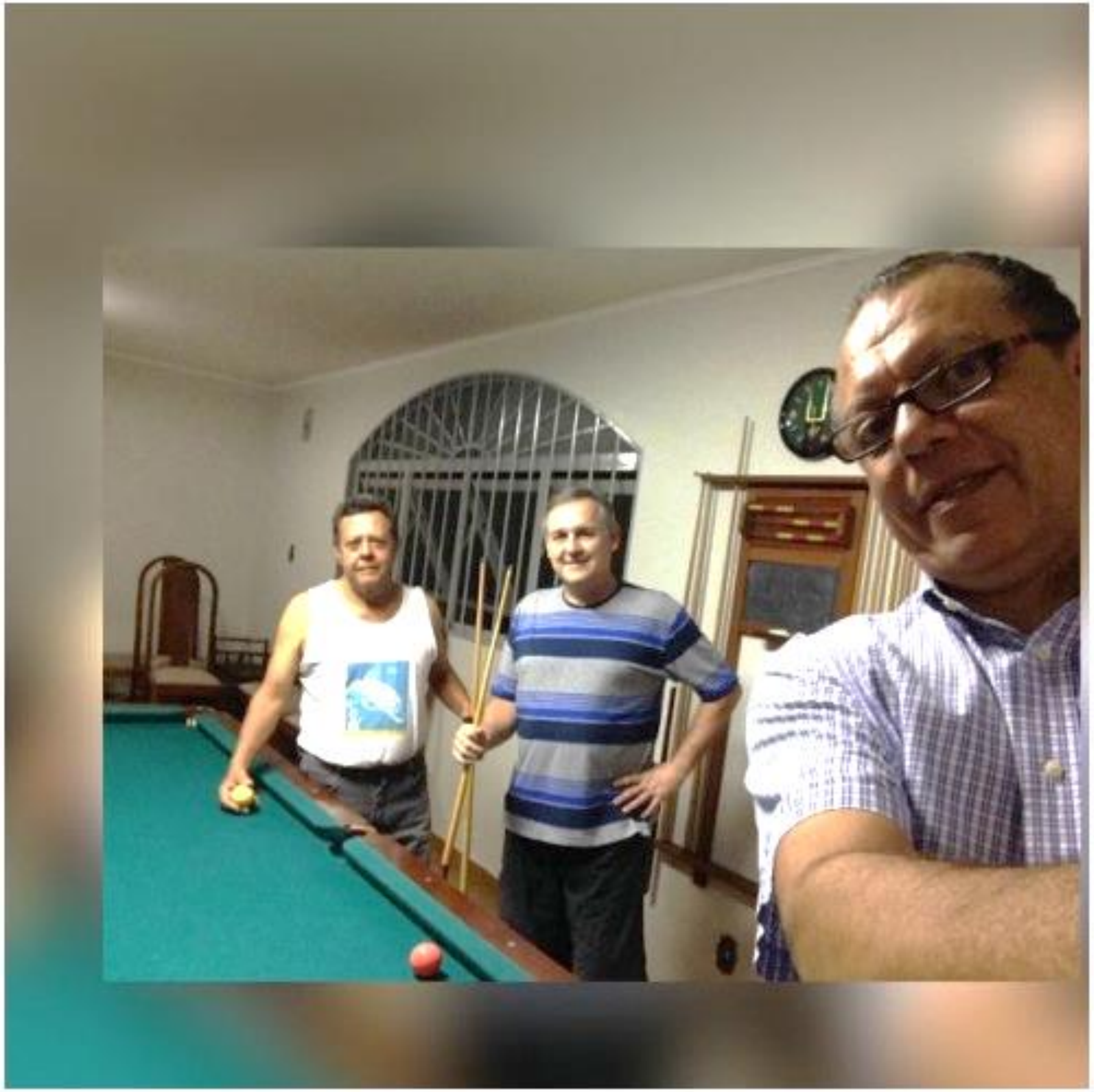
UNIVERSIDADE DE SÃO PAULO
Instituto de Física de São Carlos

Universidade de São Paulo
Brasil

WORKSHOP

GLAUCIUS 6.0

São Carlos 31 de outubro de 2019



1. Pyrano chalcones and a flavone from *Neoraputia magnifica* and their *Trypanosoma cruzi* glycosomal glyceraldehyde-3-phosphate dehydrogenase-inhibitory activities. PHYTOCHEMISTRY **55**, 643-651, 2000.

2. Strategies for the isolation and identification of trypanocidal compounds from the Rutales. PURE AND APPLIED CHEMISTRY **73**, 617-622, 2001.

3. Structure of *Trypanosoma cruzi* glycosomal glyceraldehyde-3-phosphate dehydrogenase complexed with chalepin, a natural product inhibitor, at 1.95 angstrom resolution. FEBS LETTERS **520**, 13-17, 2002.

4. Enzymatic inhibition studies of selected flavonoids and chemosystematic significance of polymethoxylated flavonoids and quinoline alkaloids in Neoraputia (Rutaceae). JOURNAL OF THE BRAZILIAN CHEMICAL SOCIETY **14**, 380-387, 2003.

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13. Anacardic acid derivatives as inhibitors of glyceraldehyde-3-phosphate dehydrogenase from *Trypanosoma cruzi*. BIOORGANIC & MEDICINAL CHEMISTRY **16**, 8889-8895, 2008.

14. Enzymatic inhibitory activity and trypanocidal effects of extracts and compounds from *Siphoneugena densiflora* O. Berg and *Vitex polygama* Cham. ZEITSCHRIFT FUR NATURFORSCHUNG SECTION C-A JOURNAL OF BIOSCIENCES **63**, 371-382, 2008.

15. Screening of *Trypanosoma cruzi* glycosomal glyceraldehyde-3-phosphate dehydrogenase enzyme inhibitors. REVISTA BRASILEIRA DE FARMACOGNOSIA-BRAZILIAN JOURNAL OF PHARMACOGNOSY **19**, 1-6, 2009.

