

open inventory

Electronic Laboratory Notebooks (ELN) have become omnipresent in chemical and pharmaceutical industry within the last decade. The electronic documentation of experiments makes the data searchable and gives researchers as well as supervisors a better overview of current and past results. In many cases, ELNs automate routine tasks, making laboratory work more productive and convenient. However, universities and public research institutes could not follow this trend as ELN software is costly or custom-made for single industrial clients.

In 2007, we therefore have started the project *open inventory* to develop an open source ELN with integrated chemical inventory, making sophisticated electronic documentation of chemical research available also to academia.

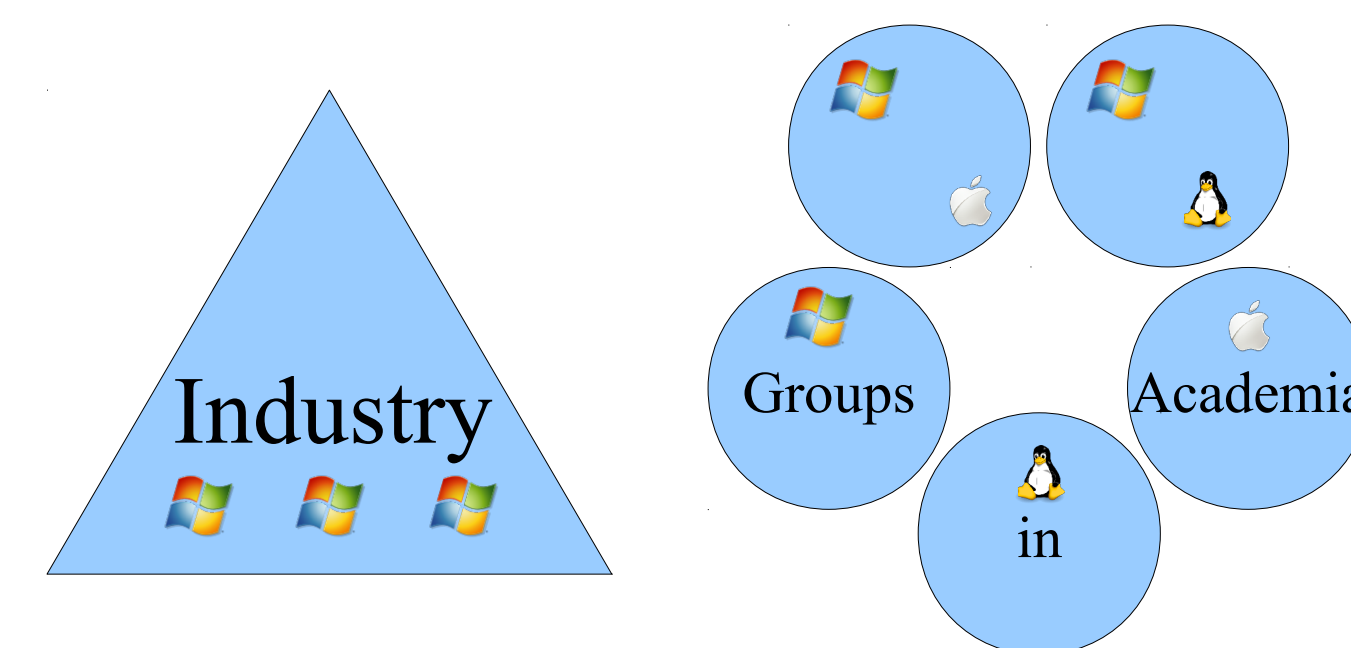
The software stores the setup of experiments, observations and all spectroscopic data, searchable by keywords, numeric parameters and chemical (sub-)structure. Researchers working on collaborative projects can easily exchange data to work in a very coordinated way, or use past projects as valuable knowledge base.

The overall design of the software particularly addresses the requirements of universities (see right), but some companies also use *open inventory* to make research more productive, convenient and resource economical.

What is different?

