A Free and Platform-independent Electronic Laboratory Notebook

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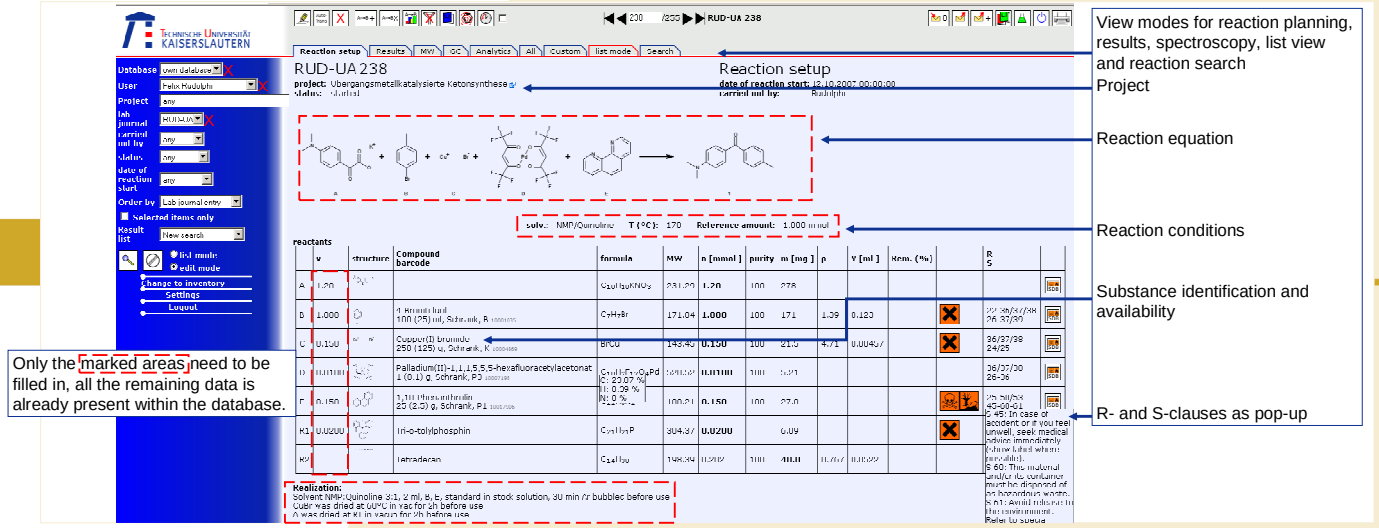
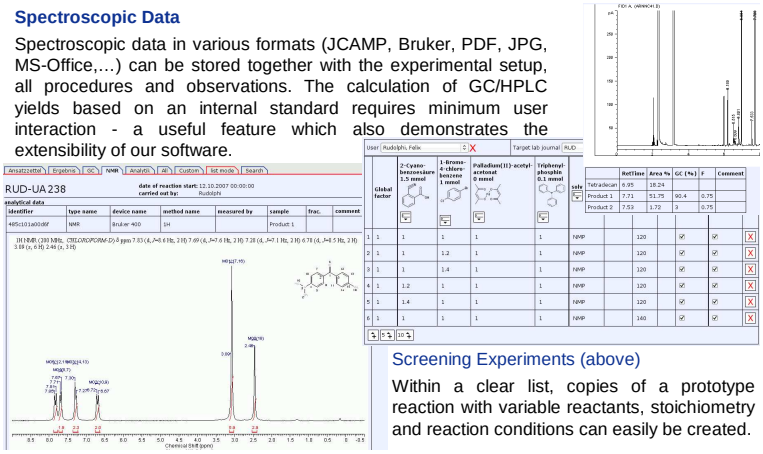
The electronic documentation of chemical reactions has become superior to hand-written laboratory notebooks in recent years as it makes work more efficient and also safer. Expensive commercial systems used in industry are not affordable for universities though. We have created a platform-independent electronic laboratory notebook as *open source* software with integrated inventory system. The inventory database makes all the required information available to researchers and can automatically extract physical and safety data from public internet sources thus maintaining an up-to-date database with a minimum amount of work. The safety instructions together with available information on molecular weight and density are used when entering a new reaction, rendering time-consuming searches within books or catalogues and following calculations obsolete. The reaction procedure and all observations are entered into the database, making this information available to present and future group members and even project partners across universities (limited to reactions belonging to the respective project for IP protection). Overall, open enventory makes laboratory work safer, more efficient and resource economical.



Spectroscopic Data

Spectroscopic data in various formats (JCAMP, Bruker, PDF, JPG, MS-Office,…) can be stored together with the experimental setup, all procedures and observations. The calculation of GC/HPLC yields based on an internal standard requires minimum user interaction - a useful feature which also demonstrates the extensibility of our software.