16. Isolation of Tiliroside from *Spiranthera odoratissima* as Inhibitor of *Trypanosoma cruzi* Glyceraldehyde-3-phosphate Dehydrogenase by Using Bioactivity-Guided Fractionation. JOURNAL OF THE BRAZILIAN CHEMICAL SOCIETY **28**, 512-519, 2017.

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Strategies for the isolation and identification of trypanocidal compounds from the Rutales. PURE AND APPLIED CHEMISTRY **73**, 617-622, 2001.

Pure Appl. Chem., 2001, Vol. 73, No. 3, pp. 617-622
http://dx.doi.org/10.1351/pac200173030617

Strategies for the isolation and identification of trypanocidal compounds from the Rutales

Paulo C. Vieira[1], Jair Mafezoli[1], Mônica T. Pupo[2], João B. Fernandes[1], M. Fátima das G. F. da Silva[1], Sérgio de Albuquerque[2], Glaucius Oliva[3] and Fernando Pavão[4,3]*

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[2] Faculdade de Ciências Farmacêuticas de Ribeirão Preto, Universidade de São Paulo, Ribeirão Preto, SP, Brazil
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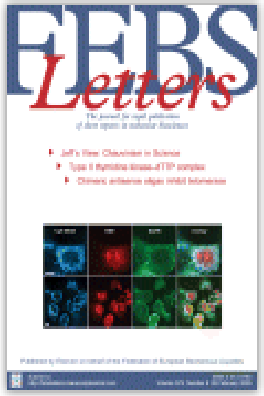
Structure of Trypanosoma cruzi glycosomal glyceraldehyde-3-phosphate dehydrogenase complexed with chalepin, a natural product inhibitor, at 1.95 angstrom resolution. FEBS LETTERS **520**, 13-17, 2002.

FEBS Letters



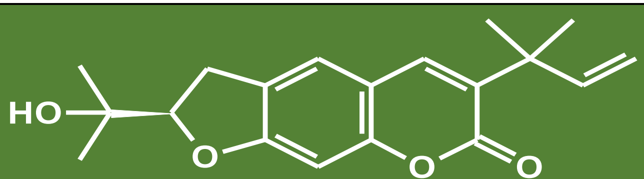
Volume 520, Issue 1-3
June 05, 2002
Pages 13-17

Structure of *Trypanosoma cruzi* glycosomal glyceraldehyde-3-phosphate dehydrogenase complexed with chalepin, a natural product inhibitor, at 1.95 Å resolution

F. Pavão, M.S. Castilho, M.T. Pupo, R.L.A. Dias, A.G. Correa, J.B. Fernandes, M.F.G.F. da Silva, J. Mafezoli, P.C. Vieira, G. Oliva

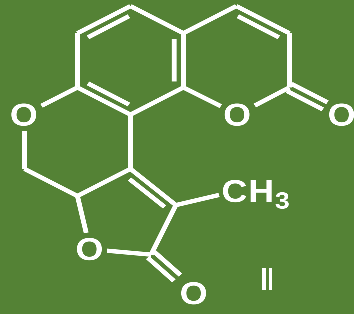
		Inibition of GAPDH (%)			
	Lysis (%)	concentration (μg/mL)			
Compound	250μg/mL	20	30	50	100
Shoreic acid	9.2				6.8
Ocotillone	34.9				32.5
Scopoletin	52.2		14.4		27.5
Steroids	20				13.1
Isoangenomalin	22.7				24.2
Xanthyletin	21.3		24.4	75.1	98.8
Chalepin	13.9	44.8	75.1	97.4	99.1
Dictamnine	17.6				30.0
Lichexanthone	22.7			20.0	
Arborinin	45.6				34.1
Xanthoxolin	66.4				8.4
New alkaloid	63.6				17.4
Tetramethoxyacridone	55.8				4.5
methylarborinin	63.2				8.0

Coumarins



I

IC_{50} = 64 µM



II

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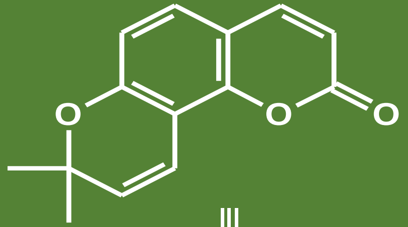
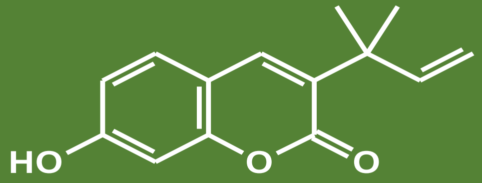


