

DAFTAR PUSTAKA

- Abramson, J., Adler, J., Dunger, J., Evans, R., Green, T., Pritzel, A., Ronneberger, O., Willmore, L., Ballard, A.J., Bambrick, J., Bodenstein, S.W., Evans, D.A., Hung, C.-C., O'Neill, M., Reiman, D., Tunyasuvunakool, K., Wu, Z., Žemgulytė, A., Arvaniti, E., Beattie, C., Bertolli, O., Bridgland, A., Cherepanov, A., Congreve, M., Cowen-Rivers, A.I., Cowie, A., Figurnov, M., Fuchs, F.B., Gladman, H., Jain, R., Khan, Y.A., Low, C.M.R., Perlin, K., Potapenko, A., Savy, P., Singh, S., Stecula, A., Thillaisundaram, A., Tong, C., Yakneen, S., Zhong, E.D., Zielinski, M., Židek, A., Bapst, V., Kohli, P., Jaderberg, M., Hassabis, D., Jumper, J.M., 2024. Accurate structure prediction of biomolecular interactions with AlphaFold 3. *Nature* 630, 493–500. <https://doi.org/10.1038/s41586-024-07487-w>
- Böckenhauer, H.-J., Bongartz, D., 2007. *Algorithmic Aspects of Bioinformatics*, Natural Computing Series. Springer Berlin Heidelberg, Berlin, Heidelberg. <https://doi.org/10.1007/978-3-540-71913-7>
- Bohr, H., Bohr, J., Brunak, S., Cotterill, R.M.J., Lautrup, B., Nørskov, L., Olsen, O.H., Petersen, S.B., 1988. Protein secondary structure and homology by neural networks The α -helices in rhodopsin. *FEBS Lett.* 241, 223–228. [https://doi.org/10.1016/0014-5793\(88\)81066-4](https://doi.org/10.1016/0014-5793(88)81066-4)
- Bourne, P., Berman, H., McMahon, B., Watenpugh, K., 1997. The Macromolecular Crystallographic Information File (mmCIF).
- Branden, C.I., Tooze, J., 2012. *Introduction to Protein Structure*, 2nd ed. Garland Science, New York. <https://doi.org/10.1201/9781136969898>
- Chou, P.Y., Fasman, G.D., 1974. Prediction of protein conformation. *Biochemistry* 13, 222–245. <https://doi.org/10.1021/bi00699a002>
- Dai, L., Zhou, Y., 2011. Characterizing the Existing and Potential Structural Space of Proteins by Large-Scale Multiple Loop Permutations. *J. Mol. Biol.* 408, 585–595. <https://doi.org/10.1016/j.jmb.2011.02.056>
- Fang, C., Shang, Y., Xu, D., 2018. MUFOLD-SS: New deep inception-inside-inception networks for protein secondary structure prediction. *Proteins Struct. Funct. Bioinforma.* 86, 592–598. <https://doi.org/10.1002/prot.25487>
- Finkelstein, A.V., Ptitsyn, O.B., 1971. Statistical analysis of the correlation among amino acid residues in helical, β -structural and non-regular regions of globular proteins. *J. Mol. Biol.* 62, 613–624. [https://doi.org/10.1016/0022-2836\(71\)90160-4](https://doi.org/10.1016/0022-2836(71)90160-4)
- Görmez, Y., Sabzekar, M., Aydın, Z., 2021. IGPRED: Combination of convolutional neural and graph convolutional networks for protein secondary structure prediction. *Proteins Struct. Funct. Bioinforma.* 89, 1277–1288. <https://doi.org/10.1002/prot.26149>
- Guo, Y., Li, W., Wang, B., Liu, H., Zhou, D., 2019. DeepACLSTM: deep asymmetric convolutional long short-term memory neural models for protein secondary structure prediction. *BMC Bioinformatics* 20, 341. <https://doi.org/10.1186/s12859-019-2940-0>
- Guo, Y., Wang, B., Li, W., Yang, B., 2018. Protein secondary structure prediction improved by recurrent neural networks integrated with two-dimensional convolutional neural networks. *J. Bioinform. Comput. Biol.* 16, 1850021. <https://doi.org/10.1142/S021972001850021X>
- Guo, Z., Hou, J., Cheng, J., 2021. DNSS2: Improved ab initio protein secondary

