

Scientific Programming

Practical 10

Introduction

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Biopython

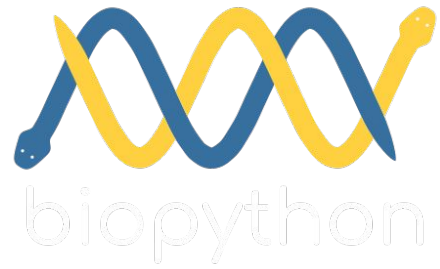


FROM Biopython's website:

The Biopython Project is an international association of developers of freely available **Python tools for computational molecular biology**.

The goal of Biopython is to make it as easy as possible to use **Python for bioinformatics** by creating high-quality, reusable modules and classes.

Biopython



Biopython:

1. Provides tools to **parse several common bioinformatics formats** (e.g. FASTA, FASTQ, BLAST, PDB, Clustalw, Genbank,...).
2. Provides an **interface towards biological data repositories** (e.g. NCBI, Expasy, Swiss-Prot, ...)
3. Provides an **interface towards some bioinformatic tools** (e.g. clustalw, MUSCLE, BLAST,...)
4. **Implements some tools** like pairwise alignment **and data structures** to deal with biological data.

Seq objects

Seq objects are more powerful than string to deal with sequences and are defined in the module Bio.Seq.

They have two information:

1. SEQUENCE

2. ALPHABET

(optional, but useful to check things)

defined in

`Bio.Alphabet.IUPAC`

Some options:

`Bio.Alphabet.generic_dna`,
`Bio.Alphabet.generic_protein`,
`Bio.Alphabet.ThreeLetterProtein`, ...

They are **immutable objects**. The mutable version is **MutableSeq**.

```
from Bio.Seq import Seq
from Bio.Alphabet import IUPAC

#No alphabet specified
s = Seq("GATTACATAATA")
dna_seq = Seq("GATTATACGTAC", IUPAC.unambiguous_dna)
print("S:", s)
print("S's alphabet:", s.alphabet)
print("dna_seq:", dna_seq)
print("dna_seq's alphabet:", dna_seq.alphabet)

my_prot = Seq("MGNAAAAKKGSEQE", IUPAC.protein)
print("my_prot:", my_prot)
print("my_prot's alphabet:", my_prot.alphabet)
```

```
S: GATTACATAATA
S's alphabet: Alphabet()
dna_seq: GATTATACGTAC
dna_seq's alphabet: IUPACUnambiguousDNA()
my_prot: MGNAAAAKKGSEQE
my_prot's alphabet: IUPACProtein()
```

Seq objects

Seq objects behave like strings, but the consistency of the alphabet is checked too.

For example we cannot concatenate a **unambiguous_dna** with a **IUPAC.protein** sequence.

```
my_mess = dna_seq + my_prot
```

```
S: GATTACATAATA
S's alphabet: Alphabet()
dna_seq: GATTATACGTAC
dna_seq's alphabet: IUPACUnambiguousDNA()
my_prot: MGNAAAARKKGSEQE
my_prot's alphabet: IUPACProtein()
```

```
-----
TypeError                                Traceback (most recent call last)
<ipython-input-20-4c1f6d65a691> in <module>()
    14 print("my_prot's alphabet:", my_prot.alphabet)
    15
--> 16 my_mess = dna_seq + my_prot

/usr/local/lib/python3.5/dist-packages/Bio/Seq.py in __add__(self, other)
    296         raise TypeError(
    297             "Incompatible alphabets {0!r} and {1!r}".format(
--> 298                 self.alphabet, other.alphabet))
    299         # They should be the same sequence type (or one of them is generic)
    300         a = Alphabet._consensus_alphabet([self.alphabet, other.alphabet])
```

```
TypeError: Incompatible alphabets IUPACUnambiguousDNA() and IUPACProtein()
```

Seq objects

Seq objects behave like strings, but the consistency of the alphabet is checked too.

For example we cannot concatenate a **unambiguous_dna** with a **IUPAC.protein** sequence.

```
from Bio.Seq import Seq
from Bio.Alphabet import generic_alphabet

dna_seq = Seq("GATTATACGTAC", IUPAC.unambiguous_dna)
my_prot = Seq("MGNAAAAKKGSEQE", IUPAC.protein)

my_prot.alphabet = generic_alphabet

#Does it really make sense though!?
print(dna_seq + my_prot)
```

GATTATACGTACMGNAAAAKKGSEQE

Seq objects

Seq objects behave like strings, but the consistency of the alphabet is checked too.

We can loop through the elements of the sequence and perform slicing...

```
from Bio.Seq import Seq
from Bio.Alphabet import IUPAC

dna_seq = Seq("GATTATACGTACGGCTA", IUPAC.unambiguous_dna)

for base in dna_seq:
    print(base, end = " ")

print("")

sub_seq = dna_seq[4:10]
print(sub_seq)

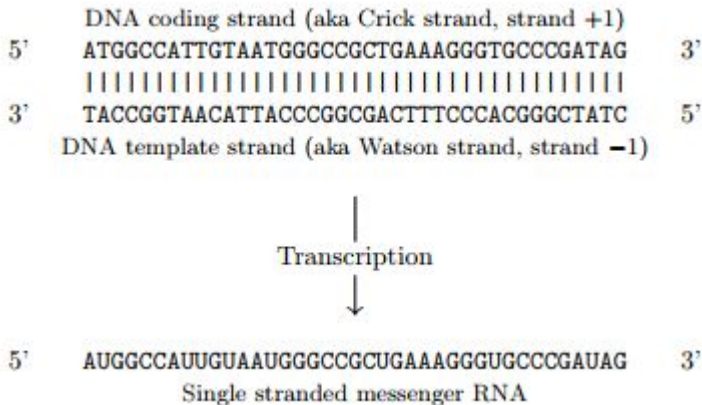
#Let's reverse the string:

print("Reversed: ", dna_seq[::-1])
#from Seq to string:
dna_str = str(dna_seq)
print("As string:", dna_str)
print(type(dna_str))
```

```
G A T T A T A C G T A C G G C T A
ATACGT
Reversed:  ATCGGCATGCATATTAG
As string: GATTATACGTACGGCTA
<class 'str'>
```

Seq objects

Biopython provides several methods working on Seq objects (remember Seq are immutable!)



General methods (return int and Seq objects):

`Seq.count(s)` : counts the number of times s appears in the sequence;

`Seq.upper()` : makes the sequence of the object Seq upper case

`Seq.lower()` : makes the sequence of the object Seq lower case

Only for DNA/RNA (return Seq objects):

`Seq.complement()` to complement the sequence

`Seq.reverse_complement()` to reverse complement the sequence.

