Universidad Nacional de San Agustín

Tópicos en Computación Gráfica

Final project proposal

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- Protein structure prediction
- Contact map
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Overview

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Definitions

Proteomics is the large-scale study of proteins [1]

Proteins are large, complex molecules that play many critical roles in the body. They do most of the work in cells. [1]

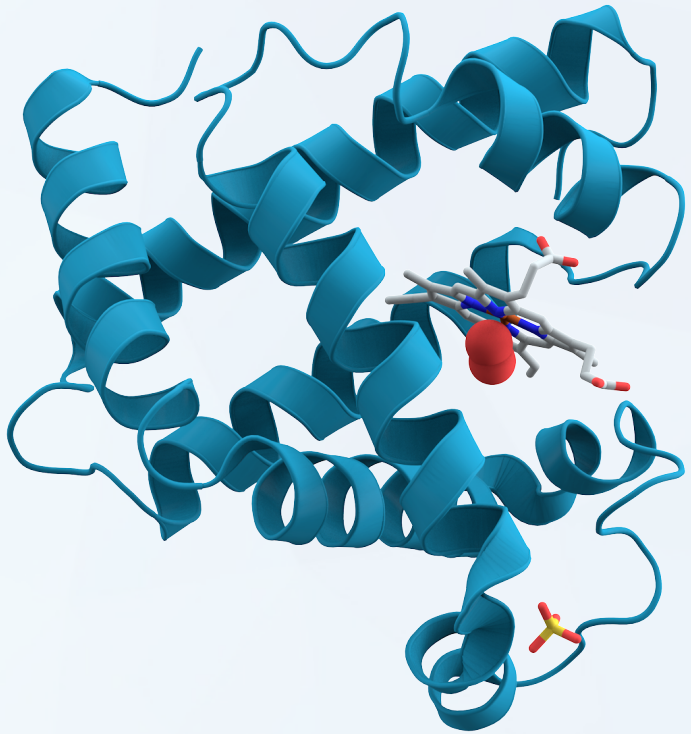


Figure: A representation of the 3D structure of the protein myoglobin. Source: PDB .

