

CHEMISTRY DATA STANDARDS SUPPORTED BY THE BEILSTEIN-INSTITUT

Dr. Wendy Patterson

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Royal Society of Chemistry
ChemSpider Webinar 2025
October 21, 2025 / 3 PM BST

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



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QUALITY OPEN SCIENCE

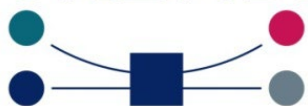
Non-profit foundation

founded in 1951 by the Max Planck Society
based in Frankfurt, Germany

Supports the advancement of the chemical sciences

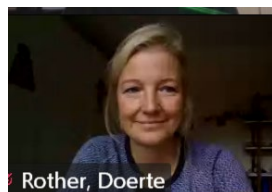
focus on communication, information and networking
long-term projects
open science

STREND



Standards for REporting ENzymology Data

Founded in 2004 under the auspices of the Beilstein-Institut



Rother, Doerte



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 STREND website.

STREND 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

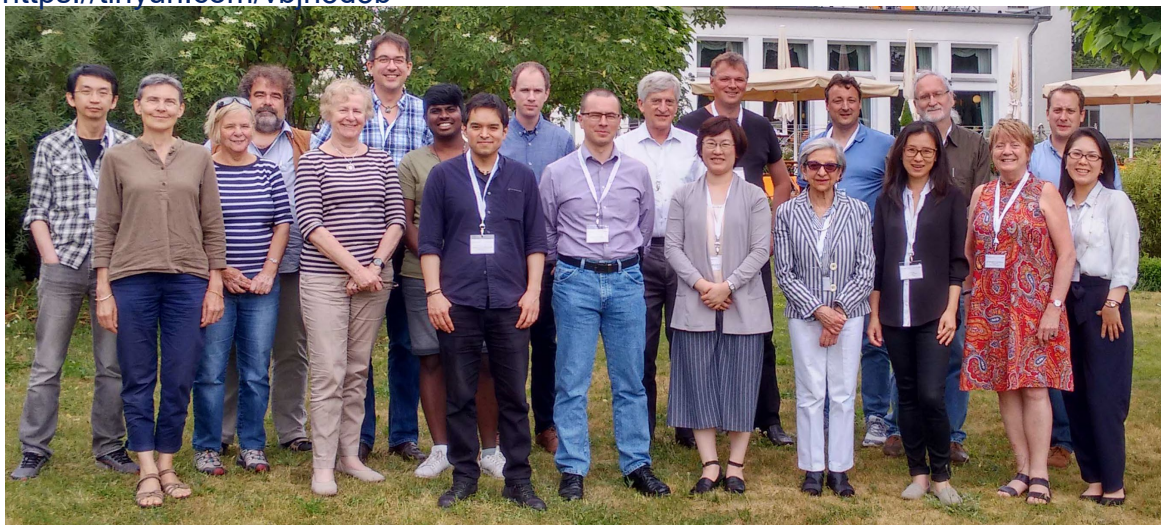


Minimum Information Required for A Glycomics Experiment

Founded 2011 under the auspices of the Beilstein-Institut



<https://tinyurl.com/vbjn5d3b>



Guideline	Version	Published
Sample Preparation	1.0; 18 Feb., 2016	<i>Glycobiology</i> , 2016, 26(9):907-910
Mass Spectrometric Analysis	1.0; 24 Apr., 2013	<i>Mol. Cell. Proteomics</i> , 2013, 12:991-995
Glycan Microarray Analysis	1.0; 22 June, 2016	<i>Glycobiology</i> , 2017, 27(4):280-284
Liquid Chromatography Analysis	1.0; 1 Mar., 2018	<i>Glycobiology</i> , 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	<i>Glycobiology</i> , 2022, 32(7):580-587
Lectin Microarray Analysis	1.0, 10 April, 2023	<i>Glycobiology</i> , 2025

<https://tinyurl.com/3z2mh64c>



Questions about STRENDa or MIRAGE?
Contact: [Carsten Kettner](#)

FAIR Data in the Beilstein Journals Publishing Workflow



1. **Extraction** of chemical structures
2. **Conversion** to and **validating** using InChI
3. **Embedding** of InChIs and 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=C3)N(C(=O)N4)C2",
    "inChI": "InChI=1S/C27H29N06/c1-25(2)19-12-21(30)34-27",
    "@type": "MolecularEntity",
    "molecularFormula": "C27H29N06",
    "inChIKey": "OYYZMRLGAAQTPV-WZCPEYNJSA-N"
  }
]
```

```
"@type": "ChemicalSubstance",
"@id": "1860-5397-21-75-0YYZMRLGAAQTPV-WZCPEYNJSA-N"
```

