VPython Drug Design

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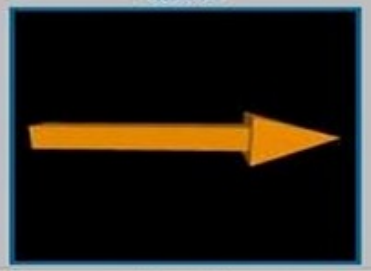
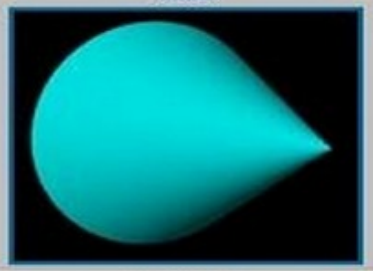
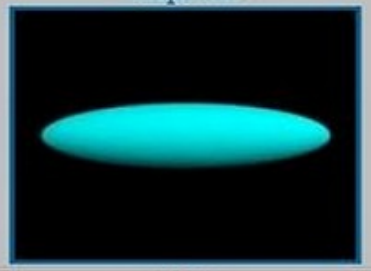
David Scherer invented Vpython while an undergrad at CMU

The VPython 3D Objects (click for details)

arrow 	box 	cone 
convex 	curve 	cylinder 
ellipsoid 	faces 	helix 
label 	points 	pyramid 
ring 	sphere 	frame Group objects together

Hello World

Physics in Action

Bouncing Ball

Gas atoms

use of Numpy and Graphing

Controls and Lambda Functions

```
button(pos=(-40,-20),height=20,width=50,text='COPY',
    action=lambda: atomcopy())
```

