

## List of ResNet NPND Publications (2021-2024)

Original research papers, [Reviews](#), [Books](#); [Edited journal volumes/collections/special issues & editorials](#)

2024

Abd Algaffar SO, Seegers S, Satyal P, [Setzer WN](#), [Schmidt TJ](#), [Khalid SA](#). Sandalwood Oils of Different Origins Are Active In Vitro against *Madurella mycetomatis*, the Major Fungal Pathogen Responsible for Eumycetoma. *Molecules* 2024, 29, 1846; DOI: 10.3390/molecules29081846

Ajayi, O., Metibemu, D.S., Crown, O., Adeyinka, O.S., [Kaiser, M.](#), Shoji, N., Silva, M., Rodriguez, A. and [Ogungbe, I.V.](#), Discovery of an orally active nitrothiophene-based antitrypanosomal agent. *European journal of medicinal chemistry*, 263, p.115954.

Amaral M, Romanelli MM, Asiki H, Bicker J, Lage DP, Freitas CS, Taniwaki NN, [Lago JHG](#), Coelho EAF, Falcão A, Fortuna A, Anderson EA, [Tempone AG](#). Synthesis of a dehydrodieugenol B derivative as a lead compound for visceral leishmaniasis- mechanism of action and *in vivo* pharmacokinetic studies. *Antimicrob Agents Chemother.* 2024 Nov 6;68(11):e0083124. doi: 10.1128/aac.00831-24. Epub2024 Oct 9. PMID: 39382276; PMCID: PMC11539218.

B. Souza, Gabriella ; M. Pontes, Carime L. ; De O. Costa, Geovanna ; F. De Sousa, Natália ; Tizziani, Tiago ; E. Pollo, Luiz Antonio ; Dambrós, Bibiana P. ; [Scotti, Marcus T.](#) ; [Steindel, Mario](#) ; Braga, Antonio L. ; Schirmeister, Tanja ; F. De Assis, Francisco ; [Sandjo, Louis P.](#) . Inhibitory Effects of *Mangifera indica* Secondary Metabolites and Their Synthetic Derivatives against SARS-CoV-2 M pro and NS2B/NS3 (ZIKV and DENV-2). *ACS Omega*, v. 9, p. 44624-44638, 2024.

Baltazar FN, Amaral M, Romanelli MM, de Castro Levatti EV, Ramos FF, Paulo Melchior de Oliveira Leão L, Chagas-Paula DA, Soares MG, Dias DF, Aranha CMSQ, Dos Santos Fernandes JP, [Lago JHG](#), [Tempone AG](#). Toward New Therapeutics for Visceral Leishmaniasis: Efficacy and Mechanism of Action of Amides Inspired by Gibbilimbol B. *ACS Omega.* 2024 Oct ;9(44):44385-44395. doi:10.1021/acsomega.4c05510. PMID: 39524621; PMCID: PMC11541474.

Brito IA, Castro Levatti EV, Regasini LO, Ferreira EA, Lopes FB, Fernandes JPS, Batista JM Jr, [Tempone AG](#), [Lago JHG](#). Homologous acetylenic acetogenins from *Porcelia macrocarpa* R.E. (Fries) displayed potent activity against amastigotes from *Trypanosoma cruzi*. *Phytochemistry.* 2024 Dec 12;231:114360. doi:10.1016/j.phytochem.2024.114360. Epub ahead of print. PMID: 39672219.

da Silva GHO, Dos Santos KF, Barcellos AF, de Sousa RMF, [Tempone AG](#), [Lago JHG](#), Caseli L. Exploring the selective incorporation of 15 $\beta$ -seneciyoxyloxi-ent-kaurenoic acid methyl ester in Langmuir monolayers mimicking cell membranes. *Bioorg Chem.* 2024 Dec;153:107941. doi: 10.1016/j.bioorg.2024.107941. Epub 2024 Nov 4. PMID: 39522426.

de M Gonçalves M, Totini CH, De Castro EV, Albuquerque V, Antar GM, [Tempone AG](#), [Lago JHG](#). Lignans Isolated from *Piper truncatum* Act as New Potent Antitrypanosomal Compounds. *Chem*

Biodivers. 2024 May;21(5):e202400547. doi: 10.1002/cbdv.202400547. Epub 2024 Apr 12. PMID: 38507773

Maria Neto R, Di Fabio E, de Monroe Gonçalves M, Mamián López MB, FigueiredoAngolini CF, Carvalho Veggi P, Tempone AG, Martin do Prado J, Lago JHG, da Silva BG. Steam distillation, supercritical fluid extraction, and anti-*Trypanosoma cruzi* activity of compounds from pink pepper (*Schinus terebinthifolius* Raddi). Nat Prod Res. 2024 Jun 22:1-9. doi:10.1080/14786419.2024.2371108. Epub ahead of print. PMID: 38907673.

