

## Getting personalised medicine to the market faster

### HPC-Competence Center

High Performance Computing (HPC) Wales is Wales' national super-computing service provider. Host to the UK's largest national distributed supercomputing network, HPCWales provides businesses and researchers with local access to world-class technology and the support to fully exploit it.



### Enterprise

Moleculomics is the only company offering open-ended lead discovery, toxicity screening and protein network identification, that is completely unlimited in reach, and that is applied across multiple genomes. With offices in both the UK and North America, the Swansea headquartered company employs 8 people and has established itself as one of the leading commercial structural bioinformatics system teams.

### How HPC makes the difference

Moleculomics' core business is focused on developing new computational tools that take genetic information and automatically convert this into detailed three-dimensional models of all of the proteins within our bodies.

Access to high performance computing (HPC) is vital in enabling Moleculomics' pipeline to run fast enough to be useful to a pharmaceutical company.

As a result of its work with HPC Wales, Moleculomics has been able to compute structures for all variants of proteins that are present in the population and has run screening experiments using docking algorithms to investigate the interaction of these variant structures with candidate compounds for drugs.



*Fig: Dr Jonathan Mullins, founder of Moleculomics and an Associate Professor at Swansea University's Institute of Life Sciences*