Protein structure

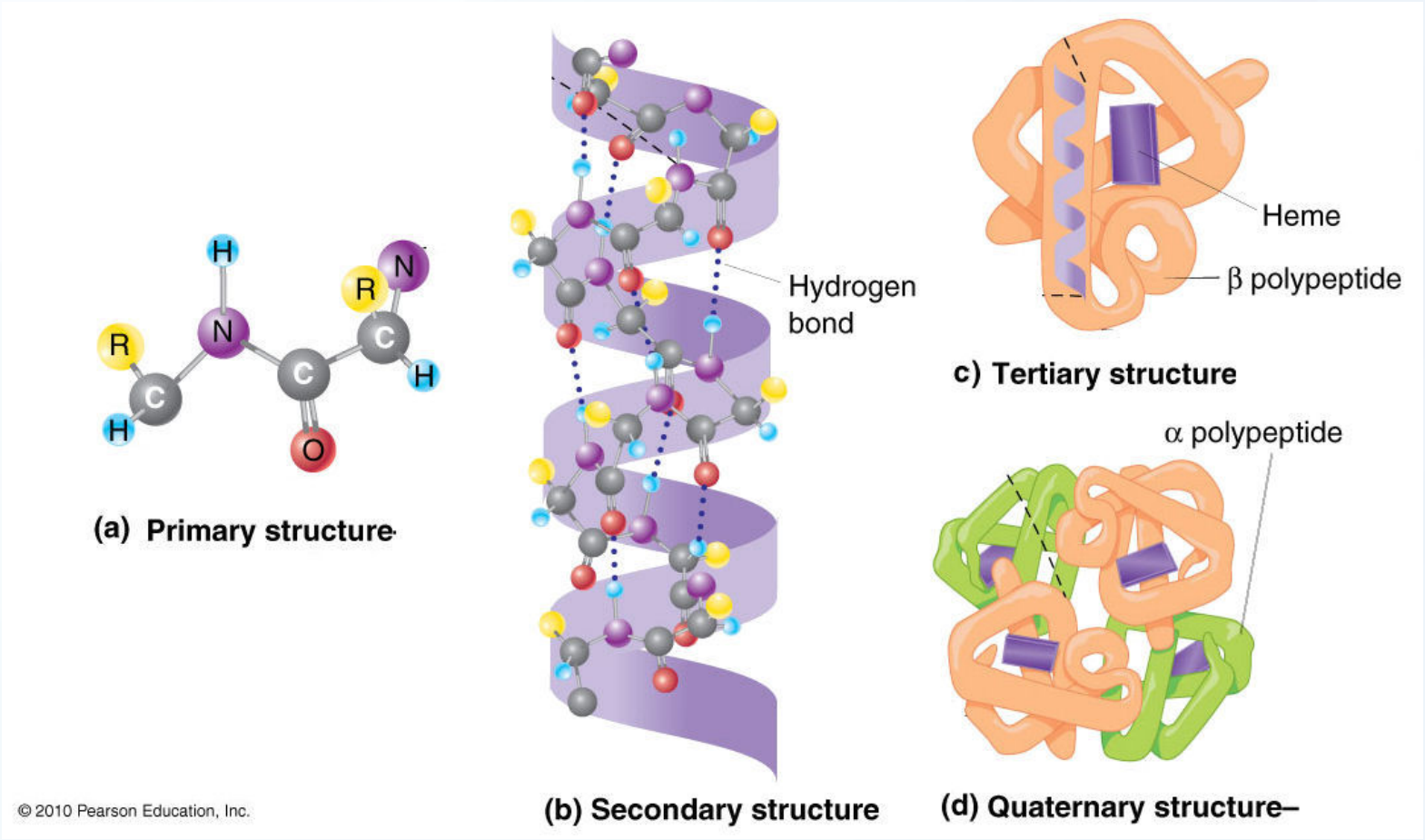


Figure: Types of protein structures. Source: [2].