Monzote, L.; Machín, L.; González, A.; Scull, R.; Gutiérrez, Y.I.; Satyal, P.; Setzer, W.N. Eugenol-rich essential oil from *Pimenta dioica*: *In-vitro* and *in-vivo* potentialities against *Leishmania amazonensis*. *Pharmaceuticals*, **2024**, 17(1) 64 (16 pages). DOI: 10.3390/ph17010064

Moreira Costa, Monalisa A. ; De Sousa, Natália F. ; Mansur Pontes, Carime L. ; Scotti, Marcus T. ; De Assis, Francisco F. ; Braga, Antonio L. ; Sandjo, Louis P. . Inhibitory effects against SARS-CoV-2 main protease (Mpro) of biflavonoids and benzophenones from the fruit of *Platonia insignis*. FITOTERAPIA, v. 173, p. 105784, 2024.

Muñoz-Vega, Maria Camila ; López-Hernández, Sofía ; Sierra-Chavarro, Adrián ; Scotti, Marcus Tullius ; Scotti, Luciana ; Coy-Barrera, Ericsson ; Herrera-Acevedo, Chonny . Machine-Learning- and Structure-Based Virtual Screening for Selecting Cinnamic Acid Derivatives as *Leishmania major* DHFR-TS Inhibitors. MOLECULES, v. 29, p. 179, 2024.

Peres N, Silva ML, Ueno AK, Antar GM, Levatti EVC, Tempone AG, Lago JHG. Highly selective alkylcoumarates and diterpenoids isolated from leaves of *Baccharis quitensis*: a search for new hit compounds against *Trypanosoma cruzi*. Nat Prod Res. 2024 Mar 27:1-7. doi: 10.1080/14786419.2024.2335362. Epub ahead of print. PMID: 38538549.

Rosa ME, Tristão DC, Barbosa H, Mendes VM, Tempone AG, Lago JHG, Caseli L. Exploring the antileishmanial activity of dicentrine from *Ocotea puberula* (Lauraceae) using biomembrane models. Bioorg Chem. 2024 Jun;147:107408. doi:10.1016/j.bioorg.2024.107408. Epub 2024 Apr 27. PMID: 38678776.

Santos Ferreira DA, de Castro Levatti EV, Santa Cruz LM, Costa AR, Migotto ÁE, Yamada AY, Camargo CH, Christodoulides M, Lago JHG, Tempone AG. Saturated Iso-Type Fatty Acids from the Marine Bacterium *Mesoflavibacter zeaxanthinifaciens* with Anti-*Trypanosomal* Potential. *Pharmaceuticals (Basel)*. 2024 Apr 13;17(4):499. doi: 10.3390/ph17040499. PMID: 38675459; PMCID:PMC11053438.

[Sülsen V., Coy-Barrera E., Konigheim B., Cáceres A. Special Issue "Potential Antimicrobial Agents Occurred in Edible and Non-edible Plants. Molecules/MDPI, Basel, 2024. ISSN 1420-3049](#)  
[Molecules | Special Issue: Potential Antimicrobial Agents Occurred in Edible and Non-edible Plants](#)

[Sülsen V., Sandjo L., Monzote L.. Special Issue "Bioactive Metabolites from Plants as Potential Treatments for Global Diseases". Plants/MDPI, Basel, 2024. ISSN 2223-7747](#)

Plants | Special Issue: Bioactive Metabolites from Plants as Potential Treatments for Global Diseases

Tristão DC, Barbosa H, de Castro Levatti EV, Andrade BA, Romanelli MM, Antar GM, Tempone AG, Lago JHG. Selective Activity Against Amastigote Forms of *Trypanosoma cruzi* and *Leishmania infantum* of Diastereomeric Dicentrine N-oxides. *Chem Biodivers*. 2024 Sep;21(9):e202401247. doi: 10.1002/cbdv.202401247. Epub 2024 Aug 11. PMID: 38896778.

