Biocomputing

Lab Assignment –2

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. v

```
shreyakathuria@Shreyaa:~/Lab_session2$ wc -m notes.txt
15 notes.txt
shreyakathuria@Shreyaa:~/Lab_session2$ vi notes.txt
shreyakathuria@Shreyaa:~/Lab_session2$ wc -l notes.txt
1 notes.txt
```

Part 2 - Pattern Matching in FASTA Files

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

```
shreyakathuria@Shreyaa:~/Lab_session2$ tail -n 4 sequence.fasta
TAACTACTGATAAGTTACAAAACTGTTTTCTATCCTAAAGGGCAATACAGCCCTAGACTCTCCCAGGTAT
TTGACTCCTGCAGCAAAAAAGGGAAATTGAGGAAATAGAGCAAGCTATTTCTCAGAGGCAACTATATCACA
TAGACACCCCG
shreyakathuria@Shreyaa:~/Lab_session2$ |
```

3. In sequence 5. fasta, print all header lines (lines starting with >).

```
shreyakathuria@Shreyaa:~/Lab_session2$ grep "^>" sequence5.fasta
>ahr
>clock
>hif1a
>hif2a
>hif3a
>npas1
>npas2
>npas3
>npas4
>sim1
>sim2
>arnt1
>bmal1
shreyakathuria@Shreyaa:~/Lab_session2$
```

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.

shreyakathuria@Shreyaa:~/Lab_session2\$ grep 'VV' sequence5.fasta AANFREGLNLQEGEFLLQALNGFVLVVTTDALVFYASSTIQDYLGFQQSDVIHQSVYELIHTEDRAEFQR IWLQTHYYITYHQWNSRPEFIVCTHTVVSYAEVRAE TVIYNTKNSQPQCIVCVNYVVSGIIQHDL QMDNLYLKALEGFIAVVTQDGDMIFLSENISKFMGLTQVELTGHSIFDFTHPCDHEEIRENLSSTERDFF KFTYCDDRITELIGYHPEELLGRSAYEFYHALDSENMTKSHONLCTKGOVVSGOYRMLAKHGGYVWLETO DRIAEVAGYSPDDLIGCSAYEYIHALDSDAVSKSIHTLLSKGQAVTGQYRFLARSGGYLWTQTQAT<mark>VV</mark>SG QTHYYITYHQWNSKPEFIVCTHS<mark>VV</mark>SYADVRVE DYVHPGDHVEMAEQLGMTLERSFFIRMKSTLTKRGVHIKSSGYKVIHITGRLRLRMGL<mark>VV</mark>VAHALPPPTI ISESVLIYLGFERSELLCKSWYGLLHPEDLAHASAQHYRLLAESGDIQAEMVVRLQAKTGGWAWIYCLLY EKSKNAARTRREKENSEFYELAKLLPLPSAITSQLDKASIIRLTTSYLKMRVVFPEGLGEAWGHSSRTSP LDNVGRELGSHLLQTLDGFIFVVAPDGKIMYISETASVHLGLSQVELTGNSIYEYIHPADHDEMTAVLTA LDGVAKELGSHLLQTLDGFVF<mark>VV</mark>ASDGKIMYISETASVHLGLSQVELTGNSIYEYIHPSDHDEMTAVLTA SYATVVHNSRSSRPHCIVSVNYVLTEIEYKEL ELKHLILEAADGFLFIVSCETGR<mark>VV</mark>YVSDSVTPVLNQPQSEWFGSTLYDQVHPDDVDKLREQLSTSRMCM GSRRSFICRMRCGSSEPHF<mark>VV</mark>VHCTGYIKAKFCLVAĬGŘLQVTSSPNCTĎMSNVCQPTEFIŠRHNIEGIF TFVDHRCVATVGYQPQELLGKNIVEFCHPEDQQLLRDSFQQ<mark>VV</mark>KLKGQVLSVMFRFRSKNQEWLWMRTSS DELKHLILRAADGFLF<mark>VV</mark>GCDRGKILFVSESVFKILNYSQNDLIGQSLFDYLHPKDIAKVKEQLSSSRLC SGARRSFFCRMKCNRPRKSFCTIHSTGYLKSNLSCLVAIGRLHSHVVPQPVNGEIRVKSMEYVSRHAIDG **RWFSFMNPWTKEVEYIVSTNTVVL** shreyakathuria@Shreyaa:~/Lab_session2\$

