

Göttingen eResearch Toolbox Series - Electronic Note Keeping

Nicole Jung

INSTITUTE OF ORGANIC CHEMISTRY - Stefan Bräse Group Karlsruhe



Chemotion

funded by

DFG

Access to research data: Key challenges

Digital Data



Almost no digital data

- Only written lab journals
- Not searchable
- Analytics >> syntheses
- Processing

Databases



Commercial databases

- Limited access
- Limited availability of data

Open Access databases

Only few data

Journals



Limited content

- No primary data
- Almost no additional info
- Accessibility

Academia-specific challenges:

Strategic issues:

- Sustainable, interdisciplinary research
- project management vs community network
- Collecting data as a basic instrument for research
- Acceptance in the community

Access to research data: Key challenges

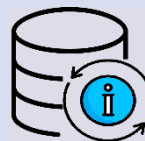
Digital Data



Almost no digital data

- Only written lab journals
- Not searchable
- Analytics >> synthesis
- Processing

Databases



Commercial databases

- Limited access
- Limited availability of data

Open Access databases

Only few data

Journals



Limited content

- No primary data
- Almost no additional info
- Accessibility

Academia-specific challenges:

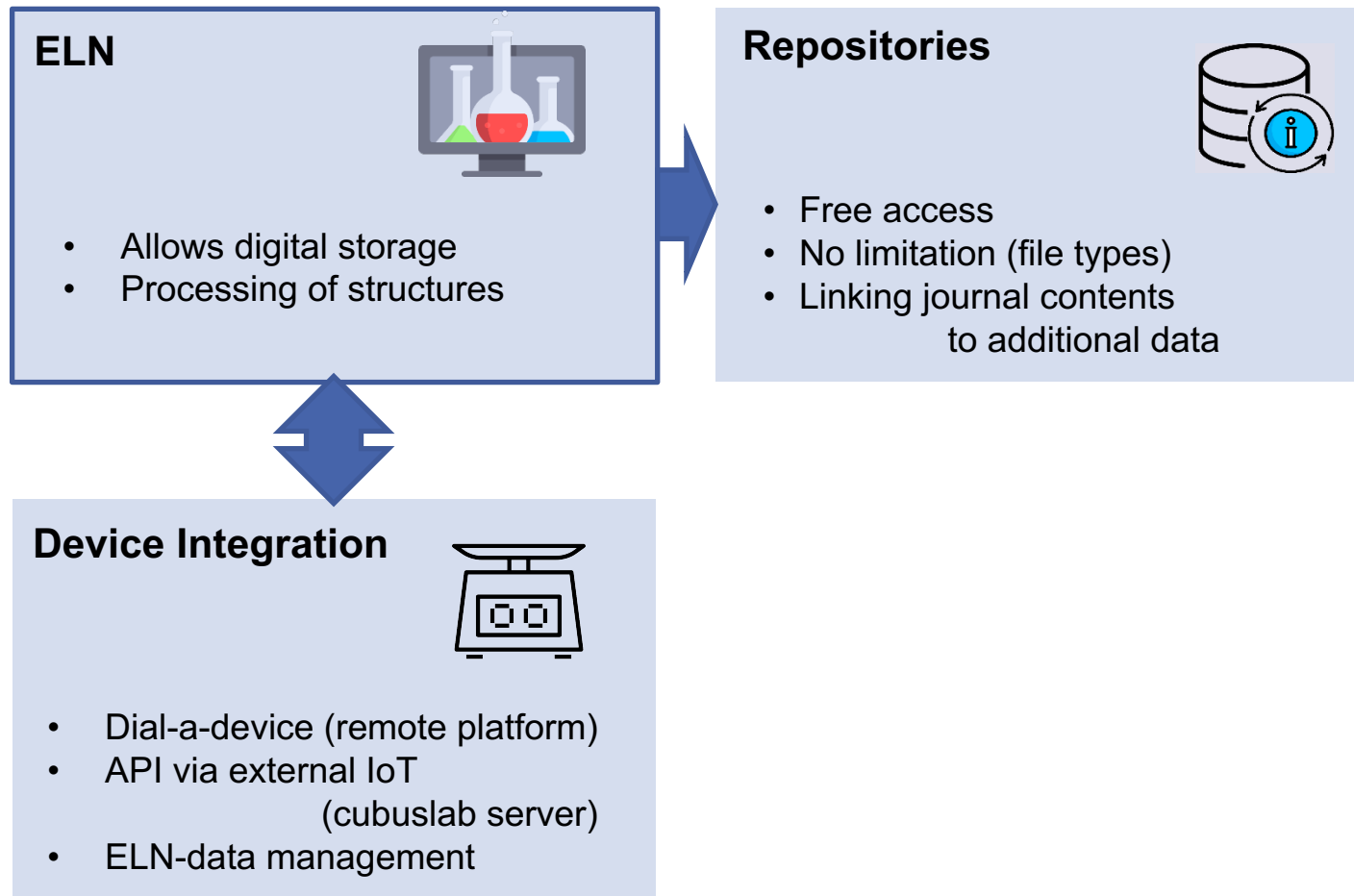
Strategic issues:

- Sustainable, interdisciplinary research
- project management vs community network
- Collecting data as a basic instrument for research
- Acceptance in the community

Technical issues:

- Infrastructure and processes differ
- Equipment and devices in general very old
- High flexibility necessary

Access to research data: Key challenges



Key instrument: ELN implementation I

Electronic Lab Notebook (ELN)

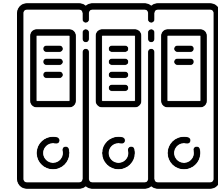


Generic Functions

Adaptable to other fields of research
Management and systematic structure

Management and Organization

- Management for projects and subprojects (flexible structure)
- Organization according to lists and detail tabs
- User defined settings, BarCodes and QR-Codes
- Items are linked, ancestries are summarized and visualized



