

Making open science a reality, from a researcher perspective

Egon Willighagen

[http://chem-bla-ics.blogspot.com/
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*AgreenSkills+ Annual Meeting
Paris, 2017-02-15*

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Maastricht University



**My background: chemist, chemometrician,
data analyst: metabolomics, drug discovery,
toxicology, drug discovery, metabolomics**



Data 20 years ago (student)

Woordenboek Organische Chemie 2.2 - Kooqooqoo

Location Edit View Go Bookmarks Tools Settings Window Help

Woordenboek Organische Chem...

Woordenboek Organische Chemie

ABCDEFGHIJKLMNOPQRSTUVWXYZ

Algemeen

- Homepage
- Nieuws
- English Homepage
- Zoekmachine

Indices

- AZ woordenlijst
- Afkortingen
- Bruto Formulelijst
- Vertalingen
- E-Nummers
- VN-Nummers
- Animaties

Informatie

- Help
- Over deze site
- Stel Vragen
- Stuur Reactie

Statistieken

- Data Stats
- Topic Map Stats
- Pagina Stats

Interface

3.0 Interface

azijnzuur (64-19-7)

structuurformule: CH3COOH

IUPAC naam: ethaanzuur

engelse vertaling: acetic acid, ethanoic acid

duitse vertaling: Essigsäure

Groepen: oplosmiddelen, alkaanzuren

CAS Nummer: 64-19-7

NSC Nummer: 406306

E-Nummer: E260

UN Nummer: 2789

Kleurloos zuur.

Samenhang:

azijnzuur is de homolog met een koolstof meer van methaanzuur

azijnzuur is de homolog met een koolstof minder van propionzuur

azijnzuur is een alkaanzuur

azijnzuur heeft als zuurrest acetaat

azijnzuur behoort tot de groep alkaanzuren

azijnzuur behoort tot de groep oplosmiddelen

Databases

NB: Hieronder staan links naar andere databases. Een link betekent NIET dat de andere database ook echt informatie heeft.

Dictionary on Organic Chemistry

Fysische Eigenschappen

2127 woorden :

naar indeling :

606 chemicaliën
11 mengsels
12 polymeren
68 reacties
17 groepen van woorden
0 nomenclatuur-regels
1413 overigen

naar woordsoort :

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

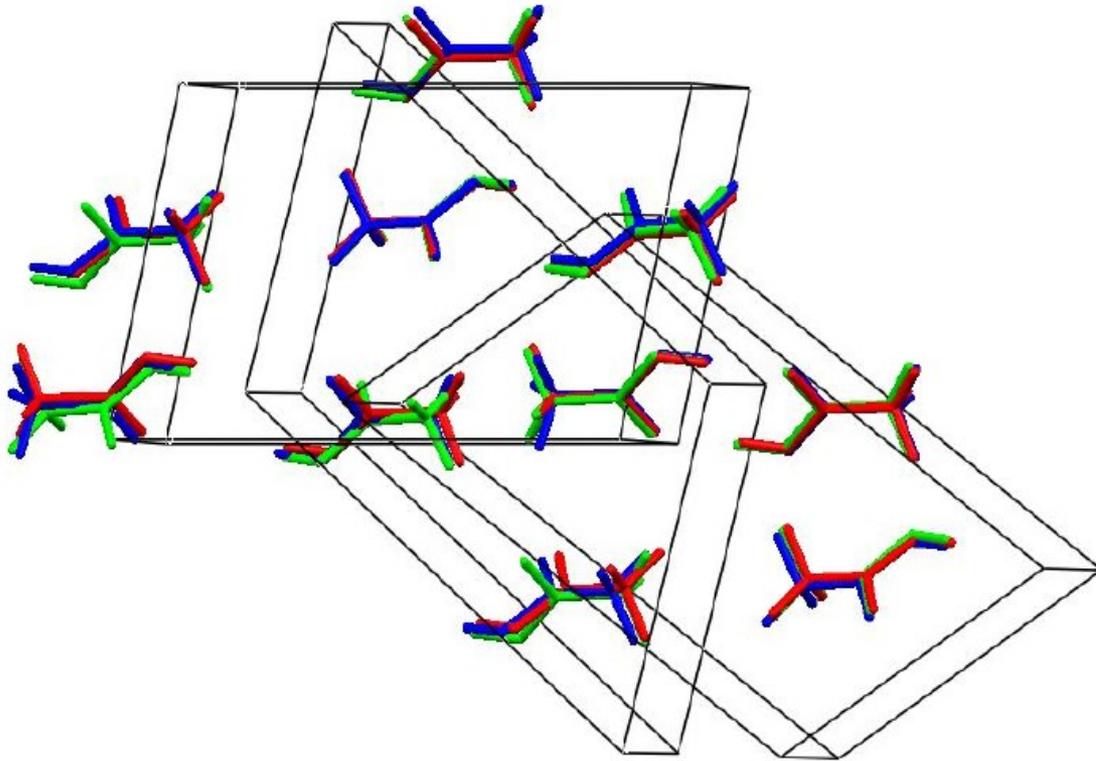
3D-structuren :

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

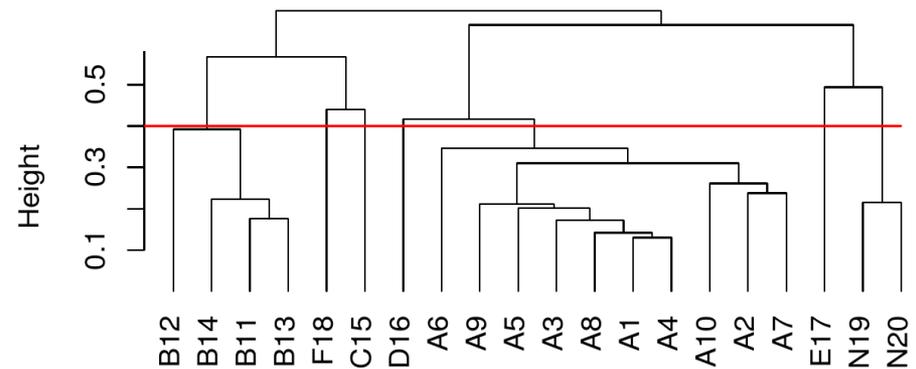
fysische gegevensbestanden :

