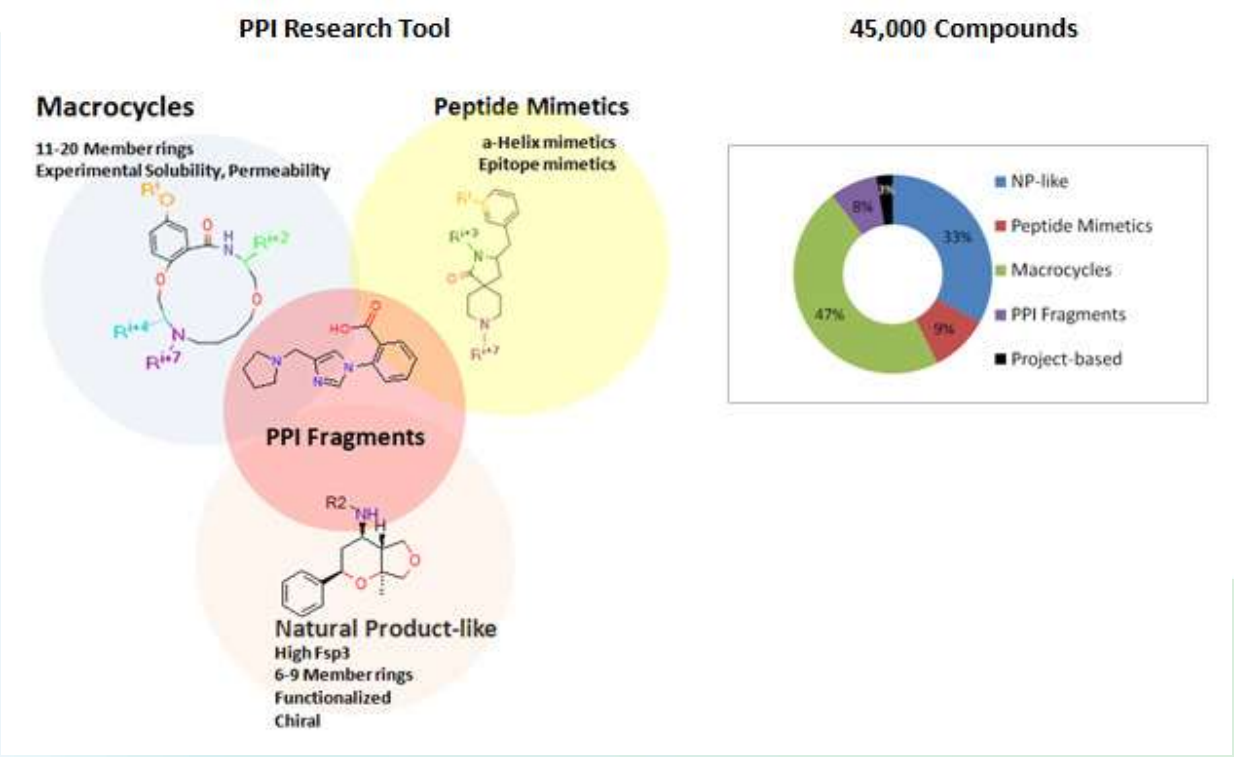
Small Molecules & Macrocycles for Protein-Protein Interactions

ASINEX has been working on the design and synthesis of protein-protein interaction (PPI) libraries since 2008. The latest generation of ASINEX PPI Library comprises molecules of various sizes, frameworks, and shapes ranging from fragment-like entities to macrocyclic derivatives designed as secondary structure mimetics or as epitope mimetics.

In the structural mimetics category we have designed small molecule and macrocyclic scaffolds that mimic the backbone geometry and the projection of side chains as observed in peptide structures at PPI interfaces. The designs cover b-turn / loop mimetics and a-helix mimetics. Since helices present at the interface in 62% of all protein-protein interactions [1], we have focused on designs including mimics with the substitution geometry of an a-helices, as well as designs that mimic the location of "hot-spot" side chains in helix-mediated PPIs. Epitope mimetics have been designed using structure based designs focusing on the locations of hot-spot residues at the PPI interfaces



References:

1. B. N. Bullock, A. L. Jochim, P. S. Arora, "Assessing helical protein interfaces for inhibitor design", JACS 2011, 133, 14220 – 14223

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