Bioinformatics against COVID-19

Bioinformatics Research Group

MSc. Vicente Machaca Arceda

June 13, 2020

Overview

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Presentation

- MSc. Vicente Enrique Machaca Arceda.

Presentation

- MSc. Vicente Enrique Machaca Arceda.
- Professor at UNSA university.

Presentation

- MSc. Vicente Enrique Machaca Arceda.
- Professor at UNSA university.
- Full time researcher at La Salle university.

Presentation

- MSc. Vicente Enrique Machaca Arceda.
- Professor at UNSA university.
- Full time researcher at La Salle university.
- Leader of Bioinformatics Research Group in Arequipa.

Presentation
Publications

Year	Country	Title
2018	Brasil	Fast Car Crash Detection in Video
2016	Chile	Fast Face Detection in Violent Video Scenes
2016	Costa Rica	Real Time Violence Detection in Video with ViF and Horn-Schunck
2016	Costa Rica	Optimization model for face detection in video sequences
2015	Chile	Real Time Violence Detection in Video

Presentation
Publications

Year	Country	Title
2020		DNA sequence similarity analysis using Chaos Game Representation
2020		Machine Learning and Chaos Game Representation for rapid classification of novel pathogens COVID-19 case study
2020	Canada	An analysis of k-mer frequency features with machine learning models for viral subtyping of Polyomavirus and HIV-1 genomes
2020	Canada	Forecasting time series with Multiplicative Trend Exponential Smoothing and LSTM: COVID-19 case study
2020	USA	Small Ship Detection on Optical Satellite Imagery with YOLO and YOLT

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The purpose of Bioinformatics

Why a person has cancer?

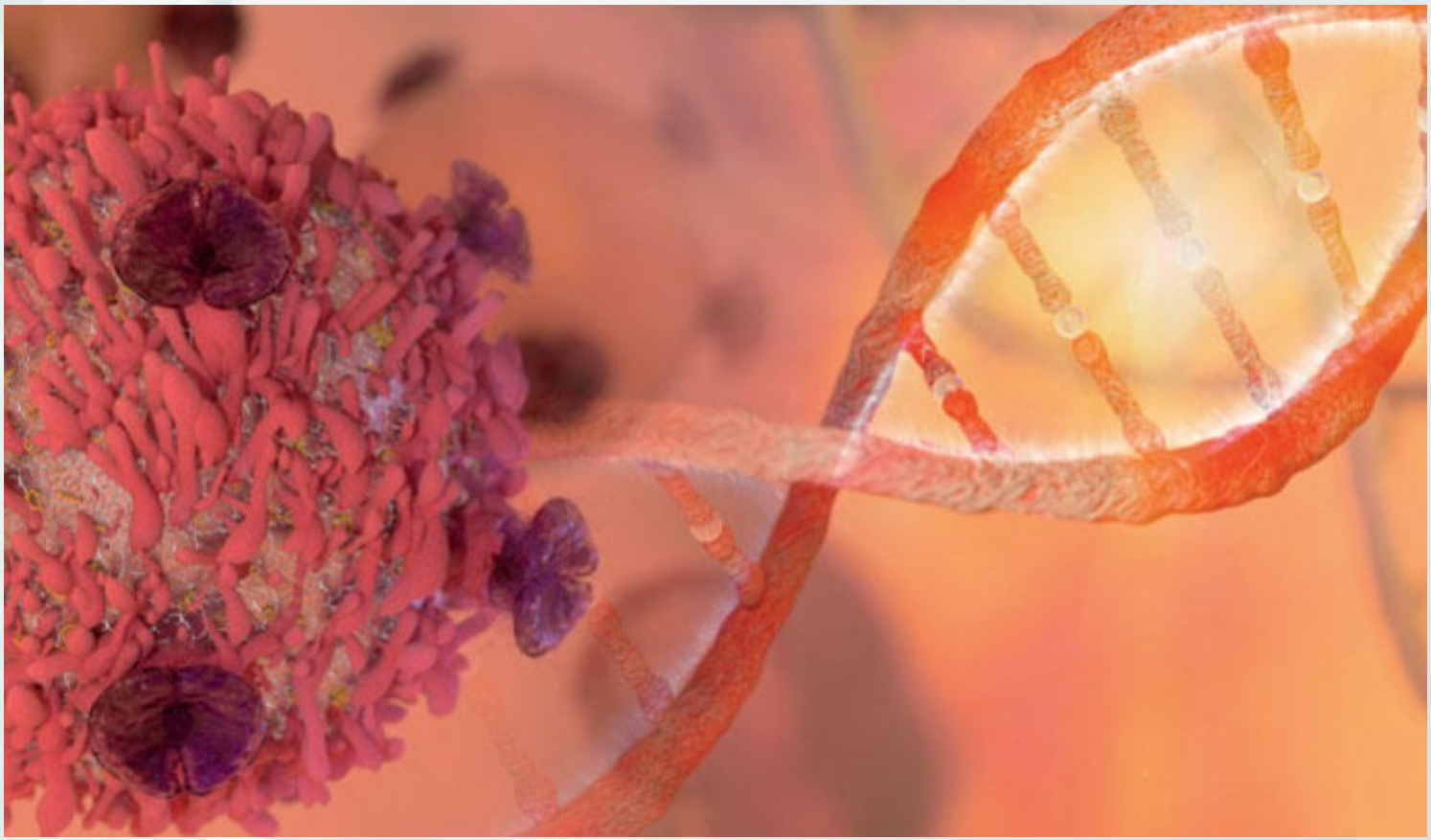

Figure: Why a person has cancer?

The purpose of Bioinformatics

Why some medicines no work in some persons?

Figure: Why some medicines no work in some persons?