`Seq.transcribe()` transcribes the DNA into mRNA

`Seq.back_transcribe()` back transcribes mRNA into DNA

`Seq.translate()` translates mRNA or DNA into proteins

Other functions are in **SeqUtils**

(ex. use `from Bio.SeqUtils import molecular_weight`):

`SeqUtils.GC(Seq)` computes GC content

`SeqUtils.molecular_weight(Seq)` computes the molecular weight of the sequence

....

Seq objects

Biopython provides several methods working on Seq objects (remember Seq are immutable!)

```
ATGGCCATTGTAATGGGCCGCTGAAAGGGTGCCCGATAG
AUGGCCAUUGUAAUGGGCCGCUGAAAGGGUGCCCGAUAG
```

```
IUPACUnambiguousRNA()
```

```
... and back
ATGGCCATTGTAATGGGCCGCTGAAAGGGTGCCCGATAG
```

```
Translation to protein:
MAIVMGR*KGAR*
```

```
Up to first stop:
MAIVMGR
```

```
Mitochondrial translation: (TGA is W!)
MAIVMGRWKGAR*
```

```
from Bio.Seq import Seq
from Bio.Alphabet import IUPAC

coding_dna = Seq("ATGGCCATTGTAATGGGCCGCTGAAAGGGTGCCCGATAG",
                  IUPAC.unambiguous_dna)
print(coding_dna)

mrna = coding_dna.transcribe()
print(mrna)
print("")
print(mrna.alphabet)
print("")
print("... and back")
print(mrna.back_transcribe())
print("")
print("Translation to protein:")
prot = mrna.translate()
print(prot)
print("")
print("Up to first stop:")
print(mrna.translate(to_stop = True))
print("")
print("Mitochondrial translation: (TGA is W!)")
mit_prot = mrna.translate(table=2)
print(mit_prot)
```

Sequence annotations

The **SeqRecord** object is used to store annotations associated to sequences

1. `SeqRecord.seq` : the sequence (the Seq object)
2. `SeqRecord.id` : the identifier of the sequence, typically an accession number
3. `SeqRecord.name` : a "common" name or identifier sometimes identical to the accession number
4. `SeqRecord.description` : a human readable description of the sequence
5. `SeqRecord.letter_annotations` : a per letter annotation using a restricted dictionary (e.g. quality)
6. `SeqRecord.annotations` : a dictionary of unstructured annotation (e.g. organism, publications,...)
7. `SeqRecord.features` : a list of SeqFeature objects with more structured information (e.g. genes pos).
8. `SeqRecord.dbxrefs` : a list of database cross references.

Sequence annotations

Read a fasta file [NC005816.fna](#) containing the whole sequence for *Yersinia pestis* biovar *Microtus* str. 91001 plasmid pPCP1 and retrieve some information about the sequence.

```
>gi|45478711|ref|NC_005816.1| Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete sequence
```

```
TGTAACGAACGGTGCAATAGTGATCCACACCCAACGCCTGAAATCAGATCCAGGGGTAATCTGCTCTCC  
TGATTCAGGAGAGTTTATGGTCACTTTTGGACAGTTATGAAATTAAAACTCTGCACAAGCAGGGAATG  
AGTAGCCGGGCGATTGCCAGAGAACTGGGGATCTCCCGCAATACCGTTAAACGTTATTTGCAGGCAAAAT  
CTGAGCCGCCAAAATATACGCCGCGACCTGCTGTTGCTTCACTCCTGGATGAATACCGGGATTATATTGCG  
TCAACGCATCGCCGATGCTCATCTTACAAAATCCCGCAACGGTAATCGCTCGCGAGATCAGAGACCAG  
GGATATCGTGGCGGAATGACCACTTCTCAGGGCATTCACTCGTTCTCTCTCGGTTCCCTCAGGAGCAGGAGC  
CTGCCGTTTCGGTTCGAACTGAACCCGGACGACAGATGCAGGTTGACTGGGGCACTATGCGTAATGGTCTG  
CTCACCCTTTCACGTGTTTCGTTGCTGTTCTCGGATACAGCCGAATGCTGTACATCGAATTCAGTACAAT  
ATGCGTTATGACACGCTGGAGACCTGCCATCGTAATGCGTTCCGCTTCTTTGGTGGTGTGCCGCGCGAAG  
TGTTGTATGACAATATGAAAACGTGG...|
```

← → ↻ 🔒 https://www.ncbi.nlm.nih.gov/nucleotide/NC_005816

NCBI Resources How To

Nucleotide NC005816
Advanced

[Learn more](#) about upcoming changes to the Nucleotide, EST, and GSS databases.

GenBank Send to: ▼

Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete sequence

NCBI Reference Sequence: NC_005816.1

[FASTA](#) [Graphics](#)

[Go to: ▼](#)

LOCUS	NC_005816	9609 bp	DNA	circular	CON 11-JAN-2018
DEFINITION	Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete sequence.				
ACCESSION	NC_005816				
VERSION	NC_005816.1				
DBLINK	BioProject: PRJNA224116 BioSample: SAMN02602970 Assembly: GCF_000007885.1				
KEYWORDS	RefSeq.				
SOURCE	Yersinia pestis biovar Microtus str. 91001				
ORGANISM	Yersinia pestis biovar Microtus str. 91001 Bacteria; Proteobacteria; Gammaproteobacteria; Enterobacterales; Yersiniaceae; Yersinia.				
REFERENCE	1 (bases 1 to 9609)				
AUTHORS	Zhou,D., Tong,Z., Song,Y., Han,Y., Pei,D., Pang,X., Zhai,J., Li,M., Cui,B., Qi,Z., Jin,L., Dai,R., Du,Z., Wang,J., Guo,Z., Wang,J., Huang,P. and Yang,R.				
TITLE	Genetics of metabolic variations between Yersinia pestis biovars				

