# Expanding Adverse Outcome Pathway knowledge by creating AOP-Wiki RDF with semantic annotations to facilitate risk assessment of chemicals

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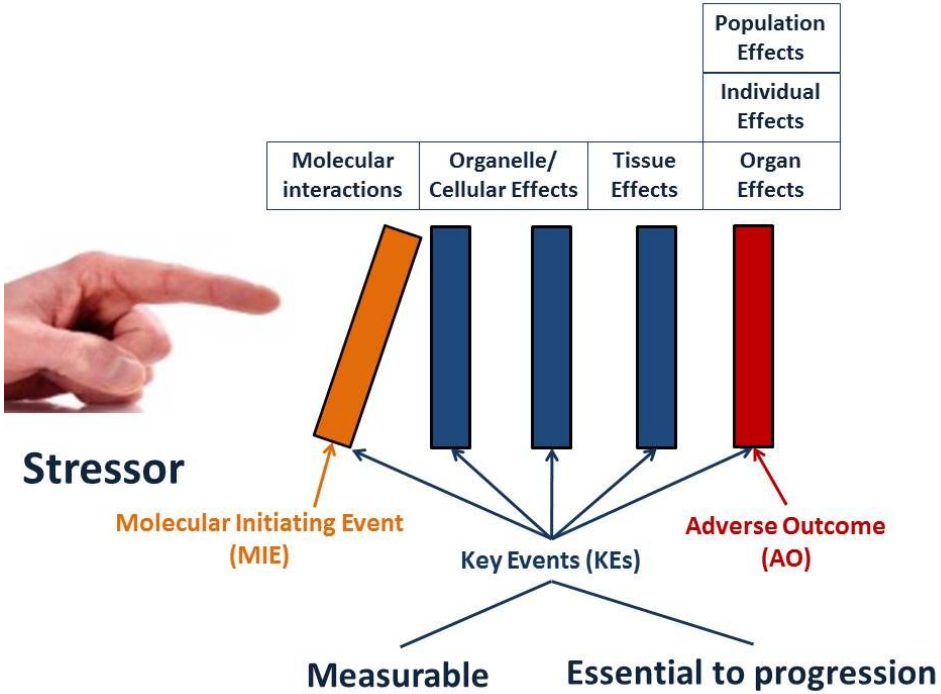
# Adverse Outcome Pathway (AOP) concept

Framework that captures mechanistic knowledge of toxicological processes to support decision making in risk assessments




Ankley et al. 2010: https://doi.org/10.1002/etc.34
Leist et al. 2017: https://doi.org/10.1007/s00204-017-2045-3

# Vision: Connect scientists and regulators

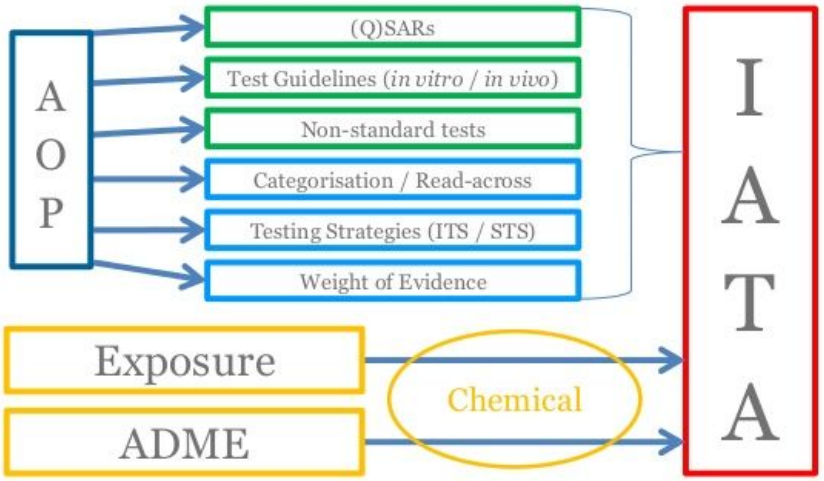
Toxicology data

Knowledge-based regulatory risk assessment

# AOPs can play major role in risk assessment

Aid **I**ntegrated **A**pproaches to **T**esting and **A**ssessment (IATA)

