

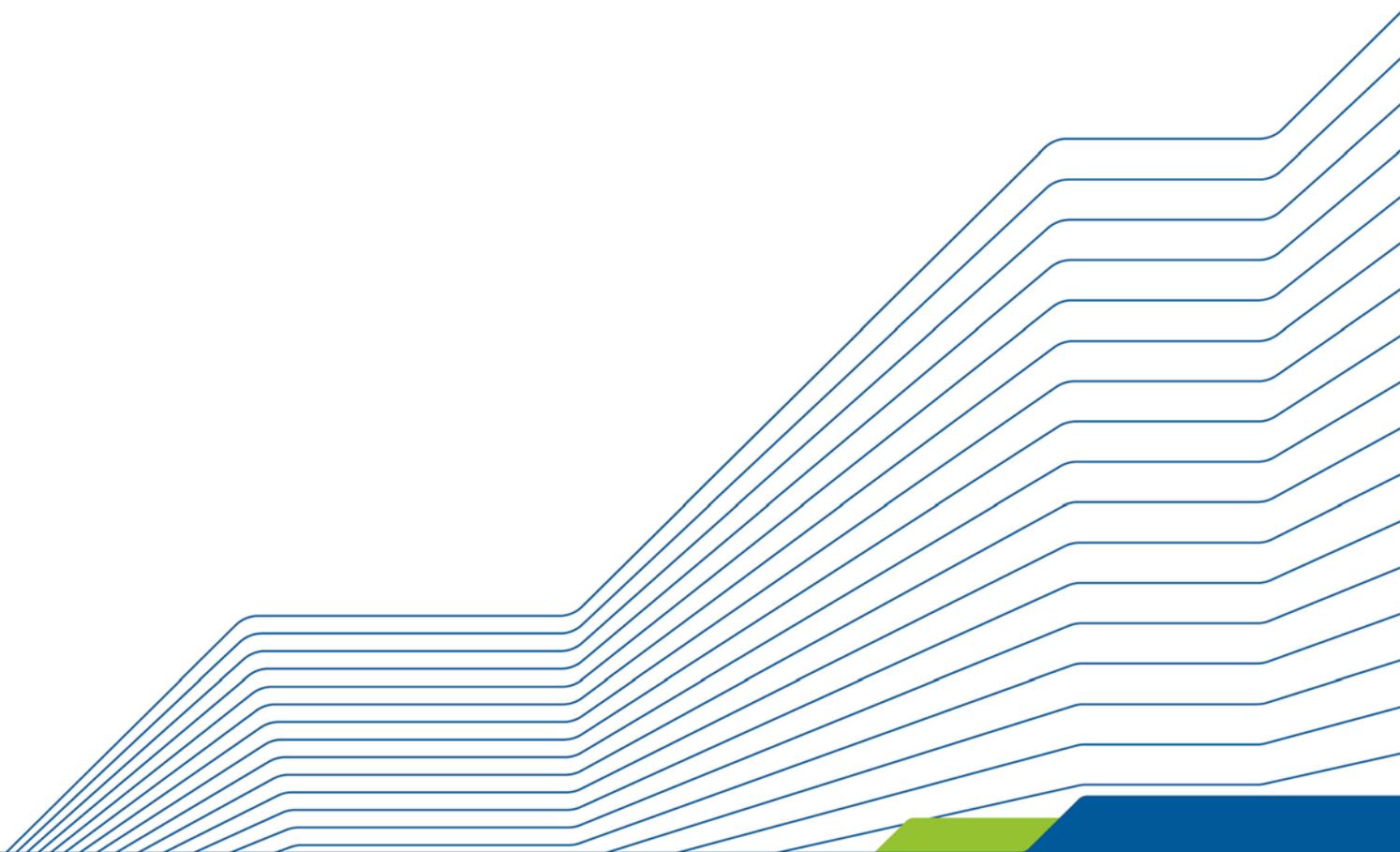
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Open Science

Helmholtz Open Science Workshop „Elektronische Laborbücher“

Braunschweig, 13.-14. September 2018

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Helmholtz Open Science Workshop „Elektronische Laborbücher“

Braunschweig, 13.-14. September 2018

Der [Helmholtz Open Science Workshop „Elektronische Laborbücher“](#) wurde vom [Helmholtz Open Science Koordinationsbüro](#) in Zusammenarbeit mit der Bibliothek des [Helmholtz-Zentrums für Infektionsforschung \(HZI\)](#) veranstaltet.

Mehr als 90 Teilnehmer/-innen aus Helmholtz-Zentren, Universitäten und weiteren Forschungseinrichtungen kamen im September 2018 in Braunschweig am [Helmholtz-Zentrum für Infektionsforschung \(HZI\)](#) zusammen um sich beim [Helmholtz Open Science Workshop „Elektronische Laborbücher“](#) über aktuelle Möglichkeiten zum Umstieg von traditionellen Laborbüchern aus Papier auf elektronische Geräte zu informieren. Durch einen Videostream konnten die Vorträge auch an HZI-Außenstandorte und weitere Helmholtz-Zentren übertragen werden.

Gerade in biologischen und chemischen Laboren sind Laborbücher die Grundlage für die Protokollierung von Arbeitsabläufen, Ergebnissen und Forschungsdaten. Elektronische Laborbücher haben gegenüber der Papierversion verschiedene Vorteile, z. B. können sie die Datenarchivierung erleichtern, die Zusammenarbeit im Team fördern und als [Open-Science-Tool](#) dienen.

Am ersten Tag des Workshops konnten die Teilnehmer/-innen während einer Demosession mit verschiedenen Anbietern elektronische Laborbücher am Rechner testen und Hilfestellung bei der Entscheidung über die Einführung und Auswahl einer Open-Source-Software oder eines kommerziellen Produkts erhalten. Beim Workshop gab es spannende Vernetzungen zwischen Teilnehmer/-innen aus unterschiedlichen Forschungsgebieten und Funktionsbereichen. Die Vortragsfolien des Workshops werden im Folgenden dokumentiert.

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Wolfgang zu Castell, AK Open Science / HMGU: Begrüßung

HZI-OSKB Workshop Elektronisches Laborbuch

Wolfgang zu Castell

Wissenschaft kann immer wieder begeistern

Erwin-Schrödinger-Preis 2018

Prostatakrebs besser erkennen und therapieren

Erwin-Schrödinger-Preis 2018

Der Erwin-Schrödinger-Preis geht in diesem Jahr an ein interdisziplinäres Forscherteam aus Heidelberg. Die Wissenschaftler Matthias Eder, Michael Eisenhut, Uwe Haberkorn und Klaus Kopka haben gemeinsam eine Methode entwickelt, mit der sich Prostatakrebs nicht nur zuverlässiger diagnostizieren, sondern auch gezielt bekämpfen lässt.



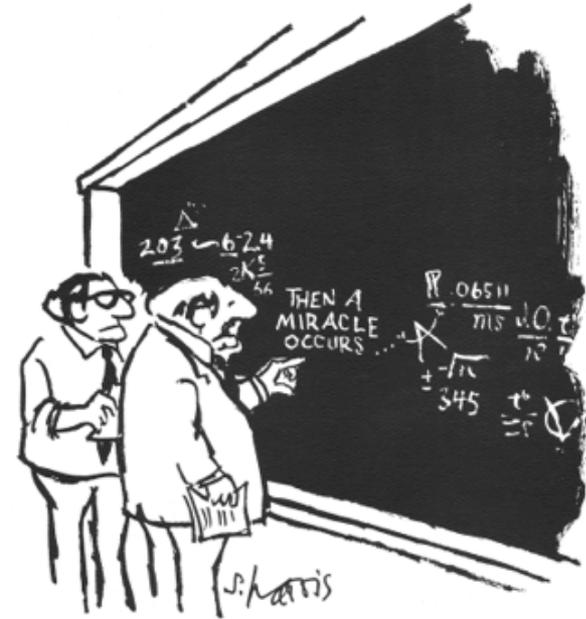
Source: www.helmholtz.de

Reproduzierbarkeitskrise

Wissenschaft lebt von Vertrauen



Source: www.scottdmiller.com



"I THINK YOU SHOULD BE MORE EXPLICIT HERE IN STEP TWO."

Source: dailyquotes99.com/s/verifiable

Fake News hoffähig machen?

Wahrheit definiert den Kern des wissenschaftlichen Anliegens



Source: www.spiegel.de

Ursachen sind vielfältig

Forderung nach Reproduzierbarkeit hat einen tiefen Grund

Essay

Why Most Published Research Findings Are False

John P. A. Ioannidis

Summary

There is increasing concern that most current published research findings are false. The probability that a research claim is true may depend on study power and bias, the number of other studies on the same question, and, importantly, the ratio of true to no relationships among the relationships probed in each scientific field. In this framework, a research finding

Ioannidis, PLoS Medicine 2005

factors that influence this problem and some corollaries thereof.

Modeling the Framework for False

Pos

Seven
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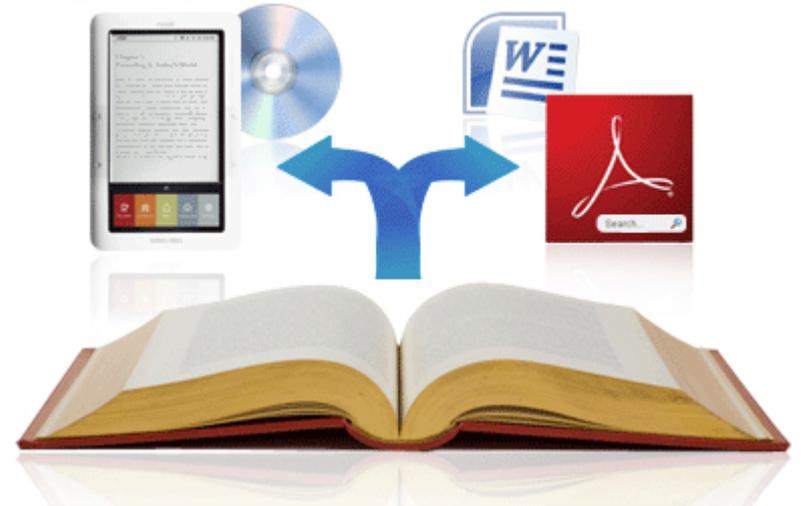
is characteristic of the field and can vary a lot depending on whether the field targets highly likely relationships or searches for only one or a few

There is increasing concern that most current published research findings are false. The probability that a research claim is true may depend on **study power** and **bias**, the **number of other studies** on the same question, and, importantly, the **ratio of true to no relationships**.

Worum geht es bei diesem Workshop?

Laborbücher sind eine (un-)erschlossene Quelle

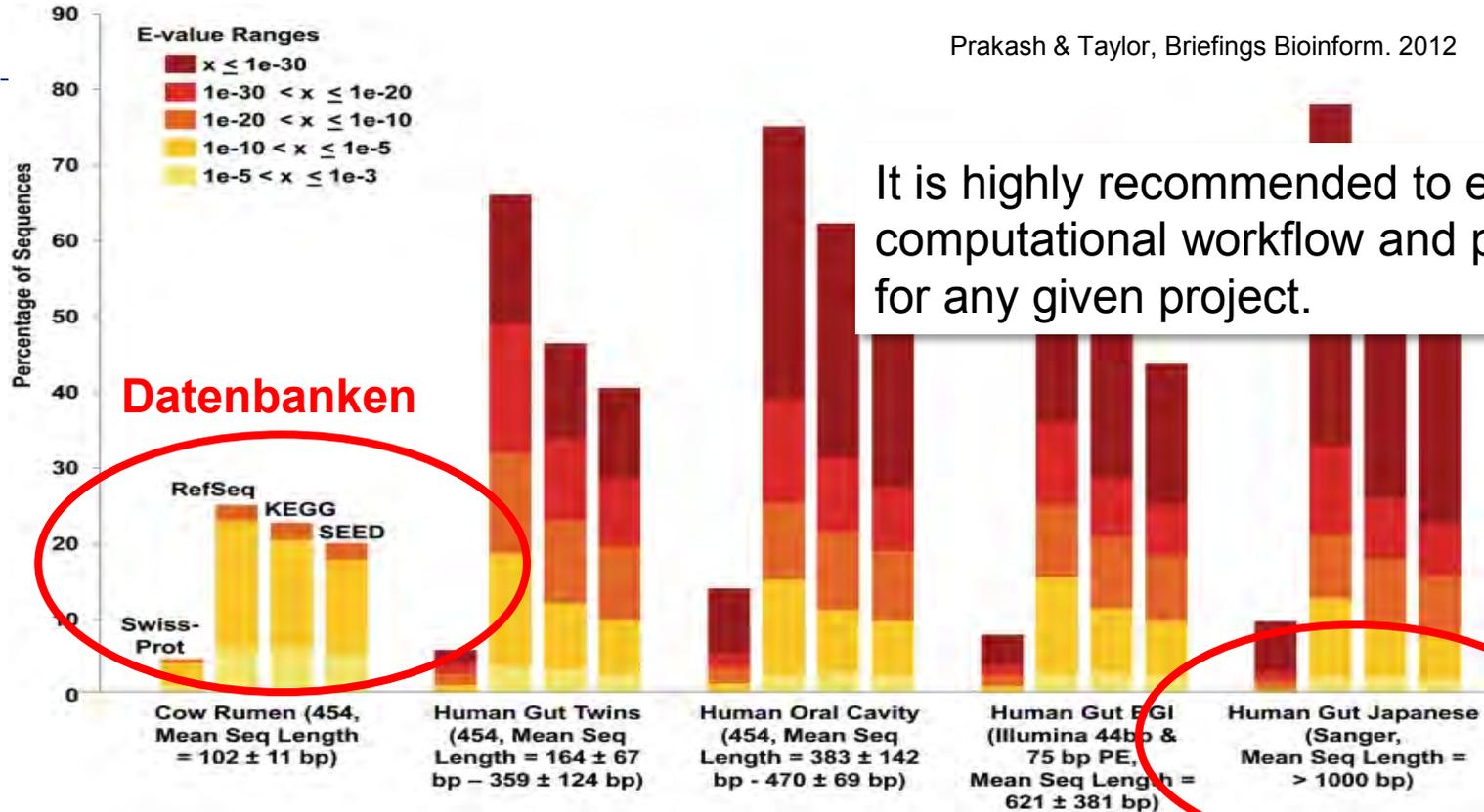
- Die Dokumentation der Arbeitsschritte im Labor sind der Anfang der wissenschaftlichen Wertschöpfung.
- Transparenz und Nachvollziehbarkeit fangen bereits im Labor an.
- Die Publikation der Ergebnisse reicht heute oft nicht mehr aus.



Source: www.e-book-news.de

Wo sind Probleme ... (zwei technische Beispiele)

Prakash & Taylor, Briefings Bioinform. 2012



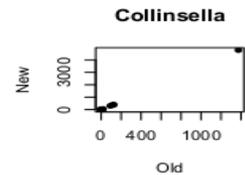
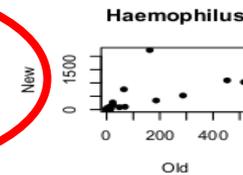
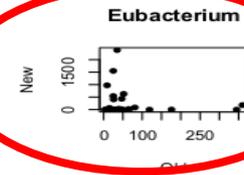
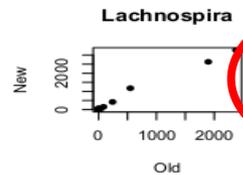
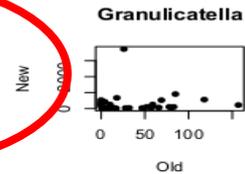
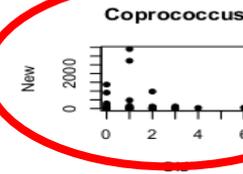
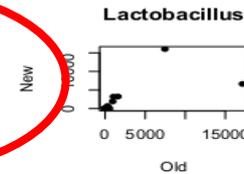
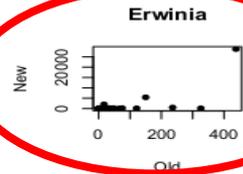
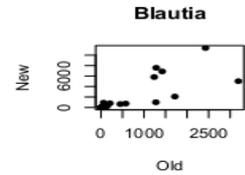
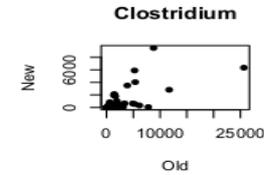
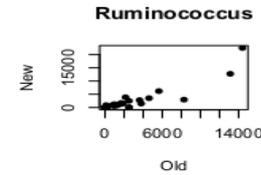
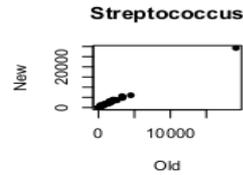
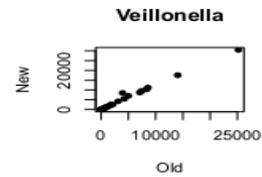
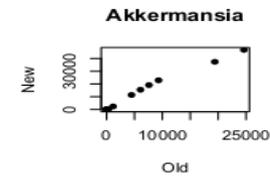
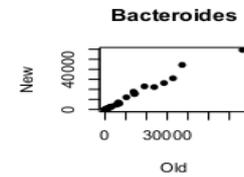
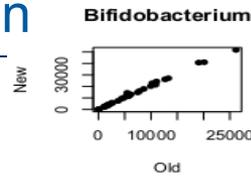
Details sind von Bedeutung !

Abhängigkeit von Datenbanken

Beispiel:

taxonomische
Bestimmung
von OTUs

hier:
RDP vs. GG



Digitalisierung erschließt die Verknüpfung

Sackgassen blockieren das Weitergehen

Digitalisierung von Inhalten ermöglicht die Verlinkung und macht die Inhalte damit für automatisierte Verfahren zugänglich.



Source: www.bayernkurier.de

microbiome analysis. Total bacterial genomic DNA was extracted using NucleoSpin for Soil Kit (Macherey-Nagel, Dueren, Germany) following the manufacturer's instructions. Amplification of the

Walker et al., ISME 2014

Digitalisierung ist nicht frei von Ängsten

Ideenklau vs. Synergie

Schutz von Ideen ist keine Frage der Speicherungsform sondern des Managements von Rechten!



Source: de.toonpool.com

Potenzial durch Vernetzung

Digitalisierung des wissenschaftlichen Wertschöpfungsprozesses

- Idee
- Experiment
- Daten
- Publikation

Wo hatte ich
das Zitat
gleich
nochmal
her?

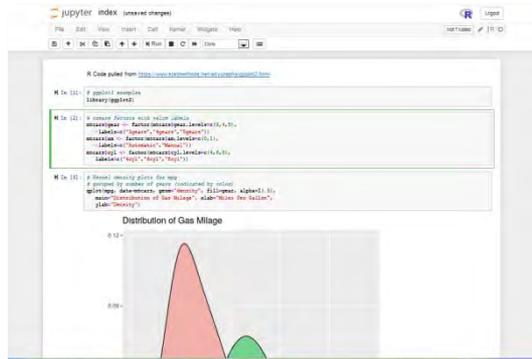


Foto: Cornelis Golhardt, www.kna-bild.de

**Viel Spaß beim Workshop und
viele anregende Gespräche!**

Heiko Rosenfelder, DKFZ: Einführung und Betrieb eines elektronischen Laborbuchs im DKFZ

Abstract

„Gute wissenschaftliche Praxis“ sind Stichworte welche immer wieder dafür sorgen, dass Organisation, Abläufe, Dokumentationen immer wieder auf den Prüfstand gestellt werden. Technischer und organisatorischer Fortschritt sorgen immer wieder für Änderungen bei den Abläufen in der täglichen Arbeit im Labor oder bei den Verfahren der Dokumentation. Unter anderem stießen einige Wissenschaftler und technische Mitarbeiter immer wieder an Grenzen, wenn es darum ging elektronische Dokumentationen oder Ergebnisse im klassischen Laborbuch zu notieren. Diese Medienbrüche aber auch die immer größer werdende Menge an Daten lieferten die Motivation ein elektronisches Laborbuch am DKFZ einzuführen.

Im Vortrag werden die Kriterien zur Auswahl des Produktes, die Vorbereitung mit einem Proof of Concept, sowie verschiedene organisatorische Rahmenbedingungen wie Datenschutz und Dienstvereinbarungen betrachtet.

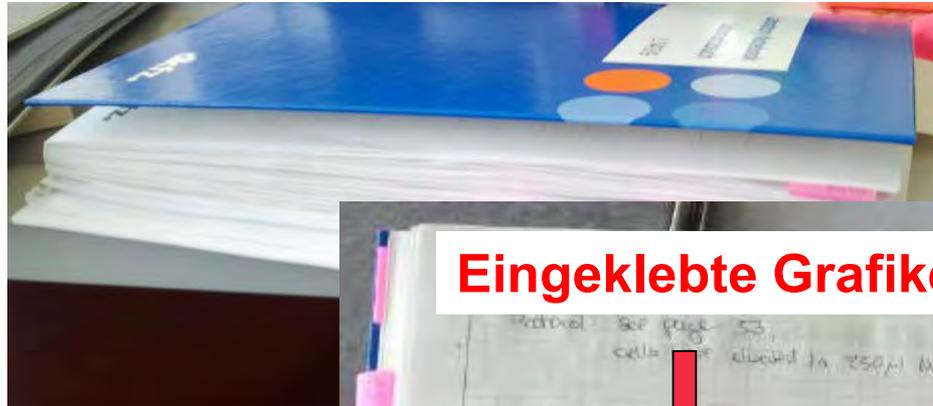


Elektronisches Laborbuch

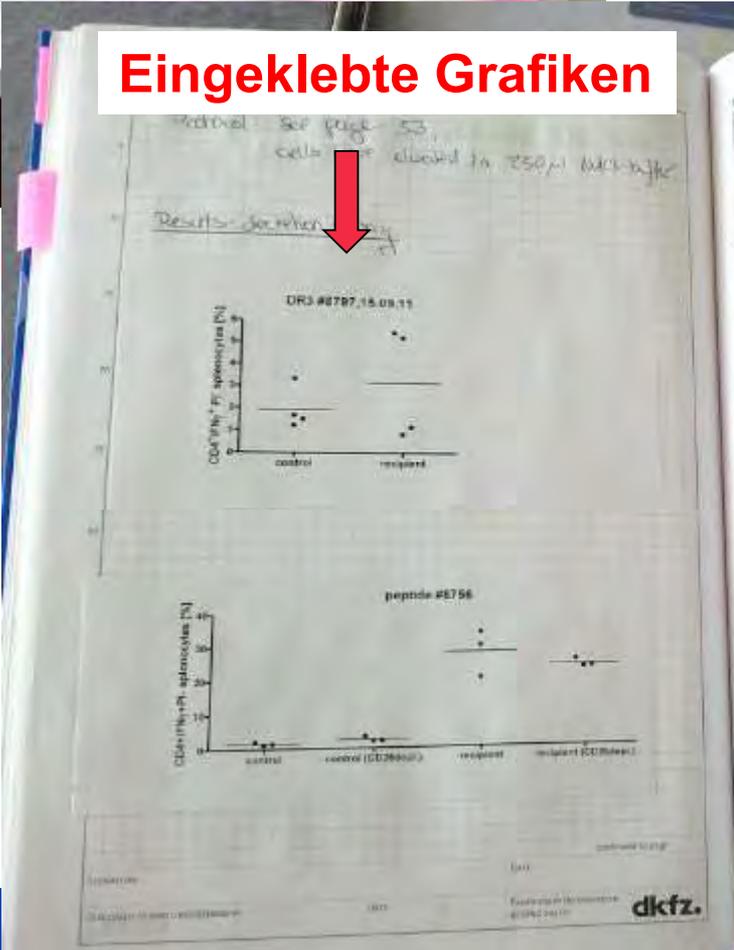
Motivation – Projektierung - Einführung

Heiko Rosenfelder

Laborbuch - Papier



Eingeklebte Grafiken



Eingeklebte Tabelle

→ alles wert in Kultur die zwei drauf
in 200 µl MACH-lyse

Expt. data

| | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| 1 | | | | | | |
| 2 | | | | | | |
| 3 | | | | | | |
| 4 | | | | | | |
| 5 | | | | | | |
| 6 | | | | | | |

2. ED4 =

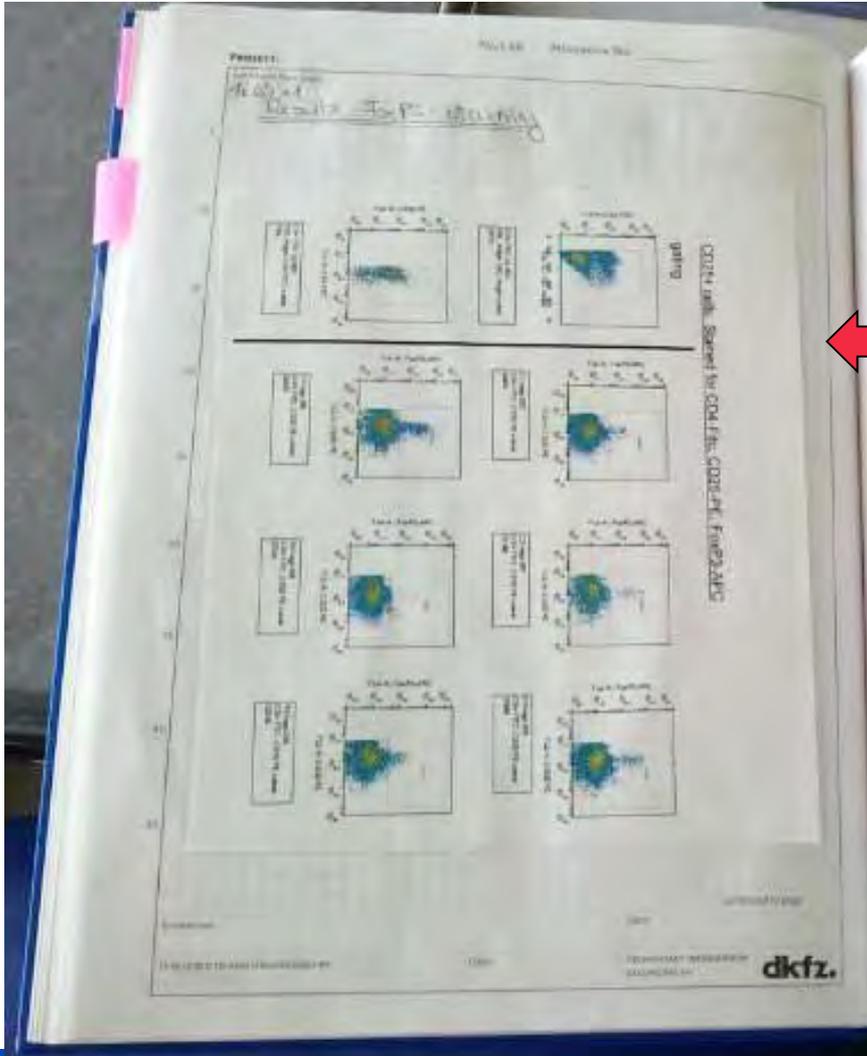
antibody 2 ml, 4°C

40 µl CD25-PE (aus dem list) + 20 µl FACS-lyse

- 100 µl FACS-lyse, spin, wash again
- 50 µl Cytofix/cytoperm, 20 min, 4°C
- spin 2000 rpm, wash with Perm Wash
- FOXP3 staining 1 µl antibody + 35 µl FACS-lyse, 30 min, 4°C
- 150 µl Perm Wash, wash again
- Transfer cells to FACS-tube, with 200 µl FACS-lyse

dkfz.

Klassisches Papier



Eingeklebte
FACS Auswertung

- Ausdrucken auf Farbdrucker
- Ausschneiden
- Einkleben

Elektronisches Laborbuch

Medienbruch verhindern:

- Viele Daten und Auswertungen werden am PC generiert
- Sollen dann auch dort gespeichert werden

➔ Daher ...

Bedeutung der Dokumentation mit einem Laborbuch

- Nachvollziehbarkeit der Experimente
- Alle notwendigen Informationen, um ein Experiment zu wiederholen oder Daten später zu analysieren
- Arbeiten nach Standards
- Experimente, die nicht dokumentiert wurden, haben gar nicht stattgefunden!

- Nachfragen von Zeitschriften
- Patent-Streitigkeiten



Chronologie

Mitte 2010: Arbeitsgruppe ELN

- Wissenschaftler
- Studentische Hilfskraft
- Später IT-Abteilung

Auswahlverfahren der div. damals vorhandener Anbieter bis ca. Mitte 2011

Februar 2012 bis August 2012

- Pilotprojekt mit 5 Gruppen in 4 Abteilungen

Ab Oktober 2012 Vorbereitung des „rollout“

- Dienstvereinbarung (Personalrat, Vorstand)
- Definition des Service (ITCF)
- IT-Umgebung installieren (ITCF)
- Ankündigungen
- Veranstaltungen

Voraussetzungen für die Auswahl des Programmes

- **Einfach** zu bedienen, intuitiv
- Es sollten möglichst Daten der gängigen Programme eingefügt werden können (Word, Excel, PDF, Bilder)
- **Datensicherheit:** Speicherung der Daten im DKFZ, nicht in der Cloud
- **Datenkapselung:** Experimente gehören dem Experimentator
- **Authentizität** der Daten: Daten müssen zu einem Zeitpunkt eingefroren werden können, und dann nicht mehr veränderbar sein
- Datum darf nicht einfach geändert werden (Lösung: auf zentralem Server des DKFZ)
- **Einbinden ins DKFZ:** Einloggen mit dem AD – Zugang
- PC und Mac kompatibel

Zwei Kandidaten

- e-Notebook (PerkinElmer, ehem. Cambridge Soft.)
 - Windowslösung (Citrix bei Mac)
 - Sehr chemielastig (kam aus Zweitmeinung)
 - Integration MS Office
 - Hoher Lernaufwand, aber sehr flexibel zu Konfigurieren
 - Probleme beim Drucken *
- iLabber (contur Software, Accelrys) heute BioVia ELN
 - Guter Kundenservice (bestätigt!)
 - Kompatibilität mit Marvin, ChemDraw, PDF, MS Office
 - Sehr intuitiv zu bedienen (ähnlich Word)
 - Anfügen von Attachements
 - Probleme beim Drucken *

ELN – Version von 2011

Bibliotheksfunktion –
Liste mit allen
einsehbaren
Journals

Erstellung von
Templates

„My Notebook“;
Überblick über
Aufgaben/Journale

Selbst-erstellte
Journale

Journale, die auf
Abzeichnung
warten

The screenshot displays the ELN 2011 interface. At the top, there is a navigation bar with tabs for 'File', 'View', and 'Help'. Below this, a menu contains icons for 'My Notebook', 'Library', 'Templates', 'Search', 'Administration', 'Help', and 'iLabber Webinar'. The main content area is divided into two panes. The left pane, titled 'My Notebook', shows a tree view of the user's notebook, including a folder for 'Lab notebook of Schoch, Arne (SCHOCH)' and a sub-folder for '2011'. The right pane, titled 'Lab Notebook of Schoch, Arne (SCHOCH)', displays a list of 'Current experiments (3)'. Below this is a 'Start new experiment' button. Further down, there is a 'Reminder lists' section with a sub-section 'Waiting for your submission (12)'. This section contains a list of experiments with their submission dates and names.

| Current experiments (3) | | |
|-------------------------|--------------|--|
| EXP-11-AR5711 | Test | |
| EXP-11-AR5710 | (untitled) | |
| EXP-11-AR5706 | Präsentation | |

| Waiting for your submission (12) | | |
|----------------------------------|---------------|--------------|
| Today | EXP-11-AR5711 | Test |
| Today | EXP-11-AR5710 | (untitled) |
| 26 days | EXP-11-AR5706 | Präsentation |
| 26 days | EXP-11-AR5709 | (untitled) |
| 26 days | EXP-11-AR5708 | (untitled) |
| 27 days | EXP-11-AR5707 | (untitled) |
| 27 days | EXP-11-AR5702 | Testing |
| 33 days | EXP-11-AR5705 | (untitled) |
| 33 days | EXP-11-AR5704 | (untitled) |
| 35 days | EXP-11-AR5703 | Test |
| 35 days | EXP-11-AR5701 | Test |
| 39 days | EXP-11-AR5700 | (untitled) |

ELN – Version von 2011

The screenshot displays the ELN 2011 interface. At the top, there is a toolbar with icons for Submit, Print, Clone, Share, and E-mail. Below this is a sidebar menu with the following sections:

- Symbol
- My Sections
- Sections
 - Body text
 - Image
 - Excel worksheet
 - Chemical sketch
 - Chemical reaction
 - PDF Document
 - Accord For Excel
 - Text field
 - File Attachment
 - Date
 - Page Break
 - User Defined Reference
 - Errata Section
 - SDFile
 - CombiChem
 - Project
 - Related experiments

The main editing area contains the following content:

- Experiment no.:** EXP-11-AR5711
- Author:** Schoch, Arne (SCHOCH)
- Date Started:** 2011-10-04 10:06
- Title: *** Test
- Project: *** Präsentation
- Body text:** Test Test Test
- Excel worksheet:**

| A1 | B1 | C1 | D1 | E1 |
|------|-----|-----|-----|----|
| -0,5 | 0,1 | 0,3 | 0,2 | 0 |
| 1,3 | 1,2 | 1,1 | 1,4 | 1 |
- Image:** A landscape image of mountains under a blue sky.

On the right side of the image section, there is a small toolbar with icons for image manipulation (crop, rotate, zoom, etc.).

Gegenzeichnung
/Locking

Sectionauswahl

„Briefkopf“

Textfeld;
integriertes
Excel- und
Bilddokument



Voraussetzungen

- Standard PC > 2GB Ram, 100 MB HDD
- Screenres. 1280 x 1024
- Webclient (Windows, Mac geprüft, Linux fehlende Officeintegration)
- Windows-Fullclient (ab Win XP) ->.NET ab 2.0
- Browser (HTML 5)
 - Mac – Firefox ,Safari
 - Windows (IE , Firefox)

Erwartungen an ein elektronisches Laborbuch

- ~~Labormanagementsystem (LIMS)~~
- ~~Container für Rohdaten~~
- ~~Datawarehouse~~
- ~~Auswertung von Daten (Assays)~~
- **Werkzeug zur Beobachtung und Nachverfolgung von Laborexperimenten**

Pilotphase – Voraussetzungen

- zur Untersuchung und zum Testen
- Reale Daten wegen Akzeptanz verwenden
- Daten aus Pilot müssen abgeschlossen werden
- Es findet nur in eigenen Projekten ein Übertrag in die Produktionsphase statt (nicht aus dem Training)
- Gruppen können bestehen bleiben
- Trainings-Projekte werden nicht zentral übernommen
- Daten/Experimente können bei nicht bestehen des Pilots in PDF/A überführt werden.

Pilotphase

- Art der Experimente
 - Ergebnis der prePilotphase
- Auswertung
 - Fragebogen
 - Fragen/Antworten über die Einführungsschulungen
 - Ausdrücklich auch Meinungen außerhalb des Fragebogen erwünscht und berücksichtigt
- Mitglieder
 - Projektteam (Wissenschaftler, PL aus IT, PR)
 - 5 Pilotgruppen aus 4 Abteilungen (ca 20 Mitarbeiter)

ELN Trial Program

Introduction

Dear participants in the iLabber pilot.

As part of our agreement with Accelrys who are providing access to the iLabber ELN you are invited to complete short surveys at the start and end of the pilot period.

The start survey may be completed using the link below. It should take less than 10 min.

Kind regards

Questions

Section 1: About yourself

1. What is your current position?
 - a. Graduate Student
 - b. Early Career Researcher (PDRA)
 - c. Academic Staff
 - d. Other (please specify) _____
2. What is the area of science you work in? _____
3. Do you currently routinely use a computer at work?
 - No
 - Yes – I have been allocated my own computer
 - Yes – I share the use of a computer
 - Yes – I use my own computer at work
4. What operating system does your (primary) computer use?
 - Linux
 - Mac OS
 - Windows

Section 2: About your research

1. How important are the following to your interest in using an ELN. (1-5 scale)
 - Saving time over the paper notebook process
 - Improved ability to search and re-use documented information
 - Better ability to collaborate and share information
 - Better protection of IP
 - Improved quality of record keeping
 - Improved access to data as linked through ELN
 - Improved group / project management

1 | Start Survey

[link](#)

Dienstvereinbarung – 1

§ 2 Grundsätze der Vereinbarung

Stiftungsvorstand und Personalrat stimmen darin überein, dass

- der Einsatz von iLabber nicht zum Abbau oder Herabgruppierung von Personal genutzt wird,
- iLabber nicht zur Arbeitszeit- und Verhaltenskontrolle der Arbeitnehmer eingesetzt wird.

Dies sichert der Stiftungsvorstand den Beschäftigten zu.

Zum Schutze der Beschäftigten vor den Gefahren einer technischen Überwachung gelten insbesondere entsprechend den vom Bundesverfassungsgericht in seiner Entscheidung vom 15.12.1983 (BVerfGE 65,1/43) zum informationellen Selbstbestimmungsrecht entwickelten Rechtsregeln:

- der Grundsatz der strikten Zweckbindung der Verarbeitung personenbezogener Daten; jeder Beschäftigte muss jederzeit die Möglichkeit haben zu erfahren, welche Daten über ihn gespeichert sind und zu welchen Zwecken sie verwendet werden,
- der Grundsatz der Verhältnismäßigkeit der Datenspeicherung, d.h. nur in dem zur Wahrnehmung der nachfolgenden Verarbeitungszwecke erforderlichen Umfang werden personenbezogene Daten erfasst und gespeichert.

Dienstvereinbarung – 2

§ 3 Systembeschreibung

In Anlage 1 sind die IT-Komponenten, die Zugriffsrechte sowie die Rollen des elektronischen Laborbuchs beschrieben.

§ 4 Nutzung des Systems

1. Die Nutzung des Systems iLabber ist für die Beschäftigten grundsätzlich freiwillig. Wenn das Laborbuch nicht mit dem System iLabber geführt wird, gilt die Maßgabe das DKFZ-Papier-Laborbuch – zu beziehen über die Zentralbibliothek – zu nutzen
2. Sofern die Nutzung des Systems iLabber vom Leiter der betrieblichen Einheit gewünscht wird, hat er für die entsprechende technische und räumliche Ausstattung Sorge zu tragen. Diese muss so ausgestaltet sein, dass es jedem Nutzer möglich ist, seine Eintragungen während der Arbeitszeit an seinem Arbeitsplatz im DKFZ zu tätigen.
3. Die Eintragungen im elektronischen Laborbuch iLabber unterliegen wie auch beim Papier-Laborbuch der Verantwortung des Beschäftigten. Es gelten hierfür die Bestimmungen des DKFZ-Laborbuchs – diese sind als Anlage 2 beigefügt.

§ 5 Schulungen

Für die Nutzer werden mit der Einführung des Systems entsprechende Schulungsmaßnahmen angeboten.

Wesentliche Änderungen im System werden den Beschäftigten rechtzeitig bekannt gegeben. Sollte hierzu Schulungsbedarf bestehen, wird eine entsprechende Schulung angeboten.

Dienstvereinbarung – 3

§ 6 Rechte des Personalrats

Über wesentliche Änderungen des hier beschriebenen Systems iLabber wird der Personalrat rechtzeitig und umfassend vor der geplanten Durchführung informiert.

Die Anlage 1 wird in Bezug auf die IT-Komponenten auf dem aktuellen Stand gehalten, nur sonstige Änderungen bedürfen der vorherigen Zustimmung des Personalrats.

Ausgenommen von der Mitbestimmung sind Änderungen bzw. Erweiterungen, soweit sie der Erfüllung einer durch Gesetz, Rechtsverordnung, Tarifvertrag oder Dienstvereinbarung festgelegten Aufgabe dienen. Über diese ist im Vorfeld umfassend zu informieren und gegebenenfalls Einigkeit herzustellen.

Weitergehende Rechte nach LPVG bleiben hiervon unberührt.

Anlage Dienstvereinbarung – Organisatorische Rollen

- Benutzer
- Keyuser
- Abteilungsleiter
- IT-Systembetreuer

Anlage DV – Technische Rollen

- Benutzer (B)
- Gruppenadministrator (GA)
- Superuser (SU)
- User (B)
- ITCF
- BioVia/Contur*

Sichtbarkeit und Zugriffsmatrix

| Rolle | Eigene Experimente | Fremde Experimente | Eigene Gruppe | Fremde Gruppe | Eigene Projekte | Fremde Projekte | Server | Datenbank |
|----------------|--------------------|--------------------|---------------|---------------|-----------------|-----------------|--------|-----------|
| B | Ja | Nein | Ja | Nein | Ja | Nein | Nein | Nein |
| GA | Ja | Nein | Ja | Nein | Ja | Nein | Nein | Nein |
| SU | Nein | Nein | Ja | Ja | Ja | Ja | Nein | Nein |
| User | Nein | Nein | Nein | Nein | Nein | Nein | Nein | Nein |
| ITCF | Nein | Nein | Nein | Nein | Nein | Nein | Ja | Ja |
| *Contur | Nein | Nein | Nein | Nein | Nein | Nein | Nein | Nein |

*Contur erhält im Wartungsfalle vollständigen Zugang, welcher sonst geschlossen ist.

Rollout

- Schulungsplan ([link](#))
- Rolloutplan ([link](#))

Zentrale Vorstellung und Demo von iLabber

PRO

Suche

Lesbar (auch für andere)

Kein Medienbruch

Einfach zusätzliche Infos
anfügen

Vorlagen (Templates)

Einfach zu bedienen

Gemeinsame Experimente

Datenspeicherung

CONTRA

PC nötig

Notiz-Zettel an Sterilbank?

Lösung: Ausdrücke!

Einarbeitung

Abhängig von PC-Konfiguration:
Software kann auch mal
Probleme geben

... kurz vor der Einführung!



- Einführungsveranstaltung im Kommunikationszentrum
- Ankündigung via Newsletter
- Aushängen von Plakaten/Postern

Elektronisches Laborbuch

am Dienstag, den 15.1.2013 um 10:00 Uhr findet im Hörsaal H1 im Kommunikationszentrum eine Infoveranstaltung zum elektronischen Laborbuch statt. Es handelt sich um das Produkt „iLabber“ der Fa. Accelrys/Contur und wird als ein neuer Service der IT Core Facility angeboten. Sie sind alle herzlich dazu eingeladen. Es besteht die Möglichkeit, dass Accelrys am Nachmittag konkrete Fragen mit Ihnen in Ihrer Abteilung klärt.



Mitmachen

Im Intranet finden sie ein Formular unter IT-Core Facility. Bitte lesen sie dazu den Artikel im Wiki. Geben sie das ausgefüllte Formular im Servicezentrum ab. Damit sie bei der Praxis-einführung am 15.01.2013 mitwirken können, geben sie es bitte bis spätestens 28.12.2012 12:00 Uhr ab.

Vorteile

- Medienbrüche werden vermieden
 - Import von Bildern und Grafiken und PDF-Dokumenten
 - Einbinden von Excel-Tabellen
 - Verlinkung auf alle Arten von Daten
- Daten werden auf zentralem Server im DKFZ gesichert

Startveranstaltung für iLabber

15.01.2013 im

Kommunikationszentrum H1

10:00 Einführungsvortrag und Vorstellung
11:00 iLabber in Action
13:30 Praxiseinführung in den Abteilungen



iLabber

Es ist eine recht einfach zu bedienende Software. Das Bedienkonzept ähnelt geläufigen Textverarbeitungs- oder Gestaltungsprogrammen, wodurch ein übersichtliches und ein sauberes Erscheinungsbild entsteht. Damit ist eine intuitive Bedienung gewährleistet. Die Einsatzfähigkeit wurde mit einigen Projektgruppen innerhalb eines Pilotprojekts überprüft.

Erfahren Sie mehr:

Hersteller und original Produktinformation :
www.contur.com
ITCF-Wiki: <https://wiki.inet.dkfz-heidelberg.de/zdvwiki/index.php/iLabber>
IT-Systembetreuer und Projektleiter:
Heiko Rosenfelder (h.rosenfelder@dkfz.de)

Hilfen bei der Einführung

- Flyer
- Mailing Listen
- Hilfe Forum (SharePoint)
- Vorträge zentral
- Vorstellungsveranstaltungen in den Abteilungen
- Schwerpunktschulungen im Labor für Gruppen
- Schulung/Einweisung für Gruppenadministratoren

Newsletter – Flyer - Poster

Electronic Laboratory Notebook iLabber

check the connection to the webinterface

The standard computer which are delivered from ITCF are ready for using iLabber. See the article at our ITCF-Wiki, about the technical requirements. You can check your computer with following instructions:

Open your prevered webbrower with: <http://dkfz-eln01/ria>

1.) Login with your computer account



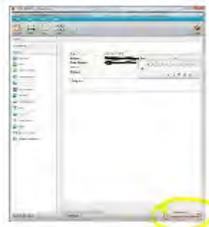
2.) Klick on bitton (start experiment)



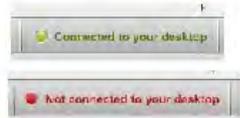
3.) Klick at following dialog on OK



4.) Check the message:



The message should be in green letters:



The version of Java is not compatible.
Please call the ITCF- service center at
2376

- Flyer
- Newsletter (Email)
- Hilfe Forum (SharePoint)

WIKI - Eintrag

The screenshot shows a web browser window displaying a wiki page. The browser's address bar shows the URL: https://itcfwiki.inet.dkfz-heidelberg.de/itcfwiki/index.php/ELN_-_elektronisches_Labornotizbuch. The page title is "Wiki der ITCF" and the subtitle is "Zentrale Einheit für Informationstechnologie". The main heading of the page is "ELN - elektronisches Labornotizbuch". Below the heading, there is a reference to "Deutsch" and a translation link to "English". A table of contents is displayed, listing sections from 1.1 to 1.10. The left sidebar contains navigation links such as "Start", "Home", "Service:", "UserIDs", "Hardwa", "Softwa", "Vorgabe", "Sonstigi", "Getting", and "Suche". At the bottom left, there is a "Servicezentrum" section with contact information and a list of services.

Wiki der ITCF
Zentrale Einheit für Informationstechnologie

ELN - elektronisches Labornotizbuch

ELN - elektronisches Labornotizbuch Reference: **Deutsch** – Translations: [English](#)

Inhalt [ausblenden]

- 1 ELN- ein elektronisches Labornotizbuch
 - 1.1 [Was ist ELN ?](#)
 - 1.2 [Vorteile](#)
 - 1.3 [Voraussetzung des Rechners vor Ort](#)
 - 1.4 [Administration und Rollen des ELN](#)
 - 1.5 [Die personelle Organisation einer "ELN" Umgebung](#)
 - 1.6 [Technischer Hintergrund](#)
 - 1.7 [Wie mache ich beim elektronischen Labornotizbuch ELN mit ?](#)
 - 1.8 [Verlassen des DKFZ oder Beenden der Aktivität im elektronischen Labornotizbuch, wie übergebe ich meine Daten und Experimente?](#)
 - 1.9 [Einstieg und Informationen über den Hersteller](#)
 - 1.10 [Weitere Information](#)

Servicezentrum
Gebäude: INF281 (Doku.)
Raum: D030

- gut lesbares und sauberes „Look and Feel“ in Dokumentenform, schön präsentieren!
- PDF-Export
- regelmäßiges Backup durch Speichern der Daten auf Servern (stehen im DKFZ I)
- Möglichkeiten des Teilens oder Freigeben von Inhalten

BioVia – elektronisches Laborbuch - aktuell

- 1000 Lizenzen
- Zur Zeit 600 belegt
- In 112 Gruppen
- 980 Projekte
- Webclient
- Windowsclient
- Nur intern!

[Antrag](#)



dkfz.

dkfz.

DEUTSCHES
KREBSFORSCHUNGSZENTRUM
IN DER HELMHOLTZ-GEMEINSCHAFT



Forschen für ein Leben ohne Krebs

Tobias Duden, Physikalisch-Technische Bundesanstalt (PTB): Das beweissichere elektronische Laborbuch (BeLab) in der Physikalisch-Technischen Bundesanstalt (PTB)

Abstract

Das beweissichere elektronische Laborbuch (BeLab) in der Physikalisch-Technischen Bundesanstalt (PTB) ist eine prototypische Umsetzung des erfolgreich abgeschlossenen DFG-Projekts BeLab. Der Vortrag geht auf rechtliche und funktionale Grundlagen des BeLab ein und stellt dar, worauf es bei der Beweiswerterhaltung von Dokumenten im Rahmen der Langzeitspeicherung ankommt. Im weiteren wird die prototypische Umsetzung in der PTB erläutert.

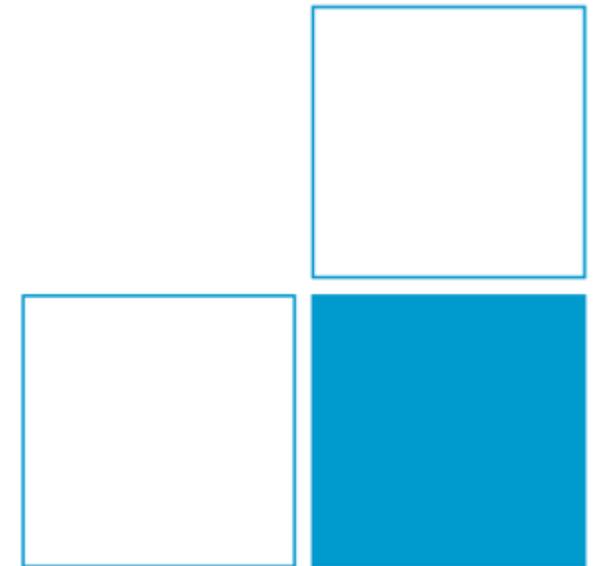
Jede Institution, die elektronische Dokumente dauerhaft aufbewahren und dabei deren Beweiswert erhalten muss, sollte sich mit dem vorgestellten Thema beschäftigt haben.



Physikalisch-Technische Bundesanstalt
Braunschweig und Berlin
Nationales Metrologieinstitut

Das beweissichere elektronische Laborbuch in der PTB

BeLab



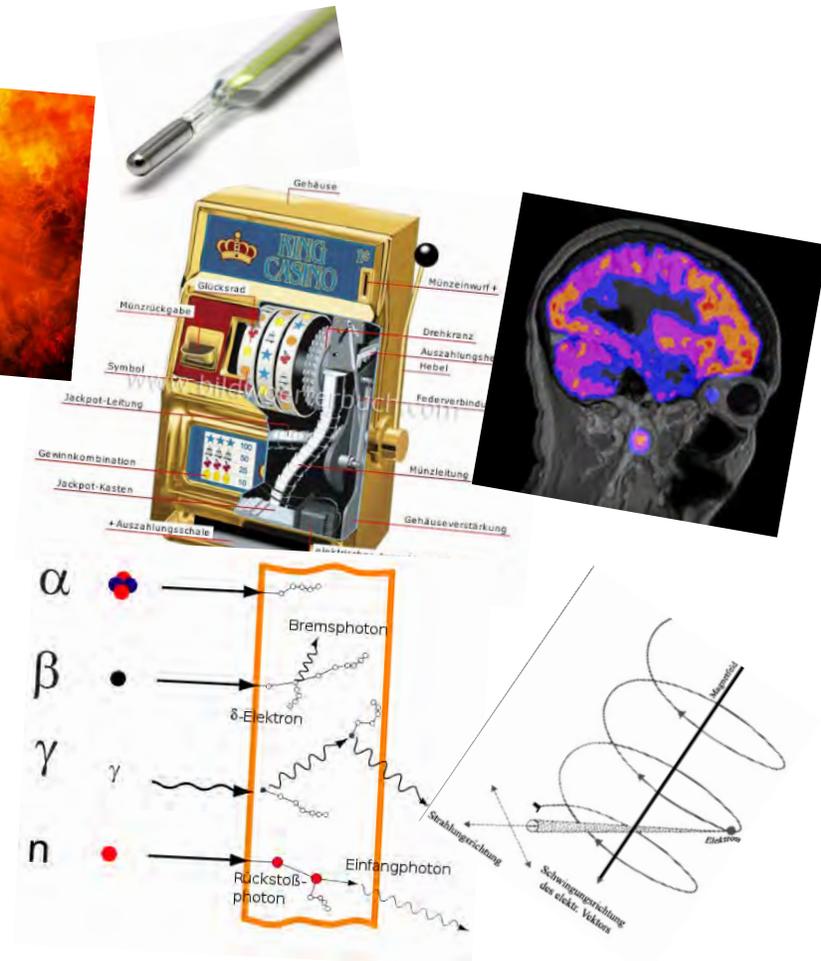
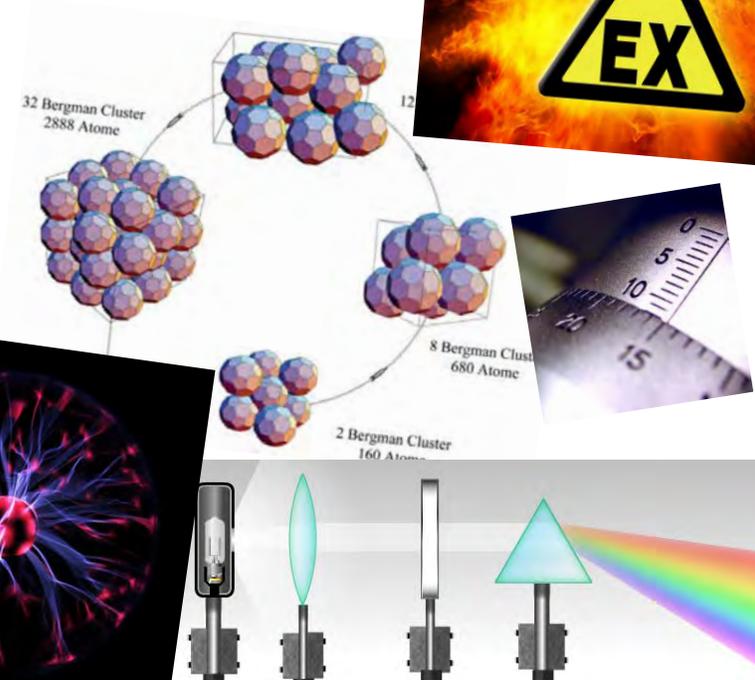
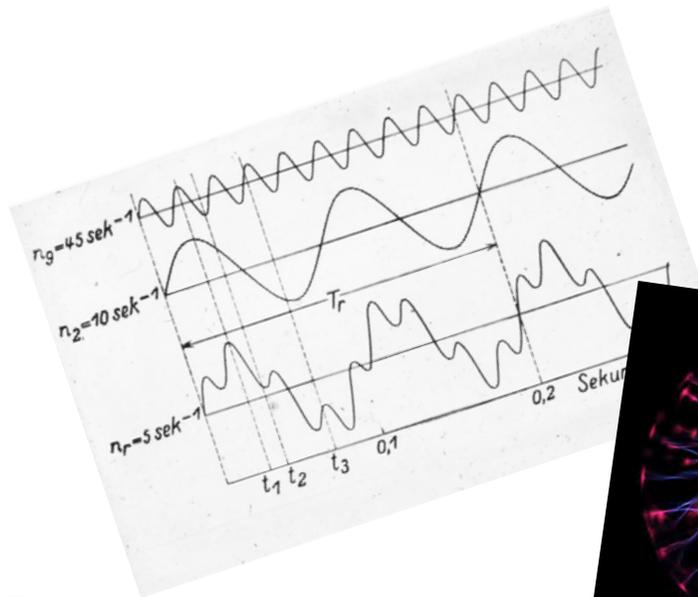


**Physikalisch-Technische Bundesanstalt
Braunschweig und Berlin**

Zielstellung

Beweisichere, langfristige Speicherung von experimentellen Primär- und Sekundärdaten

...wie sie in der PTB vorkommen.