- structure prediction using advanced deep learning architectures. *Proteins Struct. Funct. Bioinforma.* 89, 207–217. <https://doi.org/10.1002/prot.26007>
- Hanson, J., Paliwal, K., Litfin, T., Yang, Y., Zhou, Y., 2019. Improving prediction of protein secondary structure, backbone angles, solvent accessibility and contact numbers by using predicted contact maps and an ensemble of recurrent and residual convolutional neural networks. *Bioinformatics* 35, 2403–2410. <https://doi.org/10.1093/bioinformatics/bty1006>
- Heffernan, R., Paliwal, K., Lyons, J., Singh, J., Yang, Y., Zhou, Y., 2018. Single-sequence-based prediction of protein secondary structures and solvent accessibility by deep whole-sequence learning. *J. Comput. Chem.* 39, 2210–2216. <https://doi.org/10.1002/jcc.25534>
- Heffernan, R., Yang, Y., Paliwal, K., Zhou, Y., 2017. Capturing non-local interactions by long short-term memory bidirectional recurrent neural networks for improving prediction of protein secondary structure, backbone angles, contact numbers and solvent accessibility. *Bioinformatics* 33, 2842–2849. <https://doi.org/10.1093/bioinformatics/btx218>
- Holley, L.H., Karplus, M., 1989. Protein secondary structure prediction with a neural network. *Proc. Natl. Acad. Sci.* 86, 152–156. <https://doi.org/10.1073/pnas.86.1.152>
- Ismi, D.P., Pulungan, R., Afiahayati, 2024. Self-attention and asymmetric multi-layer perceptron-gated recurrent unit blocks for protein secondary structure prediction. *Appl. Soft Comput.* 159, 111604. <https://doi.org/10.1016/j.asoc.2024.111604>
- Ismi, D.P., Pulungan, R., Afiahayati, 2022. Deep learning for protein secondary structure prediction: Pre and post-AlphaFold. *Comput. Struct. Biotechnol. J.* 20, 6271–6286. <https://doi.org/10.1016/j.csbj.2022.11.012>
- IUPAC-IUB Commission on Biochemical Nomenclature, 1984. Nomenclature and Symbolism for Amino Acids and Peptides. *Eur. J. Biochem.* 138, 9–37. <https://doi.org/10.1111/j.1432-1033.1984.tb07877.x>
- Jumper, J., Evans, R., Pritzel, A., Green, T., Figurnov, M., Ronneberger, O., Tunyasuvunakool, K., Bates, R., Židek, A., Potapenko, A., Bridgland, A., Meyer, C., Kohl, S.A.A., Ballard, A.J., Cowie, A., Romera-Paredes, B., Nikolov, S., Jain, R., Adler, J., Back, T., Petersen, S., Reiman, D., Clancy, E., Zielinski, M., Steinegger, M., Pacholska, M., Berghammer, T., Bodenstein, S., Silver, D., Vinyals, O., Senior, A.W., Kavukcuoglu, K., Kohli, P., Hassabis, D., 2021. Highly accurate protein structure prediction with AlphaFold. *Nature* 596, 583–589. <https://doi.org/10.1038/s41586-021-03819-2>
- Kabsch, W., Sander, C., 1983. Dictionary of protein secondary structure: Pattern recognition of hydrogen-bonded and geometrical features. *Biopolymers* 22, 2577–2637. <https://doi.org/10.1002/bip.360221211>
- Khan, S., Qayyum, A., 2007. Measures of monetary policy stance: The case of Pakistan. *PIDE Work. Pap.* 1–18.
- Klausen, M.S., Jespersen, M.C., Nielsen, H., Jensen, K.K., Jurtz, V.I., Sønderby, C.K., Sommer, M.O.A., Winther, O., Nielsen, M., Petersen, B., Marcatili, P., 2019. NetSurfP-2.0: Improved prediction of protein structural features by integrated deep learning. *Proteins Struct. Funct. Bioinforma.* 87, 520–527. <https://doi.org/10.1002/prot.25674>
- Kotowski, K., Smolarczyk, T., Roterman-Konieczna, I., Stapor, K., 2021.

