Open Science in Chemistry The Past and the Next 20 Years

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Jülich Open Science Speaker Series, 2024-01-30







Acknowledgements

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https://scholia.toolforge.org/author/Q20895241





Abstract

Building on two decades of dedicated effort, Open Science in Chemistry has garnered renewed momentum. This personal perspective will sketch its evolutionary trajectory starting with Jmol and JChemPaint, via The OpenScience Project, the Chemistry Development Kit and the Blue Obelisk Movement. These developments will be compared with publishing models and the FAIR principles with a focus on their differences. Examples of the state of the art will include recent research from projects like NanoCommons, SbD4Nano, Scholia, and WikiPathways, leading us to current challenges. The talk will end with a vision of the next phase in Open Science in Chemistry."







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 - How can we encourage reuse and learning?







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- Open
 - Not just theoretical reuse, real reuse
 - Needed rights: use, modify, reshare







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 - Not just theoretical reuse, real reuse
 - Needed rights: use, modify, reshare
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 - Findable and Accessible







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 - Findable and Accessible
- Make it easy
 - Interoperable: we need more
 - Reusable: we need a lot more







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- Repeat
 - reproducible, repeatable, ...
- Peer review
 - journals, testing guidances, recommendations, etc







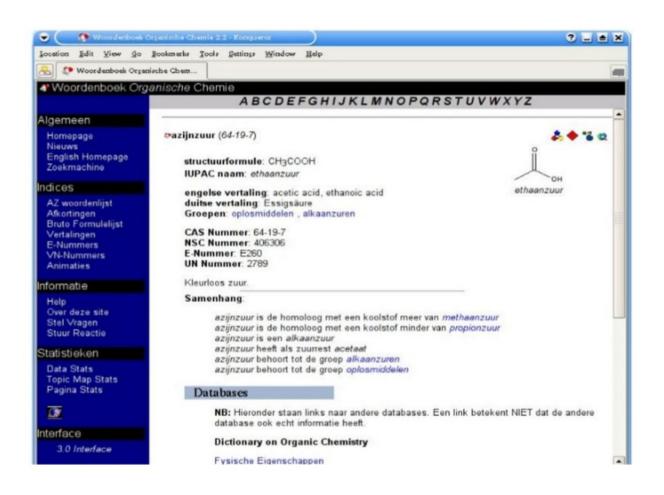
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Data 28 years ago (student)







See e.g. doi:10.3390/50100093

2127 woorden:

naar indeling:

606 chemicaliën
11 mengsels
12 polymeren
68 reacties
17 groepen van woorden
0 nomenclatuur-regels

naar woordsoort:

1413 overigen

223 afkortingen 1329 nederlandstalige woorden 982 engelse vertalingen 199 duitse vertalingen

2756 gegevensbestanden:

woorden:

1401 XML-bestanden

2D-structuren:

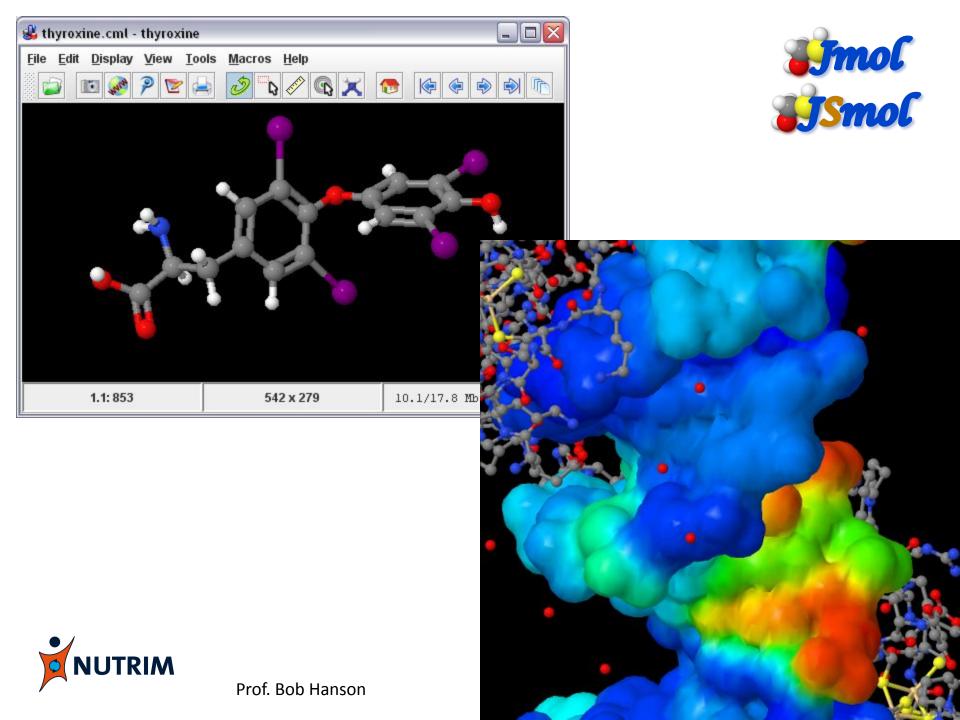
123 CML-bestanden 451 GIF-bestanden 66 (MDL) MOL-bestanden

3D-structuren:

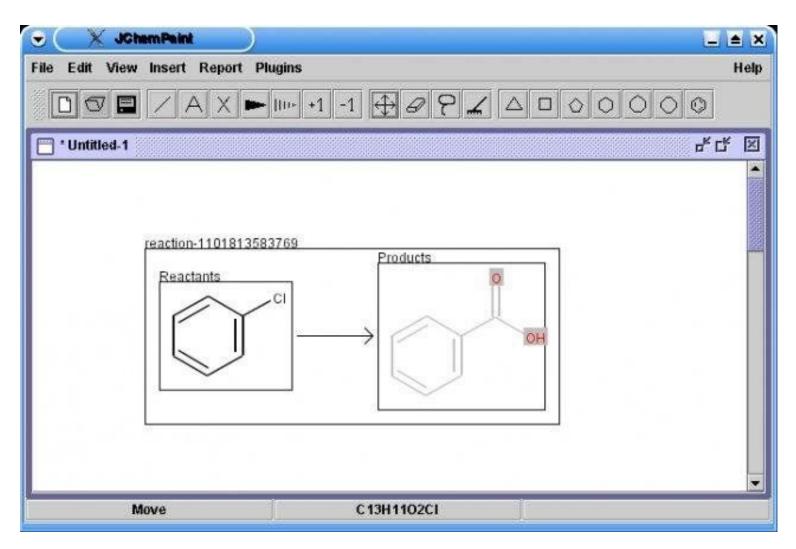
67 CML-bestanden 109 (MDL) MOL-bestanden 96 PDB-bestanden 0 VRML-bestanden 13 XYZ-bestanden

fysische gegevensbestanden:

