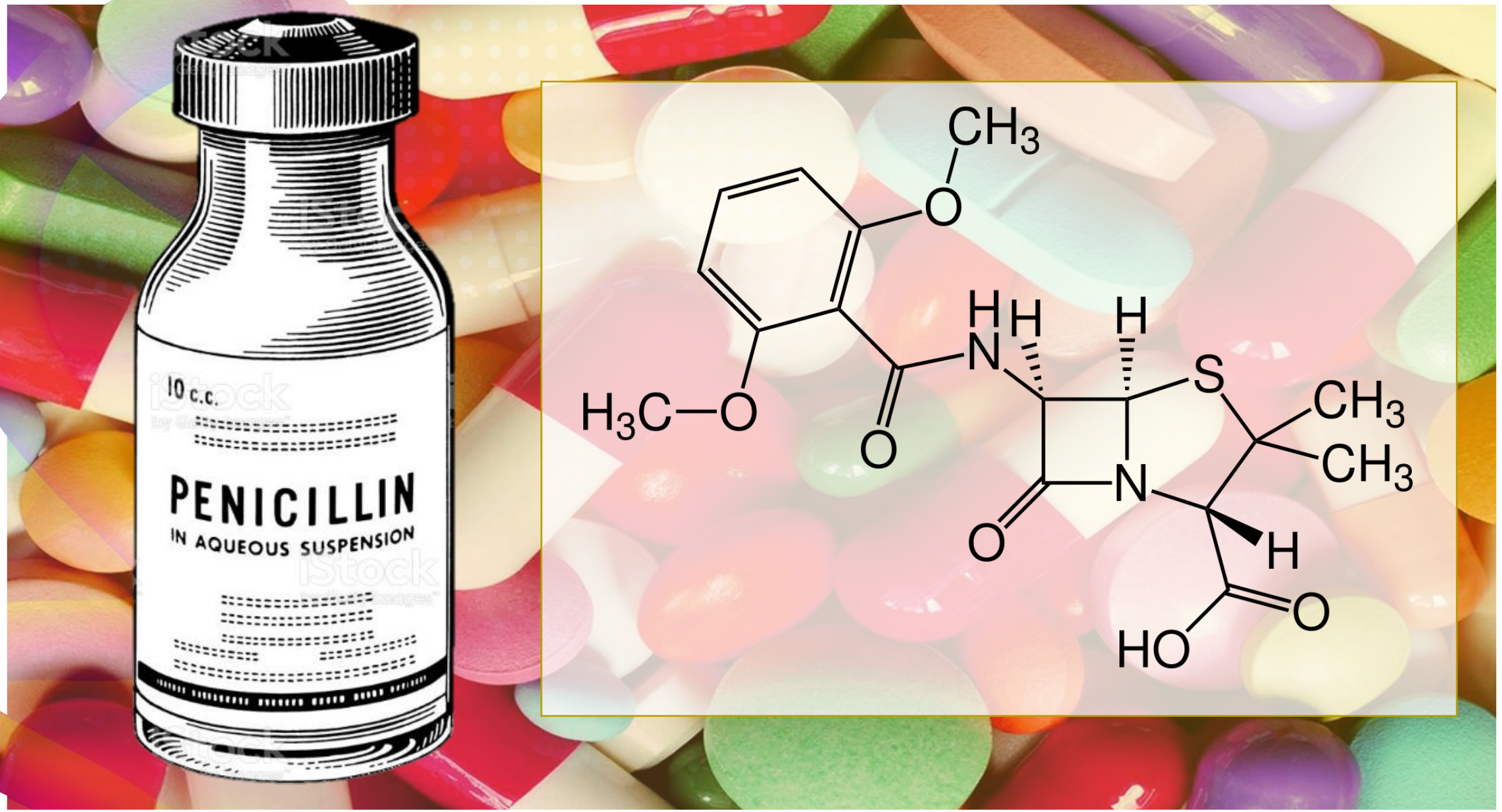
Complemento contra resistencia bacteriana a la meticilina

