

Bibliographie — Louis-Félix Nothias

Ordre chronologique (récent→ancien)

Types : **art.** revue à comité de lecture · **ac** communication/abstract de conférence · **pp** pré-print · **thèse**. Totaux : 86 art., 24 ac, 19 pp, 1 thèse.

- (2026) **art.** Caraballo-Rodríguez A.M., Cumsille A., Magyari S., Taboada-Alquerque M., Behsaz B., Leão T.F., Broders K., El Abiead Y., Clement J.A., Charron-Lamoureux V., et al.. The undiscovered natural product potential of Actinomycetes. *The Journal of Antibiotics*, 79(2), 80–92. doi :10.1038/s41429-025-00876-x
- (2026) **pp** Bekbergenova M., Jiang T., **Nothias L.F.**, Bittremieux W.. Positive-Unlabeled Learning for Predicting Small Molecule MS2 Identifiability from MS1 Context and Acquisition Parameters. *bioRxiv*, 2026–01. doi :10.64898/2026.01.23.701093
- (2026) **pp** Taghzouti Y., Jiang T., Juigné C., Navet B., Gandon F., Michel F., **Nothias L.F.**. T2S-Metrics : Unified Library for Evaluating SPARQL Queries Generated From Natural Language. *arXiv preprint arXiv :2604.26971*. doi :10.48550/arxiv.2604.26971
- (2026) **pp** Legrand M., Jiang T., Feraud M., Navet B., Taghzouti Y., Gandon F., Dumont E., **Nothias L.F.**. Mimosa Framework : Toward Evolving Multi-Agent Systems for Scientific Research. *arXiv preprint arXiv :2603.28986*. doi :10.48550/arxiv.2603.28986
- (2026) **ac** Gezer E., Bilgi E., Wolfender J., Büyükkileci A., Bedir E., **Nothias L.**, Cuendet M.. Integrating Box-Behnken experimental design with metabolomics to navigate microbial metabolite production. *Planta Medica*, 92(03), P377.
- (2026) **pp** Féraud M., Boukhajou D., Gandon F., **Nothias L.F.**. MetaboKG : An Analysis-centric Knowledge Graph Framework for Untargeted Metabolomics. *arXiv preprint arXiv :2605.24706*.
- (2026) **ac** Bekbergenova M., Pradi L., Feraud M., Jiang T., **Nothias L.**. AI-powered literature mining & metabolomics for accelerated molecular exploration. *Planta Medica*, 92(03), KL7.
- (2025) **art.** Quiros-Guerrero L.M., Burdet F., Kirchhoffer O., Haemmerli P., **Nothias L.F.**, Allard P.M., Gaudry A., Nitschke J., Hanna N., Moretti S., et al.. Enhancing prioritization strategies of natural extracts : integrating heterogeneous data from metabolomics datasets and biological screenings into knowledge graphs. *Phytochemistry Letters*, 69, 103905. doi :10.1016/j.phytol.2025.103905
- (2025) **art.** Kirchhoffer O.A., Quirós-Guerrero L., Nitschke J., **Nothias L.F.**, Burdet F., Marcourt L., Hanna N., Mehl F., David B., Grondin A., et al.. Prioritization of novel anti-infective stilbene derivatives by combining metabolomic data organization and a stringent 3R-infection model in a knowledge graph. *RSC advances*, 15(17), 13010–13030. doi :10.1039/d4ra08421g
- (2025) **art.** Kirchhoffer O.A., Nitschke J., Luscher A., **Nothias L.F.**, Marcourt L., Hanna N., Grondin A., Köhler T., Ferreira Queiroz E., Soldati T., et al.. Phenylalkyl Acetophenones and Anacardic Acids from *Knema oblongifolia* with Synthetic Analogues as Anti-infectives and Antibacterial Agents. *ACS Bio & Med Chem Au*, 5(4), 650–664. doi :10.1021/acsbiomedchemau.5c00052
- (2025) **art.** Quinlan Z.A., Nelson C.E., Koester I., Petras D., **Nothias L.F.**, Comstock J., White B.M., Aluwihare L.I., Bailey B.A., Carlson C.A., et al.. Microbial community metabolism of coral reef exometabolomes broadens the chemodiversity of labile dissolved organic matter. *Environmental Microbiology*, 27(3), e70064. doi :10.1111/1462-2920.70064
- (2025) **art.** Kirchhoffer O.A., Nitschke J., **Nothias L.F.**, Quiros-Guerrero L., Marcourt L., Hanna N., Grondin A., Queiroz E.F., Soldati T., Wolfender J.L.. Navigating Experimental Metabolomics Knowledge Graphs for Targeted Isolation of Anti-Infective Natural Products. *Phytochemistry Letters*, 69, 103476. doi :10.1016/j.phytol.2025.103476
- (2025) **art.** Wolfender J.L., Gaudry A., Rutz A., Quiros-Guerrero L., Kirchhoffer O.A., Marcourt L., David B., Grondin A., Queiroz E.F., **Nothias L.F.**, et al.. Pharmacognosy in the digital era : exciting opportunities offered by metabolomics and accessible digitised data. *Phytochemistry Letters*, 69, 103150. doi :10.1016/j.phytol.2025.103150
- (2025) **art.** Brungs C., Schmid R., Heuckeroth S., Mazumdar A., Drexler M., Šácha P., Dorrestein P.C., Petras D., **Nothias L.F.**, Veverka V., et al.. MSnLib : efficient generation of open multi-stage fragmentation mass spectral libraries. *Nature Methods*, 22(10), 2028–2031. doi :10.1038/s41592-025-02813-0
- (2025) **ac** Taghzouti Y., Michel F., Jiang T., **Nothias L.F.**, Gandon F.. Q²Forge : Minting Competency Questions and SPARQL Queries for Question-Answering Over Knowledge Graphs. *Proceedings of the 13th Knowledge Capture Conference 2025*, 74–81.

