

Other OASIS software platforms

ADVANCED AGENDA

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I. MEPS software

MEPS is a software for predicting explosive properties of chemicals considering the thermodynamics and kinetics of the explosion reaction. Two main modeling parameters are used for that purpose. The first one is “Power index” which is associated with the thermodynamics predictions discriminating explosive from non-explosive chemicals. The second one is “Sensitivity” associated with the ease with which an explosive chemical could explode, discriminating the sensitive from non-sensitive explosives.

II. Oncologic

OncoLogic is an expert system developed by U.S. EPA for predicting the carcinogenicity concern of chemicals based on empirical rules. The initial version - OncoLogic 8 - was migrated to a completely new standalone platform - OncoLogic 9. Standalone Oncologic 9 uses Toolbox knowledge to provide expert input in the Oncologic system.

III. SaaS

For more intensive tasks and for offloading client's local servers, LMC is able to provide a SaaS (software as a service) solution. In such scenario client's software send calculation requests to our server (via web services) and don't need that much computing resources at their end. The performance of this solution is guaranteed by servers optimized for the specific calculation/profiling tasks. Network traffic between the client and the LMC server is encrypted and the calculations are available to the requesting party only.

IV. MetaPath platform

The MetaPath platform is developed to collect, organize and analyse experimental data on metabolism or catabolism, observed biotransformation pathways and crucial supporting metadata. Thus, the results from metabolism studies are compiled and organized into a systematic database. The system provides a set of tools for managing and accessing the information, including powerful search engine that can extract information based on chemical structure, biotransformation, experimental metadata and specific proteins responsible for a given biotransformation.

V. UVCBs Explorer

UVCB explorer, developed by LMC, is a software for coding, generation and selection of constituents of substances of unknown or variable composition, complex reaction products, or biological materials (UVCBs). The potential UVCB constituents are coded and generated

based on preliminary literature search, expert analysis and/or analytical data for the phys-chem properties of the target substance, its manufacturing process and structural specifics. The selection of representatives could be 1) endpoint driven selection - based on ranges of a characteristic physicochemical property, e.g. logKow values are critical when assessing bioaccumulation potential and 2) endpoint independent selection – allowing objective selection of the minimum number of constituents that properly reflect the structural diversity of the entire UVCB substance. The generated constituents and/or selected representatives could be saved in a text file allowing their further analysis with other software.