

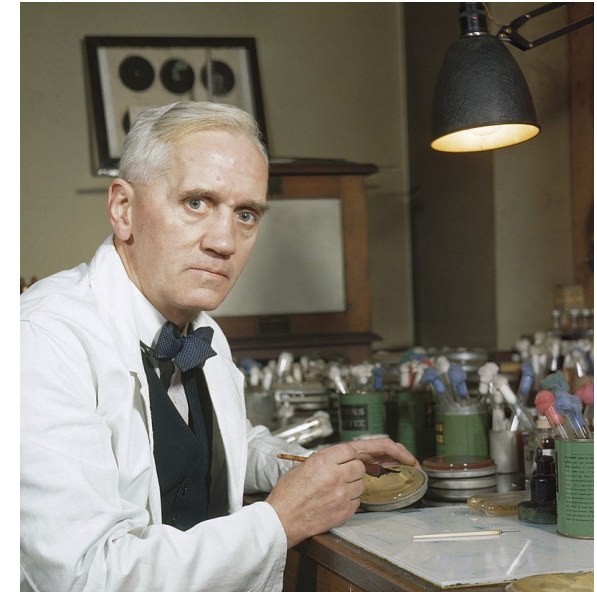
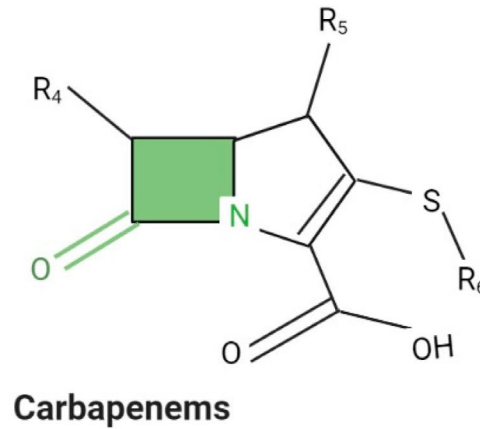
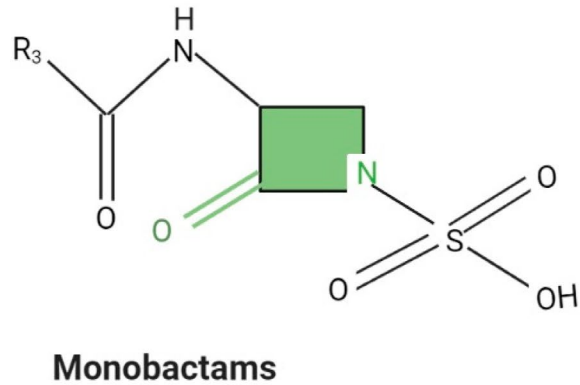
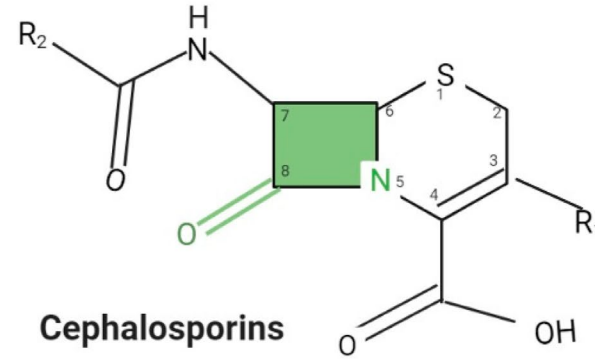
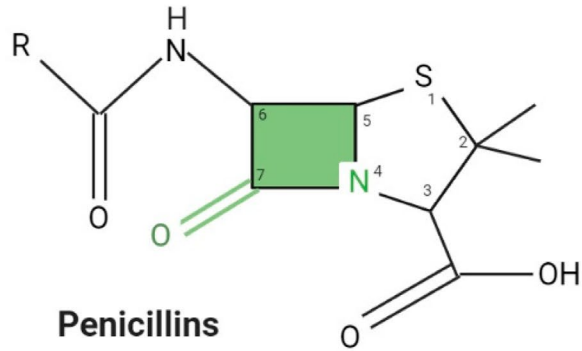
DTU