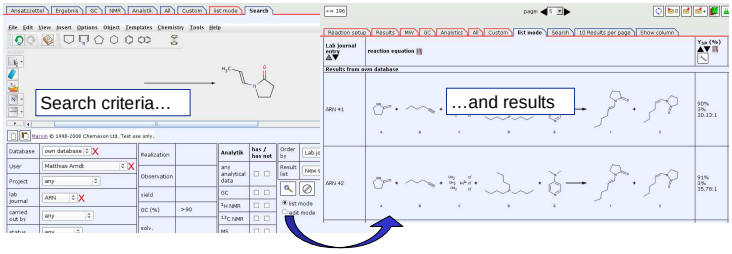


Screening Experiments (above)

Within a clear list, copies of a prototype reaction with variable reactants, stoichiometry and reaction conditions can easily be created.

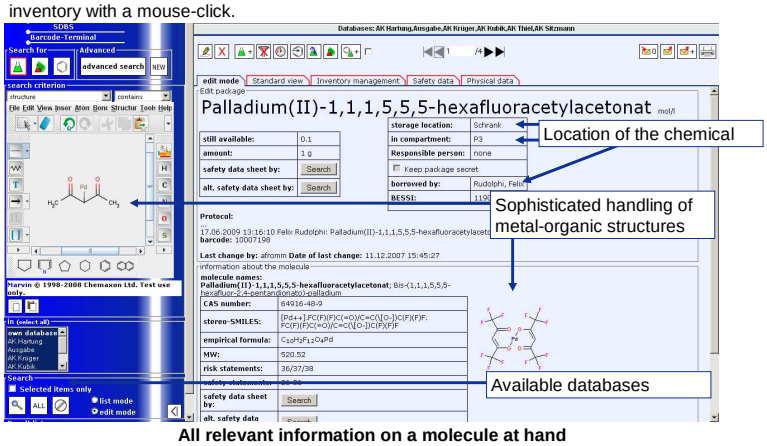
Highly Improved Efficiency for Laboratory Work and Publishing

Project members can act in a very coordinated way as all experimental and spectroscopic data is present within the database. The search function leads directly to the relevant information, which can easily be compared in the customizable list view. Past experiments can be reproduced easily and when writing publications, all available data is ready at hand. Project members can exchange project-related literature references with the integrated citation management. Overall, the accumulated knowledge and its good accessibility help to reach the goal in a more directed way.

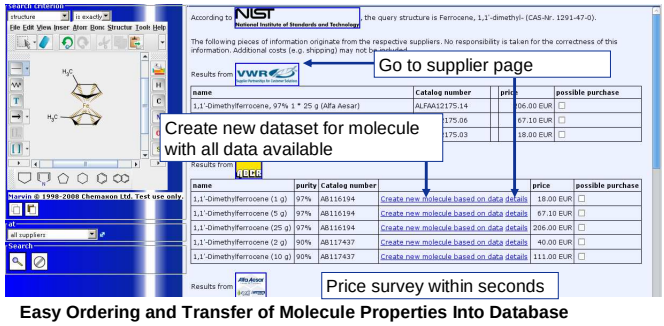


Integrated Inventory Database

The barcode-enhanced inventory database keeps track of all chemicals in the laboratory. It provides safety information (also GHS) and can be searched by name, CAS number, sub-structure, physical properties and even compound queries, thus minimizing search time. Physical and safety data can be transferred automatically from public internet sources making manual data entry practically obsolete. The inventory system allows to search for molecules at commercial sources and creates a price survey within seconds. The molecular structure together with physical and safety data for a molecule can be imported into the inventory with a mouse-click.



All relevant information on a molecule at hand



Easy Ordering and Transfer of Molecule Properties Into Database

Outlook

The system follows standards like MOLFILE and JCAMP and is currently available in English, German, French and Spanish, with more languages coming soon. The extension of the system by an integrated in-house ordering system is possible and a free, easy-to-use yet powerful structure editor is included. The community is invited to contribute to the maintenance and the development of extensions while keeping up the standardized data structures that are required for exchange between research projects.

Technical data

License: AGPL v3; Client: Internet Explorer 7, Firefox 3, Google Chrome, Opera, Safari; Server: Apache, PHP5, MySQL; open enventory and the logo are registered trademarks of F. Rudolphi and L. Gooßen. The applet to edit structures is interchangeable (ChemDraw Plugin can also be used), 3rd-party software may require separate license. Find more information on http://www.open-enventory.de

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