BIBLIOGRAPHY

Goal 1

- **Explore profound significance of Deep Learning**
- **Introduce AlphaFold for structure prediction.**
- **Application of AlphaFold in competitive binding studies**

1. Senior, A. W. *et al.* Improved protein structure prediction using potentials from deep learning. *Nature* **577**, 706–710 (2020).
2. Jumper, J. *et al.* Highly accurate protein structure prediction with AlphaFold. *Nature* **596**, 583–589 (2021).
3. Chang, L. & Perez, A. Ranking Peptide Binders by Affinity with AlphaFold**. *Angew. Chem. Int. Ed.* **62**, e202213362 (2023).
4. Tsaban, T. *et al.* Harnessing protein folding neural networks for peptide–protein docking. *Nat Commun* **13**, 176 (2022).
5. Kryshtafovych, A., Schwede, T., Topf, M., Fidelis, K. & Moult, J. Critical assessment of methods of protein structure prediction (CASP)—Round XIII. *Proteins Struct Funct Bioinform* **87**, 1011–1020 (2019).

Goal 2

- **Understand why Peptides as drugs.**
- **Pros and cons of peptide-based drugs compared to small molecules.**

1. Fosgerau, K. & Hoffmann, T. Peptide therapeutics: current status and future directions. *Drug Discov Today* **20**, 122–128 (2015)
2. Muttenthaler, M., King, G. F., Adams, D. J. & Alewood, P. F. Trends in peptide drug discovery. *Nat Rev Drug Discov* **20**, 309–325 (2021).

Goal 3

- **Learn why we need rational design approach.**

1. Vanhee, P. *et al.* Computational design of peptide ligands. *Trends Biotechnol* 29, 231–239 (2011).
2. Farhadi, T. & Hashemian, S. M. Computer-aided design of amino acid-based therapeutics: a review. *Drug Des Dev Ther* **12**, 1239–1254 (2018).

Goal 4

- **Read previous research on the system they will work to understand the chemistry and biology.**

A) BRD4 ET : LANA

1. Filippakopoulos, P. *et al.* Selective inhibition of BET bromodomains. *Nature* **468**, 1067–1073 (2010).
2. Crowe, B. L. *et al.* Structure of the Brd4 ET domain bound to a C-terminal motif from γ-retroviral integrases reveals a conserved mechanism of interaction. *Proc National Acad Sci* **113**, 2086–2091 (2016).
3. Zhang, Q. *et al.* Structural Mechanism of Transcriptional Regulator NSD3 Recognition by the ET Domain of BRD4. *Structure* **24**, 1201–1208 (2016).
4. Wang, N., Wu, R., Tang, D. & Kang, R. The BET family in immunity and disease. *Signal Transduct Target Ther* **6**, 23 (2021).
5. Cheung, K. L., Kim, C. & Zhou, M.-M. The Functions of BET Proteins in Gene Transcription of Biology and Diseases. *Frontiers Mol Biosci* **8**, 728777 (2021).
6. Mondal, A. *et al.* Structure Determination of Challenging Protein–Peptide Complexes Combining NMR Chemical Shift Data and Molecular Dynamics Simulations. *J Chem Inf Model* **63**, 2058–2072 (2023).

B) MDM2 : p53

1. Kussie, P. H. *et al.* Structure of the MDM2 oncoprotein bound to the p53 tumor suppressor transactivation domain. *Science (New York, NY)* **274**, 948 (1996).
2. MDM2/X: 1.Morrone, J. A. *et al*. Molecular Simulations Identify Binding Poses and Approximate Affinities of Stapled α-Helical Peptides to MDM2 and MDMX. *J Chem Theory Comput* **13**, 863–869 (2017).
3. Jiang, L. & Zawacka-Pankau, J. The p53/MDM2/MDMX-targeted therapies—a clinical synopsis. *Cell Death Dis* **11**, 237 (2020).
4. ElSawy, K. M., Lane, D. P., Verma, C. S. & Caves, L. S. D. Recognition Dynamics of p53 and MDM2: Implications for Peptide Design. *J Phys Chem B* **120**, 320–328 (2016).
5. Khoo, K. H., Hoe, K. K., Verma, C. S. & Lane, D. P. Drugging the p53 pathway: understanding the route to clinical efficacy. *Nat Rev Drug Discov* **13**, 217–236 (2014).
6. Moll, U. M. & Petrenko, O. The MDM2-p53 interaction. *Molecular cancer research : MCR* **1**, 1001–1008 (2003).

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