The purpose of Bioinformatics
Treatment Development

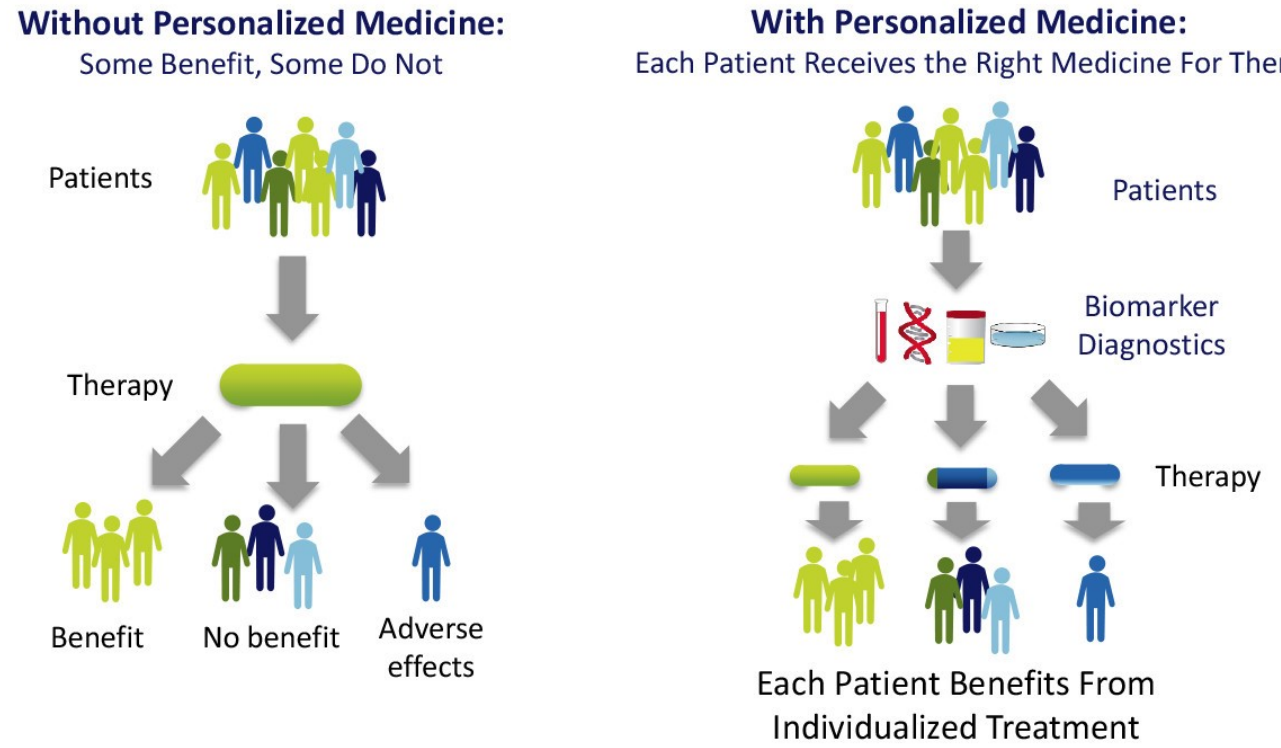

Figure: Personalized Medicine: New Approach to Treatment of Disease

The purpose of Bioinformatics

Protein structure prediction

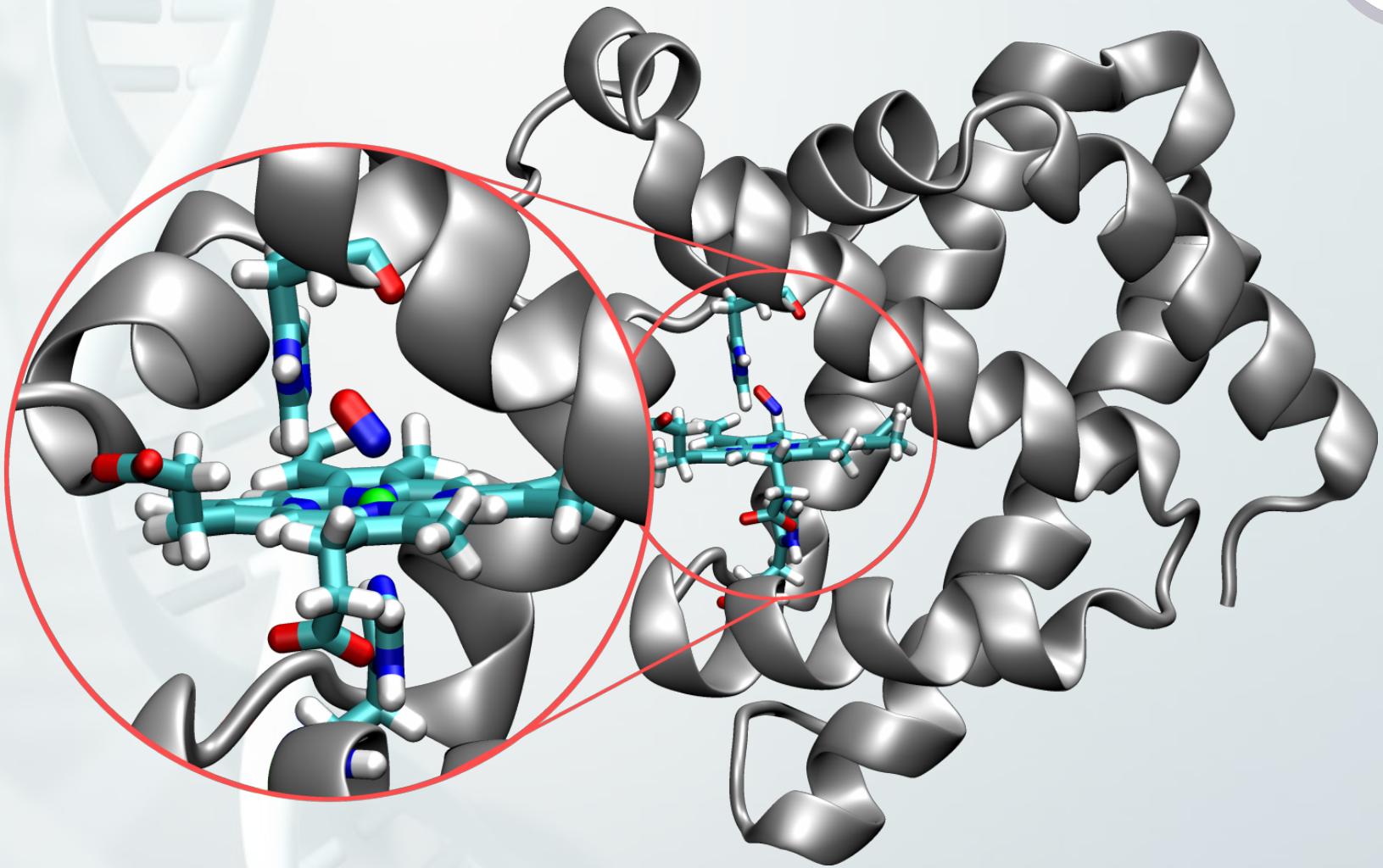

Figure: Computer simulation of protein-ligand.

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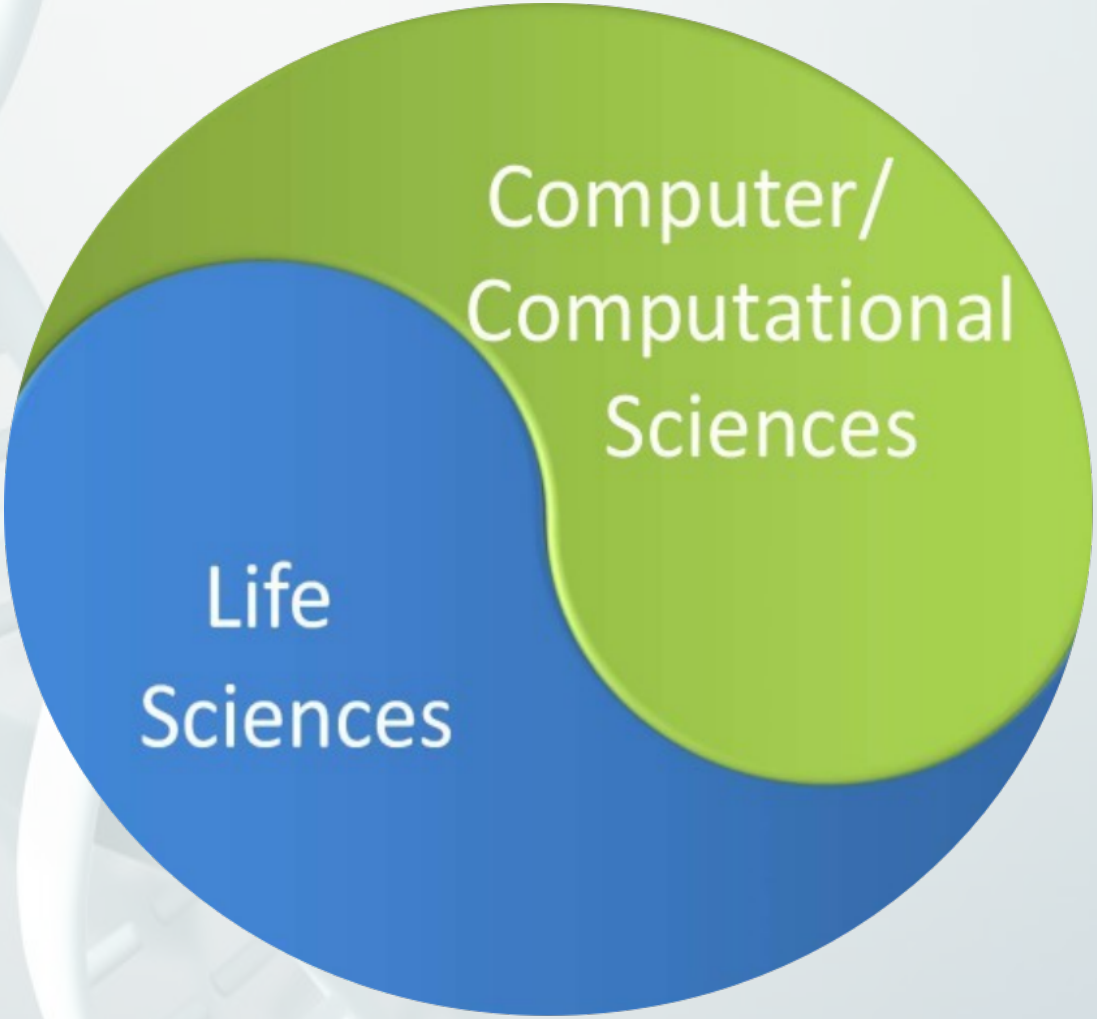
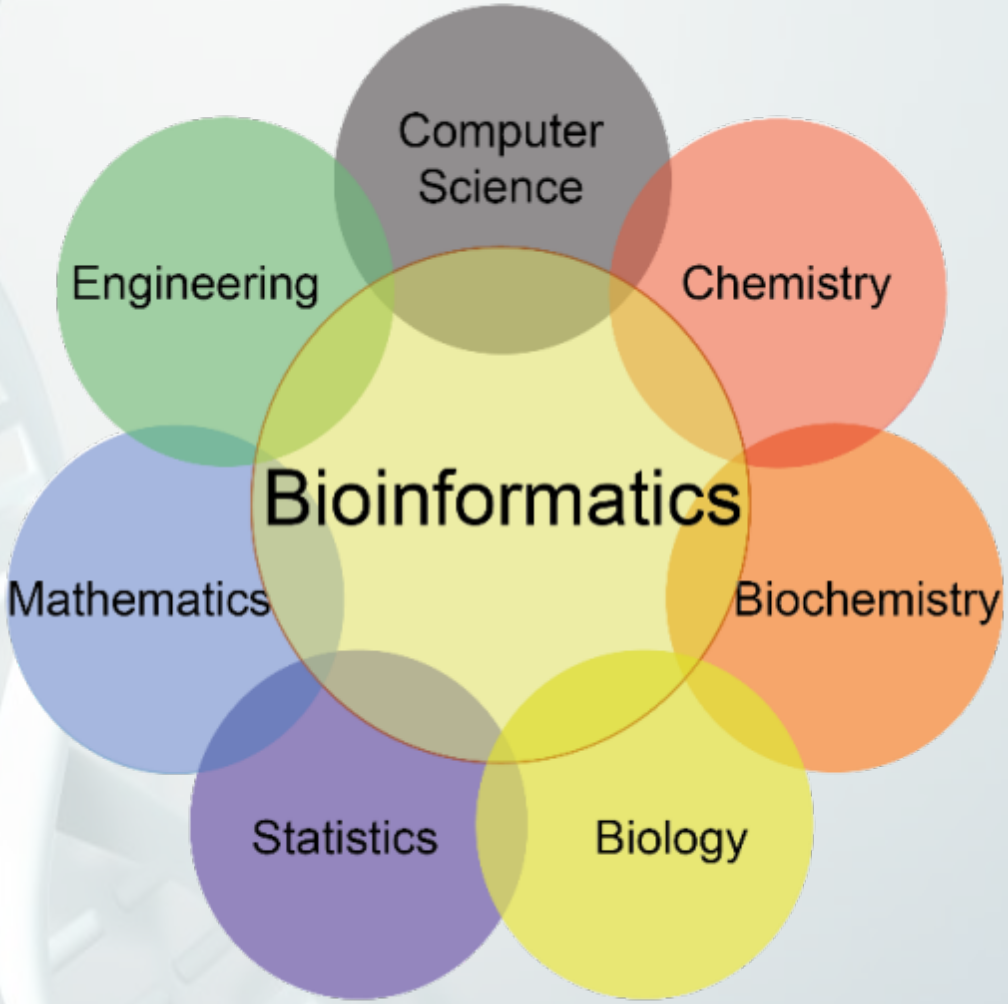
According to Luscombe et al.: **Bioinformatics** involves the technology that uses computers for storage, retrieval, manipulation, and distribution of information related to biological macromolecules such as DNA, RNA, and proteins [1].

Bioinformatics



Bioinformatics



Bioinformatics
Where is DNA located?