The requirements of academic users differ from those of the chemical and pharmaceutical industry:

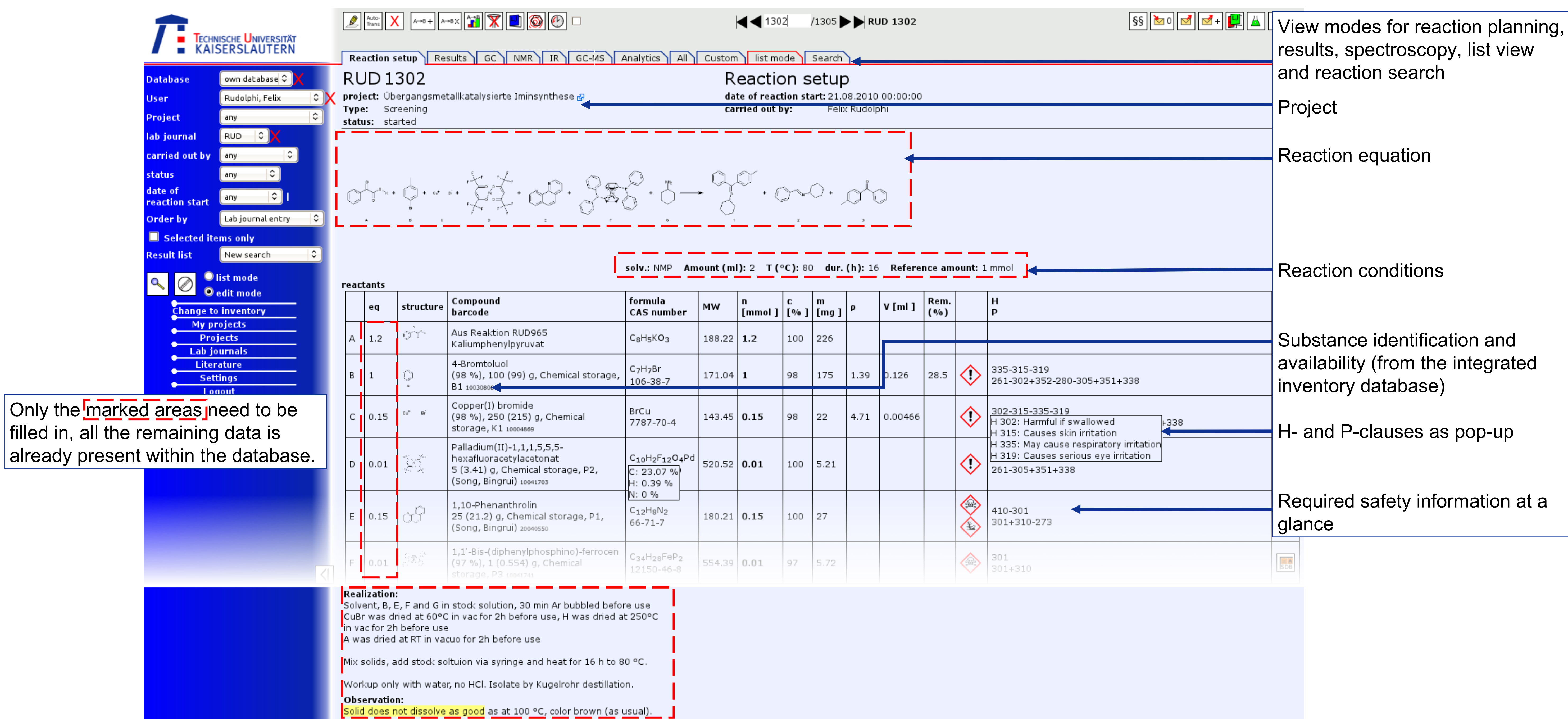
- decentralized organization
- independent workgroups
- heterogeneous IT environment
- financial limitations



An ELN suitable for application in academia must address these differences. Therefore, *open inventory* is designed as platform-independent web application, built completely on the basis of open source software (PHP, MySQL). The transparent process of data handling and storage ensures that data is not locked within a "black box" of proprietary software. By modifying or extending the source code, groups can address specific requirements of special areas of research.

As research groups are highly independent, they can store their data within separate databases. For collaborative projects and the exchange of chemicals, other groups' databases may be accessed read-only, forming a mesh.

In academic environments, an ELN must directly increase every researcher's productivity, otherwise students will not use it. Therefore, we use screen scraping techniques to extract physical and safety data from public internet sources, maintaining an up-to-date chemical database at minimum effort.



View modes for reaction planning, results, spectroscopy, list view and reaction search

Project

Reaction equation

Reaction conditions

Substance identification and availability (from the integrated inventory database)

H- and P-clauses as pop-up

Required safety information at a glance

Only the marked areas need to be filled in, all the remaining data is already present within the database.

