



Bioinformática

Curso de Especialização na Área da Saúde – 2025/2026 Bases Técnicas em Vacinas e Biofármacos

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Bioinformatics, Systems Biology, and Biostatistics

Instituto Butantan – CENTD - Bioinformática



O que vimos até aqui?

Constituição de um organismo eucarioto

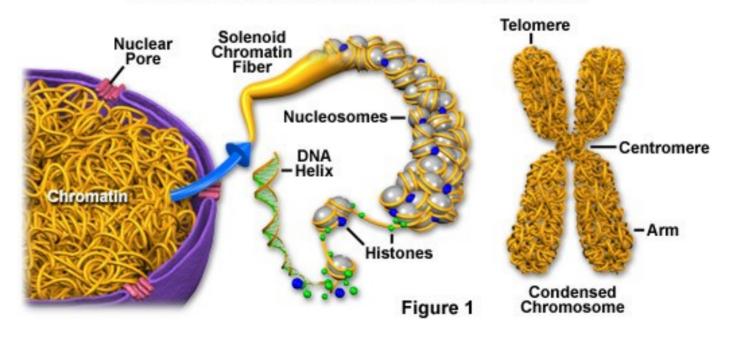
- O corpo é constituído de órgãos
- Os órgãos não são homogêneos e dividios em diferentes tecidos
- Os tecidos são constituídos de células
- Há diferentes tipos de células
- As células têm vários organelas
 - Núcleo
 - Mitocôndria
 - Retículo endoplasmático
 - Lisossomo
 - Endossomo
 - Vacúolos
 - Golgi
 - etc

O que não vimos!

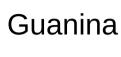
- O cromossomo é uma fita contendo material genético
- Os cromossomos estão enovelados dentro do núcleo
- Cada organismo (homem, coelho, abelha, etc) tem um número de cromossomos diferente
- O cromossomo tem milhões de nucleotídeos
- O cromossomo é formado de 2 fitas em forma de hélice
- Eles se pareiam via interações fracas ligando a fita dupla de DNA.

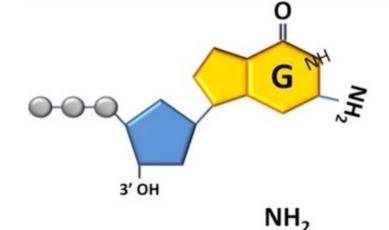
Os cromossomos estão enovelados dentro do núcleo

Chromatin and Condensed Chromosome Structure



Os quatro nucleotídeos existenste no cromossomo





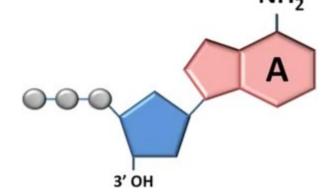
T

NH₂

3' OH

Timina

Adenina



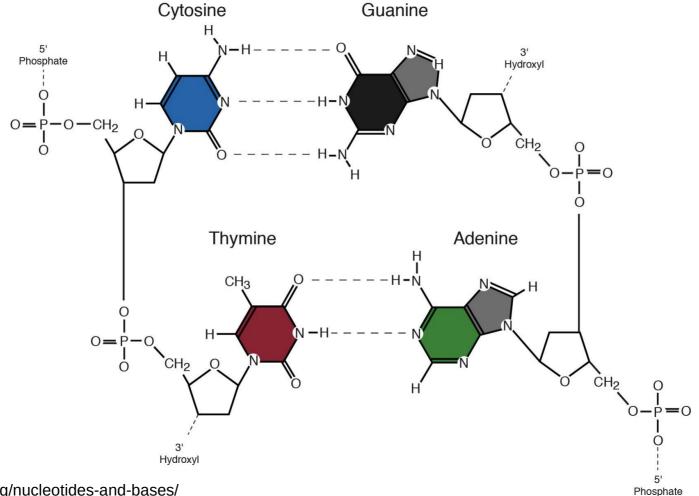
Pyrimidine Deoxyribonucleotides

3' OH

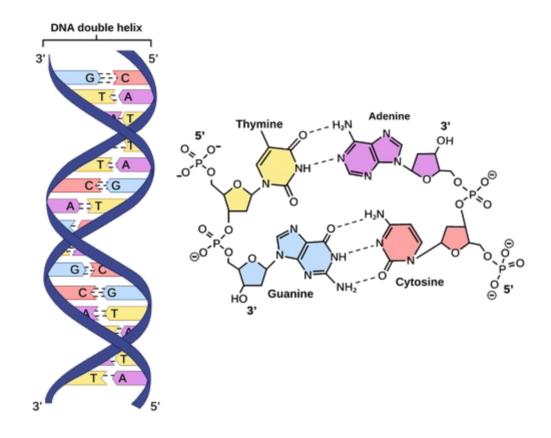
Citosina

Purine Deoxyribonucleotides Ahmad, M., Panicker, N., Rizvi, T. et al. Electrical detection and quantification of single and mixed DNA nucleotides in suspension. Sci Rep 6, 34016 (2016). https://doi.org/10.1038/srep34016

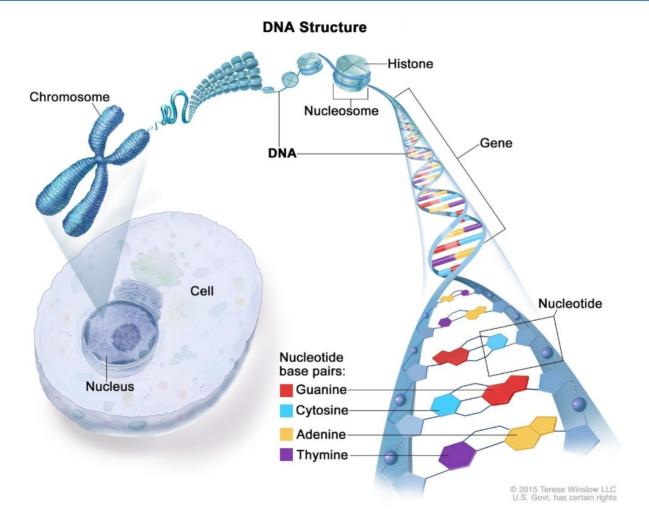
A interação fraca (ponte de hidrogênio) que segura as duas fitas de DNA



Fita dupla de DNA ~ dupla hélice



Hierarquia do cromossomo



Como estudar tudo isto?