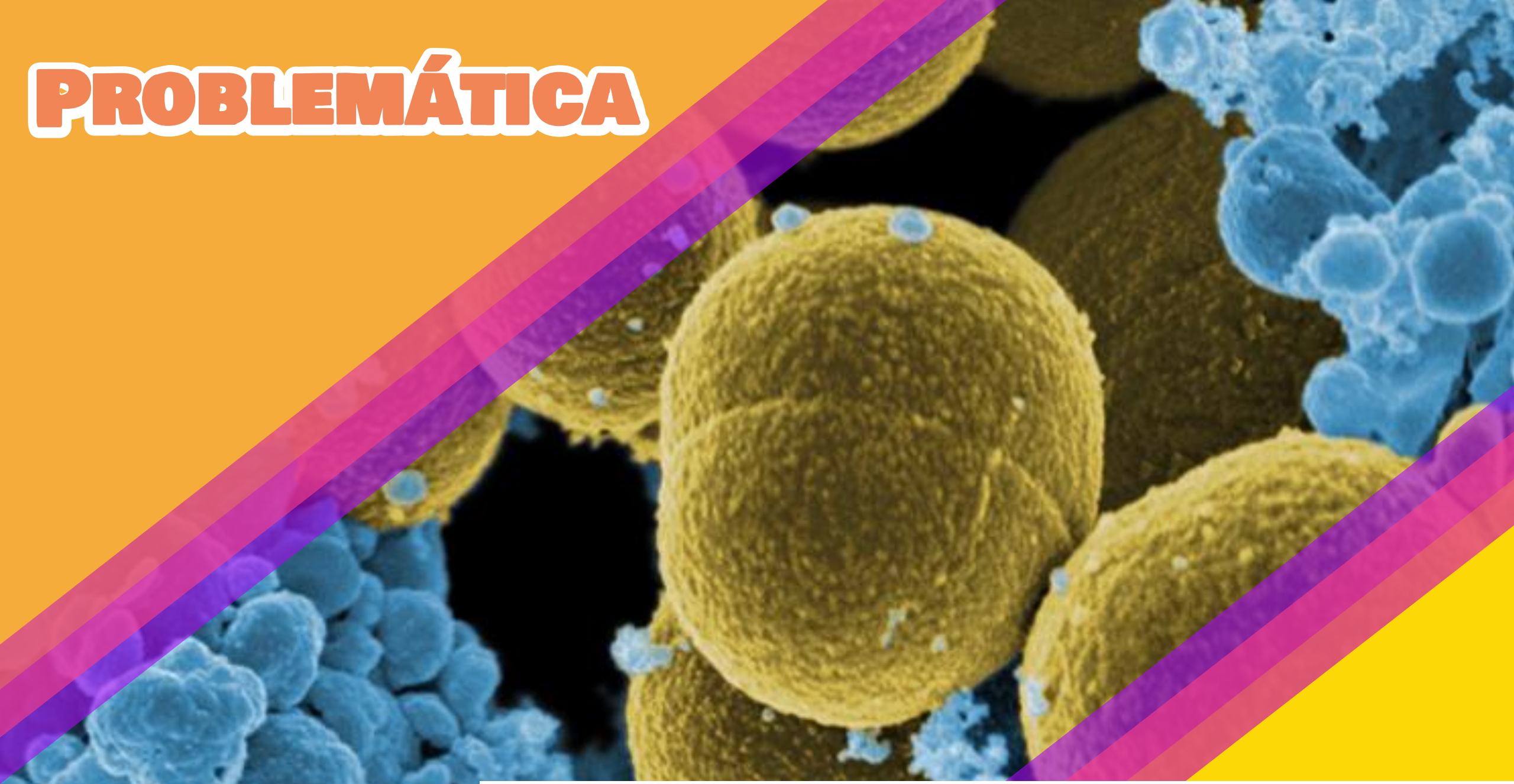
Clubes de Ciencia
México

INTRODUCCIÓN

¿Qué es la penicilina?


