Presentation in the EFMC International Symposium on Advances in Synthetic and Medicinal Chemistry

Mimicking Nature's complexity with 3D-Fragments Assembly

EDELRIS had the opportunity in August 2017 to present the work carried out in collaboration with Merck. This collaboration is a perfect example of the relevance and complementarity of EDELRIS' Services.

In continuation of a high-throughput screening strategy (650k compounds tested), Merck chose to reorient its project on Fragment Based Drug Discovery (FBDD). This FBDD program started from several libraries, included EDELRIS'.

EDELRIS' Library (**Keymical Fragments™**) stands out from other libraries by the diversity of 3D structures over traditionally flat heterocyclic structures. Thereby this program has delivered significant successes from the screening of relatively small sets of fragments (1000-2000).

Our efforts to build original collections maximizing chemical diversity in terms of shape, maximizing topological diversity, pharmacophore display and synthetic tractability were presented.

A case study of "drug design" allowed us to reveal a new binding pocket and propose new molecules. This work resulted in the identification of a highly potent small molecule inhibitor of the peptidyl-prolyl isomerase Cyclophilin-D.

It should be noticed that the originality of the proposed structures allows us to generate intellectual property. Two patents will be published soon.

This project has thus highlighted the history of our company with a library of complex molecules coupled with know-how in drug design and synthesis.

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Reference
1) Daniel A. Erlanson and Wolfgang Jahnke, Fragment-based Drug Discovery: Lessons and outlook, **2016**, *67*, Wiley-VCH