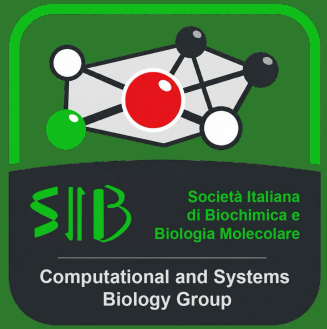
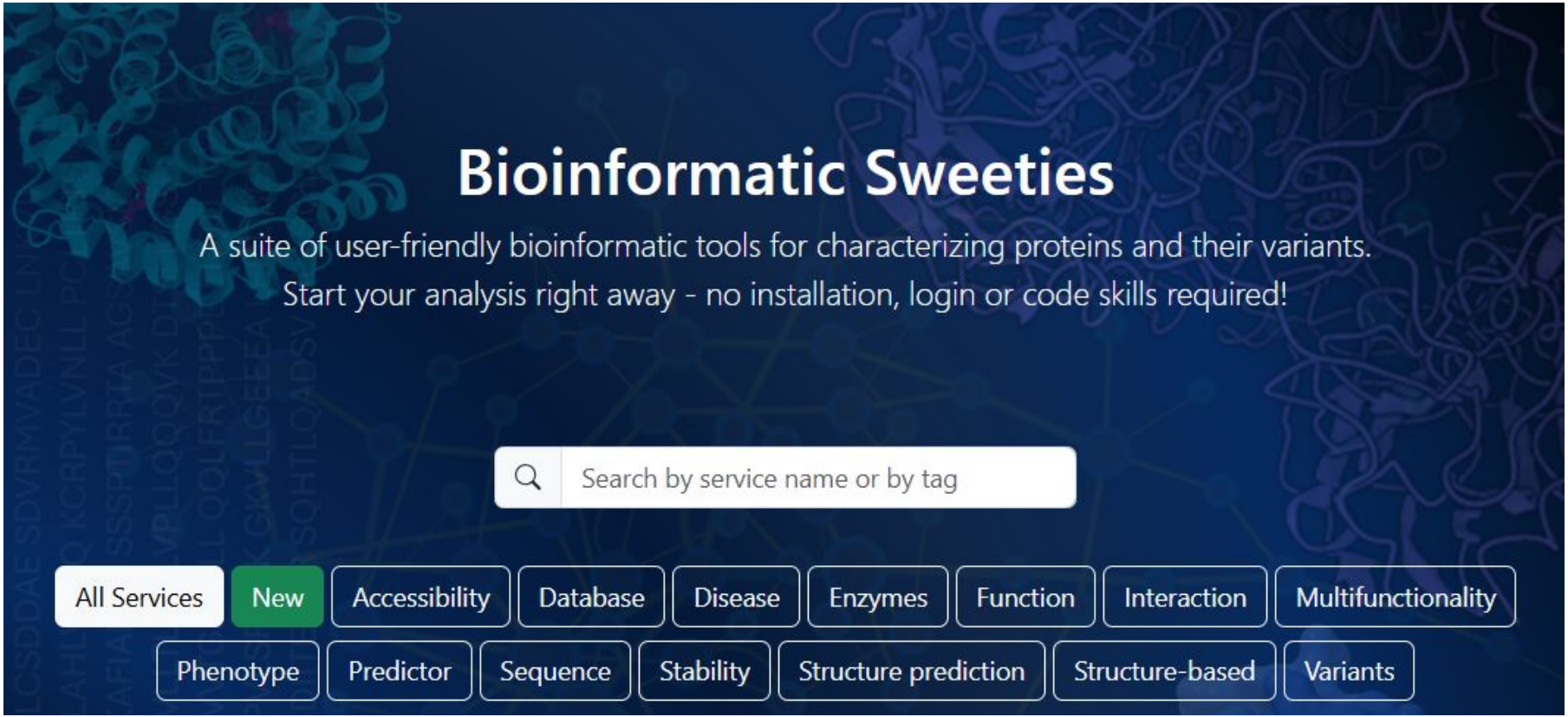
S4 · 16:30–16:45