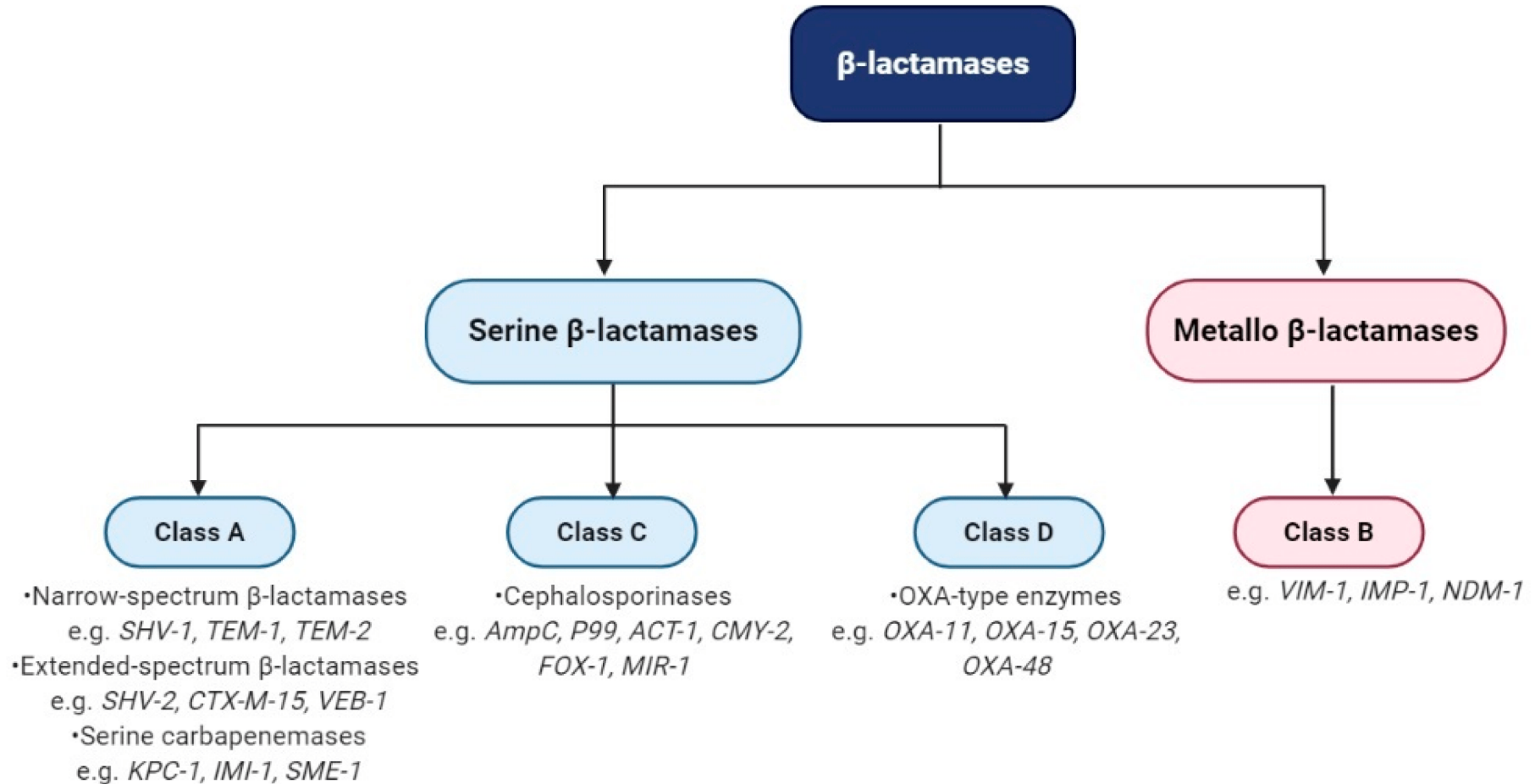
Attila Beleon
MSc. Bioinformatics

Identification of known and novel beta-lactamases through a multipronged bioinformatic approach

What is a beta-lactam?



What is a beta-lactamase?

