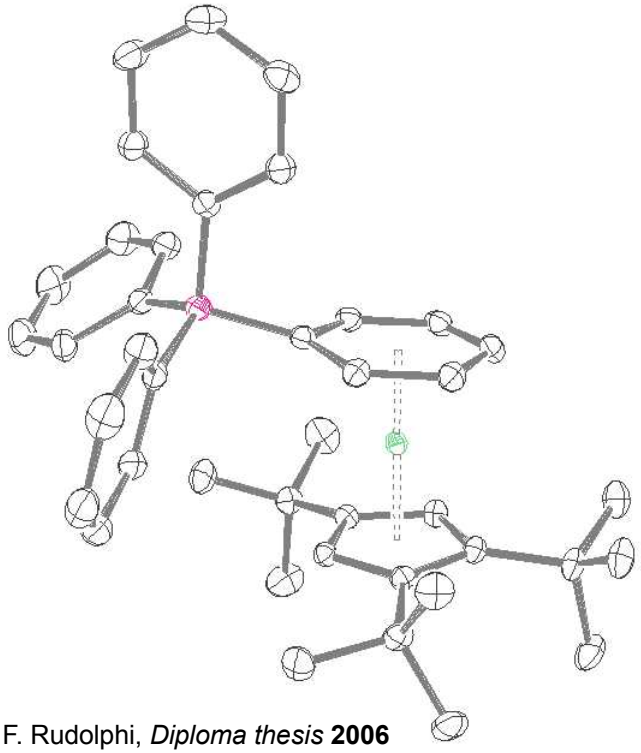
sciformation ELN

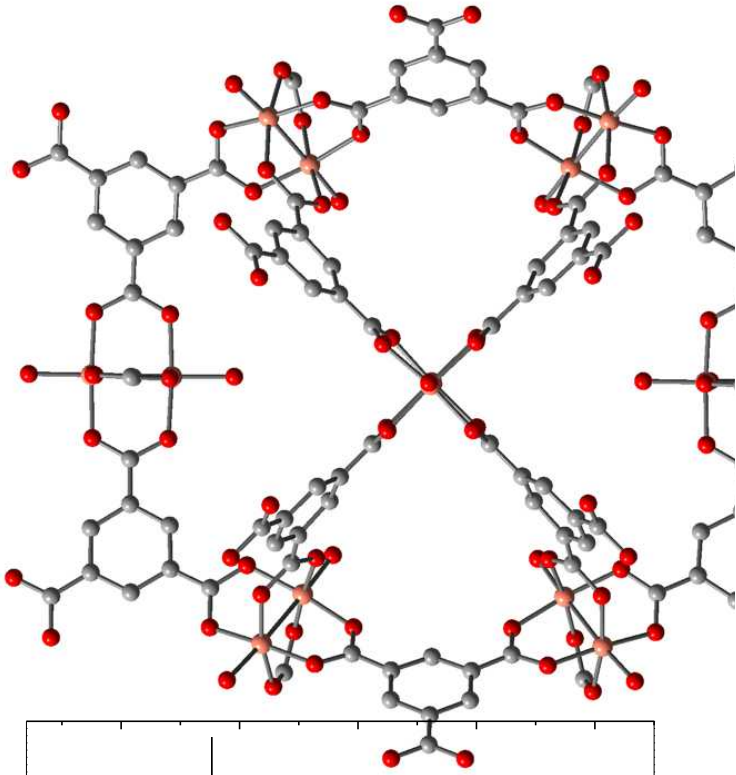
Electronic Laboratory Notebook

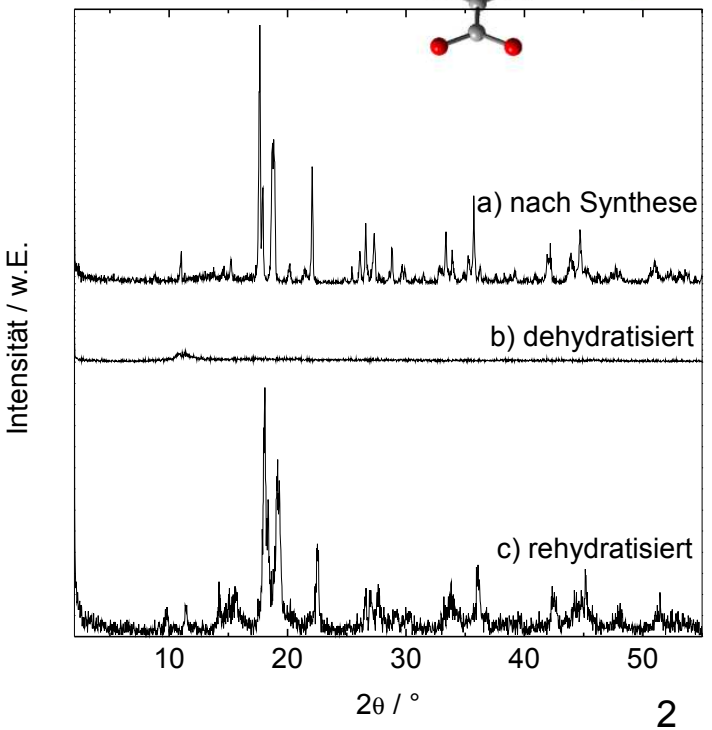
Dr. Felix Rudolphi
Sciformation Consulting GmbH

Chem. Research I



F. Rudolphi, *Diploma thesis* **2006**





A. Wagener, M. Schindler, F. Rudolphi, S. Ernst, *Chem. Ing. Tech.*, **2007**, *79(6)*, 851-855

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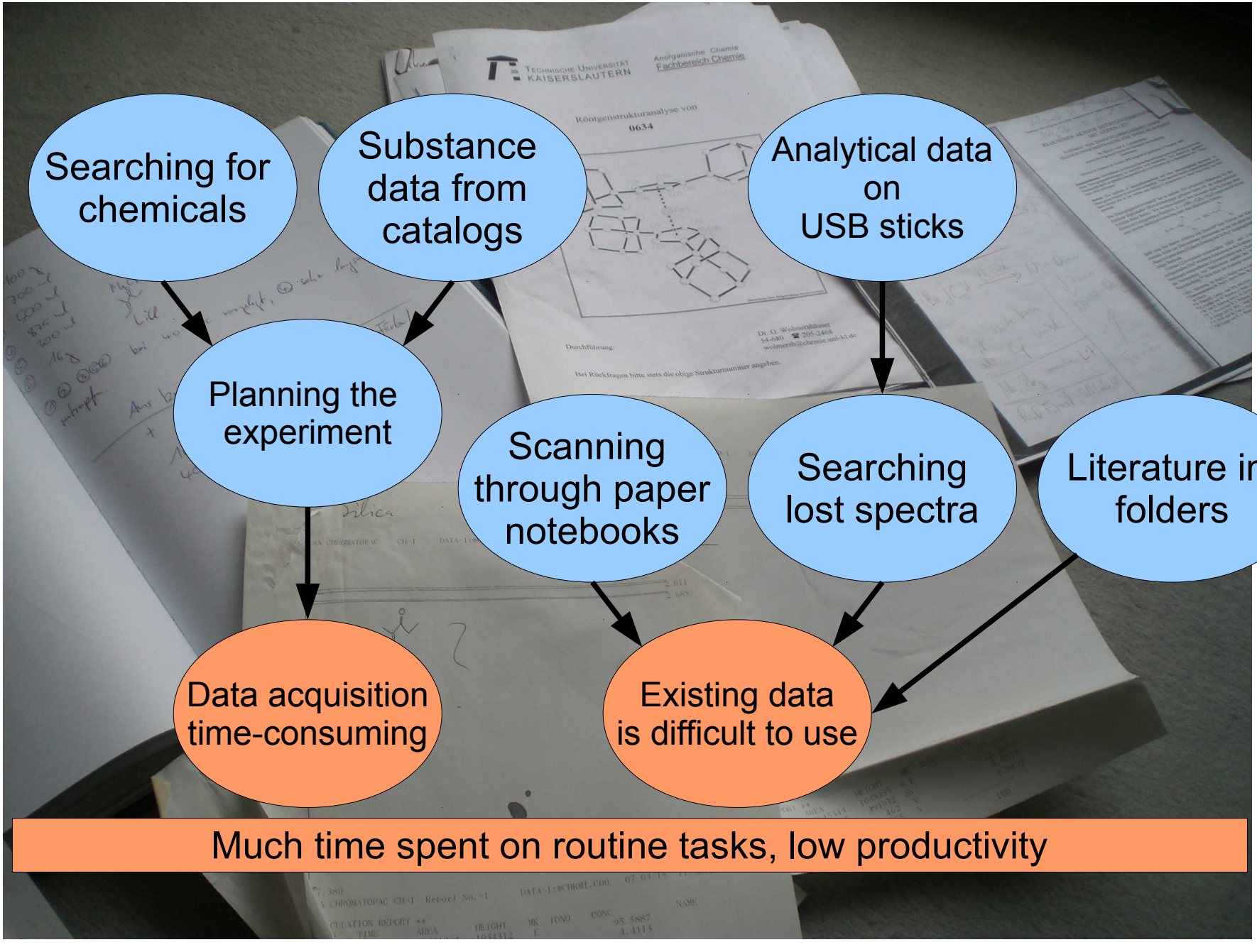
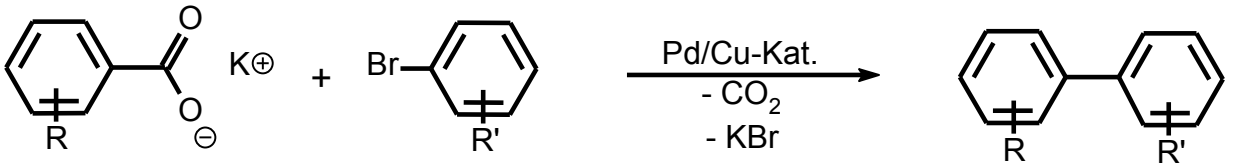
Traditional workflow

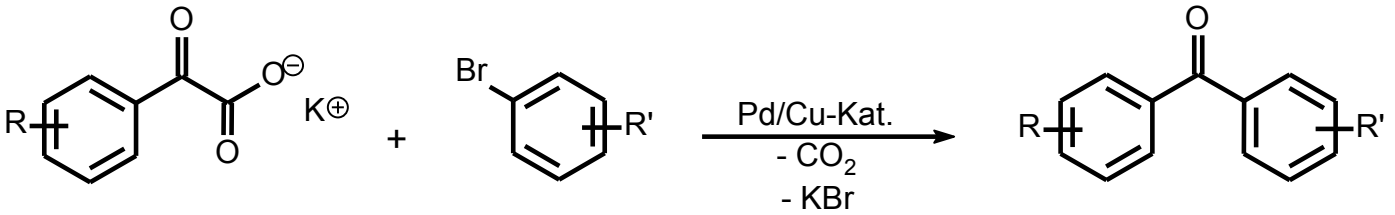


Chem. Research II

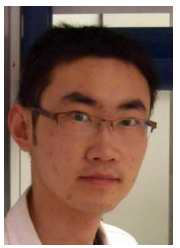
Decarboxylative cross-coupling (min 10 000 experiments)

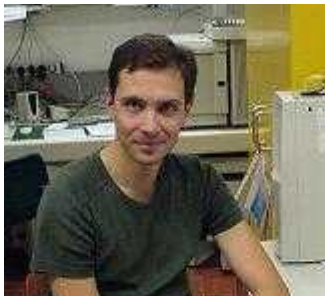


L. J. Gooßen, G. Deng, L. M. Levy, *Science* **2006**, *313*, 662-664;
L. J. Gooßen, N. Rodríguez, B. Melzer, C. Linder, G. Deng, L. M. Levy, *J. Am. Chem. Soc.* **2007**, *129*, 4824-4833;
L. J. Gooßen, N. Rodríguez, C. Linder, B. Zimmermann, T. Knauber, *Org. Synth.* **2008**, *85*, 196-204;
L. J. Gooßen, B. Zimmermann, T. Knauber, *Angew. Chem. Int. Ed.* **2008**, *47*, 7103-7106



L. J. Gooßen, F. Rudolphi, C. Oppel, N. Rodríguez, *Angew. Chem. Int. Ed.* **2008**, *47*, 3043-3045





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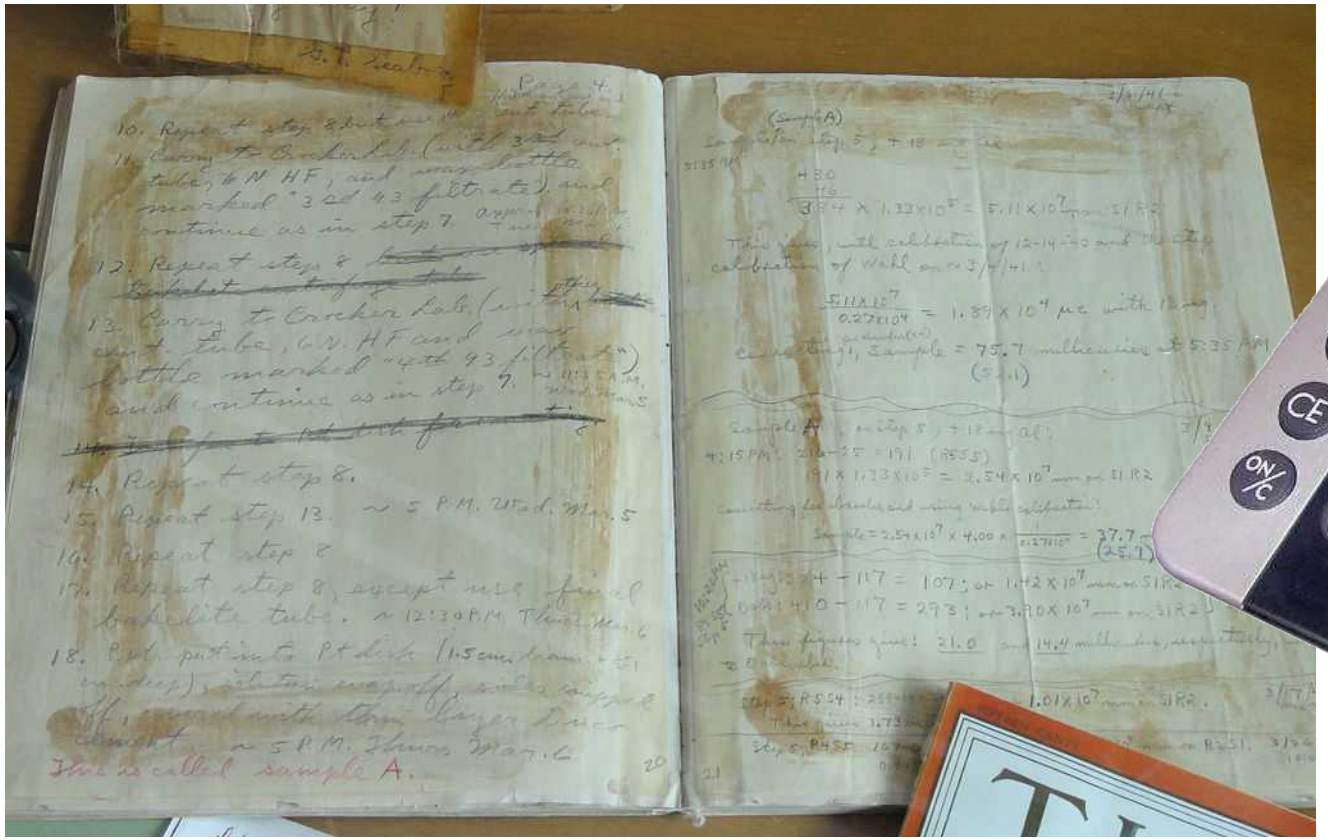
How can I plan and analyze 10 000 experiments?