2023

Araujo SC, de Angelo RM, Barbosa H, Costa-Silva TA, Tempone AG, Lago JHG, Honorio KM. Identification of inhibitors as drug candidates against Chagas disease. *Eur J Med Chem*. 2023 Feb 15;248:115074. doi: 10.1016/j.ejmech.2022.115074. Epub 2022 Dec 31. PMID: 36623331.

Barbosa H, Espinoza GZ, Amaral M, de Castro Levatti EV, Abiuzi MB, VeríssimoGC, Fernandes PO, Maltarollo VG, Tempone AG, Honorio KM, Lago JHG. Andrographolide: A Diterpenoid from *Cymbopogon schoenanthus* Identified as a New Hit Compound against *Trypanosoma cruzi* Using Machine Learning and Experimental Approaches. *J Chem Inf Model*. 2024 Apr 8;64(7):2565-2576. doi: 10.1021/acs.jcim.3c01410. Epub 2023 Dec 26. PMID: 38148604.

Barbosa H, Thevenard F, Quero Reimão J, Tempone AG, Honorio KM, Lago JHG. The Potential of Secondary Metabolites from Plants as Drugs or Leads against *Trypanosoma cruzi*-An Update from 2012 to 2021. *Curr Top Med Chem*. 2023;23(3):159-213. doi: 10.2174/1568026623666221212111514. PMID: 36515019.

Brunetti AE; Lyra ML; Bauermeister A; Bunk B; Boedeker C; Müsken M; Neto FC; Mendonça JN; Caraballo-Rodríguez AM; Melo WGP; Pupo MT; Haddad CFB; Cabrera GM; Overmann J; Lopes NP. Host macrocyclic acylcarnitines mediate symbiotic interactions between frogs and their skin microbiome. *Iscience* 2023, 26, 108109. <https://doi.org/10.1016/j.isci.2023.108109>

Coy-Barrera E, Ogungbe VI, Schmidt TJ (Guest Editors). Special Issue "Natural Products for Drug Discovery in the 21st Century: Innovations for Novel Therapeutics, 2<sup>nd</sup> Edition". *Molecules*, MDPI, Basel, 2023; ISSN 1420-3049. [https://www.mdpi.com/journal/molecules/special\\_issues/B2C57VIP5U](https://www.mdpi.com/journal/molecules/special_issues/B2C57VIP5U)

Da Silva, Layzon A. Lemos ; Sandjo, Louis P. ; Assunção, Laura S. ; Prigol, Anne N. ; De Siqueira, Carolina D. ; Creczynski-Pasa, Tânia B. ; Scotti, Marcus T. ; Scotti, Luciana ; Filippin-Monteiro, Fabíola B. ; Biavatti, Maíque W. . Semisynthetic Sesquiterpene Lactones Generated by the Sensibility of Glaucolide B to Lewis and Brønsted-Lowry Acids and Bases: Cytotoxicity and Anti-Inflammatory Activities. *MOLECULES*, v. 28, p. 1243, 2023.

de Castro Levatti EV, Costa-Silva TA, Morais TR, Fernandes JPS, Lago JHG, Tempone AG. Lethal action of Licarin A derivatives in *Leishmania (L.) infantum*: Imbalance of calcium and bioenergetic metabolism. *Biochimie*. 2023 May;208:141-150. doi: 10.1016/j.biochi.2022.12.018. Epub 2022 Dec 29. PMID:36586562.

Gonçalves GEG, Oliveira S, de Souza Gomes K, Costa-Silva TA, Tempone AG, Lago JHG, Caseli L. Effect of partial O-methylation in dehydrodieugenol on its antitrypanosomal activity -correlation with the toxicity using cell membrane models. *Biophys Chem.* 2023 May;296:106975. doi: 10.1016/j.bpc.2023.106975. Epub 2023 Feb 17. PMID: 36842251.