430 CML-bestanden













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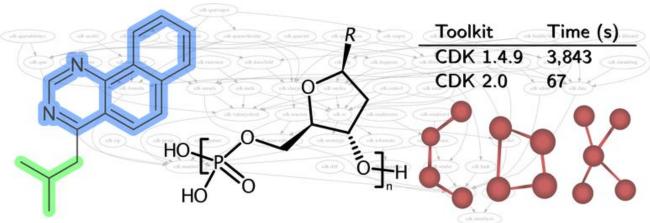
The Chemistry Development Kit (CDK) v2.0: atom typing, depiction, molecular formulas, and substructure searching

Egon L. Willighagen , John W. Mayfield, Jonathan Alvarsson, Arvid Berg, Lars Carlsson, Nina Jeliazkova, Stefan Kuhn, Tomáš Pluskal, Miquel Rojas-Chertó, Ola Spjuth, Gilleain Torrance, Chris T. Evelo, Rajarshi Guha & Christoph Steinbeck

Journal of Cheminformatics 9, Article number: 33 (2017) | Download Citation

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7825 Accesses | 50 Citations | 55 Altmetric | Metrics >>







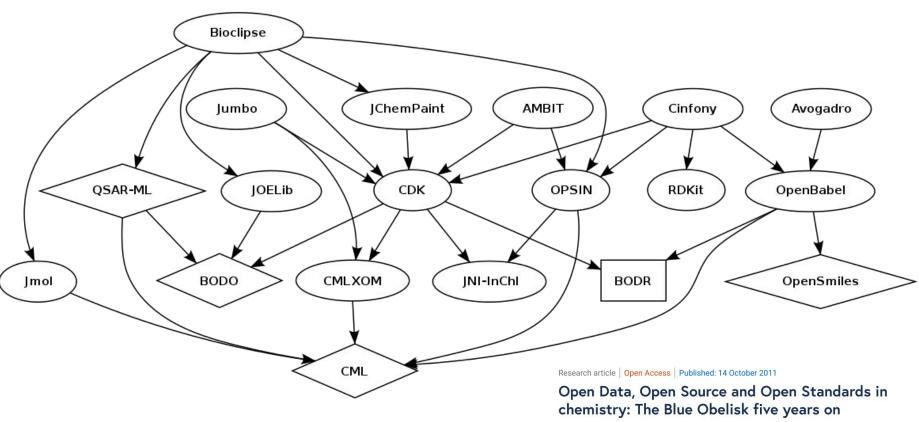
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The Blue Obelisk Movement





Noel M O'Boyle , Rajarshi Guha, Egon L Willighagen, Samuel E Adams, Jonathan Alvarsson, Jean-Claude Bradley, Igor V Filippov, Robert M Hanson, Marcus D Hanwell, Geoffrey R Hutchison, Craig A James, Nina Jeliazkova, Andrew SID Lang, Karol M Langner, David C Lonie, Daniel M Lowe, Jérôme Pansanel, Dmitry Pavlov, Ola Spjuth, Christoph Steinbeck, Adam L Tenderholt, Kevin J Theisen & Peter Murray-Rust

Journal of Cheminformatics 3, Article number: 37 (2011) | Cite this article

33k Accesses | 43 Citations | 72 Altmetric | Metrics

Abstract

Background

The Blue Obelisk movement was established in 2005 as a response to the lack of Open Data, Open Standards and Open Source (ODOSOS) in chemistry. It aims to make it easier to carry

Application Programming Interfaces



Open Source Software in Life Science Research

Practical Solutions to Common Challenges in the Pharmaceutical Industry and Beyond



Woodhead Publishing Series in Biomedicine

2012, Pages 35-61

2 - Interactive predictive toxicology with Bioclipse and OpenTox

Egon Willighagen, Roman Affentranger, Roland Grafström, Barry Hardy, Nina Jeliazkova, Ola Spjuth



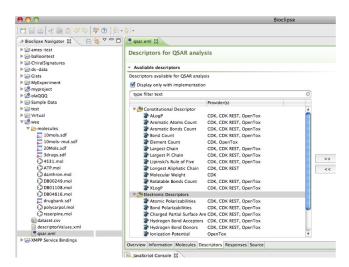
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https://doi.org/10.1533/9781908818249.35

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Abstract:

Computational predictive toxicology draws knowledge from many independent sources, providing a rich support tool to assess a wide variety of toxicological properties. A key example would be for it to complement alternative testing methods. The integration of Bioclipse and OpenTox permits toxicity prediction based on the analysis of chemical structures, and visualization of the substructure contributions to the toxicity prediction. In analogy of the decision support that is already in use in the pharmaceutical industry for designing new drug leads, we use this approach in two case studies in malaria research, using a combination of local and remote predictive models. This way, we find drug leads without predicted toxicity.

