



TWIN2PIPSA

<https://twin2pipsa.campus.ciencias.ulisboa.pt/>

On-site training
Ciências ULisboa
01–02 Feb 2024

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Computational tools to analyse protein stability and abundance

List of links to tools and references

Example protein: PTEN
Uniprot: P60484
PDB: 1d5r

- **ColabFold**

<https://colab.research.google.com/github/sokrypton/ColabFold/blob/main/AlphaFold2.ipynb#scrollTo=kObIAo-xetgx>

- **DSSP webserver**

<https://swift.cmbi.umcn.nl/gv/dssp/>
<https://www3.cmbi.umcn.nl/xssp/>

A series of PDB related databases for everyday needs. Wouter G Touw, Coos Baakman, Jon Black, Tim AH te Beek, E Krieger, Robbie P Joosten, Gert Vriend. Nucleic Acids Research 2015 January; 43(Database issue): D364-D368.

Dictionary of protein secondary structure: pattern recognition of hydrogen-bonded and geometrical features. Kabsch W, Sander C, Biopolymers. 1983 22 2577-2637. PMID: 6667333; UI: 84128824.

- **DEPTH webserver**

<http://cospi.iiserpune.ac.in/depth/>

Depth: a web server to compute depth, cavity sizes, detect potential small-molecule ligand-binding cavities and predict the pKa of ionizable residues in proteins. Kuan Pern Tan, Thanh Binh Nguyen, Siddharth Patel, Raghavan Varadarajan and M. S. Madhusudhan Nucl. Acids Res. (1 July 2013) 41 (W1): W314-W321.

DEPTH: a web server to compute depth and predict small-molecule binding cavities in proteins. Kuan Pern Tan; Raghavan Varadarajan; M. S. Madhusudhan Nucleic Acids Research 2011

Residue depth: a novel parameter for the analysis of protein structure and stability. Suvobrata Chakravarty and Raghavan Varadarajan(1999). Structure 7,723-732.



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- **Depth Colab notebook**

https://colab.research.google.com/drive/1DSTgTWQBazMERk4iD-9G0LfcSYe_oZXK?usp=sharing

- **RaSP Colab notebook**

https://colab.research.google.com/github/KULL-Centre/2022_ML-ddG-Blaabjerg/blob/main/RaSPLab.ipynb

Lasse M Blaabjerg, Maher M Kassem, Lydia L Good, Nicolas Jonsson, Matteo Cagiada, Kristoffer E Johansson, Wouter Boomsma, Amelie Stein, Kresten Lindorff-Larsen (2023) Rapid protein stability prediction using deep learning representations eLife 12:e82593.

- **QCDpred Colab notebook**

<https://colab.research.google.com/github/KULL-Centre/papers/blob/main/2022/degron-predict-Johansson-et-al/QCDpred.ipynb>

<https://github.com/KULL-Centre/papers/tree/main/2022/degron-predict-Johansson-et-al>

Johansson KE, Mashahreh B, Hartmann-Petersen R, Ravid T, Lindorff-Larsen K. Prediction of Quality-control Degradation Signals in Yeast Proteins. J Mol Biol. 2023 Jan 30;435(2):167915. doi: 10.1016/j.jmb.2022.167915. Epub 2022 Dec 7. PMID: 36495918.

- **Colab notebooks for plotting**

Notebook for plotting DSSP output, depth calculations output and QCDpred output:

<https://colab.research.google.com/drive/1t0f0Qiv7stMrfhu3GiMyKmgctpehDF5o?usp=sharing>

Matteo's notebook for plotting RaSP output:

https://colab.research.google.com/drive/1aWUDVvCQxRXYwZjCmQJ_2avbXrtzTnQW?usp=sharing



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