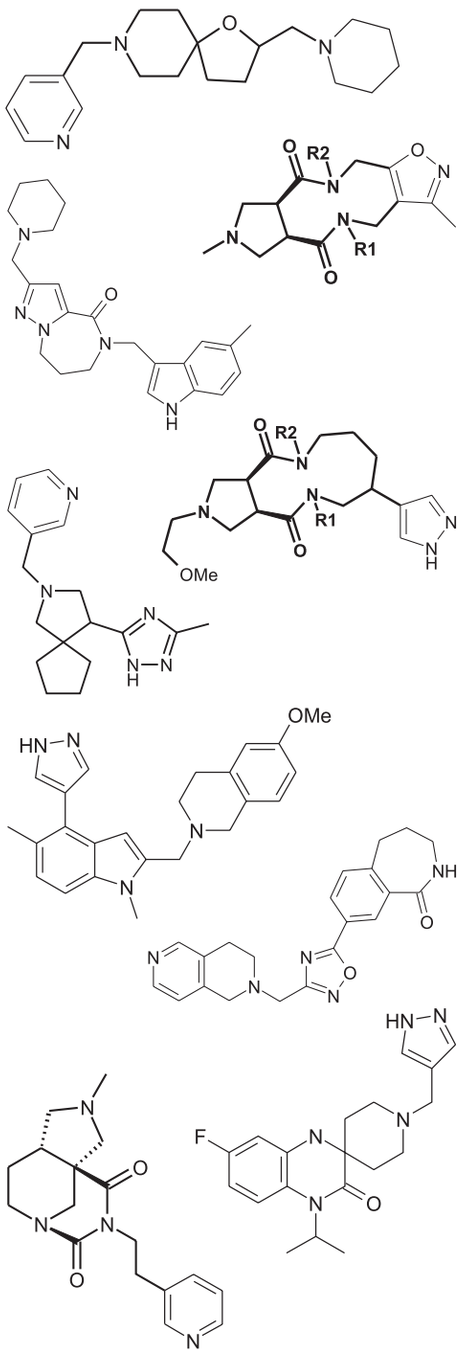
ChemDiv
The chemistry of cures℠

Protein-protein Interactions (PPI) Library

*PPI focused library contains about **142K** compounds, **2250** templates*
number of unique heterocycles: 810, diversity coefficient: 0,805 , number of screens: 10669



Principles of Design:

- **Diversity**
- **3D-Shape**
- **Escape from flatland, High SP3**
- **Drug-likeness**
- **Natural product likeness**
- **Targeted Diversity**

Structure of the library

- **Library consists of several complementary parts: Nonpeptide Peptidomimetics (based on the PPI biased substructures) ~25K compounds**
- **Set of Recognition Elements (gamma-, beta-turns, dipeptide mimetics) ~30K compounds**
- **Tripeptide mimetics ~3K compounds**
- **Shape (helix, beta-sheet, strand, loop) mimetics ~10K compounds**
- **3D-mimetics (single Isomers, caged compounds, etc.) ~3K compounds**
- **Set of Spiro-compounds ~5.5K compounds**
- **Set of Unusual compounds ~7K compounds**
- **Set of cyclic Ugi-compounds ~40K compounds**
- **Set "Escape from Flatland" ~30K compounds**
- **PDZ-domain inhibitors ~ 5K compounds**
- **MDM2 binding inhibitors ~8K compounds**
- **CD16a binding inhibitors ~2K compounds**
- **pGPCRs Focused sub-libraries:**
- **Chemokines ~10K compounds**
- **Hedgehog pathway ~10K compounds**
- **Neurotensin ~2K compounds**

154< MW < 863; 420 on average
0 < H-bond acceptors < 15; 5 on average
0 < H-bond donors < 9 1 on average
0 < rotatable bonds < 20; 6 on average
-8.0 < logD (pH 7.4) < 12.2; 3.7 on average
-14.4 < log of solubility in water (pH 7.4) < 15.3;
-3.9 on average 0<persentSP3<100; 34.8 on average

Chemical Diversity (ChemDiv, Inc.)
6605 Nancy Ridge Drive
San Diego, CA 92121, USA
Tel.: 858 794 4860 Fax: 858 794 4931
Email: chemdiv@chemdiv.com

Discovery™ outSource

TARGET TO LEAD
LEAD TO CANDIDATE
CANDIDATE TO POC
POC TO MARKET