

Curriculum Vitae and Track Record

PERSONAL DETAILS: Family name, First name: NOTHIAS, Louis-Félix (*Married, 3 children*). Date of birth: 05 April 1985 (French citizen). Researcher identifiers: [GoogleScholar link](#), ORCID [0000-0001-6711-6719](#). Website: <https://lfnothias.github.io> & <https://holobiomicslab.cnrs.fr/>

• EDUCATION

- 2011 – 2015 PhD in Organic Chemistry (*Université de Corse, France*).
Thesis in co-direction between 1) the *Laboratoire Sciences pour l'Environnement, Université de Corse & Centre National de la Recherche Scientifique (CNRS)*.
PhD Supervisors: Prof. J. Costa (*Univ. de Corse*) and Dr. Marc Litaudon (CNRS)
- 2009 – 2011 Master in Phytochemistry, with high honors. *Université de Corse*.
- 2007 – 2009 Bachelor's in Chemistry. *Université de Corse*.

• CURRENT POSITION

- Since 2023/06 *Chaire de Prof. Junior Centre National de la Recherche Scientifique (CNRS),*
« [Experimental & Computational Metabolomics & HolobiomicsLab](#) »,
Institut de Chimie de Nice (ICN), Université Côte d'Azur, Nice, France.
- Since 2024/01 Affiliated chair *Institut Interdisciplinaire d'Intelligence Artificielle Côte d'Azur*
Sophia-Antipolis, France.

• PREVIOUS POSITIONS

- 2021 – 2023 | Research associate in analytical and computational chemistry. Dept. of Pharmaceutical Sciences, University of Geneva, Geneva, Switzerland.
- 2016 – 2021 | Post-doctoral researcher in experimental and computational metabolomics, with Prof Pieter Dorrestein. Collaborative Mass Spectrometry Innovation Center, Center for Microbiome Innovation, University of California San Diego, USA.
- 2017 – 2018 | MSCA Global postdoct. researcher. Institut de Chimie des Substances Naturels, CNRS, Gif-sur-Yvette, FR.

RESEARCH FOCUS

Louis-Felix Nothias coordinates the HolobiomicsLab group at ICN (*équipe D'Intelligence Artificielle pour les sciences Moléculaires, eDIAM*), an interdisciplinary group working at the interface of experimental mass spectrometry-(MS) based metabolomics, integrative multi-omics, and AI-enabled data analysis. His research group operates over two main pillars: (i) deep metabolomics — developing and applying state-of-the-art MS methods for metabolite annotation, molecular networking, and metabolic profiling of complex biological systems; and (ii) AI for metabolomics and multi-omics: designing knowledge graphs, multi-agent LLM architectures, and AI-assisted research workflows for data exploration, literature mining, and hypothesis generation at multi-omics scale.

Five selected publications and narrative (last 3 years only)

Computational Mass Spectrometry and Open-Access Metabolomics Infrastructure

A major contribution of LFN's research program is the co-development and dissemination of open computational tools and spectral resources that have become community standards for untargeted metabolomics. Most recent contribution include MZmine 3 — developed in international collaboration — provides a complete, reproducible pipeline for mass spectrometry data processing, compound annotation via molecular networking and spectral library matching, and multimodal data integration [1, 2]. As well as the open-access nearest-neighbor suspect spectral library (GNPS/MassIVE), co-developed with the Dorrestein lab at University of California San Diego, enables repository-scale spectral propagation and dramatically extends metabolite annotation beyond curated reference compounds [2]. MS2Planner introduced iterative MS² acquisition strategies for maximizing fragmentation spectral coverage in untargeted experiments [see project references]. MSnLib provides efficient generation of multi-stage (MSⁿ) fragmentation spectral libraries, extending metabolite characterization to deeper structural resolution [3]. These tools collectively constitute the computational metabolomics layer on which the present PhD project will rely for *Nve* metabolomics data processing and annotation.

[1] Schmid R, Heuckeroth S, Korf A, et al (2023). Integrative analysis of multimodal mass spectrometry data in MZmine 3. *Nature Biotechnology*, 41(4), 447–449. <https://doi.org/10.1038/s41587-023-01690-2>

[2] Bittremieux W, Wang M & Dorrestein PC (2023). Open access repository-scale propagated nearest neighbor suspect spectral library for untargeted metabolomics. *Nature Communications*, 14(1), 8488. <https://doi.org/10.1038/s41467-023-44035-y>

[3] Brungs C, Schmid R, (2025). MSnLib: efficient generation of open multi-stage fragmentation mass spectral libraries. *Nature Methods*, 22(10), 2028–2031. <https://doi.org/10.1038/s41592-025-02813-0>

