Indian Institute of Technology Gandhinagar

BE623 Biocomputing

Sem1 2025-2026

Lab Assignment –2

Linux & Shell Scripting with Biological Data Files

Part 1 - vi Basics & File Editing

1. Open a new file called notes.txt in vi.

- Insert exactly one line of text:

Have a nice day

(Make sure there is no trailing space at the end.)

- Save and exit.

- Verify that the file contains exactly one line and 15 characters.

I tried many times but got the same results yet again for the number of characters as 16 only.

But then with the help of chatgpt and google AI Mode search I got one code which I tried and got the number of characters as 15

I got the reason behind it was the trailing space or new line character which by default gets counted

So we need an extra command to not let it get counted as a character

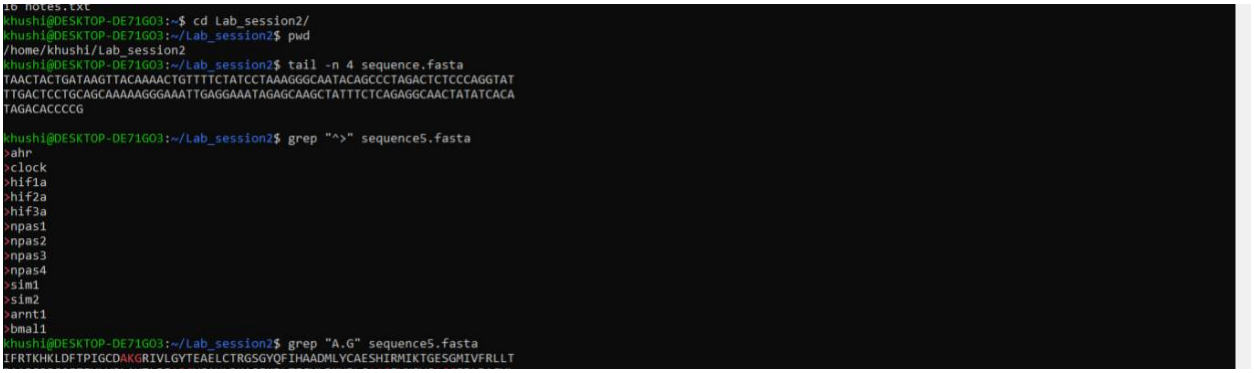
I used the command head -c -1 filename | wc -m file name

In this command they only consider all the characters except of the last one which was supposingly the new line character and I got result as 15.

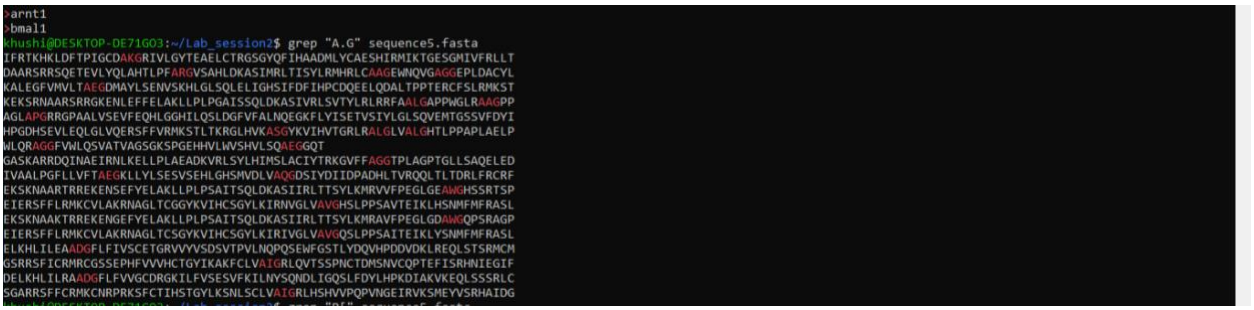
Part 2 - Pattern Matching in FASTA Files