Áreas de estudo

- Bioquímica & Química
- Biofísica
- Biologia Molecular
- Biologia Celular
- Genética
- ●...
- e onde entra a metemática?

Biologia x Matemática

- Biomatemática (mathematical biology)
- Matemática aplicada à Biologia de evolução ~ populações



- ●Bioinformática (ômicas) 🤡
- Imunoinformática
- ●Biologia de Sistemas (redes networks) ❤️
- Bioestatística
- ●Engenharia e Matemática aplicada a medicina 🤒



Qual o comprimento do genoma mitocondrial?

Quantos genes existem no genoma mitocondrial?

O que é transferência horizontal e vertical de genes?

O que é bioinformática?

O que é imunoinformática?

O que é bioinformática

Bioinformática é o estudo de algoritmos matemáticos, aprendizado de máquina e bioestatística aplicados para melhor compreender sequências de nucleotídeos e proteínas e os resultados de experimentos das ômicas.

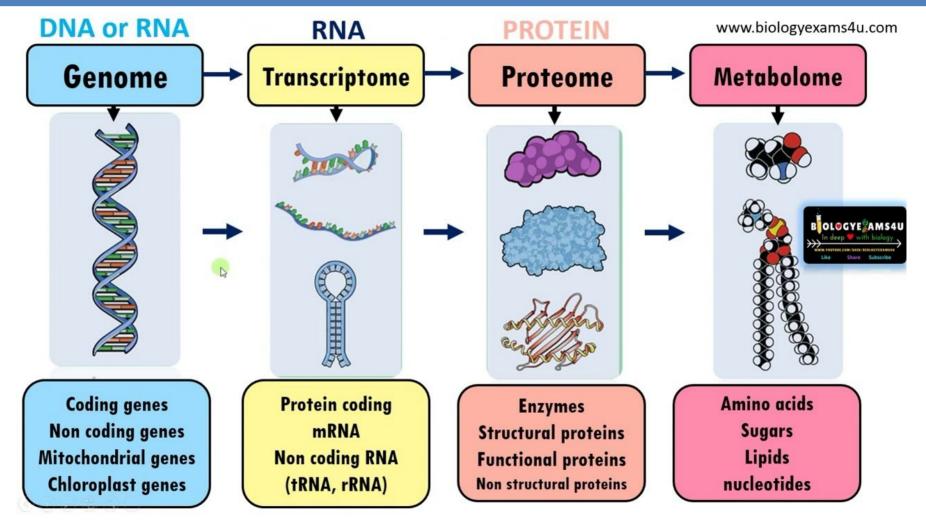
O que são ômicas? São estudos e experimentos relacionados a:

- Genômica
- ●Exômica
- Transcriptômica
- Epigenética

- Proteômica
- Metabolômica
- Single-cell



Qual a diferença entre Genoma, Transcriptoma, Proteoma and Metaboloma?



... me contaram que o COX2 é um gene interessante, será?

... me contaram que o COX2 é um gene interessante, será?

O que posso fazer?

Busca de genes / proteínas

Posso perguntar:

- Onde tem uma boa descrição deste gene?
- ●Em que vias ele participa?
- ●Como posso localizá-lo?

Busca de genes / proteínas

Posso perguntar:

Onde tem uma boa descrição deste gene?

Genecards.org/

Em que vias ele participa?

KEGG"

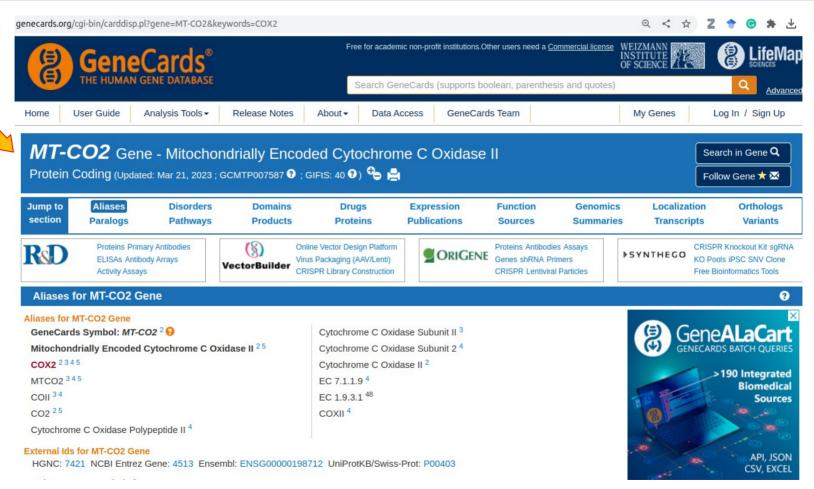
KEGG: procure no google "COX2 pathway https://www.genome.jp/dbget-bin/www_bget?dha:cox2

●Como posso localizá-lo? https://genome.ucsc.edu/

UCSC genome browser

COX2 na verdade é MT-CO2

Genecard







Debaryomyces hansenii: cox2

[66	Debaryomyces hansenii: cox2
Entry	cox2 CDS T01026
Name	(RefSeq) cytochrome c oxidase subunit 2
K0	K02261 cytochrome c oxidase subunit 2
Organism	dha Debaryomyces hansenii
Pathway	dha00190 Oxidative phosphorylation dha01100 Metabolic pathways
Module	dha_M00154 Cytochrome c oxidase
Brite	KEGG Orthology (KO) [BR:dha00001] 09100 Metabolism 09102 Energy metabolism 00190 Oxidative phosphorylation cox2 09180 Brite Hierarchies 09182 Protein families: genetic information processing 03029 Mitochondrial biogenesis [BR:dha03029] cox2 Mitochondrial biogenesis [BR:dha03029] Mitochondrial DNA transcription, translation, and replication fac Mitochondrial DNA-encoded proteins Cytochrome c oxidase cox2 BRITE hierarchy BRITE hierarchy
SSDB	Ortholog Paralog Gene cluster GFIT
Motif	Pfam: COX2 COX2 TM DUF6169
110111	Motif
	NCBI-GeneID: 5845854 NCBI-ProteinID: YP_001621413 UniProt: A9RAG1
Position	MT: 26033343 Genome browser
AA seq	246 aa AAseq DB search MIWTDVPTPWGMRFQDAATPNAEGMHELYDHMMYYLALMLGLVSYMLYVMMKDYKNNTFA YKYIKHGQTLEIMWTMFPAVMLLLMAFPSFMLLYLCDEVLTPAMTVKVVGLQWYWKYEYS DFVSETGETVEYESYVMPEDMLEEGQLRLLDTDTSMVVPVDTHVRFMVTANDVLHCFTMP SLGIKVDACPGRLNQVSALMQRTGVYYGQCSELCGVNHGLMPIKTECVPIGDFVEWLGEQ ENVYVA
NT seq	741 nt NT seq +upstream o nt +downstream o nt atgatttgactagatgtaccaacaccttgaggaatacgtttccaagatgccgcaacacct