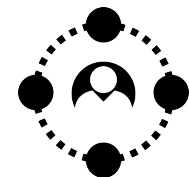
Reporting

- Reports for single elements and projects
- User defined detail level
- Settings for formatting



Share & Synchronize

- Share a selected group of information
- Synchronize to allow access to projects, support of collaboration
- User defined detail level
- Definition of groups for sharing and synchronization



Key instrument: ELN implementation II

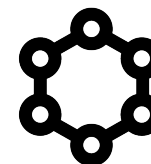
Electronic Lab Notebook (ELN)



Chemistry Specific Functions
 Application in molecule based research
 Processing of chemical data

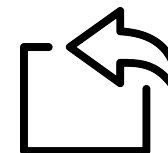
Structure Editor (Ketcher)

- Standard functions + support of polymers/surfaces
- User defined templates and general accepted templates
- Information function for structures and substructures
- Implementation of abbreviations



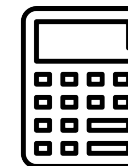
Export and Import functions

- Import and export of Excel and sdf
- User defined export scheme (detail level)



Calculations

- Calculations for elemental analysis (e.g. polymer supported material)
- Calculations of yield, control for „impossible values“



Search functions

- Text search and structure (substructure/similarity) search



Key instrument: ELN implementation II

Electronic Lab Notebook (ELN)



Chemistry Specific Functions
 Application in molecule based research
 Processing of chemical data

Additional Information: Database integration

- OpenBabel
- PubChem, SciFinder
- NMRbd
- Direct visualization in lists



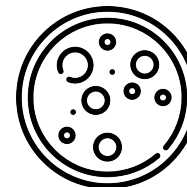
Datasets and File attachment

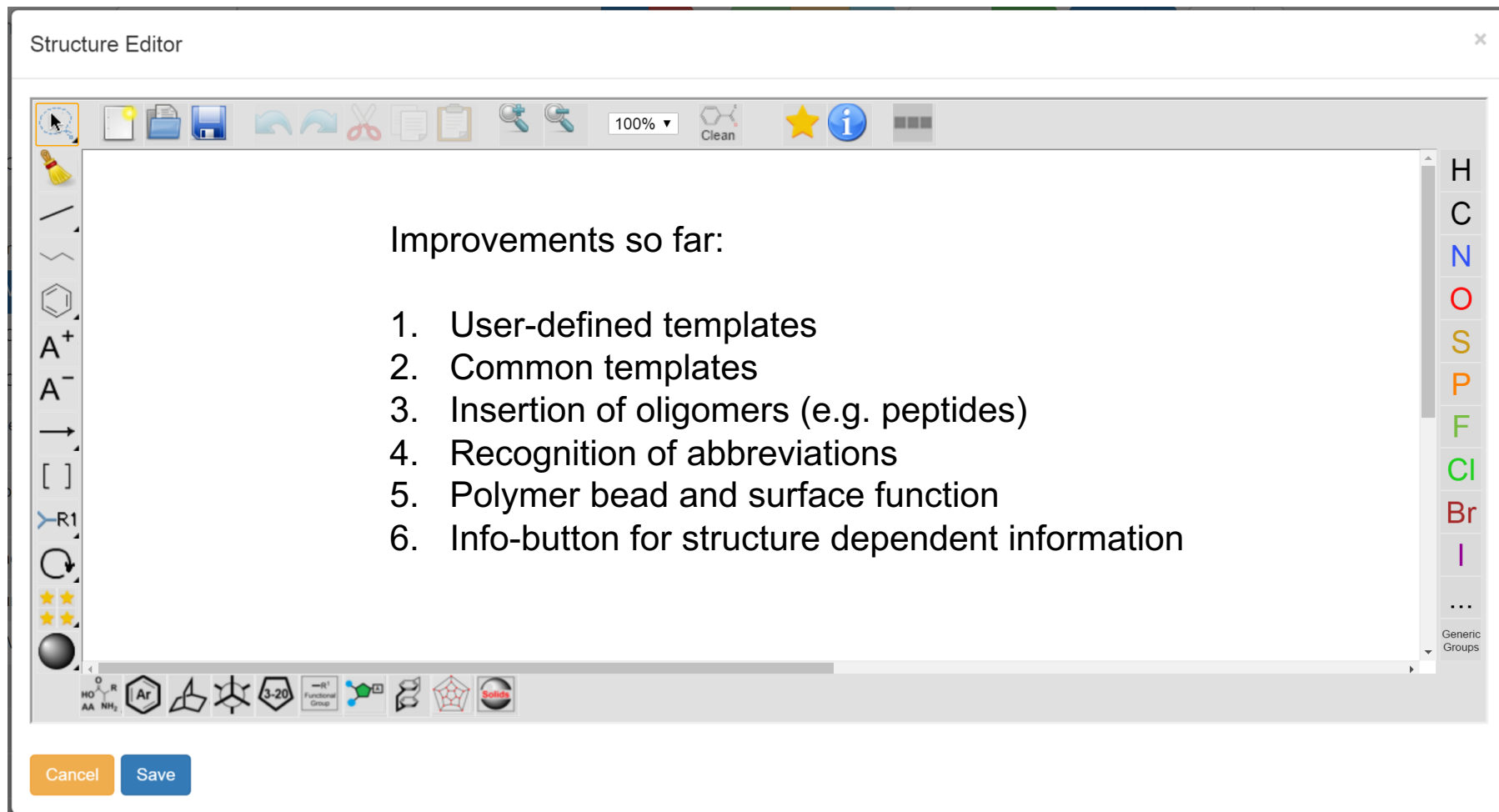
- Description of metadata (dropdown and freetext)
- Labeling (approved, not approved)
- All file formats, no limitation



