

USP

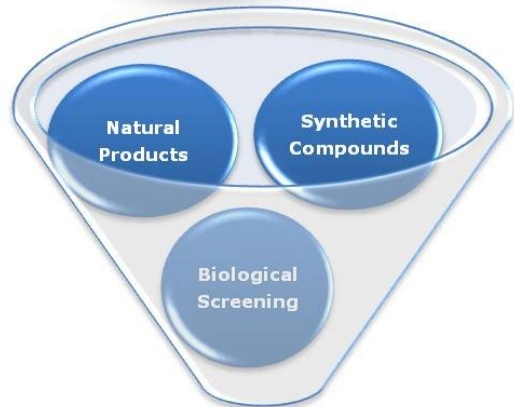


Medicinal Chemistry and Drug Discovery

Adriano D. Andricopulo



TARGET



**DRUG DESIGN
APPROACH**

**Pharmacokinetics
Metabolism
Toxicity**



**Potency
Affinity
Selectivity**

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IFSC

USP

NATIONAL E INTERNATIONAL PARTNERSHIPS

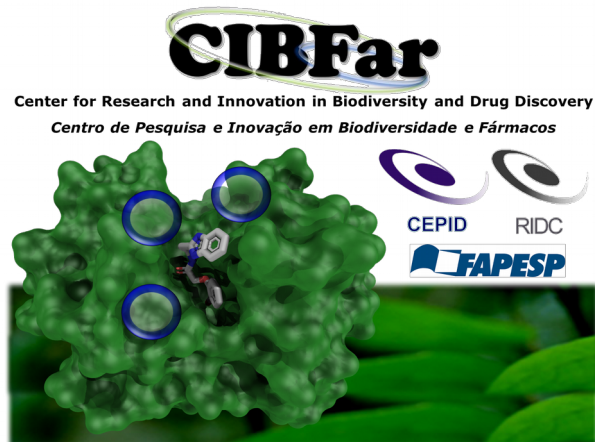
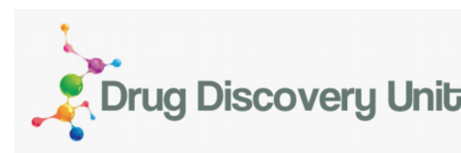


Medicinal Chemistry Centre for Chagas Disease in Brazil

World Health Organization

New Medicinal Chemistry Centers to Join Drug Discovery Networks
T24/181/136 ID No. A80141

The Special Programme for Research and Training in Tropical Diseases
TDR/UNICEF/UNDP/WB/WHO



abbvie



Lead Optimisation Latin America "LOLA"

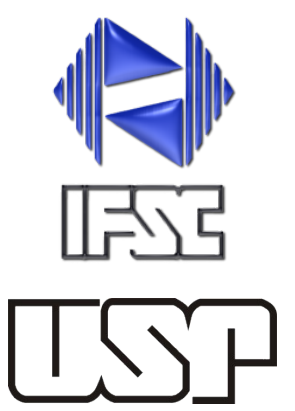
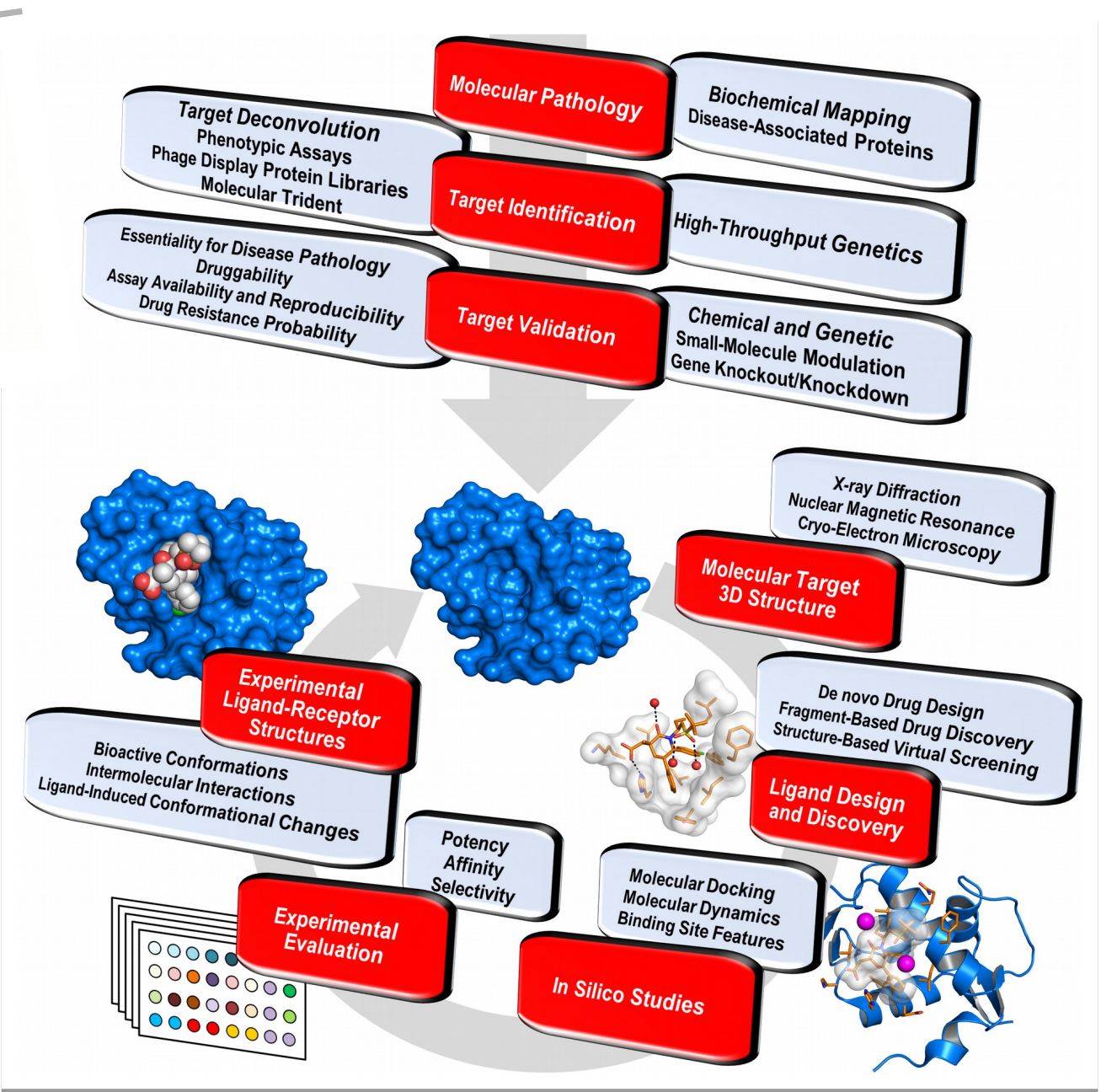


