Pierre-Marie **ALLARD**

Natural Products Chemist (PhD) | Pharmacist (PharmD)

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Google Scholar - Pierre-Marie Allard · Rue A.-Gockel 3, 1700 Fribourg, Switzerland
COMMONS Lab Website · Born 17 November 1984 in Quimper, France

Fascinated by Nature's complexity, I am a passionate researcher. I see chemodiversity as a direct reflection of biodiversity, just expressed at another granularity. I believe that a better characterization of chemodiversity combined with Open Research knowledge sharing strategies can help us to establish the value of biodiversity and, ultimately, participate in it's conservation ... a critical issue of our time.

"Understanding life will never be an easy task. But it is always a fascinating exercise." Claus Emmeche

Education

Dec. 2018	Innosuisse Start-up Training Business Concept - 14 weeks Swiss Federal program for startup founders
17 Dec 2011	Ph.D in Chemistry Université Paris Sud 11 *"Search for antiviral compounds in the Neo-Caledonian biodiversity"* - Institut de Chimie des Subsances Naturelles - CNRS. Gif-sur-Yvette, France. Under the supervision of Dr. Françoise Guéritte & Dr. Marc Litaudon. *First Class Hons.*
27 Oct 2010	Pharm.D State Diploma of Pharmacy - Université de Rennes 1
5 Sept 2008	Research Master in Life Sciences "Valuation of Natural Ressources" - Université de la Réunion. *Hons.*

Employment History

Today – Apr. 2021 — Group Leader - COMMONS Lab - COmputational Mass spectroMetry and Open Natural products reSearch, University of Fribourg, Switzerland

- Investigation in the field of computational mass spectrometry and Open Science oriented strategies for Natural Products research

Open Science · Natural Products · Computational Mass Spectrometry · Knowledge Management · Knowledge Graphs · Linked Open Data

Today – Apr. 2021 — Head of the Metabolomics Platform, University of Fribourg, Switzerland

- Management and organization of the Mass Spectrometry based Metabolomics Platform at the Department of Biology

Sample preparation · Data Acquisition · Data Analysis · Data Interpretation · Reporting · Instrument Maintenance · Method Development

Today – Jun. 2017 — Independant Scientific Consultant, MetaboMaps, Europe

- Implementation of tailored bioinformatic pipeline and in silico databases.
- Training in computational metabolite identification and molecular networking.
- Mass-spectrometry, Natural Products chemistry and general scientific consulting activities.

Consulting · Computational Mass Spectrometry · Training · Software deployment

Apr. 2021 – Aug. 2016 — Research & Teaching Assistant - Pr. Wolfender's lab, University of Geneva, Switzerland

- Development of computational metabolite identification solutions. Development of computational strategies for the treatment, organization and visualization of large mass-spectrometry datasets.
- Metabolomics applied to Natural Products chemistry, chemical-ecology, pathogenic micro-organisms studies, analytical toxicology
- Management of the High-Resolution Mass Spectrometry platform (QE Focus Orbitrap) calibration, maintenance, method development

Python · R · MZmine · molecular-networking · Jupyter Notebooks · HRMS Orbitrap · UHPLC · multivariate data analysis · Cytoscape · Plotly · Git

Sept. 2013 – Jul. 2016 — Postdoctoral Researcher - Pr. Wolfender's lab, University of Geneva, Switzerland

- Metabolomics applied to Natural Products chemistry and chemical-ecology
- Epigenetics modification of fungal strains (culture, scale-up, isolation, metabolomics, structural identification)
- High-Resolution Mass Spectrometry analysis (QE Plus Orbitrap) calibration, maintenance, method development

MZmine · R · Cytoscape · molecular-networking · HRMS Orbitrap · UHPLC · multivariate data analysis

Aug. 2013 – Jul. 2012 | **Postdoctoral Researcher - Pr. Berlinck's lab - FAPESP Fellowship, University of São-Paulo, Brazil**

- Epigenetic induction of cryptic biosynthetic gene clusters in marine fungi
- Synthesis of epigenetic modificators
- Cultivation of fungal strains (small and medium-scale
- Isolation & structural determination of Natural Products

Epigenetic modifications | Synthesis | HPLC | Mass-Spectrometry | NMR | structural determination | microorganisms cultivation techniques