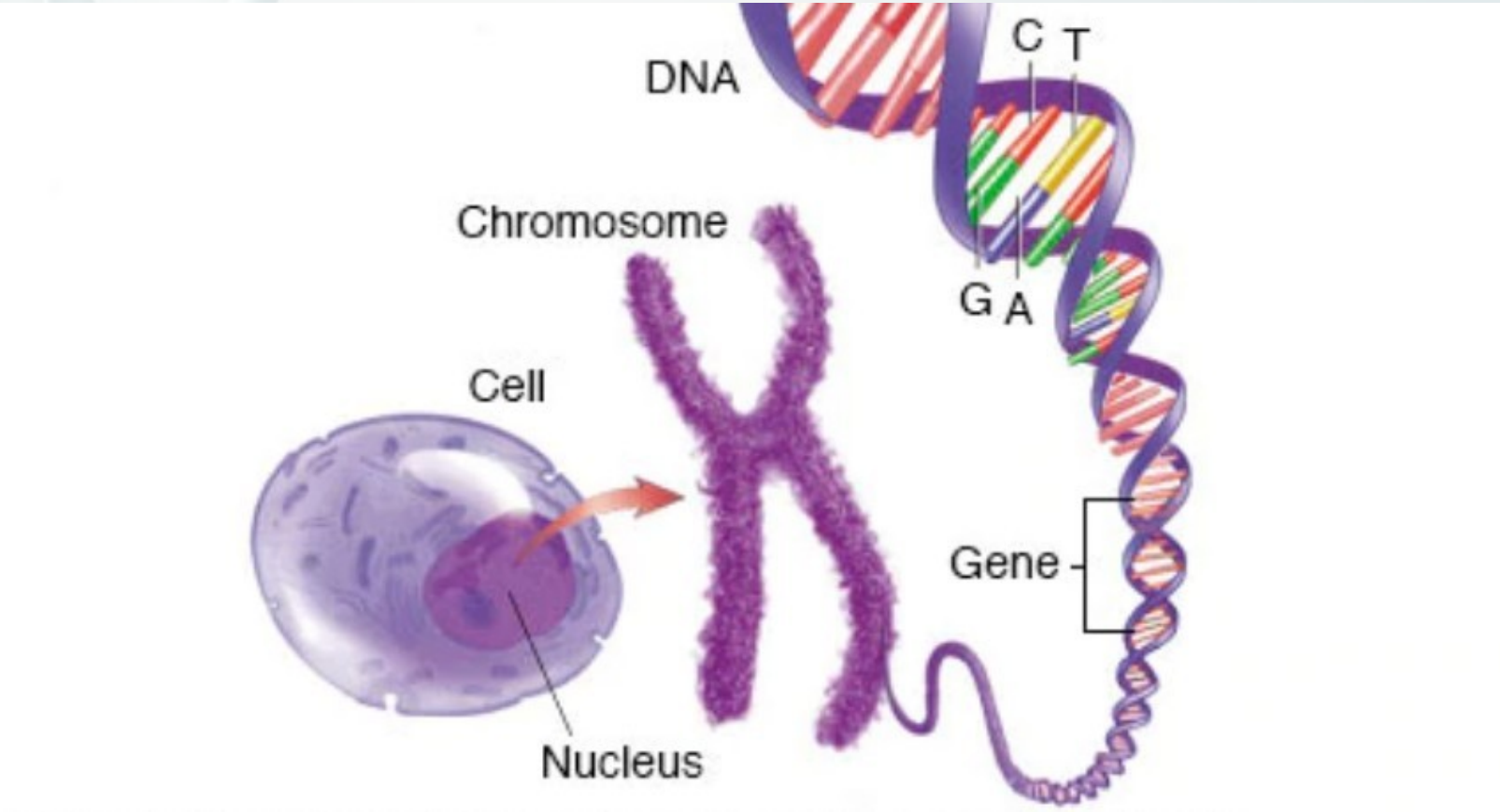


Figure: Where DNA is located [2].

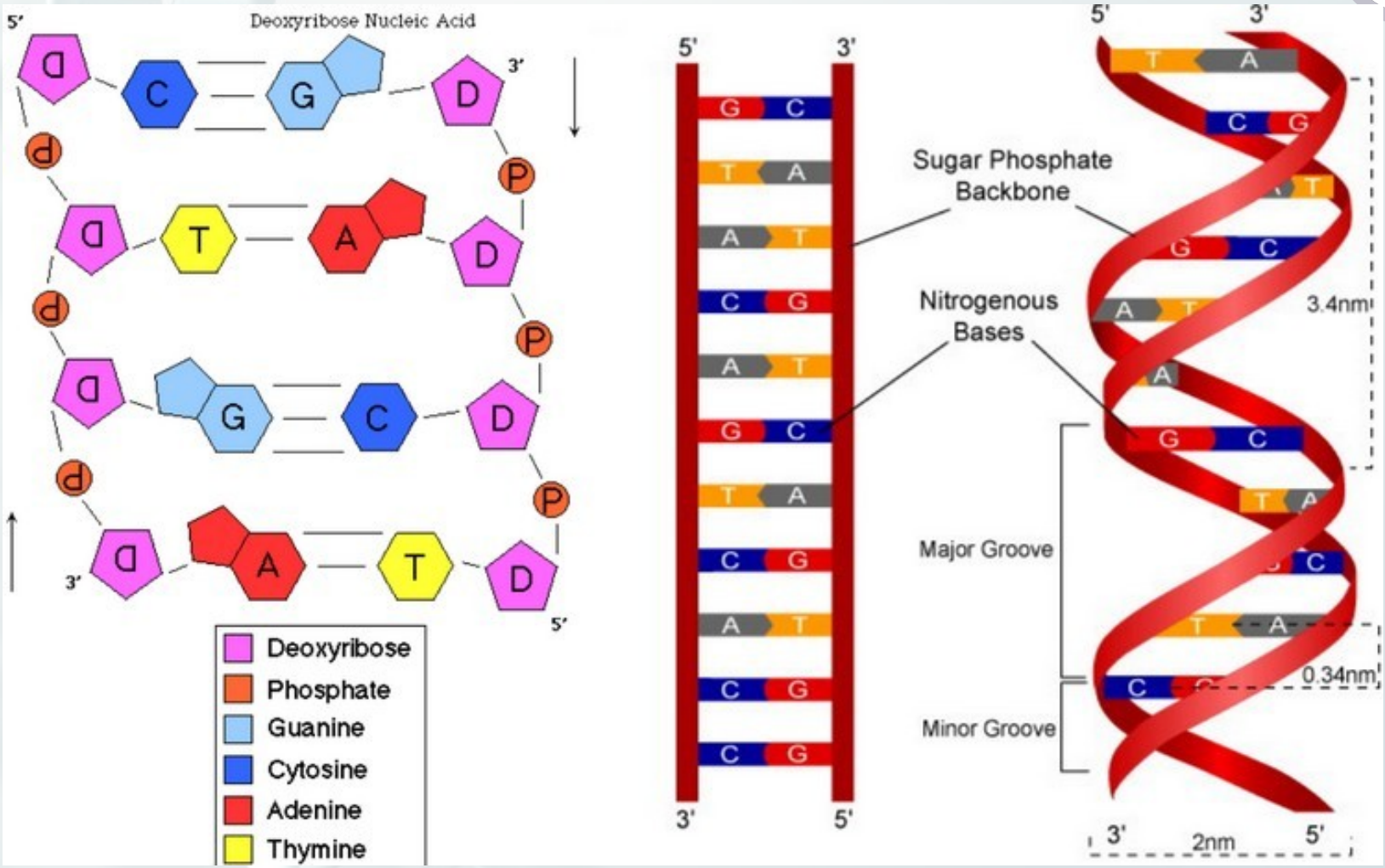


Figure: DNA structure [3].

The human genome is made of ~**3.2 billions bp** of DNA.
~6.4 billions of nucleotides [4].

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The HIV-1 genome is made of ~**20k bp** of DNA.
Meanwhile, the COVID-19 is made of ~**32k bp** [5].

The human genome is made of ~**3.2 billions bp** of DNA.
~6.4 billions of nucleotides [4].

The HIV-1 genome is made of ~**20k bp** of DNA.
Meanwhile, the COVID-19 is made of ~**32k bp** [5].

There are approximately **19000** to **25000** genes.
No one knows for sure [4].

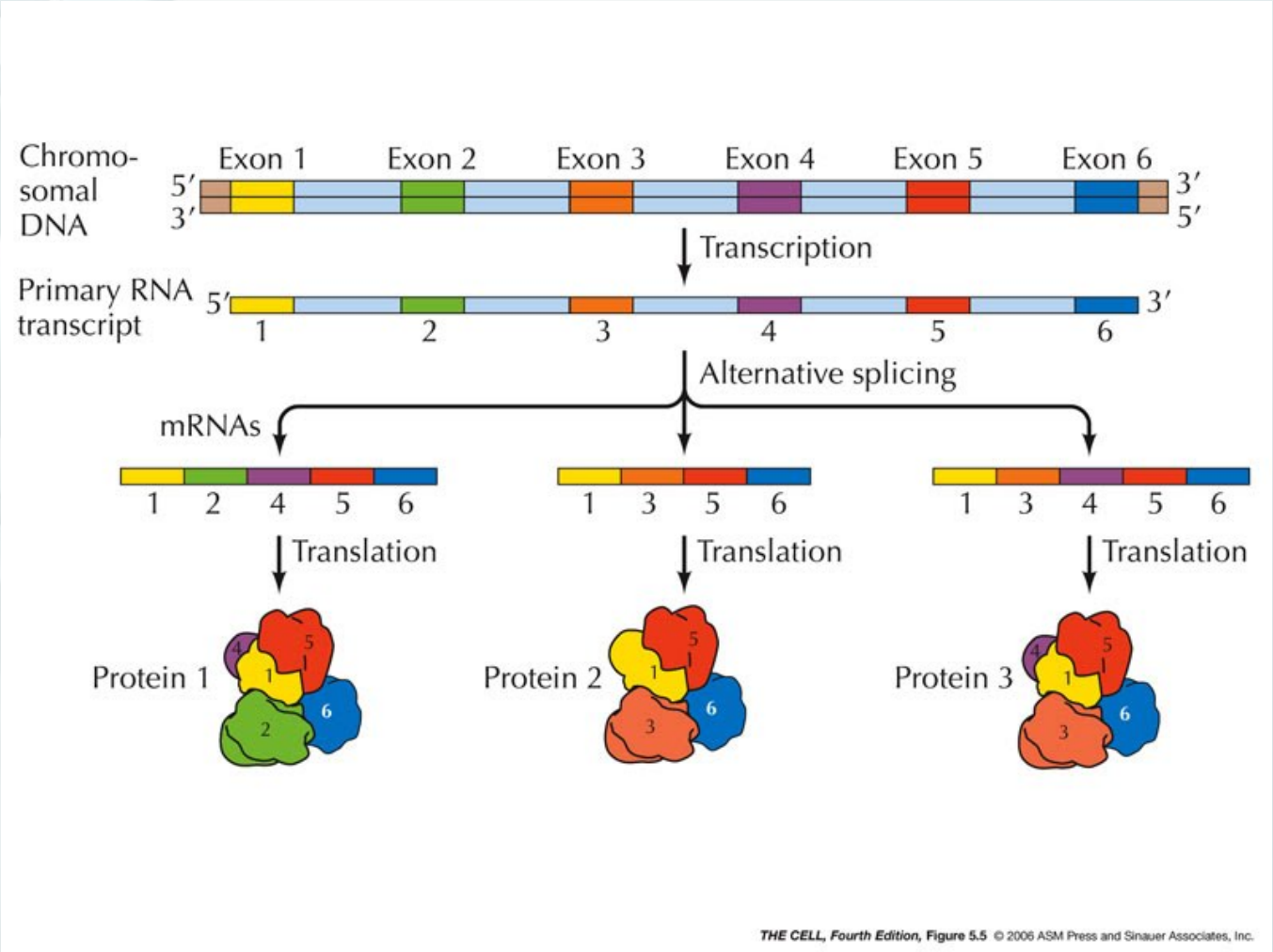

Figure: Alternative splicing [6].

