Universidade de São Paulo - USP
Faculdade de Medicina de Ribeirão Preto - FMRP
Ciências Biomédicas - Turma IX
RCB300 - Tópicos em Biotecnologia III (2024)

Desenvolvimento de vacina de mRNA contra Sars-CoV-2 atual

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Matheus de Lima Ortega (13657995)
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Sumário

1) Introdução: Covid-19 e vacinas de mRNA e proteína Spike
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4) Identificação de HBA1 (região cromossômica, estrutura e etc).
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6) Otimização de códons (o que é e resultado)
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8) Expasy (tradução do cDNA) da com mutação e sem mutação; Sequência de AA com a região RBD e mutações;
9) Predição de epítopos de anticorpos: http://tools.iedb.org/bcell/. Determinar a predição de epítopos da proteína spike codificada por ambas vacinas de mRNA, antes e após a adição das mutações missense 2P. Pergunta: há diferença no número de epítopos?
10) Predição de epítopos de MHC classe I: http://tools.iedb.org/mhci/. Coloque a sequência da proteína Spike e clique em Select HLA allele reference set e em seguida clique em submit;
11) predição de epítopos de MHC classe II + resultados
12) Conclusão e recap

1. Introdução

Anna Beatriz

Pandemia COVID-19

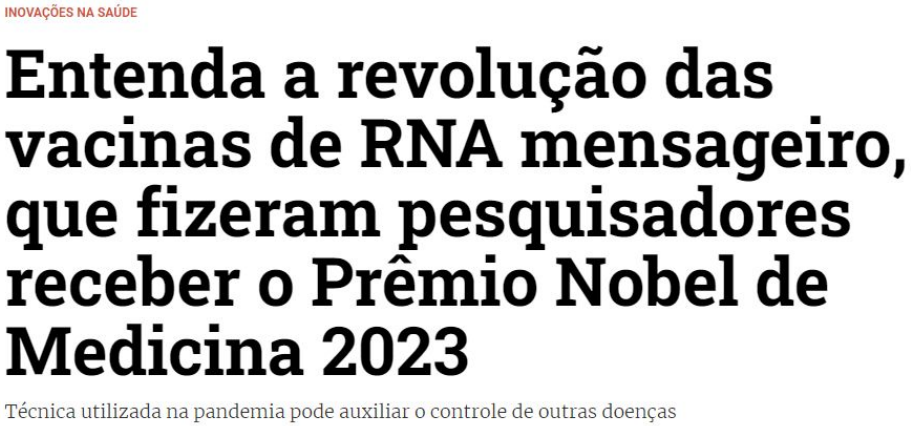
31/12/2019 - a Organização Mundial da Saúde (OMS) foi alertada sobre vários casos de pneumonia na República Popular da China. Tratava-se de uma nova cepa de coronavírus.

07/01/2020 - autoridades chinesas confirmaram que haviam identificado um novo tipo de coronavírus.

Anna Beatriz

Vacinas de RNA

As vacinas de RNA utilizam uma molécula de RNA para fornecer instruções ao corpo sobre como produzir proteínas específicas, desencadeando uma resposta imunológica capaz de produzir anticorpos contra o antígeno, garantindo imunização contra futuras infecções do patógeno.



INOVAÇÕES NA SAÚDE

Entenda a revolução das vacinas de RNA mensageiro, que fizeram pesquisadores receber o Prêmio Nobel de Medicina 2023

Técnica utilizada na pandemia pode auxiliar o controle de outras doenças

Anna Beatriz

Vacinas de RNA

Análise > Alvo de transdução de sinal.23 de março de 2022;7(1):94.
doi: 10.1038/s41392-022-00950-y.

Avanços no desenvolvimento da vacina mRNA contra a COVID-19

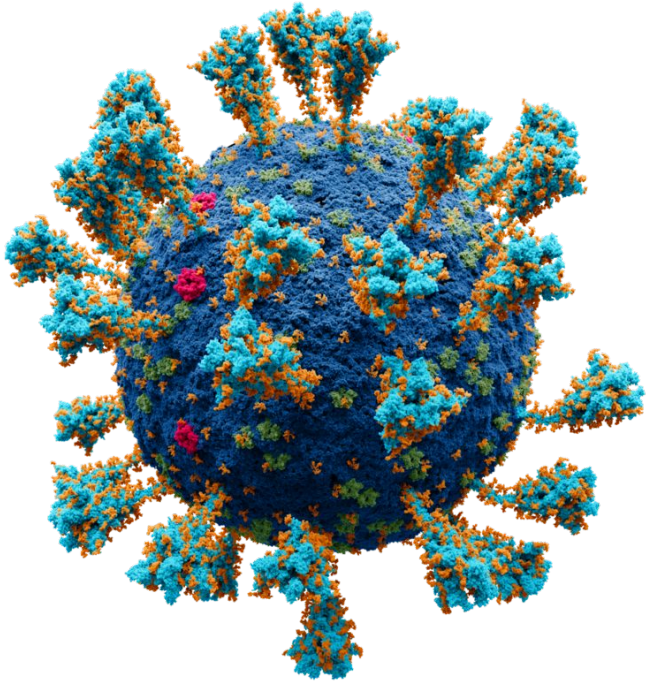
Enyue Fang [# 1 2], Xiao Hui Liu [# 1], Miao Li [# 1], Zelun Zhang [1], Canção de Lifang [1], Bai Yu Zhu [3], Xiaohong Wu [1], Jing Jing Liu [1], Danhua Zhao [1], Yuhua Li [4]

Vantagens: curto ciclo de desenvolvimento, fácil industrialização, processo de produção simples, flexibilidade para responder a novas variantes e capacidade para induzir uma melhor resposta imunológica.

Anna Beatriz

Proteína Spike

- 1.200 a 1.400 resíduos de aminoácidos de comprimento;
- Glicoproteína Spike é altamente imunogênica;
- A função da glicoproteína spike é mediar a entrada viral na célula hospedeira, primeiro interagindo com moléculas na superfície externa da célula e depois fundindo as membranas viral e celular



Solodovnikov, Alexei; Arkhipova, Valeria (29 de julho de 2021)

Anna Beatriz

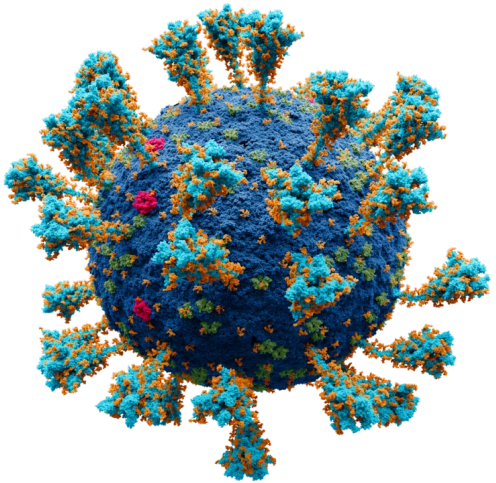
Proteína Spike

Covid: vacinas Pfizer e Moderna são as mais eficazes para reforço, indica estudo

Philippa Roxby
Repórter de saúde

3 dezembro 2021

BBC News, 2021



Solodovnikov, Alexei; Arkhipova, Valeria (29 de julho de 2021)

2. Metodologia

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Gisaid

GISAID

Virus detail	
Virus name:	hCoV-19/Belgium/rega-47745/2023
Accession ID:	EPI_ISL_18492450
Type:	betacoronavirus
Clade:	GRA
Pango Lineage:	JN.1.1 (Pango v.4.3.1 consensus call), Omicron (BA.2-like) (Scorpio)
AA Substitutions:	Spike A27S, Spike A264D, Spike A570V, Spike D405N, Spike D614G, Spike D796Y, Spike E484K, Spike E554K, Spike F157S, Spike F486P, Spike G142D, Spike G339H, Spike G446S, Spike H69del, Spike H245N, Spike H655Y, Spike I332V, Spike ins16MPLF, Spike K356T, Spike K417N, Spike L24del, Spike L212I, Spike L216F, Spike L452W, Spike L455S, Spike N211del, Spike N440K, Spike N450D, Spike N460K, Spike N481K, Spike N501Y, Spike N679K, Spike N764K, Spike N969K, Spike P25del, Spike P26del, Spike P621S, Spike P681R, Spike P1143L, Spike Q498R, Spike Q954H, Spike R21T, Spike R158G, Spike R403K, Spike R408S, Spike S50L, Spike S371F, Spike S373P, Spike S375F, Spike S477N, Spike S939F, Spike T19I, Spike T376A, Spike T478K, Spike V70del, Spike V127F, Spike V213G, Spike V445H, Spike V483del, Spike Y144del, Spike Y505H, E T9I, M A63T, M A104V, M D3H, M Q19E, M T30A, N E31del, N G204R, N P13L, N Q229K, N R32del, N R203K, N S33del, N S413R, NS3 T223I, NS7a R25K, NS7b F19L, NSP1 S135R, NSP2 A31D, NSP2 F319L, NSP3 A1892T, NSP3 G489S, NSP3 K1155R, NSP3 N1708S, NSP3 T24I, NSP3 V238L, NSP4 L264F, NSP4 T327I, NSP4 T492I, NSP5 P132H, NSP6 F108del, NSP6 G107del, NSP6 R252K, NSP6 S106del, NSP6 V24F, NSP9 T35I, NSP12 P323L, NSP13 R392C, NSP14 I42V, NSP15 T112I
Variant:	VOI GRA (JN.1+JN.1.*) first detected in Luxembourg/Iceland
Passage details/history:	Original
Sample information	
Collection date:	2023-11-04
Location:	Europe / Belgium / Lubbeek
Host:	Human
Additional location information:	Other: Postal Code:3210
Gender:	Female
Patient age:	87
Patient status:	unknown
Specimen source:	Oropharyngeal swab
Additional host information:	
Sampling strategy:	baseline surveillance
Outbreak:	
Last vaccinated:	
Treatment:	
Sequencing technology:	Nanopore MinION
Assembly method:	Artic Network methods
Coverage:	140x (average)x
Comment:	ⓘ Insertion of 12 nucleotides when compared to the reference WIV04 sequence. Gap of 42 nucleotides when compared to the reference WIV04 sequence.

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TAGAGAAAACAACAGAGTTGTTATTTCTAGTGATGTTCTTGTTAACAACTAAACGAACAATGTTTGTTTTTCTTGTTTTA
TTGCCACTAGTCTCTAGTCAGTGTGTCATGCCGCTGTTTAATCTTATAACTACAACTCAATCATACACTAATTCTTTCAC
ACGTGGTGTTTATTACCCTGACAAAGTTTTCAGATCCTCAGTTTTACATTTAACTCAGGACTTGTTCTTACCTTTCTTTT
CCAATGTTACTTGGTTCCATGCTATCTCTGGGACCAATGGTACTAAGAGGTTTGATAACCCTGTCCTACCATTTAATGAT
GGTGTTTATTTTGCTTCCACTGAGAAGTCTAACATAATAAGAGGCTGGATTTTTGGTACTACTTTAGATTCGAAGACCCA

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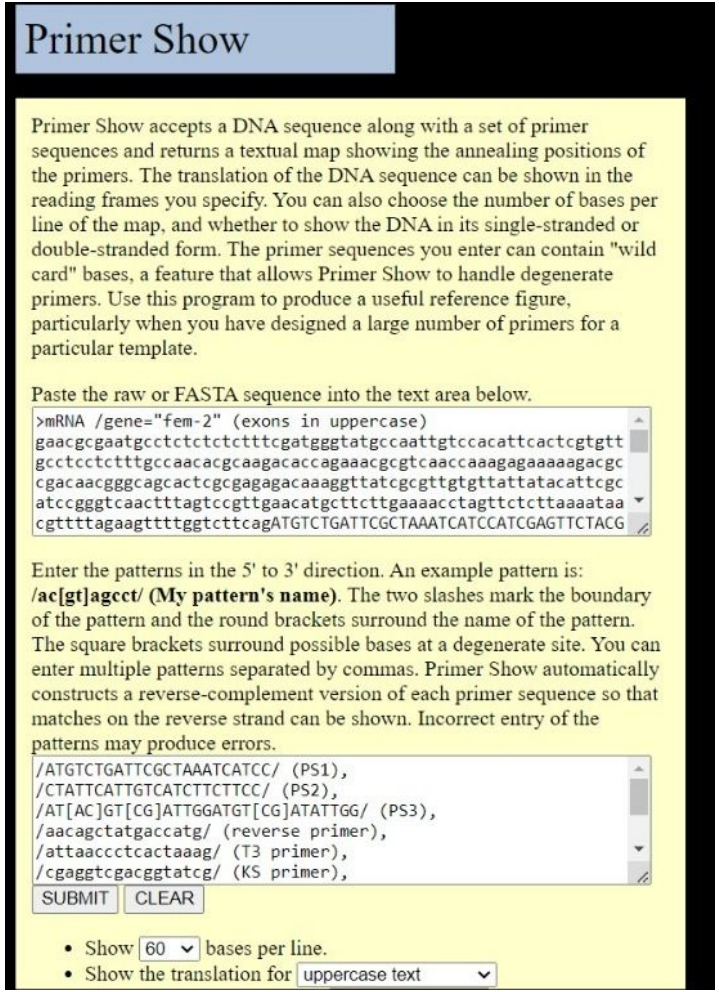
Primer Show



