

Towards a National Research Data Infrastructure for Chemistry in Germany



Christoph Steinbeck*

Friedrich-Schiller-University Jena

Nicole Jung

Karlsruhe Institute of Technology (KIT)

Matthias Razum

FIZ Karlsruhe - Leibniz Institute for Information
Infrastructure

Johannes Liermann

Johannes Gutenberg University Mainz

on behalf of 27 participants of
NFDI4Chem

Oliver Koepler*

TIB Leibniz Information Centre of Science and
Technology

Sonja Herres-Pawlis

RWTH Aachen University

Felix Bach

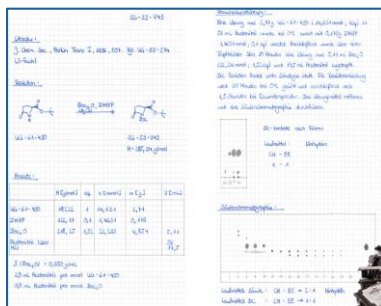
Karlsruhe Institute of Technology (KIT)

Steffen Neumann

Institut für Pflanzenbiochemie, Halle

Status Quo

Analogue / Digital



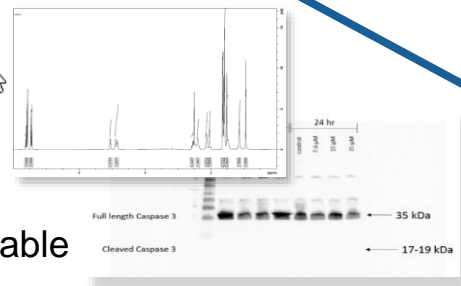
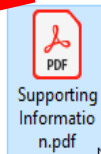
3,3'-Diaminobenzidine Tetrahydrochloride (DAB-4HCl)

Structure: Nc1ccc(N)cc1

Parameter	Value	Unit	Reference
Molecular Weight	198.15	g/mol	[1]
Boiling Point	267	°C	[2]
Melting Point	165	°C	[3]



UnFAIR



Digital



Not machine-readable

Forces and Needs



Leitlinien zur Sicherung
guter wissenschaftlicher Praxis

Kodex

DFG

Practical questions in the organisation of a working group:

? Where are the NMR data from 10 years ago?

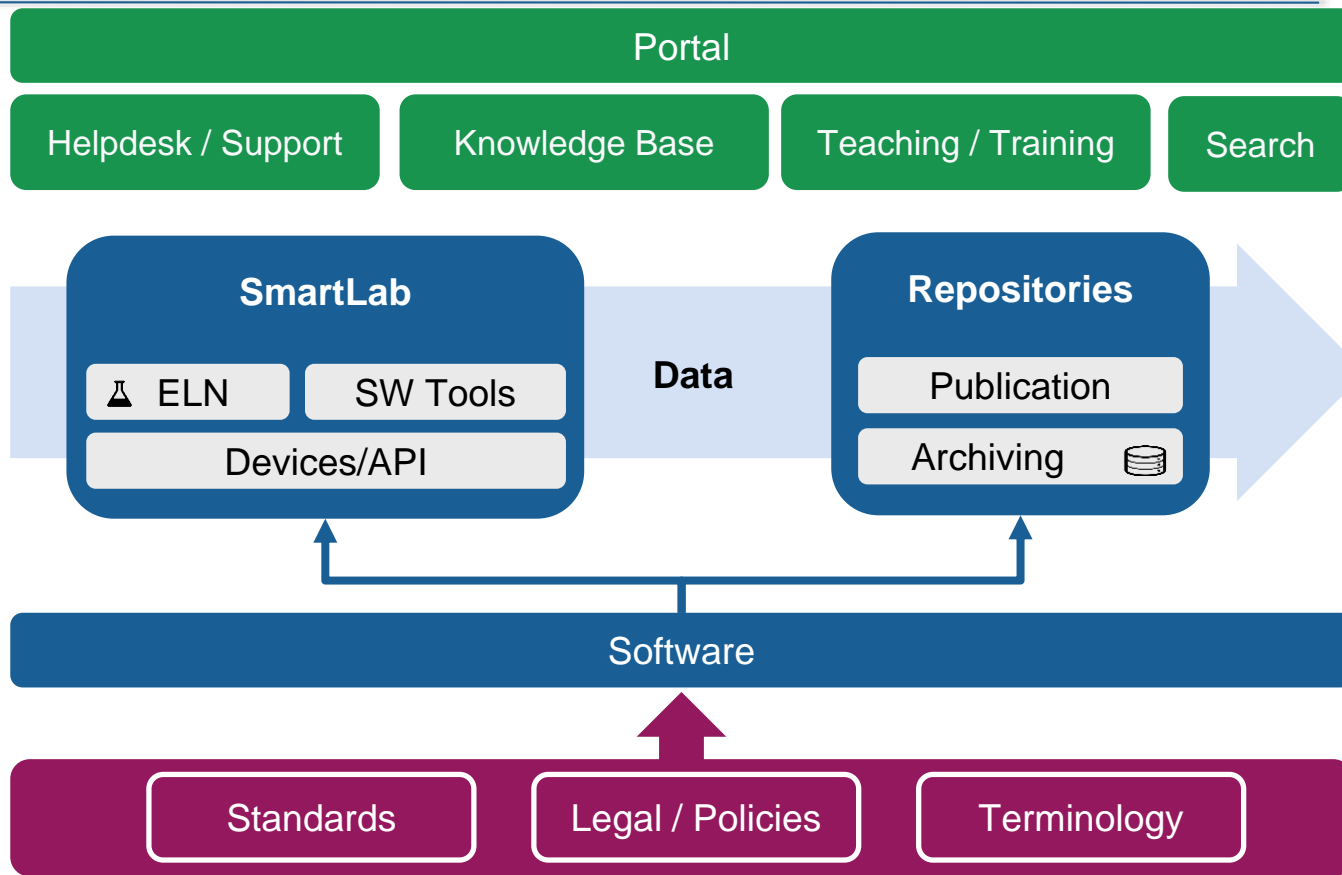
? Where are the synthesis details from 15 years ago?

