CHEMISTRY DATA STANDARDS SUPPORTED BY THE BEILSTEIN-INSTITUT

Dr. Wendy Patterson

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BEILSTEIN INSTITUT

Royal Society of Chemistry

ChemSpider Webinar 2025

October 21, 2025 / 3 PM BST

Beilstein – Biochemistry Standards – Publishing – ChemInfo Labs – InChI – Chemistry Data Standards Coalition

BEILSTEIN INSTITUT

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QUALITY OPEN SCIENCE

Non-profit foundation
founded in 1951 by the Max Planck Society
based in Frankfurt, Germany

Supports the advancement of the chemical sciences
focus on communication, information and networking
long-term projects
open science

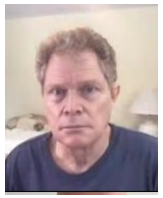
STRENDA

STandards for REporting ENzymology Data

Founded in 2004 under the auspices of the Beilstein-Institut

Contact:
Carsten Kettner

https://tinyurl.com/54xfnsvc

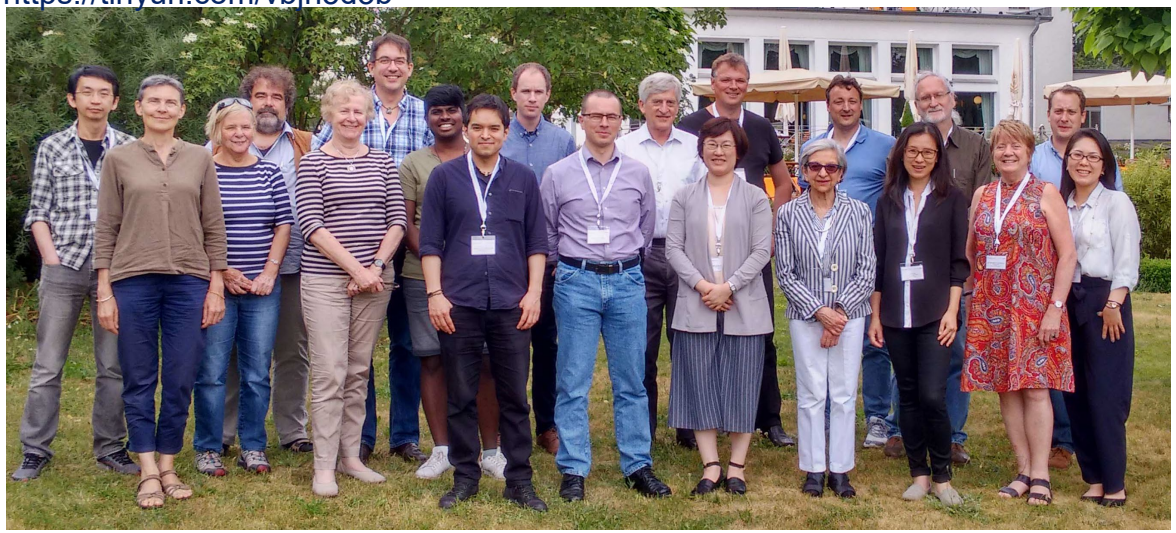


Enzymology	• Reporting Guideline: Description of assay conditions and enzyme kinetics • Recommended by >60 biochemistry journals
Biocatalysis	• Reporting Guideline: Description of the setup of biocatalysis experiments • Software-driven development of a metadata catalogue
Thermodynamics	• Guideline for design and execution of experiments to obtain the apparent equilibrium constants • Reporting Guideline of results
Thermotables	• chemical and metabolic potential of biochemical (sub'd) • Python tool for online "calculation" (retrieval of data from file) soon available on STRENDA website.
STRENDA DB	• Web-based open platform, data evaluation (compliance check) and storage • Recommended by >20 journals, core repo of NFDI4Chem
EnzymeML	• Data exchange format – "from bench to publication" • Software platform for acquisition and transfer of data