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HGNC

HUGO Gene Nomenclature Committee

The resource for approved human gene nomenclature

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- Databases
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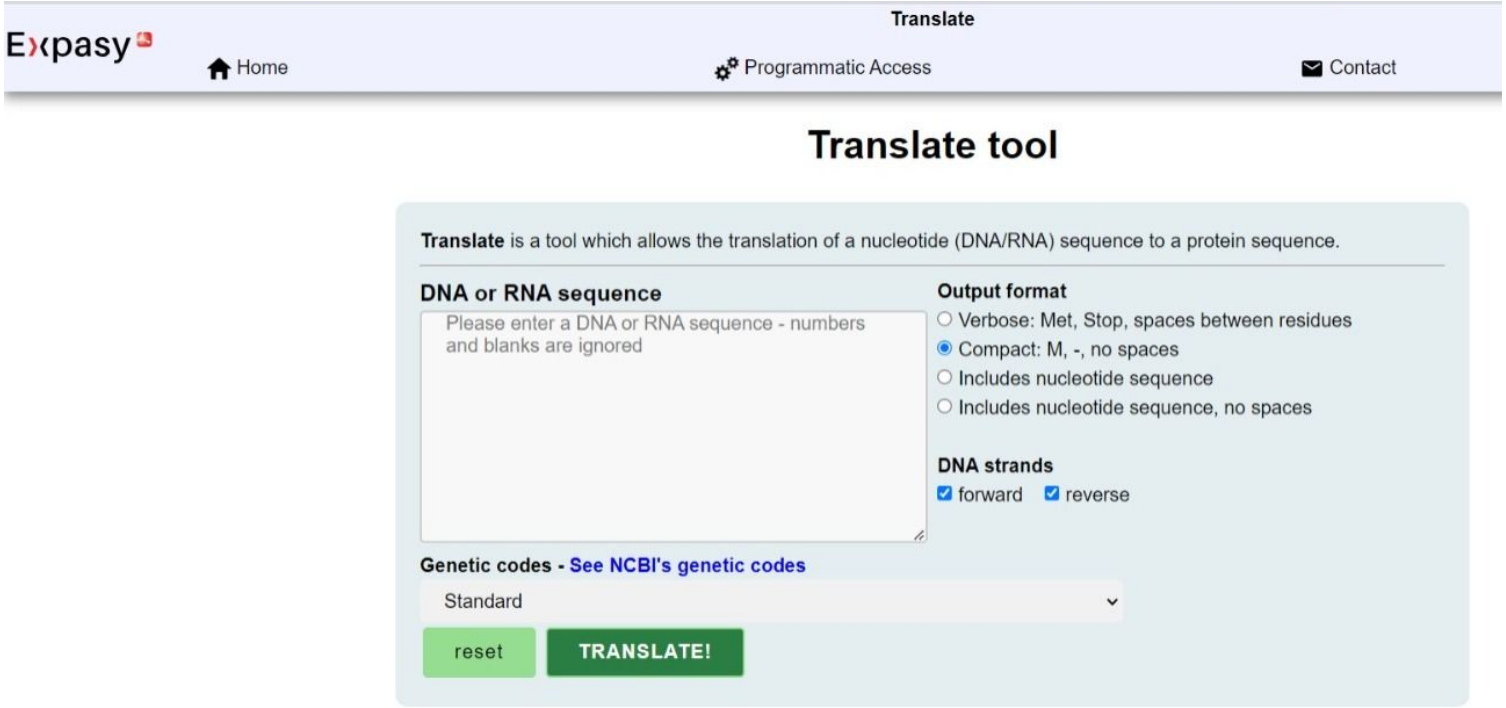
The Codon Optimization Tool converts the DNA, or protein sequence, from one organism for expression to another. The IDT algorithm provides the best sequence option by screening and filtering sequences to lower complexity and minimize secondary structures.

ExPasy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Translate is a tool which allows the translation of a nucleotide (DNA/RNA) sequence to a protein sequence.
DNA or RNA sequence
Please enter a DNA or RNA sequence - numbers and blanks are ignored
Output format
Verbose: Met, Stop, spaces between residues
Compact: M, -, no spaces
Includes nucleotide sequence
Includes nucleotide sequence, no spaces
DNA strands
forward
reverse
Genetic codes - See NCBI's genetic codes
Standard
reset
TRANSLATE!

Letícia Yumi

3. Resultados

Identificação da Spike no genoma

Virus detail	
Virus name:	hCoV-19/Belgium/rega-47745/2023
Accession ID:	EPI_ISL_18492450
Type:	betacoronavirus
Clade:	GRA
Pango Lineage:	JN.1.1 (Pango v.4.3.1 consensus call), Omicron (BA.2-like) (Scorpio)
AA Substitutions:	Spike A27S, Spike A264D, Spike A570V, Spike D405N, Spike D614G, Spike D796Y, Spike E484K, Spike E554K, Spike F157S, Spike F486P, Spike G142D, Spike G339H, Spike G446S, Spike H69del, Spike H245N, Spike H655Y, Spike I332V, Spike ins16MPLF, Spike K356T, Spike K417N, Spike L24del, Spike L212I, Spike L216F, Spike L452W, Spike L455S, Spike N211del, Spike N440K, Spike N450D, Spike N460K, Spike N481K, Spike N501Y, Spike N679K, Spike N764K, Spike N969K, Spike P25del, Spike P26del, Spike P621S, Spike P681R, Spike P1143L, Spike Q498R, Spike Q954H, Spike R21T, Spike R158G, Spike R403K, Spike R408S, Spike S50L, Spike S371F, Spike S373P, Spike S375F, Spike S477N, Spike S939F, Spike T19I, Spike T376A, Spike T478K, Spike V70del, Spike V127F, Spike V213G, Spike V445H, Spike V483del, Spike Y144del, Spike Y505H, E T9I, M A63T, M A104V, M D3H, M Q19E, M T30A, N E31del, N G204R, N P13L, N Q229K, N R32del, N R203K, N S33del, N S413R, NS3 T223I, NS7a R25K, NS7b F19L, NSP1 S135R, NSP2 A31D, NSP2 F319L, NSP3 A1892T, NSP3 G489S, NSP3 K1155R, NSP3 N1708S, NSP3 T24I, NSP3 V238L, NSP4 L264F, NSP4 T327I, NSP4 T492I, NSP5 P132H, NSP6 F108del, NSP6 G107del, NSP6 R252K, NSP6 S106del, NSP6 V24F, NSP9 T35I, NSP12 P323L, NSP13 R392C, NSP14 I42V, NSP15 T112I
Variant:	VOI GRA (JN.1+JN.1.*) first detected in Luxembourg/Iceland
Passage details/history:	Original

Matheus

S surface glycoprotein [*Severe acute respiratory syndrome coronavirus 2*]

Download Datasets

Gene ID: 43740568, updated on 7-May-2024

Summary

Gene symbol	S
Gene description	surface glycoprotein
Locus tag	GU280_gp02
Gene type	protein coding
RefSeq status	PROVISIONAL
Organism	Severe acute respiratory syndrome coronavirus 2 (isolate: Wuhan-Hu-1, nat-host: Homo sapiens)
Lineage	Viruses; Riboviria; Orthornavirae; Pisuviricota; Pisoniviricetes; Nidovirales; Cornidovirineae; Coronaviridae; Orthocoronavirinae; Betacoronavirus; Sarbecovirus
Also known as	spike glycoprotein
Summary	Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) is an enveloped, positive-sense, single-stranded RNA virus that causes coronavirus disease 2019 (COVID-19). Virus particles include the RNA genetic material and structural proteins needed for invasion of host cells. Once inside the cell the infecting RNA is used to encode structural proteins that make up virus particles, nonstructural proteins that direct virus assembly, transcription, replication and host control and accessory proteins whose function has not been determined.~ The structural proteins of SARS-CoV-2 include the envelope protein (E), spike or surface glycoprotein (S), membrane protein (M) and the nucleocapsid protein (N). The spike glycoprotein is found on the outside of the virus particle and gives coronavirus viruses their crown-like appearance. This glycoprotein mediates attachment of the virus particle and entry into the host cell. S protein is an important target for vaccine development, antibody therapies and diagnostic antigen-based tests.

NEW **Try the new Gene table**

Try the new Transcript table

NCBI

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hCoV-19/Belgium/rega-47745/2023     GTTAACAACTAAACGAACAATGTTTGTTTTTCTTGTTTTATTGCCACTAGTCTCTAGTC 21540
NC_045512.2:21563-25384             -------------------ATGTTTGTTTTTCTTGTTTTATTGCCACTAGTCTCTAGTC 41
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hCoV-19/Belgium/rega-47745/2023     CAATGGTACTAAGAGGTTTGATAACCCTGTCCTACCATTTAATGATGGTGTTTATTTTG 21774
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hCoV-19/Belgium/rega-47745/2023   AATCATTACTACAGACAACACATTTGTGTCTGGTAACTGTGATGTTGTAATAGGAATTGT  24886
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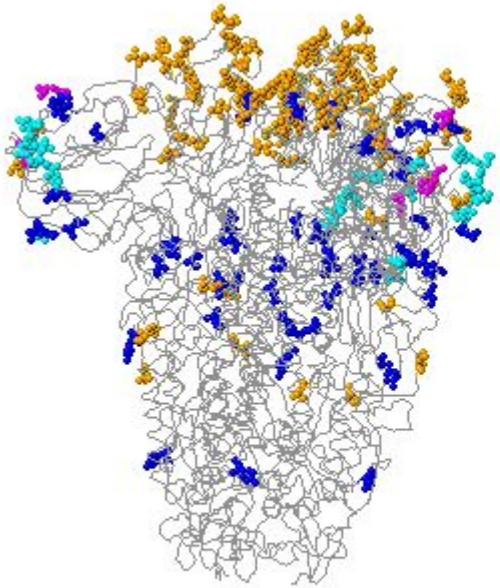
hCoV-19/Wuhan/WIV04/2019



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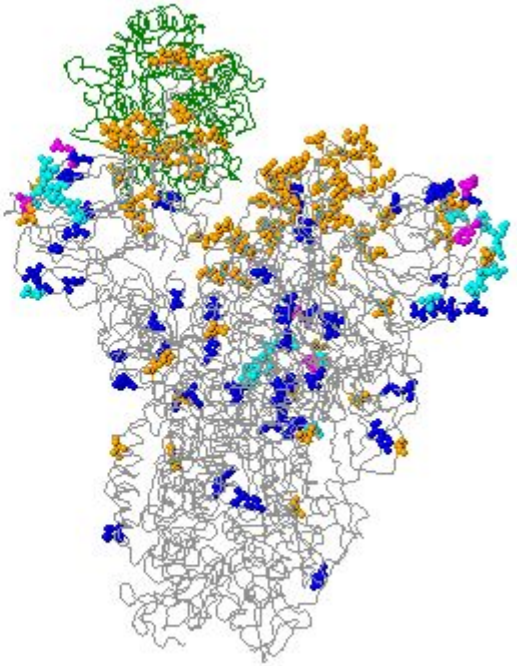

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Introdução das mutações 2P

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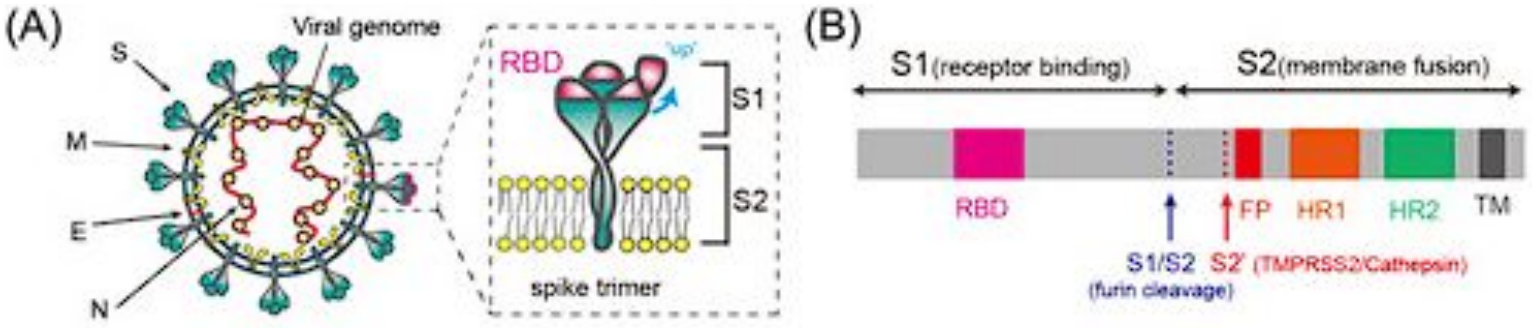

Li X, Yuan H, Li X, Wang H. Spike protein mediated membrane fusion during SARS-CoV-2 infection. J Med Virol. 2023 Jan;95(1):e28212. doi: 10.1002/jmv.28212. Epub 2022 Oct 25. PMID: 36224449; PMCID: PMC9874878.

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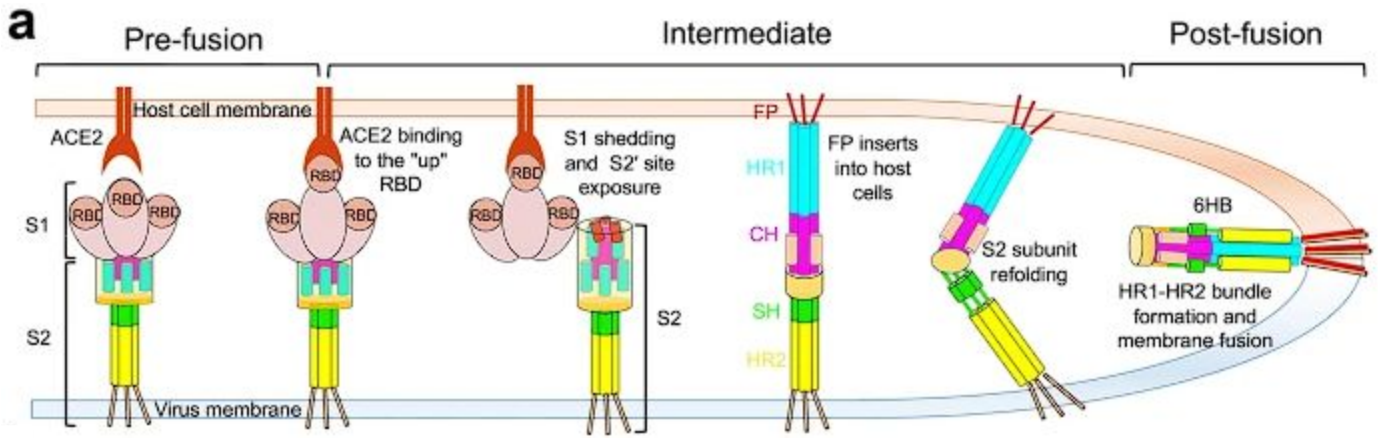

Guo L, Lin S, Chen Z, Cao Y, He B, Lu G. Targetable elements in SARS-CoV-2 S2 subunit for the design of pan-coronavirus fusion inhibitors and vaccines. Signal Transduct Target Ther. 2023 May 10;8(1):197. doi: 10.1038/s41392-023-01472-x. PMID: 37164987; PMCID: PMC10170451.