<https://www.ncbi.nlm.nih.gov>

Sequence annotations

Read a fasta file [NC005816.fna](#) containing the whole sequence for *Yersinia pestis* biovar *Microtus* str. 91001 plasmid pPCP1 and retrieve some information about the sequence.

```
ID: gi|45478711|ref|NC_005816.1|
Name: gi|45478711|ref|NC_005816.1|
Description: gi|45478711|ref|NC_005816.1| Yersinia
pestis biovar Microtus str. 91001 plasmid pPCP1,
complete sequence
Number of features: 0
Seq('TGTAACGAACGGTGCAATAGTGATCCACACCCAACGCCTGAAATCAGAT
CCAGG...CTG', SingleLetterAlphabet())
```

```
Sequence [first 30 bases]:
TGTAACGAACGGTGCAATAGTGATCCACAC
```

```
The id:
gi|45478711|ref|NC_005816.1|
```

```
The description:
gi|45478711|ref|NC_005816.1| Yersinia pestis biovar
Microtus str. 91001 plasmid pPCP1, complete sequence
```

```
The record is a: <class 'Bio.SeqRecord.SeqRecord'>
```

```
from Bio import SeqIO

record =
SeqIO.read("file_samples/NC_005816.fna",
"fasta")

print(record)
print("")
print("Sequence [first 30 bases]:")
print(record.seq[0:30])
print("")
print("The id:")
print(record.id)
print("")
print("The description:")
print(record.description)
print("")
print("The record is a: ", type(record))
```

SeqIO.parse

The `Bio.SeqIO` module aims to provide a simple way to work with several different sequence file formats

Formats available:
<https://biopython.org/wiki/SeqIO>

The method `Bio.SeqIO.parse` is used to parse some sequence data into a `SeqRecord` iterator. In particular, the basic syntax is:

```
SeqRecordIterator = Bio.SeqIO.parse(filename, file_format)
```

where `filename` is typically an open handle to a file and `file_format` is a lower case string describing the file format. Possible options include **fasta**, **fastq-illumina**, **abi**, **ace**, **clustal...** all the

Note that `Bio.SeqIO.parse` returns an iterator, therefore it is possible to manually fetch one `SeqRecord` after the other with the `next(iterator)` method.

WARNING: When dealing with very large FASTA or FASTQ files, the overhead of working with all these objects can make scripts too slow. In this case `SimpleFastaParser` and `FastqGeneralIterator` parsers might be better as they which return just a tuple of strings for each record.

SeqIO

Example: Let's get the first 3 entries of the .fasta file `contigs82.fasta` printing off the length of the sequence and the first 50 bases of each sequence followed by "...".

```
In [12]: from Bio import SeqIO

seqIterator = SeqIO.parse("file_samples/contigs82.fasta", "fasta")

labels = ["1st", "2nd", "3rd"]
for l in labels:
    seqRec = next(seqIterator)
    print(l, "entry:")
    print(seqRec.id, " has size ", len(seqRec.seq))
    print(seqRec.seq[:50]+"...")
    print("")
```

```
1st entry:
MDC020656.85  has size  2802
GAGGGGTTTAGTTCCTCACTCGCAAAGCAAAGATACATAAATTTAGAA...
```

```
2nd entry:
MDC001115.177  has size  3118
TGAATGGTGAAAATTAGCCAGAAGATCTTCTCCACACATGACATATGCAT...
```

```
3rd entry:
MDC013284.379  has size  5173
TATCGTTTCCTCTGAGTAGAATATCGTTATAACAAGATTTTTTTTTTCCT...
```

SeqIO

The module `Bio.SeqIO` also has three different ways to allow random access to elements:

1. `Bio.SeqIO.to_dict(file_handle/iterator)` : builds a dictionary of all the SeqRecords keeping them in memory and allowing modifications to the records. **This potentially uses a lot of memory but is very fast;**
2. `Bio.SeqIO.index(filename, file_type)` : builds a sort of read-only dictionary, parses the elements into SeqRecords on demand (i.e. it returns an iterator!). **This method is slower, but more memory efficient;**
3. `Bio.SeqIO.index_db(indexName.idx, filenames, file_format)` : builds a read-only dictionary, but stores ids and offsets on a SQLite3 database. **It is slower but uses less memory.**

SeqIO.write

The module `Bio.SeqIO` provides also a way to write sequence records to files in various formats (like fasta, fastq, genbank, pfam...)

SeqRecords can be written out to files by using

```
N = Bio.SeqIO.write(records, out_filename, file_format)
```

where **records** is a list of the SeqRecords to write, **out_filename** is the string with the filename to write and **file_format** is the format of the file to write. **N** is the number of sequences written.

WARNING: If you write a file that is already present, `SeqIO.write` will just rewrite it without telling you.

Multiple sequence alignment

Multiple Sequence Alignments are a collection of **multiple sequences which have been aligned together** – usually with the insertion of gap characters, and addition of leading or trailing gaps – such that all the sequence strings are the same length.

