



OHD papers published during YEAR 3 (November 2024-October 2025)

Number of the paper	Details of the publication
1	Bertram, M.G., Wong, B.B.M., Kümmerer, K., Jörg, M. In press. Development of environmentally biodegradable drugs: what are the key challenges? Expert Opin. Drug Discov. https://doi.org/10.1080/17460441.2024.2442746
2	Baz-Lomba, J.A., van Nuijs, A.L.N., Lenart-Boroń, A., Péterfi, A., de l'Eprevier, A., Löve, A.S.C., Kasprzyk-Hordern, B., Ort, C., Simeoni, E., Heath, E., Pridotkiene, E., Lai, F.Y., Béen, F., Oberacher, H., Bodík, I., Valenčić, I., Slobodnik, J., Strandberg, J., Sheeran, K., Smit-Rigter, L.A., Barron, L.P., Bijlsma, L., Psichoudaki, M., Savvidou, M., Edland-Gryt, M., Helminen, M., Busch, M., Jandl, M., Bertram, M.G., López de Alda, M., Berndt, N., Daglioglu, N., Thomaidis, N., Fabien, L., Chomynova, P., Oertel, R., Castiglioni, S., Mercan, S., Akgür, S.A., Schneider, S., Gunnar, T., ter Laak, T., Thiebault, T., Matias, J.P. 2025. Bridging the gap between research and decision making: a European survey to enhance cooperation in wastewater-based epidemiology (WBE) for illicit drugs. Public Health 241, 158–163. https://doi.org/10.1016/j.puhe.2025.02.009
3	Bayraktar, G., Marchand, P., Barbosa, E. G., da Silva, M. C., Weber, K. C., Cojean, S., ... & Istanbulu, H. (2024). Biological properties and in silico studies of thiazolopyrimidine derivatives active against visceral and cutaneous Leishmania spp. amastigote forms. European Journal of Medicinal Chemistry Reports, 12, 100228. https://doi.org/10.1016/j.ejmcr.2024.100228
4	Santos T.T., Lages E.B., Ricotta T.N.Q., de Oliveira L.G., Ramos G.S., Burlot J., Abreu S., Chaminade P., Legrand F.X., Tran P., Deloménie C., Vallejos V.M.R., Helou D.G., de Almeida R.M., Queiroz-Junior C.M., Teobaldo G.B.M., de Oliveira C.L.P., Ferreira L.A.M., Aguiar M.M.G., Pomel S., Frézard F. (2025). Long-circulating liposomes co-delivering amphotericin B and reticnoic acid for cutaneous leishmaniasis treatment. ACS Omega, in press.
5	Sustainable Antiparasitic Agents from an Agro-Industrial Waste: Mitochondria-Targeting Cashew Nutshell Liquid-Derived Phosphonium and Ammonium Salts Bianca Martinengo, Cecilia Baldassarri, Kayhan Ilbeigi, Hamed E. Alkhalaf, Aditya Sarode, Ehab Kotb Elmahallawy, Ba Reum Kwon, Amos Sarpong Agyei, Aigerim Abdimanova, Ludmila Ferreira de Almeida Fiuza, Raquel Azevedo, Ketlym da Conceição, Marcos Meuser Batista, Ellyêssa Nascimento Borges, Kleber Santiago Freitas e Silva, Éder Jéferson Souza Cardoso, Natália Cipriano Monteiro, Lais Flavia Nunes Lemes, Luiz Antonio Soares Romeiro, Antonio Alonso, Maria de Nazaré Correia Soeiro, Guy Caljon, Bryan W. Brooks, Harry P. De Koning, and Maria Laura Bolognesi Journal of Medicinal Chemistry 68(18):19438-19462 DOI: 10.1021/acs.jmedchem.5c01617
6	Ebiloma GU, Alhejely AS, De Koning HP (2025) Interventions for Neglected Diseases Caused by Kinetoplastid Parasites: A One Health Approach to Drug Discovery, Development, and Deployment. Pharmaceuticals 18:1415
7	Hrcková, G.; Mudronová, D.; Reiterová, K.; Cavallero, S.; Bellini, I. :Human Dialyzable Leukocyte Extract Enhances Albendazole Efficacy and Promotes Th1/Th2-Biased Lymphocyte and Antibody Responses in Peritoneal Cavity of