430 CML-bestanden

Data 15 years ago (PhD in chemometrics)



See e.g.
[doi:10.1107/S0108768104028344](https://doi.org/10.1107/S0108768104028344)



Data 10 years ago (#OpenScience)

Home / Browse / The Blue Obelisk Data Repository / Files



The Blue Obelisk Data Repository

Brought to you by: [egonw](#)

Summary | [Files](#) | Reviews | Support | Wiki | Tickets ▼ | Code

Looking for the latest version? [Download bodr-10.tar.bz2 \(225.7 kB\)](#)

Home / bodr

Name ↕	Modified ↕	Size ↕	Downloads / Week ↕
↑ Parent folder			
10	2013-08-23		32
9	2010-04-25		1
8	2008-03-02		0
7	2008-03-01		0
6	2007-03-10		0
5	2007-02-27		0

Totals: 6 Items

33

NMRShiftDB **Current usage is:**
Registered Users: 653
Structures: 42380
Spectra: Measured 50517, calculated 549

Welcome to nmrshiftdb2

[Personal Page \(egonw\)](#)

[Impressum](#)

[Home](#) | [Search](#) | [Results](#) | [Predict](#) | [Assignment](#) | [Submit](#) | [Review](#) | [Help](#)

Search Results
There were more than 300 results. The rest was cut off!

Bookmarks
No bookmarks!

Type of search	Mode	Value	Type
my spectra	--	egonw	

[Spectral Data](#) | [Additional Data](#) | [Download](#)

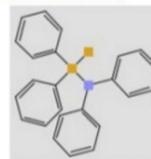
This spectrum has been reviewed as valid by [C. Steinbeck](#)

Results: 300
Browse: [1](#) [2](#) [3](#) [4](#) [5](#) [6](#) [7](#) [8](#) [9](#) [10](#) >>

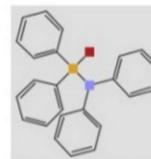
Type: 29Si

Atom No.	↓	Mult. (coupling const.)	Meas. Shift
25		5	-23.4

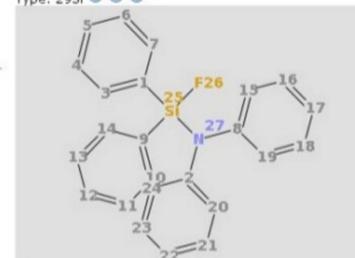
Next structure



OK:1, U:0, R:0, E:0, P:0 *



OK:1, U:0, R:0, E:0, P:0 *



See e.g. [doi:10.1021/ci050400b](https://doi.org/10.1021/ci050400b)



Maastricht University



Open Data now: eNanoMapper

Nanomaterials by contributor Download

Showing 1 to 6 of 6 entries

Nanomaterial contributor name	Nanomaterials	Table view	Nanomaterial contributor UUID
FP7 MARINA	Substances [6]	Substances and data Chemical structures	XLSX-4BBS1F08-059D-32AD-B5FD-71C6BCC6E0DB
Ideaconsult Ltd. / Sofia / Bulgaria	Substances [1]	Substances and data Chemical structures	
InterTest3	Substances [2]	Substances and data Chemical structures	
MODENA	Substances [59]	Substances and data Chemical structures	
NanoWiki	Substances [389]	Substances and data Chemical structures	
Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Substances [121]	Substances and data Chemical structures	



NANoREG search page (demo)

Search

- ▶ Data sources (79)
- ▶ Nanomaterial type (15)
- ▶ P-CHEM (15)
- ▶ Medium (0)
- ▶ Dispersion protocol (0)
- ▶ Results
- ▶ References (15)
- ▼ Protocols (15)
- SUPPLIER
- ▶ Instruments (0)

NanoSafety Cluster

Show collection details

+ Add new items Sort Filter search articles

Hits list Selection

FRAUNHOFER Particle size distribution (Granulom... Clear

< 1 > displaying 1 to 15 of 15

- JRCNM01001a (NM-101) (TiO2 6 nm) titanium oxide nanoparticle**

 P-CHEM.Particle size distribution (Granulometry) [SUPPLIER] [0]

[Material](#) [Composition](#) [Study](#) [External database](#) [Add to Selection](#)
- NM100 (TiO2 110 nm) titanium oxide nanoparticle**

 P-CHEM.Particle size distribution (Granulometry) [SUPPLIER] [0]

[Material](#) [Composition](#) [Study](#) [External database](#) [Add to Selection](#)
- NM101 (TiO2 6 nm) titanium oxide nanoparticle**

 P-CHEM.Particle size distribution (Granulometry) [SUPPLIER] [0]

[Material](#) [Composition](#) [Study](#) [External database](#) [Add to Selection](#)
- NM103 (TiO2 24.7 nm) titanium oxide nanoparticle**

doi:10.3762/bjnano.6.165

WikiPathways: capturing the full diversity of pathway knowledge

Martina Kutmon^{1,2,*}, Anders Riutta³, Nuno Nunes¹, Kristina Hanspers³,
Egon L. Willighagen¹, Anwasha Bohler¹, Jonathan Mélius¹, Andra Waagmeester^{1,4},
Sravanthi R. Sinha⁵, Ryan Miller¹, Susan L. Coort¹, Elisa Cirillo¹, Bart Smeets¹,
Chris T. Evelo^{1,2} and Alexander R. Pico^{3,*}

 Author Affiliations

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Received September 16, 2015.

Accepted September 28, 2015.

