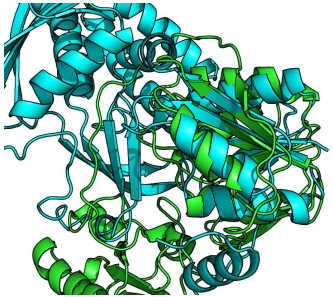
Meet-U
a meeting story

université PARIS DIDEROT PARIS 7

Upstream team Group 2



Daniel DE MURAT, **Madeleine** DE SOUSA VIOLANTE, **Mei-shiue** KUO, **Sonia** TIEO

Introduction

- **Problematic:** Find the most probable/stable 3D fold adopted by the protein in solution, given a protein primary sequence

- The project has **two steps**:
    - (*i*) domain annotation based on profile-profile comparison
    - (*ii*) identification of the most stable 3D fold by threading.

Psi-blast + Mafft alignment

PSI-BLAST 2.2.31+ vs
Uniref90

QUERY (fasta) :
ETF-alpha
(307 res)

Psipred

Output
PSI-BLAST

1	A	C	0.998	0.001	0.003
2	V	E	0.420	0.012	0.495
3	L	E	0.176	0.018	0.756
4	L	E	0.171	0.063	0.702
5	L	C	0.430	0.076	0.390
6	G	C	0.350	0.255	0.325
7	E	E	0.174	0.118	0.646
8	V	E	0.279	0.067	0.638
9	T	C	0.562	0.217	0.281

Homologs Sequences extraction
+ Multiple alignment: MAFFT

Psi-blast + Mafft alignment

PSI-BLAST 2.2.31+ vs Uniref90

Output PSI-BLAST

Homologs Sequences extraction + Multiple alignment: MAFFT

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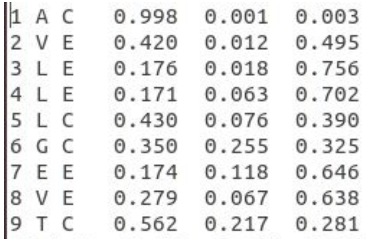

```
1 A C   0.998  0.001  0.003
2 V E   0.420  0.012  0.495
3 L E   0.176  0.018  0.756
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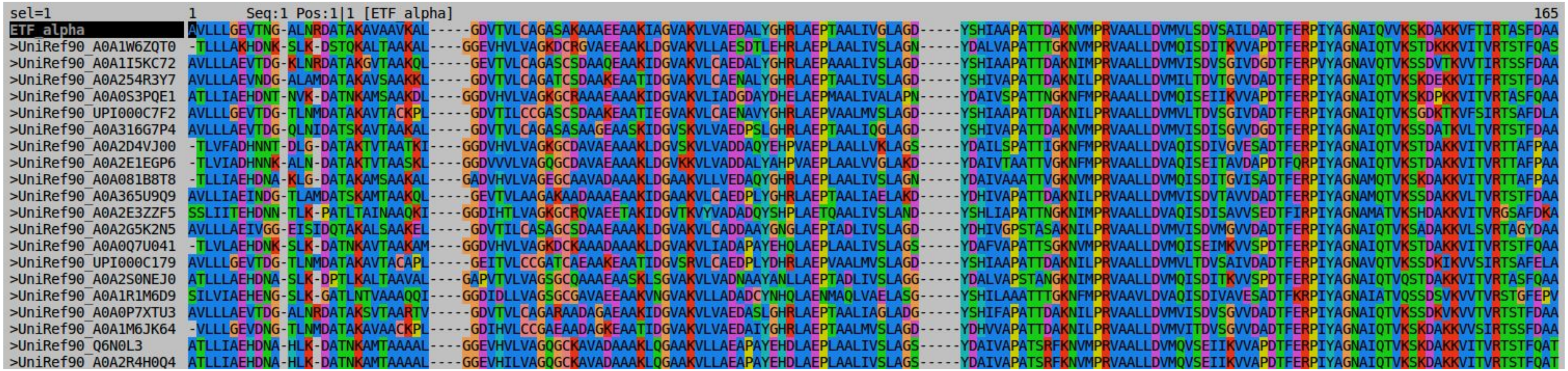
```



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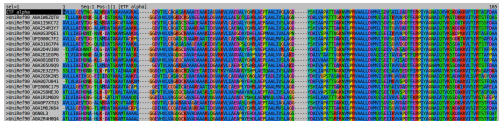
Matrix Construction

Multiple Alignement

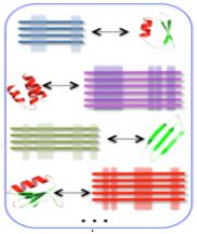


Profil

Profil creation

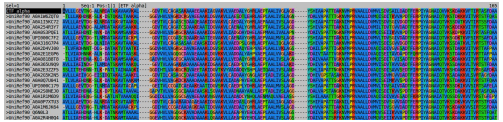
Profil : Matrix length of the input x 24 columns (20 amino acids + 1 gap + 3 secondary structure prediction : C, H et E)

