O que é possível fazer sabendo o básico de Python?

V Workshop de Python para Dados Biológicos

Beatriz Rodrigues Estevam

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Sumário

- Introdução
- Sequências conservadas
- Sequence Logos
- CoCoView: A codon conservation viewer
- Exemplos e aplicações

Por que "O que é possível fazer sabendo o básico de Python?"?

2020

Iniciação científica

Bioinformática

2021

Contato com Python

2022

Publicação do artigo

CoCoView

Por que "O que é possível fazer sabendo o básico de Python?"?

Ferramenta para visualização da conservação de sequências de códons.

Publicação do artigo

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estevam BR, Riaño-Pachón, DM, CoCoView - A codon conservation viewer via sequence logos. https://doi.org/10.1016/j.mex.2022.101803, 2022.

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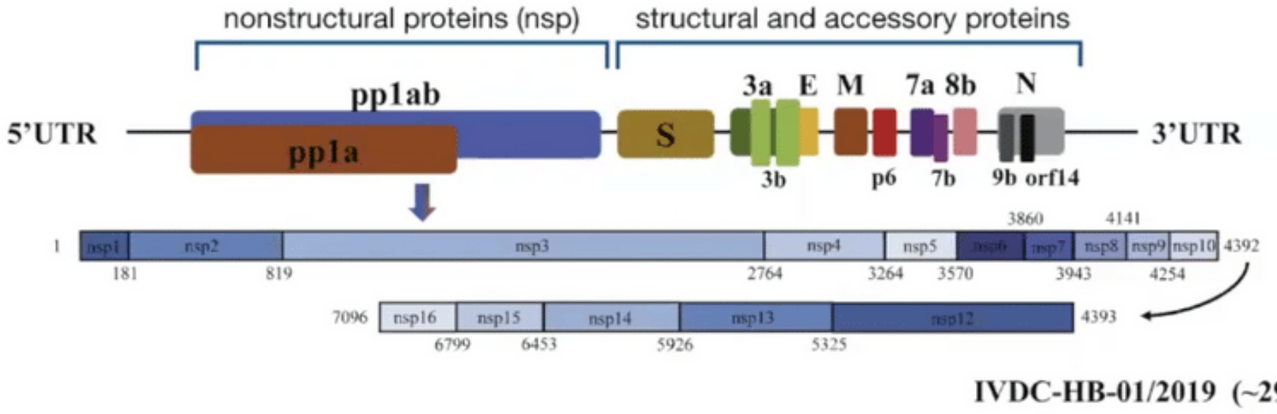
Como separar as proteínas?

Transcrição, Tradução e pós-processamento



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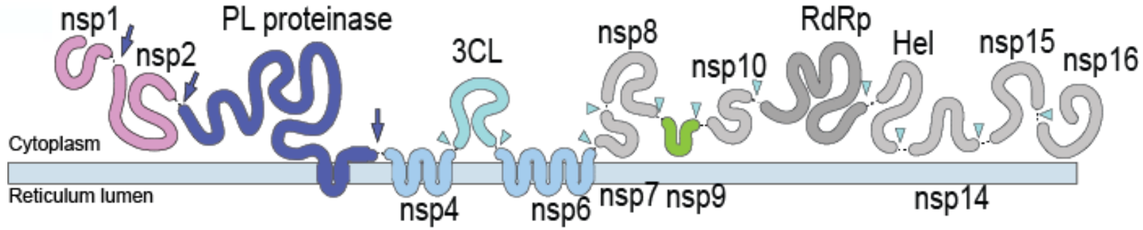
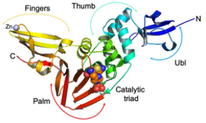
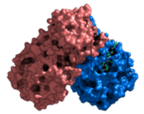


...VKLQNNEL...

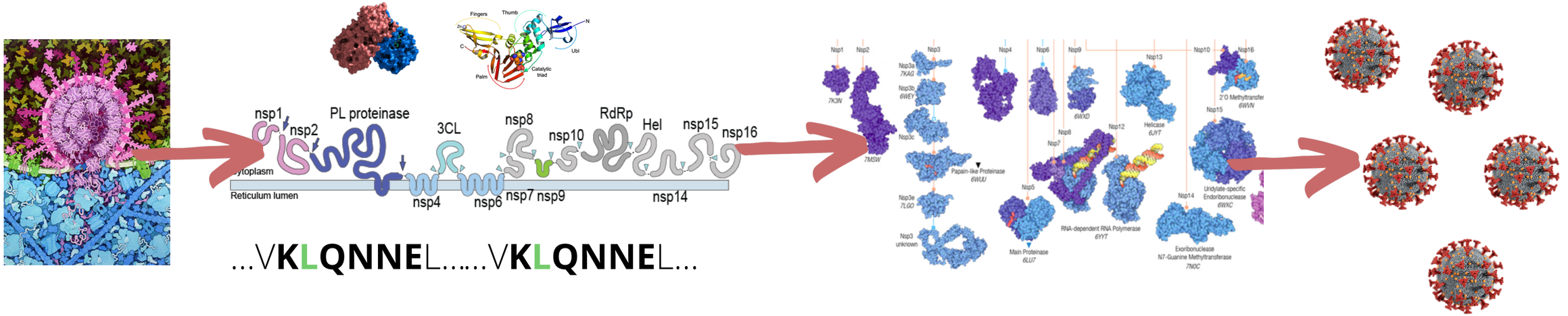
nível de aminoácido





Wu et al, 2020. https://doi.org/10.1016/j.chom.2020.02.001
Ullrich, S. Nitsche, C. 2020. https://doi.org/10.1016/j.bmcl.2020.127377
SARS coronavirus 2 /Covid-19 genome expression. ViralZone - SIB Swiss Institute of Bioinformatics, https://viralzone.expasy.org/9076. Acesso em 2022.
Osipiuk J, et al. https://doi.org/10.1038/s41467-021-21060-3, 2021 (PLprotease)
Jin Z et al. https://doi.org/10.1038/s41586-020-2223-y. 2020 (Mprotease)

Sequências conservadas



SARS coronavirus 2 /Covid-19 genome expression. ViralZone - SIB Swiss Institute of Bioinformatics, https://viralzone.expasy.org/9076. Acesso em 2022.
COVID-19/SARS-CoV-2 Resources, PDB. https://www.rcsb.org/news/feature/5e74d55d2d410731e9944f52. Acesso em 2022.
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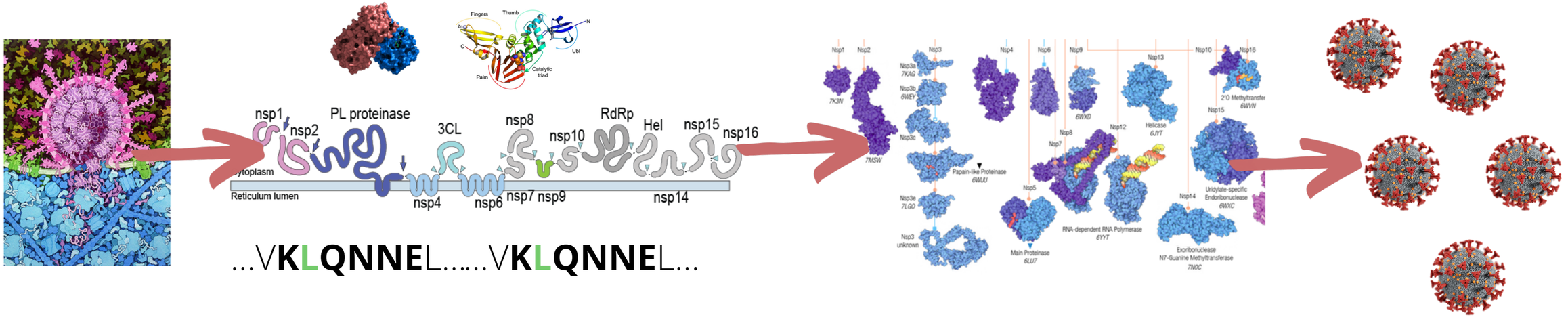
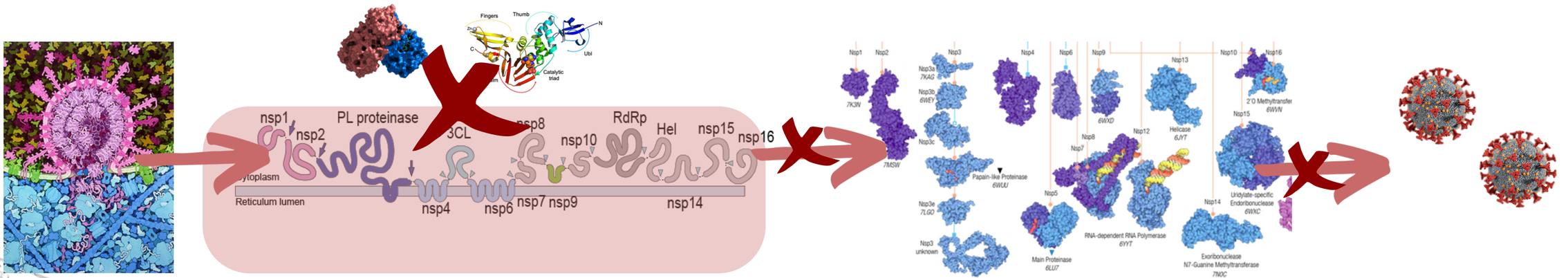
Sequências conservadas



...V**KL**Q**NNE**L.....V**KL**Q**NNE**L...



...V**KL**C**KNE**L... ...V**LN**Q**K**N**E**L...

SARS coronavirus 2 /Covid-19 genome expression. ViralZone - SIB Swiss Institute of Bioinformatics, https://viralzone.expasy.org/9076. Acesso em 2022.
COVID-19/SARS-CoV-2 Resources, PDB. https://www.rcsb.org/news/feature/5e74d55d2d410731e9944f52. Acesso em 2022.
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Jin Z et al. https://doi.org/10.1038/s41586-020-2223-y. 2020 (Mprotease)

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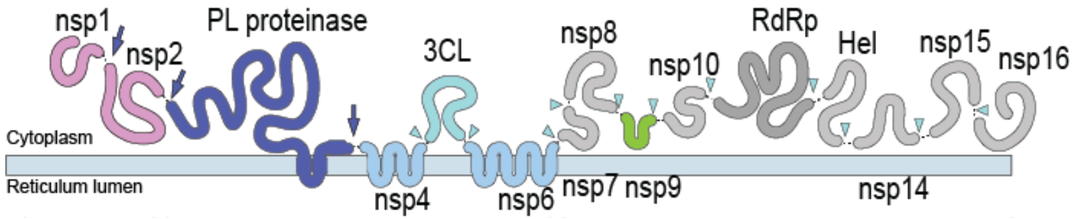
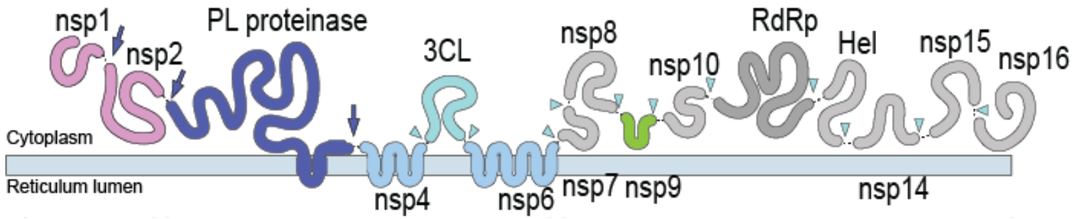
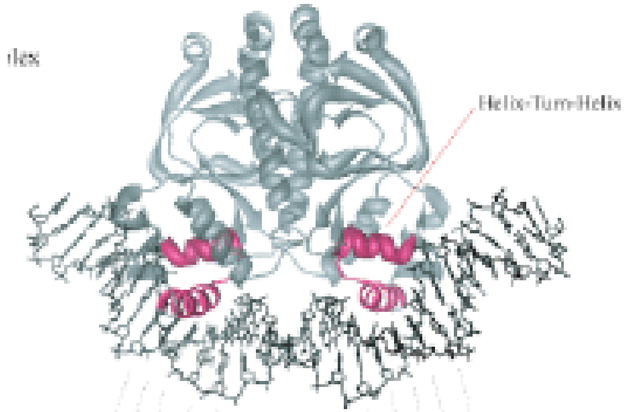


