

# 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.