Verwaltungsrechtlicher Rahmen

§18 Abs. 1 S. 2 Registraturrichtlinie Bundesministerien (RegR):

„Bei elektronisch gespeichertem Schriftgut sind die Vollständigkeit, Integrität, Authentizität und Lesbarkeit durch geeignete Maßnahmen zu gewährleisten.“

BeLab

Anforderungen, Konzepte und Umsetzung zur langfristigen, beweiswerterhaltenden Archivierung elektronischer Forschungsdaten und –dokumentation



Gefördert durch:
DFG Deutsche
Forschungsgemeinschaft

U N I K A S S E L
V E R S I T Ä T



BeLab - rechtliche Kriterien (1/2)

- Zurechenbarkeit
 - Identifizierung, Zuordnung, Zugriff, Protokollierung
- Verwertbarkeit
 - Nachnutzung, Übertragbarkeit, Verkehrsfähigkeit
- Durchsetzung von Rechten
 - Beweismittleignung, Beweismitteltransparenz
- Aufbewahrung
 - Langzeitarchivierung, Beweiswerterhaltung



Gefördert durch:
DFG Deutsche
Forschungsgemeinschaft

U N I K A S S E L
V E R S I T Ä T



BeLab - rechtliche Kriterien (2/2)

- Freie Forschungsgestaltung
 - Wissenschaftliche Selbstbestimmung
 - Arbeitserleichterung
- Datenschutz
 - Datenschutz Dritter
 - Datenschutz des Wissenschaftlers
- Vertraulichkeit und Integrität der Systeme
 - Mandantenfähigkeit und Organisationsflexibilität
 - Technische Sicherungen



Gefördert durch:
DFG Deutsche
Forschungsgemeinschaft

U N I K A S S E L
V E R S I T Ä T



BeLab – funktionale Anforderungen (1/2)

- Integritäts- und Authentizitätssicherung
- Automatisierte Sicherung der Datenerhebung
- Zugriffskontrolle, Zugriffsrechte, Mandantenfähigkeit
- Bewertung und Klassifikation
- Langfristige Verfügbarkeit



Gefördert durch:
DFG Deutsche
Forschungsgemeinschaft

U N I K A S S E L
V E R S I T Ä T



BeLab – funktionale Anforderungen (2/2)

- Langfristige Sicherheit und Überprüfbarkeit elektronischer Signaturen und Zeitstempel
- Metadatenkonzept
- (Vermeiden von) Datenkonvertierung (→Transidoc)
- Nachnutzung



Gefördert durch:
DFG Deutsche
Forschungsgemeinschaft

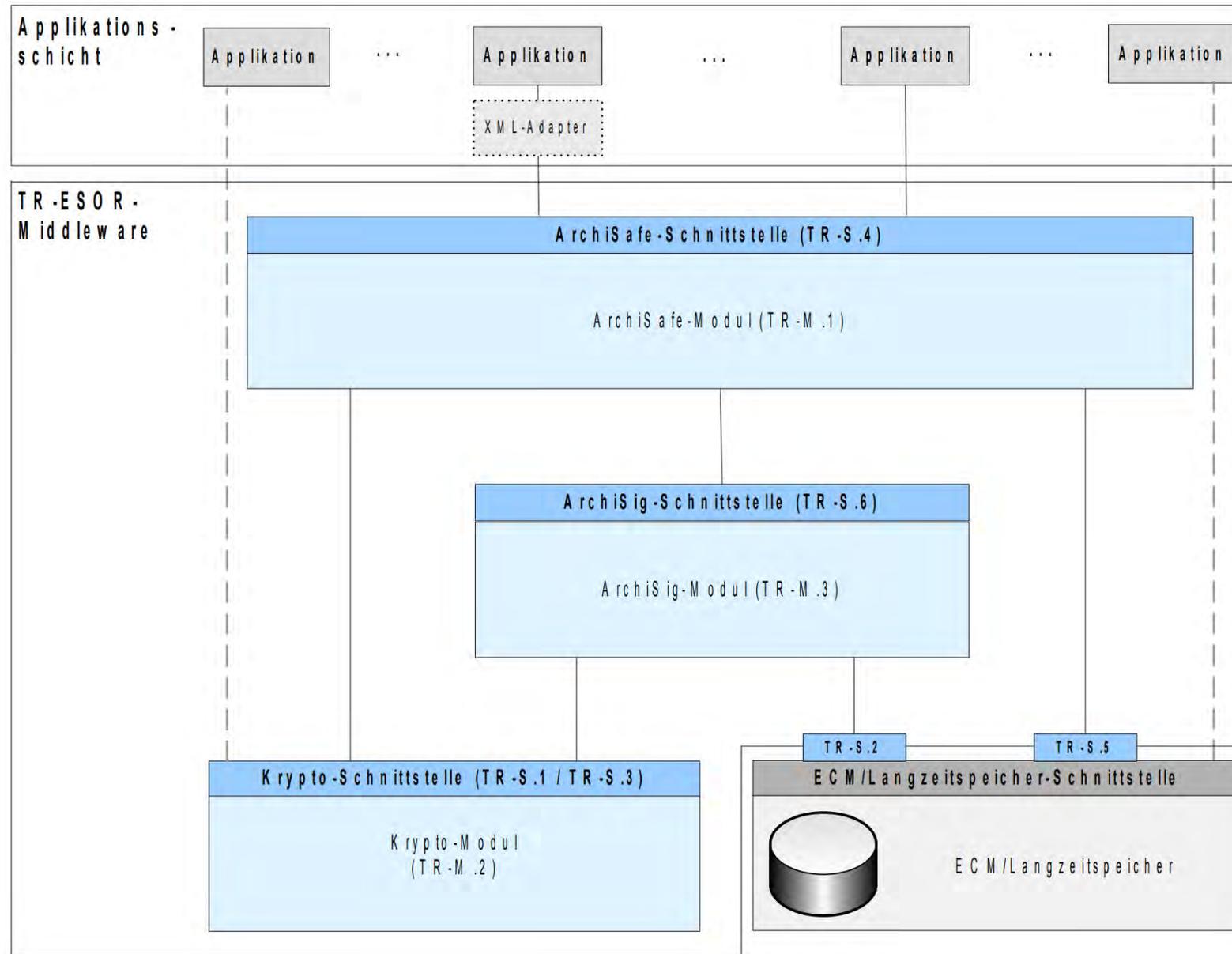
U N I K A S S E L
V E R S I T Ä T



Beweiswerterhaltung

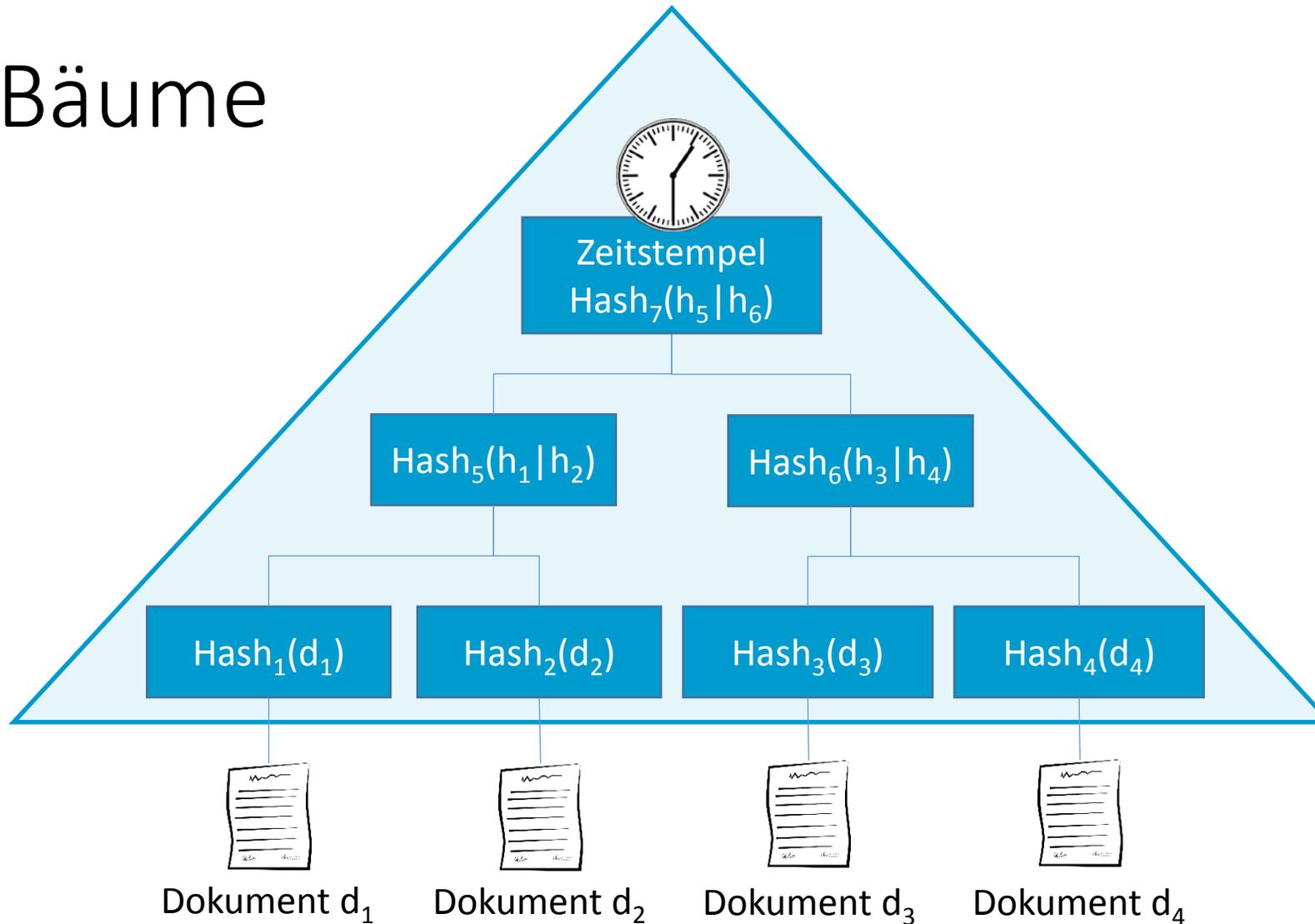
- Qualifizierte elektronische Signaturen nach Verordnung (EU) Nr. 910/2014 des Europäischen Parlaments und des Rates vom 23. Juli 2014 (eIDAS)
- BSI TR-03125 (TR-ESOR): Beweiswerterhaltung kryptographisch signierter Dokumente
- BSI-CC-PP-0049-2014 (ArchiSafe)





Quelle: BSI TR-03125

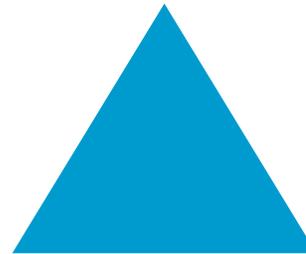
Hash-Bäume



Beweis-Dokument



Dokument d_1



Reduzierter Hash-Baum



Zeitstempel

Das BeLab-Konzept in der PTB

**Elektronisches
Laborbuch**



**Middleware
zur Langzeit-
speicherung**



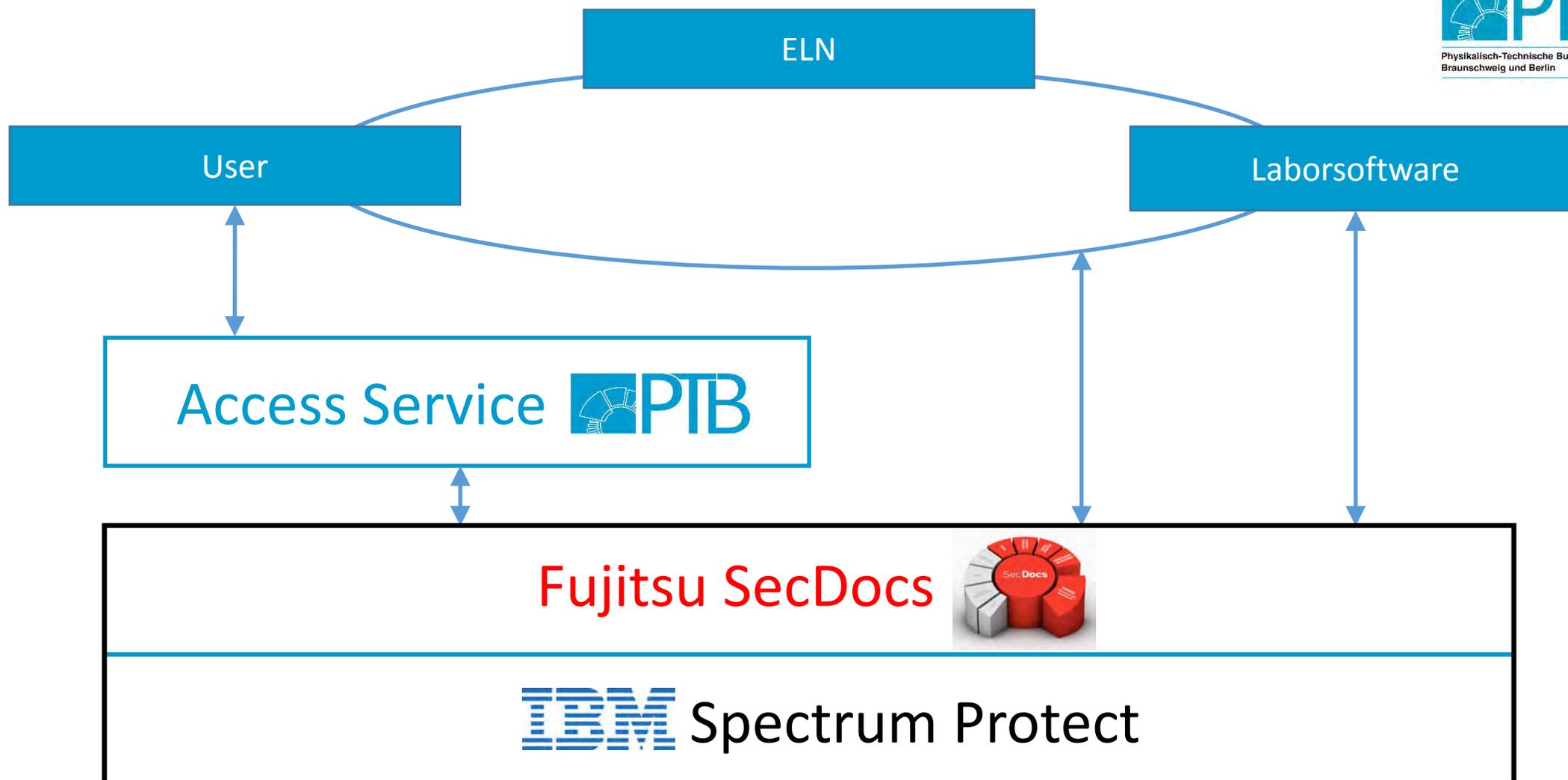
**Physisches
Speichersystem**

Das BeLab-Konzept in der PTB

Access Service

**Middleware zur
Langzeit-
speicherung**

**Physisches
Speichersystem**



SecDocs Archive Service

Search | Archive

Not for productive use

Login

Username

Password

 Remember Me[LOGIN](#)[FORGOT YOUR PASSWORD?](#)

Archivar

Select an Organisation

Abteilung 1

Select an archivescheme

Abteilung_1

[> WEITER](#)

Add MetaData and Files

* = Pflichtfeld

Id

2017-11-18-ID002

Author*

EUROPEAN COMMISSION DIRECTORATE-GENERAL FOR RESEARCH & INNOVATION

Abteilung

Q,4

Company

PTB

Description

Declaration document of european open science cloud

Keywords

EOSC, Declaration

creationDate*

26.10.2017

creationDate*

26.10.2017

lastChangedDate*

26.10.2017

lastChangeBy*

DIRECTORATE-GENERAL FOR RESEARCH & INNOVATION

Tags

carriedOutBy

Titel*

EOSC Declaration

Files

eosc_declaration.pdf

 ARCHIVE DATA



SAS

[Dashboard](#)

[Search for SciELN-Entry](#)

[Archive](#)

[Help](#)

[Tobias Duden](#)

SDO submitted successfully

Search SecDocs via MetaData

Author

Complete Match

Abteilung

Complete Match

lastChangedDate

to

Titel

EOSC

Complete Match

Results

| AOID | Author | Abteilung | lastChangedDate | Titel | Select |
|--------------------------------------|---------------------|-----------|-------------------------|------------------|---|
| b302b505-06d1-436f-b822-721010753657 | EUROPEAN COMMISSION | Q.4 | 2017-10-26T00:00:00.00Z | EOSC Declaration |  |

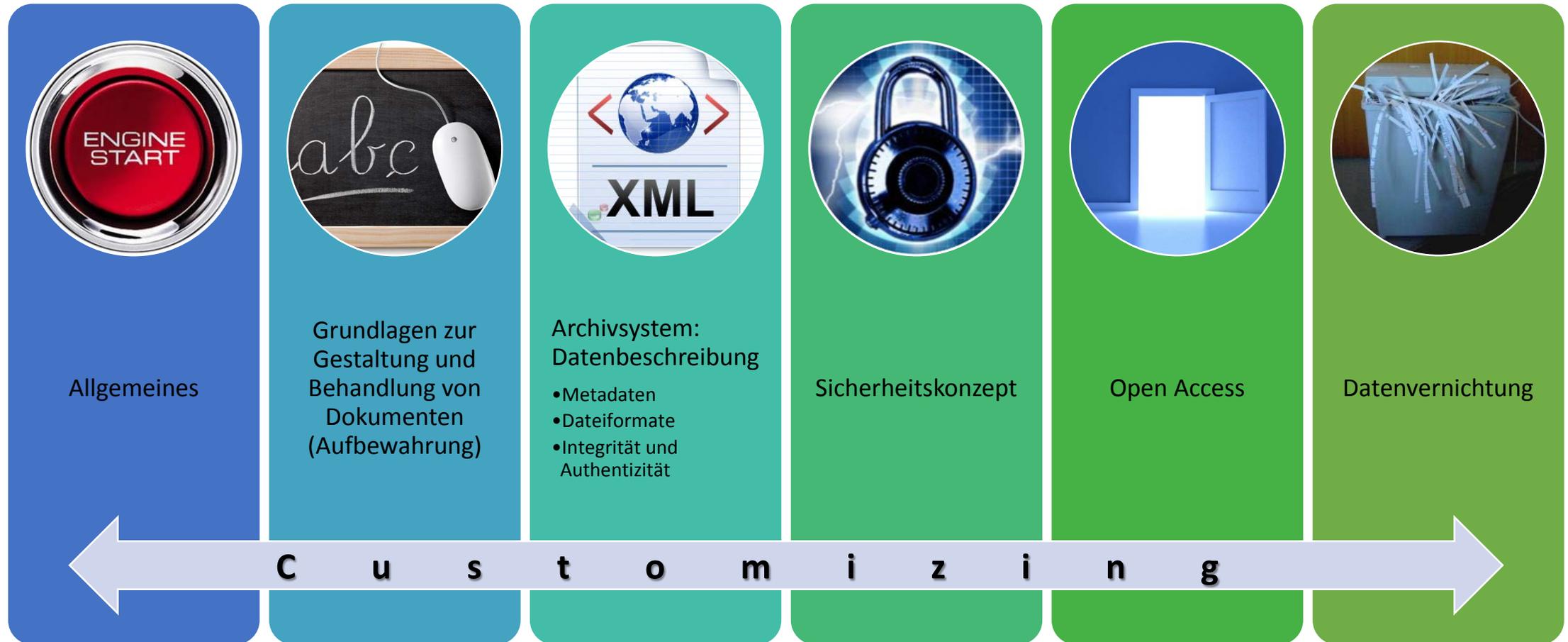
View SDO

| | |
|------------------------|--|
| Id | 2017-11-18-ID002 |
| Author | EUROPEAN COMMISSION |
| Abteilung | Q.4 |
| Company | PTB |
| Description | Declaration document of european open science cloud. |
| Keywords | EOSC, Declaration |
| creationDate | 2017-10-26T00:00:00+00:00 |
| lastChangedDate | 2017-10-26T00:00:00+00:00 |
| lastChangeBy | DIRECTORATE-GENERAL FOR RESEARCH AND INNOVATION |
| Titel | EOSC Declaration |
| File | EOSC_DECLARATION.PDF |

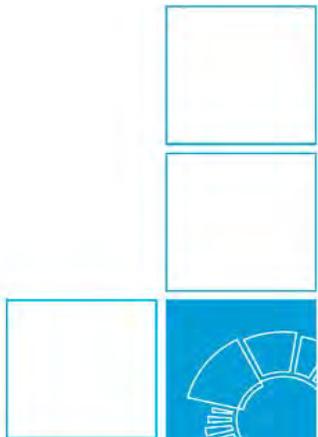
Bewertung

- Erfüllung der rechtlichen Aspekte (z.B. Integrität, Authentizität der Daten, Beweistransparenz, Aufbewahrungsfristen)
- Datenschutz und freie Forschungsgestaltung sind gewährleistet
- Vertraulichkeit in die Integrität des Systems durch Dokumentation
- Durchsetzbarkeit von Rechten: Erfolgreiche Simulationsstudie
- Policy als Klammer der technischen Umsetzung

Policy zur Langzeitspeicherung



Vielen Dank für die Aufmerksamkeit!



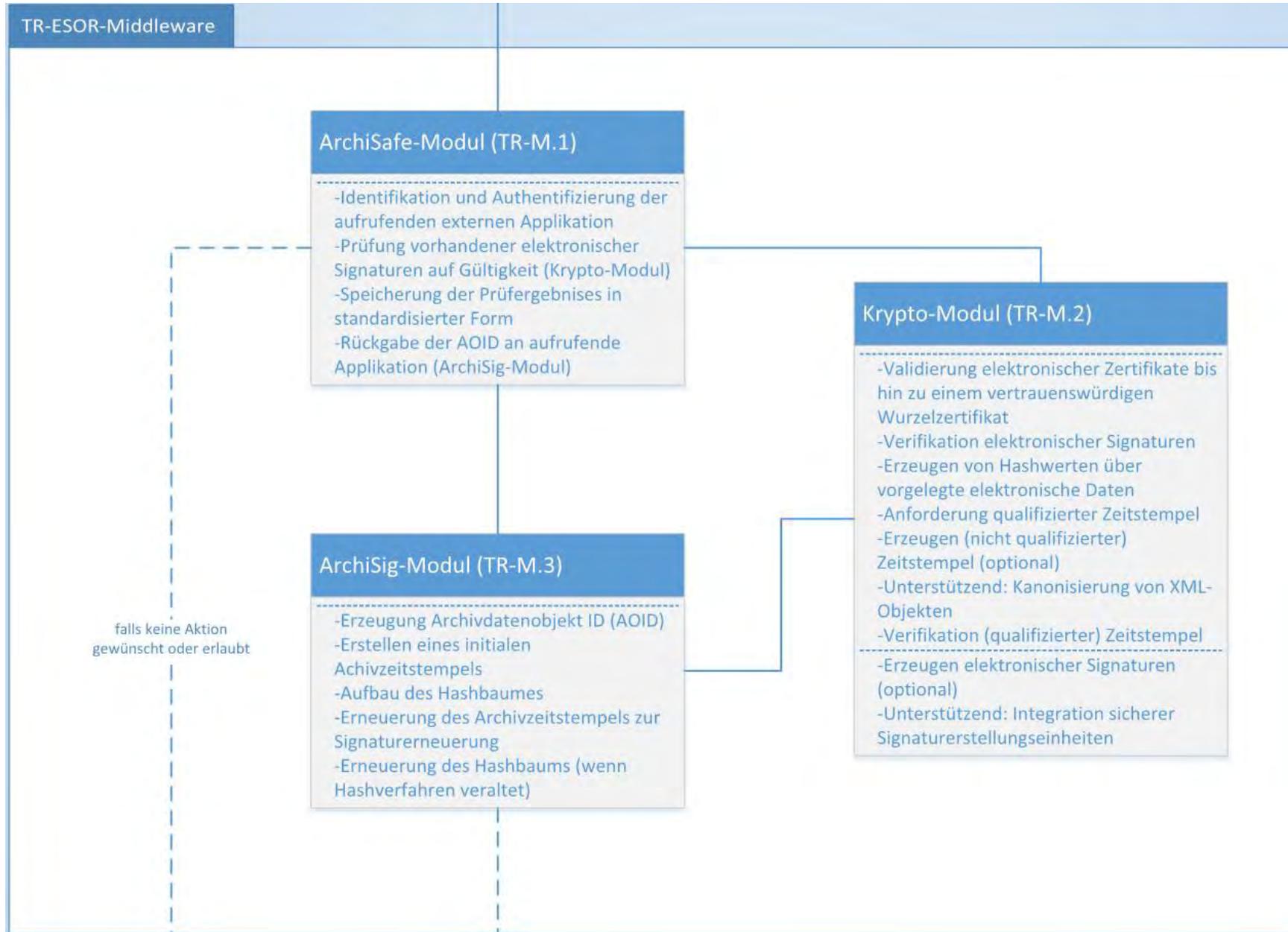
Physikalisch-Technische Bundesanstalt
Braunschweig und Berlin
Q.4 – Informationstechnologie
Bundesallee 100
38116 Braunschweig

Tobias Duden

tobias.duden@ptb.de

0531/592-8407

Backup



| Ende | | Experimentierung | | | |
|------|---|--|---|--|-------------------|
| 1 | <p>15.08.2014 12:51:42 </p> <p>15.08.2014 14:45:46 </p> | <p>Hotplate temp: 160 °C</p> <p>Lack: PMMA 200k 2% 641.02 </p> <p>Suchen</p> | <p>Hotplate soll: 160 °C</p> <p>rpm: 2000</p> | <p>Zeit: 1,5 min</p> <p>Prog: 1</p> <p>innerhalb von 1 Stunde, 54 Minuten</p> | <p>↑</p> <p>×</p> |
| 2 | <p>15.08.2014 15:00:00 </p> <p>15.08.2014 15:34:09 </p> | <p>Congovac</p> <p>Material: 1.0x Aufdampfmaterial Au </p> <p>Suchen</p> <p>Rate: 0,200 nm/s</p> <p>Leistung: 3 %</p> <p>P-Start: 20 *10-3 mbar</p> | | <p>Dicke: 30 nm</p> <p>Tooling Faktor: 94 %</p> <p>Strom: 20 A</p> <p>P-Betrieb: 10 *10-3 mbar</p> | <p>↑</p> <p>×</p> |
| 3 | <p> </p> <p> </p> | <p>Belichtung mit</p> <p>Kommentar</p> | | <p>EBPG 5000+ (Linux)</p> <p></p> | <p>↑</p> <p>×</p> |
| 4 | <p> </p> <p> </p> | <p>Waschen mit</p> <p>nicht gesetzt </p> <p>Suchen</p> | <p>3 x </p> <p>ml </p> <p>Kommentar </p> | | <p>↑</p> <p>×</p> |
| 5 | <p> </p> <p> </p> | <p>Entwicklung</p> <p>Entwickler: nicht gesetzt </p> <p>Suchen</p> <p>Stopper: nicht gesetzt </p> <p>Suchen</p> <p>Abgeschleudert? <input type="checkbox"/></p> | | <p>Dauer: sec</p> <p>Dauer: sec</p> <p>Spulen? <input type="checkbox"/> sec</p> | <p>↑</p> <p>×</p> |

Add object

Prozessschritt hinzufügen +

Durchführung

Die Arbeiten konnten problemlos durchgeführt werden.

Link einfügen

nicht gesetzt

Laborjournaleintrag

Bild einfügen

Harald Kusch, Georg-August-Universität Göttingen: Pilot-Integration eines elektronischen Laborbuchs und eines Open-Source-Forschungsdaten-Repositorys als Bestandteil einer modularen biomedizinischen Forschungsdatenplattform

Abstract

In den biomedizinischen Sonderforschungsbereichen (SFB) 1002 („Modulierende Einheiten bei Herzinsuffizienz“) und 1190 („Kompartiment- und Kontaktstellen in Zellen“), koordiniert durch die Universitätsmedizin Göttingen, wird die Organisation von Forschungsdaten durch eine integrierte und langfristig zugängliche Forschungsdatenplattform unterstützt (RDP). Als zentrales RDP-Modul haben wir vor einiger Zeit ein Elektronisches Laborbuch (ELN) implementiert, um eine strukturierte Vernetzung der großen Heterogenität digitaler biomedizinischer Forschungsdaten mit der primären experimentellen Dokumentation „am Arbeitsplatz“ zu ermöglichen. Das ausgewählte kommerzielle ELN „RSpace“ ist konzipiert als ein kooperatives und konnektives Werkzeug mit Schnittstellen zu einer Vielzahl von vorhandenen Forschungsdaten-Repositoryn. Um die Vorteile einer einfach zu handhabenden Integration des ELN und eines Open-Source-Forschungsdaten-Repositorys zu demonstrieren, hat die Göttinger eResearch Alliance eine Pilot-Implementierung von „Dataverse“, unterstützt vom Entwicklerteam der Harvard University, durchgeführt.

ELN und das Repository spielen komplementäre und sich gegenseitig verstärkende Rollen bei der langfristigen und nachhaltigen Datenhaltung. Das ELN bietet Forschern eine einfach zu bedienende, praktische Plattform zum Erfassen und Beschreiben der täglichen Arbeit und der dabei erzeugten Forschungsdaten sowie deren Verknüpfung, wenn sie auf zentralen Labor- und institutionellen Servern gespeichert sind. Die Zentralisierung von Forschungsdaten im ELN reduziert die Menge an unnötigen Medienunterbrechungen und vereinfacht dadurch die Datenverfügbarkeit, für den Transfer in Open-Source-Repositoryn (z. B. „Dataverse“). Sobald die Forschungsdaten in Dataverse registriert sind, stehen sie für eine gemeinsame Untersuchung und Abfrage im Sinne der FAIR-Prinzipien zur Verfügung. Die einfach zu bedienende ELN-Repository-Schnittstelle erleichtert diesen Prozess und ermöglicht die gemeinsame Nutzung von Forschungsdaten zwischen Forschungseinrichtungen und unabhängig von Lizenzverfügbarkeiten für ein bestimmtes ELN-Produkt.

Pilot integration of an electronic lab notebook and an open source research data repository as part of a modular biomedical research data platform

Harald Kusch, orcid.org/0000-0002-9895-2469

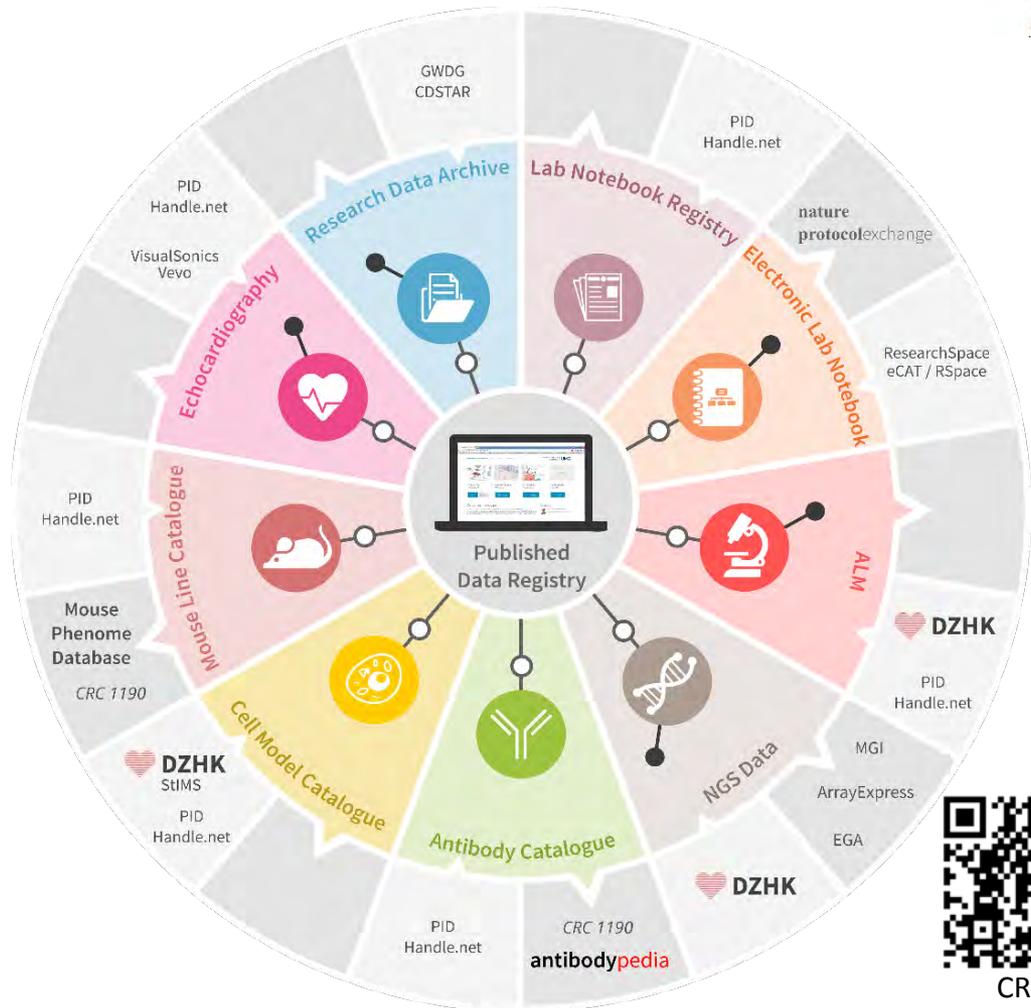
Sara Nußbeck, orcid.org/0000-0003-1223-6494

Péter Király, orcid.org/0000-0002-8749-4597

Rory Macneil

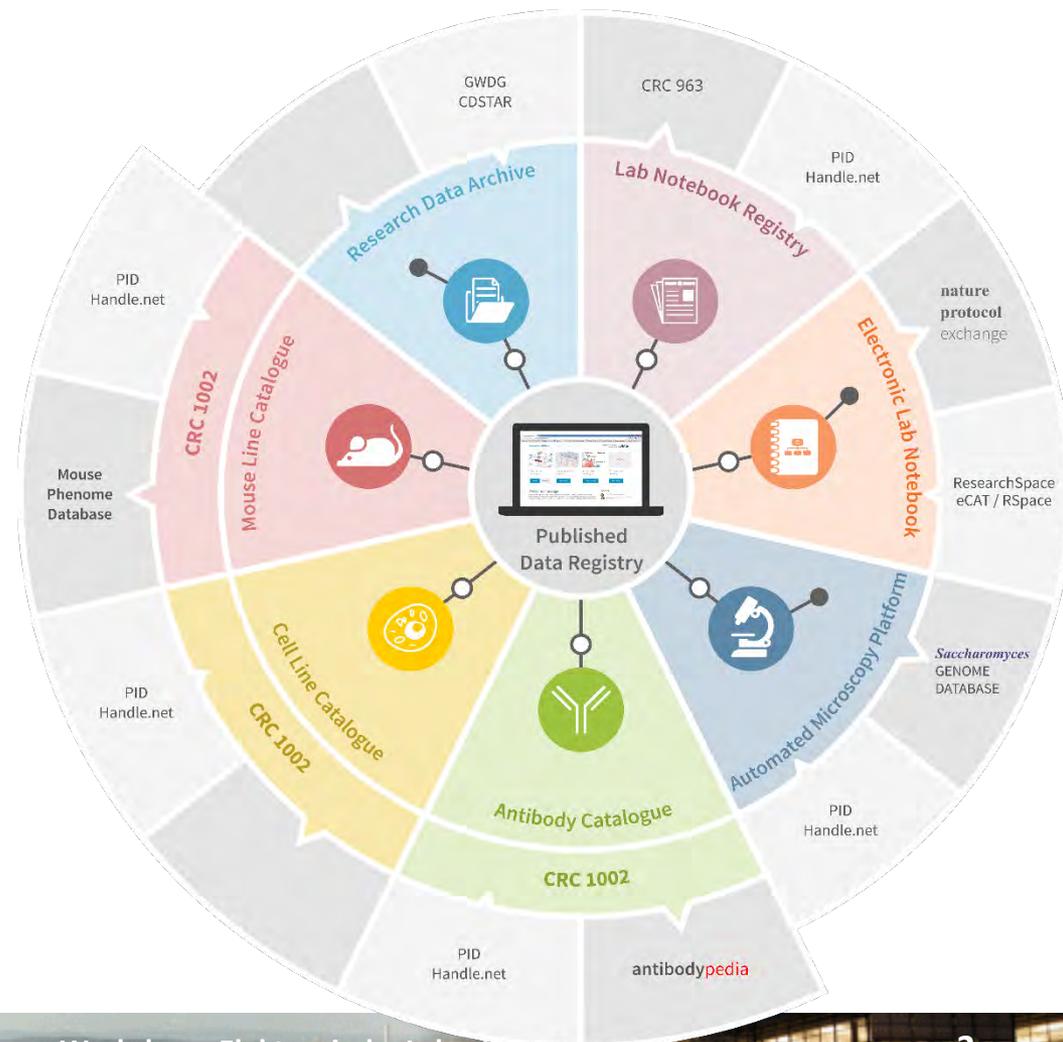
Mercè Crosas, orcid.org/0000-0003-1304-1939

- Collection and interconnection of research data used in publications
- Persistent resolvable access and long-term re-usability of CRC 1002 data
- Data standardization for submission to public repositories
- Data access: Development of Use & Access Policies



CRC 1002
Research Data Platform

RDP Modules are re-used and shared in **CRC 1190** Research Data Platform



- No routine workflows (basic research)
- Dynamic working structures (heterogeneous methodology)
- High dynamics of interdisciplinary team composition
- Data management/access policies rarely defined

- Hard to follow rapid changes on overwhelming ELN market
- Acceptance of users (time and resource investment plus changing century old habits)
- Supplying 24/7 professional support
- Individual vs. institutional requirements

CRC 1002 (Scientific Consortium)

Research Group 1

1. Community (optional)
2. PI
3. Lab Manager
4. User (Scientist)

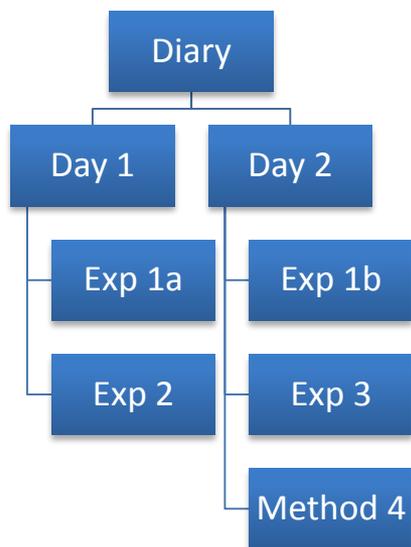


Research Group 2

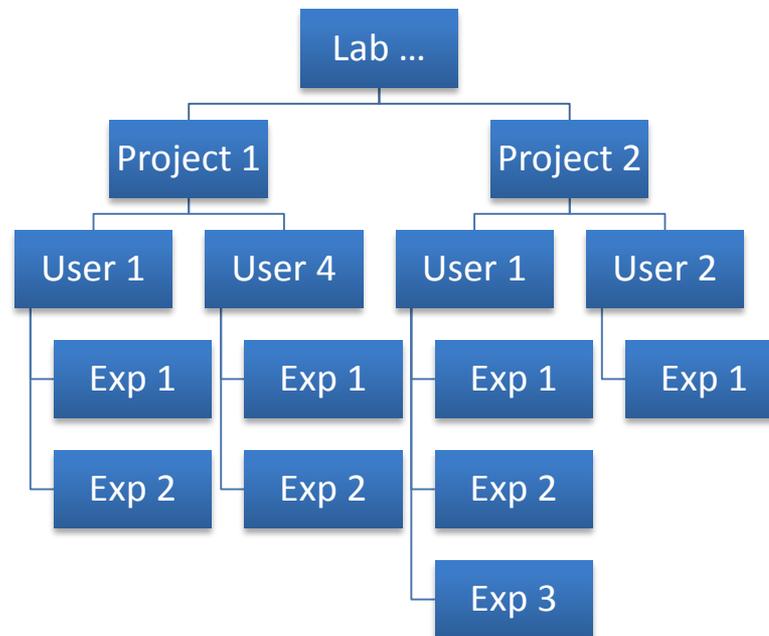
1. Community (optional)
2. PI
3. Lab Manager
4. User (Scientist)



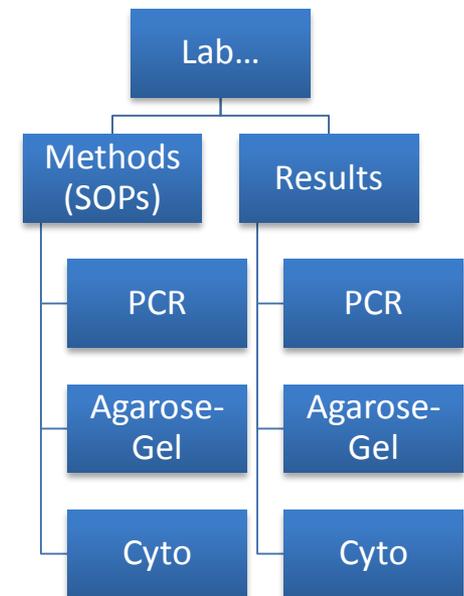
a. Chronologically



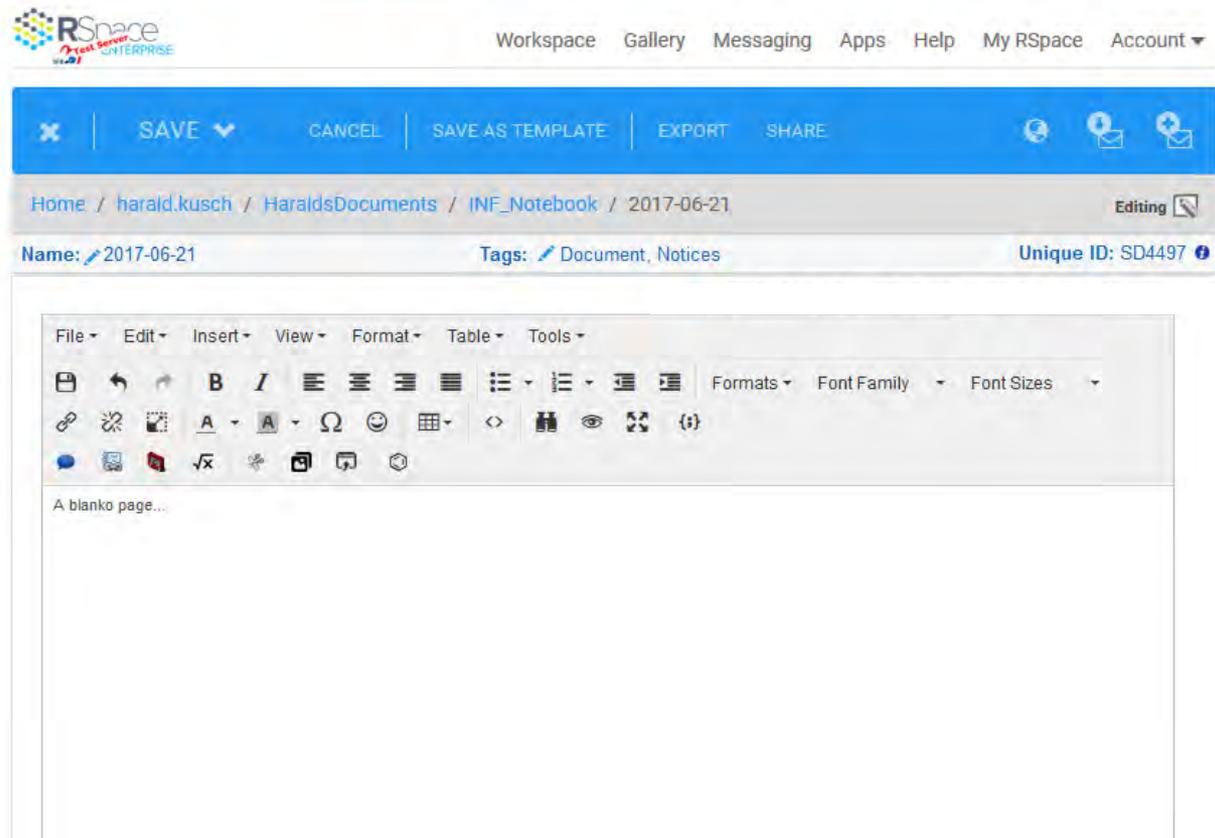
b. Project-oriented



c. Method-oriented



- New methods
- Room for “creativity”



The screenshot displays the RSpace web interface. At the top, there is a navigation bar with links for Workspace, Gallery, Messaging, Apps, Help, My RSpace, and Account. Below this is a blue action bar with buttons for SAVE, CANCEL, SAVE AS TEMPLATE, EXPORT, and SHARE. The breadcrumb path is Home / harald.kusch / HaraldsDocuments / INF_Notebook / 2017-06-21. The document name is 2017-06-21, and it is tagged as Document and Notices. The Unique ID is SD4497. The main editing area features a rich text editor with a menu bar (File, Edit, Insert, View, Format, Table, Tools) and a toolbar with various icons for text formatting, alignment, and insertion. The text area currently contains the placeholder text "A blanko page...".

- Centralized protocols
- Learning tool
- Quickly shared
- Metadata recording facilitated

Name: Western blot Tags: Unique ID: SD5059

Field 17/01/2017

Samples

Sample cells 1
Sample cells 2
Sample cells 3

Block solution

250 ml 25 ml 10 X TBS, 12.5 g milk powder

Block solution date

17/01/2017

Primary antibody

GST 1mg/ml, Rohn 3998.1

Link to research data platform

<https://fb1002.mad.uni-goettingen.de/reduction/>

Primary antibody dilution

1:1000

Primary antibody incubation time in min

60 min
 90 min
 overnight
 other

Primary antibody incubation temperature

RT

Secondary antibody

IRDye 800 CW Donkey anti-Rabbit IgG

Secondary antibody supplier

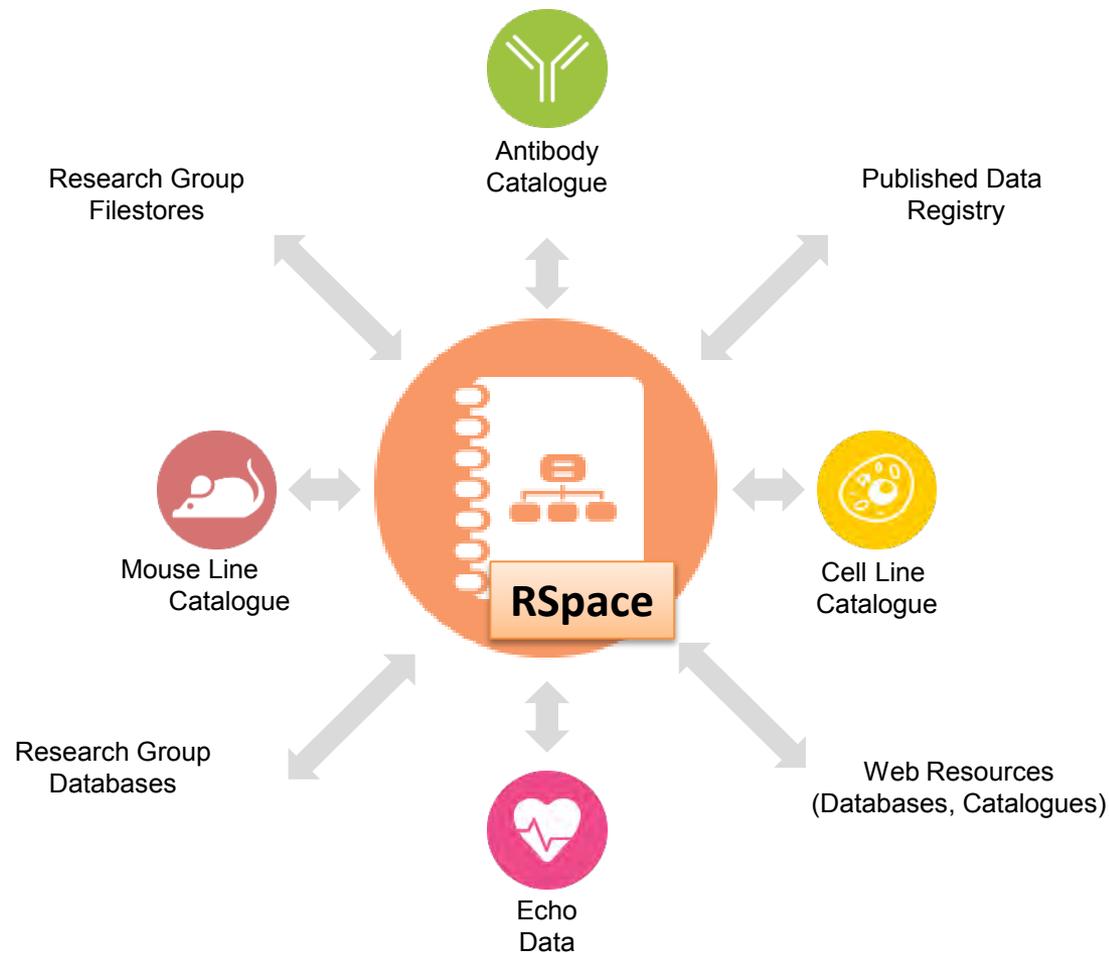
PN 928-32213, LI-COR INC.

Secondary antibody dilution

1:5000

ELN data organization

Cross-linking data in a connected ELN



Name:  Manual antibody description

Tags: 

Unique ID: SD6216 



The antibody used in the experiment is p115 (BD Biosciences Catalog no. 612261). It is highly specific and stored at -20°C.

View primary antibody

Basic data

| | |
|----------------|---|
| PID | umg-sfb1002-antibody-primary-656 |
| EPIC PID | https://hdl.handle.net/11022/umg-sfb1002-antibody-primary-656 |
| Research group | AG Lehners |
| Quality (mean) | no score (0.00) |
| Sharing level | Group |

Name:  Cross-linked antibody description

Tags: 

Unique ID: SD6218 



Used Antibody: <https://hdl.handle.net/11022/umg-sfb1002-antibody-primary-656>

Antibody data

| | |
|-------------------------|-------------------------------|
| Antigen symbol | |
| Antibody Registry ID(s) | AB_399578 |
| Name | p115 |
| Alternative name | Golgi Marker |
| Tag / Fluorophore | |
| Raised in | Mouse |
| Reacts with | Mouse |
| Clone | |
| Isotype | IgG1 |
| Clonality | monoclonal |
| Demasking | unknown |
| Antigen | rat p115 aa 843-955 |
| Crafted By | company |
| Company / Manufacturer | BD Biosciences |
| Catalog no. | 612261 |
| Lot no. | |
| Description | high specific |
| Localization | |
| Storage instruction | -20°C |
| Receipt date | 2017-11-06 00:00:00 |
| Preparation date | 2017-11-06 00:00:00 |
| Created by | AuHenbrandt, Georg |
| | AuHenbrandt, Georg |



- Cross-linking of primary research data
- Enables remote access to lab data
- Exports contain automatic lists of cross-linked data

Owner: Harald Kusch | Calculation Table Example | Page: 3

Network files

| File System id | File System URL | Path |
|----------------|--|--------------------------------|
| 1 | smb://filer4.be-mrz.med.uni-goettingen.de/Gruppenlaufwerk_ML_Prak/Projekte/SFB1002/ELN_Filestore | eCAT-Schulung/ImportExcel.xlsx |

Export date: 2018-02-27, Exported by: Harald Kusch

File details:

Name: ImportExcel.xlsx
Full path: eCAT-Schulung/ImportExcel.xlsx
Stored on a File System:
Name: Mltest
URL: smb://filer4.be-mrz.med.uni-goettingen.de/Gruppenlaufwerk_ML_Prak/Projekte/SFB1002/ELN_Filestore

Download

Order by: Select None

Insert

Filestores

Filestore: Test

- FirstFolder
- ImportExcel.xlsx
- Journal.pone.0025290.pdf
- Microscopy.PNG
- PCR-Wiki.png
- SecondFolder
- Test
- TestImportRSpace.docx
- Thumbs.db
- westernblot.jpg

File Explorer: eCAT-Sch... | ELN... | eCAT-Sch...

Name

- FirstFolder
- SecondFolder
- Test
- ImportExcel.xlsx
- Journal.pone.0025290.pdf
- Microscopy.PNG
- PCR-Wiki.png
- TestImportRSpace.docx
- Thumbs.db
- westernblot.jpg

10 Elemente

) must be protected from light.

| | D | E | F | G | H |
|-----|---|----------------------------|---|---|---|
| 1 | | I RIPA Buffer | | | |
| 150 | | ml NaCl stock solution | | | |
| 50 | | ml Tris HCl stock solution | | | |

Implemented ORCID integration



Workspace Gallery Messaging Apps Help My RSpace Account ▼



My Profile - Username: harald.kusch

First Name: Harald

Last Name: Kusch

Optionally, add any information about you or your research.

E-Mail: harald.kusch@med.uni-goettingen.de

ORCID:  <http://orcid.org/0000-0002-9895-2469>

Manage API key

Harald Kusch

ORCID ID

 orcid.org/0000-0002-9895-2469

Country

Germany

Keywords

Forschungsdatenmanagement, e-Science, Digital Medicine, Digital transformation, Biomedical informatics

Websites

UMG Medizinische Informatik
CRC 1002 Research Data Platform
Mendeley profile
Linked In Profile
Researchgate Profile
RDA Profile

Other IDs

ResearcherID: I-5912-2015

▼ Employment (4)

IT Sort

Universitätsmedizin Göttingen: Göttingen, Niedersachsen, Germany
2014-08 to present

Scientist (Institut für Medizinische Informatik)

Source: Harald Kusch

Created: 2015-05-06

Georg-August-Universität Göttingen: Göttingen, Niedersachsen, Germany
2010-08 to 2014-08

Scientist (Institut für Mikrobiologie und Genetik)

Source: Harald Kusch

Created: 2015-05-06

Ernst-Moritz-Arndt Universität Greifswald: Greifswald, Mecklenburg-Vorpommern, Germany
2005 to 2010

(Institut für Mikrobiologie)

Source: Harald Kusch

Created: 2016-10-27

Julius-Maximilians-Universität Würzburg: Würzburg, Bayern, Germany
2000 to 2004

Audit Trail

Signing/Whitnessing

Audit: My RSpace Activity

You can filter this audit by [Actions](#) and Date Range

Select date range to audit From To

Found 160 hits.

| User | Action | Type | Resource | Name |
|------|--------------------------|----------------|-----------------------------|--|
| | Modification Date | | Modification Details | Options |
| | 2017-01-31 14:22:00 | RENAME | | View Restore |
| | 2017-01-31 14:22:18 | RENAME | | View Restore |
| | 2017-01-31 14:25:04 | FIELD_CHG-Data | | View Restore |
| | 2017-01-31 14:28:39 | FIELD_CHG-Data | | View Restore |

[Show more ...](#)

Signing Document

Choose a signing statement:

I affirm that this document is a true and accurate description of work performed by me on the dates indicated in the system records.

This is the final version of this document and I have locked it to prevent additional edits.

Easy additional re-usable archiving strategies:

Regular Data-Exports

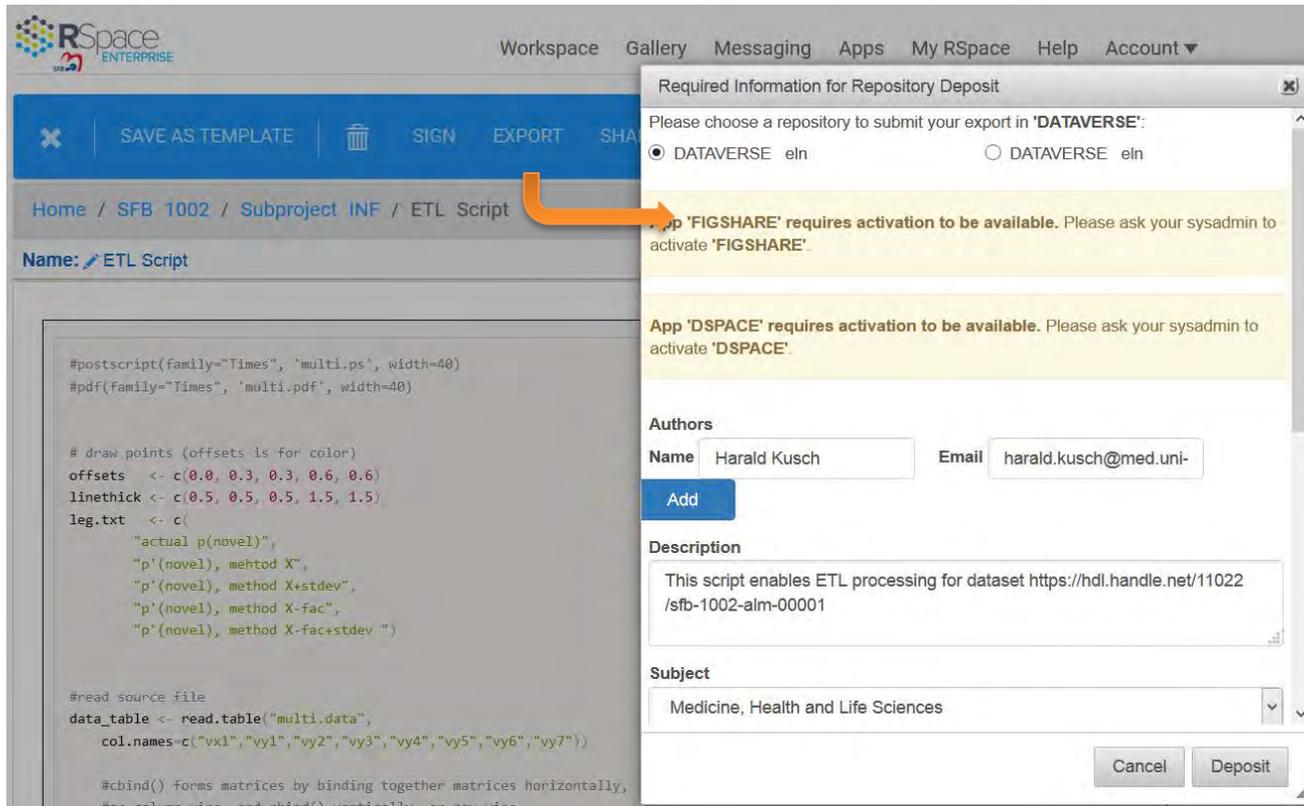
Most similar to paper, partially interactive => PDF-Format

Most similar to ELN (Rspace), interactive => HTML-Format

Interoperability, human and machine readability => XML-Format

Interfaces to repository software (e.g. Dataverse, DSPACE)

Three-click action: Data export into Dataverse repository



Required Information for Repository Deposit

Please choose a repository to submit your export in 'DATAVERSE':

DATAVERSE eln DATAVERSE eln

App 'FIGSHARE' requires activation to be available. Please ask your sysadmin to activate 'FIGSHARE'.

