To calculate logP, logS and FA in SLIPPER-2001 the following method is used:

1. For every structure the nearest neighbors are found in the SLIPPER-2001 internal databases or user own databases.

Note: The number of neighbors can be set from 1 to 10.

2. The program carries out prediction using its own algorithm on the basis of structure similarity and physico-chemicals factors of compound.
3. Results of prediction you can print or save as a *.doc file (in case of a single structure) or save as *.sdf file (in case of databases)

SLIPPER-2001 contains the following internal databases for prediction logP, logSw and FA:

- on lipophilicity – 10,950 compounds.
- on solubility – 1,960 compounds
- on absorption – 260 compounds

How SLIPPER works

1. For prediction for a single compound user introduces information about name or ID of compound and sets pH values, for which he wants to receive predicted characteristics. Then he introduces structure formula of the compound and get the calculated values of lipophilicity in the system octanol/water (logP) and aqueous solubility (logSw) for introducing pH and FA for pH=7.4. He gets the full profile of these characteristics in depend of pH. Sliding with the mouse cursor along these curves user can watch a changing of the correspondent values of lipophilicity /solubility against pH in the correspondent information windows with accuracy of thousandth of percent.
2. For prediction from *.sdf file user should introduce pH values and then get results for the whole database
3. Prediction for a database is the same as from *.sdf file

The program can import/export files (in *.sdf format) and export information in *.txt or *.xls formats for further statistical analysis.