Bioinformatic Sweeties: A Suite of User-Friendly Bioinformatic Tools for Characterizing Proteins and Their Variants



Giulia Babbi

University of Bologna


Bioinformatic Sweeties
A suite of user-friendly bioinformatic tools for characterizing proteins and their variants.
Start your analysis right away - no installation, login or code skills required!
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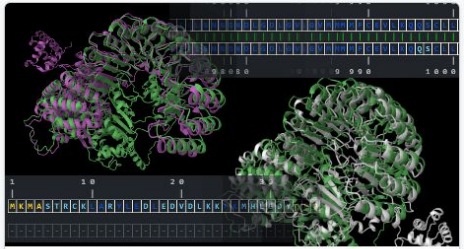
Variants

Resources for protein analysis



Alpha&ESM hFolds

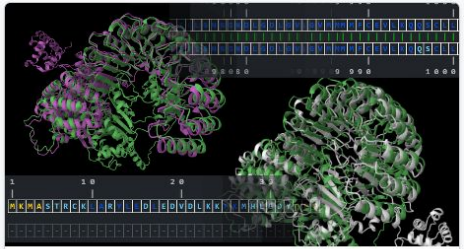
New | Structure prediction | Database

Comparison of structural models predicted by ESMFold and AlphaFold

paper direct link

Structural models comparison

Resources for protein analysis



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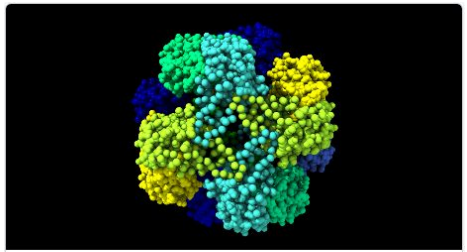

MultifacetedProtDB

Multifunctionality | Database | Function

Database providing a comprehensive collection of multifunctional human proteins with annotation

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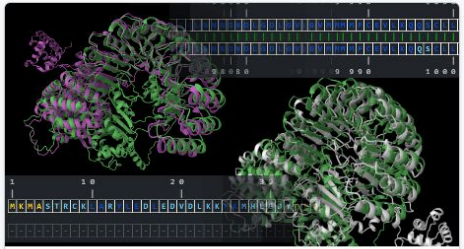
Multifunctionalities

Resources for protein analysis



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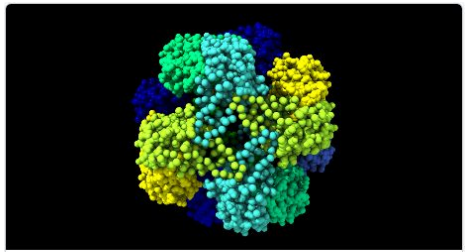

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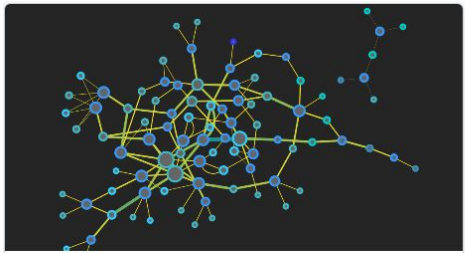

DAR

Enzymes | Database | Disease

Database mapping disease-associated enzyme into Reactome pathways

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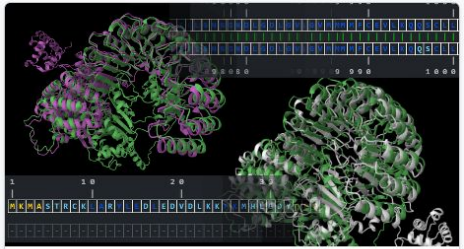
Enzymes and Reactome Pathways

Resources for protein analysis

CSB Meeting 2026



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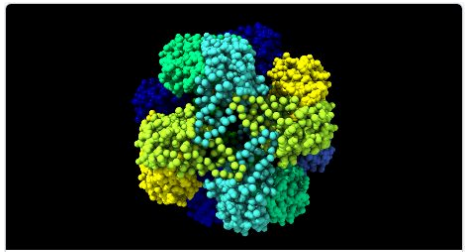