- ProteinUnet—An efficient alternative to SPIDER3-single for sequence-based prediction of protein secondary structures. *J. Comput. Chem.* 42, 50–59. <https://doi.org/10.1002/jcc.26432>
- Kumar, P., Bankapur, S., Patil, N., 2020. An enhanced protein secondary structure prediction using deep learning framework on hybrid profile based features. *Appl. Soft Comput.* 86, 105926. <https://doi.org/10.1016/j.asoc.2019.105926>
- Li, B., Krishnan, V.G., Mort, M.E., Xin, F., Kamati, K.K., Cooper, D.N., Mooney, S.D., Radivojac, P., 2009. Automated inference of molecular mechanisms of disease from amino acid substitutions. *Bioinformatics* 25, 2744–2750. <https://doi.org/10.1093/bioinformatics/btp528>
- Liu, Z., Gong, Y., Bao, Y., Guo, Y., Wang, H., Lin, G.N., 2021. TMPSS: A Deep Learning-Based Predictor for Secondary Structure and Topology Structure Prediction of Alpha-Helical Transmembrane Proteins. *Front. Bioeng. Biotechnol.* 8. <https://doi.org/10.3389/fbioe.2020.629937>
- Lyu, Z., Wang, Z., Luo, F., Shuai, J., Huang, Y., 2021. Protein Secondary Structure Prediction With a Reductive Deep Learning Method. *Front. Bioeng. Biotechnol.* 9, 687426. <https://doi.org/10.3389/fbioe.2021.687426>
- Moffat, L., Jones, D.T., 2021. Increasing the accuracy of single sequence prediction methods using a deep semi-supervised learning framework. *Bioinformatics* 37, 3744–3751. <https://doi.org/10.1093/bioinformatics/btab491>
- Mohamed Mufassirin, M.M., Newton, M.A.H., Rahman, J., Sattar, A., 2023. Multi-S3P: Protein Secondary Structure Prediction With Specialized Multi-Network and Self-Attention-Based Deep Learning Model. *IEEE Access* 11, 57083–57096. <https://doi.org/10.1109/ACCESS.2023.3282702>
- Murzin, A.G., Brenner, S.E., Hubbard, T., Chothia, C., 1995. SCOP: A structural classification of proteins database for the investigation of sequences and structures. *J. Mol. Biol.* 247, 536–540. [https://doi.org/10.1016/S0022-2836\(05\)80134-2](https://doi.org/10.1016/S0022-2836(05)80134-2)
- Ozkan, S.B., Wu, G.A., Chodera, J.D., Dill, K.A., 2007. Protein folding by zipping and assembly. *Proc. Natl. Acad. Sci.* 104, 11987–11992. <https://doi.org/10.1073/pnas.0703700104>
- Plaxco, K.W., Simons, K.T., Baker, D., 1998. Contact order, transition state placement and the refolding rates of single domain proteins1. *J. Mol. Biol.* 277, 985–994. <https://doi.org/10.1006/jmbi.1998.1645>
- Radivojac, P., Iakoucheva, L.M., Oldfield, C.J., Obradovic, Z., Uversky, V.N., Dunker, A.K., 2007. Intrinsic Disorder and Functional Proteomics. *Biophys. J.* 92, 1439–1456. <https://doi.org/10.1529/biophysj.106.094045>
- S., G., E.r., V., 2023. Protein Secondary Structure Prediction Using Cascaded Feature Learning Model. *Appl. Soft Comput.* 140, 110242. <https://doi.org/10.1016/j.asoc.2023.110242>
- Schaffhausen, J., 2012. Advances in structure-based drug design. *Trends Pharmacol. Sci.* 33, 223. <https://doi.org/10.1016/j.tips.2012.03.011>
- Schlessinger, A., Rost, B., 2005. Protein flexibility and rigidity predicted from sequence. *Proteins Struct. Funct. Bioinforma.* 61, 115–126. <https://doi.org/10.1002/prot.20587>
- Senior, A.W., Evans, R., Jumper, J., Kirkpatrick, J., Sifre, L., Green, T., Qin, C., Židek, A., Nelson, A.W.R., Bridgland, A., Penedones, H., Petersen, S., Simonyan, K., Crossan, S., Kohli, P., Jones, D.T., Silver, D., Kavukcuoglu, K., Hassabis, D., 2019. Protein structure prediction using multiple deep

- neural networks in the 13th Critical Assessment of Protein Structure Prediction (CASP13). *Proteins Struct. Funct. Bioinforma.* 87, 1141–1148. <https://doi.org/10.1002/prot.25834>
- Singh, Jaspreet, Litfin, T., Paliwal, K., Singh, Jaswinder, Hanumanthappa, A.K., Zhou, Y., 2021. SPOT-1D-Single: improving the single-sequence-based prediction of protein secondary structure, backbone angles, solvent accessibility and half-sphere exposures using a large training set and ensembled deep learning. *Bioinformatics* 37, 3464–3472. <https://doi.org/10.1093/bioinformatics/btab316>
- Stevens, A.O., He, Y., 2022. Benchmarking the Accuracy of AlphaFold 2 in Loop Structure Prediction. *Biomolecules* 12, 985. <https://doi.org/10.3390/biom12070985>