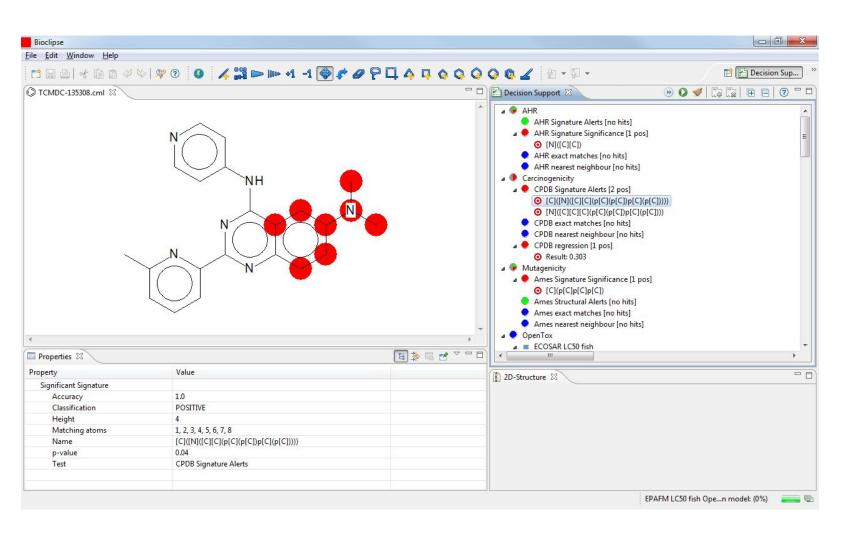




https://github.com/egonw/chapterBCOT





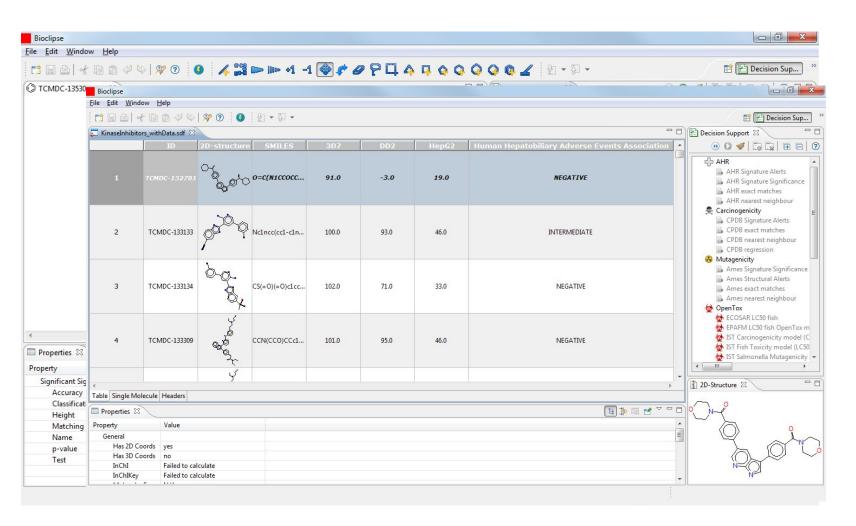










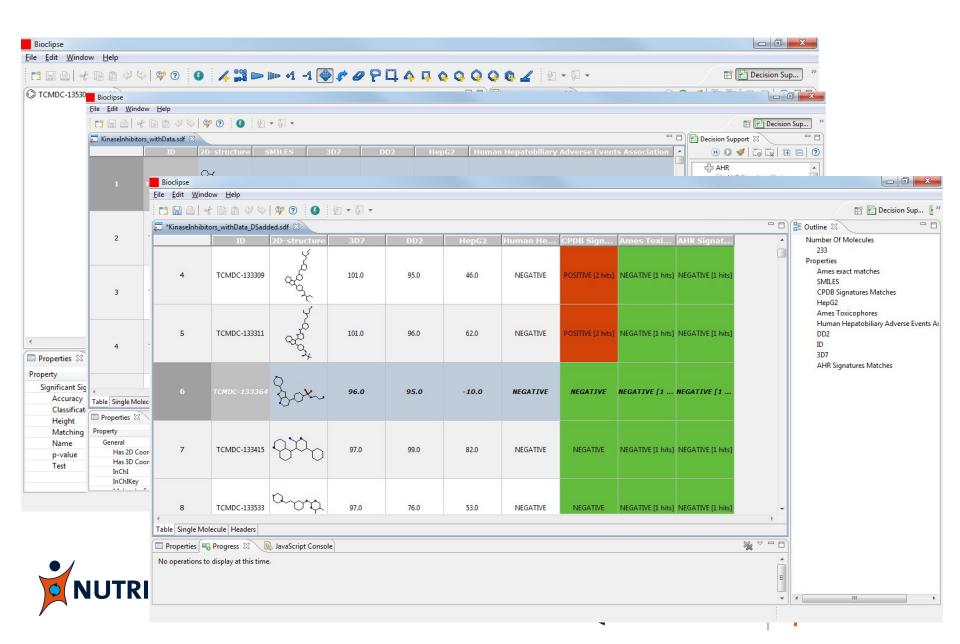




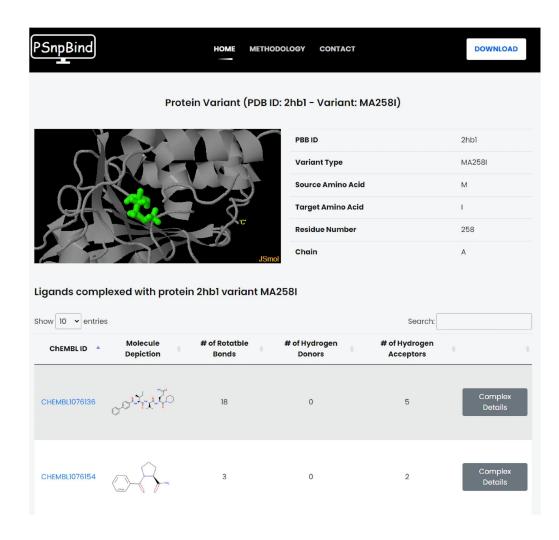








Massive sharing of docking experiments





Ammar et al. PSnpBind: [..]. J Cheminform 14, 8 (2022). 10.1186/s13321-021-00573-5





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Ontologies







PLOS ONE





PEER-REVIEWED

RESEARCH ARTICLE

The Chemical Information Ontology: Provenance and Disambiguation for Chemical Data on the Biological Semantic Web

Janna Hastings 🖾, Leonid Chepelev, Egon Willighagen, Nico Adams, Christoph Steinbeck, Michel Dumontier