Protein structure
SARS-CoV-2

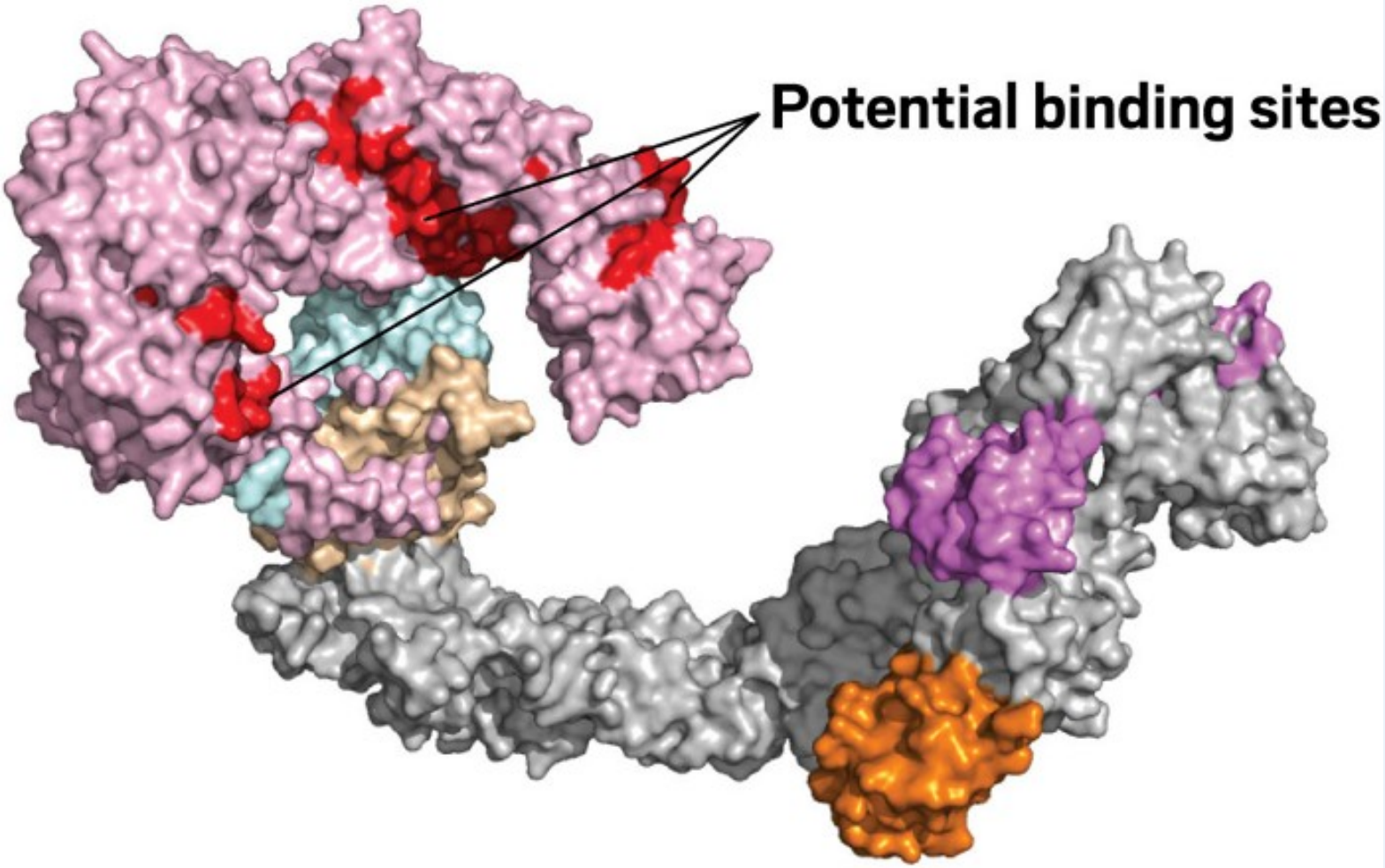


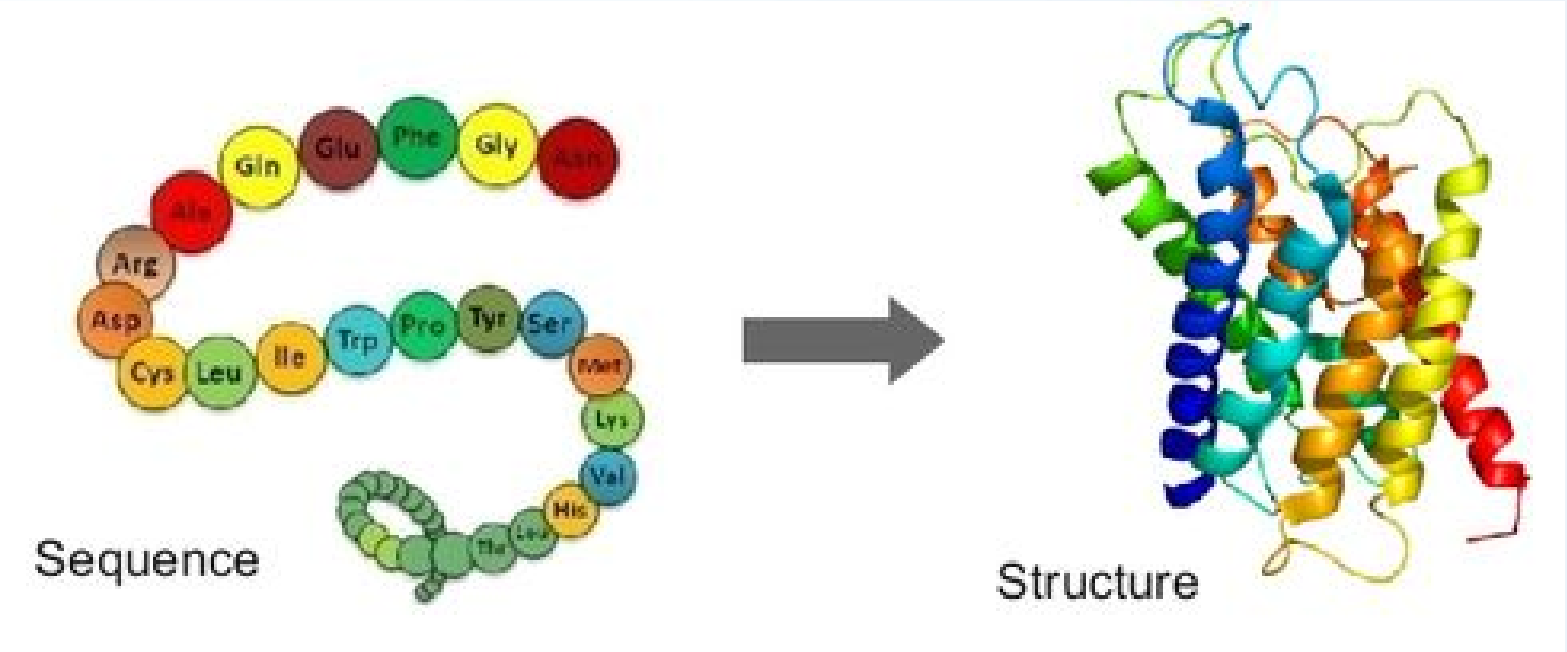
Figure: Example of SARS-CoV-2 protein structure. Source: CEn .