- (2025) **pp** Bekbergenova M., Pradi L., Navet B., Tysinger E., Michel F., Feraud M., Taghzouti Y., Chen Y.Z., Kirchhoffer O., Mehl F., et al.. MetaboT : AI-based agent for natural language-based interaction with metabolomics knowledge graphs. *arXiv preprint arXiv :2510.01724*.
- (2025) **ac** Taghzouti Y., Michel F., Jiang T., **Nothias L.F.**, Gandon F.. Building Questions and Queries Datasets for Knowledge Graphs : a Demo of Q²Forge Pipeline. *ISWC 2025 : The 24th International Semantic Web Conference*.
- (2025) **ac** Taghzouti Y., **Nothias L.F.**, Michel F., Gandon F.. Gen²KGBot : Generic Generative Knowledge Graph Robot. *AI Action Summit*.
- (2025) **ac** Pradi L., Jiang T., Féraud M., Bekbergenova M., Taghzouti Y., **Nothias L.F.**. Perspicacité-AI. *Metabolomics Symposium*.
- (2025) **pp** Bekbergenova M., Pradi L., Navet B., Tysinger E., Michel F., Feraud M., Taghzouti Y., Chen Y.Z., Kirchhoffer O., Mehl F., et al.. MetaboT : An LLM-based Multi-Agent Framework for Interactive Analysis of Mass Spectrometry Metabolomics Knowledge.. doi :10.21203/rs.3.rs-6591884/v1
- (2025) **pp** Taghzouti Y., Michel F., Jiang T., **Nothias L.F.**, Gandon F.. Q²Forge : Générer des Collections de Questions de Compétences et Requêtes SPARQL pour Interroger des Graphes de Connaissances en Langue Naturelle..
- (2025) **pp** Taghzouti Y., Michel F., Jiang T., **Nothias L.F.**, Gandon F.. User Interface and Agent Interface for Online Generation of Knowledge Graph's Competency Questions and Question-Query Training Sets..
- (2025) **pp** Pradi L., Jiang T., Feraud M., Bekbergenova M., Taghzouti Y., **Nothias L.F.**. An AI Pipeline for Scientific Literacy and Discovery : a Demonstration of Perspicacité-AI Integration with Knowledge Graphs..
- (2024) **art.** Quiros-Guerrero L.M., Allard P.M., **Nothias L.F.**, David B., Grondin A., Wolfender J.L.. Comprehensive mass spectrometric metabolomic profiling of a chemically diverse collection of plants of the Celastraceae family. *Scientific Data*, 11(1), 415. doi :10.1038/s41597-024-03094-6
- (2024) **art.** Heuckeroth S., Damiani T., Smirnov A., Mokshyna O., Brungs C., Korf A., Smith J.D., Stinson P., Dreolin N., **Nothias L.F.**, et al.. Reproducible mass spectrometry data processing and compound annotation in MZmine 3. *Nature protocols*, 19(9), 2597–2641. doi :10.1038/s41596-024-00996-y
- (2024) **pp** Burdet F., Quiros-Guerrero L.M., Kirchhoffer O., Nitschke J., Allard P.M., **Nothias L.F.**, Gaudry A., Moretti S., Engler R., Queiroz E.F., et al.. Application of the RDF framework to integrate heterogeneous experimental data of a large chemo-and biodiverse collection from a collaborative research project.. *SWAT4HCLS*, 149–152. doi :10.26434/chemrxiv-2023-4hlgd
- (2024) **ac** **Nothias L.F.**. MetaboT : A Conversational AI-Agent for Accessible Mass Spectrometry Metabolomics Data Mining. *72nd Conference on Mass Spectrometry and Allied Topics*.
- (2024) **ac** Pradi L., Bekbergenova M., **Nothias L.F.**. ScienceXGuide Pipeline : An AI-Pipeline for Accelerating Scientific Education and Research. *Benelux Metabolomics Days 2024*.
- (2024) **ac** **Nothias L.F.**. Discovering Microbially Conjugated Bile Acids with Computational Metabolomics. *2024 6th Labex SIGNALIFE Meeting*.
- (2024) **art.** Functional metabolomics of the human scalp : a metabolic niche for *Staphylococcus epidermidis*.. *mSystems*. doi :10.1128/msystems.00356-23
- (2023) **art.** Bittremieux W., Avalon N.E., Thomas S.P., Kakhkhorov S.A., Aksenov A.A., Gomes P.W.P., Aceves C.M., Caraballo-Rodríguez A.M., Gauglitz J.M., Gerwick W.H., et al.. Open access repository-scale propagated nearest neighbor suspect spectral library for untargeted metabolomics. *Nature communications*, 14(1), 8488. doi :10.1038/s41467-023-44035-y
- (2023) **art.** Ferreira Queiroz M.M., Huber R., Marcourt L., Guénée L., Allard P.M., Rutz A., **Nothias L.F.**, Carlotta De Ruvo C., Kissling J., Gupta M.P., et al.. Phytochemical study of *Alzatea verticillata*, the sole species belonging to the Alzateaceae family. *Frontiers in Natural Products*, 2, 1147195. doi :10.3389/fntpr.2023.1147195
- (2023) **art.** Kim H.W., Zhang C., Reher R., Wang M., Alexander K.L., **Nothias L.F.**, Han Y.K., Shin H., Lee K.Y., Lee K.H., et al.. DeepSAT : learning molecular structures from nuclear magnetic resonance data. *Journal of Cheminformatics*, 15(1), 71. doi :10.1186/s13321-023-00738-4
- (2023) **art.** Schmid R., Heuckeroth S., Korf A., Smirnov A., Myers O., Dyrland T.S., Bushuiev R., Murray K.J., Hoffmann N., Lu M., et al.. Integrative analysis of multimodal mass spectrometry data in MZmine 3. *Nature biotechnology*, 41(4), 447–449. doi :10.1038/s41587-023-01690-2
- (2023) **art.** Koester I., Quinlan Z., **Nothias L.F.**, White M., Rabines A., Petras D.. 'Illuminating the dark metabolome of Pseudo-nitzschia-microbiome associations (vol 24, pg 5408, 2022). *ENVIRONMENTAL*

- (2023) **art.** Kirchhoffer O., Nitschke J., **Nothias L.F.**, Hanna N., Marcourt L., Allard P.M., Grondin A., Queiroz E.F., Soldati T., Wolfender J.L.. Short Lecture. *Planta Medica*, 89(14), SL–A05.