Q5E940_BOVIN	-----MPREDRATWKSNYFLKIIQLDDYPKCFIVGADNVGSKOMQIIRMSLRGK-AVYLMGKNTMMRKAIRGHLNNH--PALE	76
RLA0_HUMAN	-----MPREDRATWKSNYFLKIIQLDDYPKCFIVGADNVGSKOMQIIRMSLRGK-AVYLMGKNTMMRKAIRGHLNNH--PALE	76
RLA0_MOUSE	-----MPREDRATWKSNYFLKIIQLDDYPKCFIVGADNVGSKOMQIIRMSLRGK-AVYLMGKNTMMRKAIRGHLNNH--PALE	76
RLA0_RAT	-----MPREDRATWKSNYFLKIIQLDDYPKCFIVGADNVGSKOMQIIRMSLRGK-AVYLMGKNTMMRKAIRGHLNNH--PALE	76
RLA0_CHICK	-----MPREDRATWKSNYFMKIIQLDDYPKCFIVGADNVGSKOMQIIRMSLRGK-AVYLMGKNTMMRKAIRGHLNNH--PALE	76
RLA0_RAMSY	-----MPREDRATWKSNYFLKIIQLDDYPKCFIVGADNVGSKOMQIIRMSLRGK-AVYLMGKNTMMRKAIRGHLNNH--PALE	76
Q7ZUG3_BRARE	-----MPREDRATWKSNYFLKIIQLDDYPKCFIVGADNVGSKOMQIIRMSLRGK-AVYLMGKNTMMRKAIRGHLNNH--PALE	76
RLA0_ICTPU	-----MPREDRATWKSNYFLKIIQLDDYPKCFIVGADNVGSKOMQIIRMSLRGK-AVYLMGKNTMMRKAIRGHLNNH--PALE	76
RLA0_DROME	-----HYRENKAAKKAQYFIKVVFLDFEPPKCFIVGADNVGSKOMQIIRMSLRGK-AVYLMGKNTMMRKAIRGHLNNH--PALE	76
RLA0_DICDI	-----MSGAG-SKREKLFIEKATKLFITTDKMIYAEADVFVGSOLQIKRSIRGI-GAVLMGKNTMIKKVIRDLADSK--PELD	75
Q54LP0_DICDI	-----MSGAG-SKRENVFIEKATKLFITTDKMIYAEADVFVGSOLQIKRSIRGI-GAVLMGKNTMIKKVIRDLADSK--PELD	75
RLA0_PLAFB	-----MAKLSKQKKQMYIEKLSSLIQQYKSLIIVVDNVGSGMASVKKSLRGK-ATILMGKNTIRIALTKKNLQAV--DOIE	76
RLA0_SULAC	-----HIGLAVTTTKIAKWKYDEVAELTKLTKNTIIIANIIGFPADKLHEIRKKLRGK-ADIKVTKNLFPNIALKNAG--YDK	79
RLA0_SULTO	-----MRIMAVITQERKIAKWKIEVKELEKLRRENTIIIANIIGFPADKLHDIRKKMRGM-AEIKVTNTLFGIAKNAG--LDVS	80
RLA0_SULSO	-----MKRLALALQQRKVASWKELEVKELEIKNSNTILGNLEGFPADKLHEIRKKLRGK-ADIKVTNTLFGIAKNAG--LDIE	80
RLA0_AERPE	MSVYSIVGQMYKREKPIPEKNTLMRLKLELFSKRRVYFLADLTCTPFFVVRVYKKKLWKK-YFMVVAKRILBAMKAAGLE--LDDN	86
RLA0_PYRAE	HMHLAIGKRRYVTRQYPAKRYKIVSEATLLQKYPYVFLFDLHLSIRILHEVRYRLRY-GVIRIIRDLFKIAFTKYVGG--IPAE	85
RLA0_METAC	-----MAEERNHTEHIPQWKDEIENIKELIQSHKVFCHVRIEGILATKMKIRRDLDV-AVLKVSNTLTERALNQLG--ETIP	78
RLA0_METMA	-----MAEERNHTEHIPQWKDEIENIKELIQSHKVFCHVRIEGILATKMKIRRDLDV-AVLKVSNTLTERALNQLG--ESIP	78
RLA0_ARCFU	-----MAAVRGS--PPEYKVRAVEEIKRMISSEYVAIVSRNVFAGOMKIRREFGK-AEIKVVKNTLTERALDALG--GDYL	75
RLA0_METKA	MAYKAKGQPPSYEPKVAENRREVKELEMDIEYNGVLDLEGIAPOLQEIYAKLRERDIIRMBRNTLMRIALKEELDER--PELE	88
RLA0_METTH	-----MAHYVAENKKKEVQELHDLIKSEVYVGIANLADIPAROLQKMQTLRDS-ALIMMKKTLISIALKKNAGREL--ENVD	74
RLA0_METTL	-----MITASEHKIAPWKIEEVNKLKLLKNGQIYALVDMMEYPAROLQEIIRDKIR-GTMTLKMRNTLIEIAIKVAETGNPEFA	82
RLA0_METYA	-----MIDAKSEHKIAPWKIEEVNKLKLLKNGQIYALVDMMEYPAROLQEIIRDKIR-GTMTLKMRNTLIEIAIKVAETGNPEFA	82
RLA0_METJA	-----METKYAHVAPWKIEEVNKLKLLKNGQIYALVDMMEYPAROLQEIIRDKIR-GTMTLKMRNTLIEIAIKVAETGNPEFA	81
RLA0_PYRAB	-----MAHYVAENKKKEVEELANLIKSPYVIALVDVSSMPAYPLSQMRRLIRENGLLVSRNTLIEIAIKKAAQELGKPELE	77
RLA0_PYRHO	-----MAHYVAENKKKEVEELAKLIKSPYVIALVDVSSMPAYPLSQMRRLIRENGLLVSRNTLIEIAIKKAAQELGKPELE	77
RLA0_PYRFU	-----MAHYVAENKKKEVEELANLIKSPYVIALVDVSSMPAYPLSQMRRLIRENGLLVSRNTLIEIAIKKAAQELGKPELE	77
RLA0_PYRKO	-----MAHYVAENKKKEVEELANLIKSPYVIALVDVSSMPAYPLSQMRRLIRENGLLVSRNTLIEIAIKKAAQELGKPELE	76
RLA0_HALMA	MSAESERKTETIPEWQEEVDIVMIESYESGVYVNIAGIPRGLDMRDLHGT-AELVSRNTLIEIAIKKAAQELGKPELE	79
RLA0_HALVO	MSSEVSRQTEVIPQWKREEVDIVFIESYESGVYVNIAGIPRGLDMRDLHGT-AELVSRNTLIEIAIKKAAQELGKPELE	79
RLA0_HALSA	MSAEQRTEETEEVPEWQRQVAYELVDILETDSYGVYVNIAGIPRGLDMRDLHGT-AELVSRNTLIEIAIKKAAQELGKPELE	79
RLA0_THEAC	-----MKESVQKKELVNEITQIKASRSVAIVDTAGIRTRQIDIRGKNGRK-INLVKIKTLIFKALENLGD--EKLS	72
RLA0_THEVO	-----MRKINPKKEIVSELAQDITKSKAVAIVDIKGVRTRQIDIRAKNHDK-VKIKVVKTLIFKALDSIND--EKLT	72
RLA0_PICTO	-----MTPEAQWKIDFVKNLENEINRKKVAAIVSIKELRNNTFKIKNSIRDK-ARIKVRARLIRLALENLGG--NNIV	72
ruler	1.....10.....20.....30.....40.....50.....60.....70.....80.....90	

Parsing MSAs: AlignIO

The function `Bio.AlignIO.parse()` returns an iterator of `MultipleSeqAlignment` objects that is a collection of `SeqRecords`.

In the frequent case that we have to deal with a single multiple alignment we will have to use the `Bio.AlignIO.read()` function.