Numbers

Protein structures are complex systems with several tens, hundreds and **thounsand** of residues (amino acids).

Only about **1%** of the total number of sequenced proteins has experimentally determined. [3].

Protein structure prediction



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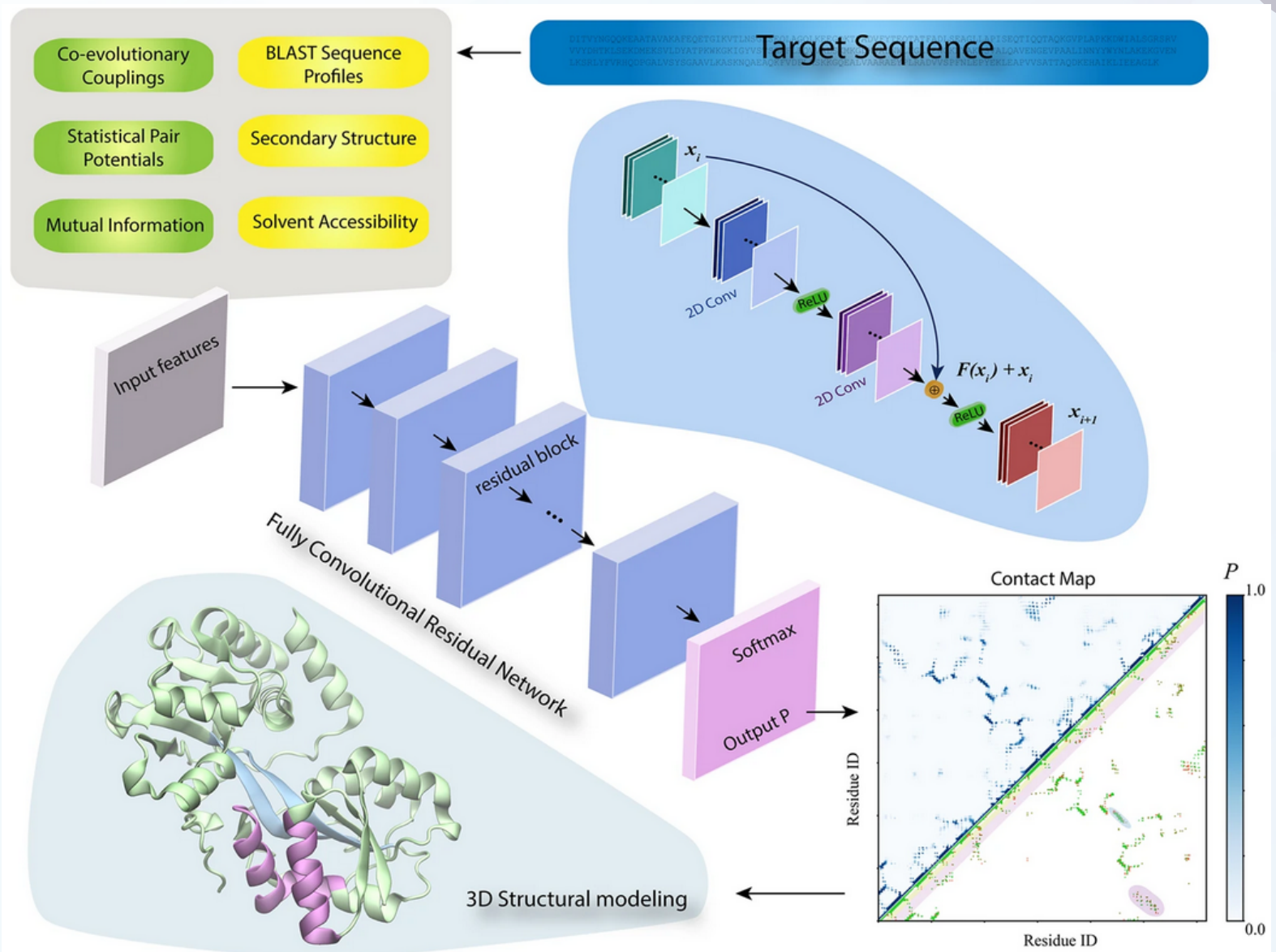
Protein structure prediction

