

## MassBank – Progress report 2023

Tobias Schulze, UFZ / UBA

Steffen Neumann, IPB

Michael Stravs, Eawag

Rene Meier, IPB

Emma Schymanski, LCSB



07.11.2023

NORMAN NTS CWG meeting

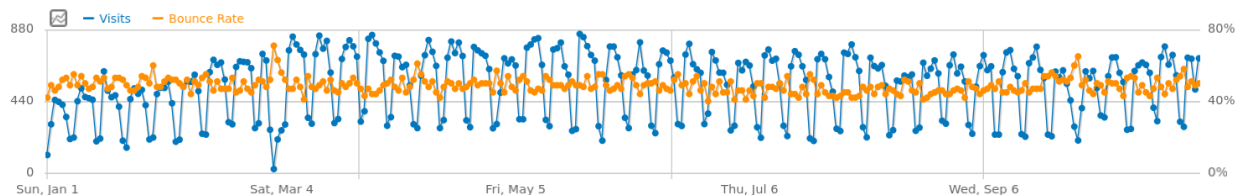
Online

DOI: 10.5281/zenodo.10078328



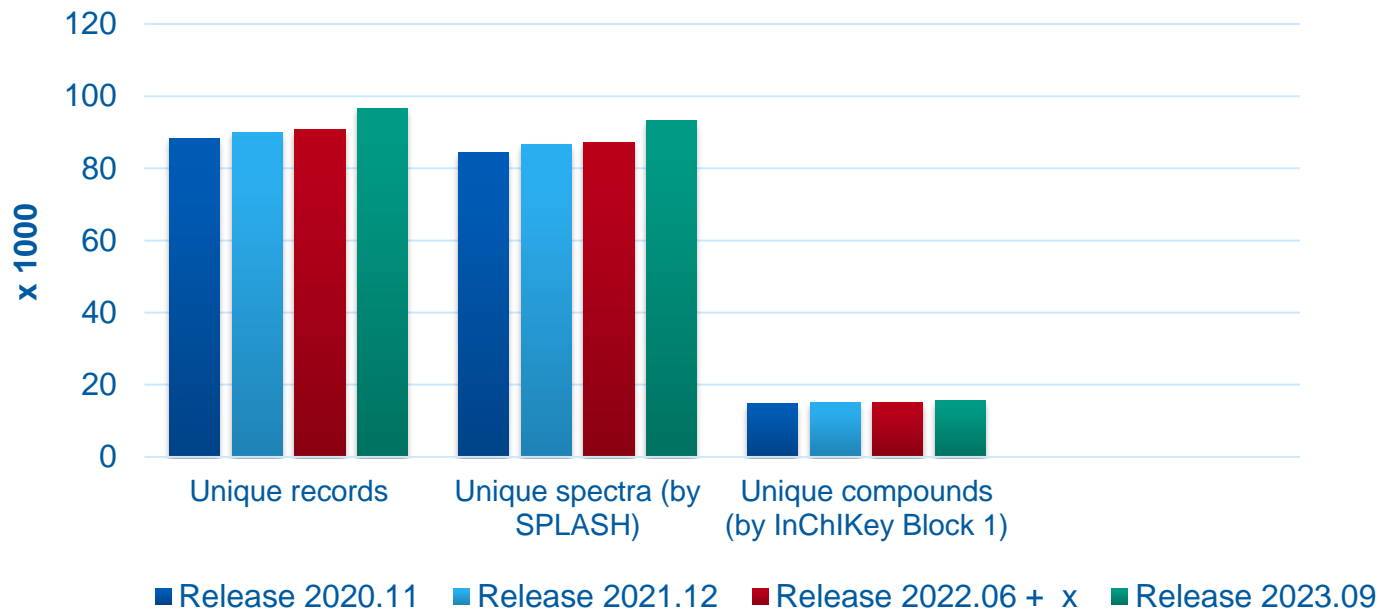
## Visits November 2022 to November 2023

Visits Over Time



- ~190 k visits (increase by 30 k compared to 2021)
- 48% bounces (left after first page) -> still fantastic for a content site
- ~790 k pageviews ~ 4 actions per visit with 2460 maximum actions per one visit!

## Development of contributions



## Findability

Criterion	Description	Fullfillment	Comment
F1	Global identifier	Yes	MassBank Accession, Universal Spectrum Identifier
F2	Rich metadata	Yes	MassBank Record Format
F3	Tailored metadata	Yes, partially	Not complete in all records
F4	Metadata registered and indexed in searchable resource	Yes	MassBank.eu Repos mirroring / mapping (e.g. PubChem, MoNA, Wikipedia)

## Accessible

Criterion	Description	Fullfillment	Comment
A1	Metadata are retrievable by their identifier by a standardised protocol	Yes	Massbank.eu
A1.1	Protocol is open, free and universal	Yes	MassBank Record Format
A2	Metadata are accessible forever	Yes	GitHub

## Interoperable

Criterion	Description	Fulfillment	Comment
I1	Metadata use a formal, accessible, shared, and broadly applicable language for knowledge representation	Yes	Structured data representation (schema.org)
I2	Metadata use vocabularies that follow FAIR principles	Yes	MassBank Record Format, HUPO-PSI
I3	Metadata include qualified references to other metadata	Yes	Links to PubChem etc.

