20.10.2010

SARomics Biostructures provides key complex structures in a drug design project.

Press release

Lund, Sweden, October 20, 2010 – SARomics Biostructures is pleased to announce the publication of its latest scientific results. The paper, which highlights the work of SARomics Biostructures and its co-founder Prof. Mikael Akke describes state-of-the-art investigations of the fundamental driving forces behind drug binding to proteins.

Diehl et al. (2010) "Conformational entropy and protein flexibility in ligand design targeting the carbohydrate recognition domain of galectin-3" J. Am. Chem. Soc. 132, 14577-14589, (Open access; freely available).

SARomics Biostructures provided crystallization and structure determination services within this exciting project. High-resolution protein structures are a prerequisite for detailed investigations of drug binding in molecular terms. In the present project, SARomics Biostructures determined the crystal structure of the carbohydrate recognition domain of galectin-3 in complex with a designed ligand at a resolution of 1.20 Å. The high-resolution structure made it possible for our clients to interpret experimental data from nuclear magnetic resonance relaxation and thereby explore the role of protein conformational entropy in modulating drug–target affinity.

The β-galactoside-binding protein galectin-3 is involved in the regulation of apoptosis, intracellular trafficking, cell signalling and cell adhesion. It is a potential target for treatments of cancer and inflammation.

Reference:

Diehl C, Engström O, Delaine T, Håkansson M, Genheden S, Modig K, Leffler H, Ryde U, Nilsson UJ, Akke M. (2010). Protein flexibility and conformational entropy in ligand design targeting the carbohydrate recognition domain of galectin-3. J Am Chem Soc. 2010 Oct 20;132(41):14577-89.

View the paper (open access).