Bioinformatics
Example of DNA sequence


```
>J01859.1 Escherichia coli 16S ribosomal RNA, complete sequence
AAATTGAAGAGTTTGATCATGGCTCAGATTGAACGCTGGCGGCAGGCCTAACACATGCAAGTCGAACGGT
AACAGGAAGAAGCTTGCTCTTTGCTGACGAGTGGCGGACGGGTGAGTAATGTCTGGGAAACTGCCTGATG
GAGGGGGATAACTACTGGAAACGGTAGCTAATACCGCATAACGTCGCAAGACCAAAGAGGGGGACCTTCG
GGCCTCTTGCCATCGGATGTGCCCAGATGGGATTAGCTAGTAGGTGGGGTAACGGCTCACCTAGGCGACG
ATCCCTAGCTGGTCTGAGAGGATGACCAGCCACACTGGAACTGAGACACGGTCCAGACTCCTACGGGAGG
CAGCAGTGGGGAATATTGCACAATGGGCGCAAGCCTGATGCAGCCATGCCGCGTGTATGAAGAAGGCCTT
CGGGTTGTAAAGTACTTTCAGCGGGGAGGAAGGGAGTAAAGTTAATACCTTTGCTCATTGACGTTACCCG
CAGAAGAAGCACCGGCTAACTCCGTGCCAGCAGCCGCGGTAATACGGAGGGTGCAAGCGTTAATCGGAAT
TACTGGGCGTAAAGCGCACGCAGGCGGTTTGTTAAGTCAGATGTGAAATCCCCGGGCTCAACCTGGGAAC
TGCATCTGATACTGGCAAGCTTGAGTCTCGTAGAGGGGGGTAGAATTCCAGGTGTAGCGGTGAAATGCGT
AGAGATCTGGAGGAATACCGGTGGCGAAGGCGGCCCCCTGGACGAAGACTGACGCTCAGGTGCGAAAGCG
TGGGGAGCAAACAGGATTAGATACCCTGGTAGTCCACGCCGTAAACGATGTCGACTTGGAGGTTGTGCCC
TTGAGGCGTGGCTTCCGGAGCTAACGCGTTAAGTCGACCGCCTGGGGAGTACGGCCGCAAGGTTAAAACT
CAAATGAATTGACGGGGGCCCGCACAAGCGGTGGAGCATGTGGTTTAATTCGATGCAACGCGAAGAACCT
TACCTGGTCTTGACATCCACGGAAGTTTTCAGAGATGAGAATGTGCCTTCGGGAACCGTGAGACAGGTGC
TGCATGGCTGTCGTCAGCTCGTGTTGTGAAATGTTGGGTTAAGTCCCGCAACGAGCGCAACCCTTATCCT
TTGTTGCCAGCGGTCCGGCCGGGAACTCAAAGGAGACTGCCAGTGATAAACTGGAGGAAGGTGGGGATGA
CGTCAAGTCATCATGGCCCTTACGACCAGGGCTACACACGTGCTACAATGGCGCATACAAAGAGAAGCGA
CCTCGCGAGAGCAAGCGGACCTCATAAAGTGCGTCGTAGTCCGGATTGGAGTCTGCAACTCGACTCCATG
AAGTCGGAATCGCTAGTAATCGTGGATCAGAATGCCACGGTGAATACGTTCCCGGGCCTTGTACACACCG
CCCGTCACACCATGGGAGTGGGTTGCAAAAGAAGTAGGTAGCTTAACCTTCGGGAGGGCGCTTACCACTT
TGTGATTCATGACTGGGGTGAAGTCGTAACAAGGTAACCGTAGGGGAACCTGCGGTTGGATCACCTCCTT
```

Figure: 16S ribosomal DNA of Escherichia coli with FASTA Format.

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COVID origin
Phylogenetic tree and BLAST

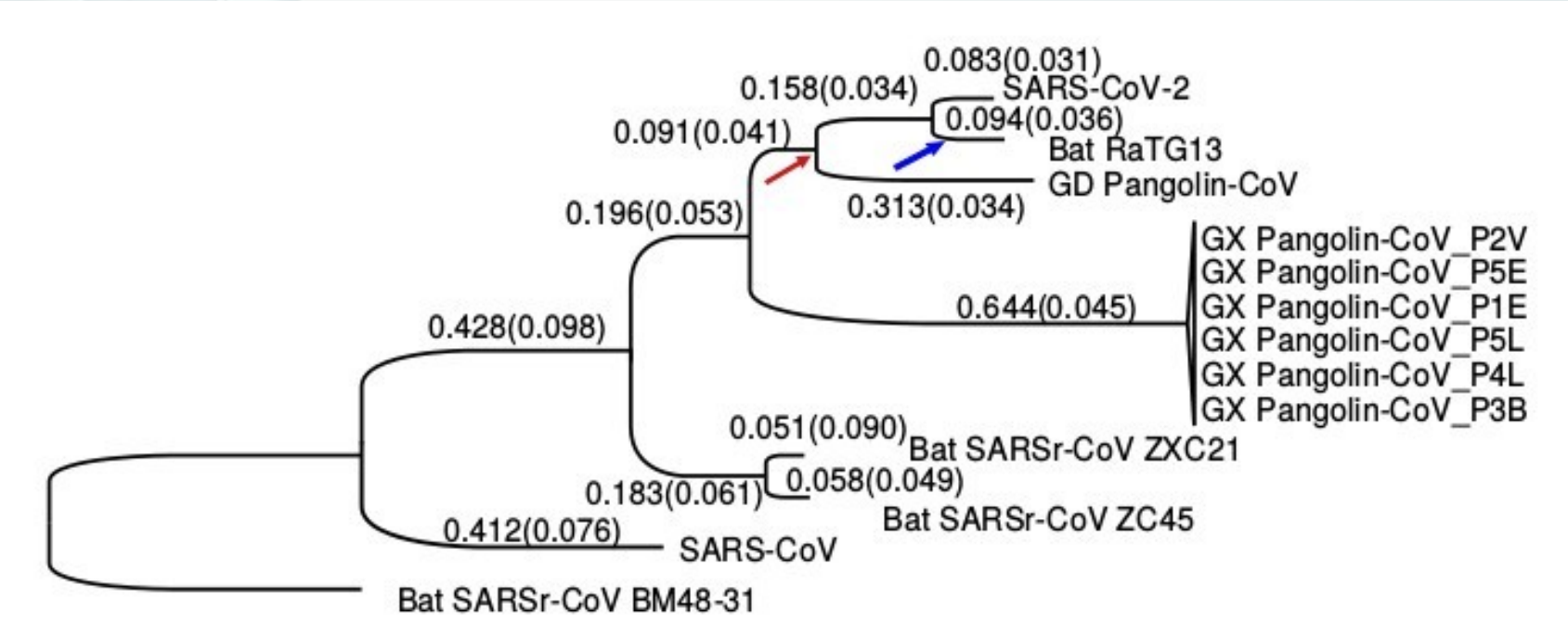

Figure: The phylogenetic tree of SARS-CoV-2 (COVID-19) and the related Coronaviruses [7].

COVID origin

Novel virus classification using alignment-free methods

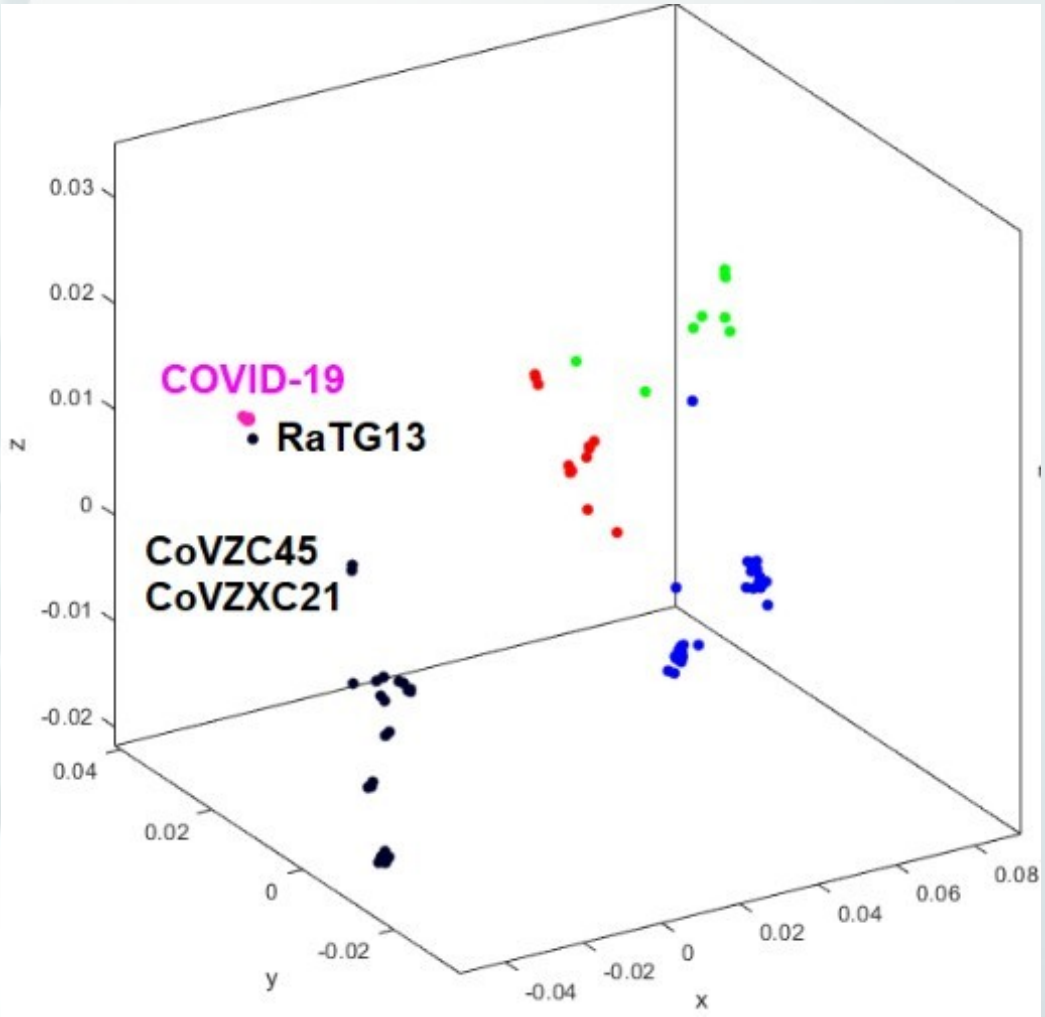

Figure: MoDMap3D of 124 Betacoronavirus sequences and COVID-19 [5].