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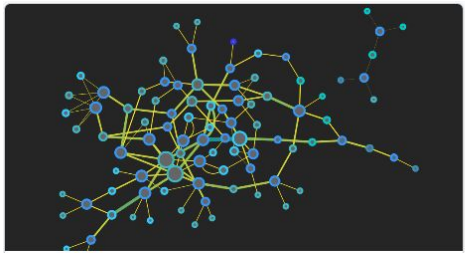

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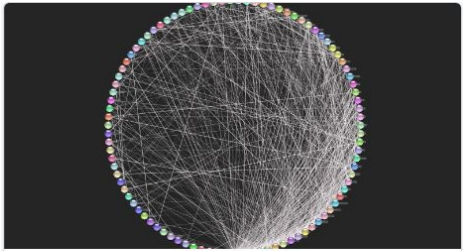

eDGAR

Disease | Database

Web-server for Disease-Gene Associations with annotated Relationships among genes

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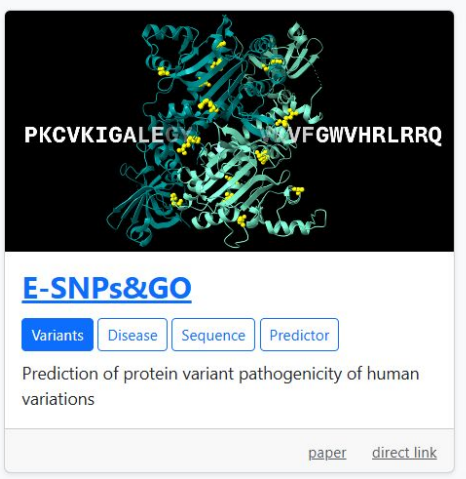
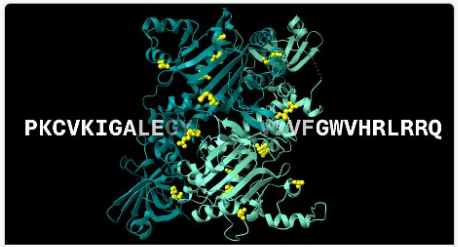
Diseases and gene relations

Tools for variants analysis starting from protein sequence



Pathogenicity class and probability

Tools for variants analysis starting from protein sequence



E-SNPs&GO

Variants | Disease | Sequence | Predictor

Prediction of protein variant pathogenicity of human variations

paper direct link

Pathogenicity class and probability

E-pRSA

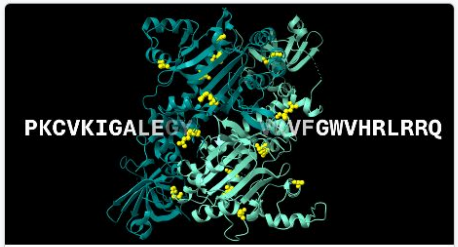
Accessibility | Sequence | Predictor

Prediction of residue Relative Solvent Accessibility starting from protein sequence

paper direct link

Relative Solvent Accessibility (RSA)

Tools for variants analysis starting from protein sequence



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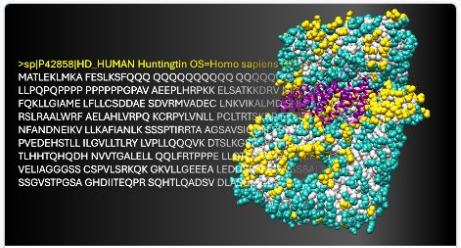

ISPRED-SEQ

Interaction | Sequence | Predictor

Prediction of Interaction Sites starting from protein sequence

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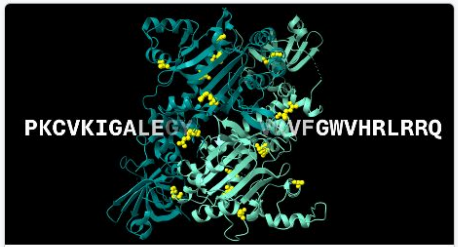
Interaction sites

