MEDEA

A data mining solution for medicinal chemistry.

INTELLIGENT PHARMA

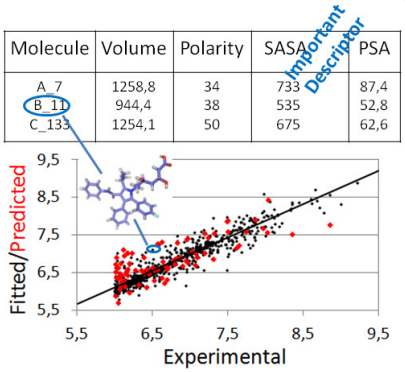
Developing solutions. Discovering drugs.

MEDEA is a data mining solution for the identification of biological patterns and the prediction of biological properties of groups of molecules.
MEDEA 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 MEDEA

We need any type of biological or physico-chemical data (e.g. activity or absorption) of a group of molecules. MEDEA extracts patterns or SAR (Structure Activity Relationship) from this data and creates QSAR (Quantitative SAR) models to predict the data for new compounds.

How does MEDEA work?



- For each molecule of the group, MEDEA determines the same set of properties/descriptors.
- Different descriptor sets may be determined as property related ones (MW, PSA, etc.), MACCs[1], Lingo's[2], ECFP[3] & Molprint2D[4].
- 2D molecular field descriptors[5] are also available.
- The relationship between these descriptors and the biological or physico-chemical data is determined using mathematical tools like PCA, SVM, PLS or Bayesian classification.
- MEDEA automatically creates QSAR models that predict the data of interest for new compounds.
- MEDEA analyses 3D-structural information and other physico-chemical properties of compounds to facilitate your design of new compounds with the desired pharmacologic properties.
- Property related descriptors include Lipinski characteristics and may be used for ADME studies or screening.

1 JL Durant, B Leland, D Henry, JG Nourse *J. Chem. Inf. Comp. Sci.* **2002**, *42*, 1273-80.
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.
5 M Pastor, G Cruciani, I McLay, S Pickett, S Clementi *J. Med. Chem.* **2000**, *43*, 3233-43.

Competitive Advantages

- MEDEA may also use public data, which we search for you.
- MEDEA can already work with small datasets of 30 molecules.
- Our experts test different approaches (descriptors /mathematical tools) to come up with the best predictions.
- MEDEA predictions can be optimized as new data becomes available, a general task during Hit optimization.

MEDEA's Applications

- Prediction and Reasoning for:
  - Activity.
  - Toxicological properties.
  - ADME properties.
  - Physicochemical properties.
- Hit optimization.
- Lead optimization.
- Extracting biological patterns / SAR.

INTELLIGENT PHARMA

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

MEDEA predicts any measurable property for new compounds.

Other technologies

CHIRON
Computer-aided hit to lead optimization.

SELENE
Receptor-based virtual screening solution.

HERCULES
3D Ligand-based virtual screening solution.

PEGASUS
2D Ligand-based virtual screening solution.

HYPERION
Allosteric site detector.

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