

Graz University of Technology

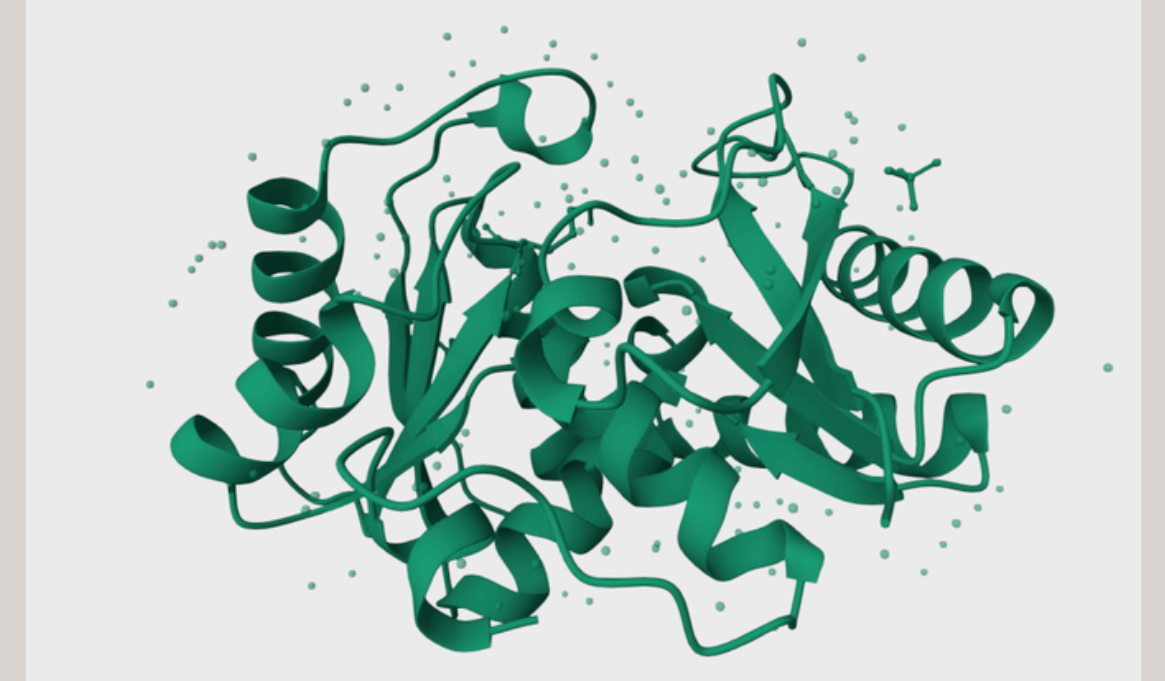
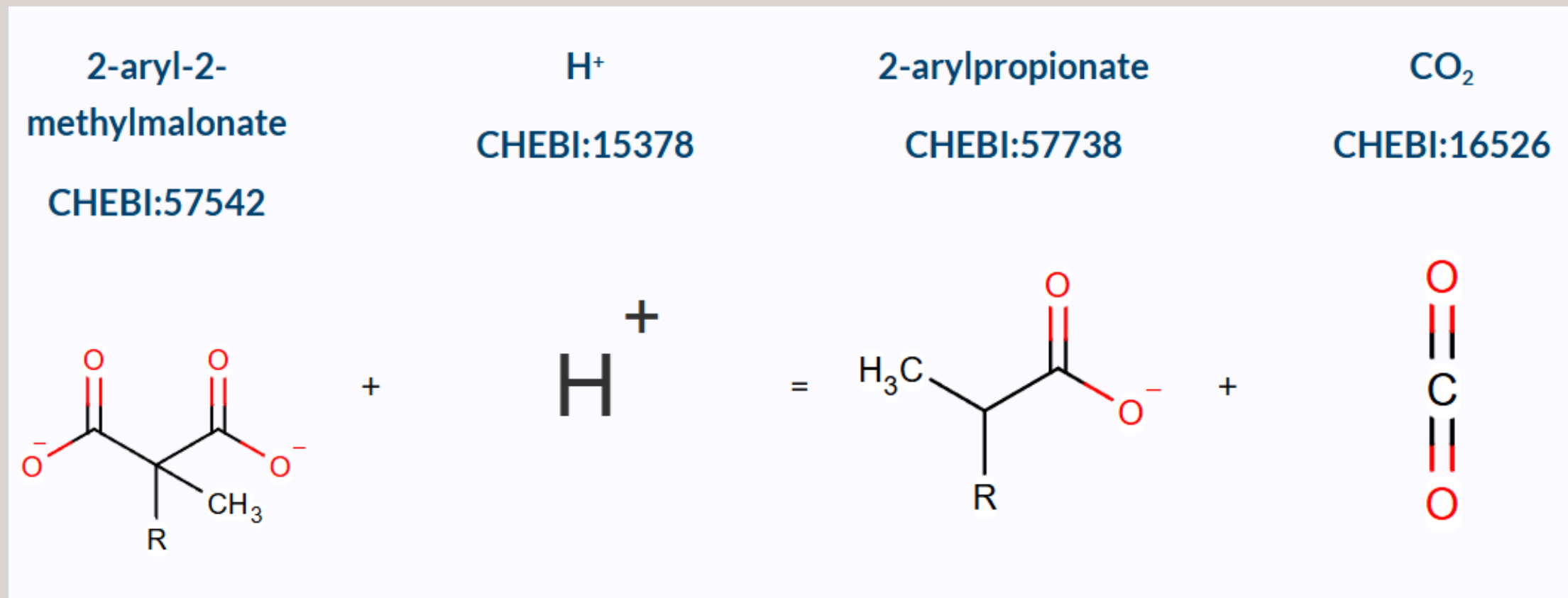
BLAST and Foldseek with Arylmalonate decarboxylase