HOMSTRAD DATABASE + Psipred



Matrix Construction

Multiple Alignement



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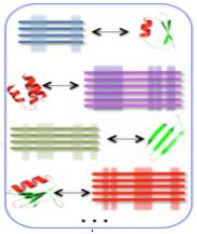

Profil

ETF_alpha

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0.299315 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.144565 0.025000 0.025000 0.025000 0.025000	0.106055	0.998 0.001 0.003
0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.211475 0.025000 0.025000 0.025000 0.025000 0.025000 0.028515 0.086155 0.025000 0.025000 0.258710	0.015080	0.420 0.012 0.495
0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.524935 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000	0.000000	0.176 0.018 0.756
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0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.025000 0.345515 0.065925 0.028560 0.025000 0.030910 0.025000 0.025000 0.025000 0.032185 0.025000 0.028330 0.143510	0.000000	0.279 0.067 0.638
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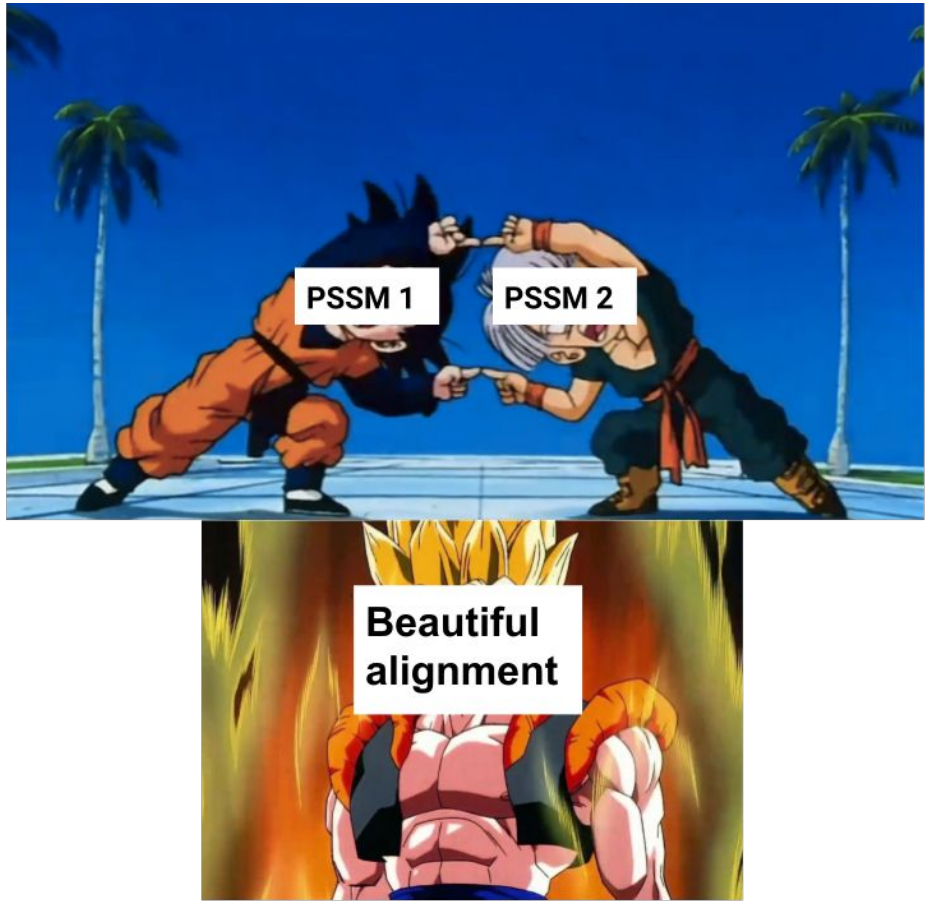
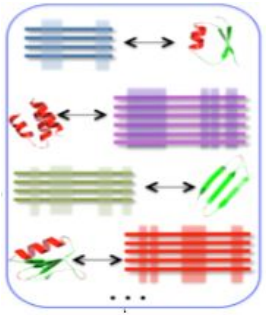
Profile-Profile Comparison



Profile-Profile Comparison

profil-profil alignment
semi-global (**dot product** & **Pearson correlation**)



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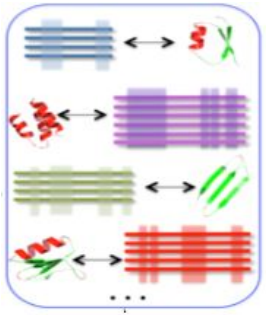