App 'DSpace' requires activation to be available. Please ask your sysadmin to activate 'DSpace'.

Authors

Name: Harald Kusch Email: harald.kusch@med.uni-

Add

Description

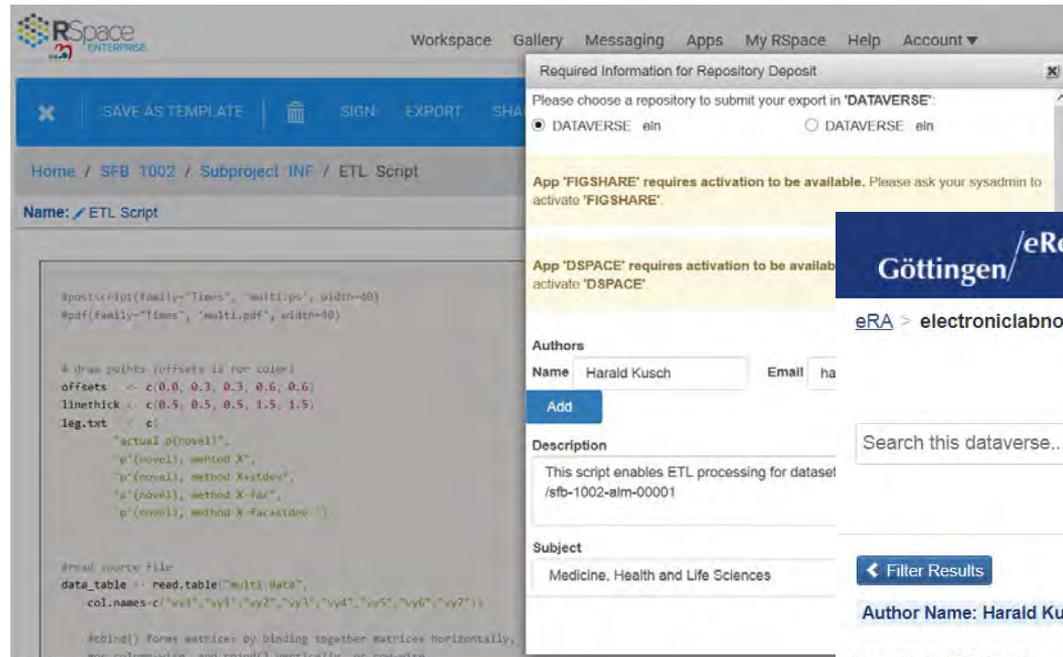
This script enables ETL processing for dataset <https://hdl.handle.net/11022/sfb-1002-alm-00001>

Subject

Medicine, Health and Life Sciences

Cancel Deposit

Persistent identification via DOI and ORCID integration



Required Information for Repository Deposit

Please choose a repository to submit your export in 'DATAVERSE':

DATAVERSE eln DATAVERSE eln

App 'FIGSHARE' requires activation to be available. Please ask your sysadmin to activate 'FIGSHARE'.

App 'DSpace' requires activation to be available. Please ask your sysadmin to activate 'DSpace'.

Authors

Name: Harald Kusch Email: ha

Add

Description

This script enables ETL processing for dataset /sfb-1002-elm-00001

Subject

Medicine, Health and Life Sciences

Göttingen/eResearch Alliance

eRA > electroniclabnotebook

Contact Share Edit

Search this dataverse... Find Advanced Search Add Data

Citation Metadata

Dataset Persistent ID
doi:10.5072/ITXS37

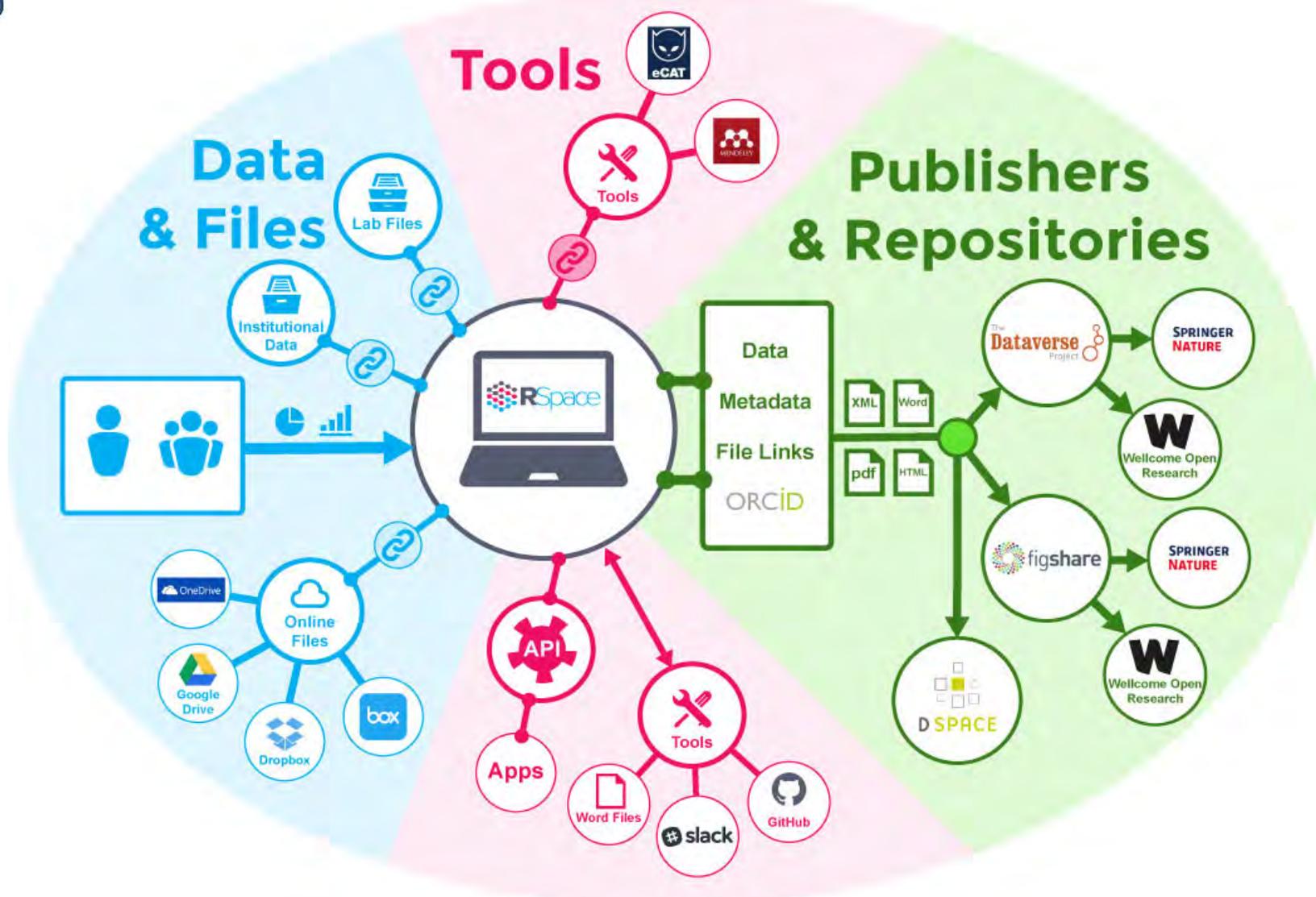
Title
ETL Script 0.1

Author
Harald Kusch (University Medical Center Göttingen) - ORCID: 0000-0002-9895-2469

Contact
Use email button above to contact.

1 to 10 of 15 Results

ETL Script 0.1 **Draft** **Unpublish**
Nov 17, 2017
Harald Kusch, 2017, "E..."
This is the RSpace-Doc



- ELN facilitates digital data organization
- Metadata schema application easily configurable and re-usable
- Existing interfaces to repository software tools facilitate vendor-independent data sharing
- Dataverse repository enables easy publishing of persistently identifiable datasets

- Extend and standardize APIs (Use case collection)
- Further improve sustainability (Use case collection)
- New / Improve interfaces with other RDM tools (rather than new ELN features)
- Establish ELN user community / communication platforms (product independent)

Please come to our demo for further discussions!



Dr. Sara Nußbeck

(TP INF-Leader IT)

orcid.org/0000-0003-1223-6494



Prof. Dr. Blanche Schwappach

(TP INF-Leader Research)

orcid.org/0000-0003-0225-6432

Georg Aschenbrandt

Luca Freckmann

Christian Henke

Sophia Rheinländer

Björn Hansen



Dr. Evelina De Laurentiis

(PostDoc)

orcid.org/0000-0002-6469-1627



Dr. Harald Kusch

(PostDoc)

orcid.org/0000-0002-9895-2469



Markus Suhr

(B.Sc. Inf)

orcid.org/0000-0002-6307-3253



Visit <http://www.eresearch.uni-goettingen.de/content/eresearch-toolbox-electronicnote-keeping> for further information.

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Caterina Barillari, Juan M. Fuentes-Serna & Bernd Rinn, ETH Zürich: openBIS – an open resource for academic laboratories

Abstract

Nowadays funding agencies, journals and academic institutions increasingly require research data to be published according to the FAIR data principles.¹ This can only be achieved if data are correctly documented and stored throughout the lifetime of a project. The use of a combined Electronic Laboratory Notebook (ELN) with a data management platform and a Laboratory Information Management System (LIMS) for samples and protocols management, allows scientists to keep track of the complete history of the work performed in the lab, a pre-requisite to achieve data FAIRness. The Scientific IT Services of ETH Zurich develop such open-source platform, openBIS,^{2,3} specifically tailored to academic research laboratories.

openBIS is a web-based application that comes with a default configuration suitable for most biological labs. This can be easily modified and tailored to the needs of each single lab. Relationships between all entities in the database ensure full history tracking. The storage manager allows tracking of biological and chemical samples. Data can be uploaded manually or automatically, directly from measuring devices.

For data analysis, openBIS is integrated with the Jupyter notebooks, which are documents that combine code, equations, output and text. Furthermore, openBIS has several APIs that allow integration with workflow managers, such as Snakemake and KNIME, for distributed data analysis. With the BigDataLink module, openBIS can be used as metadata repository for existing large datasets (hundreds of TBs to PBs) that cannot be moved conveniently to the openBIS-managed storage.

In summary, openBIS is an open and flexible platform for managing the ever increasing amount of data generated in academic scientific labs.

References

1. Wilkinson, M.D. et al. 2016: The FAIR Guiding Principles for scientific data management and stewardship. *Scientific Data* 3: 160018.
<https://doi.org/10.1038/sdata.2016.18>
2. Barillari, C. et al. 2016: openBIS ELN-LIMS: an open-source database for academic laboratories. *Bioinformatics* 32: 638–640.
<https://doi.org/10.1093/bioinformatics/btv606>
3. Bauch, A. et al. 2011: openBIS: a flexible framework for managing and analyzing complex data in biology research. *BMC Bioinformatics* 12: 468.
<https://doi.org/10.1186/1471-2105-12-468>

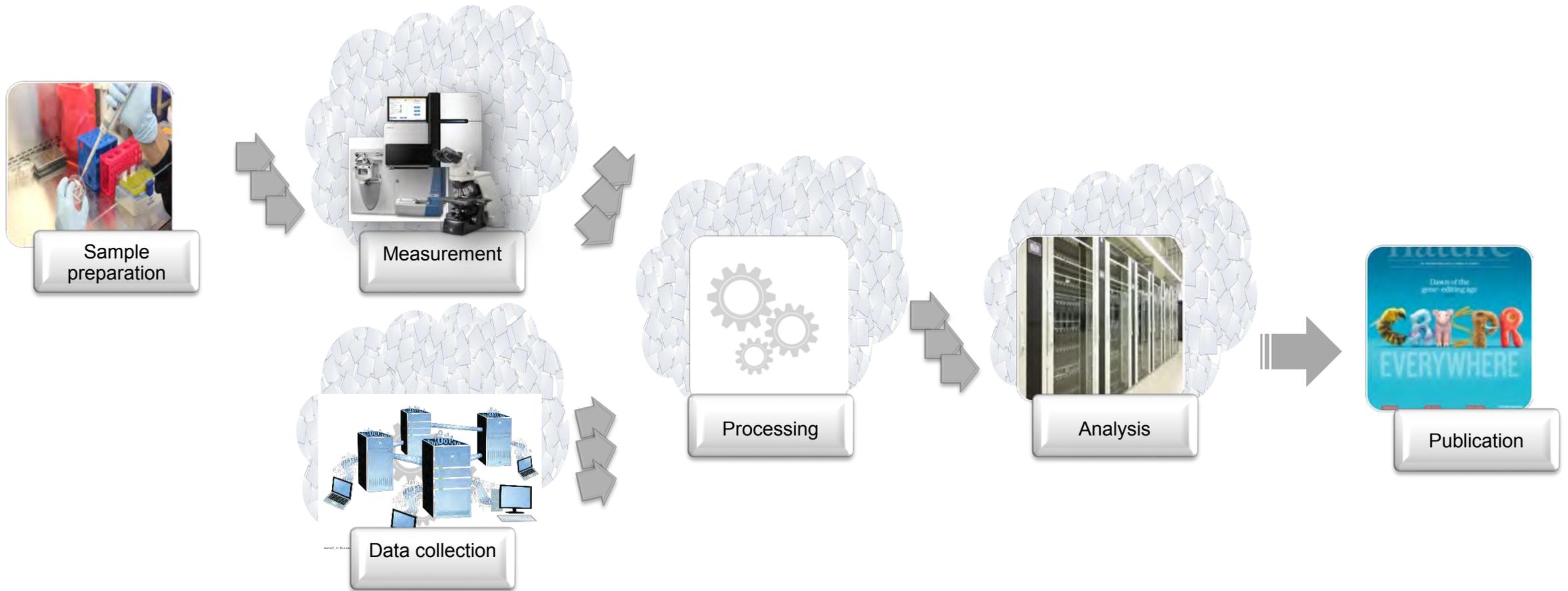


openBIS – an open resource for academic laboratories

Caterina Barillari

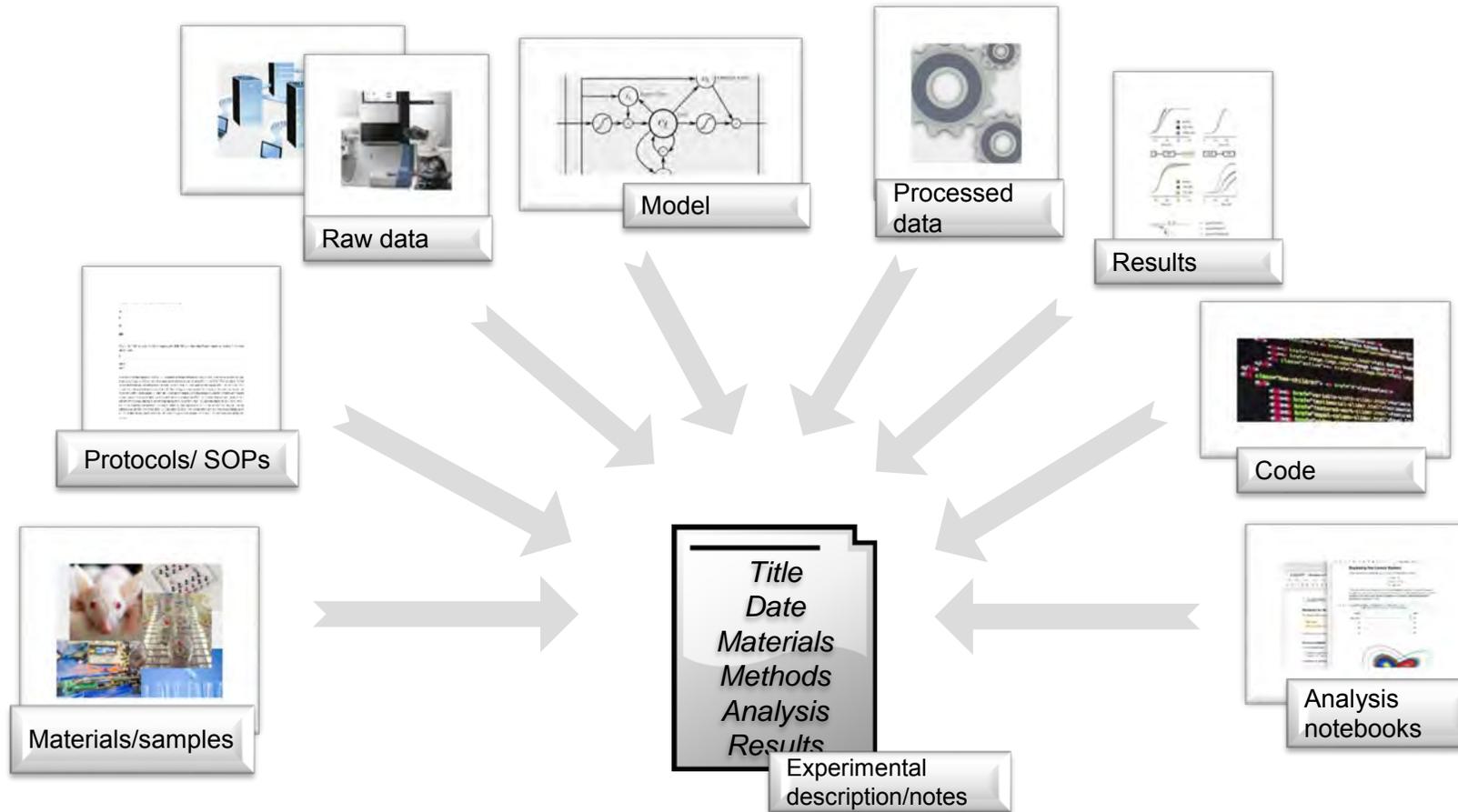
Scientific IT Services, ETH Zurich

Research workflow in experimental & computational labs

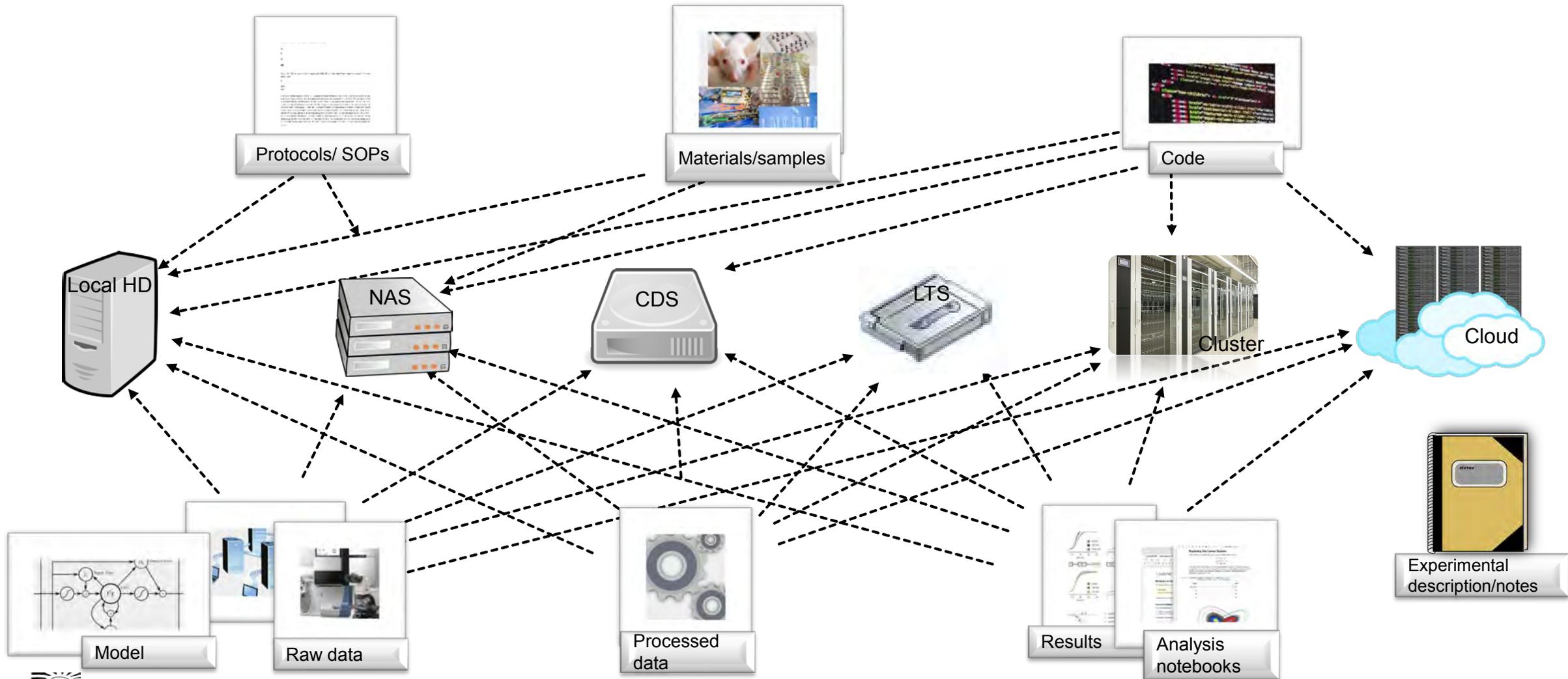


What does it take to manage research data?

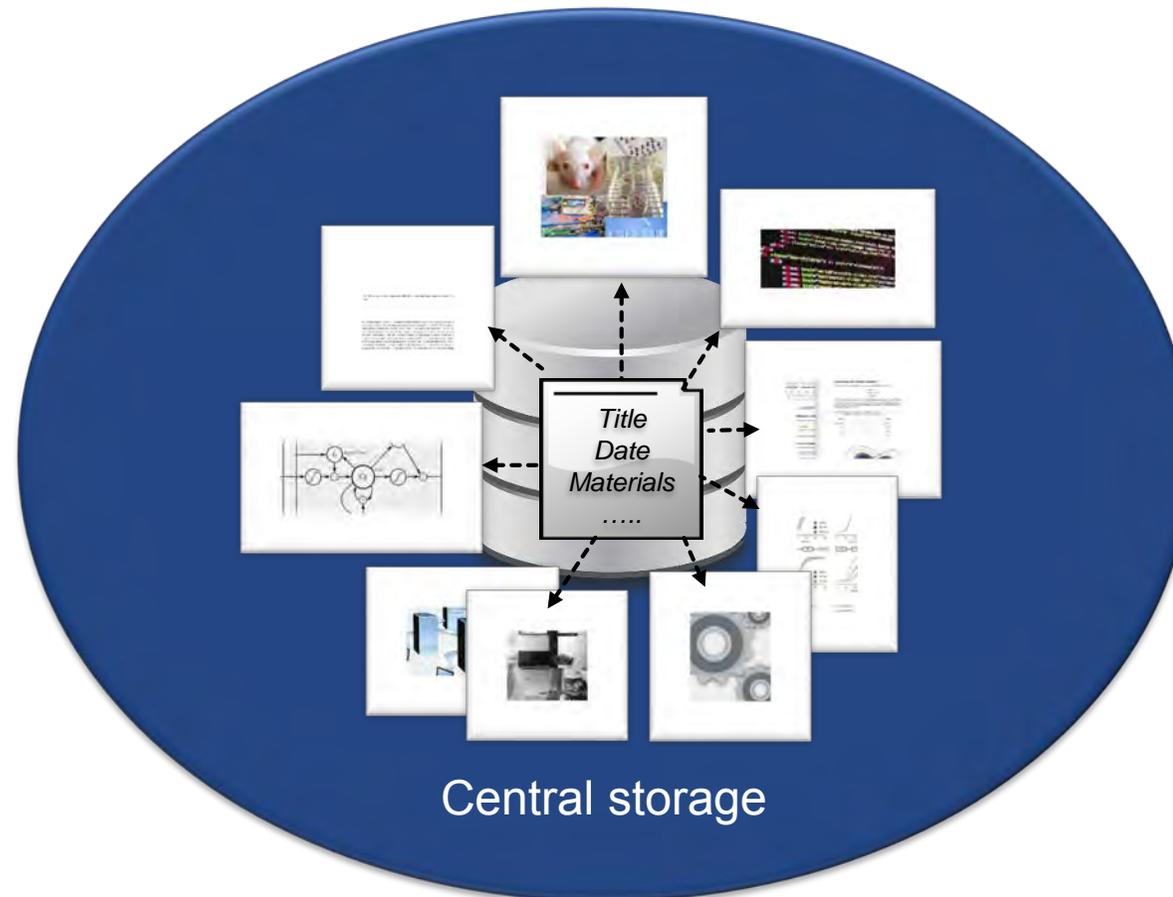
Complex process that requires tracking and linking different types of information



A very common scenario @ ETH

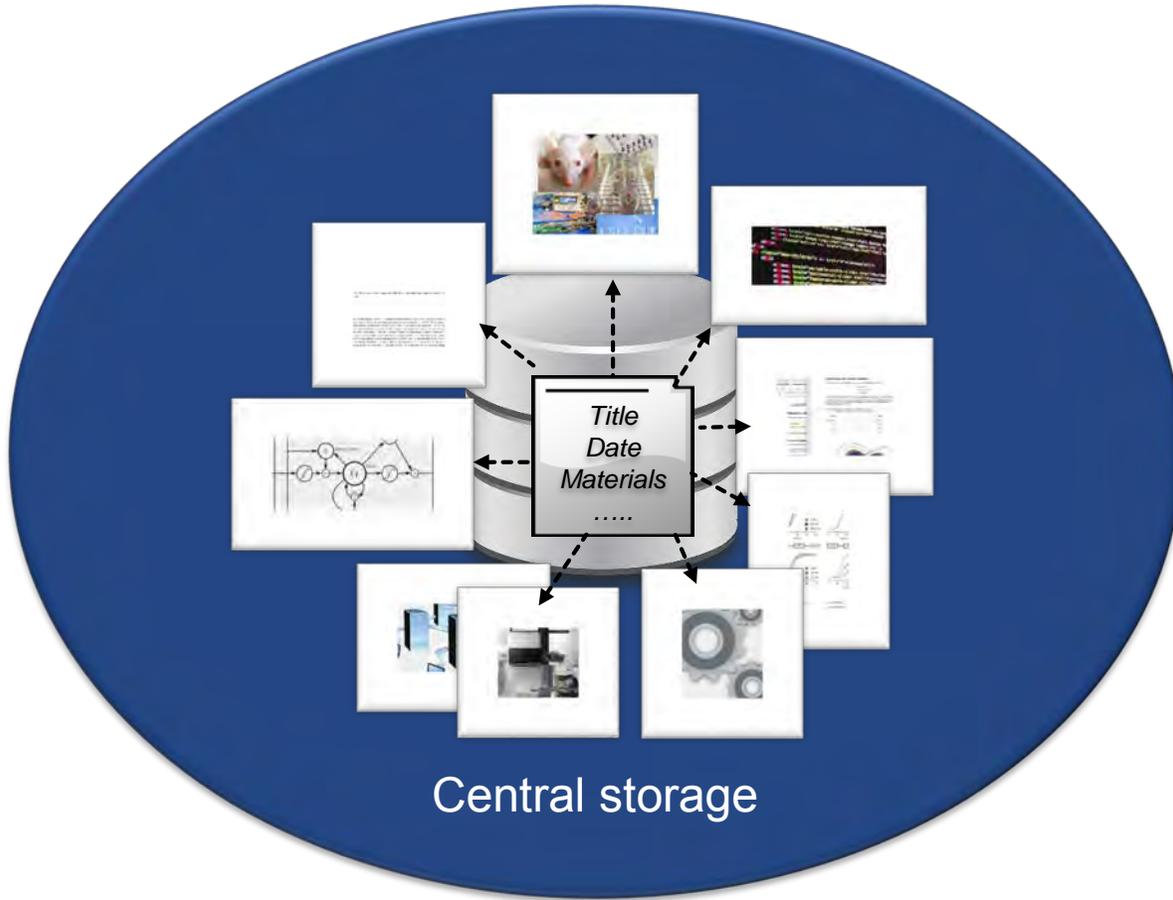


The ideal scenario



A combined ELN/LIMS can provide such solution

The ideal scenario



A combined ELN/LIMS can provide such solution

openBIS facts

Platform for managing scientific information and supporting research data workflows from “bench” to publication

Can be used in most quantitative science fields (e.g. life sciences, physics, env. sciences, etc)

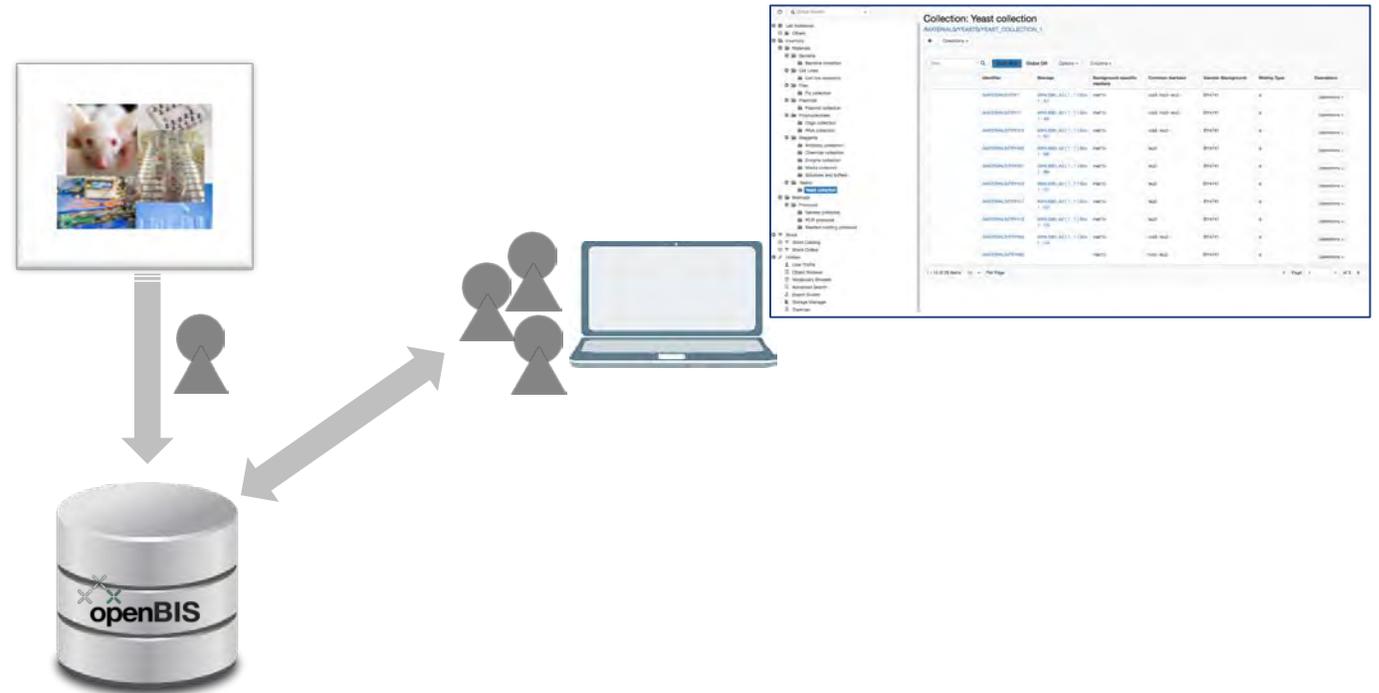
Used by research groups and facilities @ ETH, Swiss & European Universities, a few companies



- Summer 2007**
 - openBIS development start (SystemsX)
- April 2008**
 - first openBIS release (v08.04)
- Summer 2009**
 - SystemsX projects start using openBIS
- Summer 2013**
 - openBIS ELN-LIMS UI start
- Spring 2014**
 - first ELN-LIMS beta version
- May 2015**
 - first downloadable ELN-LIMS plugin
- May 2016**
 - first ELN-LIMS official release
- May 2017**
 - BigDataLink v.1
- December 2017**
 - JupyterHub integration

openBIS in a nutshell

- openBIS is a solution for research labs



Collection: Yeast collection

/MATERIALS/YEASTS/YEAST_COLLECTION_1

+ Operations -

Filter Global OR Options Columns

| Identifier | Storage | Endogenous 2micron plasmid in yeast | Genetic modifications | Mating Type | Origin | Publication | Source |
|-----------------------------------|-------------------------------|-------------------------------------|--|-------------|--------------------|--|-------------------------------|
| /MATERIALS/FRY1 | | cir+ | | a | | Brachmann, et al., Yeast, 1998 | Euroscarf |
| /MATERIALS/FRY11 | | cir+ | FRP235 INTEGRATION "ADH1 terminator" | a | negative selection | Ottoz et al., Nucleic Acids Research, 2014 | |
| /MATERIALS/FRY312 | MINUS80_A2 [1, 3] 3 - NoPos | cir+ | FRP718 INTEGRATION "HIS3" FRP235 INTEGRATION "ADH1 terminator" | a | transformation | Ottoz et al., Nucleic Acids Research, 2014 | |
| /MATERIALS/FRY400 | MINUS80_A2 [1, 3] 3 - NoPos | cir+ | FRP791 INTEGRATION "URA3" FRP718 INTEGRATION "HIS3" FRP235 INTEGRATION "ADH1 terminator" | a | transformation | Ottoz et al., Nucleic Acids Research, 2014 | |
| /MATERIALS/FRY401 | MINUS80_A2 [1, 3] 3 - NoPos | cir+ | FRP792 INTEGRATION "URA3" FRP718 INTEGRATION "HIS3" FRP235 INTEGRATION "ADH1 terminator" | a | transformation | Ottoz et al., Nucleic Acids Research, 2014 | |
| /MATERIALS/FRY403 | MINUS80_A2 [1, 3] 3 - NoPos | cir+ | FRP795 INTEGRATION "URA3" FRP718 INTEGRATION "HIS3" FRP235 INTEGRATION "ADH1 terminator" | a | transformation | Ottoz et al., Nucleic Acids Research, 2014 | |
| /MATERIALS/FRY417 | MINUS80_A2 [1, 3] 3 - NoPos | cir+ | FRP800 INTEGRATION "URA3" FRP718 INTEGRATION "HIS3" FRP235 INTEGRATION "ADH1 terminator" | a | transformation | Ottoz et al., Nucleic Acids Research, 2014 | |
| /MATERIALS/FRY418 | MINUS80_A2 [1, 3] 3 - A2 | cir+ | FRP793 INTEGRATION "URA3" FRP718 INTEGRATION "HIS3" FRP235 INTEGRATION "ADH1 terminator" | a | transformation | Ottoz et al., Nucleic Acids Research, 2014 | |
| /MATERIALS/FRY460 | MINUS80_A2 [1, 3] 3 - NoPos | cir+ | FRP467 INTEGRATION "HIS3" FRP235 INTEGRATION "ADH1 terminator" | a | transformation | Ottoz et al., Nucleic Acids Research, 2014 | |
| /MATERIALS/FRY482 | | cir+ | FRP795 INTEGRATION "URA3" FRP235 INTEGRATION "ADH1 terminator" | a | transformation | Ottoz et al., Nucleic Acids Research, 2014 | Caterina Barilari, 2018-09-13 |

- Lab Notebook
- Others
- Inventory
 - Materials
 - Bacteria
 - Bacteria collection
 - Cell Lines
 - Cell line collection
 - Flies
 - Fly collection
 - Plasmids
 - Plasmid collection
 - Polynucleotides
 - Oligo collection
 - RNA collection
 - Reagents
 - Antibody collection
 - Chemical collection
 - Enzyme collection
 - Media collection
 - Solutions and buffers
 - Yeasts
 - Yeast collection**
 - Methods
 - Protocols
 - General protocols
 - PCR protocols
 - Western blotting protocols
- Stock
 - Stock Catalog
 - Stock Orders
- Utilities
 - User Profile
 - Object Browser
 - Vocabulary Browser
 - Advanced Search
 - Export Builder
 - Storage Manager
 - User Manager
 - Trashcan
 - Settings

openBIS in a nutshell

- openBIS is a solution for research labs



- Lab Notebook
- Others
- Inventory
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 - Yeast collection
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 - Protocols
 - General protocols**
 - PCR protocols
 - Western blotting protocols
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 - Stock Catalog
 - Stock Orders
- Utilities
 - User Profile
 - Object Browser
 - Vocabulary Browser
 - Advanced Search
 - Export Builder
 - Storage Manager
 - User Manager
 - Trashcan
 - Settings
 - About

Object: Yeast transformation

/METHODS/PROTOCOLS/GENERAL_PROTOCOLS/FRPROT1



General

Name:

Yeast transformation

For what:

1. Transform plasmids in a yeast strain. 2. Integrate linearized DNA in yeast genome. 3. Knock-out and knock-in genes in yeast genome. 4. Yeast gap repair.

Protocol type:

yeast basic method

Links to materials & methods

| Code | Name | Quantity | Comments |
|---------|---------------------------|-----------------------|----------|
| FRC31 | Dimethyl sulfoxide (DMSO) | 10% | |
| FRSOB20 | PEG mix | 600 µl/transformation | |
| FRSOB21 | LiAc mix | 100 µl/transformation | |
| FRSOB22 | Salmon sperm DNA (ssDNA) | 10 µl/transformation | |

1 - 4 of 4 items | 10 Per Page | Page 1 of 1

Materials

Materials:

Centrifuge min 1000 g Orbital shaker with regulated temperature Incubator with regulated temperature Wheel or mild shaker for 1.5 ml tubes Thermomixer

Method

Time requirement:

1 day pre-culture + 2 hours bech work + 2 days incubation

Procedure:

1. Inoculate 5 ml of appropriate medium with yeast. 2. Incubate overnight at the appropriate temperature (usually 30°C). 3. Dilute the overnight culture in appropriate medium (10 ml per transformation). 4. Grow cells to OD600=0.4-0.8. 5. Harvest cells by centrifugation at max 1000 g for 5 min at room temperature. 6. Throw away supernatant. 7. Re-suspend cells in 5 ml water. 8. Harvest cells by centrifugation at max 3000 g for 5 min at room temperature. 9. Throw away supernatant. 10. Re-suspend in LiAc mix. 11. Use 100 µl cells per transformation. Transfer this volume to a 1.5 ml tube. 12. Add 1000 ng of DNA to the mix. 13. Add 10 µl ssDNA (Boil ssDNA at 95°C for 5 min every 4th time, cool down to room temperature). 14. Add 600 µl of PEG mix, and mix. 15. Incubate on the wheel at room temperature for 30 min. 16. Add 70 µl DMSO to reach final concentration of 10%. 17. Heat shock for 15 min at 42°C, shaking at max speed. 18. Harvest cells by centrifugation at max 1000 g for 2 min at room temperature. 19. Throw away the supernatant. 20. Re-suspend cell in 300 µl YPD. 21. Incubate on the wheel at room temperature for 20 min (auxotrophic markers) or 3-4 hours (drugs resistance markers). 22. Plate 150 µl on appropriate plate. 23. Incubate 2-4 days at the appropriate temperature.

Protocol evaluation:

Small yeast colonies appear on the plate after a couple of days at the appropriate temperature.

Select a dataset type

Files Uploader



Select files to upload

Create

Auto upload on drop

Projects
Experiments
Experimental
steps

- Lab Notebook
 - Others
 - Caterina
 - Diana Ottoz
 - Inducible Transcription Factor
 - Induction of the transcription factor
 - Detection of LexA-ER-B42 induction
 - Flow cytometry files
 - scripts
 - Analysis results
 - Detection of LexA-ER-B42 induction
 - Detection of LexA-ER-B112 induction
 - Analysis of the abundance of the factor
- Inventory
 - Materials
 - Methods
- Stock
 - Stock Catalog
 - Stock Orders
- Utilities
 - User Profile
 - Object Browser
 - Vocabulary Browser
 - Advanced Search
 - Export Builder
 - Storage Manager
 - User Manager
 - Trashcan
 - Settings
- About

Object: Detection of LexA-ER-B42 induction by flow cytometry

/DIANA_OTTOZ/INDUCIBLE_TRANSCRIPTION_FACTOR/INDUCTION_OF_TF/FC_LEXA-ER-B42



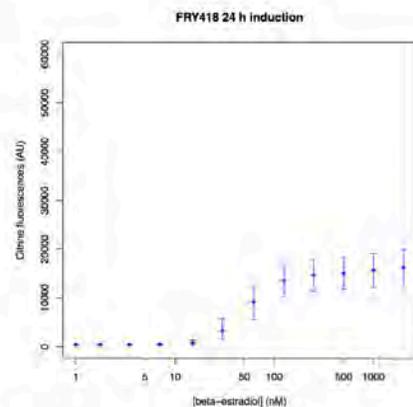
General

Name:
Detection of LexA-ER-B42 induction by flow cytometry

Owner:
Diana Ottoz

Experimental goals:
Analyze the induction of **LexA-ER-B42** in a concentration series of beta-estradiol using a fluorescence readout

Experimental results:
The LexA-ER-B42 induction can be measured by using a target gene encoding a fluorescence protein. *LexA-ER-B42 induction is different at different concentrations of inducer.*



Links to materials & methods

Filter OR

| Code | Name | Comments | Details |
|---------|---------------------|--|----------------------------|
| FRM11 | liquid S media | SDC at 25°C | |
| FRSOB34 | 1000X Cycloheximide | diluted 1/1000, treated for 1/2 hour | Dissolve in DMSO. Aliquot. |
| FRSOB37 | beta-estradiol | 1:2 concentration series with 2000 nM maximum for 24 | Dissolve in EtOH. |

Select a dataset type

Files Uploader

Auto upload on drop

openBIS in a nutshell

➤ openBIS is a solution for research labs



Object: Detection of LexA-ER-B42 induction by flow cytometry

/DIANA_OTTOZ/INDUCIBLE_TRANSCRIPTION_FACTOR/INDUCTION_OF_TF/FC_LEXA-ER-B42



- Lab Notebook
 - Others
 - Caterina
 - Diana Ottoz
 - Inducible Transcription Factor
 - Induction of the transcription factor
 - Detection of LexA-ER-B42 indu**
 - Flow citometry files
 - scripts
 - Analysis results
 - Detection of LexA-ER-B42 indu
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 - Settings
- About

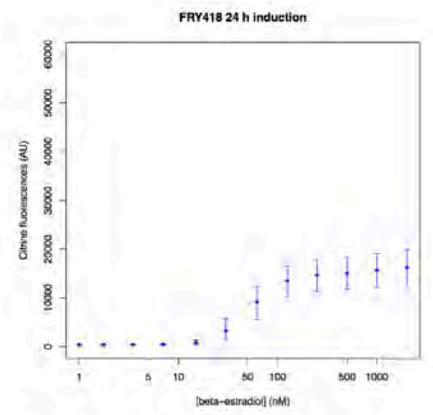
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- RAW_DATA : Flow citometry files
 - FC_LEXA-ER-B42-raw
 - FC_LEXA-ER-B42-raw
 - 1.fcs (510.3Kb)
 - 10.fcs (510.4Kb)
 - 11.fcs (510.4Kb)
 - 12.fcs (510.3Kb)
 - 2.fcs (510.3Kb)
 - 3.fcs (510.3Kb)
 - 4.fcs (510.3Kb)
 - 5.fcs (510.3Kb)
 - 6.fcs (510.3Kb)
 - 7.fcs (510.3Kb)
 - 8.fcs (510.3Kb)
 - 9.fcs (510.3Kb)
 - ANALYSIS_SCRIPTS : scripts
 - FC_LEXA-ER-B42-script.R (2.9Kb)
 - ANALYZED_DATA : Analysis results
 - FC_LEXA-ER-B42-analyzed
 - FC_LEXA-ER-B42-analyzed
 - FRY418t24hCitrine.pdf (5.2Kb)
 - FRY418t24hmKate2.pdf (5.2Kb)

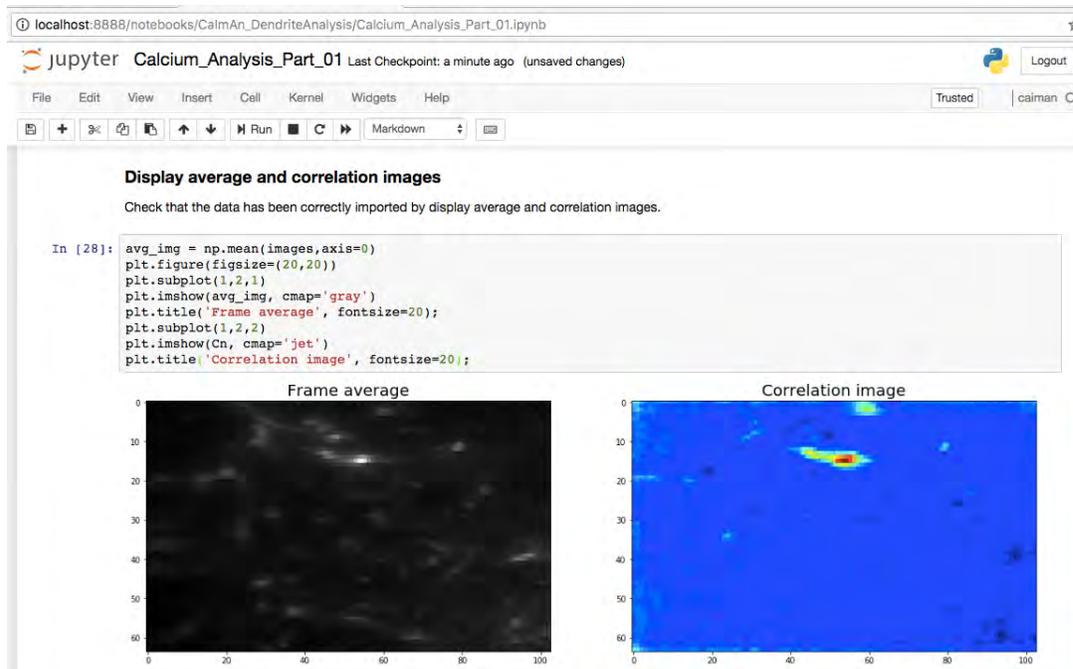
Select a dataset type

Files Uploader



Jupyter notebooks

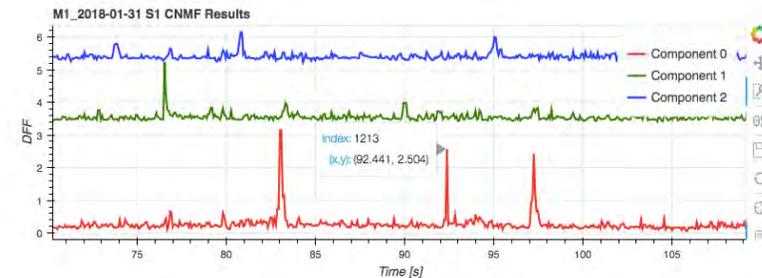
- Application that combine documentation, code, input and output generated by the code, e.g. graphs, plots ([Nature 515, 151–152](#))
- Useful for exploratory data analysis and reproducibility
- >40 programming languages supported (Python, R, Scala, Julia, etc)
- Notebooks can be shared



Plot calcium traces

The next cell plots the figure. The **interactive toolbar** on the right of the figures allows panning, zooming, saving etc. To **save figure**, click the disk icon in the plotting toolbar. With the default `output_backend` ('`canvas`'), a png file will be saved. To save to `svg` format, change `output_backend` to '`svg`'.

```
In [23]: p = Figure(plot_width=800, plot_height=300,
                    title='%s %s CNMF Results' % (date_folder, session_folder))
legend_text = ['Component %id' % (x) for x in range(len(idx_comps))]
# this is the call to the plotting function (change args. as required)
plotTimeseries(p, t, F_dff,
               legend=legend_text,
               stack=True,
               xlabel='Time [s]', ylabel='DFF',
               output_backend='canvas'
               )
```



Object: Detection of LexA-ER-B42 induction by flow cytometry

/BARILLAC/INDUCIBLE_TRANSCRIPTION_FACTOR/INDUCTION_OF_TF/FC_LEXA-ER-B42



- Lab Notebook
 - My Space (Caterina)
 - Others
 - Barillac
 - Ch2018
 - Inducible Transcription Factor
 - Induction of the transcription factor
 - Detection of LexA-ER-B42 indu**
 - Flow cytometry data
 - R script
 - Final figures
 - Jupyter test
 - Detection of LexA-ER-B42 indu
 - Detection of LexA-ER-B112 indu
- Inventory
- Stock
 - Stock Catalog
 - Stock Orders
- Utilities
 - Jupyter Workspace**
 - New Jupyter Notebook**
 - User Profile
 - Object Browser
 - Vocabulary Browser
 - Advanced Search
 - Export Builder
 - Storage Manager
 - Trashcan
 - Settings
 - About

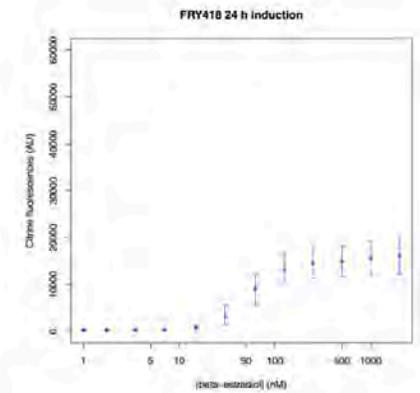
General

Name:
Detection of LexA-ER-B42 induction by flow cytometry

Show in project overview:
true

Experimental Goals:
Analyze the induction of **LexA-ER-B42** in a concentration series of beta-estradiol using a fluorescence readout

Experimental Results:
The LexA-ER-B42 induction can be measured by using a target gene encoding a fluorescence protein. *LexA-ER-B42 induction is different at different concentrations of inducer.*



Start date:
2018-07-17 17:00:23 +0200

End date:
2018-07-17 18:00:54 +0200

Readout details

- RAW_DATA : Flow cytometry data
- ANALYZED_DATA : R script
- ANALYZED_DATA : Final figures
- ANALYZED_DATA : Jupyter test**
 - flow cytometry test.ipynb (26.6Kb)
 - flow cytometry test.ipynb.html (257.1Kb)

Select a dataset type

Files Uploader

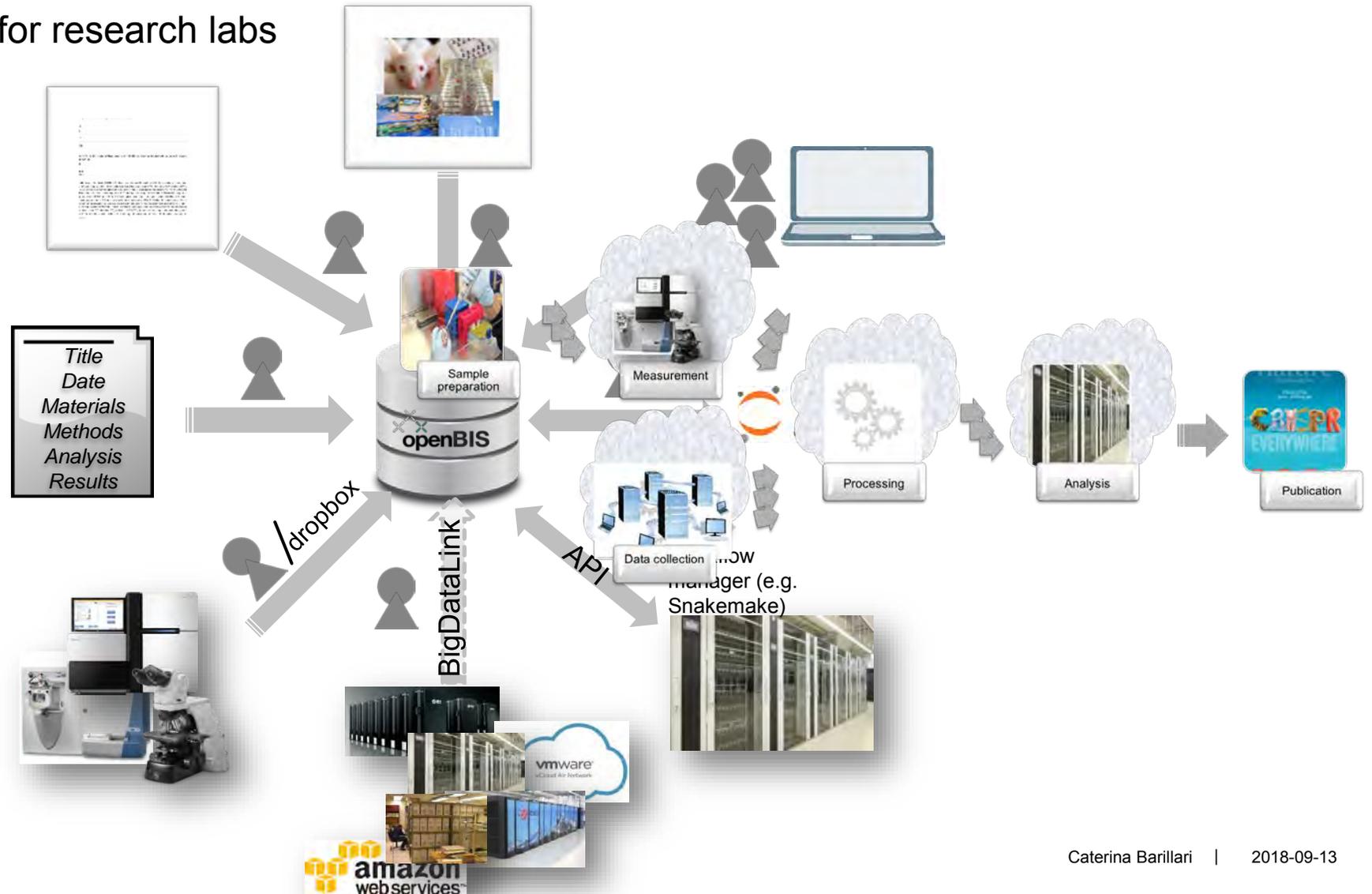
Select files to upload

Create

Auto upload on drop

openBIS in a nutshell

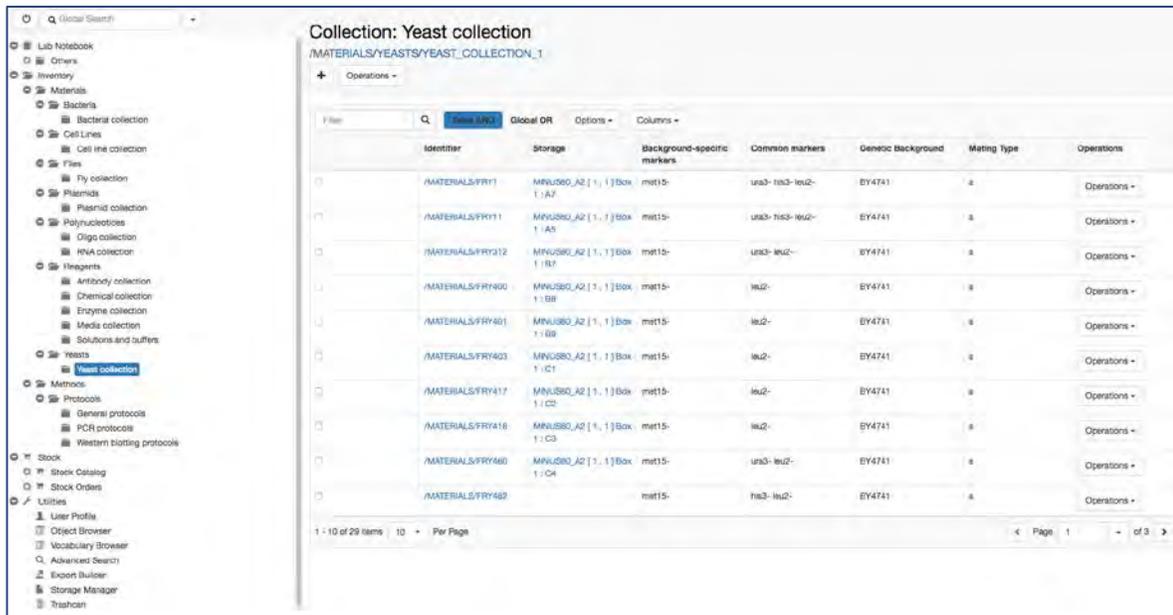
➤ openBIS is a solution for research labs



openBIS solutions

openBIS ELN-LIMS is available in two flavors:

For life sciences: customizable predefined types and fields suitable for most biological labs



The screenshot displays the 'Collection: Yeast collection' interface. The main content is a table with the following columns: Identifier, Storage, Background-specific markers, Common markers, Genetic background, Mating type, and Operations. The table contains 10 rows of yeast collection items.

| Identifier | Storage | Background-specific markers | Common markers | Genetic background | Mating type | Operations |
|-------------------|------------------------------|-----------------------------|-------------------|--------------------|-------------|--------------|
| /MATERIALS/FRY1 | MNU80_A2 [1, 1] Box 1 : A7 | mat15- | ura3- his3- leu2- | EY4741 | α | Operations - |
| /MATERIALS/FRY11 | MNU80_A2 [1, 1] Box 1 : A5 | mat15- | ura3- his3- leu2- | EY4741 | α | Operations - |
| /MATERIALS/FRY312 | MNU80_A2 [1, 1] Box 1 : B7 | mat15- | ura3- leu2- | EY4741 | α | Operations - |
| /MATERIALS/FRY400 | MNU80_A2 [1, 1] Box 1 : B8 | mat15- | his2- | EY4741 | α | Operations - |
| /MATERIALS/FRY401 | MNU80_A2 [1, 1] Box 1 : B9 | mat15- | his2- | EY4741 | α | Operations - |
| /MATERIALS/FRY403 | MNU80_A2 [1, 1] Box 1 : C1 | mat15- | his2- | EY4741 | α | Operations - |
| /MATERIALS/FRY417 | MNU80_A2 [1, 1] Box 1 : C2 | mat15- | his2- | EY4741 | α | Operations - |
| /MATERIALS/FRY418 | MNU80_A2 [1, 1] Box 1 : C3 | mat15- | his2- | EY4741 | α | Operations - |
| /MATERIALS/FRY460 | MNU80_A2 [1, 1] Box 1 : C4 | mat15- | ura3- leu2- | EY4741 | α | Operations - |
| /MATERIALS/FRY482 | | mat15- | his3- leu2- | EY4741 | α | Operations - |

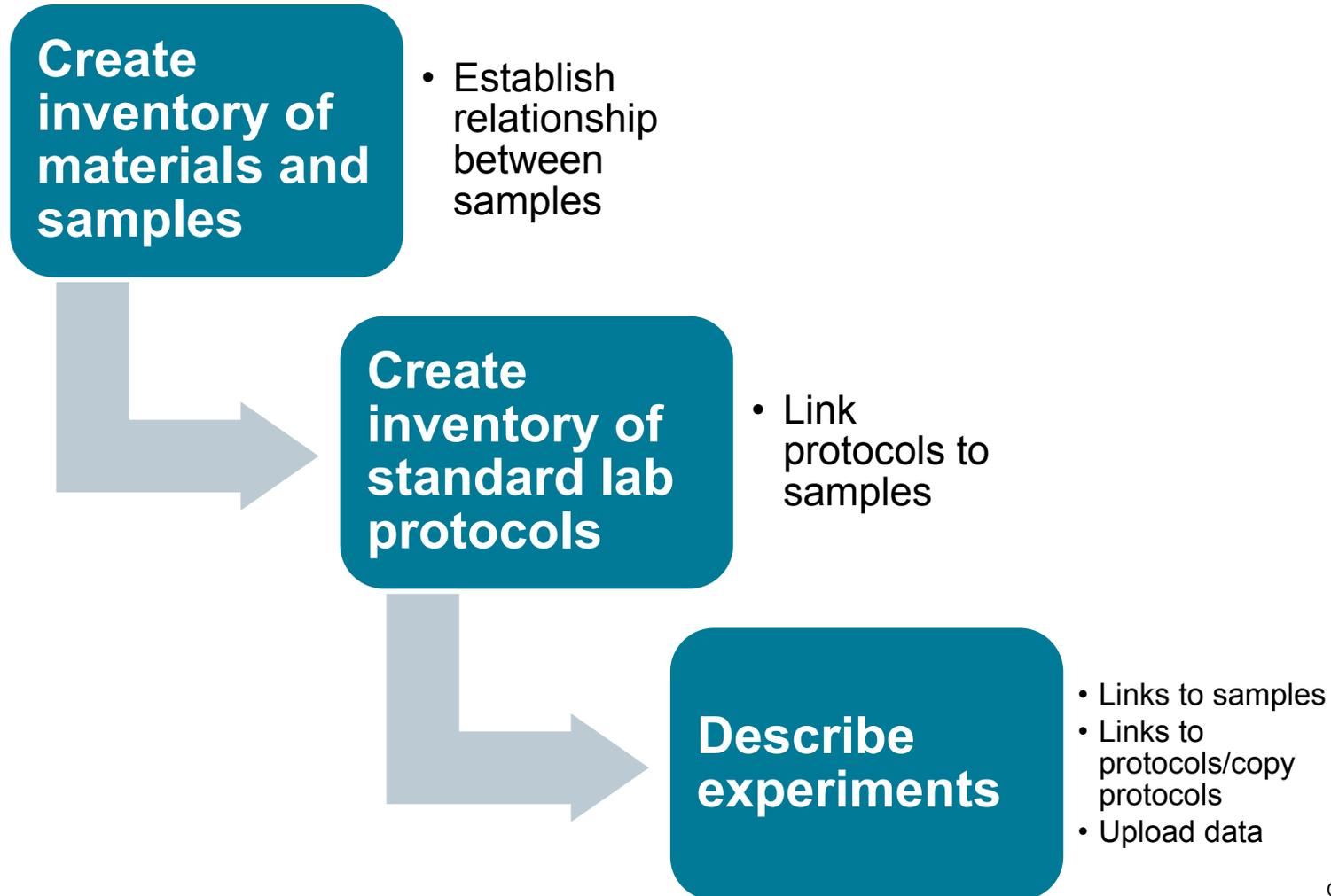
Generic: only basic generic types predefined. To be fully customized by users.