10 c.c.
PENICILLIN
IN AQUEOUS SUSPENSION
CH3
O
H3C—O
O
H
N
H
H
S
CH3
CH3
N
O
H
O
HO

PROBLEMÁTICA

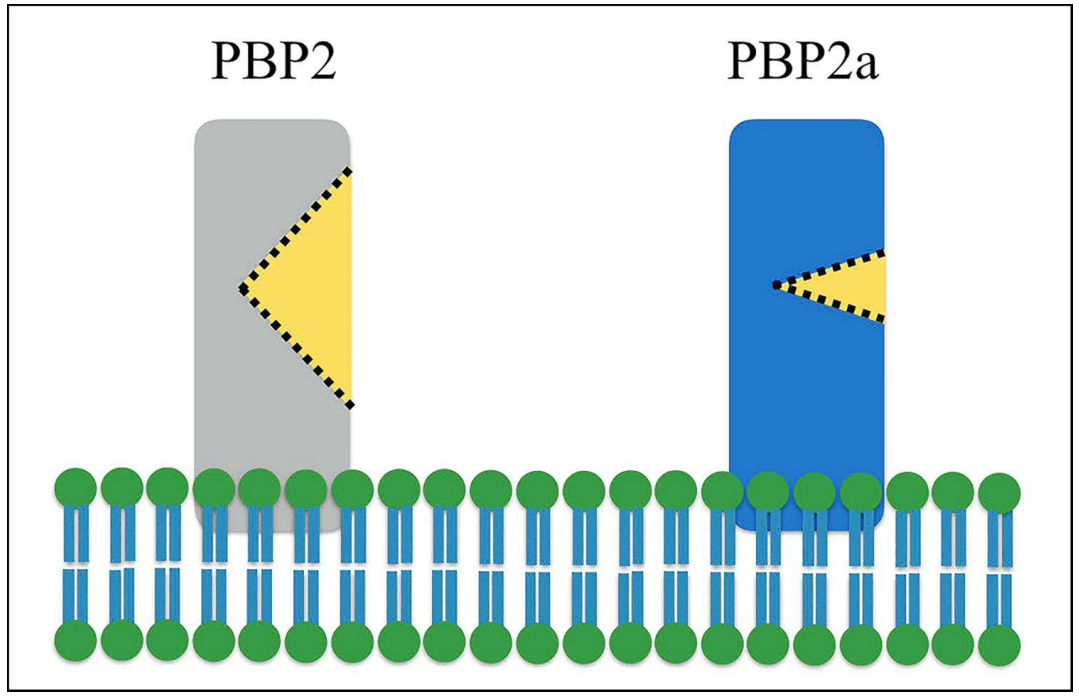


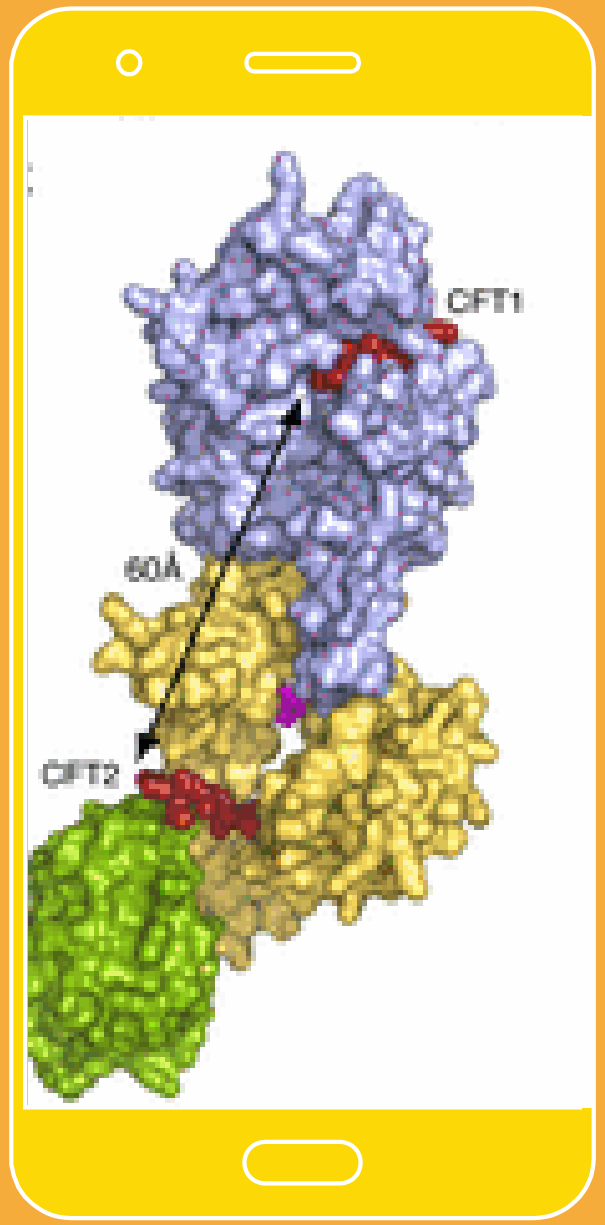
¿Y cuál es el problema con esta bacteria?


