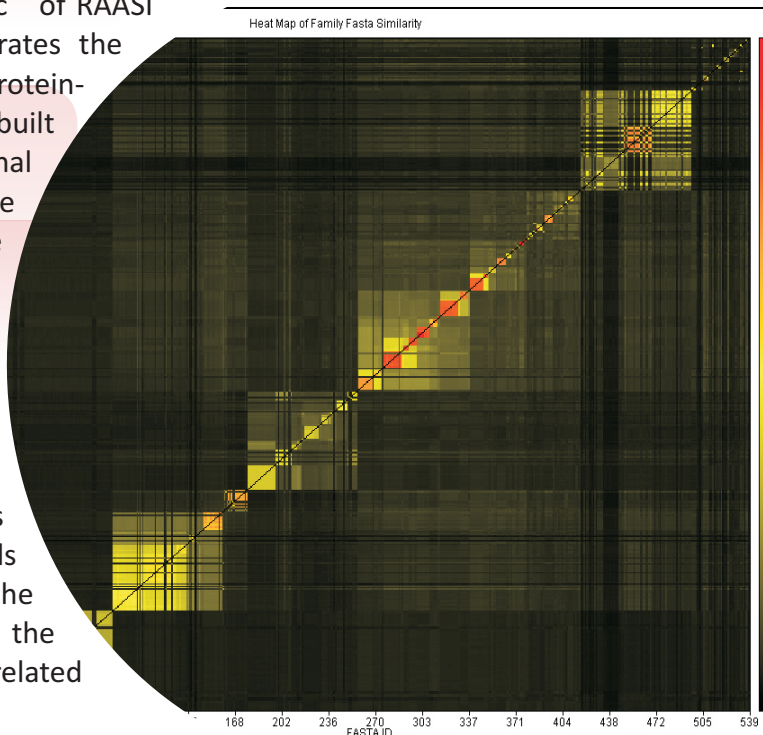


## Protein-Ligand Network Analysis

Currently available protein-ligand complex analyzing tools reveal the relationship between protein and its native ligand (complexed ligand). But no tool can predict the connection among the other proteins and ligands. Analysis of Protein-ligand complexes plays an important role in drug discovery research. Knowledge based inhibitor design based on the information or analysis of protein-ligand complexes likely to be an efficient approach.

To solve this bottleneck we introduce ProtSpec<sup>TM</sup> of RAASI<sup>TM</sup> suite. ProtSpec<sup>TM</sup> builds a network which demonstrates the protein-protein, ligand-ligand, ligand-scaffold and protein-ligand interactions. ProtSpec<sup>TM</sup> employs an in-house built scaffold extraction method and several conventional similarity analysis and clustering tools to cluster the proteins and ligands. ProtSpec<sup>TM</sup> can be used to generate the relationship between proteins, ligands and scaffolds. The alignment scores among proteins is calculated by sequence similarity methods utilizing local, global and multiple alignments whereas the ligand similarity score between ligands are identified using fingerprint based scores, namely the Tanimoto co-efficient and Euclidian Distance. ProtSpec<sup>TM</sup> specializes in building a connected network of proteins and ligands thereby enabling the users to get a better view of the related proteins and ligands, which in turn reduces the quantum of work required to find a suitable/ related ligand/protein for in-silico drug designing.



### Deliverables

- A detailed delivery report for Protein-Ligand Network Analysis consists of:
- The alignment score of the proteins sequences, generated through the alignment algorithms.
- The similarity score of the ligands calculated using tanimoto Co-efficient and Euclidian Distance.
- Detailed network showing all possible connections between all the protein and ligand entities.
- Heat map

### Required Input Data

- PDB IDs
- Organism Name