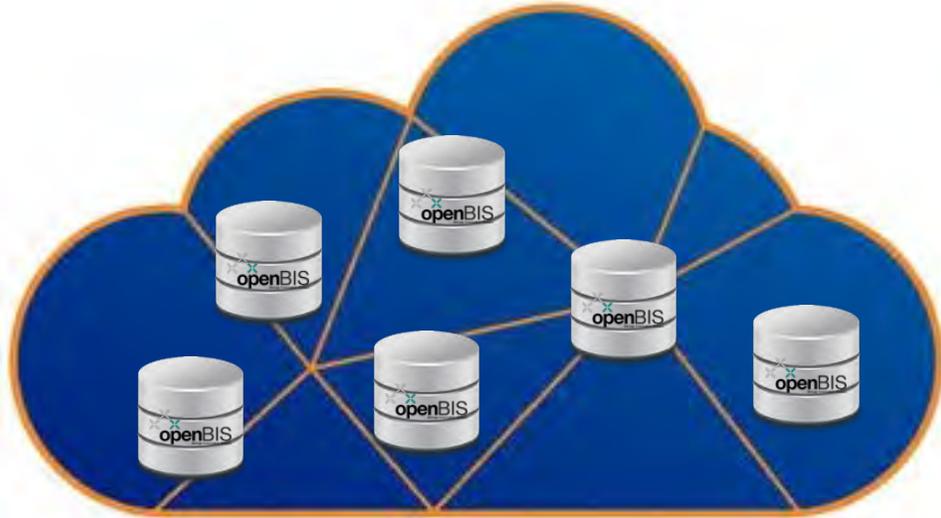
The screenshot displays the 'Welcome to openBIS ELN-LIMS.' dashboard. The left sidebar contains a navigation menu with the following items:

- Lab Notebook
- My Space (Caterina)
- Others
- Inventory
- Materials
- Methods
- Stock
- Stock Catalog
- Stock Orders
- Utilities
 - Jupyter Workspace
 - New Jupyter Notebook
 - User Profile
 - Object Browser
 - Vocabulary Browser
 - Advanced Search
 - Export Builder
 - Storage Manager
 - Trashcan
 - Settings
 - About

Best practices for openBIS introduction as ELN/LIMS in a biology lab



openRDM.swiss - National ARDM Service



Cloud-hosted openBIS ELN-LIMS

- Virtual servers per research group, institute or institution
- Generic or life-science ‘flavor’
- Optionally with JupyterHub server for analytics
- Automated deployment (Ansible)
- Integration with Community Service Hub

Training & user support (‘best effort’)

Service Marketing & Business Model

- Infrastructure & service charges for sustainable long-term operation

Connection with repositories

- Covering the entire data life cycle

SWITCHengines



University of
Zurich ^{UZH}

zh
aw

Acknowledgements

The SIS team

Bernd Rinn (Section Head)

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High-Performance Computing

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- Steven Armstrong
- Christian Bolliger
- Urban Borstnik
- Samuel Fux
- Bruno Löpfe
- Eric Müller
- Allen Neeser
- Christiane Pousa Ribeiro

Scientific Software and Data Management

- **Matthew Baker (Group Head)**
- Franz-Josef Elmer
- Juan Fuentes
- Antti Luomi
- Yves Noirjean
- Althea Parker
- Mikolaj Rybinski
- Uwe Schmitt
- Swen Vermeul
- Cezary Czernecki

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- **Thomas Wüst (Group Head)**
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- Vincenzo Capece
- Tarun Chadha
- Diana Coman Schmid
- Henry Lütcke
- Michal Okoniewski
- Jarunan Panyasantisuk
- Emanuel Schmid
- Cristian Scurtescu

Marlis Zeitler & Claire Wallace, Dotmatics Ltd: The use of an ELN to accelerate efficiency in research

Abstract

Dotmatics is one of the leaders in scientific informatics solutions. Our ELN (Electronic Lab Notebook) is a web-based application for Chemists and Biologists with flexible templating to capture, store and search experiments from all scientific disciplines.

It allows to:

- Manage the creation of your experimental data as well as handling analytical, formulations and synthesis experiments
- Implement a fully audited digital signature process to support compliance across the organization
- Save time due to cloning of experiments with standardized templates
- Have consistency in data capturing
- Track in real time the experimental data across groups

We will give an overview of our ELN along with additional related functionalities such as registration of chemical and biological entities, an idea of inventory, searching across all scientific database as well as generating reports with one button click. This simple integrated workflow provided by the Dotmatics suite allows scientists to work more efficiently and to share data across different teams and organizations in the context of collaborations.

d

Introduction to Dotmatics

d

Why Transition to an Electronic Laboratory Notebook?

d

ELN Data Entry Considerations

d

Biology vs Chemistry

- Privately owned
 - Founded in 2005 with technology from Merck UK
 - 135+ employees, 40%+ Scientists
- Rapidly growing customer base
 - ~530 customer organizations
 - 30 countries
- Revenue £17.2 M (2017)
- 30-40% annual growth
- Scottish Equity partners Investment

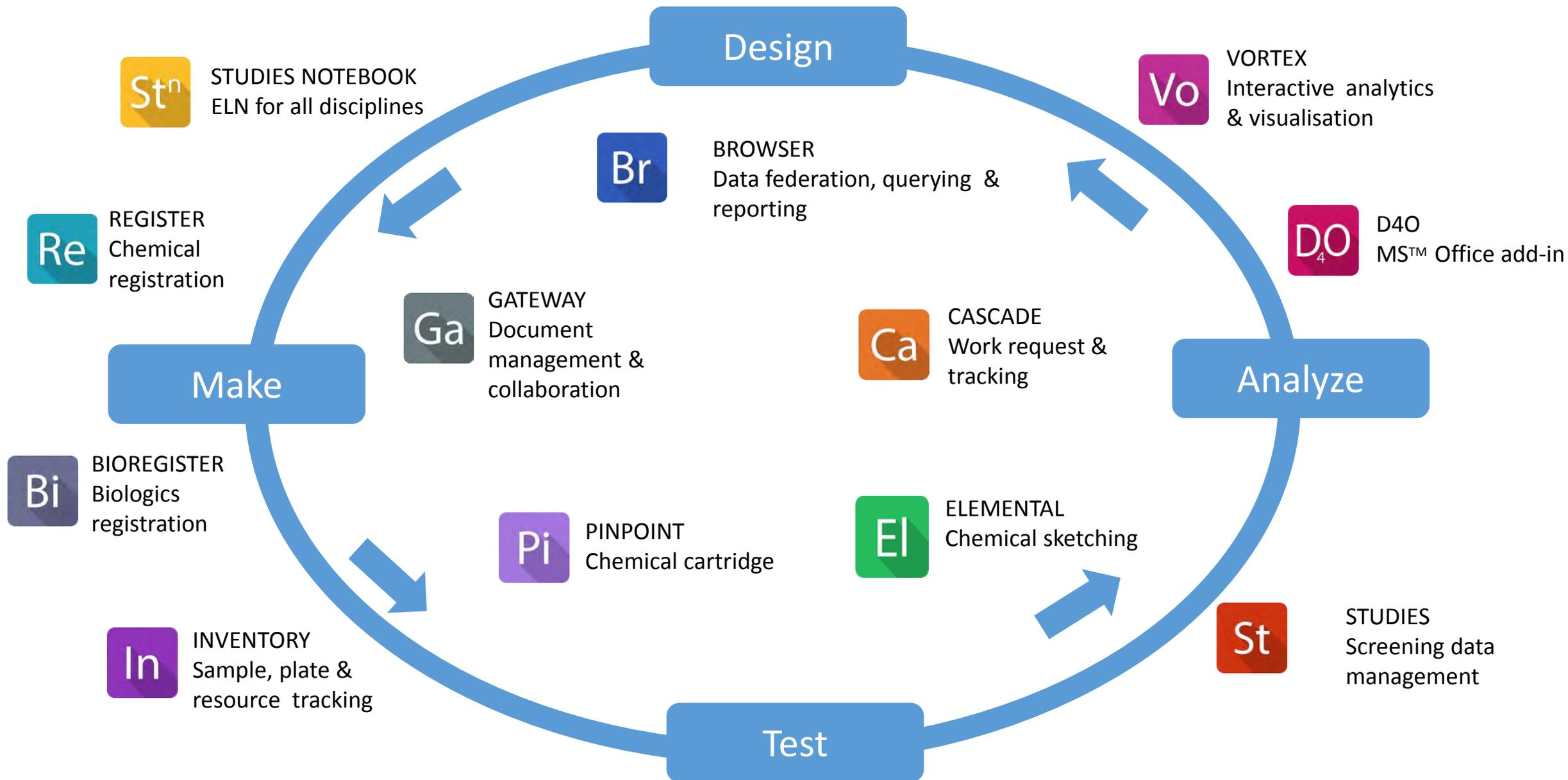


Our software supports your research teams to help you produce better drug candidates or formulated products faster.

We do this by providing

- Simple real-time access to all research data, allowing your scientific teams to make **better informed decisions** faster
- Fully-integrated scientifically-aware informatics solutions that expedite laboratory workflows and capture experiments and data, making your research teams **more efficient**





d

Introduction to Dotmatics

d

Why Transition to an Electronic Laboratory Notebook?

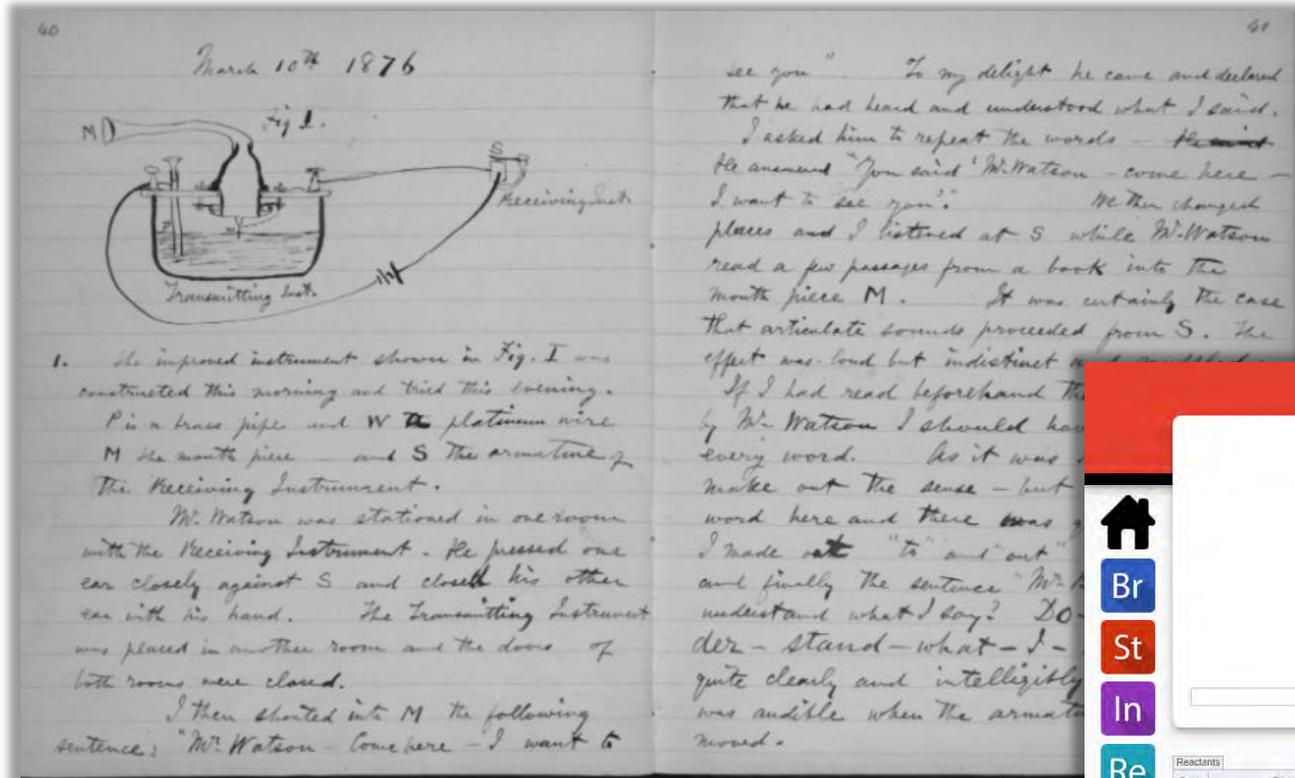
d

ELN Data Entry Considerations

d

Biology vs Chemistry

Why Transition to an Electronic Laboratory Notebook?



dotmatics
knowledge solutions

Unique ID: 139628
Notebook Ref: CHEMELN-1-237
Project: PNKP
User: testadmin
Date Created: 29/08/2018

Chemical reaction: c1ccccc1C(=O)Cl + C1CCCN1 >> c1ccccc1C(=O)N1CCCN1

save open tools

| Reactants | | | | | | | | | | | | | | |
|-----------|------------------|-------------|--------------|--------|----------|----------|----------------|-------------|------|--------|--------------|---------|--------|---------------|
| Order | Reactant Name | Reactant ID | Hazard Codes | MW | Limiting | Quantity | Quantity Units | Equivalents | mmol | Volume | Volume Units | Density | Purity | Concentration |
| 1 | benzoyl chloride | ABC030530 | H314 | 140.57 | Y | | mg | 1 | | | mL | | | |
| 2 | pyrrolidine | H200 | H200 | 71.12 | N | | mg | 1 | | | mL | | | |
| 3 | Benzoic Acid | ABC027091 | H318, H335 | 122.1 | N | | mg | 1 | | | mL | | | |

| Solvents | | | | | | | | | | Conditions | |
|--------------------|--------|---------|-------------------------------|--------|--------------|------|---------|-------------|--|------------|--|
| Solvent Name | MW | Formula | Hazard Codes | Volume | Volume Units | mmol | Density | Temperature | | | |
| 1,2-dichloroethane | 98.959 | C2H4Cl2 | H225-H302-H315-H319-H335-H350 | | mL | | 1.256 | 40 | | | |

| Products | | | | | | | | | | |
|--------------------------------|-----------------|--------|----------|----------|-------|--------|--------|------------------|-------|--|
| Product Name | Product ID | MW | Formula | Quantity | Units | mmol | Purity | Theoretical Mass | Yield | |
| phenylpyrrolidin-1-ylmethanone | CHEMELN-1-237-1 | 175.23 | C11H13NO | 100 | mg | 0.5421 | 95 | | | |

Why Transition to an Electronic Laboratory Notebook?

The screenshot displays the dotmatics E-Lab Notebook interface. At the top, the dotmatics logo is visible. The main area shows a chemical reaction: benzoyl chloride reacting with pyrrolidine to form N-benzoylpyrrolidine. Below the reaction, there are 'save' and 'open tools' buttons. To the right, a metadata panel includes fields for Unique ID (139628), Notebook Ref (CHEMELN-1-237), Project (PNKP), User (testadmin), and Date Created (29/08/2018). On the left, a vertical toolbar contains icons for Home, Br, St, In, Re, and a flask icon. Below the reaction, there are three data tables: Reactants, Solvents, and Products.

| Order | Reactant Name | Reactant ID | Hazard Codes | MW | Limiting | Quantity | Quantity Units | Equivalents | mmol | Volume | Volume Units | Density | Purity | Concentration |
|-------|------------------|-------------|--------------|--------|----------|----------|----------------|-------------|------|--------|--------------|---------|--------|---------------|
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| Solvent Name | MW | Formula | Hazard Codes | Volume | Volume Units | mol | Density |
|--------------------|--------|---------|-------------------------------|--------|--------------|-----|---------|
| 1,2-dichloroethane | 98.959 | C2H4Cl2 | H225-H302-H315-H319-H335-H350 | | mL | | 1.256 |

| Product Name | Product ID | MW | Formula | Quantity | Units | mmol | Purity | Theoretical Mass | Yield |
|----------------------------------|-----------------|--------|----------|----------|-------|--------|--------|------------------|-------|
| phenyl(pyrrolidin-1-yl)methanone | CHEMELN-1-237-1 | 175.23 | C11H13NO | 100 | mg | 0.5421 | 95 | | |

Organizational efficiencies

Quality improvement

Searchable

Scalable

Secure

Collaborative

Personal productivity

Knowledge preservation

Improved decision making

Mining and visualizing data
across the organization

Diverse data sources across many labs

Instruments

Manual Annotations

References

Standard Documents

Laboratories collecting data in multiple data formats

Excel

Word

Access

Oracle

Instrument Files

Data is stored on different file servers

Communication is done via exchange of files

Email

SharePoint

No systematic electronic tracking of information

Analysis and reporting takes considerable time

TIME

- Project initiation/transfer/witnessing
- Cloning of experiments
- Automatic calculations
- Preparing reports and presentations
- 5 “extra” weeks per year

COST

- Storage of old notebooks, Iron Mountain
- Scanning to pdf

ENVIRONMENTAL

- 250 paper notebook users today equates to:
 - 500 notebooks per tree, so 5 trees per year
 - Or 3400 kg of CO₂ released per year
 - x1.75 for additional paper pasted in to the notebook

ORGANISATIONAL

- Cross-site collaboration
- More robust IP protection
- Enforcing better record keeping
- Searching and querying

d

Introduction to Dotmatics

d

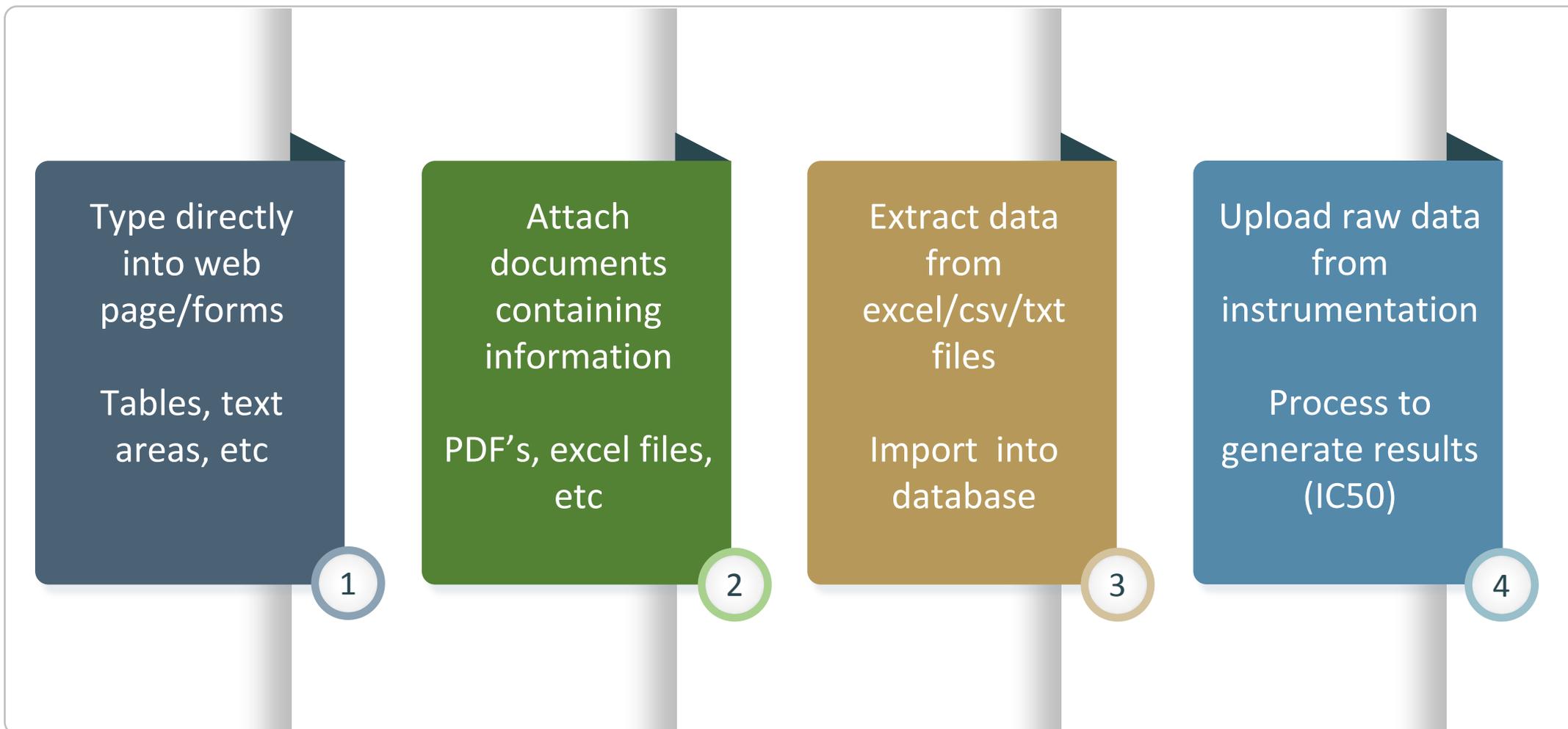
Why Transition to an Electronic Laboratory Notebook?

d

ELN Data Entry Considerations

d

Biology vs Chemistry



- Forms can be designed with any number of tables, text areas and other objects
- Provides a layout in which data can be entered using a keyboard
- Each field is linked to a database field
 - structured approach
 - good for searching later
 - ensures compliance
- Data is modified incrementally and inline throughout the lifetime of the experiment



- Drag and drop attachments
- Very flexible, any file type can be uploaded
- Documents can be previewed inline and can be opened for editing
- Appropriate for many workflows or where additional files should be associated
- Documents contents are searchable within Browser





- Use Studies to extract data from Excel, csv and txt files and place the data in a database
- This approach is useful
 - To bring order to data
 - To make it much more searchable (perfect for assay results from CROs)
 - When the data is delivered in a regular format
- This approach is less useful if
 - The files are irregular
 - The data cannot be standardised
 - It is “just for information” therefore can remain in the attachment

Studies has a plate-based screening component

- Pre-define analyses and plate layouts then combine them in a protocol
- Setting up these templates is an admin (super user) task

Possible to have multiple analyses and plate formats in any one experiment **BUT** it is designed as a robust screening tool rather than an *ad hoc* assay development tool such as Prism

ADVANTAGES

- Encourages robust practices
- Standard procedure to ensure results across different tests are comparable
- Data stored directly in the database in a structured manner
- See chemistry and biology together (and easily see SAR or drill down to raw data)



| | STRUCTURED ELN | UNSTRUCTURED ELN |
|----------------------|--|---|
| DATA UPLOAD | Form entry Extract data from files into database Screening | Leave data in attached files |
| ADVANTAGES | Guides scientist to filling out the desired information Easier to search for data | No admin overhead Easy to use Flexible |
| DISADVANTAGES | Takes a bit more effort to prepare Less flexible | Need to drill down to details (eg can be held in documents) |
| USE WHEN... | You do the same process many times “80% of my experiments are described by 20% of my workflows” | You do the process occasionally “80% of my workflows are needed to describe 20% of my experiments” |

d

Introduction to Dotmatics

d

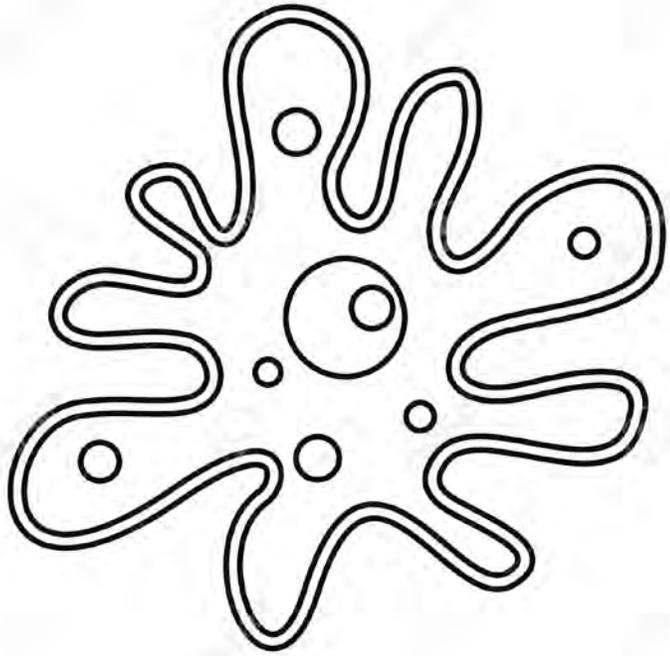
Why Transition to an Electronic Laboratory Notebook?

d

ELN Data Entry Considerations

d

Biology vs Chemistry



CHEMISTRY

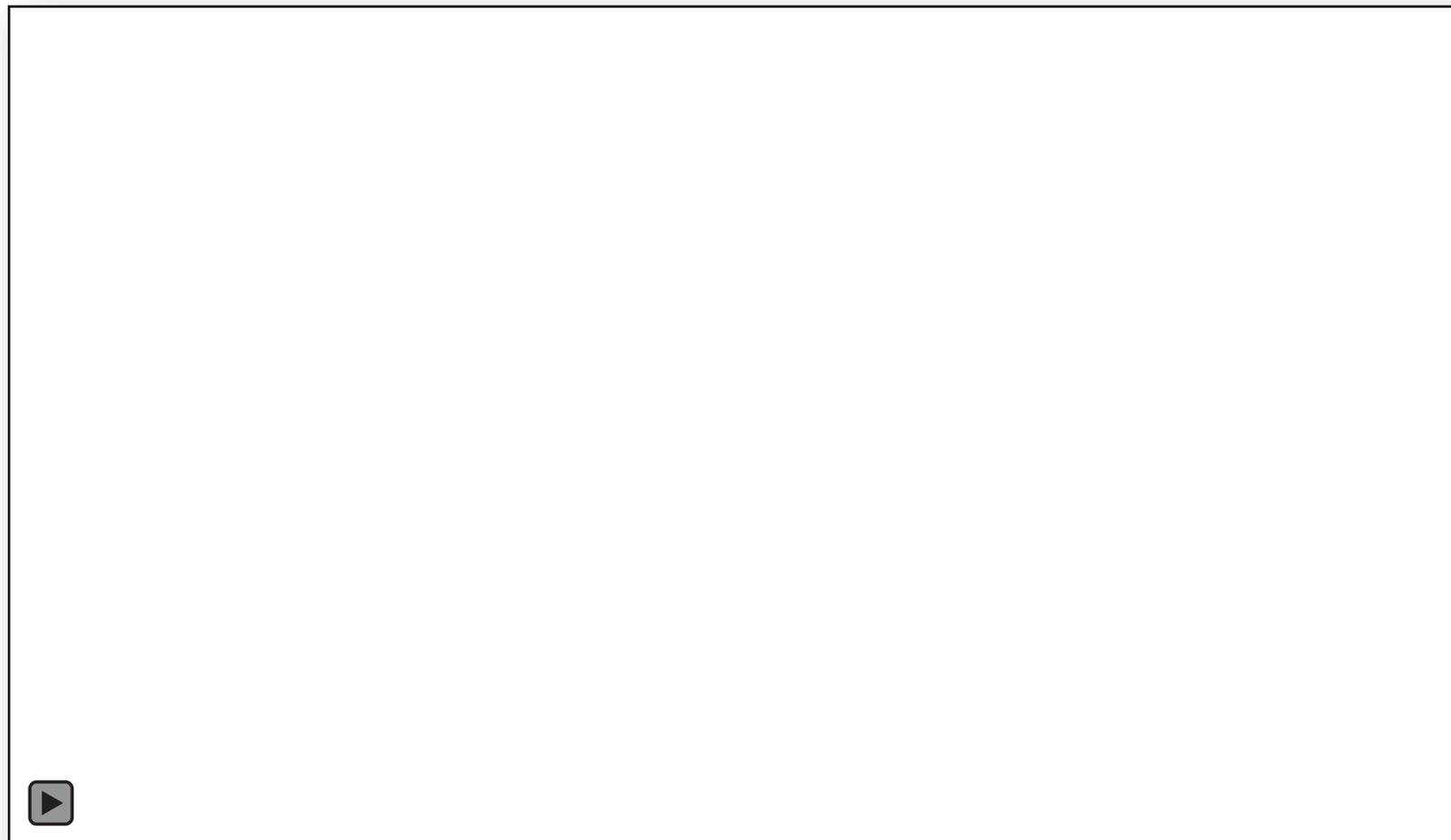


BIOLOGY

- Summary metadata
- Quick links
- Reagents table with lookup
 - Free text options possible
- Method/SOP table with lookup
 - Access the associated method selected
- Results & Conclusions section (for attaching files)



- Reagents table linked to RXN scheme
- Solvents table with lookup
- Products table linked to RXN scheme
- Procedure write up area supporting masks
- Risk assessment table
 - CAS number hyperlink to MSDS
 - Unique hazard pictograms



| | DOTMATICS ELN | |
|--------------|--|--|
| WHY AN ELN? | Efficiency Quality Productivity Collaborative Scalable | Improved visibility Secure Cost Environment Organisation |
| DATA ENTRY | Typing Directly Attaching Files | Extracting Data Screening (upload & process raw data) |
| ORGANISATION | Structured ELN Chemistry | Unstructured ELN Biology |



Alexander Minges, Heinrich-Heine-Universität Düsseldorf: eLabFTW – das freie elektronische Laborjournal

Abstract

eLabFTW ist eine freie und offene Software zur elektronischen Verwaltung und Dokumentation experimenteller Arbeiten. Weiterhin ist eine Datenbankfunktionalität implementiert, welche die Organisation unterschiedlichster Informationen wie z. B. Versuchsvorschriften vereinfacht. Durch seinen flexiblen Aufbau ist eLabFTW in praktisch allen experimentell arbeitenden Laboren einsetzbar und kann dort mit sehr geringem Aufwand auch auf eigener Hardware in Betrieb genommen werden. Zusätzlich ist die Eingliederung an zentrale Infrastrukturen, beispielsweise zur Benutzerverwaltung möglich. Über eine umfangreiche Programmierschnittstelle (API) kann weiterhin eine Anbindung an externe Programme erfolgen, worüber beispielsweise eine automatisierte Dokumentation von Messergebnissen realisiert werden kann.

eLabFTW

Das freie elektronische Laborjournal



Alexander Minges

Helmholtz Open Science Workshop „Elektronische Laborbücher“

13. September 2018

Institut für Biochemische Pflanzenphysiologie

Heinrich-Heine-Universität Düsseldorf

Einführung

Was ist eLabFTW?

eLabFTW ist ein generisches elektronisches Laborjournal (ELN)

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- Gemeinschaftliche Entwicklung durch
Freiwillige – von Wissenschaftlern, für Wissenschaftler

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- Offene und freie Software (GNU AGPL 3.0 )
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- Übersetzt in verschiedene Sprachen

eLabFTW ist eine freie und offene Software (FLOSS)

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Frei wie in „Freibier“ eLabFTW ist jederzeit **kostenlos** verfügbar

Frei wie in „Freiheit“ der **Quelltext** steht offen zur Verfügung,
kann **angepasst, verändert und weiterverbreitet**
werden



2012 Initiiert von Nicolas Carpi am *Institut Pasteur*

Feb. 2013 Erste veröffentlichte Version (0.7.0)

2018 Offiziell durch das *Institut Curie* unterstütztes
Softwareprojekt

Aug. 2018 Veröffentlichung der aktuellen stabilen Version 2.0

Vorgestern Bugfix-Release 2.0.1



- Installation auf zentralem **Server** (Webserver + PHP + MySQL/MariaDB)
- Zugriff über **Webbrowser** auf Endgeräten (Desktop, Notebook, Tablet, Smartphone)
- **Keine Installation spezieller Software** auf dem Client nötig, keine Bindung an bestimmte **Betriebssysteme**



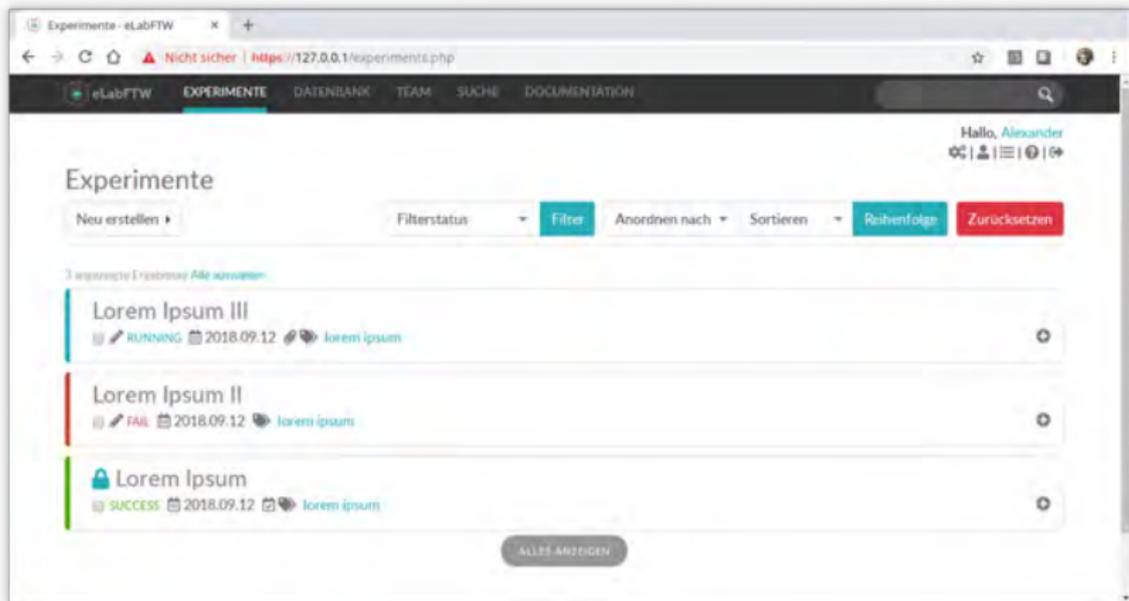
eLabFTW wird weltweit eingesetzt



Funktionsumfang

Benutzeroberfläche

eLabFTW verfügt über eine moderne und übersichtliche Benutzeroberfläche



The screenshot displays the eLabFTW web interface in a browser window. The address bar shows the URL `https://127.0.0.1/experiments.php`. The navigation menu includes 'eLabFTW', 'EXPERIMENTE' (highlighted), 'DATENBANK', 'TEAM', 'SUCHE', and 'DOCUMENTATION'. A user greeting 'Hallo, Alexander' is visible in the top right corner. The main content area is titled 'Experimente' and features a 'Neu erstellen' button. Below this, there are filter and sorting controls: 'Filterstatus' (dropdown), 'Filter' (button), 'Anordnen nach' (dropdown), 'Sortieren' (dropdown), 'Reihenfolge' (button), and 'Zurücksetzen' (button). The experiment list shows three entries:

- Lorem Ipsum III**: RUNNING status, dated 2018.09.12, with a 'lorem ipsum' tag.
- Lorem Ipsum II**: FAIL status, dated 2018.09.12, with a 'lorem ipsum' tag.
- Lorem Ipsum**: SUCCESS status, dated 2018.09.12, with a 'lorem ipsum' tag.

Each entry includes a status indicator (color bar), a pencil icon for editing, a calendar icon for dates, a tag icon for labels, and a gear icon for settings. A '3 angelegte Experimente alle anzeigen' link is positioned above the list. At the bottom of the list, there is an 'ALLES ANZEIGEN' button.



Experimente

- Frei definierbarer **Status** (z.B. „abgeschlossen“, „laufend“ ...)
- **Zeitstempel** möglich
- Definierung von **Vorlagen und Schritten**



Datenbankeinträge

- Definierung von **Vorlagen und Subtypen**
- Nutzbar für z.B. Laborinventar, Protokolle
- Definition von **buchbaren Einträgen** möglich



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Kategorisierung

- Frei definierbare Schlagwörter (*Tags*)

Erstellen von Experimenten und Datenbankeinträgen

Bearbeitung im grafischen Texteditor

Browser: <https://127.0.0.1/experiments.php?mode=edit&id=3>

Schlagwörter

Datum: 20160912

Sichtbarkeits: Only the owner

Status: Running

Experiment

Lorem ipsum dolor sit amet consectetur adipiscing elit

Lorem ipsum dolor sit amet, consectetur adipiscing elit. Aenean commodo ligula eget dolor. Aenean massa. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Donec quam felis, ultricies nec, pellentesque eu, pretium quis, sem. Nulla consequat massa quis enim. Donec pede justo, fringilla vel, aliquet nec, vulputate eget, arcu. In enim justo, rhoncus ut, imperdiet a, venenatis vitae, justo. Nullam dictum felis eu pede mollis pretium. Integer tincidunt. Cras dapibus. Vivamus elementum semper nisi. Aenean vulputate eleifend tellus. Aenean leo ligula porttitor eu, consequat vitae, eleifend ac, enim. Aliquam lorem ante, dapibus in, viverra quis, feugiat a, tellus. Phasellus viverra nulla ut metus varius laoreet. Quisque rutrum. Aenean imperdiet. Etiam ultricies nisi vel augue. Curabitur ullamcorper ultricies nisi.

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- Aenean massa cum sociis natoque penatibus

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Erstellen von Experimenten und Datenbankeinträgen

Anhängen von Dateien mit Vorschau

The screenshot shows a web browser window with the address bar displaying "https://127.0.0.1/experiments.php?mode=edit&id=3". The page content is divided into two main sections:

- # Datei anhängen**: A section with the heading "Dateien zum Hochladen hier fallen lassen".
- # Angehängte Dateien**: A section displaying three attached files, each with a preview and interactive options:
 - Substrat ZIP** (100.24 KB): Preview shows a colorful abstract image. Options: "Click to add a comment" and "Neue Version dieser Datei hochladen".
 - 101-6.pdb** (1.02 MB): Preview shows a 3D protein structure. Options: "Click to add a comment" and "Neue Version dieser Datei hochladen".
 - Struktur00 CID_2396.sdf** (7.12 KB): Preview shows a ball-and-stick molecular model. Options: "Click to add a comment" and "Neue Version dieser Datei hochladen".

Inventarverwaltung mit frei definierbaren Vorlagen

The screenshot displays a web browser window with the address bar showing 'https://127.0.0.1/database.php'. The page title is 'Datenbank - eLabFTW'. The navigation menu includes 'eLABFTW', 'EXPERIMENTE', 'DATENBANK', 'TEAM', 'SUCHE', and 'DOCUMENTATION'. The user is logged in as 'Hallo, Administrator' with a profile icon and a list of items.

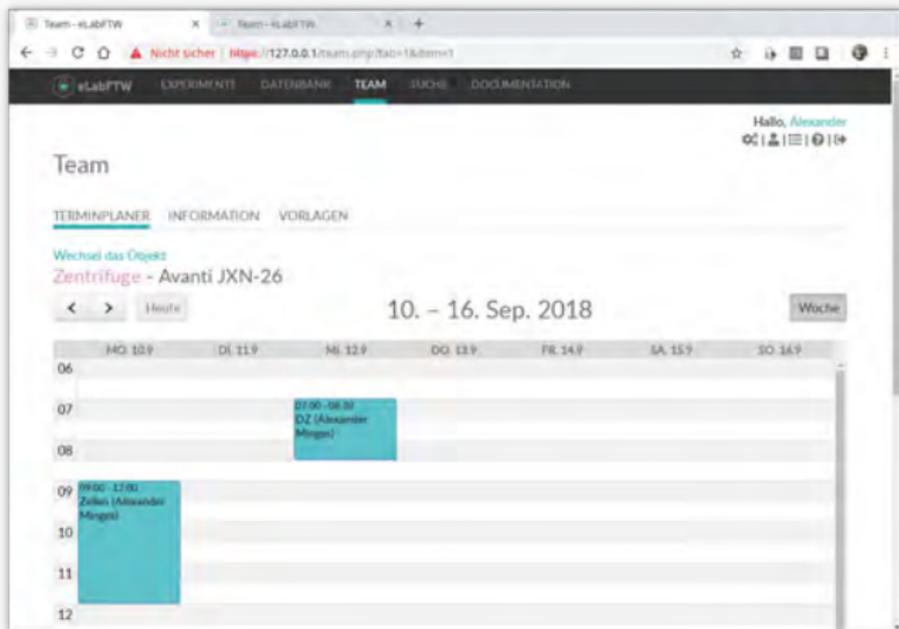
The main content area is titled 'Datenbank' and features a 'Neu erstellen' button. Below this, there are filter controls: 'Sortiere nach Typ' (with a 'Filter' button), 'Anordnen nach', 'Sortieren', 'Filterverlegen', and 'Zurücksetzen'.

The list of items includes:

- Transformation von E.coli XL1-Blue** (red bar): Includes a 'PROTOKOLL' icon, date '2018.09.13', and a 'Transformation XL1 Blue' link.
- pET-16b** (green bar): Includes a 'PLASMID' icon, date '2018.09.13', and a 'pET' link.
- Magnesiumphosphat** (blue bar): Includes a 'CHEMIKALIE' icon and date '2018.09.13'.

At the bottom of the list is a 'GUT ERSTELLEN' button. The footer contains a copyright notice for '© 2018-2019 eLABFTW eLABFTW eLABFTW' and a version number 'eLabFTW v1.12.0 (2019-09-13)'.

Buchung von Geräten über integrierten Kalender



Weitere Funktionen

- Eingabe alternativ als **strukturierter Text** (Markdown)

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- **Verlinkung** von Experimenten/Datenbankeinträgen auch untereinander
- **Freigabe** von Experimenten für andere Benutzer
- Satz **mathematischer Formeln**

Fixierung von Experimenten mittels Zeitstempel

- Nachweis eines definierten Zustandes zum Zeitpunkt „X“
- Zeitstempeldienst (TSA) nach RFC 3161 (z.B. DFN)
- Datenintegrität mittels Signatur überprüfbar



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🕒 Experiment wurde mit einem Zeitstempel versehen von Alexander Minges auf 2018-09-12 bei 22:50:11 Europe/Paris 📄 ⬇️ 🕒

- Export einzelner Experimente und Datenbankeinträge inkl. angehängter Dateien als **ZIP**
- Export als **PDF-Datei** mit Vorschau angehängter Dateien
- Massenexport als **CSV** (nur Text) und ZIP (inkl. Dateien)
- Import von Tabellen im CSV-Format als Experimente oder Datenbankeinträge



Einbindung in bestehende Infrastruktur

- Nach Installation: Lokale Benutzerkonten
- Einbindung in zentrale Identitätsmanagementsysteme möglich (SAML 2.0)
- Kombination von lokalen und zentralen Zugängen möglich



Zugriff über öffentliche REST-API

- Interaktion mit Geräten und Prozessen
- Automatisches Anlegen/Abschließen von Experimenten
- Hochladen von Daten zu eLabFTW
- Datenexport im JSON-Format

Erstellen eines Experimentes aus der *bash* heraus

```
#!/bin/bash
export API_KEY=XXXXX
curl -X POST -H "Authorization: $API_KEY" \
  "https://elabftw.example.org/api/v1/experiments"

# Datei zu Experiment 3 hochladen
curl -X POST -F "file=@your-file.jpg" -H \
  "Authorization: $API_KEY" \
  "https://elabftw.example.org/api/v1/experiments/3"
```



Python-Bibliothek zur einfachen Interaktion mit eLabFTW:

```
elabapy 0.4.0
```

```
pip install elabapy
```

Erstellen eines Experimentes mit *python*

```
#!/sbin/env python
import elabapy

manager = elabapy.Manager(endpoint="https://elab.example.org/api/v1/",
                           token="XXXX")

exp = manager.create_experiment()

files = {'file': open('report.xls', 'rb')}
print(manager.upload_to_experiment(exp["id"], files))
```

Erstellen eines Experimentes mit *python*

```
#!/sbin/env python
import elabapy

manager = elabapy.Manager(endpoint="https://elab.example.org/api/v1/",
                           token="XXXX")

exp = manager.create_experiment()

files = {'file': open('report.xls', 'rb')}
print(manager.upload_to_experiment(exp["id"], files))
```

Weitere Beispiele: <https://doc.elabftw.net/api.html>

Ausblick

- Ausbau der Vorschaufunktion (z.B. Plasmidkarten)
- Umfangreicheres Rechtemanagement
- Möglichkeit hierarchischer Verwandtschaftsbeziehungen

Wie ausprobieren?



<https://demo.elabftw.net>



<https://doc.elabftw.net/install.html>

Zum Abschluss



Website <https://www.elabftw.net>

Hilfe <https://doc.elabftw.net>

Quelltext <https://github.com/elabftw/elabftw>



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Prof. Dr. Georg Groth
Biochemische Pflanzenphysiologie
Heinrich-Heine-Universität



Nicolas Carpi
Institut Curie, Paris
Frankreich



Vielen Dank für Ihre
Aufmerksamkeit!

Abstract

Chemotion ELN ist ein elektronisches Laborbuch (ELN) für Forscher aus dem Bereich der Chemie und angrenzenden Forschungsbereichen, das von Wissenschaftlern für Wissenschaftler am Karlsruher Institut für Technologie (KIT) entwickelt wird. Das webbasierte ELN ist als Open Source verfügbar und bietet moderne Technologien für diejenigen Chemiker, die mit den derzeit verfügbaren Systemen nicht zufrieden sind und flexible Lösungen für die Zukunft suchen. Das Chemotion-ELN bietet grundlegenden Funktionen, die für die Erfassung und Verarbeitung der chemischen Forschung notwendig sind, insbesondere die Arbeit mit molekularen Strukturen und Berechnungen basierend auf molekularen Eigenschaften. Das ELN unterstützt die Planung, Beschreibung, Speicherung und Steuerung der Routinearbeit insbesondere von Organikern und wurde um Funktionen zur Kommunikation und zum Austausch von Forschungsdaten mit Kollegen erweitert. Entsprechend der Notwendigkeit einer modernen Forschungsinfrastruktur ermöglicht das ELN die Suche nach Molekülen und Reaktionen nicht nur innerhalb der Datenbank des Benutzers, sondern auch in gängigen externen Quellen wie SciFinder und PubChem. Das Chemotion ELN unterscheidet sich von ähnlichen Systemen durch die Implementierung von besonderen Anwendungen, die speziell auf die Arbeit von Wissenschaftlern in Universitäten ausgerichtet sind. Hierzu zählt die Reporting-Funktion, welche die Erstellung von formatierten Berichten oder auch einer Supporting Information für Publikationen erlaubt. Eine weitere Funktion erlaubt es, erhaltene Daten auf Wunsch direkt in ein Repositorium für Forschungsdaten zu transferieren, um die erhaltenen Informationen zugänglich zu machen. Das ELN soll insbesondere durch diese Funktion den stetig wachsenden Anforderungen an ein gutes Forschungsdatenmanagement gerecht werden und die Forscher bestmöglich unterstützen.

Chemotion ELN – Basis-Funktionen und besondere Anwendungen

Nicole Jung (Stefan Bräse group)

INSTITUTE OF ORGANIC CHEMISTRY - Stefan Bräse Group Karlsruhe



Chemotion

funded by

DFG

Intoduction group activities

**Materials
Chemistry**

**Bioactive
Molecules**

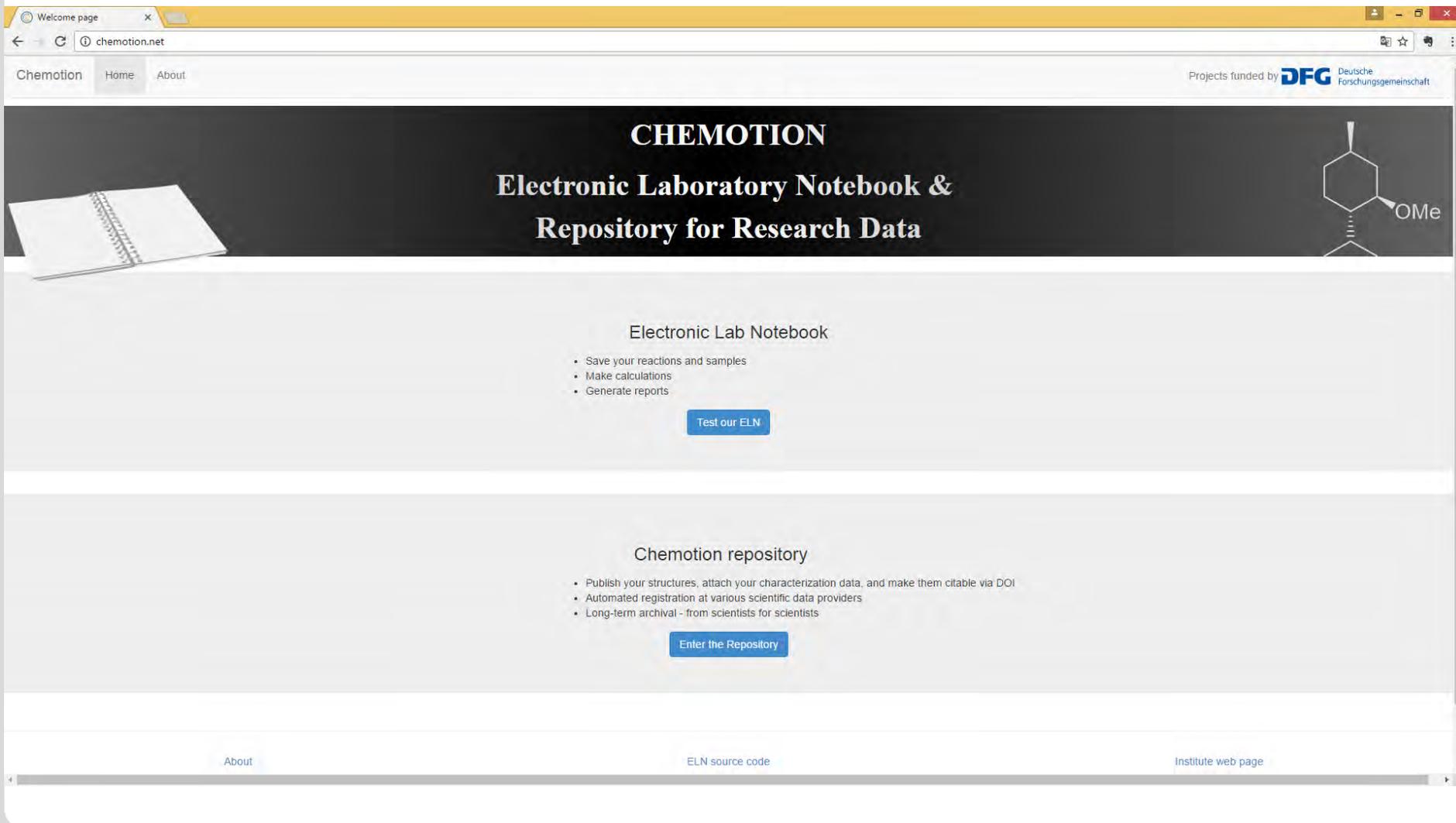
**Organometallic
Chemistry &
Catalysis**

**Solid Phase
Synthesis**

**Software
Development
*Chemotion***

**Molecule
Archive**





The screenshot shows a web browser window with the URL chemotion.net. The page features a navigation menu with 'Chemotion', 'Home', and 'About'. A banner at the top right states 'Projects funded by DFG Deutsche Forschungsgemeinschaft'. The main heading is 'CHEMOTION Electronic Laboratory Notebook & Repository for Research Data', accompanied by an image of a spiral notebook and a chemical structure of a substituted cyclohexane ring. Below this, two sections are presented: 'Electronic Lab Notebook' with a list of features and a 'Test our ELN' button, and 'Chemotion repository' with a list of features and an 'Enter the Repository' button. The footer contains links for 'About', 'ELN source code', and 'Institute web page'.