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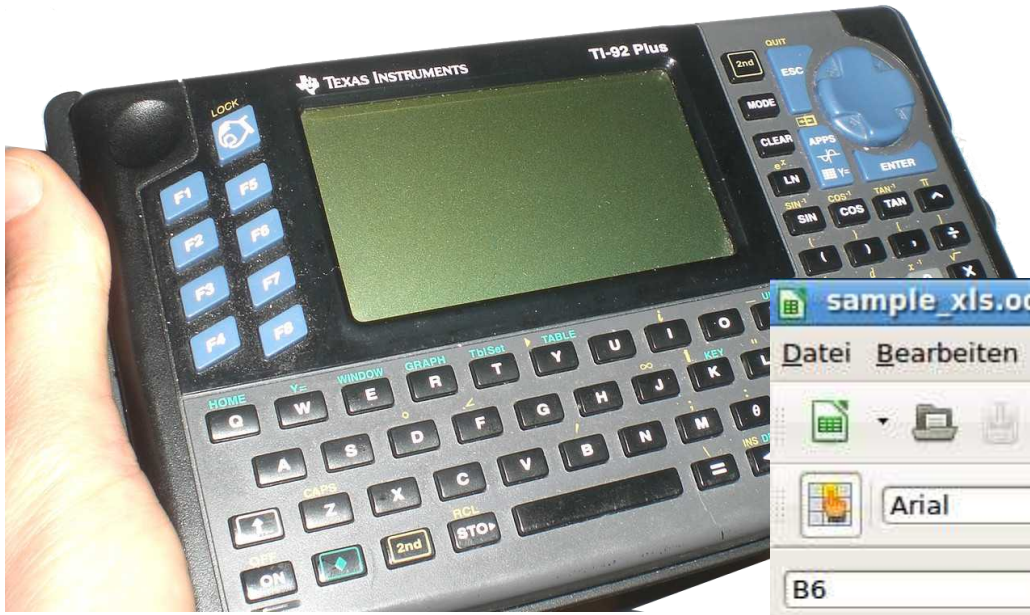

sample_xls.ods - LibreOffice Calc

Datei Bearbeiten Ansicht Einfügen Format Extras Daten Fenster Hilfe

Arial 10

B6

	A	B	C	D	E	F	G
1							
2	Component	Formula	MW	mmol	mg	g/ml	ml
3	A	C10H16	136	1	136		
4	B	C6H5Br	157	1,2	188,4	0,87	0,216551724
5	C	EtCl	74,5	2	149		
6	D						
7							
8							

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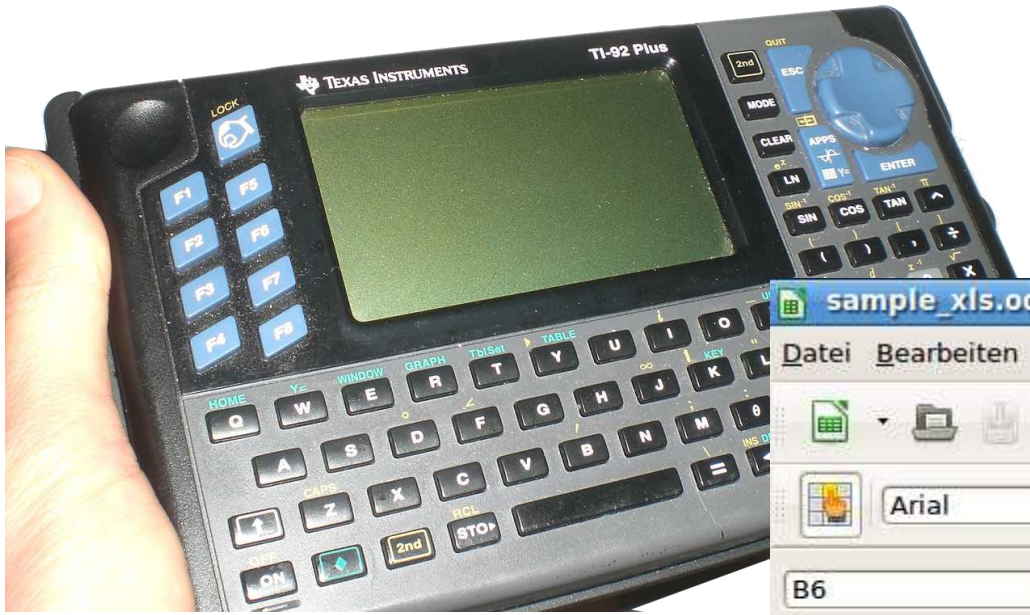

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7							
8							

No!

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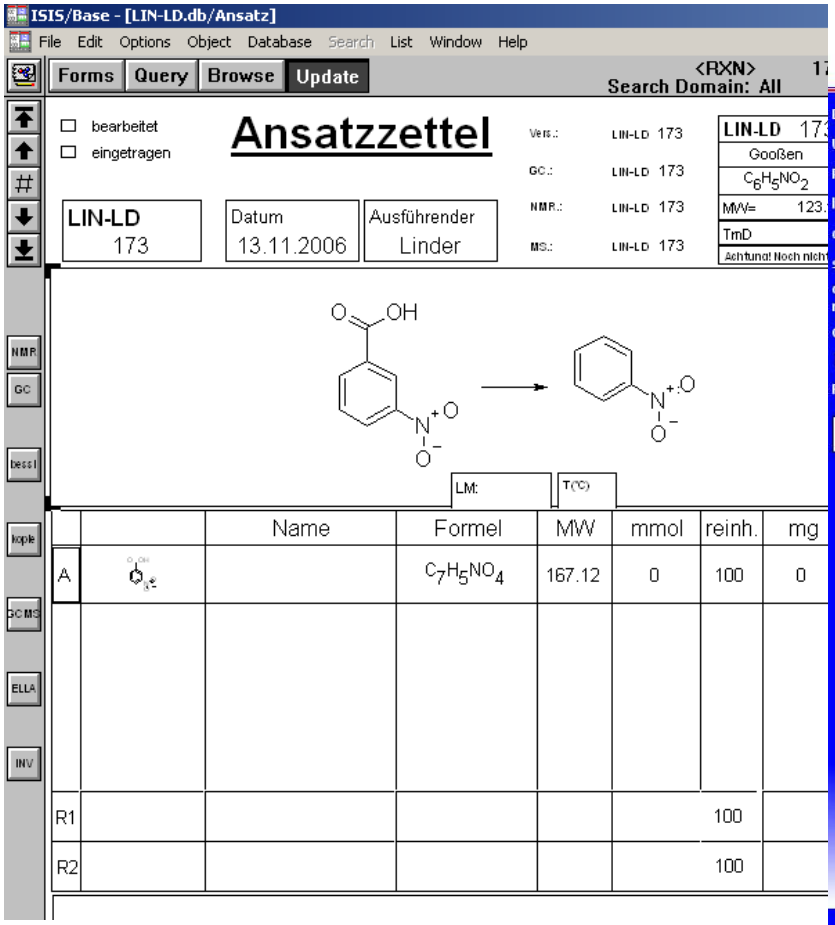
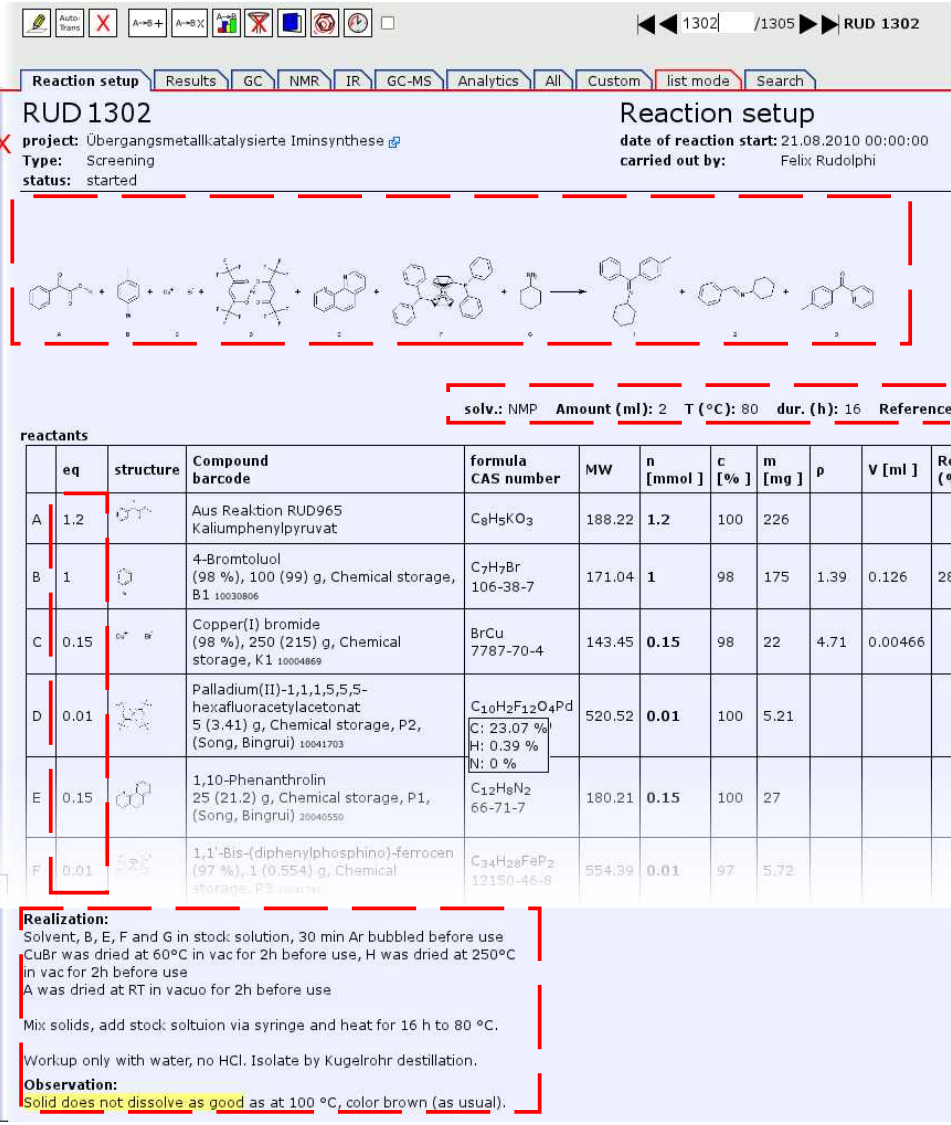
How can I plan and analyze 10 000 experiments?





Maybe...

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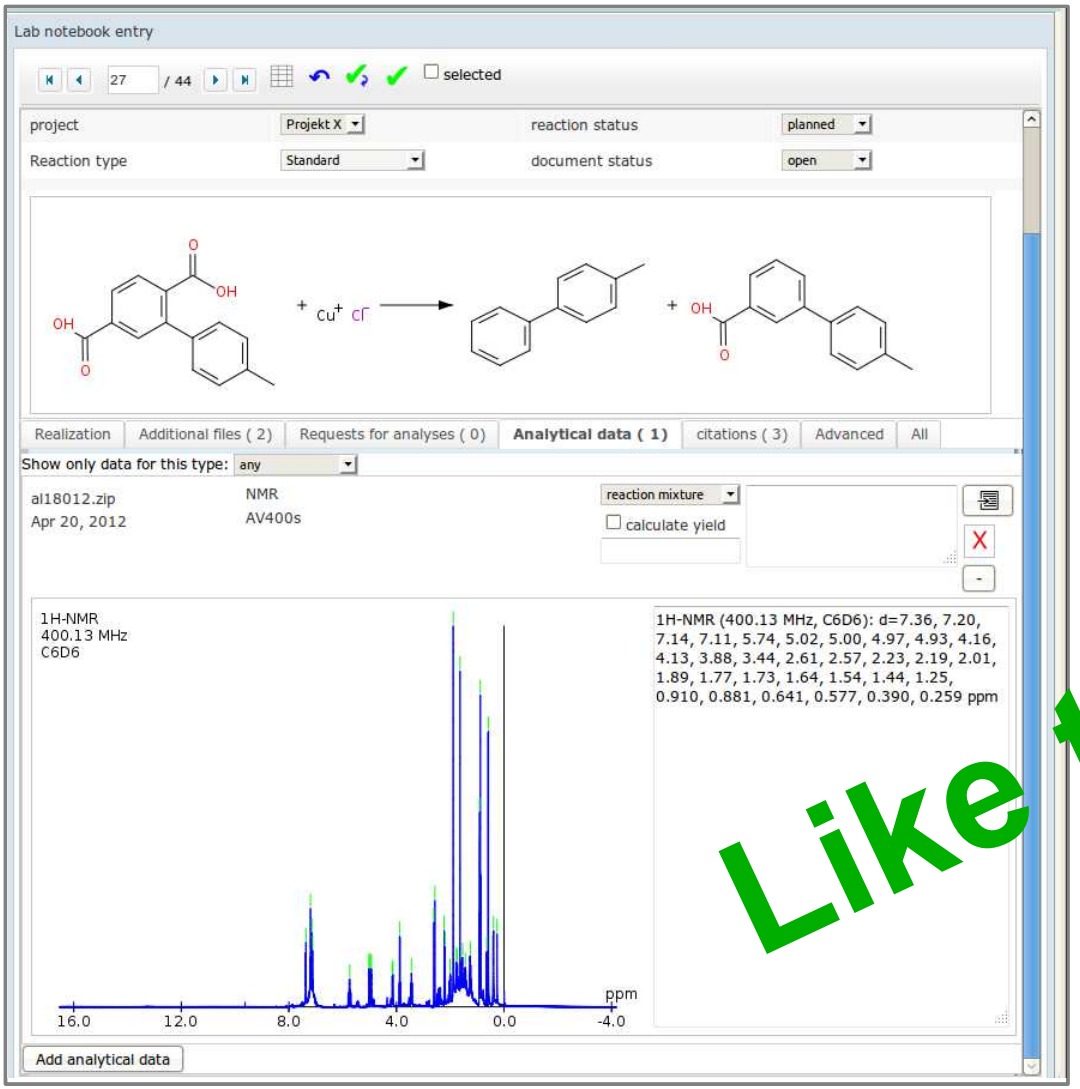
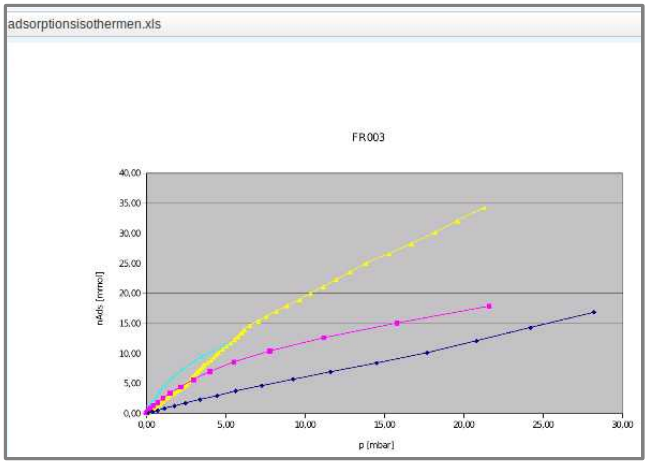
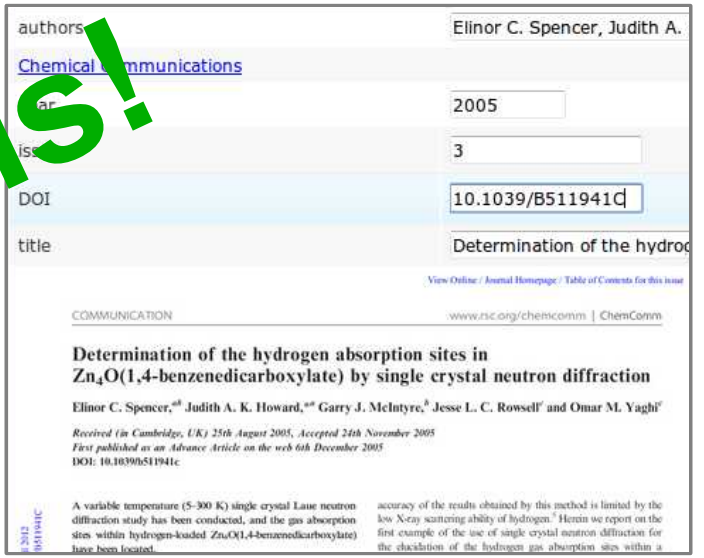
How can I plan and analyze 10 000 experiments?