? Has anyone in the group already made compound xy?

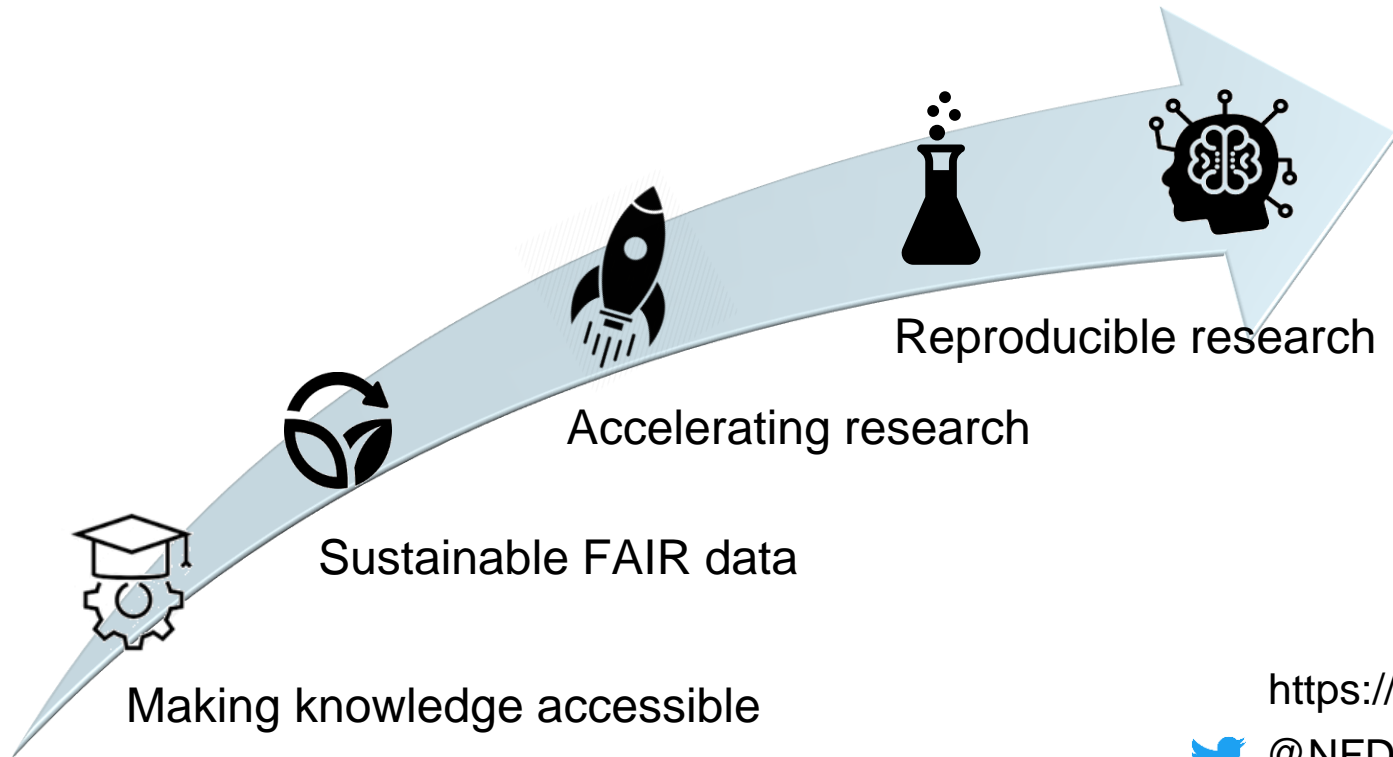
Our Vision



Strategy and Resulting Services



A Quantum Leap in Chemistry RDM



Enabling
machine-learning
on the next level

<https://nfdi4chem.de/>

 @NFDI4Chem