Virtual Worlds

Ligand Design

A Few Terms

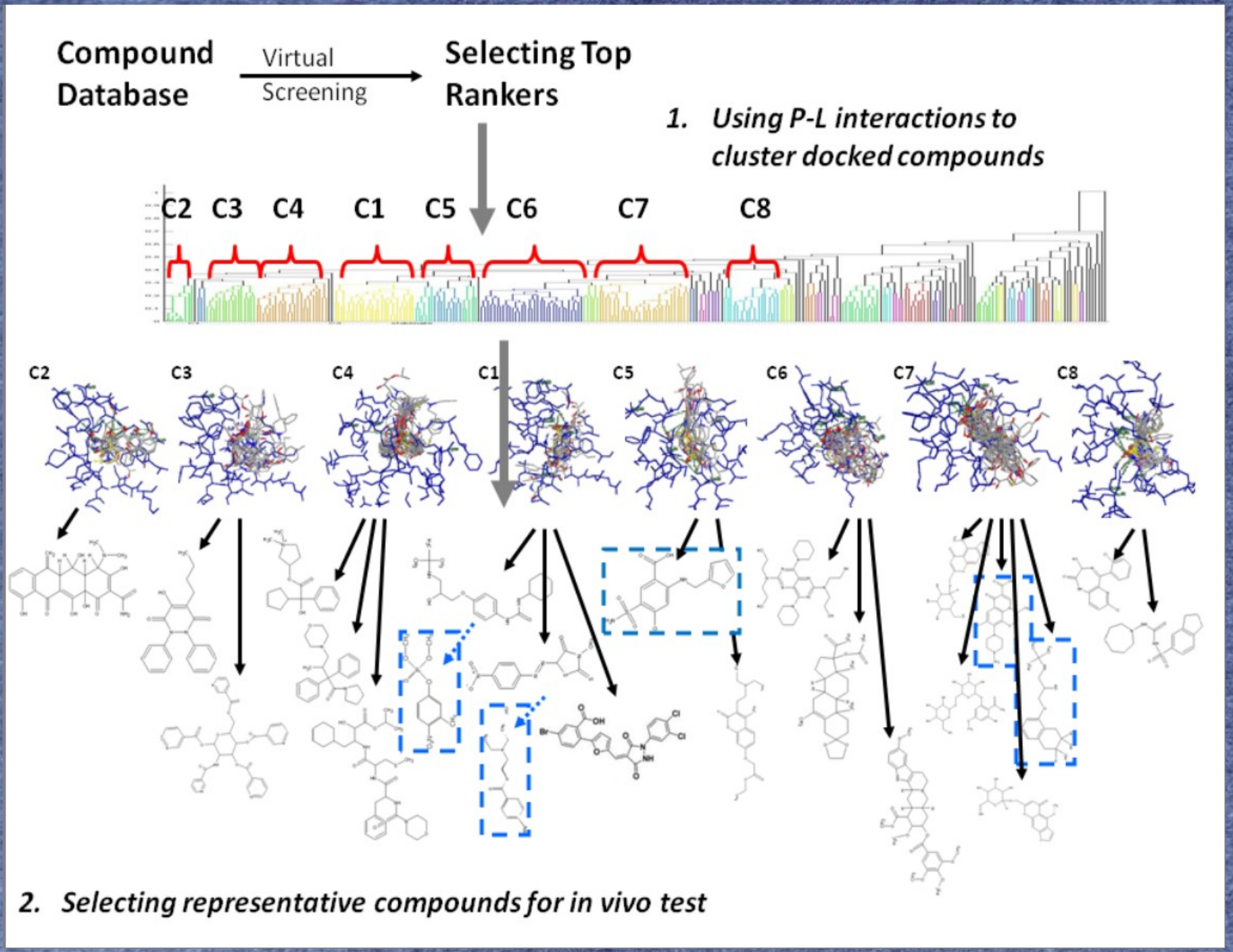
Drug / Ligand

Receptor

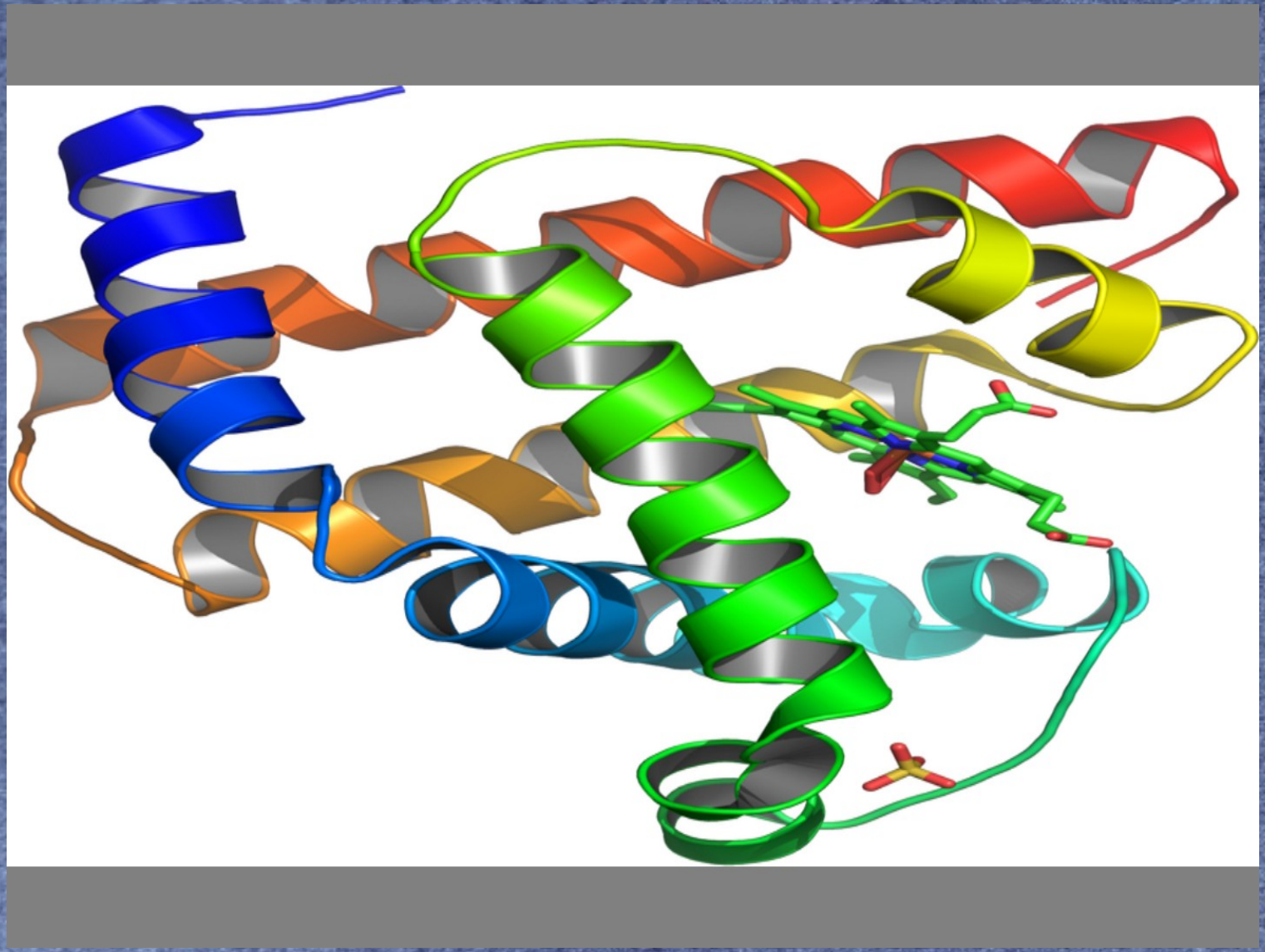
Docking