Presented by Hirschberger Anna, Jelic Ivana, Haxhi Nikol, Emilia Chua

Arylmalonate decarboxylase (3DTV)

Organism: *Bordetella bronchiseptica*

Catalytic function:



Uniprot → Q05115

BLAST – Basic Local Alignment Search Tool

→ finds regions of similarity between biological sequences



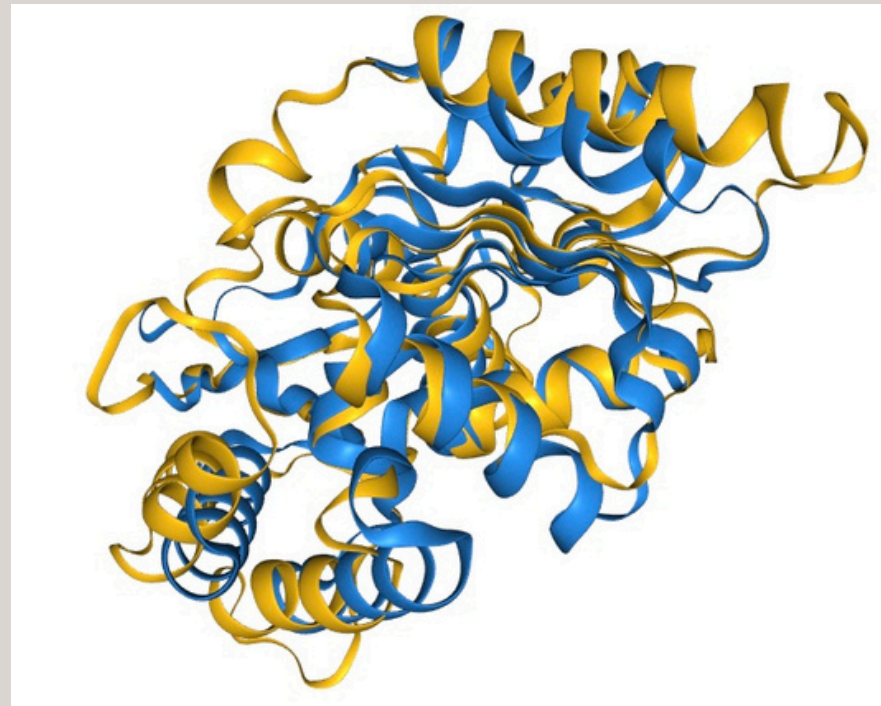
- QuickBLASTP
- BlastP
- PSI-BLAST
- PHI-BLAST
- DELTA-BLAST

Foldseek

- comparing protein structures
- 3D protein shapes
- rapid alignment
- structural searches: faster + good accuracy








simplified sequences



Foldseek Search



 Foldseek Search 



Input protein structure (PDB/CIF) or sequence (FASTA)


```
data_3DTV
#
_entry.id    3DTV
#
_audit_conform.dict_name      mmcif_pdbx.dic
_audit_conform.dict_version    5.403
_audit_conform.dict_location   http://mmcif.pdb.org/dictionaries/ascii/mmcif_pdbx.dic
#
loop_
_database_2.database_id
_database_2.database_code
```


LOAD ACCESSION


UPLOAD PDB

PREDICT

UPLOAD PREVIOUS RESULTS

 Databases & search settings

 SEARCH

 GO TO MULTIMER

Summary

Search **all available** databases with Foldseek in 3D

Reference

van Kempen M, Kim S, Tumescheit C, Mirdita M, Lee J, Gilchrist CLM, Söding J, and Steinegger M. [Fast and](#)