Abstract

WikiPathways (<http://www.wikipathways.org>) is an open, collaborative platform for capturing and disseminating models of biological pathways for data visualization and analysis. Since our last NAR update, 4 years ago, WikiPathways has experienced massive growth in content, which continues to be contributed by hundreds of individuals each year. New aspects of the diversity and depth of the collected pathways are described from the perspective of researchers interested in using pathway information in their studies. We provide updates on extensions and services to support pathway analysis and visualization via popular standalone tools, i.e.

This Article

Nucl. Acids Res. (2015)
doi: 10.1093/nar/gkv1024

First published online: October 19, 2015

This article is Open Access

Abstract *Free*

» Full Text (HTML) *Free*

Full Text (PDF) *Free*

SUPPLEMENTARY DATA

 Classifications

 Services

 Responses

 Citing Articles

 Google Scholar

 PubMed

 ORCID

Profile for Riutta, A.
<http://orcid.org/0000-0002-4693-0591>

Profile for Willighagen, E.
<http://orcid.org/0000-0001-7542-0286>

Profile for Bohler, A.
<http://orcid.org/0000-0001-7073-5852>

Profile for Mélius, J.
<http://orcid.org/0000-0001-8624-2972>

Profile for Waagmeester, A.
<http://orcid.org/0000-0001-9773-4008>

Profile for Sinha, S.

WikiPathways: capturing the full diversity of



This Article

Nucl. Acids Res. (2015)
doi: 10.1093/nar/gkv1024

First published online: October 19, 2015

This article is Open Access

Abstract *Free*

» Full Text (HTML) *Free*

Full Text (PDF) *Free*

SUPPLEMENTARY DATA

+ Classifications

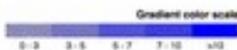
+ Services

+ Responses

+ Citing Articles

1. Select tissue of interest

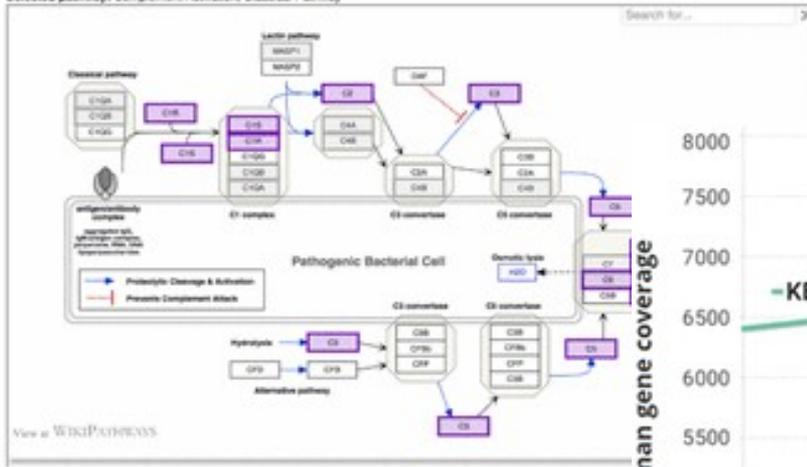
Select tissue:
 Show generic pathways
[View all...](#)



Pathways	Linkout	Median	Active genes	Measured genes	%
Ferriate Metabolism	WP2816	10.88	2	2	100
Cocaine Metabolic Pathway	WP2536	9.83	1	1	100
Lidocaine metabolism	WP2646	8.77	2	2	100
Nicotine Metabolism	WP1600	8.31	5	6	83
Polylol Pathway	WP690	7.23	3	4	75
Tamoxifen metabolism	WP681	7.22	12	21	57
Complement Activation, Classical Pathway	WP545	7.22	9	17	52
Diclofenac Metabolic Pathway	WP3491	7.21	2	4	50
Synthesis and Degradation of Ketone Bodies	WP311	6.94	3	5	60
Arachidonate Epoxidase - Epoxide Hydrolase	WP678	6.54	3	7	42
Benzo(a)pyrene metabolism	WP696	6.49	4	9	44
Folate-Alcohol and Cancer Pathway	WP1589	6.49	4	8	50
Phase I isoenzymes, non P450	WP136	6.44	3	8	37
Complement and Coagulation Cascades	WP508	6.35	28	60	48
Glycine Metabolism	WP1495	6.21	1	3	33
Blood Clotting Cascade	WP272	6.18	8	24	33
Alanine and aspartate metabolism	WP106	6.08	5	12	41

Highlighting legend
 Active gene (expression > 6) Not active gene (expression < 6)

Selected pathway: Complement Activation, Classical Pathway



2. Select pathway from table of tissue-specific results

3. View selected pathway with tissue expression data overlay

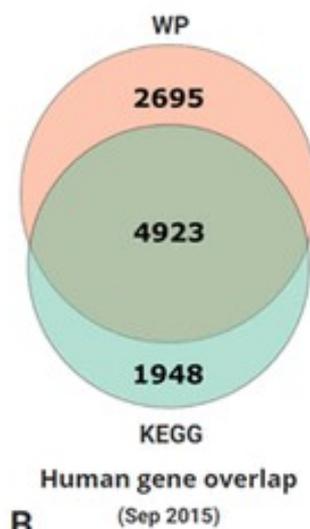
gmeester^{1,4},
Smeets¹,

3; Fax: +31 43

415 734 2741;

September 16, 2015.

September 28, 2015.



to be contributed by hundreds of individuals each year. The diversity and depth of the collected pathways are different perspectives of researchers interested in using pathway studies. We provide updates on extensions and server pathway analysis and visualization via popular standalone tools, i.e.

Profile for Sinha, S.