AI for Metabolomics and Multi-Agent Research Workflows

Since 2023, LFN's CPJ and 3iA affiliated chair programs have focused on developing AI systems for metabolomics and multi-omics interpretation, in collaboration with INRIA/Wimmics (Fabien Gandon). *MetaboT* — an LLM-based multi-agent framework for natural-language interaction with metabolomics knowledge graphs — demonstrated 83.67% accuracy in translating biological questions into SPARQL queries against a mass spectrometry knowledge graph, versus 8.16% for a baseline LLM [4]. The ANR-SNF [MetaboLinkAI](https://doi.org/10.21203/rs.3.rs-6591884) project (2025–2029) funds a full research program in metabolomics knowledge hubs, AI research assistants, graph mining, and uncertainty representation, in consortium with ETHZ, UZH, UNIGE, UNIFR, SIB, and INRIA/Wimmics. The *Mimosa* framework, the most recent methodological advance, introduces an open-source evolving multi-agent system for autonomous scientific research using MCP-based dynamic tool discovery and auditable workflow generation [5]. These developments are applied for studying marine holobiont stress response with collaboration with Eric Rottinger (IRCAN) for AI-assisted multi-omics interpretation, and provide the technical foundation for the AI-assisted research workflows proposed in the present PhD project.

[4] Bekbergenova M, Pradi P, Navet B, ..., **Nothias LF** (2025). MetaboT: An LLM-based Multi-Agent Framework for Interactive Analysis of Mass Spectrometry Metabolomics Knowledge. *Research Square*, 06 May 2025, <https://doi.org/10.21203/rs.3.rs-6591884>

[5] Legrand M, Jiang T, Feraud M, Navet B, Taghzouti Y, Gandon F, ... **Nothias LF** (2026). Mimosa Framework: Toward Evolving Multi-Agent Systems for Scientific Research. arXiv:2603.28986. Preprint — <https://arxiv.org/abs/2603.28986>

ORAL PRESENTATIONS IN PEER-REVIEWED INT. CONFERENCES

[1] Keynote speaker (KS), *Metabolomics Society Annual Meeting*, Buenos Aires, Argentina, June 2026. [2] KS, *Metabolomics Society of North America Virtual Symposium* “Metabolomics Meets AI”, online, April 2026. [3] KS, *Nontarget 2026*, Monte Verità, Ascona, Switzerland, April 2026. [4] Invited Speaker (IS), *International Conference SFEC-ICTRE 2026*, Society for Ethnopharmacology / NIPER Mohali, India, 26–28 February 2026. [5] KS, Keynote speaker at the *Metabolomics Society Annual Meeting*, Osaka, Japan, 2024. [3] KS, *Swiss Metabolomics Soc. annual conf.*, Zurich, Switzerland, 2023. [3] *Swiss Metabolomics Soc. annual conf.*, Zurich, Switzerland, 2023. [4] IS, *Swiss Metabolomics Soc. annual conf.*, Lausanne, Switzerland, 2022. [5] IS, *66th ASMS Conf. on Mass Spec.*, USA, 2018. [5] IS, *9th Joint Natural Prod. Conf.*, Denmark, 2016. [7] IS, *Annual Conf. of the Metabolomics Soc.*, Australia, 2017. [6] IS, *French Metabolomics Conf.*, FR, 2016. [9] *French Soc for MS*, FR, 2015. [10] *AFERP Int. Symposium*, FR, 2015. [11] *Trends in NPR, meeting of Phytochem. Soc. of Europe and OPhG*, Univ. of Innsbruck, Austria, 2013.

ADDITIONAL INFORMATION

• GRANTS

2025 – 2028	€450k – ANR-SNFS bilateral project, “ MetaboLinkAI “Open, integrative, and extendable, AI and knowledge graphs framework for functional and actionable metabolomics “, co-coordinator (total FR: 1.25M€ + CH: 3.2M CHF), FR and CH.
2024 – 2025	€70k – IDEX UCAJedi, 1-year postdoc funded on artificial intelligence, FR.
2023 – 2024	€50k – IDEX UCAJedi, Académie 4, Université Côte d’Azur, FR.
2025 – 2028	€191k – ANR POPS , partner of a Collaborative Research Project (total 600k€), FR.
2023 – 2028	€635k - CNRS Junior group leader (Chaire Prof. Junior), starting package, FR.
2023 – 2028	€120k – IDEX UCAJedi, Université Côte d’Azur, Welcome Package, FR.
2020 – 2021	200k USD – Contract research agreement. California Research Alliance, BASF. USA.
2017 – 2018	€247k MSCA Global postdoctoral fellow, European Commission, H2020, EU.
2011 – 2014	€120k EUR - Doctoral fellowship, French government & Univ. of Corsica, FR.

ENCADREMENT EN COURS

Madina Bekbergenova (2023–2026) Matthieu Féraud (2025–2028) Benjamin Navet (2025–2028, sur validation des acquis) et Martin Legrand (2025–2028, sur validation des acquis) ainsi qu’un·e post-doctorant·e et un ingénieur permanent. Deux stagiaires de master en 2026 (Dina Boukhajou et Deniz Ertugrul). La thèse de Lucas Pradi (débutée en 2023) a été interrompue pour raison médicale en février 2026.

RESPONSABILITE COLLECTIVE UniCA

Depuis début 2026 — membre du groupe de travail « IA générative et enseignement » Université Côte d’Azur.