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Extracting targeted sub networks from FORUM for toxicological insight

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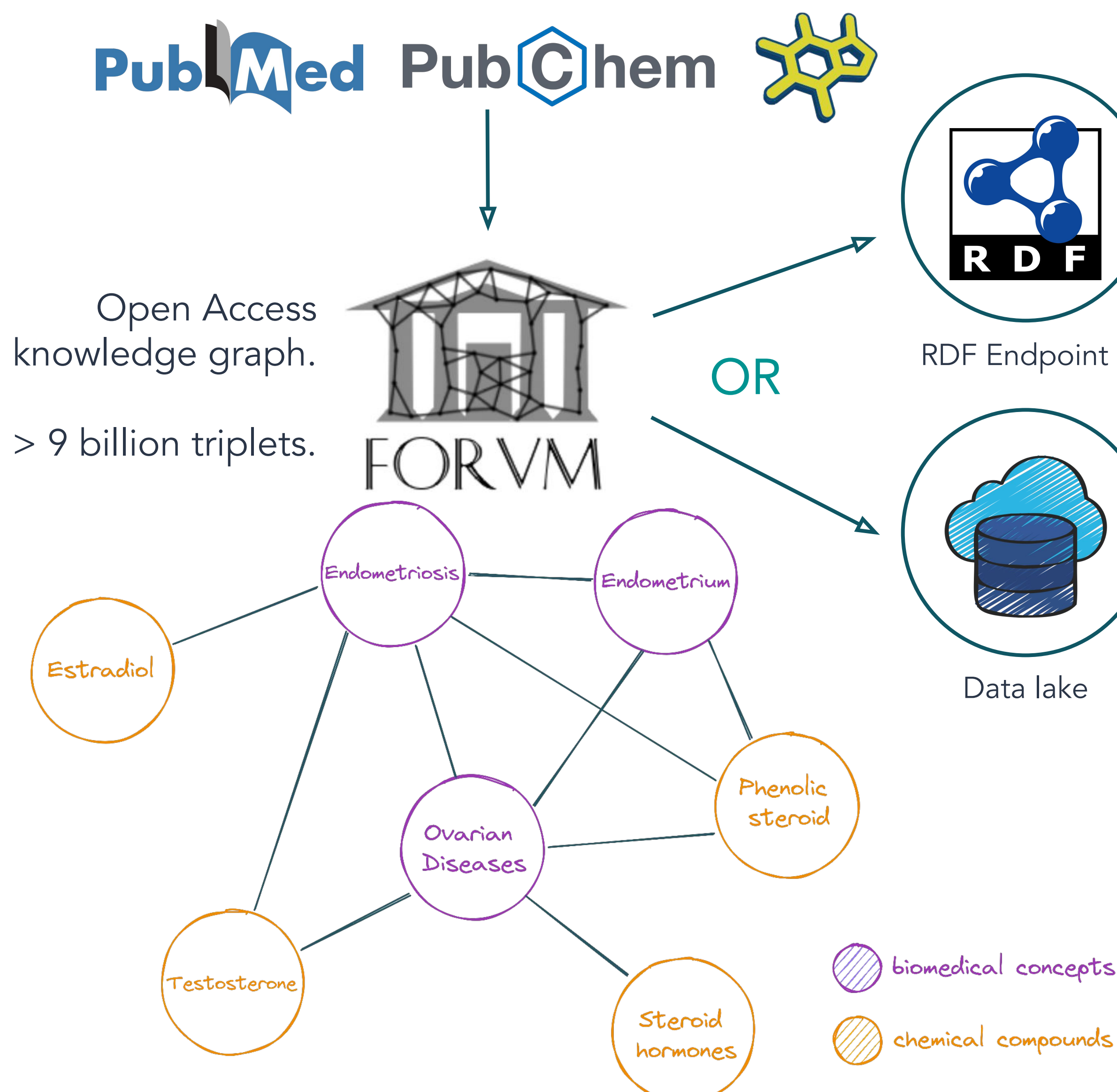
Background

To understand the connection between chemical compounds, metabolic changes, and health issues, it is necessary to connect metabolism knowledge with a broad set of modes of action leading to adverse effects on human health. FORUM, a knowledge graph (KG) with millions of associations for chemical compounds and biomedical concepts, addresses this challenge.