Sítios de clivagem de proteínas

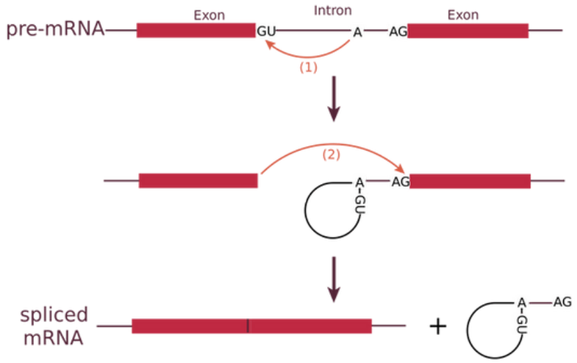
Sequências conservadas



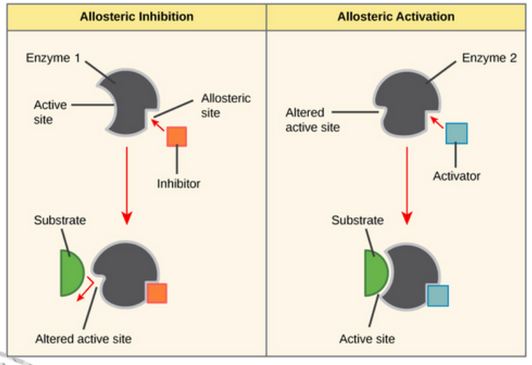
Sítios de clivagem de proteínas



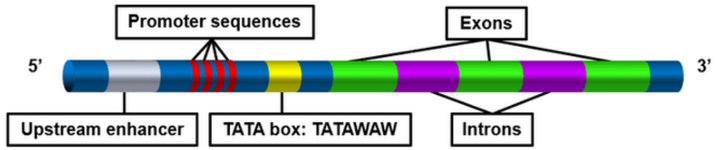
Motifs de proteína



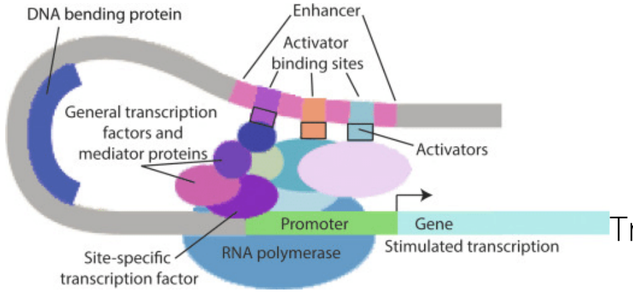
Splicing regions



Sítios alostéricos e sítios ativos de enzimas



Promotores



Transcription Factor Binding Sites

SARS coronavirus 2 /Covid-19 genome expression. ViralZone - SIB Swiss Institute of Bioinformatics, https://viralzone.expasy.org/9076. Acesso em 2022.
OpenStax College, Biology. Enzymes. https://openstax.org/books/biology/pages/6-5-enzymes (Acesso em 2022)(Sítios alostéricos e aítios ativos)
Mobley AS, Chapter 4 - Induced Pluripotent Stem Cells Imagem 4.6. https://doi.org/10.1016/B978-0-12-811014-0.00004-4 (Fatores de transcrição)
Weblogo. https://weblogo.berkeley.edu/ (Protein Motif)

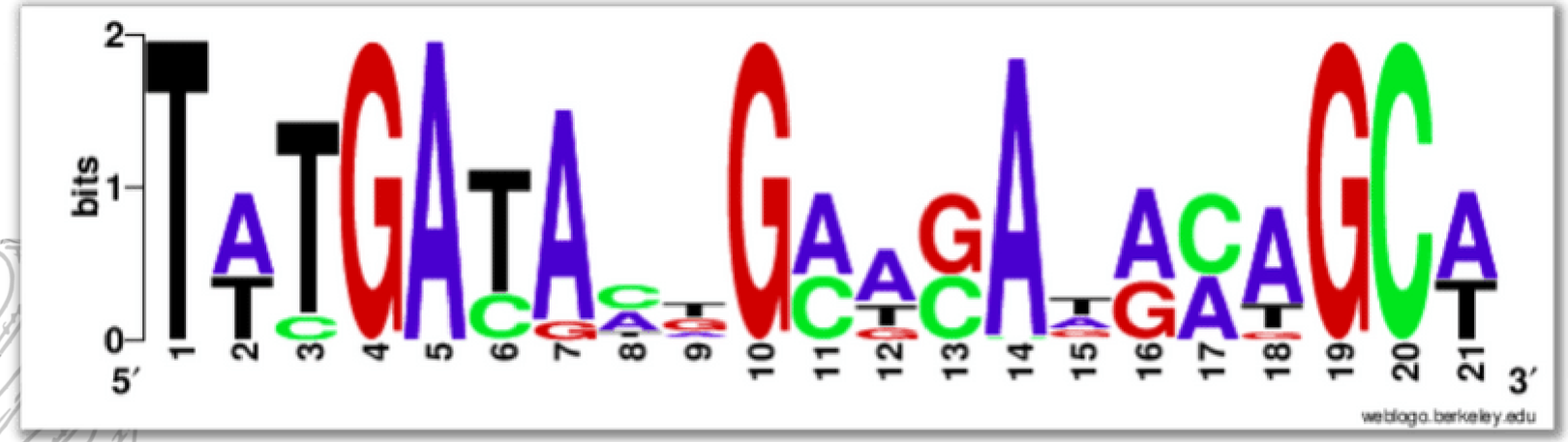
Sequências conservadas

A alta conservação de sequências indica possíveis funções relevantes (Se mudam drasticamente, são desfavorecidas)

Existe interesse em identificar e representar essas sequências

Sequence Logos

Forma de representação de sequências conservdas introduzida por Schneider and Stephens (1990)



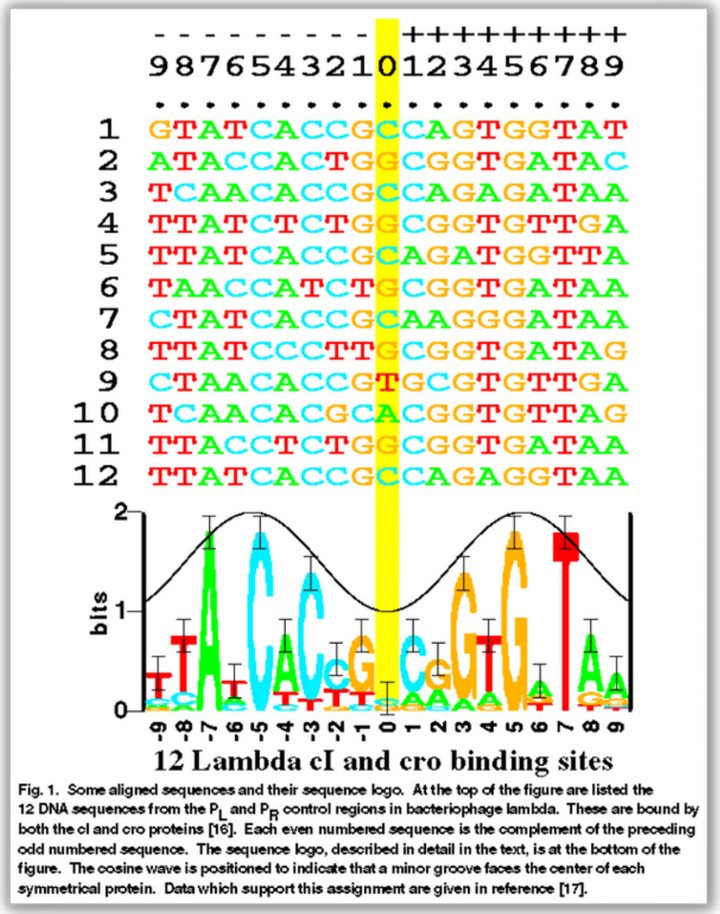


Fig. 1. Some aligned sequences and their sequence logo. At the top of the figure are listed the 12 DNA sequences from the P_L and P_R control regions in bacteriophage lambda. These are bound by both the cI and cro proteins [16]. Each even numbered sequence is the complement of the preceding odd numbered sequence. The sequence logo, described in detail in the text, is at the bottom of the figure. The cosine wave is positioned to indicate that a minor groove faces the center of each symmetrical protein. Data which support this assignment are given in reference [17].

Schneider Lab, A Gallery of Sequence Logos, http://users.fred.net/tds/lab/sequencelogo.html. 2015 (Alinhamento)
estevam BR, Riaño-Pachón, DM, CoCoView - A codon conservation viewer via sequence logos. https://doi.org/10.1016/j.mex.2022.101803, 2022.

Entendendo os Sequence Logos

Conservação
na posição 4

Conservação
Quanto maior
=
Mais conservado

Posição na sequência

Frequência
do símbolo

Conservação total

Quanto mais símbolos na posição
=
Menor é a conservação total

estevam BR, Riaño-Pachón, DM, CoCoView - A codon conservation viewer via sequence logos. https://doi.org/10.1016/j.mex.2022.101803, 2022.
Schneider TD, Stephens RM. Sequence logos: a new way to display consensus sequences. https://doi.org/10.1093/nar/18.20.6097 1990. (Teoria)

Sequence Logos

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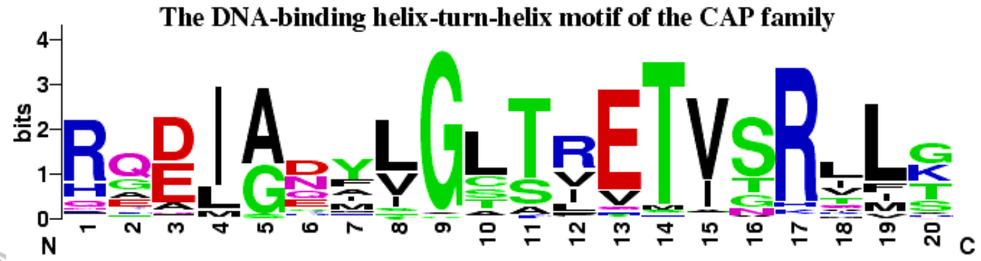
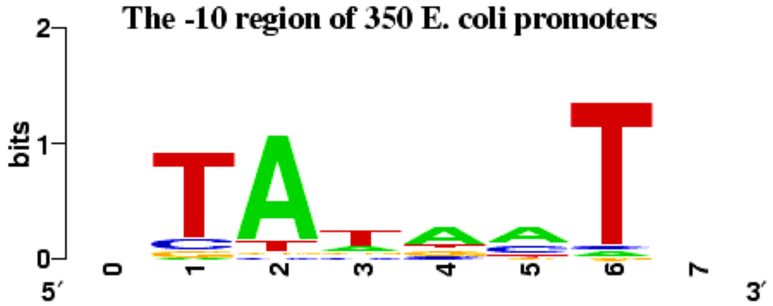
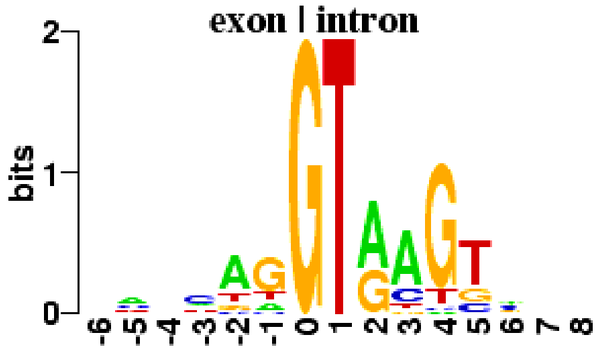
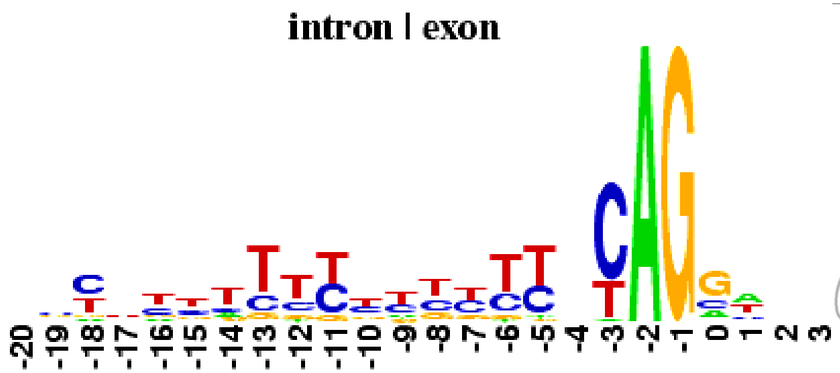


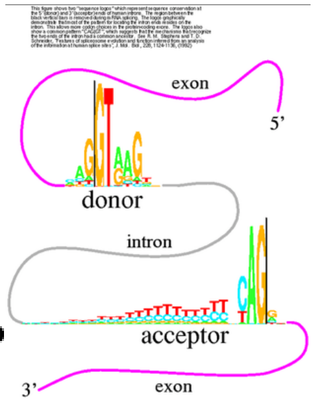
Motifs de proteína



Prototers







Splicing regions

Schneider Lab, A Gallery of Sequence Logos, http://users.fred.net/tds/lab/sequencelogo.html. 2015 (Alinhamento)

Sequence Logos

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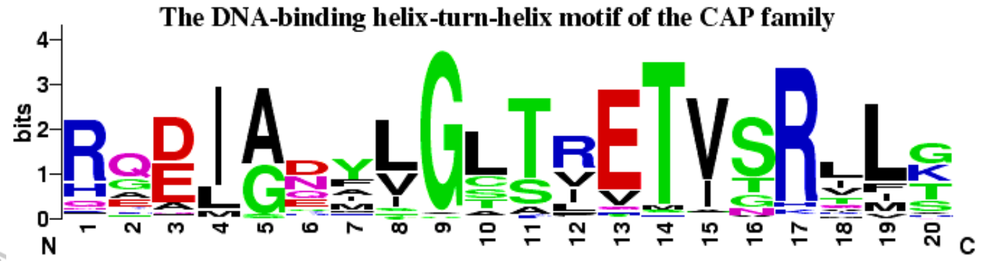
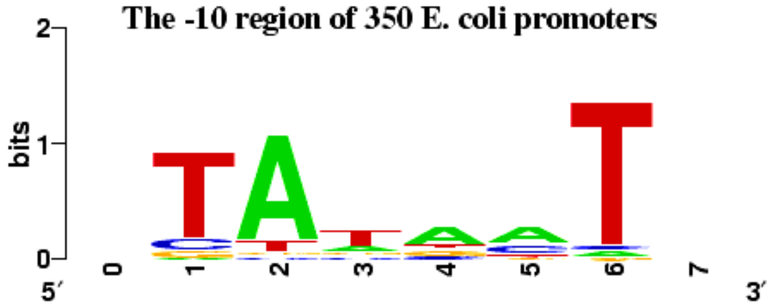
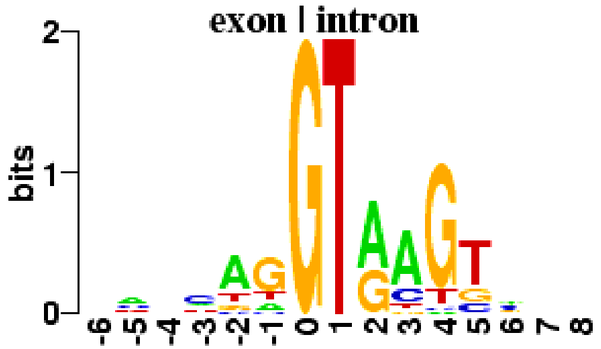


