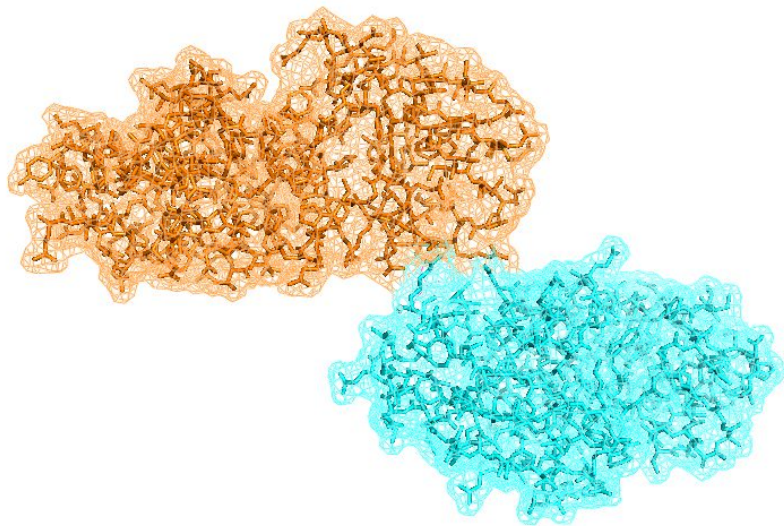# Scoring Group 1: Paula's angels

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Meet-U

PROJET COLLABORATIF
PARIS 6 - PARIS 7 - PARIS 11 - EVRY
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université
PARIS DIDEROT
PARIS 7
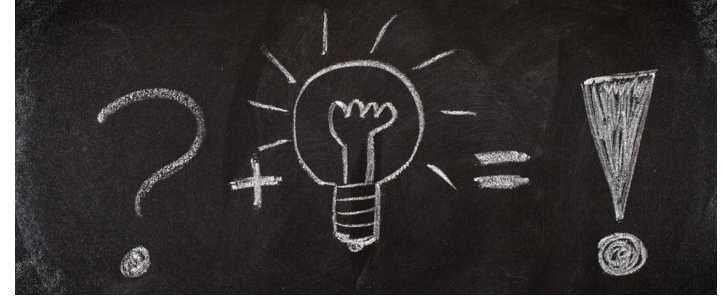
Philosophy

General scoring function

1° – **One filter** to clear up the list of pdb using **Fast Fourier Transform**

2° – Selected pdb are sorted by different scores:

- Knowledge based
- **Electrostatic** and **Van der WaAls** interactions

weight of each evaluation:

- Refine using tons of native structures and decoys
- Machine learning approaches

FILTER

Calcul of **residue depth** using 'ResidueDepth function' a MSMS library from MGlTools

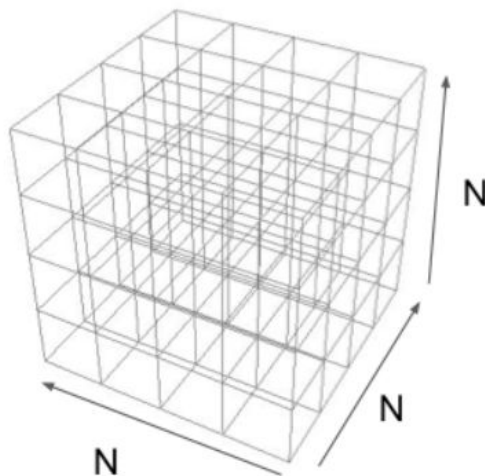**surface residues** are placed in a **grid** for both

"receptor" and "ligand" according to their

coordinates

Remove "wrong pdb" with **steric conflicts**

Allows to avoid to score some "unrealistic" docking

→ **Already coded !**

Knowledged based scoring

Electrostatic and Van der WaAls interactions

Calculation **distance** between all **residues in surface** of the two proteins

determination of the **contact interface** according to a maximal distance between two residues belonging to different proteins

calculation of Electrostatic and Van der WaAls interactions considering the **Cβ for all residues** except for glycine Cα
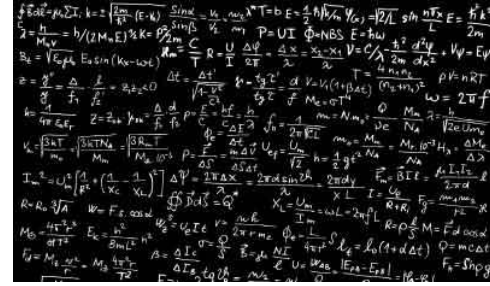
"Home made" calculations

Sorting each pdb regarding to the **liaison free energy**

In progress: Evaluation of adding more energy terms such as entropy, torsion, ... using FoldX software

FoldX

(possibly others too !)

Conclusion

General scoring function

Two steps functionality : Filter then scoring

Scoring based on energy and knowledge based approach

<u>Work in progress :</u>

- WRAP code
- Evaluation of our results
- adding others parameters ?
- MAchine-learning