

# Publications

Jia LJ<sup>#</sup>, Bernal FA, Soehnlein J, Sonnberger J, Heineking I, Rafiq M, Cseresnyes Z, Kage F, Schmidt F, Zaher R, Hortschansky P, Chaudhary S, Gong X, Schirawski J, Figge MT, Hube B, Brakhage AA<sup>#</sup> (2025) Convergent evolution of a fungal effector enabling phagosome membrane penetration. *bioRxiv* [Preprint]

Keiff F, Bernal FA, Joch M, Jacques Dit Lapierre TJW, Li Y, Liebing P, Dahse HM, Vilotijevic I, Kloss F (2024) Modulation of the Meisenheimer complex metabolism of nitro-benzothiazinones by targeted C-6 substitution. *Commun Chem* 7(1), 153.

Torres-Gómez H, Keiff F, Hortschansky P, Bernal F, Kerndl V, Meyer F, Messerschmidt N, Dal Molin M, Krüger T, Rybniker J, Brakhage AA, Kloss F (2024) Replacement of the essential nitro group by electrophilic warheads towards nitro-free antimycobacterial benzothiazinones. *Eur J Med Chem* 279, 116849.

Keiff F, Jacques dit Lapierrev TJW, Bernal F, Kloss F (2023) Design and synthesis of benzofuran- and naphthalene-fused thiazinones as antimycobacterial agents. *Arch Pharm (Weinheim)* 356(11), e2300356.

Bernal FA, Coy-Barrera E (2022) Composition and antifungal activity of the alkaloidal fraction of *Lupinus mirabilis* leaves: A biochemometrics-based exploration. *Molecules* 27(9), 2832.

Bernal FA, Hammann P, Kloss F (2022) Natural products in antibiotic development: is the success story over? *Curr Opin Biotechnol* 78, 102783. (Review)

Schieferdecker S, Bernal FA, Wojtas KP, Keiff F, Li Y, Dahse HM, Kloss F (2022) Development of predictive classification models for whole cell antimycobacterial activity of benzothiazinones. *J Med Chem* 65(9), 6748-6763.

Bernal FA, Gerhards M, Kaiser M, Wünsch B, Schmidt TJ (2020) ( $\pm$ )-trans-2-phenyl-2,3-dihydrobenzofurans as leishmanicidal agents: Synthesis, *in vitro* evaluation and SAR analysis. *Eur J Med Chem* 205, 112493.

Bernal FA, Kaiser M, Wünsch B, Schmidt TJ (2020) Structure-activity relationships of cinnamate ester analogues as potent antiprotozoal agents. *ChemMedChem* 15(1), 68-78.

Martin B, Schepmann D, Bernal FA, Schmidt TJ, Che T, Loser K, Wünsch B (2020) Enantiomerically pure quinoline-based  $\kappa$ -opioid receptor agonists: Chemoenzymatic synthesis and pharmacological evaluation. *ChemMedChem* 15(15), 1408-1420.

Sánchez-Suárez J, Bernal FA, Coy-Barrera E (2020) Colombian contributions fighting leishmaniasis: A systematic review on antileishmanials combined with chemoinformatics analysis. *Molecules* 25(23), 5704.

Bernal FA, Schmidt TJ (2019) A Comprehensive QSAR Study on Antileishmanial and Antitrypanosomal Cinnamate Ester Analogues. *Molecules* 24(23),

Guerrero-Perilla C, Bernal FA, Coy-Barrera E (2018) Insights into the interaction and binding mode of a set of antifungal azoles as inhibitors of potential fungal enzyme-based targets. *Mol Divers* 22(4), 929-942.

- Bernal FA, Orduz-Diaz LL, Coy-Barrera ED (2016) Application of PARAFAC and OPLS-DA analyses on HPLC fingerprints for the characterization of Hibiscus sabdariffa calyxes. *Quim. Nova* 39(2), 160-166.
- Bernal FA, Orduz-Diaz LL, Guerrero-Perilla C, Coy-Barrera ED (2016) Diazo coupling reaction of catechins and alkylresorcinols with diazotized sulfanilic acid for quantitative purposes in edible sources: method development and validation. *Food Analytical Methods* 9(2), 411-418.
- Bernal FA, Coy-Barrera E (2015) Molecular docking and multivariate analysis of xanthenes as antimicrobial and antiviral agents. *Molecules* 20(7), 13165-13204.
- Bernal FA, Coy-Barrera ED (2015) Chemical profile and antioxidant capacity of calyxes from commercial crops-derived Colombian Roselle (Hibiscus sabdariffa L.). *Medicinal Plants - International Journal of Phytomedicines and Related Industries* 7(2), 137-144.
- Bernal FA, Cuca LE, Fadini L (2015) A Facile approach toward 8-O-4'-neolignans: synthesis of threo-7',8'-dihydromachilin D through Jacobsen epoxidation *Revista Facultad de Ciencias Básicas* 11(1), 114-129.
- Bernal FA, Orduz-Diaz LL, Coy-Barrera E (2015) Exploitation of the complexation reaction of ortho-dihydroxylated anthocyanins with aluminum(III) for their quantitative spectrophotometric determination in edible sources. *Food Chem* 185, 84-89.
- Bernal FA, Coy-Barrera E (2014) In-silico analyses of sesquiterpene-related compounds on selected Leishmania enzyme-based targets. *Molecules* 19(5), 5550-5569.
- Orduz-Diaz LL, Bernal FA, Coy-Barrera ED (2014) Diterpenos de núcleo kaurano como inhibidores de la PTR1 de Leishmania: un estudio in silico. *Revista Facultad de Ciencias Básicas* 9(1), 142-152.
- Bernal FA, Cuca-Suárez LE, Yamaguchi LF, Coy-Barrera ED (2013) LC-DAD-UV and LC-ESI-MS-based analyses, antioxidant capacity, and antimicrobial activity of a polar fraction from Iryanthera ulei leaves. *Records of Natural Products* 7(2), 152-156.
- Bernal FA, Delgado WA, Cuca LE (2012) Fingerprint analysis of unfractionated piper plant extracts by HPLC-UV-DAD coupled with chemometric methods. *Journal of the Chilean Chemical Society* 57(3), 1256-1261.
- Bernal FA, Cuca LE (2009) Chemical constituents from Iryanthera ulei Warb. *Biochemical Systematics and Ecology* 37(6), 772-775.
- Cuca LE, Bernal FA, Coy CA, Coy ED (2009) Essential oil composition and antimicrobial activity of fruits of Iryanthera ulei W. from Colombia. *Journal of the Chilean Chemical Society* 54(4), 289-291.

\* equal contribution #corresponding author