

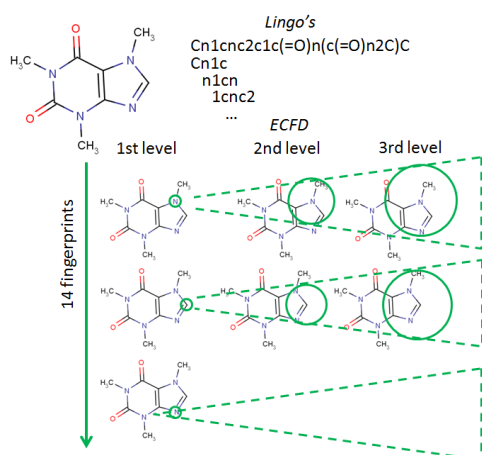
PEGASUS is a computational tool which identifies active molecules which are structurally similar to a molecule with a specific function.

PEGASUS is offered as a service, which means that Intelligent Pharma carries out the computational part of your project in order to achieve the best outcome of your objective.

### 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 work?



- PEGASUS compares the structural make-up between two molecules in 2D.

- PEGASUS can compare the structural features amongst two molecules in four different ways using the methods known as MACCS<sup>1</sup>, Lingo's<sup>2</sup>, ECFP<sup>3</sup> & MolPrint2D<sup>4</sup>.

- 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.

1 JL Durant, BA Leland, DR Henry, JG Nourse *J. Chem. Inf. Comput. Sci.* **2002**, 42, 1273-1280.

2 D Vidal, M Thormann, M Pons *J. Chem. Inf. Model.* **2005**, 45, 386-93.

3 D Rogers, M Hahn *J. Chem. Inf. Model.* **2010**, 50, 742-54.

4 A Bender, HY Mussa, RC Glen *J. Chem. Inf. Comput. Sci.* **2003**, 44, 170-88.

### Competitive Advantages

- 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 appropriate way (MACCS<sup>1</sup>, Lingo's<sup>2</sup>, ECFP<sup>3</sup> & MolPrint2D<sup>4</sup>) of doing the structural comparison for a project.

[www.intelligentpharma.com](http://www.intelligentpharma.com)

For general queries, please contact us at [info@intelligentpharma.com](mailto:info@intelligentpharma.com)

### PEGASUS Applications

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

### INTELLIGENT PHARMA

Intelligent Pharma offers different services in computation aided drug discovery. Our molecular modeling department carries out research projects to help your team in designing and developing new drugs using computational chemistry & biology expertise.

**PEGASUS is a multi-method & high throughput 2D ligand-based virtual screening solution.**

### Other technologies

#### HERCULES

3D Ligand-based virtual screening solution

#### SELENE

Receptor-based virtual screening solution

#### MEDEA

A data mining solution for medicinal chemistry

#### CHIRON

Computer aided hit to lead optimization

#### HYPERION

Allosteric site detector