

# Discovery: Empowering Access and Reusability of RDF Graphs with a Programming Query Builder

Olivier Filangi<sup>1</sup>, Nils Paulhe<sup>2</sup>, Clément Frainay<sup>3</sup>, and Franck  
Giacomoni<sup>2</sup>

<sup>1</sup> IGEPP, INRAE, Institut Agro, Université de Rennes, Domaine de la Motte, Le Rheu 35653, France <sup>2</sup> Université Clermont Auvergne, INRAE, UNH, Plateforme d'Exploration du Métabolisme, MetaboHUB Clermont, Clermont-Ferrand, France <sup>3</sup> Toxalim (Research Center in Food Toxicology), Université de Toulouse, INRAE, ENVT, INP-Purpan, UPS, Toulouse 31300, France

DOI: [10.xxxxxx/draft](https://doi.org/10.xxxxxx/draft)

## Software

- [Review](#)
- [Repository](#)
- [Archive](#)

Editor: [Open Journals](#)

## Reviewers:

- [@openjournals](#)

Submitted: 01 January 1970

Published: unpublished

## License

Authors of papers retain copyright and release the work under a Creative Commons Attribution 4.0 International License ([CC BY 4.0](#)).

## Summary

Linked data is increasingly available on the web and has been widely adopted by the bioinformatics community. However, it is not common to find APIs that enable the direct use of semantic information in web interfaces. This often leads web application designers to incorporate this information into relational databases, as they can benefit from the query builder and object-relational mapping features that are widely used in this community.

We have developed Discovery, a free software library designed to easily build intuitive and interactive user interfaces to exploit RDF data in graphical form. The API provides a dedicated query language to create and maintain complex queries to be used in a client or server side web development environment. We used Discovery to implement functionality in web decision support applications within the MetaboHUB consortium (French national Metabolomics and Fluxomics infrastructure) : FORUM (Delmas et al., 2021) (Metabolism Knowledge Network Portal) and PeakForest (Paulhe et al., 2022) (The Metabolomics spectral database web portal).

## Statement of need

Nowaday, the use of semantic web technologies into bioinformatics has become ubiquitous across all domains of life sciences (Wu & Yamaguchi, 2014). Many bioinformatics resources is now organized according to the FAIR (Findable, Accessible, Interoperable, and Reusable) principles (Wilkinson et al., 2016), enabling efficient management and reuse of data in both research and industrial settings. This implementation was made possible by the standardized languages and protocols defined by the World Wide Web Consortium (W3C) such as the Resource Description Framework (RDF) which provides a versatile framework for representing data and knowledge in a machine-readable format and the SPARQL query language to exploit these data known as knowledge graphs.

Bioinformatics communities are encouraged to develop ontologies that adhere to the principles of the Basic Formal Ontology (Otte et al., 2022) and the Open Biological and Biomedical Ontology Foundry (Otte et al., 2022). These ontologies aim to structure the modelling of knowledge in a common conceptual framework and allow the reuse of existing ontologies, favouring collaboration between different research communities. The datasets, now structured, use controlled vocabularies and taxonomies to use unambiguous standard terms.

Effective tools (BioPortal (Noy et al., 2009), EMBL-EBI Ontology Lookup Service (Côté et al., 2006) and AgroPortal (Jonquet et al., 2018)) exist to access ontologies and datasets. In addition, these resources can be imported into RDF data store, also known as triplet store,

41 to be exploited using the SPARQL query language. In conclusion, semantic web technologies  
42 have greatly facilitated the integration and exploitation of bioinformatics data, allowing the  
43 efficient management of large and complex datasets.

44 [MetaboHUB](#) is a French national infrastructure dedicated to research in metabolomics and  
45 fluxomics, with the aim of providing an integrated platform for the study of metabolic  
46 pathways and networks. This initiative brings together a wide range of academic and industrial  
47 partners, including experts in analytical chemistry and bioinformatics, to develop cutting-edge  
48 technologies and methodologies for metabolomics research. One of the key objectives of  
49 MetaboHUB is to ensure data and software interoperability within the consortium. In this  
50 context, our working group “Creating FAIR resources for knowledge mining” aims to organize  
51 data and metadata in RDF format, as well as to structure consortium software products into  
52 web components, allowing for better reuse and integration of resources within the scientific  
53 community. Presently, this has led to the establishment of a specialized infrastructure aimed  
54 at harnessing knowledge bases. Within these resources, we provide the metabolic community  
55 access to a knowledge graph that delineates connections between chemical compounds and  
56 the scientific literature([Delmas et al., 2021](#)). Additionally, we have introduced an expanded  
57 knowledge graph using a Bayesian framework, encompassing overlooked metabolites lacking  
58 annotated literature([Delmas et al., 2023](#)).