- Predictive value
- Less need for animal testing
- Identify knowledge gaps

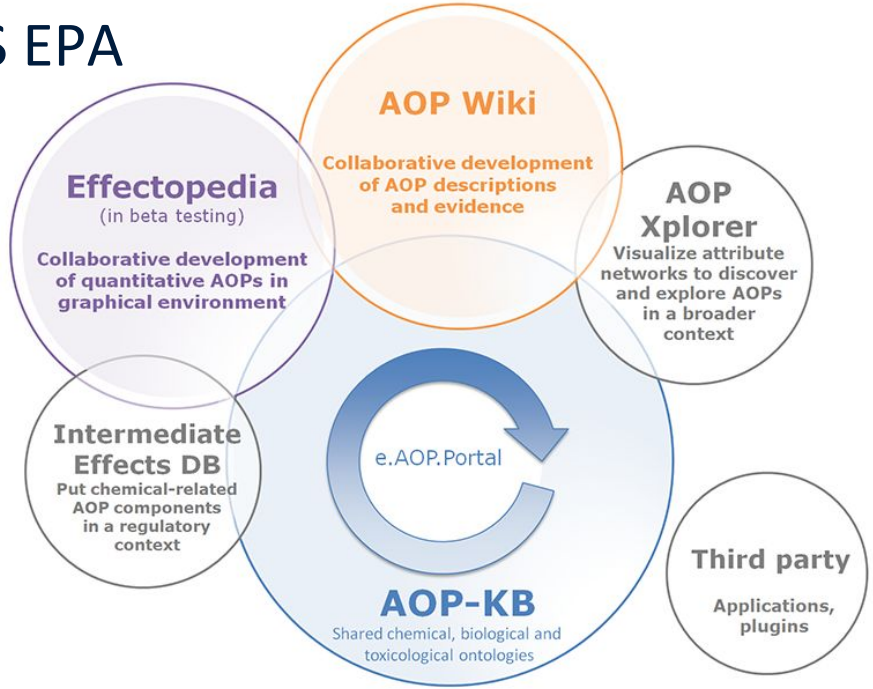


# Main AOP repository: AOP-Wiki

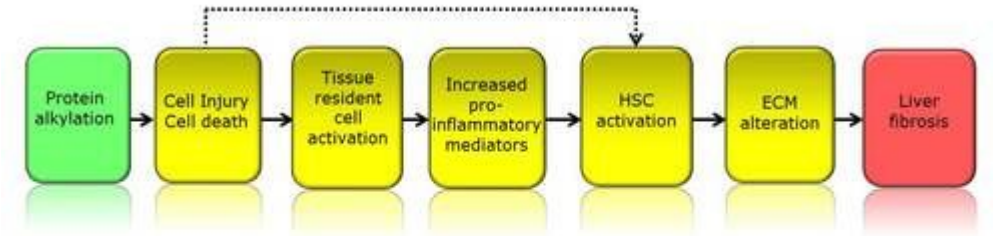
AOP-Wiki is the main qualitative AOP repository of the AOP-KB

Joint effort between EC-JRC and US EPA

| Element | Number |
|---|---|
| Adverse Outcome Pathways | 246 |
| Key Events | 1190 |
| Key Event Relationships | 1493 |
| Stressors | 438 |