Sept. 2008 – Dec. 2011 | **PhD candidate - Dr. Gueritte's lab, ICSN-CNRS, France**

- Isolation and purification of Natural Products (HPLC, MPLC, SFC, Chiral Phases)
- Structural determination of Natural Products (NMR 1D, 2D, Mass Spectrometry)
- Absolute configuration determination techniques (ECD, quantum chemistry for ECD calculations)
- Bioassays on NS5 polymerase of the Dengue Virus

HPLC | MPLC | UHPLC | SFC | ECD | NMR1D and 2D | Gaussian03

Institutional Responsibilities

Dec. 2020 – Sept.2016 | **Responsible of Practicals - Phytochemistry & Natural Products - Bachelor in Pharmacy, University of Geneva, Switzerland**

- Management and organization of Practicals in 3rd year of pharmaceutical studies with Dr. Emerson F. Queiroz.

Apr. 2020 – Sept.2016 | **Responsible of HRMS analytical platform - Pr. Wolfender's lab, University of Geneva, Switzerland**

- Management of the analytical team, formation of power users, analysis requests management. Communication with constructors.

Jan. 2017 | **Coordinate Teaching Module - Bachelor in Pharmacy, University of Geneva, Switzerland**

- Member of the Coordinate Teaching Module and advisor of group of students.

Research Projects

2020 Fond National Suisse de la Recherche Scientifique - Sinergia Grant - *"An in silico and chemo-biological approach to identify anti-infective and pro-metabolic natural products"*

2013 Fondation for Natural Products Chemistry Development | Académie des Sciences - Postdoctoral Grant - *"Triggering Diverse and New Natural Product Biosynthesis by Diversity Oriented Synthesis of Bio-inspired Histone Deacetylase Inhibitors"*

2012 FAPESP São-Paulo Research Foundation - Postdoctoral Fellowship - *"New approaches for the production of secondary metabolites by marine-derived fungi."*

Academic - Industry partnerships

2017 - today Pierre Fabre laboratories - Green Mission - *"Chemical characterisation and drug discovery program from the Pierre Fabre Nature Open Libraries"*

2019 Firmenich - *"Metabolomics and chemical characterization of commercial extracts."*

2017-2018 Nestlé Institute of Health Sciences - *"Metabolomics and chemical characterization of commercial extracts. Bioinformatics pipeline development"*

2017 Nestlé Research Center - *"Metabolomics and chemical characterization of commercial extracts"*

2017 Alpinia Institute - *"Consulting services in metabolomics and bioinformatics for natural products research"*

2016 Pierre Fabre laboratories - *"Metabolomics and chemical characterization of commercial extracts"*

Supervision of Junior Researchers

Jun.2022 – Fev.2022 | **Bachelor work Edouard Brüelhart, University of Fribourg, Switzerland**

- Pilot project for the Digital Botanical Gardens Initiative (DBGI)

Today – Sept.2018 | **Ph.D candidate Luis Manuel Quiroz Guerrero, University of Geneva, Switzerland**

- Development of computational metabolite identification solutions. Development of computational strategies for the treatment, organization and visualization of large mass-spectrometry datasets.

Today – Jun. 2017 | **Ph.D candidate - Arnaud Gaudry, University of Geneva, Switzerland**

- Development of computational metabolite identification solutions. Development of computational strategies for the treatment, organization and visualization of large mass-spectrometry datasets.

Jul. 2018 – Fev. 2018 | MSc. candidate - Lisa Ansechi, University of Geneva, Switzerland
- Discovery of antiparasitic compounds via molecular networking - Application to the study of *Zanthoxylum decaryi*

Aug. 2016 – Apr. 2016 | MSc. candidate - Damien Olivier, University of Geneva, Switzerland
- Screening of environmental filamentous fungi for anti-microbials discovery - Miniaturized cultures and bioinformatics approaches.

Jun. 2015 – Fev. 2015 | Diploma Research Internship - Juliette Joubert, University of Geneva, Switzerland
- Study of cryptic biosynthetic pathways in filamentous fungi : epigenetic modification, bioinformatic and metabolomic tools.

Jun. 2014 – Fev. 2014 | Diploma Research Internship - Marija Perisic, University of Geneva, Switzerland
- Co-cultivation and epigenetic modification strategies for the induction of new soecialized metabolites.

