
Tools for 3D molecule interactive visualization (115 mins)

— Hugo Samano - Marta Strumillo —

- 1.) Marta - let's play
- 2.) Hugo - let's work

Intro - hands on!

".ent", ".pdb", ".mol", ".xplor", ".mmod", ".ccp4", ".r3d", ".trj" and ".pse".

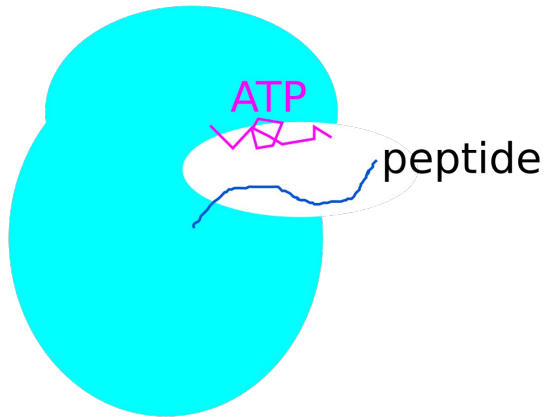
Intro - hands on!

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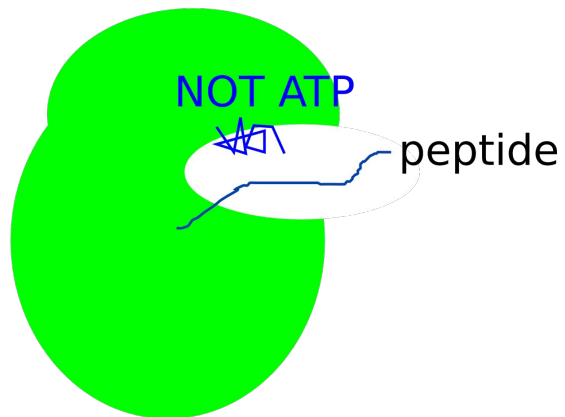
https://sites.google.com/site/afonsomduarte/pymol_tut

What do we have?

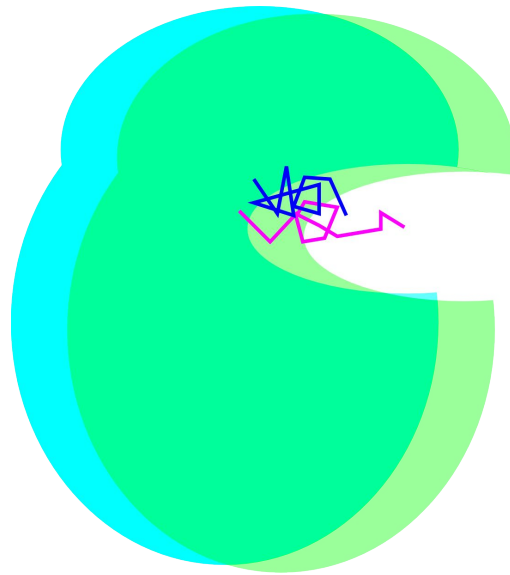
4WB8 (PKA kinase)



3QKL (AKT1 kinase)

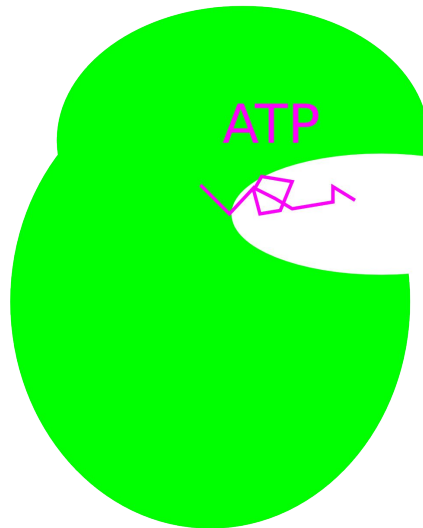


What are we going to do?



What do we want?

3QKL (AKT1 kinase)



Let's go!