Guterres Fernandes, Octavio L.; Tizziani, Tiago ; Dambrós, Bibiana P. ; Ferreira De Sousa, Natália ; Mansur Pontes, Carime L. ; Da Silva, Layzon A. L. ; Escorteganha Pollo, Luiz A. ; De Assis, Francisco F. ; Scotti, Marcus T. ; Scotti, Luciana ; Braga, Antonio L. ; Steindel, Mario; Sandjo, Louis P. Studies of Cytotoxicity Effects, SARS-CoV-2 Main Protease Inhibition, and in Silico Interactions of Synthetic Chalcones. *CHEMISTRY & BIODIVERSITY*, v. 20, p. e202201151, 2023.

Leão LPMO, de B Vieira N, Oliveira PPS, Chagas-Paula DA, Soares MG, Souza TB, Baldim JL, Costa-Silva TA, Tempone AG, Dias DF, Lago JHG. Structure-activity relationship study of antitrypanosomal analogues of gibbilimbol B using multivariate analysis and computation-aided drug design. *Bioorg Med Chem Lett.* 2023 Mar 1;83:129190. doi: 10.1016/j.bmcl.2023.129190. Epub 2023 Feb 19. PMID:36805048.

Londero VS, Rosa ME, Baitello JB, Costa-Silva TA, Cruz LMS, Tempone AG, Caseli L, Lago JHG. Barbellatonic acid, a new antitrypanosomal pseudo-disesquiterpenoid isolated from *Nectandra barbellata*, displayed interaction with protozoan cell membrane. *Biochim Biophys Acta Biomembr.* 2023 Oct;1865(7):184184. doi: 10.1016/j.bbamem.2023.184184. Epub 2023 Jun 9. PMID: 37301246.

Silva ML, Sales FS, Levatti EVC, Antar GM, Tempone AG, Lago JHG, Jerz G. Evaluation of anti-*Trypanosoma cruzi* activity of chemical constituents from *Baccharis sphenophylla* isolated using high-performance countercurrent chromatography. *Molecules* 2024, 29, 212; <https://doi.org/10.3390/molecules29010212>

Thevenard F, Brito IA, Costa-Silva TA, Tempone AG, Lago JHG. Enyne acetogenins from *Porcelia macrocarpa* displayed anti-*Trypanosoma cruzi* activity and cause a reduction in the intracellular calcium level. *Sci Rep.* 2023 Jun 24;13(1):10254. doi: 10.1038/s41598-023-37520-3. PMID: 37355735; PMCID:PMC10290671.

## 2022

Albani C. M., Borgo J., Fabbri J., Pensel P., Fasciani L., Paladini A., Beer M.F., Laurella L., Elso O., Farias N.E., Elissondo N., Gambino G., Sülsen V., Elissondo M.C. Antiparasitic effects of Asteraceae species extracts on *Echinococcus granulosus* s.s. *Evidence-Based Complementary and Alternative Medicine* 2022, 2022:6371849. doi: 10.1155/2022/6371849.

Barros De Menezes, Renata Priscila ; Scotti, L. ; Scotti, Marcus Tullius ; García, Jesús ; González, Rosalia ; Monzote, Lianet ; Setzer, William N. . Machine Learning Analysis of Essential Oils from Cuban Plants: Potential Activity against Protozoa Parasites. *MOLECULES*, v. 27, p. 1366, 2022.

BrITO IA, Thevenard F, Costa-Silva TA, Oliveira SS, Cunha RLOR, de Oliveira EA, Sartorelli P, Guadagnin RC, Romanelli MM, Tempone AG, Lago JHG. Antileishmanial Effects of Acetylene

Acetogenins from Seeds of *Porcelia macrocarpa* (Warm.) R.E. Fries (Annonaceae) and Semisynthetic Derivatives. *Molecules*. 2022 Jan 28;27(3):893. doi: 10.3390/molecules27030893. PMID: 35164158; PMCID: PMC8838408.

Da Cunha, Luana N.O. Leal ; Tizziani, Tiago ; Souza, Gabriella B. ; Moreira, Monalisa A. ; Neto, José S.S. ; Dos Santos, Carlos V.D. ; De Carvalho, Maryelle G. ; Dalmarco, Eduardo M. ; Turqueti, Leonardo B. ; Scotti, Marcus Tullius ; Scotti, Luciana ; De Assis, Francisco F. ; Braga, Antonio Luiz ; Sandjo, Louis Pergaud. Natural Products with Tandem Anti-inflammatory, Immunomodulatory and Anti-SARS-CoV/2 Effects: A Drug Discovery Perspective against SARS-CoV-2. *CURRENT MEDICINAL CHEMISTRY*, v. 29, p. 2530-2564, 2022.