- (2023) **pp** **Nothias L.F.**, Schmid R., Garlet A., Cameron H., Leoty-Okombi S., André-Frei V., Fuchs R., Dorrestein P.C., Ternes P.. A multi-omics strategy for the study of microbial metabolism : application to the human skin’s microbiome. *BiorXiv*.
- (2023) **ac** Tysinger E., Pagni M., Kirchhoffer O., Mehl F., Gandon F., Wolfender J.L., **Nothias L.F.**. An Artificial Intelligence Agent for Navigating Knowledge Graph Experimental Metabolomics Data. *2023 Swiss Metabolomics Society Annual Meeting*.
- (2022) **art.** Wegley Kelly L., Nelson C.E., Petras D., Koester I., Quinlan Z.A., Arts M.G., **Nothias L.F.**, Comstock J., White B.M., Hopmans E.C., et al.. Distinguishing the molecular diversity, nutrient content, and energetic potential of exometabolomes produced by macroalgae and reef-building corals. *Proceedings of the National Academy of Sciences*, 119(5), e2110283119. doi :10.1073/pnas.2110283119
- (2022) **art.** Wolfender J.L., Gaudry A., Rutz A., Quiros-Guerrero L.M., **Nothias L.F.**, Queiroz E.F., De-fosse E., Allard P.M.. Metabolomics in ecology and bioactive natural products discovery : challenges and prospects for a comprehensive study of the specialised metabolome. *Chimia*, 76(11), 954–963. doi :10.2533/chimia.2022.954
- (2022) **art.** Yu J.S., **Nothias L.F.**, Wang M., Kim D.H., Dorrestein P.C., Kang K.B., Yoo H.H.. Tandem mass spectrometry molecular networking as a powerful and efficient tool for drug metabolism studies. *Analytical chemistry*, 94(2), 1456–1464. doi :10.1021/acs.analchem.1c04925
- (2022) **art.** Zhang S., Song W., **Nothias L.F.**, Couvillion S.P., Webster N., Thomas T.. Comparative metabolomic analysis reveals shared and unique chemical interactions in sponge holobionts. *Microbiome*, 10(1), 22. doi :10.1186/s40168-021-01220-9
- (2022) **art.** Shaffer J.P., **Nothias L.F.**, Thompson L.R., Sanders J.G., Salido R.A., Couvillion S.P., Brejnrod A.D., Lejzerowicz F., Haiminen N., Huang S., et al.. Standardized multi-omics of Earth’s microbiomes reveals microbial and metabolite diversity. *Nature microbiology*, 7(12), 2128–2150. doi :10.1038/s41564-022-01266-x
- (2022) **art.** Quiros-Guerrero L.M., **Nothias L.F.**, Gaudry A., Marcourt L., Allard P.M., Rutz A., David B., Queiroz E.F., Wolfender J.L.. Inventa : A computational tool to discover structural novelty in natural extracts libraries. *Frontiers in Molecular Biosciences*, 9, 1028334. doi :10.3389/fmolb.2022.1028334
- (2022) **art.** Hoffmann M.A., **Nothias L.F.**, Ludwig M., Fleischauer M., Gentry E.C., Witting M., Dorrestein P.C., Dührkop K., Böcker S.. High-confidence structural annotation of metabolites absent from spectral libraries. *Nature Biotechnology*, 40(3), 411–421. doi :10.1038/s41587-021-01045-9
- (2022) **art.** Gaudry A., Huber F., **Nothias L.F.**, Cretton S., Kaiser M., Wolfender J.L., Allard P.M.. MEMO : Mass Spectrometry-based Sample Vectorization to Explore Chemodiverse Datasets. *Front. Bioinform.*, 2, 842964. doi :10.3389/fbinf.2022.842964
- (2022) **art.** Wolfender J., Gaudry A., Quiros-Guerrero L., Kirchhoffer O., Rutz A., Marcourt L., David B., Grondin A., **Nothias L.**, Queiroz E.F., et al.. Keynote Lecture “Strategies to prioritize the discovery of bioactive natural products–Chemical space exploration based on massive multi-informative metabolite networks”. *Planta Medica*, 88(15), KL–16.
- (2022) **art.** Quiros-Guerrero L., **Nothias L.**, Gaudry A., Marcourt L., Allard P., David B., Queiroz E.F., Wolfender J.. INVENTA : a workflow for discovering chemical novelty in natural products extracts libraries. *Planta Medica*, 88(15), P–302.
- (2022) **pp** Shaffer J.P., **Nothias L.F.**, Thompson L.R., Sanders J.G., Salido R.A., Couvillion S.P., Brejnrod A.D., Huang S., Lejzerowicz F., Lutz H.L., et al.. Multi-omics profiling of Earth’s biomes reveals that microbial and metabolite composition are shaped by the environment. *bioRxiv*.