Like this!



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How can I plan and analyze 10 000 experiments?

#	Glob	Bromobenzene 200.0 mmol >>	Magnesium 200.0 mmol >>	Iodine 20.0 mg >>	Neues Edukt <<	Struktur ändern	Komponente suc	Neues Reagenz >>	Titel	Durc	T (°C)	Menge (ml)	Dauer (h)	LöMi	Phenylmagnesiu >>	Neues Produkt >>	
1	1.0	1.0	1.0	1.0			Name, CAS-No		Referenz	☑	30 => 70	200	2	THF	1.0		X
2	1.0	1.0	1.0	1.0			Name, CAS-No		Et2O stat	☑	30 => 70	200	2	Et2O	1.0		X
3	1.0	1.0	1.0	1.0			Name, CAS-No		wärmer	☑	50 => 70	200	2	THF	1.0		X
4	1.0	1.0	1.0	1.0			Name, CAS-No N,N,N',N&ap 250.0 ml - Verbra...		mit TMDE	☑	30 => 70	200	2	THF	1.0		X

Eintrag hinzufügen | 5 Einträge hinzufügen | 10 Einträge hinzufügen

TMEDA

TMEDA
TMEDA
TMEDA
TMEDA
Cu-TMEDA-Katalysator
(TMEDA)PdMe2
Cu-TMEDA catalyst

Laborjournaleintrag

27 / 58 Ausgewählt Schnellsuche Reaktion kopieren Auto-Trans DOI

Ansatzgröße

Retrosynthesebaum für LAU-LC-0024 - LAU-LC-0027-A

Retrosynthesebaum	Struktur	Titel	isol. %	Kategorie
LAU-LC-0024 - LAU-LC-0027-A			78.0%	ELN Reaktionskomp
2-Bromoterephthalic acid - 586-35-6 - LAU-LC-0024-A				ELN Reaktionskomp
2-Bromoterephthalic acid - C8H5BrO4 - 586-35-6				Molekül
Keine Suchergebnisse				
4-Tolylboronic acid - 5720-05-8 - LAU-LC-0024-B				ELN Reaktionskomp
Palladium(II) acetylacetonate - 14024-61-4 - LAU-LC-0024-C				ELN Reaktionskomp
Triphenylphosphine - 603-35-0 - LAU-LC-0024-D				ELN Reaktionskomp
andere Reaktionen, die zu dieser Struktur führen				

Edukte

#	eq	Stru
A	1.0	
B	0.0	Cu+

Durchführung

Retrosyn

About Sciformation ELN

- Electronic Laboratory Notebook (ELN)
  - for chemistry
  - for other research disciplines
- Laboratory Information Management System (LIMS)
- Chemical inventory
- Literature database

- fully web-based
- not bound to any platform or OS version

Info for scientists

Info for managers

Info for IT department

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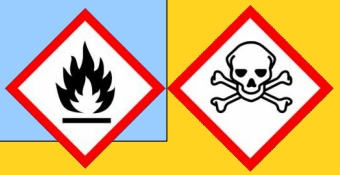
Benefits

1. Helps to generate and analyze big data
2. Routine tasks get automated
3. Better team coordination
4. Higher work safety, avoids errors and mistakes



5. Avoids redundant work
6. Higher quality of documentation (complete, readable)
7. Research data becomes valuable resource for future employees

8. Full control over your data
9. Easy deployment

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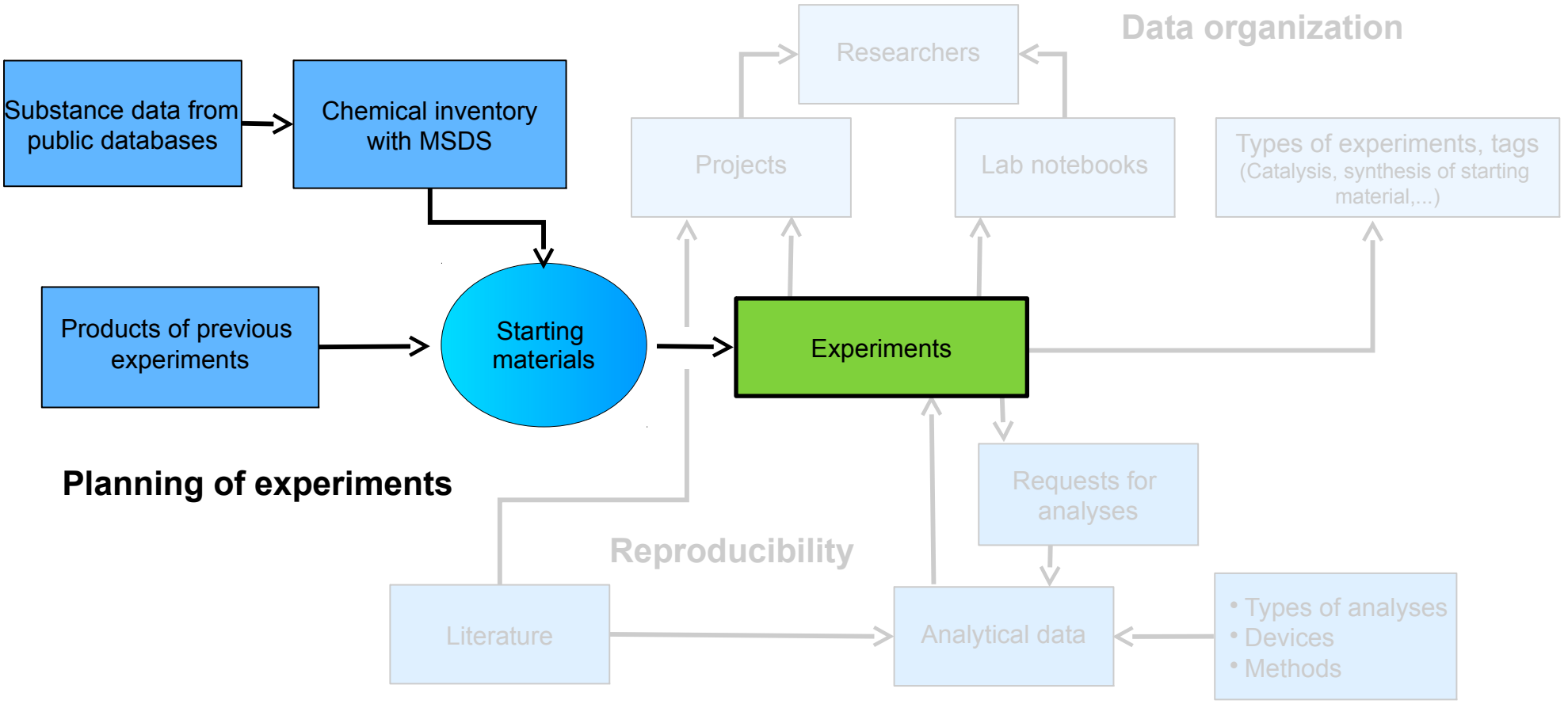
Sciformation ELN integrates all aspects of research



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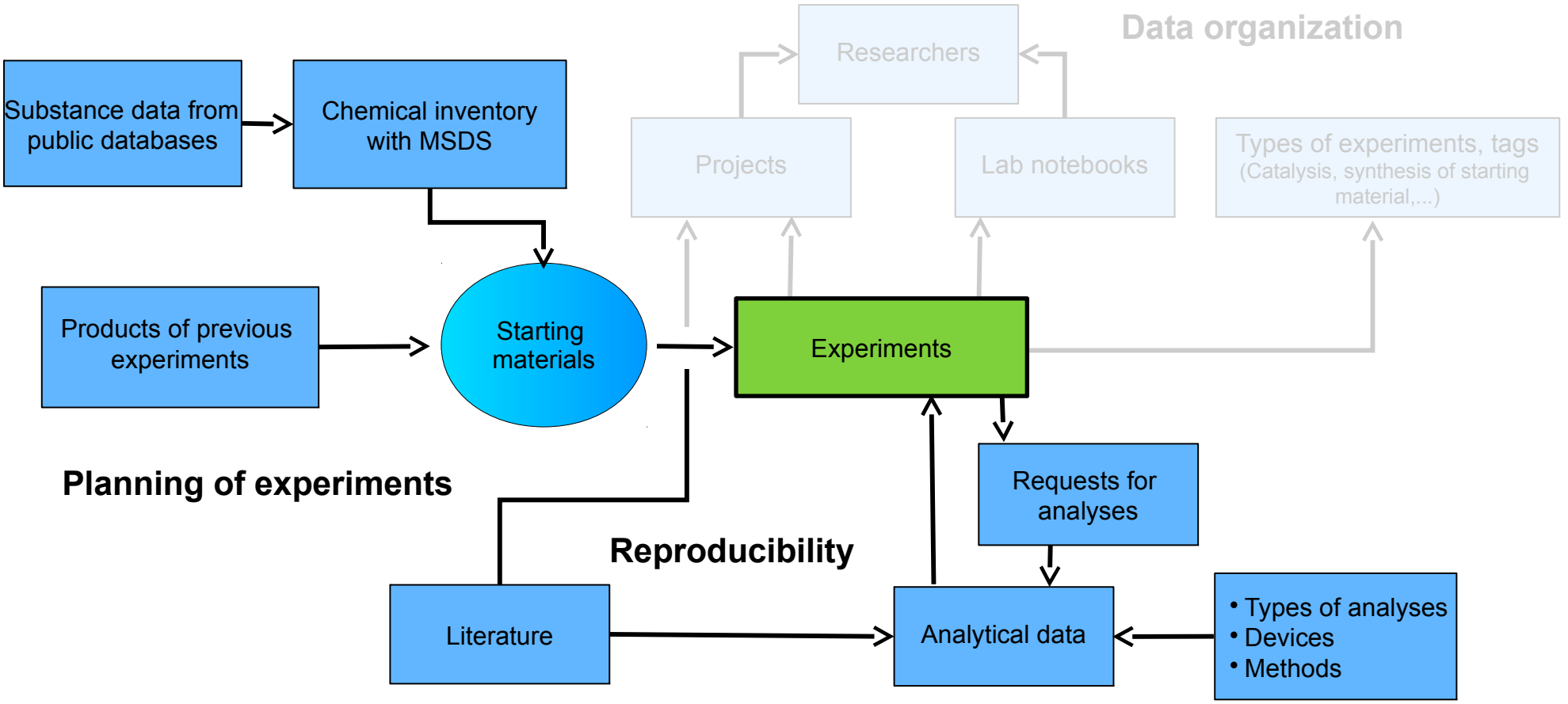
Sciformation ELN integrates all aspects of research



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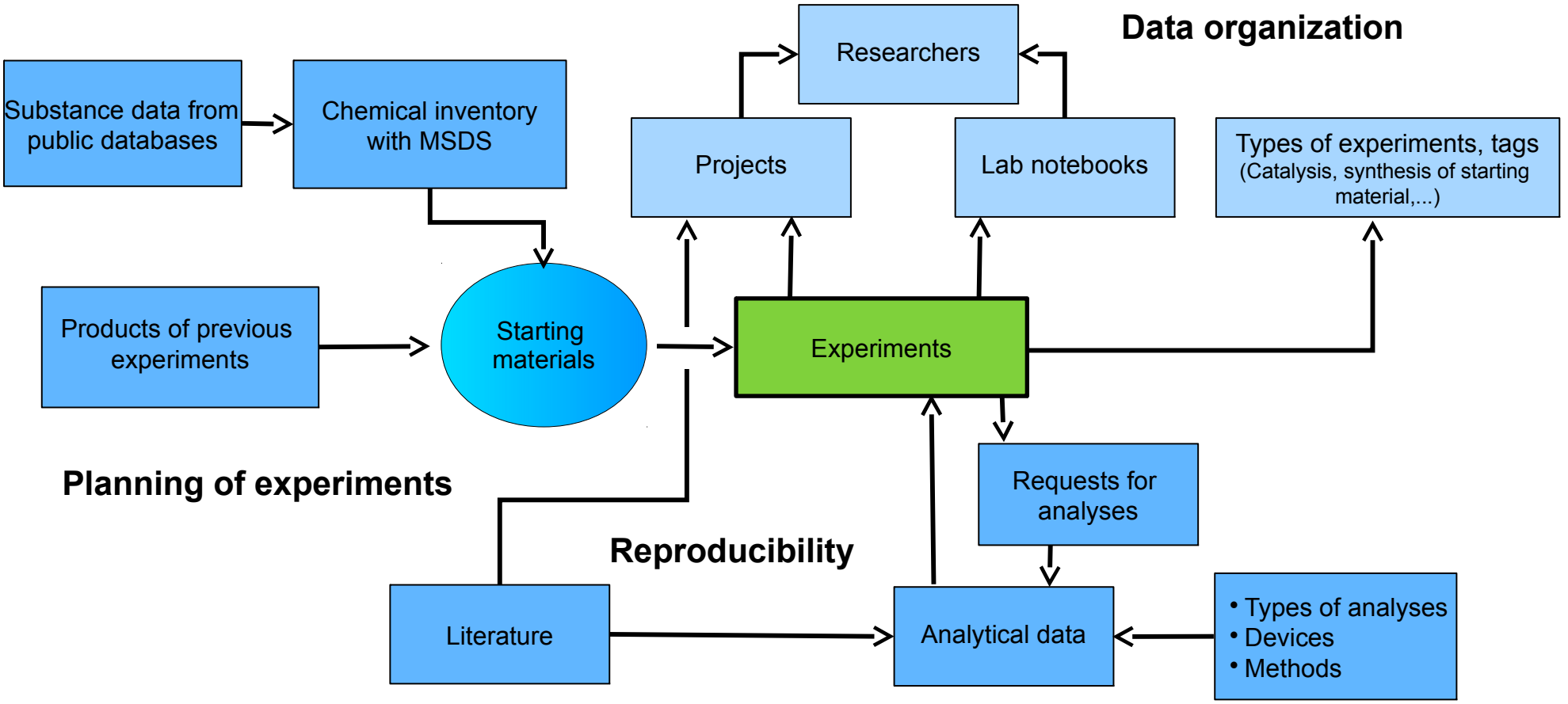
Sciformation ELN integrates all aspects of research



