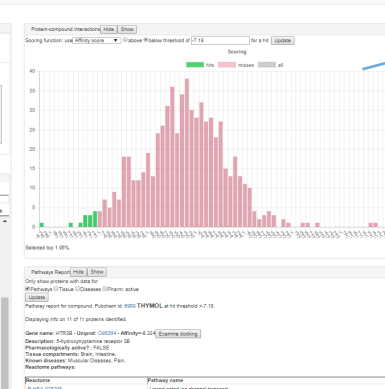
Search
panels



Genome
browser

3D viewer

Statistical
analysis of
hits



Heat
maps

Pivot Table [Hide] [Show]

Substance	AMYL_ALUMINA	AMYLUMINA	AMPUMINA	ETUMINA	DOXUMINA	TRUMINA	KOLUMINA	KOLUMINA
Substance	417	418	419	420	421	422	423	424
Substance	425	426	427	428	429	430	431	432
Substance	433	434	435	436	437	438	439	440
Substance	441	442	443	444	445	446	447	448
Substance	449	450	451	452	453	454	455	456
Substance	457	458	459	460	461	462	463	464
Substance	465	466	467	468	469	470	471	472
Substance	473	474	475	476	477	478	479	480
Substance	481	482	483	484	485	486	487	488
Substance	489	490	491	492	493	494	495	496
Substance	497	498	499	500	501	502	503	504
Substance	505	506	507	508	509	510	511	512
Substance	513	514	515	516	517	518	519	520
Substance	521	522	523	524	525	526	527	528
Substance	529	530	531	532	533	534	535	536
Substance	537	538	539	540	541	542	543	544
Substance	545	546	547	548	549	550	551	552
Substance	553	554	555	556	557	558	559	560
Substance	561	562	563	564	565	566	567	568
Substance	569	570	571	572	573	574	575	576
Substance	577	578	579	580	581	582	583	584
Substance	585	586	587	588	589	590	591	592
Substance	593	594	595	596	597	598	599	600

Register for free demo at
www.Human3DProteome.com

What we have

- 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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Thank You

www.moleculomics.com

www.human3dproteome.com

www.proteomestructure.com

