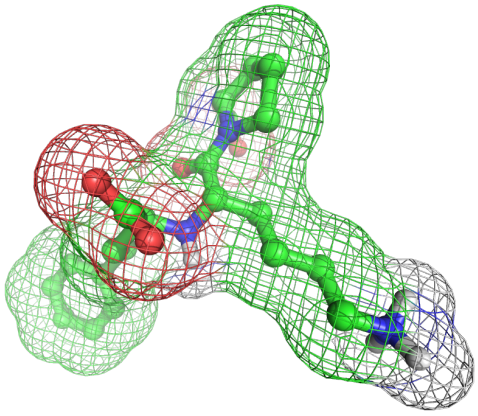
PEGASUS

2D ligand-based virtual screening solution



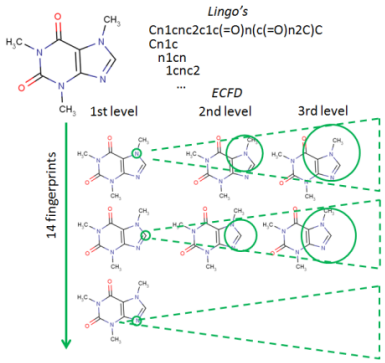
PEGASUS is a computational tool which identifies active molecules which are structurally similar to a molecule with a specific function.

Working with PEGASUS

- We need at least one molecule with a desired function and a data base containing molecules of interest. The data base can either be your proper one, provided by Intelligent Pharma or newly created in respect to your needs.

How does PEGASUS works?

- **PEGASUS** compare the structural make-up between two molecules in 2D.
- **PEGASUS** compare the structural features amongst two molecules in four different ways using the methods known as MACCS, Lingo, ECFP and MOLPRINT2D.
- **PEGASUS** ranks compounds according to the expected activity represented by the similarity score.



- **PEGASUS** organizes molecules into families or clusters, which allows one to choose the best molecule backbones (scaffolds) for testing.

PEGASUS's applications

- Determination of new active molecules
- Clustering of molecules into families
- Drug reprofiling
- Prediction of Mechanisms of action.
- Determination and selection of backups.

Competitive Advanges

- **PEGASUS** can determine the structural similarity of millions of compounds in a short time.
- The four comparison methods cover many different aspects of molecular structures allowing for high project success.
- **PEGASUS** is run by Intelligent Pharma's experts who determine the most appropiate way (MACCS, Lingo, ECFP and MOLPRINT2D) of doing the structural comparison for a project

Visit us!

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