Motifs de proteína

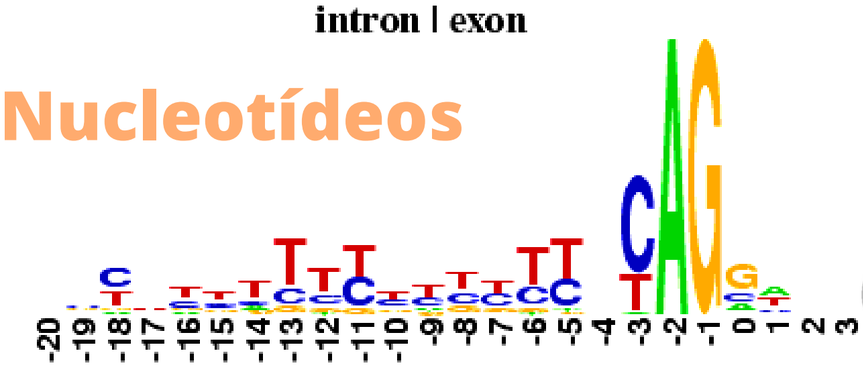
Aminoácidos

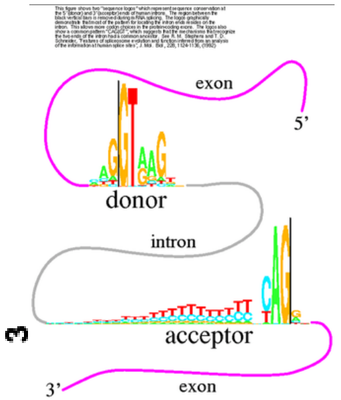


Prototers



Nucleotídeos





Splicing regions

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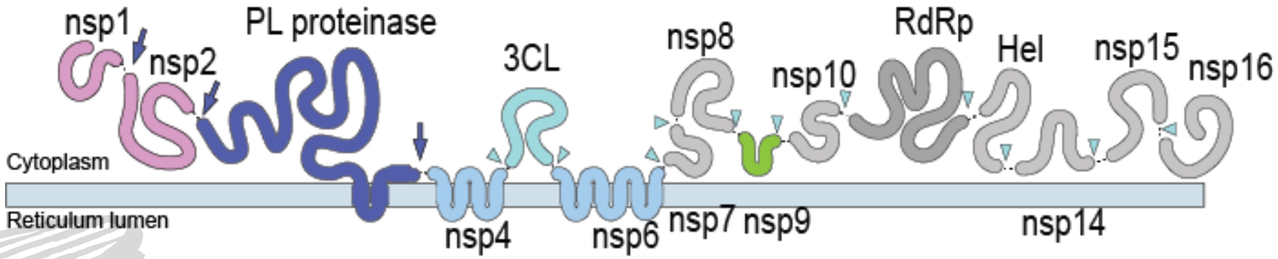
Um caso especial

Vírus recente

nível de aminoácido



Mutações sinônimas

AGT (Ser) → AGC (Ser)

Mutações não sinônimas

AGT (Ser) → AGA (Arg)

SARS coronavirus 2 /Covid-19 genome expression. ViralZone - SIB Swiss Institute of Bioinformatics, https://viralzone.expasy.org/9076. Acesso em 2022.

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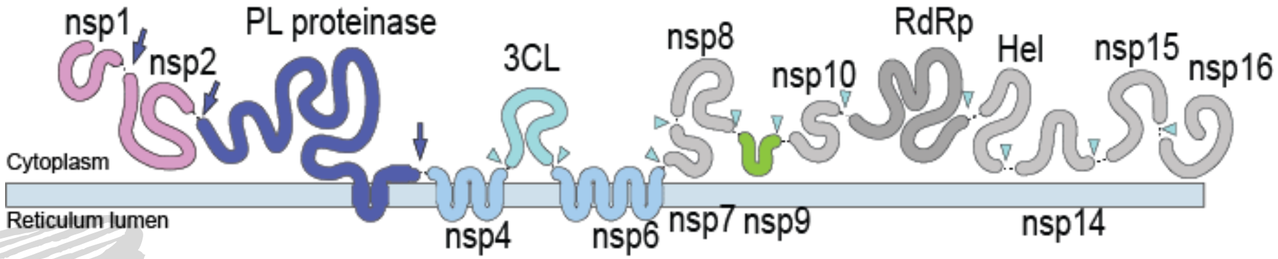
nível de aminoácido



Mutações sinônimas

AGT (Ser) → AGC (Ser)

Mutações não sinônimas

AGT (Ser) → AGA (Arg)

Unir o nível de aminoácidos ao nível de nucletídeos = **Códons**

SARS coronavirus 2 /Covid-19 genome expression. ViralZone - SIB Swiss Institute of Bioinformatics, https://viralzone.expasy.org/9076. Acesso em 2022.

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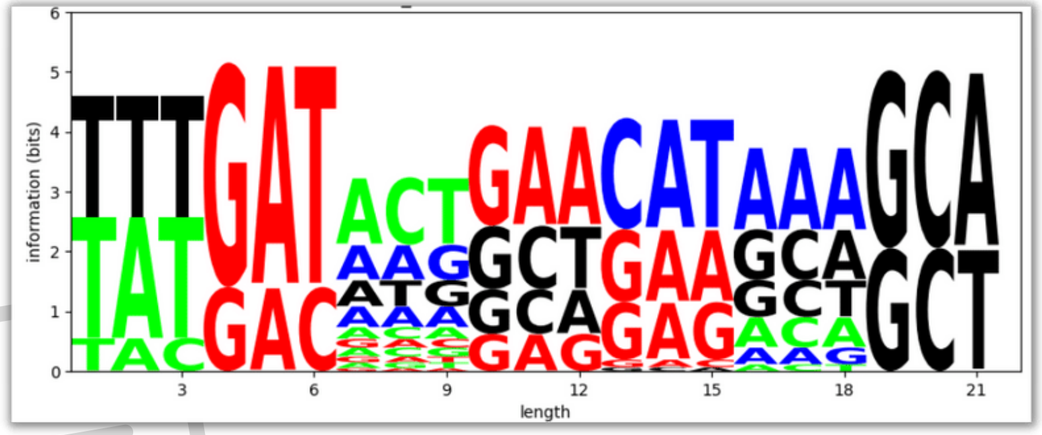
CoCoView

estevam BR, Riaño-Pachón, DM, CoCoView - A codon conservation viewer via sequence logos. https://doi.org/10.1016/j.mex.2022.101803, 2022.

Codon Sequence logo

CoCoView: A Codon Conservation Viewer



labbces/**CoCoView**

BCEr

2 Contributors · 0 Issues · 1 Star · 0 Forks

labbces/CoCoView

Contribute to labbces/CoCoView development by creating an account on GitHub.

MethodsX

Log in

METHOD ARTICLE | VOLUME 9, 101803, JANUARY 01, 2022

CoCoView - A codon conservation viewer via sequence logos

Beatriz Rodrigues Estevam • Diego Mauricio Riaño-Pachón

Open Access • Published: July 30, 2022 • DOI: https://doi.org/10.1016/j.mex.2022.101803 •

Check for updates

PlumX Metrics

Abstract

Sequence logos are a simple way to display a set of aligned sequences, and they are useful to identify conserved patterns. Since their introduction, several tools have been developed for generating these representations at the single residue level (amino acids or nucleotides). We have developed a tool to build sequence logos of protein-coding sequences at the codon level, allowing more accurate analysis of coding-sequences as they represent synonymous and non-synonymous changes instead of showing only changes that imply on acid substitutions. We built CoCoView on top of the Logomaker Python s codon sequence logos from a multiple sequence alignment of protein-

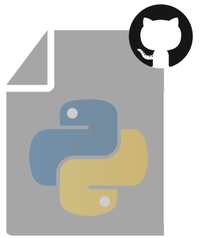
CoCoView: A Codon Conservation Viewer

Visualização geral

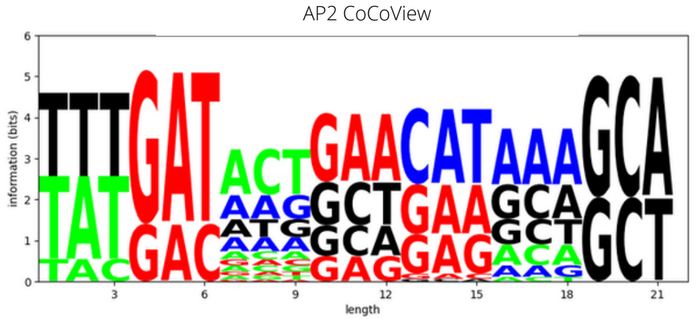
External Libraries

Mandatory


```
I> sequence ID 1
AATGGCTGCATGCATGCTGATCGA
> sequence ID 2
AATGGCTGCATGCATGCTGATCGA
> sequence ID 3
AATGGCTGCATGCATGCTGATCGA
> sequence ID 4
AATGGCTGCATGCATGCTGATCGA
> sequence ID 5
AATGGCTGCATGCATGCTGATCGA
```



CoCoView.py



Graphic features

Optional

prefixFileName (-p)	degreeOfUncertainity (-d)
imageTitle (-i)	matrixLogoType (-m)
alphaColor (-a)	datasetType (-t)
customPalletFile (-c)	logoFormat (-l)

```
python3 CoCoView.py file.fasta [-p FilesPrefixName] [-i AP2]
[-a custom]  [-c customPaletteFile.json][-d 0.0] [-m bit]
[-t nonredundant] [-l png]
```

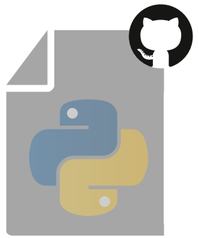
CoCoView: A Codon Conservation Viewer

Visualização geral

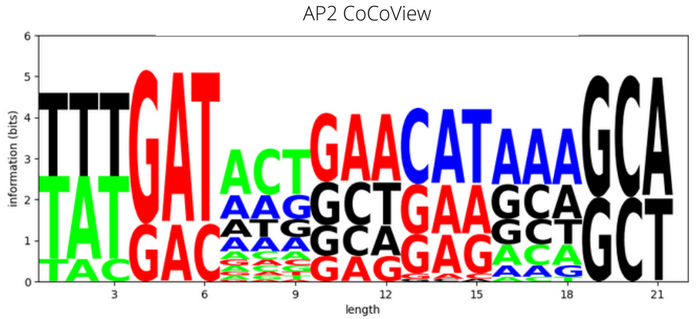
External Libraries

Mandatory


```
I> sequence ID 1
AATGGCTGCATGCATGCTGATCGA
> sequence ID 2
AATGGCTGCATGCATGCTGATCGA
> sequence ID 3
AATGGCTGCATGCATGCTGATCGA
> sequence ID 4
AATGGCTGCATGCATGCTGATCGA
> sequence ID 5
AATGGCTGCATGCATGCTGATCGA
```



CoCoView.py



Graphic features

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prefixFileName (-p)	degreeOfUncertainity (-d)
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alphaColor (-a)	datasetType (-t)
customPalletFile (-c)	logoFormat (-l)

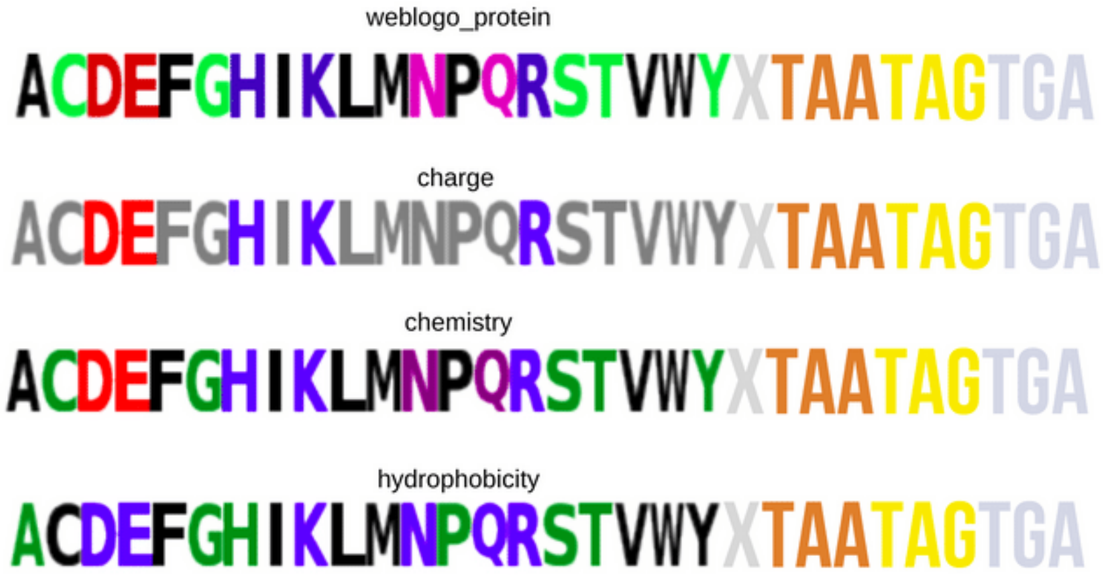
```
python3 CoCoView.py file.fasta [-p FilesPrefixName] [-i AP2]
[-a custom]  [-c customPaletteFile.json][-d 0.0] [-m bit]
[-t nonredundant] [-l png]
```

estevam BR, Riaño-Pachón, DM, CoCoView - A codon conservation viewer via sequence logos. https://doi.org/10.1016/j.mex.2022.101803, 2022.