<https://www.go-fair.org/fair-principles/>

# FAIRness of MassBank

## Reusable

Criterion	Description	Fullfillment	Comment
R1	Metadata are richely described	Yes	MassBank Record Format, Not machine readable
R1.1	Metadata are released with a clear and accessible data license	Yes	All CC licences
R1.2	Metadata are associated with detailed provenance	Yes	Github
R1.3	Metadata meet domain-relevant community standards	Yes	

```
{
  "@context": "https://schema.org",
  "@type": "ChemicalSubstance",
  "http://purl.org/dc/terms/conformsTo": {
    "@type": "CreativeWork",
    "@id": "https://bioschemas.org/profiles/ChemicalSubstance/0.4-REL"
  },
  "@id": "https://massbank.eu/MassBank/RecordDisplay?id\u003dMSBNK-AA",
  "identifier": "MSBNK-AAFC-AC000372",
  "name": "15-Acetyldeoxyynivalenol",
  "url": "https://massbank.eu/MassBank/RecordDisplay?id\u003dMSBNK-AA",
  "chemicalComposition": "C17H22O7",
  "alternateName": [
    "15-Acetyldeoxyynivalenol",
    "15-monoacetyldeoxyynivalenol"
  ],
  "hasBioChemEntityPart": [
```

Diclofenac; LC-ESI-Q; MS; NEG; 30 V

Mehr unter: [MassBank | massbank.eu](https://massbank.eu)

43 wissenschaftliche Artikel zitieren diesen Datenpool ([In Google Scholar ansehen](#))

Datensatz aktualisiert

Jan 19, 2016

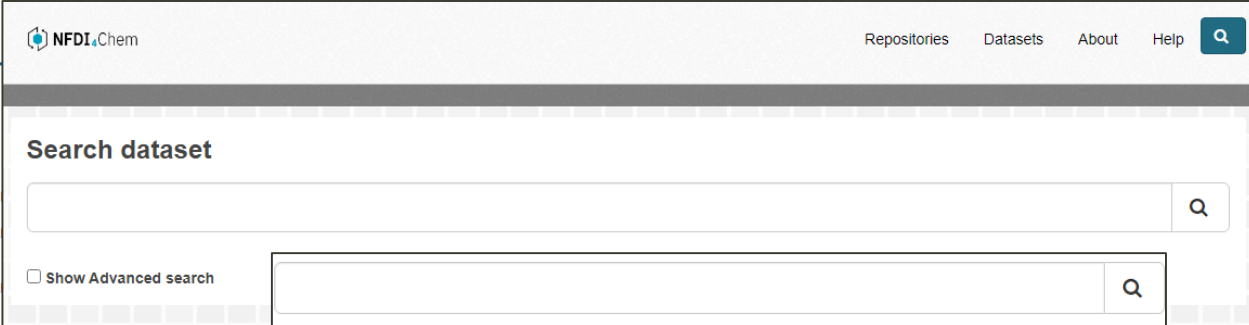
Lizenz

[Attribution-NonCommercial 4.0 \(CC BY-NC 4.0\)](#)

Lizenzinformationen wurden automatisch abgeleitet

Beschreibung

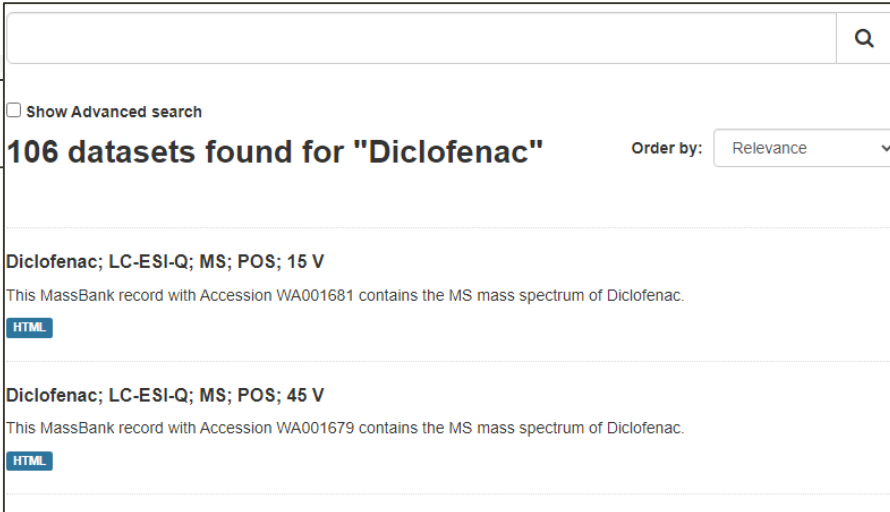
This MassBank record with Accession MSBNK-Waters-WA001682 contains the MS mass spectrum of Diclofenac with the InChIkey DCOPUUMXTXDBNB-UHFFFAOYSA-N.



NFDI4Chem

Repositories Datasets About Help

### Search dataset



Show Advanced search

## 106 datasets found for "Diclofenac"

Order by: Relevance

**Diclofenac; LC-ESI-Q; MS; POS; 15 V**

This MassBank record with Accession WA001681 contains the MS mass spectrum of Diclofenac.

[HTML](#)

**Diclofenac; LC-ESI-Q; MS; POS; 45 V**

This MassBank record with Accession WA001679 contains the MS mass spectrum of Diclofenac.

[HTML](#)

<https://search.nfdi4chem.de>  
<https://datasetsearch.research.google.com/>



# Acknowledgements

- New contributors: US EPA, BfG, Univ. Antwerp, LfU Bayern, Univ. Birmingham, SLU
- Hannes Mohring, Martin Krauss, Werner Brack, RDM Team (UFZ)
- Takaaki Nishioka, Yoshito Nihei (Japan)
- Evan Bolton and PubChem team (NIH)
- MassBank community

**contact:**  
**emma.schymanski@uni.lu**  
**sneumann@ipb-halle.de**

 @massbank\_consortium@a.gup.pe #MassBank

 @ESchymanski

 @schymane@mstdn.social

 @sneumann@mastodon.online