DESTINI: A deep-learning approach to contact-driven protein structure prediction [4].

- **Year**: 2019
- **Authors**: Gao, Mu and Zhou, Hongyi and Skolnick, Jeffrey
- **Event**: Journal of Scientific reports

Protein structure prediction



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Contact map

3D model from contact map

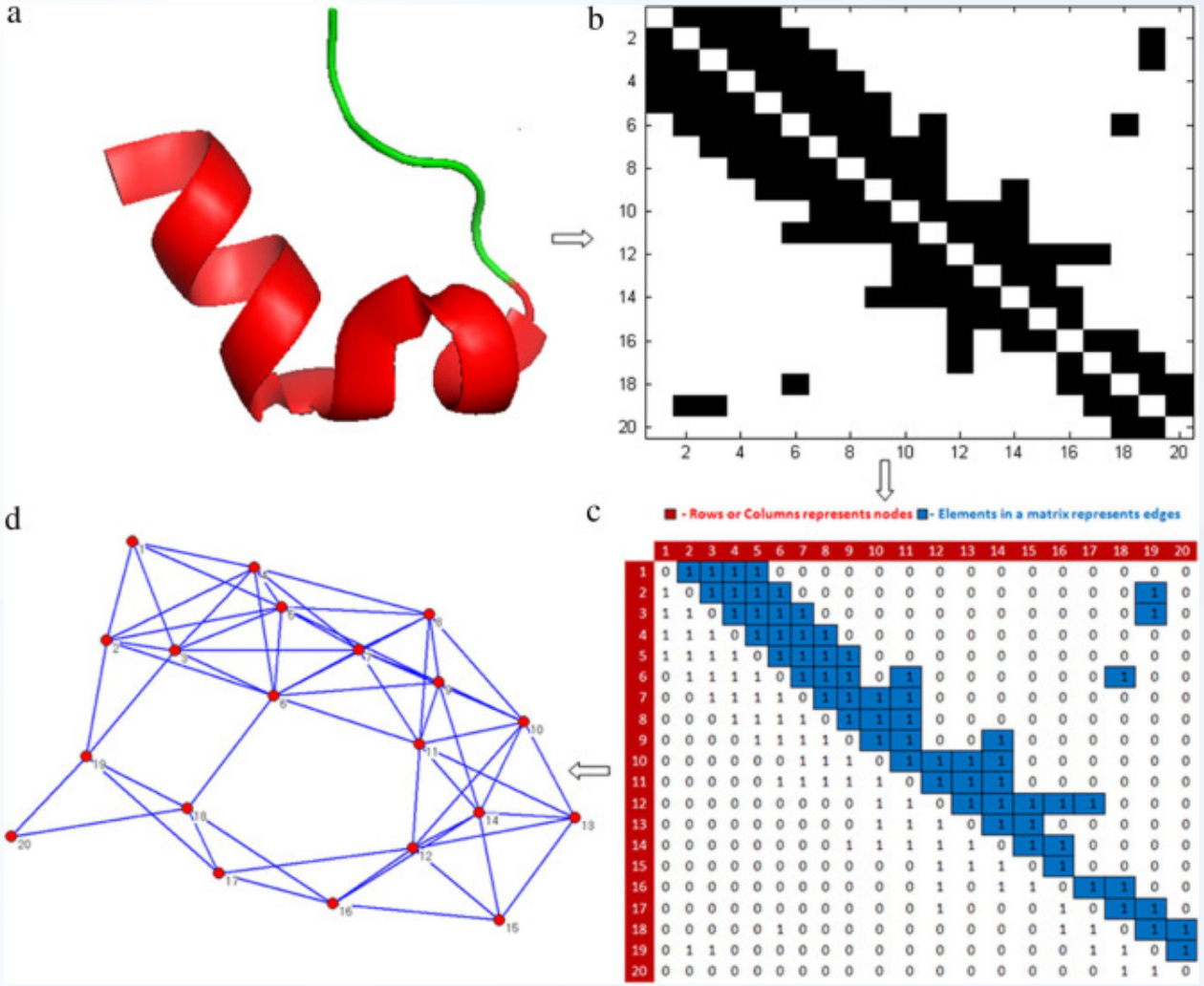

Figure: Contact map derive from 3D protein model. Source: [6].

Contact map
3D model from contact map

Reconstruct a 3D protein model from the contact map is challenging [6].

Methods are divided into *ad initio* and template-based [6].

Reconstruction of 3D Structures from Protein Contact Maps [7].

- **Year**: 2008
- **Authors**: Transactions on Computational Biology and Bioinformatics
- **Event**: BMC Bioinformatics

CONFOLD2: improved contact-driven ab initio protein structure modeling [8].

- **Year**: 2018
- **Authors**: Adhikari, Badri and Cheng, Jianlin
- **Event**: BMC Bioinformatics

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Deep learning extends de novo protein modelling coverage of genomes using iteratively predicted structural constraints [9].

- **Year**: 2019
- **Authors**: Greener, Joe G and Kandathil, Shaun M and Jones, David T
- **Event**: Nature communications
- **Repository**: git

Protein structure prediction using multiple deep neural networks in the 13th Critical Assessment of Protein Structure Prediction (CASP13) [10].

- **Year**: 2019
- **Authors**: Senior, Andrew W and Evans, ...
- **Event**: CASP13

References I

[1] N. L. Anderson and N. G. Anderson, “Proteome and proteomics: new technologies, new concepts, and new words,” *Electrophoresis*, vol. 19, no. 11, pp. 1853–1861, 1998.