## 59 Overview of the General Design

60 The query generator relies on the manipulation of immutable data structures, a fundamental  
61 tenet of functional programming. Once created, these structures persist unaltered throughout  
62 the application’s execution, providing advantages such as improved code clarity and the  
63 avoidance of unintended side effects. Developers can effortlessly construct intricate SPARQL  
64 queries by combining merging immutable query fragments. This immutability is crucial for  
65 reducing bugs linked to unforeseen alterations in object state, thereby simplifying long-term  
66 code maintenance.

67 The Discovery API utilizes the [Scala.js](#) compiler to ensure compatibility with established  
68 JavaScript libraries, a critical aspect in the realm of web development. This functionality  
69 facilitates the smooth assimilation of widely-used JavaScript libraries, allowing for tasks like  
70 DOM manipulation and other UI-related functions within web components.

71 Furthermore, [Scala.js](#) produces optimized JavaScript code, a critical consideration in web  
72 applications where responsiveness and a seamless user interface are imperative. The synergy  
73 between functional programming in Scala and transpilation through [Scala.js](#) facilitates the  
74 manipulation of a high-level API, enabling developers to focus exclusively on the concepts  
75 dedicated to the construction of a query in the end.

76 Discovery incorporates a Query Builder (QB) to streamline the construction and generation of  
77 SPARQL queries. The queries are crafted iteratively, facilitated by a dedicated Query Language  
78 (DSL). This module is paired with a second module enabling the selection of the data source,  
79 be it a SPARQL endpoint or an RDF resource.

## Key Features

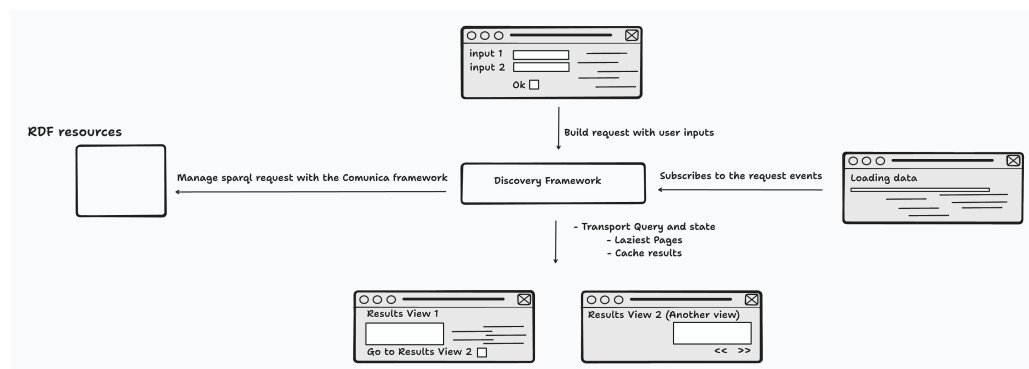


Figure 1: Interaction of the API Discovery with Web Components

## Elementary Building Blocks

A distinctive quality of the QB module is the categorization of construction elements, such as resources and qualifiers. Immutability is deliberately imposed, fortifying the security of the development process and simplifying debugging. This intentional structure promotes stability in query creation, a critical factor for precise and error-free development.

## Data Flow Management and Pagination

Addressing scalability concerns, the QB module incorporates intelligent pagination, particularly beneficial when crafting result lists with a significant number of elements. This optimization ensures the efficiency of queries and responses, enhancing the overall performance.

## Request Transport via String Serialization in a Web Architecture

Tailored for web development, Discovery's Query Builder introduces features such as string transport, simplifying component communication. Additionally, developers can enhance user queries by embedding metadata, providing contextual information within graphical representations for a more enriched user experience.

