Protein-Protein Interaction Library

Designed for discovery of novel PPI modulators

40 640 pre-plated compounds

Having a pivotal role in multiple cellular processes, protein-protein interactions (PPIs) are responsible for the effects linked to the blockage of the substrate binding site. There are numerous examples of drug candidates withdrawn from clinical trials due to unexpected side effects of direct antagonist. This fact outlines the importance of developing new potent protein-protein interactions inhibitors.

We have carefully selected 59 370 diverse compounds specifically targeting PPIs. All compounds are stored as dry materials and they can be acquired in diverse custom formats. Using our PPI Library for hit discovery you receive multiple benefits allowing you to save on time and costs in lead generation:

- Dry stock of over 2.6 M compounds for hit resupply and hit expansion.
- Low-cost synthesis of analogues within only 3 weeks through our REAL Database technology
- Medicinal chemistry support enhanced with on-site broad ADME/T panel

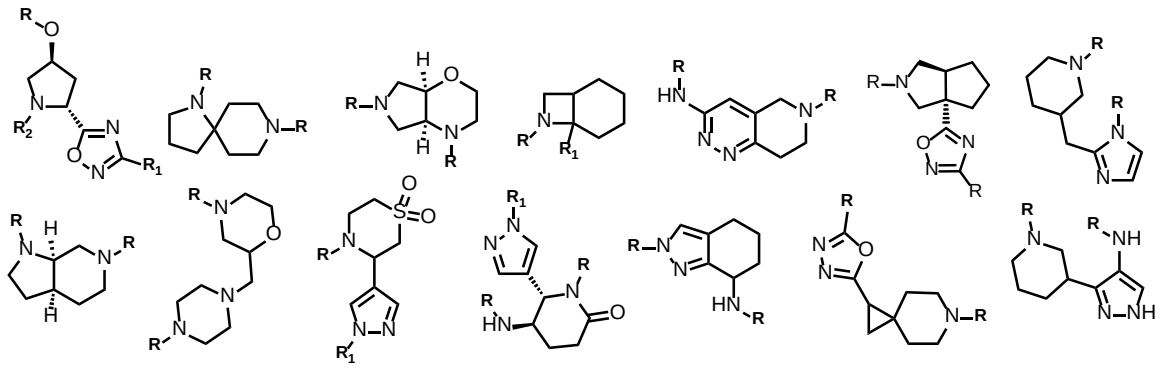
You have also an option to screen the Library directly at Enamine. In this case, we will be happy to offer discount on library cost depending on the collaboration scope.

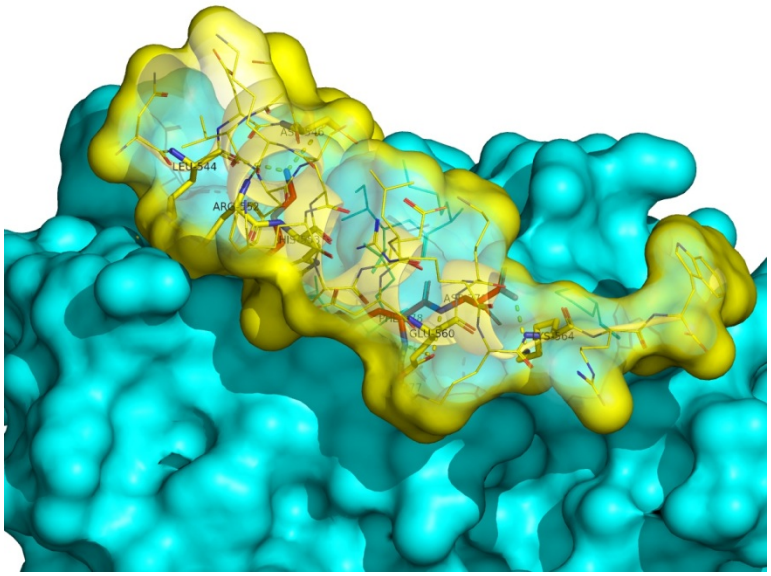
Library Design

Systemic analysis of available structural data of numerous PPIs allowed us to develop dedicated approach to the library design. We have analyzed more than 20 different protein-protein complexes to highlight specific features of majority of potent inhibitors in this area. Several specific recognition patterns, like α-helix, β-sheet, PDZ-, PBD and bromodomains were used in the library design. As a result of *Ligand- and Structure based in silico screening,* we created the selection of compounds featuring:

- Specific recognition patterns, including hot spots analysis, key amino acids, secondary/tertiary structures, α-helices, 'hot loops' and specific protein domains affinity.
- Lead-like properties and sp3-rich core structural motifs. Compounds passed all including affiliated MedChem filters including PAINS.
- Latest chemistry and novel building blocks. Identified hits can be readily followed with synthesis of new analogs through REAL Database technology.

