

Igor V. Tetko,<sup>1,\*</sup> J. Gasteiger,<sup>2</sup> R. Todeschini,<sup>3</sup> A. Mauri,<sup>3</sup> D.J. Livingstone,<sup>4</sup> P. Ertl,<sup>5</sup>  
V.A. Palyulin,<sup>6</sup> E.V. Radchenko,<sup>6</sup> N.S. Zefirov,<sup>6</sup> A.S. Makarenko,<sup>7</sup> V.Yu. Tanchuk,<sup>8</sup> V.V. Prokopenko,<sup>8</sup>

1- GSF – Centre for Environment and Health, Institute for Bioinformatics (MIPS), 2-University of Erlangen-Nürnberg, Computer-Chemie-Centrum, Erlangen, Germany,  
3-Milano Chemometrics and QSAR Research Group, Department of Environmental Sciences, Università di Milano - Bicocca, Milano, Italy,  
4-Centre for Molecular Design, Portsmouth and ChemQuest, UK, 5-Novartis Institute for BioMedical Research, Cheminformatics, Switzerland,  
6-Moscow State University, Department of Chemistry, Moscow, Russia, 7-Institute of Applied System Analysis, Kyiv, Ukraine,  
8- Institute of Bioorganic & Petroleum Chemistry, National Ukrainian Academy of Sciences, Kyiv, Ukraine

## Calculation of Descriptors

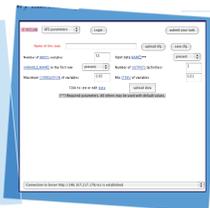
*E-DRAGON* is the electronic remote version of the DRAGON, which is an application for the calculation of molecular descriptors developed by the Milano Chemometrics and QSAR Research Group of Prof. Todeschini. DRAGON provides more than 1,600 molecular descriptors that are divided into 20 logical blocks. The user can calculate not only the simplest atom types, functional group and fragment counts, but also several topological and geometrical descriptors. If the 3D atom coordinates are not available for molecules, the user can calculate 3D coordinates using CORINA, provided by the group of Prof. Gasteiger.



*Parameter Client* (PCLIENT) is an extension of E-Dragon and encloses three different index generation programs, namely DRAGON, atom-type and bond-type E-state indices and Fragment-based indices. The conversion of molecules to 3D structure is provided using CORINA. This software makes it possible to generate more than 3000 indices.

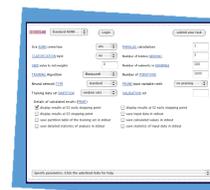
## Dimensionality Reduction

*Unsupervised Forward Selection* (UFS) is a data reduction algorithm that selects from a data matrix a maximal linearly independent set of columns with a minimal amount of multiple correlation. This software can be used to process indices generated by index calculation programs in order to decrease data redundancy.



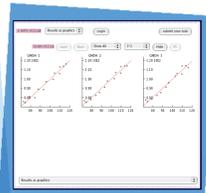
## Data Analysis

*Partial Least Squares* (PLS) uses a two-step descriptor selection procedure to significantly increase the predictive ability of the obtained models. The first step eliminates low-variable descriptors and the second step optimises the descriptor subset using a Q2-guided descriptor selection by means of a genetic algorithm. The computational experiments demonstrate the stability and good prediction accuracy of models.



*Associative Neural Network* (ASNN) represents an innovative method to calculate non-linear models between indices and molecular properties. The method represents a combination of an ensemble of feed-forward neural networks and the k-nearest neighbour technique. If new data become available, the network further improves its predictive ability and provides a reasonable approximation of the unknown function without a need to retrain the neural network ensemble.

*Polynomial Neural Network* (PNN) correlates input and target variables using (non) linear regression. In this particular software the user can define the desired properties of the solution such as the number of terms and the maximum degree of polynomials. The PNN calculates analytical models that could be easily interpreted. This is a substantial advantage of this method over other neural network approaches. Both approaches were recently compared to several other neural network methods using several QSAR datasets.



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on-line software

- ALOGPS 2.1\* is the most accurate program to predict lipophilicity and aqueous solubility of molecules
- ASNN\* calculates highly predictive non-linear neural network models
- BABEL is molecular structure information interchange hub
- PNN produces clearly interpretable analytical non-linear models
- PCLIENT generates more than 3000 descriptors
- E-DRAGON calculates DRAGON molecular indices
- PLS implements original two-step descriptors selection procedure
- UFS produces a reduced data set that contains no redundancy and a minimal amount of multicollinearity

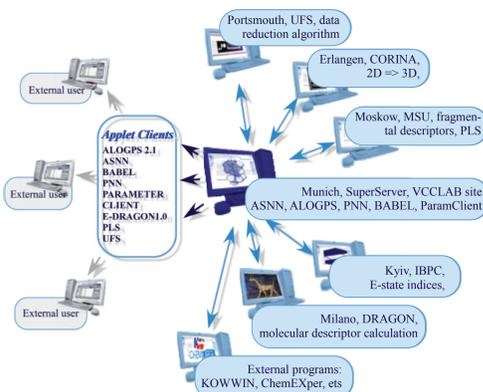
If you have any questions, problems to run applets, please, contact Dr. Igor V. Tetko.  
\*standalone version is free for academic and non for profit organisations.