De Menezes, R.P.B.; Scotti, L.; Scotti, M.T.; García, J.; González, R.; Monzote, L.; Setzer, W.N. Machine learning analysis of essential oils from Cuban plants: Potential activity against protozoa parasites. *Molecules*, 2022, 27(4), 1366. DOI: 10.3390/molecules27041366

Dos Santos AL, Amaral M, Hasegawa FR, Lago JHG, Tempone AG, Sartorelli P. Corrigendum: (-)-T-Cadinol, a Sesquiterpene Isolated From *Casearia sylvestris* (Salicaceae)-Displayed *In Vitro* Activity and Causes Hyperpolarization of the Membrane Potential of *Trypanosoma cruzi*. *Front Pharmacol*. 2022 Mar 14;13:865432. doi: 10.3389/fphar.2022.865432. Erratum for: *Front Pharmacol*. 2021 Nov 03;12:734127. doi: 10.3389/fphar.2021.734127. PMID: 35370638; PMCID: PMC8964361.

Galhardo TS, Ueno AK, Costa-Silva TA, Tempone AG, Carvalho WA, Fischmeister C, Bruneau C, Mandelli D, Lago JHG. New derivatives from dehydrodieugenol B and its methyl ether displayed high anti-*Trypanosoma cruzi* activity and cause depolarization of the plasma membrane and collapse the mitochondrial membrane potential. *Chem Biol Interact*. 2022 Oct 1;366:110129. doi: 10.1016/j.cbi.2022.110129. Epub 2022 Sep 5. PMID: 36067825.

Jürgens FM, Behrens M, Humpf H-U, Robledo SM, Schmidt TJ. In Vitro Metabolism of Helenalin Acetate and 11 $\alpha$ ,13-Dihydrohelenalin Acetate: Natural Sesquiterpene Lactones from Arnica. *Metabolites* 2022, 12, 88. DOI: 10.3390/metabo12010088

Jürgens FM, Herrmann FC, Robledo SM, Schmidt TJ. Dermal Absorption of Sesquiterpene Lactones from Arnica Tincture. *Pharmaceutics* 2022, 14, 742. DOI: 10.3390/pharmaceutics14040742

Jürgens FM, Robledo SM, Schmidt TJ. Evaluation of Pharmacokinetic and Toxicological Parameters of Arnica Tincture after Dermal Application In Vivo. *Pharmaceutics* 2022, 14, 2379. DOI: 10.3390/pharmaceutics14112379

Perera, W.H.; Scherbakov, A.M.; Buravchenko, G.I.; Mikhaevich, E.I.; Leitão, S.G.; Cos, P.; Shchekotikhin, A.E.; Monzote, L.; Setzer, W.N. *In vitro* pharmacological screening of essential oils from *Baccharis parvidentata* and *Lippia origanoides* growing in Brazil. *Molecules*, 2022, 27(6), 1926. DOI: 10.3390/molecules27061926

Robledo SM, Murillo J, Arbeláez N, Montoya A, Ospina V, Jürgens FM, Vélez ID, Schmidt TJ. Therapeutic efficacy of *Arnica* in hamsters with cutaneous leishmaniasis caused by *Leishmania braziliensis* and *L. tropica*. *Pharmaceuticals* 2022, 15, 776; DOI: 10.3390/ph15070776

Rodríguez-Ferreiro, A.O.; Ochoa-Pacheco, A.; Méndez-Rodríguez, D.; Ortiz-Beatón, E.; Font-Salmo, O.; Guisado-Bourzac, F.; Molina-Bertrán, S.; Monzote, L.; Cos, P.; Foubert, K.; Pieters, L.; Perez-Novo, C.; Vanden Berghe, W.; Escalona-Arranz, J.C.; Setzer, W.N. LC-MS characterization and biological activities of Cuban cultivars of *Plectranthus neochilus* Schltr. *Plants*, **2022**, 11(1), 134. DOI: 10.3390/plants11010134

Romanelli MM, Amaral M, Thevenard F, Santa Cruz LM, Regasini LO, Migotto AE, Lago JHG, Tempone AG. Mitochondrial Imbalance of *Trypanosoma cruzi* Induced by the Marine Alkaloid 6-Bromo-2'-de-N-Methylaplysinopsin. *ACS Omega*. 2022 Aug 4;7(32):28561-28570. doi: 10.1021/acsomega.2c03395. PMID:35990437; PMCID: PMC9387129.