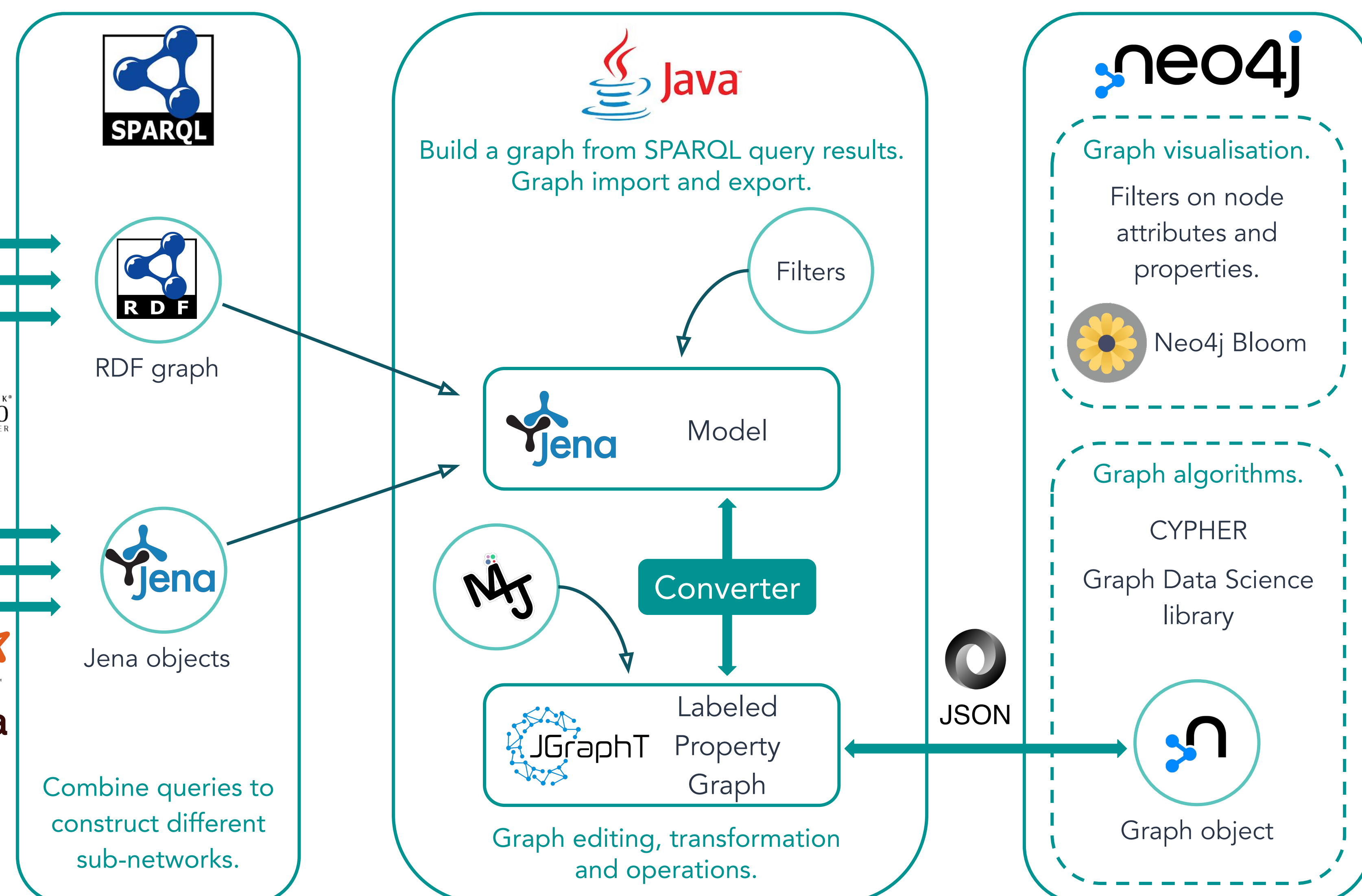
Our project focuses on developing a pipeline for creating knowledge graphs in biological studies, simplifying the analysis of toxicological pathways amidst big data. Through applying this pipeline to projects like Endoxomics [1], we aim to uncover key events linking persistent organic pollutants (POPs) to endometriosis pathophysiology, advancing our understanding of this complex condition.

