

# Clémence Réda | Marie Skłodowska-Curie Postdoctoral Fellow @ Universität Rostock

(updated on 25/01/2024)

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## Biography & Major Achievements

The researcher's research journey led her to consider several aspects of drug development and repurposing, and got her acclimated to working in an interdisciplinary environment. In particular, her PhD was about the integration of a model of gene regulation into a drug repurposing pipeline, in order to properly assess the efficacy of a drug. In order to deal with the intrinsically stochastic regulatory mechanisms, she has designed a recommender system with multi-armed bandit algorithms which can deal with this stochasticity to estimate the most promising drug candidates in a sample-efficient way:

1. The researcher has worked on a method to automatically build disease-specific regulatory networks. This method allowed to retrieve in a transparent and reproducible way a cell-line-specific network from open-access databases. This method was applied to brain cell lines, on a subset of genes strongly coexpressed with epileptic phenotypes. She introduced for the first time a method which incorporates regulatory cascades and disease-specific transcriptomic information to detect master regulators, which can be targeted for better understanding the mechanisms behind the disease. This work led to a publication in the proceedings of the 20<sup>th</sup> *International Conference on Computational Methods in Systems Biology (CMSB 2022)* and an open-source software which was accepted by the *Journal of Open-Source Software (JOSS)* in 2023.
2. Multi-armed bandit algorithms were introduced by the researcher for the first time for drug repurposing, by tackling the problem of the identification of the  $N$  best arms/treatments in a set of  $K$  ones, using the known side information about these arms. In practice, this information is set of the drug signatures built upon transcriptomic data from the LINCS L1000 database. She introduced and studied a generic family of algorithms which solve this identification problem, that encompasses all prior adaptive sampling-based algorithms in the literature. Her co-authors and herself were able to study theoretically and empirically the effect of the model structure, especially linear models, on the performance of the algorithms. This work was published in the proceedings of the 24<sup>th</sup> *International Conference on Artificial Intelligence and Statistics (AISTATS 2021)*. This problem was tackled for non-linear models in a subsequent work published at the *Advances in Neural Information Processing System Conference (NeurIPS 2021)*, one of the most prestigious conferences in machine learning) with other co-authors.
3. She has contributed to the design of a framework integrating non-coding elements in gene regulatory networks. These non-coding elements were shown both theoretically and empirically to effectively structure and constraint the regulatory dynamics across the network, and increase the interpretability and understanding the regulatory mechanisms that lead to a specific transcriptomic phenotype. The corresponding work was published in the *Journal of Theoretical Biology* in 2020.

## Education

### Université Paris Cité, Inserm UMR 1141 & CNRS UMR 9189

PhD in Genetics

09/2019 – 09/2022

Doctorate Degree in Science. Title: **Combination of gene regulatory networks and sequential machine learning for drug repurposing**, supervised by [Pr. Andrée Delahaye-Duriez](#) (Inserm UMR 1141) & [Dr. Émilie Kaufmann](#) (CNRS UMR 9189).

Viva: 09/09/2022.

### École Normale Supérieure<sup>†</sup> (ENS) Paris-Saclay

M2 Master Vision, Apprentissage (MVA)

(ex-École Normale Supérieure de Cachan)

09/2018 – 09/2019

Master's degree in Machine Learning. (*summa cum laude*, Grade: 16.17/20, no ranking)

### ENS Paris-Saclay

M1 Master Parisien en Recherche en Informatique (MPRI)

09/2016 – 09/2017

Master's degree in Computer Sciences. (*summa cum laude*, Grade: 16.72/20, rank: 3/25)

### École Normale Supérieure de Cachan

L3 Licence informatique fondamentale ENS Cachan

09/2015 – 09/2016

Bachelor's degree in Computer Sciences. (*cum laude*, Grade: 14.64/20, rank: 10/26)

† *École Normale Supérieures are selective French schools for research and teaching.*

## Professional Experience

### Research Positions

**Marie Skłodowska-Curie Postdoctoral Fellow | Pr. Olaf Wolkenhauer** **Rostock, Germany**  
*Universität Rostock (SBI Rostock)* 05/2023–present

Development of the RECeSS project, focusing on the development of new, improved techniques for drug development based on collaborative filtering approaches.

**Skills** Collaborative Filtering · Python (Programming Language) · Applied Machine Learning

**Marie Skłodowska-Curie Postdoctoral Fellow (secondment) | Dr. Jill-Jênn Vie** **Saclay, France**  
*Inria Saclay (SODA team)* 07/2023–10/2023

Development of the RECeSS project, focusing on the development of new, improved techniques for drug development based on collaborative filtering approaches.

