

Scientific Publications

1. Gomes, P. W. P. *et al.* plantMASST - Community-driven chemotaxonomic digitization of plants. *bioRxiv* 2024.05.13.593988 (2024) doi:10.1101/2024.05.13.593988.
2. Quiros-Guerrero, L. *et al.* Integration of Wnt-inhibitory Activity and Structural Novelty Scoring Results to Uncover Novel Bioactive Natural Products: New Bicyclo[3.3.1]non-3-ene-2,9-diones from the Leaves of *Hymenocardia punctata*. *ChemRxiv* (2024) doi:10.26434/chemrxiv-2024-96nz6.
3. Quiros-Guerrero, L.-M. *et al.* Comprehensive mass spectrometric metabolomic profiling of a chemically diverse collection of plants of the Celastraceae family. *Sci Data* **11**, 415 (2024).
4. Zuffa, S. *et al.* microbeMASST: a taxonomically informed mass spectrometry search tool for microbial metabolomics data. *Nat Microbiol* **9**, 336–345 (2024).
5. Escudero-Leyva, E. *et al.* Differential Volatile Organic Compound Expression in the Interaction of *Daldinia eschscholtzii* and *Mycena citricolor*. *ACS Omega* (2023) doi:10.1021/acsomega.3c03865.
6. Gaudry, A. *et al.* A Sample-Centric and Knowledge-Driven Computational Framework for Natural Products Drug Discovery. *ACS Cent. Sci.* (2024) doi:10.1021/acscentsci.3c00800.
7. Sevik Kilicaslan, O. *et al.* Antiprotozoal activity of natural products from Nigerien plants used in folk medicine. *Front. Pharmacol.* **14**, 1190241 (2023).
8. Hammerle, F., Quirós-Guerrero, L., Wolfender, J.-L., Peintner, U. & Siewert, B. Highlighting the Phototherapeutical Potential of Fungal Pigments in Various Fruiting Body Extracts with Informed Feature-Based Molecular Networking. *Microb. Ecol.* (2023) doi:10.1007/s00248-023-02200-2.
9. Allard, P.-M. *et al.* Open and reusable annotated mass spectrometry dataset of a chemodiverse collection of 1,600 plant extracts. *Gigascience* **12**, (2023).

10. Saraux, N. *et al.* Isolation and Structure Elucidation of Compounds from *Sesamum alatum* and Their Antiproliferative Activity against Multiple Myeloma Cells. *J. Nat. Prod.* **85**, 2706–2713 (2022).
11. Wolfender, J.-L. *et al.* Metabolomics in ecology and bioactive natural products discovery: Challenges and prospects for a comprehensive study of the specialised metabolome. *Chimia* **76**, 954 (2022).
12. Quiros-Guerrero, L.-M. *et al.* Inventa: A computational tool to discover structural novelty in natural extracts libraries. *Front Mol Biosci* **9**, 1028334 (2022).
13. Huber, R. *et al.* Chiral Separation of Stilbene Dimers Generated by Biotransformation for Absolute Configuration Determination and Antibacterial Evaluation. *Front Chem* **10**, 912396 (2022).
14. Sevik Kilicaslan, O. *et al.* Isolation and Structural Elucidation of Compounds from *Pleiocarpa bicarpellata* and Their In Vitro Antiprotozoal Activity. *Molecules* **27**, 2200 (2022).
15. Saraux, N. *et al.* Phytochemical Investigation of the Roots of *Ipomoea asarifolia* and Antiproliferative Activity of the Isolated Compounds against Multiple Myeloma Cells. *J. Nat. Prod.* **85**, 56–62 (2022).
16. Hammerle, F. *et al.* Feature-Based Molecular Networking-An Exciting Tool to Spot Species of the Genus *Cortinarius* with Hidden Photosensitizers. *Metabolites* **11**, (2021).
17. Conserva, G. A. *et al.* Kaempferol-3-O- α -(3,4-di-E-p-coumaroyl)-rhamnopyranoside from *Nectandra oppositifolia* releases Ca^{2+} from intracellular pools of *Trypanosoma cruzi* affecting the bioenergetics system. *Chem. Biol. Interact.* **349**, 109661 (2021).
18. Pellissier, L. *et al.* Characterization of *Pseudomonas aeruginosa* Quorum Sensing Inhibitors from the Endophyte *Lasiodiplodia venezuelensis* and Evaluation of Their Antivirulence Effects by Metabolomics. *Microorganisms* **9**, 1807 (2021).
19. Magliocco, G. *et al.* Metabolomics reveals biomarkers in human urine and plasma to predict cytochrome P450 2D6 (CYP2D6) activity. *Br. J. Pharmacol.* **178**, 4708–4725 (2021).

20. Gomes, P. *et al.* Constituents of *Chamaecrista diphylla* (L.) Greene Leaves with Potent Antioxidant Capacity: A Feature-Based Molecular Network Dereplication Approach. *Pharmaceutics* **13**, 681 (2021).
21. Gomes, P. *et al.* Feature-Based Molecular Network-Guided Dereplication of Natural Bioactive Products from Leaves of *Stryphnodendron pulcherrimum* (Willd.) Hochr. *Metabolites* **11**, 281 (2021).
22. Gomes, P. W. P. *et al.* Chemical composition and antibacterial action of *Stryphnodendron pulcherrimum* bark extract, “barbatimão” species: Evaluation of its use as a topical agent. *Arabian Journal of Chemistry* **14**, 103183 (2021).
23. Alves Conserva, G. A. *et al.* Metabolite profile of *Nectandra oppositifolia* Nees & Mart. and assessment of antitrypanosomal activity of bioactive compounds through efficiency analyses. *PLoS One* **16**, e0247334 (2021).
24. Pellissier, L. *et al.* Isolation and Identification of Isocoumarin Derivatives With Specific Inhibitory Activity Against Wnt Pathway and Metabolome Characterization of *Lasiodiplodia venezuelensis*. *Front Chem* **9**, 664489 (2021).
25. Azuama, O. C. *et al.* Tackling *Pseudomonas aeruginosa* Virulence by Mulinane-Like Diterpenoids from *Azorella atacamensis*. *Biomolecules* **10**, (2020).
26. Quirós-Guerrero, L. *et al.* Phenolic variation among *Chamaecrista nictitans* subspecies and varieties revealed through UPLC-ESI(-)-MS/MS chemical fingerprinting. *Metabolomics* **15**, 14 (2019).
27. Protti-Sánchez, F. *et al.* Toxicity and Alkaloid Profiling of the Skin of the Golfo Dulcean Poison Frog *Phyllobates vittatus* (Dendrobatidae). *J. Chem. Ecol.* **45**, 914–925 (2019).
28. Mayorga-Gross, A. L., Quirós-Guerrero, L. M., Fourny, G. & Vaillant, F. An untargeted metabolomic assessment of cocoa beans during fermentation. *Food Res. Int.* **89**, 901–909 (2016).