Published: October 3, 2011 • https://doi.org/10.1371/journal.pone.0025513

Article	Authors	Metrics	Comments	Media Coverage
*				

Abstract

Introduction

Results

Discussion

Methods

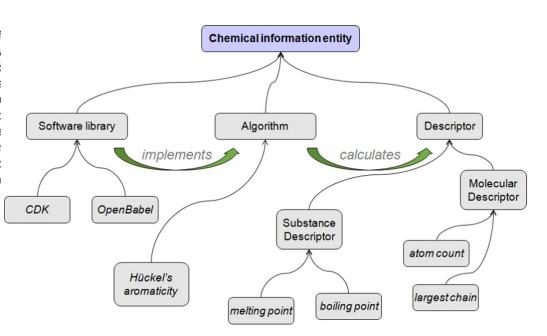
Acknowledgments

Author Contributions

References

Abstract

Cheminformatics is the application of inf silico. There are many areas in biology v computational research, including metal aspect in the application of cheminforms which is increasingly accomplished throus representations of objects and their proposuch ontologies are currently being devescience. Ontologies enable the definition particular domain, enabling intelligent co of scientists both within the domain of in







Journal of Biomedical Semantics

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Research Open Access Published: 21 March 2015

eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment

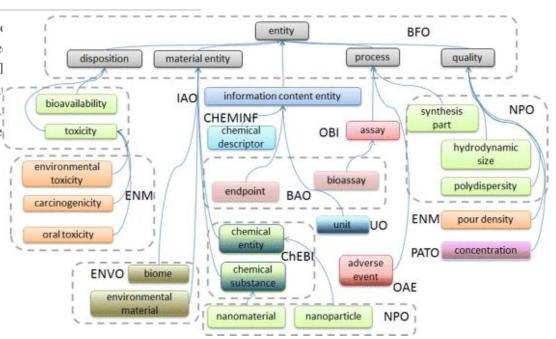
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Journal of Biomedical Semantics 6, Article number: 10 (2015) | Cite this article

5469 Accesses | 44 Citations | 48 Altmetric | Metrics

Abstract

Engineered nanomaterials (ENMs) are being developed to mediverse domains across the engineering and biomedical science accompanying the exciting proliferation of novel nanomaterial understand and predict their possibly detrimental effects on his environment. The eNanoMapper project (www.enanomapper.tomputational infrastructure for toxicological data management)







Interoperability







Application Programming Interfaces



Open Source Software in Life Science Research

Practical Solutions to Common Challenges in the Pharmaceutical Industry and Beyond



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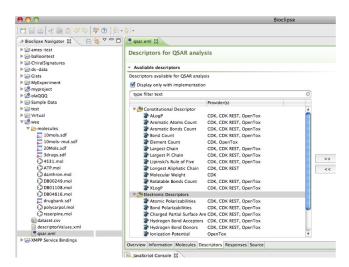
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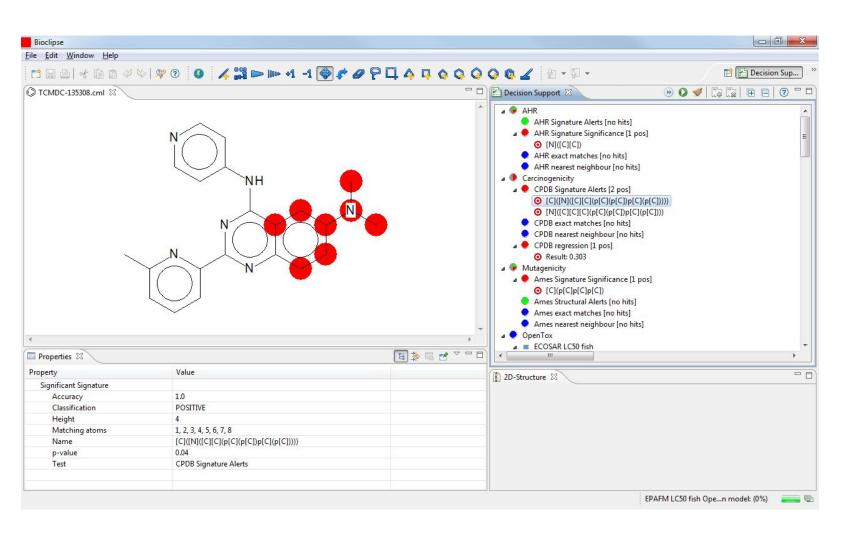




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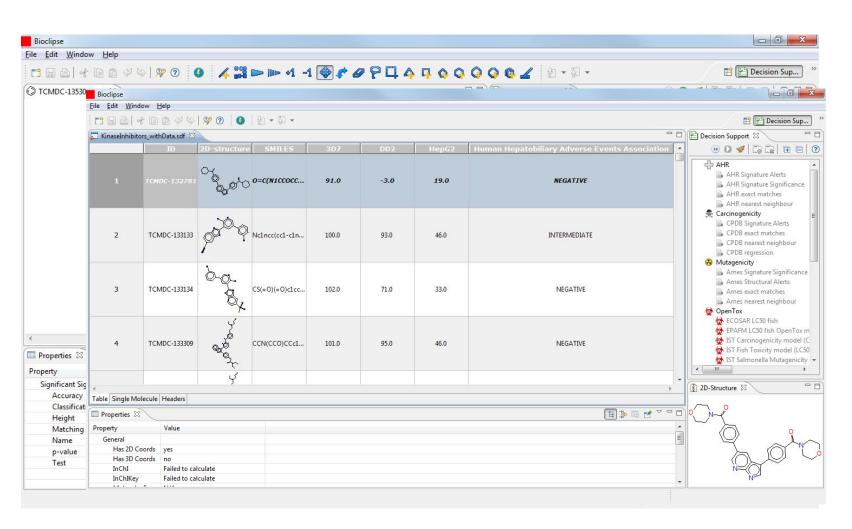