Functions for biology and chemical biology

- Wellplate function for sample management
- Organizer for biological assays and their description
- Correlation of molecules, wellplates and assays





Structure Editor

Improvements so far:

1. User-defined templates
2. Common templates
3. Insertion of oligomers (e.g. peptides)
4. Recognition of abbreviations
5. Polymer bead and surface function
6. Info-button for structure dependent information

Cancel Save

Template categories

- Image selection
- Define and approve or reject

Templates

- Image selection
- Import SDF or Molfile

Abbreviations


















- Name definition
- Define attachment point
- Use of molfile for database requests

Monomer generation for oligomers

- Definition of name and abbreviation
- Definition of two attachment points
- Use of molfile for database requests
- Reverse order of monomers

Listing template categories

New Template category

Image	Name	Show	Edit	Destroy
	Amino Acids	Show	Edit	Destroy
	Aromatics	Show	Edit	Destroy
	Bicyclics	Show	Edit	Destroy
	Common bases	Show	Edit	Destroy
	Conformers	Show	Edit	Destroy
	Cycloalkanes	Show	Edit	Destroy
	Diverse heterocycles	Show	Edit	Destroy
	Functional group	Show	Edit	Destroy
	Hexoses	Show	Edit	Destroy
	Metallocenes	Show	Edit	Destroy
	Nucleic Acids	Show	Edit	Destroy
	Paracyclophanes	Show	Edit	Destroy
	Polyhedra	Show	Edit	Destroy
	Polypeptides	Show	Edit	Destroy
	Rings View	Show	Edit	Destroy
	Schlegel	Show	Edit	Destroy
	Solid Supports	Show	Edit	Destroy

Reporting function in brief:

- Project reports
- Supporting information for publications
- Exchange of information

Report Generation

Config Sample Setting Reaction Setting Order Report Archive [Generate Report](#)

File Name

ELN_Report_2017-3-28H14M36S34

File description

Selected all

Page Break

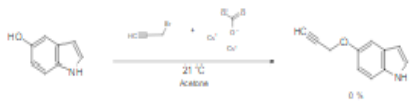

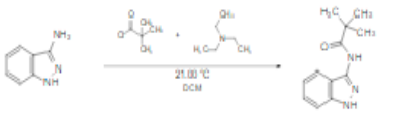

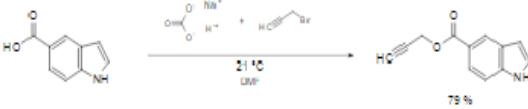

Show all material in diagrams (unchecked to show Products only)

