

# SPARQL access to linked data



NanoCommons  
Nano-Knowledge Community



## Presentation – linked data

- ▶ WikiPathways & AOP-Wiki
- ▶ SNORQL User Interface
- ▶ SPARQL

## Demo

- ▶ WikiPathways
- ▶ AOP-Wiki

## Take home

- ▶ Q&A

*NanoCommons & NanoSolveIT Webinar, 2021-03-23, #nanocommons*

*by **Marvin Martens & Ammar Ammar**, Uni Maastricht, NL*

*This projects have received funding from the European Union Horizon 2020 Programme (H2020) under grant agreements no. 731032 & 814572.*

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Martin Himly (PLUS)  
Chair WG-A Education,  
Training, Communication

[www.nanosafetycluster.eu](http://www.nanosafetycluster.eu)



## User Guidance Handbook @ [www.nanocommons.eu](http://www.nanocommons.eu)

- ▶ <https://www.nanocommons.eu/e-infrastructure/user-guidance-handbook/>

## Training events and materials @ NanoCommons infrastructure

- ▶ <https://infrastructure.nanocommons.eu/events/>

- ↳ NSC Education Day Session 1
- ↳ SmartNanoTox Final Conference

## NanoCommons @ ELIXIR TeSS

- ▶ [https://tess.elixir-europe.org/content\\_providers/nanocommons#events](https://tess.elixir-europe.org/content_providers/nanocommons#events)

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# NanoCommons User Guidance Handbook

Home / e-Infrastructure / NanoCommons User Guidance Handbook



NanoCommons  
Nano-Knowledge Community



Overview Data management Nanoinformatics Workflows Electronic lab notebooks Ontologies

**NanoCommons**  
Nano-Knowledge Community

**The European Nanotechnology Community Informatics Platform: Bridging data and disciplinary gaps for industry and regulators**

The project has received funding from the European Union Horizon 2020 Programme (1010220) under grant agreement No. 721502

**Overview**

- H2020 research infrastructure project
- Call topic: NPM-NI-02-2019-2021: Integrating Activities for Advanced Communities

Download [2.19 MB]

**US - EU**  
Collaborative Community of Research

2020 U.S.-EU NanoEHS COR Workshop: Bridging Insights and Perspectives  
September 16-17, 2020

Workshop Report

2020 U.S.-EU NanoEHS COR Workshop:  
Bridging Insights and Perspectives  
September 16-17, Virtual Meeting

NanoCommons Desktop Hackathon - M...

**NanoCommons**  
Knowledge Community

zenodo

## NanoCommons – How can we help you?

## Working Towards a Harmonized Nanosafety E-Infrastructure for Data and In Silico Tools, 2020 U.S.-EU NanoEHS COR Workshop: Bridging Insights and Perspectives, September 16-17, Virtual Meeting

You can still register to see the recordings.

## Intro to NanoCommons by Martin Himly, PLUS (at the Jaqpot Hackathon)

Online training tools for nanosafety assessment – NanoCommons for





# Events

Event	Organisations involved
<p>11th World Congress on Alternatives and Animal Use in the Life Science Conference</p> <p>22 – 26 Aug 2021 / Maastricht, NL</p>	<p>Universiteit Maastricht (UM)</p>
<p>Online SPARQL Access to WikiPathway and AOP-Wiki Webinar</p> <p>Webinar, Hackathon, Training, Workshop (organized by NanoCommons)</p> <p>23 Mar 2021</p>	<p>United Kingdom Research and Innovation (UKRI)</p> <p>BioNanoNet (BIONANONET)</p> <p>Universitat Salzburg / Paris Lodron University of Salzburg (PLUS)</p> <p>Universiteit Maastricht (UM)</p>
<p>European Researchers Night 2020</p> <p>Trade show / Exhibition, Webinar, Workshop (co-organized by NanoCommons)</p> <p>27 Nov 2020</p>	<p>Universitat Salzburg / Paris Lodron University of Salzburg (PLUS)</p>
<p>EU Nanosafety Cluster Training Day @ NanoSAFE 2020 Digital Conference</p> <p>Trade show / Exhibition, Webinar, Hackathon, Training, Workshop (organized by NanoCommons)</p> <p>23 Nov 2020 / Online</p>	<p>The University of Birmingham (UoB)</p> <p>Edelweiss Connect GmbH (EWC)</p> <p>United Kingdom Research and Innovation (UKRI)</p> <p>National Technical University of Athens (NTUA)</p> <p>National University of Ireland Dublin - University College Dublin (NUID-UCD)</p> <p>LEITAT - LEITENDE INSTITUTIONEN FÜR FÜR SENSITIVE ASSOCIATION (LEITAT)</p>