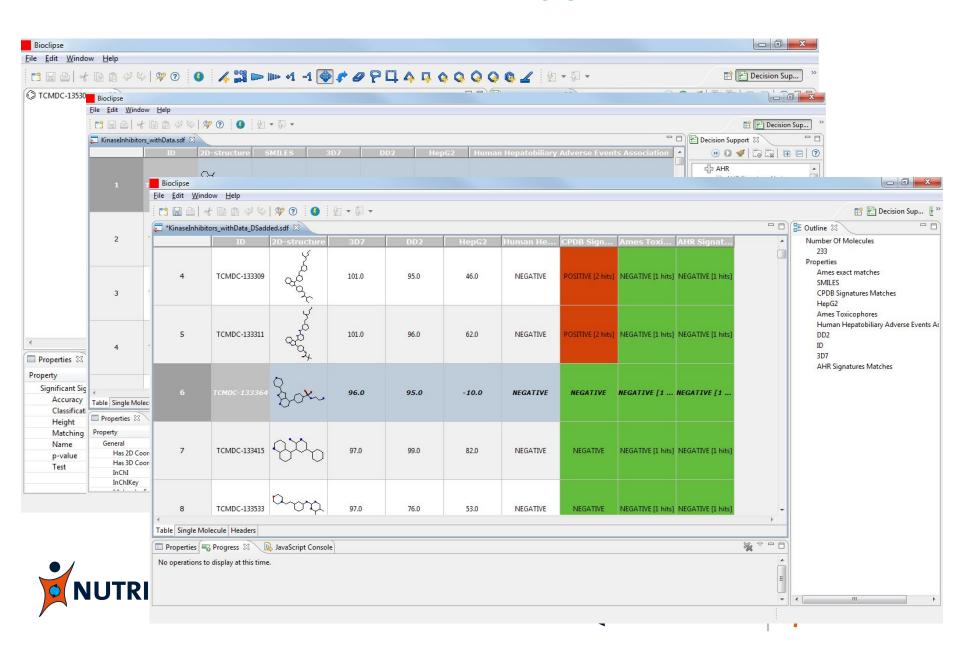












Standards







928 J. Chem. Inf. Comput. Sci. 1999, 39, 928-942

Chemical Markup, XML, and the Worldwide Web. 1. Basic Principles

Peter Murray-Rust*,† and Henry S. Rzepa*

Virtual School of Molecular Sciences, School of Pharmaceutical Sciences, University of Nottingham, U.K., and Department of Chemistry, Imperial College of Science, Technology and Medicine, London SW72AY, U.K.

Received May 26, 1999

Chemical markup language (CML) is an application of XML, the extensible markup lang for containing chemical information components within documents. Its design supports inte the XML family of tools and protocols. It provides a base functionality for atomic, crystallographic information and allows extensibility for other chemical applications. Leg imported into CML without information loss and can carry any desired chemical ontology. So of CML (Markush structures, chemical searching) will be discussed in later articles. An type declaration (DTD) for CML is included as a Chart.

INTRODUCTION TO XML TERMINOLOGY AND SYNOPSIS OF TERMS

Prior to introducing XML (extensible markup language) and CML (chemical markup language), ¹ we feel it important to define some key XML terminology (Table 1). ² We assume the reader is familiar with the basis of HTML (hypertext markup language) and its application in chemistry. ³ XML uses the same syntactic approach but, deliberately, has less flexibility and requires more precise application. This makes it much easier to write parsing software for well-formed documents (first three rules below). The most important parts of the XML syntax and name space specifications are as follows:

(1) All tags must be balanced ((FOO)...(/FOO)). Tags can contain any alphanumeric character and "-", "_" and ":" but must not contain white space.

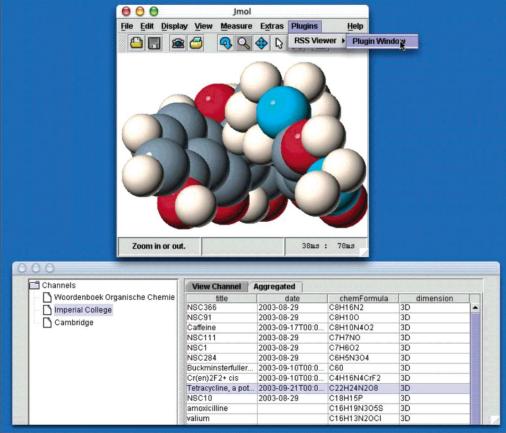
(2) The shorthand /EOOA is agriculant to /EOO\//EOO\

(9) Name spaces can be nested a with a name space declaration deta (10) A DTD may, but need document instance. If it is, a val whether the document is valid (i.e.

A number of related applications ment,² all expressed in XML itse this article are as follows:

XSL. An XML-based language formation (filtering, reordering, etc ing. Modern browsers will provide has a UNIX-like syntax for nav descendants.

XQL. A powerful XML-based q designed for structured documents any combination of (a) element na (c) attribute values and (d) element









QSAR Markup Language - QSAR-ML

Methodology | Open Access | Published: 30 June 2010

Towards interoperable and reproducible QSAR analyses: Exchange of datasets

Ola Spjuth , Egon L Willighagen, Rajarshi Guha, Martin Eklund & Jarl ES Wikberg

Journal of Cheminformatics 2, Article number: 5 (2010) Cite this article

14k Accesses 32 Citations 16 Altmetric Metrics

Abstract

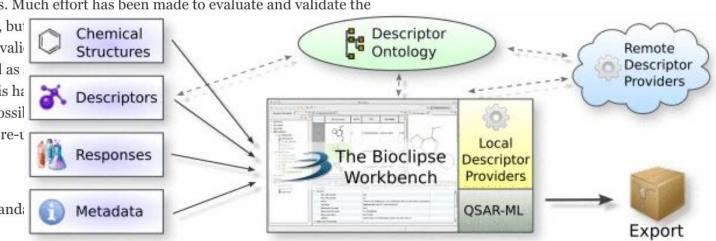
Background

QSAR is a widely used method to relate chemical structures to responses or properties based on experimental observations. Much effort has been made to evaluate and validate the

statistical modeling in QSAR, but highly important issue is the valiof chemical structures as well as to calculations. This process is ha field, making it virtually impossil constrain collaborations and re-

Results

We present a step towards stand:



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JRC representative industrial nanomaterials and Wikidata/Scholia



Ontology IRIs for the JRC representative indu

NanoCommons Working Draft 02 July 2021

This version:

http://nanocommons.github.io/specifications/2021/WD-jrc-20210702/

Latest published version:

http://nanocommons.github.io/specifications/jrc/

Previous version:

http://nanocommons.github.io/specifications/2020/WD-jrc-20200626/

Editor:

Egon Willighagen, Maastricht University

Author:

Jiakang Chang, EMBL-EBI

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Abstract

The <u>JRC representative industrial nanomaterials</u> are a series of nanomaterial This document links the JRC materials to specific terms in the ontology and The sources can be found at https://github.com/nanocommons/specification