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Definition

The prediction of protein three-dimensional structure from amino acid sequence [8].

Definition

The prediction of protein three-dimensional structure from amino acid sequence [8].

Methods

- X-ray crystallography.
- Nuclear magnetic resonance.
- Cryo-electron microscopy.

Protein structure prediction
Using computers

There are two aproaches to predicting protein structures:

- Homology modeling.
- Physical modeling.

Figure: Graphical view of COVID-19 structure. Source: [9]

Protein structure prediction
Proteins in COVID-19

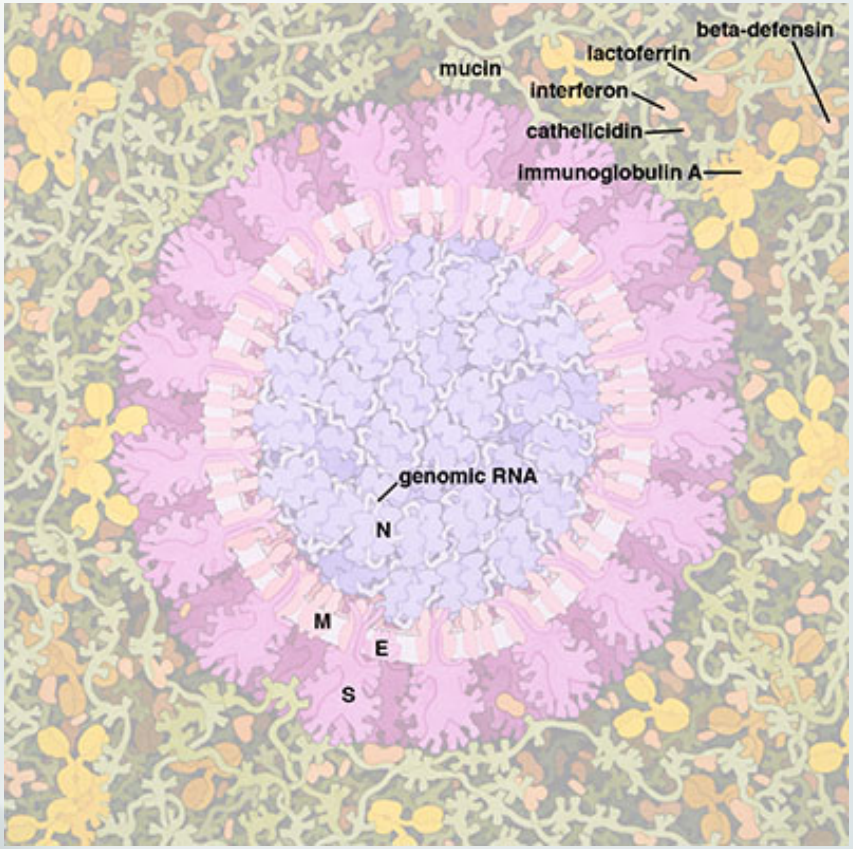

Figure: Membrane S (spike) protein, M (membrane) protein, membrane channel E (envelope) protein and the N (nucleocapsid) protein bound to the genomic RNA. Source: [9]

Protein structure prediction
AlphaFold method

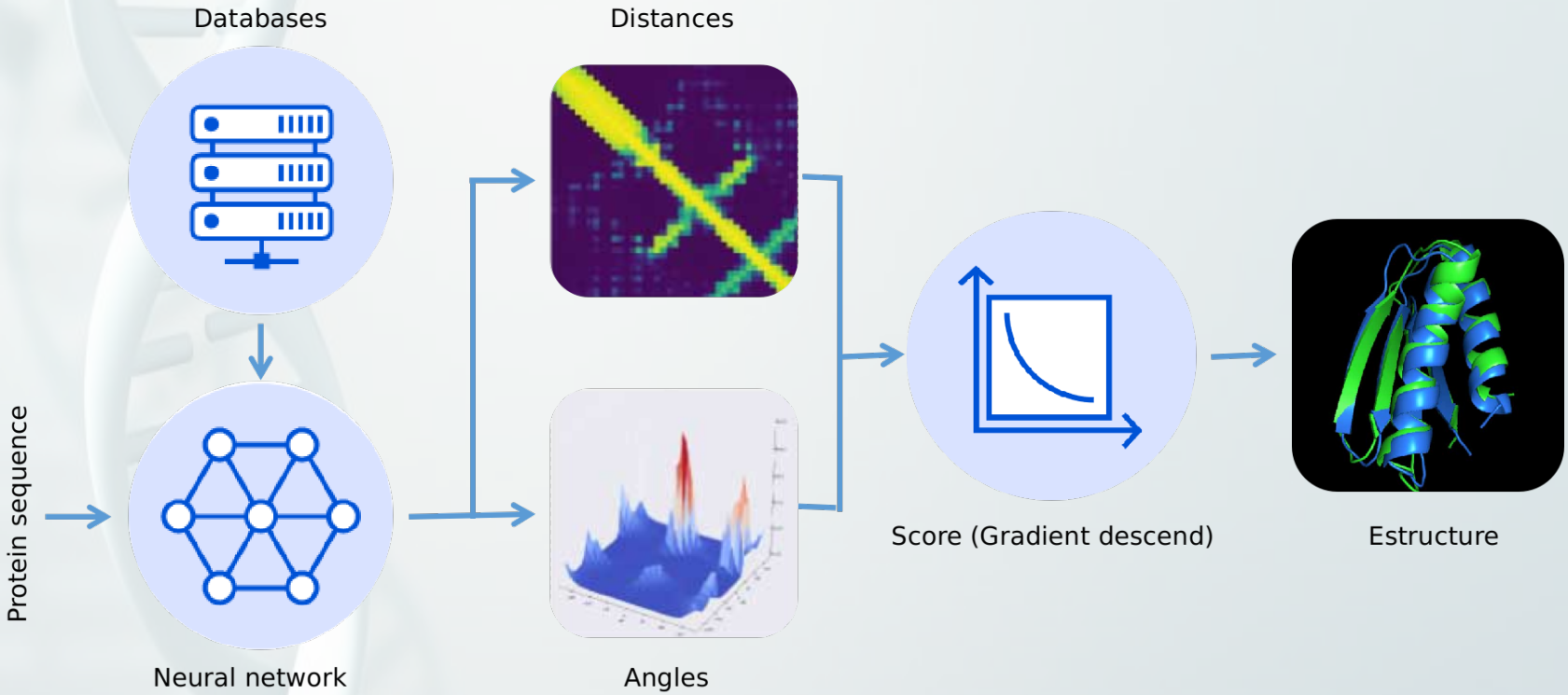

Figure: Protein structure prediction method proposed by AlphaFold. Source: [10]

Protein structure prediction
COVID-19 membrane protein

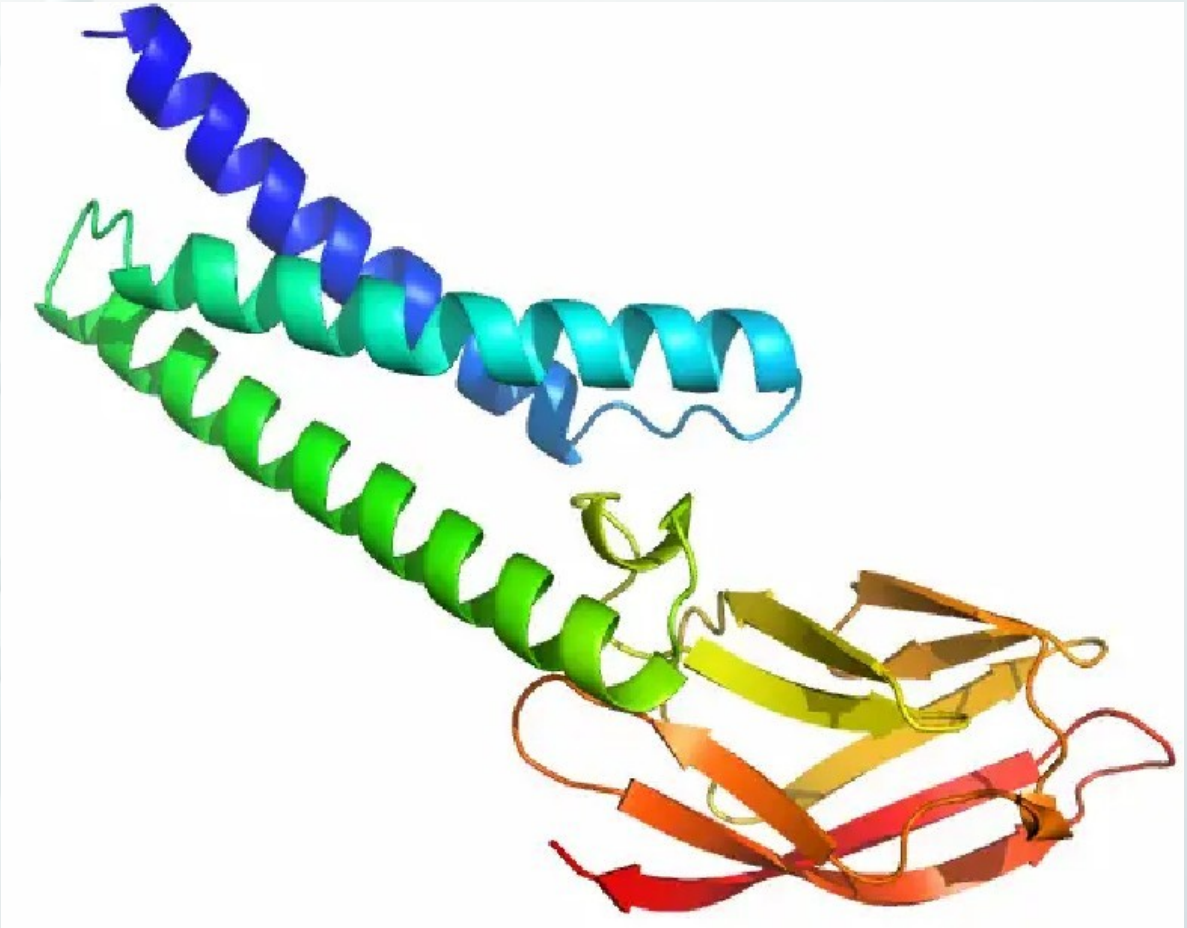

Figure: COVID-19 membrane protein. Source: [10]