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

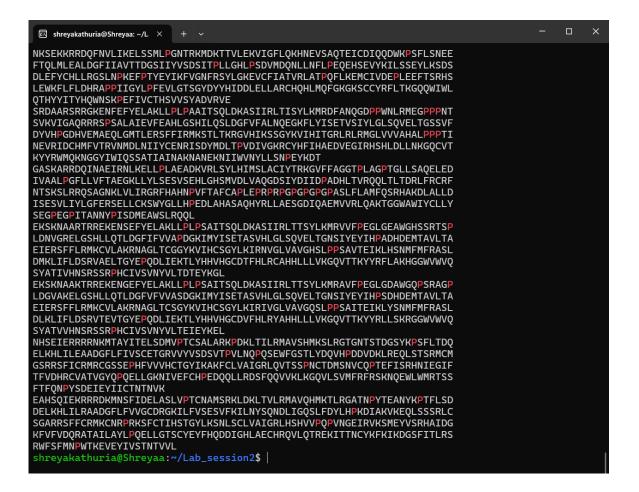
shreyakathuria@Shreyaa:~/Lab_session2\$ egrep 'AA|DD' sequence5.fasta **AANFREGLNLQEGEFLLQALNGFVLVVTTDALVFYASSTIQDYLGFQQSDVIHQSVYELIHTEDRAEFQR** IFRTKHKLDFŤPIGCDAKGRIVLGYTEAELCTRGSGYQFIHAADMLÝČAESHIRMIKTGESGMIVFRLĽT RHSLEWKFLFLDHRAPPIIGYLPFEVLGTSGYDYYHVDDLENLAKCHEHLMQYGKGKSCYYRFLTKGQQW KEKSRDAARSRRSKESEVFYELAHOLPLPHNVSSHLDKASVMRLTISYLRVRKLLDAGDLDIEDDMKAOM NCFYLKALDGFVMVLTDDGDMIYISDNVNKYMGLTOFELTGHSVFDFTHPCDHEEMREMLTHNTORSFFL KEKSRDAARCRRSKETEVFYELAHELPLPHSVSSHLDKASIMRLAISFLRTHKLLSSVCSENESEAEADO KFTYCDDRITELIGYHPEELLGRSAYEFYHALDSENMTKSHQNLCTKGQVVSGQYRMLAKHGGYVWLETQ DAARSRRSQETEVLYQLAHTLPFARGVSAHLDKASIMRLTISYLRMHRLCAAGEWNQVGAGGEPLDACYL LTSRGRTLNLKAATWKVLNCSGHMRAYEPPLQCLVLICEAIPHPGSLEPPLGRGAFLSRHSLDMKFTYCD DRIAEVAGYSPDDLIGCSAYEYIHALDSDAVSKSIHTLLSKGQAVTGQYRFLARSGGYLWTQTQATVVSG KEKSRNAARSRRGKENLEFFELAKLLPLPGAISSQLDKASIVRLSVTYLRLRRFAALGAPPWGLRAAGPP AGLAPGRRGPAALVSEVFEQHLGGHILQSLDGFVFALNQEGKFLYISETVSIYLGLSQVEMTGSSVFDYI LEWKFLFLDHRAPPIIGYLPFEVLGTSGYDYYHIDDLELLARCHOHLMOFGKGKSCCYRFLTKGOOWIWL SRDAARSRRGKENFEFYELAKLLPLPAAITSQLDKASIIRLTISYLKMRDFANQGDPPWNLRMEGPPPNT IVAALPGFLLVFTAEGKLLYLSESVSEHLGHSMVDLVAQGDSIYDIIDPADHLTVRQQLTLTDRLFRCRF EKSKNAARTRREKENSEFYELAKLLPLPSAITSQLDKASIIRLTTSYLKMRVVFPEGLGEAWGHSSRTSP EKSKNAAKTRREKENGEFYELAKLLPLPSAITSQLDKASIIRLTTSYLKMRAVFPEGLGDAWGQPSRAGP ELKHLILEAADGFLFIVSCETGRVVYVSDSVTPVLNQPQSEWFGSTLYDQVHPDDVDKLREQLSTSRMCM DELKHLILRAADGFLFVVGCDRGKILFVSESVFKILNYSQNDLIGQSLFDYLHPKDIAKVKEQLSSSRLC KFVFVDQRATAILAYLPQELLGTSCYEYFHQDDIGHLAECHRQVLQTREKITTNCYKFKIKDGSFITLRS shreyakathuria@Shreyaa:~/Lab_session2\$ |