Matheus

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GIYQTSNFRVQPTESIVRFPNITNLCPFGEVFNATRFASVYAWNRKRISNCVADYSVLYNSA
SFSTFKCYGVSPTKLNDLCFTNVYADSFVIRGDEVRQIAPGQTGKIADYNYKLPDDFTGCVI
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PVAIHADQLTPTWRVYSTGSNVFQTRAGCLIGAEHVNNSYECDIPIGAGICASYQTQTNSPR
RARSVASQSIIAYTMSLGAENSVAYSNNSIAIPTNFTISVTTEILPVSMTKTSVDCTMYICG
DSTECSNLLLQYGSFCTQLNRALTGIAVEQDKNTQEVFAQVKQIYKTPPIKDFGGFNFSQIL
PDPSKPSKRSFIEDLLFNKVTLADAGFIKQYGDCLGDIAARDLICAQKFNGLTVLPPLLTDE
MIAQYTSALLAGTITSGWTFGAGAALQIPFAMQMAYRFNGIGVTQNVLYENQKLIANQFNSA
IGKIQDSLSSTASALGKLQDVVNQNAQALNTLVKQLSSNFGAISSVLNDILSRLDKVEAEVQ
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SAPHGVVFLHVTYVPAQEKNFTTAPAICHDGKAHFPREGVFVSNGTHWFVTQRNFYEPQIIT
TDNTFVSGNCDVVIGIVNNTVYDPLQPELDSFKEELDKYFKNHTSPDVDLGDISGINASVVN
IQKEIDRLNEVAKNLNESLIDLQELGKYEQYIKWPWYIWLGFIAGLIAIVMVTIMLCCMTSC
CSCLKGCCSCGSCCKFDEDDSEPVLKGVKLHYT

K982P
V983P

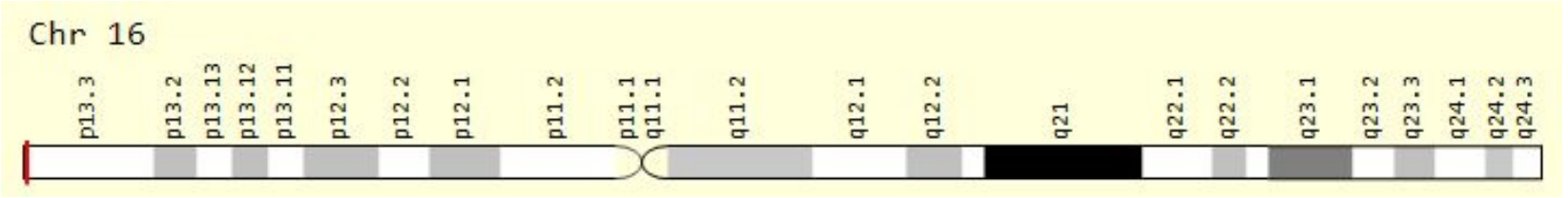
Matheus

Identificação de HBA1

Lorena

HBA1 (NM_000558.5)

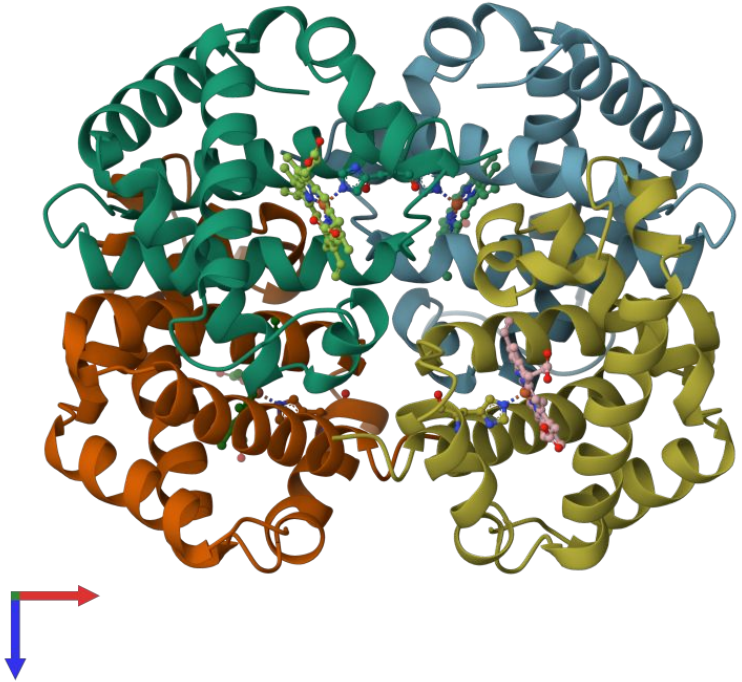
- Subunidade alfa da hemoglobina;
- Região cromossômica: 16p13.3;
- 1 isoforma; transcrito maduro contendo 577pb;
- Deleções ou mutações no gene HBA1 → hemoglobinopatias.

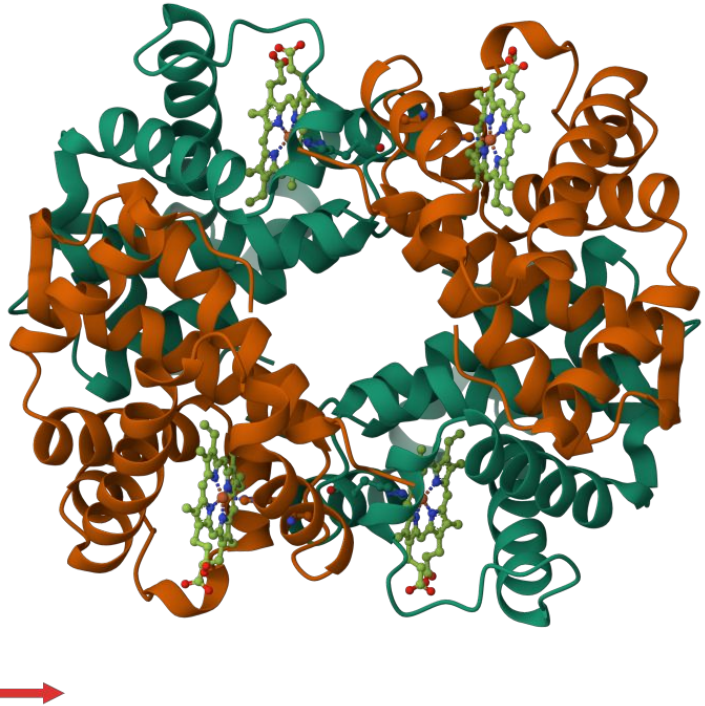


Gene Cards, 2023

Lorena

Hemoglobina



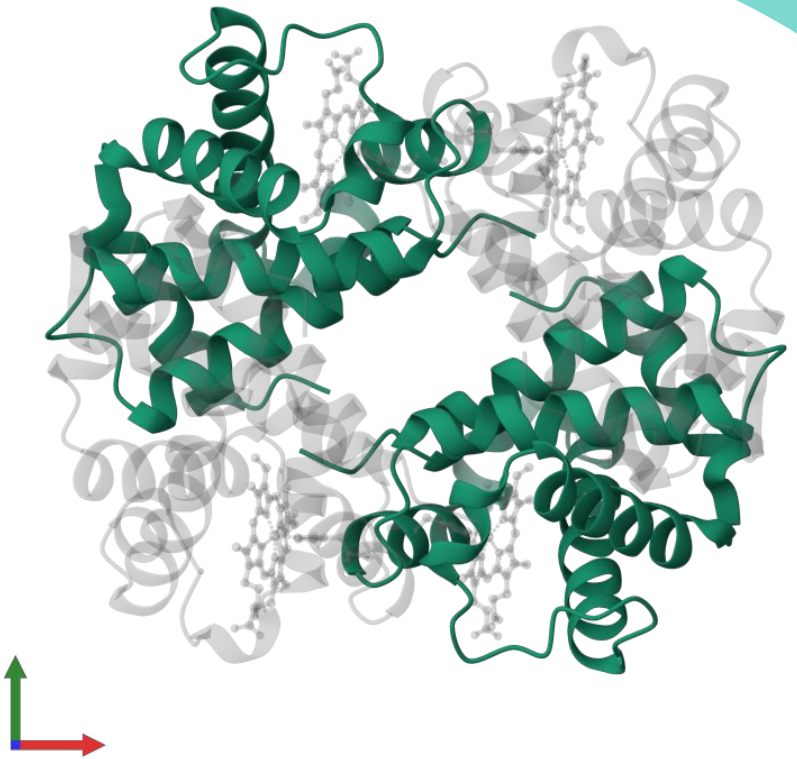


Protein Data Bank, 2023

Lorena

Proteína HBA1

- Tamanho: 142 aminoácidos
- Massa molecular: 15258 Da
- Estrutura quaternária



Protein Data Bank, 2023

Pietra Buratto De Santis

Regiões 5'UTR e 3'UTR da HBA1

Regiões UTR

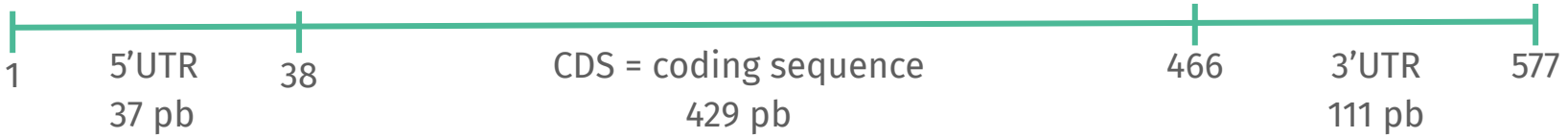
- Regiões UTR são *untranslated regions*, ou seja, regiões não traduzidas do RNA mensageiro.
- Envolvidos em mecanismos de regulação pós transcricional (Estabilidade, associação de miRNA);
- A região 5'UTR ocorre entre o CAP e o códon de iniciação;
- A região 3'UTR ocorre entre o códon de parada e a cauda Poli-A.

Pietra Buratto De Santis

(ALBERTS, et al; 2008)

Regiões UTR da HBA1

- Análise do mRNA linear da subunidade alfa da hemoglobina humana (NM_000558);
- 577 bp,



Pietra Buratto De Santis

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>NM_000558.5 Homo sapiens hemoglobin subunit alpha 1 (HBA1), mRNA

ACTCTTCTGGTCCCCACAGACTCAGAGAGAACCCACCATGGTGCTGTCTCCTGCCGACAAGACCAACGTC

AAGGCCGCCTGGGGTAAGGTCGGCGCGCACGCTGGCGAGTATGGTGCGGAGGCCCTGGAGAGGATGTTCC

TGTCCTTCCCCACCACCAAGACCTACTTCCCGCACTTCGACCTGAGCCACGGCTCTGCCCAGGTTAAGGG

CCACGGCAAGAAGGTGGCCGACGCGCTGACCAACGCCGTGGCGCACGTGGACGACATGCCCAACGCGCTG

TCCGCCCTGAGCGACCTGCACGCGCACAAGCTTCGGGTGGACCCGGTCAACTTCAAGCTCCTAAGCCACT

GCCTGCTGGTGACCCTGGCCGCCCACCTCCCCGCCGAGTTCACCCCTGCGGTGCACGCCTCCCTGGACAA

GTTCCTGGCTTCTGTGAGCACCGTGCTGACCTCCAAATACCGTTAAGCTGGAGCCTCGGTGGCCATGCTT

CTTGCCCCTTGGGCCTCCCCCCAGCCCCTCCTCCCCTTCCTGCACCCGTACCCCCGTGGTCTTTGAATAA

AGTCTGAGTGGGCGGCA

Pietra Buratto De Santis

Região 5'UTR

>NM_000558.5 Homo sapiens hemoglobin subunit alpha 1 (HBA1), mRNA

ACTCTTCTGGTCCCCACAGACTCAGAGAGAACCCACCATGGTGCTGTCTCCTGCCGACAAGACCAACGTC

AAGGCCGCCTGGGGTAAGGTCGGCGCGCACGCTGGCGAGTATGGTGCGGAGGCCCTGGAGAGGATGTTCC

TGTCCTTCCCCACCACCAAGACCTACTTCCCGCACTTCGACCTGAGCCACGGCTCTGCCCAGGTTAAGGG

CCACGGCAAGAAGGTGGCCGACGCGCTGACCAACGCCGTGGCGCACGTGGACGACATGCCCAACGCGCTG

TCCGCCCTGAGCGACCTGCACGCGCACAAGCTTCGGGTGGACCCGGTCAACTTCAAGCTCCTAAGCCACT

GCCTGCTGGTGACCCTGGCCGCCCACCTCCCCGCCGAGTTCACCCCTGCGGTGCACGCCTCCCTGGACAA

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AGTCTGAGTGGGCGGCA

Pietra Buratto De Santis

Região 5’UTR

>NM_000558.5 Homo sapiens hemoglobin subunit alpha 1 (HBA1), mRNA

ACTCTTCTGGTCCCCACAGACTCAGAGAGAACCCACCATGGTGCTGTCTCCTGCCGACAAGACCAACGTC

AAGGCCGCCTGGGGTAAGGTCGGCGCGCACGCTGGCGAGTATGGTGCGGAGGCCCTGGAGAGGATGTTCC

TGTCCTTCCCCACCACCAAGACCTACTTCCCGCACTTCGACCTGAGCCACGGCTCTGCCCAGGTTAAGGG

CCACGGCAAGAAGGTGGCCGACGCGCTGACCAACGCCGTGGCGCACGTGGACGACATGCCCAACGCGCTG

TCCGCCCTGAGCGACCTGCACGCGCACAAGCTTCGGGTGGACCCGGTCAACTTCAAGCTCCTAAGCCACT

GCCTGCTGGTGACCCTGGCCGCCCACCTCCCCGCCGAGTTCACCCCTGCGGTGCACGCCTCCCTGGACAA

GTTCCTGGCTTCTGTGAGCACCGTGCTGACCTCCAAATACCGTTAACTGGAGCCTCGGTGGCCATGCTT

CTTGCCCCTTGGGCCTCCCCCCAGCCCCTCCTCCCCTTCCTGCACCCGTACCCCCGTGGTCTTTGAATAA

AGTCTGAGTGGGCGGCA

Região 3’UTR

Região 5’UTR DA HBA1

PROTEÍNA SPIKE ATUAL 2P

ACTCTTCTGGTCCCCACAGACTCAGAGAGAACCCACCAATGTTTGTTTTTCTTGTTTTATTGCCACTAGTCTCTAGTCAGTGTGTCATGCCGCTGTTTAATCTTATAACTACAACTCAATCATACA
CTAATTCTTTCACACGTGGTGTTTATTACCCTGACAAAGTTTTCAGATCCTCAGTTTTACATTTAACTCAGGACTTGTTCTTACCTTTCTTTTCCAATGTTACTTGGTTCCATGCTATCTCT
GGGACCAATGGTACTAAGAGGTTTGATAACCCTGTCCTACCATTTAATGATGGTGTTTATTTTGCTTCCACTGAGAAGTCTAACATAATAAGAGGCTGGATTTTTGGTACTACTTTAGATTC
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TTTAGAGTCCAACCAACAGAATCTATTGTTAGATTTCCTAATGTTACAAACTTGTGCCCTTTTCATGAAGTTTTAACGCCACCAGATTTGCATCTGTTTATGCTTGGAACAGGACGAGAAT
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CTGCACCCGTACCCCCGTGGTCTTTGAATAAAGTCTGAGTGGGCGGCA

Região 3’UTR DA HBA1

Pietra Buratto De Santis

Cassiana Mathias F. dos Santos

Otimização de códons

O que é?