2. Display the last four lines of sequence.fasta without opening the file in an editor.

3. In sequence5.fasta, print all header lines (lines starting with >).

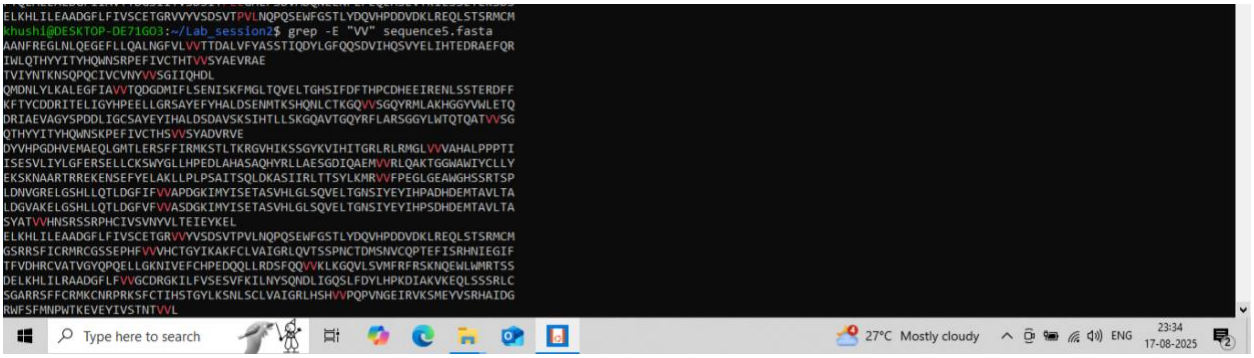


4. Find all matches in sequence5.fasta where A is followed by any single character and then G.

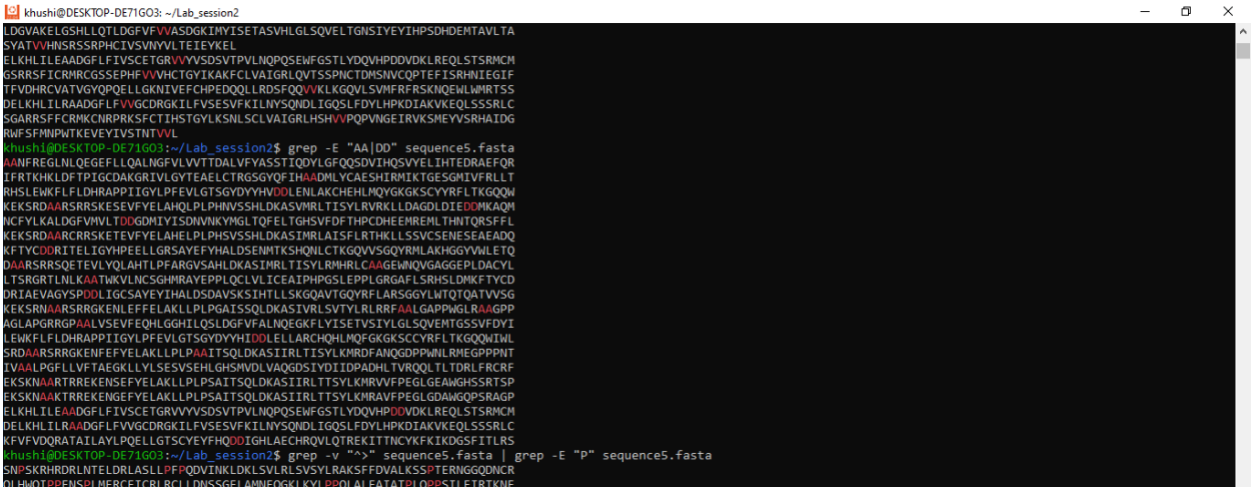


5. Find all matches in sequence5.fasta where P is followed by any character except A, then L.

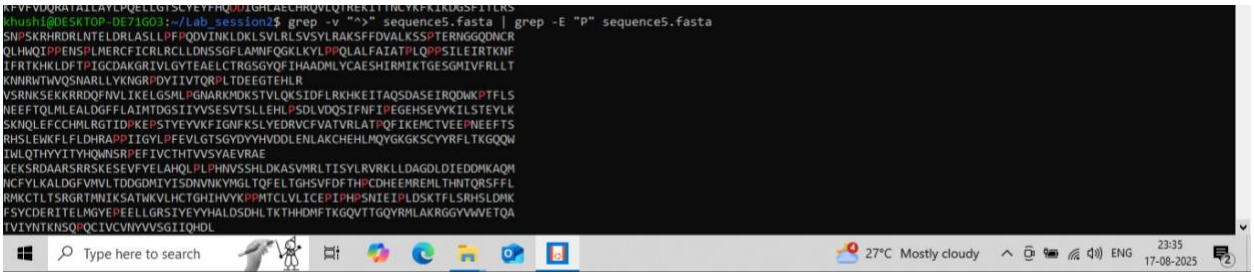
6. Print all lines in sequence5.fasta that have exactly 2 consecutive Vs anywhere in the line.

