

Escuela Profesional de Ciencia de la Computación

ICC Fase 1

Bioinformatics

Alignment tools

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- Introduction
 - Objectives
- Alignment tools
 - BioPython
 - Muscle
 - Clustal
 - BLAST
 - Mega

- Introduction
 - Objectives
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 - BioPythor
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 - a RI AST
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Introduction

Objectives

 Learn the alignment tools and databases used in Bioinformatics. Introduction

- Objectives
- Alignment tools
 - BioPython
 - Muscle

 - Mega

BioPython

Definition

Biopython is a set of freely available tools for biological computation written in Python by an international team of developers.

BioPython

Pairwise global alignment

Documentation.

```
from Bio import pairwise2
from Bio.pairwise2 import format_alignment

alignments = pairwise2.align.globalxx("ACCGT", "ACG")
print(format_alignment(*alignments[0]))
```

Results:

```
ACCGT
| | | |
A - CG -
Score=3
```

BioPython

Pairwise local alignment

Documentation.

```
from Bio import pairwise2
from Bio.pairwise2 import format_alignment

alignments = pairwise2.align.localxx("ACCGT", "ACG")
print(format_alignment(*alignments[0]))
```

Results:

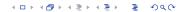
```
1 ACCG
| | | |
3 1 A-CG
Score=3
```

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Muscle

Multiple sequence alignment

It is a tool for multiple sequence alignment. Download page: link.



Muscle

Multiple sequence alignment

Samples: seqs2.fasta, seqs3.fasta

Basic usage

2

| muscle -in <inputfile> -out <outputfile>

Muscle

Multiple sequence alignment

seqs3.fasta after alignment.

- | >sp|P13786|HBAZ_CAPHI Hemoglobin subunit zeta OS=Capra hircus GN=HBZ1 PE=3 SV=2
- 2 MSLTRTERTIL --- WSKISTQADVIGTETLERLFSCYPQAKTYFPHFDLHSGSAQLRAHG SKVVAAVGDAVKSIDNVTSALSKLSELHAYVLRVDPVNFKFLSHCLLVTLASHFPADFTA
- 4 DAHAAWDKFLSIVSGVLTEKYR
 - >sp|P69905|HBA_HUMAN Hemoglobin subunit alpha OS=Homo sapiens GN=HBA1 PE=1 SV=2
- 6 MVLSPADKTNVKAAWGKVGAHAGEY-AEALERMFLSFPTTKTYFPHFDLSHGSAQVKGHG KKVADALTNAVAHVDDMPNALSALSDLHAHKLRVDPVNFKLLSHCLLVTLAAHLPAEFTP
- 8 AVHASLDKFLASVSTVLTSKYR
 - >sp|P01942|HBA_MOUSE Hemoglobin subunit alpha OS=Mus musculus GN=Hba PE=1 SV=2
- MVLSGEDKSNIKAAWGKIGGHGAEYGAEALERMFASFPTTKTYFPHFDVSHGSAQVKGHG KKVADALASAAGHLDDLPGALSALSDLHAHKLRVD-VNFKLLSHCLLVTLASHHPADFTP
- 12 AVHASLDKFLASVSTVLTSKYR



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Clustal

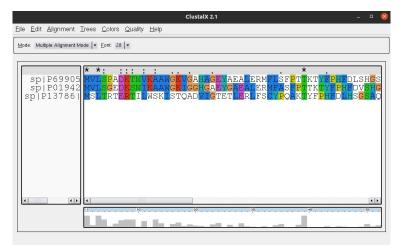
Multiple sequence alignment

It is a tool for multiple sequence alignment like Muscle. Download page: link.



Clustal

Samples: seqs2.fasta, seqs3.fasta



Clustal

Results

Results:

CLUSTAL 2.1 multiple sequence alignment

```
sp|P69905|HBA HUMAN
                        MVLSPADKTNVKAAWGKVGAHAGEY-
AEALERMFLSFPTTKTYFPHFDLSHGSAOVKGHG
sp|P01942|HBA MOUSE
MVLSGEDKSNIKAAWGKIGGHGAEYGAEALERMFASFPTTKTYFPHFDVSHGSAOVKGHG
sp|P13786|HBAZ CAPHI
                        MSLTRTERT---
ILWSKISTOADVIGTETLERLFSCYPOAKTYFPHFDLHSGSAOLRAHG
                        * *: :::
                                                 **** **
sp|P69905|HBA HUMAN
KKVADALTNAVAHVDDMPNALSALSDLHAHKLRVDPVNFKLLSHCLLVTLAAHLPAFFTP
sp|P01942|HBA MOUSE
                        KKVADALASAAGHLDDLPGALSALSDLHAHKLRVD-
VNFKLLSHCLLVTLASHHPADFTP
sp|P13786|HBAZ CAPHI
SKVVAAVGDAVKSIDNVTSALSKLSELHAYVLRVDPVNFKFLSHCLLVTLASHFPADFTA
                        ** * * * * ** ** ***
**** ******** * ** **
sp|P69905|HBA HUMAN
                        AVHASLDKFLASVSTVLTSKYR
sp|P01942|HBA MOUSE
                        AVHASLDKFLASVSTVLTSKYR
sp|P13786|HBAZ CAPHI
                        DAHAAWDKFLSIVSGVLTEKYR
                         ** **** ** ***
```

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BLAST

Web page.

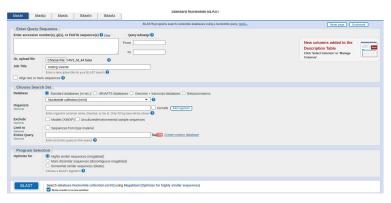






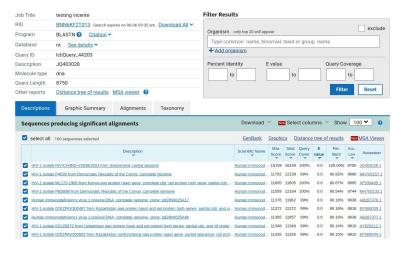
BLAST

Evaluate BLAST with this sample: HIVGRPCG.fasta.



BLAST

Results:



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Mega

Web page.

The objective of the MEGA software has been to provide tools for exploring, discovering, and analyzing DNA and protein sequences from an evolutionary perspective.

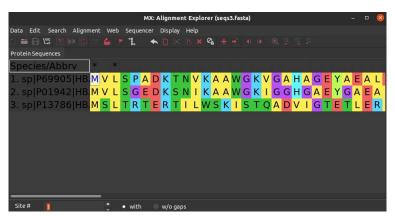
Mega

Main window.



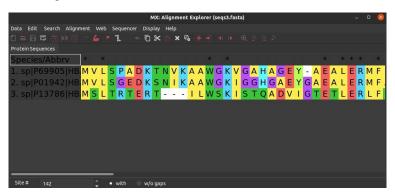
PROTOTYPE

Multiple sequence alignment.



Mega

After alignment.



Questions?



References I



J. Xiong, Essential bioinformatics. Cambridge University Press, 2006.