SCOPE

Structure Based Compound Optimization, Prioritization & Evolution (SCOPE)

SCOPE is an innovative methodology from VLife Sciences Technologies Pvt. Ltd. to overcome challenges in lead optimization. It helps to identify key residues in the active site that are involved in modulating activity of a series of molecules. SCOPE utilizes residue-wise ligand interactions calculated in terms of:

- Steric and hydrogen bond components based on a PLP scoring function
- Electrostatic and steric components based on coulombic function and van der Waals function respectively

These residue-wise interactions are used to build quantitative models to understand the relative importance of active site residues influencing the activity.

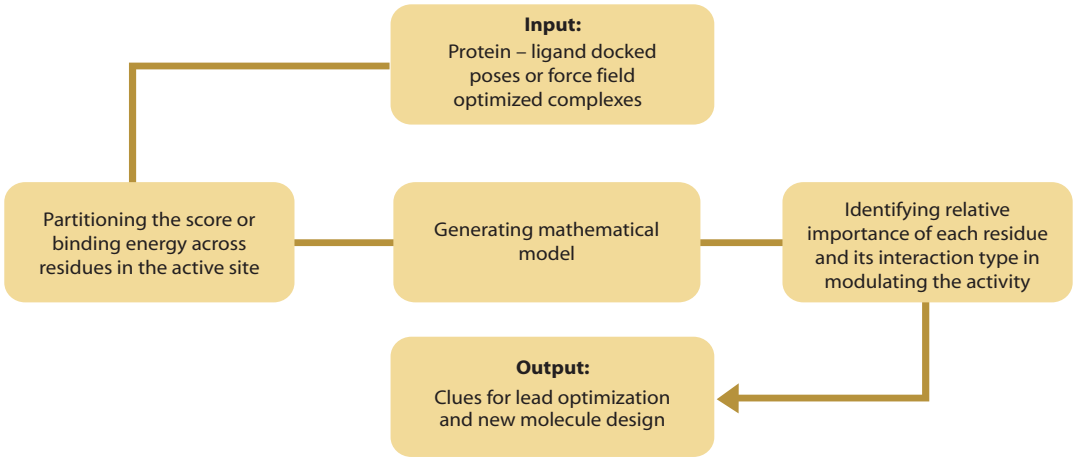
Advantages of SCOPE:

- Helps to identify the key residues important in modulating activity
- Can contribute to lead optimization by providing clues for maximizing favorable interactions with key residues
- Helps in screening of lead compounds based on the required properties that interact favorably with the key residues
- Predict activity of newly designed compounds

What does SCOPE provide:

- Insight into the relative importance of each residue in the active site of protein, which could be useful for lead optimization
- A mathematical function to estimate the activity of docked ligands

SCOPE flowchart:



References:

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