Chemotion Home About

Projects funded by **DFG** Deutsche Forschungsgemeinschaft

CHEMOTION

Electronic Laboratory Notebook & Repository for Research Data

Electronic Lab Notebook

- Save your reactions and samples
- Make calculations
- Generate reports

[Test our ELN](#)

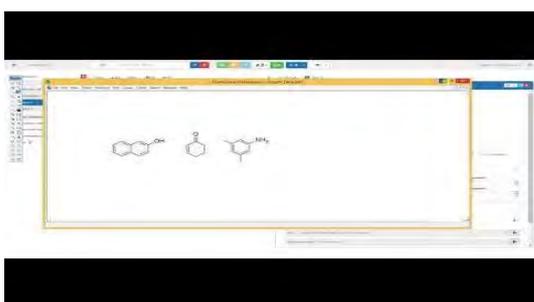
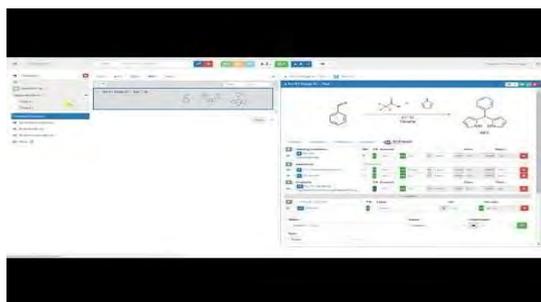
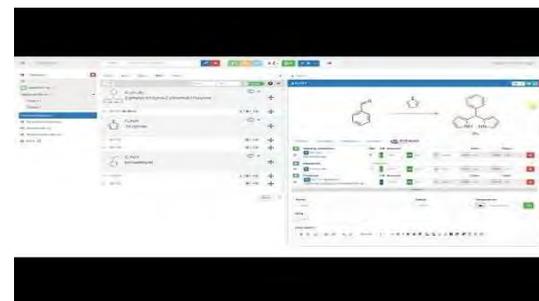
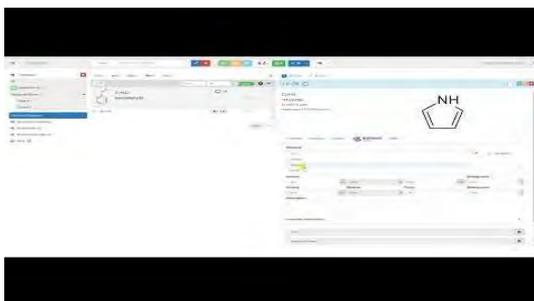
Chemotion repository

- Publish your structures, attach your characterization data, and make them citable via DOI
- Automated registration at various scientific data providers
- Long-term archival - from scientists for scientists

[Enter the Repository](#)

[About](#) [ELN source code](#) [Institute web page](#)

Chemotion ELN - Youtube



Access to research data: Key challenges

AIMS: Infrastructure: Access to research data
Improve reproducibility of scientific work
Accelerate and facilitate scientific work

Device Integration



- Remote work
- Data transfer



Electronic Lab Notebook

- Digital storage
- Processing of data

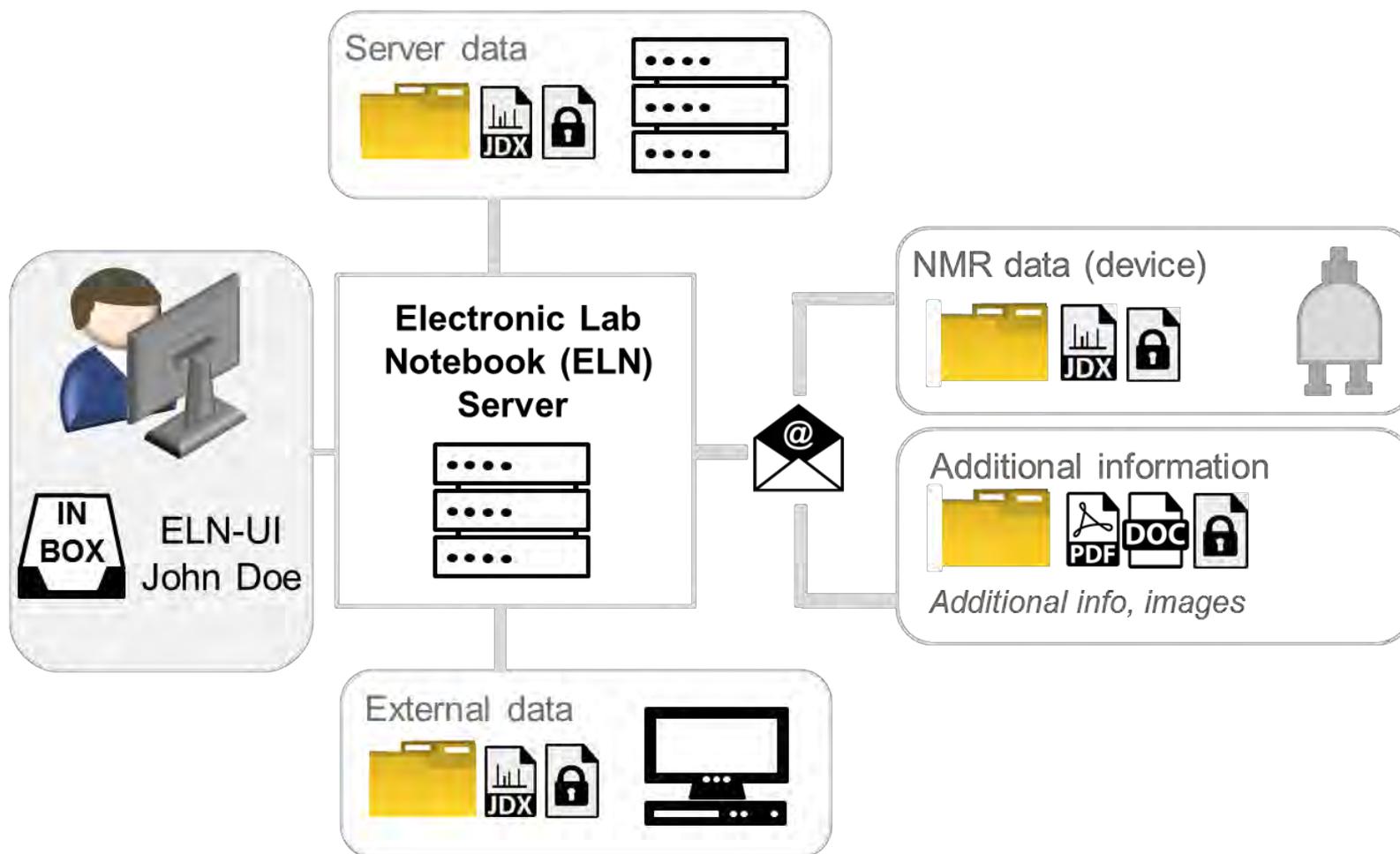


Repository

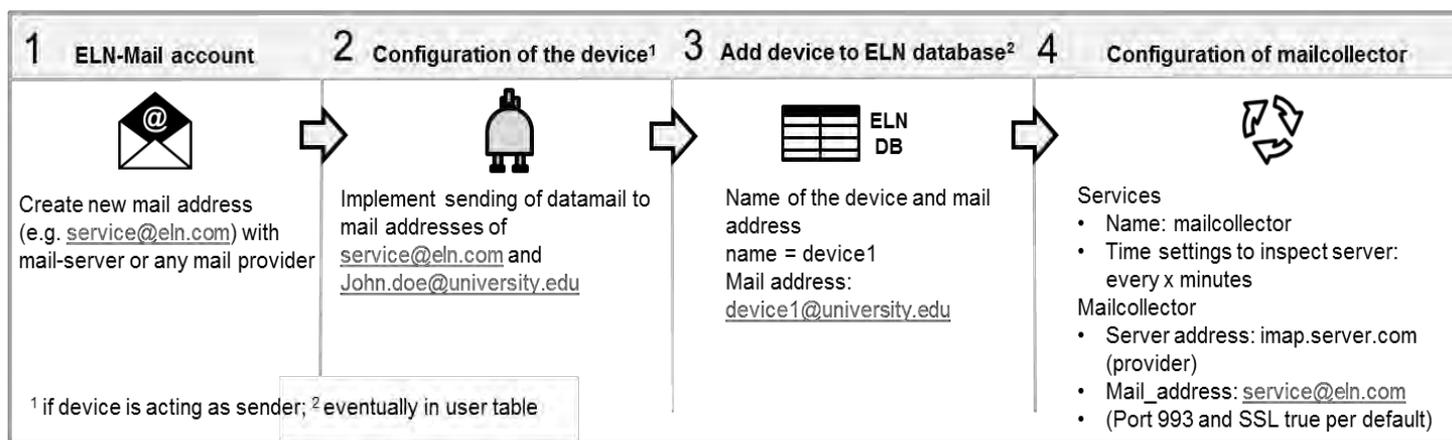
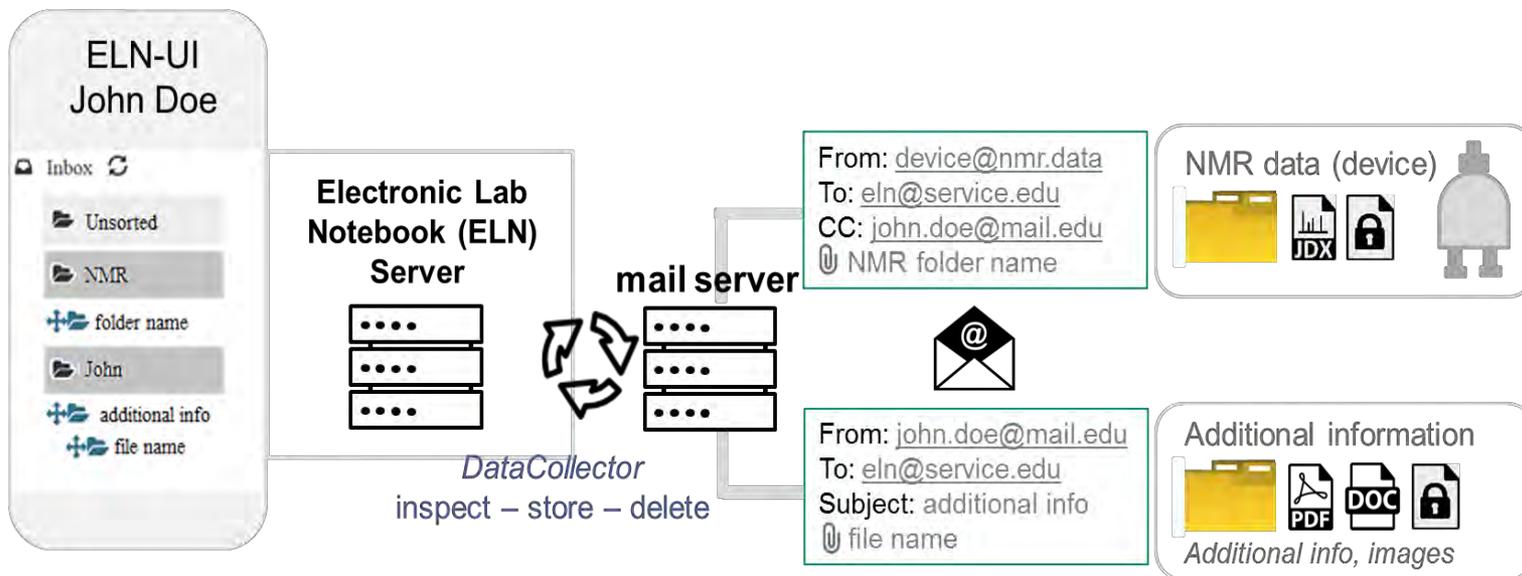
- Open Access
- No limitation (file types)
- Interoperability



Access to research data: DEVICES



Access to research data: DEVICES (example)



Access to research data: Key challenges

AIMS: Infrastructure: Access to research data
Improve reproducibility of scientific work
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Device Integration



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- Data transfer



Electronic Lab Notebook

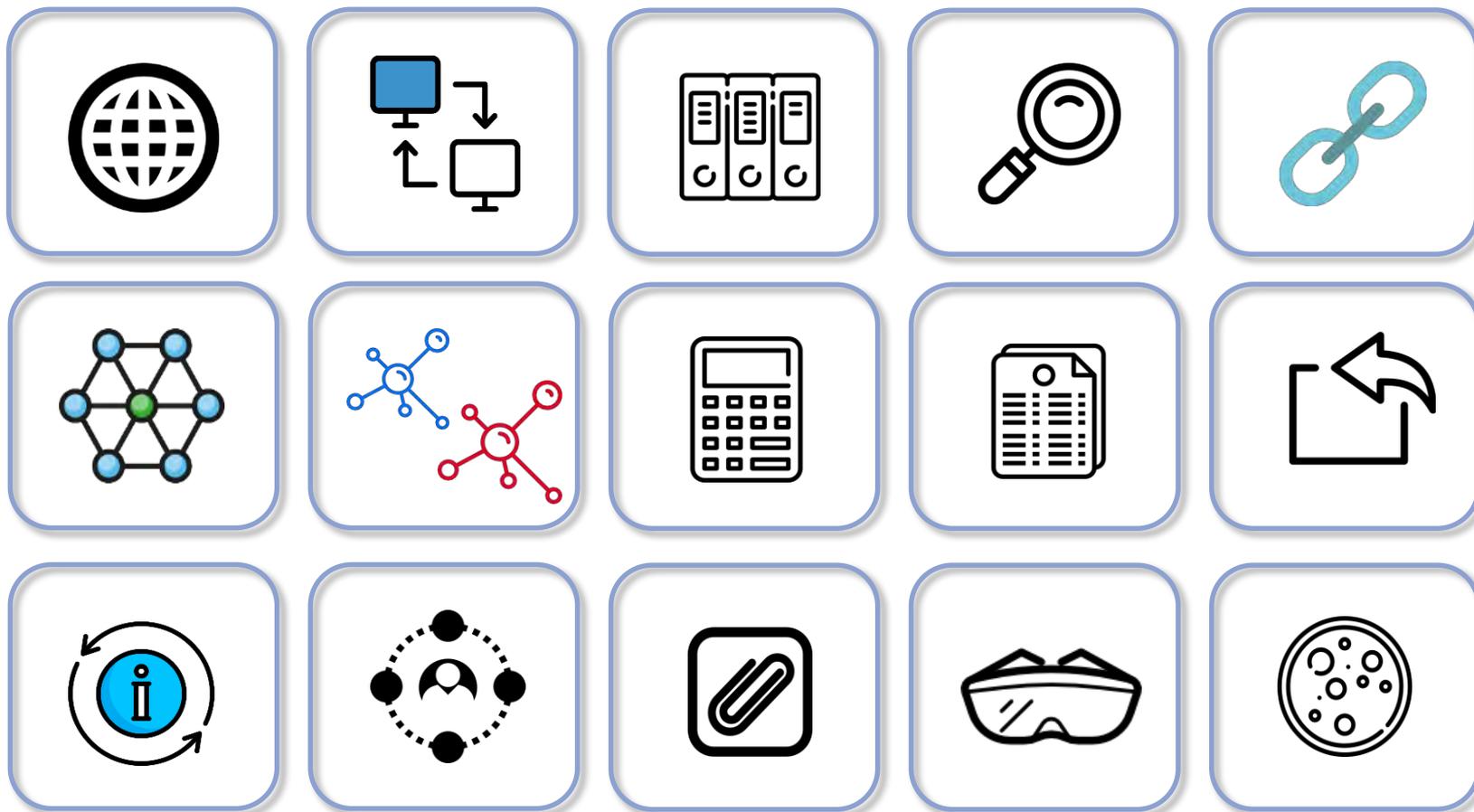
- Digital storage
- Processing of data



Repository

- Open Access
- No limitation (file types)
- Interoperability





OPEN SOURCE

Source: Our findings &
S. Kanza, C. Willoughby, N. Gibbins, R. Whitby, J.G. Frey, J. Erjavac, K. Zupanic, M. Hren, K. Kovac, *J Cheminfo*. **2017**, 9:31.

Electronic Lab Notebook - Samples

Secure | <https://eln.chemotion.net/#/collection/192/sample/1194> | Logged in as Nicole Jung

Chemotion - All - IUPAC, InChI, SMILES, ...

Collections: 219(0) 62(0) 1(0) 1(0) 1(0) | NJu-145 NJu-R24-A

chemotion.net

Collection 1

BJOC data

Collection 2

Collection 3

Test Import

My shared collections

Shared with me

Synchronized with me

inbox

From To Samples

C11H16OS2
3-[1-(1,3-dithiolan-2-ylidene)ethyl]cyclohexan-1-one

NJu-145 NJu-R24-A | 2-0

C10H13OS2

NJu-667 NJu-R162-A | 1-0

C26H24OS2
4-(1,3-dithian-2-ylidene)-1,3,4-triphenylbutan-1-one

NJu-743 NJu-R229-A | 2-0

C16H20OS2
6-(1,3-dithian-2-ylidene)-6-phenylhexan-3-one

NJu-766 NJu-R240-A | 2-0

C16H20OS2

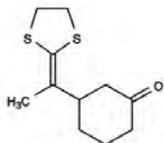
Show 15

NJu-145 NJu-R24-A | 2-0

C11H16OS2
3-(1-(1,3-dithiolan-2-ylidene)ethyl)cyclohexan-1-one
Exact mass: 228.064267 g/mol



9510758634



Properties Analyses Results NMR

Molecule: 3-(1-(1,3-dithiolan-2-ylidene)ethyl)cyclohexan-1-one

Stereo Abs: Select... Stereo Rel: Select... Top secret

| Name | External label | Location | Solvent |
|-----------|----------------|----------|-----------|
| NJu-R24-A | | | Select... |

| Amount | Bolting point |
|--------------------------------|---------------|
| 130.3 mg 0.0000 ml 0.5706 mmol | 0.0000 °C |

| Density | Molarity | Purity | Melting point |
|-------------|----------|--------|---------------|
| 0.0000 g/ml | 0.0000 M | 0.0000 | 0.0000 °C |

Description

Elemental composition

Electronic Lab Notebook - Reactions

Secure | https://eln.chemotion.net/#/collection/192/reaction/336

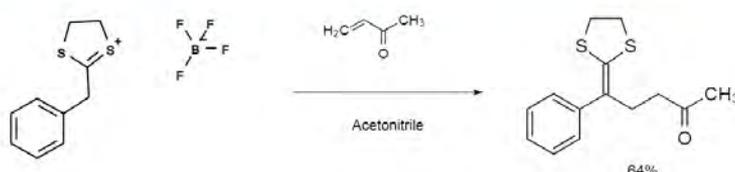
Chemotion - All | IUPAC, InChI, SMILES, ...

Logged in as Nicole Jung

Collections: 219(0) 62(0) 1(0) 1(0)

NJu-145 NJu-R24-A NJu-R243 According to General Procedure 2a

NJu-R243 According to General Procedure 2a



Scheme Properties References Analyses Green Chemistry Zotero

| Starting materials | Ref | T/R | Amount | Conc | Equiv |
|--|-----|-----|---------|---------|------------|
| NJu-772 2-benzyl-4,5-dihydro-1,3-dithiol-1- | | | 1000 mg | 0.00 ml | 3.544 mmol |

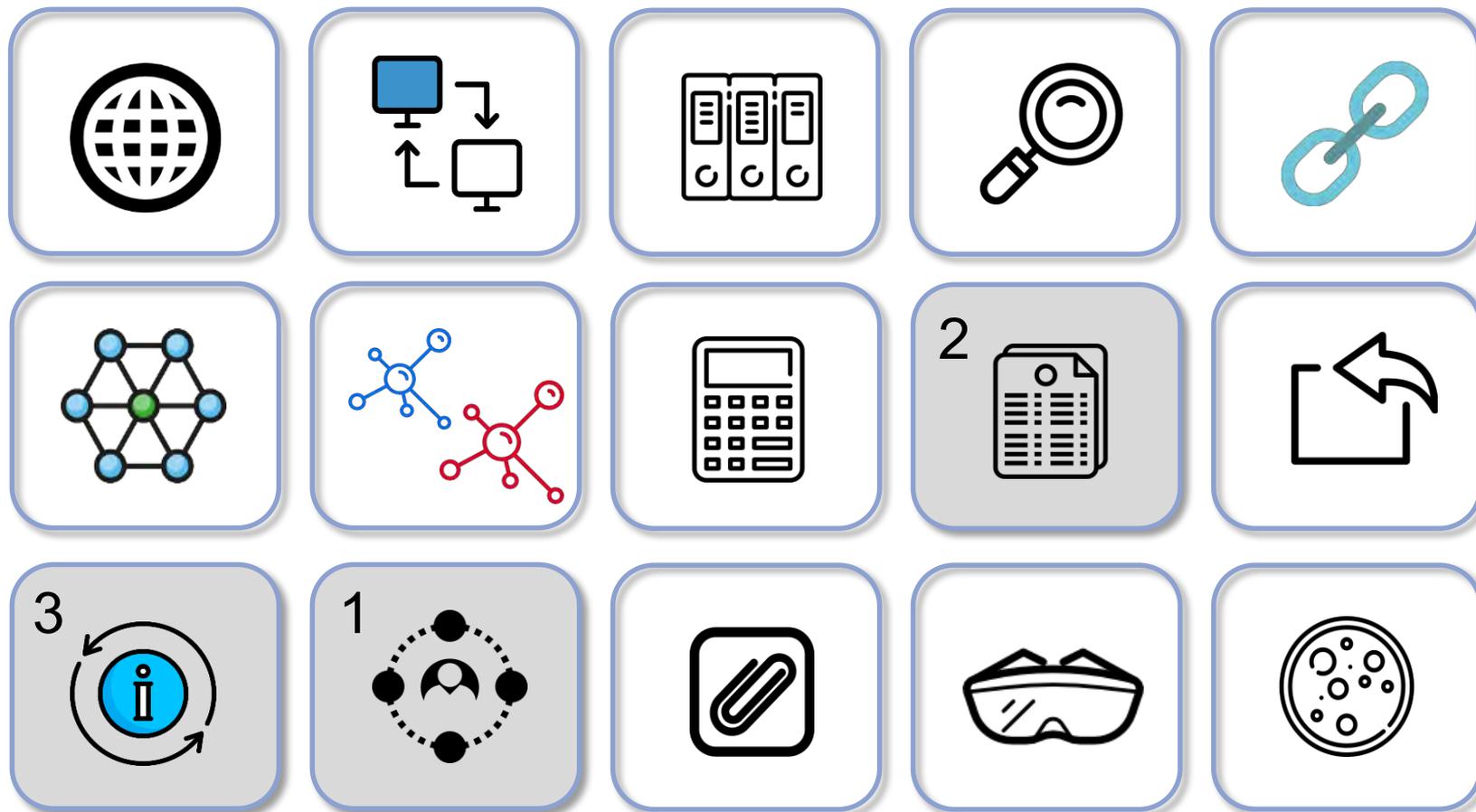
| Reactants | Reagents | T/R | Amount | Conc | Yield |
|----------------|----------|-----|----------|---------|------------|
| but-3-en-2-one | | | 298.1 mg | 0.00 ml | 4.253 mmol |

| Products | T/R | Amount | Conc | Yield | |
|---|-----|--------|----------|---------|------------|
| NJu-773 NJu-R243-A 5-(1,3-dithiolan-2-ylidene)-5-phen... | | | 599.8 mg | 0.00 ml | 2.268 mmol |

Solvents

| Name | Status | Temperature |
|-----------------------------------|--------|----------------|
| According to General Procedure 2a | Select | Temperature °C |

Role: Parts of GP According to



OPEN SOURCE

Source: Our findings &
S. Kanza, C. Willoughby, N. Gibbins, R. Whitby, J.G. Frey, J. Erjavac, K. Zupanic, M. Hren, K. Kovac, *J Cheminfo*. **2017**, 9:31.

Electronic Lab Notebook - Sharing

Secure | https://eln.chemotion.net/#/collection/192/reaction/336

Chemotion - All | IUPAC, InChI, SMILES, ...

Logged in as Nicole Jung

Collections: 219(0) 62(0) 1(0) 1(0) 1(0)

NJu-145 NJu-R24-A NJu-R243 According to General Procedure 2a

NJu-R243 According to General Procedure 2a 1-0

My shared collections

Shared with me

Synchronized with me

Inbox

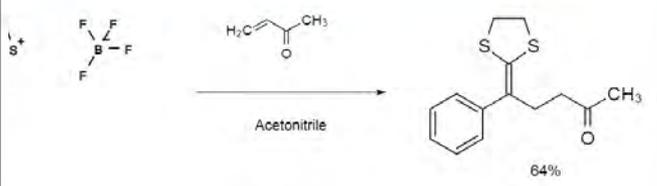
3-dithiol-1-...
Reagents
T/R Amount Conc Equiv
599.8 mg 0.00 ml 2.268 mmol 453.7 mmol 64%

3-A
te)-S-phen...
T/R Amount Conc Yield
599.8 mg 0.00 ml 2.268 mmol 453.7 mmol 64%

Solvents

Name: According to General Procedure 2a Status: Select... Temperature: °C

Role: Parts of GP According to



Electronic Lab Notebook - Sharing Data

Sharing

Role
Pick a sharing role (optional)

Permission level
Read

Sample detail level
Molecular mass of the compound, external label

Reaction detail level
Observation, description, calculation

Select Users to share with
Select...

Create Shared Collection

My Groups

Create new Group

| Name group | xxx | Name abbrev |
|---------------------|-----|-------------|
| user group S. Bräse | | UG-SB |

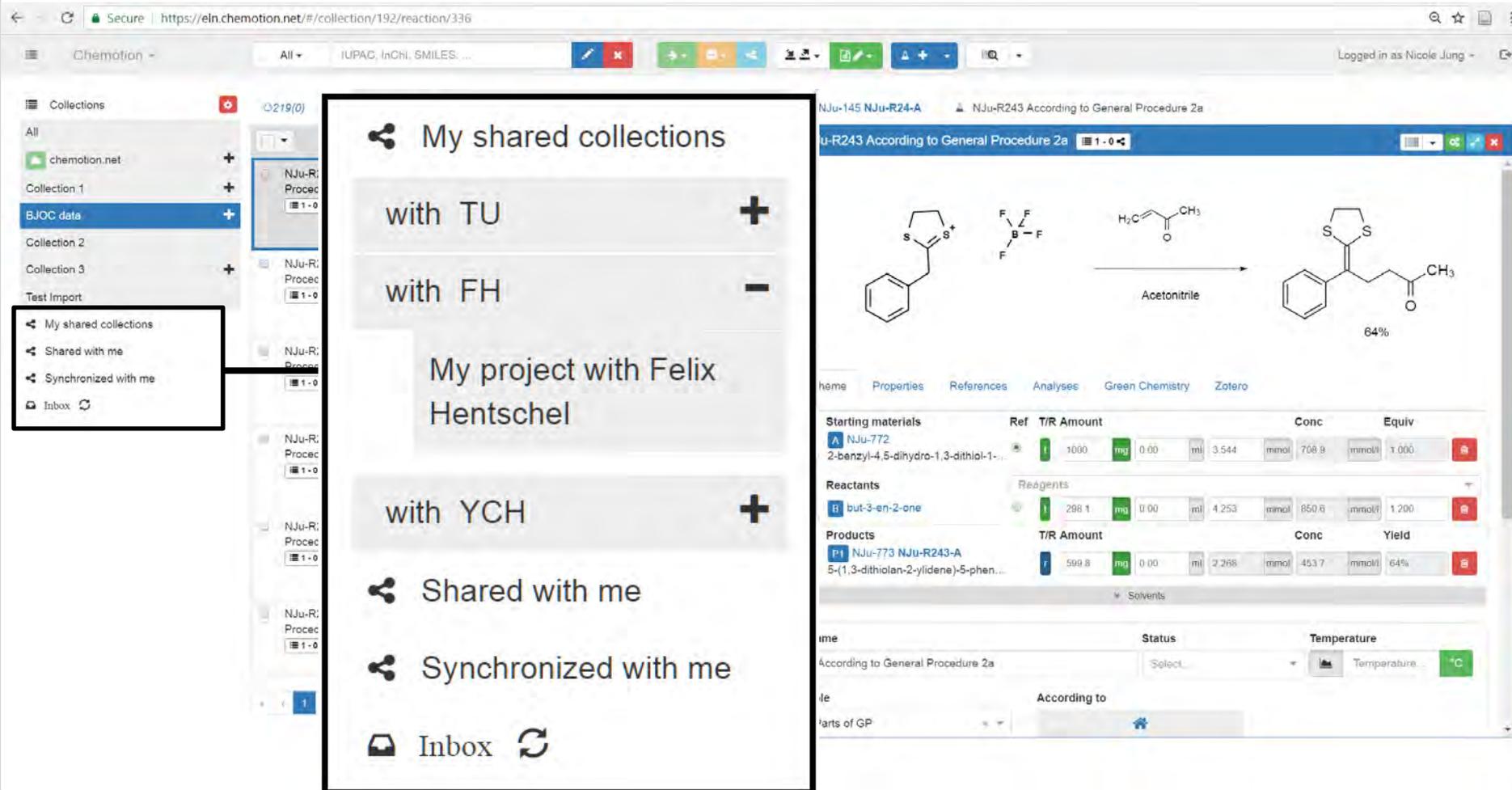
Back

Add more users

- Serhii Kotov - SK
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- Dominic Lütjohann - DL
- Jason Huang - JHX
- An Nguyen - AN
- database user - DU

Icons: List, Edit, Delete

Electronic Lab Notebook - Sharing



The screenshot displays the Chemotion ELN interface. On the left, a sidebar shows a list of collections, with 'My shared collections' highlighted. A central pop-up menu is open, listing sharing options: 'My shared collections', 'with TU', 'with FH', 'My project with Felix Hentschel', 'with YCH', 'Shared with me', 'Synchronized with me', and 'Inbox'. On the right, a reaction scheme is shown for the synthesis of 5-(1,3-dithiolan-2-ylidene)-5-phenylpentan-3-one. The reaction involves a cyclic sulfur ylide, a boron trifluoride reagent, and methyl vinyl ketone in acetonitrile, yielding the product in 64% yield. Below the reaction, a table lists starting materials, reactants, and products with their respective amounts and concentrations.

| Starting materials | Ref | T/R | Amount | Conc | Equiv |
|---|-----|------|------------|------------|------------------|
| NJu-772 2-benzyl-4,5-dihydro-1,3-dithiol-1-... | A | 1000 | mg 0.00 ml | 3.544 mmol | 708.9 mmol 1.000 |

| Reactants | Reagents |
|-------------------|---|
| li but-3-en-2-one | 298.1 mg 0.00 ml 4.253 mmol 850.0 ummol 1.200 |

| Products | T/R | Amount | Conc | Yield |
|--|-----|------------------|------------|-----------------|
| P1 NJu-773 NJu-R243-A 5-(1,3-dithiolan-2-ylidene)-5-phen... | f | 599.8 mg 0.00 ml | 2.268 mmol | 453.7 ummol 64% |

| Time | Status | Temperature |
|-----------------------------------|-----------|-------------------|
| According to General Procedure 2a | Select... | Temperature... °C |

ELN – reporting and Supporting Information

Chemotion - All - IUPAC_InChI, SMILES...

Logged in as Nicole Jung

Collections: 215(0) 62(0) 1(0) 1(0) 1(0)

Report

chemotion.net

BJOC data

Collection_J. Parsch

Rxn GP recov

My shared collections

Shared with me

Synchronized with me

Inbox

NJu-R243 According to General Procedure 2a

NJu-R242 According to General Procedure 2a

NJu-R241 According to General Procedure 2a

NJu-R240 According to General Procedure 2a

NJu-R239 According to General Procedure 2a

Report Generation

Config Setting Order Label Preview Archive

Template Selection

Supporting Information

File Name

Supporting_Information_2018-1-10H17M29S46

File description

Deselect all

Show all chemicals in schemes (unchecked to show products only)

Show 15



ELN – reporting and Supporting Information

Report Generation Reset Generate Report X

Config **Setting** Order Label Preview Archive

Template Selection

Supporting Information

File Name

Supporting_Information_2018-1-10H17M29S46

File description

Deselect all

Show all chemicals in schemes (unchecked to show products only)



ELN – reporting and Supporting Information

Report Generation Reset Generate ✕

[Config](#) **Setting** [Order](#) [Label](#) [Preview](#) [Archive](#)

Synthesis Products Information

Deselect all

| | | | |
|--|---|--|--|
| <input checked="" type="checkbox"/> Name | <input checked="" type="checkbox"/> Formula | <input checked="" type="checkbox"/> InChI | <input checked="" type="checkbox"/> Exact Mass |
| <input checked="" type="checkbox"/> CAS | <input checked="" type="checkbox"/> Smiles | <input checked="" type="checkbox"/> Molecular Mass | <input checked="" type="checkbox"/> EA |

Report Generation Reset Generate Report X

Config Setting **Order** Label Preview Archive

| |
|---|
| NJu-R243 According to General Procedure 2a X |
| |
| NJu-R242 According to General Procedure 2a X |
| |
| NJu-R241 According to General Procedure 2a X |
| |
| NJu-R240 According to General Procedure 2a X |



ELN – reporting and Supporting Information

Report Generation Reset Generate Report X

Config **Setting** Order Label Preview Archive

| | | | |
|---|--|--------------------|-----|
| 1 | | $C_{14}H_{16}OS_2$ | 16 |
| 2 | | $C_{15}H_{18}OS_2$ | 17 |
| 3 | | $C_{15}H_{18}OS_2$ | 18a |
| 4 | | $C_{16}H_{20}OS_2$ | XX |



Report Generation Reset Generate Report X

[Config](#) [Setting](#) [Order](#) [Label](#) [Preview](#) [Archive](#)

4 Synthesis

4.1 5-(1,3-dithiolan-2-ylidene)-5-phenylpentan-2-one (16)

Name: 5-(1,3-dithiolan-2-ylidene)-5-phenylpentan-2-one; Formula: C₁₄H₁₆OS₂; CAS: -; Smiles: CC(=O)CCC(=C1SCCS1)c1ccccc1; InCHI: L XKWSUYFYQCLR X-UHFFFAOYSA-N; Molecular Mass: 264.4062; Exact Mass: 264.0643; EA: C, 63.6; H, 6.1; O, 6.05; S, 24.25.

According to General Procedure 2a: {A}xx} 2-benzyl-4,5-dihydro-1,3-dithiol-1-ium tetrafluoroborate (1.00 g, 3.54 mmol, 1.00 equiv); {B}xx} but-3-en-2-one (0.298 g, 4.25 mmol, 1.20 equiv); {C} acetonitrile (5.0 ml); Yield: {D}16} = 64% (0.600 g, 2.27



ELN – reporting and Supporting Information

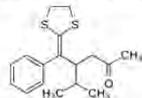
Report Generation Reset Generate Report X

[Config](#) [Setting](#) [Order](#) [Label](#) [Preview](#) [Archive](#)

| | | | |
|--|--|--|--|
| Supporting_Information_2018-1-10H17M45S44 SI | | | |
| Supporting_Information_2017-10-24H17M36S45 SI | | | |
| Supporting_Information_2017-10-24H17M30S10 SI | | | |
| Supporting_Information_2017-10-24H15M54S59 SI | | | |
| Supporting_Information_2017-10-11H7M50S15 SI | | | |



4.9 4-((1,3-Dithiolan-2-ylidene)(phenyl)methyl)-5-methylhexan-2-one (4e)



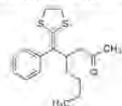
Name: 4-((1,3-Dithiolan-2-ylidene)(phenyl)methyl)-5-methylhexan-2-one; Formula: $C_{17}H_{22}OS_2$; CAS: -; Smiles: CC(C(C(=C1SCCS1)c1ccccc1)CC(=O)C)C; InChI: A1JUPLBXPXRSZPK-UHFFFAOYSA-N; Molecular Mass: 306.4860; Exact Mass: 306.1112; EA: C, 66.62; H, 7.24; O, 5.22; S, 20.92.

According to General Procedure 2b: {A1a} 2-benzyl-4,5-dihydro-1,3-dithiol-1-ium tetrafluoroborate (0.156 g, 0.551 mmol, 1.00 equiv); {B3e} (E)-5-methylhex-3-en-2-one (0.074 g, 0.660 mmol, 1.20 equiv); {C} acetonitrile (5.00 mL); Yield {D4e} = 85% (0.144 g, 0.471 mmol).

The obtained crude product was purified via flash-chromatography on silica gel using cyclohexane/ethyl acetate 10:1. $R_f = 0.63$ (cyclohexane/ethyl acetate 2:1).

1H NMR (500 MHz, $CDCl_3$, ppm) δ = 0.90 (d, J = 6.6 Hz, 3H), 1.12 (d, J = 6.6 Hz, 3H), 1.60–1.69 (m, 1H), 2.16 (s, 3H), 2.37 (dd, J = 16.6 Hz, J = 8.9 Hz, 1H), 2.53 (dd, J = 16.6 Hz, J = 4.8 Hz, 1H), 3.04 (td, J = 9.3 Hz, J = 4.7 Hz, 1H), 3.20–3.24 (m, 2H), 3.36–3.40 (m, 2H), 7.13–7.16 (m, 2H), 7.27–7.31 (m, 1H), 7.33–7.37 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ = 20.6, 21.2, 29.8, 31.1, 37.1, 37.7, 45.8, 50.3, 127.1, 128.1 (2C), 129.1, 129.3 (2C), 136.8, 141.2, 207.9; EI (m/z , 70 eV, 60 °C): 306 (38) [M]⁺, 263 (100), 221 (52), 191 (11), 113 (13), 69 (19); HRMS–EI (m/z): [M]⁺ calcd for $C_{17}H_{22}OS_2$: 306.1107; found, 306.1108; IR (ATR, $\bar{\nu}$): 2964, 2924, 1710, 1586, 1472, 1440, 1404, 1369, 1301, 1278, 1169, 1110, 1071, 1026, 917, 889, 843, 816, 793, 749, 702, 652, 590, 563, 501, 425, 400 cm^{-1} .

4.10 4-((1,3-dithiolan-2-ylidene)(phenyl)methyl)octan-2-one (4f)



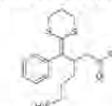
Name: 4-((1,3-dithiolan-2-ylidene)(phenyl)methyl)octan-2-one; Formula: $C_{18}H_{24}OS_2$; CAS: -; Smiles: CCCCC(C(=C1SCCS1)c1ccccc1)CC(=O)C; InChI: XLPWXCGXHOGTNX-UHFFFAOYSA-N; Molecular Mass: 320.5126; Exact Mass: 320.1269; EA: C, 67.45; H, 7.55; O, 4.99; S, 20.01.

According to General Procedure 2a: {A1a} 2-benzyl-4,5-dihydro-1,3-dithiol-1-ium tetrafluoroborate (0.156 g, 0.553 mmol, 1.00 equiv); {B3f} (E)-oct-3-en-2-one (0.084 g, 0.666 mmol, 1.21 equiv); {C} acetonitrile (5.00 mL); Yield {D4f} = 90% (0.160 g, 0.498 mmol). The obtained crude product was purified via flash-chromatography on silica gel using cyclohexane/ethyl acetate 10:1 = NEt₃ (1%). $R_f = 0.45$ (cyclohexane/ethyl acetate 2:1).

1H NMR (500 MHz, $CDCl_3$, ppm) δ = 1.04–1.09 (t, J = 7.2 Hz, 3H), 1.44–1.63 (m, 6H), 2.29 (s, 3H), 2.49 (dd, J = 16.6 Hz, J = 7.0 Hz, 1H), 2.63 (dd, J = 16.4 Hz, J = 7.0 Hz, 1H), 3.37–

3.41 (m, 2H), 3.41–3.48 (m, 1H), 3.54–3.57 (m, 2H), 7.24–7.28 (m, 2H), 7.43–7.48 (m, 1H), 7.49–7.54 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ = 13.9, 22.6, 29.6, 30.0, 33.2, 37.1, 37.8, 43.2, 47.9, 127.1, 128.2 (2C), 129.3 (2C), 129.4, 135.9, 140.7, 207.6; EI (m/z , 70 eV, 120 °C): 320 (58) [M]⁺, 263 (100), 221 (22), 195 (20), 152 (49); HRMS–EI (m/z): [M]⁺ calcd for $C_{18}H_{24}OS_2$: 320.1265; found, 320.1265; IR (ATR, $\bar{\nu}$): 2953, 2923, 2855, 1711, 1597, 1580, 1489, 1438, 1420, 1356, 1278, 1159, 1105, 1072, 1031, 978, 847, 750, 702, 645, 541 cm^{-1} .

4.11 4-((1,3-dithian-2-ylidene)(phenyl)methyl)octan-2-one (5f)

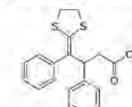


Name: 4-((1,3-dithian-2-ylidene)(phenyl)methyl)octan-2-one; Formula: $C_{18}H_{24}OS_2$; CAS: -; Smiles: CCCCC(C(=C1SCCSC1)c1ccccc1)CC(=O)C; InChI: UOHJUSHNULFLRZ-UHFFFAOYSA-N; Molecular Mass: 334.5391; Exact Mass: 334.1425; EA: C, 68.21; H, 7.83; O, 4.78; S, 19.17.

According to General Procedure 2a: {A2a} 2-benzyl-5,6-dihydro-4H-1,3-dithian-1-ium tetrafluoroborate (0.156 g, 0.525 mmol, 1.00 equiv); {B3f} (E)-oct-3-en-2-one (0.080 g, 0.630 mmol, 1.20 equiv); {C} acetonitrile (5.00 mL); Yield {D5f} = 64% (0.113 g, 0.337 mmol). The obtained crude product was purified via flash-chromatography on silica gel using cyclohexane/ethyl acetate 10:1. $R_f = 0.73$ (cyclohexane/ethyl acetate 2:1 = 1% NEt₃).

1H NMR (500 MHz, $CDCl_3$, ppm) δ = 0.90–0.96 (m, 3H), 1.26–1.45 (m, 6H), 2.05–2.15 (m, 2H), 2.12–2.15 (m, 3H), 2.27–2.42 (m, 2H), 2.75–2.86 (m, 2H), 2.91–2.98 (m, 1H), 2.99–3.06 (m, 1H), 3.80–3.88 (m, 1H), 6.99–7.04 (m, 2H), 7.28–7.39 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ = 14.0, 22.6, 24.4, 29.5, 29.5, 29.6, 30.0, 33.0, 38.7, 47.7, 127.0, 127.6, 128.0 (2C), 129.2 (2C), 138.8, 142.6, 207.6; EI (m/z , 70 eV, 60 °C): 334 (33) [M]⁺, 277 (61), 235 (22), 208 (70), 195 (26), 169 (22), 152 (100), 134 (80), 119 (29), 109 (33), 105 (37), 95 (28), 91 (21), 81 (26), 69 (55), 55 (28); HRMS–EI (m/z): [M]⁺ calcd for $C_{18}H_{24}OS_2$: 334.1420; found, 334.1421; IR (ATR, $\bar{\nu}$): 2921, 2852, 1703, 1596, 1560, 1487, 1419, 1354, 1301, 1279, 1160, 1121, 1072, 1031, 914, 878, 783, 751, 727, 707, 645, 609, 541, 444 cm^{-1} .

4.12 (E)-5-(1,3-dithiolan-2-yl)-4,5-diphenylpent-4-en-2-one (4g)

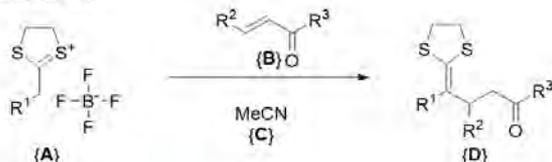


Name: (E)-5-(1,3-dithiolan-2-yl)-4,5-diphenylpent-4-en-2-one; Formula: $C_{20}H_{16}OS_2$; CAS: -; Smiles: CC(=O)CC(C(=C1SCCS1)c1ccccc1)c1ccccc1; InChI: LRVYWKWBWOILOMV-UHFFFAOYSA-N; Molecular Mass: 340.5022; Exact Mass: 340.0956; EA: C, 70.55; H, 5.92; O, 4.7; S, 18.83.



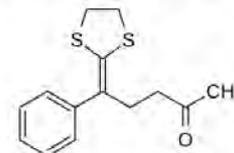


3.2 General Procedure 2a



The dithi(ol)anylium tetrafluoroborate {A} (1.00 equiv.) was dissolved in dry acetonitrile {C} in a glass vial at room temperature if not otherwise stated. The α,β -unsaturated ketone {B} (1.20 equiv.) was added in one portion, the reaction was stirred at room temperature if not otherwise stated and was observed via TLC control. To all reactions, silica gel (3 g) was added after 1 h of reaction time and the solvent was removed via evaporation under reduced pressure. Even though some of the reactions were observed to be finished faster, all of them were reacted for 1 h to allow a good comparison of the results.

4.1 5-(1,3-dithiolan-2-ylidene)-5-phenylpentan-2-one (4a)



Name: 5-(1,3-dithiolan-2-ylidene)-5-phenylpentan-2-one; Formula: $C_{14}H_{16}OS_2$; CAS: - ; Smiles: CC(=O)CCC(=C1SCCS1)c1ccccc1; InChI: L XKWSUYFYQCLRX-UHFFFAOYSA-N; Molecular Mass: 264.4062; Exact Mass: 264.0643; EA: C, 63.6; H, 6.1; O, 6.05; S, 24.25.

According to General Procedure 2a: {A|1a} 2-benzyl-4,5-dihydro-1,3-dithiol-1-ium tetrafluoroborate (1.000 g, 3.544 mmol, 1.00 equiv); {B|3a} but-3-en-2-one (0.298 g, 4.253 mmol, 1.20 equiv); {C} acetonitrile (5.00 mL); Yield {D|4a} = 64% (0.600 g, 2.268 mmol). The obtained crude product was purified via flash-chromatography on silica gel using cyclohexane/ethyl acetate 10:1. R_f = 0.44 (cyclohexane/ethyl acetate 4:1). 1H NMR (400 MHz, $CDCl_3$, ppm) δ = 1.99 (s, 3H), 2.40–2.45 (m, 2H), 2.73–2.79 (m, 2H), 3.18–3.23 (m, 2H), 3.32–3.37 (m, 2H), 7.15–7.21 (m, 3H), 7.23–7.29 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ = 29.8, 32.8, 37.8, 37.9, 41.5, 126.3, 127.1, 128.0 (2C), 128.3 (2C), 134.3, 142.0, 208.1; EI (m/z , 70 eV, 50 °C): 264 (70) $[M]^+$, 207 (100), 181 (33), 131 (33), 69 (51); HRMS–EI (m/z): [M] calcd for $C_{14}H_{16}OS_2$, 264.0643; found, 264.0642; IR (ATR, $\tilde{\nu}$): 2923, 1710, 1595, 1489, 1439, 1420, 1357, 1278, 1158, 1073, 1027, 899, 849, 791, 761, 700, 642, 597, 534, 472, 430 cm^{-1} .

- Automated generation and collection
- Sorting of contents (according to chapters)
- Assignment of reactions to General Procedure and labeling e.g. {A}
- Listing of identifiers
- Listing of calculated/expected analysis
- ACS Standard for analysis details



ELN – reporting and Supporting Information

3.2 General Procedure 2a

4.1 5-(1,3-dithiolan-2-ylidene)-5-phenylpentan-2-one (4a)



NJu-R243 According to General Procedure 2a

The reaction scheme shows the synthesis of 5-(1,3-dithiolan-2-ylidene)-5-phenylpentan-2-one (4a). The starting materials are a dithiolane ylide (1,3-dithiolan-2-ylidene) and a boron trifluoride complex (BF₃·OEt₂). The reaction is carried out in acetonitrile with but-3-en-2-one as a reactant. The product is 5-(1,3-dithiolan-2-ylidene)-5-phenylpentan-2-one (4a) with a yield of 64%.

| Category | Item | Ref | T/R | Amount | Conc | Equiv |
|--------------------|--------------------|-----|-----|----------|------------|-------|
| Starting materials | NJu-772 | | | 1000 mg | 3.544 mmol | 1.000 |
| Reactants | but-3-en-2-one | | | 298.1 mg | 4.253 mmol | 1.200 |
| Products | NJu-773 NJu-R243-A | | | 599.8 mg | 2.268 mmol | 64% |
| Solvents | Acetonitrile | | | 5.00 ml | 100.0% | |

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- Sorting of contents (according to chapters)
- Assignment of reactions to General Procedure and labeling e.g. {A}
- Listing of identifiers
- Listing of calculated/expected analysis
- ACS Standard for analysis details



ELN – reporting and Supporting Information

NJu-773 NJu-R243-A

$C_{14}H_{16}OS_2$
5-(1,3-dithiolan-2-ylidene)-5-phenylpentan-2-one
264.406240 g/mol
Exact mass: 264.064257 g/mol

2731035047

Properties Analyses Results NMR

Edit mode Add analysis

new Add to Report

Type: 1H NMR
Status:
Content: 1H NMR (400 MHz, $CDCl_3$, ppm) δ = 1.99 (s, 3H), 2.40–2.45 (m, 2H), 2.73–2.79 (m, 2H), 3.18–3.23 (m, 2H), 3.32–3.37 (m, 2H), 7.15–7.21 (m, 3H), 7.23–7.29 (m, 2H).

new Add to Report

Type: ^{13}C NMR
Status:
Content: ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ = 29.8, 32.8, 37.8, 37.9, 41.5, 126.3, 127.1, 128.0 (2C), 128.3 (2C), 134.3, 142.0, 208.1.



ELN – reporting and Supporting Information

[Edit mode](#) [Add analysis](#)



new Add to Report  

Type: 1H NMR
Status:

Content: ¹H NMR (400 MHz, CDCl₃, ppm) δ = 1.99 (s, 3H), 2.40–2.45 (m, 2H), 2.73–2.79 (m, 2H), 3.18–3.23 (m, 2H), 3.32–3.37 (m, 2H), 7.15–7.21 (m, 3H), 7.23–7.29 (m, 2H).

| Name | Type | Status |
|----------------------------------|-------------------------------------|---------------------------------------|
| <input type="text" value="new"/> | <input type="text" value="1H NMR"/> | <input type="text" value="Select.."/> |

Content

B I U   **x₂ x²** Normal   **- H C IR EI HR HR1 HR2 UV EA**

¹H NMR (400 MHz, CDCl₃, ppm) δ = 1.99 (s, 3H), 2.40–2.45 (m, 2H), 2.73–2.79 (m, 2H), 3.18–3.23 (m, 2H), 3.32–3.37 (m, 2H), 7.15–7.21 (m, 3H), 7.23–7.29 (m, 2H).

Description

Datasets

Drop File(s) for new Dataset.

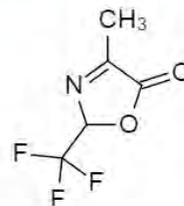
Electronic Lab Notebook - CAS_SciFinder

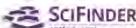
NJ-313 NJ-R146-A 1-0 4 hits (2017-02-28)

C₅H₄F₃NO₂

167.085970 g/mol

Exact mass: 167.019411 g/mol



Properties Analyses Results  NMR

Molecule

C5H4F3NO2

Top secret

Name

NJ-R146-A

External label

Location

Amount

1600

mg

1.6000

ml

9.576

mmol

Density

1.0000

g/ml

Boiling point

0.0000

°C

Melting point

0.0000

°C

Description

Purity

1.0000

Impurities

Solvent

Select

Elemental composition

InChI InChI=1S/C5H4F3NO2/c1-2-3(10)11-4(9-2)5(6,7)8/n4H,1H3

Canonical Smiles O=C1OC(N=C1C)C(F)(F)F

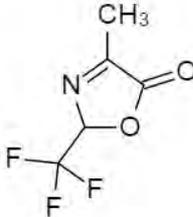
Close

Save

Electronic Lab Notebook - CAS_SciFinder

NJ-313 NJ-R146-A 1 - 0 4 hits (2017-02-28)

$C_5H_4F_3NO_2$
167.085970 g/mol
Exact mass: 167.019411 g/mol



Properties Analyses Results **SciFinder** NMR

exact substructure similarity

NJ-313 on scifinder.cas.org



Search History

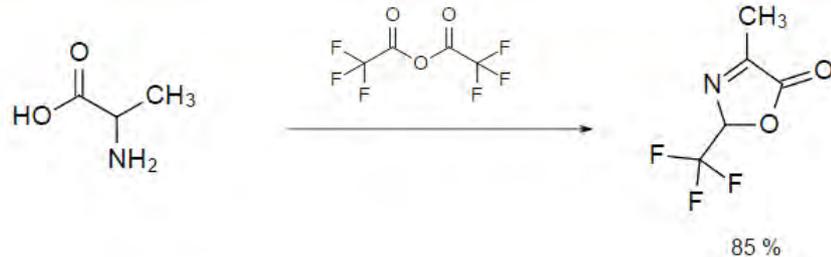
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Browser address bar: https://scifinder.cas.org/scifinder/view/link_v1/workflow.jstf?source=enjung&id=58Tigo10tNUnBkpeIQprX-mfpALdgPDf8g47lb_jmc8cY31g5WIC3piPHR5cDxAL3ZHotTsuAWw7acdy4VsyWkJSrc8C2r6OZseP9PjenK-40D90GZIRFOVA-ZIwDXRELTfzVyCktGxp9PHQ4

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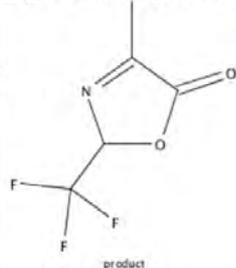
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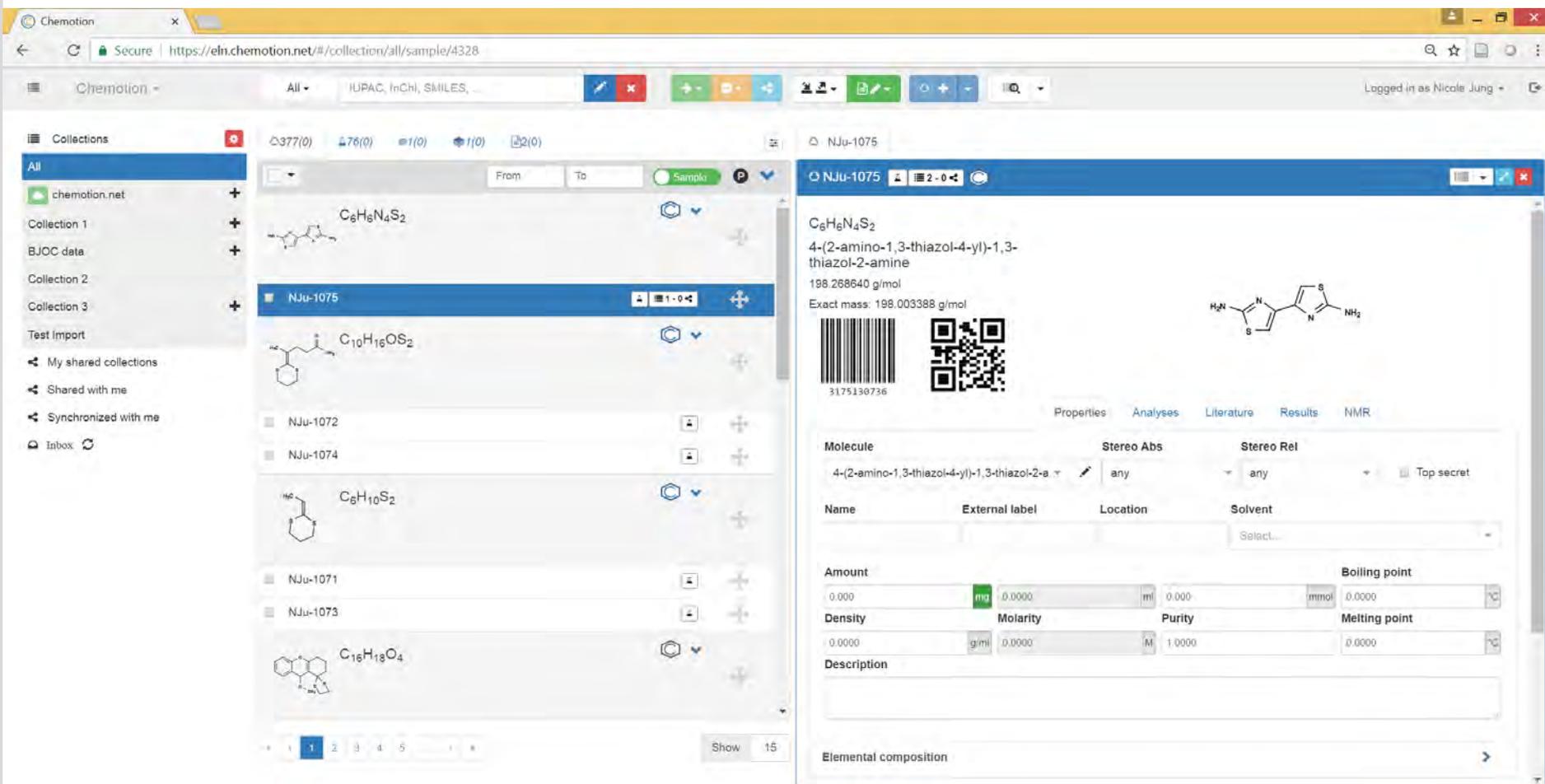


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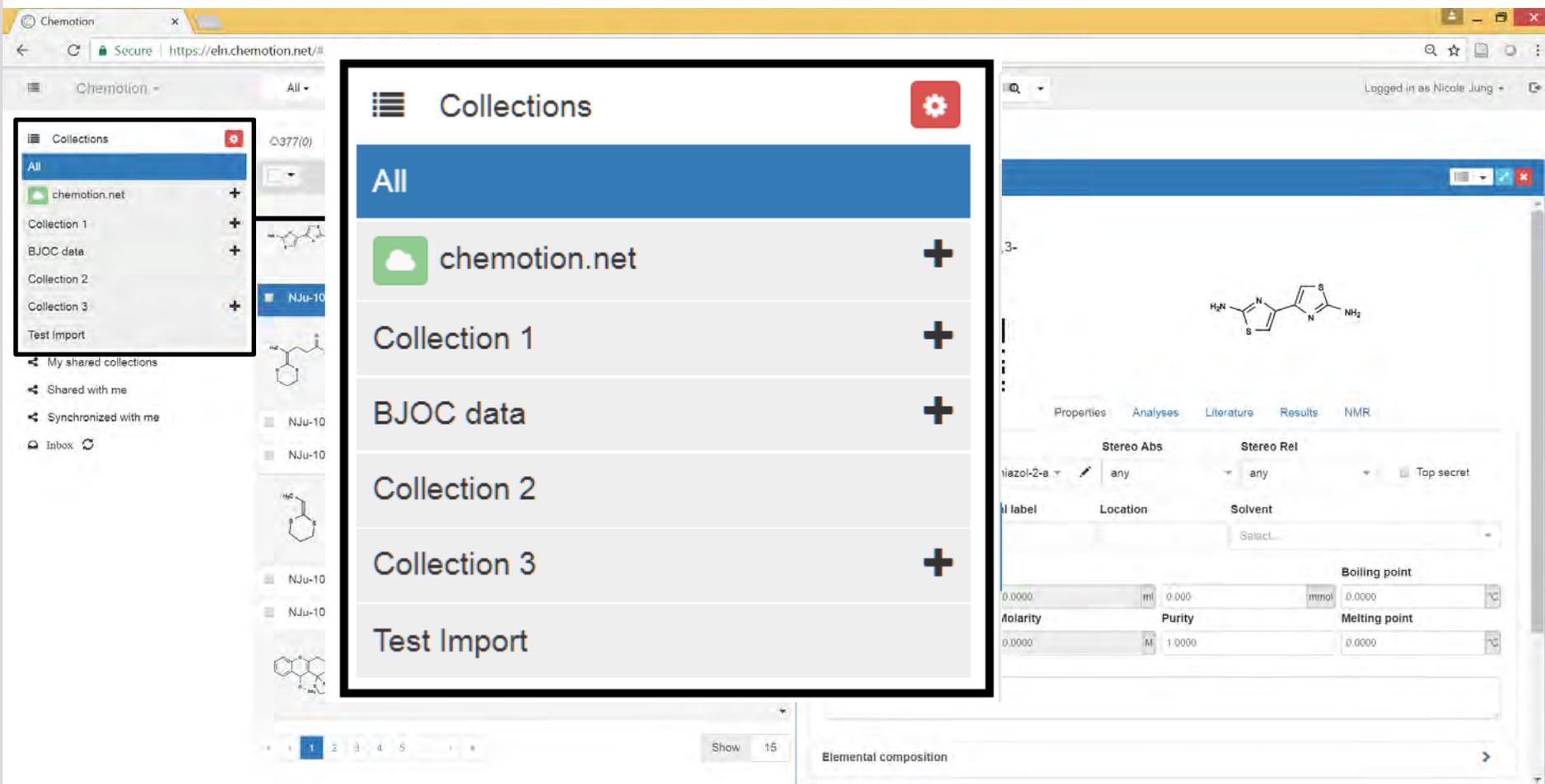
Electronic Lab Notebook - Management



The screenshot displays the Chemotion web interface for managing an Electronic Lab Notebook. The browser address bar shows the URL <https://eln.chemotion.net/#/collection/all/sample/4328>. The interface is divided into several sections:

- Left Panel (Collections):** Lists various collections including 'All', 'chemotion.net', 'Collection 1', 'BJOC data', 'Collection 2', 'Collection 3', 'Test Import', 'My shared collections', 'Shared with me', 'Synchronized with me', and 'Inbox'.
- Center Panel (Sample List):** Shows a list of samples with their chemical formulas and structures. The selected sample is NJu-1075, with the formula $C_6H_6N_4S_2$ and a chemical structure of 4-(2-amino-1,3-thiazol-4-yl)-1,3-thiazol-2-amine.
- Right Panel (Sample Detail):** Provides a detailed view of sample NJu-1075. It includes the chemical formula $C_6H_6N_4S_2$, the full name '4-(2-amino-1,3-thiazol-4-yl)-1,3-thiazol-2-amine', the molar mass '198.268640 g/mol', and the exact mass '198.003388 g/mol'. It also features a barcode with the number '5175130736' and a QR code. Below this, there are tabs for 'Properties', 'Analyses', 'Literature', 'Results', and 'NMR'. The 'Properties' tab is active, showing fields for 'Molecule', 'Stereo Abs', 'Stereo Rel', 'Name', 'External label', 'Location', 'Solvent', 'Amount', 'Boiling point', 'Density', 'Molarity', 'Purity', and 'Melting point'. The 'Amount' field is set to 0.000 mg, and the 'Boiling point' is 0.0000 °C. The 'Molarity' is 0.0000 g/ml, and the 'Purity' is 1.0000 M. The 'Melting point' is 0.0000 °C. There is also a 'Description' field and an 'Elemental composition' section.