FORUM: metabolism - biomedical KG

Automatic extraction of associations between compounds and biomedical concepts using metadata from scientific literature [2].



Workflow for building context specific KG

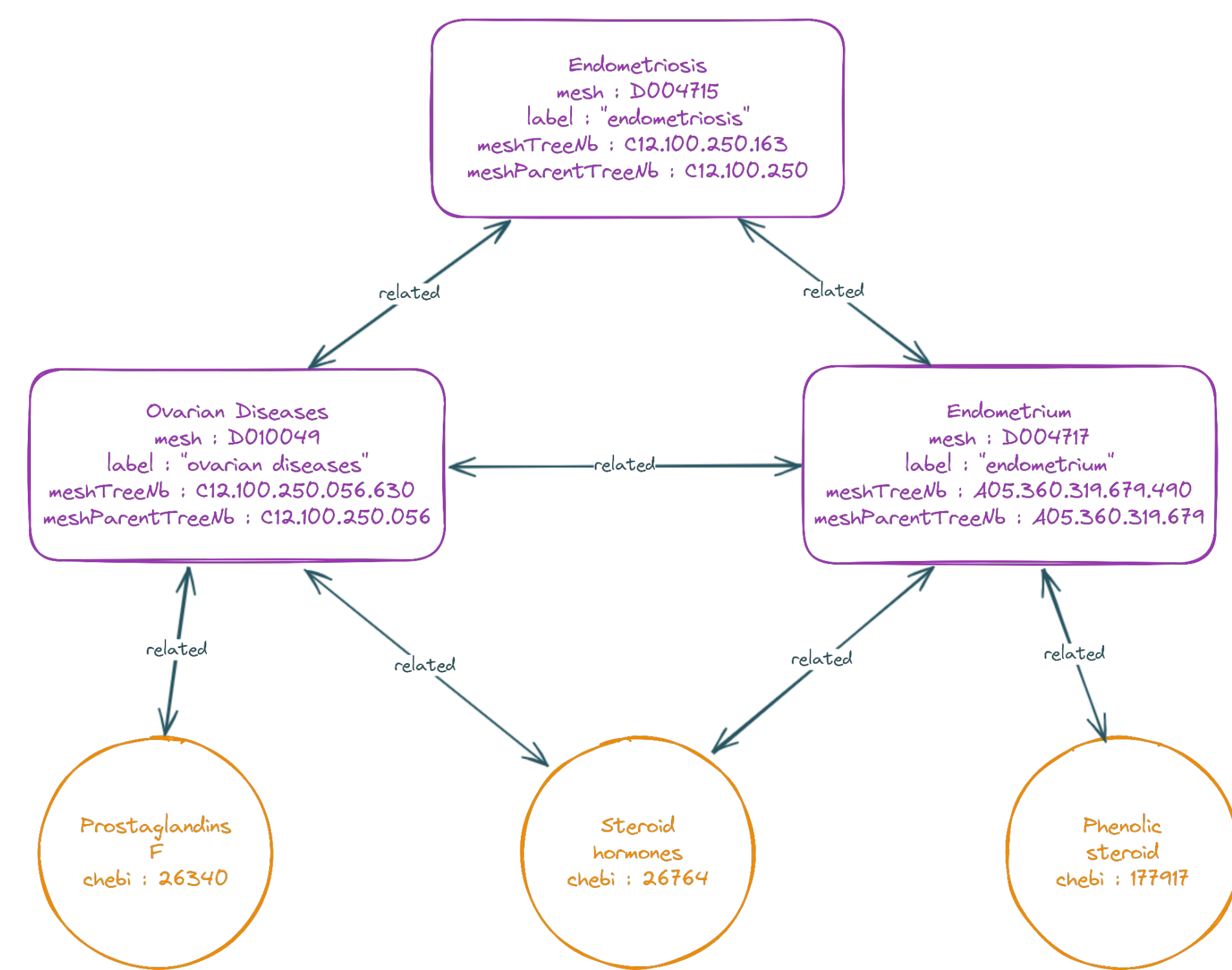


Converting a Resource Description Framework (RDF) graph to a Label Property Graph (LPG) transforms RDF triples into a lightweight model with nodes, relationships, and properties, making the graph easier to understand and more intuitive for querying specific graph patterns.

