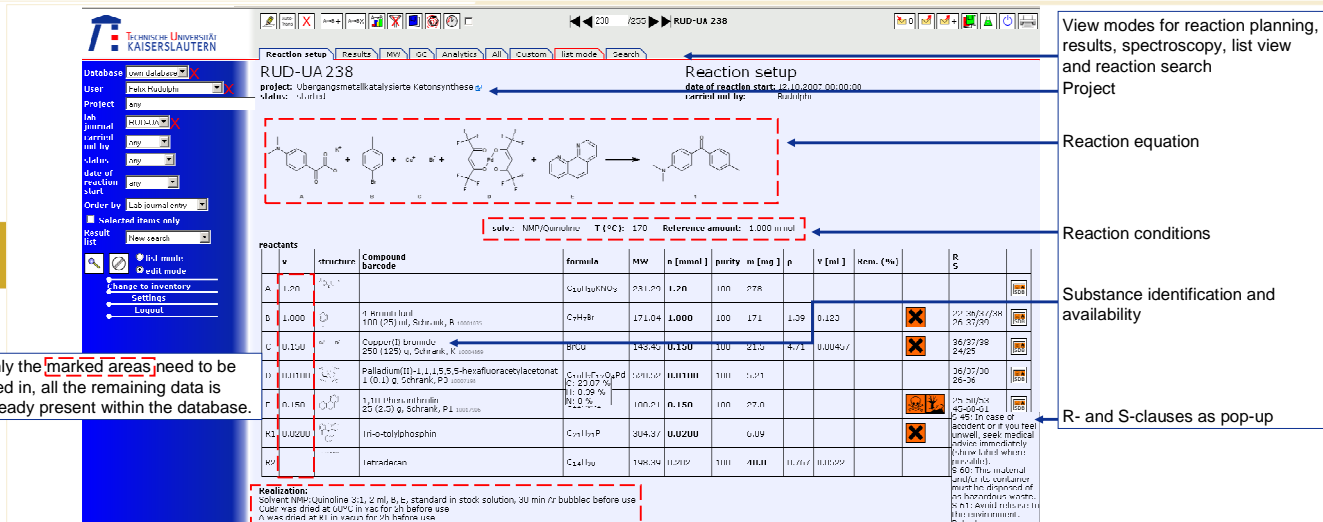


Lukas J. Gooßen*, F. Rudolphi

Institut für Organische Chemie, TU Kaiserslautern, Erwin-Schrödinger-Straße, 67663 Kaiserslautern, Tel +49 631 205 2067, goossen@chemie.uni-kl.de

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 inventory makes laboratory work safer, more efficient and resource economical.



Reaction setup
RUD-UA 238
project: Übergangsmetallkatalysierte Ketonsynthese
date of reaction start: 12.11.2007 09:00:00
current mol. eq.: Realtime

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

Reaction equation

Reaction conditions
solv.: NMF/Quinoline T (°C): 170 Reference amount: 1.000 mmol

Substance identification and availability

R- and S-clauses as pop-up

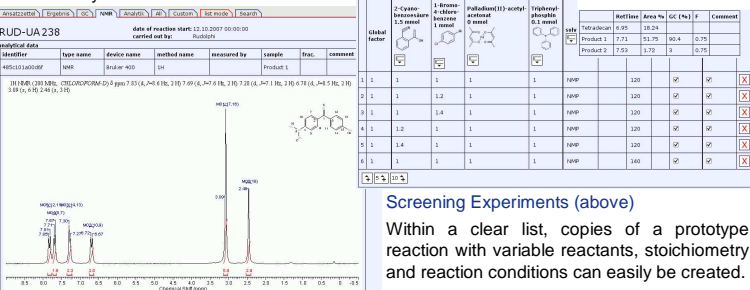
Only the marked areas need to be filled in, all the remaining data is already present within the database.

reactants	v	structure	Compound barcode	formula	MW	n [mmol]	purity	m [mg]	ρ	V [ml]	Rem. (%)	R	S
A	1.20			C ₁₀ H ₁₀ N ₂ O ₂	231.27	1.20	100	278					
D	1.000		9 899 816 100 (P5) (M) Schrank, R	C ₇ H ₈	174.04	1.000	100	174	1.39	0.123			
C	0.100		Copper(II) bromide 250 (E20) M. Schrank, R	BrCu	153.40	0.100	100	21.0	4.71	0.00447			
D	0.100		Palladium(II)-1,1,1,5,5,5-hexafluoroacetylacetonat 1 (O.1) M. Schrank, P3	C ₁₂ H ₆ F ₆ O ₄ Pd	509.10	0.100	100	10.1					
E	0.100		1,11-Herzshornite 20 (E.2) M. Schrank, P1	C ₁₂ H ₁₀ N ₂	198.21	0.100	100	27.1					
K1	0.0200		tri-n-butylphosphin	C ₁₂ H ₂₈ P	204.37	0.0200	100	4.09					
K2			tributylcarborane	C ₁₄ H ₁₆ B ₂	196.94	0.0200	100	41.1	11.61	0.1009			

Realization:
solvent: NMF/Quinoline 1:1, 2 ml, 3, 6, standard in stock solution, 30 min / 7 bubbles before use
cuber was dried at 60°C in vac. for 2h before use
A was dried at 60°C in vac. for 2h before use

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.



user: Rudolphi, Felix
target lab journal: RUD...

