



## Drug design enters a new dimension

**An American company is set to become the exclusive distributor of a new software tool developed by Chemotargets, the IMIM's first spin-off.**

*Barcelona, 6 October 2011.-* Certara ([www.certara.com](http://www.certara.com)), a US-based company and a leader in the provision of translational medicine services and solutions, is set to be **the exclusive distributor of the software developed by Chemotargets the first spin-off of the IMIM (Instituto de Investigación Hospital del Mar, 'Hospital del Mar Research Institute')** dedicated to the design of new drugs.

In recent years, Chemotargets' activity ([www.chemotargets.com](http://www.chemotargets.com)) has focused on the development and validation of the interactions established between small molecules and thousands of different proteins. The fruit of this research is the development of a **software tool which is able to predict, and build prediction models of, the activity of millions of small molecules against thousands of proteins, in a highly efficient manner**. One of the applications of this technology is the ability to predict the potential adverse effects of a pharmacologically active compound.

This exclusive distribution agreement with Certara marks the recognition of Chemotargets on the international biotechnological map and a turning point in the growth of a company which, without any outside help from venture capital firms, has tripled its turnover in 5 years. This will contribute to enabling Certara's customers to gain access to a wide range of modelling and prediction tools, which is becoming crucial with regard to making advances in the design of safer, more effective pharmaceutical compounds in a more efficient manner.

According to **Jordi Mestres, CEO of Chemotargets and coordinator of the Chemogenomics Research Group of the Research Unit on Biomedical Informatics (GRIB) of the IMIM-UPF**, *"in recent years, it has been evidenced that pharmaceutical compounds are not as selective as they were believed to be, and that in fact, they happen to have an affinity for multiple biological targets. Hence, having access to a software tool capable of predicting the affinity of small molecules for proteins adds a whole new dimension to drug design"*. *"Moreover"*, Mestres adds, *"identifying small molecules the affinity profile of which is similar to current pharmaceutical compounds allows to anticipate common potential side-effects"*.

The software, which started being developed 5 years ago by Chemotargets, aims to model or mimic the behaviour of the interactions that take place between the various entities that make up a cell system and the potential effects changes therein may entail for this system. Within this principle, the software tools of Chemotargets support the growing field of translational science, a new concept that aims to improve the productivity of drug development.

### About Chemotargets

The company was created in 2006; it was founded by its CEO, **Jordi Mestres, coordinator of the Chemogenomics Research Group of the Research Unit on Biomedical Informatics (GRIB) of the IMIM-UPF**. Since its creation, its aim has been to become a leader in the field of computational pharmacology. The technology applies to new drug design projects, through service contracts with other companies in the chemical, pharmaceutical and biotechnology industries. It is likewise involved in the European eTOX project, the purpose of which is to develop new software tools to improve drug safety. Since 2011, its headquarters have been based in the *Almogàvers Business Factory*, a new centre for start-ups

which Barcelona City Council is launching in partnership with universities, research centres, professional associations and venture capital funds wagering for innovation and entrepreneurship. The company was recently awarded a grant from the *Agencia de Gestión de Ayudas Universitarias y de Investigación* (AGAUR, the Agency for the Management of University and Research Grants ) to recruit research staff for an R&D project due to be carried out in the frame of the *Talento Empresa* (TEM-DGR, 'Business Talent') Programme 2010.

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**For further information**

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