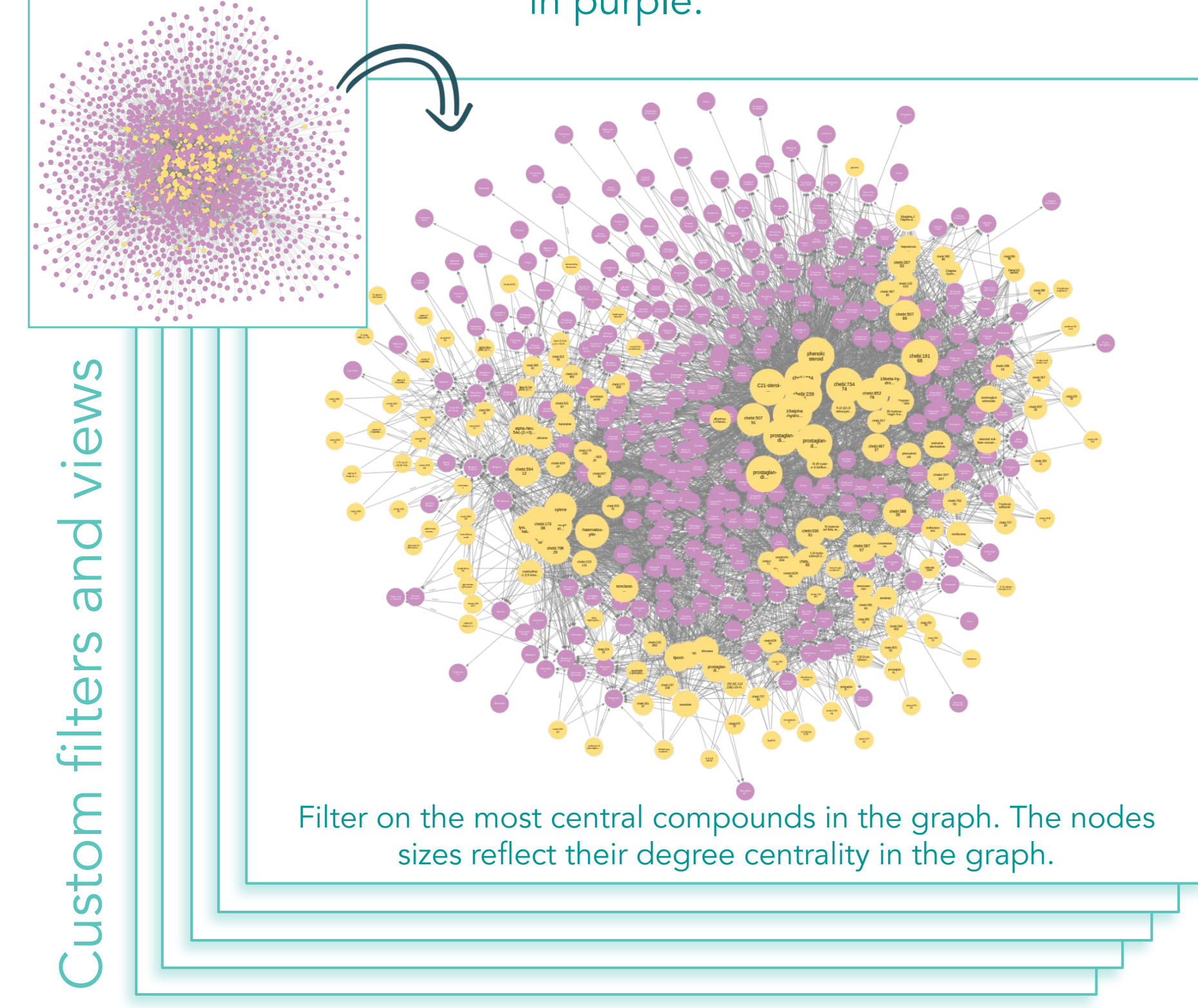
POC: links between endometriosis and pollutants

Application of the workflow to extract relevant information from FORUM and build a sub-network focused on endometriosis and persistent organic pollutants.

