Barcelona Innovation workshop: NanoBiotechnology & IT for Health

The Tropical Disease Initiative

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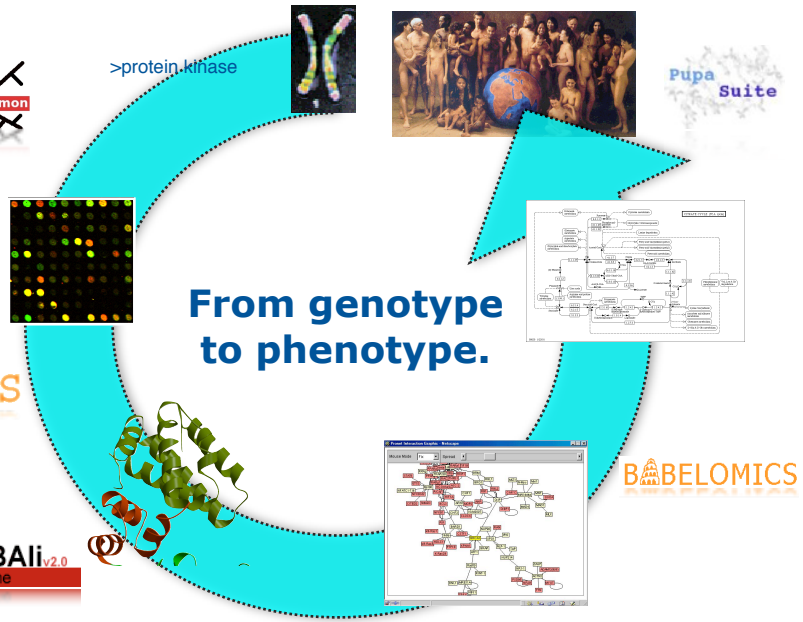
Comparative Genomics
Dr. Hernán Dopazo