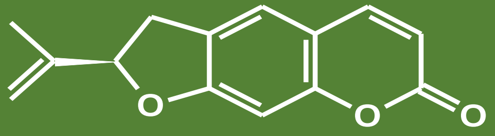
III

IC_{50} = 123 µM



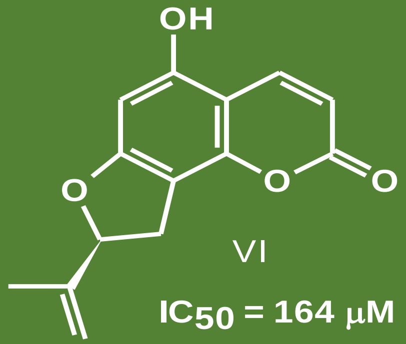
IV

IC_{50} = 130 µM



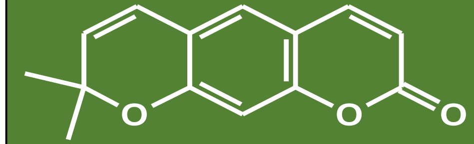
V

IC_{50} = 145 µM



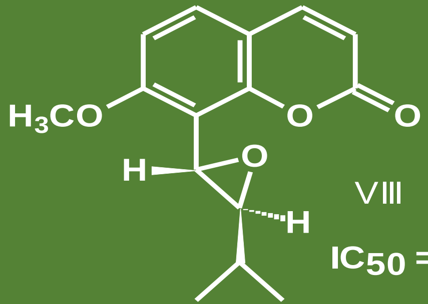
VI

IC_{50} = 164 µM



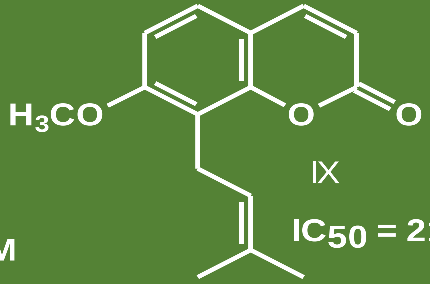
VII

IC_{50} = 175 µM



VIII

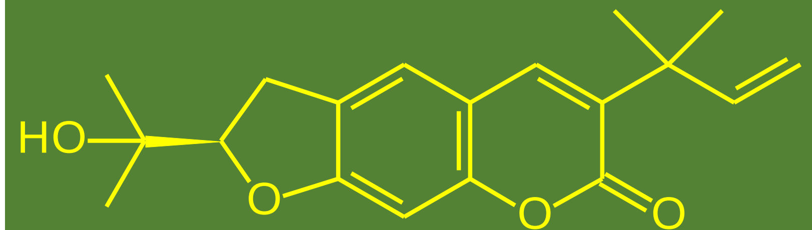
