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Poster presentation

# Online chemical modeling environment

S Novotarskyi*, I Sushko and I Tetko

Address: Helmholtz Zentrum München, Ingolstädter Landstraße 1, D-85764 Neuherberg, Germany
* Corresponding author

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Online chemical modeling environment is a web-based system, aimed to collect and organize chemical data and to provide facilities to build prediction models on the basis of this data.

The system consists of two main parts: the database of physical/chemical and biological properties, and the online modeling environment. The main goal of the database is to collect, store and manipulate chemical data. Its main features, that distinguish it from other available databases are:

• the database is open. We encourage users to submit data and to correct inaccurate submitted data

• the database is aimed at collecting high-quality data. To achieve this we encourage users to submit references to the article, where the data was published. The reference may include the article name, journal name, date of publication, page number, line number, etc.

• we provide a possibility to store measurement conditions with the data. Since the compound properties may vary greatly depending on the conditions, under which they were measured, we would like to store the measurement conditions with the data to provide the users with more accurate results.

• in exchange for the data we can provide users with valuable information, such as e-state indexes and descriptors, calculated from their data. We also provide the modeling framework, that allows a user to get quick prediction results based on his data immediately after uploading the data to our database.

The modeling framework is being developed to complement the database. Its main goal is to provide a flexible and expandable calculation environment, that would allow to create and manipulate models of arbitrary complexity. The modeling framework is integrated with the database web-interface, that allows easy transfer of database data to the models. The web interface of the modeling environment is aimed to provide to the end users easy means to create high-quality prediction models.