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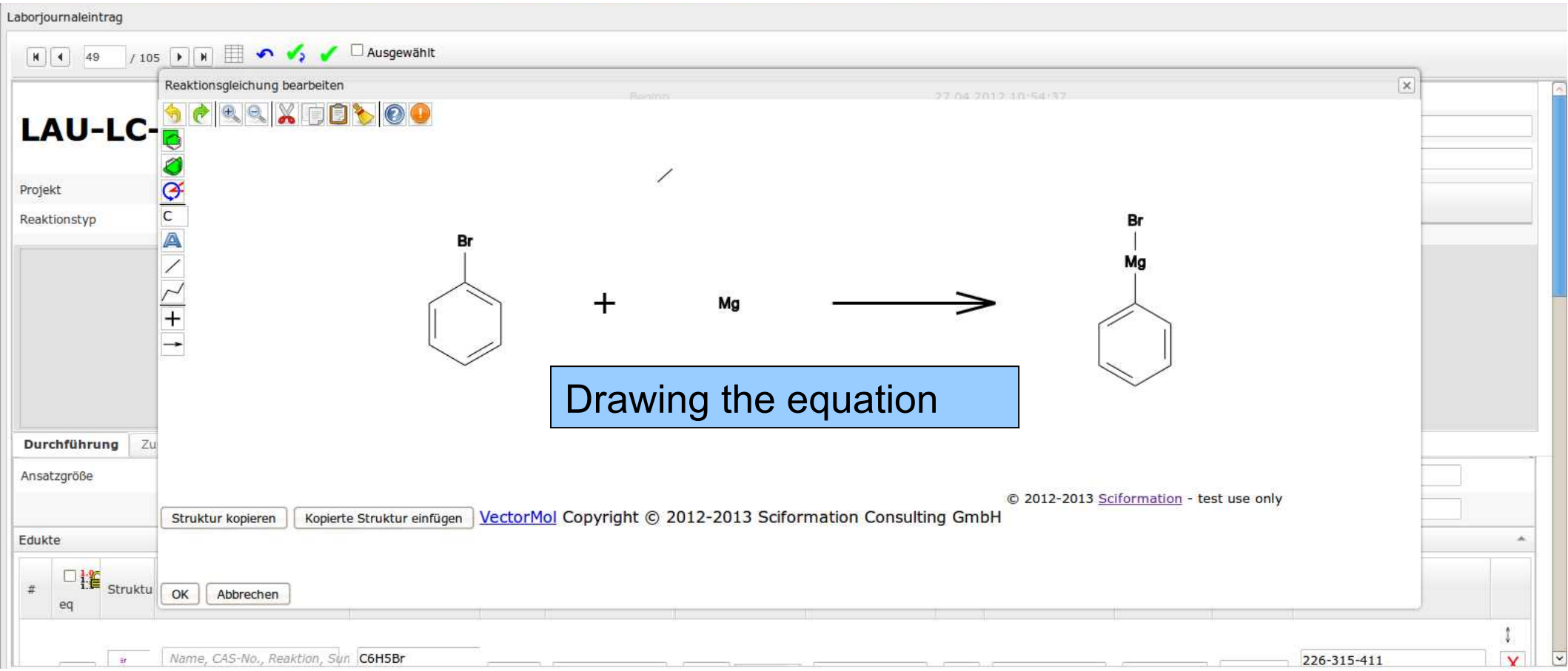
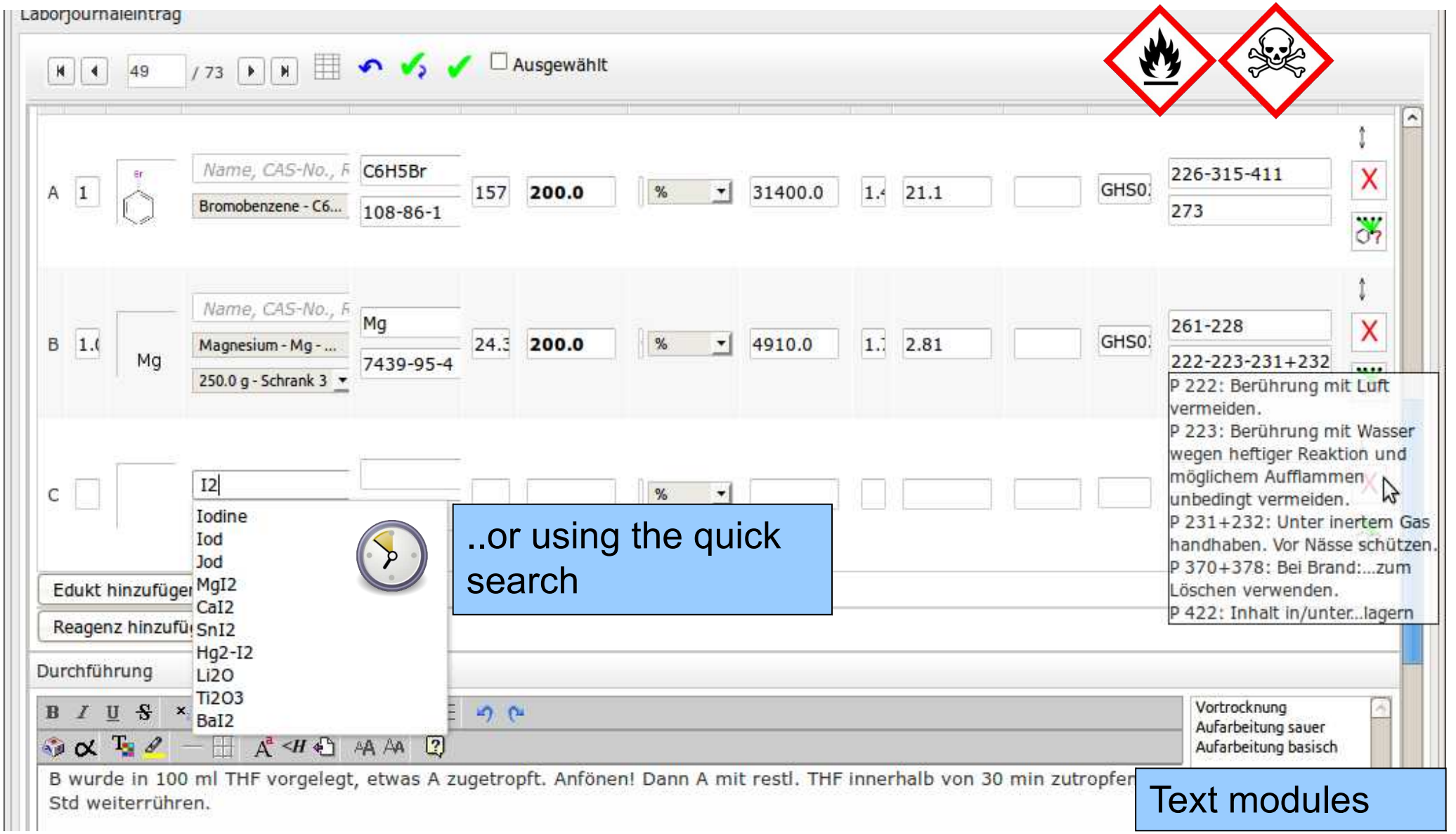
Planning experiments

Planning a chemical reaction



Planning a chemical reaction



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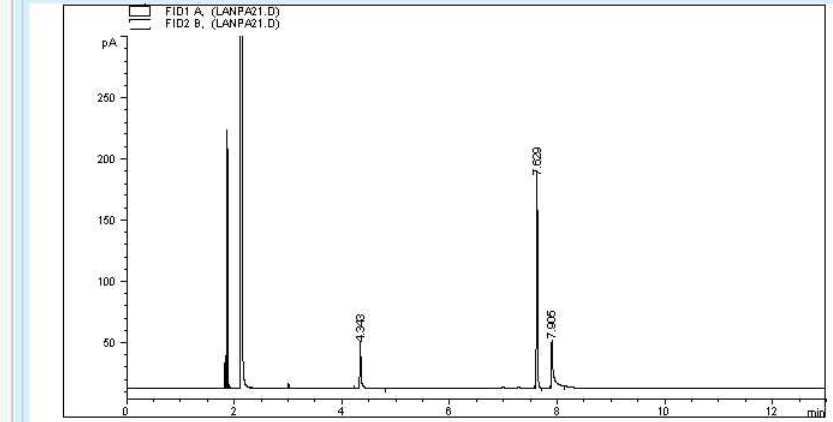
Calculating the yield

#	eq	structur	molecule names / package	sum formula / CAS No.	MW	n th [mmol]	%	m [mg]	Ysp	Yisol	comment	hazard codes	R S H P
1	1.0		4-Phenyltoluene	C13H12 644-08-6	168.24	10.0		694+76		45.8 (4.577 mmol)			24/25

Isolated



RUD-UA28.zip GC Agilent 6890 Reaktionsmischung Ausbeuteberechnung Frak. Kommentar

```
Data File D:\DATA\LANPA21.D
Instrument 1 04.04.2007 14:08:53

Injection Date : 04.04.2007 13:55:51        Seq. Line :  2
Sample Name    :                        Location : Vial 39
Acq. Operator  :                           Inj :  1
                                       Inj Volume : 1
Sequence File  : C:\HPCHEM\1\SEQUENCE\21-03-07.S
Method         : D:\METHODS\LUKASN.M
Last changed   : 27.10.2006 11:04:31

                Area Percent Report

Sorted By      :  Signal
Multiplier     :  1.0000
Dilution       :  1.0000

Signal 1: FID1 A,

Peak RetTime Type  Width    Area      Height    Area
 #  [min]       [min] [pA*s]   [pA]        %
---|-------|----|-------|---------|---------|-------|
  1  4.343 VV   0.0283  67.59409  35.31559 16.57707
  2  7.629 VV   0.0209 219.20975 171.18823 53.75994
```

Reaktionskomponente	RetTime	Area %	Y_{SP} (%)	F	Kommentar
Standard: C14H30	7,629	53,75994		1	
C6H12	4,343	16,57707	14,65	1	
C6H14	7,905	29,66299	25,6	1	
Salt - 7647-14-5					

Analytically determined (GC, etc.)

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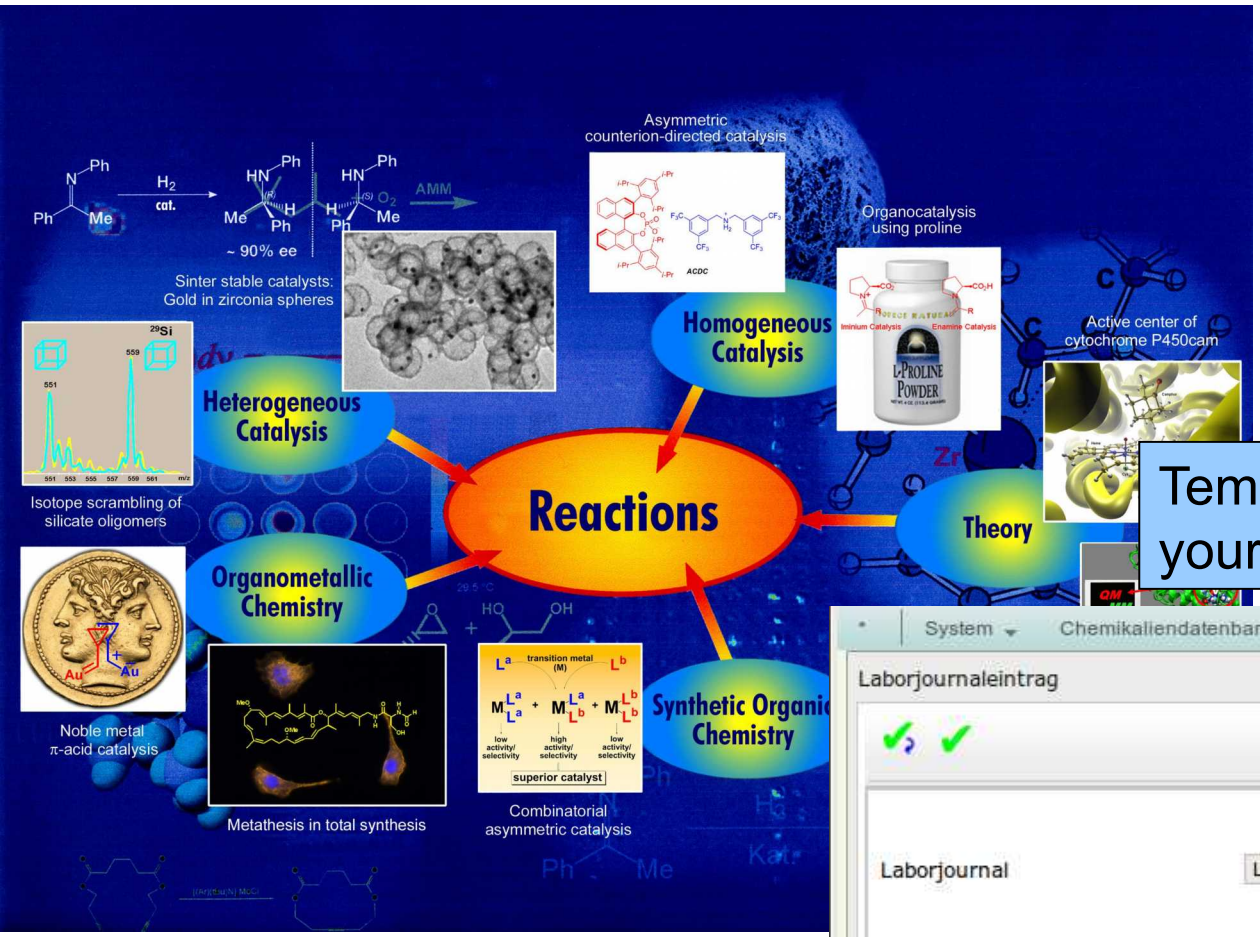
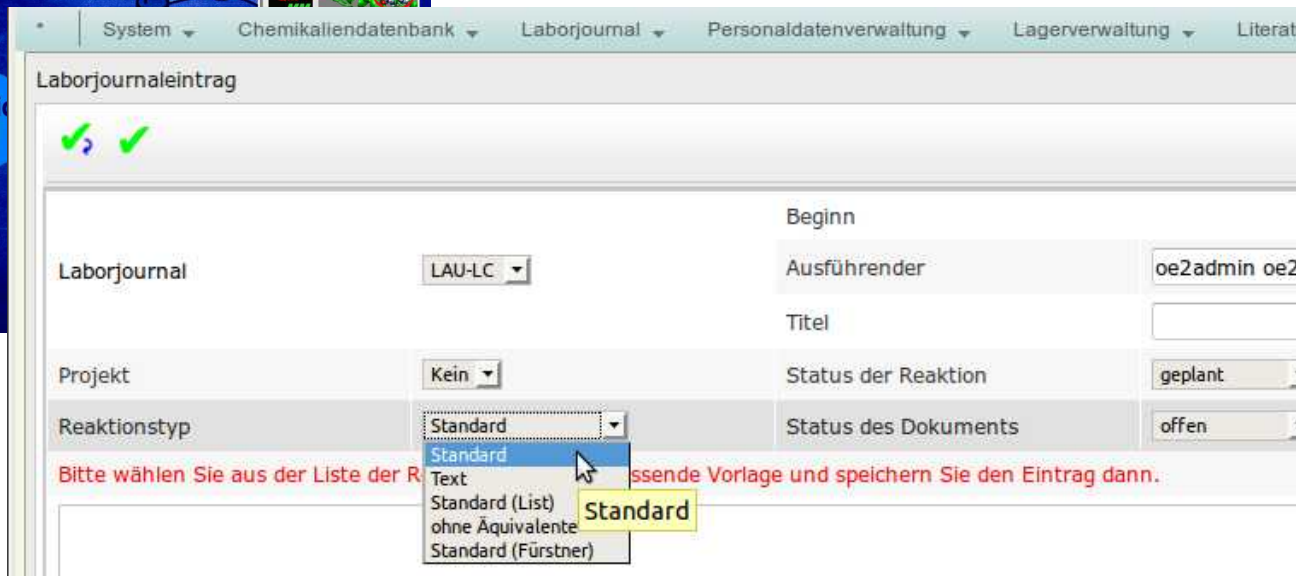
Research and experiments are heterogeneous



