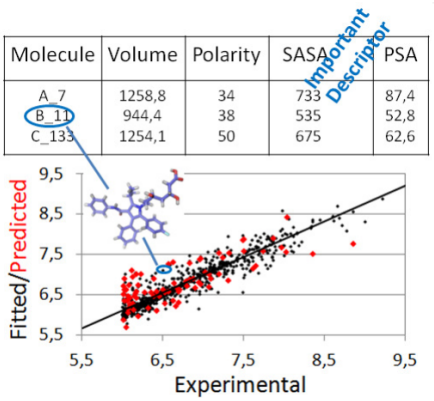
# MEDEA

## A data mining tool for medicinal chemistry




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

## 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 datafor new compounds

## How does MEDEA works?

- For each molecule of the group, MEDEA determines the same set of propertires/ descriptors.
- Different descriptor sets may be determined as property related ines (MW, PSA, etc.), MACCs, Lingo, ECFP and Molprint2D. 2D molecular field descriptors are also available. The relationship between these descriptors and the biological or physicochemical data is determined using mathematical tools like PCA, SVM, PLS or Bayesian classification.
- MEDEA automatically creates QSAR models that predict the data of the interests for new compounds.
- MEDEA analyses 3D-structural information and other physicochemical 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.

## SELENE's applications

- Prediction and reasoning for:
  - Activity
  - Toxicology properties
  - ADME properties
  - Physicochemical properties
- Hit optimization
- Lead optimization
- Extracting biological patterns / SAR

## Competitive Advanges

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