

Laboratório de Bioquímica Experimental e Computacional de Fármacos

2015

Indexado (fator de impacto >= 7,51)

doi: JRA Santos-Pinto , LD Santos , HA Arcuri , ARS Menegasso , KS Santos , P Napoleão-Pego, FM Castro, JE Kalil, De-Simone SG, MS Palma 2015. B-cell linear epitopes mapping of antigen-5 allergen from Polybia paulista wasp venom. *J Allergy Clin Immun* 135(1): 264-267.

Indexado (fator de impacto >=1 e < 2,71)

doi: Alem D, Díaz-Dellavalle P, Leoni C, De-Simone SG, Correa, Agustin, Oppezzo P, Dalla-Rizza M 2015. In search of topical agricultural biofungicides: properties of the recombinant antimicrobial peptide TrxAq-AMP obtained from Amaranthus quitensis.. *J Microbiol Biotechn* 6: 268-273.

doi: Seibt KJ, da Luz Oliveira R, Bogo MR, Senger MR, Bonan CD 2015. Investigation into effects of antipsychotics on ectonucleotidase and adenosine deaminase in zebrafish brain. *Fish Physiol Biochem* 41: 1383-1392.

Indexado (fator de impacto >=4,35 e < 7,51)

doi: Senger MR, Souza CSF, Calabrese KS, Silva Jr FPS, Gasparotto J, Kunzler A, Degrossoli A, de Simone SG, Bortolin RC, Somensi N, Girardi CS,, Dal-Pizzol F, Moreira JC, Gelain DP 2015. Increased tau phosphorylation and receptor for advanced glycation endproducts (RAGE) in the brain of mice infected with Leishmania amazonensis. *Brain Behav Immun* 43: 37-45.

2016

Indexado (fator de impacto >=1 e < 2,71)

doi: Neves BJ, Dantas RF, Senger MR, Valente WCG, Neto JMR, Chaves WT, Kamentsky L, Carpenter A, Silva Jr FPS, Andrade CH 2016. The antidepressant drug paroxetine as a new lead candidate in schistosome drug discovery. *MedChemComm* 7: 1176-1182.

Indexado (fator de impacto >=2,71 e < 4,35)

doi: Costa, I.B., Cardoso MV, de Oliveira Filho GB, de Moraes Gomes PA, Espíndola JW, de Jesus Silva TG, Torres PH, Silva Jr FPS, Martin J, de Figueiredo RC, Leite AC 2016. Compound profiling and 3D-QSAR studies of hydrazone derivatives with activity against intracellular Trypanosoma cruzi. *Bioorgan Med Chem* 24: 1608-1618.

doi: Melo-Filho CC, Dantas RF, Senger MR, Braga RC, Neves BJ, Valente WCG, Neto JMR, Chaves WT, Muratov EN, Paveley RA, Furnham N, Kamentsky L, Carpenter AE, Silva Jr FPS, Andrade CH 2016. QSAR-Driven Discovery of Novel Chemical Scaffolds Active Against Schistosoma mansoni. *J Chem Inf Model* 56 (7): 1357-1372.

doi: Souza ALM, Faria RX, Calabrese KS, Hardoim DJ, N Taniwaki , Alves LA, De-Simone SG 2016. Temporizin and Temporizin-1 peptides as novel candidates for eliminating Trypanosoma cruzi. *Plos One* 11(7): - .

Indexado (fator de impacto >=4,35 e < 7,51)

doi: Neves BJ, Dantas RF, Senger MR, Melo-Filho CC, Valente WCG, Almeida ACM, Neto JMR, Lima EFC, Paveley R, Furnham N, Muratov E, Kamentsky L, Carpenter AE, Braga RC, Silva Jr FPS, Andrade CH 2016. Discovery of New Anti-Schistosomal Hits by Integration of QSAR-Based Virtual Screening and High Content Screening. *J Med Chem* 59(15): 7075-7088.

doi: Senger MR, Fraga, C.A., Dantas RF, Silva Jr FPS 2016. Filtering promiscuous compounds in early drug discovery: is it a good idea?. *Drug Discov Today* 21: 868-872.