# AOPs in AOP-Wiki contain many types of info



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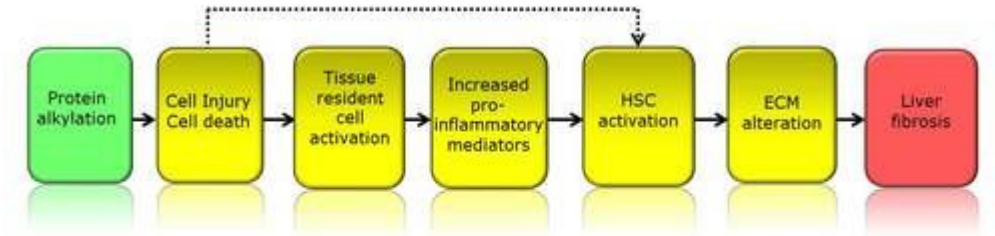
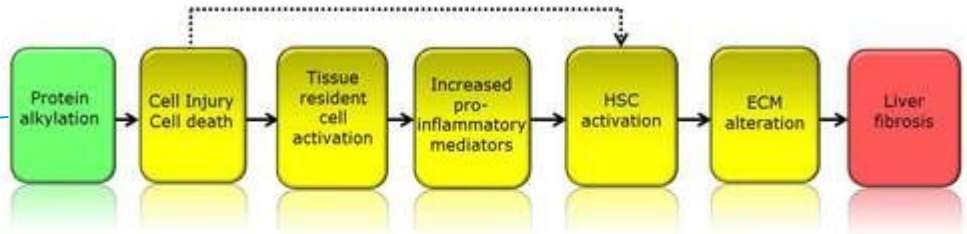



**Adverse Outcome Pathway:**
- Abstract
- Background
- Applicability
- Key Events
- Key Event Relationships
- Stressors
- Assessment

https://aopwiki.org/aops/38

# AOPs in AOP-Wiki contain many types of info

**Stressor:**
- Chemical
  - CAS
  - DSStox
  - InchiKey
  - Names
- Evidence
- Description

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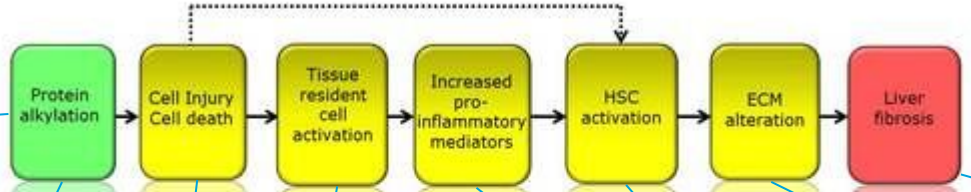