CoCoView: A Codon Conservation Viewer

Funcionalidades

--alphaColor



--customPaletteFile

-a custom -c file.json

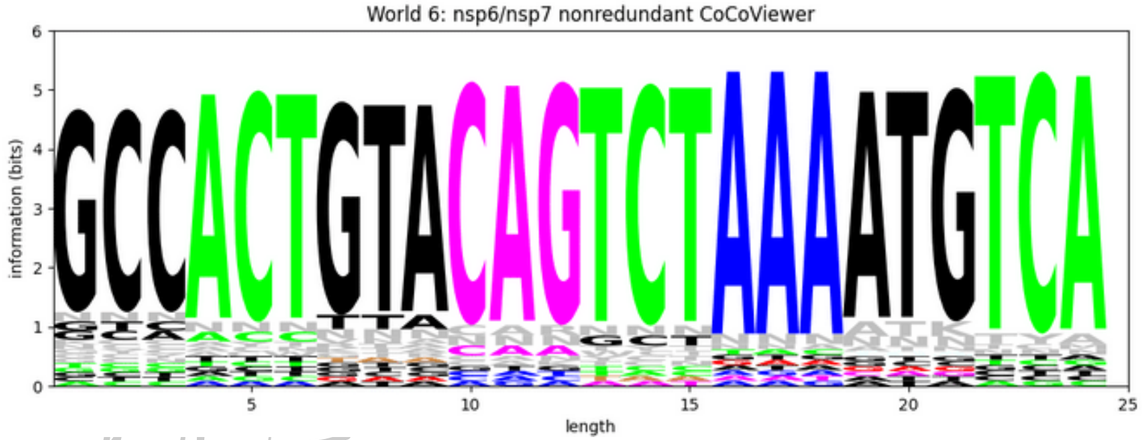
```
{ "custom" :{
    "GCT" : "dimgray",
    "GCC" : "black",
    "GCA" : "lightcoral",
    "GCG" : "brown",
    "TTT" : "red",
    "TTC" : "salmon",
    "ATT" : "tomato",
    "ATC" : "bisque",
    "ATA" : "burlywood",
    "TTA" : "tan",
    "TTG" : "orange",
    "CTT" : "wheat",
    "CTC" : "gold",
    "CTA" : "khaki",
    "CTG" : "olive",
    "ATG" : "yellow",
    "CCT" : "olivedrab",
    "CCC" : "forestgreen",
```

estevam BR, Riaño-Pachón, DM, CoCoView - A codon conservation viewer via sequence logos. https://doi.org/10.1016/j.mex.2022.101803, 2022.

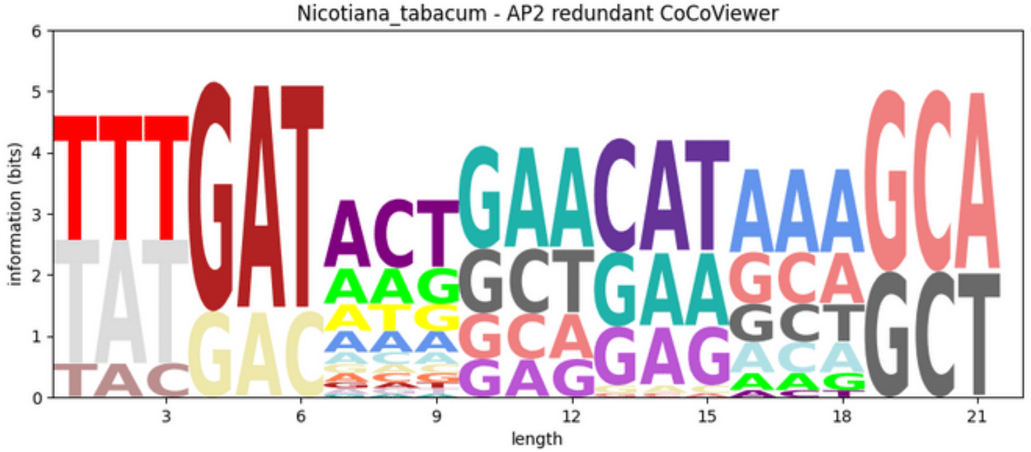
CoCoView: A Codon Conservation Viewer

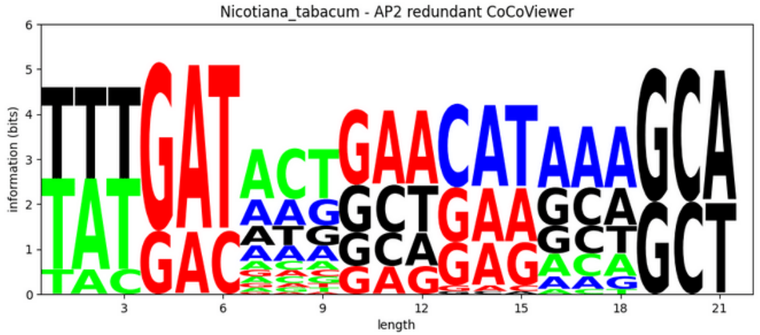
Funcionalidades

--alphaColor



--customPaletteFile



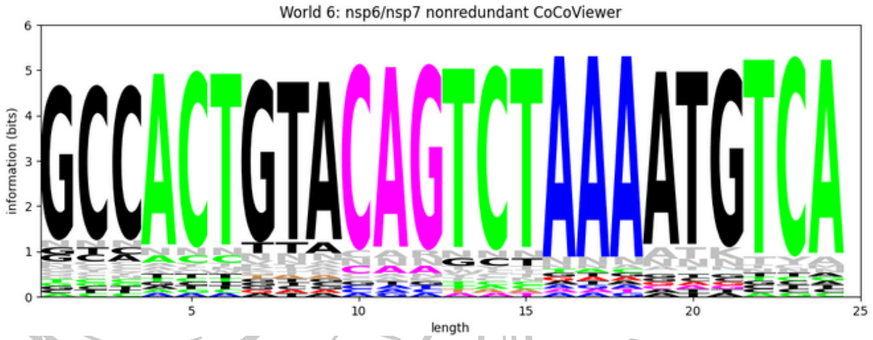


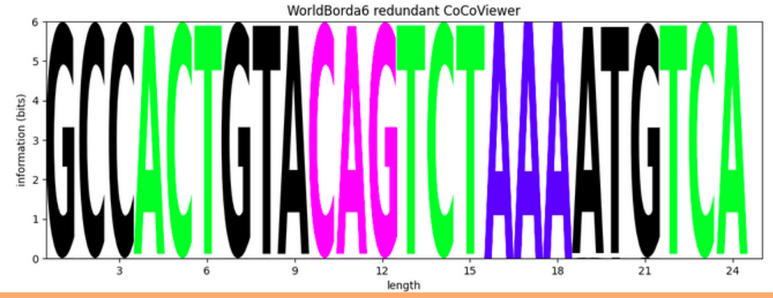
CoCoView: A Codon Conservation Viewer

Funcionalidades

--datasetType

- Datsets pequenos
- Redundante x Não redundante
- Remover sequências duplicadas





--degreeOfUncertainty

- Remover sequências (parcialmente) desconhecidas

30

AAAAAAAAAAAA

AAAAAAAAXXXX

AAAXXXXXXXXX

0

AAAAAAAAAAAA

AAAAAAAAXXXX

XXXXXXXXXXXX

100

AAAAAAAAAAAA

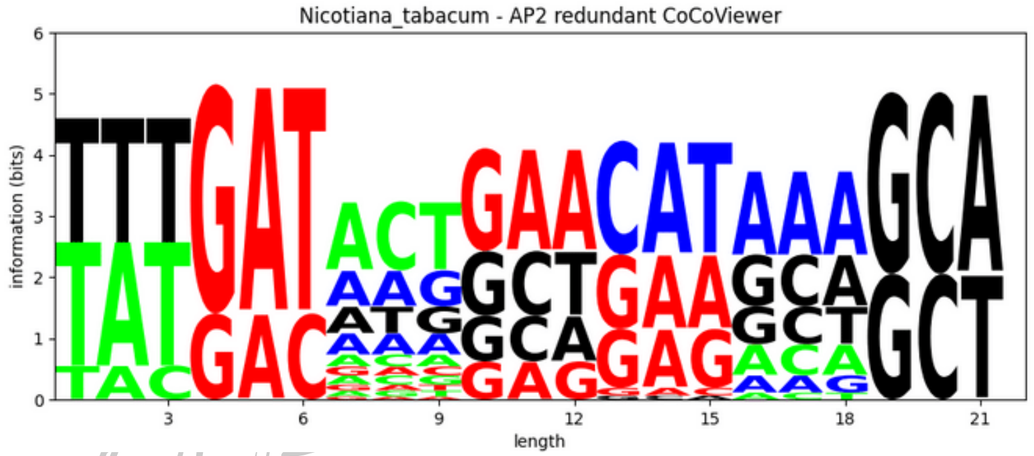
AAAAAAAAXXXX

XXXXXXXXXXXX

estevam BR, Riaño-Pachón, DM, CoCoView - A codon conservation viewer via sequence logos. https://doi.org/10.1016/j.mex.2022.101803, 2022.

Funcionalidades

--imageTitle



Nicotiana_tabacum - AP2 redundant CoCoViewer

--prefixFileName

Matriz

prefixFileName + datasetType + "bits.matrix"

Matriz

prefixFileName + datasetType + "probability.matrix"