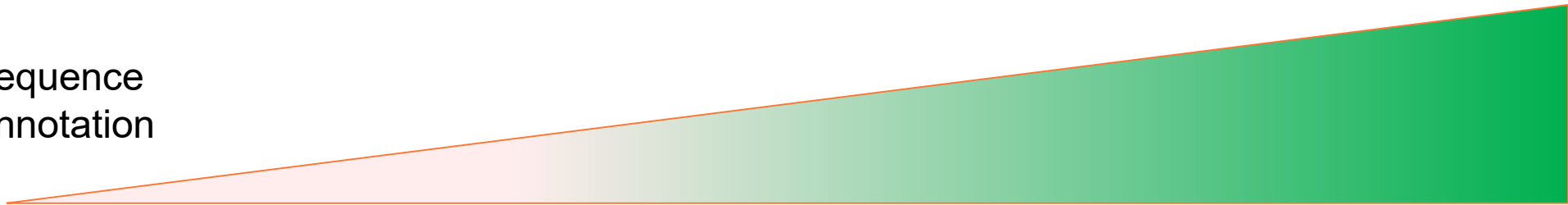


The concept

Computational complexity

3D Structural alignment

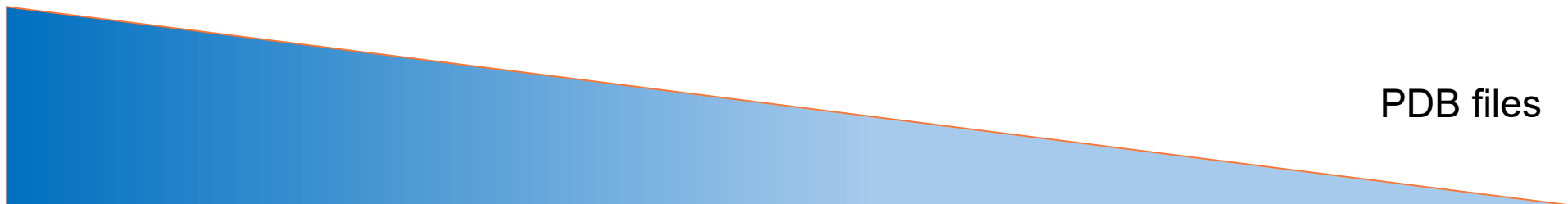
Sequence Annotation



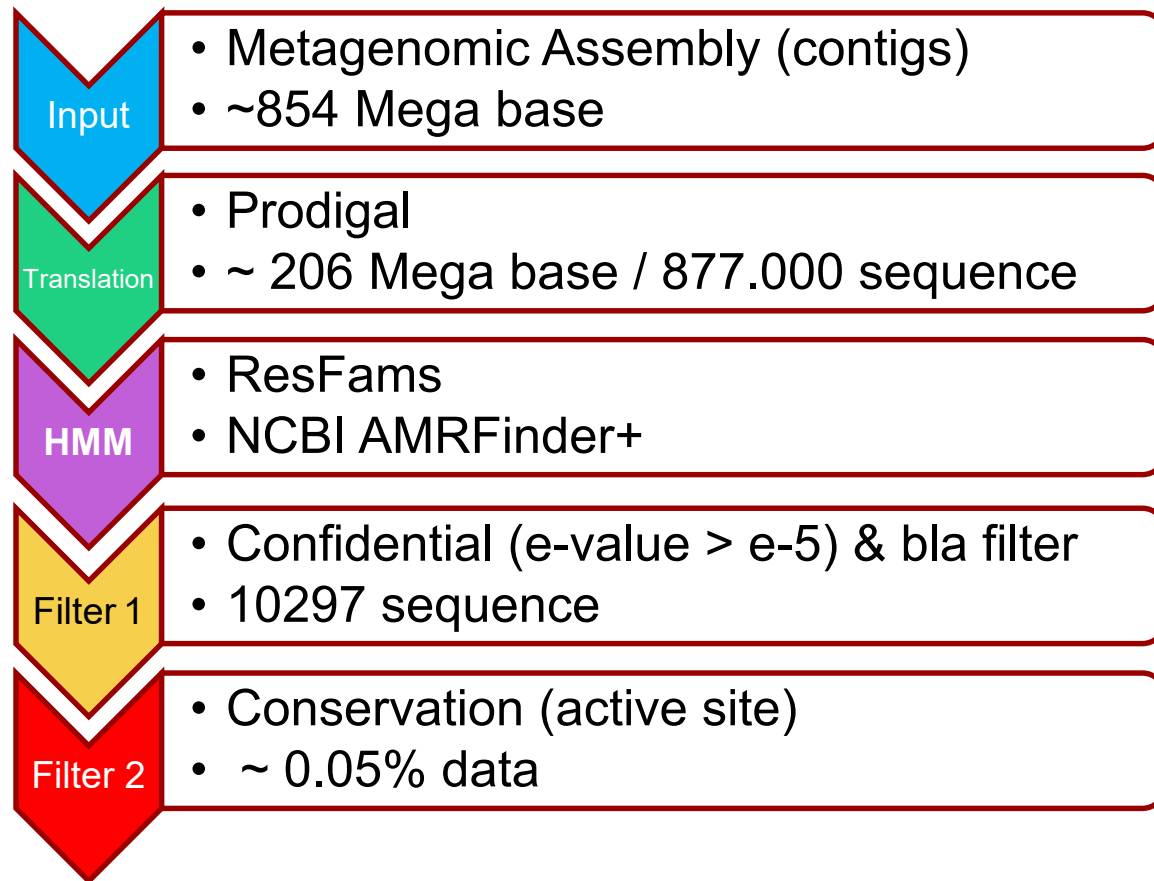
Data size

Contigs

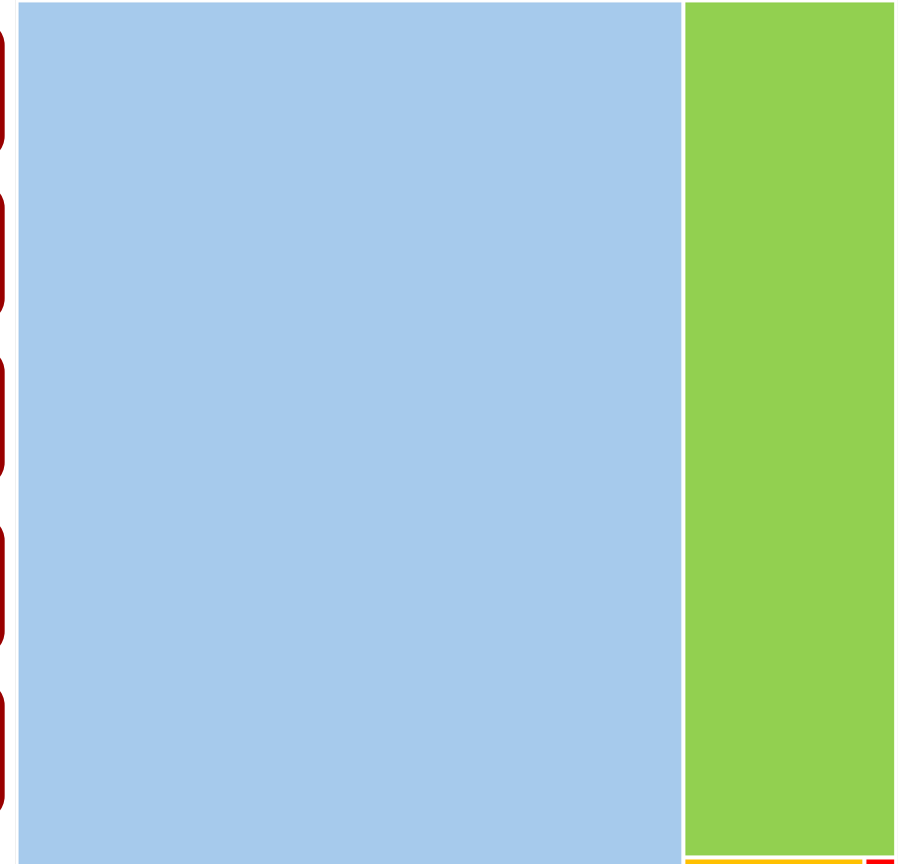
PDB files



The concept



Data Reduction



Snakemake

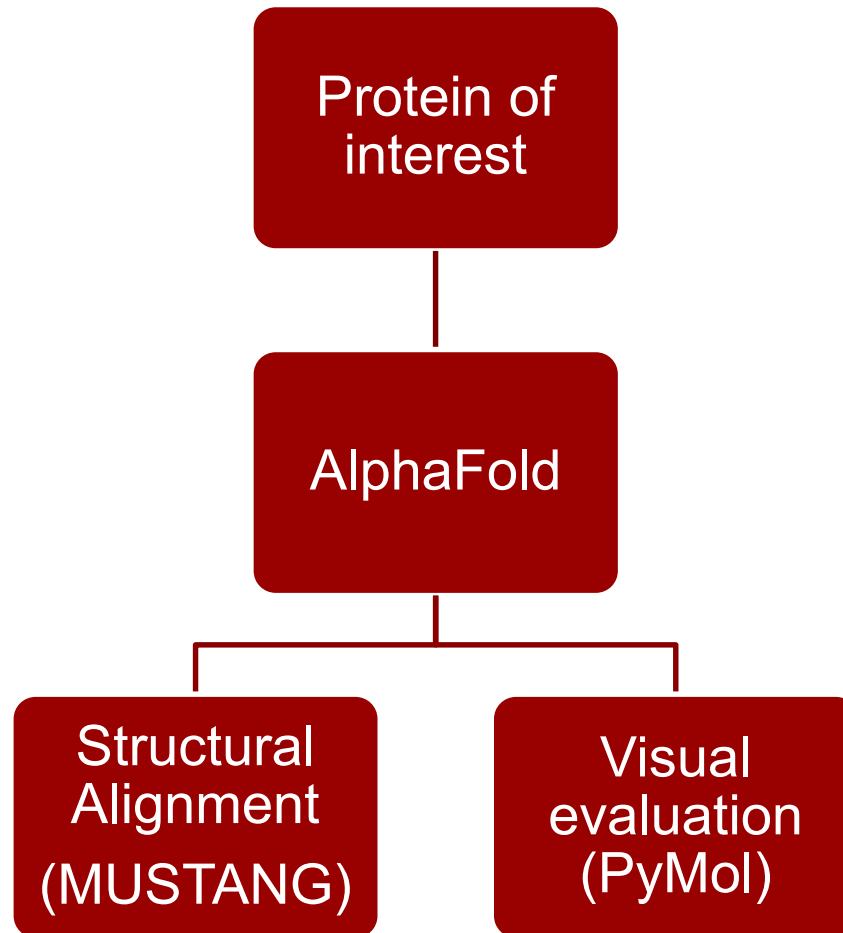


Protein of Interest (POI), priority list (HMM profile = Bla_classB_core_region)