Jul. 2013 – Fev. 2013 | MSc. - Laura P Ióca, University São-Paulo, Brazil
- Epigenetic modificators synthesis and application to the elicitation of cryptic biosynthetic pathways

Teaching activities

Today – Mar.2022 | Teaching of SBL.20004 Course & Practicals - Master of Science in Biology, University of Fribourg, Switzerland
- Class material available at https://doi.org/10.5281/zenodo.6379085 *"Introduction to metabolomics : data acquisition and processing"* - 32 h/year.

Today – Mar.2022 | Teaching - Master of Science in Bioinformatics, University of Fribourg - University of Bern, Switzerland
- Class material available at https://doi.org/10.5281/zenodo.6045962 *"Computational metabolomics and metabolite annotation"* - 4 h/year.

Today – Mar.2022 | Teaching (part of SBL.00123) - Master of Science in Biology, University of Fribourg, Switzerland
- Class material available at https://doi.org/10.5281/zenodo.6390145 *"Metabolomics, computational mass spectrometry and open science resources for the exploration of living systems metabolomes."* - 4 h/year.

Today – Sept.2021 | Teaching of SBL.00073 Course - Bachelor of Science in Biology, University of Fribourg, Switzerland
- Class material available at https://doi.org/10.5281/zenodo.6327280 *"Specialized metabolism : importance in chemical ecology and human health"* - 14 h/year.

Dec. 2020 – Sept.2016 | GC-MS Practical - Bachelor in Pharmacy, University of Geneva, Switzerland
- Teaching and orientation of students during a 2 days module. *"Identification of an unknown essential oil by GC-MS"* - 48 h/year.

Aug. 2016 – Sept. 2015 | Organic Chemistry Practicals - Bachelor in Pharmacy, University of Geneva, Switzerland
- Teaching and orientation of students in Organic Chemistry practicals - 2nd year of pharmaceutical studies - 48 h/year.

Aug. 2015 – Sept. 2013 | HPLC Practicals - Bachelor in Pharmacy, University of Geneva, Switzerland
- Teaching and orientation of students during a 2 days module. *"Analysis of Ginkgo flavonoids in a pharmaceutical speciality"* - 48 h/year.

Scientific reviewing, active membership and conference organization

Review Editor	*Frontiers in Natural Products*
Independant reviewer	*Journal of Natural Products*, *Organic Letters*, *Phytochemistry*, *Journal of Ethnopharmacology*, *Marine Drugs*, *Frontiers in Pharmacology*, *ACS Chemical Biology*
Active member	American Society of Pharmacognosy, Résau Francophone de Métabolomique et Fluxomique, Société Française d'Ethnopharmacologie, Swiss Metabolomics Society
Conference organization	Staff at the International Mass-Spectrometry Conference 2014, Geneva

Prizes & Awards

2019 **Innosuisse Business Concept Prize** - *Study trip to discover the London start-up ecosystem* - KIMIYA "the open pharmacognosy platform" team (Canwei, M.; Brillatz, T.; Houriet J. and **Allard, P.-M.**)

2015 **Best Poster Prize - RFMF Jury** - *"Mapping the chemical space of bioactive Euphorbiaceae species trough massive multi-informative molecular networks"*

2012 **Thesis prize - French National Academia of Pharmacy** *"Search for new inhibitors of emerging viruses within the neo-caledonian biodiversity."*

2011 **Oral Communication Prize - ICSN** *"Quorum-sensing : the chemical language of bacteria."*

Career Break

Jan. 2012 to Jun. 2012 Travelling with my wife in Colombia & Ecuador between Ph.D & Postdoc in Brazil

Language

French	●●●●●
Spanish	●●●●●
English	●●●●○
German	●○○○○

Forces

- Passionated
- Quick-learner
- Autonomous

References

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Major Scientific Achievements

LOTUS 2022

https://github.com/lotusnprod https://lotus.naturalproducts.net/ https://doi.org/10.7554/eLife.70780

We share the first completely Free and open database of natural products chemical structures and their biological occurrences. The data are hosted in parallel at Wikidata, allowing large-scale community curation and upload and at https://lotus.naturalproducts.net/ for more classical uses. [1]

Open Science | Natural Products Research | Metabolites Biological Occurrences | Database | Knowledge Graphs

Taxonomically informed metabolite annotation 2019

https://github.com/oolonek/taxo$_s$corer https://doi.org/10.1101/702308

We demonstrate that the integration of the taxonomical dimension drastically improves the precision and accuracy of currently available state-of-the-art computational mass spectrometry metabolite annotation solutions. We advocate for the establishment of an open and community-curated database compiling structures, spectra and biological sources.