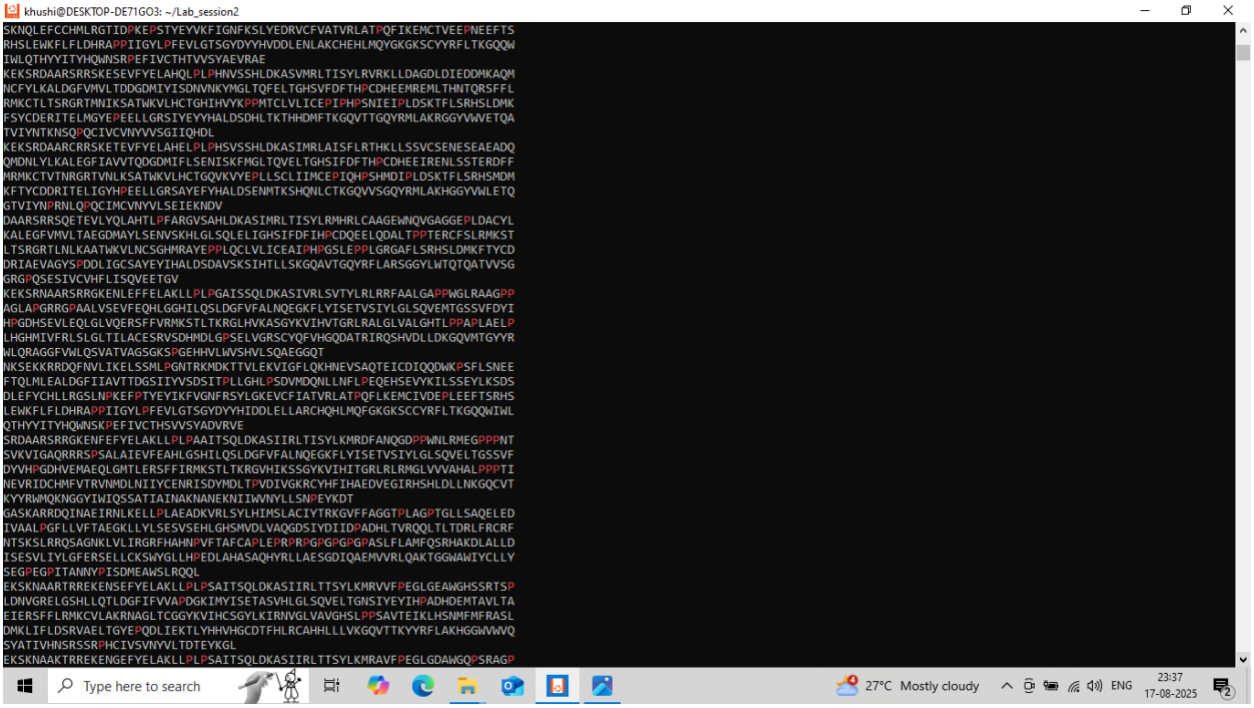


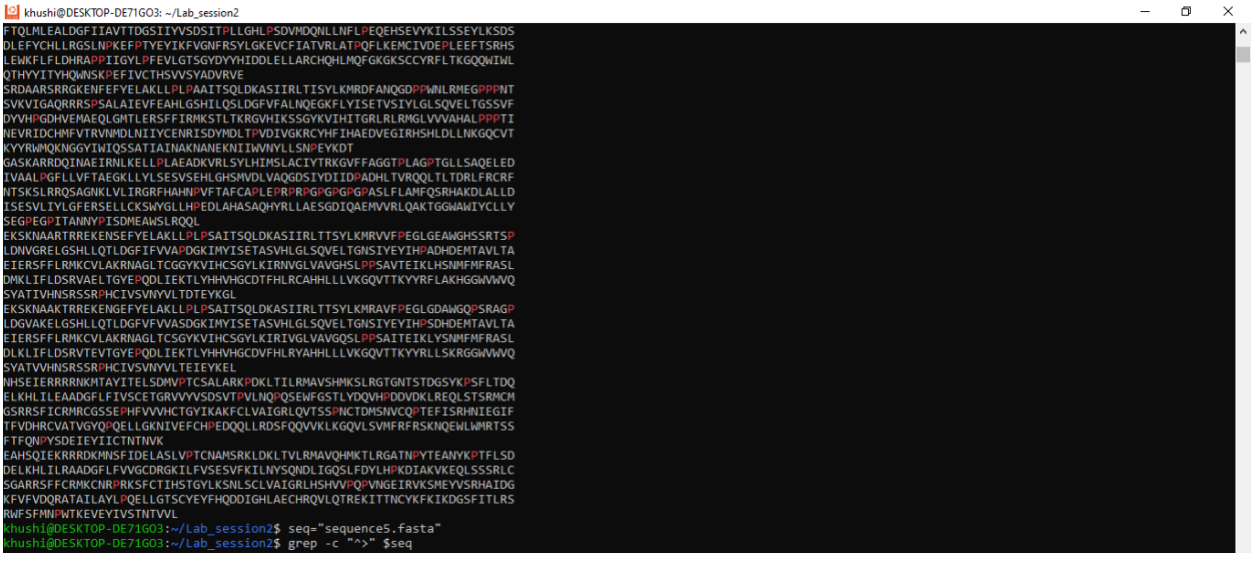
7. Print all lines in sequence5.fasta that contain either AA or DD.



