

Predict bitterness

What: Estimate the bitterness of candidate molecules.

Why: To understand the physicochemical product properties. To mask or induce bitterness.

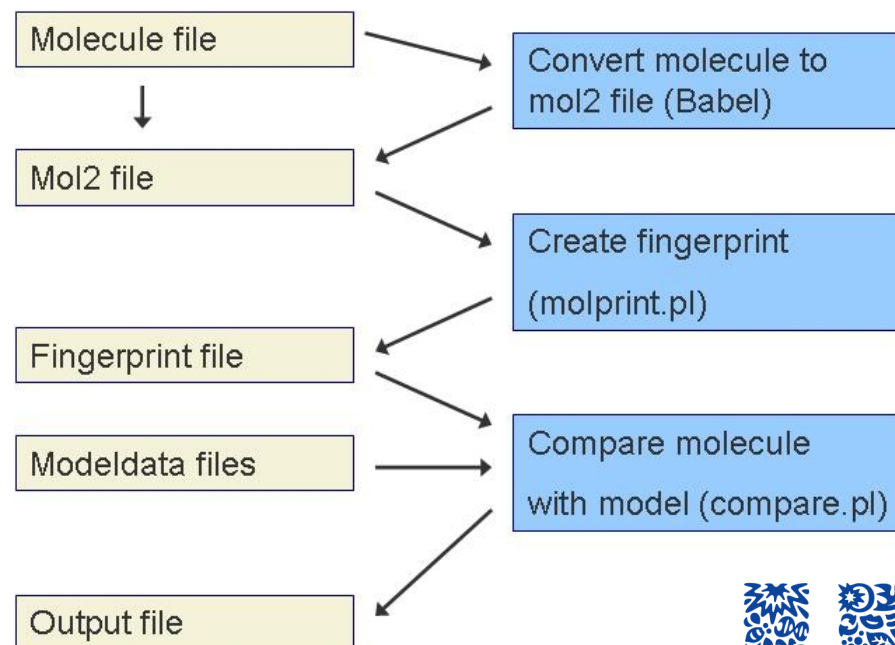
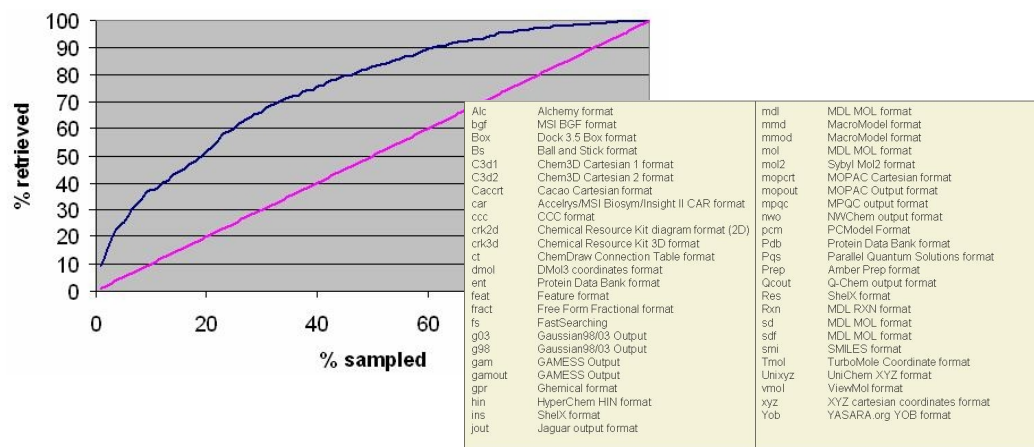
Key technologies: Machine learning, Boolean classification.

Possible applications: Automated 'taste consultant' that will reduce time to market. Use the same technique to predict different product properties (i.e. creaminess, crispness).

How: Use a training set for the Boolean classifier to learn. Choose from a wealth of molecule representation formats and feed the candidate molecule to the classifier. Get the prediction.

Note:

- The bitterness prediction tool can be utilised in Taverna as a web service.



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