## Date Added

Anytime

## Scientific topic

Ontology and terminology 1

## Event type

Workshops and courses 5

Meetings and conferences 1

## Online

 Only show online events

## Country

Greece 1

## Organizer

NanoCommons 2

www.nanocommons.eu 2

Martin Himly, PLUS, Chair o... 1

Martin Himly, PLUS, Chair o... 1

## City

Athens 1

## Sponsor

EU H2020 4

## Target audience

mixed audience 4

modellers for nanosafety pr... 2

Bench biologists 1

+ Register event

Subscribe

What are events in TeSS?

Hide past events

Search events...

## 7 events found

Content provider: NanoCommons X

Grid

Map

Earliest

Ontological Annotation of Datasets: "1st NanoCommons Hackathon"  
9 October 2018

Athens, Greece



Annotating Your Experimental Data workshop  
28 April 2020



Online Jaqpot Hackathon  
3 June 2020



EU Nanosafety Cluster Training Day @ NanoSAFE 2020 Digital Conference  
23 November 2020



EU Nanosafety Cluster Education Day @ NanoSAFE 2020 Digital Conference  
16 November 2020



Getting into using ELNs for experimental and computational workflows  
14 July 2020



Online SPARQL Access to WikiPathways and AOP-Wiki Webinar  
23 March 2021



December 10, 2020

Presentation Open Access

Edit

New version

# EU NanoSafety Cluster Education Day @ NanoSafe 2020

Dr Martin Himly

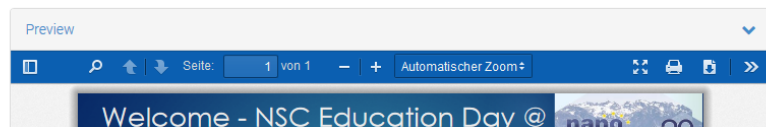
The EU NanoSafety Cluster WG-A on Education, Training, and Communication organized this Education Day on Nov 16 as satellite event of the NanoSafe Digital Congress 2020. This day acted as guidance for the entire NanoSafety community, including young researchers, to highlight how individual research projects fit as a puzzle piece into the wider picture. It was an orientation-giving and educational event depicting the overall strategy behind NanoSafe(ty).

## Means to achieve this included:

- to offer a **WG-overarching education/communication/discussion** event involving the audience *via* interactive sessions;
- to layout ways to **go beyond** with anything the nanosafety community have learned/developed to serve the emerging topics of Horizon Europe (emerging contaminants incl. microplastics, nanomedicine, safety assessment of novel/innovative/advanced materials for tomorrow along their entire life cycle);
- to foster participation in creating better sustainable materials (than e.g. nanosilver in socks), technologies, medical approaches, etc.
- to exhibit the perspectives of the NSC Working Groups and the different currently ongoing projects;
- to be **as interactive as possible** using **hands-on** activities, e.g., by showing **how-to** operate e-tools, upload/retrieve data to/from repositories & perform models;
- to facilitate vivid contribution to discussions using survey tools such as Mentimeter, WooClap, VoxVote, etc.
- to offer different perspectives in **pro/contra discussions**, e.g., by defining **challenger - defender roles taken by experts on specific topics** or evtl. by dividing attendees into zoom breakout rooms
- to show application of emerging NRG frameworks or SbD tools;
- to **request feedback** to user interfaces and enable stakeholder involvement

We herewith share and document the educational materials for later use by the scientific community.

Martin Himly, Chair of the EU NSC Working Group A with gratitude to all presenters for their contributions!



- ### Communities
- EU NanoSafety Cluster [Remove](#)
  - H2020 Infrastructure Project NanoCommons [Remove](#)
  - H2020 NMBP-15 Project SbD4Nano [Remove](#)
  - H2020 Project SABYDOMA [Remove](#)
  - Horizon2020 GRACIOUS [Remove](#)
  - Nano Risk Governance [Remove](#)
  - NanoSolveIT H2020 [Remove](#)
  - Nanoinformatics Project [Remove](#)

35

views

60

downloads

[See more details...](#)

Indexed in

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December 10, 2020

DOI:



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- Start
- Entdecken
- Abos
- Mediathek
- Verlauf
- Später ansehen
- Videos, die ich mag