8. Print only the sequence lines (ignore headers) from sequence5.fasta that contain the letter P.

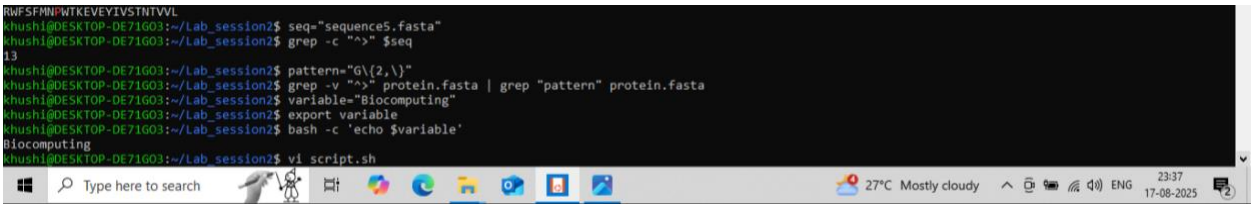



khushi@DESKTOP-DE71GO3: ~/Lab_session2
SKNQLEFCCHMLRGTIDPKEPSTYEYVKFIGNFKSLYEDRVCFVATVRLATPQFIKEMCTVEEPNEEFTS
RHSLEWKFLFLDHRAPPIIGYLPFEVLGTSGYDYYHVDDLENLAKCHEHLMQYGKGKSCYYRFLTKGQQW
IWLQTHYYITYHQWNSRPEFIVCTHTVVSYAEVRAE
KEKSRDAARSRRSKESEVFYELAHQLPLPHNVSSHLDKASVMRLTISYLRVRKLLDAGDLDIEDDMKAQM
NCFYLKALDGFVMVLTDDGDMIYISDNVNKYMGLTQFELTGHSVFDFTHPCDHEEMREMLTHNTQRSFFL
RMKCTLTSRGRTMNIKSATWKVLHCTGHIHVYKPPMTCLVLICEPIPHPSNIEIPLDSKTFLSRHSLDMK
FSYCDERITELMGYEPEELLGRSIYEYYHALDSDHLTKTHHDMFTKGQVTTGQYRMLAKRGGYVWVETQA
TVIYNTKNSQPQCIVCVNYVVSGIIQHDL
KEKSRDAARCRRSKETEVFYELAHELPLPHSVSSHLDKASIMRLAISFLRTHKLLSSVCSENESEAEADQ
QMDNLYLKALEGFIAVVTQDGDMIFLSENISKFMGLTQVELTGHSIFDFTHPCDHEEIRENLSSTERDFF
MRMKCTVTNRGRTVNLKSATWKVLHCTGQVKVYEPLLSCLIIMCEPIQHPSHMDIPLDSKTFLSRHSMDM
KFTYCDDRITELIGYHPEELLGRSAYEFYHALDSENMTKSHQNLCTKGQVVSGQYRMLAKHGGYVWLETQ
GTVIYNPRNLQPQCIMCVNYVLSEIEKNDV
DAARSRRSQETEVLYQLAHTLPFARGVSAHLDKASIMRLTISYLRMHRLCAAGEWNQVGAGGEPLDACYL
KALEGFVMVLTAEGDMAYLSENVSKHLGLSQLELIGHSIFDFIHPCDQEELQDALTPPTERCFSLRMKST
LTSRGRTLNLKAATWKVLNCSGHMRAYEPPLQCLVLICEAIPHPGSLEPPLGRGAFLSRHSLDMKFTYCD
DRIAEVAGYSPDDLIGCSAYEYIHALDSDAVSKSIHTLLSKGQAVTGQYRFLARSGGYLWTQTQATVVSG
GRGPQSESIVCVHFLISQVEETGV
KEKSRNAARSRRGKENLEFFELAKLLPLPGAISSQLDKASIVRLSVTYLRLRRFAALGAPPWGLRAAGPP
AGLAPGRRGPAALVSEVFEQHLGGHILQSLDGFVFALNQEGKFLYISETVSIYLGLSQVEMTGSSVFDYI
HPGDHSEVLEQLGLVQERSFFVRMKSTLTKRGLHVKASGYKVIHVTGRLRALGLVALGHTLPPAPLAELP
LHGHMIVFRLSLGLTILACESRVSDHMDLGPSELVGRSCYQFVHGQDATRIRQSHVDLLDKGQVMTGYYR
WLQRAGGFVWLQSVATVAGSGKSPGEHHVLWVSHVLSQAEGGQT
NKSEKKRRDQFNVLIKELSSMLPGNTRKMDKTTVLEKVIGFLQKHNEVSAQTEICDIQQDWKPSFLSNEE
FTQLMLEALDGFIIAVTTDGSIIYVSDSITPLLGHLPSDVMDQNLLNFLPEQEHSEVYKILSSEYLKSDS
DLEFYCHLLRGSLNPKEFPTYEYIKFVGNFRSYLGKEVCFIATVRLATPQFLKEMCIVDEPLEEFTSRHS
LEWKFLFLDHRAPPIIGYLPFEVLGTSGYDYYHIDDLELLARCHQHLMQFGKGKSCCYRFLTKGQQWIWL
QTHYYITYHQWNSKPEFIVCTHSVVSYADVRVE
SRDAARSRRGKENFEFYELAKLLPLPAAITSQLDKASIIRLTISYLKMRDFANQGDPPWNLRMEGPPPNT
SVKVIGAQRRRSPSALAIEVFEAHLGSHILQSLDGFVFALNQEGKFLYISETVSIYLGLSQVELTGSSVF
DYVHPGDHVEMAEQLGMTLERSFFIRMKSTLTKRGVHIKSSGYKVIHITGRLRLRMGLVVVAHALPPPTI
NEVRIDCHMFVTRVNMDLNIIYCENRISDYMDLTPVDIVGKRCYHFIHAEDVEGIRHSHLDLLNKGQCVT
KYYRWMQKNGGYIWIQSSATIAINAKNANEKNIIWVNYLLSNPEYKDT
GASKARRDQINAEIRNLKELLPLAEADKVRLSYLHIMSLACIYTRKGVFFAGGTPLAGPTGLLSAQELED
IVAALPGFLLVFTAEGKLLYLSESVSEHLGHSMVDLVAQGDSIYDIIDPADHLTVRQQLTLTDRLFRCRF
NTSKSLRRQSAGNKLVLIRGRFHAHNPVFTAFCAPLEPRPRPGPGPGPGPASLFLAMFQSRHAKDLALLD
ISESVLIYLGFERSELLCKSWYGLLHPEDLAHASAQHYRLLAESGDIQAEMVVRLQAKTGGWAWIYCLLY
SEGPEGPITANNYPISDMEAWSLRQQL
EKSKNAARTRREKENGEFYELAKLLPLPSAITSQLDKASIIRLTTSYLKMRAVFPEGLGDAWGQPSRAGP
LDGVAKELGSHLLQTLDGFVFVVASDGKIMYISETASVHLGLSQVELTGNSIYEYIHPSDHDEMTAVLTA
EIERSFFLRMKCVLAKRNAGLTCSGYKVIHCSGYLKIRIVGLVAVGQSLPPSAITEIKLVSNMFMFRASL
DLKLIFLDSRVTEVTGYEPQDLIEKTLYHHVHGCDVFHLRYAHHLLLVKGQVTTKYYRLLSKRGGWVWVQ
SYATVVHNSRSSRPHCIVSVNYVLTEIEYKEL
NHSEIERRRRNKMTAVITELSDMVPTCSALARKPDKLTILRMAVSHMKSLRGTGNTSTDGSYKPSFLTDQ
ELKHLILEAADGFLFIVSCETGRVVYVSDSVTPVLNQPQSEWFGSTLYDQVHPDDVDKLREQLSTSRMCM
GSRRSFICRMRCGSSEPHFVVVHCTGYIKAKFCLVAIGRLQVTSSPNCTDMSNVCQPTEFISRHNIEGIF
TFVDHRCVATVGYQPQELLGKNIVEFCHPEDQQLLRDSFQQVVKLKGQVLSVMFRFRSKNQEWLWMRTSS
FTFQNPYSDEIEYIICTNTNVK
EAHSQIEKRRRDKMNSFIDELASLVPTCNAMSRKLDKLTVLRMAVQHMKTLRGATNPYTEANYKPTFLSD
DELKHLILRAADGFLFVVGCDRGKILFVSESVFKILNYSQNDLIGQSLFDYLHPKDIAKVKEQLSSSRLC
SGARRSFFCRMKCNRPRKSFCTIHSTGYLKSNLSCLVAIGRLHSHVVPQPVNGEIRVKSMEYVSRHAIDG
KFVFVDQRATAILAYLPQELLGTSCYEYFHQDDIGHLAECHRQVLQTREKITTNCYKFKIKDGSFITLRS
RWFSFMNPWTKEVEYIVSTNTVVL
khushi@DESKTOP-DE71GO3:~/Lab_session2$ seq="sequence5.fasta"
khushi@DESKTOP-DE71GO3:~/Lab_session2$ grep -c "^>" $seq
Type here to search
27°C Mostly cloudy
ENG
23:37
17-08-2025