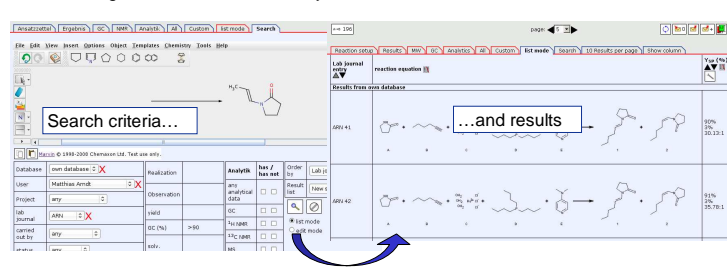
classical feature: 2-Cyano-2-bromoethyl 1,5-oxadiazole-3-carboxylate
4-oxo-2-oxo-1,5-dioxane-3-carboxylate
palladium(II)-acetate
triphenylphosphine oxide
triphenylphosphine oxide

titration: 9.75, 9.75, 9.75, 9.75, 9.75, 9.75
Product 1: 7.71, 51.75, 95.4, 0.75
Product 2: 1.53, 1.75, 9, 0.75

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.

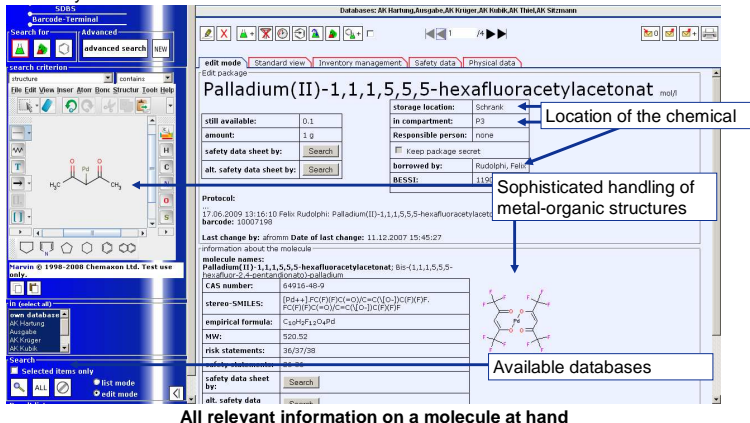


Search criteria...
...and results

Database: Matthias Anst...
User: Matthias Anst...
Project: ...
Lab journal: ...
Order by: ...

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.



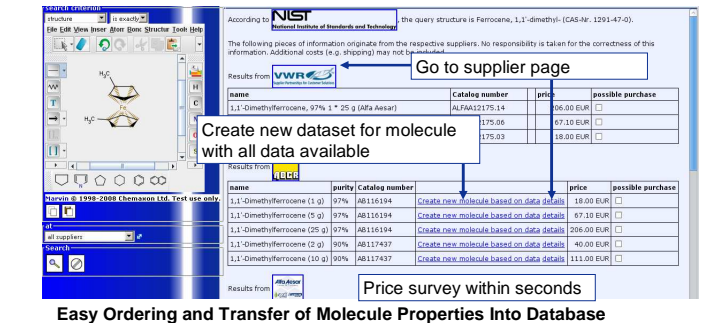
Database: AK Hartung, Amalgie, AK Prueger, AK Huber, AK Thiel, AK Strömmer

Palladium(II)-1,1,1,5,5,5-hexafluoroacetylacetonat
still available: 0.1
amount: 1 g
responsible person: none
safety data sheet by: [Search]
alt. safety data sheet by: [Search]

Protocol:
17.06.2009 13:16:10 Felix Rudolphi: Palladium(II)-1,1,1,5,5,5-hexafluoroacetylacetonat
barcode: 10007198
Last change by: afronm Date of last change: 11.12.2007 15:45:27
Information about the molecule
molecule names:
CAS number: 64916-48-9
stereo-SMILES: [P+](C)(F)(F)(F)(C)C(=O)C(F)(F)(F)F
PC(F)(F)(F)(F)(C)C(=O)C(F)(F)(F)F
empirical formula: C₁₀H₂F₆O₄Pd
MW: 520.52
risk statements: 36/37/38
safety statements: 00-00

Location of the chemical
Sophisticated handling of metal-organic structures
Available databases

All relevant information on a molecule at hand



Go to supplier page
Create new dataset for molecule with all data available
Price survey within seconds
Easy Ordering and Transfer of Molecule Properties Into Database

According to NIST
The following pieces of information originate from the respective suppliers. No responsibility is taken for the correctness of this information. Additional costs (e.g. shipping) may not be included.

name	catalog number	price	possible purchase
1,1-Dimethylferrocene, 97% (1.25 g) (Alfa Aesar)	ALFAA32175.14	265.00 EUR	<input type="checkbox"/>
		175.00	<input type="checkbox"/>
		175.00	<input type="checkbox"/>

name	quantity	Catalog number	price	possible purchase
1,1-Dimethylferrocene (1 g)	97%	AB116194	67.10 EUR	<input type="checkbox"/>
1,1-Dimethylferrocene (5 g)	97%	AB116194	266.00 EUR	<input type="checkbox"/>
1,1-Dimethylferrocene (25 g)	97%	AB116194	400.00 EUR	<input type="checkbox"/>
1,1-Dimethylferrocene (2 g)	90%	AB117437	111.00 EUR	<input type="checkbox"/>
1,1-Dimethylferrocene (10 g)	90%	AB117437	111.00 EUR	<input type="checkbox"/>

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 inventory 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-inventory.de>