Open Data now: Wikidata

Execute Clear 48 Results in 565 ms Display Download Link

wikidata	compound	pKa	source	title	doi
Q209354	2-Chloroethanol	14.31	Q22251355	Acid Ionization Constants of Alcohols. II. Acidities of Some Substituted Methanols and Related Compounds 1,2	10.1021/ja01489a008
Q4596742	2,2,2-Trichloroethanol	12.24	Q22251355	Acid Ionization Constants of Alcohols. II. Acidities of Some Substituted Methanols and Related Compounds 1,2	10.1021/ja01489a008
Q22266828	2,4-lutidine	6.46	Q22262588	Experimental determination of pKa values by use of NMR chemical shift	10.1021/ed050p510
Q23636061	2,5-lutidine	6.18	Q22262588	Experimental determination of pKa values by use of NMR chemical shift	10.1021/ed050p510
Q209284	2,6-Lutidine	6.67	Q22262588	Experimental determination of pKa values by use of NMR chemical shift	10.1021/ed050p510
Q223069	3-chloropyridine	4.09	Q22262588	Experimental determination of pKa values by use of NMR chemical shift	10.1021/ed050p510
Q22266828	2,4-lutidine	6.28	Q22262588	Experimental determination of pKa values by use of NMR chemical shift	10.1021/ed050p510

pKa

4.63±0.01

temperature

25±1 degrees Celsius

1 reference

stated in

CRC Handbook of Chemistry and Physics (1st student edition)

Observations over the years



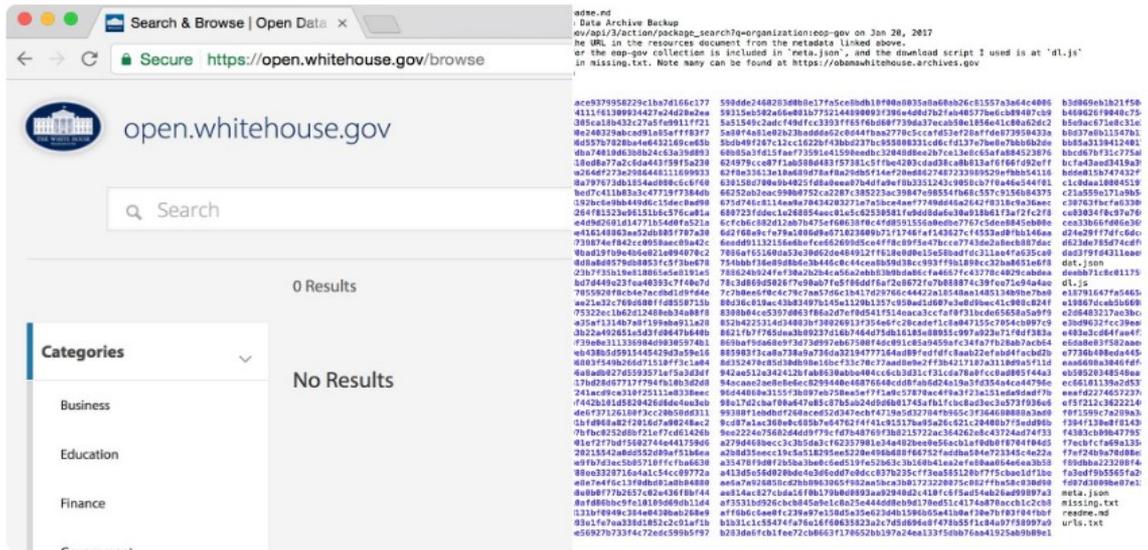
The problem



maxwell ogden
@denormalize

Follow

Today Trump removed all open data (9GB) from the White House open.whitehouse.gov/browse but I grabbed it all Jan 20! Will distribute soon



RETWEETS
749

LIKES
966



8:12 PM - 14 Feb 2017

37

749

966

The problem

Retraction Watch

Tracking retractions

Journal pulls paper with missing data, citing inquiry and legal proceedings

without comments

A journal has retracted a 2012 paper after the last author was unable to provide material to support the results presented in multiple figures.

The lack of supporting data came out during “an internal inquiry and subsequent legal proceedings,” according to the notice, issued by *Cell Cycle*.

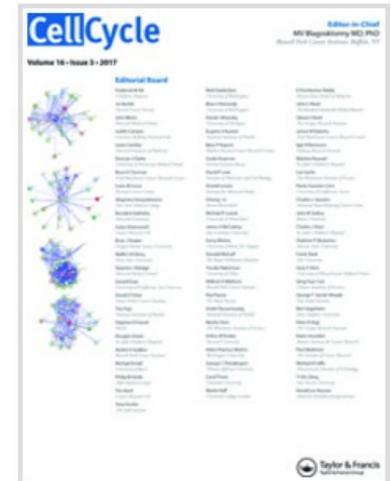
The last author on the paper is Susana Gonzalez, who was [dismissed from her position at the National Center for Cardiovascular Research \(CNIC\)](#) in Spain last year.

Here's [the full notice](#):

“

We, the Editors and Publishers of *Cell Cycle*, are retracting the following article:

Lorena Arranz, Antonio Herrera-Merchan, Jose Manuel Ligos, Antonio de Molina, Orlando Dominguez, Susana Gonzalez. “Bmi1 is critical to prevent Ikaros-mediated lymphoid priming in hematopoietic stem cells” *Cell Cycle* 11.1 (2012): 65–78 <http://tandfonline.com/doi/abs/10.4161/cc.11.1.18097>



Maastricht University



(>>>20 minutes)

Human rights debate [[edit](#)]

