

FP7 Coordination and Support Action to fund 50 technology transfer projects (TTP) in computing systems. This project has received funding from the European Union's Seventh Framework Programme for research, technological development and demonstration under grant agreement n° 609491.



## Advanced Computational Drug Discovery Technologies using High Performance Computing Architectures (ACDDT-HPC)

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### TTP Problem

In the pharmaceutical industry, the development of new drugs is crucial. To discover new drugs for a specific disease, extensive laboratory testing is needed: hundreds of thousands of chemical products have to be screened for activity against the proteins involved in the disease. This involves high costs related to:

- Purchase and storage of chemical products to be screened.
- Equipment needed for the screening.
- Residue disposal.
- Experimentation time.

High Throughput Screening equipment

### TTP Solution

Using Virtual Screenings costs can be drastically reduced:

The activity of millions of chemical compounds in respect to a specific protein can be calculated in a matter of hours by using High Performance Computing resources. These activities can be ranked, effectively filtering out thousands of inactive compounds, so that only a small list with the best candidates has to be experimentally tested in the laboratory.

ZINC  
DRUGBANK  
ChEMBL  
...



Libraries of  
chemical  
compounds

Massive processing  
in HPC clusters

Protein compound  
interaction (activity)

Activity ranking  
(best candidates)

### TTP Impact

- Speed up and cost reduction in drug discovery.
- Enhanced quality of academic studies: Development of theoretical hypothesis supporting experimental observations.
- Theoretical support for patent claims.

### TTP Facts

Contact: Horacio Pérez Sánchez  
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TETRACOM contribution: 22745€  
Duration: 01/05/2015 - 30/04/2016