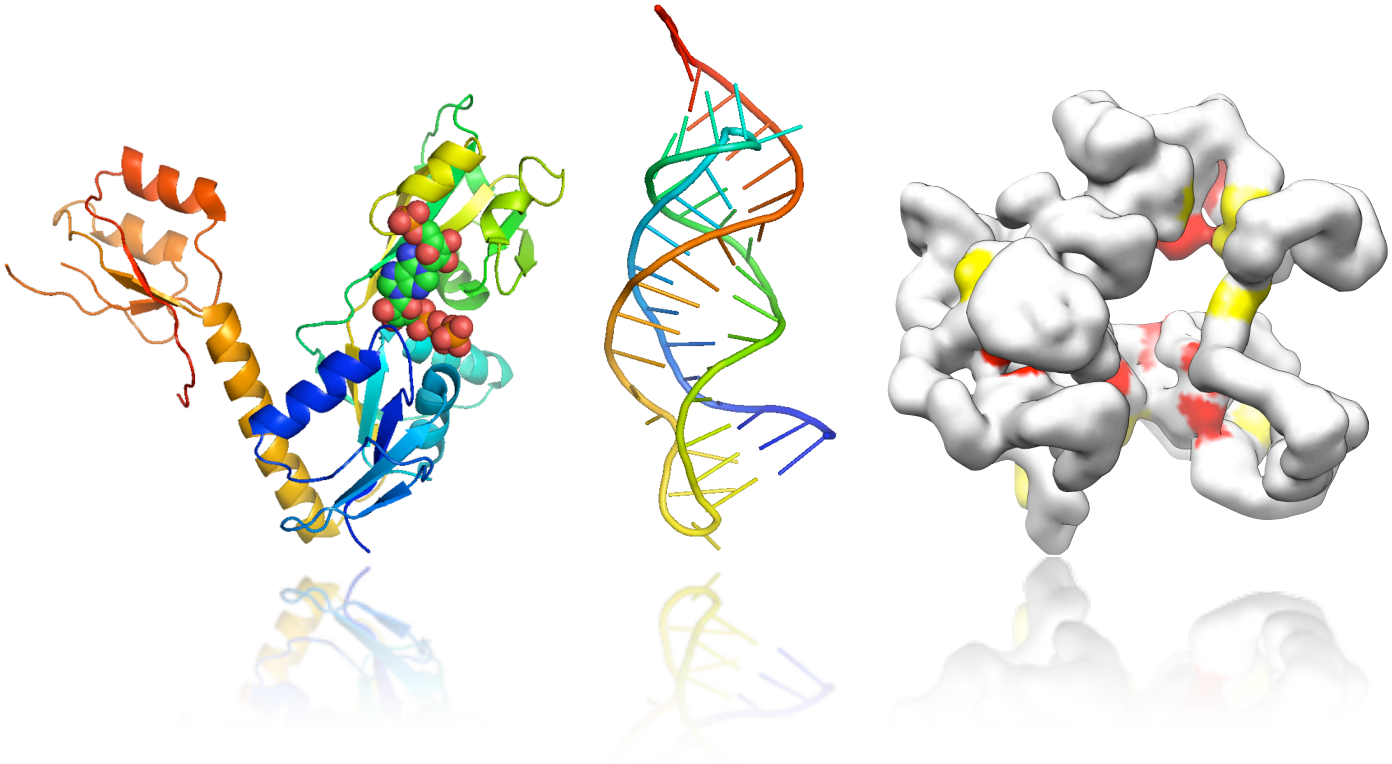


Functional Genomics
Dr. Joaquín Dopazo

Structural Genomics
Dr. Marc A. Marti-Renom

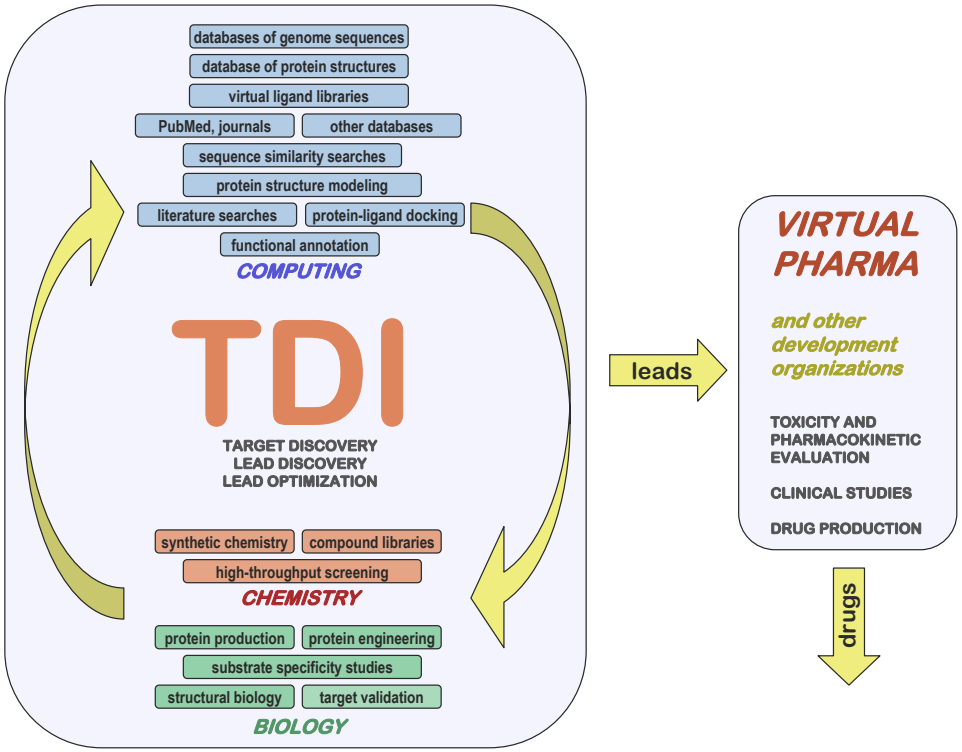
Structural Genomics Unit

Bioinformatics & Genomics Department, CIPF



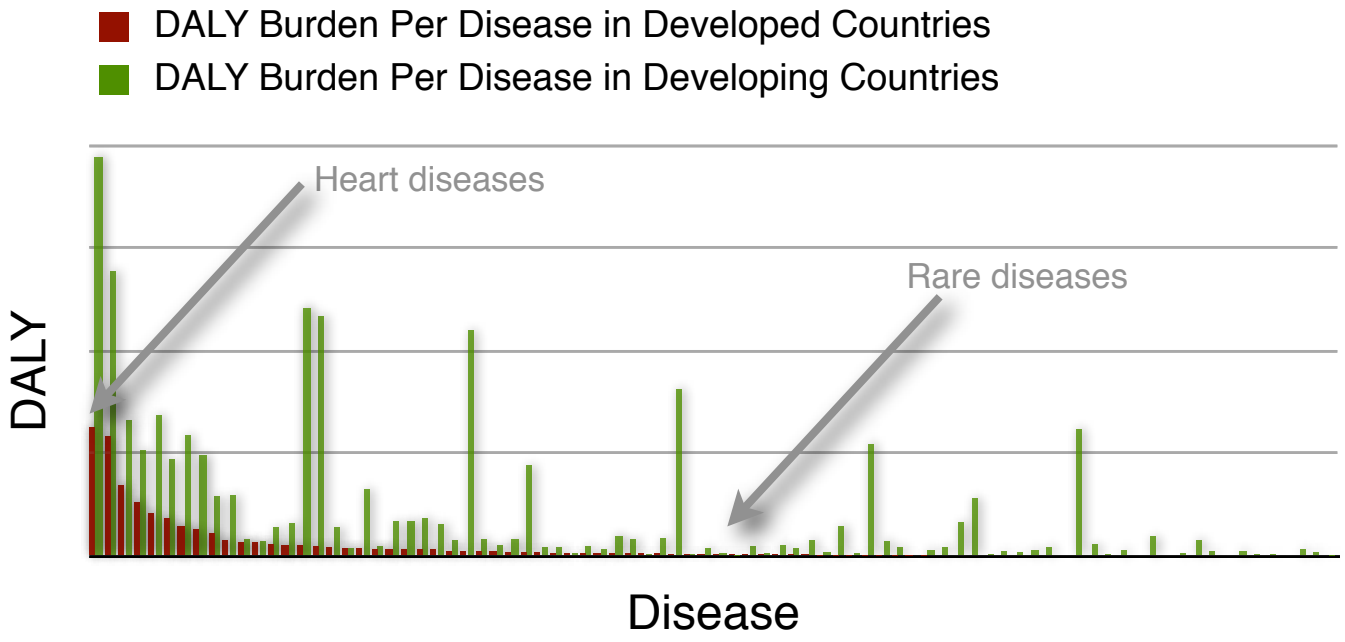
The Tropical Disease Initiative (TDI)