All links Ontology (2) KEGG BRITE (2) Pathway (3) KEGG PATHWAY (2) KEGG MODULE (1) Genome (1) KEGG GENOME (1) Gene (17) KEGG ORTHOLOGY (1) RefGene (13) NCBI-PROTEINID (1) NCBI-Gene (1) OC (1) Protein sequence (3) UniProt (1) SWISS-PROT (1) RefSeq(pep) (1) Protein domain (3) Pfam (3) All databases (29) Download RDF

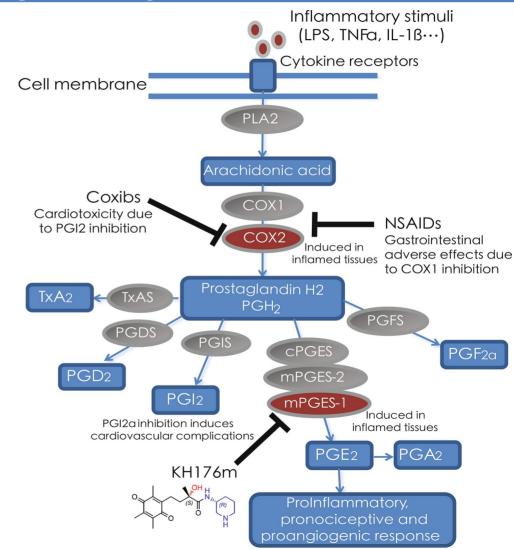
https://www.genome.jp/dbget-bin/www_bget?dha:cox2



KEGG	ORTHOLOGY: K11987	Help
Entry	K11987 K0	
Symbol	PTGS2, COX2	
Name	prostaglandin-endoperoxide synthase 2 [EC:1.14.99.1]	
Pathway	map00590 Arachidonic acid metabolism map01100 Metabolic pathways map04064 NF-kappa B signaling pathway map04370 VEGF signaling pathway map04625 C-type lectin receptor signaling pathway map04657 IL-17 signaling pathway map04668 TNF signaling pathway map04723 Retrograde endocannabinoid signaling map04726 Serotonergic synapse map04913 Ovarian steroidogenesis map04921 Oxytocin signaling pathway map04923 Regulation of lipolysis in adipocytes map05010 Alzheimer disease map05010 Alzheimer disease map05140 Leishmaniasis map05163 Human cytomegalovirus infection map05165 Human papillomavirus infection map05167 Kaposi sarcoma-associated herpesvirus infection map05200 Pathways in cancer map05204 Chemical carcinogenesis - DNA adducts map05206 MicroRNAs in cancer map05222 Small cell lung cancer	
Disease	H00017 Esophageal cancer H00025 Penile cancer H00046 Cholangiocarcinoma	
Brite	KEGG Orthology (KO) [BR:ko00001] 09100 Metabolism 09103 Lipid metabolism 00590 Arachidonic acid metabolism K11987 PTGS2, COX2; prostaglandin-endoperoxide synthase 09130 Environmental Information Processing 09132 Signal transduction 04370 VEGF signaling pathway K11987 PTGS2, COX2; prostaglandin-endoperoxide synthase 04064 NF-kappa B signaling pathway K11987 PTGS2, COX2; prostaglandin-endoperoxide synthase 04668 TNF signaling pathway K11987 PTGS2, COX2; prostaglandin-endoperoxide synthase 04605 TNF signaling pathway 09150 Organismal Systems 09151 Immune system 04625 C-type lectin receptor signaling pathway	2

https://www.genome.jp/dbget-bin/www_bget?ko:K11987

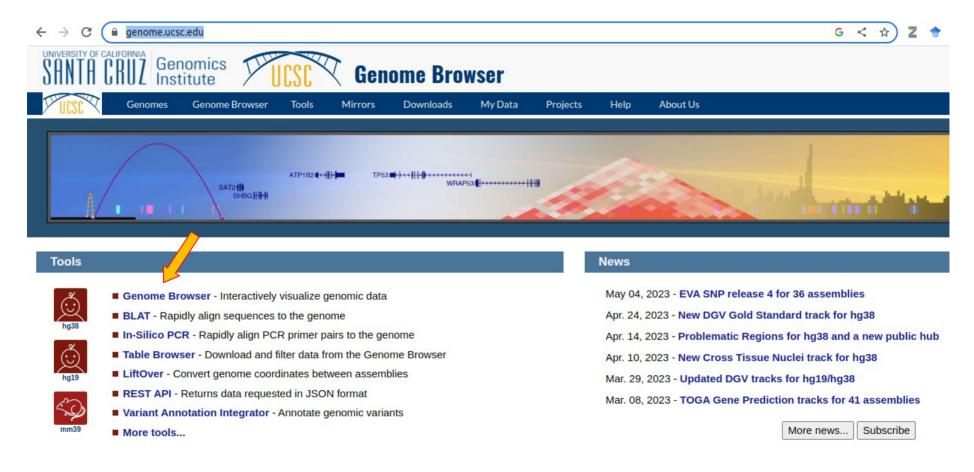
Exemplo de um pahtway contendo COX2



Jiang, X., Renkema, H., Pennings, B. et al. Mechanism of action and potential applications of selective inhibition of microsomal prostaglandin E synthase-1-mediated PGE2 biosynthesis by sonlicromanol's metabolite KH176m. Sci Rep 11, 880 (2021). https://doi.org/10.1038/s41598-020-79466-w