## Event Management for Dialog Box Notifications and User Interactions

## Asynchronous Results and Error Handling

The QB module places a premium on asynchronous result reception, ensuring the responsiveness of web applications. Developers can subscribe to events, staying abreast of specific interactions or changes and fostering a dynamic and interactive web development environment.

In essence, Discovery, as the Query Builder, serves as a pivotal guide in the intricate realm of SPARQL query generation. From streamlined configuration to categorization, scalability, and web-specific functionalities, this module empowers developers to navigate the complexities of web-based RDF data manipulation with precision and efficiency.

## Acknowledgements

## References

- Côté, R. G., Jones, P., Apweiler, R., & Hermjakob, H. (2006). The Ontology Lookup Service, a lightweight cross-platform tool for controlled vocabulary queries. *BMC Bioinformatics*, 7, 97. <https://doi.org/10.1186/1471-2105-7-97>
- Delmas, M., Filangi, O., Duperier, C., Paulhe, N., Vinson, F., Rodriguez-Mier, P., Giacomoni, F., Jourdan, F., & Frainay, C. (2023). Suggesting disease associations for overlooked metabolites using literature from metabolic neighbors. *GigaScience*, 12, giad065. <https://doi.org/10.1093/gigascience/giad065>
- Delmas, M., Filangi, O., Paulhe, N., Vinson, F., Duperier, C., Garrier, W., Saunier, P.-E., Pitarch, Y., Jourdan, F., Giacomoni, F., & Frainay, C. (2021). FORUM: Building a knowledge graph from public databases and scientific literature to extract associations between chemicals and diseases. *Bioinformatics*, 37(21), 3896–3904. <https://doi.org/10.1093/bioinformatics/btab627>
- Jonquet, C., Toulet, A., Arnaud, E., Aubin, S., Dzale-Yeumo, E., Emonet, V., Graybeal, J., Laporte, M.-A., Musen, M. A., Pesce, V., & Larmande, P. (2018). AgroPortal: A vocabulary and ontology repository for agronomy. *Computers and Electronics in Agriculture*. <https://doi.org/10.1016/j.compag.2017.10.012>
- Noy, N. F., Shah, N. H., Whetzel, P. L., Dai, B., Dorf, M., Griffith, N., Jonquet, C., Rubin, D. L., Storey, M.-A., Chute, C. G., & Musen, M. A. (2009). BioPortal: Ontologies and integrated data resources at the click of a mouse. *Nucleic Acids Research*, 37(Web Server issue), W170–173. <https://doi.org/10.1093/nar/gkp440>
- Otte, J. N., Beverley, J., Ruttenberg, A., Borgo, S., Galton, A., & Kutz, O. (2022). BFO: Basic formal Ontology1. *Appl. Ontol.*, 17(1), 17–43. <https://doi.org/10.3233/AO-220262>
- Paulhe, N., Canlet, C., Damont, A., Peyriga, L., Durand, S., Deborde, C., Alves, S., Bernillon, S., Berton, T., Bir, R., Bouville, A., Cahoreau, E., Centeno, D., Costantino, R., Debrauwer, L., Delabrière, A., Duperier, C., Emery, S., Flandin, A., ... Giacomoni, F. (2022). PeakForest: A multi-platform digital infrastructure for interoperable metabolite spectral data and metadata management. *Metabolomics*, 18(6), 40. <https://doi.org/10.1007/s11306-022-01899-3>
- Wilkinson, M. D., Dumontier, M., Aalbersberg, I. J., Appleton, G., Axton, M., Baak, A., Blomberg, N., Boiten, J.-W., Silva Santos, L. B. da, Bourne, P. E., Bouwman, J., Brookes, A. J., Clark, T., Crosas, M., Dillo, I., Dumon, O., Edmunds, S., Evelo, C. T., Finkers, R., ... Mons, B. (2016). The FAIR guiding principles for scientific data management and stewardship. *Scientific Data*, 3(1), 160018. <https://doi.org/10.1038/sdata.2016.18>
- Wu, H., & Yamaguchi, A. (2014). Semantic web technologies for the big data in life sciences. *Bioscience Trends*, 8(4), 192–201. <https://doi.org/10.5582/bst.2014.01048>