The basic syntax of the two functions:

```
Bio.AlignIO.parse(file_handle, alignment_format)
Bio.AlignIO.read(file_handle, alignment_format)
```

where `file_handle` is the handler to the opened file, while the `alignment_format` is a lower case string with the alignment format (e.g. fasta, clustal, stockholm, mauve, phylip,...).

```
from Bio import AlignIO

alignments = AlignIO.read("file_samples/PF02171_seed.sth", "stockholm")

for align in alignments:
    start = align.annotations["start"]
    end = align.annotations["end"]
    seq = align.seq
    desc = align.description
    dbref = ",".join([x for x in align.dbxrefs])
    print("{} S:{} E:{}".format(desc, start, end))
    if (len(dbref) > 0):
        print(dbref)
    print("{}".format(seq))
    print("")
```

```
AG01 SCHPO/500-799 S:500 E:799
YLFFILDK-NSPEP-YGSIKRVcntmLGVPsQCAISKHILQS-----KPQYCANLGMKINVKVGGIN-CSLIPKSNP----L

AG06 ARATH/541-851 S:541 E:851
FILCILPERKTSDI-YGPWKKICLTEEGIHtQCICPIKI-----SDQYLTnVLLKINSKLGGIN-SLLGIEYSYNIPLI

AG04 ARATH/577-885 S:577 E:885
FILCVLPDKKNSDL-YGPWKKKNLTEFGIVtQCMApTRQPND-----QYLTnLLKINAKLGGln-SMLSVERTPAFTVI

TAG76 CAEEL/660-966 S:660 E:966
CIIVVLQS-KNSDI-YMTVKEQSDIVHGIMSQCvLMKNVSRP-----TPATCANIVLKLNMKGGIN--SRIVADKITNKYL
```

Writing and converting MSAs

Biopython provides a function `Bio.AlignIO.write()` to write alignments to file and

`Bio.AlignIO.convert()` to convert one format into the other (provided that all information needed for the second format is available)

```
N = Bio.AlignIO.write(alignments, outfile, file_format)
```

where `alignments` are a `MultipleSeqAlignment` object with the alignments to write to the output file with name `outfile` that has format `file_format` (a low case string with the file format). `N` is the number of entries written to the file.

Ex.

```
my_alignments = [align1, align2, align3]
N = AlignIO.write(my_alignments, "file_samples/my_malign.phy", "phylip")
```

```
Bio.AlignIO.convert(input_file, input_file_format, output_file, output_file_format)
```

basically by passing the input file name and format and output file name and format.

Ex:

```
Bio.AlignIO.convert("PF05371_seed.sth", "stockholm", "PF05371_seed.aln", "clustal")
```


Example: Convert the seed alignment of the [Piwi \(PF02171\)](#) family stored in the pfam (stockholm) format [PF02171_seed.sth](#) into phylip format. Print some stats on the data.

N. of seq: 16
 Len of seq: 395
 1 multiple alignments converted to phylip

```
# STOCKHOLM 1.0
#=GS AG01_SCHPO/500-799 AC 074957.1
#=GS AG06_ARATH/541-851 AC 048771.2
#=GS AG04_ARATH/577-885 AC 092VDS.2
#=GS TAG76_CAEL/660-966 AC P34681.2
#=GS 016720_CAEL/566-867 AC 016720.2
#=GS 062275_CAEL/594-924 AC 062275.1
#=GS YQ53_CAEL/650-977 AC 009249.1
#=GS NRDE3_CAEL/673-1001 AC 021691.1
#=GS Q17567_CAEL/397-708 AC 017567.1
#=GS AUB_DROME/555-852 AC 076922.1
#=GS PIWI_DROME/538-829 AC 09VKM1.1
#=GS PIWL1_HUMAN/555-847 AC 096394.1
#=GS PIWI_ARCFU/110-406 AC 028951.1
#=GS PIWI_ARCFU/110-406 DR PDB: 2W42 B; 110-406;
#=GS PIWI_ARCFU/110-406 DR PDB: 1YTU B; 110-406;
#=GS PIWI_ARCFU/110-406 DR PDB: 2BGG B; 110-406;
#=GS PIWI_ARCFU/110-406 DR PDB: 1W9H A; 110-406;
#=GS PIWI_ARCFU/110-406 DR PDB: 2BGG A; 110-406;
#=GS PIWI_ARCFU/110-406 DR PDB: 1YTU A; 110-406;
#=GS PIWI_ARCFU/110-406 DR PDB: 2W42 A; 110-406;
#=GS Y1321_METJA/426-699 AC 058717.1
#=GS 067434_AQUAE/419-694 AC 067434.1
#=GS 067434_AQUAE/419-694 DR PDB: 1YVU A; 419-694;
#=GS 067434_AQUAE/419-694 DR PDB: 2F8S A; 419-694;
#=GS 067434_AQUAE/419-694 DR PDB: 2F8T A; 419-694;
#=GS 067434_AQUAE/419-694 DR PDB: 2F8S B; 419-694;
#=GS 067434_AQUAE/419-694 DR PDB: 2NUB A; 419-694;
#=GS 067434_AQUAE/419-694 DR PDB: 2F8T B; 419-694;
#=GS AG010_ARATH/625-946 AC 09XGW1.1
AG01_SCHPO/500-799
YLFFILDK..NSPEP..YGSIKRVCNTMLGVPSQCAISKHILQS.....KPQYCANLGMKINVKGGIN..CSLIPKSNP....LGNVPTL.....ILGGDVYHPG|
AG06_ARATH/541-851
FILCILPERKTSOI..YGPWKKICLTEEGIHTQCICPIKI.....SDQYLTNVLLKINSKLGGIN..SLLGIEVSYNIPLINKIPTL.....TLGMDVSHGPF
AG04_ARATH/577-885
FILCVLPDKKNSDL..YGPWKKKNLTFEGIVTQCMAPTRQPN.....QYLTNLLKINAKLGGN..SMLSVERTPAFTVISKVPTI.....ILGMDVSHGPF
TAG76_CAEL/660-966
CIIIVLQS..KNSDI..YMTVKEQSDIVHGIMSQCVLMKNVSRP.....TPATCANIVLKLNMKGGIN..SRVADKITNKYLVDPQTH.....VVGIDVTHTP|
016720_CAEL/566-867
LIVVVLPG..-KTPI..YAEVKRVGDTVLGIATQCVQAKNAIRT.....
062275_CAEL/594-924
TFVFIITD..DSITT..LHQRKYMIEKDTKMIQVQDMKLSKALSV..-IN---A
DILVGIAR..EKKPD..VHDILKYFEESIGLQTIQLCQQTVDKMMGG---Q
TIVFGIIA..EKRPD..MHDILKYFEELKQQTIQISSSETADKFMRD---H
MLVVMLAD..DNKTR..YDSLKKYLCVCEPIPNQCVNLRRLAGKSKDGENK
IVMVVMRS..PNEEK..YSCIKKRTCVDRPVPSQVVTLLKVIAPRQKQP---T
LILCLVPN..DNAER..YSSIKKRGYVDRAVPTQVVTLLKTTKNRSL-----
IVVCLLSS..NRKDK..YDAIKKYLCTDCPTPSQCVVARTLGKQQT-----
GIMLVLPE..YNTPL..YYKLKSYLINS..-IPSQFMRYDILSNRNL-----
CFALITGKEKYKNDYYEILKKQLFDLKIIISQNILWENWRKDDK-----
LVIVFLIEEYPKVDP..YKSFLLYDFVKRELLKKMIPSVQILNRTLKN---E
LLAILLPD..NNGSL..YGDCLKRICETELGLISQCLTKHVFKI-----
AG010_ARATH/625-946
AG01_SCHPO/500-799
-KPQYCANLGMKINVKGGIN..CSLIPKSNP....LGNVPTL-----
```



```
from Bio import AlignIO

alignments = AlignIO.read("file_samples/PF02171_seed.sth", "stockholm")

out = AlignIO.convert("file_samples/PF02171_seed.sth",
                      "stockholm",
                      "file_samples/PF05371_seed.aln",
                      "clustal")

print("N. of seq: {}\nLen of seq: {}".format(
    len(alignments),
    len(alignments[0])))

print("{} multiple alignments converted to phylip".format(out))
```