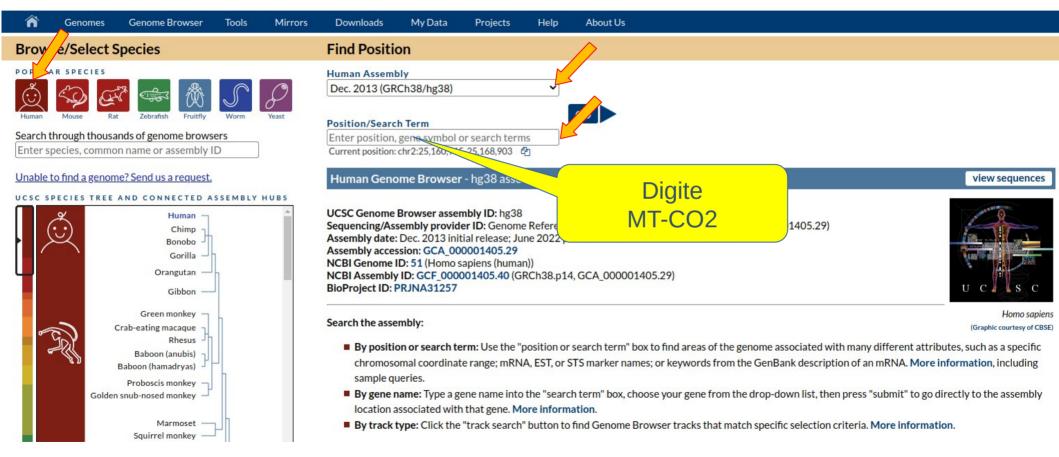
Vamos achar genes? e regiões intergênicas...

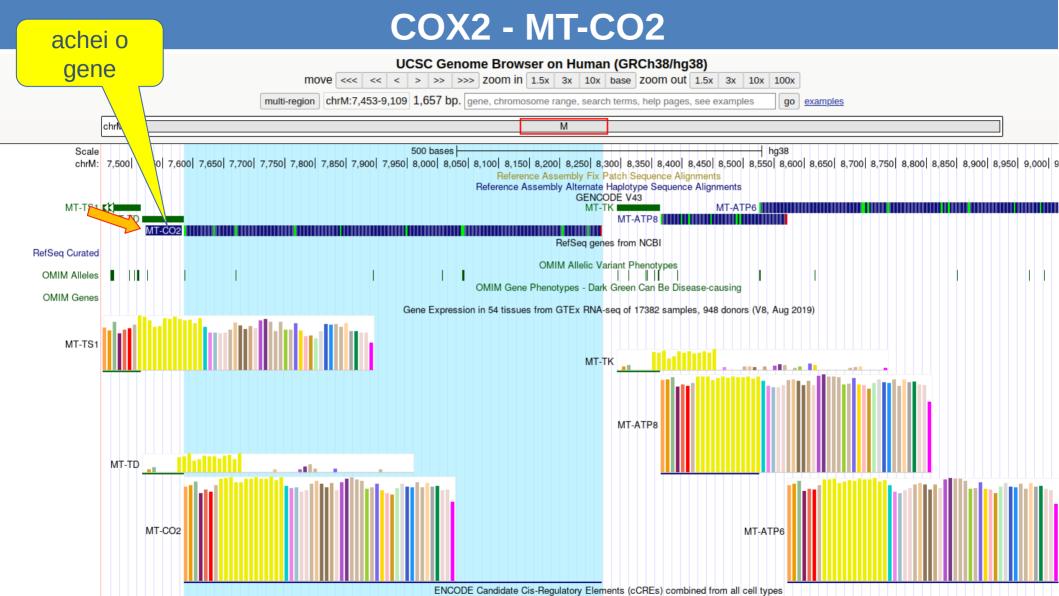
UCSC genome browser

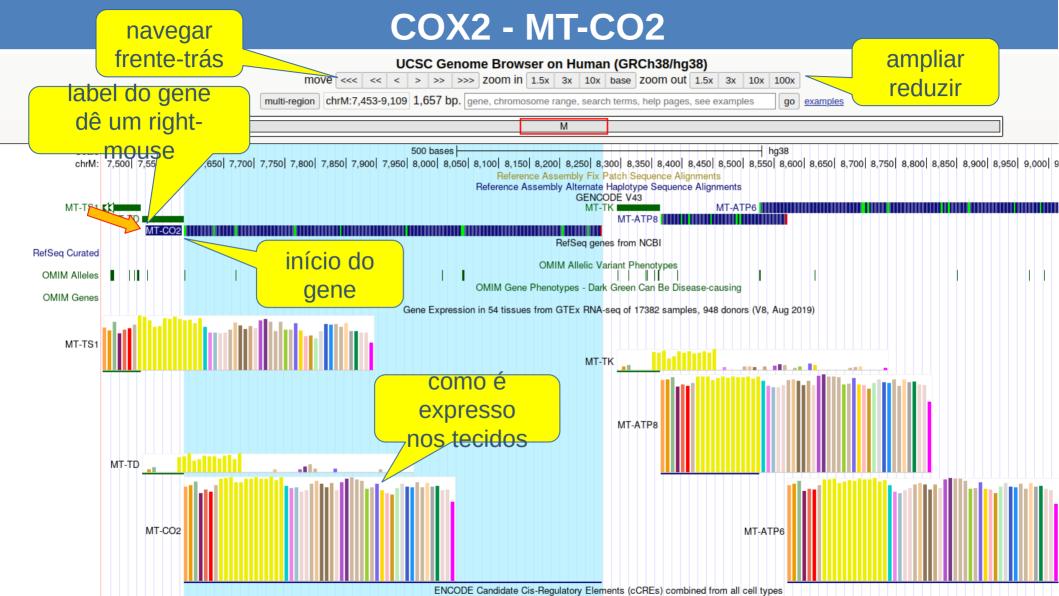


Vamos achar genes? e regiões intergênicas...

