Virtual Computational Chemistry Laboratory

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Internet technology offers an excellent opportunity for the development of tools by the cooperative effort of various groups and institutions. We have developed a multi-platform software system, Virtual Computational Chemistry Laboratory, http://www.vcclab.org, allowing the computational chemist to perform a comprehensive series of molecular indices/properties calculations and data analysis. The implemented software is based on a three-tier architecture that is one of the standard technologies to provide client-server services on the Internet. The developed software contains several popular programs, including the molecular descriptors generation program, DRAGON, a 3D structure generator, CORINA, a program to predict lipophilicity and aqueous solubility of chemicals, ALOGPS and others. All these programs are running at the host institutes located in five countries over Europe. In this article we review the main features and statistics of the developed system that can be used as a prototype for academic and industry models and discuss perspectives of development of chemoinformatics Web Tools and Services on the WWW.

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