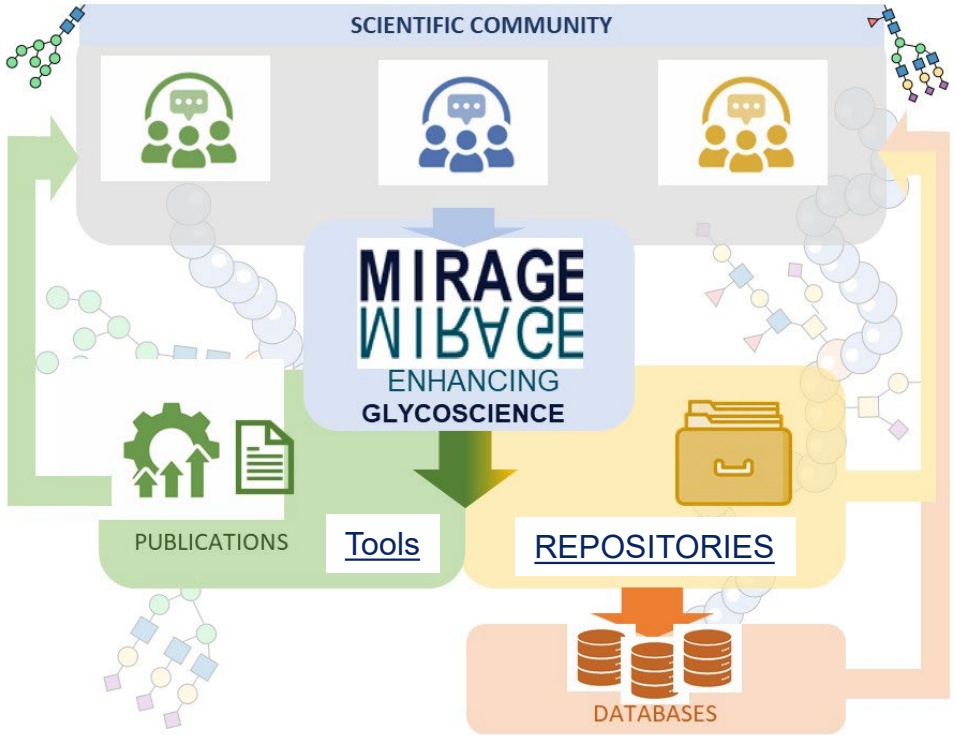
Minimum Information Required for A Glycomics Experiment

Founded 2011 under the auspices of the Beilstein-Institut

https://tinyurl.com/vbjn5d3b



Guideline	Version	Published
Sample Preparation	1.0; 18 Feb., 2016	*Glycobiology*, 2016, 26(9):907-910
Mass Spectrometric Analysis	1.0; 24 Apr., 2013	*Mol. Cell. Proteomics*, 2013, 12:991-995
Glycan Microarray Analysis	1.0; 22 June, 2016	*Glycobiology*, 2017, 27(4):280-284
Liquid Chromatography Analysis	1.0; 1 Mar., 2018	*Glycobiology*, 2019, 29(5):349-354
NMR Glycan Recognition	1.0; 21 Sept., 2020	Manuscript in preparation
NMR Glycan Structures	1.0, 21 Sept., 2020	Manuscript in preparation
Capillary Electrophoresis Analysis	1.0, 9 July, 2021	*Glycobiology*, 2022, 32(7):580-587
Lectin Microarray Analysis	1.0, 10 April, 2023	*Glycobiology*, 2025



Questions about STRENDA or MIRAGE?
Contact: Carsten Kettner

https://tinyurl.com/3z2mh64c

FAIR Data in the Beilstein Journals Publishing Workflow

1. **Extraction** of chemical structures
2. **Conversion** to and **validating** using InChI
3. **Embedding** of InChIs und further information back into the article → machine-readable chemical information in the article
4. **Dissemination** as FAIR Data