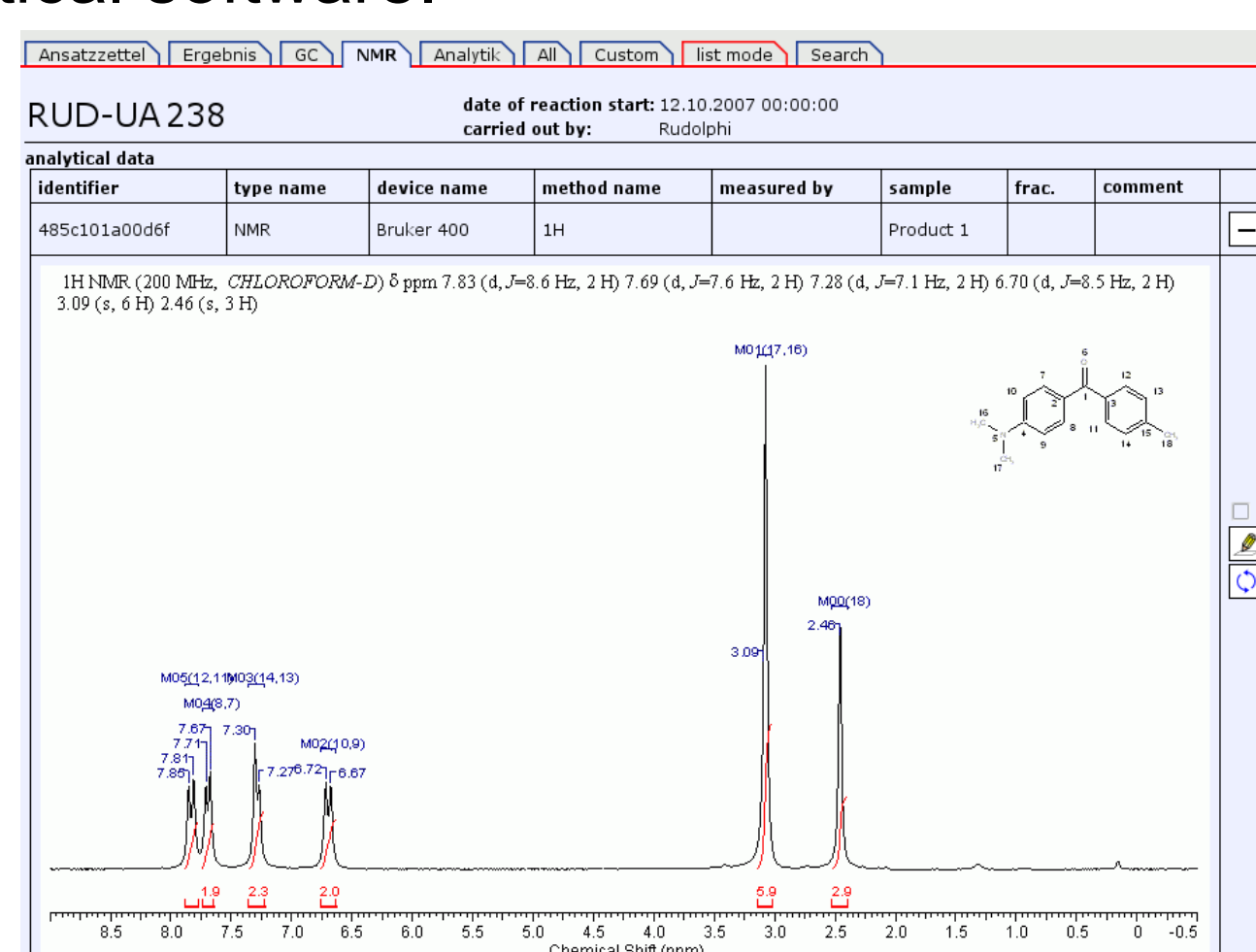
reactants	eq	structure	Compound barcode	formula	CAS number	MW	n [mmol]	C [%]	m [mg]	ρ	V [ml]	Rem. (%)	H	P
A	1.2		Aus Reation RUD965 Kaliumphenylpyruvat	C ₈ H ₈ KO ₃		188.22	1.2	100	226					
B	1		4-Bromtoluol (98%), 100 (99) g, Chemical storage, B1 10002806	C ₇ H ₇ Br	106-38-7	171.04	1	98	175	1.39	0.126	28.5	335-315-319 261-302+352-280-305+351+338	
C	0.15		Copper(I) bromide (98%), 250 (215) g, Chemical storage, K1 10004869	BrCu	7787-70-4	143.45	0.15	98	22	4.71	0.00466		302-315-335-319 H 302: Harmful if swallowed H 315: Causes skin irritation H 335: May cause respiratory irritation H 319: Causes serious eye irritation 261-305+351+338	
D	0.01		Palladium(II)-1,1,1,1,5,5,5-hexafluoroacetylacetonat 5 (3.41) g, Chemical storage, P2, (Song, Bingru) 10041703	C ₁₀ H ₂ F ₁₂ O ₄ Pd	C: 23.07 % H: 0.39 % N: 0 %	520.52	0.01	100	5.21					
E	0.15		1,10-Phenanthrolin 25 (21.2) g, Chemical storage, P1, (Song, Bingru) 20049350	C ₁₂ H ₈ N ₂	66-71-7	180.21	0.15	100	27				410-301 301+310-273	
F	0.01		1,1'-Bis-(diphenylphosphino)-ferrocen (97%), 1 (0.554) g, Chemical storage, P3 10000101	C ₃₄ H ₂₈ FeP ₂	12150-46-8	554.39	0.01	97	5.72				301 301+310	

