

NÚRIA QUERALT ROSINACH

Seeking to research on explainable AI over biomedical networks for knowledge discovery on Health

Amsterdam, NL

<https://nuriaqueralt.wordpress.com/>

github.com/NuriaQueralt

PROFESSIONAL EXPERIENCE

Researcher

Biosemantics Group at the Leiden Univeristy Medical Center

2020 – Present

Leiden, The Netherlands

- Exploit ontologies and FAIR data analytics
- Knowledge graph-based analytics with rare diseases and Covid-19

Python FAIR AI Ontology Genotype-Phenotype

Data scientist

Avillach Lab at Harvard Medical School

2019 – 2020

Boston, USA

- Implemented data access and data characterization jupyter notebooks workflows for the NIH Undiagnosed Diseases Network (UDN)
- Evaluated a new serverless cloud computing service for biomedical research on large-scale data sets

Python R API Rare diseases Patient registries AWS

Visiting researcher

The Bio-Ontology Research Group at KAUST

Aug 2019 – Nov 2019

Thuwal, Kingdom of Saudi Arabia

- Implemented a knowledge graph and a symbolic AI method for drug repurposing on metabolic rare diseases
- Developed ontology-based text mined metabolite-phenotype data sets for human and plants

Python OWLAPI Explainable AI Metabolic rare diseases

Drug repurposing Ontology-based text mining

Research associate

The Su Lab at Scripps Research

2016 – 2019

La Jolla, USA

- Developed a drug repurposing method for rare diseases
- Implemented the NGLY1 Deficiency knowledge graph for evidence-based biomedical hypothesis discovery and a Python library for its creation, use and management
- Implemented a Wikibase instance for community contribution to the NGLY1 Deficiency knowledge graph
- Created a provenance model for biomedical information in Wikidata

Python Curation Representation learning Machine Learning

Rare disease network Hypothesis generation API

Research fellow

Integrative Biomedical Informatics Group at the GRIB|UPF|IMIM

2012 – 2016

Barcelona, Spain

- Implemented the DisGeNET-RDF and nanopublication linked datasets and its accessibility and exploration, and integration to the Open PHACTS platform
- Developed a Disease Biomarker database and its Web interface for the eTOX project

RESEARCH INTERESTS

Data-knowledge integration
Networks Knowledge representation
Linked Data Hypothesis generation
Artificial intelligence Bioinformatics
Computational biology FAIR
Translational informatics BioNLP
Reproducible research Genomics
Phenomics Multi-omics integration
Precision medicine Rare diseases

EDUCATION

M.Sc. in Bioinformatics for Health Sciences

Pompeu Fabra University / Barcelona University

2006 – 2008

Barcelona, Spain

- Thesis title: *The role of a cation- π interaction in the agonist conformation of estrogen-like nuclear receptors Super-family*

PhD in Quantum Chemistry

Rovira i Virgili University

2002 – 2006

Tarragona, Spain

- Dissertation title: *Study of the magnetic coupling in hetero-metallic complexes with oxamido, oxamato, tiooxalato and analog bridged ligands*

B.Sc. in Chemistry

Rovira i Virgili University

1995 – 2001

Tarragona, Spain

- Thesis title: *Ab initio CASSCF and CASPT2 study of the photochemistry of bicyclo[3.1.0]hex-3-en-2-one*

Ongoing learning

Introduction to Logic

2019-present

Stanford University

Machine Learning

2019-present

Stanford University

Probabilistic Graphical Models

2019-present

Stanford University

LANGUAGES

Spanish, English
French



R Python Ontology Text mining Linked Data

BIOINFORMATICS PROJECTS



NGLY1 Deficiency structured review

A disease knowledge graph for hypothesis generation

Neo4j Wikibase Multi-disciplinary collaboration Motivation



DisGeNET platform

Discovery platform integrating information on gene-disease associations from several public data sources and the literature

RDF/OWL SPARQL Interoperability Team Work Flexibility



Open PHACTS platform

Open, interoperable information infrastructure for life science and drug discovery

Ontologies Nanopublications Pharmacology Professionalism
International communication FAIR