Templates adapted to your requirements



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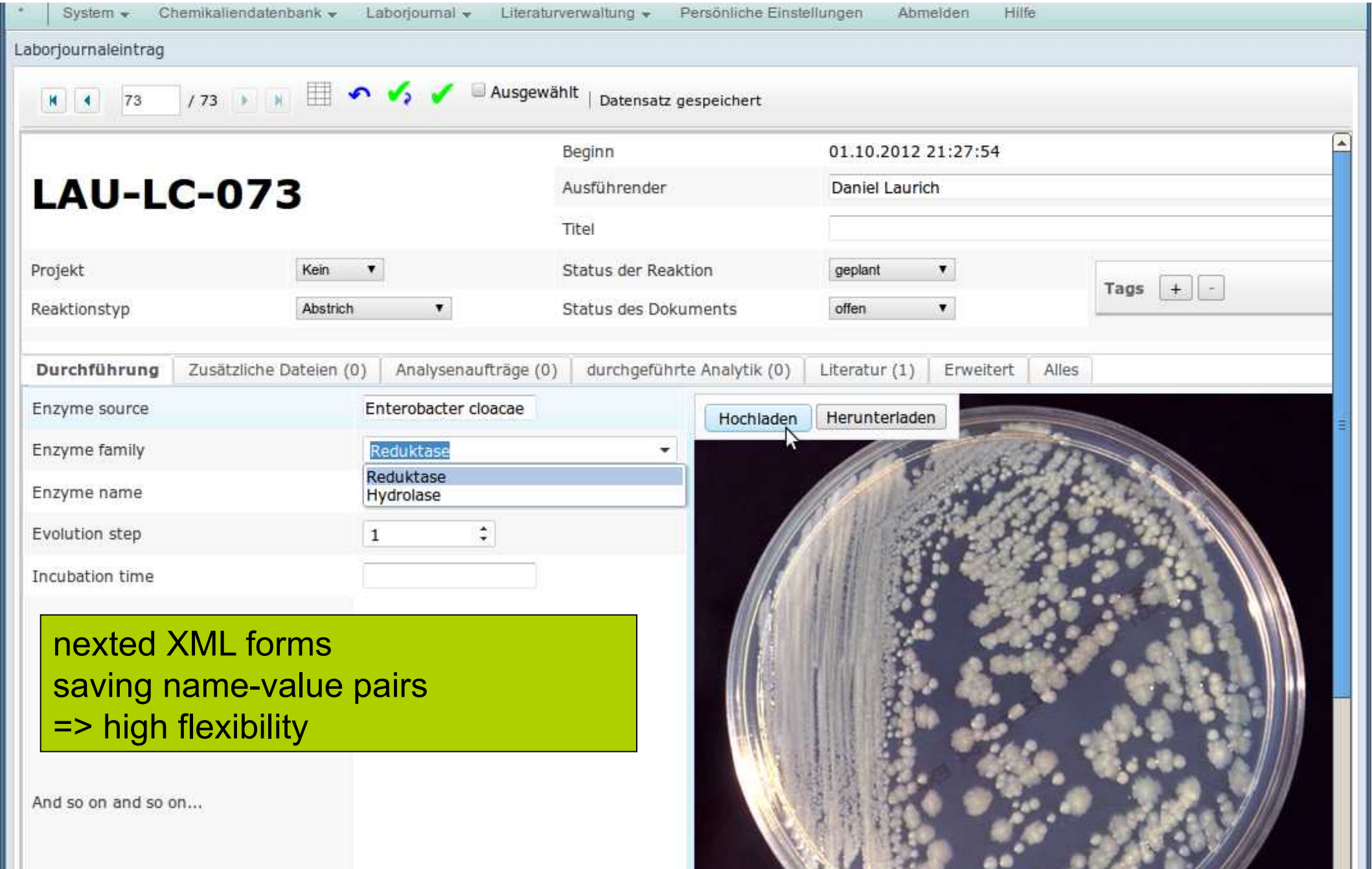
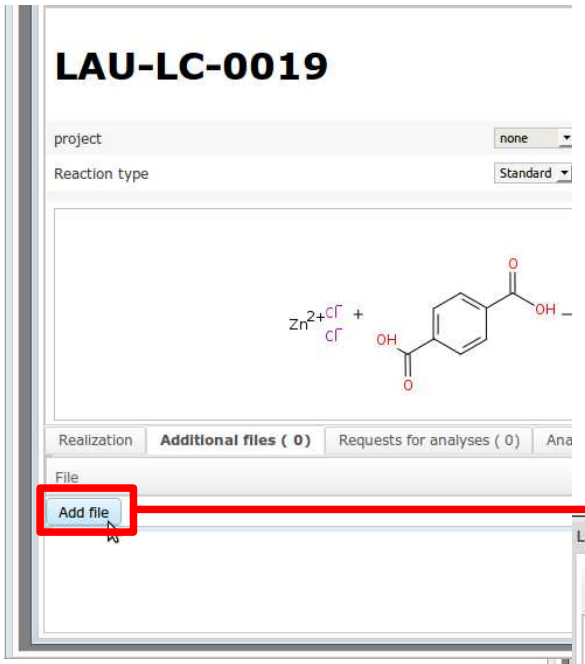
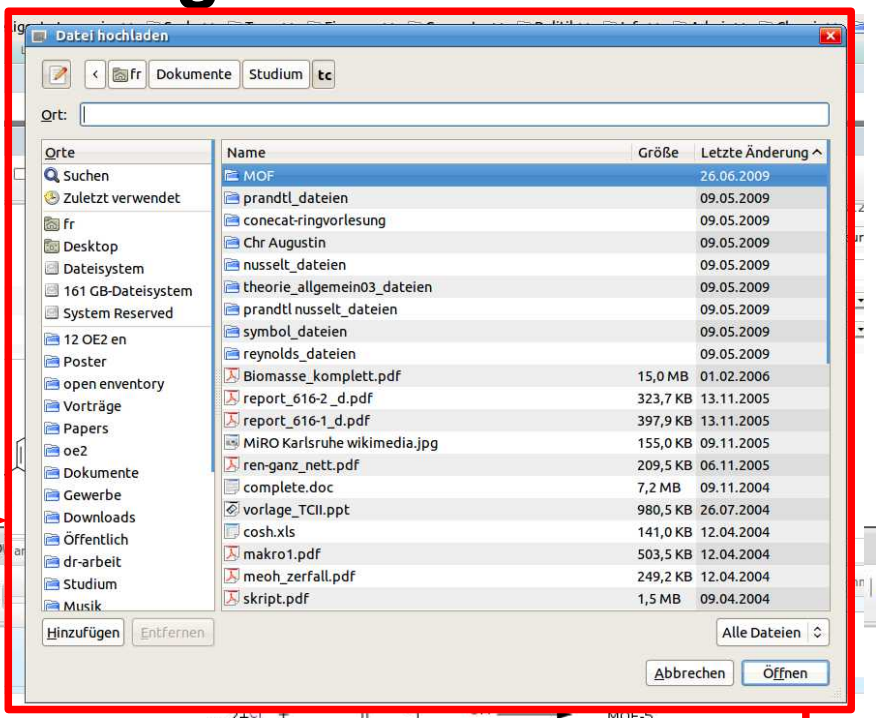
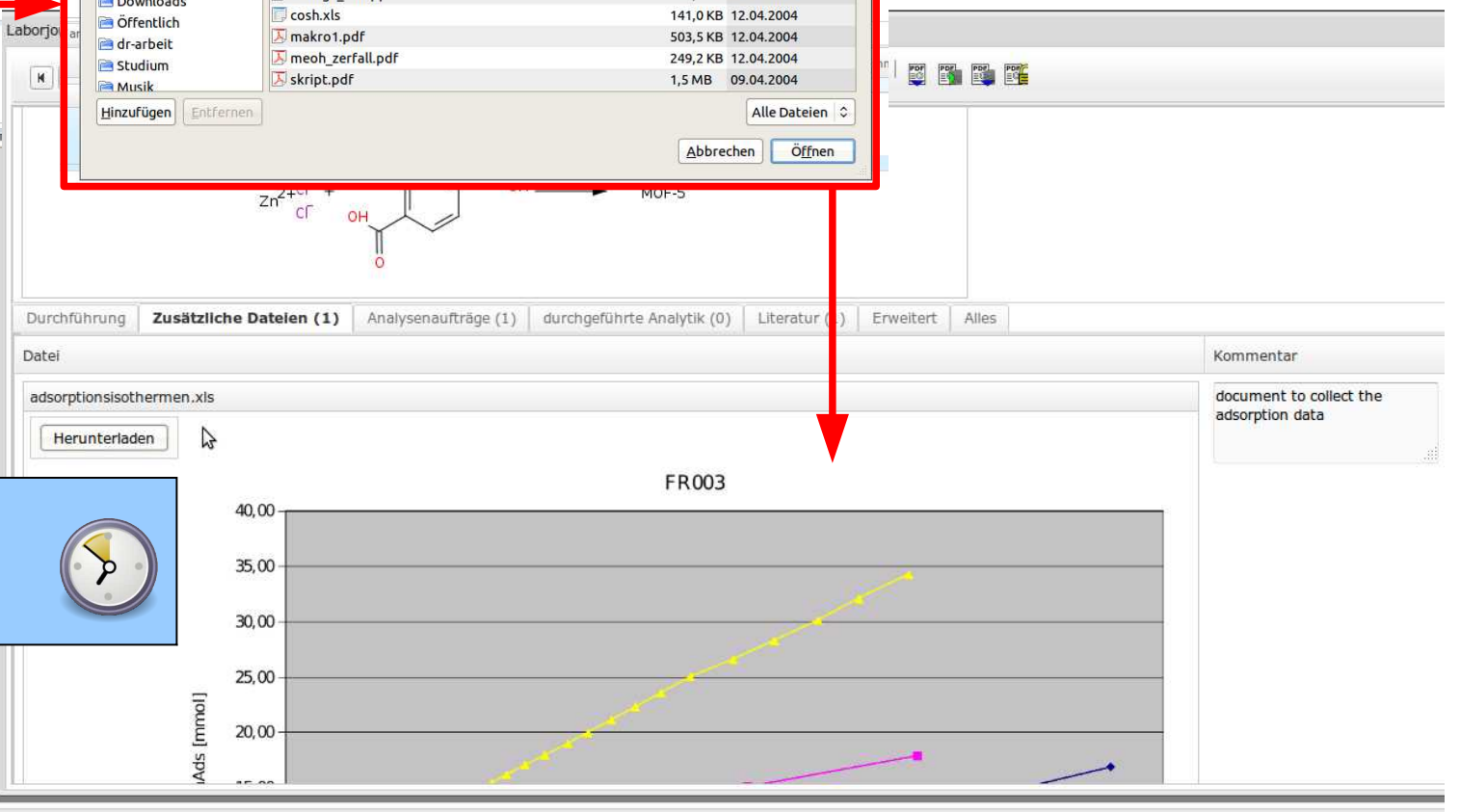
Biological or medical research



