

Compounds

Proteins

Compound
Standardization



Compound
Descriptors

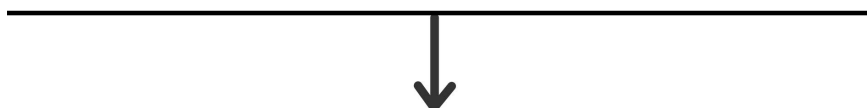
- PaDEL
- Morgan fps

Protein Sequence
from UniProt ID



Protein
Descriptors

- Amino acid
- Whole sequence



Dataset
Visualization

- Compound depiction
- PCA analysis
- Parwise Similarity ..



Dataset
Preprocessing

- Correlation
- Z-scores
- Impute missing values ..



Model
Training

- PCM / chemogenomics
- QSAR/ QSAM
- Ensemble Modeling



Prediction for
new Datapoints