CLUSTAL X (1.81) multiple sequence alignment

```
AG01_SCHPO/500-799      YLFFILDK..NSPEP..YGSIKRVCNTMLGVPSQCAISKHILQS-----
AG06_ARATH/541-851      FILCILPERKTSOI..YGPWKKICLTEEGIHTQCICPIKI-----
AG04_ARATH/577-885      FILCVLPDKKNSDL..YGPWKKKNLTFEGIVTQCMAPTRQPN-----
TAG76_CAEL/660-966      CIIIVLQS..KNSDI..YMTVKEQSDIVHGIMSQCVLMKNVSRP-----
016720_CAEL/566-867      LIVVVLPG..-KTPI..YAEVKRVGDTVLGIATQCVQAKNAIRT-----
062275_CAEL/594-924      TFVFIITD..DSITT..LHQRKYMIEKDTKMIQVQDMKLSKALSV..-IN---A
YQ53_CAEL/650-977      DILVGIAR..EKKPD..VHDILKYFEESIGLQTIQLCQQTVDKMMGG---Q
NRDE3_CAEL/673-1001      TIVFGIIA..EKRPD..MHDILKYFEELKQQTIQISSSETADKFMRD---H
Q17567_CAEL/397-708      MLVVMLAD..DNKTR..YDSLKKYLCVCEPIPNQCVNLRRLAGKSKDGENK
AUB_DROME/555-852      IVMVVMRS..PNEEK..YSCIKKRTCVDRPVPSQVVTLLKVIAPRQKQP---T
PIWI_DROME/538-829      LILCLVPN..DNAER..YSSIKKRGYVDRAVPTQVVTLLKTTKNRSL-----
PIWL1_HUMAN/555-847      IVVCLLSS..NRKDK..YDAIKKYLCTDCPTPSQCVVARTLGKQQT-----
PIWI_ARCFU/110-406      GIMLVLPE..YNTPL..YYKLKSYLINS..-IPSQFMRYDILSNRNL-----
Y1321_METJA/426-699      CFALITGKEKYKNDYYEILKKQLFDLKIIISQNILWENWRKDDK-----
067434_AQUAE/419-694      LVIVFLIEEYPKVDP..YKSFLLYDFVKRELLKKMIPSVQILNRTLKN---E
AG010_ARATH/625-946      LLLAILPD..NNGSL..YGDCLKRICETELGLISQCLTKHVFKI-----

AG01_SCHPO/500-799      -KPQYCANLGMKINVKGGIN..CSLIPKSNP....LGNVPTL-----
```

Manipulating/writing MSA

It is possible to slice alignments using the `[]` operator applied on a `SeqRecord`.

Think about it as a matrix

1. `SeqRecord[i, j]` returns the *j*th character of alignment *i* as a string;
2. `SeqRecord[:, j]` returns all the *j*th characters of the multiple alignment as a string;
3. `SeqRecord[:, i:j]` returns a `MultipleSeqAlignment` with the sub-alignments going for *i* to *j* (excluded)
4. `SeqRecord[a:b, i:j]` similar to 3. but for alignments going from *a* to *b* (excluded) only

```
YLFFILDK-NSPEP-YGSIKLVPPVYYAHLVSNLARYQDV
FILCILPERKTS DI - YGPWKIVAPVRYAHLAAAQVAQFTK
FILCVLPDKKNSDL - YGPWKVVAPICYAHLAAAQLGTFMK
CIIVVLQS-KNSDI - YMTVKIPTPVYYADLVATRARCHVK
LIVVVLPG--KTPI - YAEVKIPAPAYYAHLVAFRARYHLV
TFVFIITD-DSITT-LHQRYLPTPLYVANEYAKRGRNLWN
DILVGIAR-EKKPD-VHDILVPDVLAAENLAKRGRNNYK
TIVFGIIA-EKRPD-MHDILIPNVSYAAQNLAKRGHNNYK
MLVVMLAD-DNKTR-YDSLKVPAPCQYAHKLAFLTAQSLH
IVMVVMRS-PNEEK-YSCIKVPAVCHYAHKLAFLVAESIN
LILCLVPN-DNAER-YSSIKVPAVCQYAKKLATLVGTNLH
IVVCLLSS-NRKDK-YDAIKVPAPCQYAHKLAFLVGQSIH
GIMLVLPE-YNTPL-YYKLKLPVTVNYPKLVAGIIANVNR
CFALIIGKEKYKDNDYYEILIPAPIHYADKFVKALGKNWK
LVIVFLEEYPKVDP-YKSFLLPATVHYSKITKLMLRGIE
LLLAILPD-NNGSL-YGDLKIVPPAYYAHLAAFRARFYLE
```

`align[0,0]` is Y

`align[2,1]` is I

`align[:,0]` is YFFCLTDTMILIGCLL

`align[:,0:3]` gets first 3 rows (SeqRecords)

YLFFILDK-N...

FILCILPERK...

FILCVLPDK...

