

predict

[index](#)
</home/mpastor/soft/eTAM/src/predict.py>

```
# -*- coding: utf-8 -*-
#
# Description      eTAM component for running a predictive model
#
#
# Authors:        Manuel Pastor (manuel.pastor@upf.edu)
#
# (c) PhI 2013
```

Modules

[getopt](#) [os](#) [sys](#)

Functions

main()

predict(molecules, verID=-1, detail=False)

Top level prediction function

molecules: SDFFile containing the collection of 2D structures to be predicted
verID: version of the model that will be used. Value -1 means the last one
detail: level of detail of the prediction. If True the structure of the
 closest compound will be returned

usage()

Prints in the screen the command syntax and argument

writePrediction(pred)

Writes the result of the prediction into a log file and prints some of them in the screen