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L.G. Ferreira; **A.D. Andricopulo**. *Lancet Infectious Disease*, 19, 125-127, **2019**.
L.G. Ferreira, **A.D. Andricopulo**. *Burger's Medicinal Chemistry and Drug Discovery*, in press: 8th Edition, **2020**.

JCIMJOURNAL OF
CHEMICAL INFORMATION
AND MODELING

29-Oct-2019

*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****LQMC**
LABORATÓRIO DE QUÍMICA
MEDICINAL E COMPUTACIONAL

29-Oct-2019

*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

Imides



Violacein

N-acylhydrazones



Spirooxindoles **1,2,4-oxadiazoles**

Diarylheptanoids

Hydroxy-indoles

Dithiocarbazates

Imidazoles

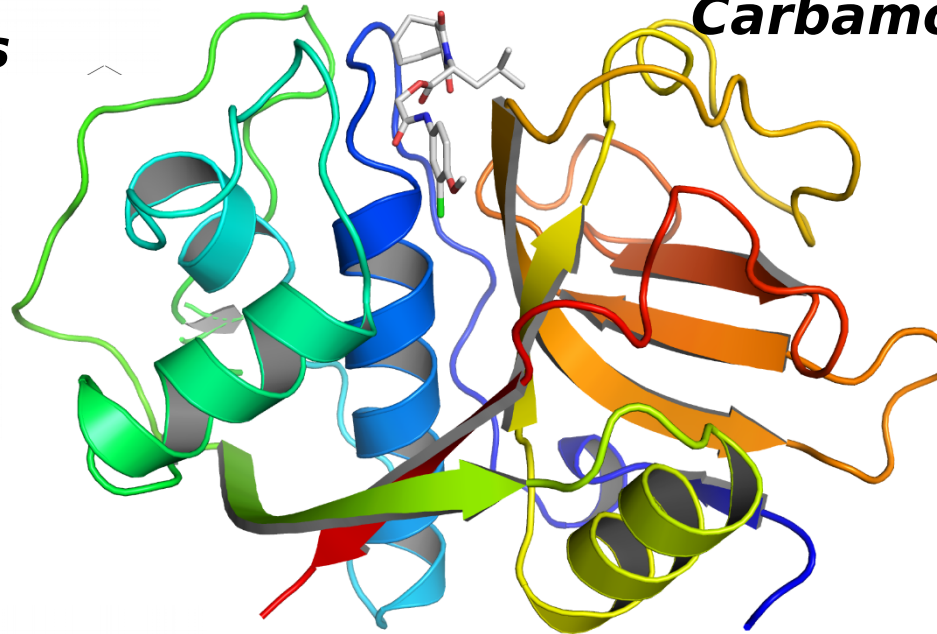
Chagas' disease - cruzain

Oxadiazoles

Carbamoyl Imidazoles

Cyclic imides

N-acylhydrazones



Chalcones

Benzimidazoles

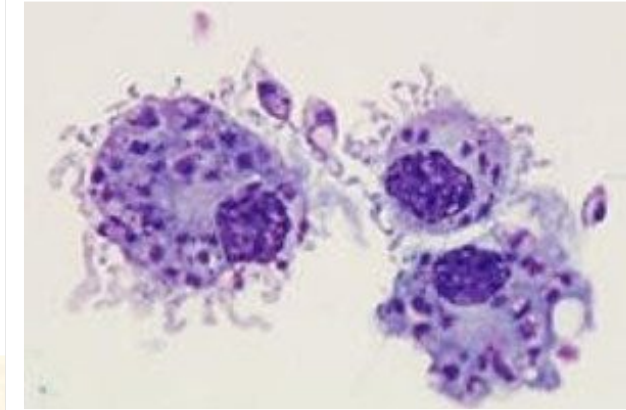
Thiosemicarbazones

Pyrimidines

CF_3

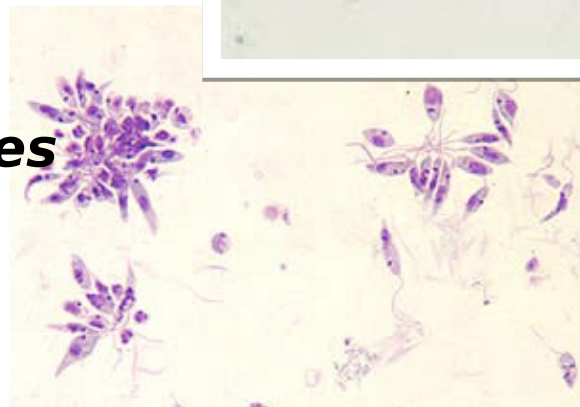
Leishmaniasis

Ptericidins



Polyketides

Hexadepsipeptides



Dinactins

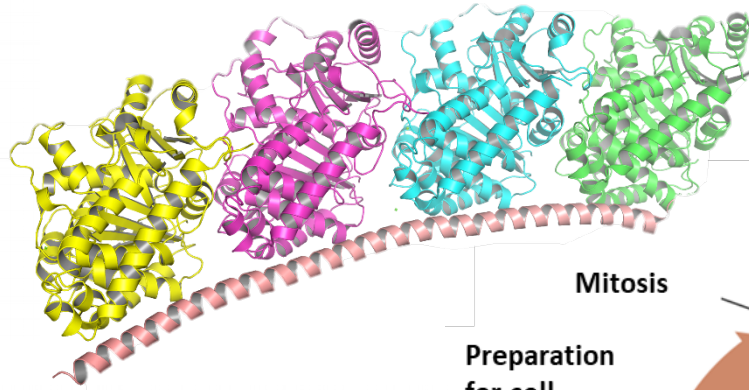
Benzodiazepines

Vinylic acids

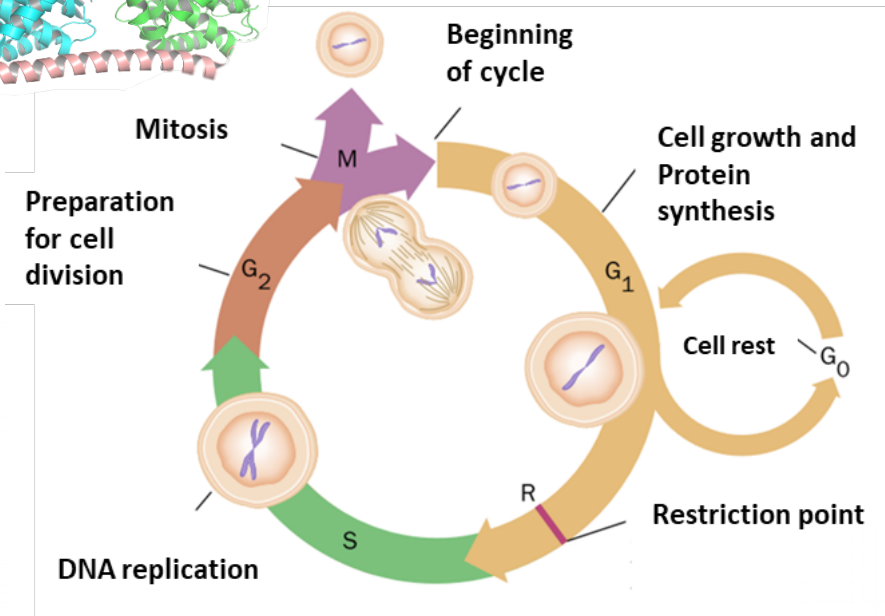
Hydrazones

Anticancer (tubulin)

Acridinones



Diarylheptanoids



Piperlongumine analogs

Acylhydrazones

Discodermolide analogs

Thiosemicarbazones

Indoles

Chalcones

Migrastatin analogs