Design of a program to evaluate the performance of a 3D protein model

DOPE
(Discrete Optimized ProteinEnergy)

- Min-yi Shen and Andrej Sali
- statistical potential used to assess homology models in protein structure prediction
- Implemented in Python and run within the MODELLER environnement

Example of a DOPE score profil

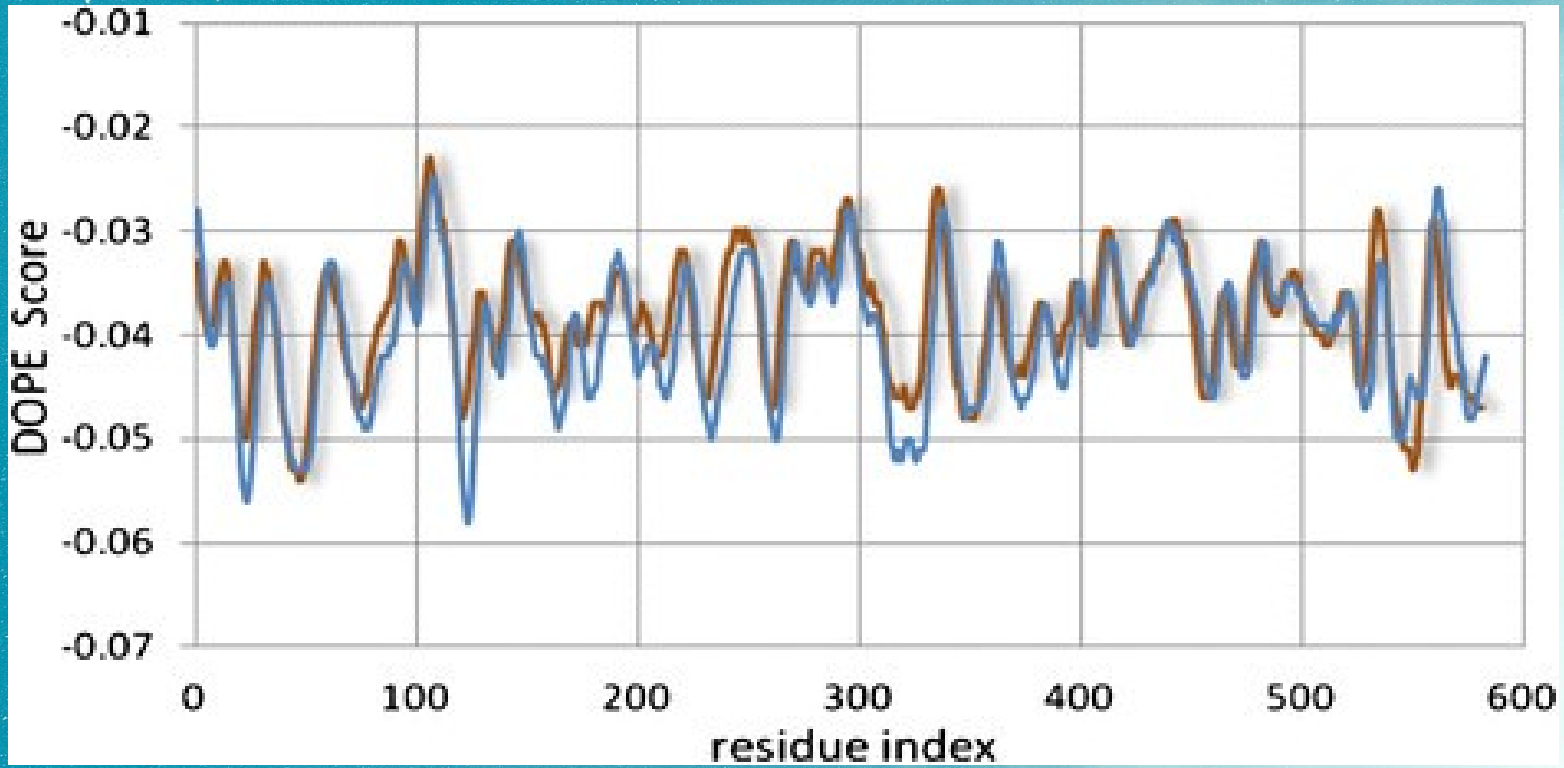

Figure 1 : Analysis of DOPE score profile of Human albumin from « *Computational investigation of inhibitory mechanism of flavonoids as bovine serum albumin anti-glycation agents » by M. Amanlou and A. Johari*

Method

- 1) Parsing of the pdb file
- 2) Calculate the distances between alpha carbons
- 3) Associate an energy to the pairs of AA according to their distance and sum them up
- 4) Using a z-score, compare to a reference result

Results

```
Enter pdb name
1n5u.pdb
energies cumulées = -1213.5199999999325
Calcul du z-score
z_score = -357.08029197077826
```

- Figure 2 : Example of resultst for the Albumin 1n5u

- Negative z-score
- Maximum wait for result : 15 sec