IC_{50} = 190 µM



IX

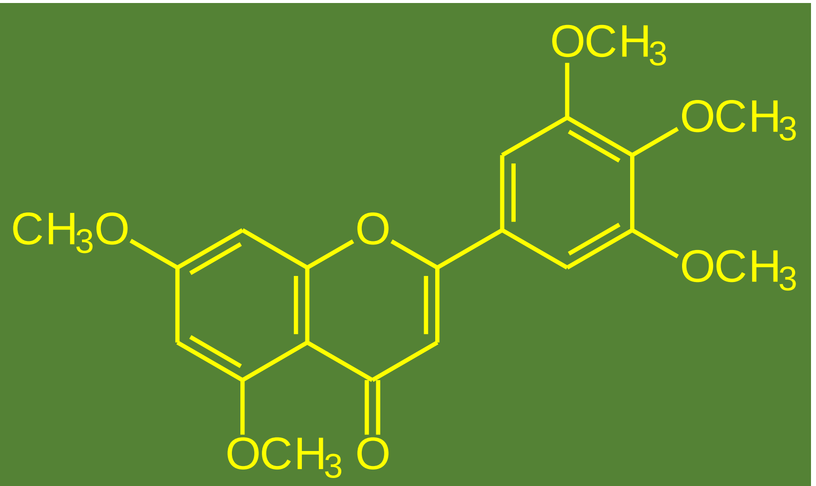
IC_{50} = 210 µM

Compounds submitted to experiments of Cocrystallization in microgravity

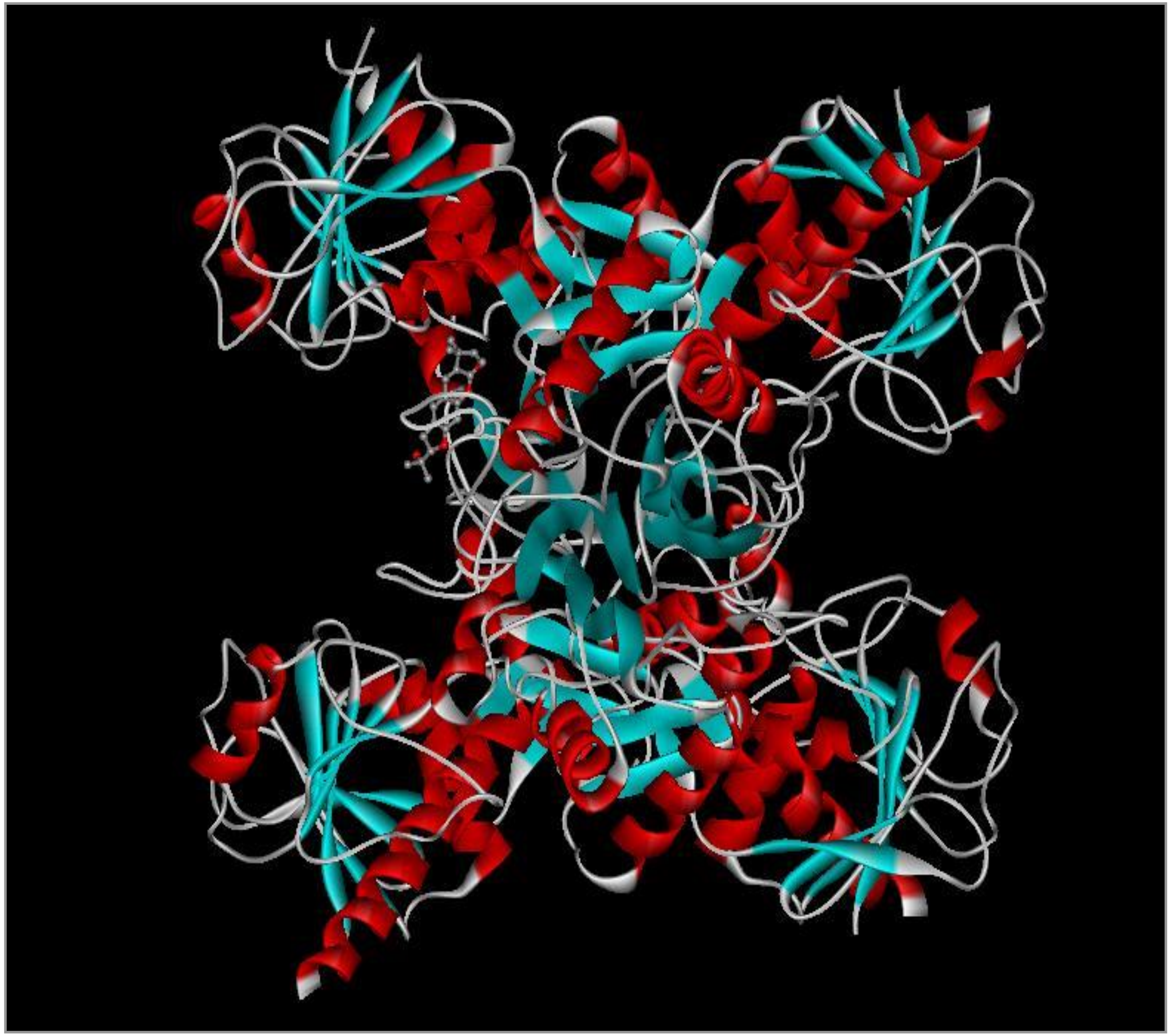


IC50 = 64 μM

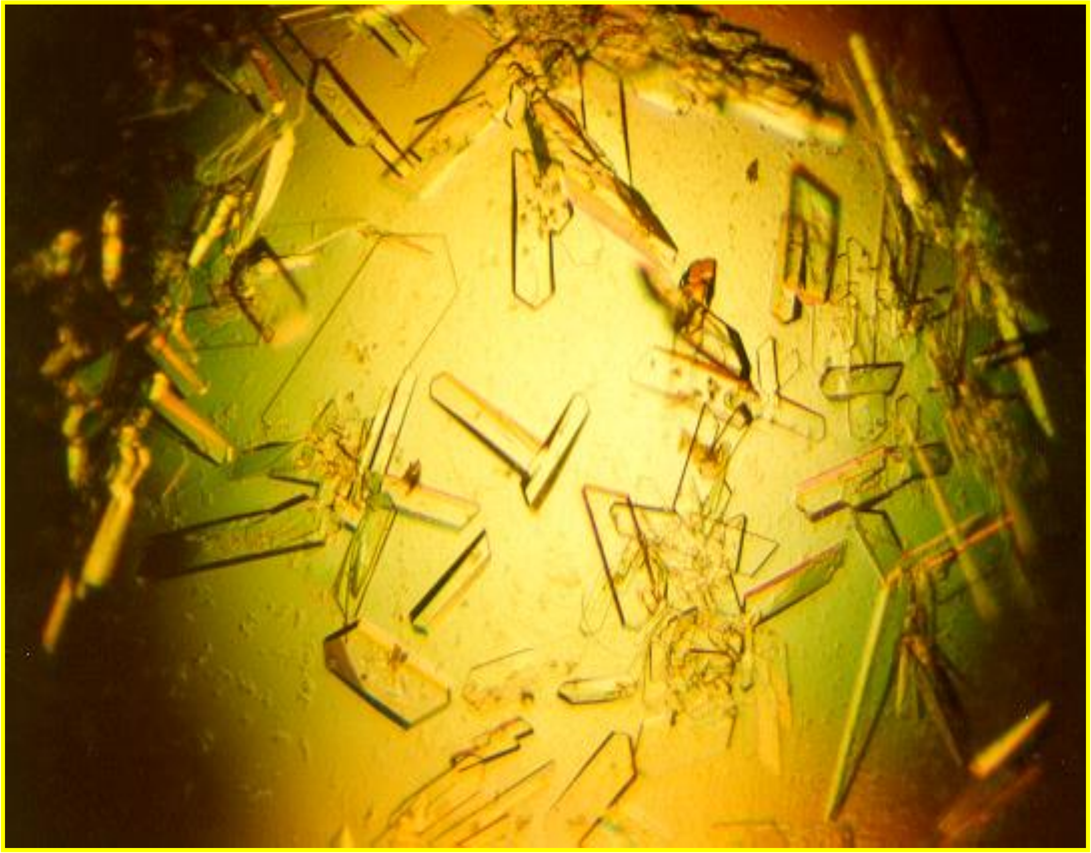
chalepin

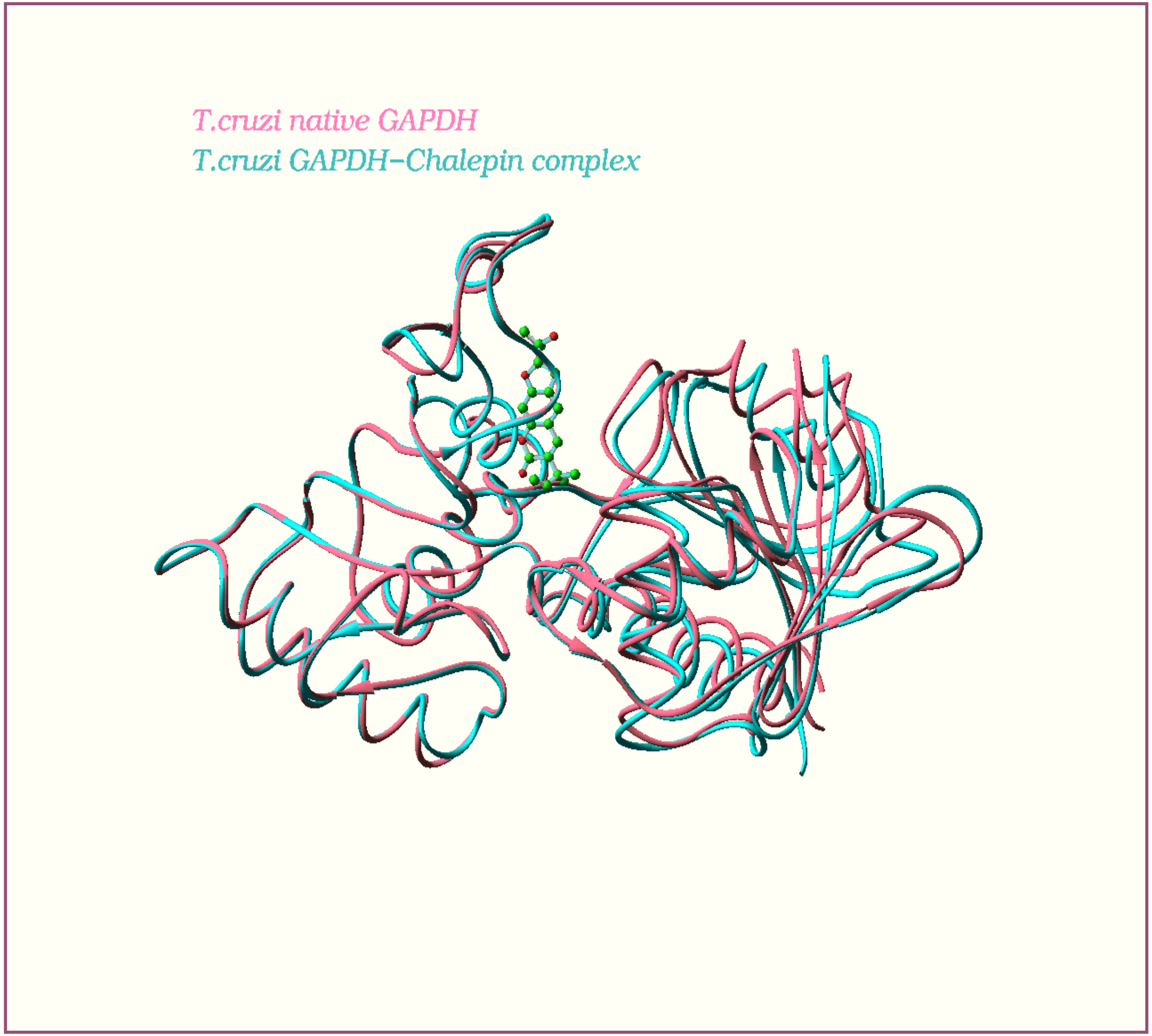


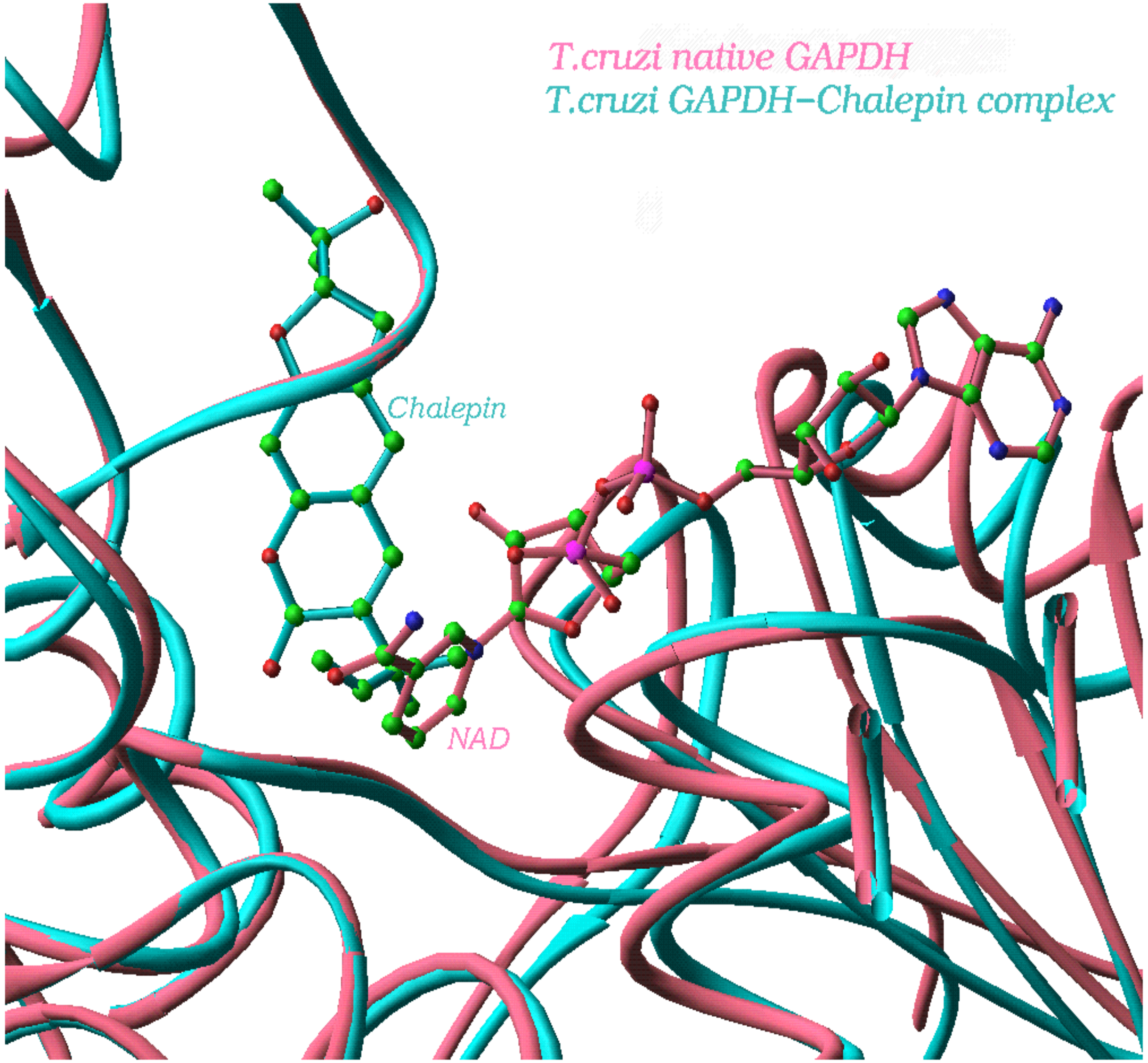
IC50 = 81 μM



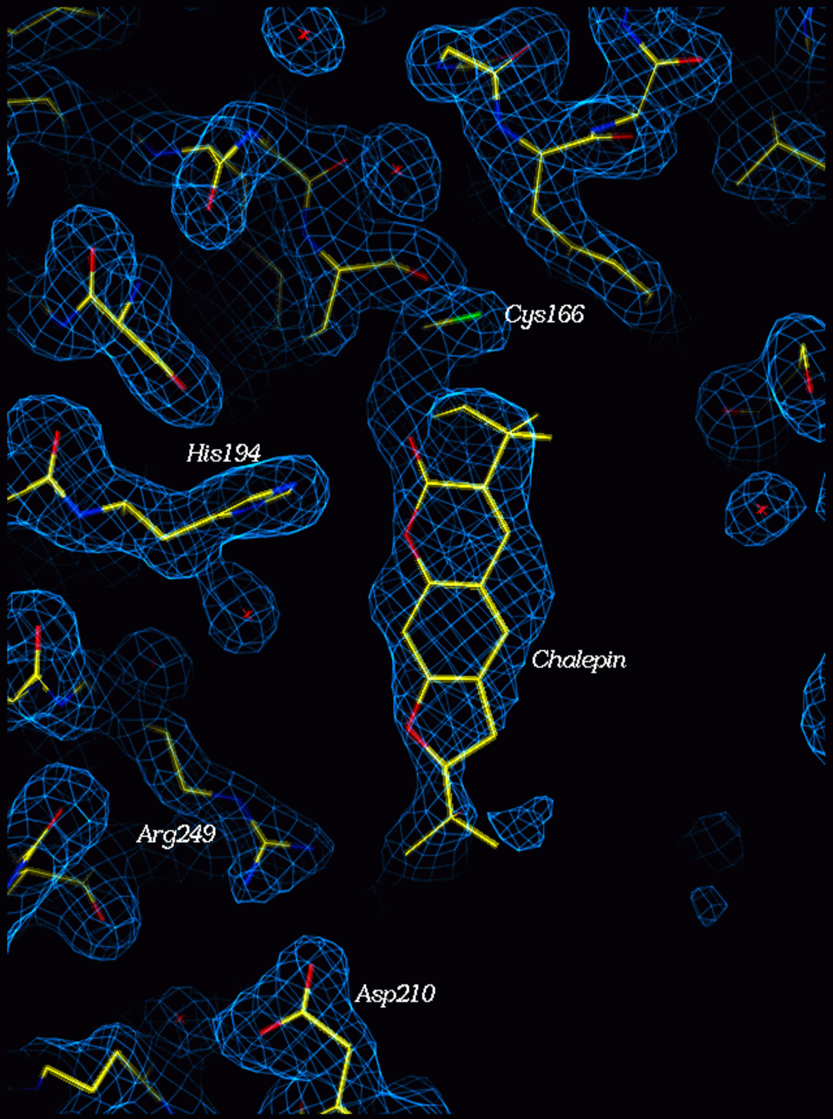