Santos CC, Zhang H, Batista MM, de Oliveira GM, Demarque KC, da Silva NL, Moreira OC, Ogungbe IV, Soeiro MD. Phenotypic investigation of 4-nitrophenylacetyl-and 4-nitro-1H-imidazolyl-based compounds as antileishmanial agents. *Parasitology*. 2022 149(4):490–495. doi: 10.1017/S0031182021002079

Schmidt TJ, Coy-Barrera E, Ogungbe VI (Guest Editors). Special Issue "Natural Products for Drug Discovery in the 21st Century: Innovations for Novel Therapeutics". *Molecules*, MDPI, Basel, 2022; ISSN 1420-3049.

[https://www.mdpi.com/journal/molecules/special\\_issues/NPs\\_Drugs](https://www.mdpi.com/journal/molecules/special_issues/NPs_Drugs)

Coy-Barrera E, Ogungbe, VI, Schmidt TJ. Editorial: Natural Products for Drug Discovery in the 21st Century: Innovations for Novel Therapeutics. *Molecules* 2023, 28, 3690. DOI: 10.3390/molecules28093690

Silva Maiolini TC, Rosa W, de Oliveira Miranda D, Costa-Silva TA, Tempone AG, Pires Bueno PC, Ferreira Dias D, Aparecida Chagas de Paula D, Sartorelli P, Lago JHG, Gomes Soares M. Essential Oils from Different Myrtaceae Species from Brazilian Atlantic Forest Biome - Chemical Dereplication and Evaluation of Antitrypanosomal Activity. *Chem Biodivers*. 2022 Jun;19(6):e202200198. doi: 10.1002/cbdv.202200198. Epub 2022 May 30. PMID: 35485995.

Tullius Scotti, Marcus; Herrera'acevedo, Chonny; Barros De Menezes, Renata Priscila; Martin, Holli'joi ; Muratov, Eugene N. ; Ítalo De Souza Silva, Ávilla ; Faustino Albuquerque, Emmanuella ; Ferreira Calado, Lucas ; Coy'barrera, Ericsson ; Scotti., Luciana. MolPredictX: Online Biological Activity Predictions by Machine Learning Models. *MOLECULAR INFORMATICS*, v. 41, p. 2200133, 2022.

Acevedo, Chonny Alexander Herrera; Mendonca-Junior, F. ; Scotti, L. ; Scotti, Marcus Tullius ; Coy-Barrera, E. . Identification of Kaurane-Type Diterpenes as Inhibitors of Leishmania Pteridine Reductase I. MOLECULES, v. 26, p. 3076, 2021.

Albani C.M., Borgo J., Fabbri J., Pensel P., Fasciani L., Elso O., Papademetrio D., Grasso D., Paladini A., Beer M.F., Farias N.E., Elissondo N., Gambino G., Zoppi J., Sülßen V., Elissondo C. Anthelmintic activity of *Stevia multiristata* extract against *Echinococcus granulosus sensu stricto*. *Parasitology* 2021, 1-10. doi:10.1017/S0031182021002109.

Alves Conserva GA, Quirós-Guerrero LM, Costa-Silva TA, Marcourt L, Pinto EG, Tempone AG, Fernandes JPS, Wolfender JL, Queiroz EF, Lago JHG. Metabolite profile of *Nectandra oppositifolia* Nees & Mart. and assessment of antitrypanosomal activity of bioactive compounds through efficiency analyses. *PLoS One*. 2021 Feb 25;16(2):e0247334. doi: 10.1371/journal.pone.0247344. PMID: 33630860; PMCID: PMC7906415.

Araujo SC, Sousa FS, Costa-Silva TA, Tempone AG, Lago JHG, Honorio KM. Discovery of New Hits as Antitrypanosomal Agents by In Silico and In Vitro Assays Using Neolignan-Inspired Natural Products from *Nectandra leucantha*. *Molecules*. 2021 Jul 6;26(14):4116. doi:10.3390/molecules26144116 . PMID: 34299391; PMCID: PMC8306904.