- (2021) **art.** Zuo Z., Cao L., Nothia L.F., Mohimani H.. MS2Planner : improved fragmentation spectra coverage in untargeted mass spectrometry by iterative optimized data acquisition. *Bioinformatics*, 37(Supplement\({}_1\)), i231–i236. doi :10.1093/bioinformatics/btab279
- (2021) **art.** Schmid R., Petras D., **Nothias L.F.**, Wang M., Aron A.T., Jagels A., Tsugawa H., Rainer J., Garcia-Aloy M., Dührkop K., et al.. Ion identity molecular networking for mass spectrometry-based metabolomics in the GNPS environment. *Nature communications*, 12(1), 3832. doi :10.1038/s41467-021-23953-9
- (2021) **art.** Dührkop K., **Nothias L.F.**, Fleischauer M., Reher R., Ludwig M., Hoffmann M.A., Petras D., Gerwick W.H., Rousu J., Dorrestein P.C., et al.. Systematic classification of unknown metabolites using high-resolution fragmentation mass spectra. *Nature biotechnology*, 39(4), 462–471. doi :10.1038/s41587-020-0740-8

- (2021) **art.** Kunyavskaya O., Tagirdzhanov A.M., Caraballo-Rodríguez A.M., **Nothias L.F.**, Dorrestein P.C., Korobeynikov A., Mohimani H., Gurevich A.. Nerpa : a tool for discovering biosynthetic gene clusters of bacterial nonribosomal peptides. *Metabolites*, 11(10), 693. doi :10.3390/metabo11100693
- (2021) **art.** Aksenov A.A., Laponogov I., Zhang Z., Doran S.L., Belluomo I., Veselkov D., Bittremieux W., **Nothias L.F.**, **Nothias-Esposito M.**, Maloney K.N., et al.. Auto-deconvolution and molecular networking of gas chromatography–mass spectrometry data. *Nature biotechnology*, 39(2), 169–173. doi :10.1038/s41587-020-0700-3
- (2021) **art.** Shaikh A.A., **Nothias L.F.**, Srivastava S.K., Dorrestein P.C., Tahlan K.. Specialized metabolites from ribosome engineered strains of *Streptomyces clavuligerus*. *Metabolites*, 11(4), 239. doi :10.3390/metabo11040239
- (2021) **art.** Caraballo-Rodríguez A.M., Puckett S.P., Kyle K.E., Petras D., da Silva R., **Nothias L.F.**, Ernst M., van der Hooft J.J., Tripathi A., Wang M., et al.. Chemical gradients of plant substrates in an *Atta texana* fungus garden. *Msystems*, 6(4), 10–1128. doi :10.1128/msystems.00601-21
- (2021) **art.** Morton J.T., McDonald D., Aksenov A.A., **Nothias L.F.**, Foulds J.R., Quinn R.A., Badri M.H., Swenson T.L., Van Goethem M.W., Northen T.R., et al.. Reply to : Examining microbe–metabolite correlations by linear methods. *Nature methods*, 18(1), 40–41. doi :10.1038/s41592-020-01007-0
- (2021) **art.** Schorn M.A., Verhoeven S., Ridder L., Huber F., Acharya D.D., Aksenov A.A., Aleti G., Moghaddam J.A., Aron A.T., Aziz S., et al.. A community resource for paired genomic and metabolomic data mining. *Nature Chemical Biology*, 17(4), 363–368. doi :10.1038/s41589-020-00724-z
- (2021) **art.** Liu J., **Nothias L.F.**, Dorrestein P.C., Tahlan K., Bignell D.R.. Genomic and metabolomic analysis of the potato common scab pathogen *Streptomyces scabiei*. *ACS omega*, 6(17), 11474–11487.
- (2020) **pp** Xie H.F., Kong Y.S., Li R.Z., **Nothias L.F.**, Zhang H., Liu L.L., An T.T., Liu R., Yang Z., Ke J.P., et al.. Feature-Based Molecular Networking Analysis of the Metabolites Produced by in vitro Solid-State Fermentation Reveals Pathways for the Bioconversion of Epigallocatechin Gallate. *J. Agric. Food Chem.*, 68, 7995–8007. doi :10.26434/chemrxiv.12124206
- (2020) **art.** De la Torre-Tarazona H.E., Jiménez R., Bueno P., Camarero S., Román L., Fernández-García J., Beltran M., **Nothias L.**, Cachet X., Paolini J., et al.. 4-Deoxyphorbol inhibits HIV-1 infection in synergism with antiretroviral drugs and reactivates viral reservoirs through PKC/MEK activation synergizing with vorinostat. *Biochemical Pharmacology*, 177, 113937. doi :10.1016/j.bcp.2020.113937
- (2020) **art.** Martin H C., Ibáñez R., **Nothias L.F.**, Caraballo-Rodríguez A.M., Dorrestein P.C., Gutiérrez M.. Metabolites from microbes isolated from the skin of the panamanian rocket frog *Colostethus panamansis* (Anura : Dendrobatidae). *Metabolites*, 10(10), 406. doi :10.3390/metabo10100406
- (2020) **art.** Ludwig M., Broeckling C.D., Dorrestein P.C., Dührkop K., Schymanski E.L., Böcker S., **Nothias L.F.**. Studying charge migration fragmentation of sodiated precursor ions in collision-induced dissociation at the library scale. *Journal of the American Society for Mass Spectrometry*, 32(1), 180–186. doi :10.1021/jasms.0c00240
- (2020) **art.** Reher R., Kim H.W., Zhang C., Mao H.H., Wang M., **Nothias L.F.**, Caraballo-Rodriguez A.M., Glukhov E., Teke B., Leao T., et al.. A convolutional neural network-based approach for the rapid annotation of molecularly diverse natural products. *Journal of the American Chemical Society*, 142(9), 4114–4120. doi :10.1021/jacs.9b13786
- (2020) **art.** Kang K.B., Woo S., Ernst M., van Der Hooft J.J., **Nothias L.F.**, da Silva R.R., Dorrestein P.C., Sung S.H., Lee M.. Assessing specialized metabolite diversity of *Alnus* species by a digitized LC–MS/MS data analysis workflow. *Phytochemistry*, 173, 112292. doi :10.1016/j.phytochem.2020.112292
- (2020) **art.** Ludwig M., **Nothias L.F.**, Dührkop K., Koester I., Fleischauer M., Hoffmann M.A., Petras D., Vargas F., Morsy M., Aluwihare L., et al.. Database-independent molecular formula annotation using Gibbs sampling through ZODIAC. *Nature Machine Intelligence*, 2(10), 629–641. doi :10.1038/s42256-020-00234-6