Fasta ID	Match Ratio	coordinates					gaps
		30	59	61	63	129	
JLJDMHNG_155446	1	D	H	H	D	H	0
JLJDMHNG_247543	1	D	H	H	D	H	0
JLJDMHNG_310222	1	D	H	H	D	H	0
JLJDMHNG_586787	1	D	H	H	D	H	0
JLJDMHNG_20588	0.8	D	H	D	D	H	0
JLJDMHNG_203055	0.8	D	H	E	D	H	0
JLJDMHNG_06878	0.8	D	H	H	D	-	1
JLJDMHNG_07094	0.8	D	H	H	D	-	1
JLJDMHNG_07422	0.8	D	H	H	D	-	1
JLJDMHNG_09829	0.8	D	H	H	D	-	1
JLJDMHNG_22047	0.8	D	H	H	D	-	1
JLJDMHNG_34022	0.8	D	H	H	D	-	1
JLJDMHNG_35291	0.8	D	H	H	D	-	1
JLJDMHNG_36649	0.8	D	H	H	D	-	1
JLJDMHNG_38394	0.8	D	H	H	D	-	1
JLJDMHNG_39939	0.8	D	H	H	D	-	1
JLJDMHNG_41927	0.8	-	H	H	D	H	1
JLJDMHNG_45742	0.8	D	H	H	D	-	1
JLJDMHNG_49556	0.8	D	H	H	D	-	1
JLJDMHNG_49846	0.8	D	H	H	D	-	1

Num of Seq		747
Match ratio	# gaps	
1	0	4
0.8	0	2
0.8	1	125
0.6	0	0
0.6	1	33
0.6	2	114
0.4	0	1
0.4	1	9
0.4	2	12
0.4	3	3
0.2	0	0
0.2	1	1
0.2	2	6
0.2	3	8
0.2	4	65
0all		364