**Skills** Collaborative Filtering · Benchmarking · Applied Machine Learning

**Postdoctoral position | Pr. Andrée Delahaye-Duriez** **Paris, France**  
*Neurodiderot (UMR 1141)* 09/2022–03/2023

Development and implementation of the NORDic pipeline for Boolean networks, Prefiguration of the multiomics workflow for the RHU FAME project led by Pr. Élie Azoulay.

**Skills** Systems Biology · Programming · Interdisciplinary Research · Bioinformatics

**PhD position | Pr. Andrée Delahaye-Duriez & Dr. Émilie Kaufmann** **Paris, France**  
*Neurodiderot (UMR 1141) & SCOOL (UMR 9189)* 09/2019–09/2022 (36 months)

Combination of gene regulatory networks and sequential machine learning for drug repurposing.

**Skills** Systems Biology · Multi-Armed Bandits · Interdisciplinary Research · Bioinformatics

**Master internship | Pr. Andrée Delahaye-Duriez & Dr. Émilie Kaufmann** **Paris, France**  
*Neurodiderot (UMR 1141) & SCOOL (UMR 9189)* 03/2019–08/2019 (4 months)

Design of a drug repurposing method through a bandit algorithm combined with the prediction of transcriptomic states by a gene regulatory network. Application to the prediction of new anti-epileptics.

**Skills** Interdisciplinary Collaboration · Interdisciplinary Research · Statistical Learning · Project Design · Bioinformatics

**Predoctoral internship | Dr. Bartek Wilczyński** **Warsaw, Poland**  
*Regulomics team (MIM UW)* 10/2017–07/2018 (10 months)

Proof-of-concept on the explicit inclusion of biological interactions in gene regulatory networks and its impact on inference and simulation of transcriptomic regulation. Led to a publication in Journal of Theoretical Biology (DOI : [10.1016/j.jtbi.2019.110091](https://doi.org/10.1016/j.jtbi.2019.110091)).

**Skills** Network Analysis · Epigenetics · Python (Programming Language) · Systems Biology · Scientific Presentation

**Master internship | Dr. Nicholas Luscombe & Dr. Garth Iles** **Onna-son, Japan**  
*Genomics and Regulatory Systems Unit (OIST)* 02/2017–07/2017 (5 months)

Design and implementation of a single-cell RNA sequencing clustering method taking into account intergene expression dependencies using a probabilistic model ; implementation in R Shiny of a web application for the visualisation and preliminary analysis of single-cell RNA sequencing data. Application to transcriptomic data analysis in *Ciona intestinalis*.

**Skills** Benchmarking · R Shiny · Unsupervised Learning · Data Visualization · Python (Programming Language)

**Bachelor internship | Dr. Macha Nikolski & Dr. Mathieu Raffinot** **Bordeaux, France**  
*Centre de Bioinformatique de Bordeaux (Université de Bordeaux)* 05/2016–07/2016 (2 months)

Design and implementation of compared analyses of taxonomic trees built from metagenomic data. Application to the analysis of data from intestinal guts of children afflicted with cystic fibrosis at Hôpital Pellegrin in Bordeaux.

**Skills** Metagenomics · Phylogenetics · Supervised Learning · Unsupervised Learning · Python (Programming Language)

### Teaching & Mentoring Experiences

**Biostatistics, programming and bioinformatics** **Université Paris Cité**  
*Doctorant Contractuel avec Mission d'Enseignement (DCME) (Teaching Assistant)* 09/2020–09/2021 (64 hours)

**References:** Dr. Anne Badel & Pr. Olivier Taboureau

**Supervision of a Master-equiv. internship** **SBI Rostock**  
*Joint supervision of Rahul Bordoloi with Pr. Olaf Wolkenhauer* 09/2023–present

Development of a linear discriminant algorithm on multivariate temporal data.

**Supervision of a Master internship** **Inserm Neurodiderot**  
*Joint supervision of Adrien Dufour with Pr. Andrée Delahaye-Duriez* 02/2020–07/2020 (6 months)

Identification of functional families of microglia cells from targeted single-cell RNA sequencing data of inflammatory microglia at a developmental stage.

### Supervision of a Masters's degree project

Joint supervision of Ariane Alix with [Dr. Émilie Kaufmann](#)

ENS Paris-Saclay

11/2019–01/2020 (2 months)

Proposal of a project on the adaptation of a published drug-target prediction method to drug repurposing using collaborative filtering in the course *Graphs in Machine Learning* taught by [Dr. Michał Valko](#) in Master Vision Apprentissage (**MVA** 2020).