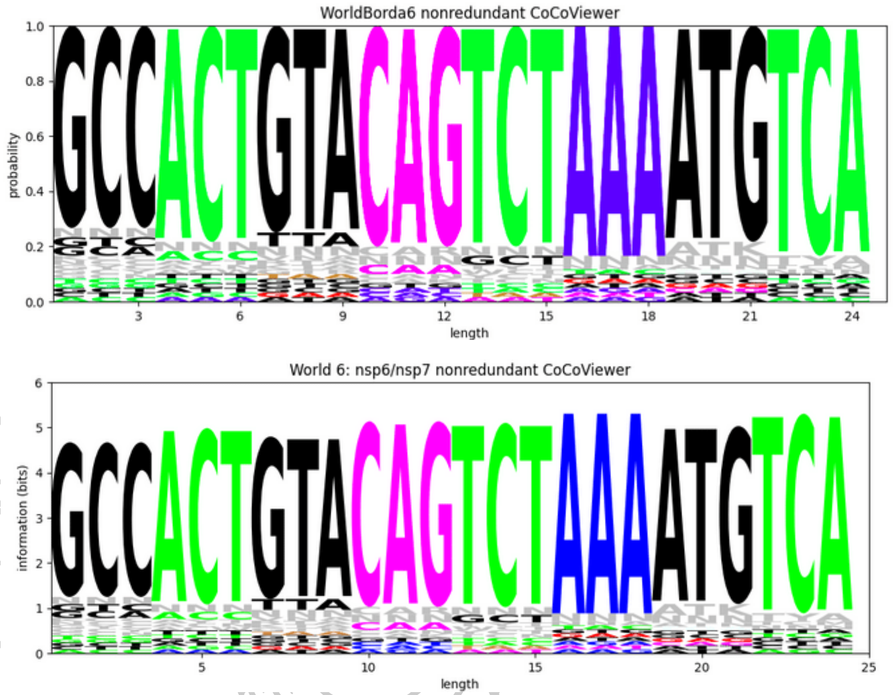
Plot

prefixFileName + datasetType + matrixLogoType + "CoCoView" + logoFormat

Funcionalidades

--matrixLogoType

- Frequência x Bits

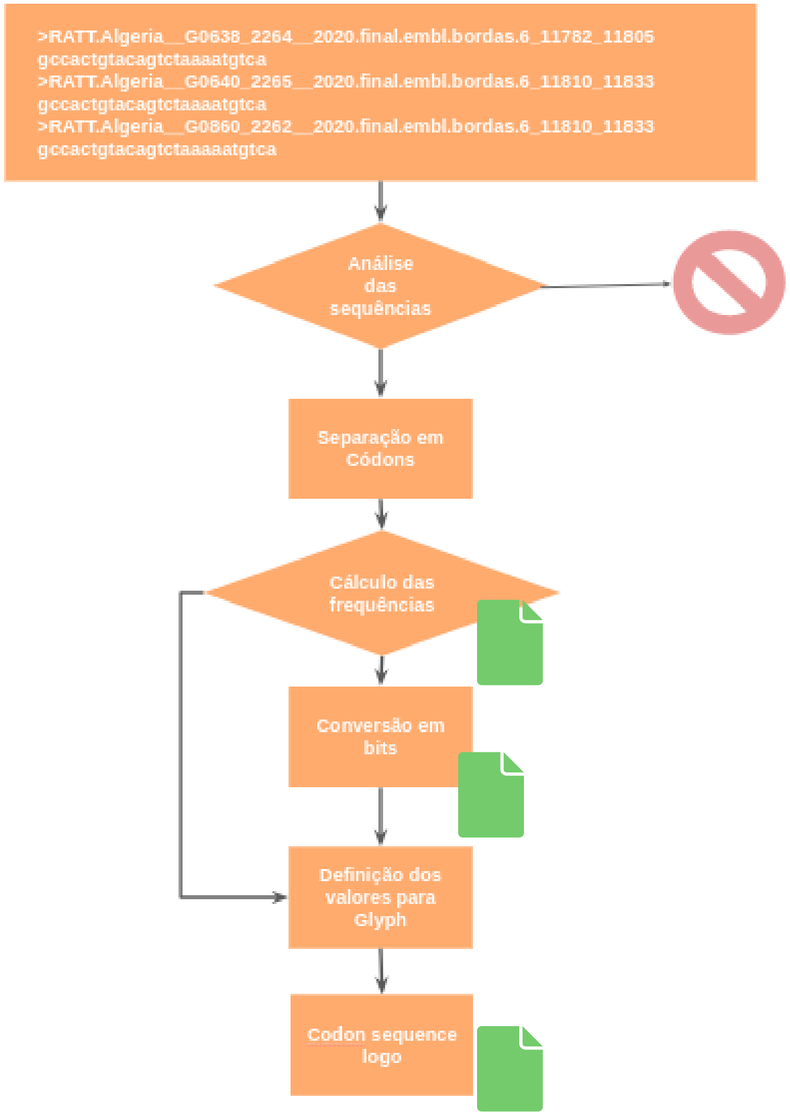


--logoFormat

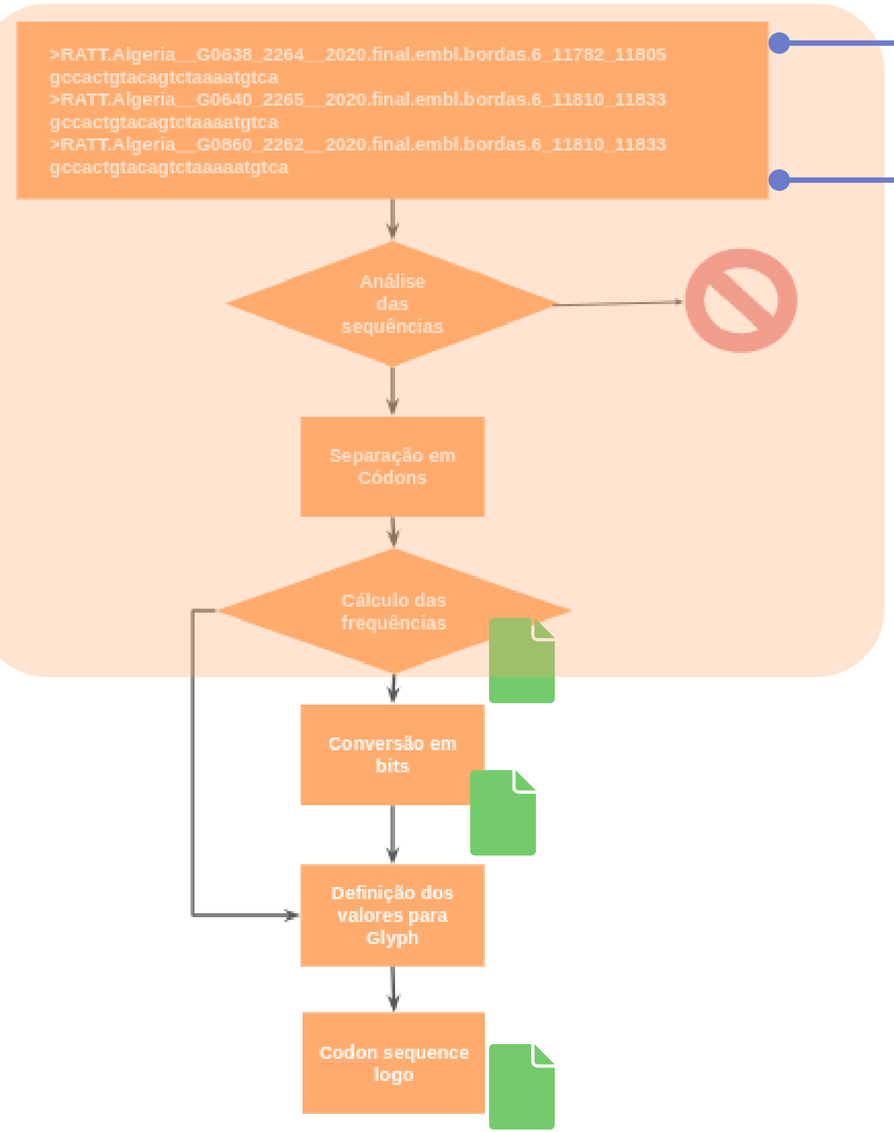
- png e pdf

Codon Sequence logo

Script overview



Codon Sequence logo
Script overview



argparse — Comunicação do script com o terminal

biopython — Operações com as seqências

MÓDULO AlignIO

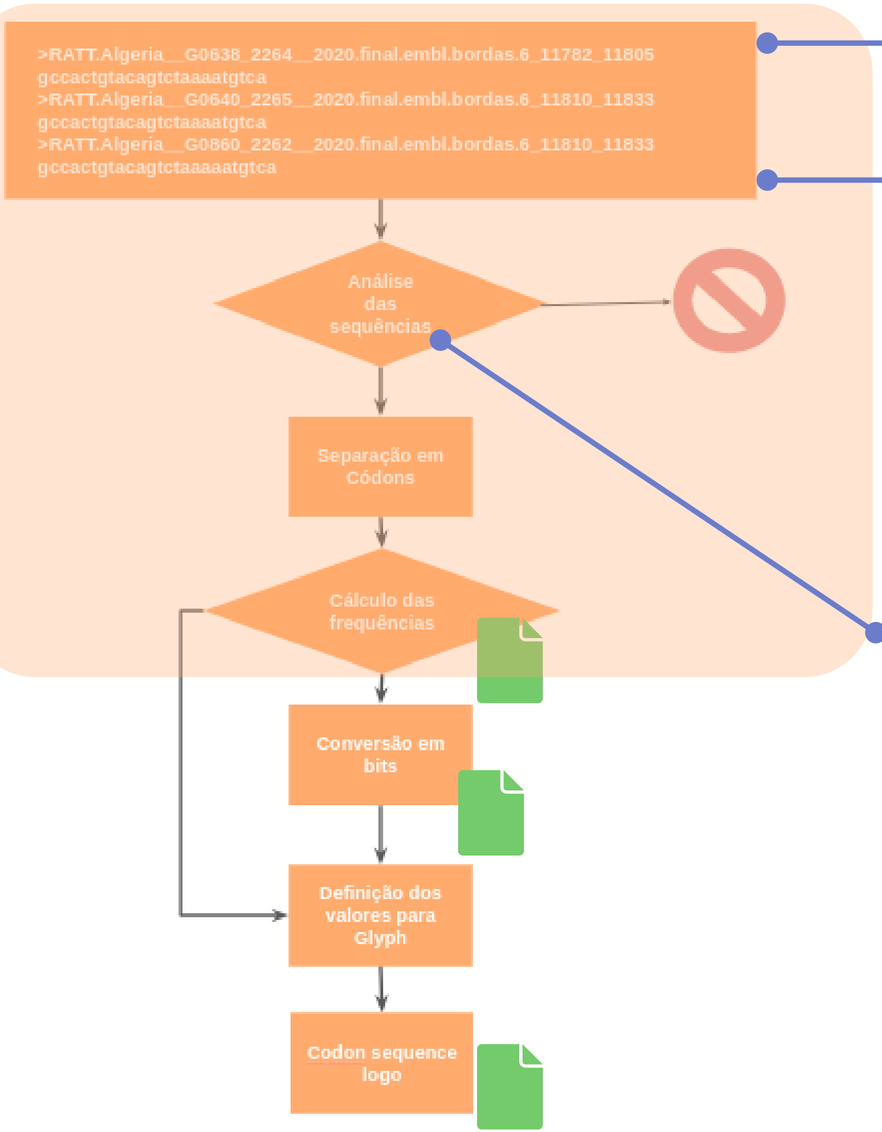
- Lê o FASTA
- Pegar o tamanho da seqência
- Seleciona as sequências dentro do FASTA

```
alignment = AlignIO.read(fastaFile, "fasta")
SeqLength = alignment.get_alignment_length()

if SeqLength % 3 != 0:
    print(f'Your sequence length {args.SeqLength} is not a multiple of 3')
    exit()


for record in alignment:
    notKnownNucleotide = 0
```

Codon Sequence logo
Script overview



argparse — Comunicação do script com o terminal

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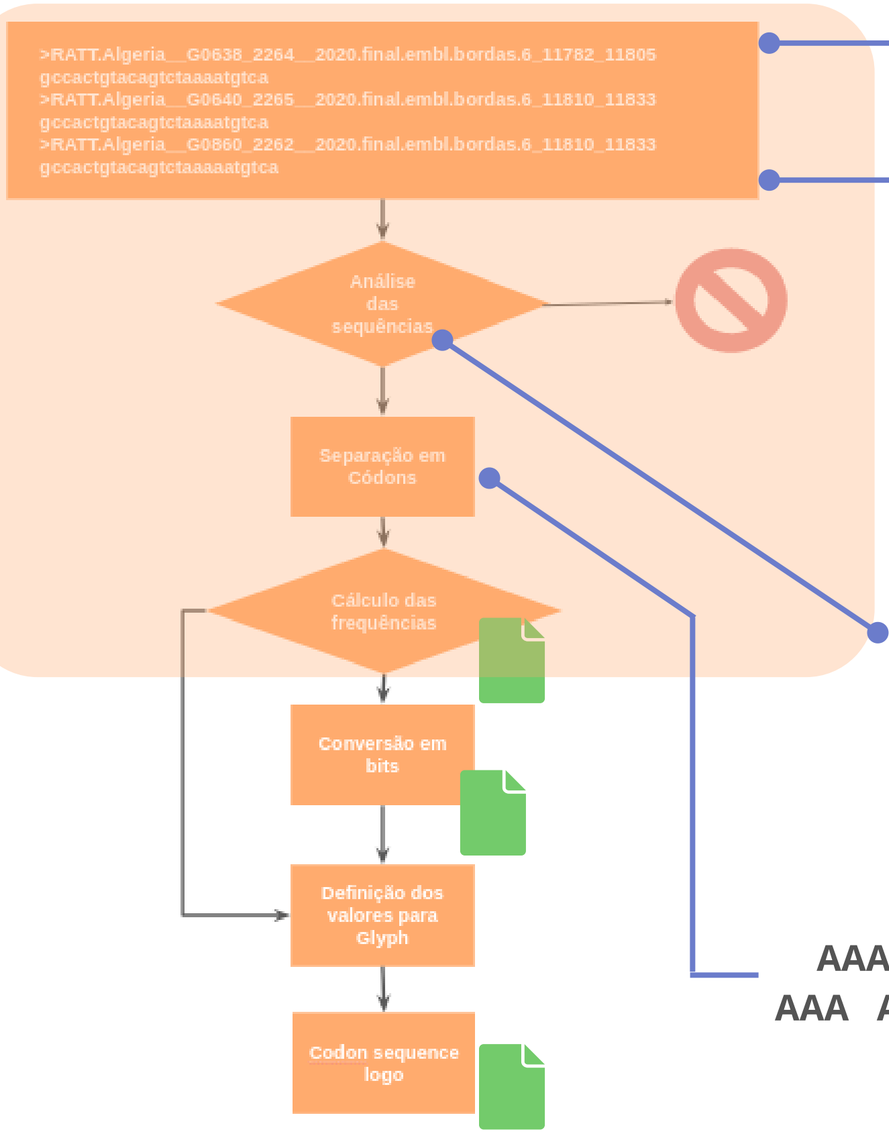
    exit()


for record in alignment:
    notKnownNucleotide = 0
```

AAAAAAAAAAAA
AAAAAAAAXXXX
AAAXXXXXXXXX

--degreeOfUncertainty
--datasetType

Codon Sequence logo
Script overview



argparse — Comunicação do script com o terminal

biopython — Operações com as seqências

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- Pegar o tamanho da seqência
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SeqLength = alignment.get_alignment_length()
if SeqLength % 3 != 0:
    print(f'Your sequence length {args.SeqLength} is not a multiple of 3')
    exit()


for record in alignment:
    notKnownNucleotide = 0
```

AAAAAAAAAAAA
AAAAAAAAXXXX
AAAXXXXXXXXX

--degreeOfUncertainty
--datasetType

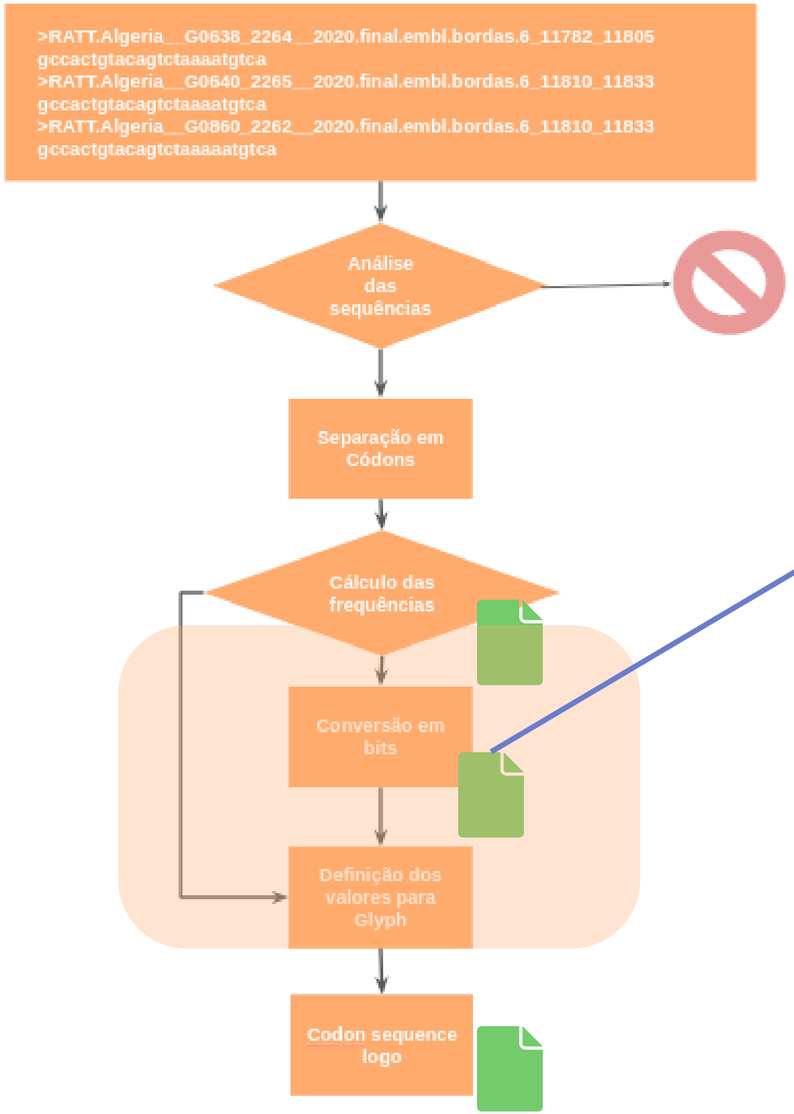
AAAAAAAAXXXX
AAA AAA AAX XXX

seq 1 AAG AAT AAX XXX
seq 2 AAG AAA AAX XXX
seq 3 AAA AAA AAX XXX
seq 4 AAA AAA AAX XXX

Dicionário=
{ posição:
{códon : frequência}
}

Codon Sequence logo

Script overview



Logomaker

--matrixLogoType

4.2.3 matrix functions

`logomaker.transform_matrix(*args, **kwargs)`

matriz de probabilidade --> Matriz de Bits

Pandas

pandas

4.2.2 Glyph class

class `logomaker.Glyph(**kwargs)`

A Glyph represents a character, drawn on a specified axes at a specified position, rendered using specified styling such as color and font_name.