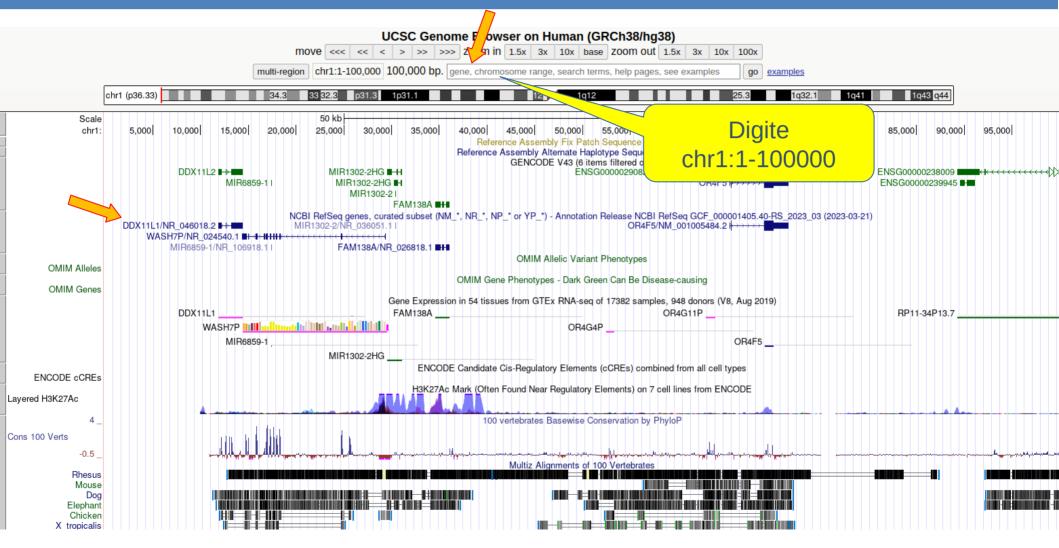
UCSC genome browser



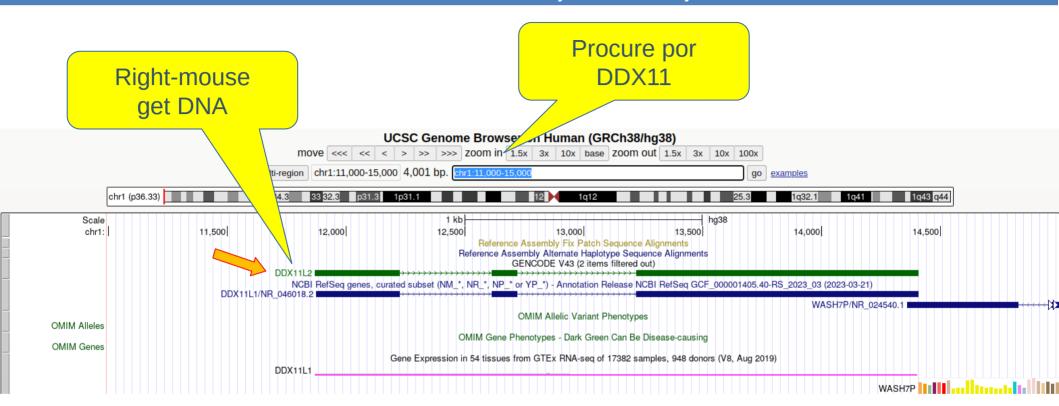




Cromossomo 1 de 1:100000



Zoom: chr1:11,000-15,000



Vamos fazer um BLAST de nucleotídeos

Basic Local Alignment Search Tool



BLAST - nucleotideos





BLAST ®

Home Recent Results Saved Strategies Help

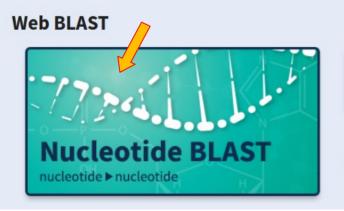
Basic Local Alignment Search Tool

BLAST finds regions of similarity between biological sequences. The program compares nucleotide or protein sequences to sequence databases and calculates the statistical significance.

Learn more

BLAST+ 2.14.0 is here!
BLASTP, BLASTX, and TBLASTN are faster than before.
Fri, 28 Apr 2023

More BLAST news...



