Medicinal Chemistry and Drug Discovery

Adriano D. Andricopulo
Affinity
PK
ADME
Potency
Selectivity
Efficacy
Toxicity
DRUG
Journal of Chemical Information and Modeling
Discovery of Potent, Reversible and Competitive Cruzain Inhibitors with Trypanocidal Activity: A Structure-Based Drug Design Approach
Manuscript ID: ci-2019-00802a

Author(s): Souza, Mariana; de Oliveira Rezende Júnior, Celso; Ferreira, Rafaela; Espinoza Chávez, Rocio; Ferreira, Leonardo; Slafer, Brian; Magalhaes, Luma; Krogh, Renata; Oliva, Glaucius; Cruz, Fabio; Dias, Luiz; Andricopulo, Adriano

Journal of Medicinal Chemistry
Discovery of Highly Potent and Selective Antiparasitic New Oxadiazole and Hydroxy-Oxindole Small Molecule Hybrids
Manuscript ID: jm-2019-017952

Authors: Fernandes, Fabio; Lima, Samia; Santos, Hugo; Conti, Caroline; Rodrigues, Manoel; Zeoly, Lucas A.; Ferreira, Leonardo; Krogh, Renata; Andricopulo, Adriano; Coelho, Fernando
Chagas’ disease

- Violacein
- N-acylhydrazones
- Diarylheptanoids
- Imides
- Aphidicolin Derivatives
- Spirooxindoles
- 1,2,4-oxadiazoles
- Dithiocarbazates
- Hydroxy-indoles
- Imidazoles
Chagas’ disease - cruzain

Oxadiazoles

Carbamoyl Imidazoles

Cyclic imides

N-acylhydrazones

Chalcones

Benzimidazoles

Thiosemicarbazones

Pyrimidines

CF$_3$
Anticancer (tubulin)

- Acridinones
- Diarylheptanoids
- Discodermolide analogs
- Indoles
- Chalcones
- Migrastatin analogs
- Piperlongumine analogs
- Acylhydrazones
- Thiosemicarbazones