Images format

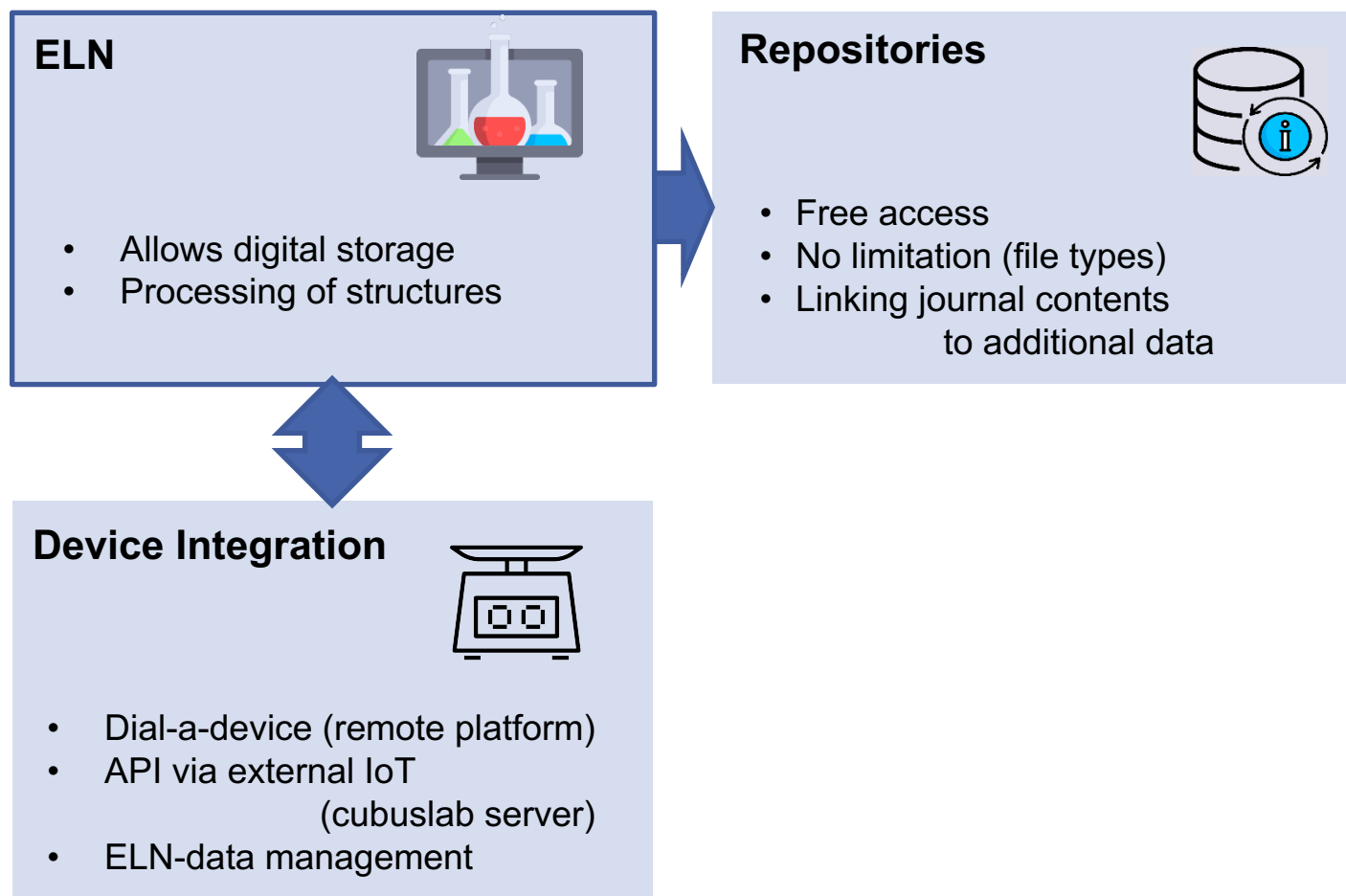
PNG

Report Generation

Config Sample Setting Reaction Setting Order Report Archive [Generate Report](#)

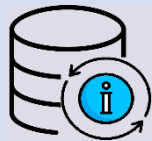
NJ-R150 5-Hydroxy indazole modification		
NJ-R149 Indazole- amidation		
NJ-R152 Indazole carboxylate modification		

Access to research data: Key challenges



Disclosure of information: Repository

Repository

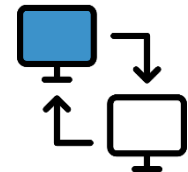


Basic Functions

Technology identical with ELN
 Generic and field specific functions identical

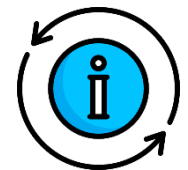
Input and Transfer of Data

- Selection of data within ELN, determination of detail level
- Transfer of data via shared folder repository-ELN
- Visibility of data after additional confirmation
- Data for molecules and reactions



Characteristics

- Search functions based on FP2-fingerprints
- Metadata defined by ELN definitions
- DOI-generation, PubChem listing, Datacite indexing



Visibility and Advertisement

- Infrastructure for repositories
- Competitions with incentives (by KIT-Stiftung)



Disclosure of information: Repository

Electronic Lab
Notebook (ELN)



Repository



External



Selection

Datasets to publish

Private Repository

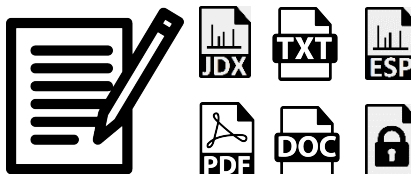
Virtual DOI from metadata
(molecule-dataset)

Open Repository

DOI – dataset/molecule url
(TIB Hannover)

DOI-resolver

Molecule - Datasets



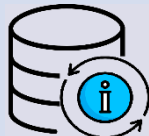
Mint and register
DOI

PubChem

Structure + DOI

Disclosure of information: Repository

Repository



Private Repository

Virtual DOI from metadata
(molecule-dataset)

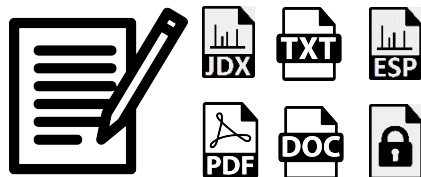
Open Repository

DOI – dataset/molecule url
(TIB Hannover)

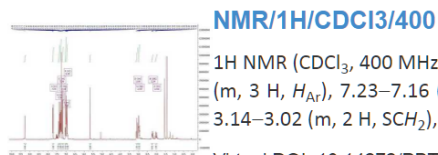
DOI-resolver



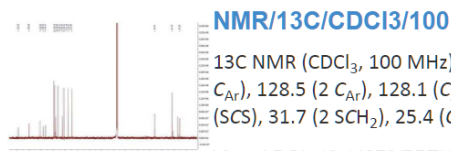
Molecule - Datasets



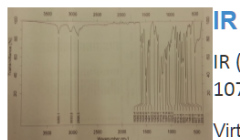
 5 Datasets



Virtual DOI: 10.14272/PBTUVUQCTONFGS-YYDJUVGSSA-N/NMR/1H/CDCI3/400

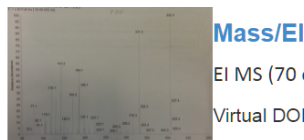


Virtual DOI: 10.14272/PBTUVUQCTONFGS-YYDJUVGSSA-N/NMR/13C/CDCI3/100



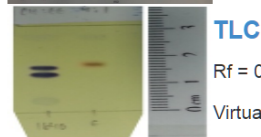
IR (ATR) ν = 3283, 3034, 2897, 1608, 1585, 1556, 1505, 1485, 1442, 1420, 1327, 1264, 1219, 1162, 1098, 1073, 1022, 900, 870, 837, 806, 782, 749, 690, 657, 588, 506 cm⁻¹.

Virtual DOI: 10.14272/PBTUVUQCTONFGS-YYDJUVGSSA-N/IR



EI MS (70 eV, 200 °C) m/z (%) = 406 [M⁺] (100), 331 (86), 184.1 (53), 141 (58), 129 (31), 119 (37), 77 (22).

