

POSTER PRESENTATION

Open Access

# Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information

I Sushko<sup>1\*</sup>, AK Pandey<sup>1</sup>, S Novotarskyi<sup>1</sup>, R Körner<sup>1</sup>, M Rupp<sup>1</sup>, W Teetz<sup>1</sup>, S Brandmaier<sup>1</sup>, A Abdelaziz<sup>1</sup>, W Prokopenko<sup>2</sup>, VY Tanchuk<sup>2</sup>, R Todeschini<sup>2</sup>, A Varnek<sup>2</sup>, G Marcou<sup>2</sup>, P Ertl<sup>2</sup>, V Potemkin<sup>2</sup>, M Grishina<sup>2</sup>, J Gasteiger<sup>2</sup>, Il Baskin<sup>2</sup>, VA Palyulin<sup>2</sup>, EV Radchenko<sup>2</sup>, WJ Welsh<sup>2</sup>, V Kholodovych<sup>2</sup>, D Chekmarev<sup>2</sup>, A Cherkasov<sup>2</sup>, J Aires-de-Sousa<sup>2</sup>, Q-Y Zhang<sup>2</sup>, A Bender<sup>2</sup>, F Nigsch<sup>2</sup>, L Patiny<sup>2</sup>, A Williams<sup>2</sup>, V Tkachenko<sup>2</sup>, IV Tetko<sup>1</sup>

From 6th German Conference on Chemoinformatics, GCC 2010  
Goslar, Germany. 7-9 November 2010

The Online Chemical Modeling Environment is a unique platform on the Web that aims to automate and simplify the typical steps required for QSAR modeling. The platform consists of two major subsystems: the database of experimental measurements and the modeling framework. The database is user-contributed and contains a set of tools for easy input, search and modification of thousands of records. The OCHEM database is based on the wiki principle and focuses on data quality and verification. The database is tightly integrated with the modeling framework, which supports all the steps required to create a predictive model: data search, calculation and selection of a vast variety of molecular descriptors, application of machine learning methods, validation, analysis of the model and assessment of the applicability domain. Our intention is to make OCHEM an ultimate platform to perform the QSPR/QSAR studies online and share it with other users on the Web. The OCHEM is free for the web users and it is available online at <http://ochem.eu>. "Computing chemistry on the web" [1] is becoming a reality.

#### Author details

<sup>1</sup>Institute of Bioinformatics and Systems Biology, Helmholtz Zentrum München - German Research Center for Environmental Health (GmbH), Ingolstädter Landstraße 1, D-85764 Neuherberg, Germany. <sup>2</sup>OCHEM consortium.

Published: 19 April 2011

#### Reference

1. Tetko IV: **Computing chemistry on the web.** *Drug Discovery Today* 2005, **10**(22):1497-1500.

doi:10.1186/1758-2946-3-S1-P20

**Cite this article as:** Sushko et al.: Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. *Journal of Cheminformatics* 2011 **3**(Suppl 1):P20.

Publish with **ChemistryCentral** and every scientist can read your work free of charge

*"Open access provides opportunities to our colleagues in other parts of the globe, by allowing anyone to view the content free of charge."*

W. Jeffery Hurst, The Hershey Company.

- available free of charge to the entire scientific community
- peer reviewed and published immediately upon acceptance
- cited in PubMed and archived on PubMed Central
- yours — you keep the copyright

Submit your manuscript here:  
<http://www.chemistrycentral.com/manuscript/>



\* Correspondence: [iurii.sushko@helmholtz-muenchen.de](mailto:iurii.sushko@helmholtz-muenchen.de)

<sup>1</sup>Institute of Bioinformatics and Systems Biology, Helmholtz Zentrum München - German Research Center for Environmental Health (GmbH), Ingolstädter Landstraße 1, D-85764 Neuherberg, Germany  
Full list of author information is available at the end of the article