Take 4WB8 kinase, and move ATP to 3QKL

4WB8 - how many chains, what's in it

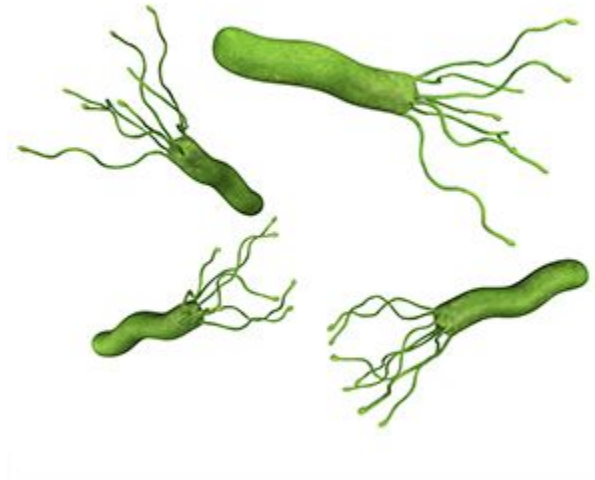
3QKL - how many chains, what's in it

Align, delete 4wb8, but not atp, delete inhibitor, but not 4wb8

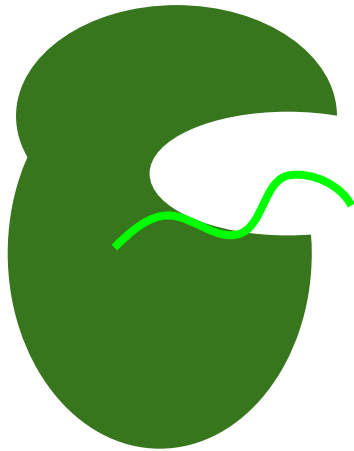
http://www-cryst.bioc.cam.ac.uk/members/zbyszek/figures_pymol best rendering overview

Helicobacter pylori

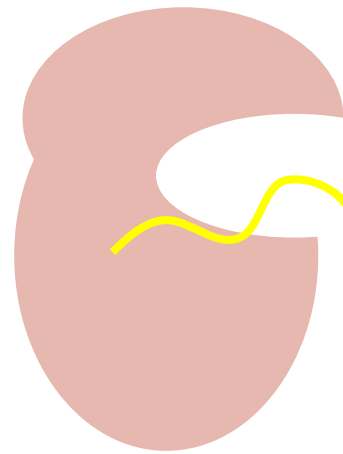
Helicobacter pylori infects more than 50% of the human population
Clinical isolates are categorized as Western or East Asian strains
They differ by polymorphisms in the CagA gene



CagA inhibits a protein kinase

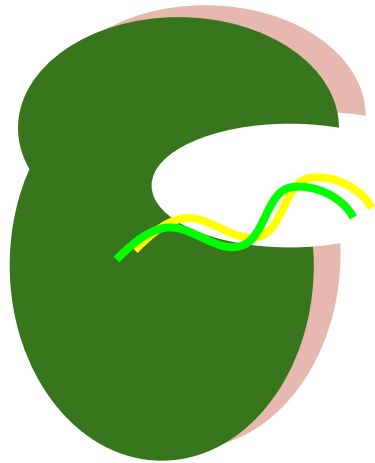


AMPK and PKI
both are endogenous
proteins



Human PAR1 is inhibited
by *Helicobacter pylori*
CagA

CagA inhibits a protein kinase

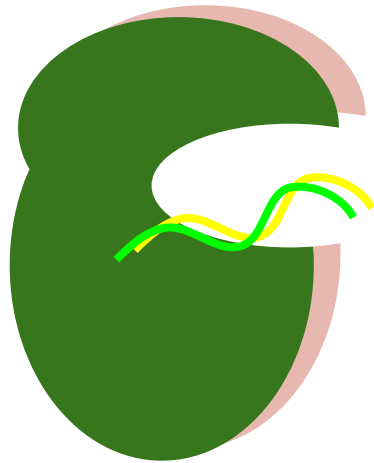


AMPK - PKI
PAR1 - Western CagA

AMPK and PAR1 are structurally very similar

Western CagA mimics PKI in the way it binds to PAR1

CagA inhibits a protein kinase



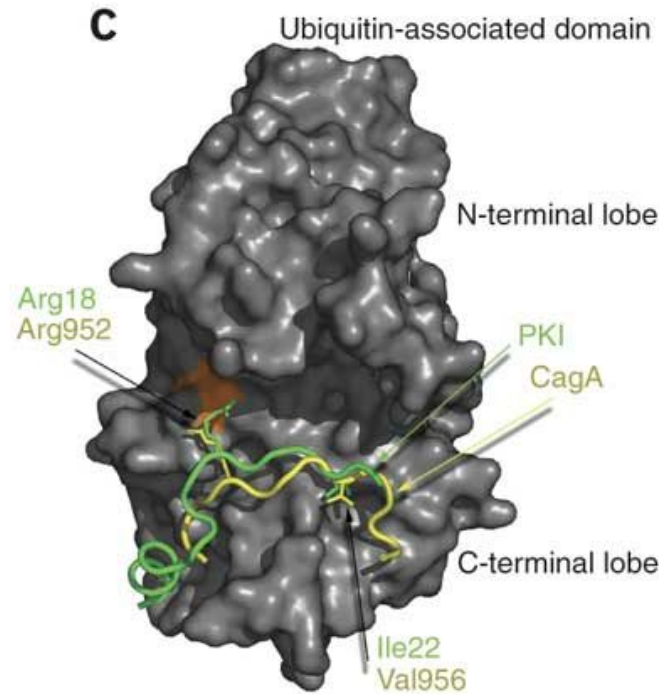
AMPK - PKI
PAR1 - Western CagA

Is this mimicry property exclusive of the Western strain?



East Asian CagA

Modeling by homology



<http://www.nature.com/nsmb/journal/v17/n1/full/nsmb.1705.html>