`align[0:3,0:3]` first 3 cols of first 3 rows (SeqRecords):

YLF

FIL

FIL

Pairwise alignment

Biopython has its own module to make pairwise alignment. It provides two algorithms: [Smith-Waterman](#) for local alignment and [Needleman-Wunsch](#) for global alignment. These methods are implemented in two Biopython functions of the `Bio.pairwise2` module:

```
pairwise2.align.globalxx()  
pairwise2.align.localxx()
```

Example:

```
alignments = pairwise2.align.globalxx("ACCGTTATATAGGCCA", "ACGTACTAGTATAGGCCA")  
for i in range(len(alignments)):  
    print(alignments[i])
```

```
('ACCGT--TA-TATAGGCCA', 'A-CGTACTAGTATAGGCCA', 15.0, 0, 19)  
('ACCGT--TA-TATAGGCCA', 'AC-GTACTAGTATAGGCCA', 15.0, 0, 19)
```

```
aligns = pairwise2.align.globalxx(seq1, seq2)  
aligns = pairwise2.align.localxx(seq1, seq2)
```

where `seq1` and `seq2` are two `str` objects. These methods return a list of alignments (at least one) that have the same **optimal score**. Each alignment is represented as tuples with the following 5 elements in order:

1. The alignment of the first sequence;
2. The alignment of the second sequence;
3. The alignment score;
4. The start of the alignment (for global alignments this is always 0);
5. The end of the alignment (for global alignments this is always the length of the alignment).

Pairwise alignment

OPTIONS FOR MATCHES/MISMATCHES AND GAP OPENS/EXTENSIONS

```
pairwise2.align.globalxx  
pairwise2.align.globalmx  
pairwise2.align.globalms  
pairwise2.align.globalmd  
pairwise2.align.globalxd  
pairwise2.align.localxx  
pairwise2.align.localmx  
pairwise2.align.localms  
pairwise2.align.localmd  
pairwise2.align.localxd  
pairwise2.align.localxs
```

Match parameters can be:

- `x` : means that a match scores 1 a mismatch 0;
- `m` : the match and mismatch score are passed as additional params after the sequence (es. `aligns = pairwise2.align.globalmx(seq1,seq2, 1, -1)` to set 1 as match score and -1 as mismatch penalty).

Gap parameters can be:

- `x` : gap penalty is 0;
- `s` : same gap open and gap extend penalties for the 2 sequences (passed as additional params after seqs).
- `d` : different gap open and gap extend penalties for the 2 seqs (additional params after the seqs).

Pairwise alignment

```
('ACCGT--TA-TATAGGCCA', 'A-CGTACTAGTATAGGCCA', 15.0, 0, 19)
('ACCGT--TA-TATAGGCCA', 'AC-GTACTAGTATAGGCCA', 15.0, 0, 19)
```

```

Looping through aligns
ACCGT--TA-TATAGGCCA
A-CGTACTAGTATAGGCCA
Score: 15.0, Start: 0, End: 19

```

ACCGT - TA-TATAGGCCA
AC-GTACTAGTATAGGCCA
Score: 15.0, Start: 0, End: 19

Match: 1, Mismatch: -1, Gap open: -0.5, Gap extend: -0.2
ACCGT--TA-TATAGGCCA
A-CGTACTAGTATAGGCCA
Score: 13.3, Start: 0, End: 19

ACCGT - -TA-TATAGGCCA
AC-GTACTAGTATAGGCCA
Score: 13.3, Start: 0, End: 19

[illegible]

http://biopython.org



biopython

Python Tools for
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Introduction

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

It is a distributed collaborative effort to develop Python libraries and applications which address the needs of current and future work in bioinformatics. The source code is made available under the [Biopython License](#), which is extremely liberal and compatible with almost every license in the world.

We are a member project of the [Open Bioinformatics Foundation \(OBF\)](#), who take care of our domain name and hosting for our mailing list etc. The OBF used to host our development repository, issue tracker and website but these are now on [GitHub](#).

This wiki will help you download and install Biopython, and start using the libraries and tools.

Get Started	Get help	Contribute
Download Biopython	Tutorial (PDF)	What's being worked on
Installation help (PDF)	Documentation on this wiki	Developing on Github
	Cookbook (working examples)	Google Summer of Code
	Discuss and ask questions	Report bugs (older issues)

The latest release is [Biopython 1.70](#), released on 10 July 2017.

http://biopython.org/DIST/docs/api/

Check:
Seq
SeqRecord
MultipleSeqAlignment

Table of Contents

[Everything](#)

Modules

[Bio](#)

[Bio.Affy](#)

[Bio.Affy.CelFile](#)

[Bio.Align](#)

[Bio.Align.AlignInfo](#)

[Bio.Align.Applications](#)

[Bio.Align.Applications.ClustalOmega](#)

[Bio.Align.Applications.Clustalw](#)

[Bio.Align.Applications.Dialign](#)

[Bio.Align.Applications.MSAProbs](#)

[Bio.Align.Applications.Mafft](#)

Everything

All Classes

[Bio.Affy.CelFile.ParserError](#)

[Bio.Affy.CelFile.Record](#)

[Bio.Align.AlignInfo.PSSM](#)

[Bio.Align.AlignInfo.SummaryInfo](#)

[Bio.Align.Applications.ClustalOmega.ClustalOmegaCommandline](#)

[Bio.Align.Applications.Clustalw.ClustalwCommandline](#)

[Bio.Align.Applications.Dialign.DialignCommandline](#)

[Bio.Align.Applications.MSAProbs.MSAProbsCommandline](#)

[Bio.Align.Applications.Mafft.MafftCommandline](#)

[Bio.Align.Applications.Muscle.MuscleCommandline](#)

[Bio.Align.Applications.Prank.PrankCommandline](#)

[Bio.Align.Applications.Probcons.ProbconsCommandline](#)

[Bio.Align.Applications.TCoffee.TCoffeeCommandline](#)

[Bio.Align.MultipleSeqAlignment](#)

[Bio.AlignIO.ClustalIO.ClustalIterator](#)

[Bio.AlignIO.ClustalIO.ClustalWriter](#)

[Bio.AlignIO.EmbossIO.EmbossIterator](#)

[Bio.AlignIO.EmbossIO.EmbossWriter](#)

[Bio.AlignIO.Interfaces.AlignmentIterator](#)

[Bio.AlignIO.Interfaces.AlignmentWriter](#)

[Bio.AlignIO.Interfaces.SequentialAlignmentWriter](#)

[Bio.AlignIO.MafftIO.MafftIndex](#)

[Bio.AlignIO.MafftIO.MafftWriter](#)

[Bio.AlignIO.MauveIO.MauveIterator](#)

[Bio.AlignIO.MauveIO.MauveWriter](#)

[Bio.AlignIO.NexusIO.NexusWriter](#)

[Bio.AlignIO.PhylipIO.PhylipIterator](#)

[Bio.AlignIO.PhylipIO.PhylipWriter](#)

[Bio.AlignIO.PhylipIO.RelaxedPhyIpIterator](#)