## Funding as Principal Recipient

### Marie Skłodowska-Curie Postdoctoral Fellowship 2022

Postdoctoral grant

[RECESS project](#), Project ID: 101102016.

Horizon 2020

2023–2025 (2 years)

### Contrat Doctoral Spécifique aux Normaliens (CDSN) 2019

PhD fellowship

French Ministry of Higher Education & Research

2019–2022 (3 years)

Around 122 fellowships (less than 50% of the candidates) are granted yearly through a selective process based on scholastic records, recommendation letters, and the project proposal.

### Élève fonctionnaire stagiaire de l'ENS Cachan

Scholarship

French Ministry of Higher Education & Research

2017, 2018 (2 years)

Intern civil servant student at ENS de Cachan (Second concours: oral admission test in Computer Sciences, rank: 2, 4 positions every year at national level). Caesura for personal convenience from 01/09/2017 to 31/08/2018.

## Research

### Peer-Reviewed Scientific Journals

#### 2023

#### stanscofi and benchcofi: a new standard for drug repurposing by collaborative filtering

[C. Réda](#), J.-J. Vie, O. Wolkenhauer

, *Under review*

#### An Anytime Algorithm for Good Arm Identification

M. Jourdan & [C. Réda](#)

, *Under review*

#### NORDic: a Network-Oriented package for the Repurposing of Drugs

[C. Réda](#) & A. Delahaye-Duriez

, *Journal of Open Source Software*, 8(90):5532, DOI: [10.21105/joss.05532](#)

#### 2021

#### Machine learning applications in drug development

[C. Réda](#), [É. Kaufmann](#) & A. Delahaye-Duriez

, *Computational and Structural Biotechnology Journal*, 18:241–252, DOI: [10.1016/j.csbj.2019.12.006](#)

#### 2020

#### Automated inference of gene regulatory networks using explicit regulatory modules

[C. Réda](#) & B. Wilczyński

, *Journal of Theoretical Biology*, 486:110091, DOI: [10.1016/j.jtbi.2019.110091](#)

#### 2019

#### Identification de cibles thérapeutiques et repositionnement de médicaments par analyses de réseaux géniques

A. Delahaye-Duriez, [C. Réda](#) & P. Gressens

, *Médecine/Sciences*, 35:515–518, DOI: [10.1051/medsci/2019108](#)

### Peer-Reviewed Conference Proceedings

#### 2022

#### Near-optimal Collaborative Learning in Bandits

[C. Réda](#), S. Vakili, [É. Kaufmann](#)

, *Proceedings of the 36<sup>th</sup> Conference on Advances in Neural Information Processing Systems (NeurIPS 2022)*

HAL: [03825099](#) [[Selected as Oral](#)]

#### Prioritization of Candidate Genes Through Boolean Networks

[C. Réda](#), A. Delahaye-Duriez

, *Proceedings of the 20<sup>th</sup> International Conference on Computational Methods in Systems Biology (CMSB 2022)*

Springer:89–121 [[Best Student Paper Award](#)]

#### 2021

## Dealing With Misspecification In Fixed-Confidence Linear Top-m Identification

C. Réda, A. Tirinzoni & R. Degenne

, *Proceedings of the 35<sup>th</sup> Conference on Neural Information Processing Systems (NeurIPS 2021)*, 34, HAL: [03409205](#)

## Top-m identification for linear bandits

C. Réda, É. Kaufmann & A. Delahaye-Duriez

, *Proceedings of the 24<sup>th</sup> International Conference on Artificial Intelligence and Statistics (AISTATS 2021)*, 130

HAL: [03172145](#)

## Oral Communications at International Conferences.....

### 2024

**C. Réda. Towards a large-scale benchmark of collaborative filtering in drug repurposing**

SMPGD 2024 (Paris, France)

02/02/2024

### 2023

**C. Réda. Benchmarking collaborative filtering approaches to drug repurposing**

e:Med Meeting 2023 on Systems Medicine (Berlin, Germany)

10/10/2023

### 2022

**C. Réda. Near-optimal Collaborative Learning in Bandits**

35<sup>th</sup> International Conference on Advances in Neural Information Processing Systems (New Orleans, USA)

07/12/2022

**C. Réda. Prioritization of Candidate Genes Through Boolean Networks**

20<sup>th</sup> International Conference on Computational Methods in Systems Biology (Bucharest, Romania)

14/09/2022

**C. Réda. Gene network oriented drug discovery: automated inference of Boolean networks (...)**

13<sup>th</sup> Conference on Dynamical Systems Applied to Biology and Natural Sciences (held virtually)