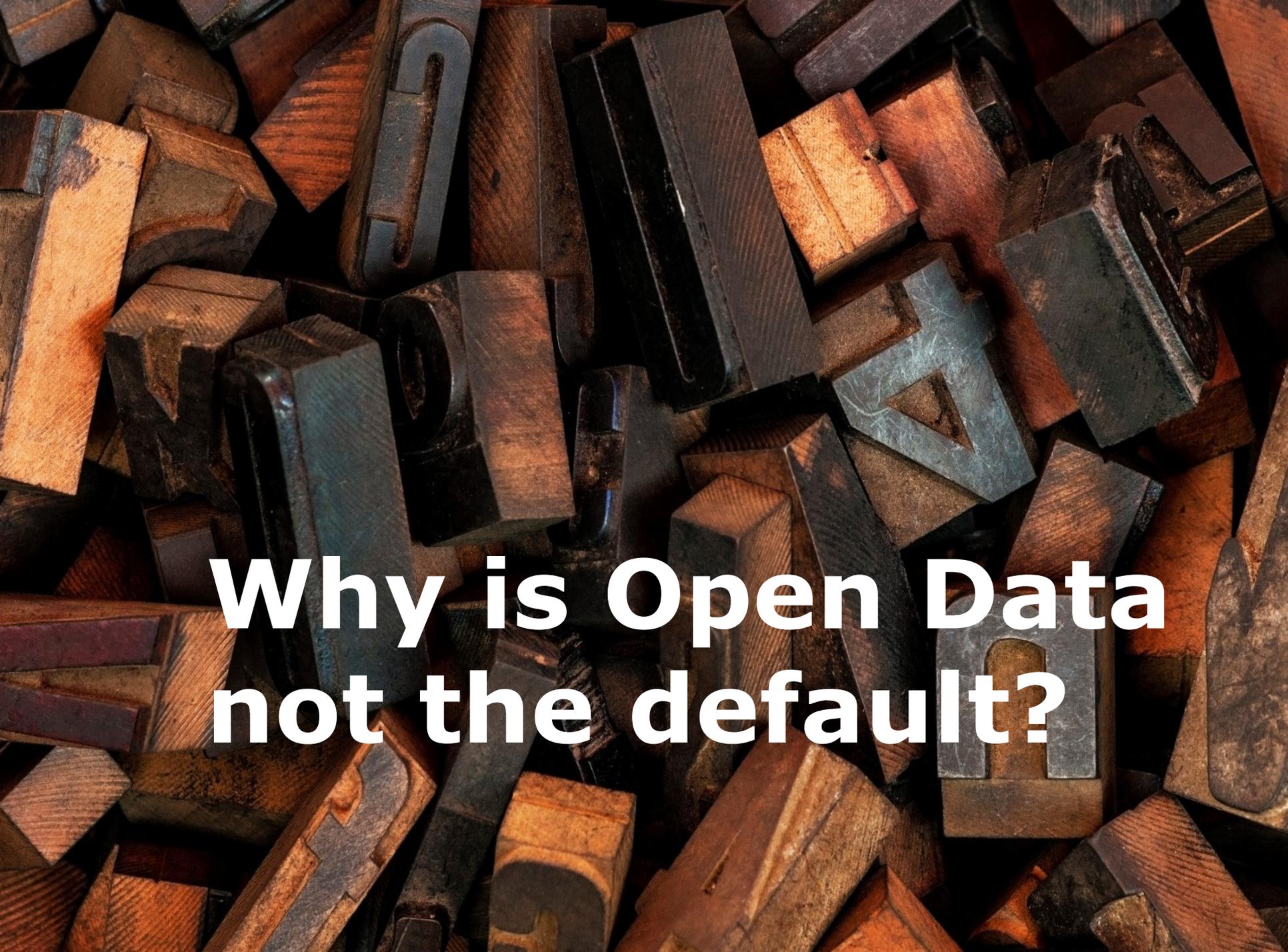
Access to knowledge and science is protected by Article 27 of the [Universal Declaration of Human Rights](#). The article balances the right of access with a right to protection of moral and material interests:

Article 27

Everyone has the right freely to participate in the cultural life of the community, to enjoy the arts and to share in scientific advancement and its benefits.

Everyone has the right to the protection of the moral and material interests resulting from any scientific, literary or artistic production of which he is the author.





**Why is Open Data
not the default?**

Complications

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THE EU SINGLE MARKET

[European Commission](#) > [The EU Single Market](#) > [Copyright and Neighbouring Rights](#) > [Protection of Databases](#)

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[News](#)

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[Management of Copyright and Related Rights](#)

[Copyright in the Information Society](#)

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[Term of Protection](#)

[Satellite and Cable](#)

Protection of Databases

- [Directive](#)
- [Evaluation report](#)
- [Stakeholder Consultation](#)
- [Related documents](#)

Directive

The Directive on the legal protection of Databases was adopted in February 1996. The Directive created a new exclusive "sui generis" right for database producers, valid for 15 years, to protect their investment of time, money and effort, irrespective of whether the database is in itself innovative ("non-original" databases). The Directive harmonised also copyright law applicable to the structure and arrangement of the contents of databases ("original" databases). The Directive's provisions apply to both analogue and digital databases.



Press and Information

Court of Justice of the European Union

PRESS RELEASE No 92/16

Luxembourg, 8 September 2016

Judgment in Case C-160/15

GS Media BV v Sanoma Media Netherlands BV,
Playboy Enterprises International Inc.,
Britt Geertruida Dekker

The posting of a hyperlink on a website to works protected by copyright and published without the author's consent on another website does not constitute a 'communication to the public' when the person who posts that link does not seek financial gain and acts without knowledge that those works have been published illegally

In contrast, if those hyperlinks are provided for profit, knowledge of the illegality of the publication on the other website must be presumed.



Julia Reda ✓

@Senficon



Following

Am I the only one who thinks this is an explosive combination of terrible ideas?
[@EU_Commission](#) [#GSMedia](#)
[#ancillarycopyright](#)

RETWEETS

33

LIKES

21



9:30 AM - 9 Sep 2016



↻ 33

♥ 21



What is Open Data?



Sharing knowledge



By Frits Ahlefeldt

Public Domain:

<http://www.publicdomainpictures.net/view-image.php?image=2568&picture=building-bridges>

What is Open Data?