- Acontece uma estruturação dos códons para leitura e tradução dos aminoácidos.

Utilizar o Codon Optimization Tool da IDT (Integrated DNA Technologies)

  - A ferramenta de otimização de códons altera as trincas do DNA, de um organismo para expressão em outro, sem mudar os aminoácidos que serão traduzidos.

Cassiana Mathias F. dos Santos

Resultado

Otimização de códons da spike atual sem as regiões 5´UTR e 3´UTR

ATG TTC GTG TTT TTG GTT TTG CTC CCC CTC GTC TCT TCA CAG TGT GTT
ATG CCT CTC TTC AAC CTG ATA ACC ACG ACC CAA TCA TAT ACC AAC TCC
TTT ACT AGG GGA GTT TAC TAC CCG GAC AAG GTG TTC CGA TCA TCA GTA
CTC CAC CTC ACA CAG GAC CTT TTC CTG CCG TTT TTT TCA AAT GTC ACC
TGG TTC CAT GCC ATA AGC GGT ACG AAC GGA ACA AAG AGA TTT GAC AAC
CCT GTA CTC CCG TTT AAT GAT GGA GTT TAT TTC GCG TCA ACG GAG AAG
TCA AAT ATC ATA AGA GGG TGG ATC TTC GGA ACA ACC CTG GAT TCC AAG
ACA CAG TCC CTT TTG ATT GTT AAC AAC GCC ACA AAT GTG TTT ATC AAG
GTC TGC GAG TTC CAA TTT TGC AAT GAT CCC TTT CTG GAC GTA TAC CAT
AAA AAT AAT AAG TCT TGG ATG GAG TCC GAA TCT GGT GTG TAC AGC TCC
GCT AAC AAT TGT ACA TTC GAA TAT GTC TCA CAG CCT TTC CTC ATG GAC
CTT GAG GGA AAG CAG GGG AAT TTC AAA AAC TTG CGA GAG TTC GTT TTT
AAG AAC ATA GAC GGC TAT TTT AAG ATC TAT AGC AAA CAC ACC CCC ATA
ATC GGC AGG GAT TTT CCG CAG GGG TTC TCA GCT CTC GAA CCG TTG GTC
GAC TTG CCC ATA GGG ATT AAC ATC ACG AGA TTC CAA ACT CTG CTT GCT
CTT AAT CGA AGC TAT CTT ACG CCT GGC GAC AGC TCC TCC GGA TGG ACC
GCC GGG GCA GCT GAT TAC TAC GTT GGT TAC TTG CAA CCA CGG ACG TTC
CTT CTT AAG TAT AAC GAA AAT GGA ACG ATA ACT GAC GCT GTA GAT TGT
GCT CTG GAC CCG TTG TCA GAG ACT AAG TGC ACC CTT AAG TCC TTT ACG
GTG GAA AAA GGA ATC TAT CAG ACA AGC AAC TTT AGA GTT CAG CCT ACC
GAG AGC ATC GTT CGA TTT CCA AAC GTC ACT AAT CTT TGT CCG TTC CAT
GAG GTA TTC AAC GCC ACA CGC TTC GCC AGT GTA TAC GCC TGG AAT AGG
ACG AGA ATT AGC AAC TGC GTA GCC GAC TAC AGT GTC CTC TAC AAT TTC
GCC CCG TTT TTT GCG TTT AAA TGT TAC GGG GTT AGT CCC ACA AAG CTG

Cassiana

Resultado

GCC CCG TTT TTT GCG TTT AAA TGT TAC GGG GTT AGT CCC ACA AAG CTG
AAT GAC CTT TGC TTC ACC AAT GTG TAC GCG GAC TCA TTC GTG ATC AAA
GGC AAC GAG GTG TCA CAG ATT GCC CCC GGT CAA ACA GGG AAT ATC GCG
GAC TAT AAT TAC AAG CTC CCC GAC GAC TTT ACT GGT TGT GTG ATC GCT
TGG AAT AGT AAT AAG CTT GAC TCT AAA CAT TCC GGC AAC TAC GAT TAC
TGG TAC CGG TCT TTC CGA AAA TCT AAG CTT AAA CCC TTT GAA CGG GAC
ATA TCC ACT GAA ATA TAC CAA GCT GGG AAC AAG CCT TGC AAG GGG AAG
GGC CCT AAT TGC TAT TTT CCG CTT CAG TCC TAT GGA TTT AGG CCG ACC
TAC GGC GTC GGC CAT CAA CCT TAT CGG GTA GTG GTA CTC AGC TTC GAG
CTC CTT CAT GCC CCA GCC ACT GTG TGC GGG CCG AAA AAA TCC ACA AAC
TTG GTG AAG AAT AAA TGC GTC AAC TTC AAC TTT AAT GGG CTT ACA GGT
ACG GGA GTA CTG ACA AAA TCT AAC AAA AAG TTT CTT CCG TTT CAG CAG
TTT GGT AGG GAC ATC GTC GAC ACG ACT GAT GCG GTT AGA GAT CCA CAG
ACA CTT GAA ATC CTC GAC ATA ACT CCA TGT TCC TTC GGG GGA GTT TCC
GTG ATA ACC CCA GGG ACC AAT ACA AGC AAC CAA GTA GCG GTA CTG TAT
CAA GGA GTT AAT TGC ACG GAA GTG AGC GTT GCA ATC CAC GCG GAC CAG
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CAA ACG AAA TCT AGA AGA AGG GCC AGG TCC GTG GCG TCC CAA AGT ATC
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AAC AAC AGC ATT GCC ATA CCC ACG AAC TTT ACG ATC AGT GTC ACA ACG
GAG ATT CTG CCG GTG TCC ATG ACC AAG ACC AGC GTG GAT TGT ACA ATG
TAT ATT TGC GGT GAT TCT ACA GAG TGT TCT AAT CTC TTG CTC CAA TAC
GGG TCA TTC TGC ACC CAA CTC AAG AGA GCC CTT ACG GGG ATC GCT GTT

Cassiana

Resultado

GAG CAA GAC AAG AAT ACT CAG GAA GTC TTC GCC CAA GTT AAA CAG ATC
TAC AAA ACA CCG CCT ATC AAA TAC TTC GGC GGT TTT AAC TTC TCT CAA
ATC CTG CCG GAT CCC TCT AAG CCC TCT AAG CGA AGC TTC ATA GAA GAC
TTG CTT TTT AAT AAA GTT ACA CTC GCG GAT GCC GGG TTT ATT AAG CAA
TAT GGC GAC TGC CTG GGG GAC ATA GCG GCT AGG GAC CTG ATA TGT GCT
CAA AAA TTT AAT GGG CTT ACA GTT TTG CCT CCG CTG CTC ACA GAC GAA
ATG ATA GCT CAG TAC ACC AGC GCC TTG CTT GCG GGC ACC ATC ACA AGC
GGT TGG ACC TTC GGG GCG GGA GCG GCG CTT CAA ATT CCA TTT GCT ATG
CAG ATG GCC TAC CGG TTT AAT GGG ATT GGT GTA ACT CAA AAC GTC CTC
TAC GAA AAC CAG AAG CTG ATT GCC AAT CAA TTC AAT TCC GCA ATT GGT
AAG ATT CAG GAT AGC CTC TTT TCC ACC GCA TCA GCA CTT GGG AAA TTG
CAG GAC GTC GTA AAT CAC AAC GCG CAA GCC CTC AAT ACA CTG GTG AAA
CAG CTG TCC TCT AAG TTC GGA GCG ATC AGT TCC GTA TTG AAT GAC ATA
TTG TCA AGG CTG GAC CCA CCC GAG GCT GAG GTG CAG ATA GAT AGA CTT
ATC ACT GGA CGC CTC CAG TCT CTT CAA ACT TAT GTT ACT CAG CAG CTG
ATA CGG GCC GCA GAA ATC CGA GCA AGT GCG AAC CTG GCT GCT ACC AAG
ATG TCT GAA TGT GTC CTC GGG CAG AGC AAG AGG GTT GAT TTC TGT GGC
AAA GGT TAC CAC TTG ATG AGC TTC CCG CAA AGT GCT CCT CAC GGG GTT
GTT TTT CTT CAC GTT ACA TAT GTC CCC GCG CAG GAA AAA AAC TTT ACA
ACC GCG CCC GCT ATC TGT CAT GAC GGA AAG GCG CAC TTT CCC AGA GAA
GGG GTT TTT GTC TCA AAT GGG ACA CAC TGG TTC GTT ACC CAG AGG AAT
TTC TAC GAG CCT CAG ATC ATC ACG ACC GAT AAT ACA TTC GTC AGT GGT
AAT TGT GAT GTG GTC ATC GGT ATT GTC AAT AAC ACT GTC TAT GAC CCG
CTG CAG CTC GAG CTT GAT TCC TTC AAG GAG GAG CTG GAT AAG TAT TTT
AAA AAC CAT ACA TCT CCC GAC GTA GAT TTG GGC GAT ATC TCA GGA ATC
AAC GCG TCC GTG GTG AAT ATC CAG AAG GAG ATA GAC CGA CTT AAT GAG
GTT GCT AAA AAC CTG AAT GAG AGT CTG ATT GAC CTG CAA GAA CTC GGG
AAA TAC GAA CAA TAT ATA AAA TGG CCC TGG TAC ATC TGG CTG GGT TTT
ATA GCG GGT CTT ATA GCC ATA GTT ATG GTC ACC ATT ATG CTT TGT TGT
ATG ACC TCC TGT TGC AGT TGC CTT AAG GGA TGT TGT TCA TGC GGT AGC
TGC TGC AAG TTT GAT GAA GAT GAT TCC GAG CCA GTC CTT AAG GGC GTC
AAA CTC CAC TAT ACT TAA

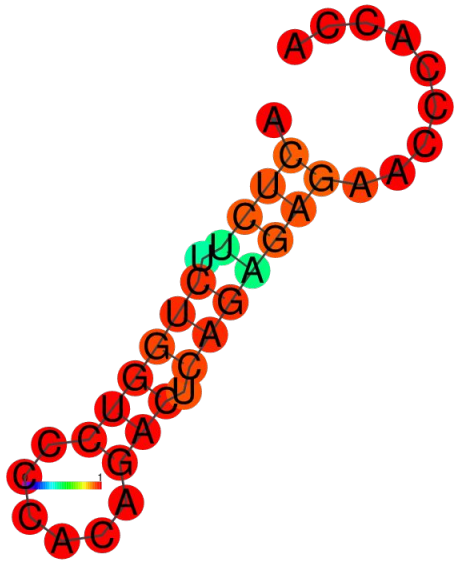
Estrutura Secundária e Energia Livre

Leticia Kaiser

Regiões 5'UTR e 3'UTR

Região 5'UTR

ACTCTTCTGGTCCCCACAGACTCAGAGAGAACCCACCA



Energia livre mínima: -10.20 kcal/mol

Região 3'UTR

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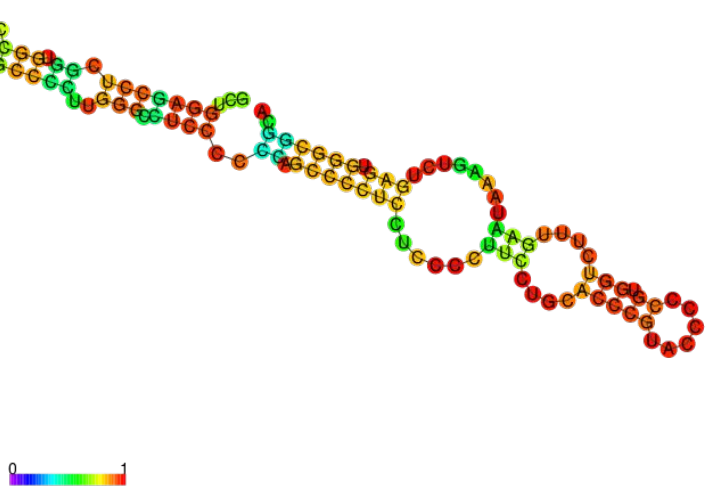

Energia livre mínima: -29.50 kcal/mol

medida de estabilidade da estrutura secundária

Fonte: ViennaRNA, 2024

(RNAfold Server)

ViennaRNA Web Services
Institute for Theoretical Chemistry

Vacina de mRNA (antes da otimização)