Barbosa H, Costa-Silva TA, Alves Conserva GA, Araujo AJ, Lordello ALL, Antar GM, Amaral M, Soares MG, Tempone AG, Lago JHG. Aporphine Alkaloids from *Ocotea puberula* with Anti-Trypanosoma Cruzi Potential - Activity of Dicentrine- $\beta$ -N- Oxide in the Plasma Membrane Electric Potentials. *Chem Biodivers*. 2021 Apr;18(4):e2001022. doi: 10.1002/cbdv.202001022. Epub 2021 Mar 1. PMID: 33635585

Conserva GA, Costa-Silva TA, Quirós-Guerrero LM, Marcourt L, Wolfender JL, Queiroz EF, Tempone AG, Lago JHG. Kaempferol-3-O- $\alpha$ -(3,4-di-E-p- coumaroyl)-rhamnopyranoside from *Nectandra oppositifolia* releases  $\text{Ca}^{2+}$  from intracellular pools of *Trypanosoma cruzi* affecting the bioenergetics system. *Chem Biol Interact*. 2021 Nov 1;349:109661. doi:10.1016/j.cbi.2021.109661. Epub 2021 Sep 16. PMID: 34537181.

Costa, Renan P. O. ; Lucena, Lucas F. ; Silva, Lorena Mara A. ; Zocolo, Guilherme Julião ; Herrera-Acevedo, Chonny ; Scotti, Luciana ; Da-Costa, Fernando Batista ; Ionov, Nikita ; Poroikov, Vladimir ; Muratov, Eugene N. ; Scotti, Marcus T. . The Sistemax Web Portal of Natural Products: An Update. *JOURNAL OF CHEMICAL INFORMATION AND MODELING (ONLINE)*, v. 61, p. 2516-2522, 2021.

da Costa-Silva TA, Silva ML, Antar GM, Tempone AG, Lago JHG. Ent-kaurane diterpenes isolated from n-hexane extract of *Baccharis sphenophylla* by bioactivity-guided fractionation target the acidocalcisomes in *Trypanosoma cruzi*. *Phytomedicine*. 2021 Dec;93:153748. doi: 10.1016/j.phymed.2021.153748. Epub 2021 Sep 11. PMID: 34628240.

Dos Santos AL, Amaral M, Hasegawa FR, Lago JHG, Tempone AG, Sartorelli P. (-)-T-Cadinol-a Sesquiterpene Isolated From *Casearia sylvestris* (Salicaceae)-Displayed In Vitro Activity and Causes Hyperpolarization of the Membrane Potential of *Trypanosoma cruzi*.

Front Pharmacol. 2021 Nov 3;12:734127. doi: 10.3389/fphar.2021.734127. Erratum in: Front Pharmacol. 2022 Mar 14;13:865432. doi: 10.3389/fphar.2022.865432. PMID: 34803682; PMCID: PMC8595124.

Flittner D, [Kaiser M](#), [Mäser P](#), [Lopes NP](#), [Schmidt TJ](#). The Alkaloid Fraction of *Pachysandra terminalis* (Buxaceae) shows prominent Activity against *Trypanosoma brucei rhodesiense*. *Molecules* 2021, 26, 591. DOI: 10.3390/molecules26030591

Greve HL, [Kaiser M](#), [Mäser P](#), [Schmidt TJ](#). Boswellic Acids Show in Vitro Activity Against *Leishmania donovani*. *Molecules* 2021, 26, 3651; DOI: 10.3390/molecules26123651

Herrera-Acevedo, Chonny ; Perdomo-Madrigal, Camilo ; Herrera-Acevedo, Kenyi ; [Coy-Barrera, Ericsson](#) ; [Scotti, L.](#) ; [Scotti, Marcus Tullius](#) . Machine learning models to select potential inhibitors of acetylcholinesterase activity from Sistemax: a natural products database. *MOLECULAR DIVERSITY*, v. 2021, p. 1553-1568, 2021

Llurba Montesino N, [Kaiser M](#), [Mäser P](#), [Schmidt TJ](#). *Salvia officinalis*: Antitrypanosomal Activity and Active Constituents against *Trypanosoma brucei rhodesiense*. *Molecules* 2021, 26, 3226. DOI: 10.3390/molecules26113226

Londero VS, Costa-Silva TA, Antar GM, Baitello JB, de Oliveira LVF, Camilo FF, Batista ANL, Batista JM Jr, [Tempone AG](#), [Lago JHG](#). Antitrypanosomal Lactones from *Nectandra barbellata*. *J Nat Prod*. 2021 May 28;84(5):1489-1497. doi: 10.1021/acs.jnatprod.0c01303. Epub 2021 Apr 15. PMID: 33857368.

