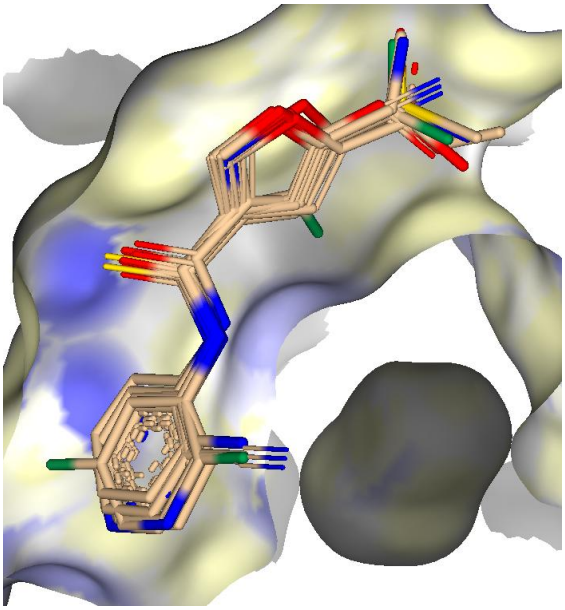
MedChemesis – Analoging

BioSolveIT
expect actives!

MedChemesis is a tool specifically designed for ligand mutation, enabling the generation of a series of closely related analogs to a given query compound by applying common medicinal chemistry reactions.

How does MedChemesis work?

MedChemesis facilitates the generation of a comprehensive series of closely related analogs to a specified query compound by leveraging prevalent medicinal chemistry reactions. MedChemesis operates in the Inspirator Mode, allowing users to explore the neighboring chemical space of a given compound and identify promising modifications. These modifications include bioisosteric replacements, such as substituting a carboxylic acid with a tetrazole group, as well as introducing halogens and methyl groups to enhance potency. Furthermore, MedChemesis enables transformations like replacing a carbon atom with a nitrogen atom, performing heteroatom walks within aromatic rings, and much more.



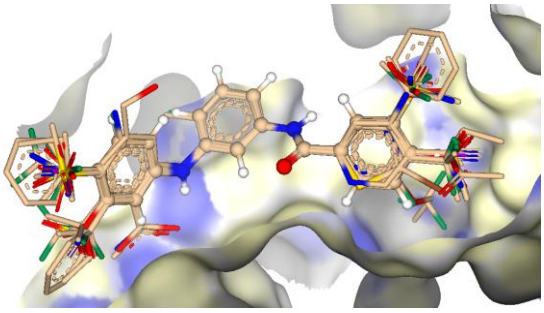
With an extensive library comprising 290 of the most commonly used medicinal chemistry transformations, MedChemesis offers a vast exploration of analogs. It achieves this while considering the binding site topology in an efficient manner, thus avoiding the exhaustive enumeration of all possible modifications. This approach not only saves valuable time but also conserves energy, allowing researchers to focus their efforts on the most promising avenues of exploration. MedChemesis serves as a valuable tool in the field of medicinal chemistry, facilitating the design and optimization of compounds through a diverse range of analog generation.

Advantages

- Only promising candidates are generated avoiding the full enumeration of all possible modifications
- Samples only small modifications to keep the molecular weight similar to the query compound
- Extremely fast and efficient

Complementing your toolbox

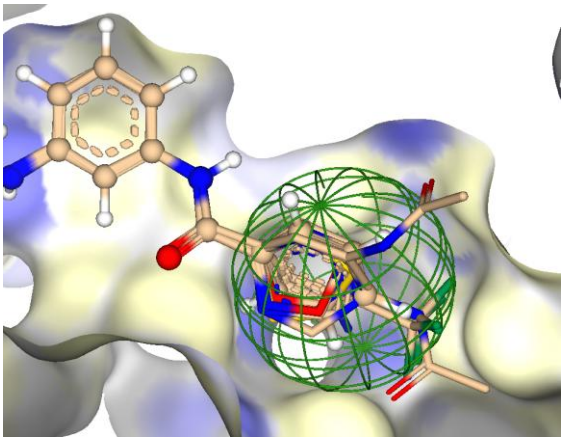
MedChemesis provides new ideas how to improve a compound or its physicochemical properties. It does so by expanding your in-house medicinal chemistry portfolio by showing you results you would have not considered otherwise.



MedChemesis, while keeping the original ligand intact, examines various modifications that can be applied to specific motifs of the molecule. It also evaluates potential clashes and eliminates unfavorable compounds. Once all potential modifications are generated, they are efficiently pre-scored to identify the most promising candidates that interact with the binding site. Ultimately, the desired number of optimal solutions is presented to you.

Guide your search

You can also apply a broad range of pharmacophore constrains to fine-tune your results for particular features and modifications.



Use this to screen for replacements of a structure that does not contribute to the overall binding affinity of your ligand.