Drug Design in the past

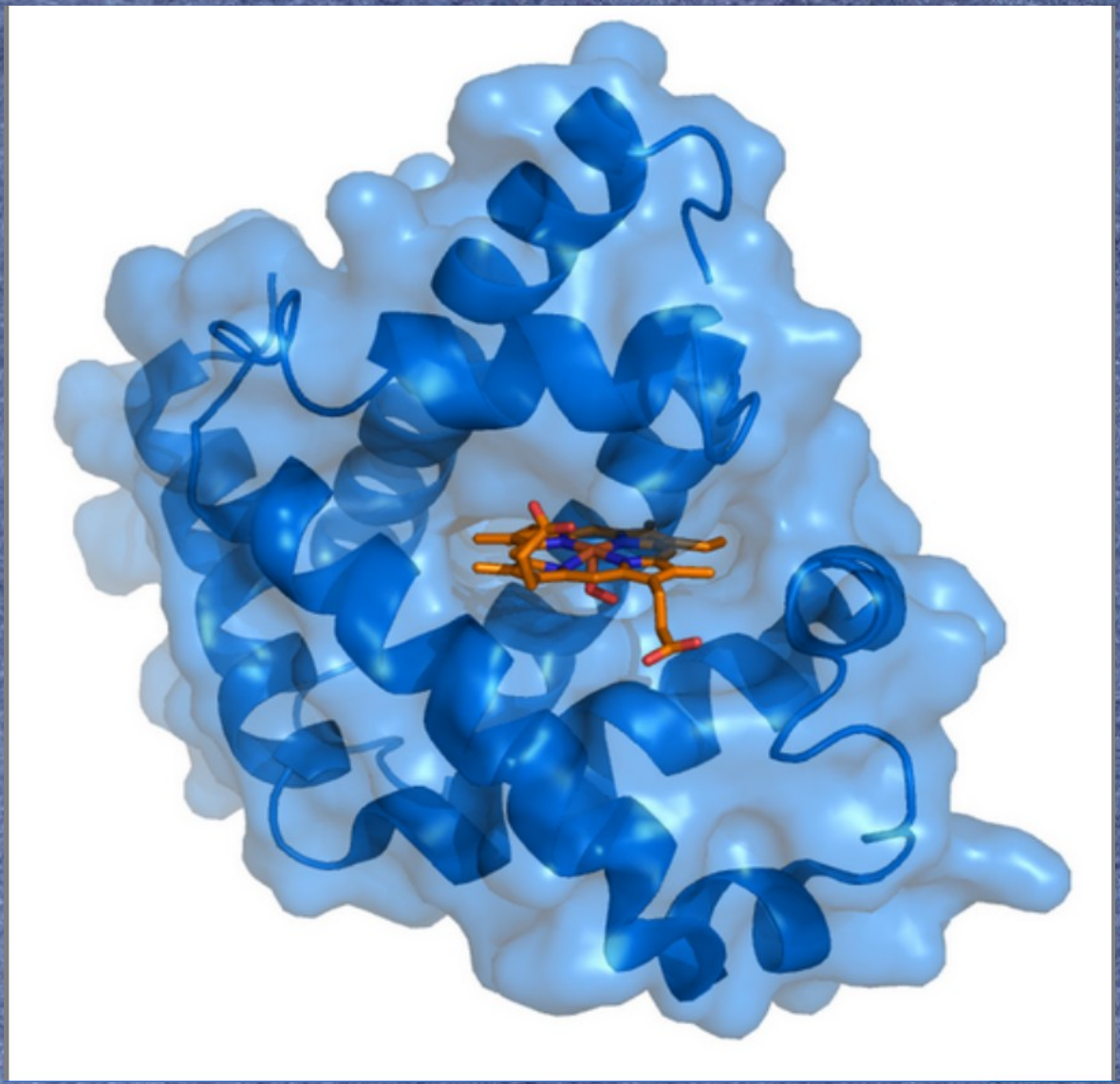
1. Random
2. Statistical


Compound Database
Virtual Screening
Selecting Top Rankers
1. Using P-L interactions to cluster docked compounds
C2 C3 C4 C1 C5 C6 C7 C8
C2 C3 C4 C1 C5 C6 C7 C8
2. Selecting representative compounds for in vivo test