- (2020) **art.** Tripathi A., Vázquez-Baeza Y., Julia M.G., Mingxun W., Kai D., Mélissa N.E.D.D.A., Madeleine E., Justin J. J. v.d.H., Qiyun Z., Daniel M., et al.. Chemically informed analyses of metabolomics mass spectrometry data with Qemistree. *Nature Chemical Biology*. doi :10.1038/s41589-020-00677-3
- (2020) **art.** Aron A.T., Gentry E.C., McPhail K.L., **Nothias L.F.**, **Nothias-Esposito M.**, Bouslimani A., Petras D., Gauglitz J.M., Sikora N., Vargas F., et al.. Reproducible molecular networking of untargeted mass spectrometry data using GNPS. *Nature protocols*, 15(6), 1954–1991. doi :10.1038/s41596-020-0317-5
- (2020) **art.** Jarmusch A.K., Wang M., Aceves C.M., Advani R.S., Aguirre S., Aksenov A.A., Aleti G., Aron A.T., Bauermeister A., Bolleddu S., et al.. ReDU : a framework to find and reanalyze public mass spectrometry data. *Nature Methods*, 17(9), 901–904. doi :10.1038/s41592-020-0916-7

- (2020) **art.** **Nothias L.F.**, Petras D., Schmid R., Dührkop K., Rainer J., Sarvepalli A., Protsyuk I., Ernst M., Tsugawa H., Fleischauer M., et al.. Feature-based molecular networking in the GNPS analysis environment. *Nature methods*, 17(9), 905–908. doi :10.1038/s41592-020-0933-6
- (2020) **art.** Wang M., Jarmusch A.K., Vargas F., Aksenov A.A., Gauglitz J.M., Weldon K., Petras D., da Silva R., Quinn R., Melnik A.V., et al.. Mass spectrometry searches using MASST. *Nature biotechnology*, 38(1), 23–26. doi :10.1038/s41587-019-0375-9
- (2020) **pp** Caraballo-Rodríguez A.M., Puckett S.P., Kyle K.E., Petras D., da Silva R., **Nothias L.F.**, Ernst M., van der Hooft J.J., Tripathi A., Wang M., et al.. The ant fungus garden acts as an external digestive system. *bioRxiv*, 2020–11. doi :10.1101/2020.11.18.389361
- (2020) **ac** Aluwihare L., Petras D., Koester I., **Nothias L.F.**, Ludwig M., Duhrkop K., Wang M., Böcker S., Dorrestein P.. Challenges and rewards of nontargeted studies of marine dissolved organic matter (DOM) composition using liquid chromatography coupled to tandem mass spectrometry (LC MS/MS) : Case studies from coastal, marine environments.. *American Geophysical Union, Ocean Sciences Meeting*, CT43A–02.
- (2020) **art.** Hyun Woo K., Wang M., Leber C., **Nothias L.F.**, Reher R., Kang K.B., van der Hooft J.J., Dorrestein P., Gerwick W., Cottrell G.. NPClassifier : A deep neural network-based structural classification tool for natural products.. doi :10.1021/acs.jnatprod.1c00399
- (2019) **art.** Martin C.H., Ibáñez R., **Nothias L.F.**, Reinert L.K., Rollins-Smith L.A., Dorrestein P.C., Gutiérrez M.. Viscosin-like lipopeptides from frog skin bacteria inhibit *Aspergillus fumigatus* and *Batrachochytrium dendrobatidis* detected by imaging mass spectrometry and molecular networking. *Scientific reports*, 9(1), 1–11. doi :10.1038/s41598-019-39583-7
- (2019) **art.** Cao L., Gurevich A., Alexander K.L., Naman C.B., Leão T., Glukhov E., Luzzatto-Knaan T., Vargas F., Quinn R., Bouslimani A., et al.. MetaMiner : a scalable peptidogenomics approach for discovery of ribosomal peptide natural products with blind modifications from microbial communities. *Cell systems*, 9(6), 600–608. doi :10.1016/j.cels.2019.09.004
- (2019) **art.** AbuSara N.F., Piercey B.M., Moore M.A., Shaikh A.A., **Nothias L.F.**, Srivastava S.K., Cruz-Morales P., Dorrestein P.C., Barona-Gómez F., Tahlan K.. Comparative genomics and metabolomics analyses of clavulanic acid-producing *Streptomyces* species provides insight into specialized metabolism. *Frontiers in Microbiology*, 10, 2550. doi :10.3389/fmicb.2019.02550
- (2019) **art.** Ernst M., Kang K.B., Caraballo-Rodríguez A.M., **Nothias L.F.**, Wandy J., Chen C., Wang M., Rogers S., Medema M.H., Dorrestein P.C., et al.. MolNetEnhancer : enhanced molecular networks by integrating metabolome mining and annotation tools. *Metabolites*, 9(7), 144. doi :10.3390/metabo9070144
- (2019) **art.** Bolyen E., Rideout J.R., Dillon M.R., Bokulich N.A., Abnet C.C., Al-Ghalith G.A., Alexander H., Alm E.J., Arumugam M., Asnicar F., et al.. Reproducible, interactive, scalable and extensible microbiome data science using QIIME 2. *Nature biotechnology*, 37(8), 852–857. doi :10.1038/s41587-019-0209-9
- (2019) **art.** Ernst M., **Nothias L.F.**, Van der Hooft J.J., Silva R.R., Saslis-Lagoudakis C.H., Grace O.M., Martinez-Swatson K., Hassemer G., Funez L.A., Simonsen H.T., et al.. Assessing specialized metabolite diversity in the cosmopolitan plant genus *Euphorbia* L.. *Frontiers in Plant Science*, 10, 846. doi :10.3389/fpls.2019.00846
- (2019) **art.** Morton J.T., Aksenov A.A., **Nothias L.F.**, Foulds J.R., Quinn R.A., Badri M.H., Swenson T.L., Van Goethem M.W., Northen T.R., Vazquez-Baeza Y., et al.. Learning representations of microbe–metabolite interactions. *Nature methods*, 16(12), 1306–1314. doi :10.1038/s41592-019-0616-3
- (2019) **pp** Morton J.T., McDonald D., Aksenov A.A., **Nothias L.F.**, Foulds J.R., Quinn R.A., Badri M.H., Swenson T.L., Van Goethem M.W., Northen T.R., et al.. Revisiting microbe-metabolite interactions : Doing better than random. *bioRxiv*, 2019–12. doi :10.1101/2019.12.10.871905
- (2019) **art.** **Nothias-Esposito M.**, **Nothias L.F.**, Da Silva R.R., Retailleau P., Zhang Z., Leyssen P., Roussi F., Touboul D., Paolini J., Dorrestein P.C., et al.. Investigation of premyrsinane and myrsinane esters in *Euphorbia cupanii* and *Euphorbia pithyusa* with MS2LDA and combinatorial molecular network annotation propagation. *Journal of Natural Products*, 82(6), 1459–1470.