http://tropicaldisease.org



Showcase

"Unprofitable" Diseases and Global DALY (in 1000's)



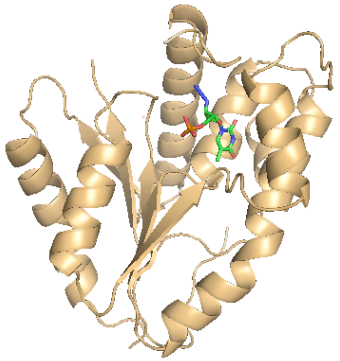
Disease data taken from WHO, *World Health Report 2004*
DALY - Disability adjusted life years

Malaria*	**46,486**
Tetanus	7,074
Lymphatic filariasis*	**5,777**
Syphilis	4,200
Trachoma	2,329
Leishmaniasis*	**2,090**
Ascariasis	1,817
Schistosomiasis*	**1,702**
Trypanosomiasis*	**1,525**
Trichuriasis	1,006
Japanese encephalitis	709
Chagas Disease*	**667**
Dengue*	**616**
Onchocerciasis*	**484**
Leprosy*	**199**
Diphtheria	185
Poliomyelitise	151
Hookworm disease	59

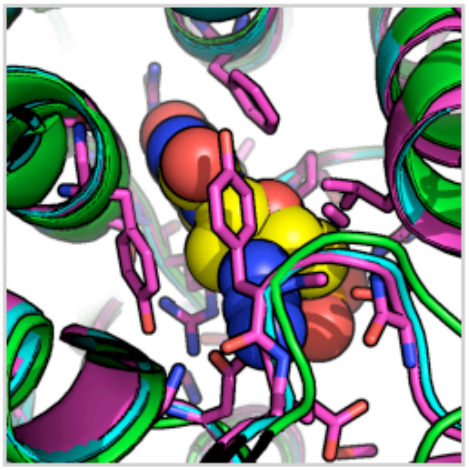
Showcase

P. falciparum tymidylate kinase + zidovudine

Template 3tmkA a yeast tymidylate kinase.



PDB		Template		Model		Ligand	Exact	SupStr	SubStr	Similar
2tmkB	100.00/100.00	3tmkA	41.00/1.49	PFL2465c.2.pdb	82.61/100.00	ATM		DB00495		DB00495

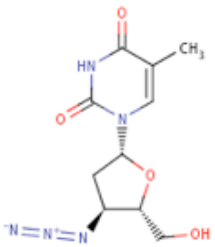


DB00495 Zidovudine

Small Molecule; Approved

Drug categories:

Anti-HIV Agents
Antimetabolites
Nucleoside and Nucleotide Reverse Transcriptase Inhibitors



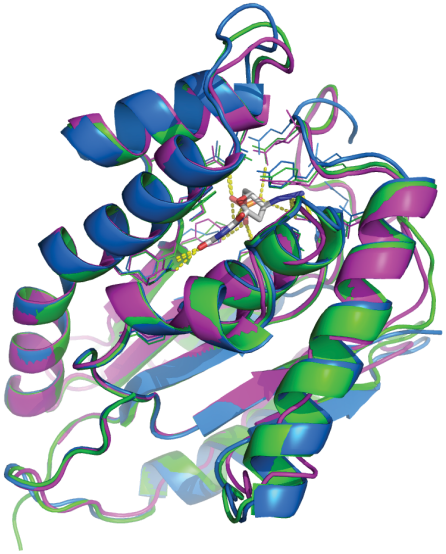
Drug indication:

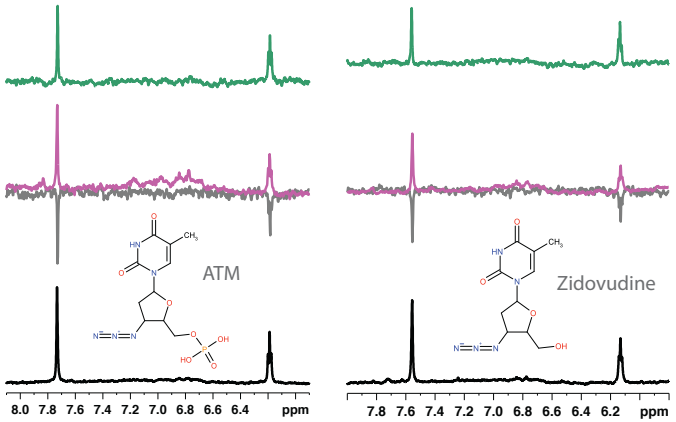
For the treatment of human immunovirus (HIV) infections.

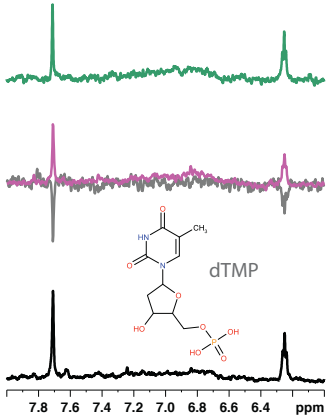
Showcase

P. falciparum tymidylate kinase + zidovudine

NMR Water-LOGSY and STD experiments





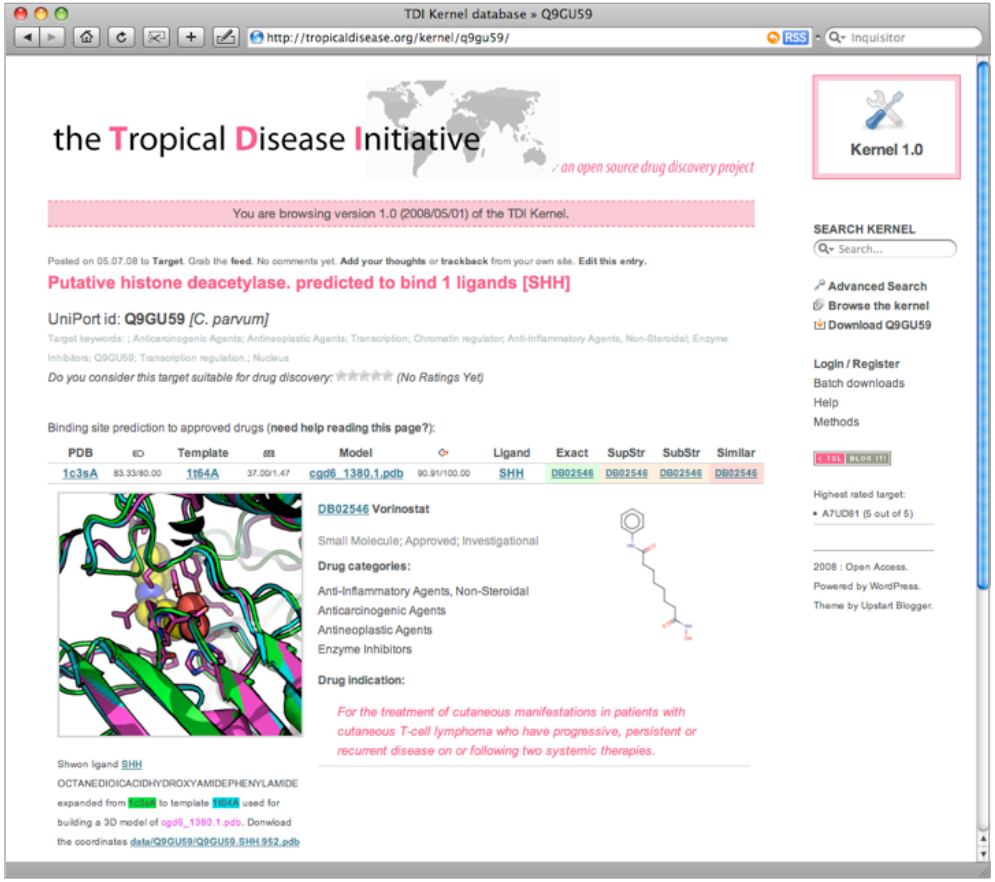


Experimental NRM data from Pineda-Lucena Lab (CIPF)

Showcase

TDI's kernel

http://tropicaldisease.org/kernel



A Kernel for Open Source Drug Discovery in Tropical Diseases

L. Orti *et al.*, *Nat Biotechnol* **27**, 320 (2009)
L. Orti *et al.*, *PLoS Negl Trop Dis* **3**, e418 (2009).

Case Study: Future