X-ray crystallography

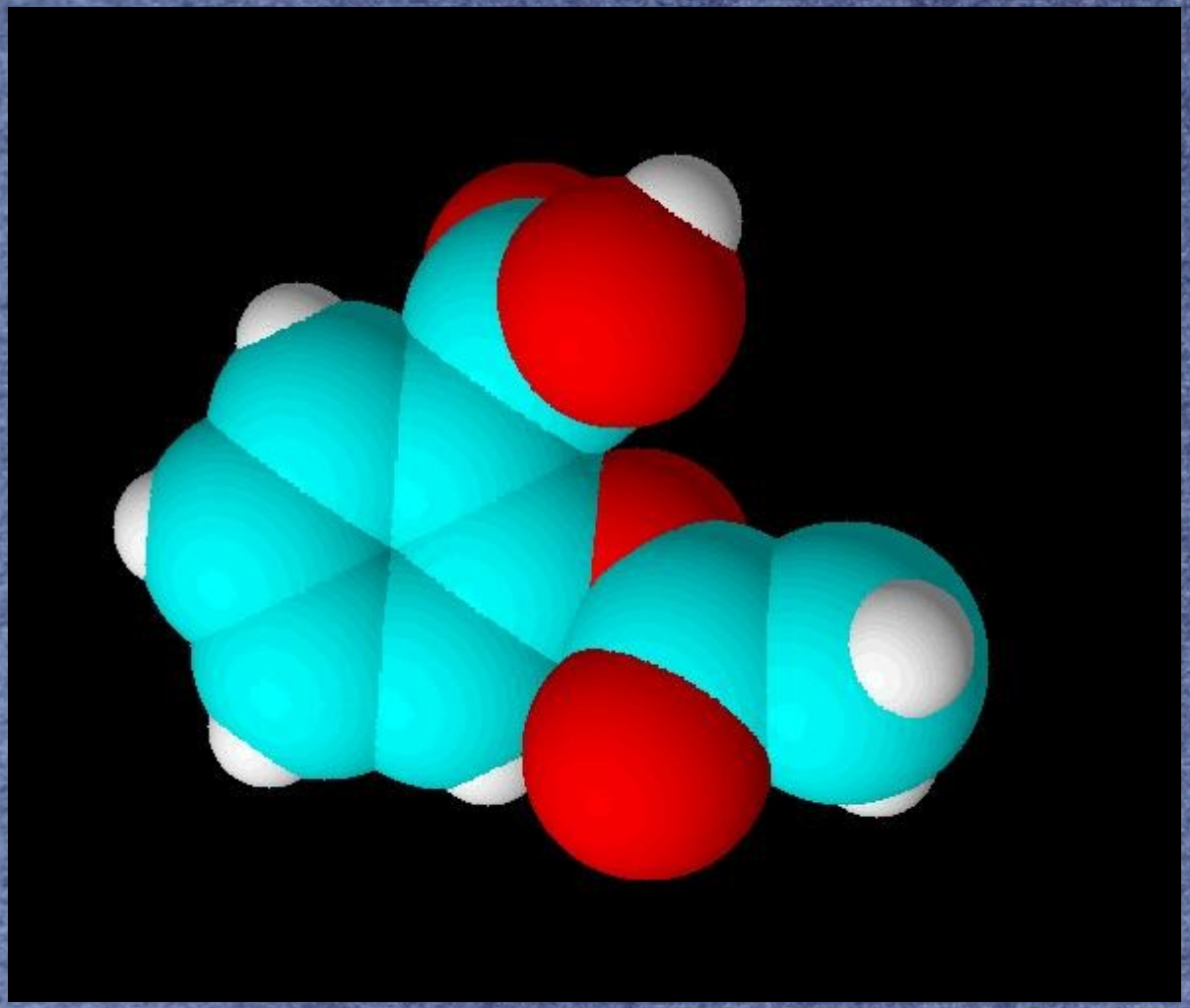


Ligand Docking

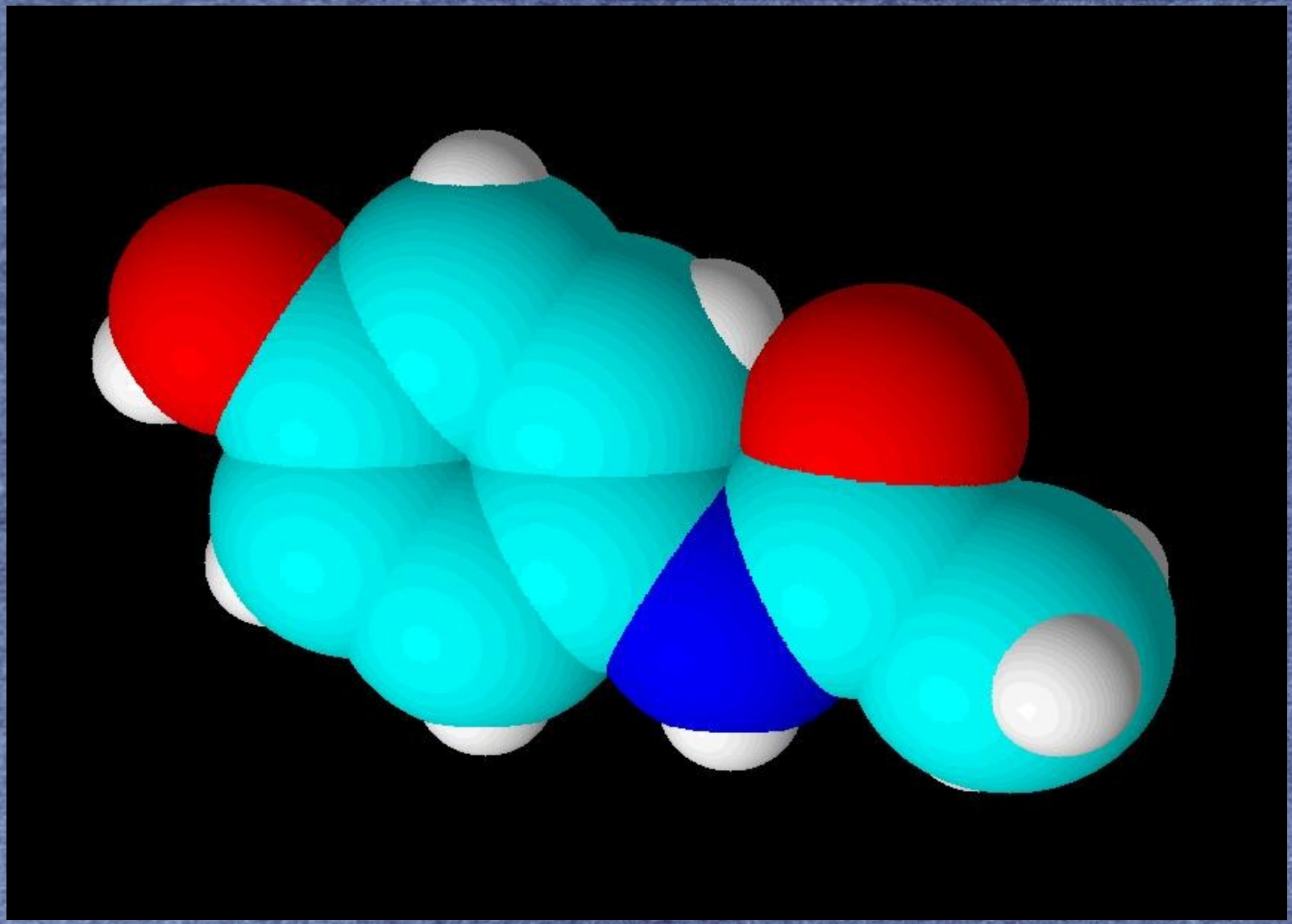


Common Drugs and their Atomic Structure