Crystals of the complex enzyme-chalepin

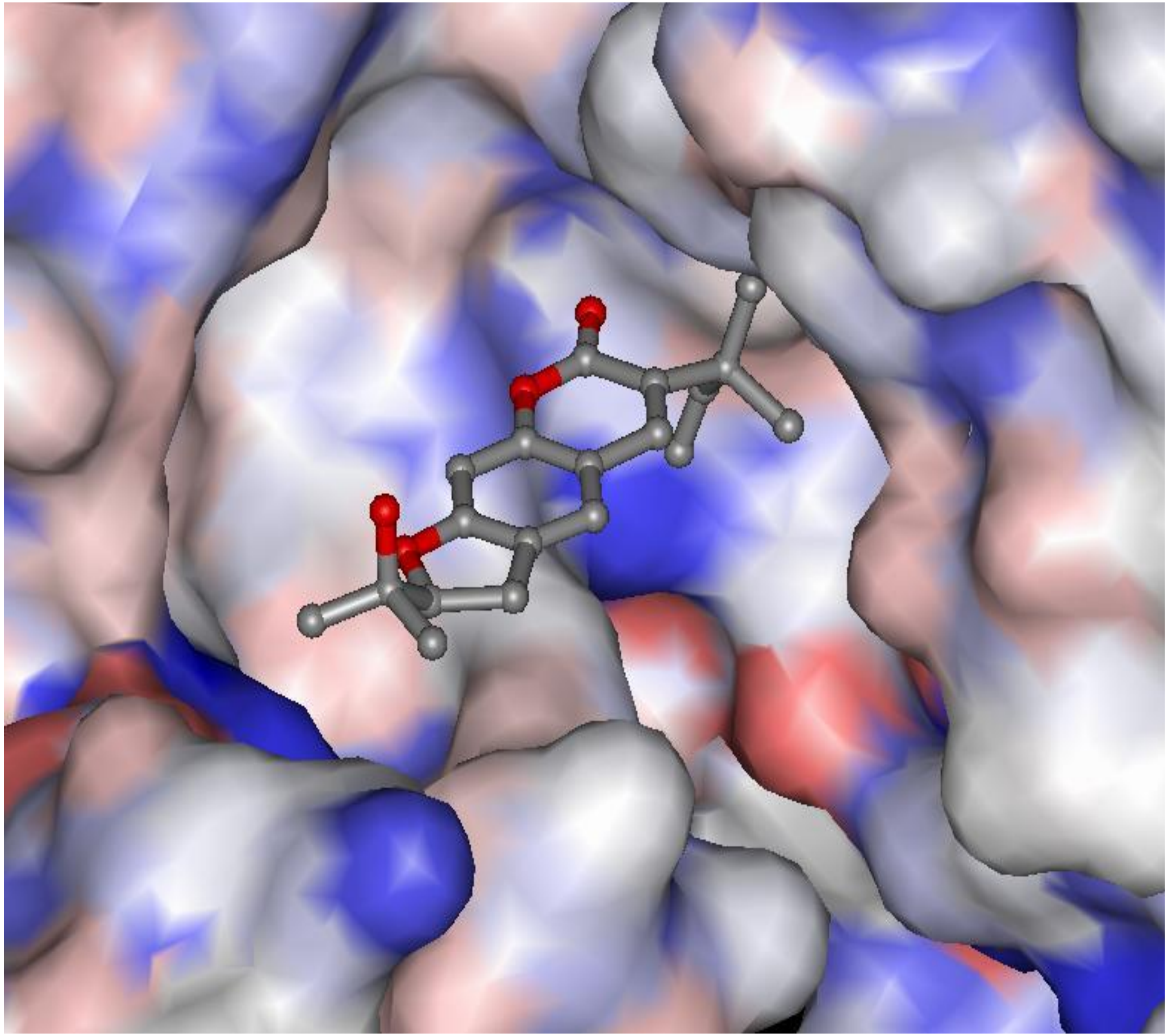


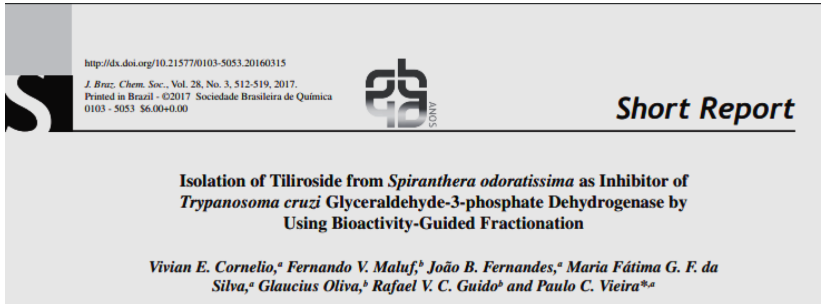

T.cruzi native GAPDH
T.cruzi GAPDH–Chalepin complex


T.cruzi native GAPDH
T.cruzi GAPDH-Chalepin complex
Chalepin
NAD

T.cruzi GAPDH–Chalepin complex






http://dx.doi.org/10.21577/0103-5053.20160315

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Short Report

Isolation of Tiliroside from *Spiranthera odoratissima* as Inhibitor of *Trypanosoma cruzi* Glyceraldehyde-3-phosphate Dehydrogenase by Using Bioactivity-Guided Fractionation

Vivian E. Cornelio,[a] Fernando V. Maluf,[b] João B. Fernandes,[a] Maria Fátima G. F. da Silva,[a] Glaucius Oliva,[b] Rafael V. C. Guido[b] and Paulo C. Vieira[*,a]*