Attaching files to ELN entries

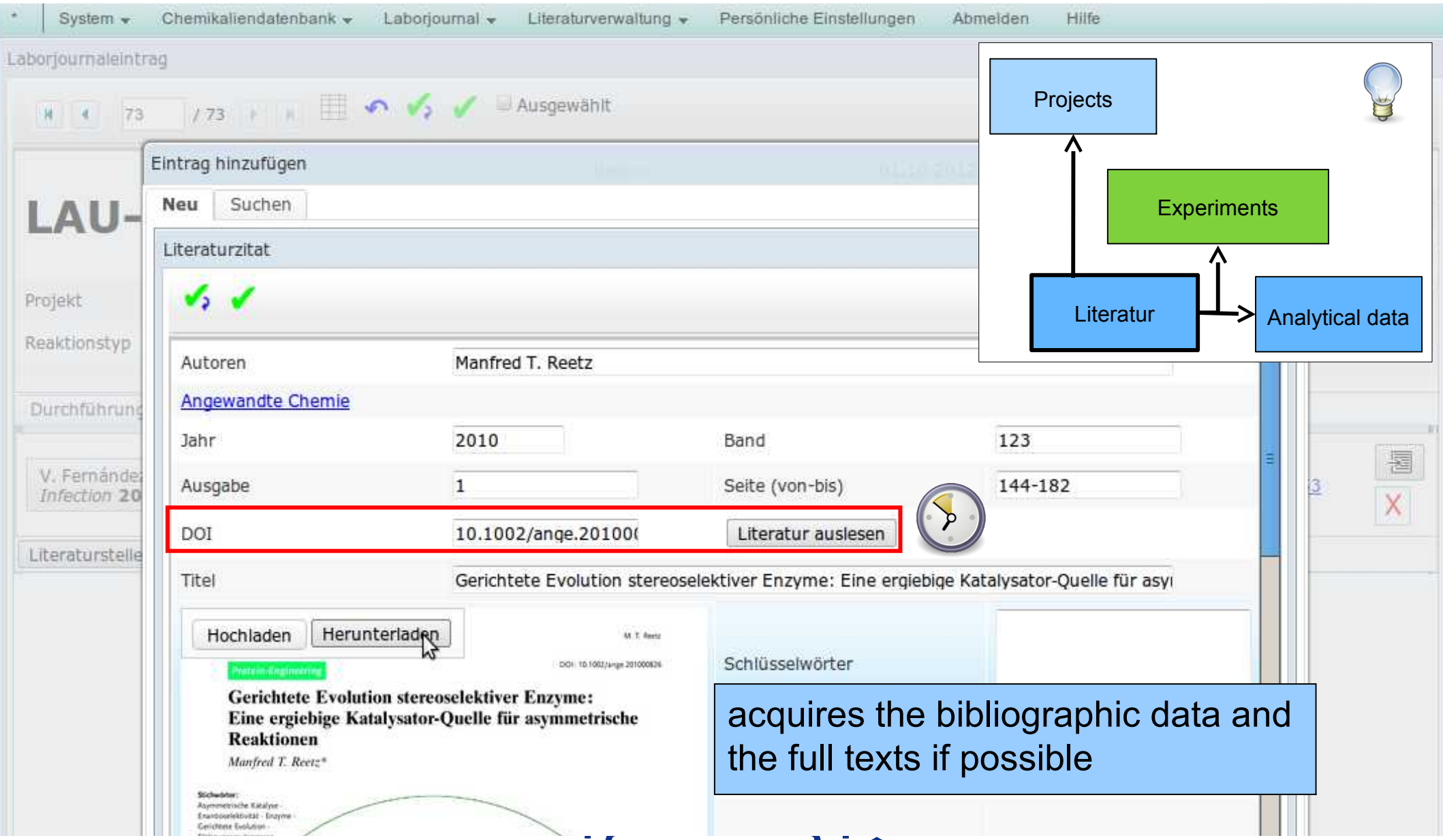






also via „drag & drop“

Adding literature



acquires the bibliographic data and the full texts if possible

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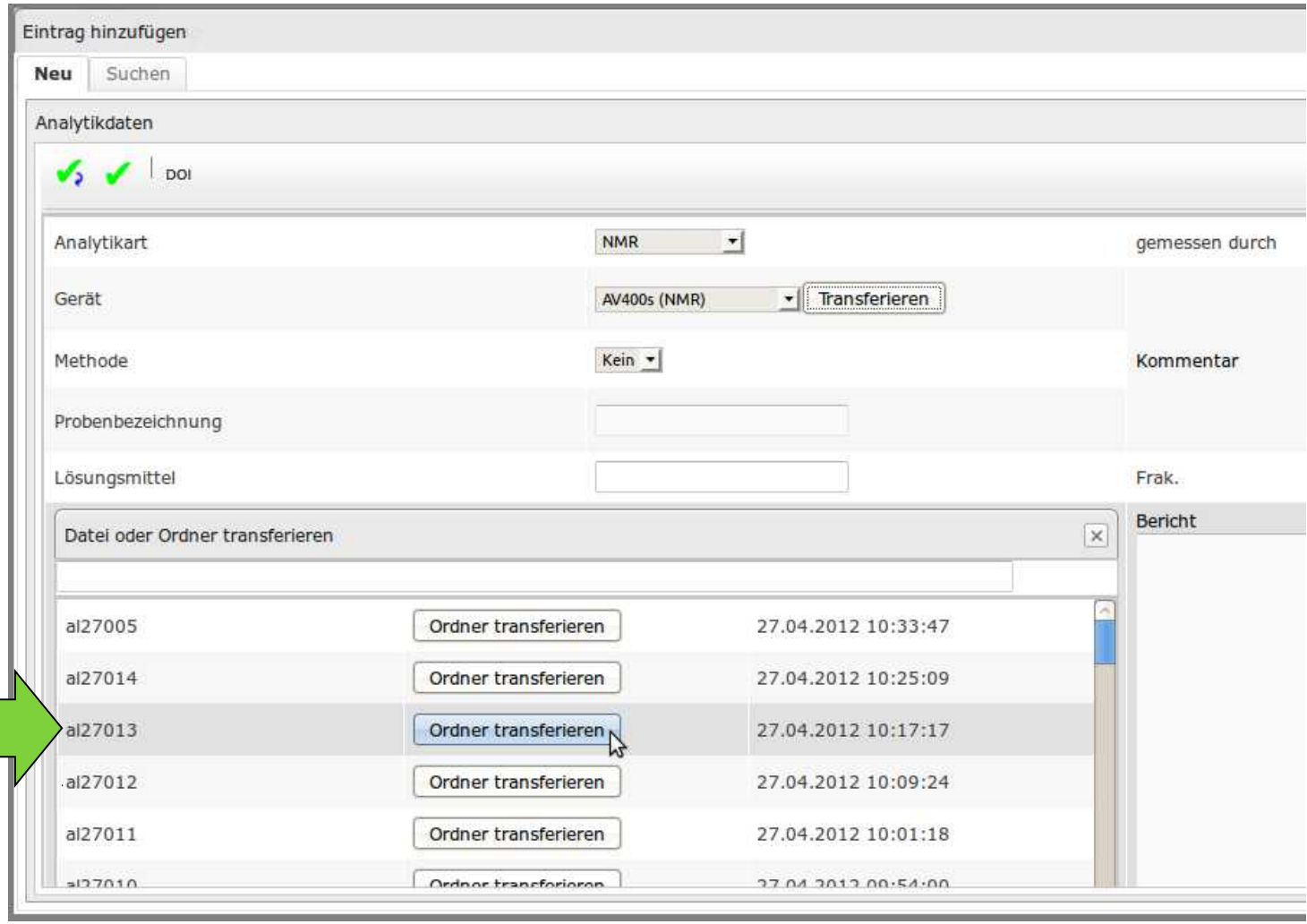
Analytical data

Analytical data

- **Transfer data from the devices to the ELN**
- Create preview images (extensible by Python modules)



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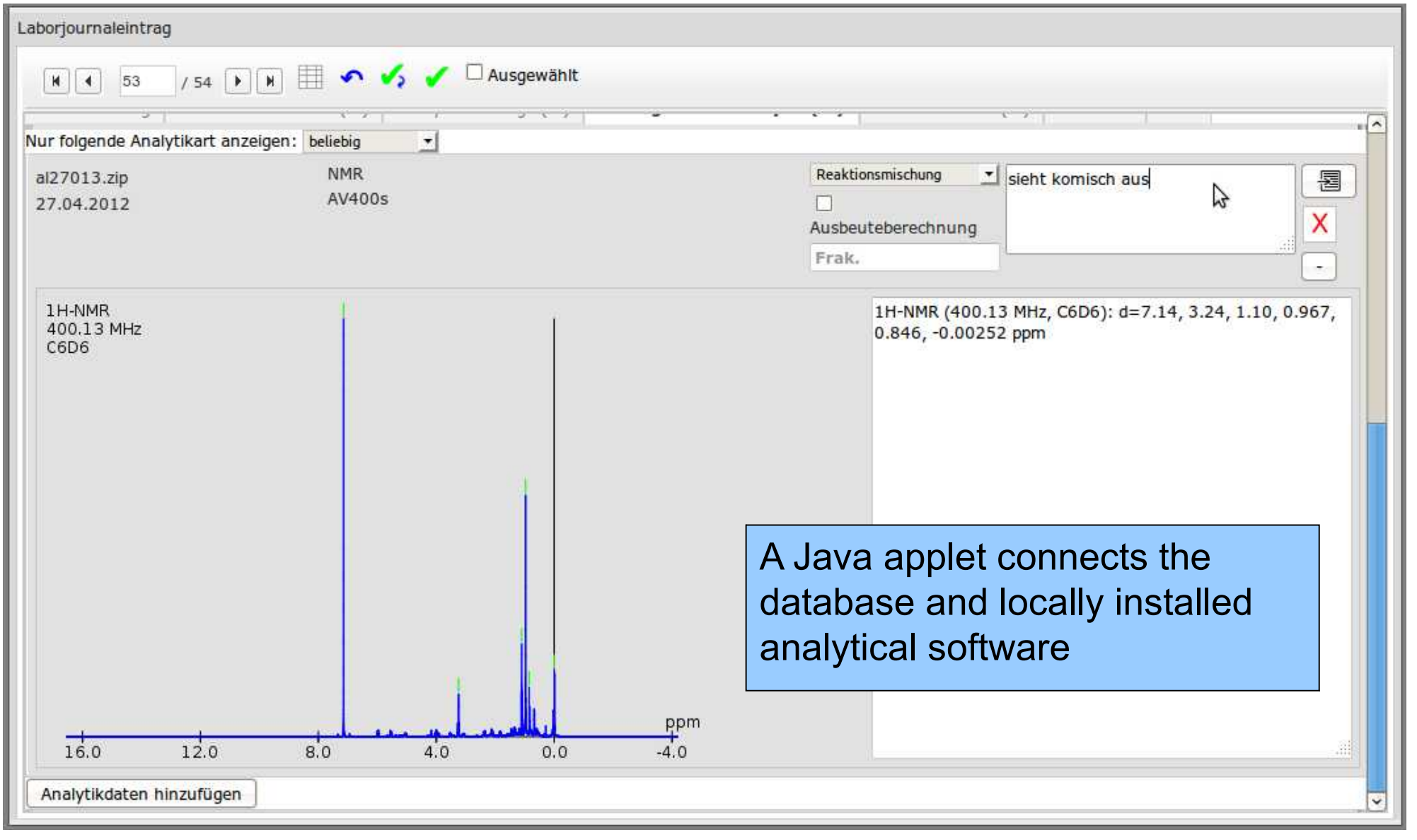
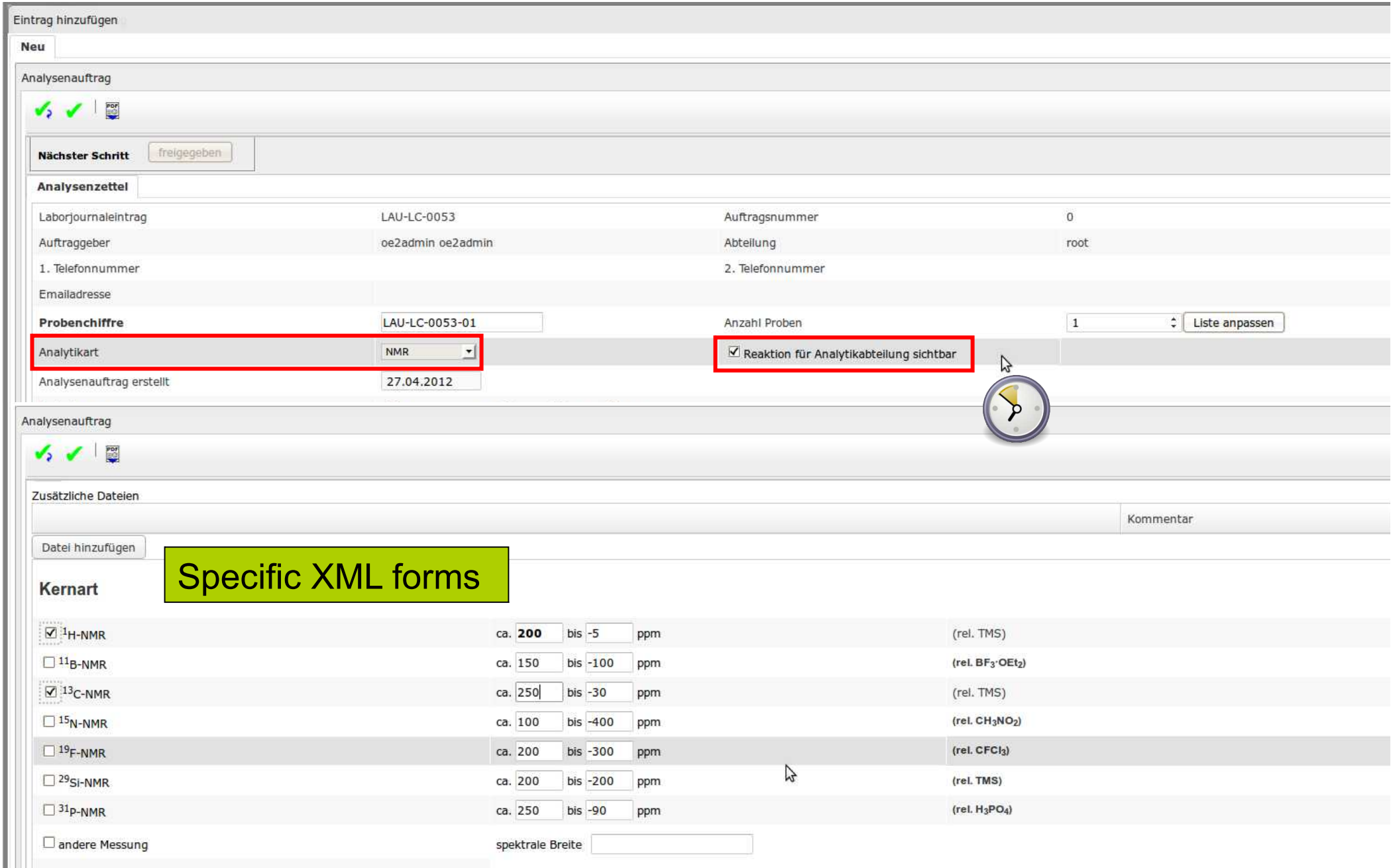
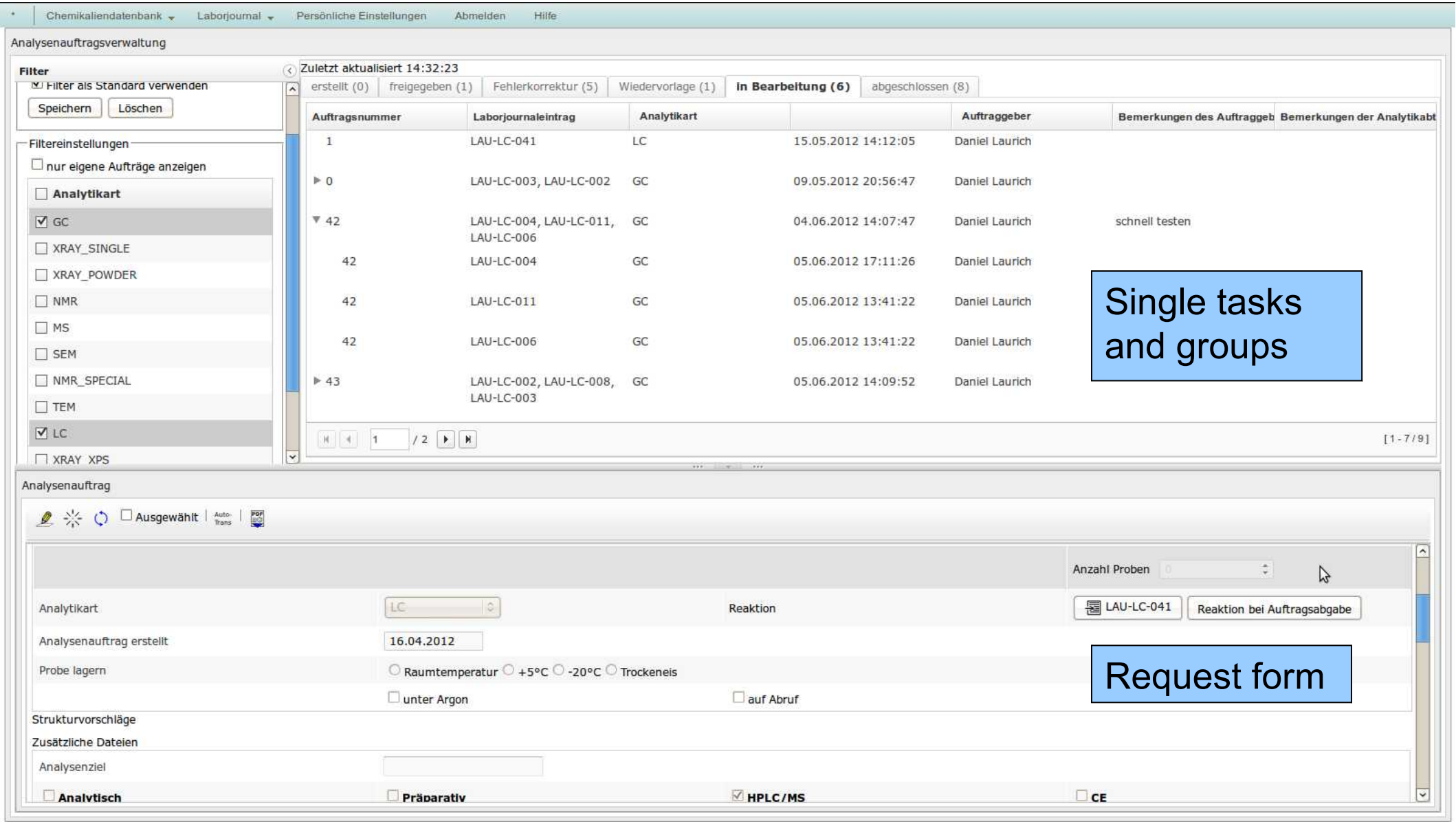


Measure and let measure



Sample inbox



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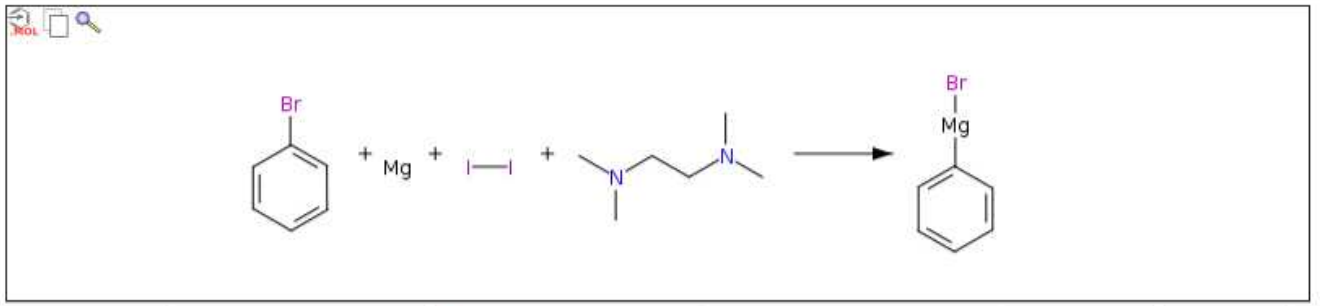
Collaboration with analytical departments



Status monitoring and communication

Durchführung | Zusätzliche Dateien (0) | **Analysenaufträge (2)** | durchgeführte Analytik (1) | Literatur (0) | Erweitert | Alles

Probenchiffre	Analytikart	Auftragsnummer	Erstellt	Bemerkungen des Auftrag	Bemerkungen der Analyti	Reaktion anzeigen	
	NMR	16	27.04.2012	**eilt wie immer sehr**		☑	in Bearbeitung
	NMR	17	30.04.2012	**urgent as usual**		☑	Fehlerkorrektur

The analytical department adds the results directly to the lab notebook entry.