ACTCTTCTGGTCCCCACAGACTCAGAGAGAACCCACCAATGTTTGTTTTTCTTGTTTTATTGCCACTAGTCTCTAGTCAGTGTGTCATGCCGCTGTTTAATCTTATAACTACAACTCAATCATACA
CTAATTCTTTCACACGTGGTGTTTATTACCCTGACAAAGTTTTCAGATCCTCAGTTTTACATTTAACTCAGGACTTGTTCTTACCTTTCTTTTCCAATGTTACTTGGTTCCATGCTATCTCT
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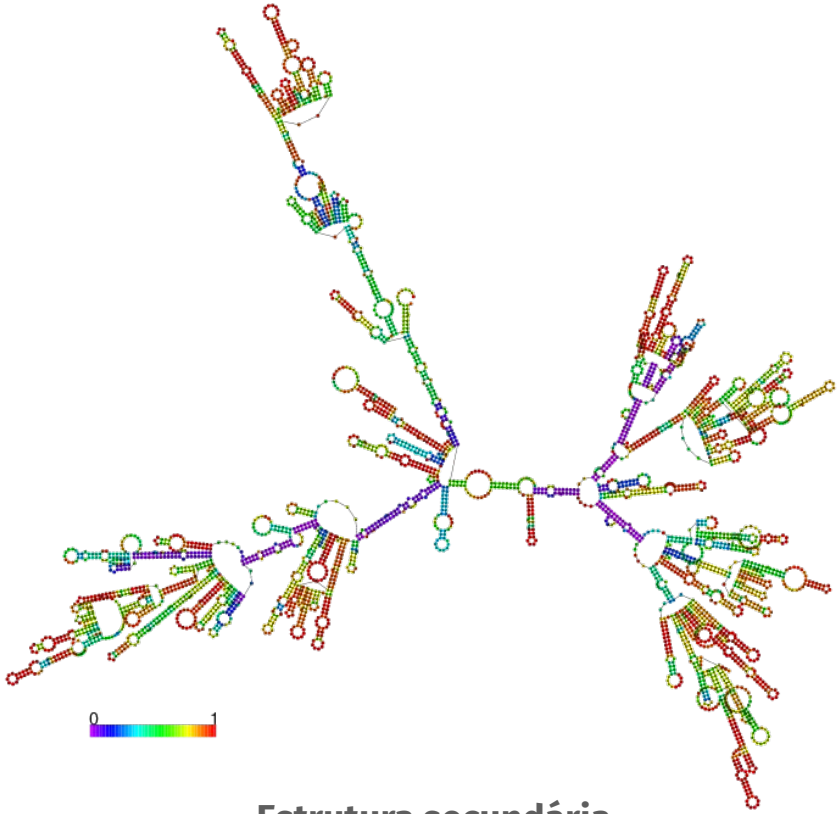
Sequência da vacina de mRNA antes da otimização de códons

RNAfold WebServer

ViennaRNA Web Services
Institute for Theoretical Chemistry

Leticia Kaiser

Vacina de mRNA (antes da otimização)



Estrutura secundária

Energia livre mínima: -1110.70 kcal/mol

Fonte: ViennaRNA, 2024

Vacina de mRNA (após a otimização)

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C TGC GAG TTC CAA TTT TGC AAT GAT CCC TTT CTG GAC GTA TAC CAT AAA AAT AAT AAG TCT TGG ATG GAG TCC GAA TCT GGT GTG TAC AGC TCC GCT AAC AAT
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TAT ACT TAAGCTGGAGCCTCGGTGGCCATGCTTCTTGCCCCTTGGGCCTCCCCCCAGCCCCTCCTCCCCTTCCTGCACCCGTACCCCCGTGGTCTTTGAATAAAGTCTGAGTGGGCGGCA

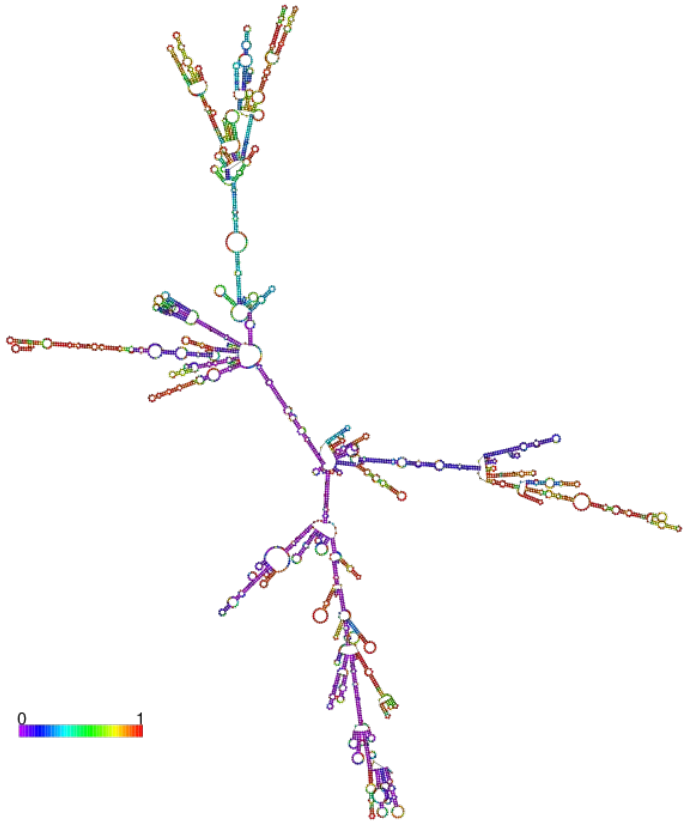
Sequência da vacina de mRNA após a otimização de códons

RNAfold WebServer

ViennaRNA Web Services
Institute for Theoretical Chemistry

Leticia Kaiser

Vacina de mRNA (após a otimização)



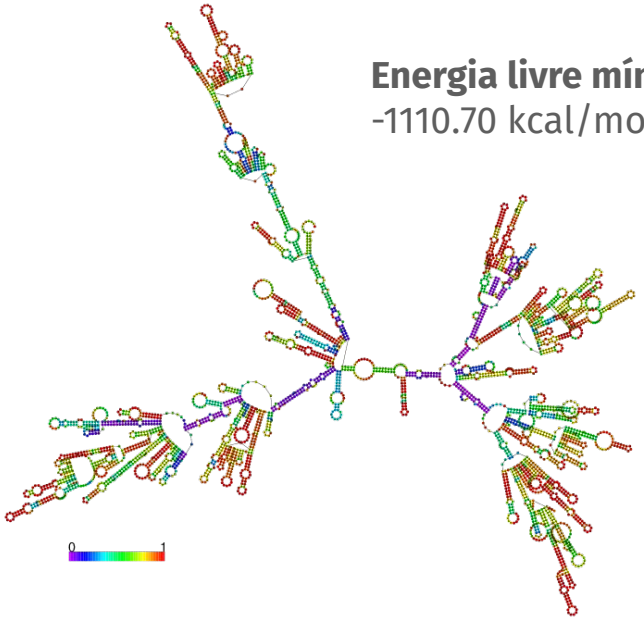
Estrutura secundária

Energia livre mínima: -1153.10 kcal/mol

Fonte: ViennaRNA, 2024

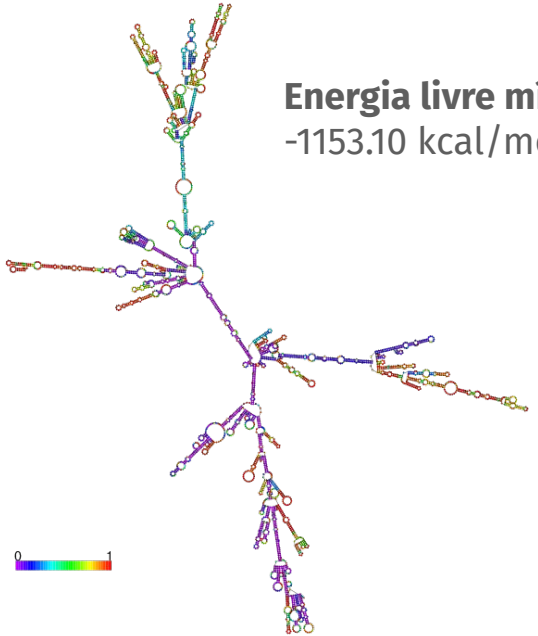
Leticia Kaiser

Estruturas Secundárias e Energia Livre



Energia livre mínima:
-1110.70 kcal/mol

Otimização de códons



Energia livre mínima:
-1153.10 kcal/mol

Vacina de mRNA antes

Vacina de mRNA depois

Otimização de códons → Aumento da estabilidade da estrutura secundária

Fonte: ViennaRNA, 2024

Helena

Sequências da Spike da linhagem JN.1 antes e após as mutações

Helena

Sequência cDNA Spike JN.1: sem mutação

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3809 bp

Helena

Sequência traduzida Spike JN.1: sem mutação

5'3' Frame 1

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1269 resíduos

Expasy
Bioinformatics Resource

Helena

Domínio RBD Spike JN.1: sem mutação

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KGVKLHYT

Segundo o roteiro disponibilizado (316-533) = 217 resíduos*

Helena

Domínio RBD Spike original: sem mutação

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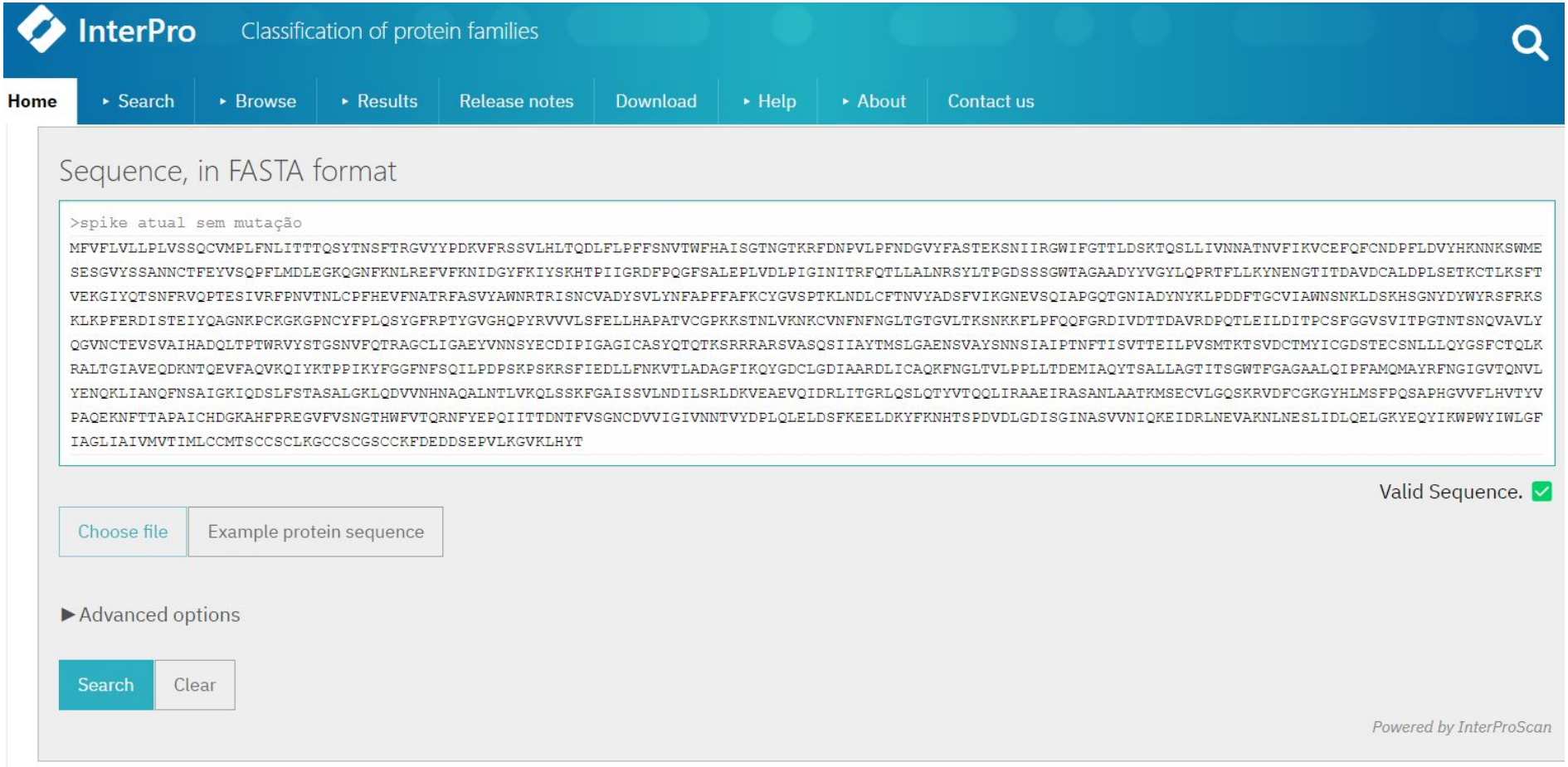
Segundo o roteiro disponibilizado (319-537) = 218 resíduos