Electronic Lab Notebook - Management

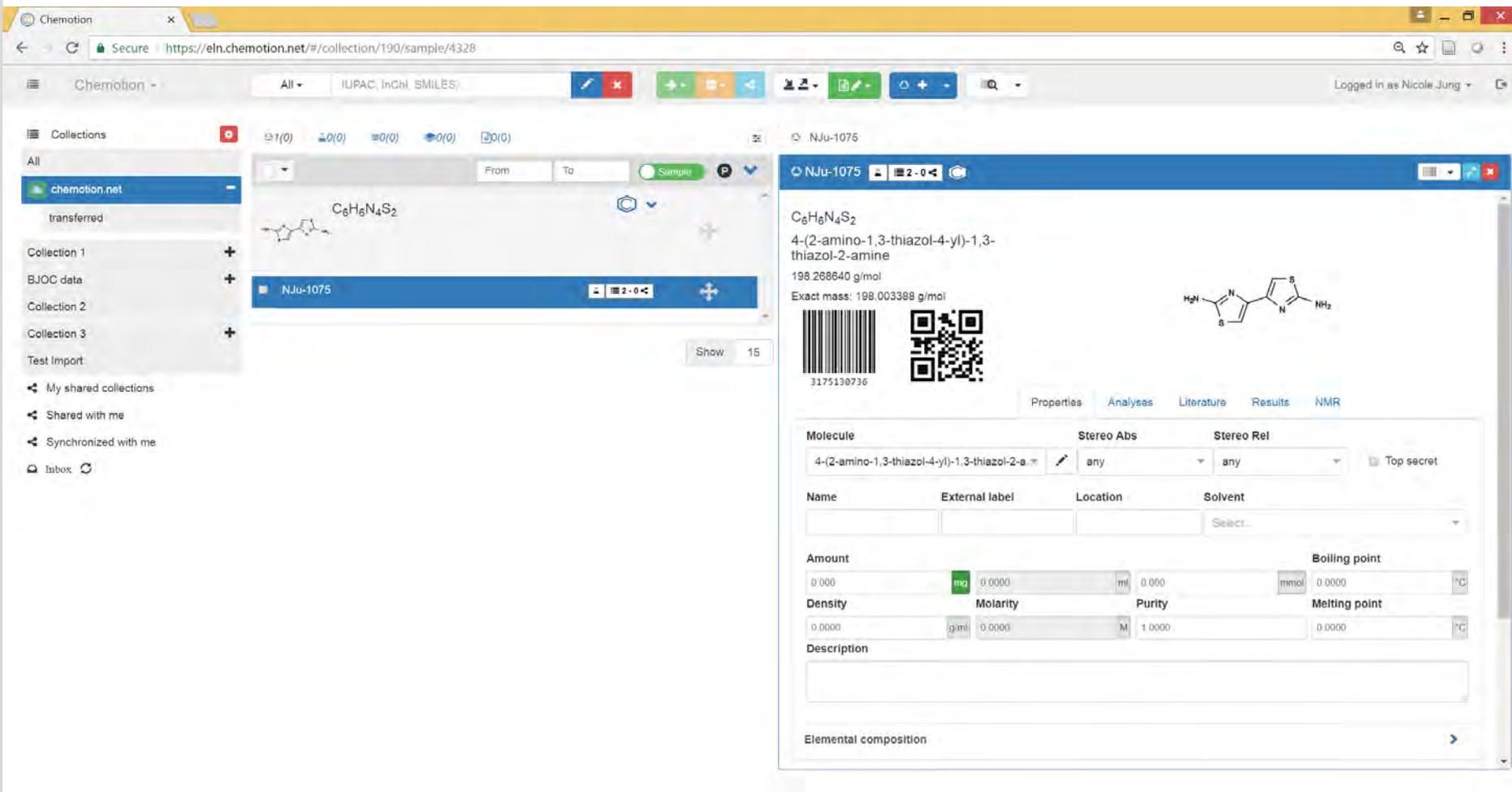


The screenshot displays the Chemotion ELN Management interface. On the left, a sidebar shows a 'Collections' menu with a red gear icon. The main area is titled 'Collections' and lists several collections: 'All', 'chemotion.net', 'Collection 1', 'BJOC data', 'Collection 2', 'Collection 3', and 'Test Import'. Each collection has a plus sign icon. The 'All' collection is highlighted in blue. Below the collections list, there is a 'Show 15' button and an 'Elemental composition' field with a right-pointing arrow.

On the right side of the interface, a chemical structure is displayed. Below the structure, there are tabs for 'Properties', 'Analyses', 'Literature', 'Results', and 'NMR'. The 'Properties' tab is active, showing a table of properties:

| Stereo Abs | | Stereo Rel | |
|---------------|-----|---------------|--------|
| any | any | any | any |
| Location | | Solvent | |
| Select... | | Select... | |
| Boiling point | | Boiling point | |
| 0.0000 | ml | 0.0000 | mmol |
| Polarity | | Purity | |
| 0.0000 | M | 1.0000 | 0.0000 |
| Melting point | | Melting point | |
| 0.0000 | | 0.0000 | |

Electronic Lab Notebook - Management



The screenshot displays the Chemotion web interface. The browser address bar shows the URL <https://eln.chemotion.net/#/collection/190/sample/4328>. The interface includes a sidebar for collections, a main workspace for sample management, and a detailed view for the selected sample, NJu-1075.

Sample Details:

- Chemical Formula:** $C_6H_6N_4S_2$
- Structure:** Nc1nc2c(nc(=S1)N)nc2
- Molecular Weight:** 198.268640 g/mol
- Exact mass:** 198.003388 g/mol
- Barcode:** 3175130736
- QR Code:** [QR Code]

Properties and Data Entry:

| Amount | Boiling point |
|----------|---------------|
| 0.000 mg | 0.000 mmol |

| Density | Molarity | Purity | Melting point |
|-------------|----------|--------|---------------|
| 0.0000 g/ml | 0.0000 M | 1.0000 | 0.0000 °C |

Description:

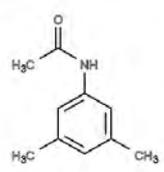
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All - IUPAC, InChI, SMILES, ...

 C10H13NO
N-(3,5-dimethylphenyl)acetamide

 C9H8N2O
N-(4-cyanophenyl)acetamide

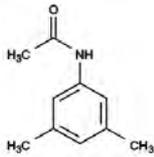
 C9H8INO
N-(4-iodophenyl)prop-2-enamide

 C11H11N3O
N-(3-pyrazol-1-ylphenyl)acetamide

 C8H8INO
N-(3-iodophenyl)acetamide

 C8H8BrNO
N-(2-bromophenyl)acetamide

Show 10



Name: N-(3,5-dimethylphenyl)acetamide (C₁₀H₁₃NO)

Canonical Smiles: CC(=O)Nc1cc(C)cc(c1)C

Inchi: InChI=1S/C10H13NO/c1-7-4-8(2)-6-10(5-7)11-9(3)12/h4-6H,1-3H3,(H,11,12)

Inchikey: HFAYQHIHBTMBI-UHFFFAOYSA-N

Mass: 163.21632

Crosslinks: 

Published on 25-6-2018

Author: Nicolai Wippert¹

¹ Stefan Bräse Group, Institute of Organic Chemistry, Karlsruhe Institute of Technology, Germany

DOI: [10.14272/HFAYQHIHBTMBI-UHFFFAOYSA-N](https://doi.org/10.14272/HFAYQHIHBTMBI-UHFFFAOYSA-N)

Type: 1H NMR

DOI: [10.14272/HFAYQHIHBTMBI-UHFFFAOYSA-N/1HNMR](https://doi.org/10.14272/HFAYQHIHBTMBI-UHFFFAOYSA-N/1HNMR)

Content:
¹H NMR (400 MHz, DMSO-d₆, ppm) δ = 9.74 (br s, 1H), 7.19 (s, 2H), 6.66–6.65 (m, 1H), 2.21 (s, 6H), 2.01 (s, 3H)

Type: 13C NMR

DOI: [10.14272/HFAYQHIHBTMBI-UHFFFAOYSA-N/13CNMR](https://doi.org/10.14272/HFAYQHIHBTMBI-UHFFFAOYSA-N/13CNMR)

Content:

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Author: Nicolai Wippert¹

1. Stefan Bräse Group, Institute of Organic Chemistry, Karlsruhe Institute of Technology, Germany

DOI: [10.14272/HFAYQHIHIBTMBI-UHFFFAOYSA-N](https://doi.org/10.14272/HFAYQHIHIBTMBI-UHFFFAOYSA-N)



Type: 1H NMR

DOI: [10.14272/HFAYQHIHIBTMBI-UHFFFAOYSA-N/1HNMR](https://doi.org/10.14272/HFAYQHIHIBTMBI-UHFFFAOYSA-N/1HNMR)



Content:

¹H NMR (400 MHz, DMSO-d₆, ppm) δ = 9.74 (br s, 1H), 7.19 (s, 2H), 6.66–6.65 (m, 1H), 2.21 (s, 6H), 2.01 (s, 3H).



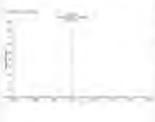
Type: 13C NMR

DOI: [10.14272/HFAYQHIHIBTMBI-UHFFFAOYSA-N/13CNMR](https://doi.org/10.14272/HFAYQHIHIBTMBI-UHFFFAOYSA-N/13CNMR)



Content:

¹³C NMR (100 MHz, DMSO-d₆, ppm) δ = 168.1, 139.2, 137.5 (2C), 124.5, 116.7 (2C), 24.0, 21.1 (2C).



Type: Mass

DOI: [10.14272/HFAYQHIHIBTMBI-UHFFFAOYSA-N/Mass](https://doi.org/10.14272/HFAYQHIHIBTMBI-UHFFFAOYSA-N/Mass)



Content:

El (m/z, 70 eV, 60 °C): 163 (50) [M]⁺, 122 (10), 121 (100), 120 (14), 106 (15).



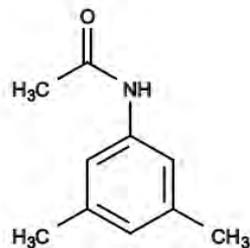
Type: IR

DOI: [10.14272/HFAYQHIHIBTMBI-UHFFFAOYSA-N/IR](https://doi.org/10.14272/HFAYQHIHIBTMBI-UHFFFAOYSA-N/IR)



Content:

IR (ATR) $\tilde{\nu}$ = 3316 (w), 3290 (w), 3266 (w), 3214 (w), 3161 (w), 3098 (w), 3016 (w), 2964 (w), 2916 (w), 2856 (w), 2729 (w), 2466 (w), 1727 (vw), 1661 (m), 1613 (m), 1550 (m), 1468 (m), 1438 (m), 1414 (s), 1366 (m), 1326 (m), 1298 (m), 1278 (m), 1254 (m), 1168 (m), 1157 (m), 1050 (w), 1036 (m), 999 (m), 986 (m), 951 (w), 918 (w), 890 (w), 874 (w), 839 (m), 758 (m), 725 (m), 718 (m), 686 (m), 611 (m), 569 (w), 563 (w), 526 (m) cm⁻¹.



Formula: C₁₀H₁₃NO

Canonical Smiles: CC(=O)Nc1cc(C)cc(C)c1C

Inchi: InChI=1S/C10H13NO/c1-7-4-8(2)6-10(5-7)11-9(3)12/h4-6H,1-3H3,(H,11,12)

Inchikey: HFAYQHIHIBTMBI-UHFFFAOYSA-N

Mass: 163.21632

Crosslinks: 

Type: 1H NMR

DOI: [10.14272/HFAYQHIHIBTMBI-UHFFFAOYSA-N/1HNMR](https://doi.org/10.14272/HFAYQHIHIBTMBI-UHFFFAOYSA-N/1HNMR)



Content:

¹H NMR (400 MHz, DMSO-d₆, ppm) δ = 9.74 (br s, 1H), 7.19 (s, 2H), 6.66–6.65 (m, 1H), 2.21 (s, 6H), 2.01 (s, 3H).

Datasets

1H NMR



Solid-Supported Odorless Reagents for the Dithioacetalization of Aldehydes and Ketones

pubs.acs.org/doi/abs/10.1021/ol403313h

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Solid-Supported Odorless Reagents for the Dithioacetalization of Aldehydes and Ketones

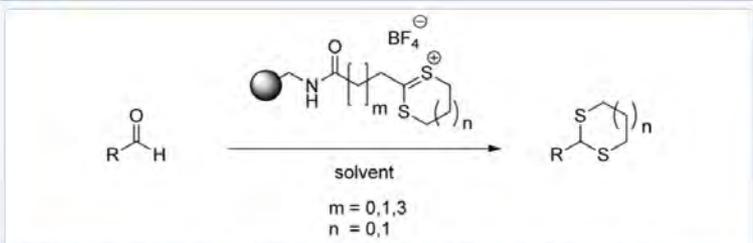
N. Jung*, S. Grässle, D. S. Lütjohann, and S. Bräse*

Karlsruhe Institute of Technology, Campus North, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany
Karlsruhe Institute of Technology, Campus South, Fritz-Haber-Weg 6, 76131 Karlsruhe, Germany

Org. Lett., 2014, 16 (4), pp 1036–1039
DOI: 10.1021/ol403313h
Publication Date (Web): January 31, 2014
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*E-mail: nicole.jung@kit.edu, *E-mail: stefan.braese@kit.edu

Abstract



A solid supported, odorless reagent for the dithioacetalization of aldehydes and ketones has been developed. The new reagent provides the dimercaptoalkane equivalent in combination with stoichiometric amounts of immobilized acid and enables the formation of dithianes and dithiolanes from aldehydes without any additives in good to very good yields with high purities. The reaction is chemoselective for aldehydes, but ketones can be reacted to the corresponding dithioacetals if an

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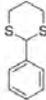
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2. Individual compounds and analysis

2-Phenyl-1,3-dithiane (2a), CAS: 5425-44-5; Smiles: C1(SCCC1)c1ccccc1



Benzaldehyde (**1a**) (10.6 mg, 75% purity, 0.075 mmol, 1.00 equiv.) is dissolved in MeCN and 250 mg of the dithianylum resin **8** (0.81 mmol/g, 0.203 mmol, 2.7 equiv.) are added. The reaction is heated to 80 °C and is shaken for 8 h until complete conversion of the starting material is shown via TLC control (see TLC support). The resin is filtered according to work-up procedure A and conversion and purity have been checked via NMR spectroscopy. The obtained filtered product is further purified via a short column chromatography to get 14.7 mg (0.075 mmol) of the target compound in quantitative yield. – R_f = 0.66 (cyclohexane/ethyl acetate; 4:1). – ^1H NMR (250 MHz, CDCl_3 , ppm), δ = 7.49–7.44 (m, 2 H), 7.38–7.28 (m, 3 H), 5.17 (s, 1 H), 3.16–2.87 (m, 4 H), 2.23–1.84 (m, 2 H). – ^{13}C NMR (62.5 MHz, CDCl_3 , ppm), δ = 25.3, 32.3 (2 C), 51.6, 127.9 (2 C), 128.6, 128.9 (2 C), 139.2. – EI (m/z (%), 70 eV, 80 °C): 196.2 (100), 153.1 (20), 131.2 (70), 122.1 (84), 121.1 (94), 105.1 (37). – HRMS ($\text{C}_{10}\text{H}_{12}\text{S}_2$): calc 196.0380; found 196.0382. – IR (ATR, v): 2928, 2890, 1648, 1519, 1494, 1450, 1422, 1411, 1274, 1233, 1170, 1026, 908, 882, 831, 723, 695, 673, 594, 502 cm^{-1} .

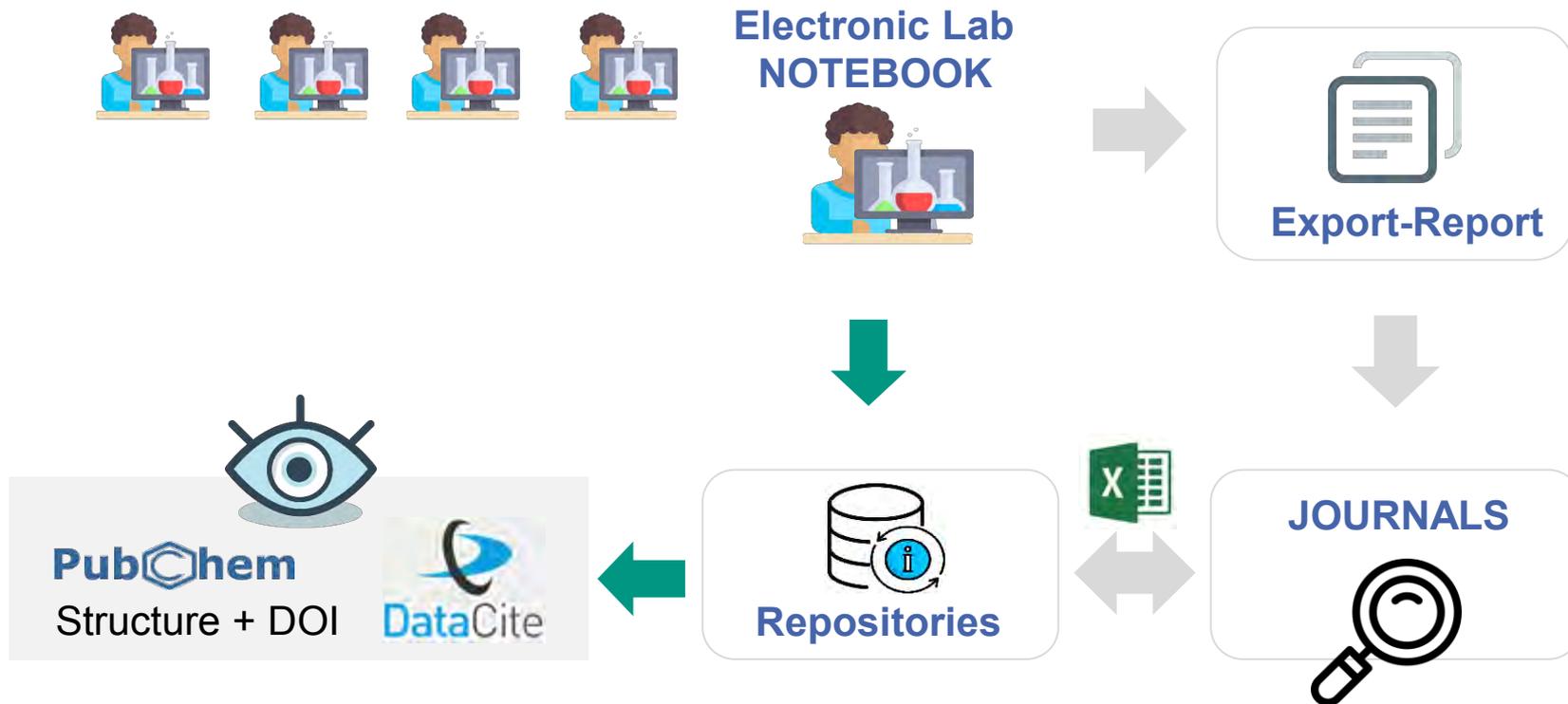
For the conversion in a larger scale, the reaction was repeated with 1.30 mmol of benzaldehyde, giving 221.6 mg (1.128 mmol) of the target 2-phenyl-1,3-dithiane **2a** in 87% yield.

Further supporting information is available via DOI-referencing to the Chemotion-repository:
DOI: [10.14272/GXKPARDRBFURON-UHFFFAOYSA-N](https://doi.org/10.14272/GXKPARDRBFURON-UHFFFAOYSA-N)

| analytics | DOI | My* or others** |
|-----------------|---|-----------------|
| NMR | | |
| ^1H | 10.14272/GXKPARDRBFURON-UHFFFAOYSA-N/NMR/1H/CDCL3/250 | M |
| ^{13}C | 10.14272/GXKPARDRBFURON-UHFFFAOYSA-N/NMR/13C/CDCL3/62.5 | M |
| MASS | | |
| EI | 10.14272/GXKPARDRBFURON-UHFFFAOYSA-N/Mass/EI | M |
| IR | | |
| ATR | 10.14272/GXKPARDRBFURON-UHFFFAOYSA-N/IR | M |
| TLC | 10.14272/GXKPARDRBFURON-UHFFFAOYSA-N/TLC | M |

My* = the spectra that are available via the chemotion repository have been measured and added by the authors; or others** = we refer herein to spectra that have been provided by other researchers

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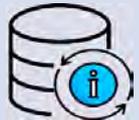
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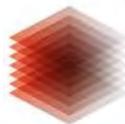


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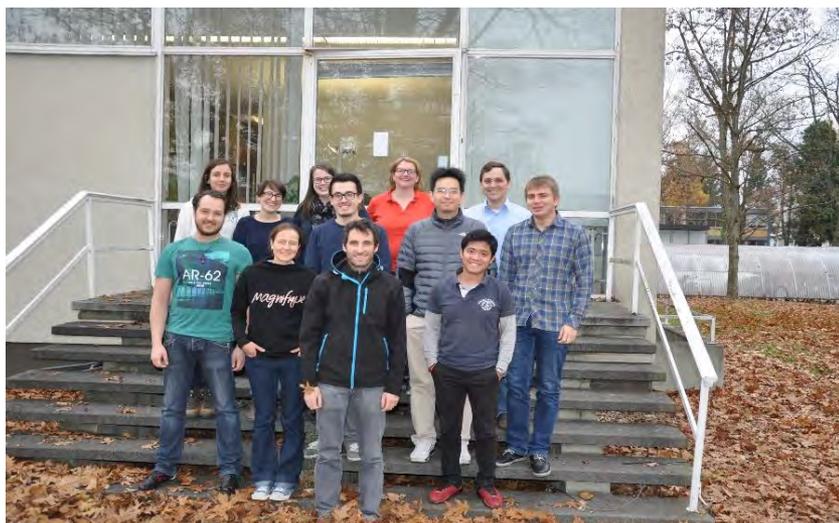
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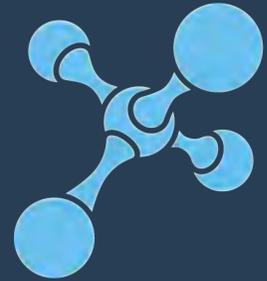


Florian Hauer, Labfolder GmbH: Digital in die Zukunft – elektronische Laborbücher als zentraler Bestandteil des Forschungsdatenmanagements

Abstract

Sowohl die Anforderungen als auch die Möglichkeiten des digitalen Forschungsdatenmanagements ändern sich aktuell mit großer Geschwindigkeit. Aus der Entwicklung einer Plattform für das Labordatenmanagement möchten wir folgende Aspekte beleuchten:

1. Elektronische Laborbücher im Kontext des Forschungsdatenmanagements: Möglichkeiten und Herausforderungen
2. Rechtliche Rahmenbedingungen & Compliance
3. Trends und Entwicklungen: ein Blick in die Zukunft



labfolder

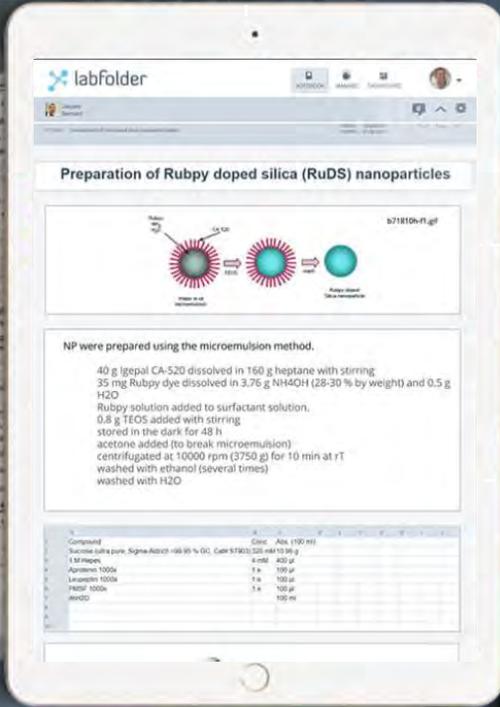
Helmholtz Open Science Workshop **„Elektronische Laborbücher“**

Dr. Florian Hauer Co-Founder & CPO labfolder GmbH
14.09.2018



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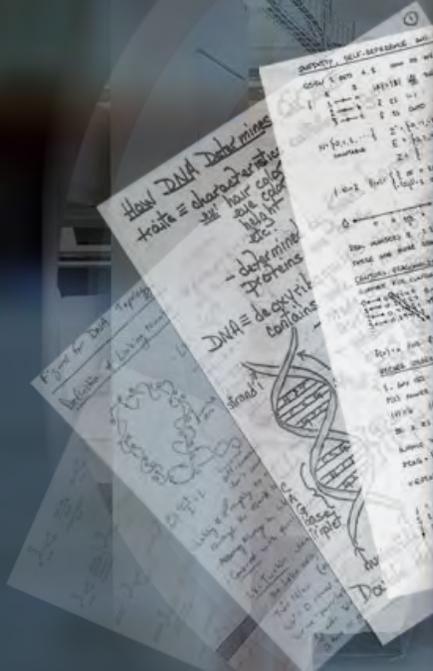


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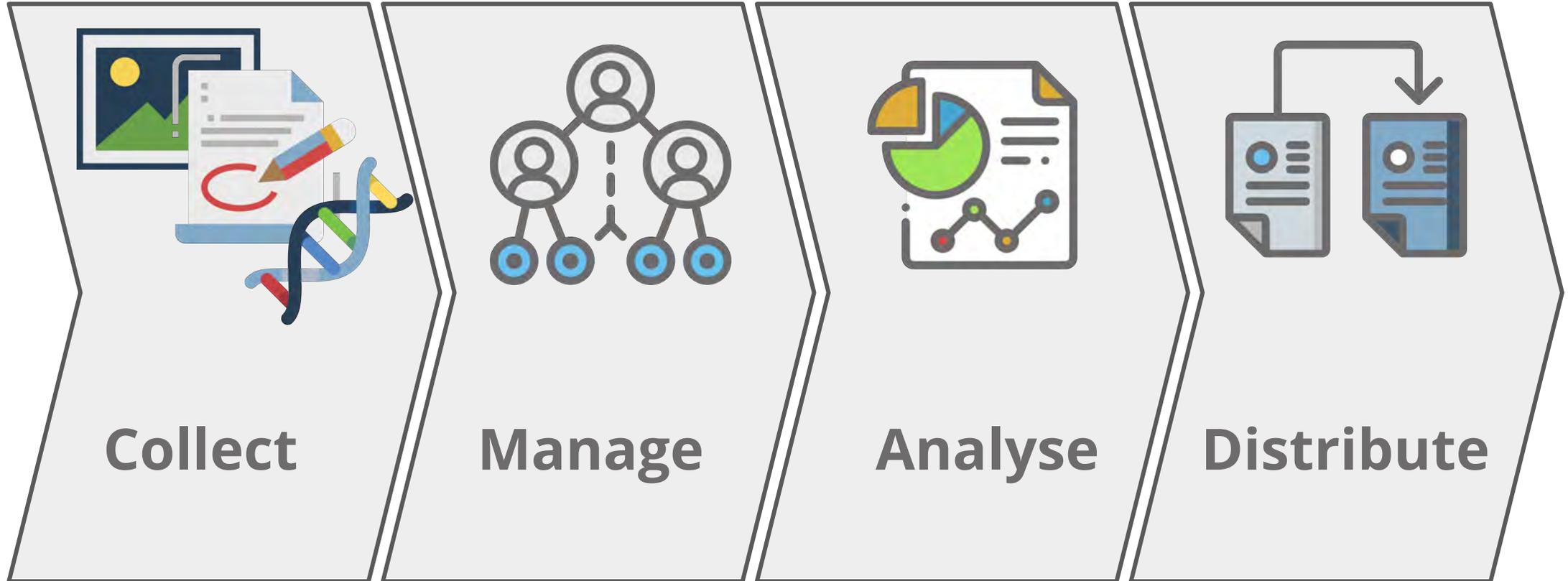
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NiNTA_gel.tif

Anti-alpha Tubulin

Measuring_Protein_Concentration.xlsx

| uL in Assay | Sample 1 | Sample 2 | Sample 3 | Sample 4 | Sample 5 | Sample 6 |
|-------------|----------|----------|----------|----------|----------|----------|
| 2 uL | 0.861 | 0.742 | 0.588 | 0.609 | 0.861 | 0.742 |
| 1 uL | 0.583 | 0.492 | 0.429 | 0.448 | 0.583 | 0.492 |
| 0.5 uL | 0.45 | 0.418 | 0.359 | 0.367 | 0.45 | 0.418 |

BSA Std Curve 570 nm Abs Values

| uL in Assay | ug in Assay | Abs |
|-------------|-------------|-------|
| 0 | 0 | 0.213 |
| 0.5 | 1 | 0.342 |
| 1 | 2 | 0.469 |
| 2 | 4 | 0.663 |
| 3 | 6 | 0.884 |
| 4 | 8 | 1.054 |
| 5 | 10 | 1.224 |
| 6 | 12 | 1.367 |
| 10 | 20 | 1.973 |

Standard Curve Equation Values

Sheet1 Sheet2 Sheet3



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created: 13.09.2018 modified: 13.09.2018 No tags associated

Anti-alpha Tubulin

Measuring_Protein_Concentration.xlsx

| | A | B | C | D | E | F | G |
|----|--|--------------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 1 | | | | | | | |
| 2 | Unknown Samples 570 nm Abs Values | | | | | | |
| 3 | | | | | | | |
| 4 | uL in Assay | Sample 1 | Sample 2 | Sample 3 | Sample 4 | Sample 5 | Sample 6 |
| 5 | 2 uL | 0.861 | 0.742 | 0.588 | 0.609 | 0.861 | 0.742 |
| 6 | 1 uL | 0.583 | 0.492 | 0.429 | 0.448 | 0.583 | 0.492 |
| 7 | 0.5 uL | 0.45 | 0.418 | 0.359 | 0.367 | 0.45 | 0.418 |
| 8 | | | | | | | |
| 9 | BSA Std Curve 570 nm Abs Values | | | | | | |
| 10 | | | | | | | |
| 11 | uL in Assay | ug in Assay | Abs | | | | |
| 12 | 0 | 0 | 0.213 | | | | |
| 13 | 0.5 | 1 | 0.342 | | | | |
| 14 | 1 | 2 | 0.469 | | | | |
| 15 | 2 | 4 | 0.663 | | | | |
| 16 | 3 | 6 | 0.884 | | | | |
| 17 | 4 | 8 | 1.054 | | | | |



Manage Data and Access

labfolder

Groups > Department of Biochemistry

NOTEBOOK

MANAGE

DASHBOARD



+ Add

AG Andrea Claes Inventory



Share settings

Search...

- Alexander Haas
- Bayer Pharma
- Brabender Test
- Florian Hauer
- giuppi petro
- James Evans
- Jaques Bernard
- Julia Wagner
- Katie Aberra

Team members who have access to this material database ?

- A. Claes labfolder x
- Andrea R. Claes x
- Anne Kriegel x
- Carlos Perez x
- Clark Williams
- Erin Westover x
- Giulia Petrovich x
- Hakim Ahmad x
- Jack Matthews x
- Joseph Njoki x
- Li Chun x
- Mia Schmidt x
- Priscila Campuzano x
- Robert Martin x
- Sophie Dubois x
- Susan Hall x
- Tobi Grebe x
- Yannick Skop x

Close

Save

- Sung-min Yun
- Mitochondrien
- Jaques Bernard (admin)



Finding and mining data

labfolder **Advanced Search** NOTEBOOK MANAGE DASHBOARD SEARCH NOTIFICATIONS USER

Content: WT1 expression

AND Material element: C19 WT1

AND Numerical Data Element: Induction concentration: Mass concentration: Between: 0 2 pg/μL

SEARCH

[Collapse](#)

Results found in: **ENTRIES 1** **TEMPLATES 0**

| ENTRY TITLE | AUTHOR | PROJECT | MOD. DATE | CREAT. DATE |
|--|----------------|----------------|------------|-------------|
| Unfinished Entry ... MDCK stable and inducible clones - WB WT1 expression was analysed in each clone after 24h induction with 1 μg/ml Dox by WB. Tested Clones Sheet1 Isoform clone WB IF +/- 2 positive positive +/- 40 negative ... stable clones express WT1 only under Dox induction, no leakage. The protein isoforms have the expected molecular weight. Induction concentration: Mass concentration: 1 μg/mL C19 WT1 Dilution: 1:1000 Incubation: ... | Clark Williams | Helmholtz Demo | 13.09.2018 | 13.09.2018 |

support
recommend



Finding and mining data

- Latest
- Access
 - Location
 - Authentication
 - Endpoints
 - Signup - Create Account
 - Login - Generate Token
- Concepts
- Projects
 - Projects Resource
 - List Projects
 - Create Project
- Notebook
 - Entries
 - List Entries
 - Create Notebook Entry
- Material Database
- Entry Elements

Location

The API can only be accessed via HTTPS.
You can reach the API for the cloud instance at

```
https://ein.labfolder.com/api/v2/
```

Local installations can access the API using the respective domain with the path `/api/v2/` appended.
So if your server is reachable at `https://labfolder.mycompany.lan` the API endpoint is located at

```
# Note: ~/api/v2/ is appended to the standalone server url
```

```
https://labfolder.mycompany.lan/api/v2/
```

Authentication

Requests to the API have to be authenticated using an API token which is received after successfully providing your application credentials to the API.
Once acquired the token can either be provided as the username field for HTTP-Basic authentication (useful for commandline access) or set in the `Authorization` header using other tools.

The following examples illustrate the two different ways to provide the token when using `curl`

```
# via HTTP-Basic  
# Note the proceeding ':'  
  
> curl -u "$LABFOLDER_API_TOKEN:" <API_RESOURCE_PATH_GOES_HERE>
```

```
# via Authorization header  
# Note the format is "Authorization: Token xxxxxxx"  
  
> curl -H "Authorization: Token $LABFOLDER_API_TOKEN" <API_RESOURCE_PATH_GOES_HERE>
```

ENDPOINTS

```
POST /auth/signup
```



Data Sharing and Research Continuity



Figshare

Last update:
26.03.2014

[Activate](#)

Export data

New XHTML export

[Start](#)

XHTML

Export - 13.Sep.18 - 09:53:00

[Download](#)



EXPECT THE MAXIMUM

- ✓ Platform independent
- ✓ Self-hosted or Cloud
- ✓ Easy-to-use interface
- ✓ Multilingual UI
- ✓ File attachments
- ✓ MS Office Support
- ✓ Tables, calculations & graphs
- ✓ Free design of records
- ✓ Protocol templates
- ✓ Inventory & Sample Tracking
- ✓ Mobile App
- ✓ User Management
- ✓ Rights, roles & access management
- ✓ Full Audit Trail
- ✓ Data Safeguarding
- ✓ Compliance
- ✓ Digital Signatures
- ✓ PDF Export
- ✓ XHTML Export
- ✓ File export
- ✓ Linking of data
- ✓ Repository connectivity
- ✓ Team communication
- ✓ Comments
- ✓ Search & Filters
- ✓ Structured parameter recording
- ✓ Data Mining
- ✓ Unit interconversions
- ✓ Flexible API
- ✓ Device Integrations
- ✓ Support
- ✓ Onboarding & Training



COMPLIANT TO REGULATED ENVIRONMENTS

GLP

(OECD Guidelines on good laboratory practice)

| GLP requirement | Labfolder Feature | Compliance |
|-----------------------|------------------------------|------------|
| Access control | Login, project access rights | ✓ |
| Full audit trail | History function | ✓ |
| Digital signatures | Signing and witnessing | ✓ |
| Daily backups | Provided by labfolder | ✓ |
| Data center protected | Provided by data center | ✓ |

CFR 21 Part 11

(FDA guidelines for digital signatures)

| Requirement | Labfolder Feature | Compliance |
|-------------------------------------|---|------------|
| Signature (biometric / credentials) | Signing and witnessing | ✓ |
| Document integrity | Audit Trail, Controlled deletion, Hash sum | ✓ |
| Access management | Login, author control, access rights management | ✓ |



Compliance in the digital lab

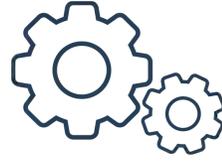
Person-centered



“Who did what and when?”

DFG-Guidelines , Gute wiss. Praxis' (GWP)

Process- and role-centered



“How does a process work and who is responsible?”

QM-Systems acc. to ISO 9001, 13485, 15189, 17025

Integrity



“How is the integrity of Data ensured?”

QM-systems acc. to GLP, GMP, GAMP



www.labfolder.com/white-papers/

White papers



Digital lab notebooks and intellectual property protection

This text explains how the patenting systems work in the US and Europe for science and how digital laboratory notebooks can aid the protection of Intellectual Property.

GET WHITEPAPER



Digital lab management in ISO certified laboratories

This whitepaper discusses the ISO Standards that are relevant to laboratory work, the principles that govern quality management systems and how the requirements can be fulfilled and made easier with labfolder.

GET WHITEPAPER



How labfolder Meets Technical Requirements of FDA's 21 CFR Part 11

This whitepaper summarizes the sections of the 21 CFR part 11 regulations which are relevant to electronic systems, also pointing out how the labfolder software implements these technical requirements.

GET WHITEPAPER





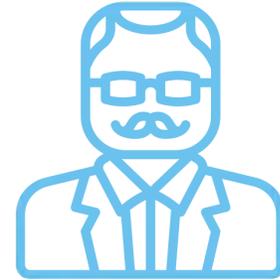
Different priorities



Lab scientist



PI



RDM, Librarian

Collect

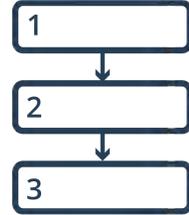
Manage

Analyse

Share



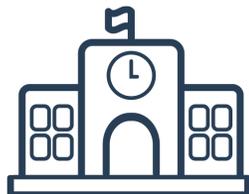
ONBOARDING DONE RIGHT



Tailor-made
onboarding process



Dedicated Account Manager
that handles initial
onboarding and support



Online webinars (user &
Admin) and on-site workshops



PROPER IMPLEMENTATION IS KEY

Coordinate with BO/IT

Kick Off



Admin Webinar

User Webinar



Fully in Production



Week 1

Week 2

Week 3

Week 4



Setup / Installation

Advanced Admin Q&A

Advanced User Q&A



Coordinate Super Users

1 Month

Goal: Per-group onboarding process of admins and users fully completed after 1 month



ORGANIZATION-WIDE COMMUNITY PORTAL

Max Planck Community Portal



User Manual
v1.17.0

[GO TO MANUAL'S PAGE](#)



Admin Manual
v1.17.0

[GO TO MANUAL'S PAGE](#)



Helpdesk

Easily find the answers you are looking for

[VISIT OUR HELPDESK](#)



Webinars

For Users and Admins

[SCHEDULE A WEBINAR](#)



Forum

Questions for MPI scientists

[ASK ANY QUESTION](#)



MPI Webinars

We have exclusive weekly Webinars for MPI scientists.

Whether you are an User or an Admin, book a webinar with us for a fast and smooth start with labfolder

| NOVEMBER 2017 | | | | | | |
|---------------|-----|-----|-----|-----|-----|-----|
| Mon | Tue | Wed | Thu | Fri | Sat | Sun |
| | | 1 | 2 | 3 | 4 | 5 |
| 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| 13 | 14 | 15 | 16 | 17 | 18 | 19 |
| 20 | 21 | 22 | 23 | 24 | 25 | 26 |
| 27 | 28 | 29 | 30 | | | |

BIH Community Portal



Group creation webinars

Note: Only for initial group creation.

[GROUP CREATION WEBINAR](#)



On-Site Events

[SEE SCHEDULE](#)



labfolder Guide

Get a complete overview of labfolder's main features

[CHECK OUR GUIDE](#)



Helpdesk

Easily find the answers you are looking for

[VISIT OUR HELPDESK](#)



Manuals

User & Admin

[GO TO MANUALS PAGE](#)



SUPPORT RESOURCES

labfolder guide

- Getting Started
- Notebook Basics
- Productivity
- Collaboration
- Team Admin
- Material Database
- Data Elements
- Advanced search
- Pro Tips

LET US HELP YOU

What are you looking for?

Popular Help Topics

- How do I restore a deleted entry?
- Can labfolder be used in a ISO certified laboratory?
- How do I add a new member to a group?
- Which image formats does labfolder support?

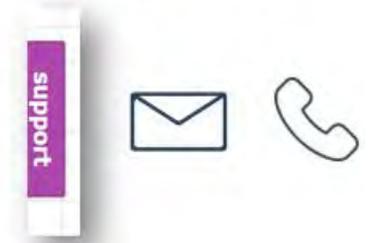
Using labfolder

- Account Settings
- Dashboard & Apps
- Data Elements & Advanced Search
- Data Import & Export
- Entries & Templates
- Group Management & Collaboration
- Material Database
- Projects & Folders
- Search & Filter
- Security & Compliance

labfolder Manuals

- User Manual
- Admin Manual

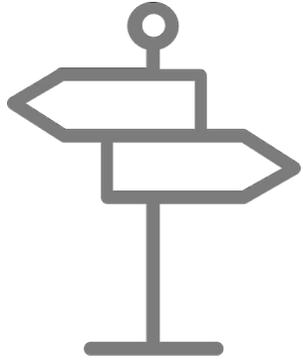
Continuous support



Average first response time: <60 min

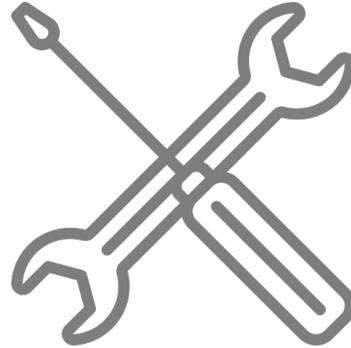


SUPPORTING ALL STAGES



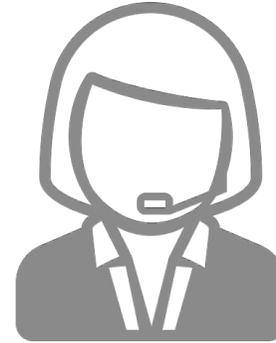
Implementation support

- Onboarding of group leaders and scientists.
- Continuous training of (new) scientists and students.



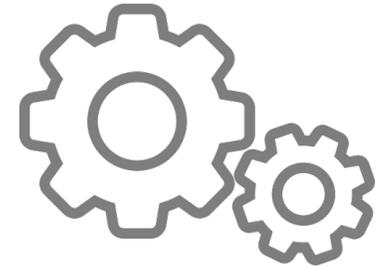
Installation & update support

- Supported installation and regular updates.
- Technical IT support above the operating system.



User support

- In-tool ticket system.
- Telephone and email support for scientists.

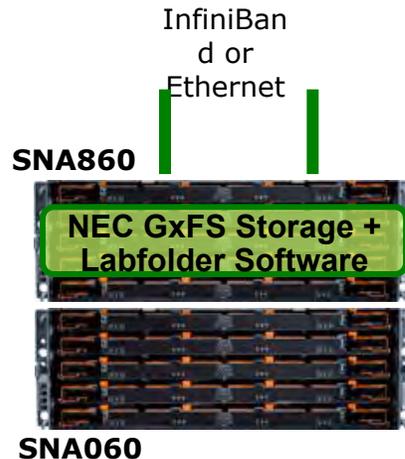


Integration support

- Supported API integration of in-house solutions for linking, long-term archiving, publication, etc.



NEC Validated Hardware Design



„Data Center-Ready“:

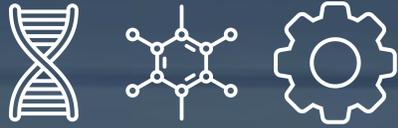
- Pre-tested Reference Architecture
- Vertically scalable:
30 TB to 480 TB (per building block)
- Horizontally scalable:
Additional building blocks
- Local High Availability Solution
- Data Replication to DR site

GxFS Price varies with Performance (GB/s) and Capacity (TB) Requirements.

Rule of Thumb:
Hardware / Software / System Service for 5 Years included:
GxFS Appliance: Approx. 0,0026 USD per GB and Month



THE ELN IS THE GATEWAY TO THE FUTURE



Various scientific & methodological fields



Inventory & Sourcing



Automatisation



R&D, Diagnostic/Testing, QM/QA



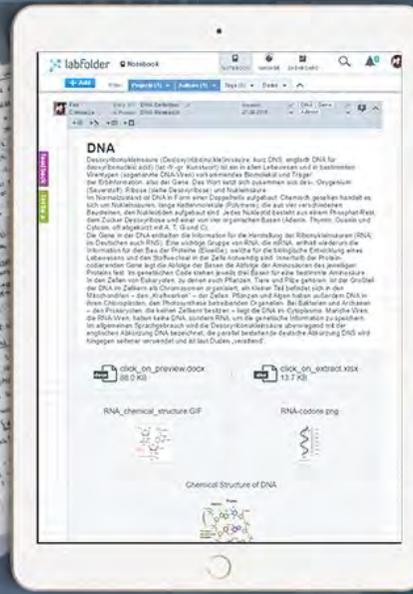
Smart devices



Sharing, publishing, IP protection



Data-mining & AI



The digital lab notebook is the central data hub, the operating system as well as the main result exploitation channel of the lab of the future.



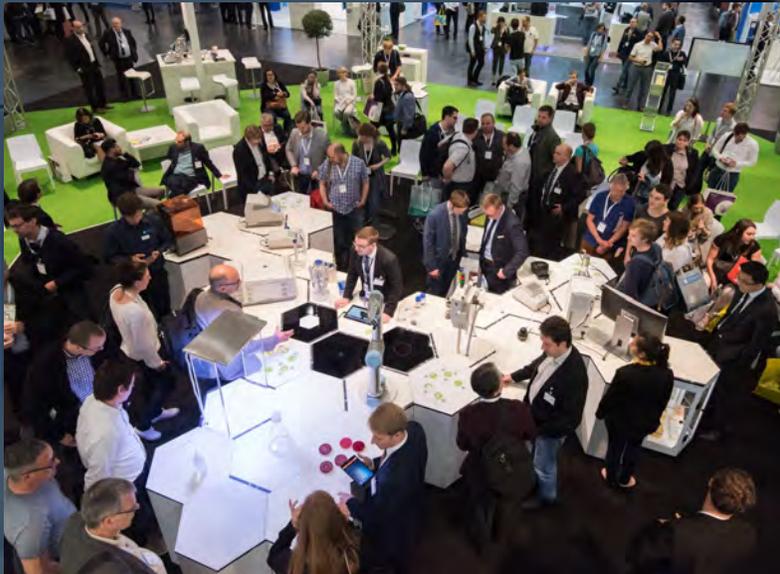
SMART WORKFLOWS

- Digital protocol: Workflows visualized step-by-step
- Execution of workflow, instructing the researcher in detail what to do
- Triggering devices and transmitting parameters
- Capturing data on the fly and sending it to ELN
- Beautiful design and ease of use ensure smooth conduct of experiment



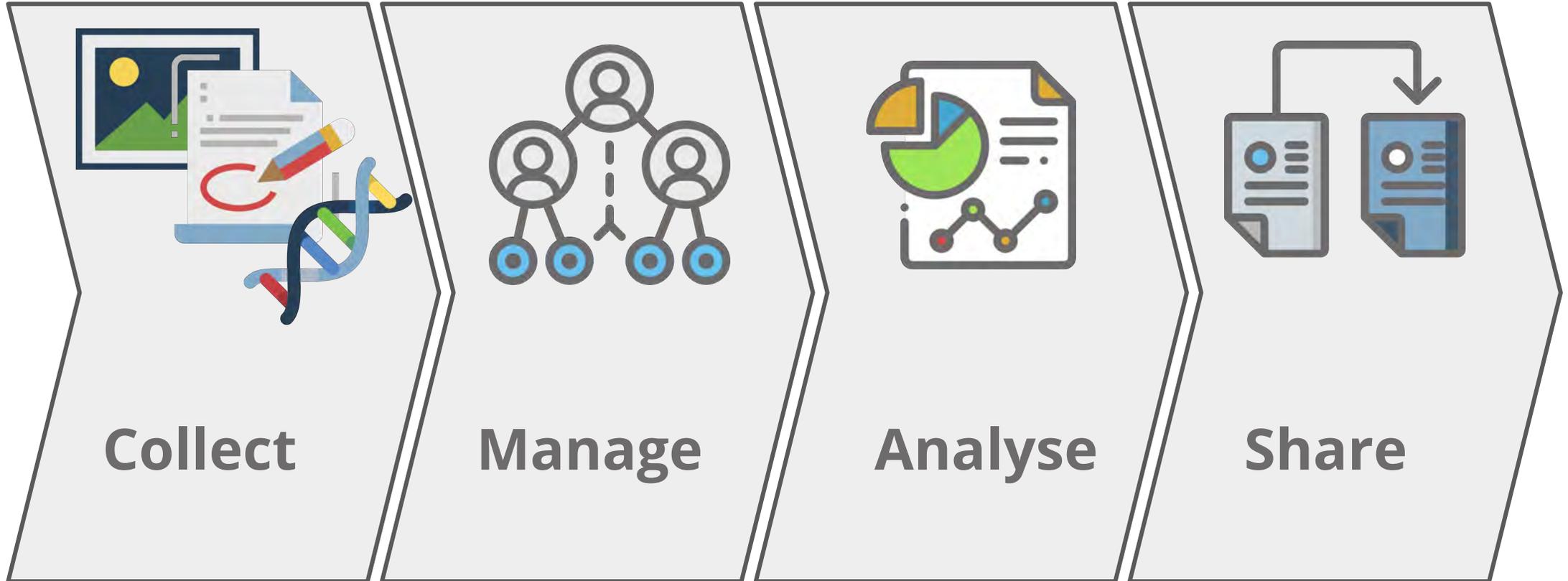


SMARTLAB - SUCCESS THROUGH PARTNERSHIPS





Life cycle of scientific data



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 contact@labfolder.com

 www.labfolder.com

Ulrich Dirnagl, Abt. für Experimentelle Neurologie, Charite Universitätsmedizin Berlin und QUEST Center for Transforming Biomedical Research, Berlin Institute of Health: Nie wieder ohne – das elektronische Laborbuch aus der Sicht eines Neurowissenschaftlers

Abstract

Aus der Sicht eines Wissenschaftlers und Leiters einer universitären, neurowissenschaftlichen Forschungsabteilung möchte ich in meinem Vortrag aufgrund mehrjähriger theoretischer Auseinandersetzung, praktischer Erfahrung und Begleitforschung zu und mit elektronischen Laborbüchern folgende vier Thesen begründen:

1. Das Papier-Laborbuch ist ein Atavismus und gehört eingemottet.
2. Das elektronische Laborbuch (eLN) kann viel mehr als ein Papierlaborbuch.
3. eLNs sollten Teil der guten wissenschaftlichen Praxis (GWP) werden.
4. Die Voraussetzungen dafür müssen von den Institutionen im Rahmen der Grundausstattung geschaffen werden (IT, Lizenzgebühren etc.).



NIE WIEDER OHNE: DAS ELEKTRONISCHE LABORBUCH AUS DER SICHT EINES EXPERIMENTELLEN NEUROWISSENSCHAFTLERS

Ulrich Dirnagl

<http://bit.ly/dirnaglbraunschweig>

Papierlaborbücher sind ein Anachronismus.....



Frederic Remington. Smoke signals;
Amon Carter Museum, Fort Worth

VS.



iPhone X

Papierlaborbücher sind ein Anachronismus.....

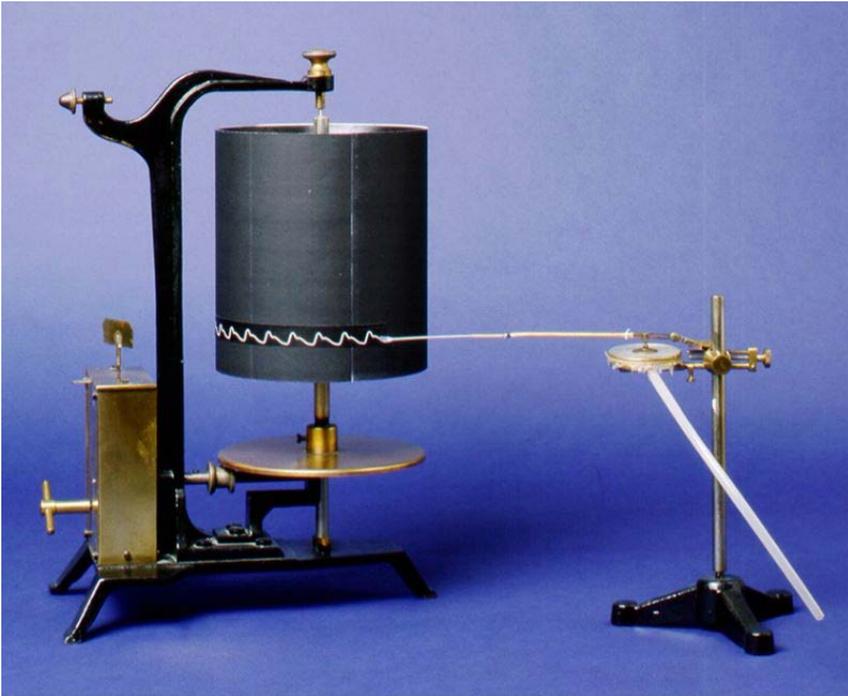


19. Jahrhundert



2018

Papierlaborbücher sind ein Anachronismus.....