**Key Event:**
- Description
- Method
- Key Event components
  - Biological process
  - Biological object
  - Biological action
- Applicability
  - Taxonomy
  - Life stage
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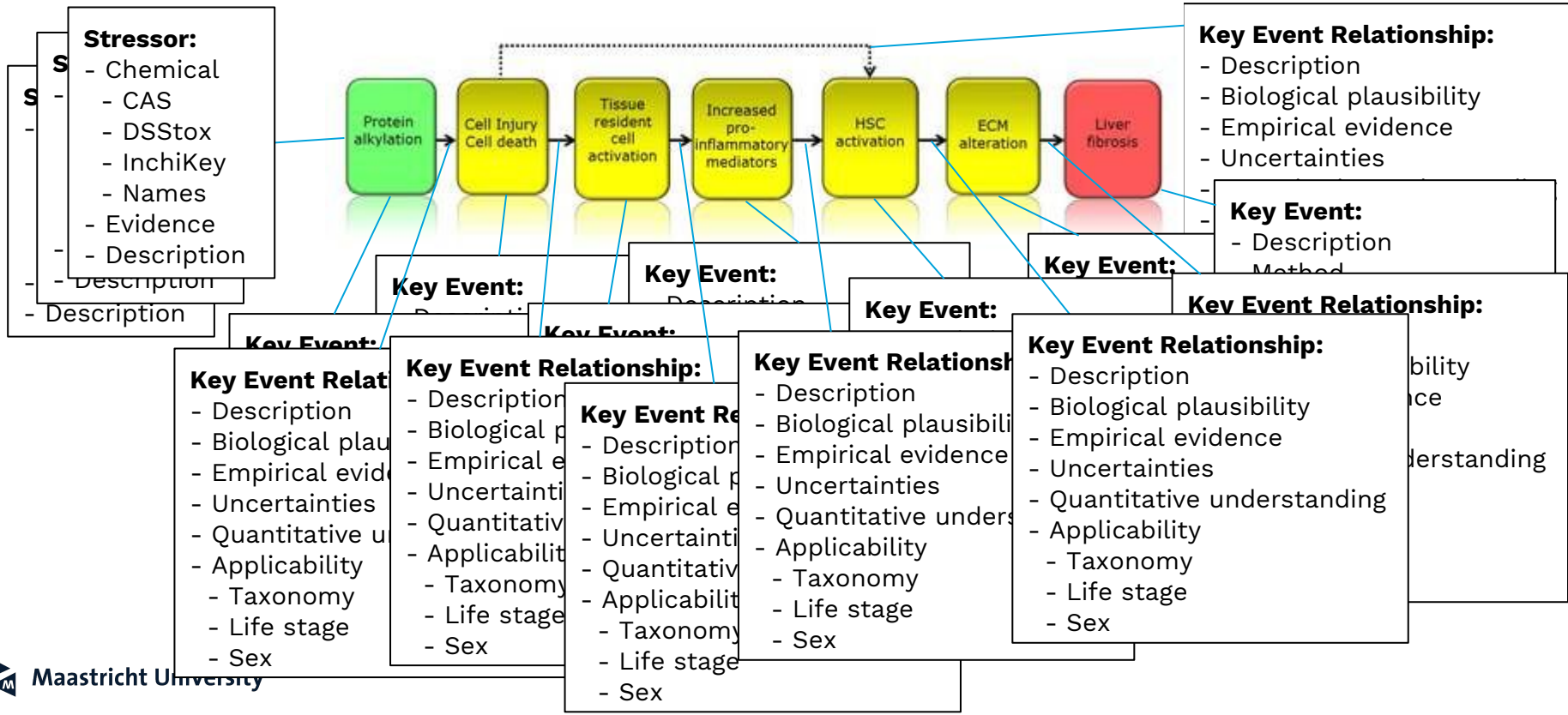
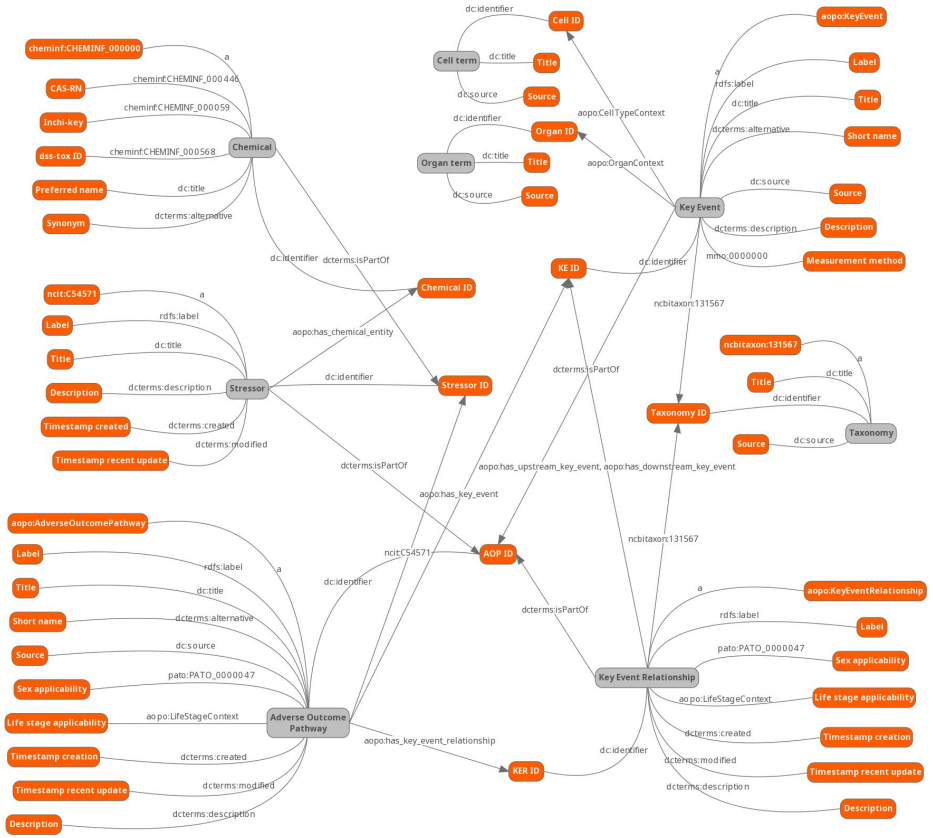