Storing and Disseminating Chemical Information


```
{
    "hasBioChemEntityPart": [
        {
            "smiles": "CC1(C)[C@]2([H])CC(=O)O[C@]2(C)C3=NC4=C(C=C
            "inChI": "InChI=1S/C27H29NO6/c1-25(2)19-12-21(30)34-27
            "@type": "MolecularEntity",
            "molecularFormula": "C27H29NO6",
            "inChIKey": "OYYZMRLGAAQTPV-WZCPEYNJSA-N"
        }
    ],
    "@type": "ChemicalSubstance",
    "@id": "1860-5397-21-75-OYYZMRLGAAQTPV-WZCPEYNJSA-N"
},
{
    "hasBioChemEntityPart": [
        {
            "smiles": "CC(=O)O[C@@H]1C[C@@]2([H])C(C)(C)C(=O)C=C[C
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```


https://pubchem.ncbi.nlm.nih.gov/source/28569

Open Source Tools for FAIR Data Publishing in Chemistry

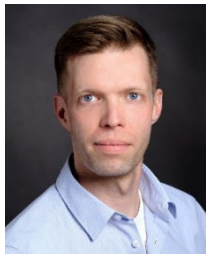
- Semi-automated extraction workflow designed for minimal user (author) input to provide **chemical semantics**
- **Stand-alone** (and soon to be **open source**) software – not limited to the Beilstein Journals (or journals in general)
- Based on open source libraries
- **Github repos**: BChemLookup (open); BChemXtract (in work)
- Call for chemistry publishing community to **join us!**

BEILSTEIN CHEMINFO LABS

BChemXtract:
(open soon)

BChemLookup:

Contact:
Felix Bänsch



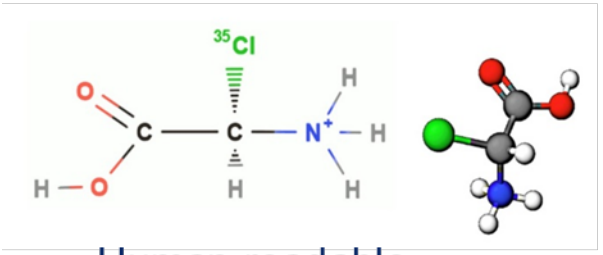
Success stories in chemical standards – InChI

https://www.inchi-trust.org/

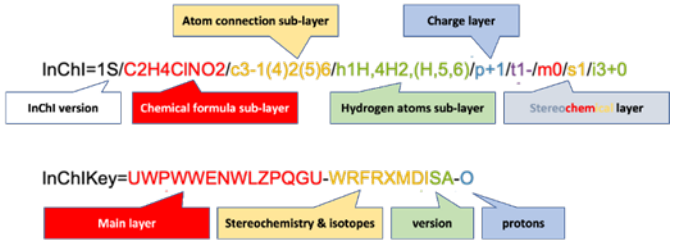
- Why we support further development of InChI with in-kind developer and cheminformatics support
- Invitation to **join us** in this community effort

Felix Bänsch

Christoph Müller



Human-readable



Machine-readable

InChI TRUST

ACD/Labs · CCDC advancing structural science · CCS Chinese Chemical Society · Chemaxon

CAS A division of the American Chemical Society · IUPAC · NIH National Institutes of Health

NIST National Institute of Standards and Technology U.S. Department of Commerce · OpenEye cadence MOLECULAR SCIENCES · ELSEVIER

Royal Society of Chemistry · Springer Nature · WILEY Publishers Since 1807

IAC Leibniz Institute for Analytical Sciences | RWTH AACHEN UNIVERSITY · BEILSTEIN INSTITUT · NFDI4Chem

VolkswagenStiftung · Data Literacy Alliance

Beilstein – Biochemistry Standards – Publishing – ChemInfo Labs – InChI – **Chemistry Data Standards Coalition**

Coalition for the Sustainability of Digital Data Standards in the Chemical Sciences

- Why is this needed?
- What have we done so far?
- Where are we headed?
- How can you get involved?

Beilstein – Biochemistry Standards – Publishing – ChemInfo Labs – InChI – **Chemistry Data Standards Coalition**

DigSustain1: Sustainable Business Modeling for Digital Standards Development

Value Proposition & Business Modeling exercise for digital chemical standards outputs and services:

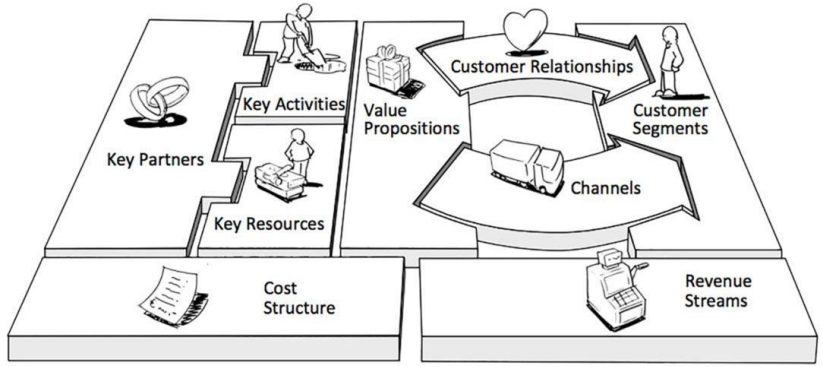
- Define community, contributors, users, and other groups