blastx translated nucleotide ▶ protein

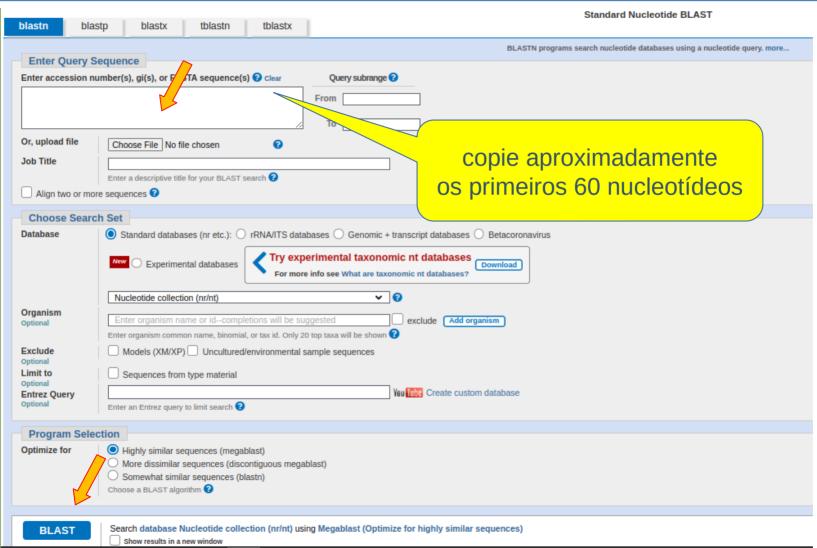
tblastn

protein ▶ translated nucleotide

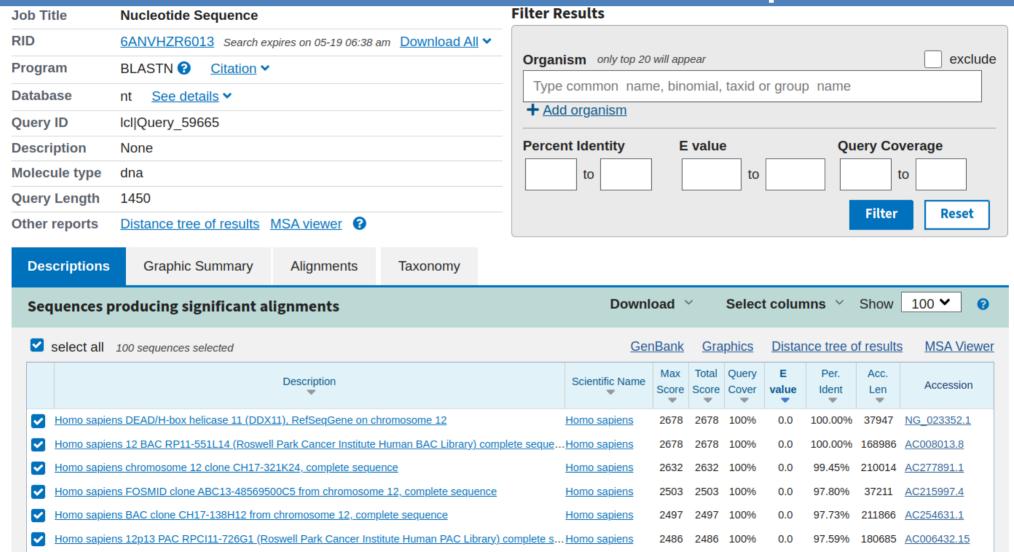


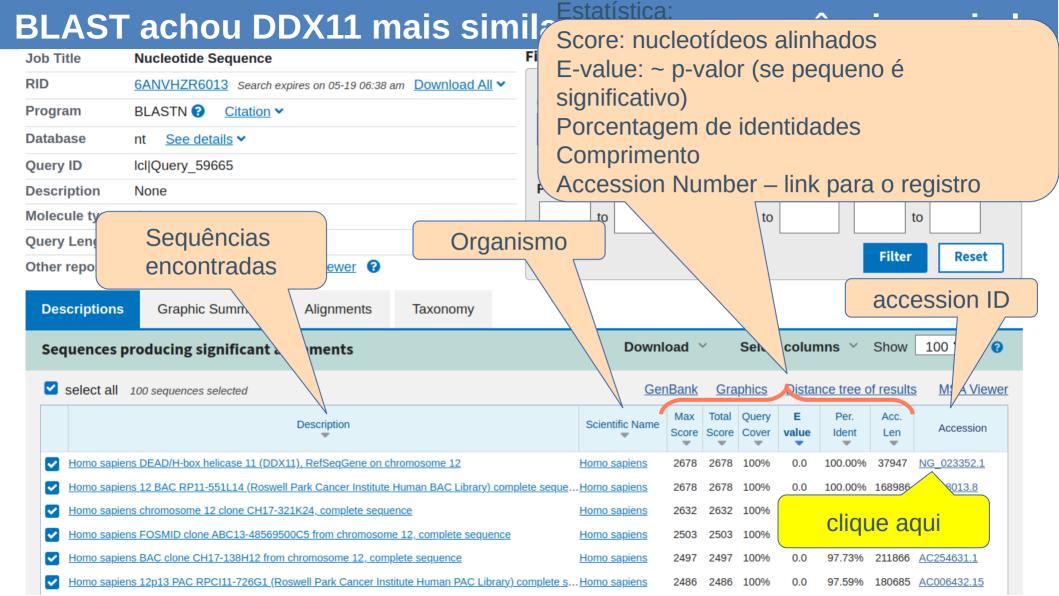


BLAST – copie a sequência e dê um blast



BLAST achou DDX11 mais similares com a sequência enviada





DDX11 registro do NG_023352 no Genbank do NCBI

GenBank → Send to: →

Homo sapiens DEAD/H-box helicase 11 (DDX11), RefSeqGene on chromosome 12

NCBI Reference Sequence: NG_023352.1

FASTA Graphics

```
Go to: ✓
LOCUS
            NG 023352
                                               DNA
                                                                PRI 25-MAR-2023
                                   37947 bp
                                                       linear
DEFINITION Homo sapiens DEAD/H-box helicase 11 (DDX11), RefSeqGene on
            chromosome 12.
ACCESSION
           NG 023352
            NG 023352.1
VERSION
KEYWORDS
            RefSea: RefSeaGene.
SOURCE
            Homo sapiens (human)
 ORGANISM Homo sapiens
            Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi;
            Mammalia; Eutheria; Euarchontoglires; Primates; Haplorrhini;
            Catarrhini; Hominidae; Homo.
           1 (bases 1 to 37947)
REFERENCE
 AUTHORS
            Alkhunaizi, E., Brosh, R.M. Jr., Alkuraya, F.S. and Chitayat, D.
 TITLE
            Warsaw Syndrome
  JOURNAL
            (in) Adam MP, Mirzaa GM, Pagon RA, Wallace SE, Bean LJH, Gripp KW
            and Amemiya A (Eds.);
            GENEREVIEWS(R);
            (1993)
   PUBMED
            31169992
COMMENT
            REVIEWED REFSEO: This record has been curated by NCBI staff. The
            reference sequence was derived from AC008013.8.
            This sequence is a reference standard in the RefSeqGene project.
            Summary: DEAD box proteins, characterized by the conserved motif
```