Realization:
Solvent, B, E, F and G in stock solution, 30 min Ar bubbled before use
CuBr was dried at 60°C in vac for 2h before use, H was dried at 250°C in vac for 2h before use
A was dried at RT in vacuo for 2h before use
Mix solids, add stock solution via syringe and heat for 16 h to 80 °C.
Workup only with water, no HCl. Isolate by Kugelrohr distillation.

Observation:
Solid does not dissolve as good as at 100 °C, color brown (as usual).

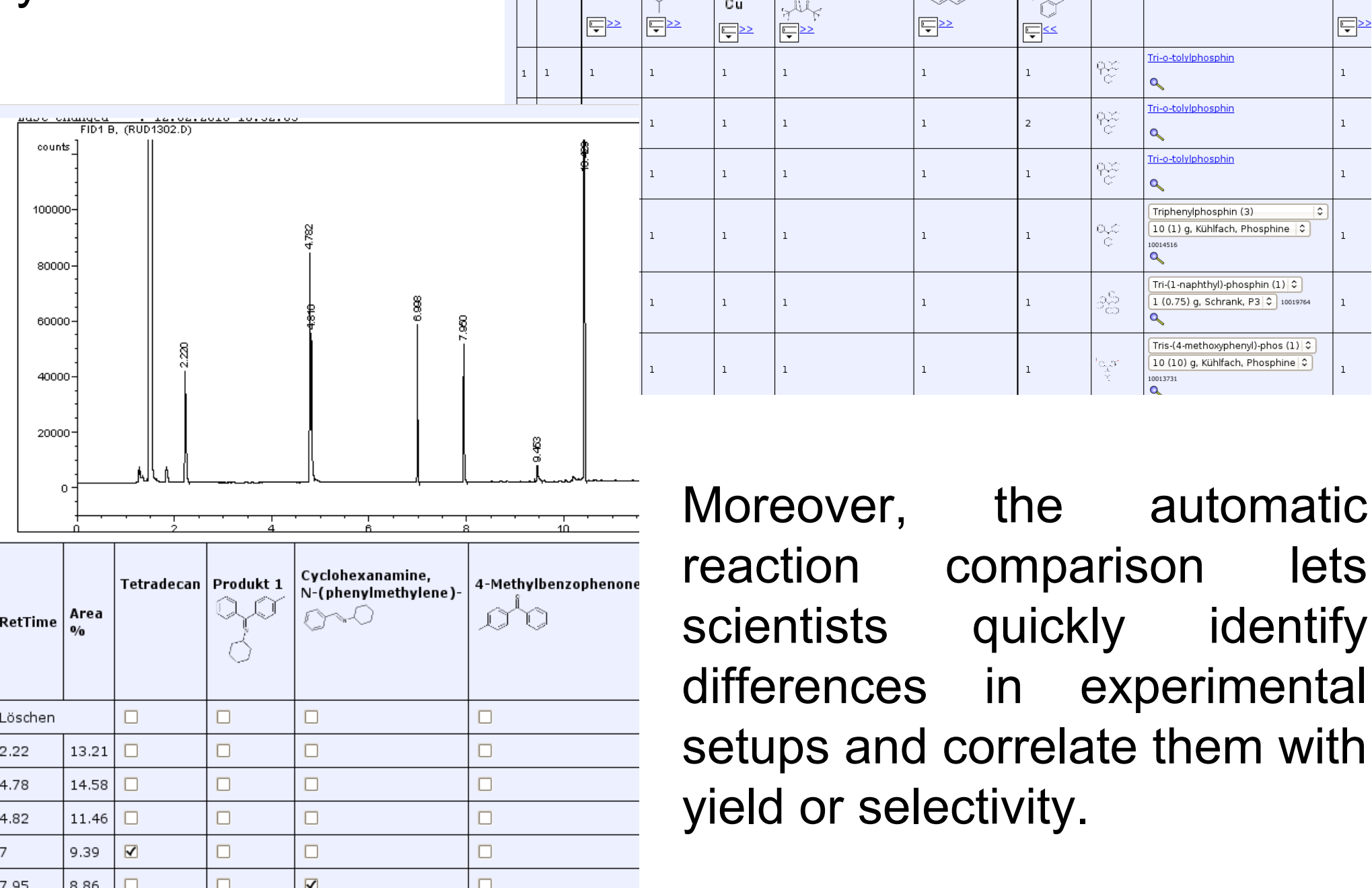
Spectroscopic Data