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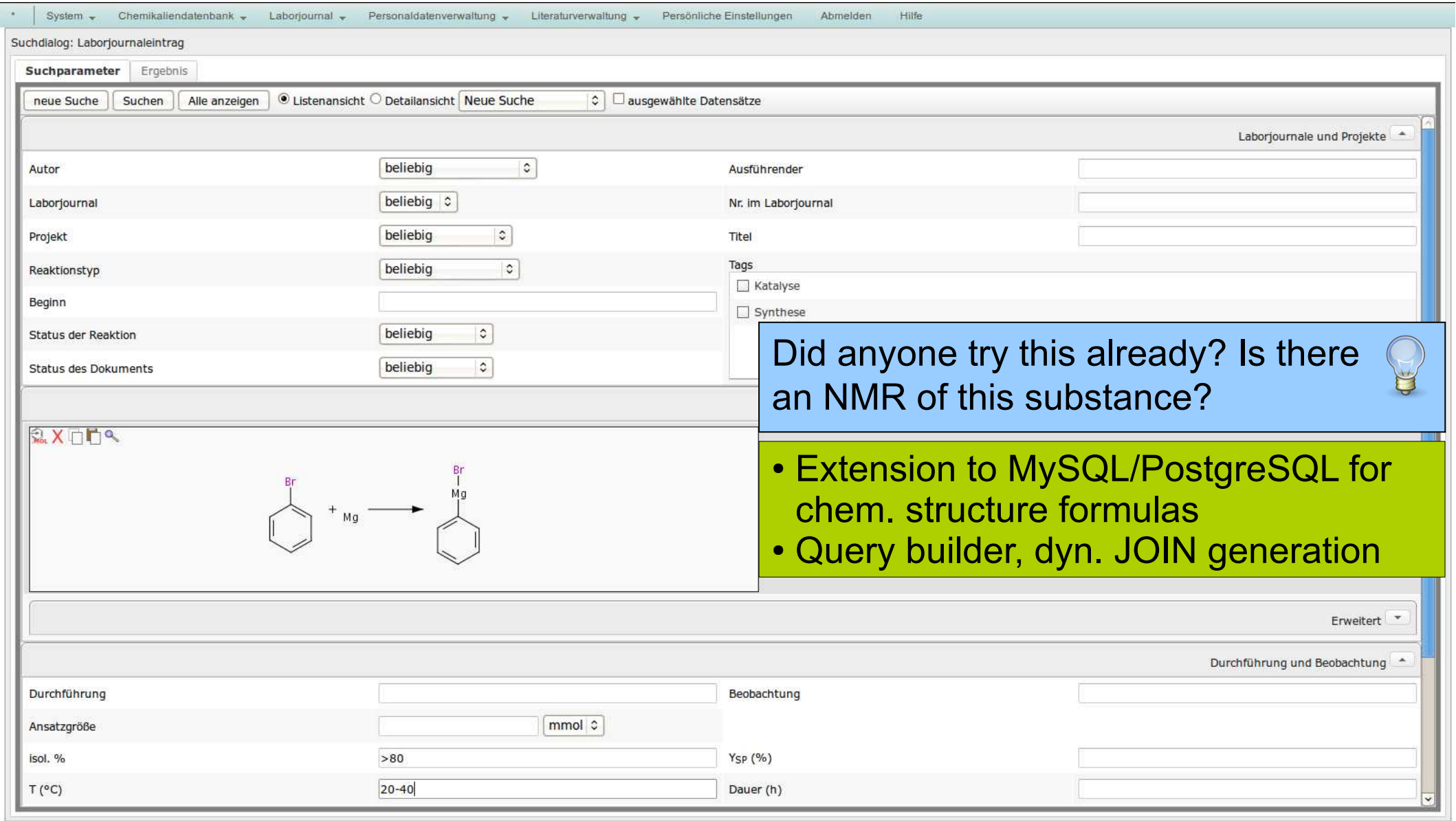
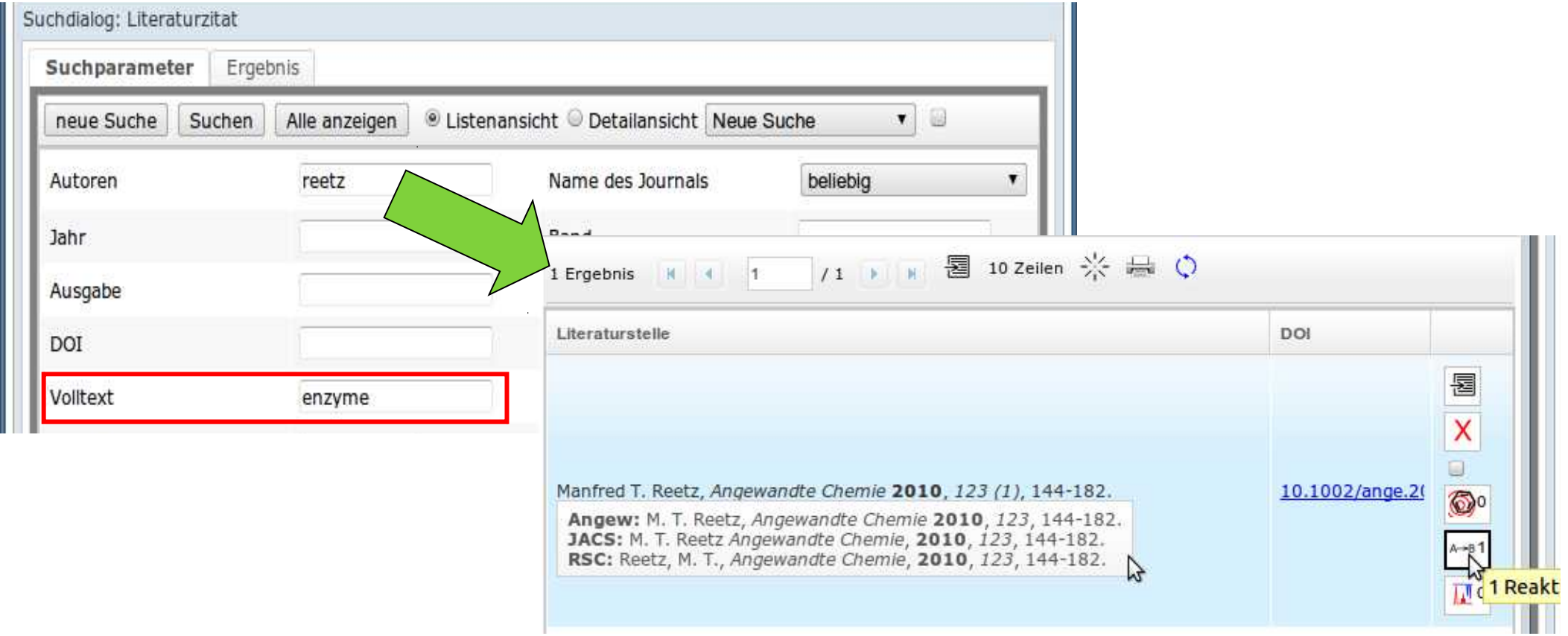
Searching within the database

Searching for chemical substructures and any other kind of information



Searching the literature database



Interesting paper! What experiment does it belong to?

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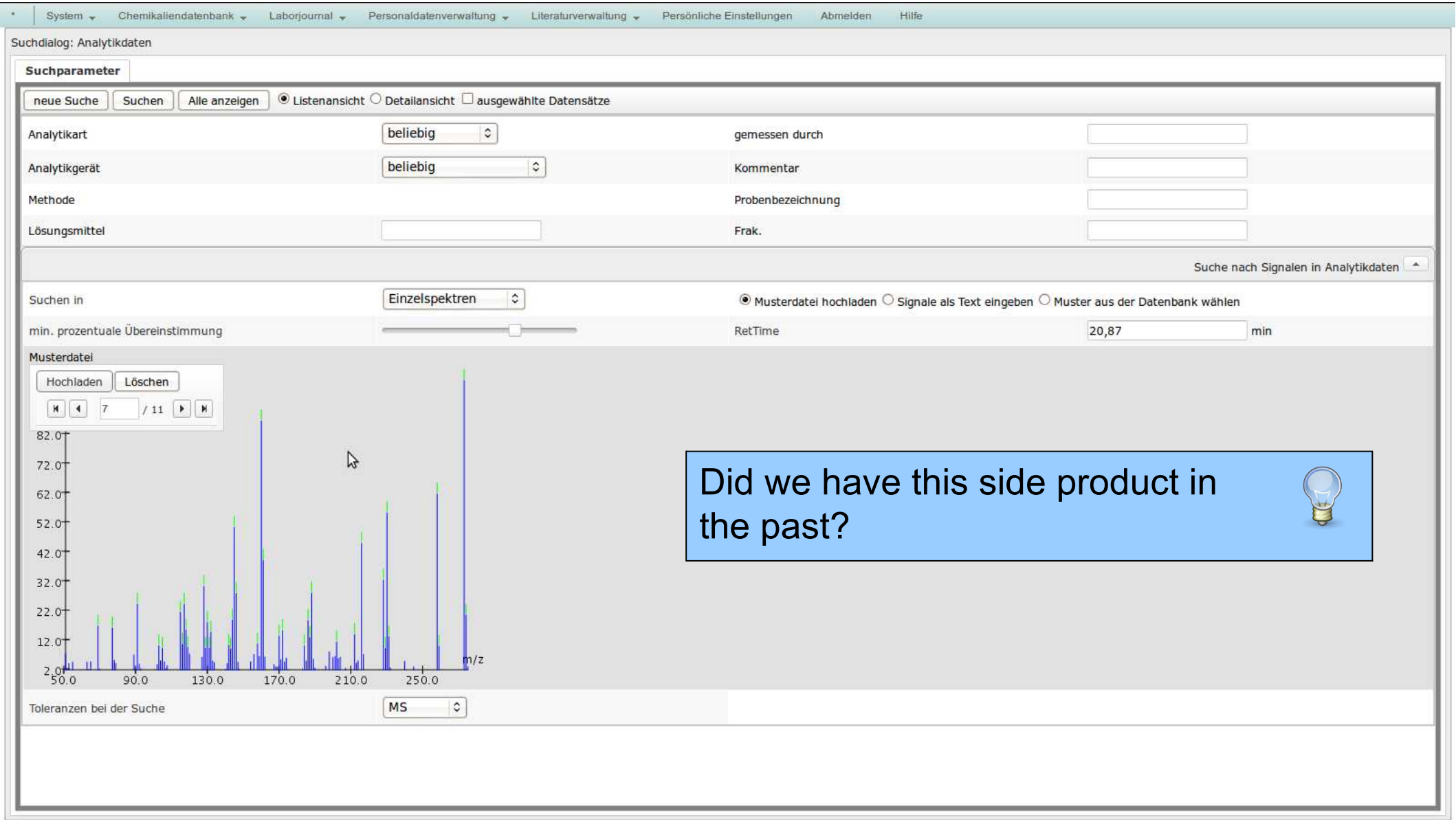
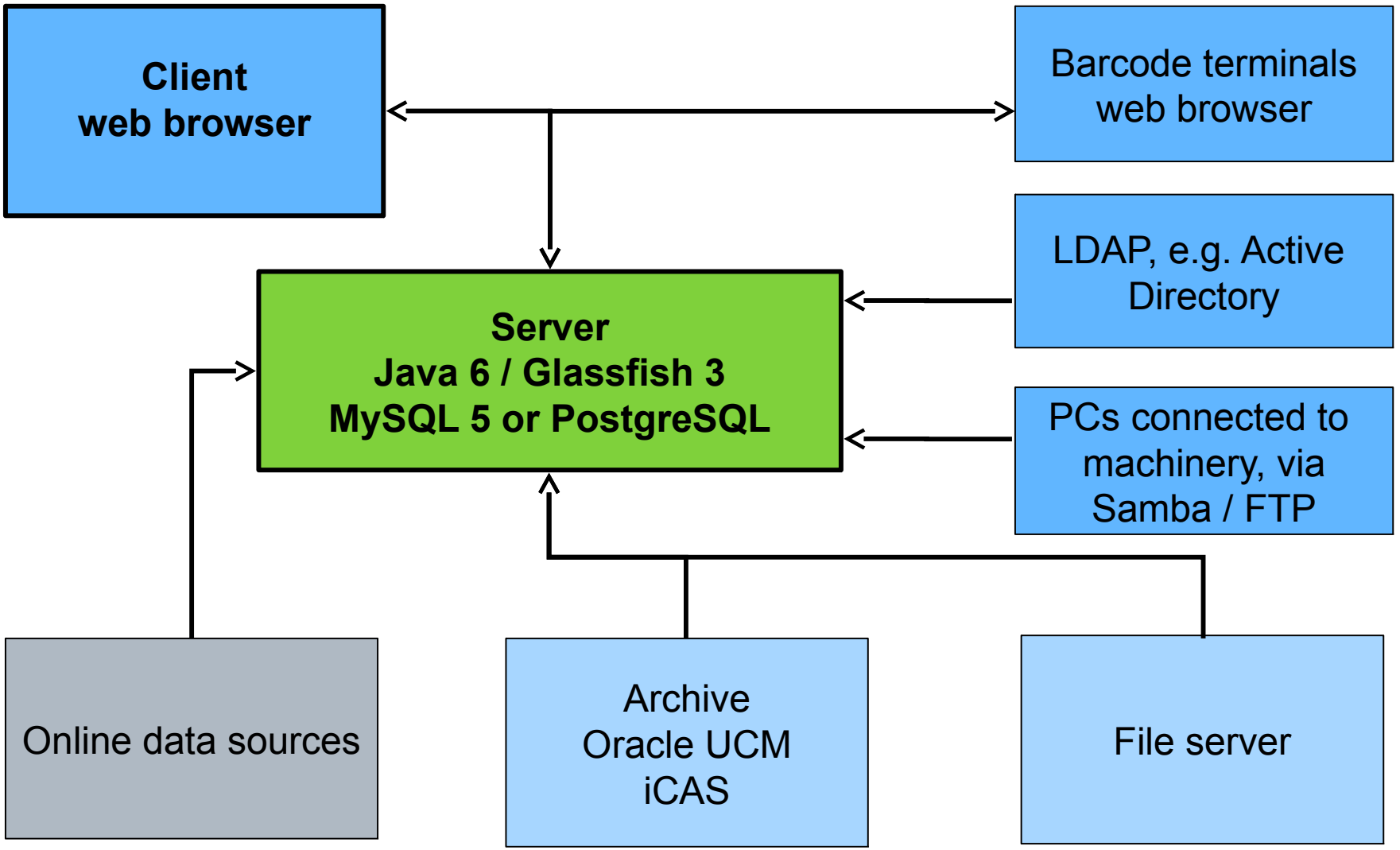
Searching for similar spectra