Helena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Contact us
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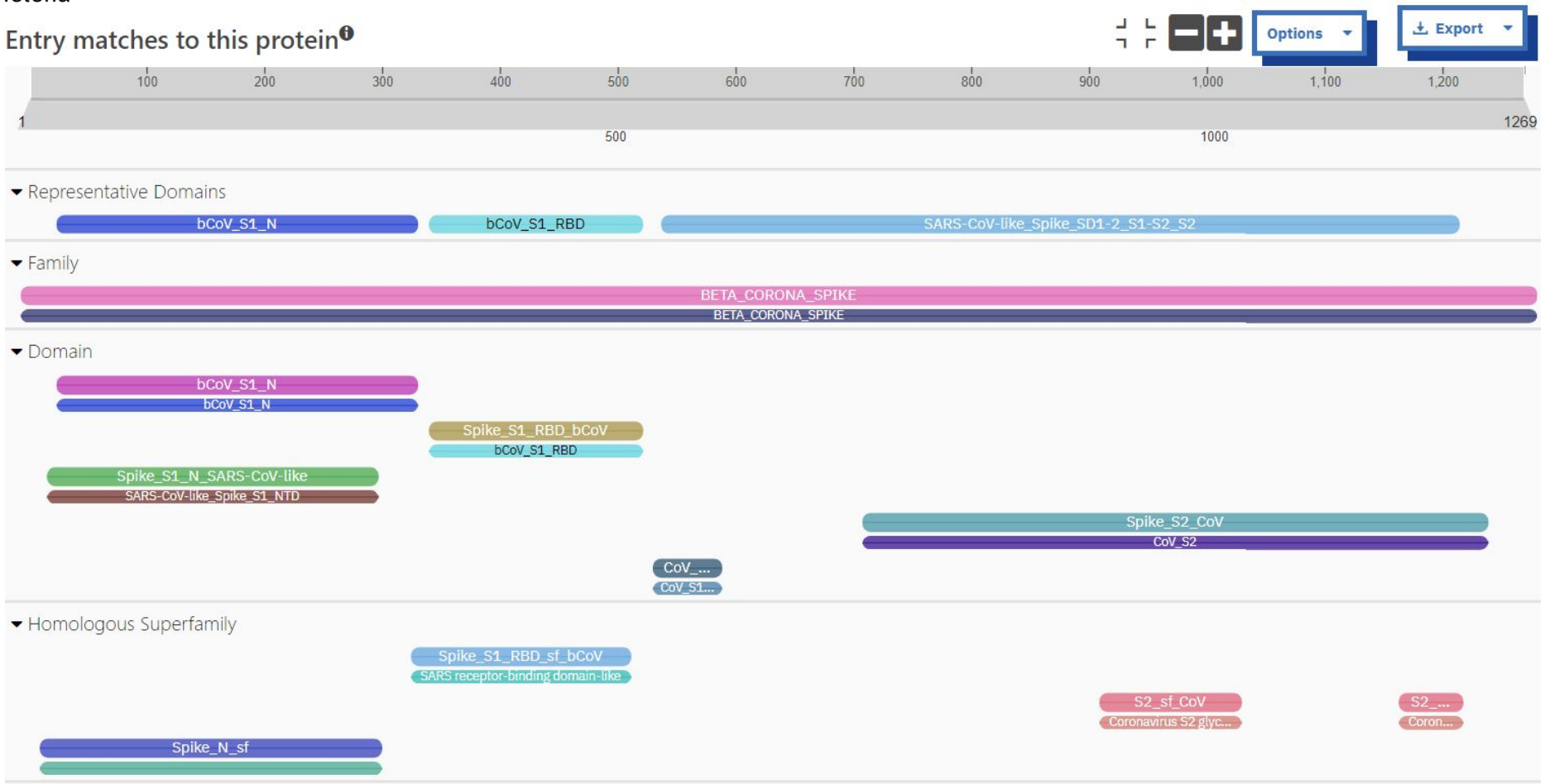
Helena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Helena

Domínio RBD Spike JN.1: sem mutação

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KGVKLHYT

Segundo o Interpro (345-522) = 177 resíduos

InterPro

Helena

Sequência cDNA Spike JN.1: com mutação

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3809 bp

CCU
CCC
CCA
CCG
Pro

Helena

Sequência traduzida Spike JN.1: com mutação

5'3' Frame 1

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1269 resíduos

Expasy
Bioinformatics Resource

Helena

Domínio RBD Spike JN.1: com mutação

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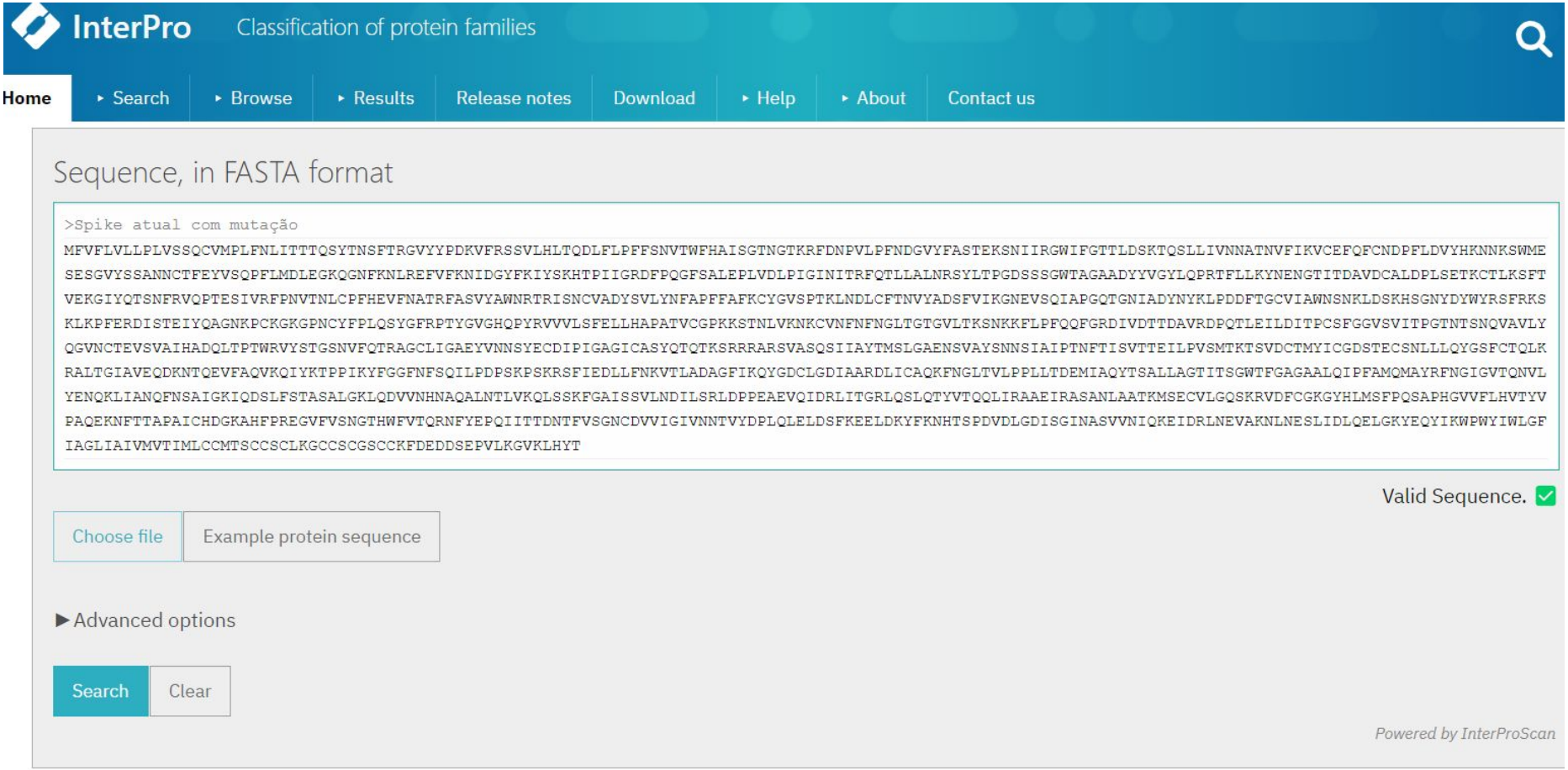
KGVKLHYT

Segundo o roteiro disponibilizado (316-533) = 217 resíduos

Helena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▶ Advanced options
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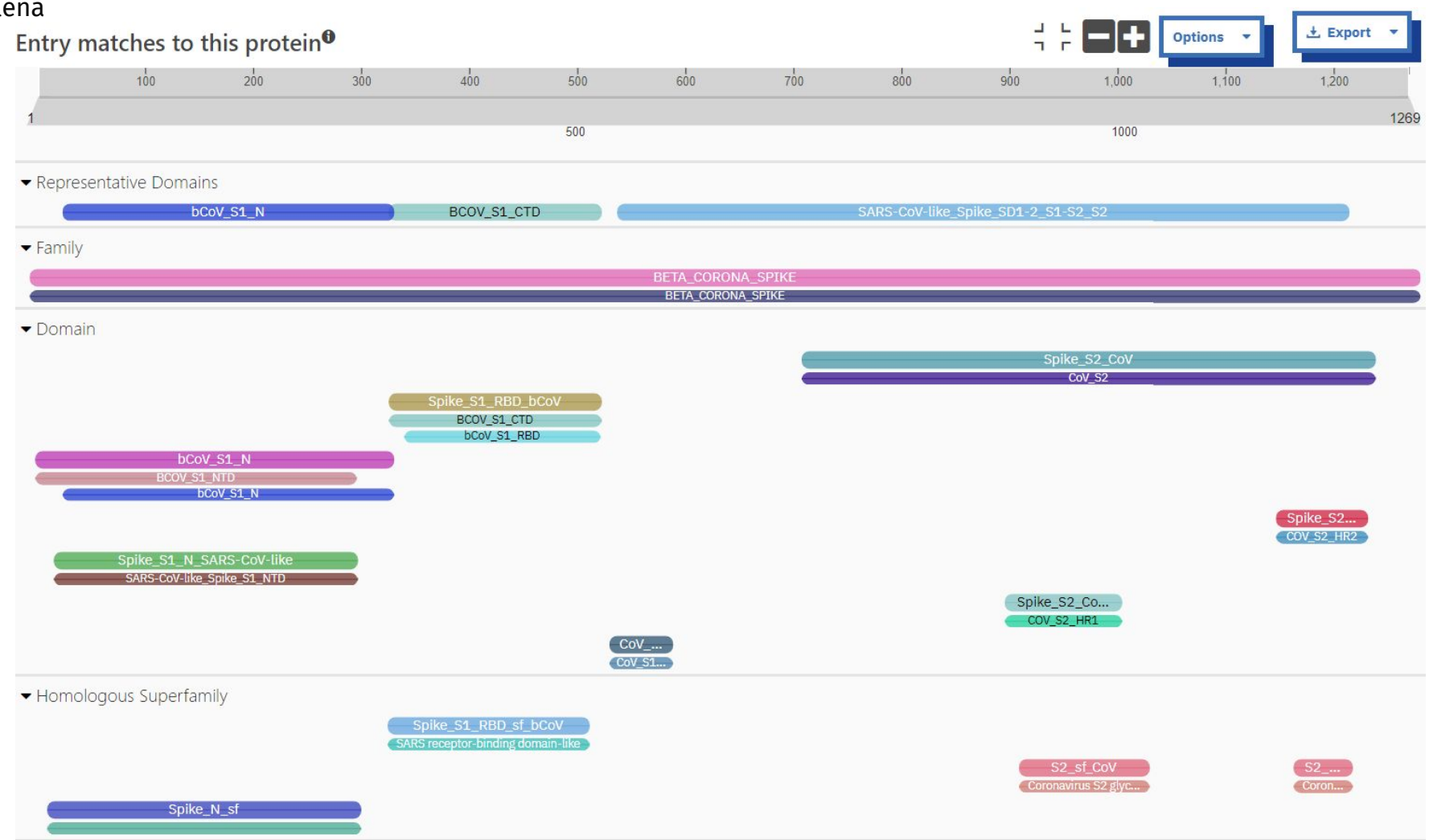
Helena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Homologous Superfamily
Spike_S1_RBD_sf_bCoV
SARS receptor-binding domain-like
S2_sf_CoV
Coronavirus S2 glyc...
S2_...
Coron...
Spike_N_sf

Helena

Domínio RBD Spike JN.1: com mutação

MFVFLVLLPLVSSQCVMPLFNLITTTQSYTNSFTRGVYYPDKVFRSSVLHLTQDLFLPFFSNVTWFHAISGTNGTKRFDNPVLPFNDGVYFASTEKS
NIIRGWIFGTTLDSKTQSLLIVNNATNVFIKVCEFQFCNDPFLDVYHKNNKSWMESESGVYSSANNCTFEYVSQPFLMDLEGKQGNFKNLREFVFKN
IDGYFKIYSKHTPIIGRDFPQGFSALEPLVDLPIGINITRFQTLLALNRSYLTPGDSSSGWTAGAADYYVGYLQPRTFLLKYNENGTITDAVDCALD
PLSETKCTLKSFTVEKGIYQTSNFRVQPTESIVRFPNVTNLCPFHEVFNATRFASVYAWNRTRISNCVADYSVLYNFAPFFAFKCYGVSPTKLNDLC
FTNVYADSFVIKGNEVSQIAPGQTGNIADYNYKLPDDFTGCVIAWNSNKLDSKHSGNYDYWYRSFRKSKLKPFERDISTEIYQAGNKPCKGKGPNCY
FPLQSYGFRPTYGVGHQPYRVVVLSFELLHAPATVCGPKKSTNLVKNKCVNFNFNGLTGTGVLTKSNKKFLPFQQFGRDIVDTTDAVRDPQTLEILD
ITPCSFGGVSVITPGTNTSNQVAVLYQGVNCTEVSVAIHADQLTPTWRVYSTGSNVFQTRAGCLIGAEYVNNSYECDIPIGAGICASYQTQTKSRRR
ARSVASQSIIAYTMSLGAENSVAYSNNSIAIPTNFTISVTTEILPVSMTKTSVDCTMYICGDSTECSNLLLQYGSFCTQLKRALTGIAVEQDKNTQE
VFAQVKQIYKTPPIKYFGGFNFSQILPDPSKPSKRSFIEDLLFNKVTLADAGFIKQYGDCLGDIAARDLICAQKFNGLTVLPPLLTDEMIAQYTSAL
LAGTITSGWTFGAGAALQIPFAMQMAYRFNGIGVTQNVLYENQKLIANQFNSAIGKIQDSLFSTASALGKLQDVVNHNAQALNTLVKQLSSKFGAIS
SVLNDILSRLDPPEAEVQIDRLITGRLQSLQTYVTQQLIRAAEIRASANLAATKMSECVLGQSKRVDFCGKGYHLMSFPQSAPHGVVFLHVTYVPAQ
EKNFTTAPAICHDGKAHFPREGVFVSNGTHWFVTQRNFYEPQIITTDNTFVSGNCDVVIGIVNNTVYDPLQLELDSFKEELDKYFKNHTSPDVDLGD
ISGINASVVNIQKEIDRLNEVAKNLNESLIDLQELGKYEQYIKWPWYIWLGFIAGLIAIVMVTIMLCCMTSCCSCLKGCCSCGSCCKFDEDDSEPVL
KGVKLHYT