Protein structure prediction

Tertiary representations of the S1 and S2 subunits of the spike protein

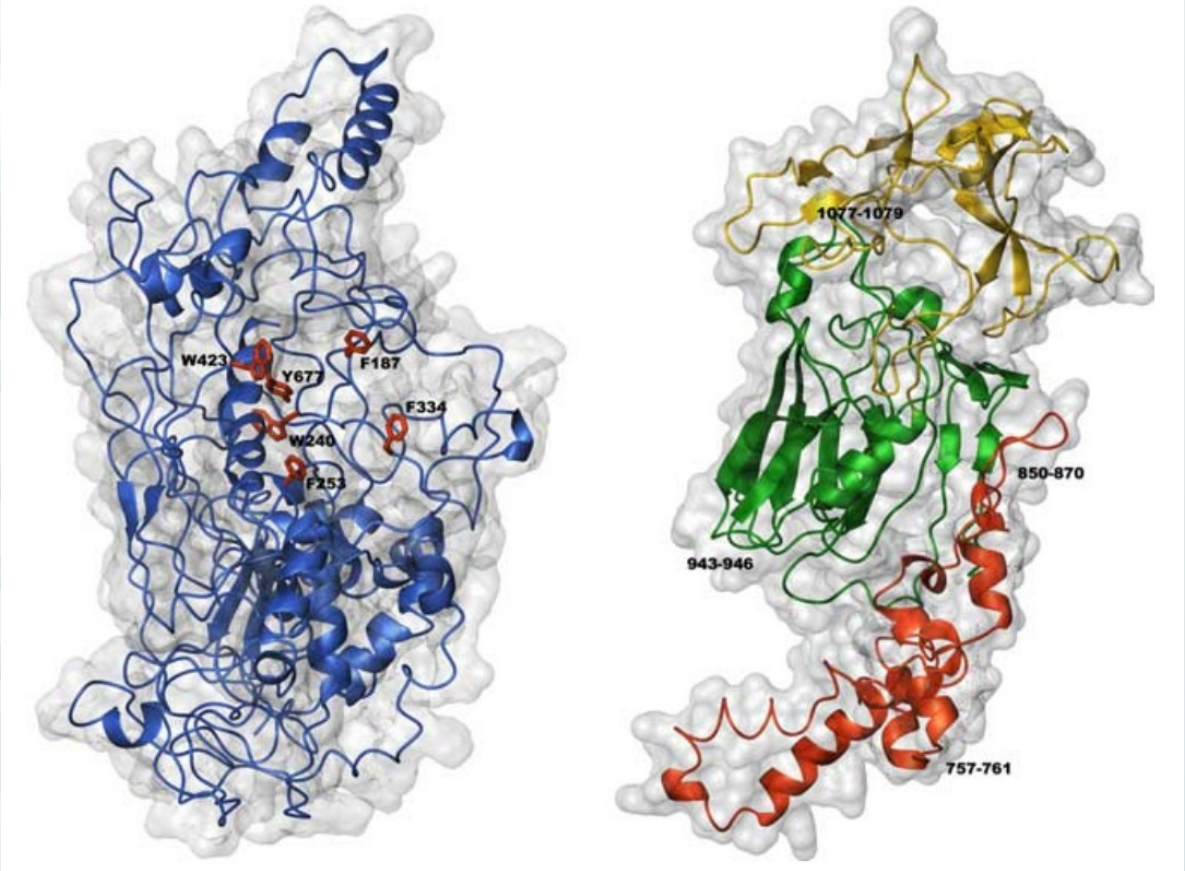

Figure: Tertiary representations of the S1 and S2 subunits of the spike protein using PsiPred. Source: [11]

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Definition

Drug discovery is the process by new candidate medications are discovered [12].

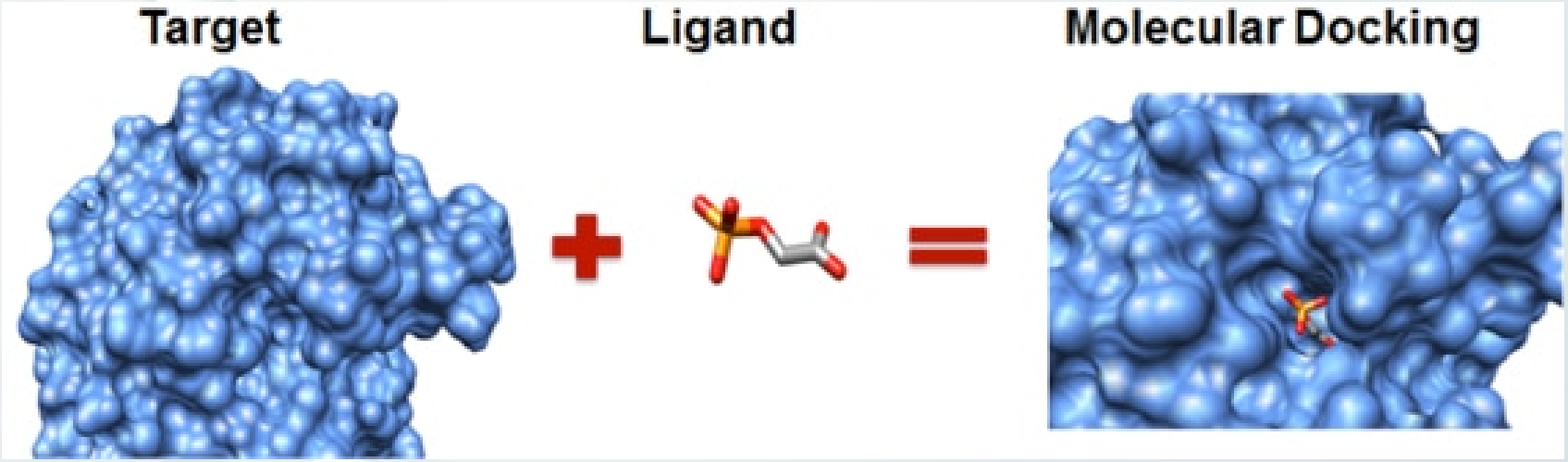
Molecular docking

Molecular docking is a computer simulation procedure to predict the conformation of a receptor-ligand complex [13]

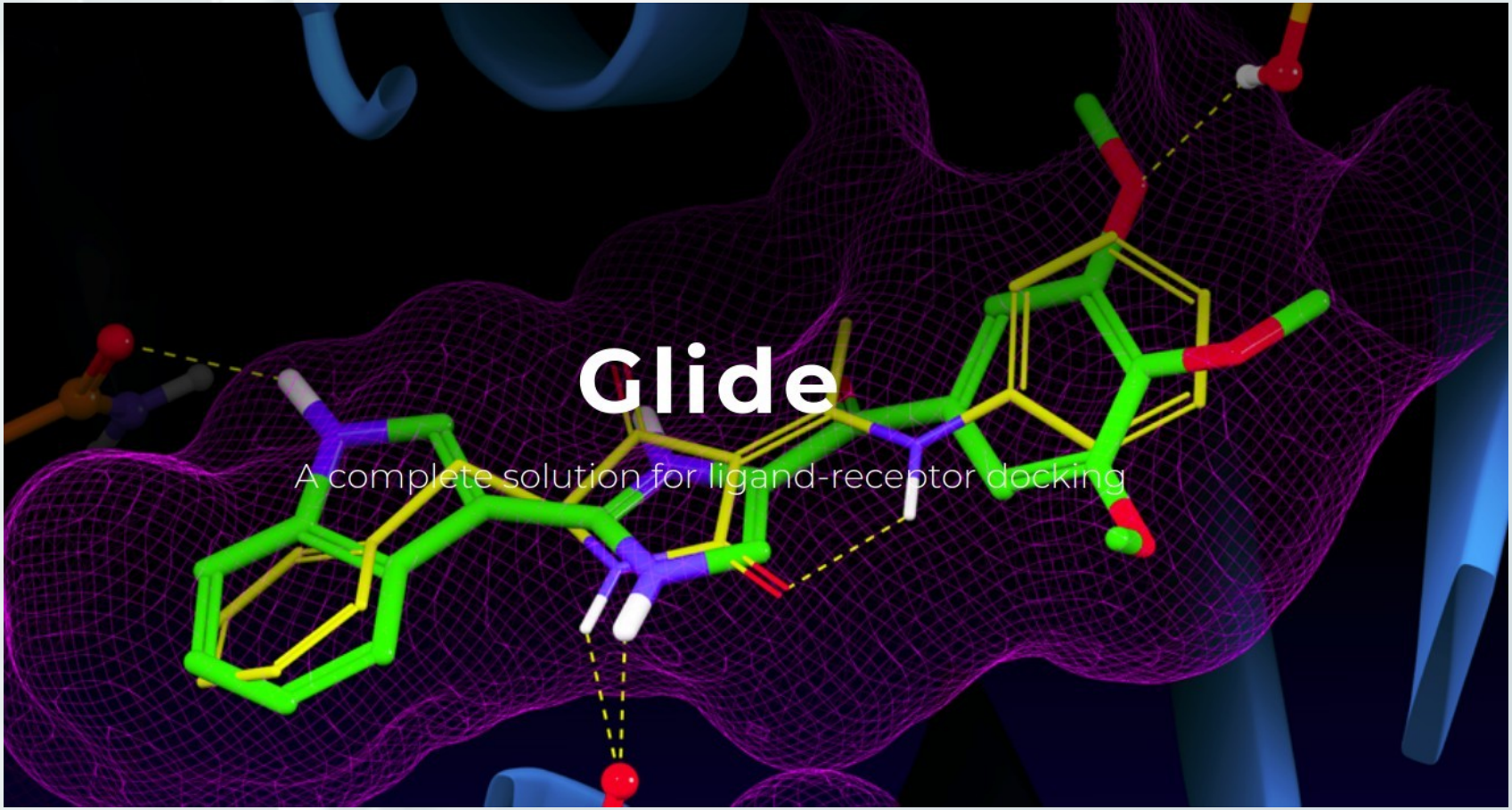
Algorithms used:

- Fast shape matching (take into account the geometric).
- Simulated Anneling.
- Genetic algorithms.
- Tabu search.