- Su, C., 2006. *Bioinformatics: A Practical Guide to the Analysis of Genes & Proteins*, (third edition). Edited by Andreas D. Baxevanis and B.F. Francis Ouellette. New York: John Wiley & Sons; ISBN: 0471 478784; 540pp.; 2004; \$79.95. *Brief. Bioinform.* 7, 123–124. <https://doi.org/10.1093/bib/bbk012>
- Sussman, J.L., Lin, D., Jiang, J., Manning, N.O., Prilusky, J., Ritter, O., Abola, E.E., 1998. Protein Data Bank (PDB): Database of Three-Dimensional Structural Information of Biological Macromolecules. *Acta Crystallogr. D Biol. Crystallogr.* 54, 1078–1084. <https://doi.org/10.1107/S0907444998009378>
- Tai, C.-H., Bai, H., Taylor, T.J., Lee, B., 2014. Assessment of template-free modeling in CASP10 and ROLL. *Proteins Struct. Funct. Bioinforma.* 82, 57–83. <https://doi.org/10.1002/prot.24470>
- Teng, S., Wang, L., Srivastava, A.K., Schwartz, C.E., Alexov, E., 2010. Structural Assessment of the Effects of Amino Acid Substitutions on Protein Stability and Protein-Protein Interaction. *Int. J. Comput. Biol. Drug Des.* 3, 334–349. <https://doi.org/10.1504/IJCBDD.2010.038396>
- Uddin, M.R., Mahbub, S., Rahman, M.S., Bayzid, M.S., 2020. SAINT: self-attention augmented inception-inside-inception network improves protein secondary structure prediction. *Bioinformatics* 36, 4599–4608. <https://doi.org/10.1093/bioinformatics/btaa531>
- Wang, S., Peng, J., Ma, J., Xu, J., 2016. Protein Secondary Structure Prediction Using Deep Convolutional Neural Fields. *Sci. Rep.* 6, 18962. <https://doi.org/10.1038/srep18962>
- Whittle, P.J., Blundell, T.L., 1994. Protein Structure-Based Drug Design. *Annu. Rev. Biophys.* 23, 349–375. <https://doi.org/10.1146/annurev.bb.23.060194.002025>
- Wilson, C.J., Choy, W.-Y., Karttunen, M., 2022. AlphaFold2: A Role for Disordered Protein/Region Prediction? *Int. J. Mol. Sci.* 23, 4591. <https://doi.org/10.3390/ijms23094591>
- Xu, G., Wang, Q., Ma, J., 2020. OPUS-TASS: a protein backbone torsion angles and secondary structure predictor based on ensemble neural networks. *Bioinformatics* 36, 5021–5026. <https://doi.org/10.1093/bioinformatics/btaa629>
- Yang, W., Hu, Z., Zhou, L., Jin, Y., 2022. Protein secondary structure prediction using a lightweight convolutional network and label distribution aware margin loss. *Knowl.-Based Syst.* 237, 107771. <https://doi.org/10.1016/j.knosys.2021.107771>
- Yang, Y., Gao, J., Wang, J., Heffernan, R., Hanson, J., Paliwal, K., Zhou, Y., 2018. Sixty-five years of the long march in protein secondary structure prediction:



- the final stretch? *Brief. Bioinform.* 19, 482–494.
<https://doi.org/10.1093/bib/bbw129>
- Yuan, Q., Chen, S., Rao, J., Zheng, S., Zhao, H., Yang, Y., 2021. AlphaFold2-aware protein-DNA binding site prediction using graph transformer.
<https://doi.org/10.1101/2021.08.25.457661>
- Yue, P., Li, Z., Moulton, J., 2005. Loss of Protein Structure Stability as a Major Causative Factor in Monogenic Disease. *J. Mol. Biol.* 353, 459–473.
<https://doi.org/10.1016/j.jmb.2005.08.020>
- Zeng, Y., Wei, Z., Yuan, Q., Chen, S., Yu, W., Lu, Y., Gao, J., Yang, Y., 2023. Identifying B-cell epitopes using AlphaFold2 predicted structures and pretrained language model. *Bioinformatics* 39, btad187.
<https://doi.org/10.1093/bioinformatics/btad187>
- Zhang, B., Li, J., Lü, Q., 2018. Prediction of 8-state protein secondary structures by a novel deep learning architecture. *BMC Bioinformatics* 19, 293.
<https://doi.org/10.1186/s12859-018-2280-5>
- Zhou, J., Wang, H., Zhao, Z., Xu, R., Lu, Q., 2018. CNNH_PSS: protein 8-class secondary structure prediction by convolutional neural network with highway. *BMC Bioinformatics* 19, 60.
<https://doi.org/10.1186/s12859-018-2067-8>
- Zhou, Y., Duan, Y., Yang, Y., Faraggi, E., Lei, H., 2011. Trends in template/fragment-free protein structure prediction. *Theor. Chem. Acc.* 128, 3–16. <https://doi.org/10.1007/s00214-010-0799-2>
- Zhou, Y., Karplus, M., 1999. Interpreting the folding kinetics of helical proteins. *Nature* 401, 400–403. <https://doi.org/10.1038/43940>