Attributes

p: (number) x-coordinate value on which to center the Glyph.

c: (str) The character represented by the Glyph.

floor: (number) y-coordinate value where the bottom of the Glyph extends to. Must be < ceiling.

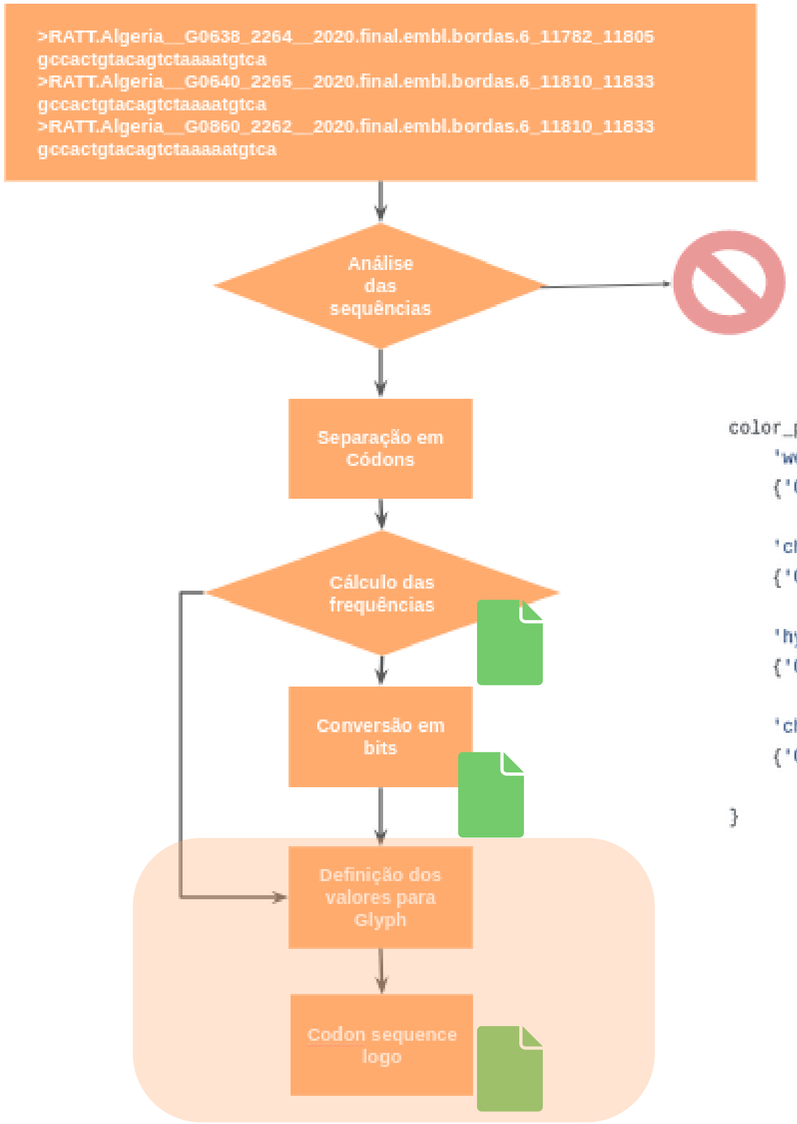
ceiling: (number) y-coordinate value where the top of the Glyph extends to. Must be > floor.

ax: (matplotlib Axes object) The axes object on which to draw the Glyph.

Tareen A, Kinney JB. Logomaker: beautiful sequence logos in Python, https://doi.org/10.1093/bioinformatics/btz921. 2019.

Codon Sequence logo

Script overview



- Onde cada símbolo entra no gráfico;
- Cor, nome, formatos (.pdf, .png).
- --alphaColor, --custonPaletteFile, --imageTitle, --prefixFileName, --logoFormat

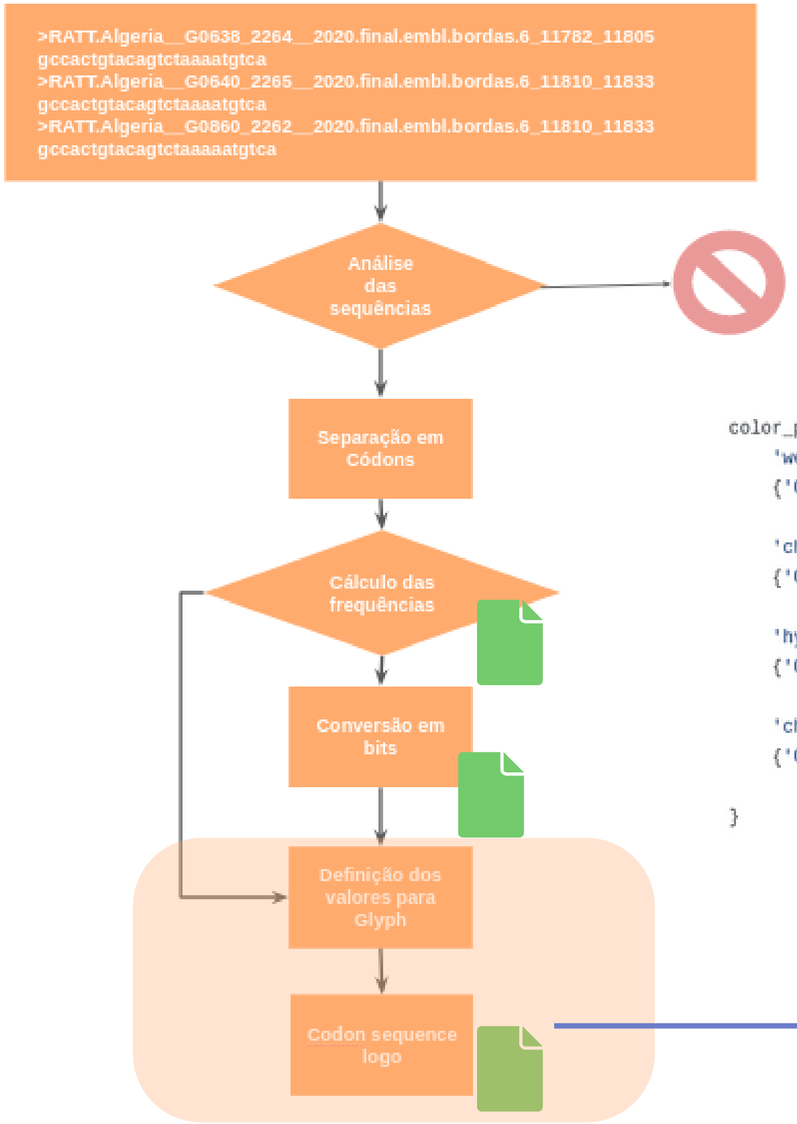
```
    ,
color_palett = {
    'weblogo_protein':
    {'GCT': 'black', 'GCC': 'black', 'GCA': 'black', 'GCG': 'black', 'TTT': 'black', 'TTC': 'black', 'ATT': 'black', 'ATC': 'black', 'ATA': 'black', 'TTA': 'bla
        'TCC': 'lime', 'TCA': 'lime', 'TCG': 'lime', 'AGT': 'lime', 'AGC': 'lime', 'ACT': 'lime', 'ACC': 'lime', 'ACA': 'lime', 'ACG': 'lime', 'TAT': 'lime', 'T
    'charge':
    {'GCT': 'dimgrey', 'GCC': 'dimgrey', 'GCA': 'dimgrey', 'GCG': 'dimgrey', 'TTT': 'dimgrey', 'TTC': 'dimgrey', 'ATT': 'dimgrey', 'ATC': 'dimgrey', 'ATA': 'dim
        'TCC': 'dimgrey', 'TCA': 'dimgrey', 'TCG': 'dimgrey', 'AGT': 'dimgrey', 'AGC': 'dimgrey', 'ACT': 'dimgrey', 'ACC': 'dimgrey', 'ACA': 'dimgrey', 'ACG': '
    'hydrophobicity':
    {'GCT': 'green', 'GCC': 'green', 'GCA': 'green', 'GCG': 'green', 'TTT': 'black', 'TTC': 'black', 'ATT': 'black', 'ATC': 'black', 'ATA': 'black', 'TTA': 'bla
        'AGT': 'green', 'AGC': 'green', 'ACT': 'green', 'ACC': 'green', 'ACA': 'green', 'ACG': 'green', 'TAT': 'black', 'TAC': 'black', 'GAT': 'mediumblue', 'GA
    'chemistry':
    {'GCT': 'black', 'GCC': 'black', 'GCA': 'black', 'GCG': 'black', 'TTT': 'black', 'TTC': 'black', 'ATT': 'black', 'ATC': 'black', 'ATA': 'black', 'TTA': 'bla
        'TCG': 'lime', 'AGT': 'lime', 'AGC': 'lime', 'ACT': 'lime', 'ACC': 'lime', 'ACA': 'lime', 'ACG': 'lime', 'TAT': 'lime', 'TAC': 'lime', 'GAT': 'red', 'GA
}
```

Tareen A, Kinney JB. Logomaker: beautiful sequence logos in Python, https://doi.org/10.1093/bioinformatics/btz921. 2019.

,

Codon Sequence logo

Script overview



- Onde cada símbolo entra no gráfico;
- Cor, nome, formatos (.pdf, .png).
- --alphaColor, --custonPaletteFile, --imageTitle, --prefixFileName, --logoFormat

```
    ,
color_palett = {
    'weblogo_protein':
    {'GCT': 'black', 'GCC': 'black', 'GCA': 'black', 'GCG': 'black', 'TTT': 'black', 'TTC': 'black', 'ATT': 'black', 'ATC': 'black', 'ATA': 'black', 'TTA': 'bla
        'TCC': 'lime', 'TCA': 'lime', 'TCG': 'lime', 'AGT': 'lime', 'AGC': 'lime', 'ACT': 'lime', 'ACC': 'lime', 'ACA': 'lime', 'ACG': 'lime', 'TAT': 'lime', 'T
    'charge':
    {'GCT': 'dimgrey', 'GCC': 'dimgrey', 'GCA': 'dimgrey', 'GCG': 'dimgrey', 'TTT': 'dimgrey', 'TTC': 'dimgrey', 'ATT': 'dimgrey', 'ATC': 'dimgrey', 'ATA': 'dim
        'TCC': 'dimgrey', 'TCA': 'dimgrey', 'TCG': 'dimgrey', 'AGT': 'dimgrey', 'AGC': 'dimgrey', 'ACT': 'dimgrey', 'ACC': 'dimgrey', 'ACA': 'dimgrey', 'ACG': '
    'hydrophobicity':
    {'GCT': 'green', 'GCC': 'green', 'GCA': 'green', 'GCG': 'green', 'TTT': 'black', 'TTC': 'black', 'ATT': 'black', 'ATC': 'black', 'ATA': 'black', 'TTA': 'bla
        'AGT': 'green', 'AGC': 'green', 'ACT': 'green', 'ACC': 'green', 'ACA': 'green', 'ACG': 'green', 'TAT': 'black', 'TAC': 'black', 'GAT': 'mediumblue', 'GA
    'chemistry':
    {'GCT': 'black', 'GCC': 'black', 'GCA': 'black', 'GCG': 'black', 'TTT': 'black', 'TTC': 'black', 'ATT': 'black', 'ATC': 'black', 'ATA': 'black', 'TTA': 'bla
        'TCG': 'lime', 'AGT': 'lime', 'AGC': 'lime', 'ACT': 'lime', 'ACC': 'lime', 'ACA': 'lime', 'ACG': 'lime', 'TAT': 'lime', 'TAC': 'lime', 'GAT': 'red', 'GA
}
```

Matplotlib

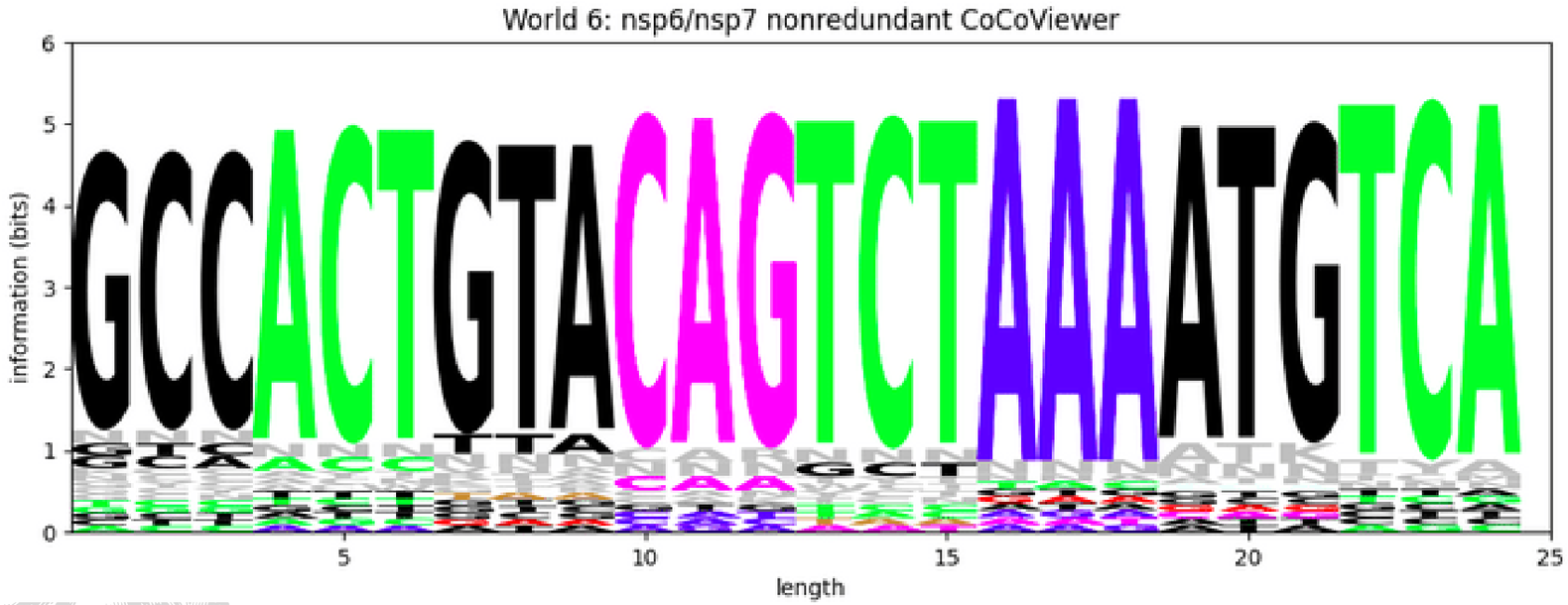
Plot

Tareen A, Kinney JB. Logomaker: beautiful sequence logos in Python, https://doi.org/10.1093/bioinformatics/btz921. 2019.