Aonde estão os Éxons? Onde começa este gene? start-codon ATG

>hq38 dna range=chr12:31073860-31104799 5'pad=0 3'pad=0 strand=+ repeatMasking=none GTTGTTCCGGCTGCCTTTCACTGAGGGGACCCGCCAGTTTCTAACTCAGT GGCGTTTGCCCTGATTCCCGGGGCCTGGCTTTCAGCGTAGCAATTCTGCC GGCGAAGAAGGTGAGCGCAGTGCTGTGTGGCAGCAGAGCTCCTTAGGACG AGGAGCAGCGGGACGAGGGAAGGGCAGACTGGTGAAATCGCAAACTGGGCG GCGGGAAAACATTCCGGAAGTGGAGGGCCGGGCCAGCGTGATTGACAAGC GGGAACCCCTGTGTGGGGACGGGTAGGCCTAGGAAGGTTGTGCCTGCGGT GGAACTGGGCGGTGCGCAGAAGTGGGCATTAACAGCAGCCGCGTGTCTGG GTCTTAGATTTGGCCCAGCTGTGTTGAGCTTTTCATGGATTATCTTACGT AGATAAGACACTGCAACAGTGAGTGAGCGCTTGTAACCCACCTGTCTCTT ACGGAAACTGAGCCCCAGCG<mark>ATG</mark>CTAACTTTAGCAAGGATACAGCTGGGA TCCTAAACTTGGCAATCAGAGCCCAGAGCCGATAAAGTTAGCTGCATGAG TCTAGCTTCCCCCAGGGCGGGAATCGAGGCGGAGCAGGGTACAGTACGGA GGCCAGGA<mark>ATG</mark>AGTGCACTTGACCAGATTGTTGACGGAAGTGTCATAAAA ATGGACTTAAATGCTGATAAGCAGCTGTTTGGGTTCCACACAGGGTGCGA GCTCAGG<mark>ATG</mark>CACGTTGGAGGGGACACAGGGCCAGAGCAAGGTGGGA<mark>ATG</mark> CGGGTATT<mark>ATG</mark>GGCCAGGCCATCCTCCAGCTGGTGGAGCACCGCAGTACT GCAGTGTGTGGCCCTGGCTTAACAGCAGTGCGGAAAAGCTTTTTTCTTGG GGCTGTGGTGCTTTCCAGGTGTGTGAAGTTAAAACATTTTAGGGCCATAC GGTAGATAGTACCTGCCACATAGTTGTCTTGGTCAGCCCCGGCTGCCATG ACAAAATACCATAAACTGGGTGGCTTAGACACAGAA<mark>ATG</mark>TGTTTTCTCAC AGTCCCAGAGGCTTGGGATGTCCAAGATCAATGTGGGGAGGACACAACTG AGCCCACAACAATAGTCTGTACTCAGTA<mark>ATG</mark>AGTGATAATTGGGGACTGA AGAAA<mark>ATG</mark>AACACGTTAAGAACTAAT<mark>ATG</mark>TTCCTGAAGTGCTTTCACAAC TCTAACCTCGTTTT<mark>ATG</mark>AGCGTGAGCTTTGCTGTCCTGGTGTGTGCCTTG GCACTGGGAGGTG<mark>ATG</mark>GTTGTCCTCCACACAGCCAACCTGAAGAGGGCTG AACAAGTCACTGCAAATGTTTTTTAATAGGGCTTAGTGAATCCGTTATACT CAGATTTATCTAAACCTCT<mark>ATG</mark>ATTTAGCCTGTGCTGCTTCTGGAATAAT GAGATCCATAATTACCACTG<mark>ATG</mark>GGGAAGTGAAATAATACTTACGTTTCT TTTTTATCCCACTTATCCTGGTGGGAGGAAAAGTGAGGAGATAGAAAGTT TCAGGTGGCTTGGGGGTCTGGCAG<mark>ATG</mark>TGGTTCAAATCCTGAGTTCAAGC ACTTGCTGAGTGACCTTGGGCAAGTCATATAAGTTTACTGAGTCTCAGTT TCTTTCTCTATAAAATAGAGCTTATAAAAATACCACACAGGGTTTTTGTG GGGTTATCTGAAAACGGTTTGAAACCATTAAAGAACTGGCCATTTAACTA

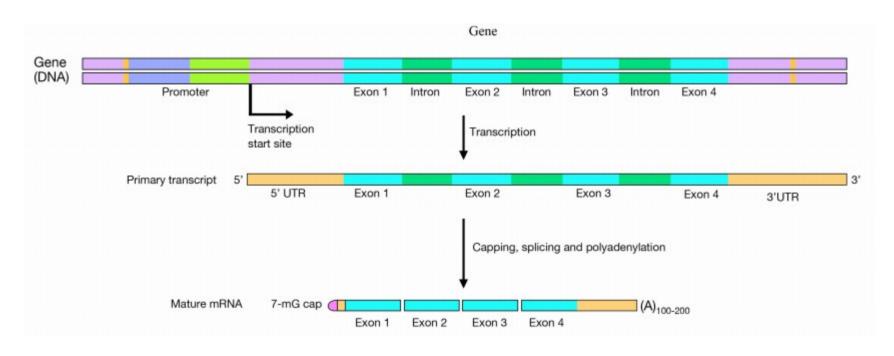
Aonde estão os Éxons? Onde começa este gene? start-codon ATG

|>hg38_dna range=chr12:31073860-31104799 5'pad=0 3'pad=0 strand=+ repeatMasking=none

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ACACGGTGAAACCCCGTCTCTACCAAAAAAAAAAAA CGTGGT AGAATGG GGCGGGCACCTGTAGTCCCAGCTACTCGGGAGGCT CACTGCA TGTGAACCCGGGAGGCGGAGCGTGCAGTGAGCCGA AAAAAAAA CTCCAGCCTGGGCGACAGAGTGAGACTCTGTCTCGA AGCTGTGC AAGATAGGGACGTGTATGTTAACTTGCGCTATCCAA TTATGGTCCTCTGCCTGTGCGTCATGATTTTCCAGG ACAACGGGA TAAAGTGAAGTAGCTTCGGCTTGTGAATGTGCATTG ACGTGGGAG AAGAAAGCTGCAAAAGTCATTATAAGCAACACCCTTO TAGGGGTGC TTAGAAAGGT TGGTCTGTGAGAAGAGAGCTCTAAGCCTTTTGTAGAG ATCGGAGCCACGGTGAAATGCAGGGGAGATTGGGTTT GGCTTTCCTG GTCTGCATTCTGCTACAGCCGTTAAATGCCGCTAGAT AGTGCGTGATT AGAACATGGTC CTGGTATGGCCTCACGTGGACCTGCTGCGAAGGATGGA TCTGCTTCCCAGAAAAAAGGAGAAATTTGGTAATAAG1,6TGGAGACTGCT CTTAAATAATGCTCCAGATTTCAAGCCACTTCTTCCTGGACCATGAGAGA GCTCCCTAATGTTGTATTTATTTTTCCTAGGTCCATGGCTAATGAAACAC AGAAGGTTGGTGCCATCCATTTTCCTTTTCCCTTCACACCCTATTCCATC

Aonde estão os Éxons? Onde começa este gene?