	Murine Model of <i>Mesocestoides vogae</i> Infection. Int. J. Mol. Sci. 2025, 26, 6994. https://doi.org/10.3390/ijms26146994
8	Ilbeigi K, Mabilie D, Matheeussen A, Hendrickx R, Claes M, Van Reet N, Anthonissen R, Hulpia F, Lin C, Maes L, Regnault C, Whitfield P, Roy R, Ungogo MA, Sterckx YG, De Winter H, Mertens B, Bundschuh M, De Koning HP, Van Calenbergh S, Caljon G. (2025) Discovery and Development of an Advanced Lead for the Treatment of African Trypanosomiasis. ACS Infectious Diseases 11:131-143. doi: 10.1021/acsinfecdis.4c00472
9	Oaikhenaa EE, Yahaya UA, Abdulsalami SM, Egbe NL, Adeyemi MM, Ungogo MA, Ebiloma GU, Zoiku FK, Fordjour PA, Elati HAA, Quashie NB, Igoli JO, Gray AI, Lawson C, Ferro VA, de Koning HP (2024) The activities of suaveolol and other compounds from <i>Hyptis suaveolens</i> and <i>Momordica charantia</i> against the aetiological agents of African trypanosomiasis, leishmaniasis and malaria. Exp Parasitol 263-264, 108807. 10.1016/j.exppara.2024.108807.
10	Lima CM, Uliassi E, Thoré ESJ, Bertram MG, Cardoso L, Cordeiro da Silva A, Costi MP, De Koning HP (2024) Environmental impacts of drugs against parasitic vector-borne diseases and the need to integrate sustainability into their development and use. Open Research Europe, 4:207. https://doi.org/10.12688/openreseurope.18008.2
11	Ebiloma GE, Balogun EO, Arai N, Otani M, Baldassari C, Alhejely A, Cueto-Diaz E, De Koning HP, Dardonville C, Shiba T (2025) Uncovering the unusual inhibition mechanism of a trypanosome alternative oxidase inhibitor displaying broad-spectrum activity against African trypanosomes. J Med Chem, 68:17115-17174 doi.org/10.1021/acs.jmedchem.5c00631
12	Dupouy B, Donzel M, Roignant M, Charital S, Keumoe R, Yamaryo-Botté Y, Feckler A, Bundschuh M, Bordat Y, Rottmann M, Mäser P, Botté CY, Blandin SA, Besteiro S, Davioud-Charvet E. 3-Benzylmenadiones and their Heteroaromatic Analogues Target the Apicoplast of Apicomplexa Parasites: Synthesis and Bioimaging Studies. ACS Infect Dis. 2024 Oct 11;10(10):3553-3576. doi: 10.1021/acsinfecdis.4c00304.
13	Cesar-Rodo E, Dupouy B, Häberli C, Strub JM, Williams DL, Mäser P, Rottmann M, Keiser J, Lanfranchi DA, Davioud-Charvet E. Regioselective Synthesis of Potential Non-Quinonoid Prodrugs of Plasmodione: Antiparasitic Properties Against Two Hemoglobin-Feeding Parasites and Drug Metabolism Studies. Molecules. 2024 Nov 7;29(22):5268. doi: 10.3390/molecules29225268.
14	Dupouy B, Cotos L, Binder A, Slavikova L, Rottmann M, Mäser P, Jacquemin D, Ganter M, Davioud-Charvet E, Elhabiri M. Click Coupling of Flavylum Dyes with Plasmodione Analogues: Towards New Redox-Sensitive Pro-Fluorophores. Chemistry. 2025 Jan 27;31(6):e202403691. doi: 10.1002/chem.202403691.
15	Dupouy B, Karpstein T, Häberli C, Cal M, Rottmann M, Mäser P, Keiser J, Elhabiri M, Davioud-Charvet E. Synthesis of 1,2,3-Triazole-Methyl-Menadione Derivatives: Evaluation of Electrochemical and Antiparasitic Properties against two Blood-Dwelling Parasites. ChemMedChem. 2025 Mar 15;20(6):e202400731. doi: 10.1002/cmdc.202400731.
16	Roignant M, Richard J, Donzel M, Rottmann M, Mäser P, Davioud-Charvet E. Design, Synthesis and Antiplasmodial Activities of a Library of Fluorine-Based 3-Benzylmenadiones. Molecules. 2025 Jun 3;30(11):2446. doi: 10.3390/molecules30112446.
17	From pan-active to parasite-selective antiparasitic agents: A scaffold hopping approach. Borsari C, Santarem N, Coertzen D, Mazzolari A, Corfu AI, Coelho C, Barbosa F, Tamborini L, Birkholtz LM, Raffellini L, Keminer O, Basilico N, Parapini S, Gul S, Cordeiro-da-Silva A, Conti P. Eur J Med Chem. 2025 Aug 29;300:118095. doi: 10.1016/j.ejmech.2025.118095.