Normal air sacs
Inflamed air sacs filled with fluid (pneumonia)
Lungs

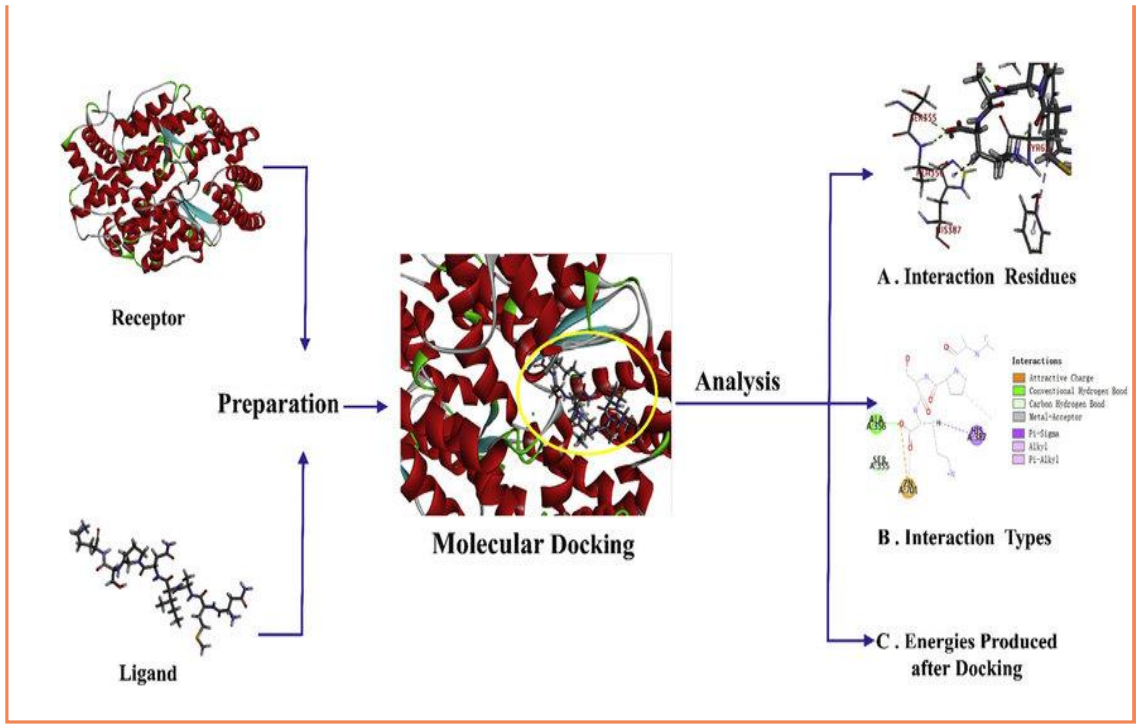
SOBRE LA PBP2A

¿Qué es la proteína PBD2a?





SOBRE EL DOCKING DE PBP2A CON INHIBIDORES



¿Inhibidores...?