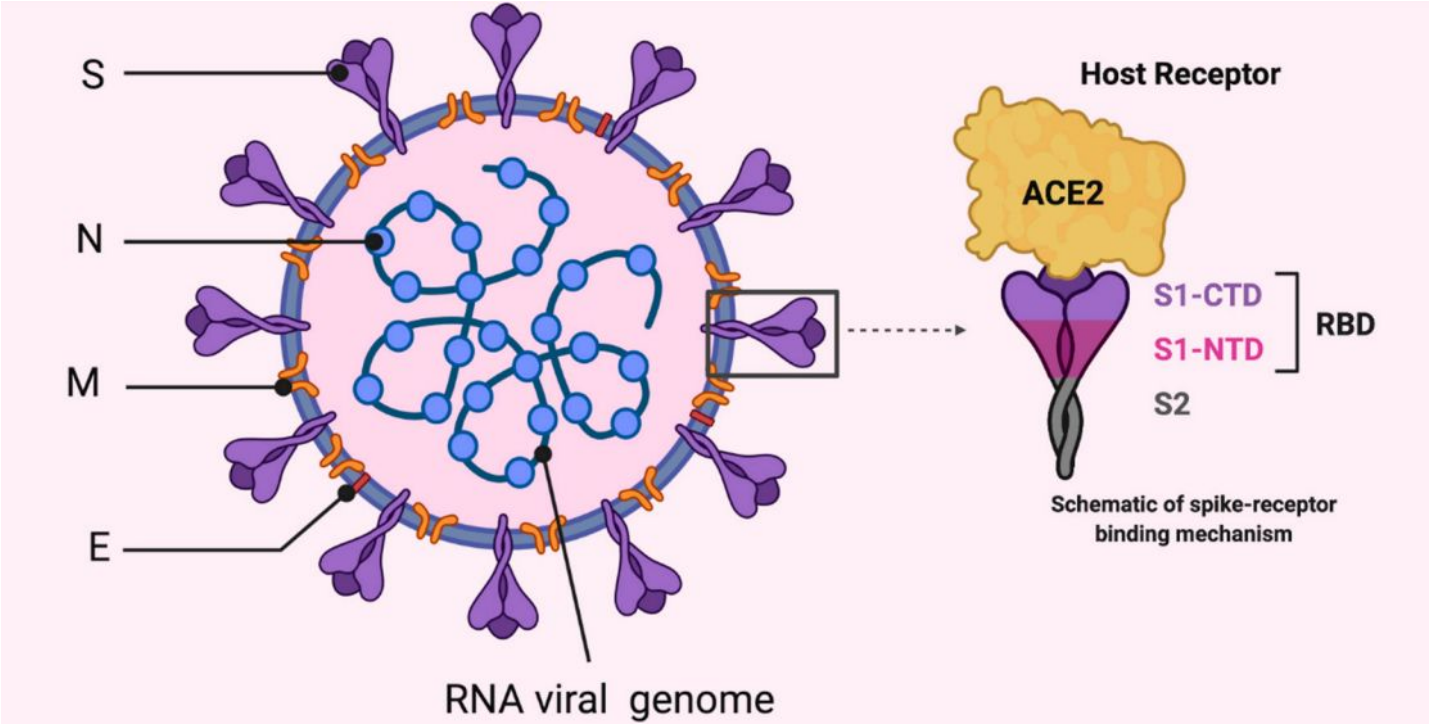
Segundo o Interpro (345-522) = 177 resíduos

InterPro

Helena

Domínio RBD

Receptor Binding Domain



Mahmood, Z. et al, 2020

4. Perfil Imunológico

IEDB
Immune Epitope Database & Tools

Predição de epítopos (pré-mutação)

Predicted peptides:

No.	Start	End	Peptide	Length
1	22	32	LITTTQSYTNS	11
2	56	77	FLPFFSNVTWFHAISGTNGTKR	22
3	137	152	DPFLDVYHKNNKSWME	16
4	173	187	FLMDLEGKQGNFKNL	15
5	206	217	TPIIGRDFPQGF	12
6	246	258	LTPGDSSSGWTAG	13
7	291	291	D	1
8	293	293	L	1
9	303	321	FTVEKGIYQTSNFRVQPTE	19
10	326	362	FPNVTNLCPFHEVFNATRFASVYAWNRTRISNCVADY	37
11	370	392	PFFAFKCYGVSPTKLNDLCFTNV	23
12	398	423	VIKGNEVSQIAPGQTGNIADYNYKLP	26
13	436	494	NKLDSKHSGNYDYWYRSFRKSKLKPFERDISTEIYQAGNKPCKGKGPNCYFPLQSYGFR	59
14	513	530	LLHAPATVCGPKKSTNLV	18
15	553	557	KKFLP	5
16	576	578	QTL	3

Obs. RBD 316-533

IEDB
Immune Epitope Database & Tools

Predição de epítopos (pré-mutação)

17	598	602	TNTSN	5
18	612	616	NCTEV	5
19	620	628	IHADQLTPT	9
20	633	643	STGSNVFQTRA	11
21	651	661	YVNNSYECDIP	11
22	669	686	SYQTQTKSRRRARSVASQ	18
23	692	705	TMSLGAENSVAYSN	14
24	744	744	E	1
25	769	775	EQDKNTQ	7
26	782	810	KQIYKTPPIKYFGGFNFSQILPDPSKPSK	29
27	824	839	LADAGFIKQYGDCLGD	16
28	984	988	EAEVQ	5
29	1031	1039	GQSKRVDFC	9
30	1104	1114	NFYEPQIITTD	11
31	1129	1170	VNNTVYDPLQLELDSFKEELDKYFKNHTSPDVDLGDISGINA	42
32	1199	1203	LGKYE	5
33	1249	1263	CCKFDEDDSEPVLKG	15
34	1265	1265	K	1

Total: 34 epítopos

IEDB
Immune Epitope Database & Tools

Predição de epítopos (pós-mutação)

Predicted peptides:

No.	Start	End	Peptide	Length
1	23	32	ITTTQSYTNS	10
2	56	77	FLPFFSNVTWFHAISGTNGTKR	22
3	137	152	DPFLDVYHKNNKSWME	16
4	173	187	FLMDLEGKQGNFKNL	15
5	206	217	TPIIGRDFPQGF	12
6	246	258	LTPGDSSSGWTAG	13
7	291	291	D	1
8	293	293	L	1
9	303	320	FTVEKGIYQTSNFRVQPT	18
10	327	351	PNVTNLCPFHEVFNATRFASVYAWN	25
11	353	353	T	1
12	355	362	ISNCVADY	8
13	368	392	FAPFFAFKCYGVSPTKLNDLCFTNV	25
14	399	418	IKGNEVSQIAPGQTGNIADY	20
15	420	423	YKLP	4
16	437	495	KLDSKHSGNYDYWYRSFRKSKLKPFERDISTEIYQAGNKPCKGKGPNCYFPLQSYGFRP	59
17	513	530	LLHAPATVCGPKKSTNLV	18
18	553	557	KKFLP	5
19	576	578	QTL	3
20	598	602	TNTSN	5
21	612	616	NCTEV	5

Obs. RBD 316-533

Maria Laura

Predição de epítopos (pós-mutação)

22	620	628	IHADQLTPT	9
23	633	643	STGSNVFQTRA	11
24	651	661	YVNNSYECDIP	11
25	669	686	SYQTQTKSRRRARSVASQ	18
26	692	705	TMSLGAENSVAYSN	14
27	744	744	E	1
28	769	775	EQDKNTQ	7
29	782	810	KQIYKTPPIKYFGGFNFSQILPDPSKPSK	29
30	824	839	LADAGFIKQYGDCLGD	16
31	981	989	DPPEAEVQI	9
32	1031	1039	GQSKRVDFC	9
33	1103	1114	RNFYEPQIITTD	12
34	1129	1170	VNNTVYDPLQLELDSFKEELDKYFKNHTSPDVDLGDISGINA	42
35	1198	1203	ELGKYE	6
36	1249	1263	CCKFDEDDSEPVLKG	15
37	1265	1265	K	1

Total: 37 epítopos

Epítopos de MHC I e II

MHC-I

	Epítopo	*Start*	*End*	Tamanho	Aminoácidos	Score	Afinidade
Sem mutação	HLA-A*11:01	446	454	9	PREGVFVSN	0.0	100%
Com mutação	HLA-A*11:01	413	422	10	PHGVVFLHVT	0.0	100%

Fonte: autoral, 2024

- ➔ Tamanho (início e fim);
- ➔ Sequência de aminoácidos;
- ➔ *Score*;
- ➔ Afinidade do epítopo ao MHC I.

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Immune Epitope Database & Tools

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MHC-II

Fonte: Autoral, 2024

	Epítopo	Start	End	Tamanho	Aminoácidos	Score	Afinidade
Sem mutação	HLA-DRB4*01:01	472	486	15	CKGKGPNCY	0.0003	100.0
Mutação 2P	HLA-DRB4*01:01	472	486	15	CKGKGPNCY	0.0003	100.0

Quantidade de epítopos:

MHC-II original
sem mutação: 27.945 epítopos
com mutação: 27.945 epítopos

MHC-II atual
sem mutação: 27.945 epítopos
com mutação: 33.885 epítopos

Audrey Beatriz

Sem mutação

Method used: netmhciipan_el

allele	seq_num	start	end	length	core_peptide	peptide	score	rank	
HLA-DRB5*01:01	1	341	354	14	FASVYAWNR	ATRFASVYAWNRTR	0.8510	0.06	
HLA-DRB3*01:01	1	459	472	14	FERDISTEI	KPFERDISTEIYQA	0.9192	0.06	
HLA-DRB3*01:01	1	458	471	14	FERDISTEI	LKPFERDISTEIYQ	0.9261	0.06	
HLA-DRB5*01:01	1	932	946	15	FSTASALGK	DSLFSTASALGKLQD	0.8472	0.08	
HLA-DRB3*01:01	1	457	472	16	FERDISTEI	KLKPFERDISTEIYQA		0.9121	0.08
HLA-DRB3*01:01	1	458	472	15	FERDISTEI	LKPFERDISTEIYQA	0.9213	0.08	
HLA-DRB5*01:01	1	340	354	15	FASVYAWNR	NATRFASVYAWNRTR	0.8232	0.1	
HLA-DRB3*01:01	1	457	470	14	FERDISTEI	KLKPFERDISTEIY	0.8715	0.1	
HLA-DRB3*01:01	1	457	471	15	FERDISTEI	KLKPFERDISTEIYQ	0.9054	0.1	
HLA-DRB5*01:01	1	932	945	14	FSTASALGK	DSLFSTASALGKLQ	0.7789	0.11	
HLA-DRB5*01:01	1	341	355	15	FASVYAWNR	ATRFASVYAWNRTRI	0.8078	0.12	
HLA-DRB5*01:01	1	931	946	16	FSTASALGK	QDSLFSTASALGKLQD		0.8292	0.12
HLA-DRB3*01:01	1	458	473	16	FERDISTEI	LKPFERDISTEIYQAG		0.8696	0.12
HLA-DRB3*01:01	1	456	471	16	FERDISTEI	SKLKPFERDISTEIYQ		0.8698	0.12
HLA-DRB3*01:01	1	459	473	15	FERDISTEI	KPFERDISTEIYQAG	0.8415	0.14	
HLA-DRB3*01:01	1	456	470	15	FERDISTEI	SKLKPFERDISTEIY	0.8108	0.16	
HLA-DRB5*01:01	1	932	947	16	FSTASALGK	DSLFSTASALGKLQDV		0.7744	0.18
HLA-DRB5*01:01	1	340	355	16	FASVYAWNR	NATRFASVYAWNRTRI		0.7884	0.18
HLA-DRB5*01:01	1	339	354	16	FASVYAWNR	FNATRFASVYAWNRTR		0.7888	0.18
HLA-DRB5*01:01	1	340	353	14	FASVYAWNR	NATRFASVYAWNRT	0.7335	0.19	
HLA-DRB5*01:01	1	775	789	15	FAQVKQIYK	QEVFAQVKQIYKTPP	0.7751	0.2	
HLA-DRB5*01:01	1	342	355	14	FASVYAWNR	TRFASVYAWNRTRI	0.7187	0.21	
HLA-DRB5*01:01	1	775	788	14	FAQVKQIYK	QEVFAQVKQIYKTP	0.7189	0.21	
HLA-DRB5*01:01	1	931	945	15	FSTASALGK	QDSLFSTASALGKLQ	0.7483	0.22	
HLA-DRB5*01:01	1	774	789	16	FAQVKQIYK	TQEVFAQVKQIYKTPP		0.7520	0.22
HLA-DRB5*01:01	1	341	356	16	FASVYAWNR	ATRFASVYAWNRTRIS		0.7394	0.24
HLA-DRB1*01:01	1	535	550	16	FNGLTGTGV	VNFNFNGLTGTGVLTK		0.9358	0.25
HLA-DRB1*01:01	1	536	550	15	FNGLTGTGV	NFNFNGLTGTGVLTK	0.9435	0.26	
HLA-DRB5*01:01	1	933	946	14	FSTASALGK	SLFSTASALGKLQD	0.6997	0.27	
HLA-DRB5*01:01	1	232	245	14	FQTLLALNR	ITRFQTLLALNRSY	0.6855	0.28	
HLA-DRB3*01:01	1	455	470	16	FERDISTEI	KSKLKPFERDISTEIY		0.7190	0.28
HLA-DRB3*01:01	1	459	474	16	FERDISTEI	KPFERDISTEIYQAGN		0.7252	0.28
HLA-DRB5*01:01	1	775	790	16	FAQVKQIYK	QEVFAQVKQIYKTPPI		0.7016	0.29
HLA-DRB1*01:01	1	312	325	14	FRVQPTESI	TSNFRVQPTESIVR	0.9072	0.34	
HLA-DRB1*01:01	1	63	77	15	FHAISGTNG	VTWFHAISGTNGTKR	0.9222	0.34	
HLA-DRB5*01:01	1	231	244	14	FQTLLALNR	NITRFQTLLALNRS	0.6566	0.35	
HLA-DRB5*01:01	1	930	945	16	FSTASALGK	IQDSLFSTASALGKLQ		0.6749	0.36
HLA-DRB3*01:01	1	1250	1263	14	FDEDDSEPV	CKFDEDDSEPVLKG	0.6972	0.36	
HLA-DRB5*01:01	1	339	353	15	FASVYAWNR	FNATRFASVYAWNRT	0.6690	0.37	
HLA-DRB5*01:01	1	774	788	15	FAQVKQIYK	TQEVFAQVKQIYKTP	0.6734	0.37	
HLA-DRB1*01:01	1	536	551	16	FNGLTGTGV	NFNFNGLTGTGVLTKS		0.9067	0.4
HLA-DRB5*01:01	1	776	789	14	FAQVKQIYK	EVFAQVKQIYKTPP	0.6383	0.42	