Virtual DOI: 10.14272/PBTUVUQCTONFGS-YYDJUVGSSA-N/Mass/EI

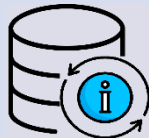


R_f = 0.48 (cyclohexane : ethyl acetate, 4:1)

Virtual DOI: 10.14272/PBTUVUQCTONFGS-YYDJUVGSSA-N/TLC

Disclosure of information: Repository

Repository



Private Repository

Virtual DOI from metadata
(molecule-dataset)

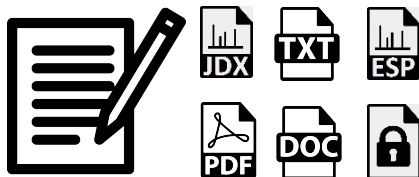
Open Repository

DOI – dataset/molecule url
(TIB Hannover)

DOI-resolver



Molecule - Datasets

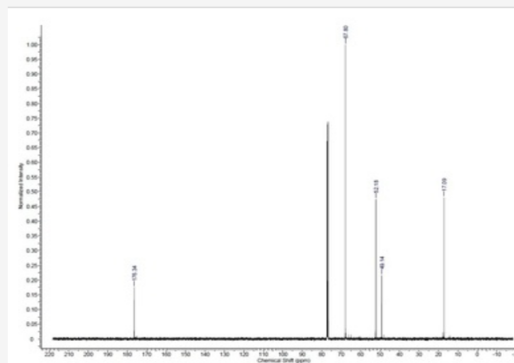


 NMR/13C/CDCl3/125

 Download as ZIP





Description: 13C NMR (125 MHz, CHLOROFORM-d, ppm) δ = 17.1, 49.1, 52.2, 67.8, 176.3.

Preview [Jdx Viewer](#)



View attached files

To edit this dataset, please fork it first.

	1433_Carbon.jpg	72.58 KB
	SSU-1433.010.001.1R.esp	529.82 KB
	SSU-1433.010.001.1R.spc	263.03 KB
	SSU-1433.010.001.1R.jdx	264.14 KB

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

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

Organic LETTERS

Search: Enter search text / DOI Anywhere Search
Org. Lett. All Publications/Website

Home Browse the Journal Articles ASAP Current Issue Submission & Review Open Access About the Journal

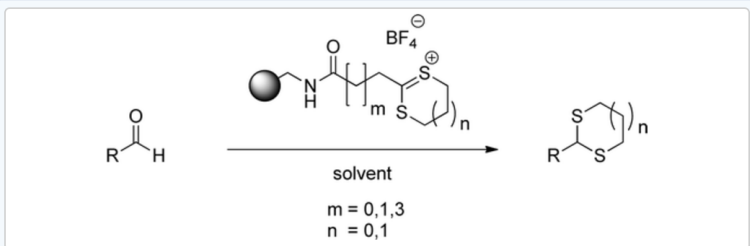
Letter < Previous Article Next Article > Table of Contents

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
Copyright © 2014 American Chemical Society
*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

Article Options

- ACS ActiveView PDF (Hi-Res Print, Annotate, Reference QuickView)
- PDF (567 KB)
- PDF w/ Links (280 KB)
- Full Text HTML

Abstract

- Supporting Info
- Figures
- References
- Citing Articles

★ Add to Favorites

- Download Citation
- Email a Colleague
- Order Reprints
- Rights & Permissions
- Citation Alerts

Add to ACS ChemWorx

SCIFINDER A CAS SOLUTION Sign in

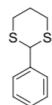
Retrieve Detailed Record of this Article

Retrieve Substances Indexed for this Article



2. Individual compounds and analysis

2-Phenyl-1,3-dithiane (2a), CAS: 5425-44-5; Smiles: C1(SCCCS1)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} .

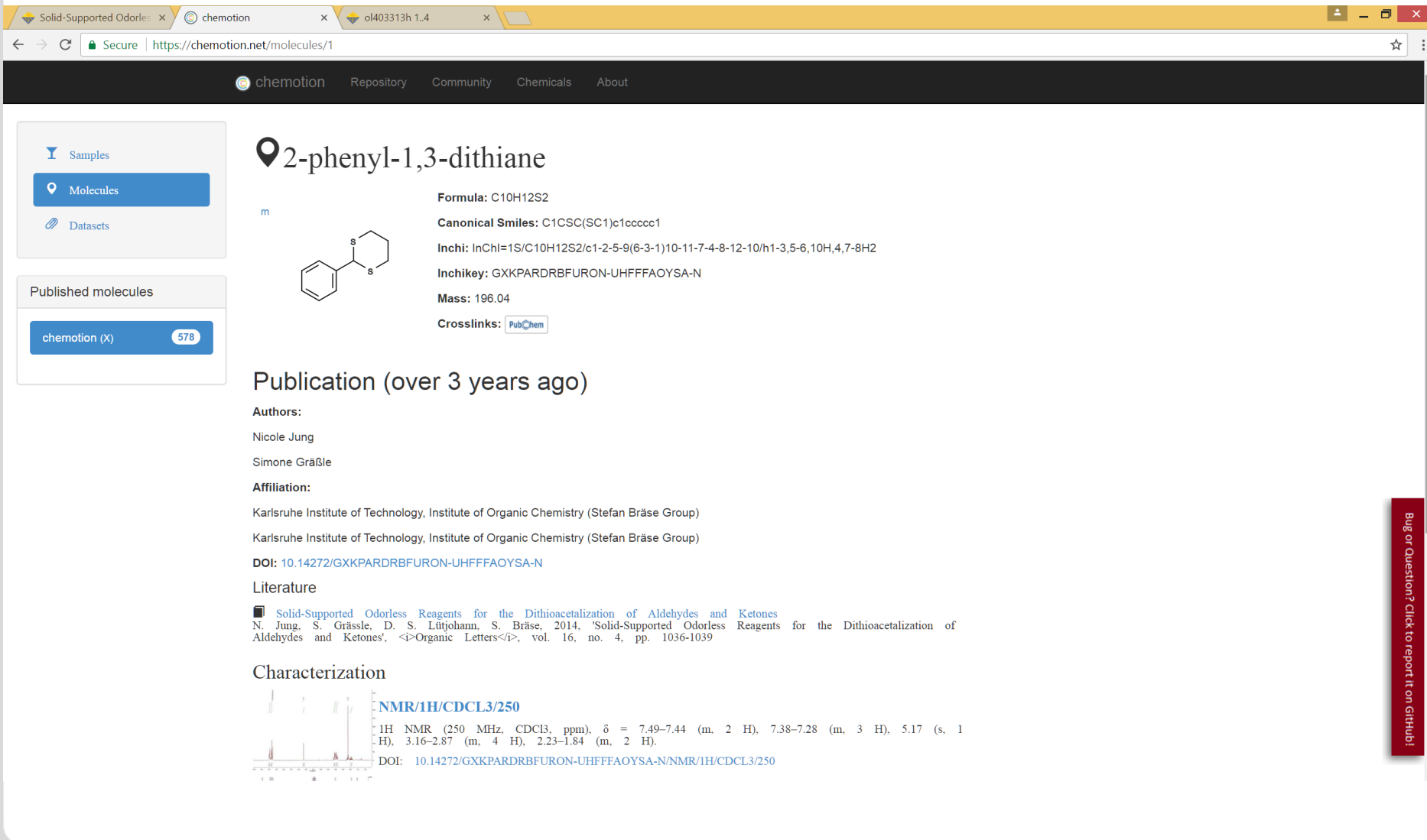
For the conversion in a larger scale, the reaction was repeated with 1.30 mmol of benzaldehyde, giving 221.6 mg (1.128 mmol) of the target 2-phenyl-1,3-dithiane **2a** in 87% yield.