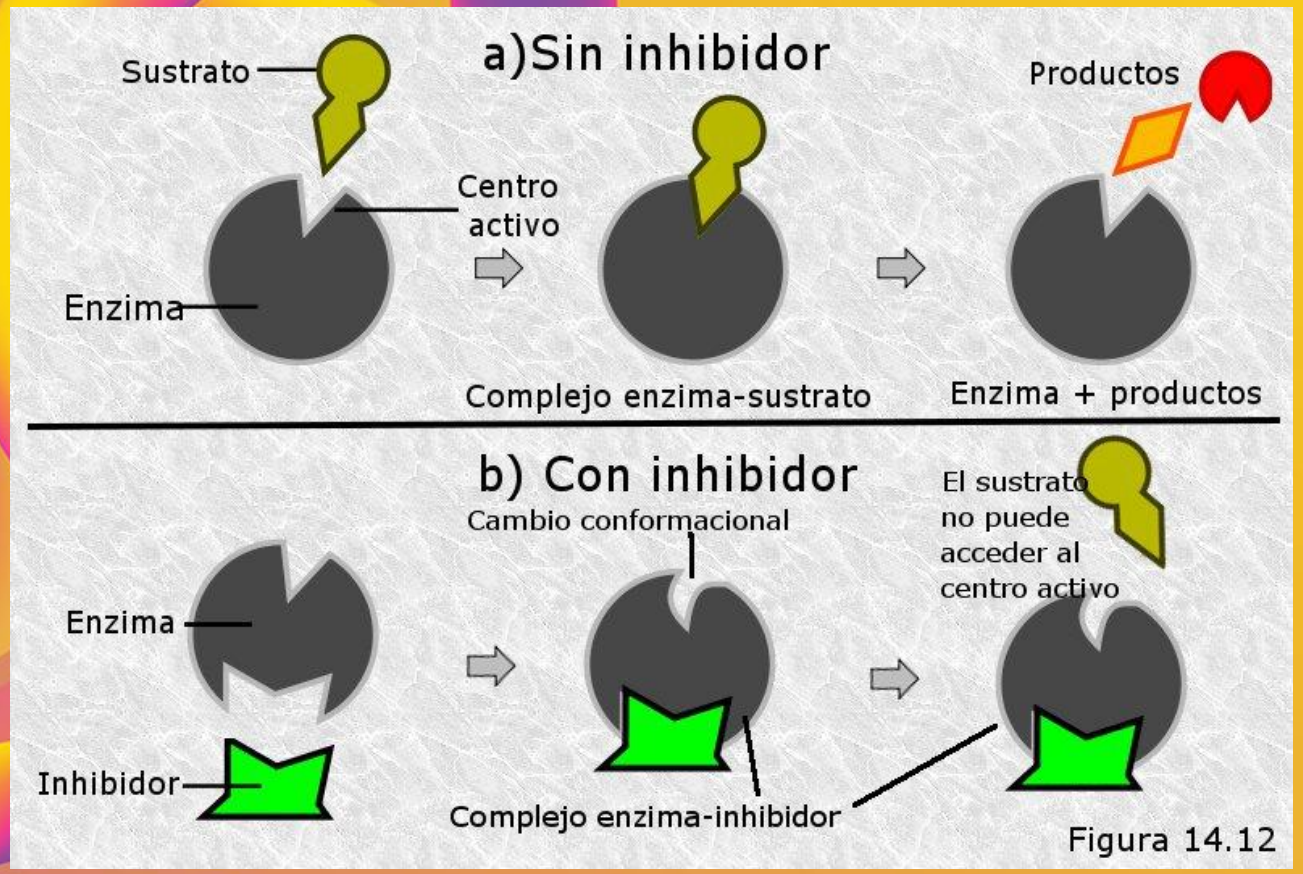
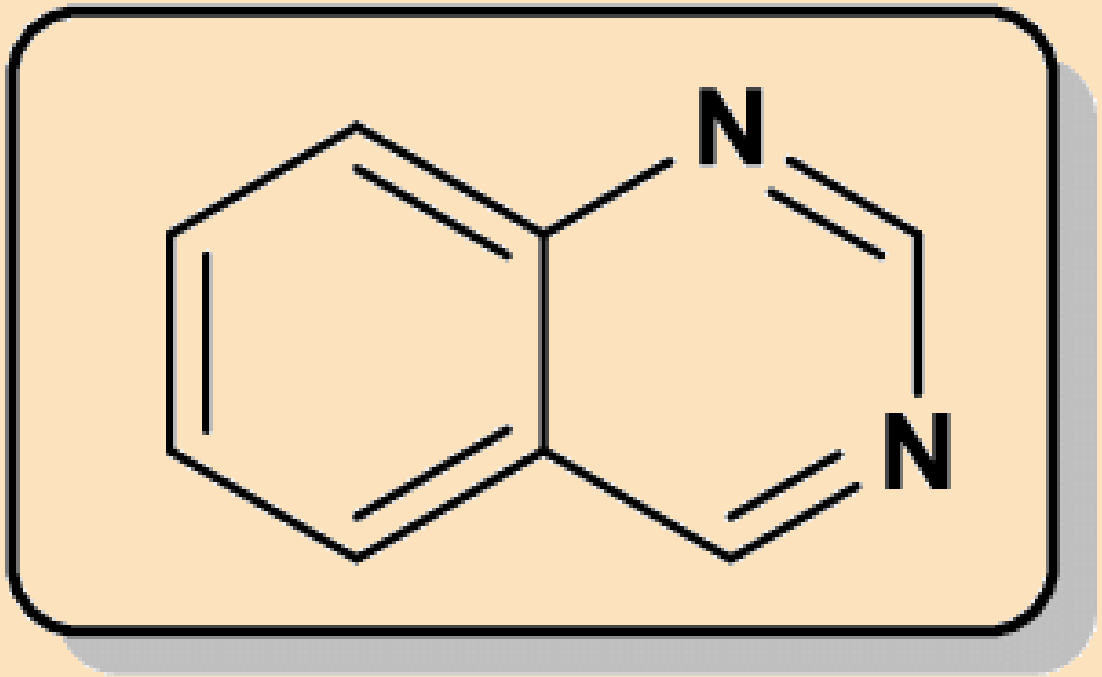
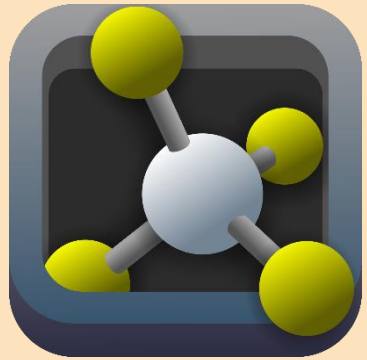

a)Sin inhibidor
Sustrato
Centro activo
Enzima
Productos
Complejo enzima-sustrato
Enzima + productos
b) Con inhibidor
Cambio conformacional
El sustrato no puede acceder al centro activo
Enzima
Inhibidor
Complejo enzima-inhibidor