- Clear copyright statement(s)
- Full provenance of where the data comes from
- An Open license
 - reuse, modify, redistribute
 - keep IP
- Or a waiver

(CLW := Copyright statement and License or Waiver)

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THE EU SINGLE MARKET

European Commission > The EU Single Market > Copyright and Neighbouring Rights > Protection of Databases

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Copyright and Neighbouring Rights

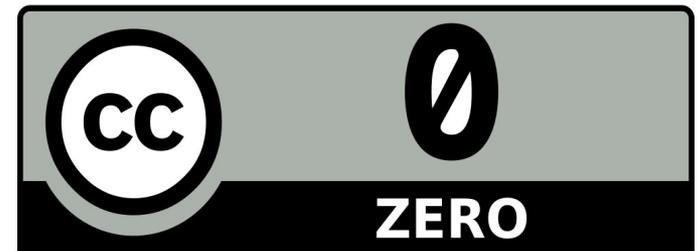
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- EU Legislation ("acquis")
 - Management of Copyright and Related Rights
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Open Data in Europe

The screenshot shows the Zenodo website interface. At the top, the Zenodo logo is on the left, and the tagline "Research. Shared." is on the right. Below the logo is a navigation menu with "Search", "Communities", "Browse", "Upload", and "Get started". On the right side of the navigation menu are "Sign In" and "Sign Up" buttons. A search bar is located below the navigation menu. The main content area is divided into several sections: "Datasets", "Recent Uploads", "Using GitHub?", and "New to Zenodo?".

Recent Uploads

03 June 2016 **Dataset** [Open access](#)

Binary Pulsar PSR B1913+16 arrival time and associated files. Ref. Weisberg & Huang ARJ 2016

[Weisberg, Joel](#); [Huang, Yuping](#)

These files contain arrival time and associated data for PSR B1913+16, which are usable as input to the tempo software program. They were used for the paper "Relativistic Measurements from Timing the Binary Pulsar PSR B1913+16," Weisberg & Huang, ...

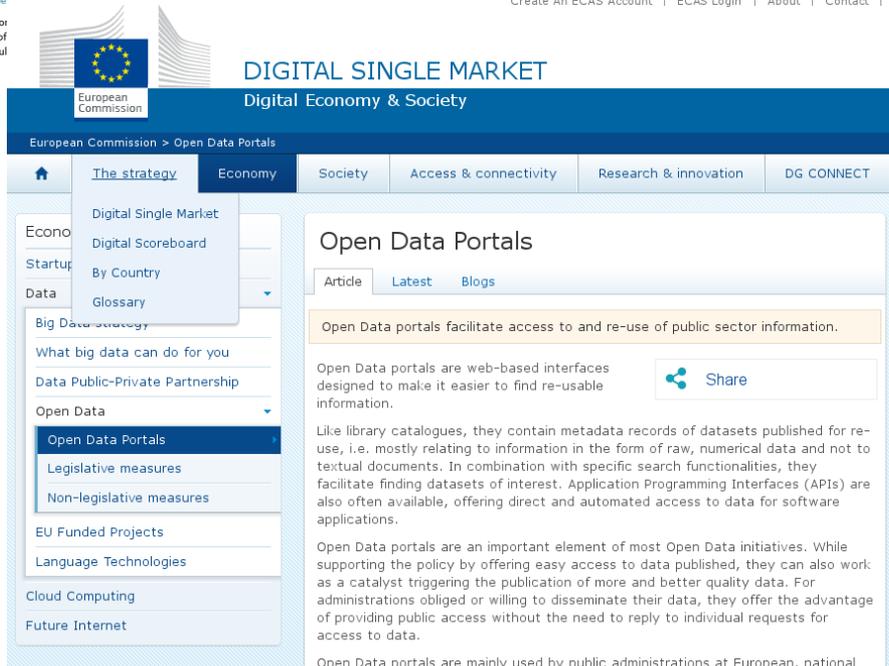
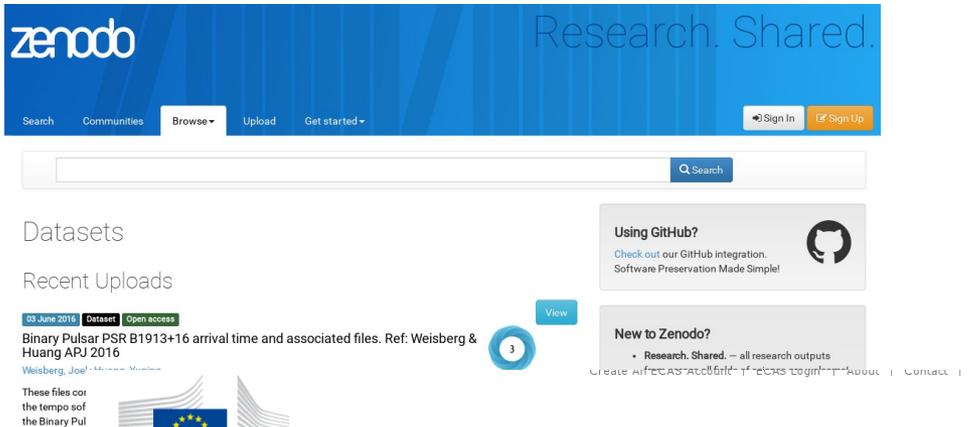
Using GitHub?

[Check out](#) our GitHub integration. Software Preservation Made Simple!

New to Zenodo?

- **Research. Shared.** – all research outputs from across all fields of science are welcome!
- **Citeable. Discoverable.** – uploads gets a Digital Object Identifier (DOI) to make them easily and uniquely citeable.
- **Community Collections** – accept or reject

Open Data in Europe



Open Data in Europe



Search [Search]

Datasets

Recent Uploads

03 June 2016 **Dataset** [Open access](#)
Binary Pulsar PSR B1913+16 arrival time and associated files. Ref. Weisberg & Huang APJ 2016

Weisberg, Joe

These files cover the tempo of the Binary Pulsar



DIGITAL SINGLE MARKET

Digital Economy & Society

European Commission > Open Data Portals

Home | **The strategy** | Economy | Society | Access & connectivity | Research & innovation | DG CONNECT

- Economy
- Startup
- Data
 - Big Data strategy
 - What big data can do for you
 - Data Public-Private Partnership
 - Open Data
 - Open Data Portals**
 - Legislative measures
 - Non-legislative measures
 - EU Funded Projects
 - Language Technologies
- Cloud Computing
- Future Internet

Open Data Portals

Article | Latest | Blogs

Open Data portals facilitate access to and re-use of public sector information.