```
"hasBioChemEntityPart": [
  {
    "smiles": "CC(=O)O[C@@H]1C[C@@]2([H])C(C)(C)C(=O)C=C[C@H]2C1",
    "inChI": "InChI=1S/C28H34O7/c1-15(29)33-20-13-18-24(2,3,4,5,6,7,8,9,10,11,12,14,16,17,19,21,22,23,25,26,27)/p-1"
  }
]
```

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A convergent synthetic approach to the tetracyclic core framework of khayanolide-type limonoids

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A non-peer-reviewed version of this article has been published as a preprint (https://doi.org/10.27426/bjoc.2020.19-1)

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Abstract

A convergent approach for the enantioselective construction of an advanced intermediate containing the [5,5,6,6]-tetracyclic core framework of the khayanolide-type limonoids was described. The strategy features an enantioselective isolation of the benzylic alcohol, a 1,2-Cigand addition and an AcOH-interrupted Nazarov cyclization.

Keywords: enantioselective synthesis; interrupted Nazarov cyclization; khayanolide-type limonoids; tetracyclic framework

Introduction

Limonoids, a class of tetracyclic compounds derived biosynthetically from oxidative truncation of isoprenoid or sesquiterpene precursors coupled with subsequent [3,3]-sigmatropic rearrangement, constitute



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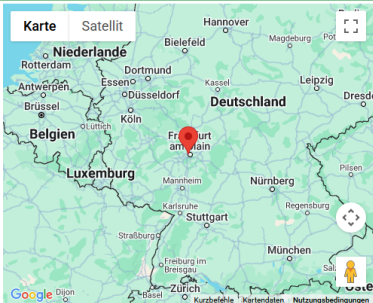


Beilstein Journals

The Beilstein-Institut is a charitable foundation whose mission is to promote the advancement of the chemical and related sciences. The communication and dissemination of high-quality information in chemistry is central to this mission. The results of all projects that the Beilstein-Institut supports are freely available to the scientific community and include diamond open access journals, data standardization projects, scientific events and digital infrastructure projects.

Organization	Beilstein-Institut zur Förderung der Chemischen Wissenschaften (Beilstein-Institut)
Category	Curation Efforts, Journal Publishers
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Data in PubChem	783 Live Substances
Last Updated	2025/05/07

Karte Satellit



<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/>

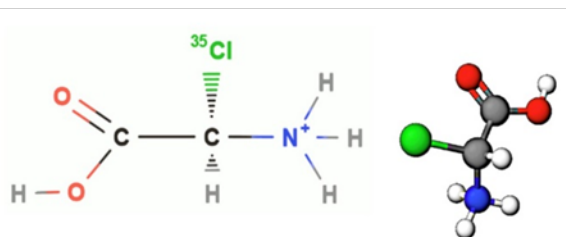
- Why we support further development of InChI with in-kind developer and cheminformatics support
- Invitation to **join us** in this community effort



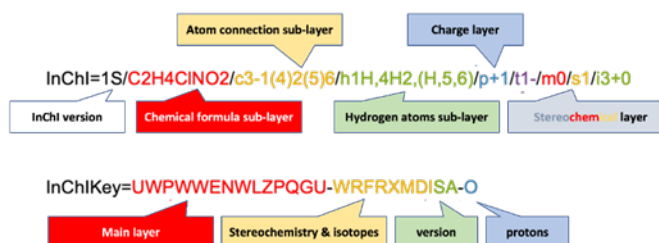
Felix Bänsch



Christoph Müller



Human-readable



Machine-readable



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?

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

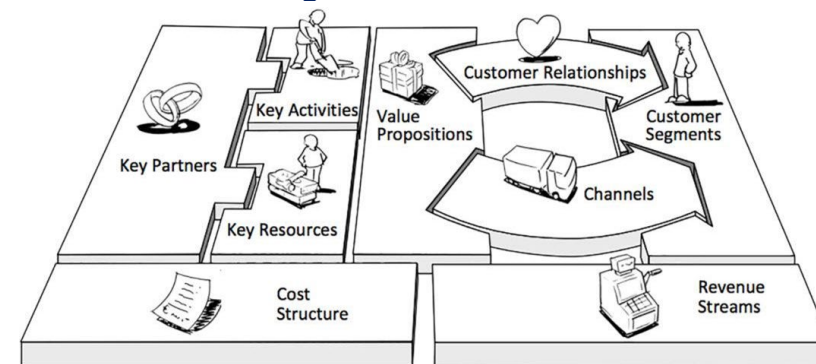
*Representatives from Scientific Unions, Industry Alliances,
Academic Infrastructure Initiatives, Data Repositories,
Publishing Organisations, Solution Developers*

Chemistry – Life Sciences – Earth Sciences – Materials

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



Cambridge, CCDC, March 2024



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

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

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>



Delitzsch, Germany, April 2025



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Transformation of
Chemistry

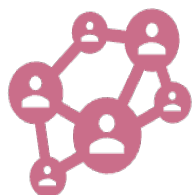


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WorldFAIR

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

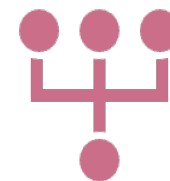


Coalition Planning Meeting, London, 6–7 Nov. 2025

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

Strengthen community collaboration – Join us!

STRENDAMIRAGE 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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