Chemotaxonomy | Computational Mass Spectrometry | Metabolite Annotation | Open Database

Integration of Molecular Networking and In Silico Databases 2016

http://oolonek.github.io/ISDB/ https://pubs.acs.org/doi/abs/10.1021/acs.analchem.5b04804

I developed a unique metabolite annotation solution which integrates molecular networking and in silico fragmentation databases. With 170 000 compounds, the generated database is today the widest spectral database available for small molecules identification, worldwide. [2] The database has been accessed by more than 1500 individual connections and the paper cited over 300 times since 2016.[3]

Molecular Networking | In Silico Fragmentation | Computational Metabolite Identification | Open Database

Bioactive Natural Products pipeline : Massive Multi-Informative Molecular Networks 2017

http://pubs.acs.org/doi/abs/10.1021/acschembio.7b00413

This bioinformatic pipeline generates multi-informative molecular networks combining bioactivity assay results, taxonomy and spectral similarity information. It allows to prioritize bioactive compounds before any physical fractionation process. It thus offers a serious alternative to the paradigmatic and labor intensive bio-guided fractionation process. This work is a co-authorship : I designed the strategy and the bioinformatic tools, Florent Olivon (PhD) has been applying the approach and isolating most of the compounds.[4]

Bioactive NPs Prioritization | Multi-Informative Molecular Networks | Drug Discovery

Global Natural Products Social molecular networking 2016

https://gnps.ucsd.edu/ http://www.nature.com/doifinder/10.1038/nbt.3597

The GNPS platform is a unique web service allowing the online generation of Molecular Networks. It is also a living reposittory of mass spectrometry data. We participated to this collective effort as beta-testers and data contributors. I implemented such approach for the first time in our lab at University of Geneva. Molecular networking is now the fundamental tool of most of our research projects. This tool as been fundamentally reshaping the manner to treat mass spectrometry data of complex matrices.[5]

GNPS | Molecular Networks | Living Mass Spectral Database

Références

[1] Rutz, A.; Sorokina, M.; Galgonek, J.; Mietchen, D.; Willighagen, E.; Gaudry, A.; Graham, J. G.; Stephan, R.; Page, R.; Vondrášek, J.; Steinbeck, C.; Pauli, G. F.; Wolfender, J.-L.; Bisson, J.; **Allard, Pierre-Marie** The LOTUS Initiative for Open Knowledge Management in Natural Products Research. *eLife* **2022**, *11*, e70780.

[2] Kind, T.; Tsugawa, H.; Cajka, T.; Ma, Y.; Lai, Z.; Mehta, S. S.; Wohlgemuth, G.; Barupal, D. K.; Showalter, M. R.; Arita, M.; Fiehn, O. Identification of small molecules using accurate mass MS/MS search. *Mass Spectrom. Rev.* **2017**, 1-20.

[3] **Allard, P.-M.**; Péresse, T.; Bisson, J.; Gindro, K.; Marcourt, L.; Pham, V. C.; Roussi, F.; Litaudon, M.; Wolfender, J.-L. Integration of Molecular Networking and In-Silico MS/MS Fragmentation for Natural Products Dereplication. *Anal. Chem.* **2016**, *88*, 3317-3323.

[4] Olivon, F.; **Allard, P.-M.**; Koval, A.; Righi, D.; Genta-Jouve, G.; Neyts, J.; Apel, C.; Pannecouque, C.; Nothias, L.-F.; Cachet, X.; Marcourt, L.; Roussi, F.; Katanaev, V. L.; Touboul, D.; Wolfender, J.-L.; Litaudon, M. Bioactive Natural Products Prioritization Using Massive Multi-informational Molecular Networks. *ACS Chem. Biol.* **2017**, *12*, 2644-2651.

[5] Wang, M. et al. Sharing and community curation of mass spectrometry data with Global Natural Products Social Molecular Networking. *Nat. Biotechnol.* **2016**, *34*, 828-837.