- Explore value propositions for using and supporting standards
- Articulate target resources & services needed to support broader community adoption of standards
- Initiate market analysis and identification of funding streams

Representatives from Scientific Unions, Industry Alliances, Academic Infrastructure Initiatives, Data Repositories, Publishing Organisations, Solution Developers

Chemistry – Life Sciences – Earth Sciences – Materials

https://www.degruyterbrill.com/document/doi/10.1515/ci-2024-0325/html

Cambridge, CCDC, March 2024



CCDC advancing structural science

InChITRUST

WorldFAIR

Beilstein – Biochemistry Standards – Publishing – ChemInfo Labs – InChI – **Chemistry Data Standards Coalition**

DigSustain2: Digital Data Standards Sustainability in Chemical Sciences Workshop

- ☞ Establishing community assets to support standards adoption, such as tools for standards mapping and data harmonization
- ☞ Identifying use cases and parameters for chemistry data reuse across sectors and disciplines
- ☞ Developing collective messaging and value propositions to promote standards adoption and sustainable business models
- ☞ **Launching a community coalition to drive ongoing collaboration and development**

Delitzsch, Germany, April 2025

Organizers and contributors: Beilstein-Institut, CTC, IUPAC, CODATA, InChI Trust, NFDI4Chem, ELIXIR, ISO, IUCr, Pistoia Alliance, PDB

Center for the Transformation of Chemistry

BEILSTEIN INSTITUT

WorldFAIR

McEwen et al. "Collaborative development and sustainability of digital chemical data standards" *Chemistry International*, vol. 47, no. 3, 2024, pp. 45-48. https://doi.org/10.1515/ci-2025-0317

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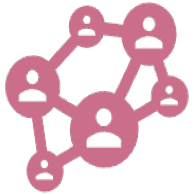
DigSustain3: Coalition for the Sustainability of Digital Data Standards in the Chemical Sciences Planning Meeting

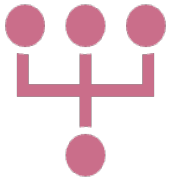


Coalition Planning Meeting, London, 6–7 Nov. 2025

Priorities for advancement, adoption, interoperability and sustainability of community digital standards

Vision paper, prospectus, statement of intent

Prioritize projects and activities



Our Questions?

- Must-haves to get started
- Critical input needed from community
- Leadership to initiate engagement and coordination
- Communication across initiatives, sectors, disciplines, coalitions
- Resources needed to advance aims

ROYAL SOCIETY OF CHEMISTRY

WorldFAIR

Beilstein – Biochemistry Standards – Publishing – ChemInfo Labs – InChI – Chemistry Data Standards Coalition

Strengthen community collaboration – Join us!

STRENDA/MIRAGE biochemistry standards
Open source project for **chemical lookup tables**
Open source projects for **extraction workflow**
InChI support
Chemistry data standards **coalition**

Thanks for your attention and please get in touch!

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