27.945 epítopos

Fonte: Autoral, 2024

Audrey Beatriz

Com mutação 2P

Method used: netmhciipan_el

allele	seq_num	start	end	length	core_peptide	peptide	score	rank
HLA-DRB5*01:01	1	341	354	14	FASVYAWNR	ATRFASVYAWNRTR	0.8510	0.06
HLA-DRB3*01:01	1	459	472	14	FERDISTEI	KPFERDISTEIYQA	0.9192	0.06
HLA-DRB3*01:01	1	458	471	14	FERDISTEI	LKPFERDISTEIYQ	0.9261	0.06
HLA-DRB5*01:01	1	932	946	15	FSTASALGK	DSLFSTASALGKLQD	0.8472	0.08
HLA-DRB3*01:01	1	457	472	16	FERDISTEI	KLKPFERDISTEIYQA	0.9121	0.08
HLA-DRB3*01:01	1	458	472	15	FERDISTEI	LKPFERDISTEIYQA	0.9213	0.08
HLA-DRB5*01:01	1	340	354	15	FASVYAWNR	NATRFASVYAWNRTR	0.8232	0.1
HLA-DRB3*01:01	1	457	470	14	FERDISTEI	KLKPFERDISTEIY	0.8715	0.1
HLA-DRB3*01:01	1	457	471	15	FERDISTEI	KLKPFERDISTEIYQ	0.9054	0.1
HLA-DRB5*01:01	1	932	945	14	FSTASALGK	DSLFSTASALGKLQ	0.7789	0.11
HLA-DRB5*01:01	1	341	355	15	FASVYAWNR	ATRFASVYAWNRTRI	0.8078	0.12
HLA-DRB5*01:01	1	931	946	16	FSTASALGK	QDSLFSTASALGKLQD	0.8292	0.12
HLA-DRB3*01:01	1	458	473	16	FERDISTEI	LKPFERDISTEIYQAG	0.8696	0.12
HLA-DRB3*01:01	1	456	471	16	FERDISTEI	SKLKPFERDISTEIYQ	0.8698	0.12
HLA-DRB3*01:01	1	459	473	15	FERDISTEI	KPFERDISTEIYQAG	0.8415	0.14
HLA-DRB3*01:01	1	456	470	15	FERDISTEI	SKLKPFERDISTEIY	0.8108	0.16
HLA-DRB5*01:01	1	932	947	16	FSTASALGK	DSLFSTASALGKLQDV	0.7744	0.18
HLA-DRB5*01:01	1	340	355	16	FASVYAWNR	NATRFASVYAWNRTRI	0.7884	0.18
HLA-DRB5*01:01	1	339	354	16	FASVYAWNR	FNATRFASVYAWNRTR	0.7888	0.18
HLA-DRB5*01:01	1	340	353	14	FASVYAWNR	NATRFASVYAWNRT	0.7335	0.19
HLA-DRB5*01:01	1	775	789	15	FAQVKQIYK	QEVFAQVKQIYKTPP	0.7751	0.2
HLA-DRB5*01:01	1	342	355	14	FASVYAWNR	TRFASVYAWNRTRI	0.7187	0.21
HLA-DRB5*01:01	1	775	788	14	FAQVKQIYK	QEVFAQVKQIYKTP	0.7189	0.21
HLA-DRB5*01:01	1	931	945	15	FSTASALGK	QDSLFSTASALGKLQ	0.7483	0.22
HLA-DRB5*01:01	1	774	789	16	FAQVKQIYK	TQEVFAQVKQIYKTPP	0.7520	0.22
HLA-DRB5*01:01	1	341	356	16	FASVYAWNR	ATRFASVYAWNRTRIS	0.7394	0.24
HLA-DRB1*01:01	1	535	550	16	FNGLTGTGV	VNFNFNGLTGTGVLTK	0.9358	0.25
HLA-DRB1*01:01	1	536	550	15	FNGLTGTGV	NFNFNGLTGTGVLTK	0.9435	0.26
HLA-DRB5*01:01	1	933	946	14	FSTASALGK	SLFSTASALGKLQD	0.6997	0.27
HLA-DRB5*01:01	1	232	245	14	FQTLLALNR	ITRFQTLLALNRSY	0.6855	0.28
HLA-DRB3*01:01	1	455	470	16	FERDISTEI	KSKLKPFERDISTEIY	0.7190	0.28
HLA-DRB3*01:01	1	459	474	16	FERDISTEI	KPFERDISTEIYQAGN	0.7252	0.28
HLA-DRB5*01:01	1	775	790	16	FAQVKQIYK	QEVFAQVKQIYKTPPI	0.7016	0.29
HLA-DRB1*01:01	1	312	325	14	FRVQPTESI	TSNFRVQPTESIVR	0.9072	0.34
HLA-DRB1*01:01	1	63	77	15	FHAISGTNG	VTWFHAISGTNGTKR	0.9222	0.34
HLA-DRB5*01:01	1	231	244	14	FQTLLALNR	NITRFQTLLALNRS	0.6566	0.35
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HLA-DRB5*01:01	1	774	788	15	FAQVKQIYK	TQEVFAQVKQIYKTP	0.6734	0.37
HLA-DRB1*01:01	1	536	551	16	FNGLTGTGV	NFNFNGLTGTGVLTKS	0.9067	0.4
HLA-DRB5*01:01	1	776	789	14	FAQVKQIYK	EVFAQVKQIYKTPP	0.6383	0.42

33.885 epítopos

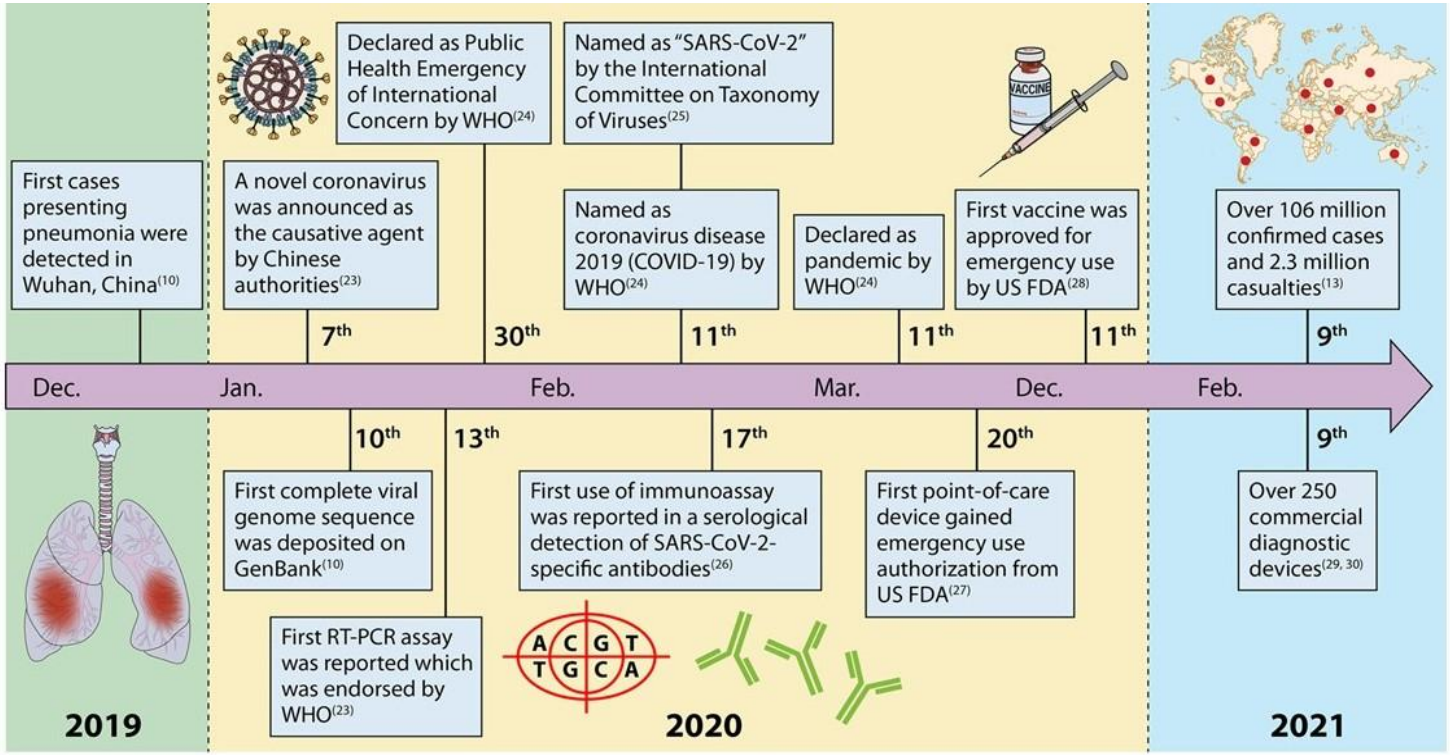
Fonte: Autoral, 2024

Thuany

5. Pontos-chave e conclusão

Panorama geral

Thuany



Fonte: Tali et al., 2021

Recapitulação

Etapa 1

Identificação da proteína Spike no genoma, das mutações 2P e da HBA1.

1º

Etapa 2

Otimização de códons.

2º

Etapa 3

Estrutura do mRNA e análise da energia livre mínima.

3º

Etapa 4

Identificação do domínio RBD.

4º

Etapa 5

Predição de epítopos de anticorpos, MHC-I e MHC-II.

5º

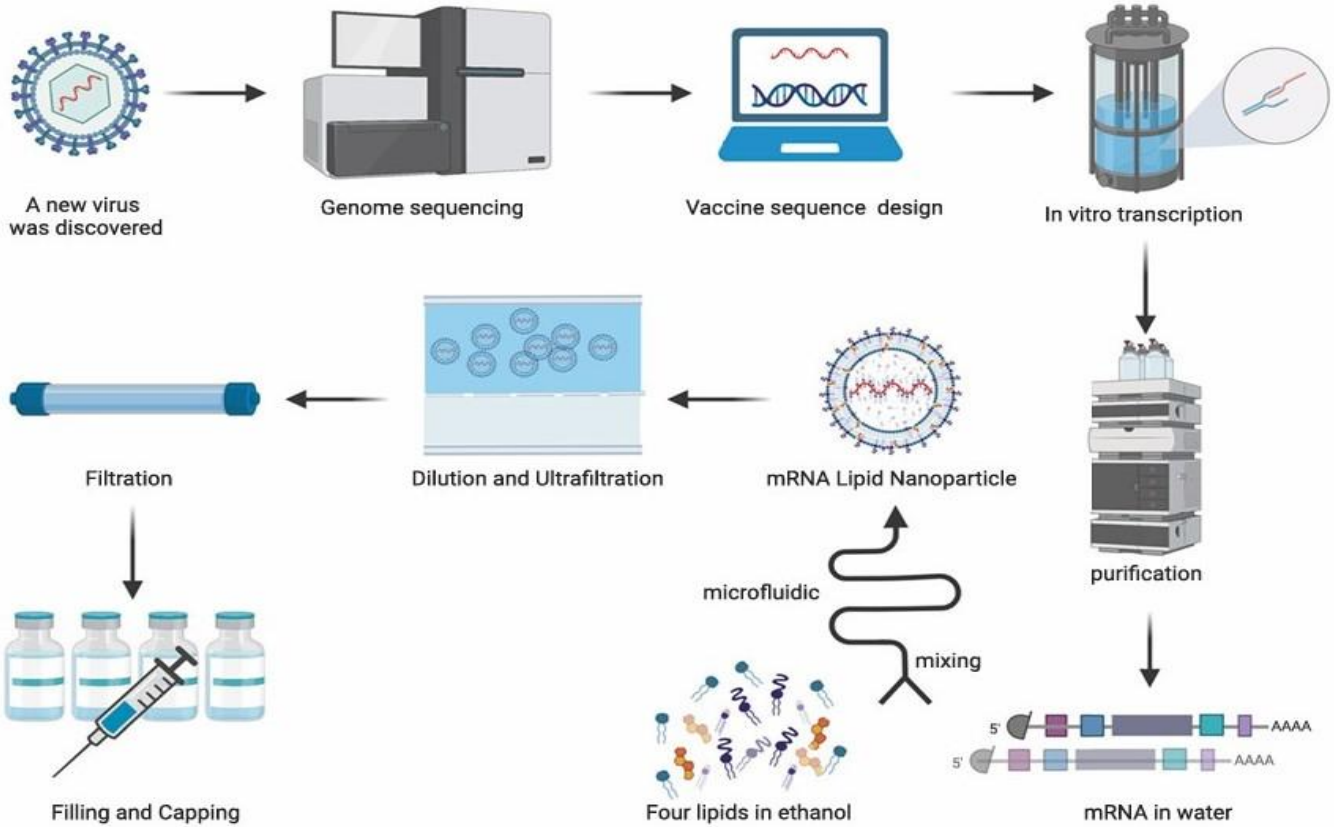
Thuany

A construção de uma vacina de mRNA contra a linhagem atual de SARS-CoV-2 apresentou desenvolvimento satisfatório.

Thuany

Thuany

Perspectivas



Fonte: Fang *et al.*, 2022

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Muito obrigado!