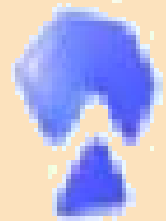
Figura 14.12

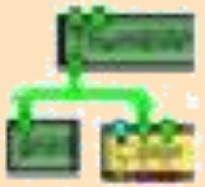

INHIBICIÓN COMPETITIVA
Sitio activo de la enzima
Sustrato
Inhibidor
Productos
El sustrato y el inhibidor pueden unirse al sitio activo
El inhibidor impide la unión del sustrato


INHIBICIÓN NO COMPETITIVA
Sitio Activo
Sitio Inhibidor
Al unirse el inhibidor se distorciona la forma de la enzima
El sustrato y el Inhibidor pueden unirse a la enzima simultáneamente
En ausencia del inhibidor, los productos pueden ser formados
La presencia del inhibidor enlentece la velocidad de la formación del producto





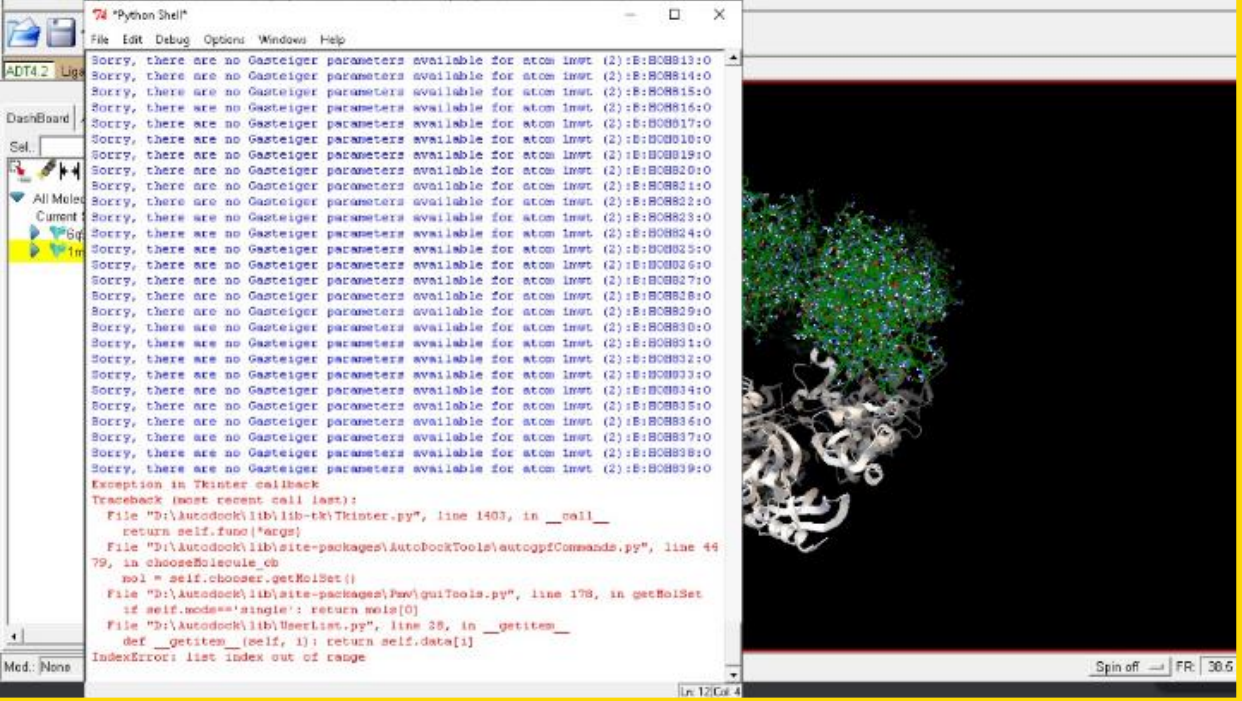




¿Qué proponemos nosotros?