Technology

Architecture



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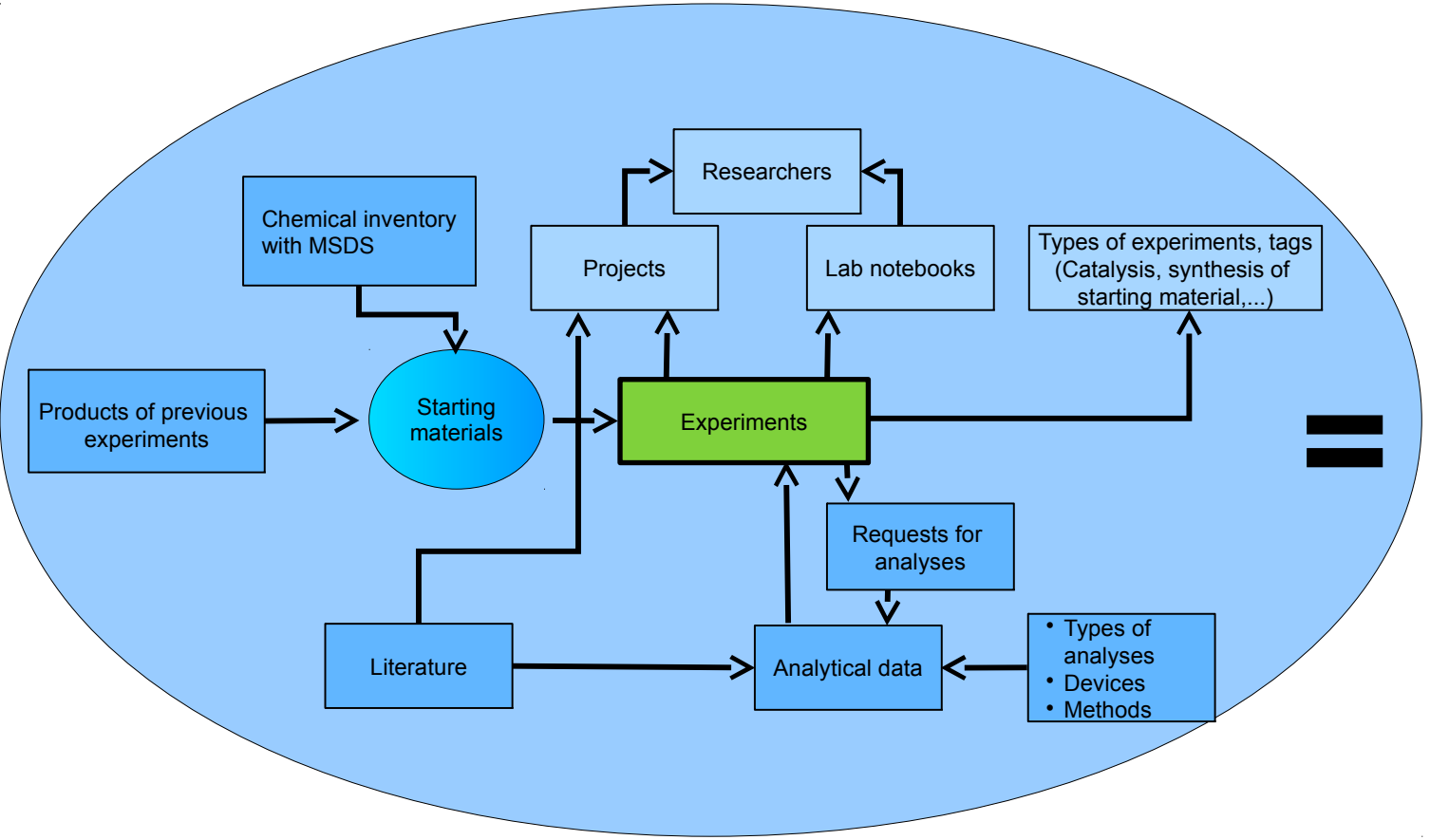
Managing permissions



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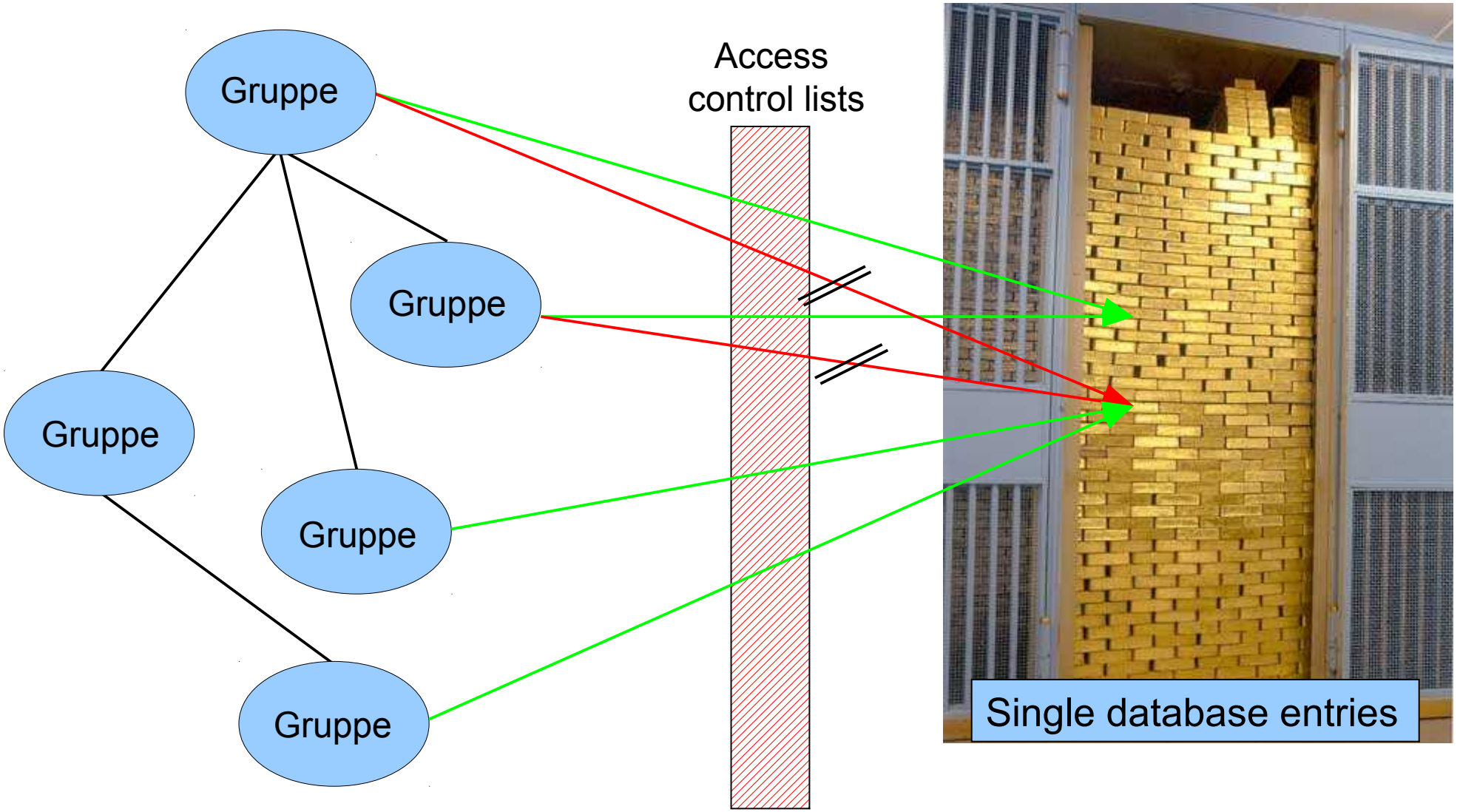
Managing permissions



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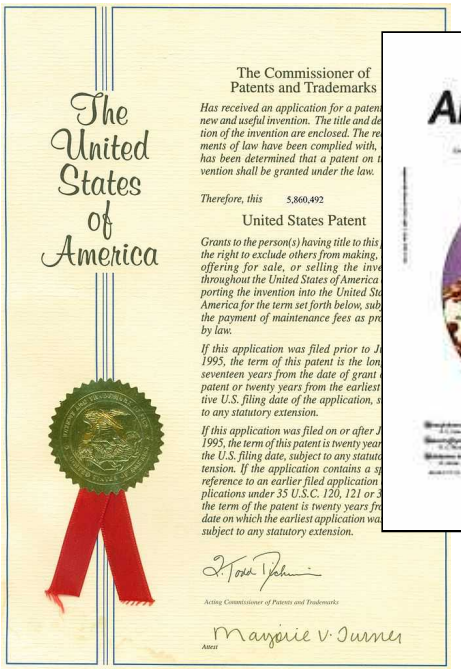
Summary

- complete documentation integrating all data
- rich and smart functionlity
- more work safety, less routine work
- shared and controlled data access
- search functionality with chemical intelligence
- flexible and extensible

Reach your goal with less effort in shorter time



Reference users

open inventory

- TU Kaiserslautern
- Univ. Düsseldorf, Hamburg, Hohenheim, Leipzig, Mainz, Saarbrücken, Tübingen
- SMEs
- Government agencies

sciformation ELN

- MPI für Kohlenforschung

UNI BASEL

CYNORA optoelectronic materials

DyStar®

TECHNISCHE UNIVERSITÄT DRESDEN

ICIQ

Technische Universität München

LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

RWTH AACHEN UNIVERSITY

TECHNISCHE UNIVERSITÄT DARMSTADT

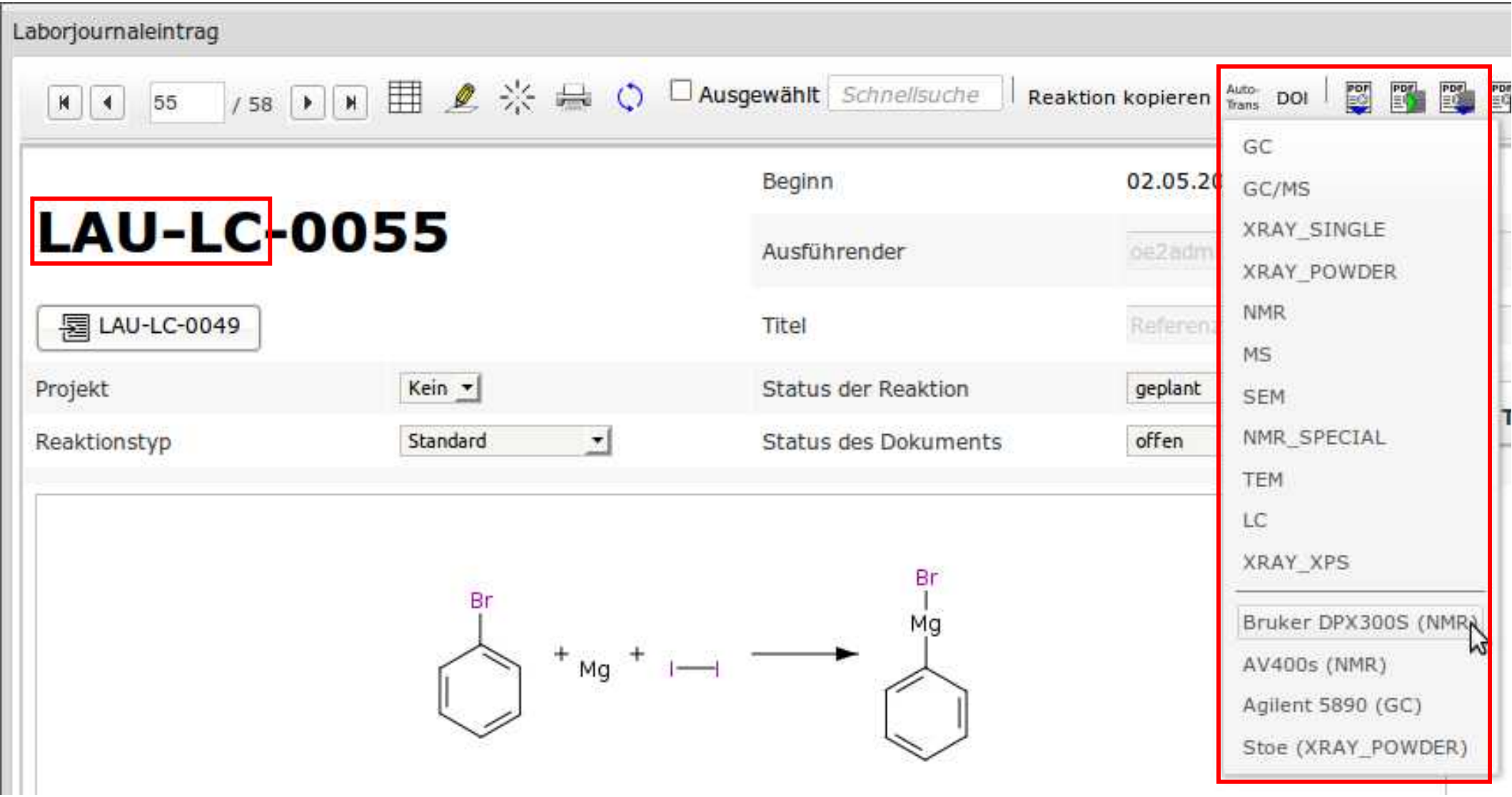
Philipps Universität Marburg

Universität zu Köln

sciformation

open inventory	sciformation ELN
• PhD project	• Project together with the MPI für Kohlenforschung
• PHP/MySQL	• Java Server Pages/PostgreSQL or MySQL
• open source	• commercial license
• ELN for chemistry	• multidisciplinary ELN
• Chemical inventory	• Chemical inventory
• Literature database	• Literature database
• 3 permission levels	• detailed permission management
• substructure search	• about 20x faster, extended search modes
	• audit trail
	• LDAP integration
	• LIMS (requests for analyses)

Automatic transfer of analytical data



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