The LIBRARY MODE of ALOGPS 2.1

The current instructions are provided to test/use the logP program in the Library mode. The very similar procedure can be used to test the logS program too.

Please, prepare a file (smiles.txt) with SMILES followed by logP values in a file, e.g.,

```
CC      1.81
CI      1.51
C=C     1.13
```

After the experimental value you can add any commentary, name of molecule, etc.

```
CC      1.81    molecule no 1
CI      1.51    molecule no 2
BrC     1.19    experimental value is from Dr. Y
C=C     1.13    molecule no 4
ClC     0.91    public molecule no 5
FC      0.51    proprietary molecule no 6
```

Run **alogps** program and on the prompt:

***** LIBRARY MODE *****

LogP LIBRARY FILE:

type smiles.txt file (or alternatively do it for prediction of logS, use $\log_{10}$(mol/L) data).

The program will calculate "BLIND PREDICTION" and "LIBRARY LOO" results for all compounds in the file. Compare both results. New experimental logP data from the smiles.txt file usually provide a significant improved performance of the program for your compounds (Tetko and Tanchuk 2002, Tetko and Poda 2004, Tetko et al. 2008, Tetko et al. 2016).

N.B. If you have original proprietary data, provide them in the **LIBRARY** mode as the first step of your analysis! Whenever you quit the program it "forgets" information about the molecules provided in the **LIBRARY** mode. This version does not save user's libraries.

N.B. If several compounds have identical SMILES codes (notice that stereochemistry is not considered in this program), only the first one will be used in the **LIBRARY**. The experimental value for the used SMILES will be an average value of all identical SMILES.

You can also test the program in several ways, e.g. select by chance and save 50% of molecules as the smiles.txt file and save the second half of the molecules as the test.txt. In this case a blind prediction of all compounds from the test.txt file will be performed. Notice, that only the experimental values of compounds provided at **LIBRARY** mode will be used to improve ALOGPS 2.1 results. The experimental values of compounds provided in the **BATCH** mode (if available) will not be considered.

The same steps can be also used to test the aqueous solubility prediction module of the program. If you have any further questions how to test program in the LIBRARY mode, do not hesitate to contact us.

The on-line demo version of ALOGPS 2.1 is available at http://vcclab.org/lab/alogps.

References

Tetko, I. V. and V. Y. Tanchuk (2002). "Application of associative neural networks for prediction of lipophilicity in ALOGPS 2.1 program." J. Chem. Inf. Comput. Sci. **42**(5): 1136-1145.
Tetko, I. V. and G. I. Poda (2004). "Application of ALOGPS 2.1 to predict log D distribution coefficient for Pfizer proprietary compounds." J. Med. Chem. **47**(23): 5601-5604.
Tetko, I. V., et al. (2008). "Calculation of lipophilicity for Pt(II) complexes: Experimental comparison of several methods." J. Inorg. Biochem. **102**(7): 1424-1437.
Tetko, I. V., et al. (2016). "Prediction of logP for Pt(II) and Pt(IV) complexes: Comparison of statistical and quantum-chemistry based approaches." J. Inorg. Biochem. **156**: 1-13.