File: **.foldrec**

*** HITS RANKED ***

SEQUENCE QUERY FILE : ETF_alpha, 307

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1	183.7905	X	X	X	X	X	X	X	X	X	X	Arginosuc_synth
2	182.5134	X	X	X	X	X	X	X	X	X	X	PGI
3	181.479	X	X	X	X	X	X	X	X	X	X	Glu_syn_central
4	181.2363	X	X	X	X	X	X	X	X	X	X	aldedh
5	180.5341	X	X	X	X	X	X	X	X	X	X	chorismate_bind
6	180.4503	X	X	X	X	X	X	X	X	X	X	psaA_psaB
7	179.8043	X	X	X	X	X	X	X	X	X	X	Trypan_glycop
8	178.3679	X	X	X	X	X	X	X	X	X	X	DNA_photolyase
9	177.9143	X	X	X	X	X	X	X	X	X	X	ATP-synt
10	177.5459	X	X	X	X	X	X	X	X	X	X	Ald_Xan_dh_2
11	177.4527	X	X	X	X	X	X	X	X	X	X	COX1
12	177.0703	X	X	X	X	X	X	X	X	X	X	Sec23_NC
13	176.9332	X	X	X	X	X	X	X	X	X	X	cytochrome_b
14	176.9118	X	X	X	X	X	X	X	X	X	X	CODH
15	176.3796	X	X	X	X	X	X	X	X	X	X	Sec1
16	175.7833	X	X	X	X	X	X	X	X	X	X	Gly_radical
17	175.3281	X	X	X	X	X	X	X	X	X	X	6PGD
18	175.2631	X	X	X	X	X	X	X	X	X	X	PK
19	173.8668	X	X	X	X	X	X	X	X	X	X	lipoxygenase
20	173.6621	X	X	X	X	X	X	X	X	X	X	AFOR
21	173.2912	X	X	X	X	X	X	X	X	X	X	RNA_dep_RNA_pol
22	173.2841	X	X	X	X	X	X	X	X	X	X	alk_phosphatase
23	173.2703	X	X	X	X	X	X	X	X	X	X	PAP2
24	172.8111	X	X	X	X	X	X	X	X	X	X	pgk
25	171.8797	X	X	X	X	X	X	X	X	X	X	lyase_1

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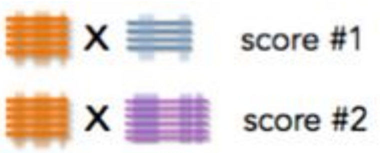

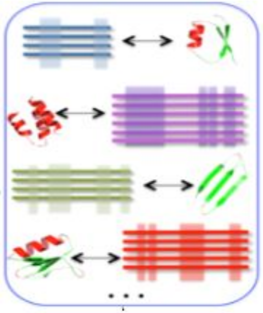

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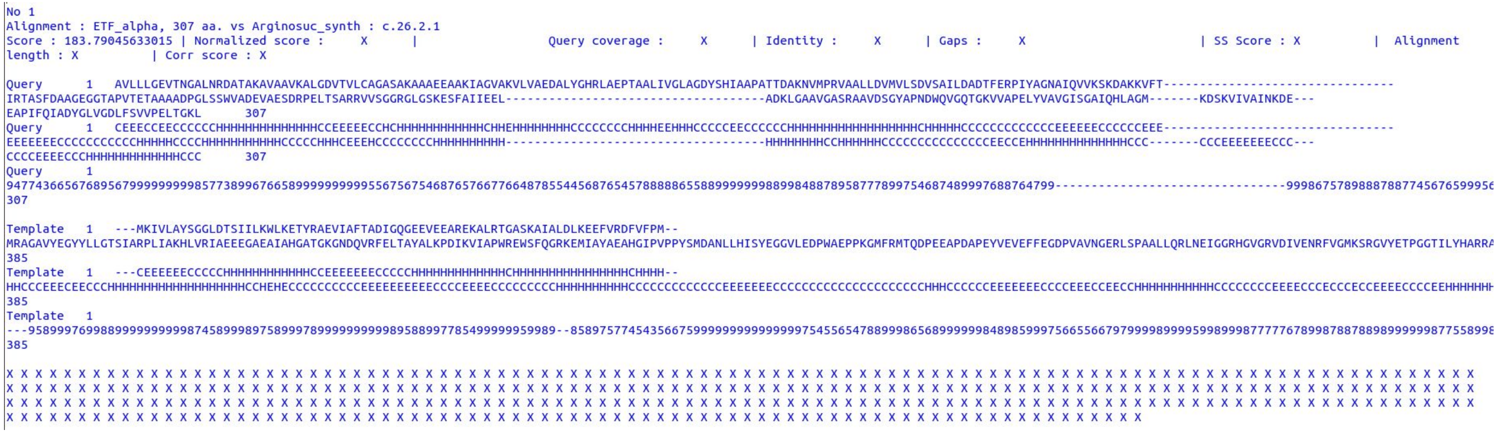

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No 1
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length : X          | Corr score : X

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EAPIFQIADYGLVGDLFSVVPELTGKL      307
Query      1   CEEECCEECCCCCCHHHHHHHHHHHHHHHCCEEEEECCHCHHHHHHHHHHHHHCHHEHHHHHHHHHCCCCCCCHHHHEEHHHCCCCCEECCCCCCHHHHHHHHHHHHHHHHHHHCHHHHHCCCCCCCCCCCCCEEEEEECCCCCCEEE-------------------------------
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CCCCEEEECCCHHHHHHHHHHHHHCCC      307
Query      1
947743665676895679999999999857738996766589999999999995567567546876576677664878554456876545788888655889999999889984887895877789975468748999768876 4799-------------------------------9998675789888788774567659995e
307

Template   1   ---MKIVLAYSGGLDTSIILKWLKETYRAEVIAFTADIGQGEEVEEAREKALRTGASKAIALDLKEEFVRDFVFPM--
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385
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385
Template   1
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385