Tools for variants analysis starting from protein sequence

CSB Meeting 2026



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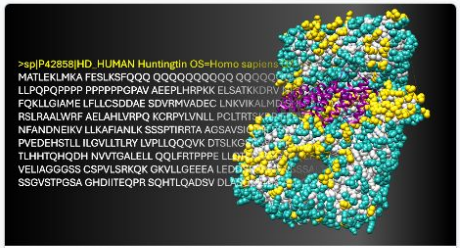

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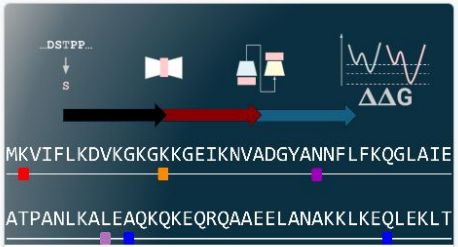

DDGEmb

New | Variants | Predictor | Sequence

Prediction of the impact of nsSNPs on protein stability starting from protein sequence

paper direct link

ΔΔG for single- and multi-point variations

Pterin-4-alpha-carbinolamine dehydratase (UniProt AC: P61457, Gene: PCBD1)

- It is associated with a rare condition called **Hyperphenylalaninemia due to dehydratase deficiency (ORPHA:1578)**, a rare genetic, transient and benign form of hyperphenylalaninemia due to tetrahydrobiopterin deficiency.

- It is characterized by muscular **hypotonia**, irritability, slow acquisition of psychomotor skills, age-dependent movement disorders, including dystonia. Neurological developement is normal with **dietary control** of blood phenyalanine.

Use case: Analysis of Pterin-4-alpha-carbinolamine dehydratase

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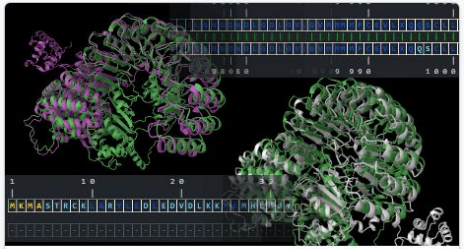

Alpha&ESM hFolds

New | Structure prediction | Database

Comparison of structural models predicted by ESMFold and AlphaFold

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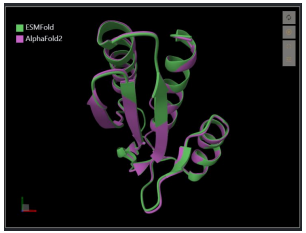
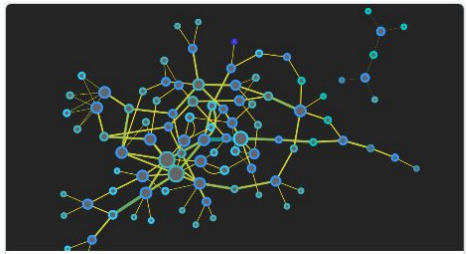
Structural models comparison
TM-score 0.96
RMSD 1.46 Å





DAR

Enzymes | Database | Disease

Database mapping disease-associated enzyme into Reactome pathways

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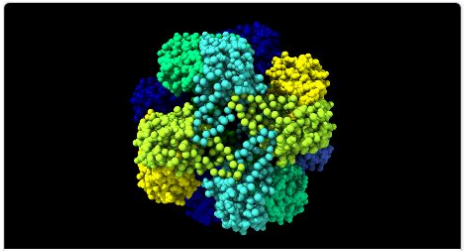
EC number (4.2.1.96)
R-HAS-8964208,
"Phenylalanine metabolism"



MultifacetedProtDB

Multifunctionality | Database | Function

Database providing a comprehensive collection of multifunctional human proteins with annotation

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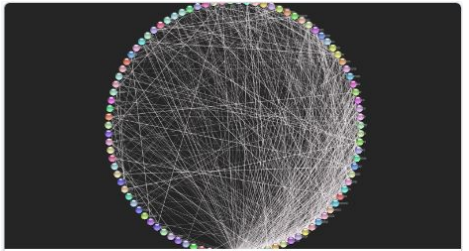
- Enzyme
- coactivator for HNF1A and HNF1B-dependent transcription



eDGAR

Disease | Database

Web-server for Disease-Gene Associations with annotated Relationships among genes