Drug discovery
Molecular docking



Drug discovery
Molecular docking with Glide



Drug discovery
From a million to one

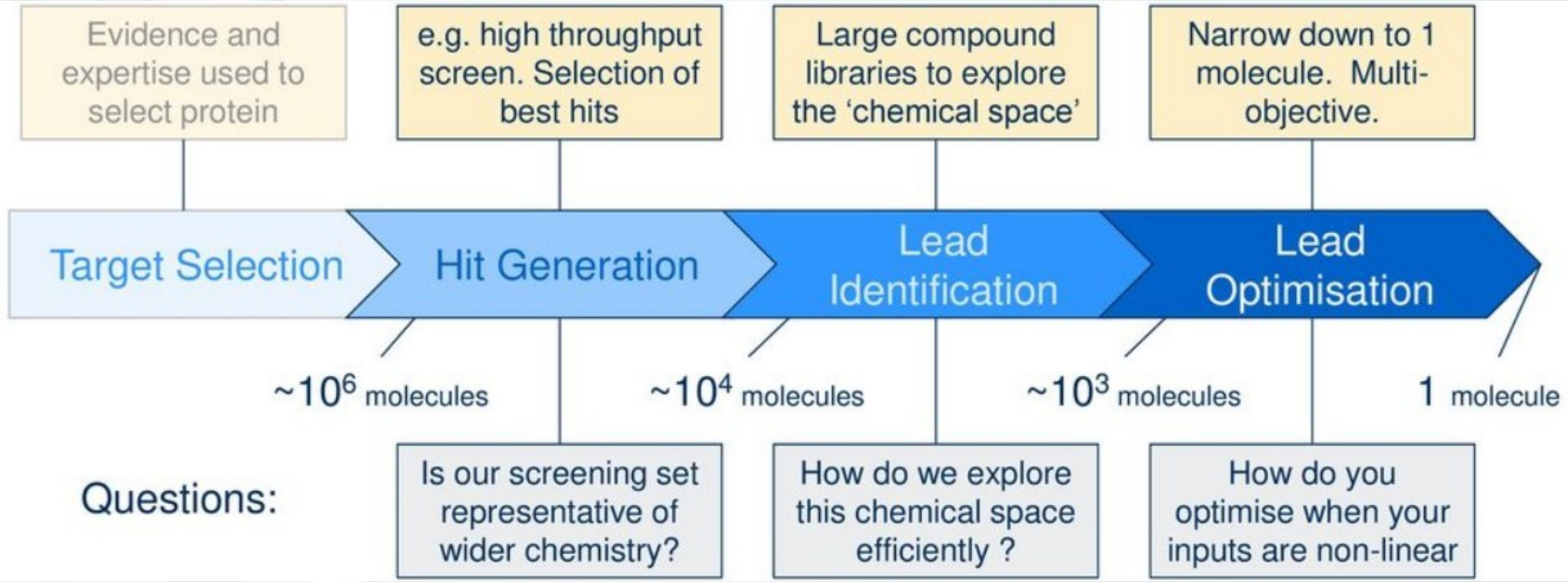


Figure: Process in drug discovery. Source: [14]

Drug discovery
COVID-19 main protease

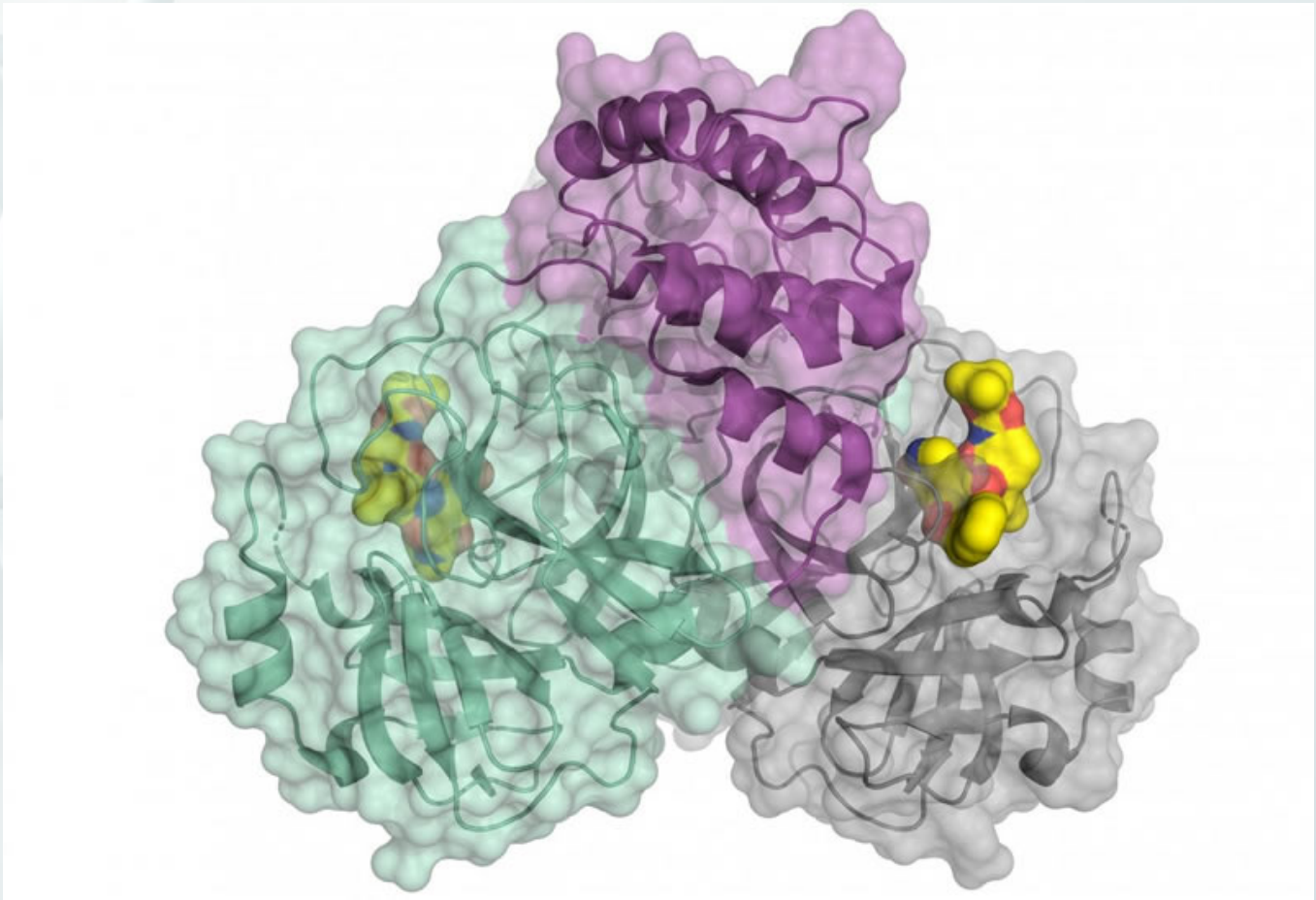


Figure: Schematic representation of the coronavirus protease. Source: [15]

Drug discovery
N3 inhibitor of main protease

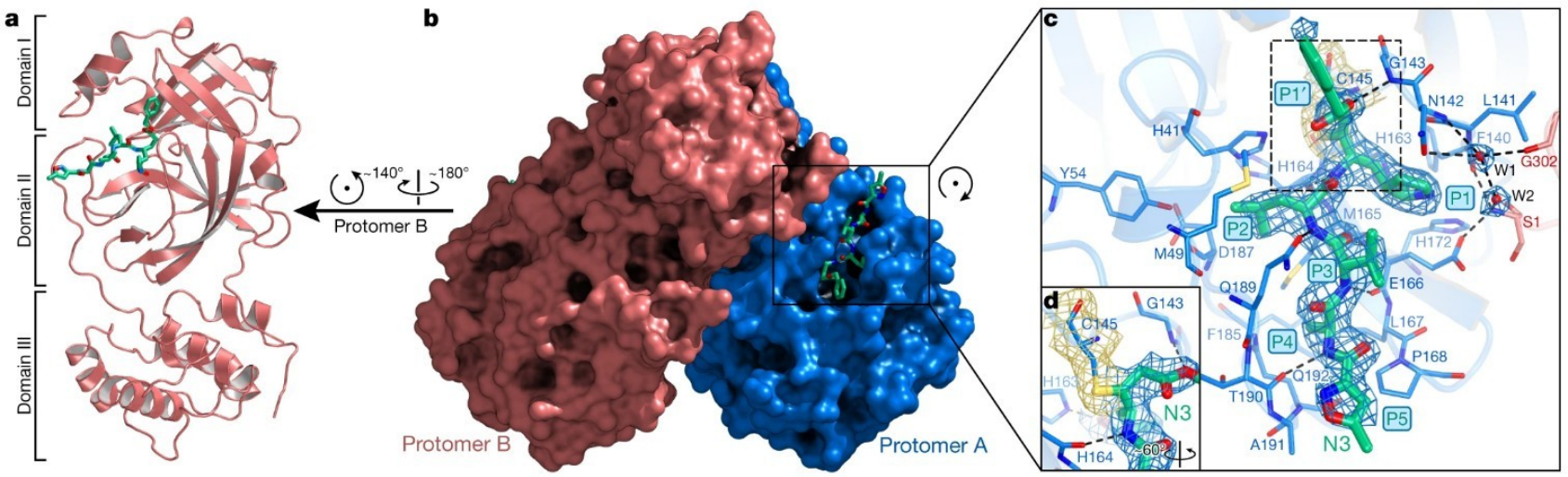


Figure: The crystal structure of SARS-CoV-2 main protease N3 inhibitor.
Source: [16]