LPG graph resulting from the SPARQL query used to construct the sub-network. We extracted biomedical concepts related to endometriosis, their hierarchical organisation in the MeSH thesaurus, and their related chemical compounds.



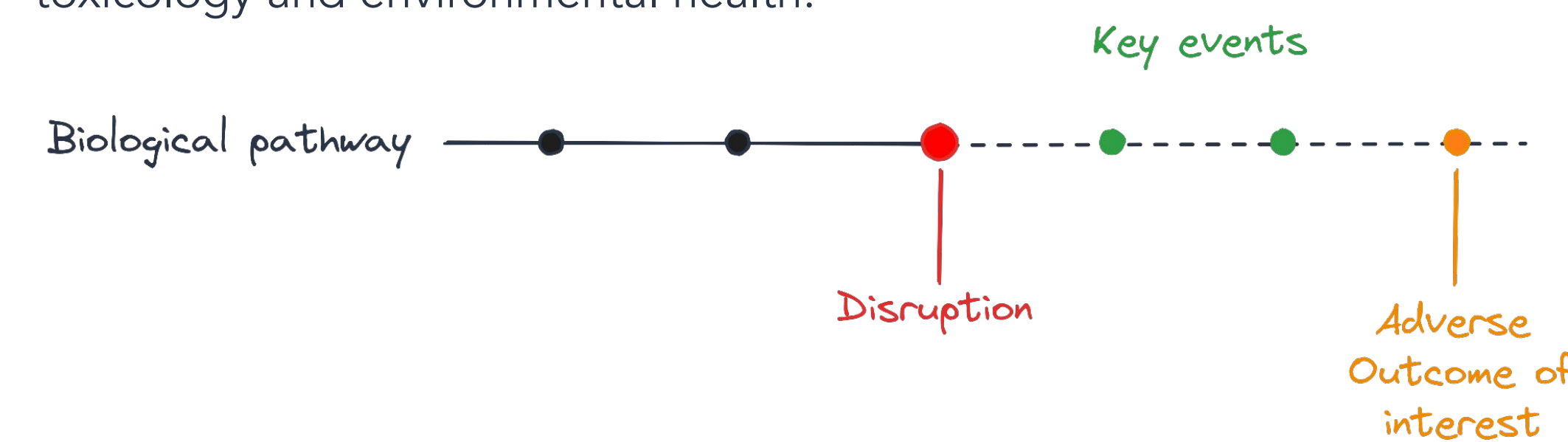
Knowledge graph focused on endometriosis. The biomedical concepts are represented in yellow and the chemical compounds in purple.



Perspectives

Adverse Outcome Pathways (AOPs)

AOPs consists of standardized and expert provided sequences of events leading to toxic effects [3]. The integration of AOPs into FORUM would enable researchers to better understand the toxicological effects of chemical compounds and their connections to metabolic pathways, thus facilitating more informed risk assessment and decision-making in toxicology and environmental health.



Scan to access the project code repository. <https://forgemia.inra.fr/metexplore/kg4j>



[1] Matta *et al.* Associations between persistent organic pollutants and endometriosis: A multiblock approach integrating metabolic and cytokine profiling. *Environ Int.* 2021 Oct 11;158:106926. doi: 10.1016/j.envint.2021.106926.

[2] Delmas *et al.* FORUM: building a Knowledge Graph from public databases and scientific literature to extract associations between chemicals and diseases. *Bioinformatics*, Volume 37, Issue 21, November 2021, Pages 3896–3904, doi: 10.1093/bioinformatics/btab627.

[3] Kleinstreuer *et al.* Adverse outcome pathways: From research to regulation scientific workshop report. *Regul Toxicol Pharmacol.* 2016 Apr;76:39–50. doi: 10.1016/j.yrtph.2016.01.007.