Kymograph, Johannes Müller, Sammlung der HU



GY 6000 - 128 channel recorder

Acknowledgment:



Potential conflict of interest:



Ca. 1000 registered users

Ca. 700 active users

Department of Experimental Neurology, Charité

- Founded in 1999
- ca. 90 PhD Students, MD-Thesis Students, Technicians, Postdocs, Clinician Scientists, Professors...
- >90% third party funded (DFG, BMBF, EU, Foundations....)
- Focus: Pathophysiology of stroke
- Techniques: Molecular biology, Biochemistry, Histochemistry, Electrophysiology, Behaviour, Imaging (SPECT, MR, CT, PET, Optical), Cell culture, In vivo modeling of disease (rodent)
- Among the leading labs in stroke research (citations, patents, transitions to clinical trials...)



Berlin Institute of Health: Charité + Max Delbrück Center



Campus Charité Mitte
(CCM)



Campus Benjamin Franklin
(CBF)



Campus Virchow-Klinikum
(CVK)



Campus Berlin Buch
(CBB)





Berlin University Alliance



THIS WEEK

EDITORIALS

NEW New agreement to tackle pharmaceutical pollution **p.164**

WORLD VIEW Vaccination: The best way to measure health care **p.165**

ANIMALS Rolling beetles fooled by look-alike seeds **p.167**

Let's think about cognitive bias

The human brain's habit of finding what it wants to find is a key problem for research. Establishing robust methods to avoid such bias will make results more trustworthy

Reproducibility: Seek out stronger science

Monya Baker

Nature 537, 703–704



DATA SHARING

An open mind on open data

The move to make scientific findings transparent can be a major boon to research, but it can be tricky to embrace the change.

Power size undermines the reliability of neuroscience

Repetitive flaws

Strict guidelines to improve the reproducibility of experiments are a welcome move.

From next week, scientists who submit grant applications to the National Institutes of Health (NIH) will be asked to take more care. As part of an increasing drive to boost the quality of research, the NIH will require applicants to explain the premise behind their proposals and defend the quality of the mental designs. They must also account for biological variability, for example, by including both male and female mice in planned experiments and describe how they will authenticate experimental materials as cell lines and antibodies.

These demands are timely, sensible and, if researchers follow the advice of their scientific societies, will sound over the past year, a string of organizations have published statements and guidelines to boost the reproducibility of research.

Collectively, the message is show your work, and don't rely on unreliable reagents or shoddy data. Updated guidelines from the Federation of American Societies for Experimental Biology, for example, call for standard ways to cite antibodies and animal-care practices. The Society for Neuroscience has asked for uniform standards of reporting.

Raise standards for preclinical cancer research

C. Glenn Begley and Lee M. Ellis propose how methods, publications and incentives must change if patients are to benefit.

Fewer numbers, better science

Scientific quality is hard to define, and numbers are easy to look at. Leaders at two institutions are trying to change how the science is done



QUALITY TIME
IT MAY NOT BE SEXY, BUT QUALITY ASSURANCE IS BECOMING A CRUCIAL PART OF LAB LIFE.

WORKPLACE CLIMATE

Metrics for ethics

Focus on perceived working conditions could help graduate schools to train responsible researchers.

ROYAL SOCIETY OPEN SCIENCE

rsos.royalsocietypublishing.org

Research



Low statistical power in biomedical science: a review of three human research domains

Confidence in preclinical research

Model organisms have provided an important reductionist approach for understanding the mechanistic basis of human diseases. With

making strides in their efforts for the complexity of the human system (see page 1334)

THE LANCET
"85% of health research is wasted."
Research: increasing value, reducing waste

Reality check on reproducibility

A survey of Nature researchers

Muddled meanings hamper efforts to fix reproducibility crisis

Researchers tease out different definitions

Monya Baker

They can help to make sure that research is not only because scientists can inspire identity and integrity.

Acknowledging and Overcoming Nonreproducibility in Basic and Preclinical Research

nature

International weekly journal of science

Home | News & Comment | Research | Careers & Jobs | Current Issue | Archive | Audio & Video | Feedback

News & Comment | News | 2016 | May | Article

REPRODUCIBILITY Twenty teams, one data set, one question, many answers

NATURE | NEWS

Missing mice: gaps in data plague animal research

Reports of hundreds of biomedical experiments lack essential information.



Hide results to seek the truth

More fields should, like particle physics, adopt blind analysis to thwart bias, urge Robert MacCoun and Saul Perlmutter.

Believe it or not: how much can we rely on published data on potential drug targets?

EDITORIAL

nature

International weekly journal of science

Home | News & Comment | Research | Careers & Jobs | Current Issue | Archive | Audio & Video

Archive | Volume 506 | Issue 7487 | News Feature | Article

NATURE | NEWS FEATURE

عربي

Scientific method: Statistical errors

Perrin S (2014) Nature 407:423-425

DUE DILIGENCE, OVERDUE

Results of rigorous animal tests by the Amyotrophic Lateral Sclerosis Therapy Development Institute (ALSTDI) are less promising than those published. All these compounds have disappointed in human testing.



Factors antagonizing research quality in preclinical biomed

In academic medicine:

- Patients, research, teaching: „Research after hours“
- Supervisors also have clinical duties
- Many students (often without formal training)
- Little supervision - lack of professionalism

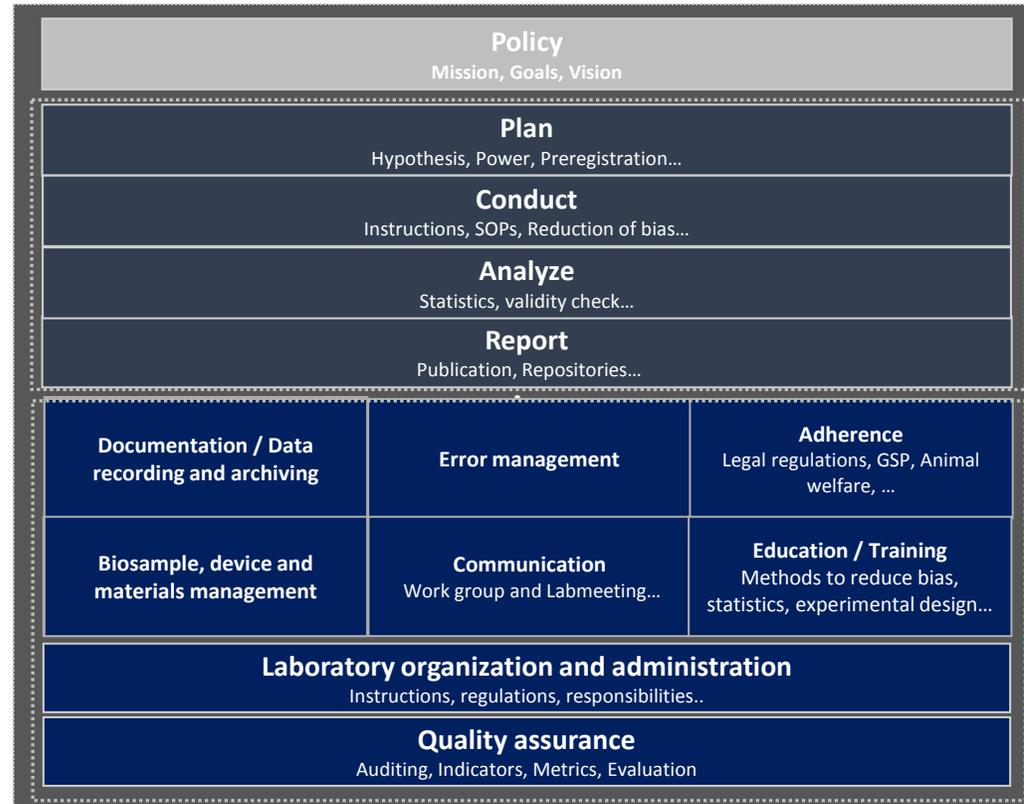
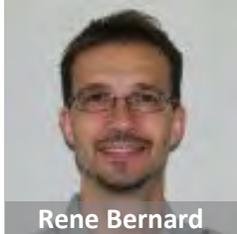
In general:

- Very complex biology, very complex methodology
- Structural underfunding (project funding often ok)
- Hypercompetition, publish or perish



PREMIER - Structured quality assurance

from and for academic preclinical biomedicine



The research process

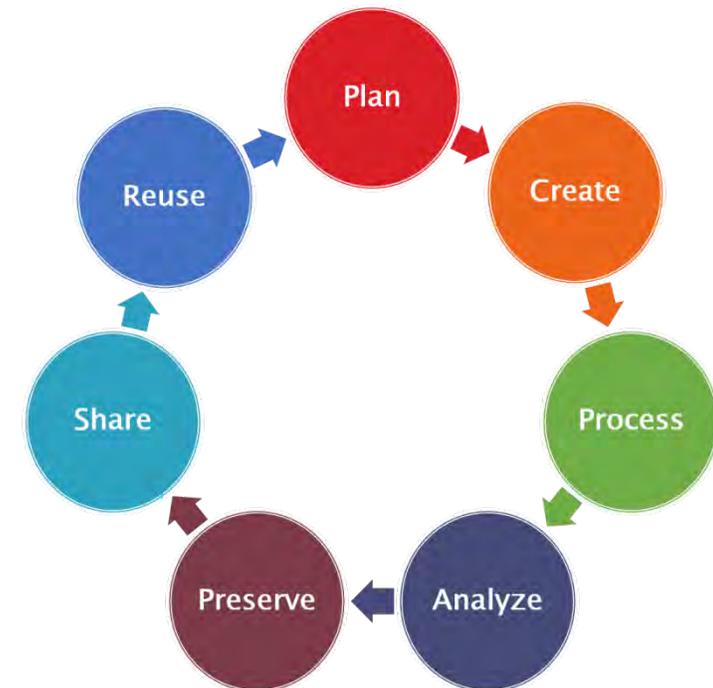
Supporting processes

Funded by

Research Data Management (RDM)

Governed by

- Standard operating procedures (SOPs)
- Guidelines
- Open Science: Open access, Open Data
- Electronic Laboratory Notebook (ELN)



Surveys

| | Group Leader | Labmanager | Postdoc | PhD Student | Technical personnel | Undergraduate |
|---|--------------|------------|---------|-------------|---------------------|---------------|
| ELN naive (n) | 4 | 1 | 12 | 13 | 10 | 10 |
| ELN user (n) | 2 | 4 | 5 | 3 | 7 | 1 |
| Sharing notes and data (naive) | | | | | | |
| Sharing notes and data (before test) | | | | | | |
| Sharing notes and data (after test) | | | | | | |
| Following progress (naive) | | | | | | |
| Following progress (before test) | | | | | | |
| Following progress (after test) | | | | | | |
| Intuitive interface (naive) | | | | | | |
| Intuitive interface (before test) | | | | | | |
| Intuitive interface (after test) | | | | | | |
| Use of mobile devices (naive) | | | | | | |
| Use of mobile devices (before test) | | | | | | |
| Use of mobile devices (after test) | | | | | | |
| Use of templates (naive) | | | | | | |
| Use of templates (before test) | | | | | | |
| Use of templates (after test) | | | | | | |
| Personal support (naive) | | | | | | |
| Personal support (before test) | | | | | | |
| Personal support (after test) | | | | | | |
| Saving time (naive) | | | | | | |
| Saving time (before test) | | | | | | |
| Saving time (after test) | | | | | | |
| Better structuring (naive) | | | | | | |
| Better structuring (before test) | | | | | | |
| Better structuring (after test) | | | | | | |
| Integration of digital content (naive) | | | | | | |
| Integration of digital content (before test) | | | | | | |
| Integration of digital content (after test) | | | | | | |
| Annotation and freehand drawing (naive) | | | | | | |
| Annotation and freehand drawing (before test) | | | | | | |
| Annotation and freehand drawing (after test) | | | | | | |

| Score | |
|--------------------|--|
| 1 = least relevant | |
| 5 = most relevant | |
| 4,75 - 5,00 | |
| 4,50 - 4,75 | |
| 4,25 - 4,50 | |
| 4,00 - 4,25 | |
| 3,75 - 4,00 | |
| 3,50 - 3,75 | |
| 3,25 - 3,50 | |
| 3,00 - 3,25 | |
| 2,75 - 3,00 | |
| 2,50 - 2,75 | |
| 2,25 - 2,50 | |
| 2,00 - 2,50 | |
| 1,75 - 2,00 | |
| 1,50 - 1,75 | |
| 1,25 - 1,50 | |
| 1,00 - 1,25 | |

| | Group Leader | Labmanager | Postdoc | PhD student | undergraduate student | Technical Assistant |
|--|--------------|------------|---------|-------------|-----------------------|---------------------|
| n naive | 22 | 9 | 39 | 47 | 8 | 34 |
| n ELN user | 3 | 8 | 16 | 7 | 2 | 6 |
| share notes and data (naive) | | | | | | |
| share notes and data (ELN user) | | | | | | |
| follow progress (naive) | | | | | | |
| follow progress (ELN user) | | | | | | |
| intuitive interface (naive) | | | | | | |
| intuitive interface (ELN user) | | | | | | |
| mobile devices (naive) | | | | | | |
| mobile devices (ELN user) | | | | | | |
| templates (naive) | | | | | | |
| templates (ELN user) | | | | | | |
| personal support (naive) | | | | | | |
| personal support (ELN user) | | | | | | |
| save time (naive) | | | | | | |
| save time (ELN user) | | | | | | |
| better structuring (naive) | | | | | | |
| better structuring (ELN user) | | | | | | |
| integration of digital content (naive) | | | | | | |
| integration of digital content (ELN user) | | | | | | |
| annotation and freehand drawing (naive) | | | | | | |
| annotation and freehand drawing (ELN user) | | | | | | |

| Rank | |
|------|--|
| 1 | |
| 2 | |
| 3 | |
| 4 | |
| 5 | |
| 6 | |
| 7 | |
| 8 | |
| 9 | |
| 10 | |

Alle Daten in einem Archiv

The screenshot shows a web browser window with the URL <https://labfolder.bihealth.org/ein/notebook?authorIds=858>. The interface is titled "labfolder Notebook" and includes a navigation bar with "NOTEBOOK", "MANAGE", and "DASHBOARD" options. A notification bubble in the top right corner says "We have a new text editor! Click to learn more!".

The main content area displays a notebook entry by Claudia Muselmann-Genschow, dated 22/29, titled "Test outerPCR_IL21_IL17a_TNF5F" in the "B-Cell" project. The entry contains the following text:

Cyclen
MasterMix + DNA

| | |
|-------|----------|
| 30min | 98°C |
| 10s | 98°C |
| 30s | 69°C 35x |
| 30s | 72°C |
| 10min | 72°C |
| hold | 4°C |

Agarose-Gel:
1% Agarose, 2log-ladder, OG

Below the text are two gel electrophoresis images, both titled "20171020_Kasia_Test_PCR_zur_Klonierung.tif". The left image shows a standard agarose gel with multiple lanes. The right image is a dark gel, possibly representing a different experimental condition or a failed run. Both images include technical metadata at the bottom, such as "App: Exp. Time: 1.26 sec. Bath: 6°C. Upper: 100.0%, Lower: 6.5%, Lin: Gamma 2" and "Date: 30.10.2017 Time: 08:45:28 Name: 20171020_Kasia_Test_PCR_zur_Klonierung.tif".

At the bottom of the notebook, there is a section for "23.10.2017 Outer-PCR für Primer mL17a; mL21; mTNFSF".

Stichwörter, Suchen (Daten, Projekte, Mitarbeiter...)

The screenshot shows the labfolder Notebook interface. The main content area displays a notebook entry titled "ELISA with serum samples of mice:" by Andreas Peitz. The entry includes a table of data, a text description of the experiment, and a graph showing OD 405 vs dilution [1:x].

| Sample | Value |
|---------------|----------|
| Fingo I, w12 | 5, 21 |
| Fingo I, w12 | 2, 11 |
| Fingo II, w12 | 1, 15, 4 |

Except 5 and 21 only 1:50 dilutions
Coated different concentrations of EColi lysate onto the plate + serum + total IgG antibody

The graph shows OD 405 on the y-axis (0 to 1500) and dilution [1:x] on the x-axis (10 to 100000). Two data series are plotted, both showing a decrease in OD as dilution increases, with a horizontal dotted line at OD 100.

Files associated with the notebook include:

- 20180103_165143.jpg (Image)
- 20160318_Ab_titer_MIR.tif (Image)
- 20160318_Ab_titer_MIR.pzfx (9.1 KB)
- 2016-03-18_ELISA_MIR_lysat.d08 (7.9 KB)
- 20160318_ELISA_MIR_Lysate.xlsx (12.4 KB)

Tags and filters are visible on the left side of the interface, including "B cells", "BZ20", "B6.129P-CX3CR1", "BAL", "BCA", "BCA-Assay", "BCA-Proteinbestimmung", "BECN1", "BIH", "BIH Curro", "BIH Curro 5xFAD", "Behaviour", "Beschichtung", "Besprechung", "Bloanalyzer", "Biocystin", "Biotin", "Bleeding", "Blinding group 1", "Blinding group 2", "BrdU", "BuGR2", "bumetanide", "C57BL/6", "CGB", "CCR2.RFP", "CD 86", "CD11b", "CD13", "CD19-FITC threshold", "CD3", "CD4", "CD45", "CHS", "COX", "CamK2a-Cre", "Catwalk", "Cerebellum", "Chat", "Circadian", and "CoCa".

Nutzung von Vorlagen

The screenshot displays the 'labfolder' website's 'Template index' page. The browser's address bar shows the URL 'https://labfolder.bihealth.org/eln/templates'. The page features a search bar, navigation tabs for 'NOTEBOOK', 'MANAGE', and 'DASHBOARD', and a sidebar with 'support' and 'recommend' buttons. The main content is a table listing templates, their creators, and timestamps.

| Template Name | Creator | Timestamp |
|--------------------------------------|---------------------|------------------|
| DNA Prep | Nasim Dokani Kh... | 28.03.2014 12:53 |
| Drug making | René Bernard | 02.03.2015 09:21 |
| DTI_Harms | Susanne Mueller | 25.04.2017 07:40 |
| Ehrlichs Reagenz Assay | Ria Uhlemann | 20.01.2016 15:27 |
| English Training Template | testgruppenadmin... | 14.12.2015 14:20 |
| FB_Protokollvorlage | Nikolas Offenhauser | 27.11.2013 10:28 |
| Field potential recording | Alienor Ragot | 07.01.2016 15:27 |
| Field_potential_recording | Alienor Ragot | 07.01.2016 15:41 |
| fire | Kristin Wendland | 29.11.2013 12:02 |
| Geb.kalender ExpNeuro | Christa Josties | 23.10.2013 11:20 |
| Geb.kalender ExpNeuro | Christa Josties | 23.10.2013 11:21 |
| Geb.kalender ExpNeuro | Christa Josties | 23.10.2013 11:22 |
| Generierung doppelsträngiger Oligos | Nasim Dokani Kh... | 29.04.2014 09:24 |
| Genotyping Andreas | Andreas Greiner | 04.01.2018 12:26 |
| GFAP Färbung DAB | Stefanie Balz | 05.01.2016 13:08 |
| GFP Färbung DAB | Stefanie Balz | 05.01.2016 12:58 |
| Glut 1 Färbung Fluoreszenz Alexa 488 | Stefanie Balz | 05.01.2016 11:15 |
| Griess-Assay | Ria Uhlemann | 06.08.2015 10:29 |
| Hippo-Präp | Tobias Schwarz | 25.10.2013 12:24 |
| Iba1 Färbung DAB | Stefanie Balz | 05.01.2016 10:40 |
| Iba1 Färbung Fluoreszenz Alexa 488 | Stefanie Balz | 05.01.2016 10:48 |
| IHC | Francisco Fernan... | 25.09.2017 11:15 |
| IHC | Christian Böttcher | 18.12.2017 11:26 |
| IHC | Christian Böttcher | 18.12.2017 11:29 |
| IL6 - ELISA | Janet Lips | 31.05.2016 13:32 |
| IL6-ELISA | Janet Lips | 07.01.2016 11:46 |
| Immuno-DAB NeuN | Petra Loge | 26.01.2016 11:06 |
| Immunostaining | BIH Admin | 13.11.2013 20:01 |
| Immunostaining | BIH Admin | 13.11.2013 20:01 |
| Immunostaining | BIH Admin | 13.11.2013 20:01 |

Nutzung von Vorlagen

The screenshot shows a web browser window with multiple tabs. The active tab is 'labfolder' showing a workspace for 'Francisco Fernandez-Klett'. The workspace contains a template for an IHC protocol. The protocol is presented as a table with 9 steps. A sidebar on the left has 'support' and 'recommended' buttons. At the bottom, a document icon indicates the template is 'Vorlage_IHC.docx' (15.0 KB).

Material:

| | | |
|----|---|--------------------------------|
| 1. | M.O.M. blocking | |
| 2. | wash in TBST | 3x5min, RT |
| 3. | Block with 20%NDS | 1h,RT |
| 4. | 1.antibodies in 1%NDS in TBST | 4degree, over two nights |
| 5. | wash in TBST | 3x20min, over night 1 and RT 2 |
| 6. | 2. antibody in 1% NDS in TBST: | 4degree, over night |
| 7. | wash in TBST | 3x20min, RT |
| 8. | Dapl 1:25.000 | 1x20min, RT |
| 9. | wash in TBST (2x) wash in TBS (1x) -Mounting with Fluorsave | 2x10min 1x10min |

Vorlage_IHC.docx
15.0 KB

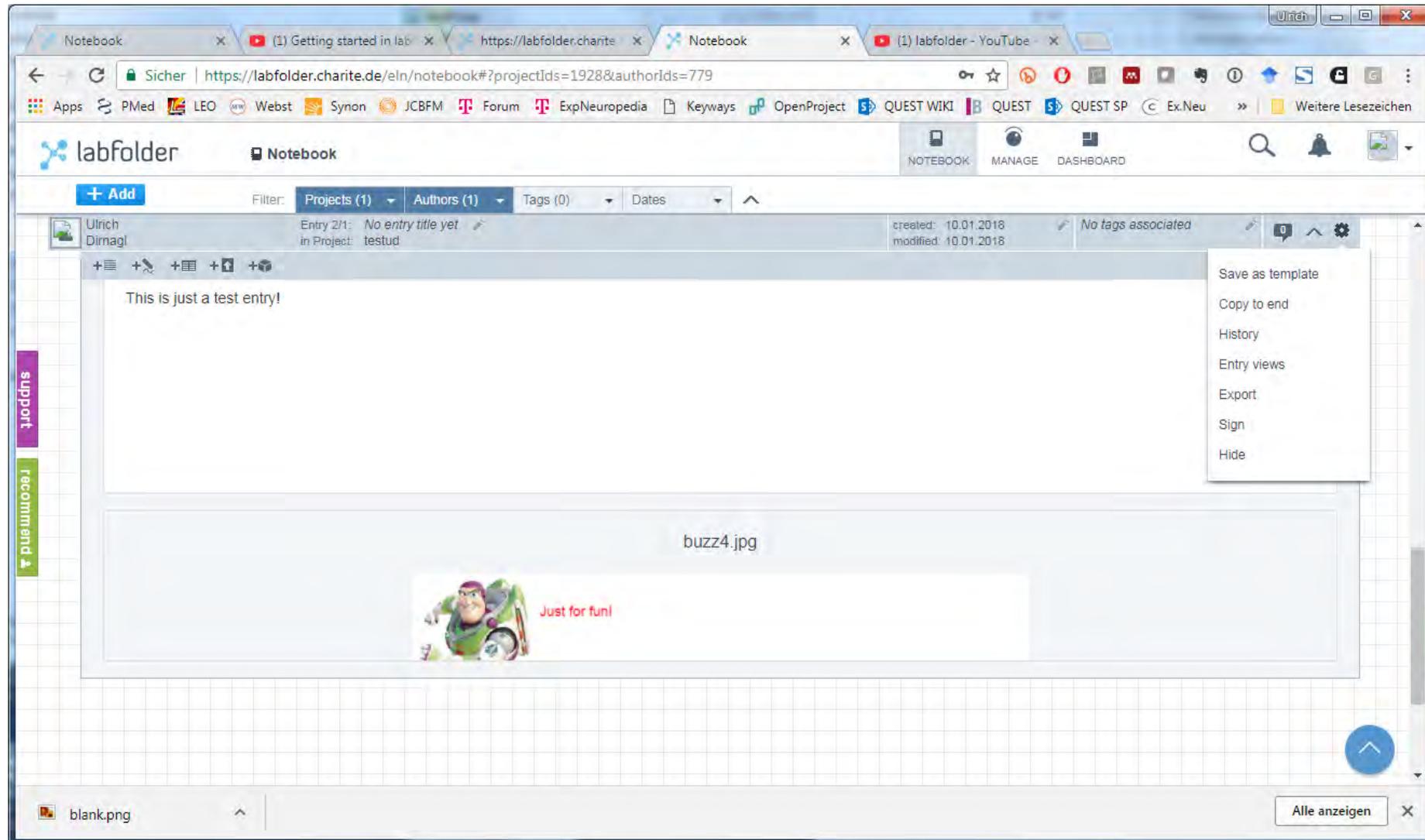
Jeder Eintrag verfolgbar, ob gelöscht, verändert....

The screenshot displays a web browser window with the URL <https://labfolder.charite.de/eln/notebook#?projectIds=1928&authorIds=779>. A modal dialog titled "History of this entry" is open, showing a list of actions:

| Timestamp | Action |
|------------------|--------------------------------|
| 10.01.2018 13:46 | Image annotated |
| 10.01.2018 13:46 | Element removed |
| 10.01.2018 13:46 | Element removed |
| 10.01.2018 13:46 | Image uploaded |
| 10.01.2018 13:46 | Element added |
| 10.01.2018 13:45 | Element removed |
| 10.01.2018 13:45 | Data Element container changed |
| 10.01.2018 13:45 | Element added |
| 10.01.2018 13:44 | Image uploaded |
| 10.01.2018 13:44 | Element added |
| 10.01.2018 13:44 | Data Element container changed |
| 10.01.2018 13:43 | Text changed |
| 10.01.2018 13:43 | Element added |
| 10.01.2018 13:43 | Element added |
| 10.01.2018 13:43 | Entry created |

The main content area of the dialog shows the current state of the entry, which includes the text "This is just a test entry!" and an image placeholder labeled "buzz4.jpg".

Exportieren, Signieren, etc.....



Arbeit im Team

The screenshot shows the labfolder web application interface. The browser address bar displays <https://labfolder.bihealth.org/ein/notebook#?null>. The application header includes the labfolder logo, a 'Notebook' title, and navigation buttons for 'NOTEBOOK', 'MANAGE', and 'DASHBOARD'. A filter bar shows 'Projects (0)', 'Authors (0)', 'Tags (0)', and 'Dates'. A search bar contains 'Find a project...'. A dropdown menu is open, listing project folders under 'Group projects: Exp Neuro':

- 7TExpMRT-CoreFacility
- AG-Harms
- Allgemein
- AP_Archiv aus Beta 02/2014 - 06/2014
- Autophagie
- Bortezomib
- Claudia MG
- Clemens Reiffurth
 - Na,K-ATPase isoform deficiency & Spreading Depolarization
- Clonierungen
- Current projects

The main content area shows a notebook page with a table and an image. The table has the following data:

| Time (s) | Mean of Force (N) | Peak Force (N) | Time to Peak (s) | Time to Relax (s) |
|----------|-------------------|----------------|------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|
| 1 | 15.4 | 15.4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 2 | 15.4 | 15.4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3 | 15.4 | 15.4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

Below the table is an image of a document titled '20180103_165227.jpg'. The document contains a table with the following data:

| Time (s) | Mean of Force (N) | Peak Force (N) | Time to Peak (s) | Time to Relax (s) |
|----------|-------------------|----------------|------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|
| 1 | 15.4 | 15.4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 2 | 15.4 | 15.4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3 | 15.4 | 15.4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

At the bottom of the notebook page, there are two files: '20160323_EAMG_Strength_Tryout.pzfx' (15.3 KB) and '20160323_EAMG_Strength_Tryout.xlsx' (16.4 KB). The left sidebar shows a user profile for 'Andreas Pelz' and a 'support' button.

Arbeit im Team: Kommentare

The screenshot displays a web browser window with multiple tabs. The active tab is a labfolder notebook page. The browser's address bar shows the URL `https://labfolder.charite.de/eln/notebook#?projectIds=1928&authorIds=779`. The labfolder interface includes a navigation bar with 'NOTEBOOK', 'MANAGE', and 'DASHBOARD' options. Below this is a filter section with 'Projects (1)', 'Authors (1)', 'Tags (0)', and 'Dates'. The main content area shows a notebook entry with a grid background. The entry header includes the author's name 'Ulrich Dimagl', the entry title 'No entry title yet', the project name 'testud', and the creation/modification date '10.01.2018'. The entry content contains the text 'This is just a test entry!' and an image labeled 'buzz4.jpg' which shows a cartoon character with the text 'Just for fun!'. A comment box on the right side of the entry shows a comment by 'Ulrich Dimagl' with the text 'To infinity and beyond!' and a 'Reply' button. The interface also features a 'support' sidebar on the left and a 'Alle anzeigen' button at the bottom right.

Nutzung von Daten ausserhalb des ELN, Export nach XHTML...

The screenshot shows the 'labfolder' ELN interface. At the top, there are browser tabs and a navigation bar with 'labfolder' and 'Apps' menus. Below the navigation bar, there is a newsletter subscription prompt. The main area displays several application tiles, each with an icon, a title, a 'Last update' date, and an 'Install' button. The tiles are:

- Dropbox**: Last update: 04.04.2017
- Figshare**: Last update: 26.03.2014
- Sign And Witness**: Last update: 04.07.2017
- Messages**: Last update: 24.03.2014
- Tasks**: Last update: 24.04.2014
- Comments**: Last update: 24.04.2014
- Todos**: Last update: 01.09.2014
- XHTML Export**: Last update: 14.03.2017
- Material Database**: Last update: 18.07.2017

On the left side of the interface, there is a vertical sidebar with a purple 'support' button and a green 'recommend 1' button. At the bottom right of the interface, there is a 3D rendering of a laboratory instrument, likely a plate reader or similar device, with a sample tray and a display screen.

Schnittstellen
zu Laborgeräten



Kompatibilität mit regulatorischen Standards

GLP

(OECD Guidelines on good laboratory practice)

| GLP requirement | Labfolder Feature | Compliance |
|-----------------------|------------------------------|------------|
| Access control | Login, project access rights | ✓ |
| Full audit trail | History function | ✓ |
| Digital signatures | Signing and witnessing | ✓ |
| Daily backups | Provided by labfolder | ✓ |
| Data center protected | Provided by data center | ✓ |

CFR 21 Part 11

(FDA guidelines for digital signatures)

| Requirement | Labfolder Feature | Compliance |
|-------------------------------------|---|------------|
| Signature (biometric / credentials) | Signing and witnessing | ✓ |
| Document integrity | Audit Trail, Controlled deletion, Hash sum | ✓ |
| Access management | Login, author control, access rights management | ✓ |

Schützt wenn in der AG oder im Institut ein Verdacht aufkommt....



Kann mitgenommen werden wenn man Institution verlässt



Löst das institutionelle Archivierungsproblem (10 Jahre!)



Quelle: Kernkraftwerk Stendal (!)

Horses for courses – different types of LNs

| Feature | Paper LN | Generic, electronic documentation system (Word, EverNote, ...) | ELNs, (iLabber, Labfolder, eCat...) | High-End ELNs (LIMS) |
|---|--|--|---|-------------------------------------|
| Digital documentation (Text, graphics)* | - | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Digital documentaion (Free hand drawing)* | - | (<input checked="" type="checkbox"/>) | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Text search* | - | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Searching projects* | - | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Exchange of data* | - | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Management of users, logging of entries, time stamp, audit trail* | (<input checked="" type="checkbox"/>) manually | - | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| 21CFR11 Compliance* | - | - | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Management of inventories (e.g. probes, chemicals) | - | - | (<input checked="" type="checkbox"/>) | <input checked="" type="checkbox"/> |
| Workflows (tasks, experiments) | - | - | (<input checked="" type="checkbox"/>) | <input checked="" type="checkbox"/> |
| Device integration (e.g. scales, readers, microscopes) | - | - | (<input checked="" type="checkbox"/>) | <input checked="" type="checkbox"/> |
| Analysis of raw data | - | - | | <input checked="" type="checkbox"/> |
| Cost | low | low | Intermed. | high |

* Minimum requirement for a state of the art eLN

Horses for courses – different types of LNs

| Feature | Paper LN | Generic, electronic documentation system (Word, EverNote, ...) | ELNs, (iLabber, Labfolder, eCat...) | High-End ELNs (LIMS) |
|---|---|--|---|-------------------------------------|
| Digital documentation (Text, graphics)* | - | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Digital documentaion (Free hand drawing)* | - | (<input checked="" type="checkbox"/>) | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Text search* | Do not meet minimum requirements | | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Searching projects* | (time stamping, copy/deletion protection, user management, 21 CFR 11, etc.) | | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Exchange of data* | | | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Management of users, logging of entries, time stamp, audit trail* | | | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| 21CFR11 Compliance* | - | - | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Management of inventories (e.g. probes, chemicals) | - | - | (<input checked="" type="checkbox"/>) | <input checked="" type="checkbox"/> |
| Workflows (tasks, experiments) | - | - | (<input checked="" type="checkbox"/>) | <input checked="" type="checkbox"/> |
| Linking instruments (e.g. scales, readers, microscopes) | - | - | (<input checked="" type="checkbox"/>) | <input checked="" type="checkbox"/> |
| Analysis of raw data | - | - | | <input checked="" type="checkbox"/> |
| Cost | low | low | Intermed. | high |

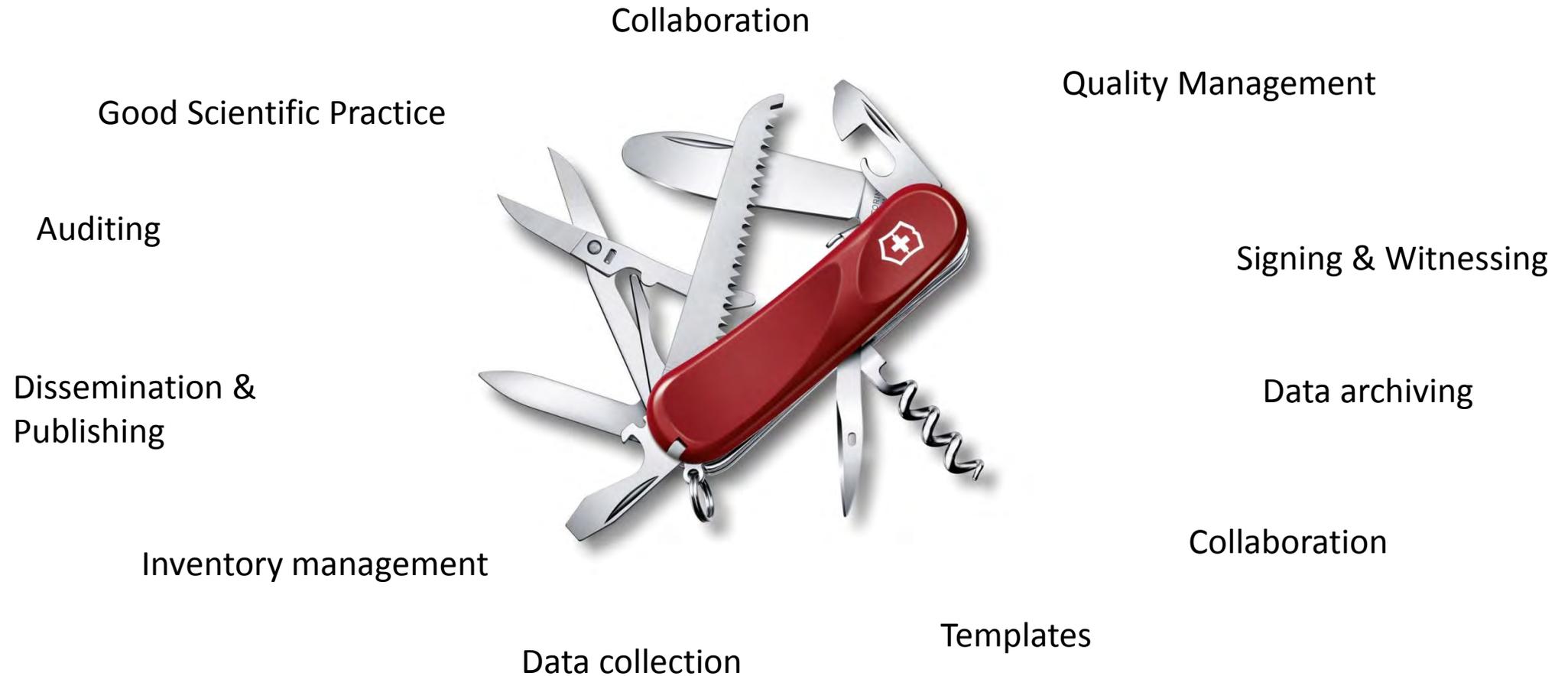
Too expensive, too many features, too complex, not user friendly

Herausforderungen (Institutionell)

- Teurer als Papierlaborbuch
- Integration in institutionelle IT
- Administration, user support
- Betriebliche und gesetzliche Vorgabe (GWP, Betriebsrat, Datenschutz)

- Einarbeitung nötig
- Neophobie: ‚Was der Bauer nicht kennt...‘ – ‚Never change a winning horse‘
- Paranoia I: Andere könnten einem in die Karten schauen
- Paranoia II: Daten gehen verloren gehen, verschwinden in ‚Cloud‘, werden von Google oder Amazon ausspioniert etc.
- Paranoia III: Firma geht bankrott, Mittel für ELN werden gestrichen, Wechsel an Institution ohne ELN
- Technophobie (insbes. bei TAs)

ELN: Swiss army knife of experimental biomedical research



Aber es hat keine Espresso-Funktion!

Espresso



Also:

1. Das Papier-Laborbuch ist ein Atavismus und gehört eingemottet
2. Das elektronische Laborbuch (eLN) kann viel mehr als ein Papierlaborbuch
3. eLNs sollten integraler Teil von Data management plans (DMP) und der guten wissenschaftlichen Praxis (GWP) werden
4. Die Hürden liegen in den Köpfen der Wissenschaftler ebenso wie bei den Institutionen
5. Die Voraussetzungen dafür müssen von den Institutionen im Rahmen der Grundausstattung geschaffen werden (IT, Lizenzgebühren, Onboarding, etc.). Auch die Fördergeber sind hier gefragt (Auflagen, Finanzmittel).

Die Zukunft

- eLN voll integriert in Datengenerierung, Kollaboration und Dissemination
- Integration in Open data Strategie
- Publikation aus dem eLN [data journals]
- Integration in strukturierte QM Systeme

Electronic laboratory notebooks – a pocket guide



OPINION ARTICLE

A pocket guide to electronic laboratory notebooks in the academic life sciences [version 1; referees: 4 approved]

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v1 First published: 04 Jan 2016, 5:2 (doi: [10.12688/f1000research.7628.1](https://doi.org/10.12688/f1000research.7628.1))
Latest published: 04 Jan 2016, 5:2 (doi: [10.12688/f1000research.7628.1](https://doi.org/10.12688/f1000research.7628.1))

Abstract

Every professional doing active research in the life sciences is required to keep a laboratory notebook. However, while science has changed dramatically over the last centuries, laboratory notebooks have remained essentially unchanged since pre-modern science. We argue that the implementation of electronic laboratory notebooks (eLN) in academic research is overdue, and we provide researchers and their institutions with the background and practical knowledge to select and initiate the implementation of an eLN in their laboratories. In addition, we present data from surveying biomedical researchers and technicians regarding which hypothetical features and functionalities they hope to see implemented in an eLN, and which ones they regard as less important. We also present data on acceptance and satisfaction of those who have recently switched from paper laboratory notebook to an eLN. We thus provide answers to the following questions: What does an electronic laboratory notebook afford a biomedical researcher, what does it require, and how should one go about implementing it?



This article is included in the [Neuroinformatics](#) channel.

Open Peer Review

Referee Status:

| Invited Referees | | | | |
|---------------------------------|--|--|--|--|
| | 1 | 2 | 3 | 4 |
| version 1 published 04 Jan 2016 | <input checked="" type="checkbox"/> report |

- 1 Thomas A. Kent**, Baylor College of Medicine USA
- 2 Christoph Kleinschnitz**, University of Würzburg Germany, **Eva Geuß**, University Hospital Würzburg Germany
- 3 Barry W. McColl**, The University of Edinburgh UK
- 4 Adam Denes**, Hungarian Academy of Sciences Hungary

Discuss this article

Comments (0)

How to pick an ELN



Published online: August 29, 2018

Science & Society

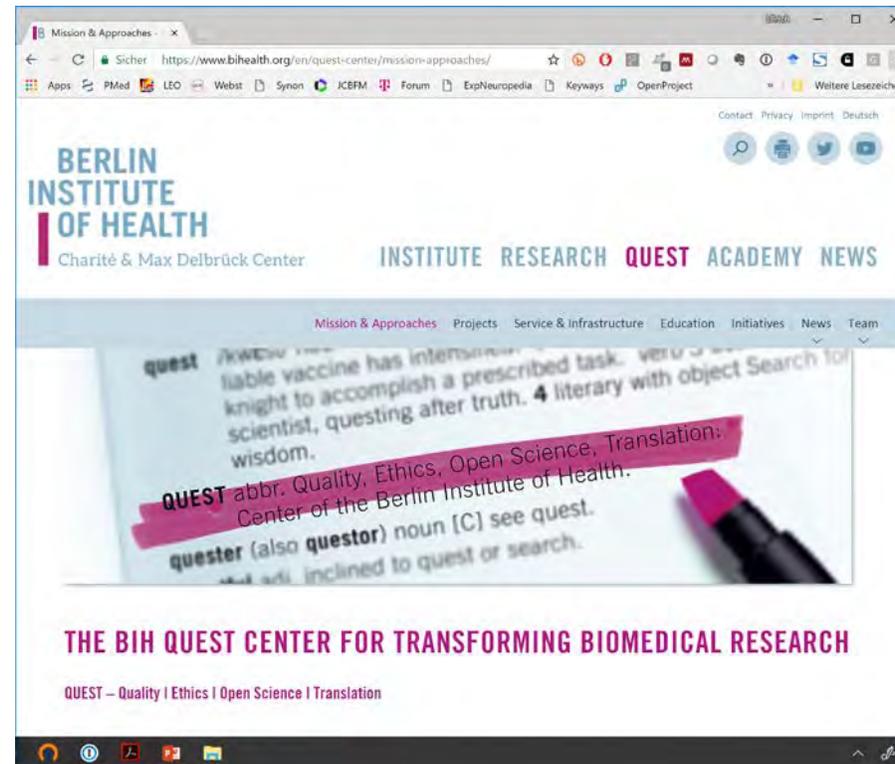
EMBO
reports

Scientific honesty and publicly shared lab notebooks

Sharing lab notebooks along with publication would increase transparency and help to improve honesty when reporting results

Bas van Steensel

<http://quest.bihealth.org>



<http://bit.ly/dirnaglbraunschweig>

Laborjournal

SERIE



Einsichten eines Wissenschaftsnarren (2)

Zu Risiken und Nebenwirkungen fragen Sie Ihren Bibliothekar

Der Übergang des wissenschaftlichen Publizierens zu Open Access ist überfällig. Doch zuerst müssen wir das Diktat des Journal-Impact-Faktors brechen.

Nahzu unbekannt von der Wissenschaft:

wir es mit Steuermitteln wieder zurück. Doch es kommt noch toller: Die Verlage geben uns unser Produkt nur leihweise, mit beschränktem Zugang, auf Widerruf und ohne Rechte auf die Artikel zurück. Der Steuerohner, der alles bezahlt hat, kommt gar nicht ran. Also nicht nur Liebchen Müller bleibt draußen, sondern auch niedergelassene Ärzte oder Kliniker und Wissenschaftler außerhalb der Universitäten.

Nach vielen Jahren als Chief Editor bei

Welche Probleme sind das? Ganz klar, wir Autoren behalten das Recht auf die Weiterverwertung unserer Artikel (zumindest im Creative-Commons-Modell), und jeder mit dem Zugang zum Internet kann sie lesen. Das wider in der Tat ein berechtigter Anspruch! Allerdings haben sich die gegenständliche Täuschung, bei dem wir unser selbstgeschriebenes Produkt verschicken, um es gleichzeitig wieder zurückzukäufen, überhaup nicht geändert. Seht über Sub-

To infinity, and beyond!
Is Translational Stroke Research Broken, and if So, How Can We Fix It?
JULY 9, 2016

Based on research, mainly in rodents, tremendous progress has been made in our basic understanding of the pathophysiology of stroke. After many failures, however, few scientists today deny that bench-to-bedside translation in stroke has a disappointing track record. I have summarized many measures to improve the predictiveness of preclinical stroke research, some of which are currently in various stages of implementation. We must reduce preclinical (behavioral) attrition. Key measures for this revolve around improving practical study design. Internal validity must be improved by reducing bias; external validity will improve by including aged, comorbid rodents of both sexes in our modeling. False-positives and inflated effect sizes can be reduced by increasing statistic of power, which necessitates increasing group sizes. Compliance to reporting guidelines and checklists needs to be enforced by journals and funders. Customizing study designs to exploratory and confirmatory studies will

Ulrich Dirnagl
@dirnagl
Tweets 283 Following 62 Followers 456

Who to follow
Kim Wever @kimwever
Justin Vothelick @justvothelick
Jon Tennant @jtennant

Trends for you
#BVP16
#GahardGP
#GahardGP

Monthly column
laborjournal.de

Blog
dirnagl.com



@dirnagl

Vorteile des Elektronischen Laborbuchs (ELN)

- Originaldaten digital verfügbar, direkte Einbindung in ELN
- Zusammenarbeit : Austausch von Infos, Protokolle und Daten zw/innerhalb von Gruppen
- Einträge und Änderungen werden getrackt mit Zeitstempel, Versionskontrolle
- Zugang zum ELN von verschiedenen Computern aus möglich
- Häufig gebrauchte Protokolle können als Vorlagen hinterlegt werden
- Projektfortschritt kann durch Gruppen-/Projektleiter einfach nachverfolgt werden
- Suchfunktion
- Kopieren von Daten und Datenarchivierung ist einfach
- Unbegrenzte eLN Archivierung in Institution
- Mitnahme des 'Originals' durch den Mitarbeiter wenn er/sie Institution verlässt

Torsten Bronger, FZJ: JuliaBase – Framework für Proben-basierte elektronische Laborbücher

Abstract

JuliaBase ist ein in Python + Django geschriebenes Framework zur Entwicklung von Browser-basierten Probandatenbanken und ELN-Lösungen. Hauptanwendungsgebiet sind Arbeitsgruppen und Institute mit Workflows, bei denen Proben eine Vielzahl von Prozess- und Charakterisierungstationen durchlaufen. Im Kern stellt JuliaBase die Proben-Chronik in Form eines Probandatenblatts zusammen. Im ELN-Bereich positioniert sich JuliaBase eindeutig bei den hochgradig anpassbaren Lösungen inklusive Visualisierung und Analyse. Das erfordert dann allerdings eigene Programmierarbeit.

JuliaBase 14 September 2018

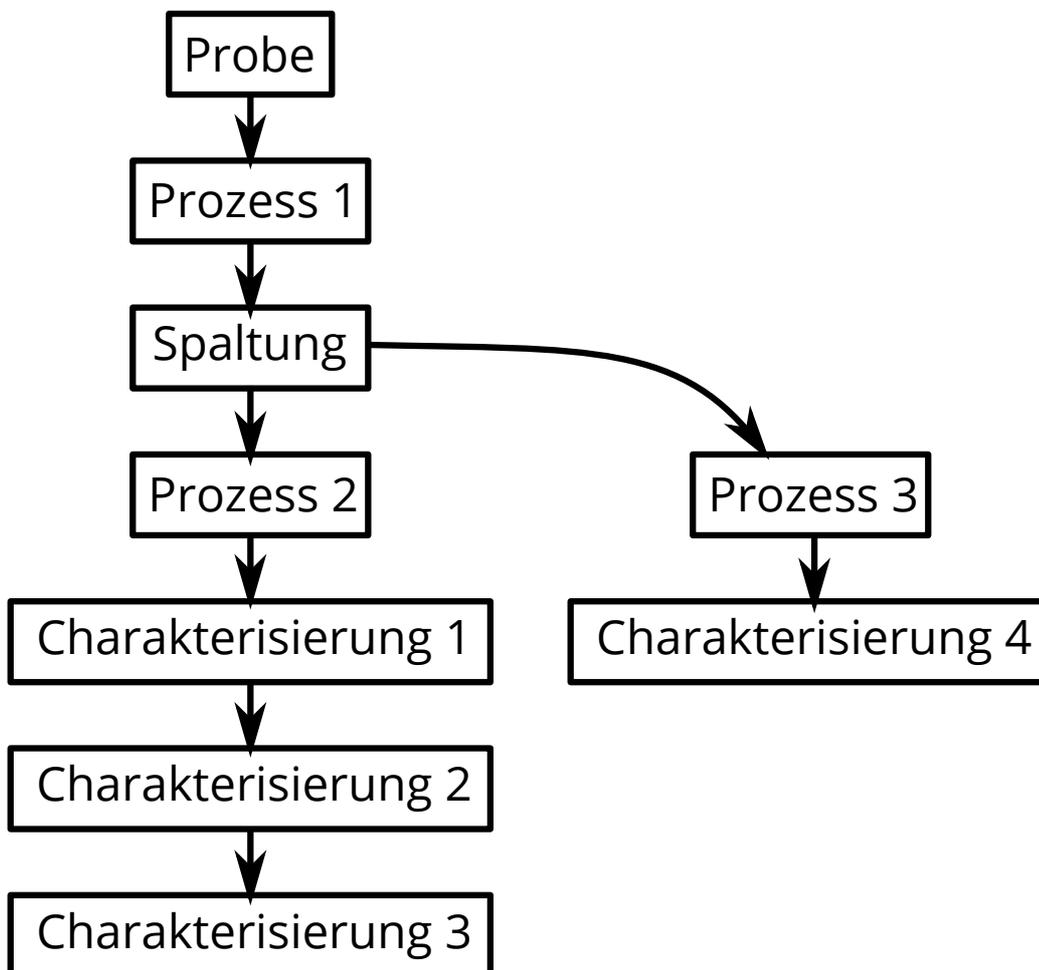
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1. Das Projekt

- Ein-Person-Projekt, derzeit kaum neue Features
- sehr gut gepflegt, stets an neueste Bibliotheken angepaßt
- sehr gut dokumentiert
- Python 3 + Django 2
- Open Source (AGPL), GitHub

<https://juliabase.org>

2. Workflow



3. Motivation

- unseren Workflow abbilden
- sehen, was mit einer **Probe** gemacht wurde
- hohe Anpassung an die jeweiligen Apparaturen
- Altdaten importieren
- mächtige Suche

- neue Daten automatisch hineinbekommen
- bisherige Datenströme nicht antasten

4. Neue Apparatur

- DB-Modell nötig
- Programmierung der Anzeigelogik nötig (mit 10–20 Zeilen ist man dabei)
- Web-Schablonen nötig (u.U. auch für's Laborbuch)
- Programmierung für den „Remote Client“

Einfache Apparatur: < 10 Python-Zeilen, DB-Model dazu: auch < 10 Zeilen Apparatur mit Subentitäten: ≈ 20 Zeilen

5. Erweiterte Features

- Vor-Auswertung
- halbautomatische Probenvisualisierung
- Themen und Unterthemen
- Aufträge
- RSS/Atom-Feeds für Benachrichtigung
- Export von allen Seiten (auch Suchergebnissen)
- responsive

6. Ausblick

- Einfaches Zusammenklicken neuer Apparaturen
- Versionierung (Öffnung der Schreibrechte)
- Rezepte
- Nicht-SQL-Backend
- Rohdaten speichern (alles, was durch's Ethernet paßt)?
- Anlagen-Reservierung?

Ralf Oeser, Jutta Schlegel & Friedhelm von Blanckenburg, GFZ: MEDUSA – über die Entdeckung einer griechischen Sagengestalt in Japan und deren Weiterentwicklung am Deutschen GeoForschungsZentrum Potsdam

Abstract

Im Zeitalter von Big Data, in denen immer mehr (geochemische) Daten generiert werden und die interdisziplinäre Nutzung dieser Daten für Wissenschaftler immer mehr zur Voraussetzung wird, wird der Bedarf an einer leicht zugänglichen Datenbasis immer deutlicher. Obwohl kommerzielle Datenbanken existieren, erfüllen sie oft nicht die speziellen Anforderungen großer wissenschaftlicher Arbeitsgruppen. Im Jahr 2012 hat eine japanische Gruppe von der Okayama University unter Yachi et al. die Open-Source-Datenbank Medusa entwickelt, um die Nachteile kommerzieller und geschlossener Datenbanken zu überwinden.

Medusa ist eine Mischung aus einem elektronischen Labor-Notizbuch (ELN) und einem Labor-Informationen-Management-System (LIMS), das alle Metadaten und Analyseergebnisse einer Probe speichert. So ist es in der Lage die Wege einer Probe von der Probennahme im Feld, über die Aufbereitung im Labor, bis hin zur anschließenden Analyse und Lagerung zurückzuverfolgen. Darüber hinaus bietet Medusa die Möglichkeit, Publikationen, Abbildungen und viele andere Arten von Daten mit den Proben zu verknüpfen, was die Kommunikation und den Datenaustausch in kollaborativen Projekten vereinfacht.

Ab 2015 wurde der Quellcode der japanischen Gruppe am GeoForschungsZentrum Potsdam (GFZ) erweitert, um den unterschiedlichen Anforderungen verschiedenster wissenschaftlicher Bereiche (i.e. Biologie, Geomorphologie, Geochemie, Geologie, Geophysik und Bodenkunde) gerecht zu werden und den Datenaustausch im Rahmen des EarthShape Projekts (DFG-SPP 1803) zu ermöglichen. Heute ist Medusa in der Lage, Daten über CSV-Dateien zu importieren und zu exportieren, IGSNs zu generieren und zu veröffentlichen und die Beprobungsstandorte in einer interaktiven Karte zu visualisieren. Darüber hinaus wird die Datensicherheit und der Zugriff durch die Implementierung eines intelligenten Gruppenmanagements gewährleistet. In diesem Vortrag werden wir Erfolge und Herausforderungen von fast 3 Jahren Medusa Entwicklung und Benutzererfahrung präsentieren und einen Einblick vor und hinter die Kulissen gewähren.

Medusa

Die Entdeckung einer griechischen Sagengestalt in Japan und
deren Weiterentwicklung am Deutschen
GeoForschungsZentrum Potsdam



by Toyomi Usami

von Jutta Schlegel

Was ist das für eine Probe?

Ist die Probe schon angesäuert?

Welche Daten wurden schon gemessen?



Ist diese Probe „M11“ die gleiche wie diese „M11“?

...und wer ist Nadine?

Wer hat Zugriff auf meine Daten?

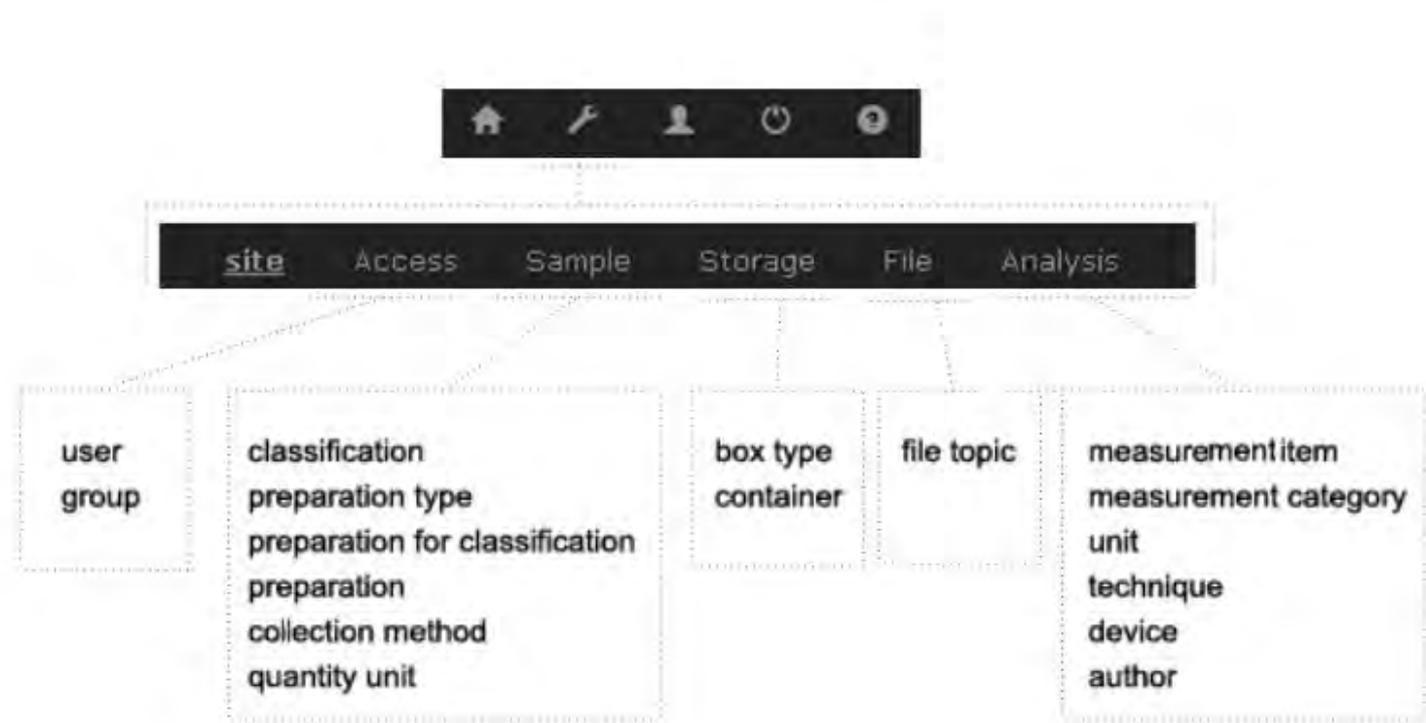
Medusa...