18	L. Misevičienė, M.-P. Golinelli-Cohen, V. Kairys, A. Marozienė, M. Lesanavičius, N. Čėnas. Reactions of <i>Plasmodium falciparum</i> Quinoidal and Nitroaromatic oxidants INADH:Ubiquinone Reductase with Nonphysiological Oxidants. Int. J. Molec. Sci. 2025, 26, 2509. doi: 10.3390/ijms26062509.
19	Picard M, Boutrais S, Rodrigues V, Fortier Y, Borde C, Soundaramourty C, Clain C, Joly-Beauparlant C, Racine G, Zghidi-Abouzid O, Droit A, Pruvost A, Costi MP, Silvestre R, Cordeiro da Silva A, MacDougall J, André S, and Estaquier J. Persistent myeloid cell reprogramming despite miltefosine treatment in Leishmania-infected macaques. ISciences 2025
20	New Trypanosoma brucei acting derivatives incorporating 1-(4-phenyl)adamantane and 1-(4-phenoxyphenyl)adamantane. K. Stavropoulou, A. Kaimaki, M. Nikolaou, A. K. Brown, A. Tsotinis, M. C. Taylor, J. M. Kelly, I. P. Papanastasiou. RSC Med. Chem., 2025, 16, 2441-2451. DOI: 10.1039/d5md00135h
21	Nanostructured Lipid Carrier for Intracellular Delivery of a Bis(pyridine-2-carboxamide) DNA Minor Groove Binder Active against Leishmania J. J. Nué-Martinez, M. Leo-Barriga, F. Herranz, Z. Koutsogiannis, P. W. Denny, G. U. Ebiloma, C. Dardonville, A. González-Paredes. ACS Omega 2025, 10 (8), 7795–7805 DOI: 10.1021/acsomega.4c08138
22	Kolařík M, Ilbeigi K, Caljon G, Brulíková L. Thiazolidinones and related analogues as efficient antitrypanosomal agents. Bioorg Med Chem. 2025 Dec 1;130:118363. doi: 10.1016/j.bmc.2025.118363. Epub 2025 Aug 21. PMID: 40885017.
23	Pinto Torres JE, Claes M, Hendrickx R, Yuan M, Smiejewska N, Van Wielendaele P, Hacisuleyman A, De Winter H, Muyldermans S, Michels PAM, Walkinshaw MD, Versées W, Caljon G, Magez S, Sterckx YG. Allosteric inhibition of trypanosomatid pyruvate kinases by a camelid single-domain antibody. Elife. 2025 Mar 31;13:RP100066. doi: 10.7554/eLife.100066. PMID: 40163365; PMCID: PMC11957543.
24	Ilbeigi K, Mabilie D, Roy R, Bundschuh M, Van de Velde E, Hulpia F, Van Calenbergh S, Caljon G. 3'-deoxytubercidin: A potent therapeutic candidate for the treatment of Surra and Dourine. Int J Parasitol Drugs Drug Resist. 2025 Apr;27:100580. doi: 10.1016/j.ijpddr.2025.100580. Epub 2025 Jan 10. PMID: 39827514; PMCID: PMC11787584.
25	Agarwal DS, Beteck RM, Mabilie D, Caljon G, Legoabe LJ. Pyrazolyl amide-chalcones conjugates: Synthesis and antiketoplastid activity. Naunyn Schmiedeberg's Arch Pharmacol. 2025 Apr;398(4):4199-4210. doi: 10.1007/s00210-024-03524-7. Epub 2024 Oct 21. PMID: 39432069; PMCID: PMC11978679.
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29	Martins, M.F.; Ribeiro, F.; Borges, A.; Calhelha, R.C.; Santarém, N.; Cordeiro-da-Silva, A.; Queiroz, M.-J.R.P. Synthesis of Tricyclic and Tetracyclic Lactone Derivatives of Thieno[2,3-b]pyrazine or Thieno[2,3-b]quinoline: Preliminary Antitumor and Antiparasitic Activity Evaluation. Molecules 2025, 30, 1999. https://doi.org/10.3390/molecules30091999



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31	Persistent myeloid cell reprogramming despite miltefosine treatment in Leishmania-infected macaques Morgane Picard ¹ · Steven Boutrais ² · Vasco Rodrigues ¹ · Yasmina Fortier ¹ · Chloé Borde ¹ · Calaiselvy Soundaramourty ¹ · Julien Clain ² · Charles Joly-Beauparlant ² · Gina Racine ² · Ouafa Zghidi-Abouzid ² · Arnaud Droit ² · Alain Pruvost ³ · Maria Paola Costi ⁴ · Ricardo Silvestre ^{5,6} · Anabela Cordeiro da Silva ^{7,8,9} · Jane MacDougall ¹⁰ · Sónia André ¹ estaquier@yahoo.fr · Jérôme Estaquier ^{1,2} , DOI: 10.1016/j.jisci.2025.113900
32	Design of 2-Aminobenzothiazole Derivatives Targeting Trypanosomatid PTR1 by a Multidisciplinary Fragment Hybridization Approach Joanna Panecka-Hofman*, Pasquale Linciano, Ina Pöhner, Edyta Dyguda-Kazimierowicz, Wiktoria Jedwabny, Giacomo Landi, Nuno Santarem, Gesa Witt, Bernhard Ellinger, Maria Kuzikov, Rosaria Luciani, Stefania Ferrari, Daniele Aiello, Stefano Mangani, Cecilia Pozzi, Anabela Cordeiro-da-Silva, Sheraz Gul, Maria Paola Costi, and Rebecca C. Wade* Journal of Medicinal Chemistry 2025, 68, 19, 20595-20618