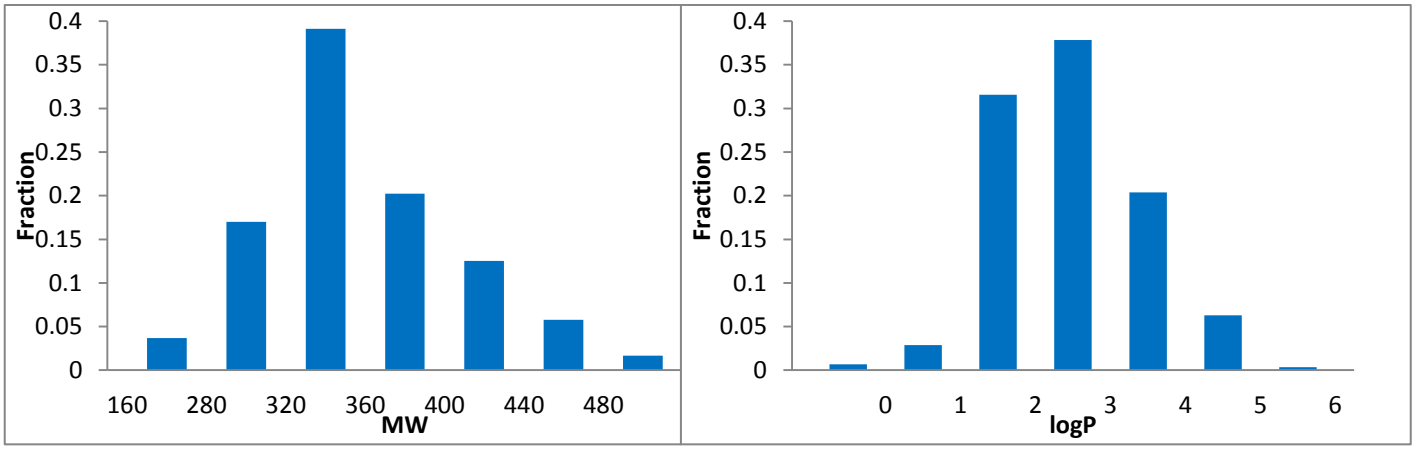
Examples of scaffolds populating PPI Library