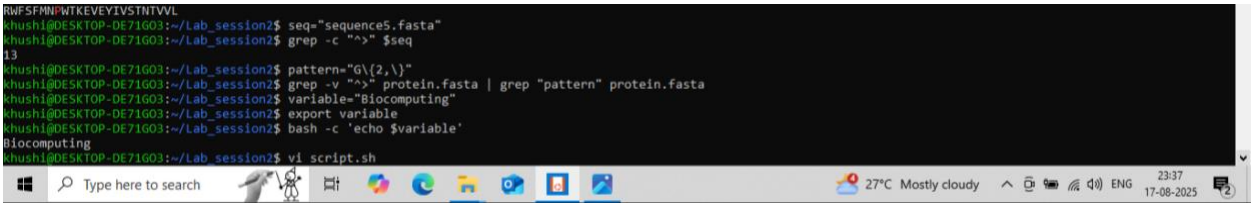

khushi@DESKTOP-DE71GO3: ~/Lab_session2
FTQLMLEALDGFIIAVTTDGSIIYVSDSITPLLGHLPSDVMDQNLLNFLPEQEHSEVYKILSSEYLKSDS
DLEFYCHLLRGSLNPKEFPTYEYIKFVGNFRSYLGKEVCFIATVRLATPQFLKEMCIVDEPLEEFTSRHS
LEWKFLFLDHRAPPIIGYLPFEVLGTSGYDYYHIDDLELLARCHQHLMQFGKGKSCCYRFLTKGQQWIWL
QTHYYITYHQWNSKPEFIVCTHSVVSYADVRVE
SRDAARSRRGKENFEFYELAKLLPLPAAITSQLDKASIIRLTISYLKMRDFANQGDPPWNLRMEGPPPNT
SVKVIGAQRRRSPSALAIEVFEAHLGSHILQSLDGFVFALNQEGKFLYISETVSIYLGLSQVELTGSSVF
DYVHPGDHVEMAEQLGMTLERSFFIRMKSTLTKRGVHIKSSGYKVIHITGRLRLRMGLVVVAHALPPPTI
NEVRIDCHMFVTRVNMDLNIIYCENRISDYMDLTPVDIVGKRCYHFIHAEDVEGIRHSHLDLLNKGQCVT
KYYRWMQKNGGYIWIQSSATIAINAKNANEKNIIWVNYLLSNPEYKDT
GASKARRDQINAEIRNLKELLPLAEADKVRLSYLHIMSLACIYTRKGVFFAGGTPLAGPTGLLSAQELED
IVAALPGFLLVFTAEGKLLYLSESVSEHLGHSMVDLVAQGDSIYDIIDPADHLTVRQQLTLTDRLFRCRF
NTSKSLRRQSAGNKLVLIRGRFHAHNPVFTAFCAPLEPRPRPGPGPGPGPASLFLAMFQSRHAKDLALLD
ISESVLIYLGFERSELLCKSWYGLLHPEDLAHASAQHYRLLAESGDIQAEMVVRLQAKTGGWAWIYCLLY
SEGPEGPITANNYPISDMEAWSLRQQL
EKSKNAARTRREKENSEFYELAKLLPLPSAITSQLDKASIIRLTTSYLKMRVVFPEGLGEAWGHSSRTSP
LDNVGRELGSHLLQTLDGFIFVVAPDGKIMYISETASVHLGLSQVELTGNSIYEYIHPADHDEMTAVLTA
EIERSFFLRMKCVLAKRNAGLTCGGYKVIHCSGYLKIRNVGLVAVGHSLPPSAVTEIKLHSNMFMFRASL
DMKLIFLDSRVAELTGYEPQDLIEKTLYHHVHGCDTFHLRCAHHLLLVKGQVTTKYYRFLAKHGGWVWVQ
SYATIVHNSRSSRPHCIVSVNYVLTDTEYKGL
EKSKNAARTRREKENGEFYELAKLLPLPSAITSQLDKASIIRLTTSYLKMRAVFPEGLGDAWGQPSRAGP
LDGVAKELGSHLLQTLDGFVFVVASDGKIMYISETASVHLGLSQVELTGNSIYEYIHPSDHDEMTAVLTA
EIERSFFLRMKCVLAKRNAGLTCSGYKVIHCSGYLKIRIVGLVAVGQSLPPSAITEIKLVSNMFMFRASL
DLKLIFLDSRVTEVTGYEPQDLIEKTLYHHVHGCDVFHLRYAHHLLLVKGQVTTKYYRLLSKRGGWVWVQ
SYATVVHNSRSSRPHCIVSVNYVLTEIEYKEL
NHSEIERRRRNKMTAVITELSDMVPTCSALARKPDKLTILRMAVSHMKSLRGTGNTSTDGSYKPSFLTDQ
ELKHLILEAADGFLFIVSCETGRVVYVSDSVTPVLNQPQSEWFGSTLYDQVHPDDVDKLREQLSTSRMCM
GSRRSFICRMRCGSSEPHFVVVHCTGYIKAKFCLVAIGRLQVTSSPNCTDMSNVCQPTEFISRHNIEGIF
TFVDHRCVATVGYQPQELLGKNIVEFCHPEDQQLLRDSFQQVVKLKGQVLSVMFRFRSKNQEWLWMRTSS
FTFQNPYSDEIEYIICTNTNVK
EAHSQIEKRRRDKMNSFIDELASLVPTCNAMSRKLDKLTVLRMAVQHMKTLRGATNPYTEANYKPTFLSD
DELKHLILRAADGFLFVVGCDRGKILFVSESVFKILNYSQNDLIGQSLFDYLHPKDIAKVKEQLSSSRLC
SGARRSFFCRMKCNRPRKSFCTIHSTGYLKSNLSCLVAIGRLHSHVVPQPVNGEIRVKSMEYVSRHAIDG
KFVFVDQRATAILAYLPQELLGTSCYEYFHQDDIGHLAECHRQVLQTREKITTNCYKFKIKDGSFITLRS
RWFSFMNPWTKEVEYIVSTNTVVL
khushi@DESKTOP-DE71GO3:~/Lab_session2$ seq="sequence5.fasta"
khushi@DESKTOP-DE71GO3:~/Lab_session2$ grep -c "^>" $seq

Part 3 - Using Variables

9. Store the filename sequence5.fasta in a variable called seq and print the number of sequences in it (headers count as sequences).

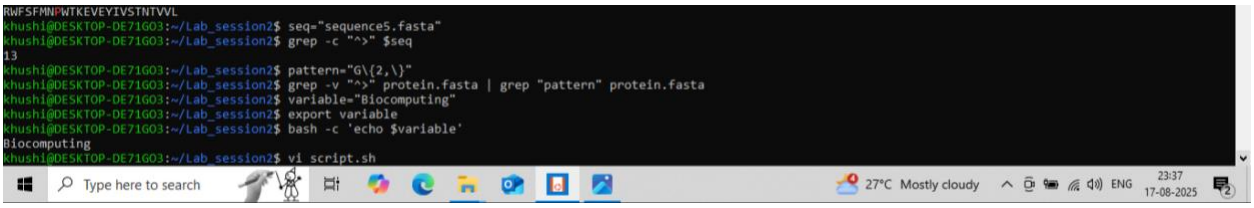


10. Store the pattern G\{2,\} in a variable and search protein.fasta for sequence lines (ignore headers) with 2 or more consecutive Gs.