The BeFree system

Text mining tool to unlock the information contained in biomedical documents

Python Dictionaries Text mining Provenance Organization

SELECTED PUBLICATIONS

[1] N. Queralt-Rosinach, R. Kaliyaperumal, C. H. Bernabé, Q. Long, S. A. Joosten, H. J. van der Wijk, E. L. A. Flikkenschield, K. Burger, A. Jacobsen, B. Mons, M. Roos, BEAT-COVID Group, COVID-19 LUMC Group, Applying the FAIR principles to data in a hospital: challenges and opportunities in a pandemic, *J Biomed Semant*, 2022, 13, 12

[2] N. Queralt-Rosinach, G.S. Stupp, T.S. Li, M.D. Mayers, M. E. Hoatlin, M. Might, B.M. Good, A.I. Su, Structured Reviews for Data and Knowledge Driven Research, *Database*, 2020

[3] M. Alshahrani, M. A. Khan, O. Maddouri, A. R. Kinjo, N. Queralt-Rosinach, R. Hoehndorf, Neuro-symbolic representation learning on biological knowledge graphs, *Bioinformatics*, 2017, 33, 2723–2730

[4] N. Queralt-Rosinach, J. Piñero, À. Bravo, F. Sanz, L.I. Furlong, DisGeNET-RDF: Harnessing the Innovative Power of the Semantic Web to Explore the Genetic Basis of Diseases, *Bioinformatics*, 2016, 32, 2236–2238

[5] D. Digles, B. Zdrzil, J.-M. Neefs, H. Van Vlijmen, C. Herhaus, A. Caracoti, J. Brea, B. Roibás, M. Loza, N. Queralt-Rosinach, L. I. Furlong, A. Gaulton, L. Bartek, S. Senger, C. Chichester, O. Engkvist, C. Evelo, G. F. Ecker and E. Jacoby, Open PHACTS Computational Protocols for *in silico* Target Validation of Cellular Phenotypic Screens: Knowing the Knowns, *Med. Chem. Commun*, 2016, 7, 1237–1244

[6] À. Bravo, M. Cases, N. Queralt-Rosinach, F. Sanz, L.I. Furlong, A knowledge-driven approach to extract disease-related biomarkers from the literature, *BioMed Research International*, 2014, 2014, 253128

SKILLS

Software development

- **Programming:** Python, R, BASH, SPARQL, CYPHER, PHP, HTML, Perl, C, Fortran
- **Development:** Git/GitHub, Jupyter Notebook, Anaconda, PyCharm, RStudio, Docker

Knowledge base creation

- **Free-text:** BioNLP, Curation
- **Data engineering:** RDF, OWL, Neo4j, Wikibase, MySQL, Apache, and Virtuoso server management

Prediction and analysis

- **Databases:** WikiData, Monarch, EBI-RDF, UMLS, GO, Swissprot, PDB, NuclearRDB
- **Bioinformatics tools:** OWLAPI, Protegé, R&Bioconductor, IPA, Cytoscape, EMBOSS, RepeatMasker, ClustalW, MAMMOTH-mult, Pymol
- **Data science:** AWS SageMaker, PyKEEN, PyTorch, sklearn, Weka
- **Cloud computing:** AWS EC2

CONFERENCES

ICBO 2022

Knowledge graphs and Explainable AI for Drug Repurposing on Rare Diseases

📅 25-28 Sep 2022 📍 Ann Arbor, USA

ISMB/ECCB 2021

COVID-19 epidemiology and monitoring ontology

📅 25-30 Jul 2021 📍 Virtual

FOIS 2021

Reuse of Design Pattern Measurements for Health Data

📅 13-17 Sep 2021 📍 Bozen-Bolzano, Italy

ISWC 2020

FAIR Data Management to Access Patient Data

📅 1-6 Nov 2020 📍 Virtual

Biomedical Linked Annotation Hackathon 6

<https://blah6.linkedannotation.org/>

📅 4-7 February 2020 📍 Tokyo, Japan

BioHackathon 2019

<http://2019.biohackathon.org/>

📅 1-7 Sep 2019 📍 Fukuoka, Japan