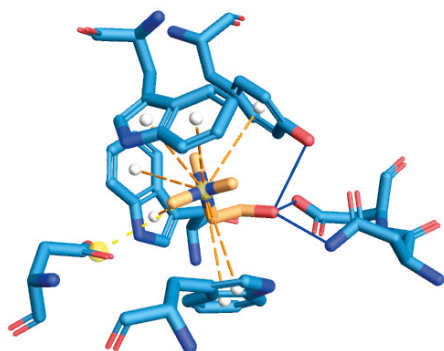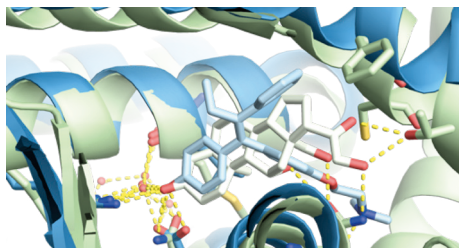# Cloud-based simulation of target drug compounds

Fortissimo Experiment Facts:
- Segment: Pharma Industry
- Application Domain: Computational Chemistry
- Application: In-house code

The Company

Transinsight is a German SME which develops software products in the area of bioinformatics where it analyses high-throughput data. This case study addresses the identification of existing drugs to treat illnesses other than those for which they are currently prescribed. This has the potential to make a significant impact in drug discovery where the costs of developing new treatments are becoming prohibitive. The assessment of target compounds requires the use of Cloud-based HPC because the search space is so large and complex. A new Cloud-based-HPC service will be offered by Transinsight to support drug discovery both by SMEs and by larger organisations.

The Challenge

The journey for a drug from invention to market is a long one. It has been estimated that the time required to develop a new drug de novo ranges between 10 and 17 years; that is, if it ever makes it. The chance for a new drug to actually make it to market is only 1:5,000. These slim chances are accompanied by the high cost for developing a new drug, which may reach an average of US$ 403 million. These rising costs threaten to make the development of new drugs increasingly unaffordable for both companies and patients.

Repositioning existing drugs for new diseases could deliver the productivity increases that the industry needs. A prerequisite for drug repurposing is drug promiscuity, a drug's ability to bind to several targets. Research indicates that there is a correlation between promiscuity and structural similarity as well as binding site similarity of protein targets. The use of this correlation has a huge potential to infer currently unknown drug-target relationships. However, such an approach requires significant computational resources. The use of Cloud-based computing can speed up drug development and reduce its costs by uncovering off-targets and thus causes of adverse drug reactions early in the development pipeline.

The Solution

The use of an HPC-Cloud infrastructure combined with algorithmic improvements enabled substantially better computational performance. This was achieved through the parallelisation of the algorithms used combined with the more efficient use of memory. This resulted in a significant reduction in the time and cost of the evaluation of a single compound. The Cloud-based approach enabled significant computational resources to be deployed without the need to purchase and maintain expensive hardware.

Fortissimo Experiment Partners:
- Transinsight (End-user)
- Technical University of Dresden
  (Domain Expert)
- Harokopio University (HPC Expert)
- UEDIN (HPC Provider)

More Information:
www.fortissimo-project.eu
E-Mail: info@fortissimo-project.eu

The Benefits

Transinsight estimates that there are hundreds of potential users of its proposed service. Each user represents a potential profit of €2,000 per annum comprising around 4,000 queries regarding protein matching. For Transinsight this represents a potential increase in profits of around 3% per annum.
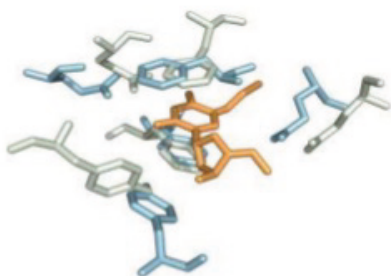
The Fortissimo Project

Fortissimo is a collaborative project that enables European SMEs to be more competitive globally through the use of simulation services running on a High Performance Computing cloud infrastructure. The project is coordinated by the University of Edinburgh and involves 123 partners including Manufacturing Companies, Application Developers, Domain Experts, IT Solution Providers and HPC Cloud Service Providers from 14 countries. These partners are engaged in 53 experiments (case studies) where business relevant simulations of industrial processes are implemented and evaluated. The project is funded by the European Commission within the 7th Framework Programme and is part of the I4MS Initiative.