11. Store "Biocomputing" in a variable, export it, and verify that it is available inside a new shell started using:

bash -c 'echo $VARIABLE_NAME'



Part 4 - File Existence & Loops

12. Write a shell script that checks if sequence3.fasta exists in the current folder. If yes, print the number of lines. If no, print "Missing file".

13. Using a for loop, go through all .fasta files in the current directory and print: filename, number of sequences, and file size in characters.

14. Modify the above loop so that it only prints files with more than 3 sequences.

khushi@DESKTOP-DE71GO3: ~/Lab_session2

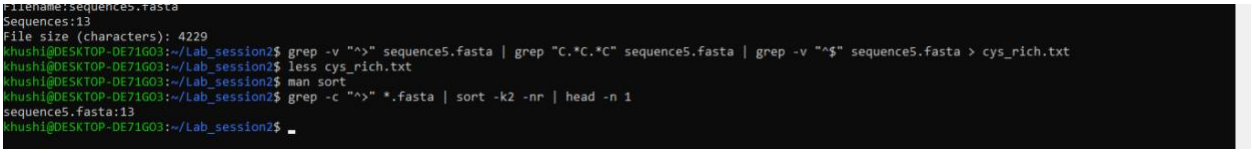
```
#!/bin/bash

if [ -f "sequence3.fasta" ]; then
        wc -l sequence3.fasta
else
        echo "Missing file"
fi


#!/bin/bas

for file in *.fasta; do
        if [ -f "$file" ]; then
                echo "Filename:$file"
                echo "Sequences:$(grep -c "^>" "$file")"
                echo "File size (characters): $(wc -c < "$file")"
        fi
done


#!/bin/bas

for file in *.fasta; do
        if [ -f "$file" ]; then
                seqs=$(grep -c "^>" "$file")
                if [ "$seqs" -gt 3 ]; then
                        echo "Filename:$file"
                        echo "Sequences:$seqs"
                        echo "File size (characters): $(wc -c < "$file")"
                fi
        fi
done

~
~
~
~
~
~
~
~
~
~
"script.sh" 33L, 536B                                                    27,17-38      All
```

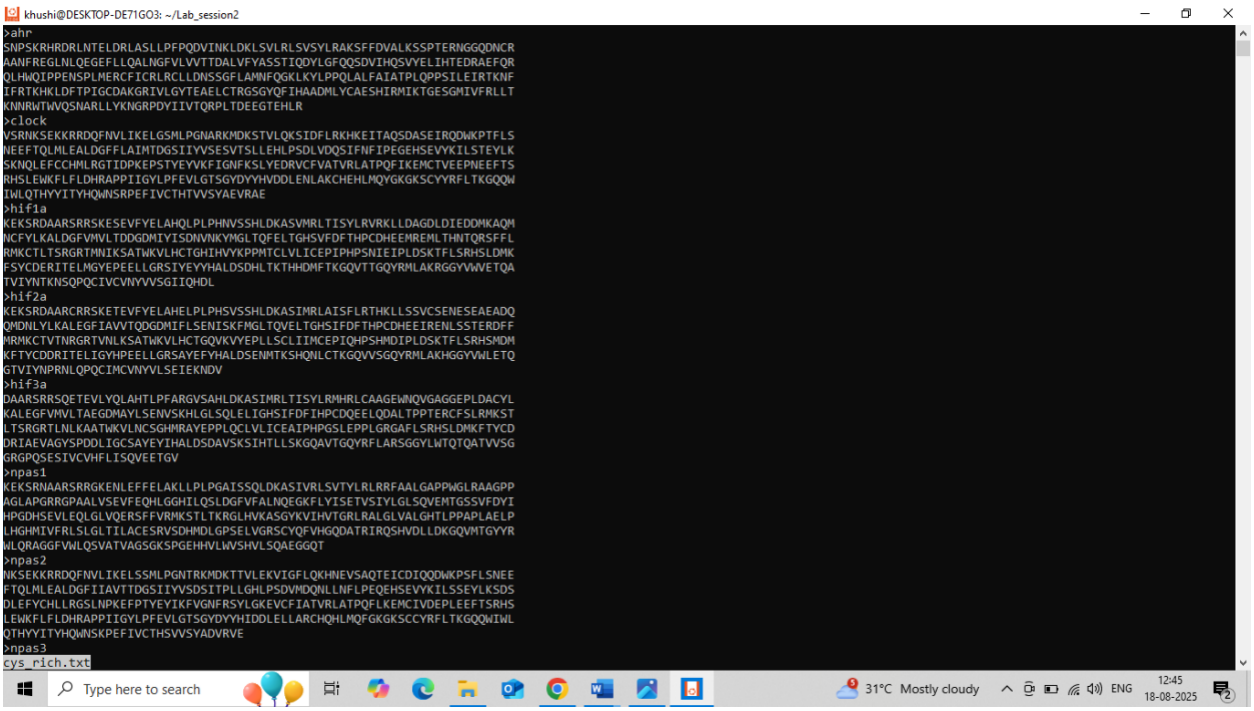
khushi@DESKTOP-DE71GO3: ~/Lab_session2

```
13
khushi@DESKTOP-DE71GO3:~/Lab_session2$ pattern="G\{2,\}"
khushi@DESKTOP-DE71GO3:~/Lab_session2$ grep -v "^>" protein.fasta | grep "pattern" protein.fasta
khushi@DESKTOP-DE71GO3:~/Lab_session2$ variable="Biocomputing"
khushi@DESKTOP-DE71GO3:~/Lab_session2$ export variable
khushi@DESKTOP-DE71GO3:~/Lab_session2$ bash -c 'echo $variable'
Biocomputing
khushi@DESKTOP-DE71GO3:~/Lab_session2$ vi script.sh
khushi@DESKTOP-DE71GO3:~/Lab_session2$ chmod +x script.sh
khushi@DESKTOP-DE71GO3:~/Lab_session2$ ./script.sh
19 sequence3.fasta
Filename:protein.fasta
Sequences:1
File size (characters): 467
Filename:sequence.fasta
Sequences:1
File size (characters): 79551
Filename:sequence1.fasta
Sequences:1
File size (characters): 974
Filename:sequence2.fasta
Sequences:4
File size (characters): 1710
Filename:sequence3.fasta
Sequences:2
File size (characters): 1000
Filename:sequence4.fasta
Sequences:4
File size (characters): 2374
Filename:sequence5.fasta
Sequences:13
File size (characters): 4229
Filename:sequence2.fasta
Sequences:4
File size (characters): 1710
Filename:sequence4.fasta
Sequences:4
File size (characters): 2374
Filename:sequence5.fasta
Sequences:13
File size (characters): 4229
khushi@DESKTOP-DE71GO3:~/Lab_session2$ grep -v "^>" sequence5.fasta | grep "C.*C.*C" sequence5.fasta | grep -v "^$" sequence5.fasta > cys_rich.txt
khushi@DESKTOP-DE71GO3:~/Lab_session2$ less cys_rich.txt
khushi@DESKTOP-DE71GO3:~/Lab_session2$ man sort
```