Structural analysis



Green: Hypothetical Protein

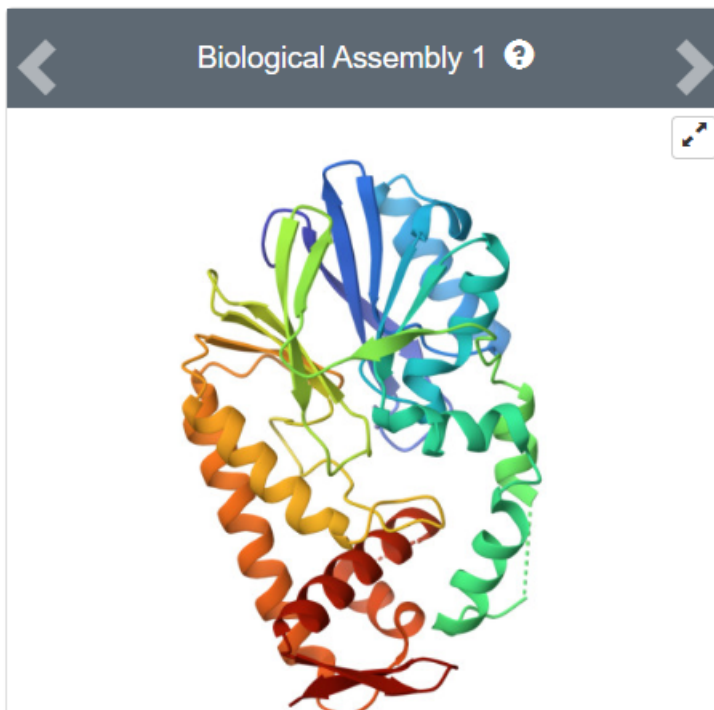
Cyan: 2ZO4 (PDB)



Green: Hypothetical Protein

Cyan: 2ZO4 (PDB)





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2ZO4

Crystal structure of metallo-beta-lactamase family protein TTHA1429 from *Thermus thermophilus* HB8

PDB DOI: <https://doi.org/10.2210/pdb2ZO4/pdb>

Classification: **HYDROLASE**

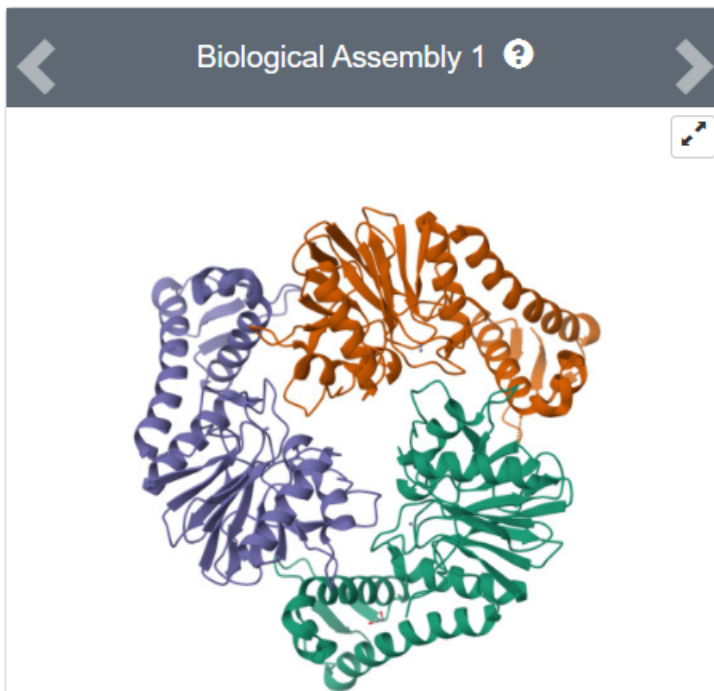
Organism(s): *Thermus thermophilus* HB8

Expression System: *Escherichia coli*

Mutation(s): No ⓘ

Deposited: 2008-05-05 **Released:** 2009-03-17

Deposition Author(s): Yamamura, A., Nagata, K., Agari, Y., Ebihara, A., Nakagawa, N., Yokoyama, S., Kuramitsu, S., Tanokura, M.



4AD9

Crystal structure of human LACTB2.

PDB DOI: <https://doi.org/10.2210/pdb4AD9/pdb>

Classification: **HYDROLASE**

Organism(s): *Homo sapiens*

Expression System: *Escherichia coli* BL21(DE3)

Mutation(s): No ⓘ

Deposited: 2011-12-22 **Released:** 2012-02-01

Deposition Author(s): Allerston, C.K., Krojer, T., Shrestha, B., Burgess Brown, N., Chalk, R., Elkins, J.M., Filippakopoulos, P., Pike, A.C.W., Muniz, J.R.C., Vollmar, M., Arrowsmith, C.H., Weigelt, J., Edwards, A., Bountra, C., von Delft, F., Gileadi, O.