ABOS

- UNIVERSAL MUSL...
- Kanäle finden

MEHR VON YOUTUBE

- YouTube Premium
- Filme
- Gaming
- Live
- Sport
- Einstellungen
- Meldeverlauf
- Hilfe
- Feedback senden

# NanoSafety Cluster



NanoSafety Cluster



NanoSafety Cluster  
28 Abonnenten

ABONNIEREN

- ÜBERSICHT
- VIDEOS
- PLAYLISTS
- KANÄLE
- KANALINFO

Uploads ▶ ALLE WIEDERGEBEN

17 Aufrufe • vor 1 Monat	13 Aufrufe • vor 1 Monat	39 Aufrufe • vor 1 Monat	15 Aufrufe • vor 1 Monat	11 Aufrufe • vor 1 Monat	15 Aufrufe • vor 1 Monat

# Online SPARQL Access to WikiPathways and AOP-Wiki

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**NanoCommons Webinar**  
**23-03-2021**



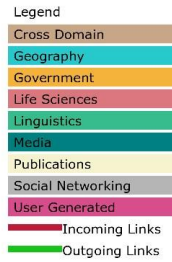
# Contents of the webinar

- Linked Data → Semantic Web Technologies → Life Sciences
- Introduction to WikiPathways and AOP-Wiki
- SNORQL User Interface (UI) for SPARQL exploration
- Brief description of SPARQL
- Demo of SNORQL UIs of WikiPathways and AOP-Wiki

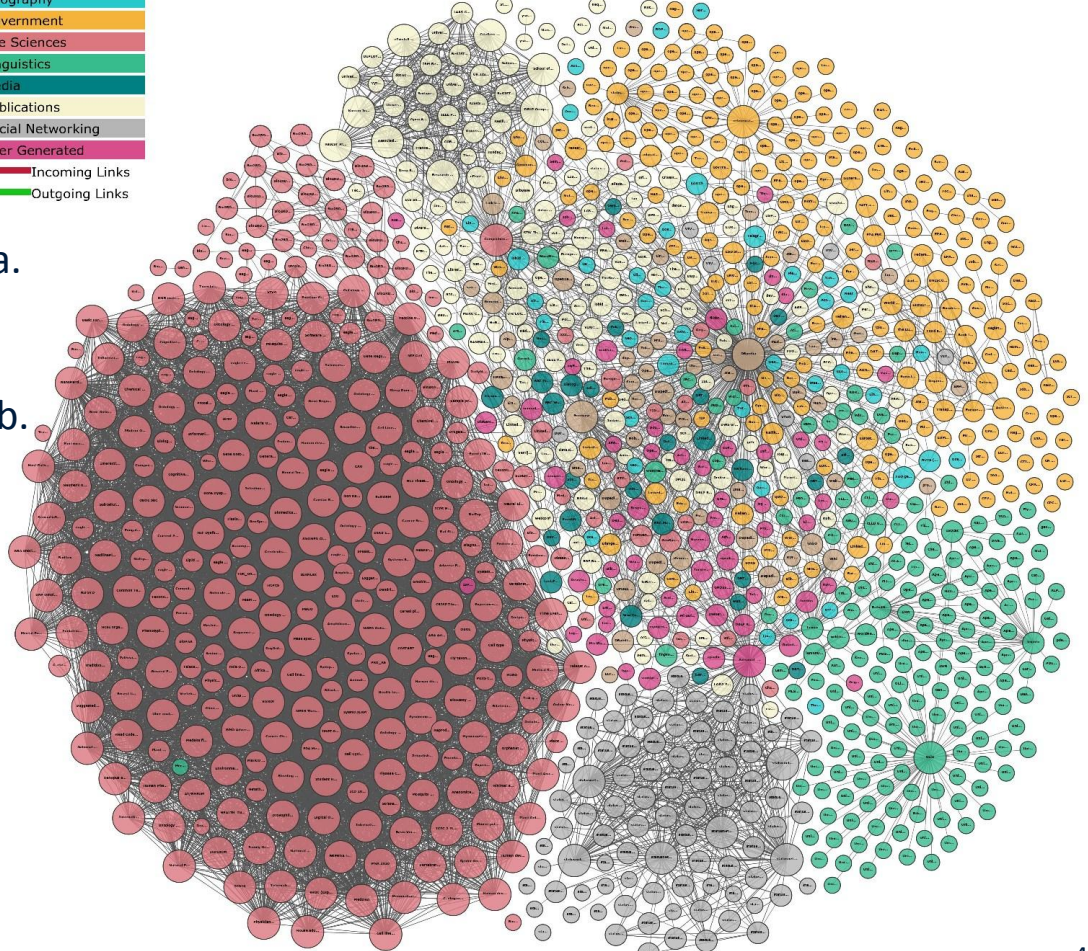
# Linked Data

# Linked data

- Moving from a web of linked documents to a web of linked data.
- Linked data is a set of design principles to share machine-readable data on the web.
- Value proposition:
  - Data integration of heterogeneous knowledge.
  - Increase data quality
  - Accessible to humans and machines
  - Enables analysis