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```

Query - First Template Aligment

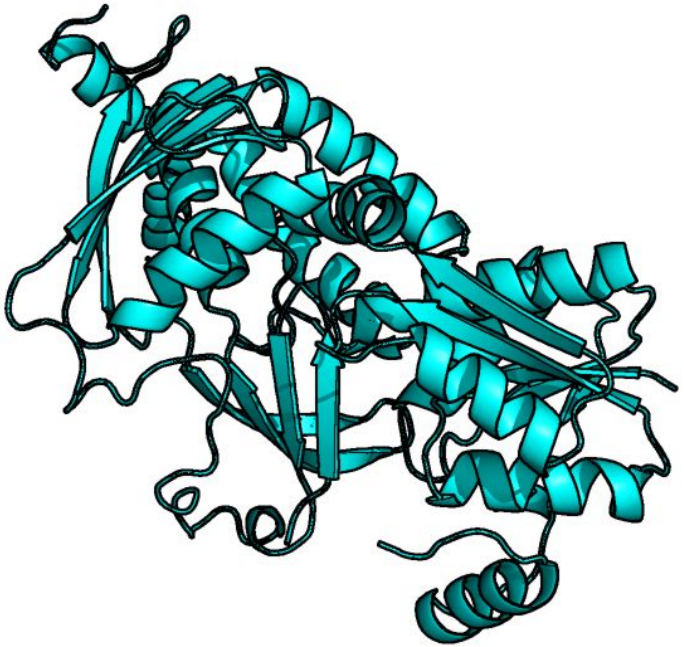
ETF-alpha

```
4 LLGEVTNGALNRDATAKAVAAVKALGDVTVLCAGASAKAAAEEAAKIAGVAKVLVAEDALYGHRLAEPTAALIVGLAGDYSHIAAPATTDAKNVMPRVAALLDVM
  VLSDVSAILDADTFERPIYAGNAIQVVKSKDAKKVF----------------------------------------TIRTASFDAAGEGGTAPVTETAAAADP
  G--------------------LSSWVADEVAESDRPELTSARRVVSGGRGL--------GSKESFAIIEELADKLGAAVGASRAAVDSGYAPNDWQVGQTGKVVA
  PELYVAVGISGAIQHLAG------MKDSKVIVAINKDE--EAPIFQIADYGLVGDLFSVVPELTGKL 307
```

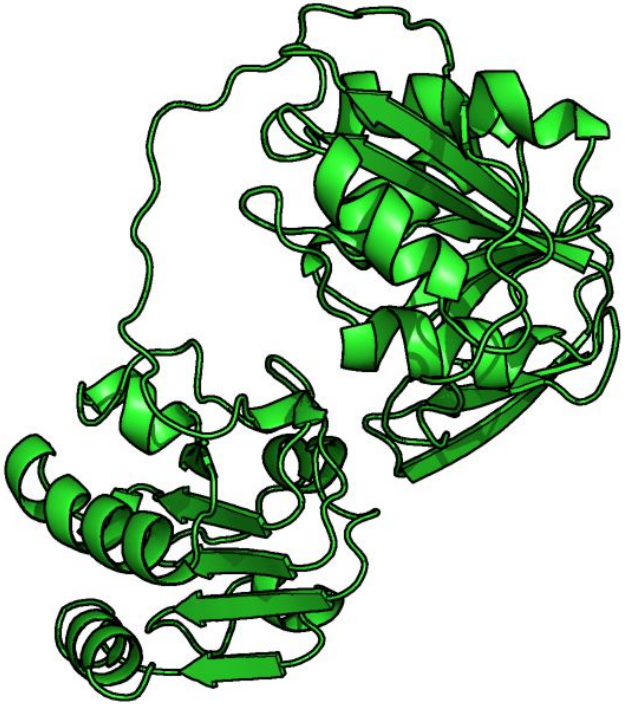
Arginosuc_synth

```
1 MKIVLAYSGGLDTSIILKWLKETYRAEVIAFTADIGQGEEVEEAREKALRTGASKAIALDLKEEFVRDFVFP--MMRAGAVYEGYYLLGTSIARPLIAKHLVRIA
  EEEGAEAIAHGATGKGNDQVRFELTAYALKPDIKVIAPWREWSFQGRKEMIAYAEAHGIPVPPYSMDANLLHISYEGGVLEDPWAEPPKGMFRMTQDPEEAPDAP
  EYVEVEFFEGDPVAVNGERLSPAALLQRLNEIGGRHGVGRVDIVENRFVGMKSRGVYETPGGTILYHARRAVESLTLDREVLHQRDMLSPKYAELVYYGFWYAPE
  REALQAYFDHVARSVTGVARLKLYKGNVYVVGRKAPKSLYRGYDQKDAEGFIKIQALRLRVRALVER 380
```