Open Data portals are web-based interfaces designed to make it easier to find re-usable information.



Like library catalogues, they contain metadata records of datasets published for re-use, i.e. mostly relating to information in the form of raw, numerical data and not to textual documents. In combination with specific search functionalities, they facilitate finding datasets of interest. Application Programming Interfaces (APIs) are also often available, offering direct and automated access to data for software applications.

Open Data portals are an important element of most Open Data initiatives. While supporting the policy by offering easy access to data published, they can also work as a catalyst triggering the publication of more and better quality data. For administrations obliged or willing to disseminate their data, they offer the advantage of providing public access without the need to reply to individual requests for access to data.

Open Data portals are mainly used by public administrations at European, national

ELIXIR

A distributed infrastructure for life-science information

ELIXIR unites Europe's leading life science organisations in managing and safeguarding the increasing volume of data being generated by publicly funded research.

It coordinates, integrates and sustains bioinformatics resources across its member states and enables users in academia and industry to access vital data, tools, standards, compute and training services for their research.

Services



Training



EU projects



Annual Report published
 Read the ELIXIR Annual Report 2015

Events

- ELIXIR Italy Training course: Exome analysis with GALAXY
19 Sep 2016 to 20 Sep 2016
 - Software faster: From months to minutes (ELIXIR Training course)
20 Sep 2016
- More events >

News

- ELIXIR Hub strengthens its industry and international outreach
26 Aug 2016
 - Germany joins ELIXIR
19 Aug 2016
- More news >

Tweets by @ELIXIREurope

Open Data in Europe



Datasets

Recent Uploads

03 June 2016 **Dataset** [Open access](#)
 Binary Pulsar PSR B1913+16 arrival time and associated files. Ref. Weisberg & Huang APJ 2016

Weisberg, Joel
 These files cor
 the tempo sof
 the Binary Pul

Using GitHub?
 Check out our GitHub integration.
 Software Preservation Made Simple!

New to Zenodo?
 • Research. Shared. – all research outputs



DIGITAL SINGLE MARKET

Digital Economy & Society

European Commission > Open Data Portals

- The strategy
- Economy
- Society
- Access & connectivity
- Research & innovation
- DG CONNECT

- Digital Single Market
- Digital Scoreboard
- By Country
- Glossary
- Big Data strategy
- What big data can do for you
- Data Public-Private Partnership
- Open Data
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Open Data Portals

Article Latest Blogs

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Like library catalogues, they contain metadata records of datasets published for re-use, i.e. mostly relating to information in the form of raw, numerical data and not to textual documents. In combination with specific search functionalities, they facilitate finding datasets of interest. Application Programming Interfaces (APIs) are also often available, offering direct and automated access to data for software applications.

Open Data portals are an important element of most Open Data initiatives. While supporting the policy by offering easy access to data published, they can also work as a catalyst triggering the publication of more and better quality data. For administrations obliged or willing to disseminate their data, they offer the advantage of providing public access without the need to reply to individual requests for access to data.

Open Data portals are mainly used by public administrations at European, national



ELIXIR unites Europe's leading life science organisations in managing and safeguarding the increasing volume of data being generated by publicly funded research.

It coordinates, integrates and sustains bioinformatics resources across its member states and enables users in academia and industry to access vital data, tools, standards, compute and training services for their research.

- ### Events
- ELIXIR Italy Training course: Exome analysis with GALAXY 19 Sep 2016 to 20 Sep 2016
 - Software faster: From months to minutes (ELIXIR Training course) 20 Sep 2016
- More events >



- ### News
- ELIXIR Hub strengthens its industry and international outreach 26 Aug 2016
 - Germany joins ELIXIR 19 Aug 2016
- More news >

Annual Report published
 Read the ELIXIR Annual Report 2015

Tweets by @ELIXREurope



Open Data in Europe

European Open Science Cloud

20 June 2016 – first draft report from the High Level Expert Group

The Commission High Level Expert Group on the European Open Science Cloud (HLEG EOOSC) has drafted their first report, which the Commission will publish shortly after the summer.

Enquiries can be made directly to members of the HLEG EOOSC and/or to the Commission at RTD-EOOSC@ec.europa.eu.