Data in various formats (image files, PDF, MS-Office, Agilent, Bruker, PE,...) can be stored together with the experiment. A macro connects centrally stored data and locally installed analytical software.



Productivity Extensions

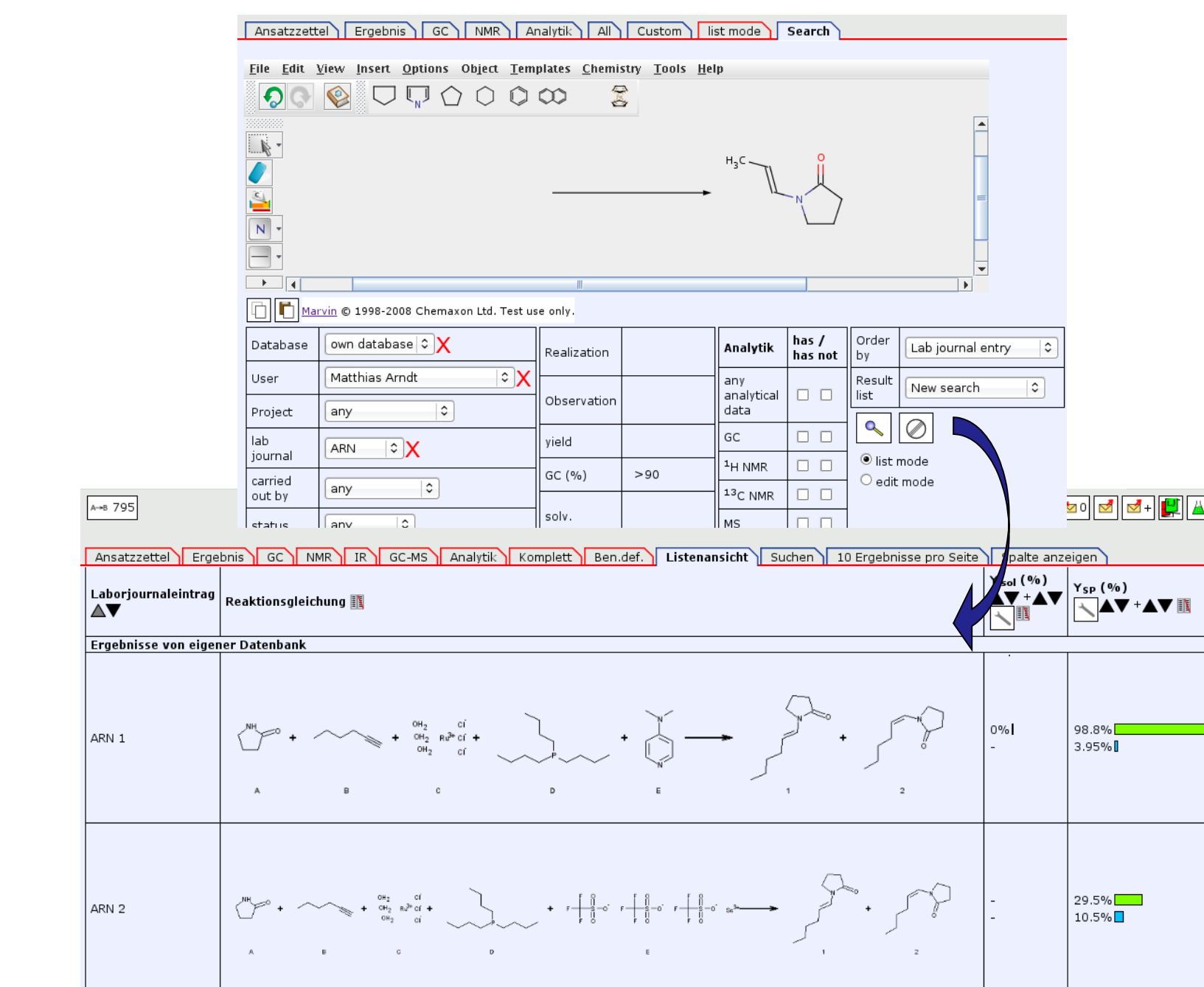
open inventory brings functionality to create series of experiments and automates data transfer from analytic instruments for high-throughput applications. It "learns" peak assignments in chromatograms and then automatically calculates GC/HPLC yields.