<https://lod-cloud.net>

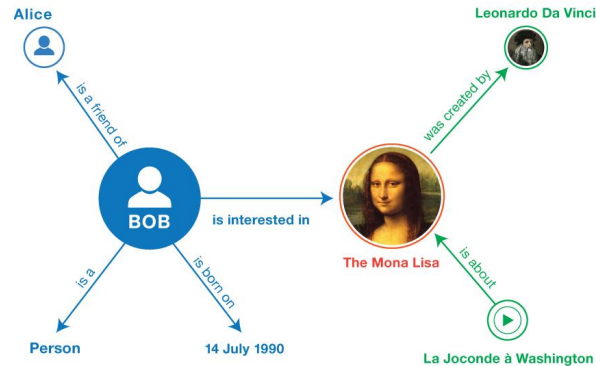
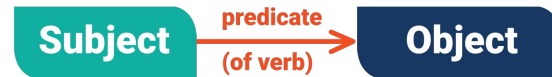


# RDF / SPARQL

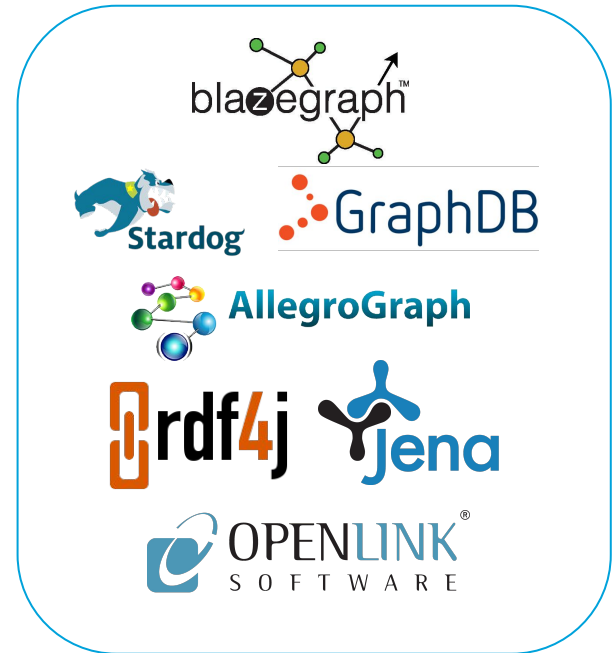
## Query Language



## Data representation/model



## Data store / Database



# RDF / SPARQL vs Relational DB / SQL

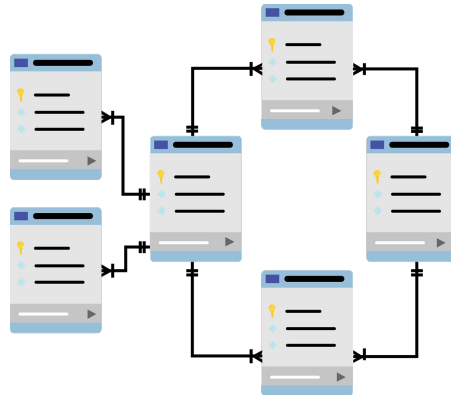
Query Language



Data representation/model

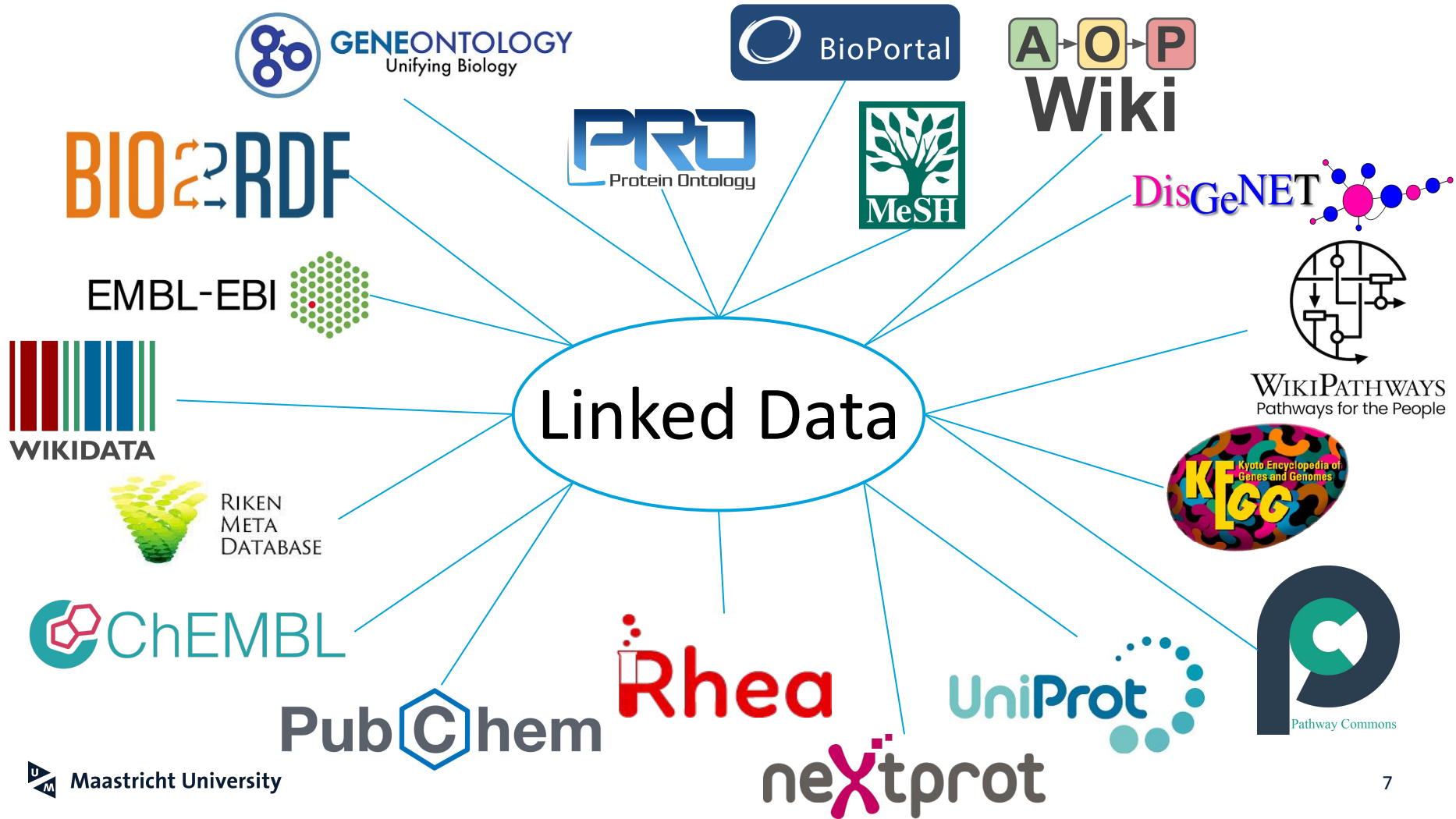


Data store / Database



Entity-Relation Diagram (ERD)