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⚙ Data API

MUSTANG

2zo4

RMSD = 15.1 Å

```
#=====
# Aligned_structures: 2
#   1: 2zo4_noH0H.pdb
#   2: ranked_0.pdb
#
# Length:          612
# Identity:         51/612 ( 8.3%)
# Similarity:       51/612 ( 8.3%)
# Gaps:             365/612 ( 59.6%)
```

RMSD = 5.8 Å

4ad9

```
#=====
# Aligned_structures: 2
#   1: 4ad9_A_noH0H.pdb
#   2: ranked_0.pdb
#
# Length:          584
# Identity:         79/584 ( 13.5%)
# Similarity:       79/584 ( 13.5%)
# Gaps:             322/584 ( 55.1%)
```

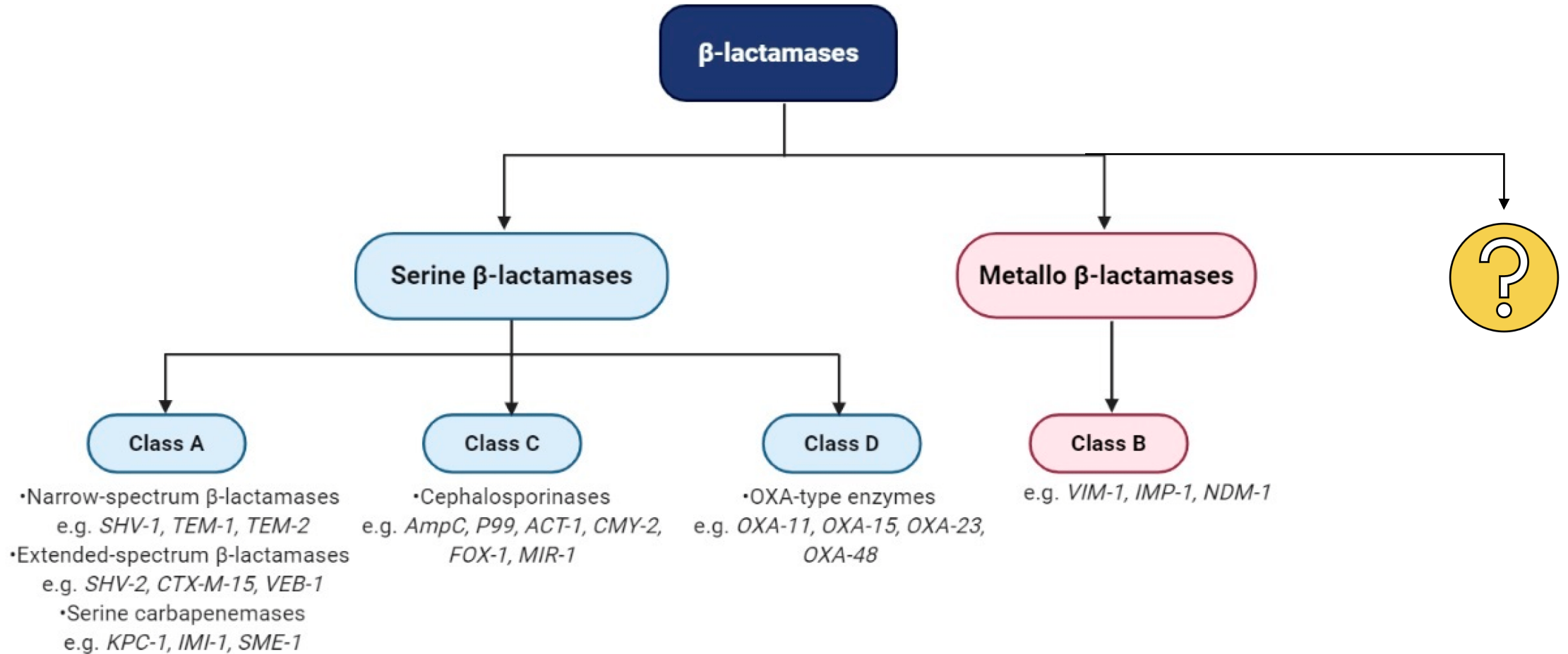
VS

PyMol

Executive: RMSD = 1.769 (124 to 124 atoms)

Executive: RMSD = 1.368 (178 to 178 atoms)

Limitations



Thank you for your attention!