- **Proponemos emplear el inhibidor Quinazolinona alostérica como inhibidor de la expresión de la enzima.**

- **Se utiliza pyMol para la representación gráfica de las enzimas y moléculas y para la simulación del docking AutoDockTools**


Python Shell
File Edit Debug Options Windows Help
Sorry, there are no Gasteiger parameters available for atom lmwt (2):B:HOH813:O
Sorry, there are no Gasteiger parameters available for atom lmwt (2):B:HOH814:O
Sorry, there are no Gasteiger parameters available for atom lmwt (2):B:HOH815:O
Sorry, there are no Gasteiger parameters available for atom lmwt (2):B:HOH816:O
Sorry, there are no Gasteiger parameters available for atom lmwt (2):B:HOH817:O
Sorry, there are no Gasteiger parameters available for atom lmwt (2):B:HOH818:O
Sorry, there are no Gasteiger parameters available for atom lmwt (2):B:HOH819:O
Sorry, there are no Gasteiger parameters available for atom lmwt (2):B:HOH820:O
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Sorry, there are no Gasteiger parameters available for atom lmwt (2):B:HOH828:O
Sorry, there are no Gasteiger parameters available for atom lmwt (2):B:HOH829:O
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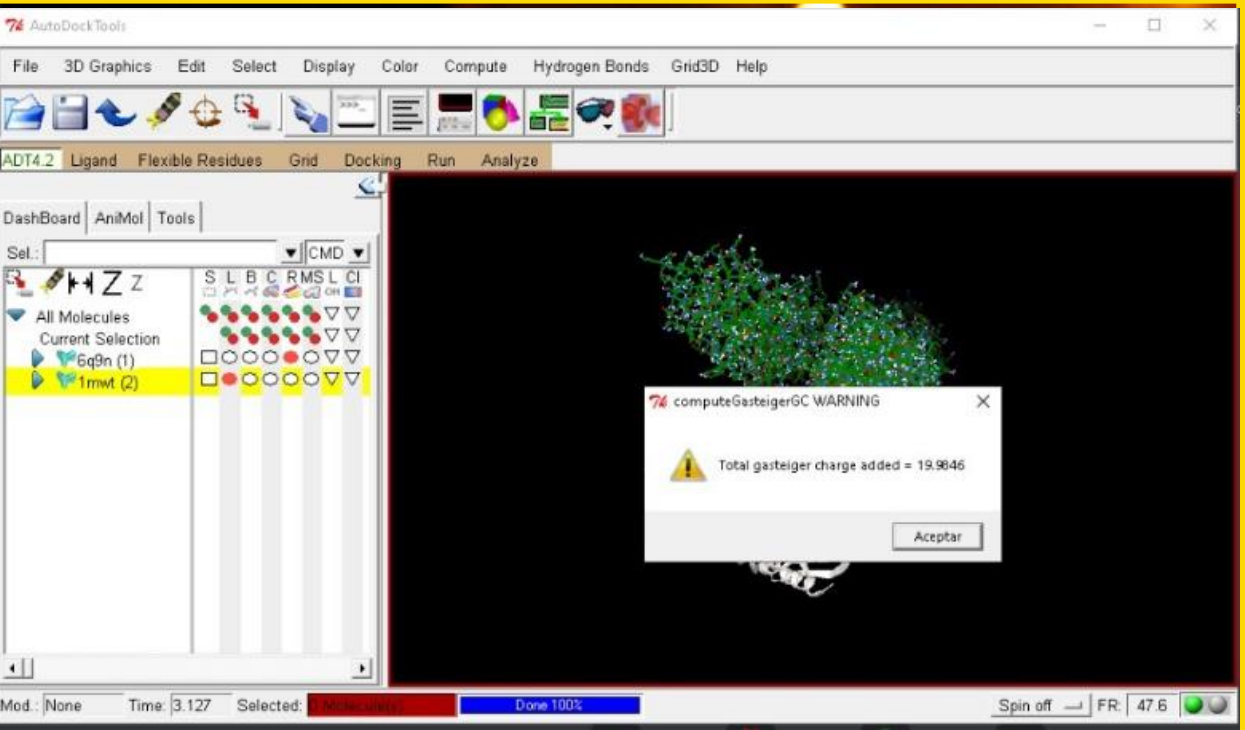
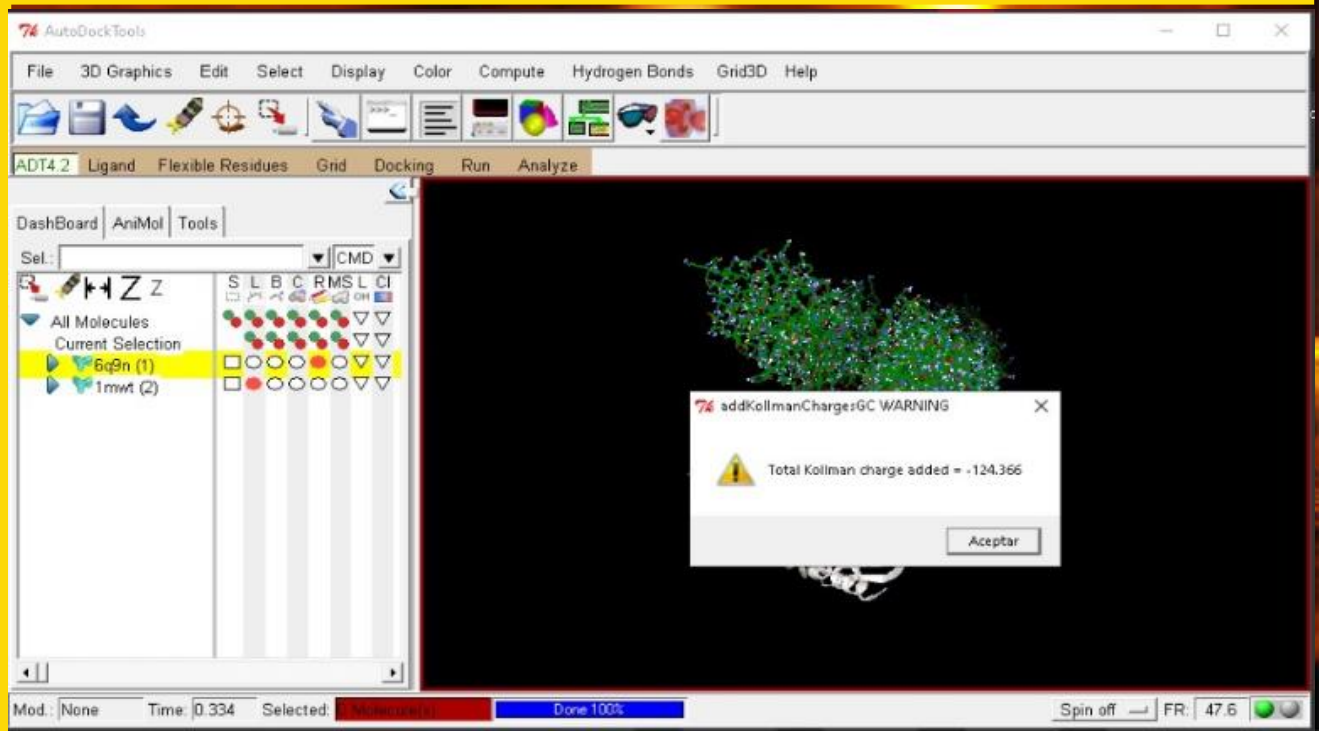
Sorry, there are no Gasteiger parameters available for atom lmwt (2):B:HOH838:O
Sorry, there are no Gasteiger parameters available for atom lmwt (2):B:HOH839:O
Exception in Tkinter callback