[2] P. J. Russell and K. Gordey, *IGenetics*. Benjamin Cummings San Francisco, 2002, no. QH430 R87.

[3] H. Rangwala and G. Karypis, *Introduction to protein structure prediction: methods and algorithms*. John Wiley & Sons, 2011, vol. 18.

[4] M. Gao, H. Zhou, and J. Skolnick, “Destini: A deep-learning approach to contact-driven protein structure prediction,” *Scientific reports*, vol. 9, no. 1, pp. 1–13, 2019.

[5] R. Ando and C. Batty, “A practical octree liquid simulator with adaptive surface resolution,” *ACM Transactions on Graphics (TOG)*, vol. 39, no. 4, pp. 32–1, 2020.

References II

[6] I. A. Emerson and A. Amala, “Protein contact maps: A binary depiction of protein 3d structures,” *Physica A: Statistical Mechanics and its Applications*, vol. 465, pp. 782–791, 2017.

[7] M. Vassura, L. Margara, P. Di Lena, F. Medri, P. Fariselli, and R. Casadio, “Reconstruction of 3d structures from protein contact maps,” *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, vol. 5, no. 3, pp. 357–367, 2008.

[8] B. Adhikari and J. Cheng, “Confold2: improved contact-driven ab initio protein structure modeling,” *BMC bioinformatics*, vol. 19, no. 1, p. 22, 2018.

[9] J. G. Greener, S. M. Kandathil, and D. T. Jones, “Deep learning extends de novo protein modelling coverage of genomes using iteratively predicted structural constraints,” *Nature communications*, vol. 10, no. 1, pp. 1–13, 2019.

References III

[10] A. W. Senior, R. Evans, J. Jumper, J. Kirkpatrick, L. Sifre, T. Green, C. Qin, A. Žídek, A. W. Nelson, A. Bridgland *et al.*, "Protein structure prediction using multiple deep neural networks in the 13th critical assessment of protein structure prediction (casp13)," *Proteins: Structure, Function, and Bioinformatics*, vol. 87, no. 12, pp. 1141–1148, 2019.