Biopython Work with biological sequence data in Python

Alexander McFarland

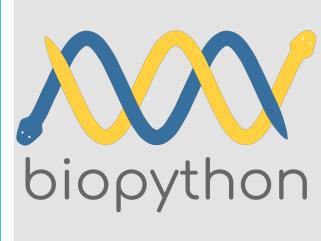
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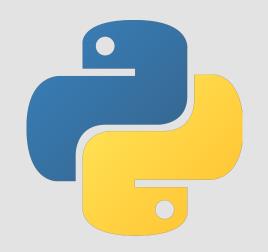
Northwestern University

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Biopython Work with biological sequence data in Python is brought to you by NUIT Research Computing Services.

Have a programming or data question about your research? We're here to help. bit.ly/rcsconsult





Running the workshop code

The contents of this workshop are available at

https://github.com/agmcfarland/biopython_workshop

Please use look over the contents of the README in github

Two ways to run the code:

- Open the main github directory in Google Colab and select the notebook (.ipynb) you wish to run (easy)
- 2. Clone the repository, go to the repository directory, open the notebook you wish to run.
 - This assumes you have a way of running a jupyter notebook already set (VScode, JupyterLab (anaconda)

Biopython is designed to work with biological sequences and their formats

- Biological sequences are DNA, RNA, and amino acids
- When working with more than a handful of sequence, manual editing becomes inefficient and time-consuming
 - Manual work can become error prone and irreproducible
- Biopython is a Python package that is built to interact with all types of sequences found in formats used by biologists, including
 - Fasta (.fasta)
 - GenBank file-format (.gbk)
- Biopython can help to make analyses efficient and reproducible

By the end of Day 3 you will know how to do all these things!

Biopython can help overcome many everyday sequence challenges

Remove the * at the end of each sequence and calculate GC content

>4_UTYA01000022_02838

MNLVGKRGVVLGVLNKKSIAAACASKLMSEGAEVICSYLPVKGDEERRHALASRAVSGLP SNYMLPCDVTSDESVKAFFDGVKDIFGSIDFIVHGVSLIPSEASVGNLVELPREAFIASM NVSVYSLILISKCAKSLMPKGGSILTFSYLSADALVPGYELLGICKAALQTSVSYLAFDL SKENIRVNVLSAPPFPSSSAIGHTAYGELSDTYSKKLQPTGTPSVNEILNVAIFLISDNS IGVTGDRIFVDGGFHNMSAAI*

>77 LT629780 01324

MDRINSLAGKKGLIVGIANDNSIAYGCARVLKSLGAEFAVTYLNEKAERFVRPLAEELES PIIAQMDVEKPGELEAVFRSIEETWGKLDFVIHSIAFCPMDDLHGRVTDCSKEGFLQAMG VSCYSLIEMARLAEPLMKDGGSIITMSYYGADKVVENYNVMGPVKAALESTVRYLAAELG QQRIRVHAVSPGPLKTRAASGIAHFDKLIEEAIERTPQHRLVDIEDVGMTAAFLISDASR AITGEVIYVDGGFHMMA*

>1 NRAU01000010 00778

MSIKESLSLAGKRGLVVGIANPHSIAWGCAQALHDMGAELAVTWLNDKARVHVEPLAQQV HASVRMPLDVTRAGELDALFEHLAVQWGSLDFVVHCLASAPKEELRGRLLDSSSSGFLQA VDISCHSFIRMARLAEPLMPRGGSLVTMSYLGAQETIEGYALMGPVKAALEASVRYLATE LGPRNIRVHAISPGPMPTRAASGLKDFDHLLETSTNRAPLRRLVTLEEVGGLCAWLVSNA SQGQTGGVHFVDGGLNILG*

Rename headers to gene name and species, count the number of times a genus is found