- ...ist ein Hybrid aus einem Elektronischen Laborbuch (ELN) und einem Labor Management Information System (LIMS)
- ...kann die Arbeitsschritte an einer Probe darstellen
- ...kann Probenlager organisieren
- ...kann (geochemische) Datensets archivieren

Architektur

- Datenbank = PostgreSQL
- Webserver = Apache
- Webframework = Ruby on Rails
- Physischer Standort = Linux Server im Rechenzentrum
 - DMZ – Zugriff auch für Institutsfremde Partner
 - Login via Browser
 - Backup via RZ



Kategorien



1 2 3 4 5 ... Next › Last »

Suche

Ergebnisse

Select all

Neuer Eintrag

View all entries

Map

Sampling Campaign

Sampling Location

Storage room/Box

Sample

Analysis

File

Bibliography

Import of CSV



1 2 3 4 5 ... Next › Last »

New Entry

Suche

Ergebnisse

Select all

bundle edit

Neuer Eintrag

Search and filter Sample

| Entries per page | name | parent | Labname | IGSN | Sampling Location | classification | group | updated-at | |
|--|--------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--|---|
| <input type="text" value="5"/>  | <input type="text" value="search:"/> | <input type="text" value="from:"/> <input type="text" value="to:"/> |  |

Ergebnisse

[Select all](#)
[bundle edit](#)

Neuer Eintrag

Interface – Seitenlayout

View all entries | Map | Sampling Campaign | Sampling Location | Storageroom/Box | **Sample** | Analysis | File | Bibliography | Import of CSV |      

1 2 3 4 5 ... Next > Last » [New Entry](#)

Search and filter Sample

Entries per page: 

| | name | parent | Labname | IGSN | Sampling Location | classification | group | updated-at | |
|--------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--|---|
| <input type="checkbox"/> | <input type="text" value="search:"/> | <input type="text" value="from:"/> <input type="text" value="to:"/> |  |
| <input type="checkbox"/> | LCPED30-06-RO-W6 | LCPED30-06-RO-W | 35226 | GFRO100FC | LCPED30 | soil | PSA Soil | 2017-01-03 | |
| <input type="checkbox"/> | SGPED40-REP-01-RO-W6 | SGPED40-REP-01-RO-W | 35183 | GFRO100GG | SGPED40-REP | soil | PSA Soil | 2017-01-03 | |
| <input type="checkbox"/> | SGPED40-04-RO-W6 | SGPED40-04-RO-W | 35181 | GFRO100GE | SGPED40 | soil | PSA Soil | 2017-01-03 | |
| <input type="checkbox"/> | SGPED40-02-RO-W6 | SGPED40-02-RO-W | 35179 | GFRO100GF | SGPED40 | soil | PSA Soil | 2017-01-03 | |
| <input type="checkbox"/> | SGPED20-REP-01-LMM-W6 | SGPED20-REP-01-LMM-W | 35171 | GFRO100GD | SGPED20 | soil | PSA Soil | 2017-01-03 | |

Select all

Neuer Eintrag

Interface – Seitenlayout

[View all entries](#) [Map](#) [Sampling Campaign](#) [Sampling Location](#) [Storageroom/Box](#) **[Sample](#)** [Analysis](#) [File](#) [Bibliography](#) [Import of CSV](#)



1 2 3 4 5 ... Next > Last » [New Entry](#)

Search and filter Sample

| Entries per page | name | parent | Labname | IGSN | Sampling Location | classification | group | updated-at | |
|--------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--|--|
| <input type="text" value="5"/> | <input type="text" value="search:"/> | <input type="text" value="from:"/> <input type="text" value="to:"/> | |

| | | | | | | | | |
|--------------------------|---------------------------------------|--------------------------------------|-------|-----------|-----------------------------|------|----------|------------|
| <input type="checkbox"/> | LCPED30-06-RO-W6 | LCPED30-06-RO-W | 35226 | GFRO100FC | LCPED30 | soil | PSA Soil | 2017-01-03 |
| <input type="checkbox"/> | SGPED40-REP-01-RO-W6 | SGPED40-REP-01-RO-W | 35183 | GFRO100GG | SGPED40-REP | soil | PSA Soil | 2017-01-03 |
| <input type="checkbox"/> | SGPED40-04-RO-W6 | SGPED40-04-RO-W | 35181 | GFRO100GE | SGPED40 | soil | PSA Soil | 2017-01-03 |
| <input type="checkbox"/> | SGPED40-02-RO-W6 | SGPED40-02-RO-W | 35179 | GFRO100GF | SGPED40 | soil | PSA Soil | 2017-01-03 |
| <input type="checkbox"/> | SGPED20-REP-01-LMM-W6 | SGPED20-REP-01-LMM-W | 35171 | GFRO100GD | SGPED20 | soil | PSA Soil | 2017-01-03 |

Select all

Create Sample here:

Identification

| | | |
|---|--|--|
| Sample Name <input type="text" value="- required -"/> | Parent <input type="text" value=""/> | IGSN <input type="text" value=""/> |
|---|--|--|

Acquisition

| | | | | |
|---|--|--|---|--|
| Collection method <input type="text" value=""/> | Classification <input type="text" value="- required -"/> | Sampling Location <input type="text" value="- required -"/> | Sampling Campaign <input type="text" value="- required -"/> | Depth (m from groundlevel) <input type="text" value="- required -"/> |
| Date <input type="text" value="- required -"/> | Quantity unit <input type="text" value="- required -"/> | Quantity (initial) <input type="text" value="- required -"/> | Quantity (current) <input type="text" value=""/> | |

Storage

| | | |
|---|---|---|
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|---|---|---|

NAPED20-02-LMM < 20160727131218-992148 >



Bild/Karte
und
Stammbaum

Aktueller Lagerort

Informationen über den Eintrag

NAPED20-02-LMM < 20160727131218-992148 >



NAPED20-02-LMM 2 1

- NAPED20-02-LMM-A
- NAPED20-02-LMM-W 8
 - NAPED20-02-LMM-W2-res
 - NAPED20-02-LMM-W5
 - NAPED20-02-LMM-W>2mm
 - NAPED20-02-LMM-W1
 - NAPED20-02-LMM-W6
 - NAPED20-02-LMM-W3 4
 - NAPED20-02-LMM-W3.1 1
 - NAPED20-02-LMM-W3.1-1
 - NAPED20-02-LMM-W3.4
 - NAPED20-02-LMM-W3.3
 - NAPED20-02-LMM-W3.2
 - NAPED20-02-LMM-W7
 - NAPED20-02-LMM-W4

Aktueller Lagerort

Informationen über den Eintrag

NAPED20-02-LMM < 20160727131218-992148 >



- ▶ NAPED20-02-LMM 2 1
- ▶ NAPED20-02-LMM-A
- ▶ NAPED20-02-LMM-W 8
- ▶ NAPED20-02-LMM-W2-res
- ▶ NAPED20-02-LMM-W5
- ▶ NAPED20-02-LMM-W>2mm
- ▶ NAPED20-02-LMM-W1
- ▶ NAPED20-02-LMM-W6
- ▶ NAPED20-02-LMM-W3 4
- ▶ NAPED20-02-LMM-W3.1 1
- ▶ NAPED20-02-LMM-W3.1-1
- ▶ NAPED20-02-LMM-W3.4
- ▶ NAPED20-02-LMM-W3.3
- ▶ NAPED20-02-LMM-W3.2
- ▶ NAPED20-02-LMM-W7
- ▶ NAPED20-02-LMM-W4



Proben sind leicht und eindeutig identifizierbar durch die Etiketten mit IGSN

NAPED20-02-LMM < 20160727131218-992148 >



NAPED20-02-LMM 2 1

- NAPED20-02-LMM-A
- NAPED20-02-LMM-W 8
 - NAPED20-02-LMM-W2-res
 - NAPED20-02-LMM-W5
 - NAPED20-02-LMM-W>2mm
 - NAPED20-02-LMM-W1
 - NAPED20-02-LMM-W6
 - NAPED20-02-LMM-W3 4
 - NAPED20-02-LMM-W3.1 1
 - NAPED20-02-LMM-W3.1-1
 - NAPED20-02-LMM-W3.4
 - NAPED20-02-LMM-W3.3
 - NAPED20-02-LMM-W3.2
 - NAPED20-02-LMM-W7
 - NAPED20-02-LMM-W4

Aktueller Lagerort

Informationen über den Eintrag

NAPED20-02-LMM < 20160727131218-992148 >



Aktueller Lagerort

at-a-glance daughter (2) analyses bib file (1) preparation



- site: -37.8077 South, -73.0135 West [more](#)
- IGSN: [GFRO10018](#) Register/Update IGSN
- Sampling Campaign: NAPED soil baseline data assessment
- material: soil
- type: soil
- container type: bag
- Preparations:
- modified at 2016-07-27
-

NAPED20-02-LMM 2 1

- NAPED20-02-LMM-A
- NAPED20-02-LMM-W 8
 - NAPED20-02-LMM-W2-res
 - NAPED20-02-LMM-W5
 - NAPED20-02-LMM-W>2mm
 - NAPED20-02-LMM-W1
 - NAPED20-02-LMM-W6
 - NAPED20-02-LMM-W3 4
 - NAPED20-02-LMM-W3.1 1
 - NAPED20-02-LMM-W3.1-1
 - NAPED20-02-LMM-W3.4
 - NAPED20-02-LMM-W3.3
 - NAPED20-02-LMM-W3.2
 - NAPED20-02-LMM-W7
 - NAPED20-02-LMM-W4

NAPED20-02-LMM < 20160727131218-992148 >











NAPED20-02-LMM 2 1

- NAPED20-02-LMM-A
- NAPED20-02-LMM-W 8
 - NAPED20-02-LMM-W2-res
 - NAPED20-02-LMM-W5
 - NAPED20-02-LMM-W>2mm
 - NAPED20-02-LMM-W1
 - NAPED20-02-LMM-W6
 - NAPED20-02-LMM-W3 4
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 - NAPED20-02-LMM-W3.1-1
 - NAPED20-02-LMM-W3.4
 - NAPED20-02-LMM-W3.3
 - NAPED20-02-LMM-W3.2
 - NAPED20-02-LMM-W7
 - NAPED20-02-LMM-W4

Aktueller Lagerort

[at-a-glance](#)
[daughter](#)
[analyses](#)
[bib](#)
[file](#)
preparation (3)

| Preparation type | Info | |
|----------------------|----------------------|---|
| extraction | ECEC | ✕ |
| oven dried | 40°C | ✕ |
| sieving | <2mm | ✕ |
| <input type="text"/> | <input type="text"/> |  |

NAPED20-02-LMM < 20160727131218-992148 >



- NAPED20-02-LMM** 2 1
 - NAPED20-02-LMM-A
 - NAPED20-02-LMM-W 8
 - NAPED20-02-LMM-W2-res
 - NAPED20-02-LMM-W5
 - NAPED20-02-LMM-W>2mm
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 - NAPED20-02-LMM-W3 4
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 - NAPED20-02-LMM-W3.1-1
 - NAPED20-02-LMM-W3.4
 - NAPED20-02-LMM-W3.3
 - NAPED20-02-LMM-W3.2
 - NAPED20-02-LMM-W7
 - NAPED20-02-LMM-W4

Aktueller Lagerort

[at-a-glance](#) [daughter](#) [analyses](#) [bib](#) [file \(1\)](#) [preparation \(3\)](#)

| Filetopic | name | global-id | |
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| | | |
|---|---|--|
| Filetopic | File upload | Group |
| - required - | <input type="button" value="Durchsuchen..."/> Keine Datei ausgewählt. | Proj111 <input type="button" value="↓"/> |
| <ul style="list-style-type: none"> - required - field measurement other publications results <li style="background-color: #e0e0e0;">sample picture sample strategy SOP (standard operational procedure) | | |

NAPED20-02-LMM < 20160727131218-992148 >



- ➔ NAPED20-02-LMM 2 1
- ➔ ➔ NAPED20-02-LMM-A
- ➔ ➔ NAPED20-02-LMM-W 8
- ➔ ➔ ➔ NAPED20-02-LMM-W2-res
- ➔ ➔ ➔ NAPED20-02-LMM-W5
- ➔ ➔ ➔ NAPED20-02-LMM-W>2mm
- ➔ ➔ ➔ NAPED20-02-LMM-W1
- ➔ ➔ ➔ NAPED20-02-LMM-W6
- ➔ ➔ ➔ NAPED20-02-LMM-W3 4
- ➔ ➔ ➔ ➔ NAPED20-02-LMM-W3.1 1
- ➔ ➔ ➔ ➔ ➔ NAPED20-02-LMM-W3.1-1
- ➔ ➔ ➔ ➔ NAPED20-02-LMM-W3.4
- ➔ ➔ ➔ ➔ NAPED20-02-LMM-W3.3
- ➔ ➔ ➔ ➔ NAPED20-02-LMM-W3.2
- ➔ ➔ ➔ NAPED20-02-LMM-W7
- ➔ ➔ ➔ NAPED20-02-LMM-W4

GFZ-Potsdam / C051 / ES-02 / me

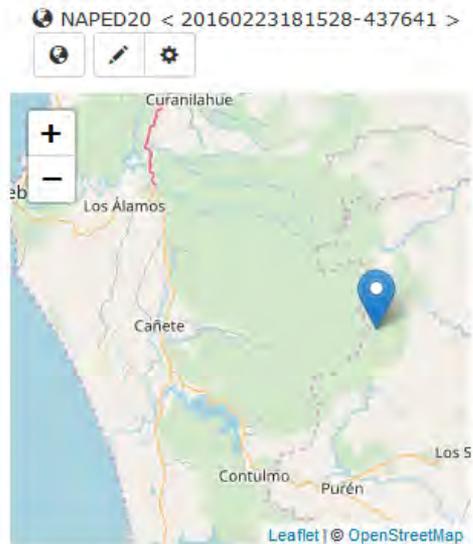
[at-a-glance](#) [daughter](#) [analyses](#) [bib](#) file (1) [preparation \(3\)](#)

| Filetopic | name | global-id | |
|--------------------------|------------|------------------|--|
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| <input type="checkbox"/> | Select All | | |

edit

Filetopic **File upload** **Group**
 - required - Keine Datei ausgewählt. Proj111

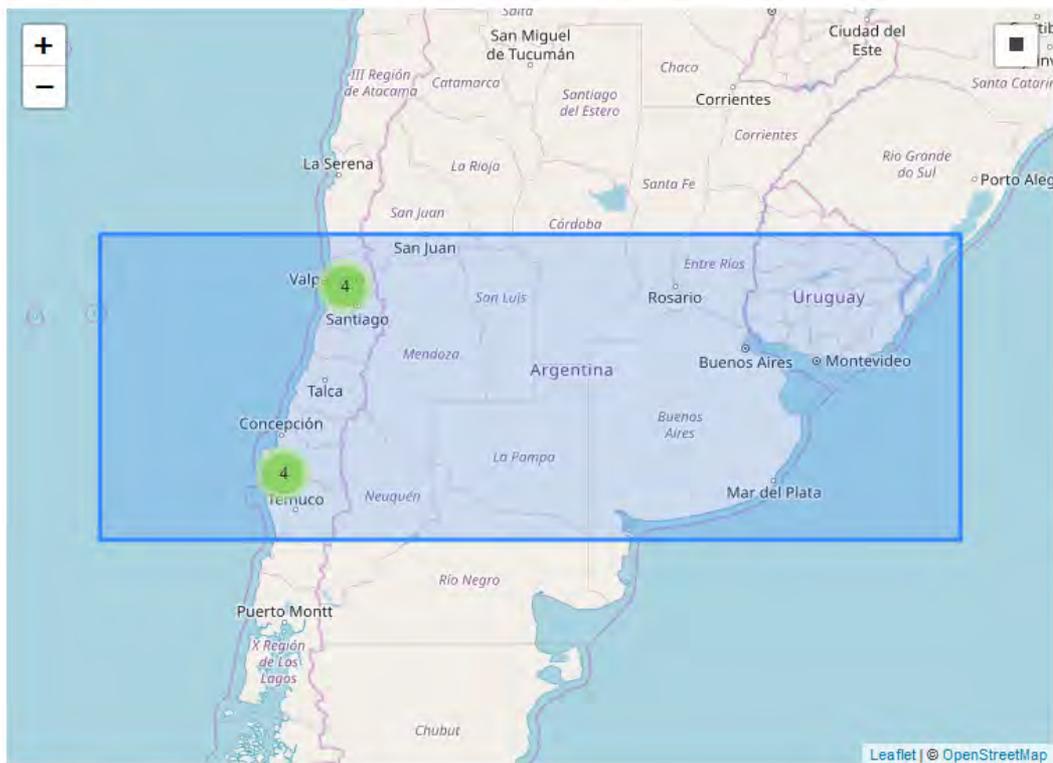
- required -
- field measurement
- other
- publications
- results
- sample picture
- sample strategy
- SOP (standard operational procedure)



[at-a-glance](#)
[sample \(430\)](#)
[neighbor](#)
[file \(1\)](#)
[geoname](#)

Link Sample to this Location

| | name | quantity | unit | global-id | |
|--------------------------|------------------------------------|----------|------|-----------------------|---|
| <input type="checkbox"/> | NAPED20-H7-NADI-W | 629.6 | g | 20160829100224-160789 | ✕ |
| <input type="checkbox"/> | NA20d | | g | 20161217133610-128722 | ✕ |
| <input type="checkbox"/> | NAPED20-H1-NADI-W | 48.7 | g | 20160720155825-401290 | ✕ |
| <input type="checkbox"/> | NAPED20-H11-NADI-W | 436.9 | g | 20160902180114-513826 | ✕ |
| <input type="checkbox"/> | NAPED20-14-LMM-A | | g | 20160727131746-111331 | ✕ |
| <input type="checkbox"/> | NAPED20-09-LMM-A | | g | 20160727131658-348788 | ✕ |
| <input type="checkbox"/> | NAPED20-H2-NADI-W | 168.5 | g | 20160811105108-528456 | ✕ |
| <input type="checkbox"/> | NAPED20-H8-NADI-W | 571.2 | g | 20160811105226-285234 | ✕ |
| <input type="checkbox"/> | NAPED20-H9-NADI | | | 20160720172359-845539 | ✕ |
| <input type="checkbox"/> | NAPED20-10-LMM-W | 646.5 | g | 20160725105849-599445 | ✕ |
| <input type="checkbox"/> | NAPED20-12-LMM-A | | g | 20160727131728-557685 | ✕ |
| <input type="checkbox"/> | NAPED20-14-LMM | | kg | 20160727132545-654511 | ✕ |
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| <input type="checkbox"/> | NAPED20-10-LMM | | kg | 20160727132513-444394 | ✕ |
| <input type="checkbox"/> | NAPED20-09-LMM | | kg | 20160727132505-607202 | ✕ |
| <input type="checkbox"/> | NAPED20-08-LMM | | kg | 20160727132457-119474 | ✕ |



Samples: 1 2 3 4 5 Next > Last >>

| Sample Name | Sample Parent | Labname | IGSN | Sampling Location | classification | Group | updated-at |
|-----------------------------------|---------------------------------|---------|-----------|-------------------------|----------------|----------|------------|
| NAPED20-H1-NADI-W | NAPED20-H1-NADI | | GFRO100SQ | NAPED20 | litter bag | PSA Soil | 2017-02-17 |
| LCPED40-H1-NADI-W | LCPED40-H1-NADI | | GFLMM00LM | LCPED40 | litter bag | PSA Soil | 2017-02-17 |
| NAPED20-H1-NADI-A | NAPED20-H1-NADI | | GFRO10078 | NAPED20 | litter bag | PSA Soil | 2017-12-14 |
| LCPED20-H1-NADI | | | GFLMM00QL | LCPED20 | litter bag | PSA Soil | 2017-12-04 |
| NAPED30-H1-NADI | | | GFLMM00PX | NAPED30 | litter bag | PSA Soil | 2017-12-04 |

25 Entries per page

Parent Location

lon

lat

from: to:

Sample name

Material

Collector

Affiliation

Campaign

Upload new entries from a CSV file

Storageroom/Box (889)

Sampling Location (889)

Sampling Campaign (889)

Sample (889)

| | | | | | | |
|-----------------------------------|---------------------------------------|----------------------------|--------------------------------------|-----------------------------|------------------------|------------------------|
| Sample Name Con_B 02-Mar-15 | Parent ▼ | IGSN | Collection method automatic sam ▼ | Material water:river ▼ | Location Conventl ▼ | Campaign Freiburg ▼ |
| Depth (m from groundlevel) 0.0 | Date 2015-03-02 | Quantity (initial) 15.0 | Quantity unit ml | Quantity (current) 15.0 | Labname CB1 | Box CON_B0 ▼ |
| Container 15ml-tube (pir ▼) | Description | | Name Jakob Sohr | Affiliation Uni Freiburg | | |
| Group Freiburg ▼ | <input type="button" value="Create"/> | | | | | |

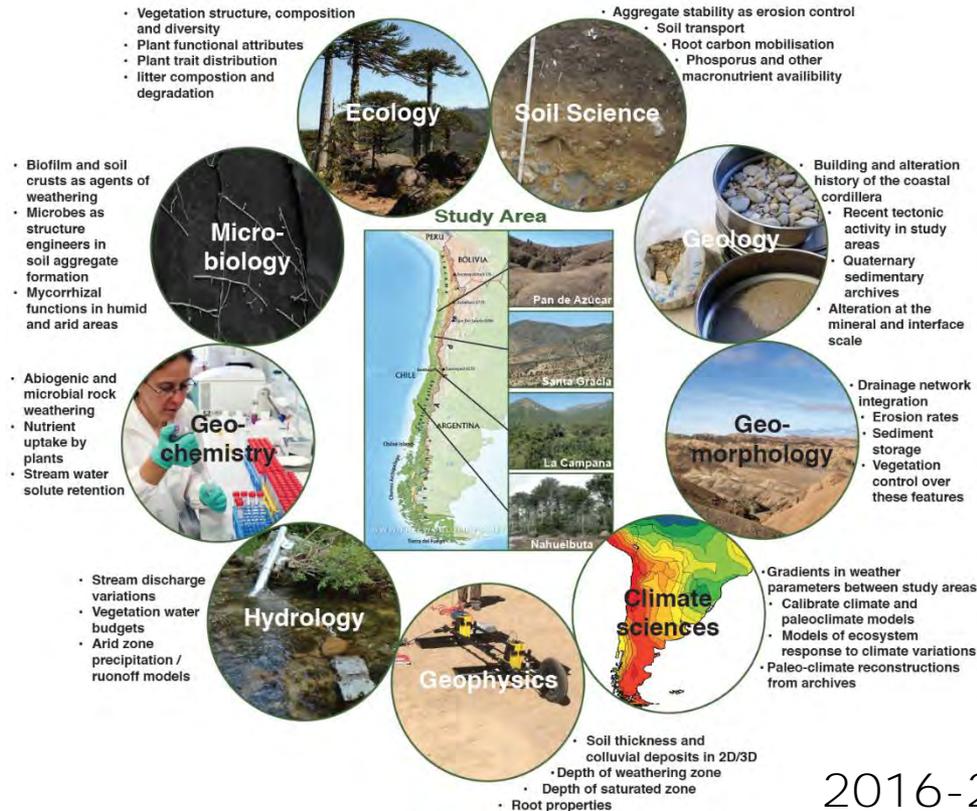
| | | | | | | |
|-----------------------------------|---------------------------------------|----------------------------|--------------------------------------|-----------------------------|------------------------|------------------------|
| Sample Name Con_B 03-Mar-15 | Parent ▼ | IGSN | Collection method automatic sam ▼ | Material water:river ▼ | Location Conventl ▼ | Campaign Freiburg ▼ |
| Depth (m from groundlevel) 0.0 | Date 2015-03-03 | Quantity (initial) 15.0 | Quantity unit ml | Quantity (current) 15.0 | Labname CB2 | Box CON_B0 ▼ |
| Container 15ml-tube (pir ▼) | Description | | Name Jakob Sohr | Affiliation Uni Freiburg | | |
| Group Freiburg ▼ | <input type="button" value="Create"/> | | | | | |

| | | | | | | |
|-----------------------------------|---------------------------------------|----------------------------|--------------------------------------|-----------------------------|------------------------|------------------------|
| Sample Name Con_B 04-Mar-15 | Parent ▼ | IGSN | Collection method automatic sam ▼ | Material water:river ▼ | Location Conventl ▼ | Campaign Freiburg ▼ |
| Depth (m from groundlevel) 0.0 | Date 2015-03-04 | Quantity (initial) 15.0 | Quantity unit ml | Quantity (current) 15.0 | Labname CB3 | Box CON_B0 ▼ |
| Container 15ml-tube (pir ▼) | Description | | Name Jakob Sohr | Affiliation Uni Freiburg | | |
| Group Freiburg ▼ | <input type="button" value="Create"/> | | | | | |

| | | | | | | |
|-----------------------------------|---------------------------------------|----------------------------|--------------------------------------|-----------------------------|------------------------|------------------------|
| Sample Name Con_B 05-Mar-15 | Parent ▼ | IGSN | Collection method automatic sam ▼ | Material water:river ▼ | Location Conventl ▼ | Campaign Freiburg ▼ |
| Depth (m from groundlevel) 0.0 | Date 2015-03-05 | Quantity (initial) 15.0 | Quantity unit ml | Quantity (current) 15.0 | Labname CB4 | Box CON_B0 ▼ |
| Container 15ml-tube (pir ▼) | Description | | Name Jakob Sohr | Affiliation Uni Freiburg | | |
| Group Freiburg ▼ | <input type="button" value="Create"/> | | | | | |

Earthshape, ein interdisziplinäres Projekt

Interdisciplinary Approach & Research Themes



Graphik: <https://esdynamics.geo.uni-tuebingen.de/earthshape/fileadmin/content/images/Disciplines.png>

Erfahrungsbericht – Herausforderungen/Probleme vor und nach der Einführung

- Welche Metadaten werden erhoben?
 - Flexibilität vs. Durchsuchbarkeit
 - Datenmanagement – Datenbank vs. Anhänge

- Wer setzt die neuen Ideen um?
 - externe Firma
 - projektangestellter Informatiker
 - interessierte Kollegen

Erfahrungsbericht – Herausforderungen/Probleme vor und nach der Einführung

- Wie sorgt man dafür, dass die Leute das Programm nutzen?
 - Einführung mit Projektstart
 - klare Richtlinien
- Wie pflegt man das Programm am Besten, damit es übersichtlich bleibt und die Daten korrekt sind?
 - Dropdown Listen
 - Administratoren
 - Kollisionsabfragen
 - Klare Zuständigkeiten
 - Kurse
 - Qualitätskontrolle bei Hiwis
 - vom Gerät in die Datenbank



Fragen?

Mehr Informationen:

Jutta.schlegel@gfz-potsdam.de

Interesse?

<https://github.com/ulbricht/medusa>

<https://dream.misasa.okayama-u.ac.jp/documentation/>

- **Campaign Name:** Give your field campaign a name. We recommend a name/abbreviation related to the sampling location.
- **Project:** Give information about which project the samples were taken for.
- **Time series:** "Yes", if you will return to this location and take further samples, else "No".
- **Sampling strategy:** Give a brief summary how the sampling is planned (e.g. "3 sediment traps installed for 5 days on river bed") Detailed information can be uploaded later via file.
- **Weather conditions:** Mention the weather if this can influence your samples.
- **Comment:** Other important information, which is missing in the campaign category.
- **Information:** After creation of an entry, detailed information about the sampling strategy can be uploaded.
- **Group:** Select a group to define read and write rights.

- **Is Parent / Parent:** “Is parent” can be selected by administrators to create a new parent location. Group Sample Locations (e.g. AZPED10, AZPED20, ...) to a bigger area (e.g. “Parque Nacional Pan de Azúcar”).
- **Site Name:** Give your sampling location a nice, meaningful name.
- **Latitude:** Use format dd. yyyy N/S or +/- dd. yyyy. The system is WGS84. Parent locations build an interval from their daughter locations.
- **Longitude:** Use format dd. xxxx E/W or +/- dd. xxxx. The system is WGS84. Parent locations build an interval from their daughter locations.
- **Elevation:** Note in m above sea level. Parent locations build an interval from their daughter locations.
- **Vegetation:** Inform about the major vegetation.
- **Topographic position:** Describe the position from your sample on the relief (e.g. toe slope, plateau)
- **Landuse:** According to Engelen and Wen (1995) inform about the major landuse.
- **Light situation:** Describe the intensity of solar radiation at your site (e.g. “exposed to open sun; canopy coverage”).
- **Hillslope:** Write down in degrees.
- **Aspect:** Inform about which direction your slope is in.
- **Description:** Other important information, which is missing.
- **Group:** Select a group to define read and write rights.

- **Name:** Give a distinct name for the Building, Room or Box.
- **Parent:** Describes where your Building, Room or Box is. The first parent is very likely an institute (Figure 1).
- **Box type:** Describes the type of the current location.
- **Group:** Select a group to define read and write rights.

- **Sample name** is a clear name to identify your sample fast. It can be the name you gave in the field.
- **Parent:** In case of a subsample you can link it to an existing sample.
- **IGSN:** Will be generated automatically according to the information in your user account.
- **Collection method:** This describes the elementary method/tool how the sample was taken.
- **Classification:** Gives information about the material (e.g. plant) and the type (e.g. twig) of your sample.
- **Sampling Location:** Link here the sampling site. Use the site of the parents for subsamples.
- **Sampling Campaign:** Link here your field campaign. Use the campaign of the parents for subsamples.
- **Depth:** above or below ground level.
- **Date:** Gives information which exact date your sample was taken or made if it is a subsample.
- **Quantity unit:** In most cases it's in g, kg, ml or l.
- **Quantity initial:** Says how much of the sample was taken.
- **Quantity current:** Says how much sample is left. Don't forget to update this, especially if you emptied the sample.
- **Labname:** Short name you use in the lab for analyses. (e.g. "Con43" instead of "CON-DC2-skel-2-3 (20-63mm)")
- **Storage Room/Box:** Link here in which box or lab this sample is stored at the moment.
- Kind of **Container** in which your sample is stored. This information helps to find your sample later easier.
- **Description:** Other important information, which is missing.
- **Group:** Select a group to define read and write rights.
- **Collector:** Gives information about who takes the sample. Multiple entries can be made.
- **Affiliation:** This is the institute of the collector at the time when he takes the sample.

International Geo Sample Number

- Weltweit einzigartige, alphanumerische Kennzeichnung für Proben
- GFZ Potsdam stellt **den Namespace "GF"** als Registrationservice zur Verfügung
- GF*XXXyyyy*
 - *X* ist ein semi-personeller Namespace
 - *y* ist ein inkrementeller, alphanumerischer Code
- semi-personelle Namespace müssen bei Kirsten Elger (GFZ) registriert werden
- <http://dataservices.gfz-potsdam.de/igsn/esg/index.php?igsn=GFRO10018>

General Identifiers

| | |
|---------------|-------------------------------------|
| Project: | 12, 13 |
| Campaign: | NAPED soil baseline data assessment |
| Type: | Specimen |
| Name: | NAPED20-02-LMM |
| IGSN: | GFRO10018 |
| Parent IGSN: | N/A |
| Release Date: | N/A |

Sampling Location

| | |
|-----------------------|-------------------|
| Latitude: | -37.8077 |
| Longitude: | -73.0135 |
| Coordinate System: | WGS84 |
| Elevation: | 1239.0 |
| Location Type: | nature protection |
| Location Name: | NAPED20 |
| Location Description: | soil pit |
| Country: | Chile |
| Province: | Araucania |
| County: | N/A |
| City: | N/A |

Acquisition

| | |
|----------------------|-------------------------------|
| Material: | Soil |
| Soil Classification: | soil |
| Collection Method: | |
| Funding Agency: | |
| Comments: | N/A |
| Chief Scientist: | Ralf Oeser, Lisa-Marie Moskwa |
| Start Date: | 2016-04-22 |
| End Date: | 2016-04-22 |

Repositories

| | |
|------------------------------|-------------|
| Current Repository: | GFZ-Potsdam |
| Current Repository Contact: | N/A |
| Original Repository: | N/A |
| Original Repository Contact: | N/A |

Sample Family



 = Specimen

The Sample Family shows a sub-sampling graph. Select entries to navigate samples.

Location Map



Drilling Start/End: 2016-04-22 / 2016-04-22 *
Latitude: -37.80770 * Longitude: -73.01350 *
NAPED20

Publications & Datasets

General Identifiers

| | |
|---------------|------------------------|
| Project: | SPP 1685 |
| Campaign: | PhD Project DavUhl |
| Type: | Specimen |
| Name: | CON-DC1-4.7-5.2 (<2mm) |
| IGSN: | GFDUH00JL |
| Parent IGSN: | GFDUH00FB |
| Release Date: | N/A |

Sampling Location

| | |
|-----------------------|-------------------|
| Latitude: | 48.020653 |
| Longitude: | 7.966067 |
| Coordinate System: | WGS84 |
| Elevation: | 770.0 |
| Location Type: | forestry |
| Location Name: | Conventforest 1 |
| Location Description: | trench |
| Country: | Germany |
| Province: | Baden-Württemberg |
| County: | N/A |
| City: | N/A |

Acquisition

| | |
|----------------------|--|
| Material: | Soil |
| Soil Classification: | soil:saprolite |
| Soil Description: | sieved aliquot <2mm, sampling period: 13.11.2013-19.11.2013 |
| Collection Method: | auger |
| Funding Agency: | |
| Comments: | N/A |
| Chief Scientist: | David Uhlig |
| Start Date: | 2013-11-19 |
| End Date: | 2013-11-19 |

Repositories

| | |
|------------------------------|-------------|
| Current Repository: | GFZ Potsdam |
| Current Repository Contact: | N/A |
| Original Repository: | N/A |
| Original Repository Contact: | N/A |

Sample Family

- CON-DC-1
 - CON-DC1-3.0-3.7
 - CON-DC1-3.7-4.0
 - CON-DC1-4.0-4.7
 - CON-DC1-4.7-5.2
 - CON-DC1-4.7-5.2 (<2mm)
 - CON-DC1-4.7-5.2 (<2mm)

= Specimen

The Sample Family shows a sub-sampling graph. Select entries to navigate samples.

Location Map



Drilling Start/End: 2013-11-19 / 2013-11-19 *
Latitude: 48.02065 * Longitude: 7.96607 *
Conventforest 1

Publications & Datasets

Heiko Rosenfelder, DKFZ: iLabber – organisatorische und technische Einführung

Abstract

„Gute wissenschaftliche Praxis“ sind Stichworte welche immer wieder dafür sorgen, dass Organisation, Abläufe, Dokumentationen immer wieder auf den Prüfstand gestellt werden. Technischer und organisatorischer Fortschritt sorgen immer wieder für Änderungen bei den Abläufen in der täglichen Arbeit im Labor oder bei den Verfahren der Dokumentation. Unter anderem stießen einige Wissenschaftler und technische Mitarbeiter immer wieder an Grenzen, wenn es darum ging elektronische Dokumentationen oder Ergebnisse im klassischen Laborbuch zu notieren. Diese Medienbrüche aber auch die immer größer werdende Menge an Daten lieferten die Motivation ein elektronisches Laborbuch am DKFZ einzuführen.

Im Vortrag geht es um die Umsetzung und Integration in das technische Umfeld der IT, sowie um organisatorische Abläufe und Strukturen für den laufenden Betrieb in den Abteilungen und Gruppe in den Laboren, sowie die entsprechenden Erfahrungen.

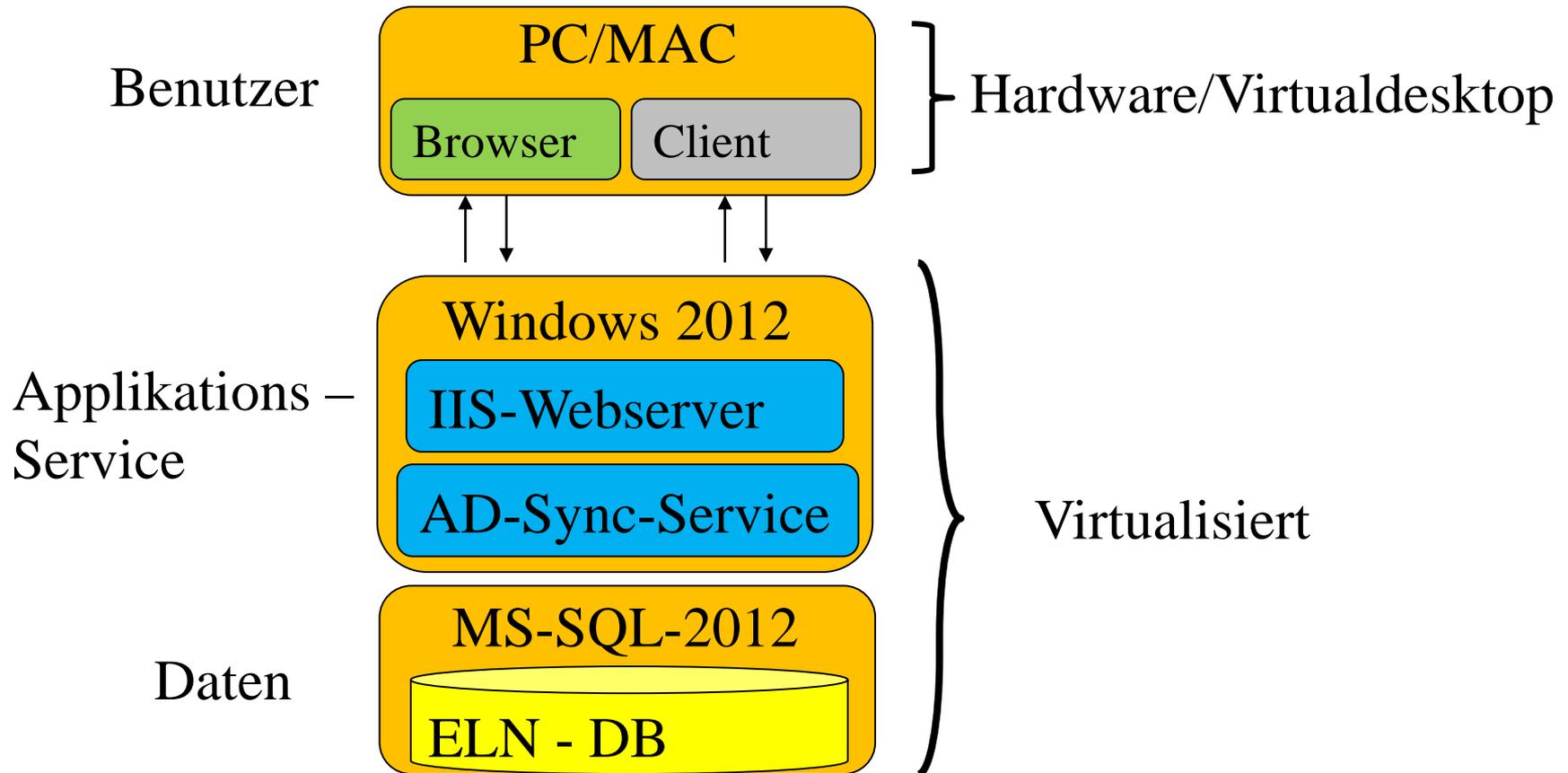


Elektronisches Laborbuch

Lebenszyklus – Organisation – Möglichkeiten - Erfahrungen

Heiko Rosenfelder

Technik – Architektur ELN



Wie komme ich zum ELN

Antrag



ITCF

Teilnahme am Elektronischen Laborbuch „iLabber“

HINWEIS: Bei einem Wechsel der Abteilung für das elektronische Laborbuch iLabber ersetzt dieses Formular NICHT das Formular zum Wechsel der Kostenstelle im DKFZ

Angaben zur Person (bitte vollständig ausfüllen):

Herr Name Vorname
Frau Last Name: First Name:

Abteilung:

1. Neuantrag
2. Wechsel in eine andere Gruppe, Gruppenname
3. Wechsel in eine andere Abteilung
4. unter Beibehaltung der alten Aufgaben und Rechte
5. neue veränderte Aufgaben und Rechte
6. neue Gruppe (Anträge für die Mitglieder müssen einzeln erfolgen)

Bemerkungen
(hauptsächlich zu Punkten 2–5):

Neue Gruppe: Alte Gruppe
Gruppenadministrator: ehem. Gruppenadmin*:

Neue Abteilung:
(* nur wenn die Punkte 2 oder 3 bzw. 4 oder 5 betroffen sind.)

Datum: _____
Unterschrift Antragsteller

Unterschrift Gruppenadministrator

Unterschrift Abteilungsleiters



Organisation of eIn iLabber

Department/Abteilung/Kostenstelle

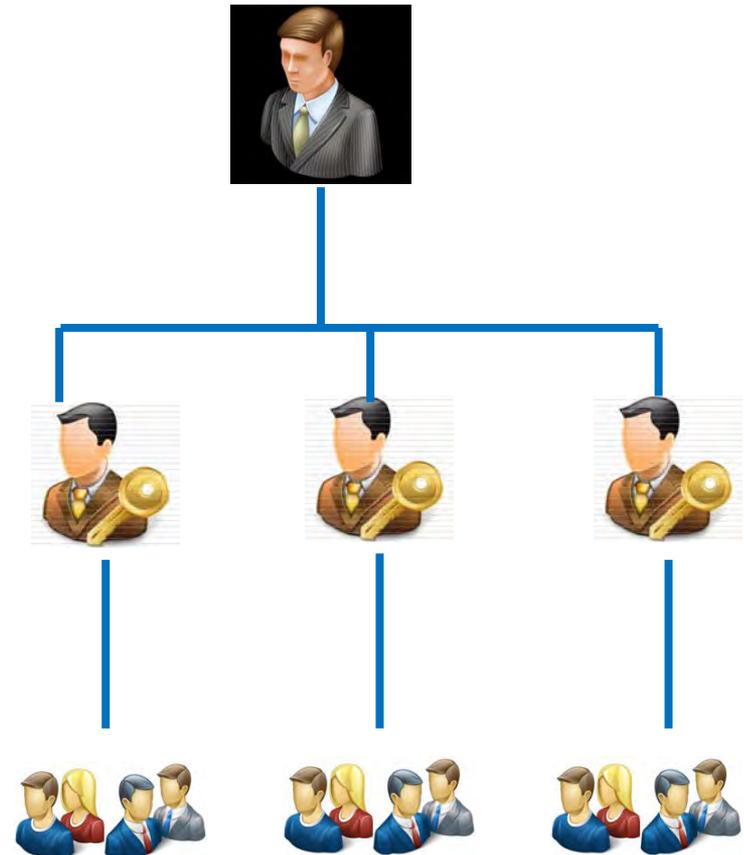
- A190

Groups/Workinggroups

- A190-groupname

User

- A... , B... C...





Roles at eIn



User

- working with documents/experiments
- print, enable/disable permission
- Member of group(s)



Groupadmin / Keyuser

- Manage the group
- Permissions to the users
- Creates Projects
- Templates



Superuser only at ITCF

- Defines (new) groups
- add new user
- Administrates common templates
- Responsible for the technical resources



Projects and groups and user



User

- Member of a group(s)
- Access to project(s)



Groups

- Organisation
- Administration



Projects

- Scope of interest, work
- Collaboration / teamwork
- Topic of research

Projekte

ElnAdminWeb

https://dkfz-eln02.dkfz-heidelberg.de/ElnAdminWeb/manageproject.aspx?id=31

Users Groups Projects Privileges Audit logs License info

Manage project Logout

Here is where you can manage the projects details, groups and users.

Project name: MusterP

Description: only for Rollout

Members_users Members_groups

Filter

Clear

BENDERN
DASK
GARDYAN
HAZIN
OSEN
WEBERCL

Add ->

<- Remove

DICKES
EICHMUE
GA_EICHM
KORONA
LUO

Permissions that user/group will get on experiments in the project:

- Browse unsubmitted
- Browse submitted
- Read unsubmitted
- Read submitted
- Counter sign
- Add

Permissions that user/group will get on the project:

- Administrate

Update permission

Experimente, Gruppen, Projekte, Dateien

- Feste Nummer, unveränderbar
- Gehören dem Ersteller, festes Datum
- Sichtbarkeit (Listen und Lesen) und Möglichkeiten zum Bearbeiten **wird im Projekt** geregelt
- Experimente können lesend oder auch bearbeitend geteilt werden („geshared“)
 - Im Gesamten
 - Nur Teile davon
- Templates können aus Experimenten erstellt werden, meist im Gruppen/Projektrahmen
- Excel, Word werden wenn importiert in ELN bearbeitet, die **Datei auf der Platte wird nicht aktualisiert**

BioVia ELN

The screenshot displays the BioVia ELN interface. The top navigation bar includes the BioVia logo, 'Notebook Experiment', and 'New for Demonstration EXP-18-AB8507'. The main content area is divided into a left sidebar, a central workspace, and a right sidebar.

Left Sidebar: Contains a 'Sections' menu with options like 'Body Text', 'Text Field', 'Image', 'Excel Workbook', 'Word Document', 'PDF Document', 'File Attachment', 'Chemical Sketch', 'Chemical Reaction', 'Date', 'Errata Section', 'Project', 'Experiment Type' (circled in red), and 'Related Experiments'. Below this is a 'My Sections' and 'Deleted Sections' section.

Central Workspace: Shows a table of experiment details and a list of experiment types.

| Experiment no. | EXP-18-AB8507 |
|----------------|-----------------------------|
| Author | Rosenfelder Heiko (MUSTER1) |
| Date Started | 12 Sep 2018 08:19 (UTC + 2) |
| Title | New for Demonstration |
| Project | MusterP [only for Rollout] |

| Name | Description |
|---------------------|--|
| Espression Analysis | incl. qPCR, RT-PCR, WB, NorthernB |
| ADMET | Absorption, Distribution, Metabolism, Elimination, Tox |
| Animal Experiment | Mouse, etc. |
| Assay | Apoptose, ..., Etablierung |
| Cell Culture | Validierung, Screening, Routine, transfection, |
| Chemistry | Chemistry, Synthesis |
| Expression Analysis | qPCR, RT-PCR, WB, Northern |
| FACS | FACS |

Right Sidebar: Contains a 'Body Text at first default' section with a text input field, a 'Text Field' section with a text input field, and an 'Image - TIFF' section with a file upload area.

Bottom Status Bar: Shows 'Last Changed Today 08:31 by Me', 'All Changes Saved', and 'Connected to Notebook'.



Excel

The screenshot displays a web-based notebook interface. The main window is titled "New for Demonstration EXP-18-AB8507". The left sidebar shows a "Sections" menu with various options like "Body Text", "Text Field", "Image", "Excel Workbook", etc. The main content area shows a section titled "Beliebiger Text" containing an "Excel Workbook" section. The Excel workbook is titled "Document.xlsx" and contains the following text:

| |
|--|
| www.dkfz.de |
| \\ad\fs\W310-Daten |
| Irgend was als eintrag ... |

At the bottom of the interface, there are status bars indicating "Last Changed Today 08:29 by Me", "All Changes Saved", and "Connected to Notebook".

Word

The screenshot displays a web-based laboratory notebook interface. The main window shows a document titled "New for Demonstration" with a table of metadata and a list of sections. The "Word Document" section is expanded, showing a document named "TOPO cloning.doc". The document content includes a title "TOPO cloning (Doumpas protocol)" and a list of steps for the cloning process. A context menu is visible over the document, and a status bar at the bottom indicates the document was last changed today at 08:39 by the user.

| Experiment no. | EXP-18-AB8507 |
|-----------------|-----------------------------|
| Author | Rosenfelder Heiko (MUSTER1) |
| Date Started | 12 Sep 2018 08:19 (UTC + 2) |
| Title | New for Demonstration |
| Project | MusterP [only for Rollout] |
| Experiment Type | Assay |

TOPO cloning (Doumpas protocol)

- PCR using cDNA and Phusion Hot Start.
- Gel extraction of the PCR product (end volume 30µl)
- Add in the PCR product:
 - 4µl 10x ThermoPol buffer
 - 1µl 10mM dNTPs
 - 1µl Taq
- 72°C for 5min
- Topo reaction:
 - 4µl of the PCR product
 - 1µl salt (from the kit)
 - 0.5µl TOPO vector
 - Incubate at **Room Temperature for 10min**Put TOP10 cells on ice for 10min
- Add 2µl of TOPO reaction to the cells
- 10min on ice
- Heat shock at 42 °C for 30sec
- Add LB medium 500µl
- Incubate at 37 °C for 30min
- Prepare LB amp plates (add 40µl X-Gal)
- Spin cells for 2min at 3000rpm

Last Changed Today 08:39 by Me | All Changes Saved | Connected to Notebook



Bilder/Grafiken

Browser address bar: <http://dkfz-eln01/notebook/experiment/EXP-13-AA1634>

Page title: **Notebook** Experiment **Virtual Experiments for Presentation** EXP-13-AA1634 (You: Author)

Table:

| Object Id | E_Cmax | EC50 | Hill | Y_min | Y_max | Data Quality | Comments |
|----------------|--------|----------|------|-------|--------|--------------|---------------------------------|
| 088248_3060001 | 100.69 | 2.47E-06 | 0.55 | 10.13 | 133.98 | 3.66E-07 | Warning Please, write a comment |
| 5HT B | 112.35 | 1.42E-09 | 0.96 | 17.32 | 112.21 | | Normal |
| 5HT B | 124.14 | 5.23E-10 | 0.93 | 7.84 | 121.63 | | Warning Please, write a comment |

Image: IOANNA_TEST-PCR1_021208.png

Word Document: Document.doc

Submission, counter sign

https://labnotebook.dkfz.de/notebook/experiment/EXP-18-AB8507

Notebook Home EXP-18-AB8507 - New for D... x

Notebook Experiment **New for Demonstration** EXP-18-AB8507 **Go to Submission**

Sections

- Body Text +
- Text Field +
- Image +
- Excel Workbook +
- Word Document +
- PDF Document +
- File Attachment +
- Chemical Sketch +
- Chemical Reaction +
- Date +
- Errata Section +
- Project +
- Experiment Type +
- Related Experiments +

My Sections

Deleted Sections

| | |
|-----------------|-----------------------------|
| Experiment no. | EXP-18-AB8507 |
| Author | Rosenfelder Heiko (MUSTER1) |
| Date Started | 12 Sep 2018 08:19 (UTC + 2) |
| Title | New for Demonstration |
| Project | MusterP [only for Rollout] |
| Experiment Type | Assay |

Word Document

TOPO cloning.doc Edit Download Delete

TOPO cloning (Doumpas protocol)

- PCR using cDNA and Phusion Hot Start.
- Gel extraction of the PCR product (end volume 30µl)
- Add in the PCR product:
 - 4µl 10x ThermoPol buffer
 - 1µl 10mM dNTPs
 - 1µl Taq
- **72°C for 5min**
- Topo reaction:
 - 4µl of the PCR product
 - 1µl salt (from the kit)
 - 0,5µl TOPO vector
 - Incubate at **Room Temperature for 10min**
- Add 2µl of TOPO reaction to the cells
- **10min on ice**
- Heat shock at **42°C for 30sec**
- Add LB medium 500µl
- Incubate at **37°C for 30min**
- Prepare LB amp plates (add 40µl X-Gal)
- Spin cells for **2min at 3000rpm**

} Put TOP10 cells on ice for **10min**

Last Changed Today 08:39 by Me All Changes Saved Connected to Notebook

Submission, counter sign

The screenshot displays the DKFZ Notebook submission interface for a 'New for Demonstration' experiment (EXP-18-AB8507). The interface is divided into several sections:

- Header:** Shows the experiment title 'New for Demonstration EXP-18-AB8507' and navigation options like 'Go to Submission'.
- Sections List:** A sidebar on the left lists various content types that can be added to the notebook, such as 'Body Text', 'Text Field', 'Image', 'Excel Workbook', 'Word Document', 'PDF Document', 'File Attachment', 'Chemical Sketch', 'Chemical Reaction', 'Date', 'Errata Section', 'Project', 'Experiment Type', and 'Related Experiments'. A red circle highlights a lock icon next to the 'Text Field' option.
- Main Content Area:** Displays the notebook content, including a 'Text Field' with the text 'einfacher Text' and an 'Image - TIFF' section containing a photograph of a PCR plate. The image shows a gel electrophoresis result with multiple lanes.
- Metadata:** A table at the bottom left provides details about the submission, including the author (DKFZ-HEIDELBERG), experiment number, date started, and project name.

At the bottom of the interface, there are status indicators: 'Last Changed Today 08:40 by Me', 'All Changes Saved', and 'Connected to Notebook'.

Diverse Erfahrungswerte

- Es bedarf eines ständig präsenten Support seitens IT
 - Word geht nicht rein (Plug-In, meist aber zu groß)
 - Dateianhang klappt nicht (immer zu groß)
 - Fragen nach Regelungen in Projekten
- Empfehlung: öfter und kürzere Sektionen submitten
- Wird auch oft zur allgemeinen Dokumentation genommen
- Archivformat, Ausdruck, Export ist PDF
- Es wird so gut wie nie das Archivieren verlangt, fast immer wird „geshared“
- Gruppen informieren sich auch über BioVia – Community (Webseite, Demo)

Zusammenfassung

- Erfolgsgeschichte
- Fokussierung auf „Laborbuch“
- „Science Management System“ ist übergeordnet (LIMS ect.)
- Hervorragender Support des Herstellers BIOVIA
- Einfache Bedienung und sehr gute Suchfunktion
- Arbeitsweise muss angepasst werden
- Einfachheit, Datenkapselung und Schulungen waren ein Schlüssel in der Akzeptanz
- In Sachen Archivierung wäre mehr Komfort wünschenswert
- Skeptiker gibt es trotzdem

Würden wir es wieder tun? JA!

Vielen Dank für die Aufmerksamkeit !

Noch Fragen ?



dkfz.

dkfz.

DEUTSCHES
KREBSFORSCHUNGSZENTRUM
IN DER HELMHOLTZ-GEMEINSCHAFT



Forschen für ein Leben ohne Krebs

Tim Henckel, HZB: Elektronisches Laborbuch am Kompetenzzentrum Dünnschicht- und Nanotechnologie für Photovoltaik Berlin (PVcomB) – Flexibilität vs. Performanz

Abstract

Das Helmholtz-Zentrum Berlin für Materialien und Energie erforscht komplexe Materialsysteme an verschiedenen Standorten, dazu gehört auch das Kompetenzzentrum Dünnschicht- und Nanotechnologie für Photovoltaik Berlin (PVcomB). Am PVcomB werden verschiedene Solarzellentechnologien entwickelt. Ein besonderer Fokus liegt dabei auf zwei Dünnschicht-Technologien zur Herstellung von Solarzellen, die sogenannte CIGS-Technologie und die Silizium-Photovoltaik.

Während der Herstellung und der anschließenden Analytik von Solarzellen fallen etliche Daten an, wie zum Beispiel Anlagenparameter oder Kennlinien. Zur Dokumentation und Archivierung der Prozessierung und der Messdaten nutzt das PVcomB zum einen ein vom HZB entwickeltes elektronisches Laborbuch, zum anderen ein vom PVcomB selbst entwickeltes Datawarehouse-System.

Das elektronische Laborbuch ist auf Flexibilität ausgelegt und ermöglicht eine schnelle und einfache Anpassung der zu speichernden Meta- und Messdaten. Durch diese Flexibilität und der dafür benötigten Datenbankstruktur ist es nur mit viel Aufwand möglich, Daten über einen langen Zeitraum abzufragen. Deshalb betreibt das PVcomB ein Datawarehouse, welches auf Performance ausgelegt ist, um viele Daten über einen großen Zeitraum performant abzufragen.

Da die Daten zwischen den beiden Systemen konsistent gehalten werden müssen, ist eine weitere Schicht („ETL“ - Extract, Transform, Load) vonnöten. Diese ETL-Schicht kopiert tagesaktuelle Daten aus dem elektronischen Laborbuch in das Datawarehouse.

Des Weiteren werde ich einen Einblick in das Nutzerverhalten geben und auf die Vor- und Nachteile, sowie eventuelle Probleme bei der Nutzung eines elektronischen Laborbuchs am PVcomB eingehen.