

ClogP_{alk} Supporting information guide

The supporting information consists of source code for ClogP_{alk} and SSProFilter, parameter files for ClogP_{alk} and the data used in the study. A valid OpenEye license will be necessary to use the software and you will also have to edit the Makefiles to build the software. Predicted values of ClogP_{alk} are included in the data files so you can use these for testing.

These files are intended to be used on linux systems:

ssprofilter.1.0.cpp
make_ssprofilter
ssprofilter.documentation.pdf

ClogPalk.1.0.cpp
make_ClogPalk
ClogPalk.documentation.pdf
ClogPalk.param.1.0 (Parameter file)
ClogPalk.vb.1.0 (Vector binding file)

external_test_data.txt
training_data.txt

The data files are also provided in DOS format (unix2dos) for Windows users:

external_test_data_dos.txt
training_data_dos.txt