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



The screenshot shows a web browser window with the URL <https://chemotion.net/molecules/1>. The page title is "2-phenyl-1,3-dithiane". The left sidebar contains navigation options: "Samples", "Molecules" (selected), and "Datasets". Below this is a "Published molecules" section with a filter for "chemotion (X)" showing 578 items. The main content area displays the chemical structure of 2-phenyl-1,3-dithiane, its formula (C₁₀H₁₂S₂), canonical SMILES (C1CSC(SC1)c1ccccc1), InChI, InChIkey, mass (196.04), and a crosslink to PubChem. A "Publication (over 3 years ago)" section lists authors (Nicole Jung, Simone Gräßle) and affiliation (Karlsruhe Institute of Technology, Institute of Organic Chemistry (Stefan Bräse Group)). The DOI is 10.14272/GXKPARDRBFURON-UHFFFAOYSA-N. The literature section cites a paper by N. Jung, S. Gräßle, D. S. Lütjohann, and S. Bräse (2014) in Organic Letters. The characterization section includes an NMR spectrum and the text: "1H NMR (250 MHz, CDCl₃, 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). DOI: 10.14272/GXKPARDRBFURON-UHFFFAOYSA-N/NMR/1H/CDCL3/250".

2-phenyl-1,3-dithiane

Formula: C₁₀H₁₂S₂
Canonical Smiles: C1CSC(SC1)c1ccccc1
Inchi: InChI=1S/C10H12S2/c1-2-5-9(6-3-1)10-11-7-4-8-12-10/h1-3,5-6,10H,4,7-8H2
Inchikey: GXKPARDRBFURON-UHFFFAOYSA-N
Mass: 196.04
Crosslinks: [PubChem](#)

Publication (over 3 years ago)

Authors:
Nicole Jung
Simone Gräßle

Affiliation:
Karlsruhe Institute of Technology, Institute of Organic Chemistry (Stefan Bräse Group)
Karlsruhe Institute of Technology, Institute of Organic Chemistry (Stefan Bräse Group)

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

Literature
Solid-Supported Odorless Reagents for the Dithioacetalization of Aldehydes and Ketones
N. Jung, S. Gräßle, D. S. Lütjohann, S. Bräse, 2014, 'Solid-Supported Odorless Reagents for the Dithioacetalization of Aldehydes and Ketones', *Organic Letters*, vol. 16, no. 4, pp. 1036-1039

Characterization
NMR/1H/CDCL3/250
1H NMR (250 MHz, CDCl₃, 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).
DOI: [10.14272/GXKPARDRBFURON-UHFFFAOYSA-N/NMR/1H/CDCL3/250](https://doi.org/10.14272/GXKPARDRBFURON-UHFFFAOYSA-N/NMR/1H/CDCL3/250)

Device Integration

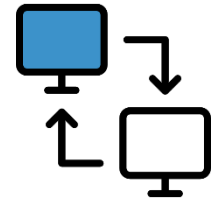


Basic Concepts

Diverse solutions and continuous extension
of basic structure: done

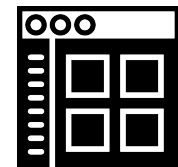
Dial a device (property: group)

- Server infrastructure managing remote access to devices implemented: e.g. HPLC, GC-MS, Raman spectrometer (10)
- Single infrastructure connecting devices Campus North and South
- Virtual machines



ELN device management (property: university)

- User interface for the submission of analysis requests
- NMR implemented (Bruker)



Device Integration

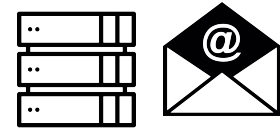


Basic Concepts

Diverse solutions and continuous extension
of basic structure: ongoing

ELN data management

- Server requests (e.g. HPLC, GC)
- Mail-Support (NMR data)
- Primary data storage and archiving



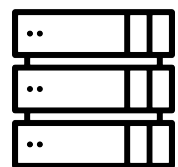
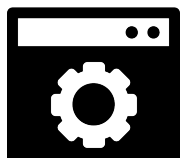
API to external IoT