- (2019) **art.** Gaudry A., Quirós L., Rutz A., Dounoue M., Kaiser M., David B., Marcourt L., Queiroz E., Wolfender J., Allard P.. Multi-informative bioactivity-based molecular networking of a large chemodiverse plant collection allows efficient identification of trypanocidal natural products. *Planta Medica*, 85(18), P–109.
- (2019) **art.** Shi D., Chahal K.K., Oto P., **Nothias L.F.**, Debnath A., McKerrow J.H., Podust L.M., Abagyan R.. Identification of Four Amoebicidal Nontoxic Compounds by a Molecular Docking Screen of *Naegleria fowleri* Sterol 8- 7-Isomerase and Phenotypic Assays. *ACS infectious diseases*, 5(12), 2029–2038.

- (2018) **art. Nothias L.F., Nothias-Esposito M.**, Da Silva R., Wang M., Protsyuk I., Zhang Z., Sarvepalli A., Leyssen P., Touboul D., Costa J., et al.. Bioactivity-based molecular networking for the discovery of drug leads in natural product bioassay-guided fractionation. *Journal of natural products*, 81(4), 758–767. doi :10.1021/acs.jnatprod.7b00737
- (2018) **art. d'Auriac I.G., Quinn R.A., Maughan H., Nothias L.F., Little M., Kapon C.A., Cobian A., Reyes B.T., Green K., Quistad S.D., et al.** Before platelets : the production of platelet-activating factor during growth and stress in a basal marine organism. *Proceedings of the Royal Society B : Biological Sciences*, 285(1884), 20181307. doi :10.1098/rspb.2018.1307
- (2018) **art. Mohimani H., Gurevich A., Shlemov A., Mikheenko A., Korobeynikov A., Cao L., Shcherbin E., Nothias L.F., Dorrestein P.C., Pevzner P.A.** Dereplication of microbial metabolites through database search of mass spectra. *Nature communications*, 9(1), 4035. doi :10.1038/s41467-018-06082-8
- (2018) **art. Protsyuk I., Melnik A.V., Nothias L.F., Rappez L., Phapale P., Aksenov A.A., Bouslimani A., Ryazanov S., Dorrestein P.C., Alexandrov T.** 3D molecular cartography using LC–MS facilitated by Optimus and ili software. *Nature protocols*, 13(1), 134–154. doi :10.1038/nprot.2017.122
- (2018) **art. da Silva R.R., Wang M., Nothias L.F., van der Hooft J.J., Caraballo-Rodríguez A.M., Fox E., Balunas M.J., Klassen J.L., Lopes N.P., Dorrestein P.C.** Propagating annotations of molecular networks using in silico fragmentation. *PLoS computational biology*, 14(4), e1006089. doi :10.1371/journal.pcbi.1006089
- (2018) **art. Quinn R.A., Comstock W., Zhang T., Morton J.T., da Silva R., Tran A., Aksenov A., Nothias L.F., Wangpraseurt D., Melnik A.V., et al.** Niche partitioning of a pathogenic microbiome driven by chemical gradients. *Science advances*, 4(9), eaau1908. doi :10.1126/sciadv.aau1908
- (2018) **art. Nothias L.F., Ballero M., Maxia A., Pollastro F., Dorrestein P., Paolini J., Litaudon M., Appendino G.** Chemodiversity or taxonomy error? A search for the true phytochemical profile of *Ferula arrigonii* Bocchieri. *ISTE OpenSci*, 1, 1–9.
- (2018) **art. Olivon F., Nothias L.F., Dumontet V., Retaillieu P., Berger S., Ferry G., Cohen W., Pfeiffer B., Boutin J.A., Scalbert E., et al.** Natural Inhibitors of the RhoA–p115 Complex from the Bark of *Meiogyne baillonii*. *Journal of natural products*, 81(7), 1610–1618.
- (2018) **ac Koester L., Petras D., Brunson J.K., Nothias L.F., White M.E., Azam F., Knight R., Allen A.E., Dorrestein P., Aluwihare L.** A Metabolomic Profile of the Pseudo-nitzschia Microbiome. *American Geophysical Union, Ocean Sciences Meeting*, BN23B–02.
- (2017) **art. Olivon F., Allard P.M., Koval A., Righi D., Genta-Jouve G., Neyts J., Apel C., Pannecouque C., Nothias L.F., Cachet X., et al.** Bioactive natural products prioritization using massive multi-informational molecular networks. *ACS chemical biology*, 12(10), 2644–2651. doi :10.1021/acscchembio.7b00413
- (2017) **art. Quinn R.A., Nothias L.F., Vining O., Meehan M., Esquenazi E., Dorrestein P.C.** Molecular networking as a drug discovery, drug metabolism, and precision medicine strategy. *Trends in pharmacological sciences*, 38(2), 143–154. doi :10.1016/j.tips.2016.10.011
- (2017) **art. Scheubert K., Hufsky F., Petras D., Wang M., Nothias L.F., Dührkop K., Bandeira N., Dorrestein P.C., Böcker S.** Significance estimation for large scale metabolomics annotations by spectral matching. *Nature Communications*, 8(1), 1494. doi :10.1038/s41467-017-01318-5
- (2017) **art. Mohimani H., Gurevich A., Mikheenko A., Garg N., Nothias L.F., Ninomiya A., Takada K., Dorrestein P.C., Pevzner P.A.** Dereplication of peptidic natural products through database search of mass spectra. *Nature chemical biology*, 13(1), 30–37. doi :10.1038/nchembio.2219
- (2017) **art. Nothias L.F., Boutet-Mercey S., Cachet X., De La Torre E., Laboureur L., Gallard J.F., Retaillieu P., Brunelle A., Dorrestein P.C., Costa J., et al.** Environmentally friendly procedure based on supercritical fluid chromatography and tandem mass spectrometry molecular networking for the discovery of potent antiviral compounds from *Euphorbia semiperfoliata*. *Journal of natural products*, 80(10), 2620–2629.