# RDF schema covers most of the AOP-Wiki

Main elements converted in RDF:

- Adverse Outcome Pathways
- Key Events
- Key Event Relationships
- Stressors
- Chemicals
- Taxonomy
- Cell-terms
- Organ-terms

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# AOP-Wiki RDF Virtuoso SPARQL endpoint

Deployed in OpenRiskNet e-infrastructure
As a SPARQL endpoint with AOP-Wiki RDF
using a Virtuoso base docker image:
(openlink/virtuoso-opensource-7)

Available from: [http://aopwiki-rdf.prod.openrisknet.org/sparql/](http://aopwiki-rdf.prod.openrisknet.org/sparql/)

Virtuoso SPARQL Query Editor

Default Data Set Name (Graph IRI)

Query Text

```
select distinct ?Concept where {[] a ?Concept} LIMIT 100
```

# SPARQL beginners course

Introduction to SPARQL in life sciences

Tomorrow, 14:00, Room 1+2

By Denise Slenter and Marvin Martens

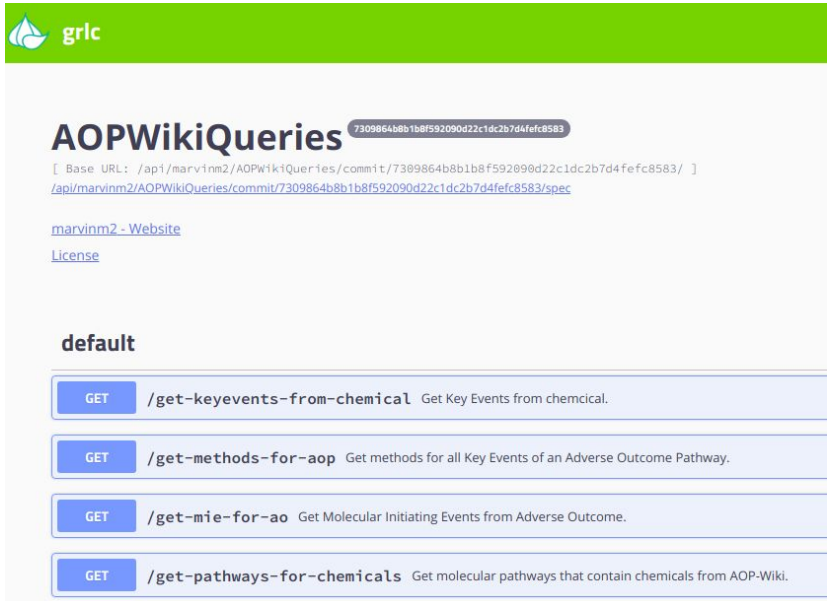
| Entity | # in Wikidata |
|---|---|
| Genes | 1044320 |
| Proteins | 744769 |
| Metabolites | 85866 |
| Chemicals | 157994 |

# SPARQL endpoint to Swagger UI:

Convert SPARQL queries into RESTful API's
Available from: [http://grlc.io/api/marvinm2/AOPWikiQueries](http://grlc.io/api/marvinm2/AOPWikiQueries)