- Support of cubuslab server
- primary application: balance integration

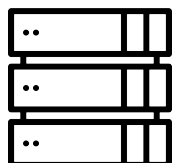


Device Integration: Part II, Data and Information

Virtual
Machine



LSDF



cubuslab



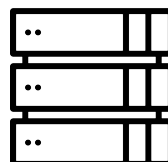
ELN



Repository



Primary Data (Archive)



Challenges and questions

Electronic Lab Notebook (ELN)



Integration of additional information systems

- OpenPhacts (server)
- Reaxys
- chemical safety data/PubChem

API to alternative archives

- bwDataDiss
- Radar

Repository



Establishment of automatic proof of analyses

Acceptance of datasets for registration processes

Device integration



ELN-interface for mass, IR, EA requests, Analysis manager

Additional instruments (Cubuslab)

Advanced



Deep learning support

- Data analyses
- Reaction prediction

Chemotion Secure <https://complat-eln.ioc.kit.edu/#/collection/7/reaction/1099> Logged in as nicole jung

Chemotion All IUPAC, InChI, SMILES, ... Search

○ 285(0) ▲ 91(0) ● 4(0) ■ 7(0) □ 1(0)

Sample

Oc1ccccc1 C₆H₆O
phenol

NJ-374 1-0

Nc1c[nH]c2ccccc12 C₇H₇N₃
1H-indazol-3-amine

NJ-349 5-Carboxylicacid indole 0-1

Cc1c(C)nc2c1c(=O)nc2 C₁₂H₁₅N₃O
N-(1H-indazol-3-yl)-2,2-dimethylpropanamide

NJ-359 NJ-R149-A 0-1

O=C(O)c1ccc2c(c1)c[nH]2 C₉H₇NO₂
1H-indole-5-carboxylic acid

NJ-366 5-Carboxylicacid indole

Cc1ccc2c(c1)c[nH]2 C₃₈H₅₉NO₅

NJ-362-2 1-0

NJ-362 1-0

Oc1ccc2ccccc12 C₁₀H₈O
naphthalen-2-ol

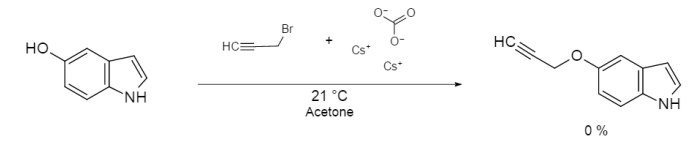
NJ-360-2 1-0


Schemes Show 15

◀ 1 2 3 4 5 ... ▶

NJ-R150 5-Hydroxy indazole modification

NJ-R150 5-Hydroxy indazole modification



Scheme Properties References Analyses 


	Ref	T/R	Amount	Conc	Equiv
Starting materials					
NJ-350	⊗	T	985.1 mg	0.985 ml	7.398 mmol
1H-indol-5-ol				n.d.	mmol 1.000
Reactants					
3-bromoprop-1-yne	⊙	T	968.1 mg	0.650 ml	8.138 mmol
dicesium carbonate	⊙	T	2652 mg	2.65 ml	8.138 mmol
Products					
NJ-352 NJ-R150-A	R		0.000 mg	0.00 ml	0.000 mmol
5-prop-2-ynoxy-1H-indole				n.d.	mmol 0%

Solvents

Name: 5-Hydroxy indazole modification Status: Select... Temperature: 21 °C

Description

B I U x_2 x^2 Normal Δ Å



Chemotion x

Secure | <https://complat-eln.ioc.kit.edu/#/collection/7/wellplate/43>

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

Logged in as nicole jung

Well Details

NJ-R146-A NJ-313-1

Designer

1 6 7 8 9 10 11 12 A B C D E F G H

Readout

Imported Readout

Close Save Export samples

Barcode: 0454857474

Chemotion Collections

chemotion.net

- My Lab journal 1
- Chemical Database 1
- Chemical Database 2
- Parvesh_Anne Compounds 1
- Export Claude Ostermann April 2017
- meine neue Datenbank
- cheung compounds
- My shared projects
- Shared with me
- Synchronized with me

285(0) 91(0) 4(0) 7(0) 1(0)

Sample

phenol Oc1ccccc1 C6H6O

NJ-374

1H-indazol-3-amine Nc1c[nH]c2ccccc12 C7H7N3

NJ-349 5-Carboxylic acid indole

N-(1H-indazol-3-yl)-2,2-dimethylpropanamide CC(C)(C)C(=O)Nc1c[nH]c2ccccc12 C12H15N3O

NJ-359 NJ-R149-A

1H-Indole-5-carboxylic acid O=C(O)c1c[nH]c2ccccc12 C9H7NO2

NJ-366 5-Carboxylic acid indole

C38H59NO5

NJ-362-2

NJ-362

naphthalen-2-ol Oc1ccc2ccccc2c1 C10H8O

NJ-360-2

Schemes Show 15

1 2 3 4 5 ...