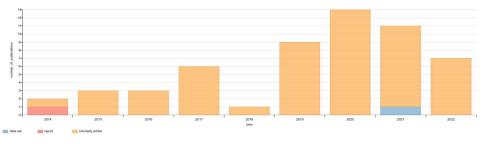
Status of This Document

This document is a specification by NanoCommons. It has no official standir

The below table gives the ontology likis for each of the JRC

	JRC nanomaterial	Code	Ontology IRI
	JRCNM01000a	ENM_9000074	http://purl.enanomapper.
	JRCNM01001a	ENM_9000075	http://purl.enanomapper.
	JRCNM01002a	ENM_9000076	http://purl.enanomapper.
	JRCNM01003a	ENM_9000083	http://purl.enanomapper.
	JRCNM01004a	ENM_9000084	http://purl.enanomapper.
	JRCNM01005a	ENM_9000077	http://purl.enanomapper.
	JRCNM01100a	ENM_9000078	http://purl.enanomapper.
	JRCNM01101a	ENM_9000086	http://purl.enanomapper.
	JRCNM02000a	ENM_9000087	http://purl.enanomapper.
	JRCNM02001a	ENM_9000088	http://purl.enanomapper.
	JRCNM02002a	ENM_9000089	http://purl.enanomapper.
	JRCNM02003a	ENM_9000090	http://purl.enanomapper.
	JRCNM02004a	ENM_9000091	http://purl.enanomapper.
	JRCNM02004b	ENM_9000092	http://purl.enanomapper.
	JRCNM02101a	ENM_9000237	http://purl.enanomapper.
	JRCNM02102a		http://purl.enanomapper.
	JRCNM03000a		http://purl.enanomapper.
	JRCNM03300a		http://purl.enanomapper.
	JRCNM03301a	ENM_9000098	http://purl.enanomapper.
	JRCNM04000a		http://purl.enanomapper.
	JRCNM04001a	ENM_9000081	http://purl.enanomapper.
	JRCNM50001a	ENM_9000256	http://purl.enanomapper.
	JRCNM10200a	ENM_9000231	http://purl.enanomapper.
	JRCNM10201a	ENM_9000094	http://purl.enanomapper.
year			





Encourage reuse with Findability

datasets

Overview of open datasets released by NanoSafety Cluster projects

This list provides an overview of archived datasets with an open license. Each one of them can be cited with DataCite and various datasets are not only downloaded from the archives but can also be interactively explored via databases.



Additional datasets and databases that provide interactive access to these datasets can be reported here.

RDF version of the data from Choi, JS. et al. Towards a generalized toxicity prediction model for oxide nanomaterials using integrated data from different sources (2018)



Twitter (4)

- Dataset Overview
- Date: 2021-11-30
- License: CC-BY 4.0
- Project: NanoSolveIT
- URL: https://zenodo.org/record/5743204
- DOI: 10.5281/zenodo.5743204

RDF version of the data from Anastasios G. Papadiamantis et al. Predicting Cytotoxicity of Metal Oxide Nanoparticles Using Isalos Analytics Platform (2020)



Twitter (1)

Twitter (1)



ioschemas

Dataset Overview

Date: 2021-11-30

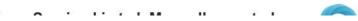
License: CC-BY 4.0

Project: NanoSolveIT

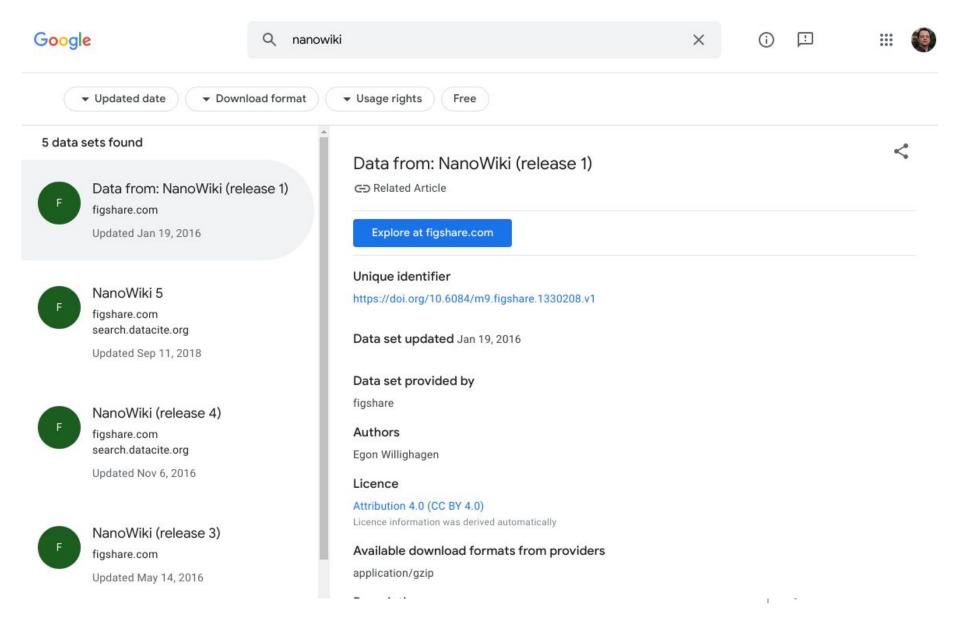
URL: https://zenodo.org/record/5743788

DOI: 10.5281/zenodo.5743788





Google Dataset Search



European Registry of Nanomaterials Journal of Cheminformatics

(ERM)

Home About Articles Submission Guidelines About The Editors Calls For Papers

Research article | Open Access | Published: 24 August 2022

European Registry of Materials: global, unique identifiers for (undisclosed) nanomaterials

Jeaphianne van Rijn ⊡, Antreas Afantitis, Mustafa Culha, Maria Dusinska, Thomas E. Exner, Nina Jeliazkova, Eleonora Marta Longhin, Iseult Lynch, Georgia Melagraki, Penny Nymark, Anastasios G. Papadiamantis, David A. Winkler, Hulya Yilmaz & Egon Willighagen

Journal of Cheminformatics 14, Article number: 57 (2022) Cite this article 350 Accesses | 16 Altmetric | Metrics

Abstract

Management of nanomaterials and nanosafety data needs to operate under the FAIR (findability, accessibility, interoperability, and reusability) principles and this requires a unique, global identifier for each nanomaterial. Existing identifiers may not always be applicable or sufficient to definitively identify the specific nanomaterial used in a particular study, resulting in the use of textual descriptions in research project communications and



Why the new ERM identifier?