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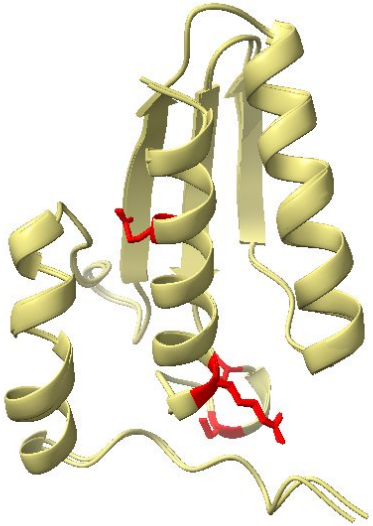
Patients may also develop hypomagnesemia and nonautoimmune diabetes mellitus during puberty

Use case: Analysis of Pterin-4-alpha-carbinolamine dehydratase

variant	E-SNPs&GO	E-pRSA	ISPRED-SEQ	DDGemb
T79I*	Pathogenic (0.89)	Buried (0.10)	Interaction Site	-1.34
C82R*	Pathogenic (0.95)	Exposed (0.25)	Interaction Site	-0.16
R88Q*	Pathogenic (0.58)	Exposed (0.34)	Interaction Site	-1.21
E97K*	Pathogenic (0.93)	Exposed (0.29)	Interaction Site	-0.56

4 known pathogenic missense variants are **correctly predicted** as pathogenic

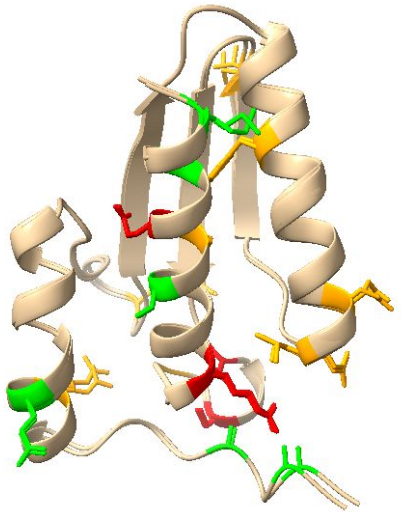


Use case: Analysis of Pterin-4-alpha-carbinolamine dehydratase

variant	E-SNPs&GO	E-pRSA	ISPRED-SEQ	DDGemb
A2D	Benign (0.37)	Exposed (0.58)	-	-0.02
A2V	Benign(0.36)	Exposed (0.58)	-	-0.30
A5T	Benign (0.13)	Exposed (0.41)	Interaction Site	0.38
R13W	Pathogenic (0.95)	Buried (0.17)	-	-0.21
Q15H	Benign (0.24)	Exposed (0.62)	Interaction Site	-0.97
R31C	Pathogenic (0.89)	Exposed (0.40)	Interaction Site	-0.95
F49C	Pathogenic (0.93)	Buried (0.06)	Interaction Site	-2.40
E58K	Pathogenic (0.93)	Exposed (0.51)	Interaction Site	-0.35
L60P	Pathogenic (0.96)	Exposed (0.31)	Interaction Site	-2.38
D61Y	Pathogenic (0.93)	Exposed (0.57)	Interaction Site	-0.55
V69M	Pathogenic (0.72)	Exposed (0.41)	Interaction Site	-0.40
G84C	Pathogenic (0.95)	Exposed (0.25)	Interaction Site	-0.53
R88W	Pathogenic (0.82)	Exposed (0.34)	Interaction Site	-0.54
S94I	Benign (0.24)	Exposed (0.38)	Interaction Site	1.37
I96V	Pathogenic (0.56)	Buried (0.06)	-	-0.66
A100V	Benign (0.24)	Buried (0.15)	-	-0.27
M103K	Benign (0.46)	Exposed (0.29)	Interaction Site	-1.15
M103V	Benign (0.13)	Exposed (0.29)	Interaction Site	-1.32

Among the 18 missense variants of uncertain significance:

- 10 predicted as pathogenic
- 8 predicted as benign



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