,

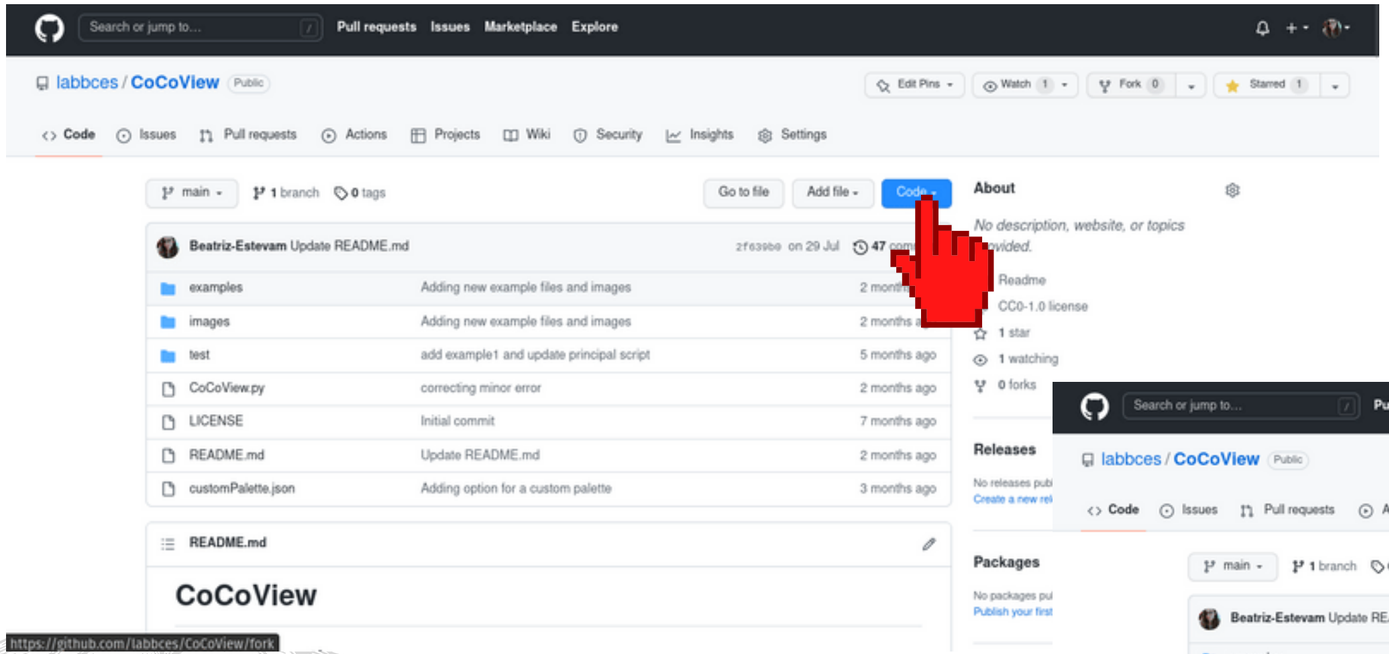
Exemplo

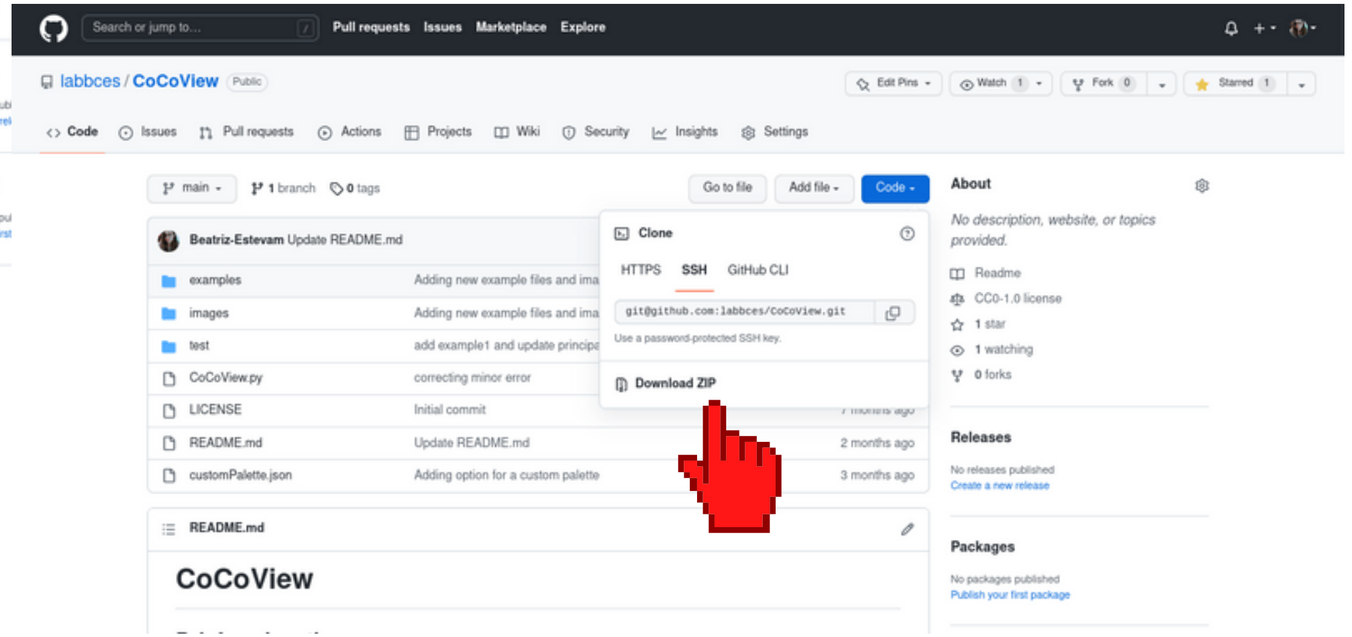
```
python3 CoCoView.py ./CoCoView/examples/example1/Bordas_World_6.nt.fasta -p "World6" -i "World 6 : nsp6/nsp7 nonredundant" -a "weblogo_protein" -d 100 -m "bit" -t "nonredundant" -l "png"
```

