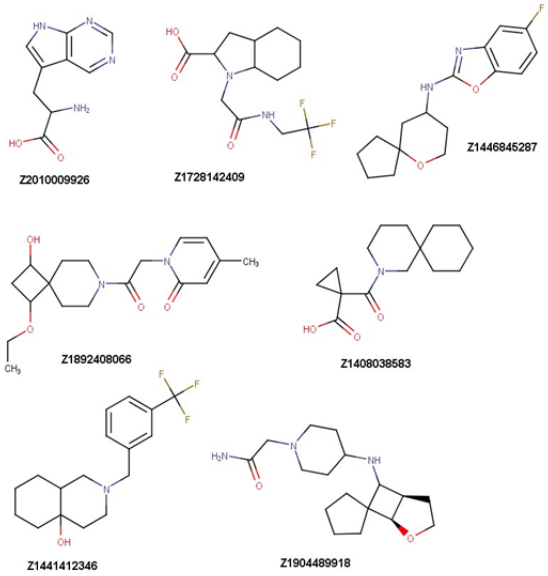
PPI Fragment Library

Protein-protein interactions regulate most aspects of life cycle thereof being the most attractive and perspective target for contemporary drug development. This field is still not well explored and is not a common feature of all the proteins involved in it. Such intricate biological systems cannot be cost-efficiently tackled using conventional high-throughput screening methods. To maximally meet purposes of i-PPI search projects we have created the library of fragments with dedicated design. The multivectoral algorithm consists of systematical knowledge on PhysChem parameters of active molecules within selection of privileged structure cores and moieties. Criteria used for the selection of PPI fragments are summarized in the table below:

Parameter	Range
Molecular weight	200 – 400
ClogP	0.0 – 4.0
TPSA	< 120 Å^2
H-acceptors	≤ 5
H-donors	≤ 4
Rotable bonds	0 – 5
Hydrophobic cores	1 – 5
RDF070m	≥ 13.31
Ui	≥ 3.95



Examples of the compounds included in the Library.