ON-LINE SOFTWARE

- ALOGPS 2.1
- ASNN
- E-BABEL
- PNN
- PCLIENT
- E-DRAGON 1.0
- PLS
- UFS

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## Lipophilicity, logP and aqueous solubility, logS

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Welcome to the ALOGPS

Provide CAS RN or SMILES of a molecule and press the "Submit"

SMILES: c1ccccc1

Upload a file with molecule(s) in 48 formats

Online

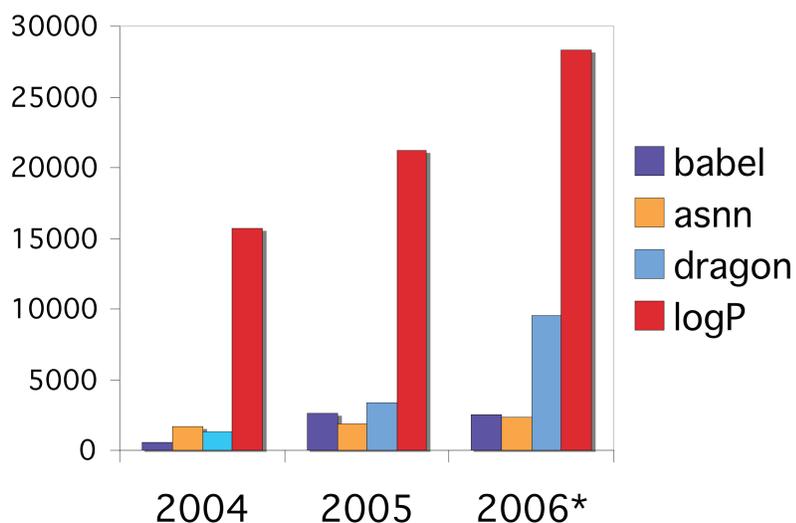
CAS RN	formula	C6H7N	
62-53-3			
SMILES	c1ccccc1N		
logP (exp)	0.90	logS (exp)	
ALOGPS	0.89 <-0.01>	ALOGPS	-0.71 (17.99 g/l) <-0.30>
IA_logP	1.07 <+0.17>	IA_logS	-0.32 (44.57 g/l) <+0.09>
CLOGP	0.92 <+0.02>		
mlogP	1.01 <+0.11>		
KOWWIN	1.08 <+0.18>	PhysProp reference	
XLOGP	1.21 <+0.31>	Sangster reference	

User's LogP LIBRARY  User's LogS LIBRARY

Click on calculated result to see details of calculations.  
Press underlined links to read about a particular method.  
Press LogP or LogS LIBRARY to read how to improve your predictions.  
If you have any suggestions or bug reports contact us at [root@vcclab.org](mailto:root@vcclab.org)  
We wish you to have only good results!

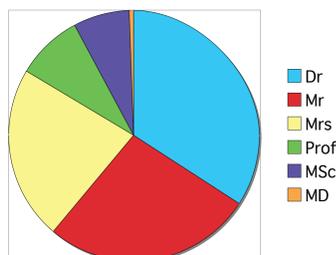
The calculated results are available.

## Popular VCCLAB tasks

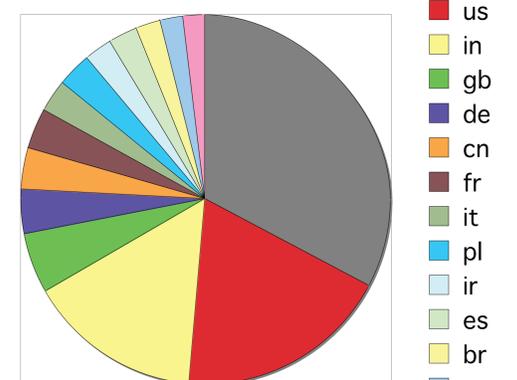


## Who are the VCCLAB users?

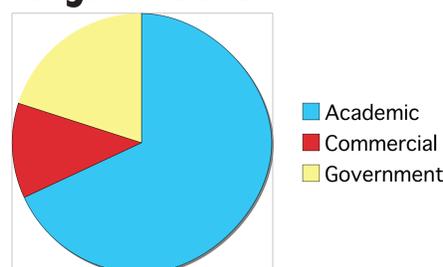
### Education



### Countries



### Organisations



## Future plans

Exporting of some tasks as Web Services  
Estimation of Applicability Domain of logP/logS predictions  
Similarity search in logP/logS spaces  
Calculation of new ADME/T properties  
HTML interface for non-Java users

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