# The focus of the webinar



# WikiPathways

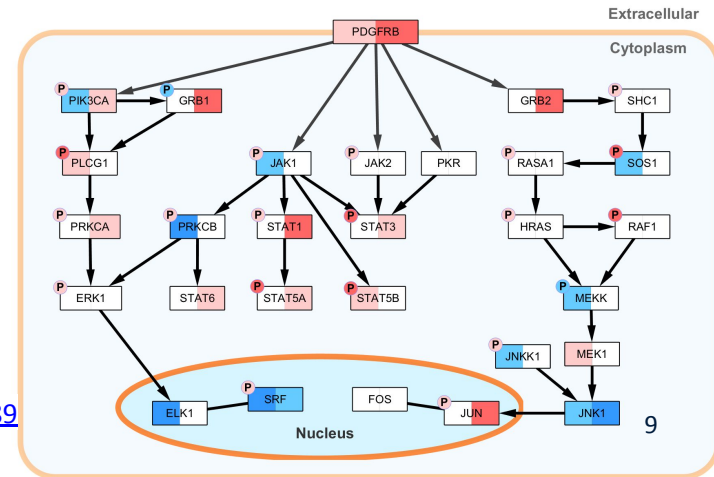
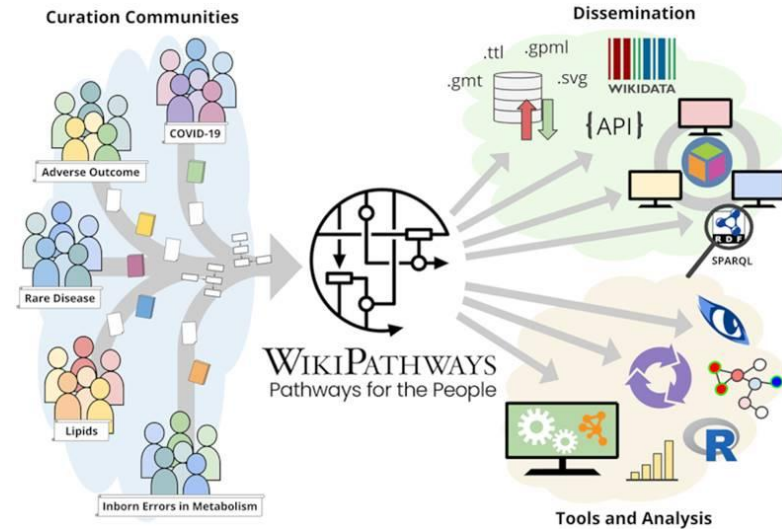
- A community resource to contribute and maintain biological knowledge in a form of pathways.
- Includes metabolic, signaling, regulatory and other types of pathways.
- Supports a variety of ways to integrate and interact with pathway content.
  - link-outs, image maps, RSS feeds and web services (e.g. REST API).
- Available as RDF and has a SPARQL endpoint

<http://sparql.wikipathways.org>

Martens M. et al. (2020) DOI: [10.1093/nar/gkaa1024](https://doi.org/10.1093/nar/gkaa1024)

Waagmeester A. et al. (2016) DOI: [10.1371/journal.pcbi.1004989](https://doi.org/10.1371/journal.pcbi.1004989)

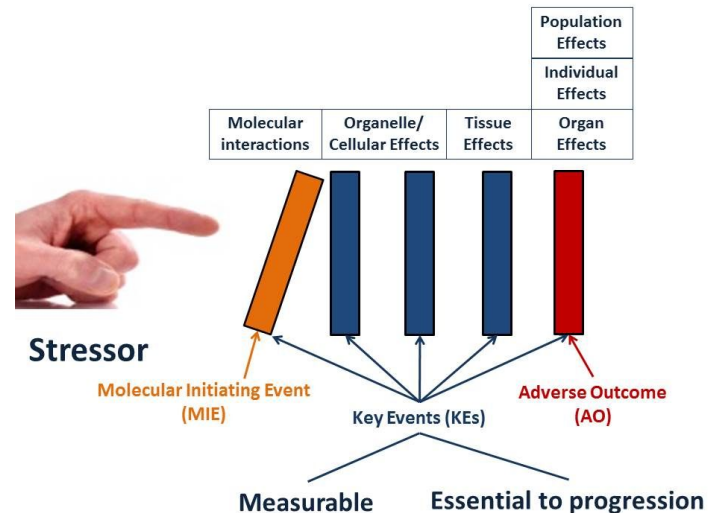
Pico A.R. et al. (2008) DOI: [10.1371/journal.pbio.0060184](https://doi.org/10.1371/journal.pbio.0060184)





# AOP Wiki

- Part of the AOP Knowledge Base
- Developed by EC JRC and US EPA
- Stores Adverse Outcome Pathways (AOPs)
  - Framework that captures mechanistic knowledge of toxicological processes to support decision making in risk assessments
- Transformed into RDF and available in SPARQL endpoint