Part 5 - Applied Data Extraction

15. From sequence5.fasta, extract only the sequence lines (no headers) that contain 3 or more cysteines (C). Save the output to a file named cys_rich.txt. Ensure the output file contains no empty lines.




khushi@DESKTOP-DE71GO3: ~/Lab_session2
>ahr
SNPSKRHRDRLNTELDRLASLLPFPQDVINKLDKLSVLRLSVSYLRAKSFFDVALKSSPTERNGGQDNCR
AANFREGLNLQEGEFLLQALNGFVLVVTTDALVFYASSTIQDYLGFQQSDVIHQSVYELIHTEDRAEFQR
QLHWQIPPENSPLMERCFICRLRCLLDNSSGFLAMNFQGKLKYLPPQLALFAIATPLQPPSILEIRTKNF
IFRTKHKLDFTPIGCDAKGRIVLGYTEAELCTRGSGYQFIHAADMLYCAESHIRMIKTGESGMIVFRLLT
KNNRWTWVQSNARLLYKNGRPDYIIVTQRPLTDEEGTEHLR
>clock
VSRNKSEKKRRDQFNVLIKELGSMLPGNARKMDKSTVLQKSIDFLRKHKEITAQSDASEIRQDWKPTFLS
NEEFTQLMLEALDGFFLAIMTDGSIIYVSESVTSLLEHLPSDLVDQSIFNFIPEGEHSEVYKILSTEYLK
SKNQLEFCCHMLRGTIDPKEPSTYEYVKFIGNFKSLYEDRVCFVATVRLATPQFIKEMCTVEEPNEEFTS
RHSLEWKFLFLDHRAPPIIGYLPFEVLGTSGYDYYHVDDLENLAKCHEHLMQYGKGKSCYYRFLTKGQQW
IWLQTHYYITYHQWNSRPEFIVCTHTVVSYAEVRAE
>hif1a
KEKSRDAARSRRSKESEVFYELAHQLPLPHNVSSHLDKASVMRLTISYLRVRKLLDAGDLDIEDDMKAQM
NCFYLKALDGFVMVLTDDGDMIYISDNVNKYMGLTQFELTGHSVFDFTHPCDHEEMREMLTHNTQRSFFL
RMKCTLTSRGRTMNIKSATWKVLHCTGHIHVYKPPMTCLVLICEPIPHPSNIEIPLDSKTFLSRHSLDMK
FSYCDERITELMGYEPEELLGRSIYEYYHALDSDHLTKTHHDMFTKGQVTTGQYRMLAKRGGYVWVETQA
TVIYNTKNSQPQCIVCVNYVVSGIIQHDL
>hif2a
KEKSRDAARCRRSKETEVFYELAHELPLPHSVSSHLDKASIMRLAISFLRTHKLLSSVCSENESEAEADQ
QMDNLYLKALEGFIAVVTQDGDMIFLSENISKFMGLTQVELTGHSIFDFTHPCDHEEIRENLSSTERDFF
MRMKCTVTNRGRTVNLKSATWKVLHCTGQVKVYEPLLSCLIIMCEPIQHPSHMDIPLDSKTFLSRHSMDM
KFTYCDDRITELIGYHPEELLGRSAYEFYHALDSENMTKSHQNLCTKGQVVSGQYRMLAKHGGYVWLETQ
GTVIYNPRNLQPQCIMCVNYVLSEIEKNDV
>hif3a
DAARSRRSQETEVLYQLAHTLPFARGVSAHLDKASIMRLTISYLRMHRLCAAGEWNQVGAGGEPLDACYL
KALEGFVMVLTAEGDMAYLSENVSKHLGLSQLELIGHSIFDFIHPCDQEELQDALTPPTERCFSLRMKST
LTSRGRTLNLKAATWKVLNCSGHMRAYEPPLQCLVLICEAIPHPGSLEPPLGRGAFLSRHSLDMKFTYCD
DRIAEVAGYSPDDLIGCSAYEYIHALDSDAVSKSIHTLLSKGQAVTGQYRFLARSGGYLWTQTQATVVSG
GRGPQSESIVCVHFLISQVEETGV
>npas1
KEKSRNAARSRRGKENLEFFELAKLLPLPGAISSQLDKASIVRLSVTYLRLRRFAALGAPPWGLRAAGPP
AGLAPGRRGPAALVSEVFEQHLGGHILQSLDGFVFALNQEGKFLYISETVSIYLGLSQVEMTGSSVFDYI
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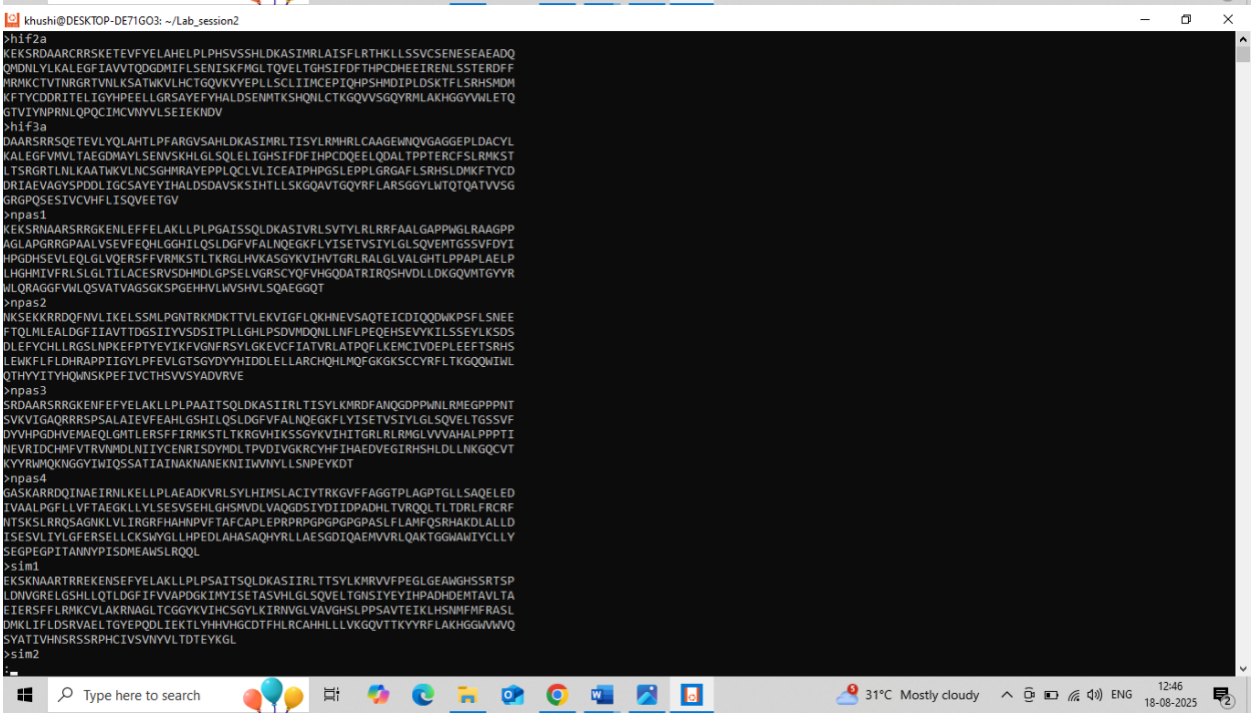
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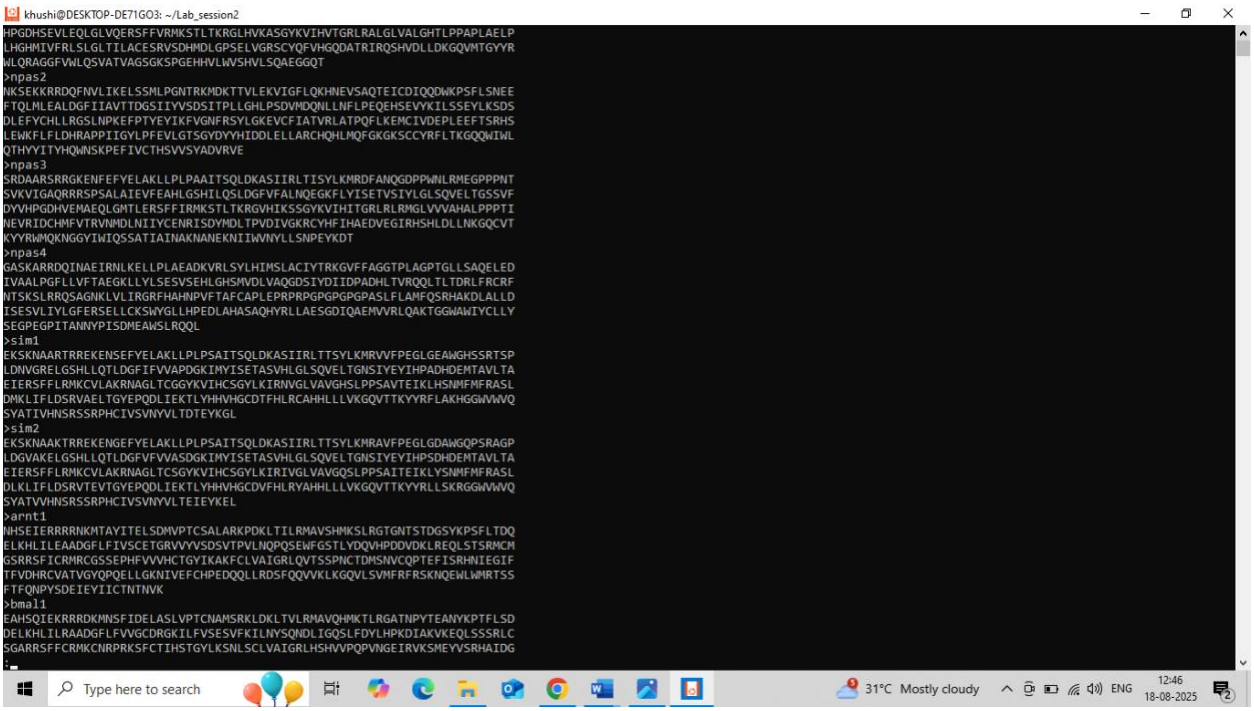