- (2017) **art. Esposito M., Nothias L.F., Retaillieu P., Costa J., Roussi F., Neyts J., Leyssen P., Touboul D., Litaudon M., Paolini J.** Isolation of premyrsinane, myrsinane, and tiglane diterpenoids from *Euphorbia pithyusa* using a Chikungunya virus cell-based assay and analogue annotation by molecular networking. *Journal of natural products*, 80(7), 2051–2059.
- (2017) **art. Esposito M., Nim S., Nothias L.F., Gallard J.F., Rawal M.K., Costa J., Roussi F., Prasad R., Di Pietro A., Paolini J., et al.** Evaluation of jatrophone esters from *Euphorbia* spp. as modulators of *Candida albicans* multidrug transporters. *Journal of natural products*, 80(2), 479–487.
- (2016) **art. Wang M., Carver J.J., Phelan V.V., Sanchez L.M., Garg N., Peng Y., Nguyen D.D., Watrous J., Kapon C.A., Luzzatto-Knaan T., et al.** Sharing and community curation of mass spectrometry data with

- (2016) **art.** Petras D., **Nothias L.F.**, Quinn R.A., Alexandrov T., Bandeira N., Bouslimani A., Castro-Falcón G., Chen L., Dang T., Floros D.J., et al.. Mass spectrometry-based visualization of molecules associated with human habitats. *Analytical chemistry*, 88(22), 10775–10784. doi :10.1021/acs.analchem.6b03456
- (2016) **art.** **Nothias L.F.**, Knight R., Dorrestein P.C.. Antibiotic discovery is a walk in the park. *Proceedings of the National Academy of Sciences*, 113(51), 14477–14479. doi :10.1073/pnas.1618221114
- (2016) **ac LF Nothias I.P.T.A.R.K.A.B.D.T.P.D.**. 3D-Plant2cells project : Spatial metabolomic, spatial metagenomic, and 3D mass spectrometry imaging, to explore the impact of pesticides on plant metabolome and microbiota. *Planta Medica*, 82(S 01), S1–S381. doi :10.1055/s-0036-1596119
- (2016) **ac** Esposito M., **Nothias-Scaglia L.**, Leyssen P., Roussi F., Touboul D., Costa J., Paolini J., Litaudon M.. Targeting new anti-CHIKV diterpenoids from two Corsican Euphorbia species using MS/MS molecular networking. *Planta Medica*, 82(S 01), P80. doi :10.1055/s-0036-1596248
- (2016) **art.** Esposito M., **Nothias L.F.**, Nedev H., Gallard J.F., Leyssen P., Retailleau P., Costa J., Roussi F., Iorga B.I., Paolini J., et al.. Euphorbia dendroides Latex as a source of jatrophone esters : isolation, structural analysis, conformational study, and anti-CHIKV activity. *Journal of natural products*, 79(11), 2873–2882.
- (2016) **art.** Petras D., **Nothias L.F.**, Quinn R.A., Alexandrov T., Bandeira N., Bouslimani A., Castro-Falcón G., Chen L., Dang T., Floros D.J., et al.. Mass Spectrometry-Based 3D Cartography Displays the Chemistry Associated with Modern Human Habitats. *Analytical chemistry*, 88(22), 10775.
- (2016) **ac Nothias-Scaglia L.**, Boutet-Mercey S., Cachet X., de La Torre H., Costa J., Paolini J., Bedoya L., Alcamí J., Leyssen P., Brunelle A., et al.. Welcoming the green metabolomic era : supercritical fluid chromatography, tandem mass spectrometry, and molecular networking, as an efficient workflow to explore metabolome and isolate targeted compound.. *9th Joint Natural Products Conference, 2016*.
- (2016) **ac** Espositoa M., **Nothias-Scagliaa L.**, Leyssen P., Roussib F., Touboulb D., Costaa J., Litaudonb M., Paolinia J.. Molecular Networking of MS/MS as a tool to target antiviral diterpenoids from Corsican Euphorbia. *10èmes Journées Scientifiques du Réseau Francophone de Métabolomique et Fluxomique*.
- (2015) **art.** **Nothias-Scaglia L.F.**, Schmitz-Afonso I., Renucci F., Roussi F., Touboul D., Costa J., Litaudon M., Paolini J.. Insights on profiling of phorbol, deoxyphorbol, ingenol and jatrophone diterpene esters by high performance liquid chromatography coupled to multiple stage mass spectrometry. *Journal of Chromatography A*, 1422, 128–139. doi :10.1016/j.chroma.2015.09.092
- (2015) **art.** **Nothias-Scaglia L.F.**, Gallard J.F., Dumontet V., Roussi F., Costa J., Iorga B.I., Paolini J., Litaudon M.. Advanced structural determination of diterpene esters using molecular modeling and NMR spectroscopy. *Journal of Natural products*, 78(10), 2423–2431. doi :10.1021/acs.jnatprod.5b00511
- (2015) **art.** **Nothias-Scaglia L.F.**, Dumontet V., Neyts J., Roussi F., Costa J., Leyssen P., Litaudon M., Paolini J.. LC-MS2-Based dereplication of Euphorbia extracts with anti-Chikungunya virus activity. *Fitoterapia*, 105, 202–209. doi :10.1016/j.fitote.2015.06.021
- (2015) **art.** **Nothias-Scaglia L.F.**, Pannecouque C., Renucci F., Delang L., Neyts J., Roussi F., Costa J., Leyssen P., Litaudon M., Paolini J.. Antiviral activity of diterpene esters on chikungunya virus and HIV replication. *Journal of natural products*, 78(6), 1277–1283. doi :10.1021/acs.jnatprod.5b00073
- (2015) **thèse Nothias-Scaglia L.F.**. Etude de l'activité antivirale d'extraits d'Euphorbia de Corse : recherche de nouveaux diterpènes d'intérêt biologique. *Université Pascal Paoli*. doi :10.70675/220f96d3zc9d0z4998zaed8z84697b65f84e
- (2015) **art.** **Nothias-Scaglia L.F.**, Esposito M., Costa J., Paolini J., Touboul D., Litaudon M.. Les réseaux moléculaires, une approche bio-informatique globale pour interpréter les données de spectrométrie de masse tandem. *Spectra Analyse*, 73–78.