2017

Indexado (fator de impacto >=1 e < 2,71)

doi: De-Simone SG, Souza ALA, Aguiar AS, Melgarejo AR, Provance Jr DW 2017. Development of an elisa for the diagnosis of reactive IgE antibodies anti-therapeutic horse sera. *Toxicon* 138: 37-42.

doi: Silva Jr FPS, Dantas RF, Azevedo LD, Mastos MM, Vasconcelos FC, Hoelz LVB, Almeida ACM, De Oliveira AP, Gomes LC, Maia RC, Boechat N 2017. Imatinib derivatives as inhibitors of K562 cells in chronic myeloid leukemia. *Med Chem Res* 26: 2929-2941.

doi: Sodero ACR, Abrahim-Vieira B, Torres PHM, Pascutti PG, Garcia CRS, Ferreira V, Rocha DR, Ferreira SB, Silva Jr FP 2017. Insights into cytochrome bc1 complex binding mode of antimalarial 2-hydroxy-1,4-naphthoquinones through molecular modelling. *Mem I Oswaldo Cruz (impresso)* 112: 299-308.

doi: Gasparotto J, Kunzler A, Senger MR, Souza CSF, De-Simone SG, Bortolin RC, Somensi N, Dall-Pizzol F, Moreira JCF, Calabrese KS, Silva Jr FPS, Gelain DP 2017. N-acetyl-cysteine inhibits liver oxidative stress markers in BALB/c mice infected with Leishmania amazonensis. *Mem I Oswaldo Cruz (impresso)* 112(2): 146-154.

doi: Prado IC, Souza ALA, Provance-Jr DW, Cassella RJ, De-Simone SG 2017. Ultrasensitive and rapid immuno-detection of human IgE anti-therapeutic horse sera using an electrochemical immunosensor. *Anal Biochem* 538: 13-19.

Indexado (fator de impacto >=2,71 e < 4,35)

doi: Santos AL, Rachel Ann Hauser Davis, Santos MJ, De-Simone SG 2017. Potentially toxic filamentous fungi associated to the economically important *Nodipecten nodosus* (Linnaeus, 1758) scallop farmed in southeastern Rio de Janeiro, Brazil. *Mar Pollut Bull* 115: 75-79.

2018

Indexado (fator de impacto < 1 ou sem FI)

doi: De-Simone SG, Souza ALM, Soares-de-Pina JL, Ivan Neves Junior, Maria Cristina Lourenço, David Provance Jr 2018. Bactericidal activity of a cationic peptide on *Neisseria meningitidis*. *Infect Disord Drug Targets* 18: 1-7.

Indexado (fator de impacto >= 7,51)

doi: Isis Campo Prado, Alcon MET, Santos AL, Souza ALM, Gomes LP, Lemos ERS, De-Simone SG 2018. Development of an electrochemical immunosensor for the diagnostic testing of spotted fever using synthetic peptides. Biosens Bioelectron 100: 115-122.

doi: Prado IC, Mendes VG, Souza ALM, Dutra RF, De-Simone SG 2018. Electrochemical immunosensor for differential diagnostic of Wuchereria Bancrofti using a synthetic peptide. Biosens Bioelectron 113: 9-15.

Indexado (fator de impacto >=1 e < 2,71)

doi: Oliveira Junior AF, Bleicher L, Scharago, Silva Jr FP 2018. Conservation analysis and decomposition of residue correlation networks in the Phospholipase A2 superfamily (PLA2s): Insights into the structure-function relationships of snake venom toxins. Toxicon 146: 50-60.

doi: Santos AL, LTF De Oliveria, Souza ALM, RA Hauser-Davis, De-Simone SG 2018. Cryptosporidium spp. contamination in Perna perna Mussels destined for human consumption in southeastern Rio de Janeiro, Brazil. Bull Environ Contam Tox 100: 240-244.

doi: Teixeira MAC, Belloze KT, Cavalcanti MC, Silva Jr FPS 2018. Data Mart Construction based on Semantic Annotation of Scientific Articles: A Case Study for the Prioritization of Drug Targets. Comput Meth Prog Bio 157: 225-235.

doi: De-Simone SG, Nascimento HJ, Prado IC, Aguiar AS, Melgarejo AR, Soares-de-Pina JL, Ferreira P, Provance Jr D 2018. Purification of equine IgG3 by lectin affinity and an interaction analysis via microscale thermophoresis. Anal Biochem 561-562: 27-31.

Indexado (fator de impacto >=2,71 e < 4,35)

doi: Lopes JPB, Silva L, da Costa Franarin G, Antonio Ceschi M, Seibert Lüdtke D, Dantas RF, de Salles CMC, Silva Jr FPS, Senger MR, Alvim Guedes I, Emmanuel Dardenne L 2018. Design, synthesis, cholinesterase inhibition and molecular modelling study of novel tacrine hybrids with carbohydrate derivatives. Bioorgan Med Chem 26: 5566-5577.

doi: Rocha-Santos C, Bastos FF, Dantas RF, Hauser-Davis RA, Rodrigues LC, Cunha Bastos VLF, Cunha Bastos JC 2018. Glutathione peroxidase and glutathione S-transferase in blood and liver from a hypoxia-tolerant fish under oxygen deprivation. Ecotox Environ Safe 163: 604-611.