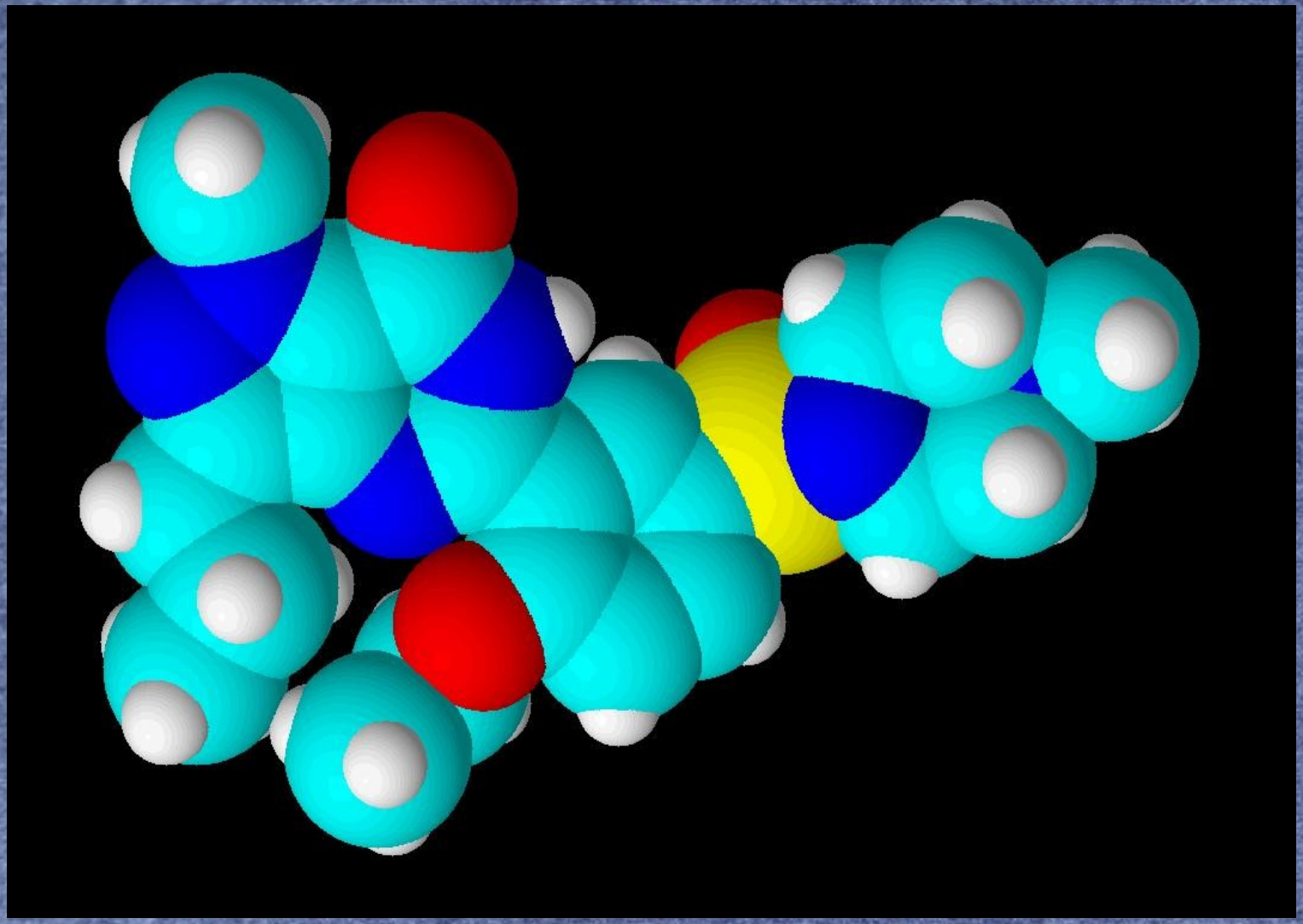
Aspirin



Paracetamol



Viagra



Demo

Problems

1. Docking versus Performance
2. Accuracy of the model
3. Search Space

Questions?

Thank You!