- (2015) **art.** **Nothias-Scaglia L.**, Esposito M., Costa J., Paolini J., Touboul D., Litaudon M.. Molecular networks, a bioinformatic tool for tandem mass spectrometry data interpretation. *Spectra Analyse*, 307, 73–78.
- (2015) **ac Nothias-Scaglia L.**, Esposito M., Cachet X., Roussi F., Costa J., Leyssen P., Paolini J., Touboul D., Litaudon M.. Accelerating Natural Products Research Workflow by MS/MS Molecular Networking : an Efficient Approach Toward the Study of Euphorbia species. *8ième édition du congrès français de Spectrométrie de Masse et d'Analyse Protéomique (SMAP)*.
- (2015) **ac Nothias-Scaglia L.**, Esposito M., Cachet X., Costa J., Roussi F., Paolini J., Touboul D., Litaudon M.. Molecular Networking, an Innovative Tool for Natural Products Research : Application to the

- (2015) **ac Nothias-Scaglia L.**, Schmitz-Afonso I., Renucci F., Roussi F., Leyssen P., Touboul D., Costa J., Litaudon M., Paolini J.. HPLC-MS² dereplication and profiling of diterpene esters from Euphorbia extracts with anti-chikungunya virus activity. *8ième édition du congrès français de Spectrométrie de Masse et d'Analyse Protéomique (SMAP)*.
- (2015) **ac Allard P., Nothias-Scaglia L.**, Cachet X., Litaudon M.. Massive multi-informative molecular networks : a map to navigate through the chemical space of bioactive Euphorbiaceae. *8ième édition du congrès français de Spectrométrie de Masse et d'Analyse Protéomique (SMAP)*.
- (2015) **ac Esposito M., Nothias-Scaglia L.**, Leyssen P., Roussi F., Touboul D., Costa J., Litaudon M., Paolini J.. A Molecular Networking Based Workflow for an Efficient Phytochemical Study of Euphorbia pithyusa L. Plant Species. *8ième édition du congrès français de Spectrométrie de Masse et d'Analyse Protéomique (SMAP)*.
- (2015) **ac Nothias-Scaglia L.**, Esposito M., Cachet X., Costa J., Roussi F., Paolini J., Touboul D., Litaudon M.. Molecular Networking for Structure-Guided Purification of Diterpene Esters from Euphorbia Species. *IX° Journées Scientifiques du Réseau Français de Métabolomique et Fluxomique*.
- (2015) **pp Nothias-Scaglia L.F.**. Study of the antiviral activity of Euphorbia extracts from Corsica : Search for new diterpenes of biological interest..
- (2014) **art. Nothias-Scaglia L.F.**, Retailleau P., Paolini J., Pannecouque C., Neyts J., Dumontet V., Roussi F., Leyssen P., Costa J., Litaudon M.. Jatrophone diterpenes as inhibitors of chikungunya virus replication : structure-activity relationship and discovery of a potent lead. *Journal of natural products*, 77(6), 1505–1512. doi :10.1021/np500271u
- (2014) **ac Nothias-Scaglia L.**, Dumontet V., Leyssen P., Retailleau P., Gallard J., Roussi F., Paolini J., Costa J., Litaudon M.. Antiviral diterpene polyesters from Corsican Euphorbia species. *Planta Medica*, 80(16), P1M5. doi :10.1055/s-0034-1394572
- (2013) **ac Litaudon M., Nothias L.**, Allard P., Bourjot M., Dumontet V., Guéritte F., Delang L., Pannecouque C., Leyssen P.. Diterpenoids from Euphorbiaceae with Potent Anti-CHIKV and Anti-HIV Activities : Are these Antiviral Properties Correlated?. *Planta Medica*, 79(10), PN44.
- (s.d.) **pp Bolyen E., Rideout J., Dillon M., Bokulich N., Abnet C., Al-Ghalith G., Alexander H., Alm E., Arumugam M., Asnicar F., et al.. Robeson II MS. Rosenthal P, Segata N, Shaffer M, Shiffer A, Sinha R, Song SJ, Spear JR, Swafford AD, Thompson LR, Torres PJ, Trinh P, Tripathi A, Turnbaugh PJ, UI-Hasan S, Hooft JJJ, Vargas F, Vázquez-Baeza Y, Vogtmann E, Hippel M, Walters W, Wan Y, Wang M, Warren J, Weber KC, Williamson CHD, Willis AD, Xu ZZ, Zaneveld JR, Zhang Y, Knight R, Caporaso JG**, 1, 852–857.
- (s.d.) **pp Wolfender J.L., Kirchhoffer A., Gaudry A., Quiros-Guerrero L., Pagni O.M., Mehl F., Burdet F., Marcourt L., David B., Grondin A., et al.. FROM BIOACTIVE NATURAL PRODUCTS TO MEGA-BYTES : HARNESSING AI'S POTENTIAL AND METABOLOMICS FOR FOR THE DIGITAL TRANSFORMATION OF PHARMACOGNOSY..**
- (s.d.) **pp Allard P.M., Nothias-Scaglia L.F.**, Cachet X., Litaudon M., Wolfender J.L.. Mapping the chemical space of bioactive Euphorbiaceae species through massive multi-informative molecular networks..