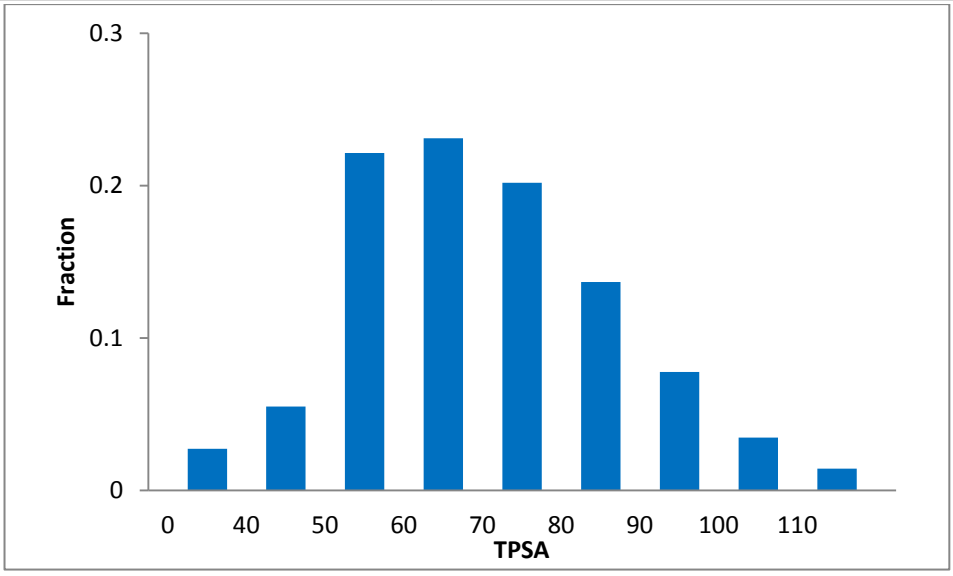


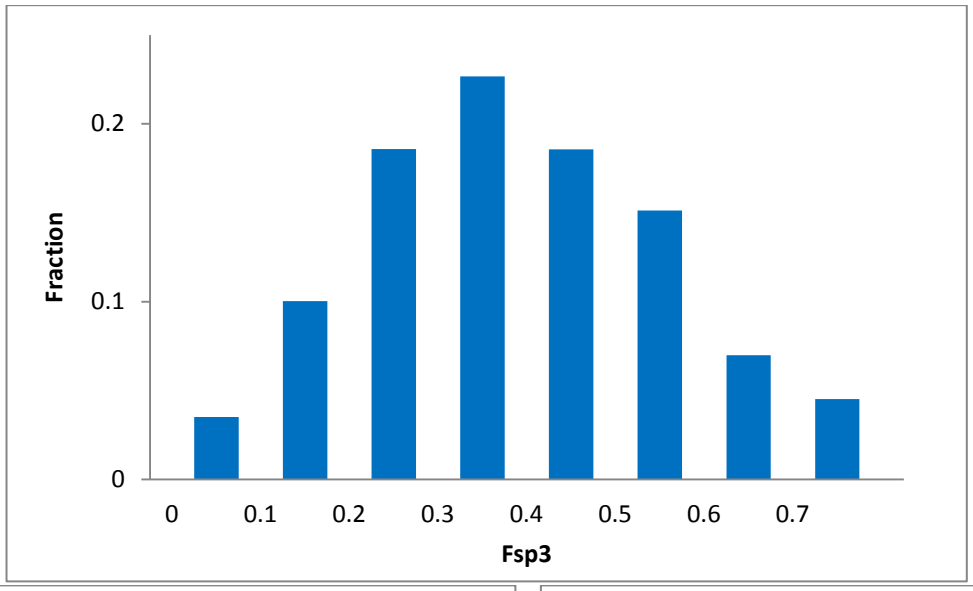


Importantly, our team of experienced computational, synthetic, medicinal chemists and biologists is ready to address your specific needs in tackling protein-protein interaction of your interest. Please, challenge us with your biological concepts, computational ideas and synthetic designs.

Molecular profile of PPI Library



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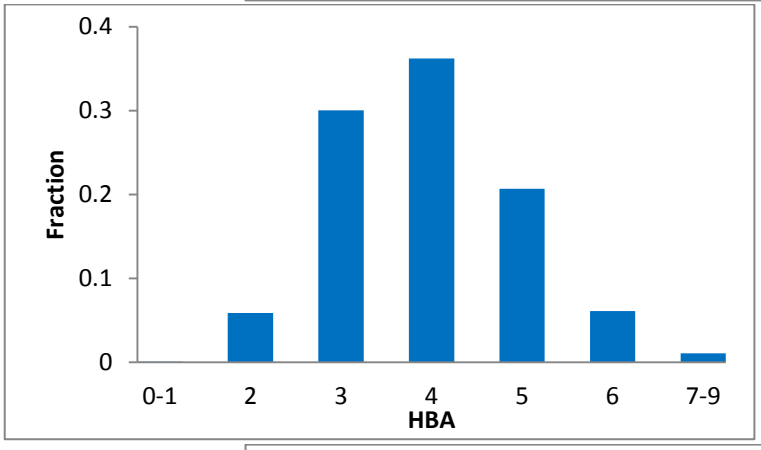
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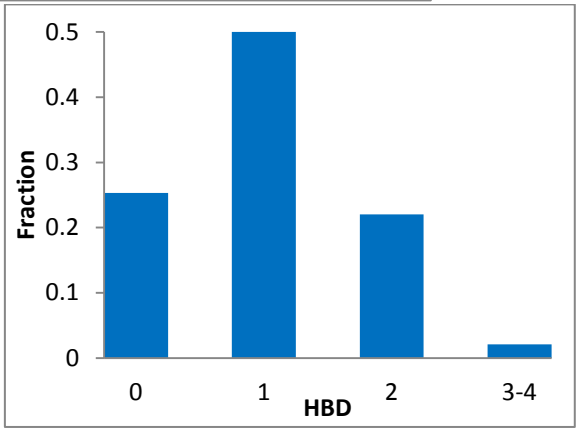
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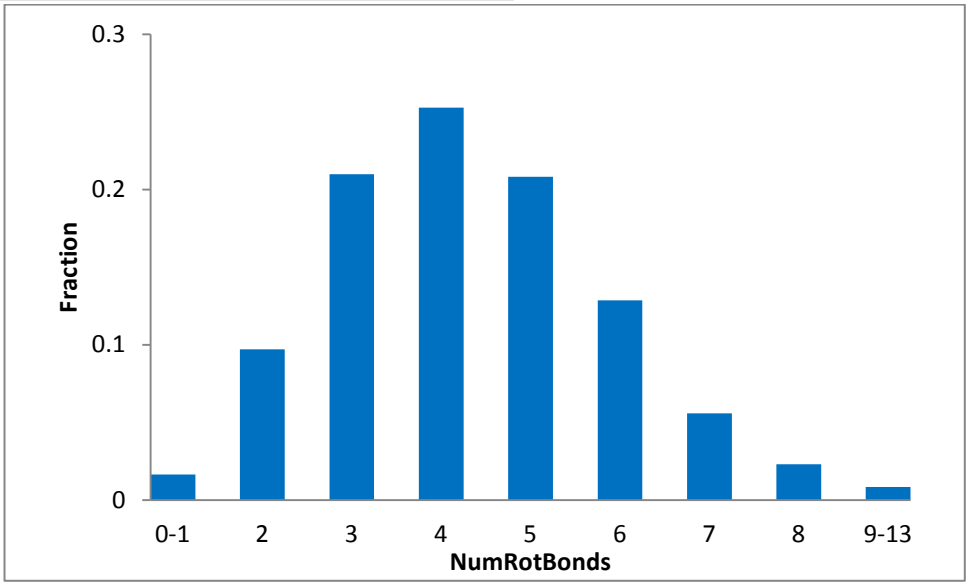
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