Registring new materials

How to register new materials

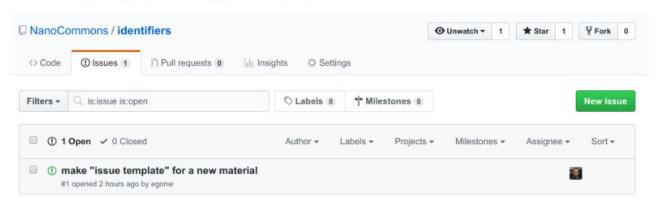
The following step explain how to register new materials. Mind you, for each material, please create a new issue.

Step 1. Aggregate the information

The first step is to aggregate the information you want to have associated with the newly minted identifier. There is required and optional information: only the name or label is required, and all other information is optional.

Step 2: Create a registry request

In the Issues section you can click the green New issue button:

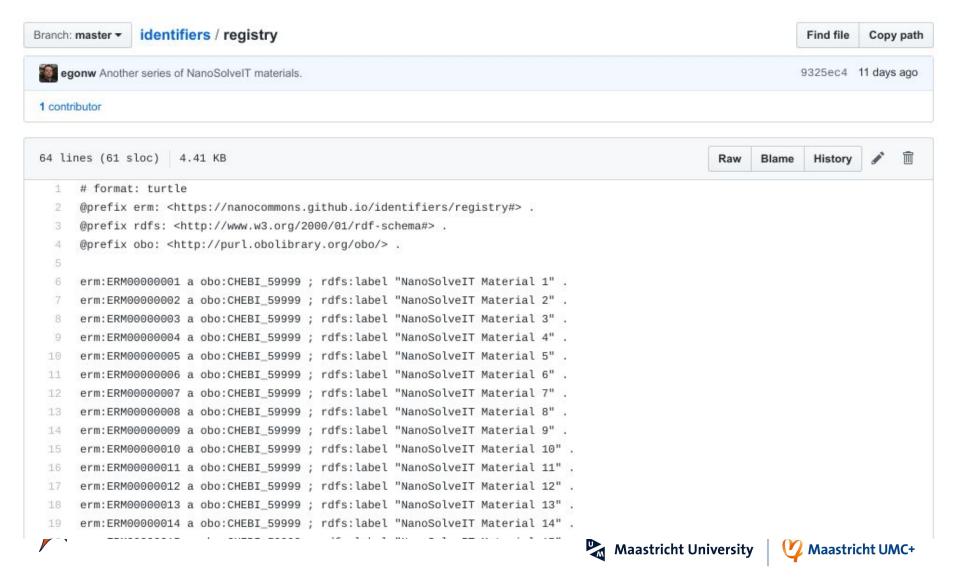


You can then select the Register Material template by clicking the green Get started bytton:



You can then fill out the template using the information aggregated in Step 1. For example:

A simple RDF format (Turtle)



ERM00000548

https://nanocommons.github.io/identifiers/registry#ERM00000548
erm:ERM00000548

Ag

Chemical composition: AgPVP Ontology class: npo:NPO_707

Blog posts

Silver nanoforms with ERM identifiers (20 Jan 2024)

Datasets

10.5281/ZENODO.7335039

Articles

10.1021/ACSANM.3C00173

Further reading

■ 10.5281/ZENODO.7335039 Furxhi, I. (2022). Extracting interpretable rules with Bayesian Networks. A case study of intrinsic human hazardous properties of silver nanoforms for the Safety Dimension of Safe and Sustainable by design paradigm. (Version 00) [Data set]. Zenodo. https://doi.org/10.5281/ZENODO.7335039 CrossRef Scholia
■ 10.1021/acsanm.3c00173 Furxhi, I., Bengalli, R., Motta, G., Mantecca, P., Kose, O., Carriere, M., Haq, E. U., O'Mahony, C., Blosi, M., Gardini, D., & Costa, A. (2023). Data-Driven Quantitative Intrinsic Hazard Criteria for

Nanoproduct Development in a Safe-by-Design Paradigm: A Case Study of Silver Nanoforms, ACS Applied Nano



Building on two decades of dedicated effort, Open Science in Chemistry has garnered renewed momentum. This personal perspective will sketch its evolutionary trajectory starting with Jmol and JChemPaint, via The OpenScience Project, the Chemistry Development Kit and the Blue Obelisk Movement. These developments will be compared with publishing models and the FAIR principles with a focus on their differences. Examples of the state of the art will include recent research from projects like NanoCommons, SbD4Nano, Scholia, and WikiPathways, leading us to current challenges. The talk will end with a vision of the next phase in Open Science in Chemistry."







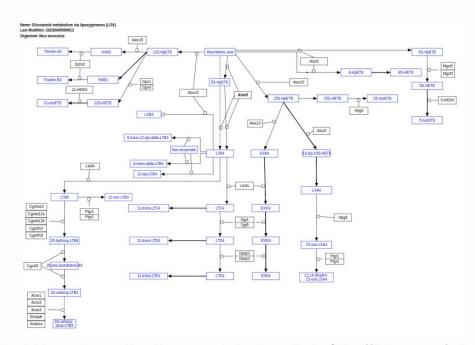
Actions-based WikiPathways website



Eicosanoid metabolism via lipoxygenases (LOX) (WP4348)

Mus musculus



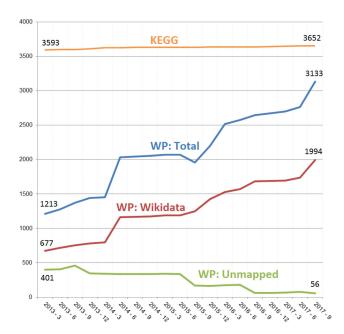




This pathway is inspired by the Lipidmaps>Eicosanoids Pathway expended pathway display [https://lipidmaps.org/pathway/pathways_maps]. Eicosanoids are a large group of compounds metabolised from arachidonic acid (AA), either via cyclooxygenases (COX) [https://www.wikipathways.org/index.php/Pathway:WP4347], lipooxygenases (LOX) [https://www.wikipathways.org/index.php/Pathway:WP4348], or cytochrome P450 monooxygenases (CYP) [https://www.wikipathways.org/index.php/Pathway:WP4349]. This pathway visualises the second route, via LOX.

