IMS-P3 **Synthetic and Cheminformatic Exploration of Macrocyclic and Peptidomimetic Medicinal Chemistry Space**

Gerhard MÜLLER[1], Jorg BENNINGSHOF[1], Pauline VAN MEURS[1], Anita WEGERT[1], Joyce VAN DEN HEUVEL[1], Sander VAN ASSEMA[1], ○Norimasa MORITA[1], Dagmar STUMPFE[2], Antonio DE LA VEGA DE LEÓN[2], Norbert FURTMANN[2], Dilyana DIMOVA[2], Jürgen BAJORATH[2]

[1]Mercachem bv., [2]Department of Life Science Informatics, B-IT, LIMES Program Unit Chemical Biology and Medicinal Chemistry, Rheinische Freidrich-Wilhelms-Universität

Matching the synthetically accessible chemical space with disease-related biological target space is one of the core activities of current medicinal chemistry. The content of today's compound collections is a reflection of the target families that have been addressed in the past. Hence, there remains a substantial risk that currently populated compound space might not match with the areas of biological target space the pharmaceutical industry will have to focus on in the near future.

In this context, we embark into a systematic exploration of fused, bridged, and spiro-cyclic systems in which a smaller ring (3 to 7 skeleton atoms) is associated with a medium-sized ring (7 to 12 skeleton atoms, figure). We will elaborate on the results of a systematic cheminformatics and data mining analysis of the charted bioactive compound space, followed by structure-based designs and synthesis bicyclic ring topologies.