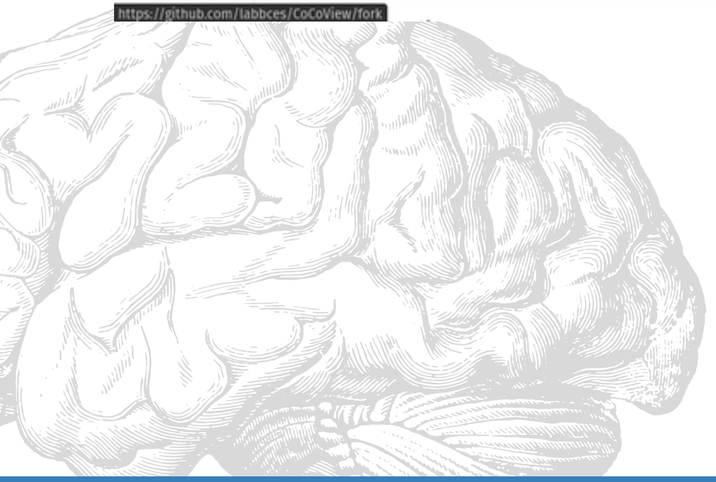


CoCoView: A Codon Conservation Viewer

Exemplo





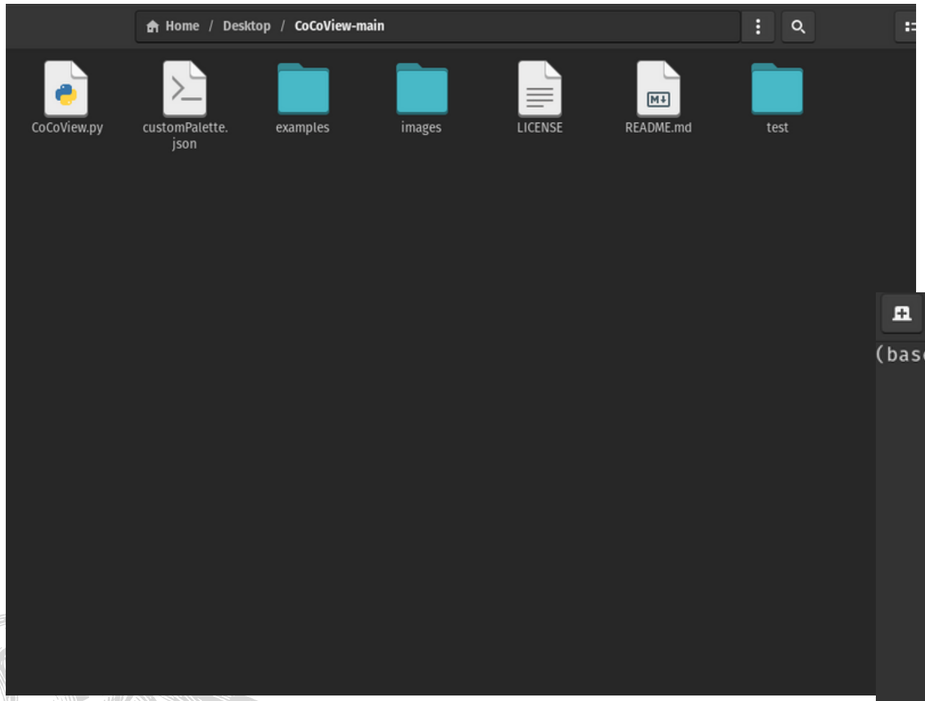


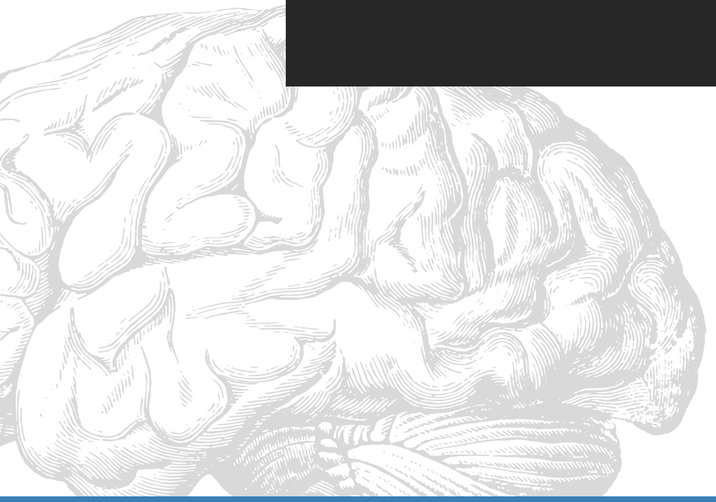
https://github.com/labbces/CoCoView

,

CoCoView: A Codon Conservation Viewer

Exemplo



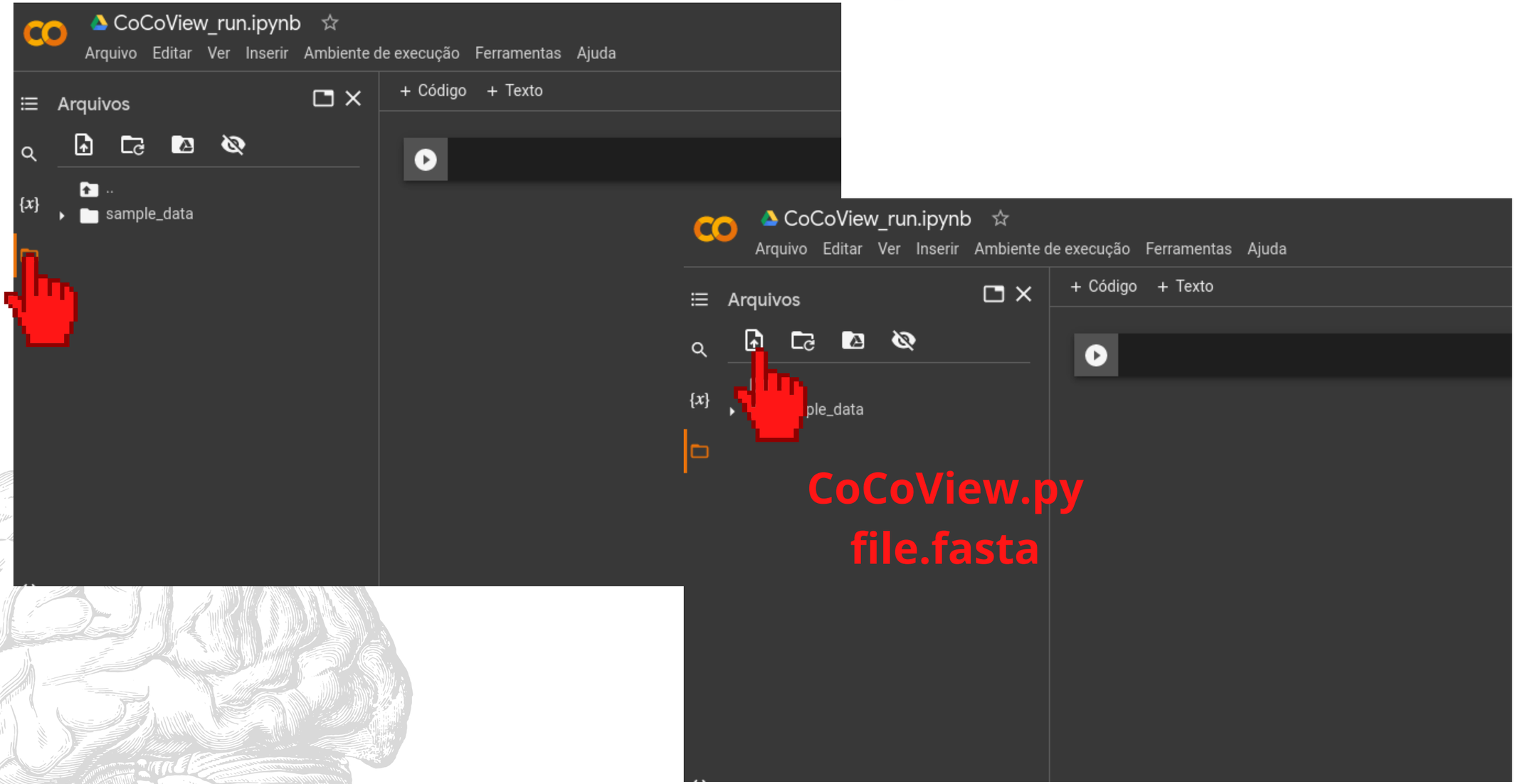


https://github.com/labbces/CoCoView

,

CoCoView: A Codon Conservation Viewer

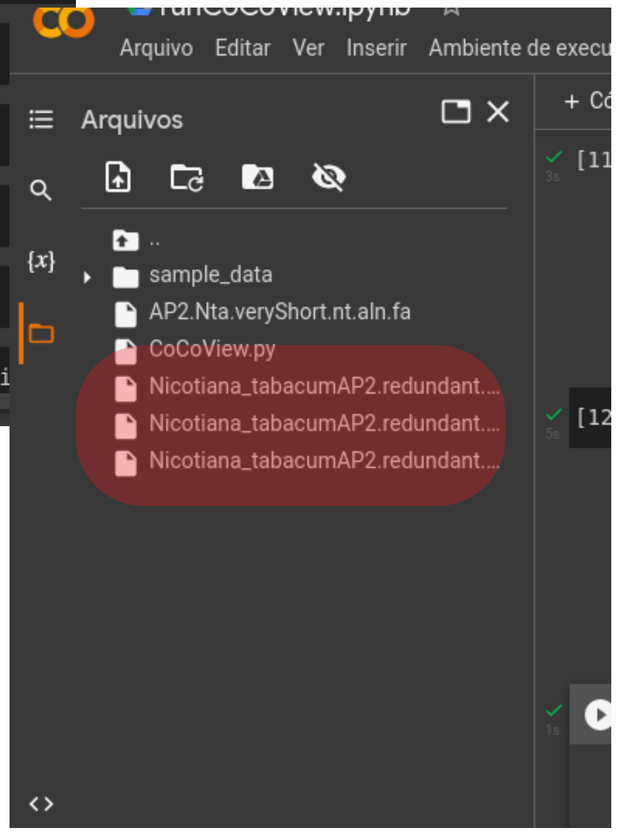
Exemplo



https://github.com/labbces/CoCoView

CoCoView: A Codon Conservation Viewer

Exemplo



https://github.com/labbces/CoCoView

CoCoView: A Codon Conservation Viewer

Validação do método

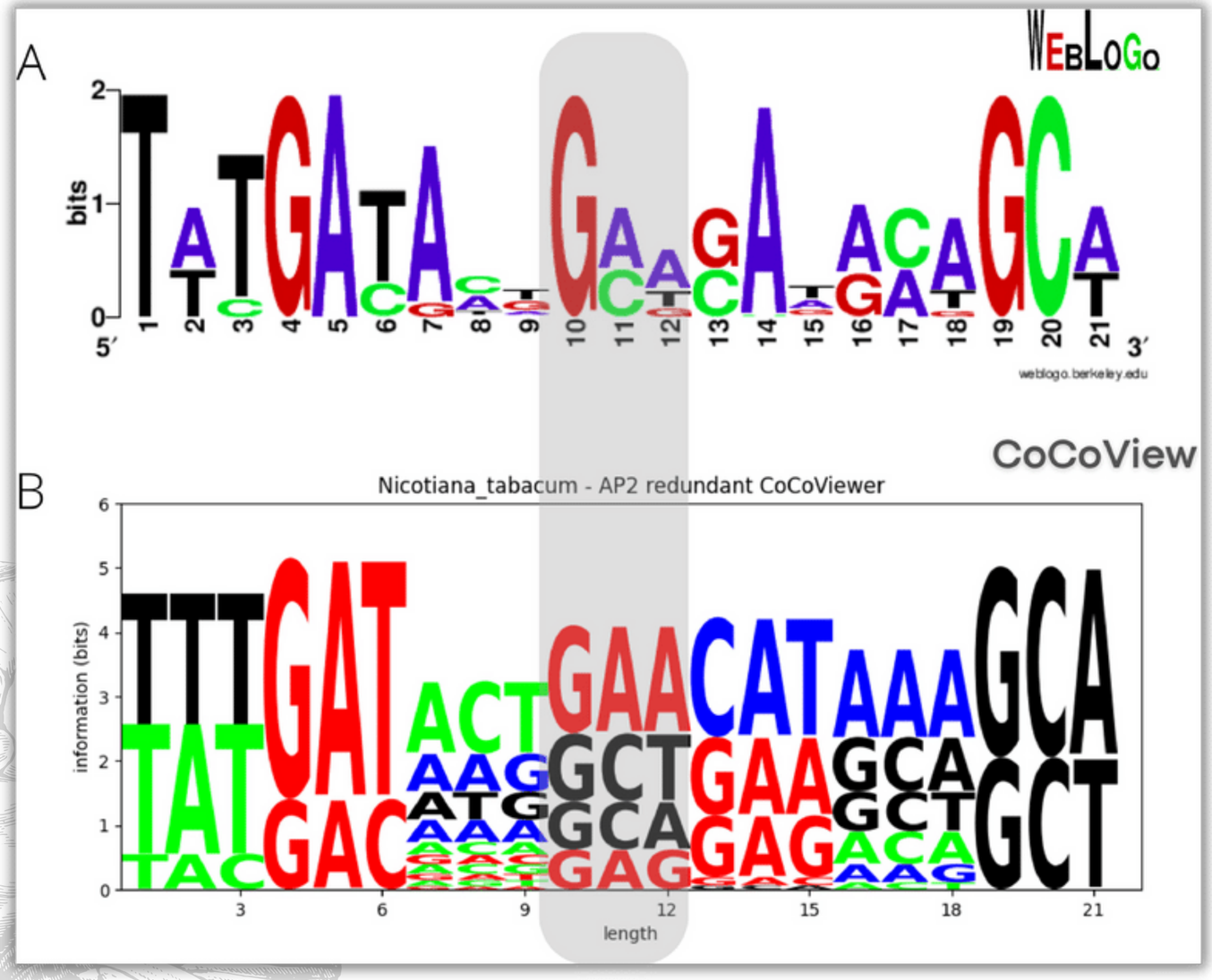
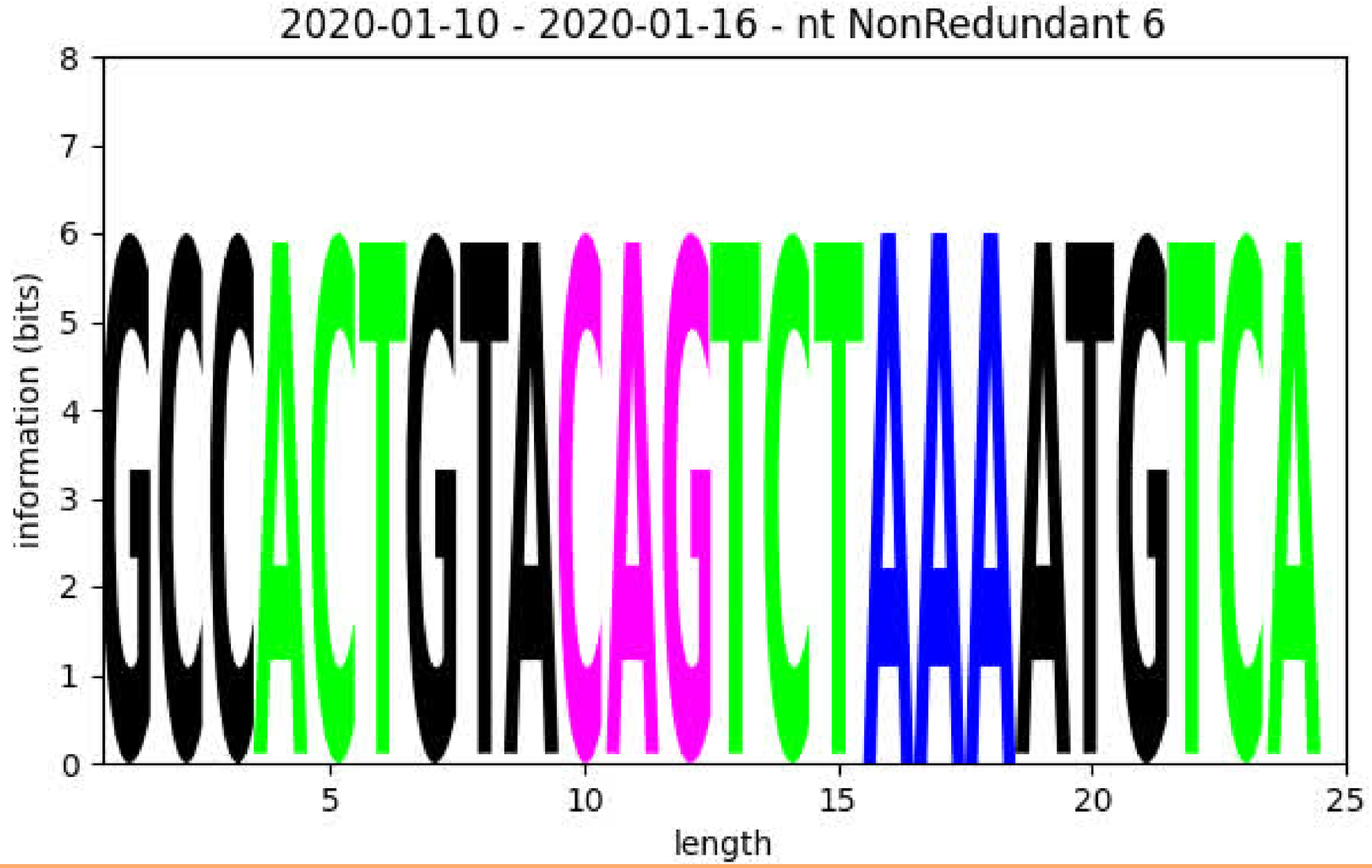


Fig. 1. CoCoView logo based on a multiple sequence alignment of a region of AP2 transcription factor coding sequences from *Nicotiana tabacum*. (A) Sequence logo generated using WebLogo [4], representing a per-nucleotide analysis. (B) Sequence logo generated using CoCoView (per-codon analysis). A per-nucleotide analysis could erroneously suggest that some codons are common, which can be ruled out on a per-codon visualization. Exemplified by the codon “GAT”, at the position highlighted in gray on both sequence logos, which can be interpreted as a common codon in the per-nucleotide analysis. However, in the per-codon analysis, this codon does not occur at this position.

estevam BR, Riaño-Pachón, DM, CoCoView - A codon conservation viewer via sequence logos. https://doi.org/10.1016/j.mex.2022.101803, 2022.

Exemplo de aplicação



Muito obrigada!

Agradecimentos

Prof. Dr. rer. nat. Diego Mauricio Riaño Pachón (Orientador)
LabBCES (Laboratório de Biologia Computacional, Evolutiva e de Sistemas)
Danilo Brito Rocha (Projeto do SARS-CoV-2)
USP/CENA
Equipe Workshop Python para Dados Biológicos

Prática!

bia.estevam.25@usp.br
@BiaREstevam

https://github.com/labbces/CoCoView

Estevam BR, Riaño-Pachón, DM. **CoCoView - A codon conservation viewer via sequence logos.** https://doi.org/10.1016/j.mex.2022.101803, 2022.

https://labbces.netlify.app/

Muito obrigada!

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Perguntas?

bia.estevam.25@usp.br
@BiaREstevam
https://github.com/labbces/CoCoView

Estevam BR, Riaño-Pachón, DM. **CoCoView - A codon conservation viewer via sequence logos.**
https://doi.org/10.1016/j.mex.2022.101803, 2022.
https://labbces.netlify.app/