Structures of Query and First Template

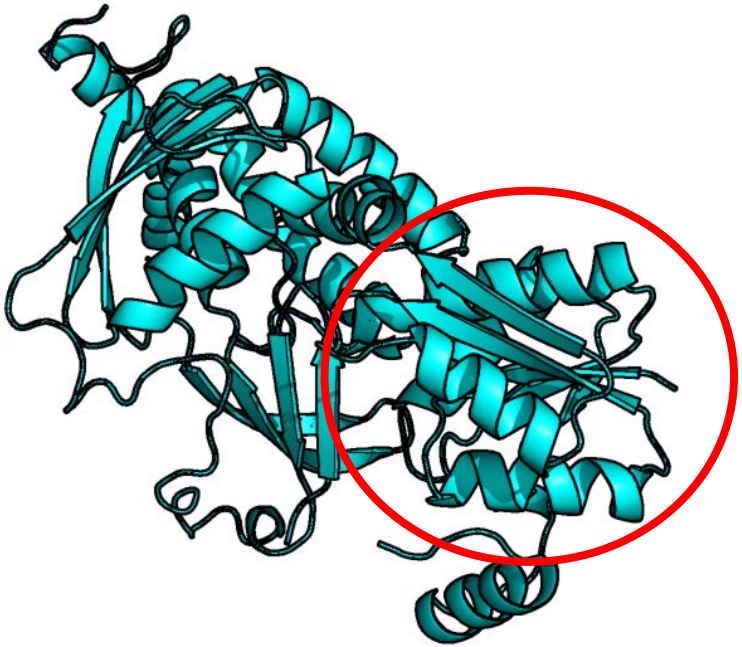


Arginosuc_synth

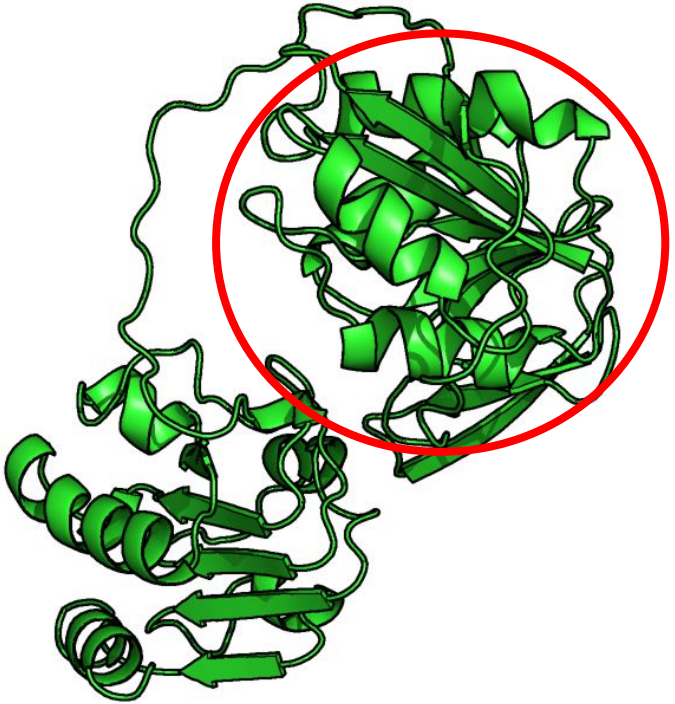


ETF-alpha

Structures of Query and First Template



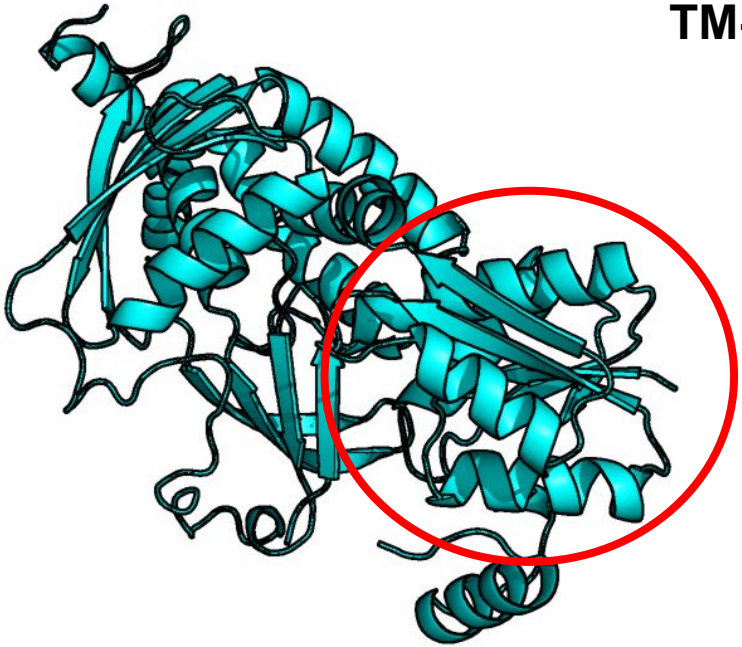
Arginosuc_synth



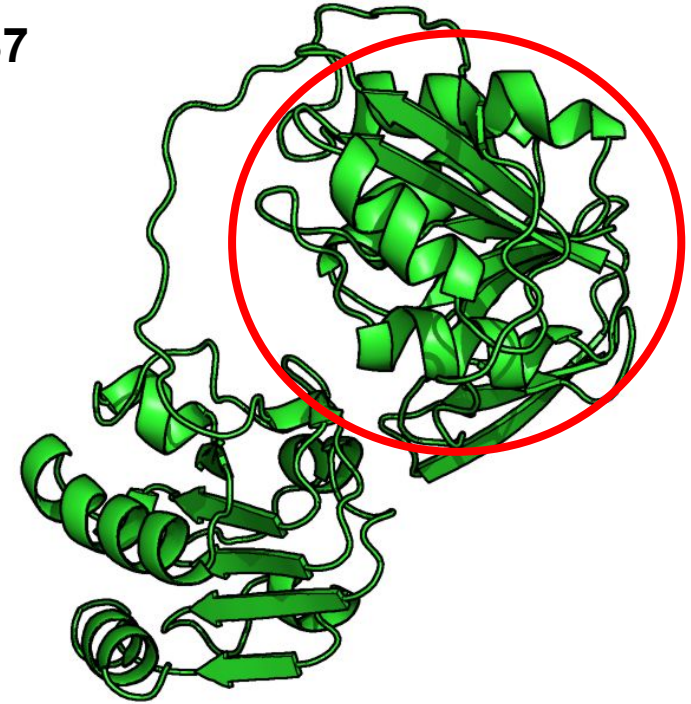
ETF-alpha

Structures of Query and First Template

TM-score = 0.37

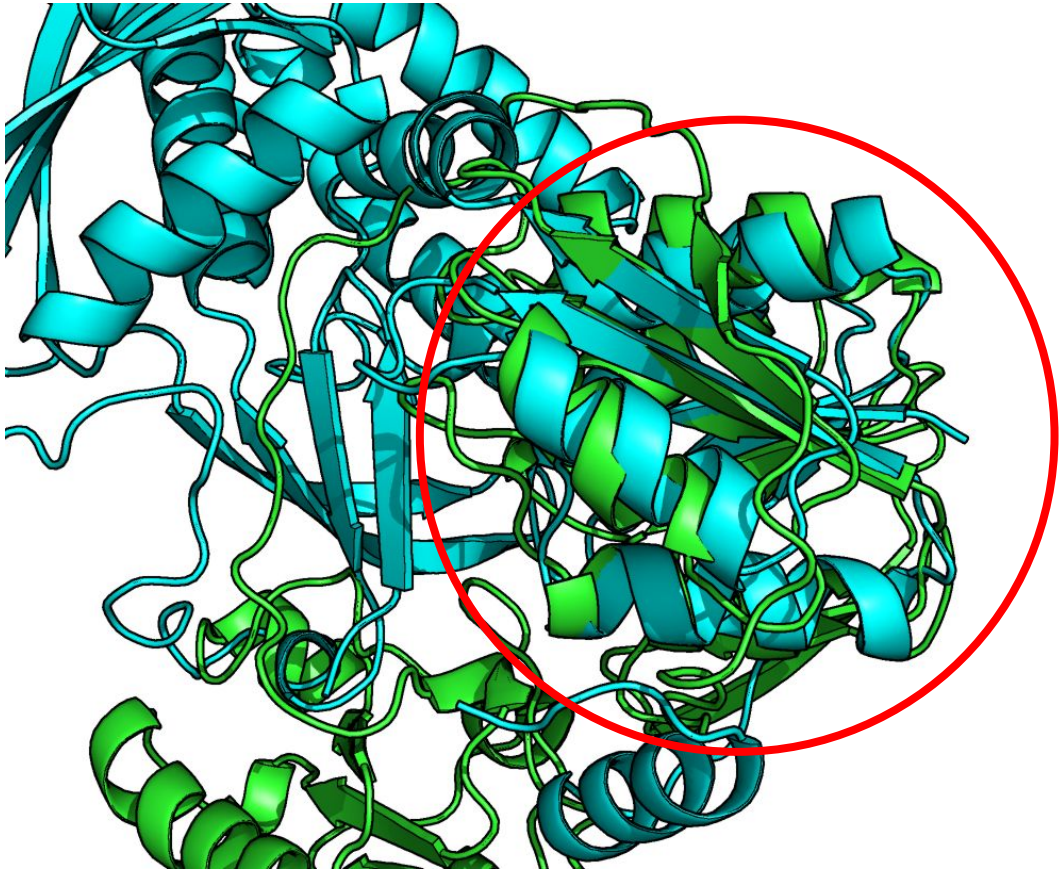