[Monzote, L.](#); [García, J.](#); [González, R.](#); [Scotti, M.T.](#); [Setzer, W.N.](#) Bioactive essential oils from Cuban plants: An inspiration to drug development. *Plants*, 2021, 10(11), 2515. DOI: 10.3390/plants10112515

[Monzote, Lianet](#) ; [García, Jesús](#) ; [González, Rosalia](#) ; [Scotti, Marcus Tullius](#) ; [Setzer, William N.](#) . Bioactive Essential Oils from Cuban Plants: An Inspiration to Drug Development. *PLANTS*, v. 10, p. 2515, 2021

Parolin GA, Gonçalves GEG, Costa-Silva TA, [Tempone AG](#), Caseli L, [Lago JHG](#), Péres LO. Evaluation of the effects in cellular membrane models of antitrypanosomal poly-thymolformaldehyde (PTF) using Langmuir monolayers. *Biochim Biophys Acta Biomembr*. 2021 Feb 1;1863(2):183500. doi:10.1016/j.bbmem.2020.183500. Epub 2020 Oct 29. PMID: 33130097.

Reis IMA, Umehara E, Conceição RS, de M Oliveira L, Coelho Dos S Junior M, Costa-Silva TA, Amaral M, [Tempone AG](#), Branco A, [Lago JHG](#).  $\gamma$ -Lactones from *Persea americana* and *Persea fulva* - in Vitro and in Silico Evaluation of *Trypanosoma cruzi* Activity. *Chem Biodivers*. 2021 Sep;18(9):e2100362. doi: 10.1002/cbdv.202100362. Epub 2021 Jul 29. PMID: 34254435.

Silva ML, Costa-Silva TA, Antar GM, [Tempone AG](#), [Lago JHG](#). Chemical Constituents from Aerial Parts of *Baccharis sphenophylla* and Effects against Intracellular Forms of *Trypanosoma cruzi*. *Chem*

Biodivers. 2021 Oct;18(10):e2100466. doi: 10.1002/cbdv.202100466. Epub 2021 Aug 4. PMID:34263530.

Souza DCS, Costa-Silva TA, Morais TR, Brito JR, Ferreira EA, Antar GM, Sartorelli P, Tempone AG, Lago JHG. Simplified Derivatives of Dibenzylbutyrolactone Lignans from *Hydrocotyle bonariensis* as Antitrypanosomal Candidates. Chem Biodivers. 2021 Oct;18(10):e2100515. doi: 10.1002/cbdv.202100515. Epub 2021 Sep 29. PMID: 34424612.

Szabó LU, Kaiser M, Mäser P, Schmidt TJ. Antiprotozoal Nor-Triterpene Alkaloids from *Buxus sempervirens* L. Antibiotics 2021, 10, 696. DOI: 10.3390/antibiotics10060696

Szabó LU, Kaiser M, Mäser P, Schmidt TJ. Identification of Antiprotozoal Compounds from *Buxus sempervirens* L. by PLS-Prediction. Molecules 2021, 26, 6181. DOI: 10.3390/molecules26206181

Tempone AG, Pieper P, Borborema SET, Thevenard F, Lago JHG, Croft SL, Anderson EA. Marine alkaloids as bioactive agents against protozoal neglected tropical diseases and malaria. Nat Prod Rep. 2021 Dec 15;38(12):2214-2235. doi: 10.1039/d0np00078g. PMID: 34913053; PMCID: PMC8672869.

Uth J-F, Börgel F, Lehmkuhl K, Schepmann D, Kaiser M, Nonato MC, Krauth-Siegel L, Schmidt TJ, Wünsch B. Synthesis and biological evaluation of natural product-inspired, aminoalkyl substituted 1-benzopyrans as novel antiplasmodial agents. J. Med. Chem. 2021, 64, 6397-6409. DOI: 10.1021/acs.jmedchem.1c00483