Under development

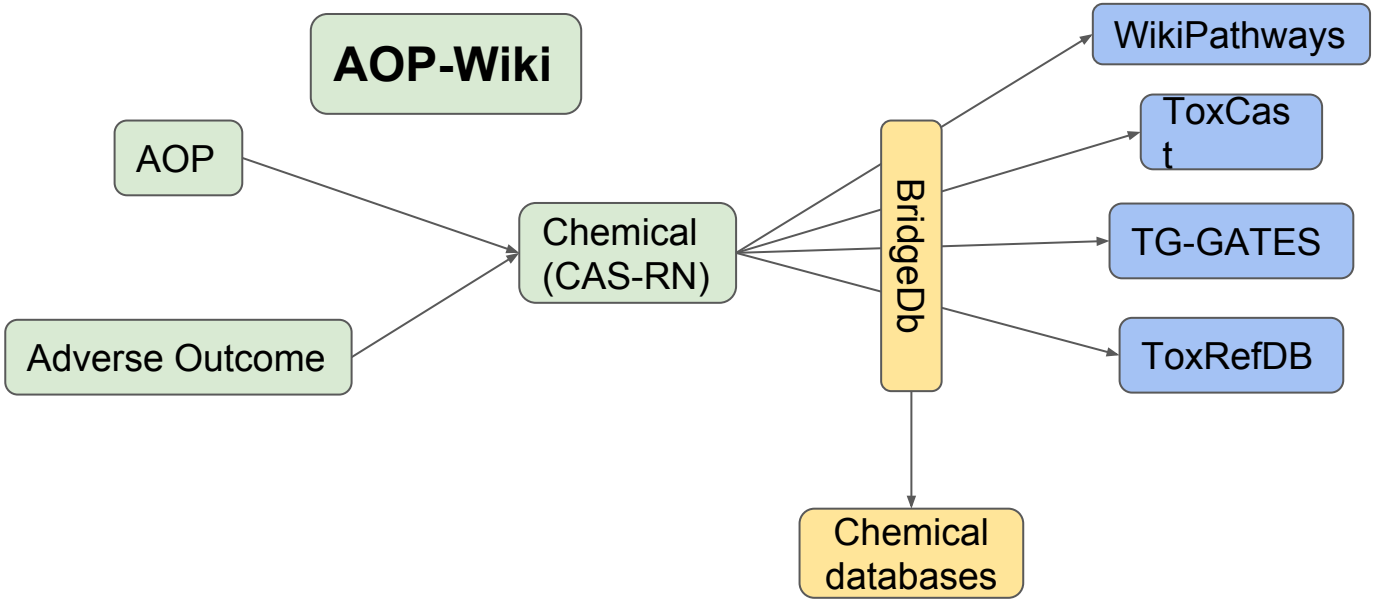
Available as Docker image






Meroño-Peñuela et al. https://doi.org/10.1007/978-3-319-47602-5_48

# AOP-Wiki in risk assessment workflows



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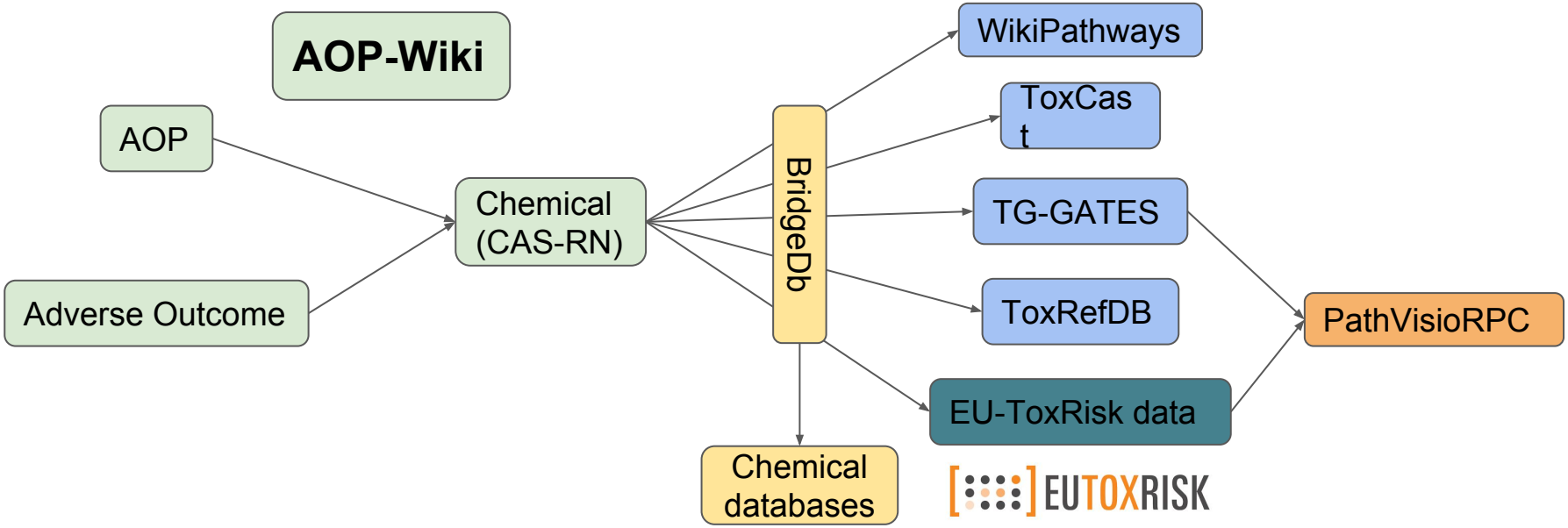


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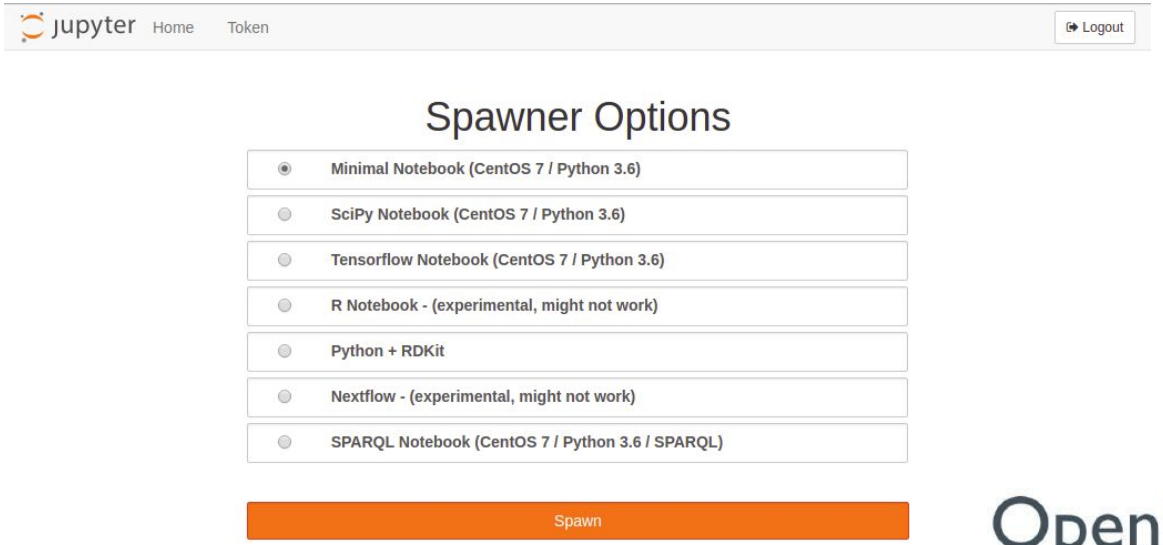
# Workflows in JupyterHub Docker

Jupyter notebooks allow systematic workflows

JupyterHub deployed in the OpenRiskNet e-Infrastructure

https://jupyterhub-jupyter.prod.openrisknet.org/hub/login



# Acknowledgements

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Chris Evelo

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