[Bio.AlignIO.PhylipIO.RelaxedPhyIpWriter](#)

[Bio.AlignIO.PhylipIO.SequentialPhyIpIterator](#)

[Bio.AlignIO.PhylipIO.SequentialPhyIpWriter](#)

Trees Indices Help

[\[Module Hierarchy | Class Hierarchy \]](#)

Module Hierarchy

- Bio:** Collection of modules for dealing with biological data in Python.
 - Bio.Affy:** Deal with Affymetrix related data such as cel files.
 - Bio.Affy.CelFile:** Reading information from Affymetrix CEL files version 3 and 4.
 - Bio.Align:** Code for dealing with sequence alignments.
 - Bio.Align.AlignInfo:** Extract information from alignment objects.
 - Bio.Align.Applications:** Alignment command line tool wrappers.
 - Bio.Align.Applications.ClustalOmega:** Command line wrapper for the multiple alignment program Clustal Omega.
 - Bio.Align.Applications.Clustalw:** Command line wrapper for the multiple alignment program Clustal W.
 - Bio.Align.Applications.Dialign:** Command line wrapper for the multiple alignment program DIALIGN2-2.
 - Bio.Align.Applications.MSAProbs:** Command line wrapper for the multiple sequence alignment program MSAProbs.
 - Bio.Align.Applications.Mafft:** Command line wrapper for the multiple alignment programme MAFFT.
 - Bio.Align.Applications.Muscle:** Command line wrapper for the multiple alignment program MUSCLE.
 - Bio.Align.Applications.Prank:** Command line wrapper for the multiple alignment program PRANK.
 - Bio.Align.Applications.Probcons:** Command line wrapper for the multiple alignment program PROBCONS.
 - Bio.Align.Applications.TCoffee:** Command line wrapper for the multiple alignment program TCOFFEE.
 - Bio.AlignIO:** Multiple sequence alignment input/output as alignment objects.
 - Bio.AlignIO.ClustalIO:** Bio.AlignIO support for "clustal" output from CLUSTAL W and other tools.
 - Bio.AlignIO.EmbossIO:** Bio.AlignIO support for "emboss" alignment output from EMBOSS tools.
 - Bio.AlignIO.FastaIO:** Bio.AlignIO support for "fasta-m10" output from Bill Pearson's FASTA tools.
 - Bio.AlignIO.Interfaces:** AlignIO support module (not for general use).
 - Bio.AlignIO.MafftIO:** Bio.AlignIO support for the "ma" multiple alignment format.
 - Bio.AlignIO.MauveIO:** Bio.AlignIO support for "mafa" output from Mauve/ProgressiveMauve.
 - Bio.AlignIO.NexusIO:** Bio.AlignIO support for the "nexus" file format.
 - Bio.AlignIO.PhylipIO:** AlignIO support for "phylip" format from Joe Felsenstein's PHYLIP tools.
 - Bio.AlignIO.StockholmIO:** Bio.AlignIO support for "stockholm" format (used in the PFAM database).
 - Bio.Alphabet:** Alphabets used in Seq objects etc to declare sequence type and letters.
 - Bio.Alphabet.IUPAC:** Standard nucleotide and protein alphabets defined by IUPAC.
 - Bio.Alphabet.Reduced:** Reduced alphabets which lump together several amino-acids into one letter.
 - Bio.Application:** General mechanisms to access applications in Biopython.
 - Bio.Blast:** Code for dealing with BLAST programs and output.
 - Bio.Blast.Applications:** Definitions for interacting with BLAST related applications.
 - Bio.Blast.NCBIStandalone:** Code for calling standalone BLAST and parsing plain text output (DEPRECATED).
 - Bio.Blast.NCBIWWW:** Code to invoke the NCBI BLAST server over the internet.
 - Bio.Blast.NCBIXML:** Code to work with the BLAST XML output.
 - Bio.Blast.ParseBlastTable:** A parser for the NCBI blastpgp version 2.2.5 output format. Currently only supports the '-m 9' option, (table w/ annotations). Returns a BlastTableRec instance
 - Bio.Blast.Record:** Record classes to hold BLAST output.
 - Bio.CAPS:** Cleaved amplified polymorphic sequence (CAPS) markers.
 - Bio.Cluster:** Cluster Analysis.
 - Bio.Cluster.cluster:** C Clustering Library
 - Bio.Compass:** Code to deal with COMPASS output, a program for profile/profile comparison.
 - Bio.Crystal:** Represent the NDB Atlas structure (a minimal subset of PDB format).
 - Bio.Data:** Collections of various bits of useful biological data.
 - Bio.Data.CodonTable:** Codon tables based on those from the NCBI.
 - Bio.Data.IUPACData:** Information about the IUPAC alphabets.
 - Bio.Data.SCOPData:** Additional protein alphabets used in the SCOP database and PDB files.
 - Bio.DocSQL:** Bio.DocSQL: easy access to DB API databases (DEPRECATED).

Installing biopython

```
import Bio
```

```
-----  
ImportError                                Traceback (most recent call last)  
<ipython-input-1-f227b1b7f7f3> in <module>()  
----> 1 import Bio  
  
ImportError: No module named 'Bio'
```

In windows installing Biopython should be as easy as opening the command prompt as administrator (typing `cmd` and then right clicking on the link choosing run as administrator) and then `pip3 install biopython`.

In linux `sudo pip3 install biopython` will install biopython for python3 up to python3.5. On python 3.6, the command is: `python3.6 -m pip install biopython`.

Exercises

1. Write a python function that reads a genebank file given in input and prints off the following information:
 1. Identifier, name and description;
 2. The first 100 characters of the sequence;
 3. Number of external references (dbxrefs) and ids of the external refs.
 4. The name of the organism (hint: check the annotations dictionary at the key "organism")
 5. Retrieve and print all (if any) associated publications (hint: annotation dictionary, key: "references")
 6. Retrieve and print all the locations of "CDS" features of the sequence (hint: check the features)

Hint: go back and check the details of the `SeqRecord` object.

Test the program downloading some files from genebank like [this](#)

Show/Hide Solution

2. Write a python program that loads a pfam file (stockholm format .sth) and reports for each record of the alignment:
 1. the id of the entry
 2. the start and end points
 3. the number of gaps and the % of gaps on the total length of the alignment
 4. the number of external database references (dbxrefs), and the first 3 external references comma separated (hint: use join).

Print these information to the screen. Finally, write this information in a tab separated file (.tsv) having the following format: `#ID\tstart\tend\tnum_gaps\tpercentage_gaps\tbdbxrefs`.