Authors



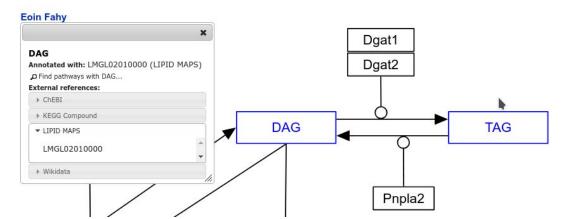


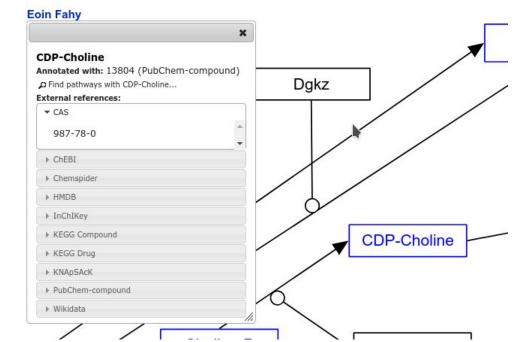
Denise Slenter *et al*, 10.1093/nar/gkx1064



School of Nutrition and Translational Research in Metabolism







SPARQL Query Language



SPARQL Endpoint

http://spargl.wikipathways.org/spargl

SPARQL Query:

```
1 PREFIX : <http://nextprot.org/rdf#>
2 select distinct ?pathwayname ?entry str(?gen) (group concat(distinct str(?loclab); SEPAR
     {?geneProduct a wp:Protein}
4
     union
     {?geneProduct a wp:GeneProduct}
6
     ?geneProduct rdfs:label ?gen .
     filter(!regex(?gen,"[ a-z-]")).
8
     ?geneProduct dcterms:isPartOf ?pathway .
9
     ?pathway a wp:Pathway .
     ?pathway wp:organism ?organism .
10
11
     filter(contains(str(?organism), "9606"))
12
     ?pathway dc:title ?pathwayname .
13
    filter(regex(?pathwayname, "Rett")).
14
     service <https://api.nextprot.org/spargl> {
15
       ?entry a :Entry ;
```

Query

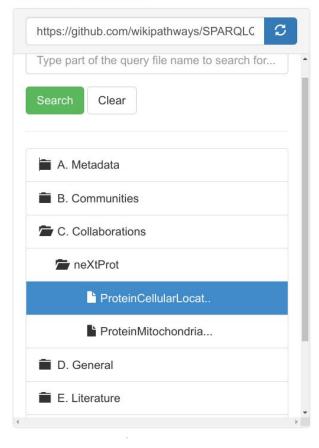
Reset

Export JSON

Get Permalink

Fullscreen Mode

SPARQL Examples:



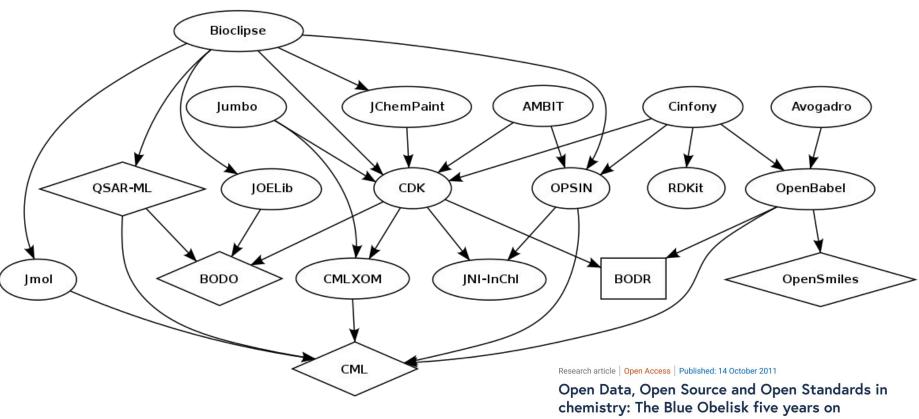
Building on two decades of dedicated effort, Open Science in Chemistry has garnered renewed momentum. This personal perspective will sketch its evolutionary trajectory starting with Jmol and JChemPaint, via The OpenScience Project, the Chemistry Development Kit and the Blue Obelisk Movement. These developments will be compared with publishing models and the FAIR principles with a focus on their differences. Examples of the state of the art will include recent research from projects like NanoCommons, SbD4Nano, Scholia, and WikiPathways, leading us to current challenges. The talk will end with a vision of the next phase in Open Science in Chemistry."







The Blue Obelisk Movement





Noel M O'Boyle , Rajarshi Guha, Egon L Willighagen, Samuel E Adams, Jonathan Alvarsson, Jean-Claude Bradley, Igor V Filippov, Robert M Hanson, Marcus D Hanwell, Geoffrey R Hutchison, Craig A James, Nina Jeliazkova, Andrew SID Lang, Karol M Langner, David C Lonie, Daniel M Lowe, Jérôme Pansanel, Dmitry Pavlov, Ola Spjuth, Christoph Steinbeck, Adam L Tenderholt, Kevin J Theisen & Peter Murray-Rust

Journal of Cheminformatics 3, Article number: 37 (2011) | Cite this article

33k Accesses | 43 Citations | 72 Altmetric | Metrics

Abstract

Background

The Blue Obelisk movement was established in 2005 as a response to the lack of Open Data, Open Standards and Open Source (ODOSOS) in chemistry. It aims to make it easier to carry



Altmetric Score



Tags



Definition rating



Research Output Management v2

Jente Houweling 1 , Egon Willighagen 2 Author(s) details \checkmark Declarations

The product of conducting research is research output. Research output management refers to the process of organising and documenting the diverse range of outputs generated during the research lifecycle. It recognises that research extends beyond the mere accumulation of data and emphasises the importance of managing not only the data but also the analytical processes, tools, and knowledge structures employed during analysis.

Research is traditionally subject to meticulous documentation, spanning from the initial







Funded projects















FAIRplus



















Open Science in Chemistry The Past and the Next 20 Years

Egon Willighagen
@egonw@social.edu.nl
0000-0001-7542-0286

Jülich Open Science Speaker Series, 2024-01-30