Toxicology data



Knowledge-based  
regulatory risk  
assessment

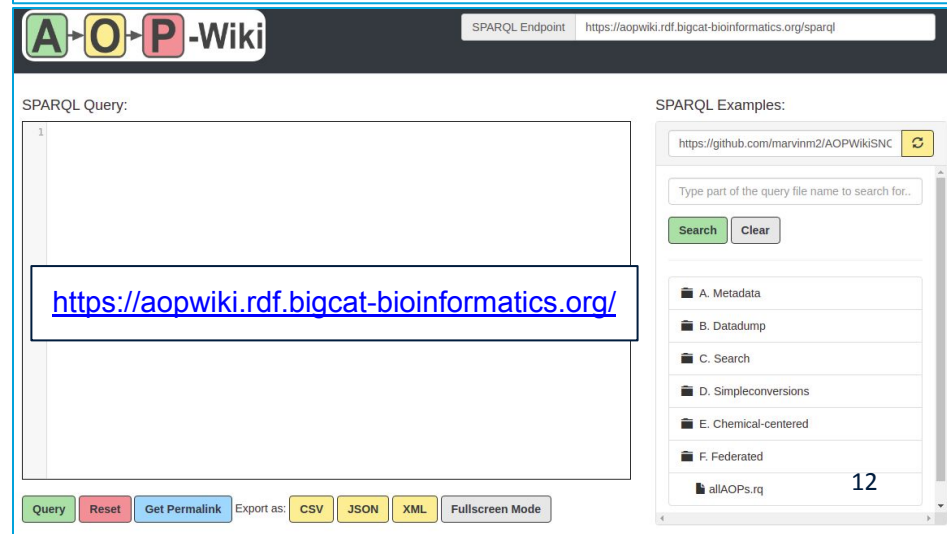
# SNORQL

# SNORQL User Interface

- It is a SPARQL explorer
- More user-friendly
- Functionalities
  - SPARQL editor
  - Query panel
  - Exports
  - Fullscreen
  - Sharing queries



The screenshot shows the SNORQL interface for the Wikidata endpoint. At the top, the logo for WIKIPATHWAYS "Pathways for the People" is visible. The SPARQL Endpoint is set to <http://sparql.wikipathways.org/sparql>. The main area is a SPARQL Query editor with a text area containing the URL <http://sparql.wikipathways.org/>. Below the editor are buttons for Query, Reset, Export CSV, Export JSON, Export XML, Get Permalink, and Fullscreen Mode. On the right, there is a sidebar for SPARQL Examples with a search bar and a list of categories: A. Metadata, B. Communities, C. Collaborations, D. General, E. Literature, F. Datadump, and G. Curation.



The screenshot shows the SNORQL interface for the AOPWiki endpoint. At the top, the logo for AOP-Wiki is visible. The SPARQL Endpoint is set to <https://aopwiki.rdf.bigcat-bioinformatics.org/sparql>. The main area is a SPARQL Query editor with a text area containing the URL <https://aopwiki.rdf.bigcat-bioinformatics.org/>. Below the editor are buttons for Query, Reset, Get Permalink, and Export as (with sub-buttons for CSV, JSON, XML), and Fullscreen Mode. On the right, there is a sidebar for SPARQL Examples with a search bar and a list of categories: A. Metadata, B. Datadump, C. Search, D. Simpleconversions, E. Chemical-centered, F. Federated, and allAOPs.rq. The number 12 is displayed at the bottom right of the sidebar.

# SPARQL editor provides SPARQL syntax highlighting



WIKIPATHWAYS  
Pathways for the People

SPARQL Endpoint

<http://sparql.wikipathways.org/sparql>

SPARQL Query:

```
1 SELECT DISTINCT ?DataNodeLabel ?PathwayTitle
2 WHERE {
3   ?DataNodes a wp:DataNode ; rdfs:label ?DataNodeLabel ; dcterms:isPartOf ?Pathway .
4   ?Pathway dc:title ?PathwayTitle .
5   FILTER (?PathwayTitle = "Apoptosis"@en) #replace to query other pathways
6 }
7
```

Query

Reset

Export CSV

Export JSON

Export XML

Get Permalink

Fullscreen Mode

SPARQL Examples:

<https://github.com/wikipathways/SPARQLC>



Type part of the query file name to search for..

Search

Clear

A. Metadata

B. Communities

C. Collaborations

D. General



## SPARQL Query:

1

[Query](#)[Reset](#)[Export CSV](#)[Export JSON](#)[Export XML](#)[Get Permalink](#)[Fullscreen Mode](#)

## SPARQL Examples:

1.

[Search](#)[Clear](#)[A. Metadata](#)[B. Communities](#)[C. Collaborations](#)[D. General](#)[E. Literature](#)[F. Datadump](#)[G. Curation](#)

- master 4 branches 0
- DeniseSl22 Update to more descri
- A. Metadata
- B. Communities
- C. Collaborations/ncExiProt
- D. General
- E. Literature
- F. Datadump
- G. Curation
- README.md