Localizando os éxons no texto do Genebank

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mRNA
                join(5016..5247,9546..9693,14969..15217,15739..15825,
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                21042...21250...22875...23027...24002...24048...24401...24480...
                25746..25790,25911..25978,27497..27535,27793..27901,
                28015..28146,29041..29153,31791..31863,32183..32286,
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                25911..25978,27497..27535,27793..27901,28015..28146,
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                33399...33467,33583...33683,34092...34176,34473...34551,
                34733..34887,34963..34992)
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                /EC number="3.6.4.12"
                                                             9721 aaaggacaac ttaacagcag ccgtactagc ttttcctgtt tgcctatcca gagattttca
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Parte do registro do Genebank refere-se a anotações

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/EC number="3.6.4.12"
/note="isoform 1 is encoded by transcript variant 1;
DEAD/H (Asp-Glu-Ala-Asp/His) box polypeptide 11 (CHL1-like
helicase homolog, S. cerevisiae); probable ATP-dependent
RNA helicase DDX11; CHL1-related helicase gene-1; DEAD/H
(Asp-Glu-Ala-Asp/His) box helicase 11; KRG-2; hCHLR1;
DEAD/H box protein 11; CHL1-related protein 1;
keratinocyte growth factor-regulated gene 2 protein:
probable ATP-dependent DNA helicase DDX11"
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```

outras bases

do NCBI

Protein

CDS

HGNC (Hugo)

MIM

clique aqui para ir para as anotações da proteína

clique aqui também para ver o conding segment CDS

Salvar a proteína em fasta no site

```
GenPept -
                                                                                                    Send to: -
ATP-dependent DNA helicase DDX11 isoform 1 [Homo sapiens]
NCBI Reference Sequence: NP 085911.2
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Identical Proteins FASTA Graphics
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Go to: ✓
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LOCUS.
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                                                               PRI 12-MAR-2023
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ACCESSION
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VERSION
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DBSOURCE
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REFERENCE
           1 (residues 1 to 906)
  AUTHORS
           Saeed M, Ibanez-Costa A, Patino-Trives AM, Munoz-Barrera L,
           Collantes Estevez E, Aguirre MA and Lopez-Pedrera C.
  TITLE
            Expression of DDX11 and DNM1L at the 12p11 Locus Modulates Systemic
           Lupus Erythematosus Susceptibility
  JOURNAL
           Int J Mol Sci 22 (14), 7624 (2021)
   PUBMED
           34299244
  REMARK
           GeneRIF: Expression of DDX11 and DNM1L at the 12p11 Locus Modulates
            Systemic Lupus Erythematosus Susceptibility.
```



Copie as sequências CDS no conversor do EMBOSS



https://www.ebi.ac.uk/ https://www.embl.org/

EMBL

The European Molecular Biology Laboratory

Service Announcement

The new Job Dispatcher Services beta website is now available at https://wwwdev.ebi.ac.uk/Tools/jdispatcher. We'd love to hear your feedback about the new webpages!

EMBOSS Transeq

EMBOSS Transeq translates nucleic acid sequences to their corresponding peptide sequences. It can translate to the three forward and three reverse frames, and output multiple frame translations at once.



https://www.ebi.ac.uk/Tools/st/emboss transeq/

Resultado do conversor do EMBOSS

https://www.ebi.ac.uk/ Tools/emboss/

EMBL

The European Molecular Biology Open Source Software

Results for job emboss_transeq-I20230518-184221-0857-82638710-p2m

Tool Output Submission Details

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>EMBOSS 001 1

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Exercício fazer um BLAST de amino ácidos

Pegue os 30 primeiros aa de DDX11 e faça um BLAST



Mas, na verdade eu gosto do Seaview



PRABI-Doua Pôle Rhône-Alpes de Bioinformatique Site Doua

Download

https://doua.prabi.fr/software/seaview

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SeaView - Multiplatform GUI for molecular phylogeny

Version 5.0.5

NEW: seaview performs reconcilation between gene and species trees using Treerecs version 1.2

NEW: bootstrap support optionally with the "Transfer Bootstrap Expectation" method

NEW: trimming-rule to shorten long sequence names in phylogenetic trees

NEW: 64-bit version for the MS Windows platform

NEW: multiple-tree windows

NEW: seaview uses PHYLIP v3.696 to compute parsimony trees

NEW: seaview can be run without GUI using a command line

NEW: seaview drives the PhyML v3.1 program to compute maximum likelihood phylogenetic trees.

NEW: seaview drives the Gblocks program to select blocks of conserved sites.

SeaView is a multiplatform, graphical user interface for multiple sequence alignment and molecular phylogeny.

- SeaView reads and writes various file formats (<u>NEXUS</u>, MSF, CLUSTAL, FASTA, PHYLIP, <u>MASE</u>, Newick) of DNA and protein sequences and of phylogenetic trees.
- SeaView drives programs <u>muscle</u> or <u>Clustal Omega</u> for multiple sequence alignment, and also allows to use any external alignment algorithm
 able to read and write FASTA-formatted files.
- . Seaview drives the Gblocks program to select blocks of evolutionarily conserved sites.
- · SeaView computes phylogenetic trees by
 - o parsimony, using PHYLIP's dnapars/protpars algorithm,
 - distance, with NJ or BioNJ algorithms on a variety of evolutionary distances,
 - maximum likelihood, driving program PhyML 3.1.
- Seaview can use the <u>Transfer Bootstrap Expectation</u> method to compute the bootstrap support of PhyML and distance trees.
- Seaview uses the Treerecs method to reconcile gene and species trees.
- SeaView prints and draws phylogenetic trees on screen, SVG, PDF or PostScript files.
- SeaView allows to download sequences from EMBL/GenBank/UniProt using the Internet.

Screen shots of the main <u>alignment</u> and <u>tree</u> windows. Dialog window to perform <u>Maximum-Likelihood</u> tree-building. On-line <u>help</u> document.Old <u>seaview version 3.2</u>

Download SeaView



Use Linux, por favor





Bioinformática

Curso de Especialização na Área da Saúde – 2025/2026 Bases Técnicas em Vacinas e Biofármacos

PhD Flavio Lichtenstein



Bioinformatics, Systems Biology, and Biostatistics

dúvidas: flavio.lichtenstein@butantan.gov.br

abril/2025 e maio/2023