10/02/2022

### 2021

**C. Réda. Dealing With Misspecification In Fixed-Confidence Linear Top-m Identification**

NeurIPS@Paris 2021 (Paris, France)

08/12/2021

### 2020

**C. Réda. Automated inference of gene regulatory networks using explicit regulatory modules**

Journées Ouvertes de Biologie, Informatique et Mathématique (JOBIM) 2020 (held virtually)

02/07/2020

### 2018

**C. Réda. Automated inference of gene regulatory networks using explicit regulatory modules**

Workshop 6 of the 17th European Conference on Computational Biology (ECCB 2018, Athens, Greece)

08/09/2018

**C. Réda. Automated inference of gene regulatory networks using explicit regulatory modules**

Bioinformatics in Toruń (BIT 2018, Toruń, Poland)

28/06/2018

## Poster presentations at International Conferences.....

**C. Réda. Drug repurposing in breast cancer by combining bandit algorithms and Boolean networks (...)**

ISMB/ECCB 2023 (Lyon France)

07/2023

**C. Réda. Prioritization of Candidate Genes Through Influence Maximization**

Journées Ouvertes de Biologie, Informatique et Mathématique (JOBIM 2022, Rennes, France)

07/2022

**C. Réda. Dealing With Misspecification In Fixed-Confidence Linear Top-m Identification**

35<sup>th</sup> International Conference on Advances in Neural Information Processing Systems (NeurIPS 2022, held virtually) 12/2021

**C. Réda. Top-m identification for linear bandits**

24<sup>th</sup> International Conference on Artificial Intelligence and Statistics (AISTATS 2021, held virtually)

04/2021

## Open-Source Softwares & Datasets

### Softwares.....

#### 2023

**BENCHmark for drug Screening with COLlaborative Filtering (benchscofi)**

C. Réda

, Zenodo, DOI: [10.5281/zenodo.8241505](#), GitHub: [recess-eu-project/benchscofi](#)

Python package implementing algorithms and methods from the state-of-the-art in drug repurposing with collaborative filtering

## STANdard for drug Screening by COllaborative FIltering (stanscofi)

C. Réda

, Zenodo, DOI: [10.5281/zenodo.8038847](https://doi.org/10.5281/zenodo.8038847), GitHub: [recess-eu-project/stanscofi](https://github.com/recess-eu-project/stanscofi)

Python package for the automation of the training and validation of drug repurposing with machine learning

## Network Oriented Repurposing of Drugs (NORDic)

C. Réda

, Zenodo, DOI: [10.5281/zenodo.7239047](https://doi.org/10.5281/zenodo.7239047), GitHub: [clreda/NORDic](https://github.com/clreda/NORDic)

Python package for the inference, analysis of Boolean networks & application to drug repurposing

## Datasets

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### 2023

#### PREDICT

C. Réda

, Zenodo, DOI: [10.5281/zenodo.7982964](https://doi.org/10.5281/zenodo.7982964)

Large drug repurposing dataset [with open-source generation](#)

#### TRANSCRIPT

C. Réda

, Zenodo, DOI: [10.5281/zenodo.7982969](https://doi.org/10.5281/zenodo.7982969)

Drug repurposing dataset on transcriptomic data [with open-source generation](#)

## Commitment to Popularization of Sciences and Law Making

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### Popularization of Sciences

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**05/2023–present:** Created and published on [RECeSS project blog](#): progress reports on the [RECeSS project](#) and introductory blog posts on drug repurposing and collaborative filtering.

**12/2016–09/2018:** Published on [Tryalgo](#) [in French] : series of blog posts on known algorithms with concrete applications, aimed at high school and college students (approx. 2,400 unique monthly users ; two of these posts constitute the Top-2 most visited pages).

**10/2016:** Published on [Binaire](#) (blog on Computer Science affiliated with French newspaper *Le Monde*) and [The Conversation](#) [in French] : “A.P.B. : La vie après le bac” (conjointly written with [Serge Abiteboul](#)). Explanation of the algorithm of Gale-Shapley which has been in use in a previous version of the French national web application for high school students' applications to college

### Popularization of Law-Making

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**12/2016–09/2018:** Published on [Réfléchir.fr](#) [in French] : series of blog posts on laws passed since 2017 in France: explanation of their content and their consequences (534 followers on February, 24 2021).

## Miscellaneous

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**2023–present:** Selection as postdoc female mentoree by **Universität Rostock** to develop her professional career: access to seminars and personalized mentoring (see the [list of selected candidates](#)).