README.md

# SPARQLQueries

Queries for the [WikiPathways Snorql UI](#) automated loading

master SPARQLQueries / A. Metadata /

egonw Create linksets.rq

- ..
- datacounts
- datasources
- species
- linksets.rq
- metadata.rq

master SPARQLQueries / A. Metadata / metadata.rq

marvinm2 restructure and more queries

1 contributor

7 lines (7 sloc) | 192 Bytes

```
1 SELECT DISTINCT ?dataset (str(?titleLit) as ?title) ?date ?license
2 WHERE {
3   ?dataset a void:Dataset ;
4   dcterms:title ?titleLit ;
5   dcterms:license ?license ;
6   pav:createdOn ?date .
7 }
```

15

# SPARQL Query Examples panel

1. GitHub repository to load queries
2. Folders are reflected in the browser
3. Search queries

The screenshot shows a web interface titled "SPARQL Examples:". It features a list of items with a search bar and a file browser. The items are:

- 1. A URL input field containing "https://github.com/wikipathways/SPARQLC" with a refresh button.
- 3. A search bar with the placeholder text "Type part of the query file name to search for..." and "Search" and "Clear" buttons.
- 2. A file browser showing a tree structure:
  - A. Metadata
    - datacounts
    - datasources
    - linksets.rq
    - metadata.rq
    - species
  - B. Communities

The page number "16" is visible in the bottom right corner.

# Exports, full screen mode, and permanent links

Download as:

Export CSV

- CSV

Export JSON

- JSON

Export XML

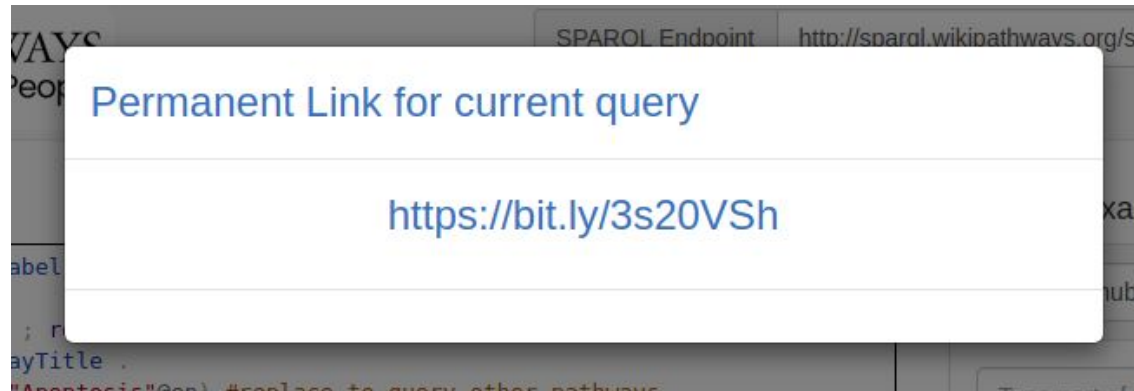
- XML

Fullscreen Mode

Enter full screen for spacious SPARQL query writing

Get Permalink

Get a sharable link for current query





# SPARQL

# SPARQL query structure (simplified)

```
1 SELECT ?variable1 ?variable2
2 # query select conditions
3 WHERE{
4     ?variabl1 ?p1 ?o1 .
5     ?variabl1 ?p2 ?variable2 .
6 }
7
8 ORDER BY ?variable
```

# SPARQL query structure (simplified)

```
1 SELECT ?variable1 ?variable2
2 # query select conditions
3 WHERE {
4     ?variabl1 ?p1 ?o1 .
5     ?variabl1 ?p2 ?variable2 .
6 }
7
8 ORDER BY ?variable
```

Keywords

End of triple (dot)

Comment

Variables in Results

# DEMO

# AOP-Wiki demo

Q1 - Number of AOPs, KEs, stressors

Q2 - KE-centered + methods + filtered for mito

Q3 - AOP-focus + all KEs

Q4 - multiple AOPs + all fibrosis AOPs + chems

Q5 - federated with WikiPathways, federated with other DBs

Q6 - switch query repo to nano-repo

# Take home messages

- RDF and SPARQL extend the databases' usability
  - Exploring data
  - Linking databases
- SNORQL creates a SPARQL workspace
  - Easier use of SPARQL queries
  - Flexible, adaptable layout
  - Ability of sharing queries quickly

# Thank you!

## Supervisors:

- Egon Willighagen
- Chris Evelo

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This project has received funding from the European Union's Horizon 2020 (EU 2020) research and innovation program under grant agreement no. 681002 (EU-ToxRisk), grant agreement no. 814572 (NanoSolveIT), and EINFRA-22-2016 program under grant agreement no. 731075 (OpenRiskNet).

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Thank you for joining our Webinar!