>gb|CDF47262.1|+|cfr(B) [Clostridioides difficile]
MQQKNKYIRIQEFLKQNKFPNYRMKQITNAIFPGRINNFNEITVLPKSLRDMLIEEFGESIL
VNMKYKAGWESFCISSQCGCNFGCKFCATGDIGLKRNLTSDEITDQILYFHLQGHSIDSISF
PRRLSISTIGIIPNIKKLTQNYPQVNLTFSLHSPFNEQRSELMPINERYPLSDVMDTLDEHI
NLLRGRYRSGNLYHVNIIRYNPTVSSRMRFEEANEKCLVNFYKELKSAGIKVTIRSQFGIDI
>gb|BAH45481.1|-|clbB [Brevibacillus brevis NBRC 100599]
MKLTSKYETIRRILSECKQPEYRYAQIMDAIFKQNIGEYERMTILPKFLRDELNRILGPNVC
VRLTYERGWKSYCISTQCGCGFRCKFCATGTIGLKRNLTADEITDQLLYFRLNGHSLDSISF
HRRITISTIGLLPGIDKLTREFPQVNLTFSLHSPFDDQRSELMPINDRFPVRDVLIALDRHI
ELLRGRGAWEHLYHVNLIPFNSTEVTPDSYRQSDPSRIKAFVRILKSRGISVTVRTQFGSDI
>gb|ACX65640.1|-|cipA [Paenibacillus sp. Y412MC10]
MKYLSKYEKIRKILSALNQPNYRYSQITEAIFKNKIGNFEAMNNLPKPVRNELIKELGNNVL
VRLSYQTGWESYCISSQCGCGFGCTFCATGTLGLKRNLTTDEITDQLLYFTLNHPLDSVSF
HRRITVSTIGLLPGVKKLTKEFPQINLTFSLHSPFHDQRSELMPINNHFPLEEVMTVLDEHI
DLLRERGSWEHLYHVNLIPYNSTDATSQSFVESDQNSINMFLRILKSKGIHVTVRTQFGSDI

Extract specific gene names and associated sequences

```
complement(2118936..2119730)
                /gene="pduF"
                /locus_tag="AV88_RS10350"
                /old locus tag="AV88 11535"
                /inference="COORDINATES: similar to AA
                sequence:RefSeq:NP 460982.1"
                /note="Derived by automated computational analysis using
                gene prediction method: Protein Homology."
                /codon start=1
                /transl table=11
                /product="propanediol diffusion facilitator PduF"
                /protein_id="WP_001000023.1"
                /translation="MNDSLKAQCGAEFLGTGLFLFFGIGCLSALKVAGASLGLWEICI
                IWGLGISLAVYLTAGISGGHLNPAVTIALWLFACFPKQKVLPYIIAQFAGAFGGALLA
                YVLYSSLFTEFETAHHMVRGSVESLOLASIFSTYPAAALNVWOAALVEVVITSILMGM
                IMALTDDGNGIPKGPLAPLLIGILVAVIGASTGPLTGFAMNPARDFGPKLFTWLAGWG
                NMAMSGGREIPYFIVPIVAPVIGACAGAAIYRYFIGKNLPCNRCEL"
                2120255..2120539
                /gene="pduA"
                /locus_tag="AV88_RS10355"
                /old locus tag="AV88 11540"
CDS
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                /gene="pduA"
                /locus_tag="AV88_RS10355"
                /old_locus_tag="AV88_11540"
                /inference="COORDINATES: similar to AA
                sequence: RefSeq:NP 460983.1"
                /note="Derived by automated computational analysis using
                gene prediction method: Protein Homology."
                /codon start=1
                /transl table=11
                /product="propanediol utilization microcompartment protein
                /protein_id="WP_001183618.1"
                /translation="MOOEALGMVETKGLTAAIEAADAMVKSANVMLVGYEKIGSGLVT
                VIVRGDVGAVKAATDAGAAAARNVGEVKAVHVIPRPHTDVEKILPKGISO'
                2120536..2121348
                /gene="pduB"
                /locus_tag="AV88_RS10360"
                /old locus tag="AV88 11545"
                2120536..2121348
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                /locus_tag="AV88_RS10360"
                /old_locus_tag="AV88_11545"
                /inference="COORDINATES: similar to AA
                sequence:RefSeq:YP_005228567.1"
                /note="Derived by automated computational analysis using
                gene prediction method: Protein Homology."
                /codon_start=1
```

Biopython applications covered by this workshop

1. Working with sequences

- Remove certain characters (*)
- Remove first or last 'X' number of nucleotides/amino acids
- Transcribe/translate DNA sequences
- Calculate GC content
- Calculate length of sequences
- Find motifs

2. Modifying headers

- Make headers more readable
- Extract information from headers

3. Extracting and storing sequences

- Write only certain sequences to new file
- Write modified sequences/headers to new file

4. BLAST-ing against the NCBI database

Set homology thresholds and store results

Workshop overview

- Five days of one-hour sessions
 - 4-5 pm July 19-23
- All code is run on a Jupyter notebook
- When necessary, Python basics will be reviewed prior to their use with Biopython
- Focus on writing code that can be adapted to workflows
- <u>Feel free to ask questions/for clarifications in the chat</u> I will read over them during examples and find the best time to address them!

Session outline

- **Monday** Introduction to strings, Biopython, and Biopython sequences
- **Tuesday** Opening, closing, and saving sequence files with Biopython
- 3. Wednesday More sequence modification and data extraction
- 4. Thursday Extracting and storing sequence data, working with GenBank files
- 5. Friday BLAST-ing against the NCBI database

Expected 'easiness'

