Virtual Computational Chemistry Laboratory http://vcclab.org

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Calculation of Descriptors

**E-DRAGON**

- Provides descriptors based on molecular fingerprints
- Supports a comprehensive set of descriptor types
- Allows for the selection of descriptor types and parameters
- Aids in identifying similar molecules

**Parameter Client**

Internal database search
- Searches for structures based on parameters
- Helps in selecting descriptors

Dimensionality Reduction

**Unsupervised Forward Selection**

- Effective method for reducing the number of descriptors
- Helps in feature selection

Data Analysis

**Partial Least Squares**

- Technique for regression and classification
- Useful for dealing with multicollinearity
- Provides a way to reduce complexity

**Polynomial Neural Network**

- Advanced method for regression and classification
- Useful for nonlinear data
- Provides a way to reduce complexity

Lipophilicity, logP and aqueous solubility, logS

Virtual Computational Chemistry Laboratory

Welcome to the ALOOPS software

Popular VCCLAB tasks

- babel
- asnn
- dragon
- logP

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

Who are the VCCLAB users?

Education

- PhD
- MS
- BS
- Other

Countries

- us
- in
- gb
- de
- cn
- fr
- it
- es
- br
- au
- ch

Organisations

- Academic
- Commercial
- Government

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