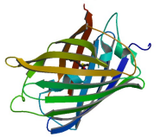
Input data

Compounds

CC(=O)Oc1ccccc

+

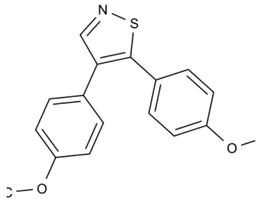
Targets

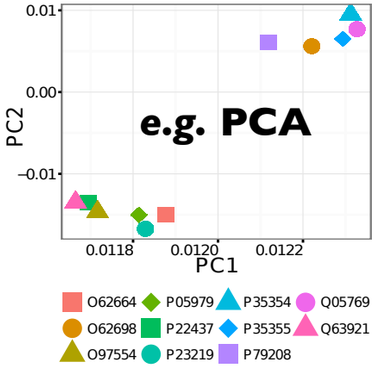


=

Bioactivities / Properties

Visualization





Descriptors

Compounds (after Standardization)

- Morgan fps
  - hashed
  - unhashed
- PaDEL (905 1D)
- PaDEL fps (13)

Targets

- Amino acid (8)
- Sequence (13)

Model Training

1. Data preprocessing

Feature selection
Centering & scaling
Data partitioning

2. Training

e.g. RF, SVM, GP, .
Ensemble Modelling

3. Validation

Metrics: R_0^2, RMSE, ..
Max. model performance

New Molecules

Preprocessing