Moreover, the automatic reaction comparison lets scientists quickly identify differences in experimental setups and correlate them with yield or selectivity.

Reaction Database for Knowledge Exchange

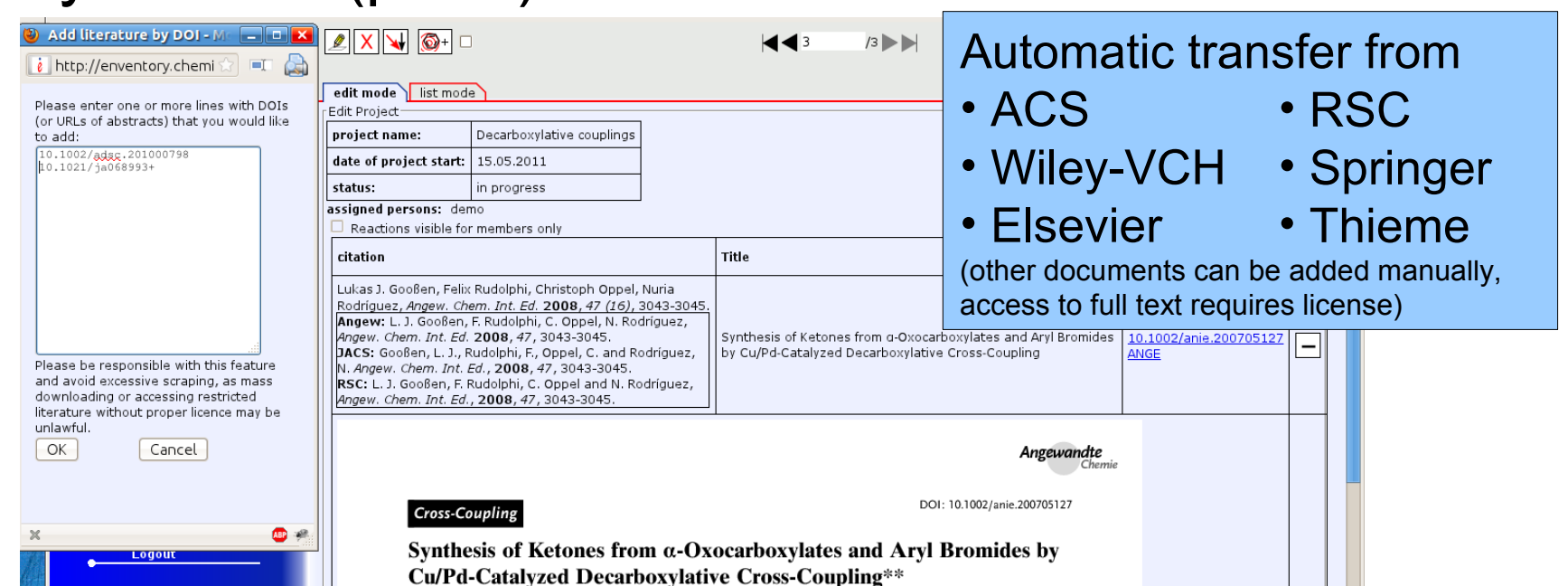
Compared to data written on paper, the practical value of structured electronic data is much higher. Within seconds, users can search thousands of reactions by (sub-)structure, keywords or numeric parameters to take advantage of this data collection. They may find useful separation procedures, reference spectra or inspiration for future experiments. When writing up theses or publications, all relevant data is instantly accessible.



open inventory makes the advantages of an ELN available to academia and helps researchers worldwide to reach their scientific target in a more directed and productive way.

Citation Management

Scientists can attach related literature to projects and reactions, making the information available to other project members. The PDFs can be searched by citation (parts) or full-text.



Automatic transfer from

- ACS
- Wiley-VCH
- Elsevier
- RSC
- Springer
- Thieme

(other documents can be added manually, access to full text requires license)