Sharing with researchers or the repository

My Groups

Add more users

- Serhii Kotov - SK
- Nicole Jung - NJ
- Daniel Knoll - DMK
- Dominic Lütjohann - DL
- Jason Huang - JHX
- An Nguyen - AN
- database user - DU

Name	Kürzel
user group S. Bräse	UG-SB

[Back](#)

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

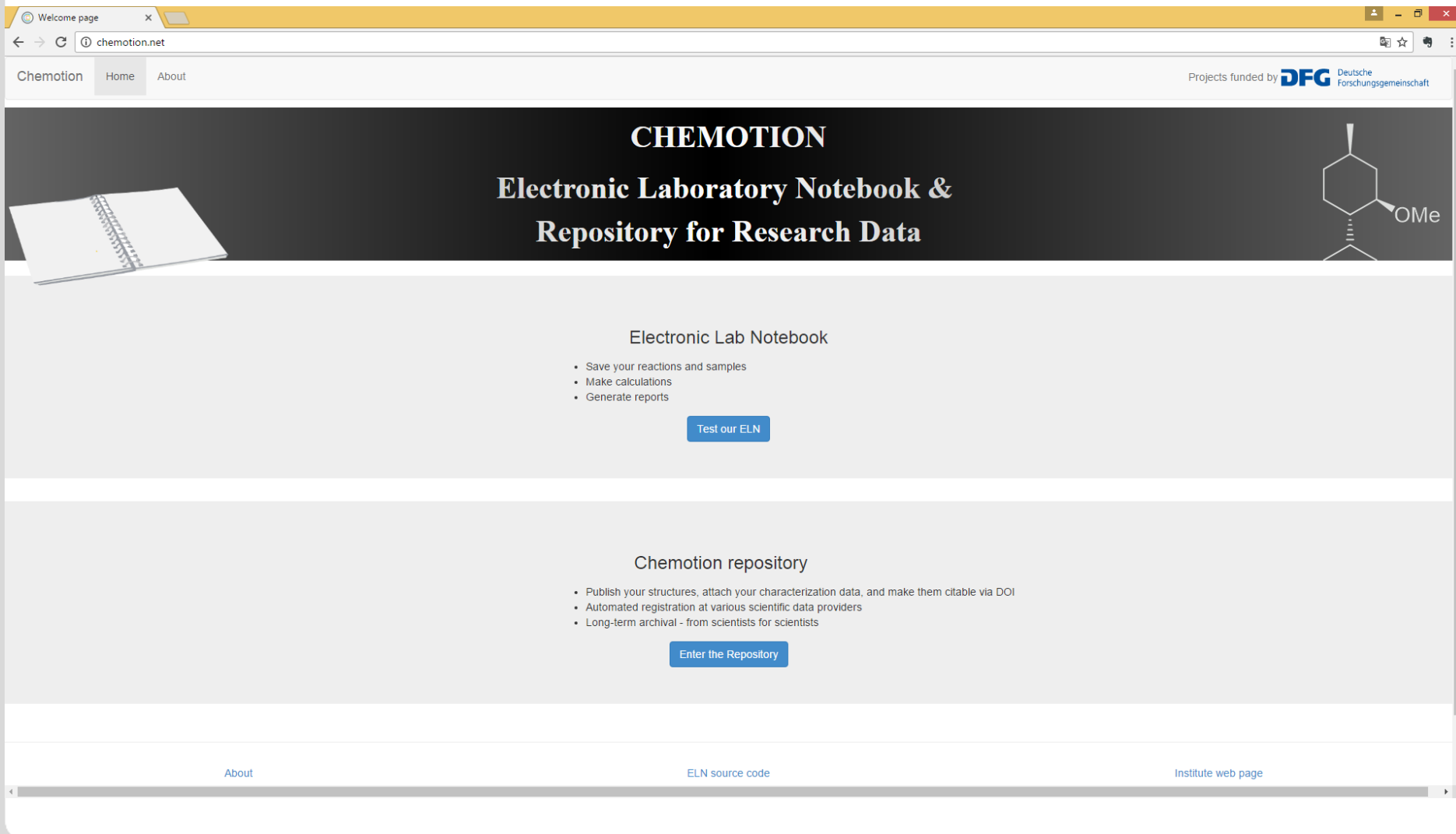
Select Data to Export

Deselect all

- | | | | |
|--|-------------------------------------|---|---|
| <input checked="" type="checkbox"/> image | <input type="checkbox"/> created at | <input type="checkbox"/> is top secret? | <input type="checkbox"/> density |
| <input checked="" type="checkbox"/> name | <input type="checkbox"/> updated at | <input type="checkbox"/> ancestry | <input type="checkbox"/> melting point |
| <input checked="" type="checkbox"/> description | <input type="checkbox"/> molfile | <input type="checkbox"/> external label | <input type="checkbox"/> boiling point |
| <input checked="" type="checkbox"/> canonical smiles | <input type="checkbox"/> purity | <input type="checkbox"/> short label | <input type="checkbox"/> molecular weight |
| <input checked="" type="checkbox"/> sum formula | <input type="checkbox"/> solvent | <input type="checkbox"/> real amount | |
| <input checked="" type="checkbox"/> inchi string | <input type="checkbox"/> impurities | <input type="checkbox"/> imported readout | |
| <input type="checkbox"/> target amount | <input type="checkbox"/> location | <input type="checkbox"/> identifier | |

Cancel

XLSX/SD Export



The screenshot shows a web browser window displaying the Chemotion website. The browser's address bar shows "chemotion.net". The website has a navigation menu with "Chemotion", "Home", and "About". A banner at the top features the text "CHEMOTION Electronic Laboratory Notebook & Repository for Research Data" next to an image of a spiral notebook and a chemical structure of a substituted cyclohexane ring. Below the banner, there are two main sections: "Electronic Lab Notebook" and "Chemotion repository". Each section includes a list of features and a corresponding button.

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](#)

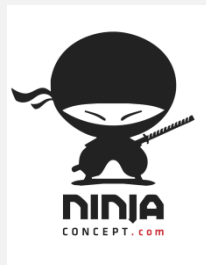
[About](#) [ELN source code](#) [Institute web page](#)

Project Partners and Supporters

Institute of Organic Chemistry

Karlsruhe Library

Steinbuch Center of Computing



Thank you for your attention

Contact: nicole.jung@kit.edu
stefan.braese@kit.edu



DFG