Load accession

Source

PDB (rcsb.org) ▼

Accession

3DTV

CANCEL

LOAD

Result

< ALL DATABASES BFVD (1000) AFDB-PROTEOME (393) AFDB-SWISSPR >

BFVD 1000 hits

SHOW TAXONOMY GRAPHICAL **NUMERIC**

Target	Scientific Name	Prob.	Seq. Id.	E-Value	Position in query	 Alignment
A0A5J6VJ33	Megaviridae enviro...	1.00	19.8	4.56e-11	 2 215	
A0A1V0S9F2	Catovirus CTV1	0.97	8.6	1.90e-4	 3 201	
V5L5T2_1	Insectomime virus	0.97	12.5	8.91e-4	 2 194	
A0A1D6Y723	Golden Marseillevirus	0.96	9.6	2.25e-3	 2 197	
A0A7T5QY57	unclassified Ishigur...	0.89	21.4	2.35e-2	 93 187	
A0A9E8S3A6	unclassified Spoun...	0.87	14	4.09e-2	 92 187	

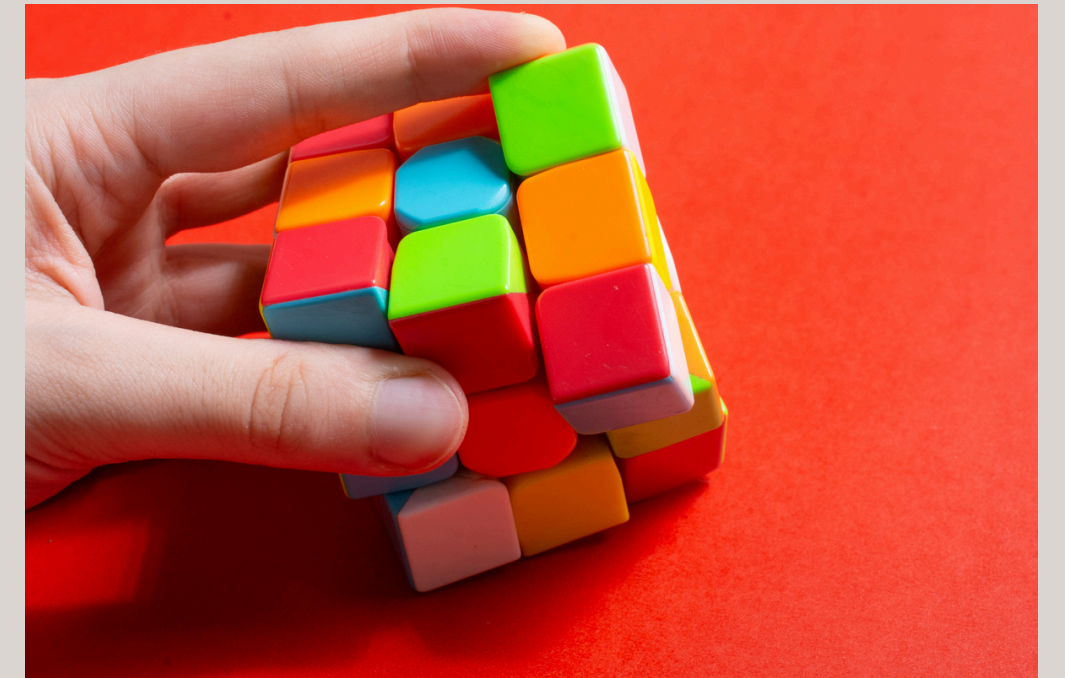
Feedback on BLAST

(-) Interface seems complicated at first

(+) Provides results quickly

(+) Easy to use

(+) Easy to save as FASTA file



Feedback on Foldseek

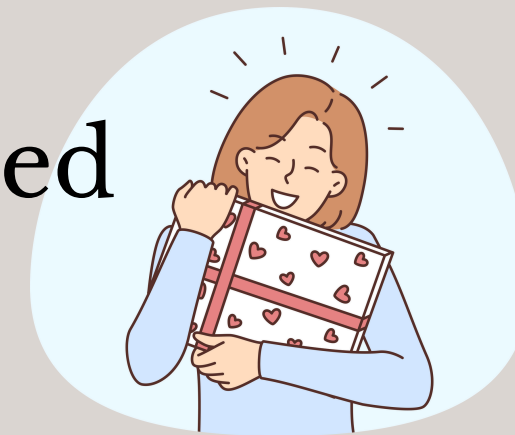
confusing: tutorials made it look easier



unexpected results: enzymes from viruses



After a while: user-friendly + well organized



Thank you for your attention!

Foldseek Search