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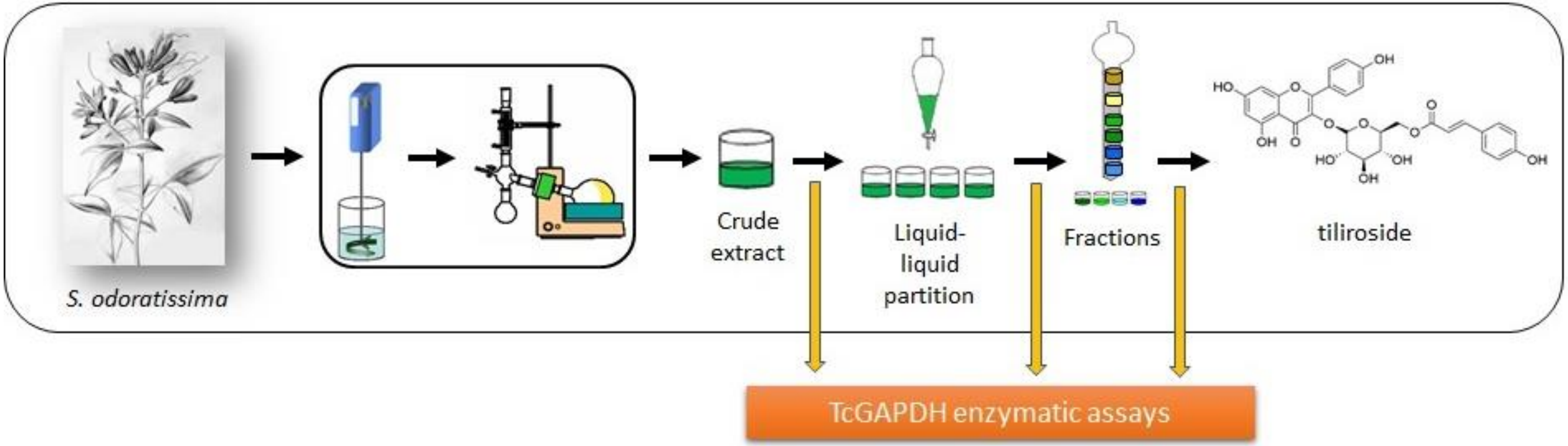
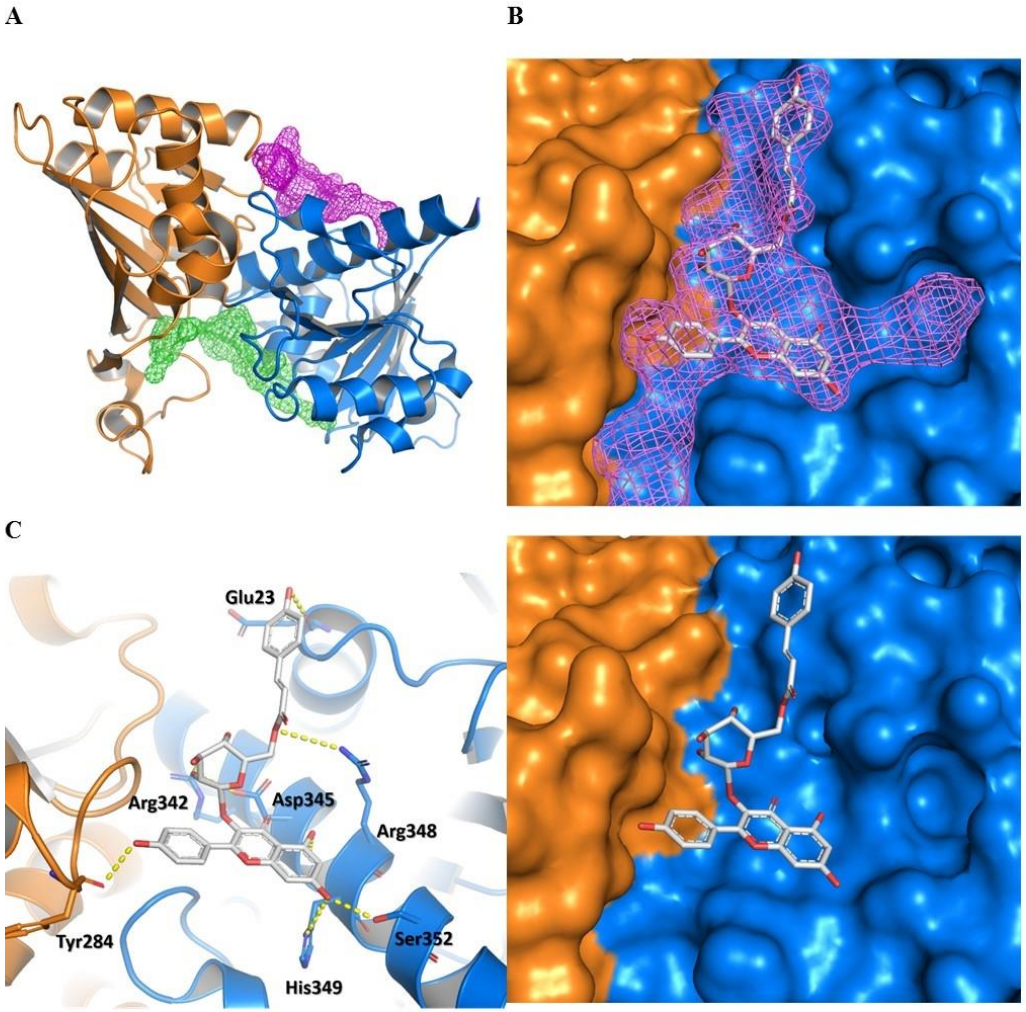
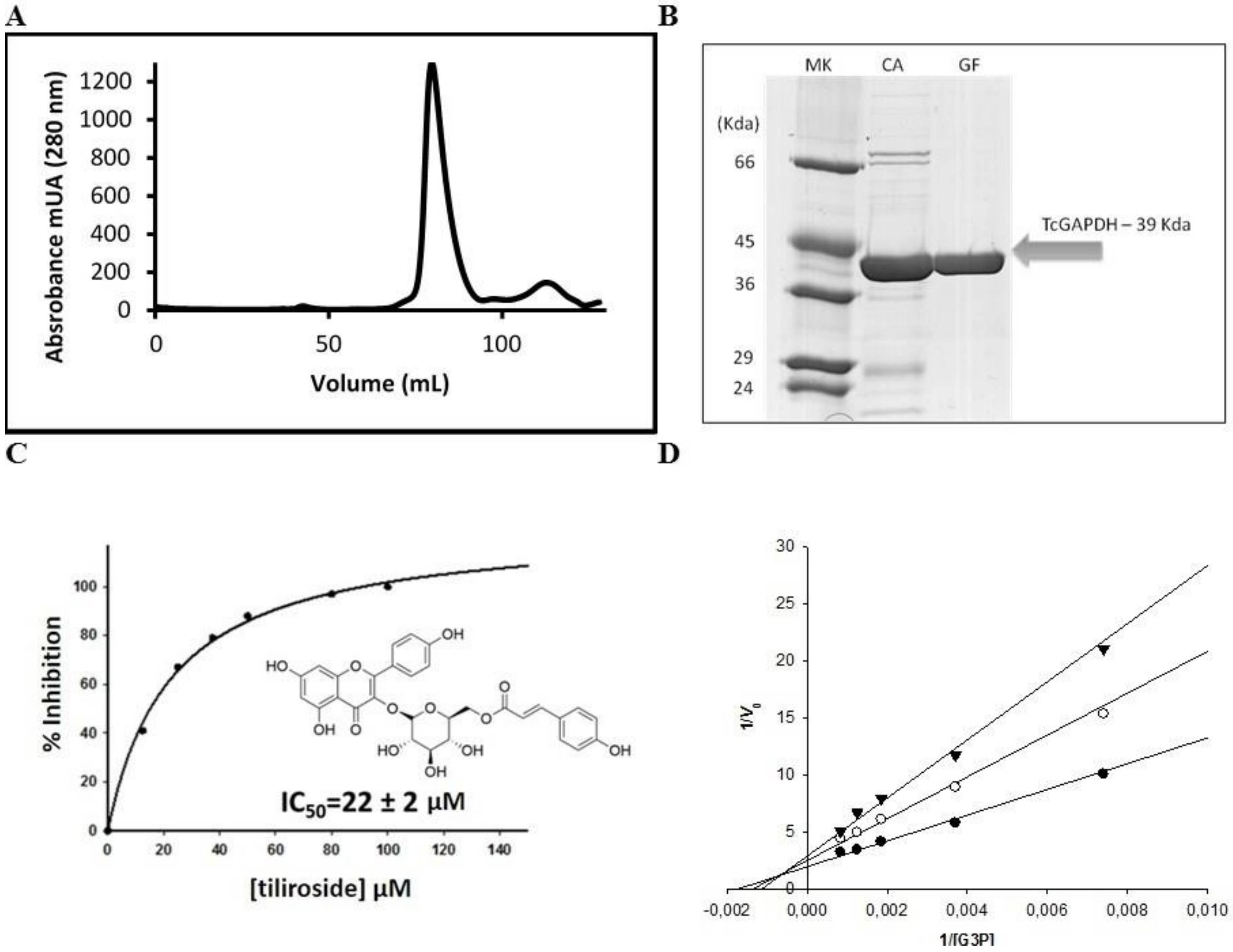



A
B
C
Glu23
Arg342
Asp345
Arg348
Tyr284
Ser352
His349


A
B
C
D
Absrobance mUA (280 nm)
Volume (mL)
MK
CA
GF
(Kda)
66
45
36
29
24
TcGAPDH – 39 Kda
% Inhibition
[tiliroside] µM
IC50=22 ± 2 µM
HO
OH
1/V0
1/[G3P]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