Traceback (most recent call last):
File "D:\Autodock\lib\lib-tk\Tkinter.py", line 1403, in __call__
return self.func(*args)
File "D:\Autodock\lib\site-packages\AutoDockTools\autogpfCommands.py", line 44
79, in chooseMolecule_cb
mol = self.chooser.getMolSet()
File "D:\Autodock\lib\site-packages\Pmw\guiTools.py", line 178, in getMolSet
if self.mode=='single': return mols[0]
File "D:\Autodock\lib\UserList.py", line 28, in __getitem__
def __getitem__(self, i): return self.data[i]
IndexError: list index out of range
Ln: 12 Col: 4
ADT4.2 Ligand Flexible Residues Grid Docking Run Analyze
DashBoard AniMol Tools
Sel.:
CMD
All Molecules
Current Selection
6q9n (1)
1mwt (2)
Mod.: None
Time: 61.306
Selected:
Done 100%
Spin off
FR: 43.6


AutoDockTools
File 3D Graphics Edit Select Display Color Compute Hydrogen Bonds Grid3D Help
ADT4.2 Ligand Flexible Residues Grid Docking Run Analyze
DashBoard AniMol Tools
Sel.:
CMD
All Molecules
Current Selection
6q9n (1)
1mwt (2)
computeGasteigerGC WARNING
Total gasteiger charge added = 19.9846
Aceptar
Mod.: None
Time: 3.127
Selected:
Done 100%
Spin off
FR: 47.6


AutoDockTools
File 3D Graphics Edit Select Display Color Compute Hydrogen Bonds Grid3D Help
ADT4.2 Ligand Flexible Residues Grid Docking Run Analyze
DashBoard AniMol Tools
Sel.:
CMD
All Molecules
Current Selection
6q9n (1)
1mwt (2)
addKollmanChargesGC WARNING
Total Kollman charge added = -124.366
Aceptar
Mod.: None
Time: 0.334
Selected:
Done 100%
Spin off
FR: 47.6