Arginosuc_synth



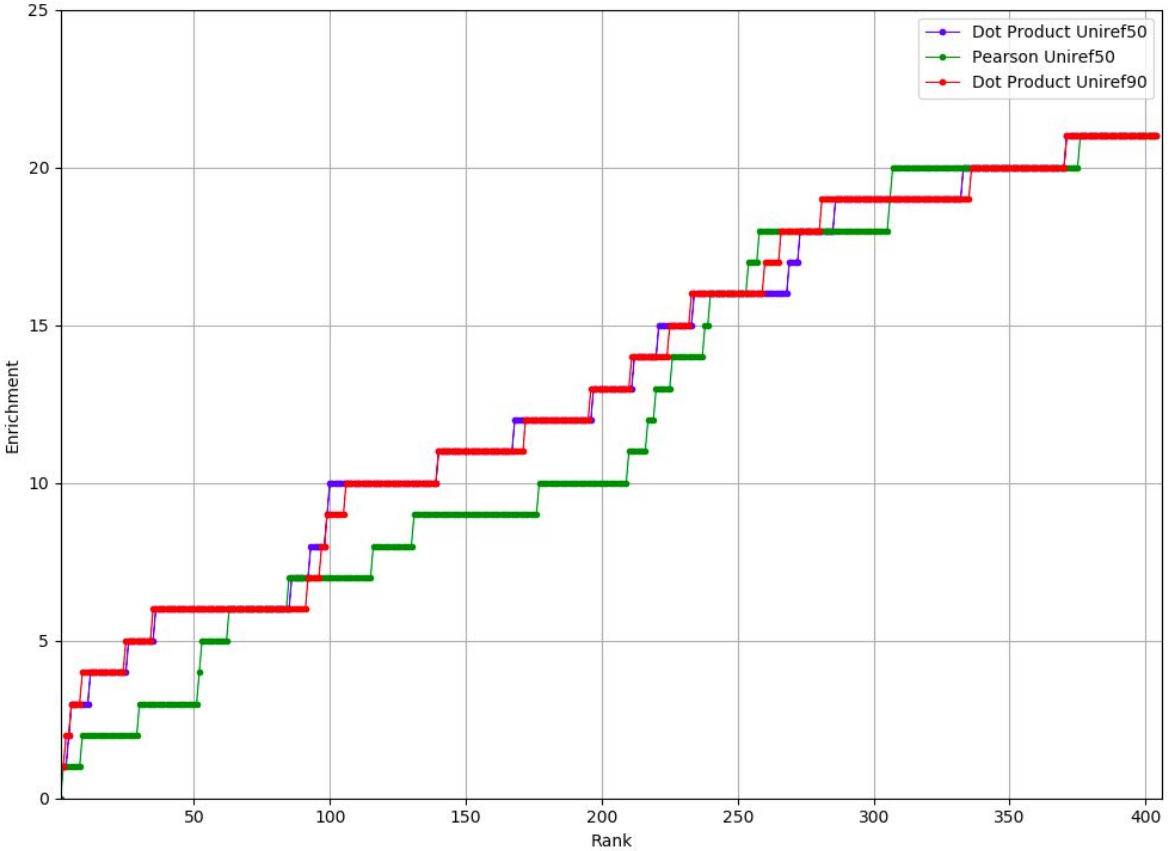
ETF-alpha

Structures of Query and First Template: Superposition



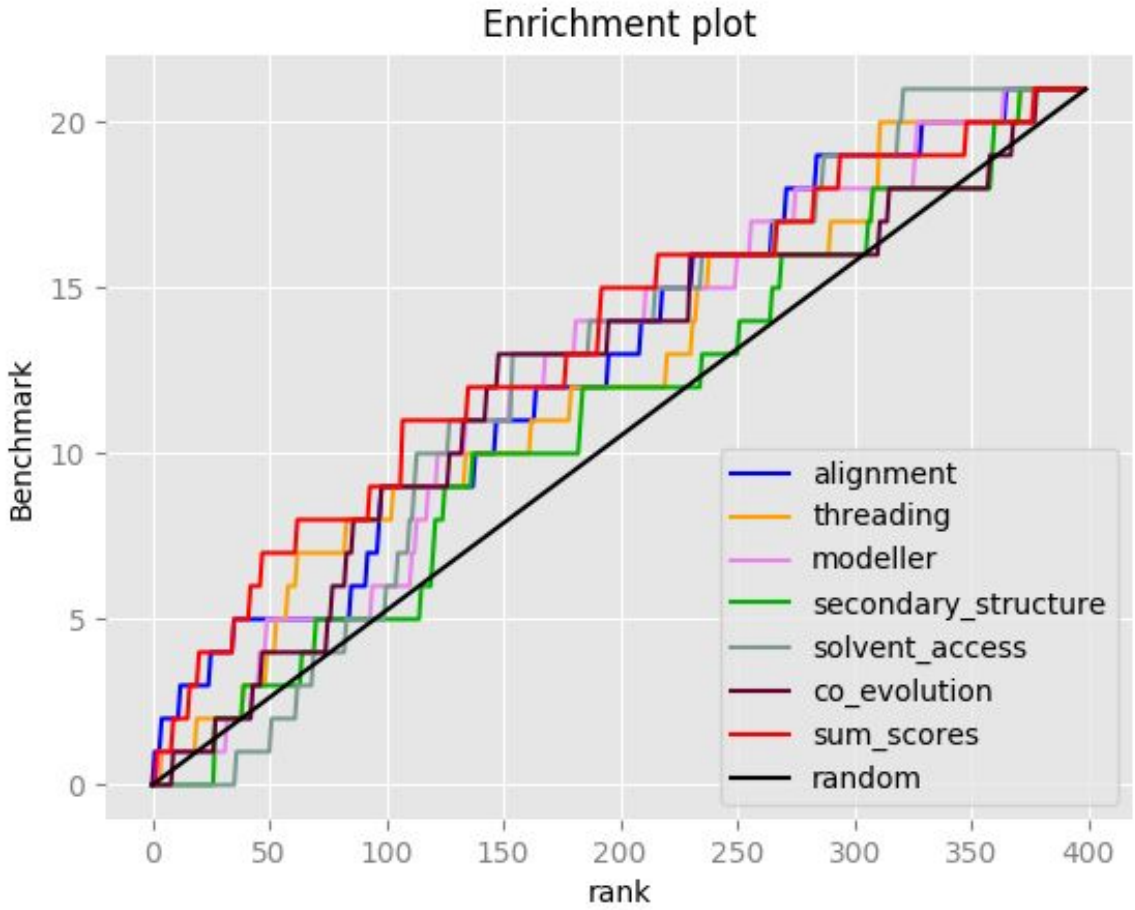
TM-score = 0.58

Results of 21 sequences (benchmark: upstream)

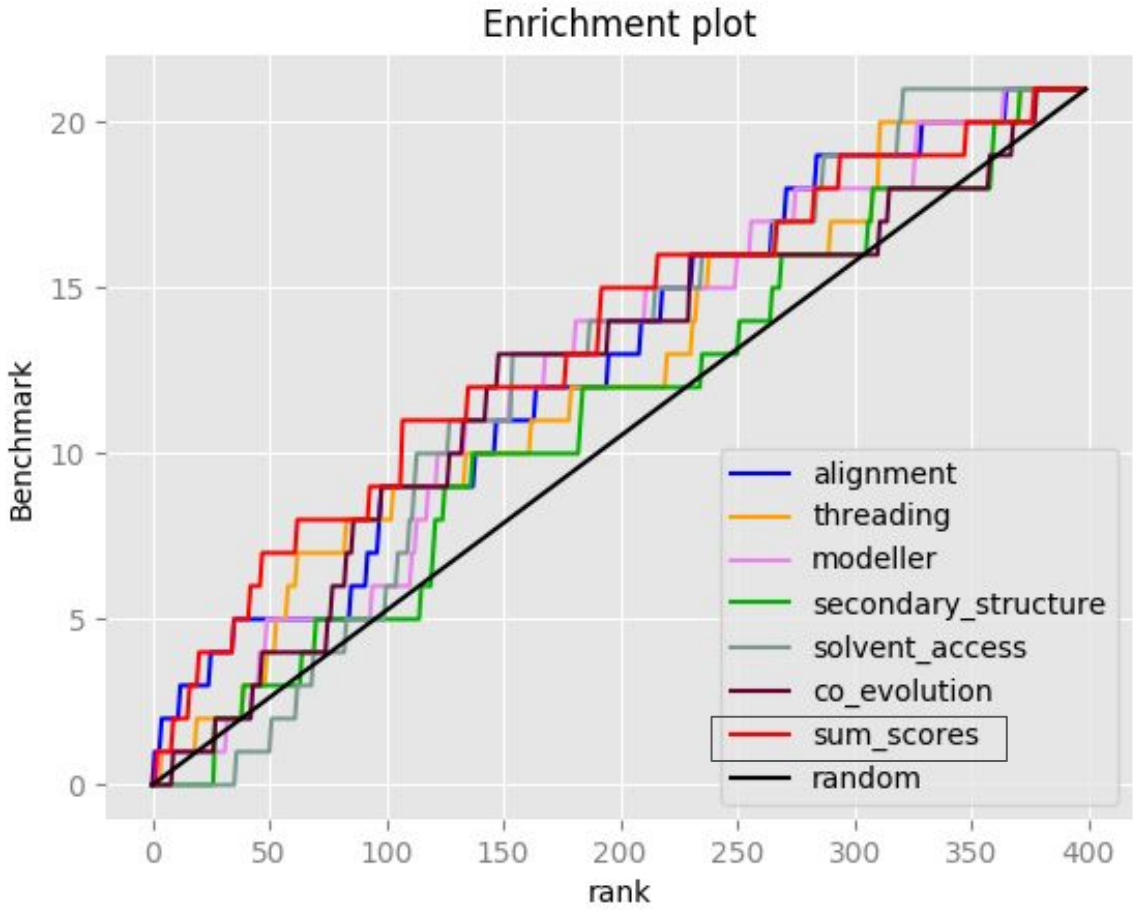


Enrichment Scores

Results of 21 sequences (upstream + downstram)



Results of 21 sequences (upstream + downstram)



Families are found at better positions

<u>Exception, ex:</u>
ETF-alpha (10th)

Results mysterious sequences

The whole pipeline was used on the **11 mysterious sequences**.

We noticed that :

- The results were **really divergent** amongst the teams
- **9 families** were found
- Amongst them :
  - **COX1** and **COX3** are subunits of the cytochrome c complexe, component of the mitochondrial respiratory chain.
  - **Cytochrome b** is the component of the ubiquinol-cytochrome c reductase complex, also part of the respiratory chain.

Discussion

PSIPRED	Prediction on multiple alignment of Query and hits
DSSP	On templates HOMSTRAD
Query Infos	Solvent Accessibility
Scoring Function (Profil-Profil)	PICASSO3Q

Thank you for your attention