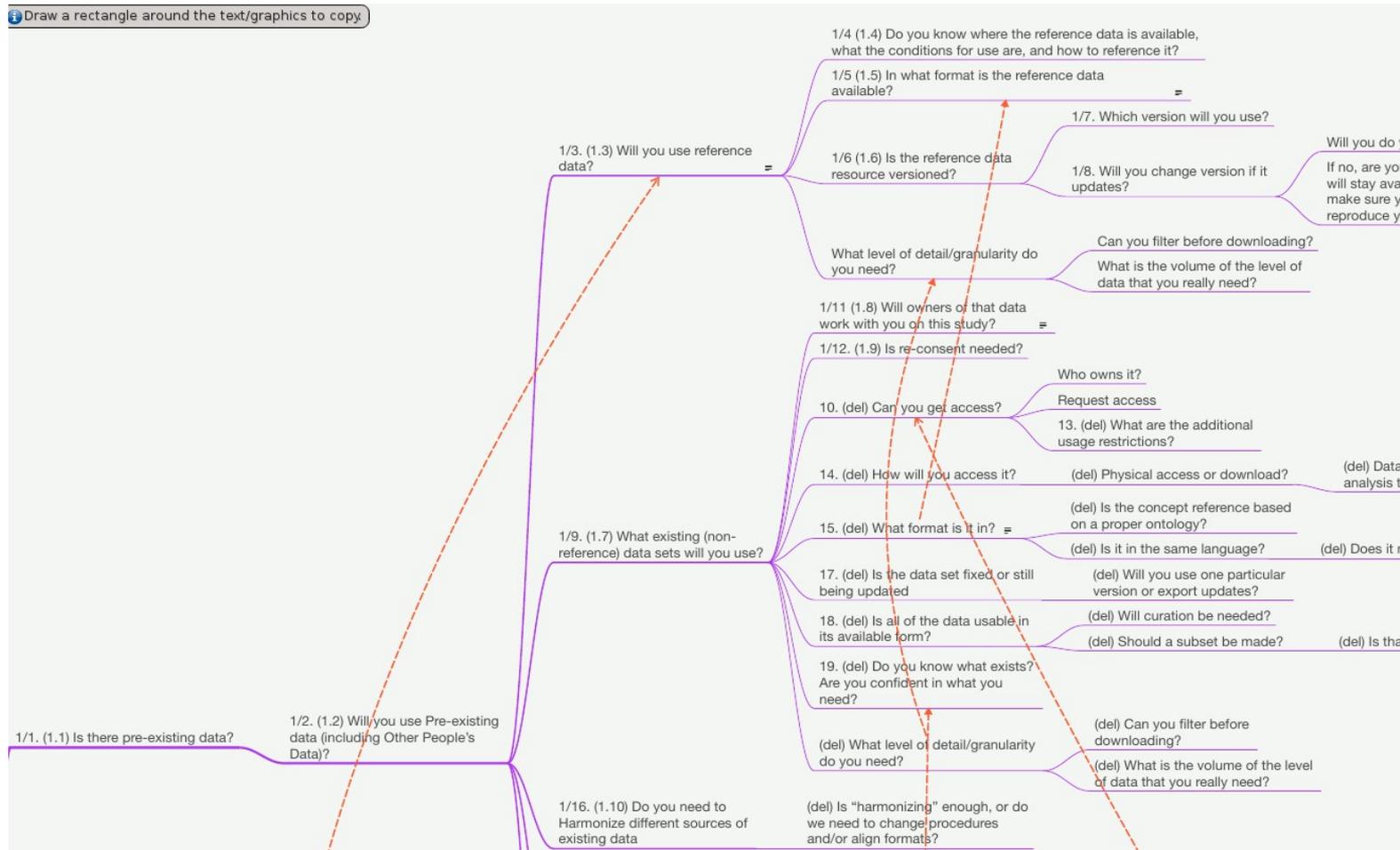
19 April 2016 – European Open Science Cloud



Giving a major boost to Open Science in Europe, the Commission today presented its blueprint for cloud-based services and world-class data infrastructure to

Open Data in Europe

Research Data Management



Roadmap: A Research Data Management Advisory Platform

▼ [Stephanie Simms](#), [Sarah Jones](#), [Kevin Ashley](#), [Marta Ribeiro](#), [John Chodacki](#), [Stephen Abrams](#), [Marisa Strong](#)

Executive summary

The DMPTool and DMPonline were developed to meet an... data policies and each is now well established as *the* resource... data management plans (DMPs) in the US and UK resp... organizations, the California Digital Library (CDL) and the D... enabling researchers to comply with funder requirements in... along the road to advancing open science.



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FAIR data

Open data
is about
MORE
THAN
DISCLOSURE
it must be
Fair

- Findable
- Accessible
- Interoperable
- Reusable

nature.com > scientific data > comment > article

SCIENTIFIC DATA

Altmetric: 454 Views: 31,944 Citations: 26 [More detail >>](#)

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The FAIR Guiding Principles for scientific data management and stewardship

Mark D. Wilkinson, Michel Dumontier [...] Barend Mons

Abstract

There is an urgent need to improve the infrastructure supporting the reuse of scholarly data. A diverse set of stakeholders—representing academia, industry, funding agencies, and scholarly publishers—have come together to design and jointly endorse a concise and measurable set of principles that we refer to as the FAIR Data Principles. The intent is that these may act as a guideline for those wishing to enhance the reusability of their data holdings. Distinct from peer initiatives that

doi:10.1038/sdata.2016.18

Reality: Research Data Management

- Unclear agreements in H2020 data pilot (many exceptions)
- Too late thinking about CLW
- No resources set aside for RDM

- The European Laws
 - Database protection
 - Hyperlinking!



What can we do?

- Start doing RDM and release Open Data
- There is a clear need to fund a research data infrastructure itself
 - this is cheaper with Open Source solutions
 - plenty of solutions exist for RDM
 - must be a scalable, distributed approach
- All stakeholders must take their responsibilities
 - Early and clear IP agreements
 - CLW, CLW, CLW, CLW



CC-BY-SA 2.0, "Protector of the sheep":
https://commons.wikimedia.org/wiki/File:Protector_of_the_sheep.jpg



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Egon Willighagen

Biography

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Assistant professor (Dutch: "universitair docent") at the Department of Bioinformatics - BiGCaT group at Maastricht University. Working on the eNanoMapper project on safety and systems biology of nanomaterials and metabolomics mashed up with WikiPathways and other data sources.

Also known as

Egon L. Willighagen

Country

Netherlands

Keywords

statistics, cheminformatics,
chemometrics, bioinformatics,
chemistry development kit,
metabolomics, predictive
toxicology, nanoqsar

Other IDs

Scopus Author ID: [6507481906](#)



Education (2)



Employment (7)



Works (80)

Funding (1)

Sort

SPLASH, a hashed identifier for mass spectra

Nature Biotechnology

2016-11-08 | journal-article

DOI: [10.1038/nbt.3689](https://doi.org/10.1038/nbt.3689)

Source: Crossref

Preferred source



XMetDB: an open access database for xenobiotic metabolism

Journal of Cheminformatics

2016-09 | journal-article

DOI: [10.1186/s13321-016-0161-3](https://doi.org/10.1186/s13321-016-0161-3)