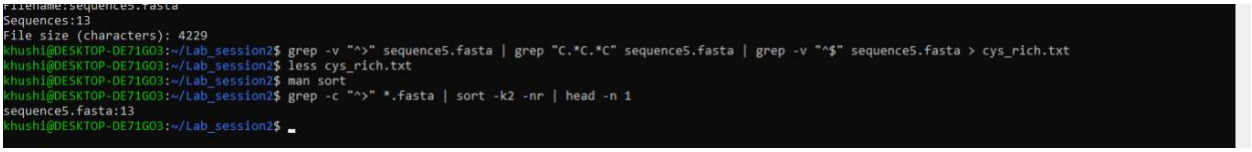
Extra Challenge (Optional)

Write a single shell command that finds the file in the current directory with the largest number of

sequences (by header count) and prints:

<filename> has <count> sequences

Hint: You will likely need wc, grep, sort, and head.



I used google AI Mode search to understand the sort command use in this question then I used command sort -k2 -nr filename from which I understood we use sort to segregate or arrange data. In this command by giving flag -k2 I specified the field which it has to look for to arrange data and by 2 I meant it has to look for 2nd column which has the number of sequences to find the file in the current directory with the largest number of sequences (by header count) then flag -nr I specified to sort numerical data and in reverse/descending order.