Drug discovery

Protease Inhibitors Designed Using Generative Deep Learning Approaches

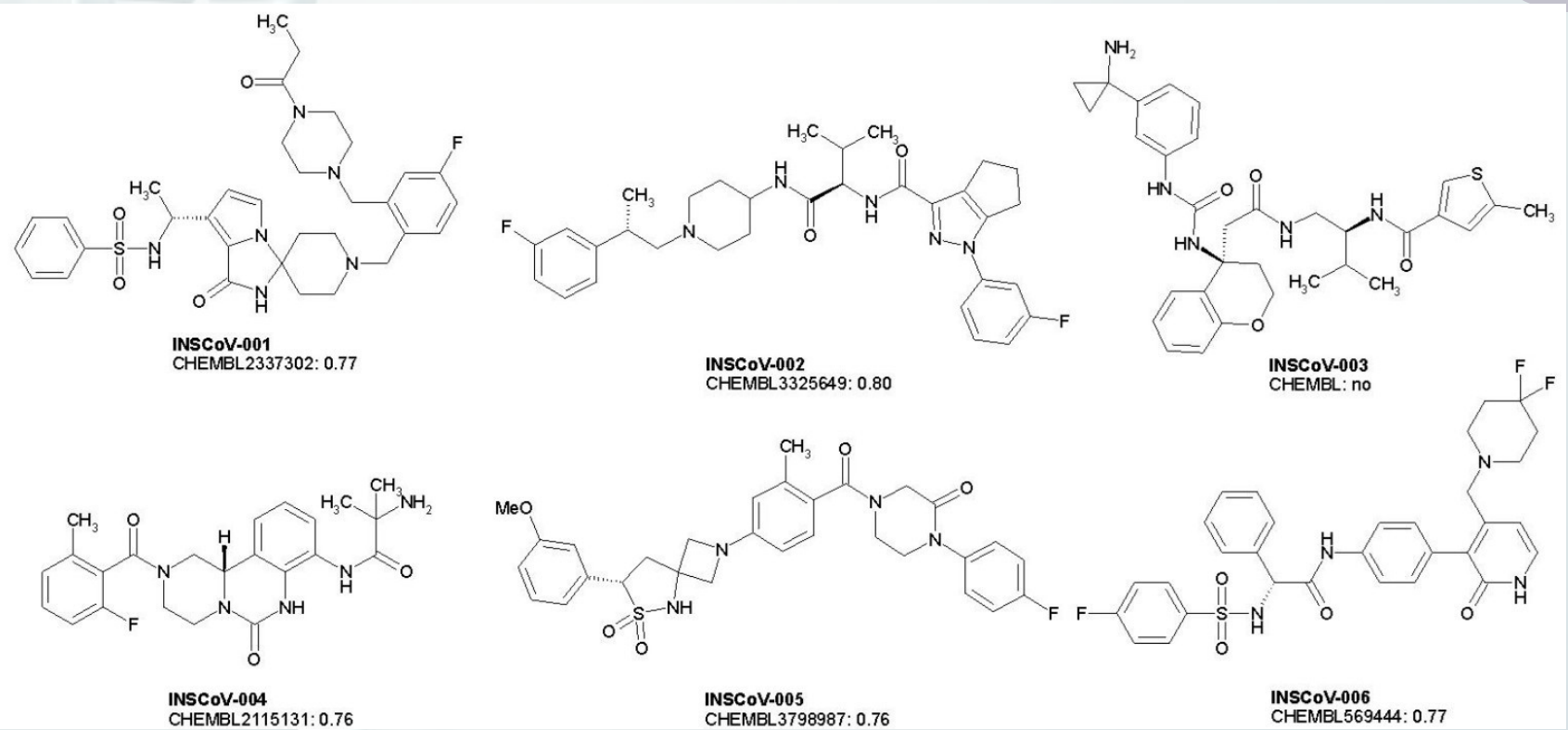


Figure: Representative examples of the structures generated to target the main protease of 2019-nCoV. Novelty was assessed using similarity search in ChEMBL Database. Source: [17]

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Funding

Coronavirus Funding Monitor

List of open funding calls and other support for researchers, non-profit organizations and commercial organizations, specifically for COVID-19 and coronavirus-related research (Link).

Coronavirus Funding Monitor

frontiers

Funding
MIT CVID-19 challenges

MIT is hosting a series of challenges to empower YOU to take action on the COVID-19 crisis (Link).

Funding
FONDECYT

CONCYTEC

FONDECYT

FONDO NACIONAL DE DESARROLLO CIENTÍFICO, TECNOLÓGICO Y DE INNOVACIÓN TECNOLÓGICA

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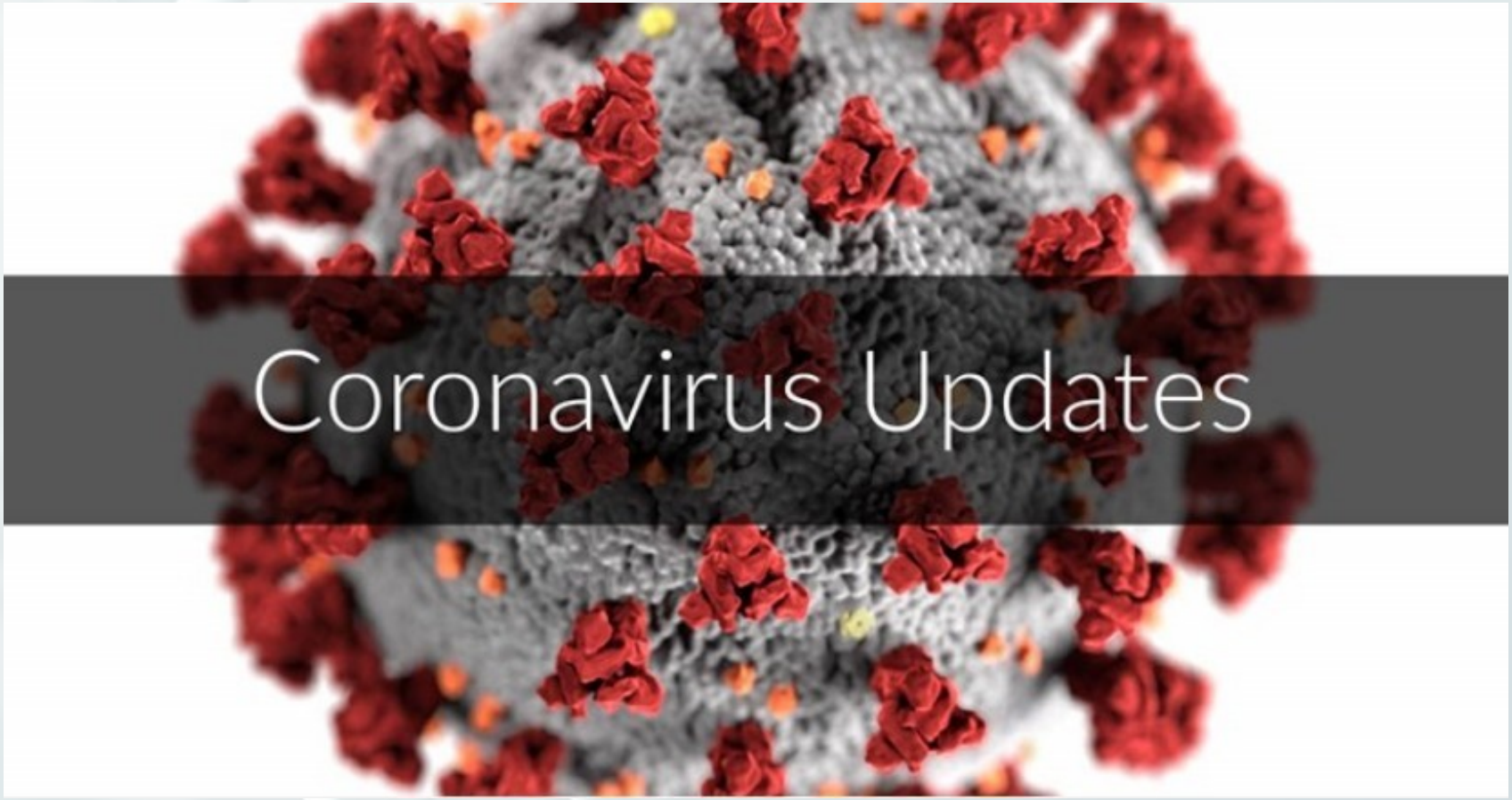
Datasets and resources
Coronavirus updates

Links to bioinformatics resources useful to track the evolution and progression as well as to manage genomics data (Link).



Datasets and resources
Institut Français de Bioinformatique (IFB)

The IFB offers expertise and computing facilities to support the involved teams on COVID-19 (Link).

Datasets and resources
The European Bioinformatics Institute (EMBL-EBI)

EMBL-EBI is gathering and sharing data resources as they become available (Link).

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T-Bio platform (Link).

How to learn Bioinformatics?
Coursera

Coursera (Link).

How to learn Bioinformatics?

Bioinformatics Research Group

Bioinformatics Research Group at la Salle university is a interdisciplinary group open for everybody who have a computer science‘ background.

References I

[1] N. M. Luscombe, D. Greenbaum, and M. Gerstein, “What is bioinformatics? a proposed definition and overview of the field,” *Methods of information in medicine*, vol. 40, no. 04, pp. 346–358, 2001.

[2] M. Clinics, “How genetic disorders are inherited,” https://www.mayoclinic.org/tests-procedures/genetic-testing/multimedia/genetic-disorders/sls-20076216?s=2, 2020, accessed: 2020-03-20.

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[17] A. Zhavoronkov, V. Aladinskiy, A. Zhebrak, B. Zagribelnyy, V. Terentiev, D. S. Bezrukov, D. Polykovskiy, R. Shayakhmetov, A. Filimonov, P. Orekhov, Y. Yan, O. Popova, Q. Vanhaelen, A. Aliper, and Y. Ivanenkov, “Potential COVID-2019 3c-like protease inhibitors designed using generative deep learning approaches,” Feb. 2020. [Online]. Available: https://doi.org/10.26434/chemrxiv.11829102.v2

Thank you