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

shreyakathuria@Shreyaa:~/Lab_session2\$ grep -v '^>' sequence5.fasta | grep 'P' SNPSKRHRDRLNTELDRLASLLPFPQDVINKLDKLSVLRLSVSYLRAKSFFDVALKSSPTERNGGQDNCR QLHWQIPPENSPLMERCFICRLRCLLDNSSGFLAMNFQGKLKYLPPQLALFAIATPLQPPSILEIRTKNF IFRTKHKLDFTPIGCDAKGRIVLGYTEAELCTRGSGYQFIHAADMLYCAESHIRMIKTGESGMIVFRLLT KNNRWTWVQSNARLLYKNGRPDYIIVTQRPLTDEEGTEHLR VSRNKSEKKRRDQFNVLIKELGSMLPGNARKMDKSTVLQKSIDFLRKHKEITAQSDASEIRQDWKPTFLS NEEFTQLMLEALDGFFLAIMTDGSIIYVSESVTSLLEHLPSDLVDQSIFNFIPEGEHSEVYKILSTEYLK SKNQLEFCCHMLRGTIDPKEPSTYEYVKFIGNFKSLYEDRVCFVATVRLATPQFIKEMCTVEEPNEEFTS RHSLEWKFLFLDHRAPPIIGYLPFEVLGTSGYDYYHVDDLENLAKCHEHLMQYGKGKSCYYRFLTKGQQW IWLQTHYYITYHQWNSRPEFIVCTHTVVSYAEVRAE KEKSRDAARSRRSKESEVFYELAHQLPLPHNVSSHLDKASVMRLTISYLRVRKLLDAGDLDIEDDMKAQM NCFYLKALDGFVMVLTDDGDMIYISDNVNKYMGLTQFELTGHSVFDFTHPCDHEEMREMLTHNTQRSFFL RMKCTLTSRGRTMNIKSATWKVLHCTGHIHVYKPPMTCLVLICEPIPHPSNIEIPLDSKTFLSRHSLDMK FSYCDERITELMGYEPEELLGRSIYEYYHALDSDHLTKTHHDMFTKGQVTTGQYRMLAKRGGYVWVETQA TVIYNTKNSQPQCIVCVNYVVSGIIQHDL KEKSRDAARCRRSKETEVFYELAHELPLPHSVSSHLDKASIMRLAISFLRTHKLLSSVCSENESEAEADQ QMDNLYLKALEGFIAVVTQDGDMIFLSENISKFMGLTQVELTGHSIFDFTHPCDHEEIRENLSSTERDFF MRMKCTVTNRGRTVNLKSATWKVLHCTGOVKVYEPLLSCLIIMCEPIOHPSHMDIPLDSKTFLSRHSMDM KFTYCDDRITELIGYHPEELLGRSAYEFYHALDSENMTKSHQNLCTKGQVVSGQYRMLAKHGGYVWLETQ GTVIYNPRNLQPQCIMCVNYVLSEIEKNDV DAARSRRSQETEVLYQLAHTLPFARGVSAHLDKASIMRLTISYLRMHRLCAAGEWNQVGAGGEPLDACYL KALEGFVMVLTAEGDMAYLSENVSKHLGLSQLELIGHSIFDFIHPCDQEELQDALTPPTERCFSLRMKST LTSRGRTLNLKAATWKVLNCSGHMRAYEPPLQCLVLICEAIPHPGSLEPPLGRGAFLSRHSLDMKFTYCD DRIAEVAGYSPDDLIGCSAYEYIHALDSDAVSKSIHTLLSKGQAVTGQYRFLARSGGYLWTQTQATVVSG GRGPQSESIVCVHFLISQVEETGV KEKSRNAARSRRGKENLEFFELAKLLPLPGAISSOLDKASIVRLSVTYLRLRRFAALGAPPWGLRAAGPP AGLAPGRRGPAALVSEVFEOHLGGHILOSLDGFVFALNOEGKFLYISETVSIYLGLSOVEMTGSSVFDYI HPGDHSEVLEQLGLVQERSFFVRMKSTLTKRGLHVKASGYKVIHVTGRLRALGLVALGHTLPPAPLAELP LHGHMIVFRLSLGLTILACESRVSDHMDLGPSELVGRSCYQFVHGQDATRIRQSHVDLLDKGQVMTGYYR

NKSEKKRRDQFNVLIKELSSMLPGNTRKMDKTTVLEKVIGFLQKHNEVSAQTEICDIQQDWKPSFLSNEE

WLQRAGGFVWLQSVATVAGSGKSPGEHHVLWVSHVLSQAEĞGQT



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

```
shreyakathuria@Shreyaa:~/Lab_session2$ pattern1="G\{2,\}"
shreyakathuria@Shreyaa:~/Lab_session2$ grep -v '^>' sequence5.fast
a | grep "$pattern1"
SNPSKRHRDRLNTELDRLASLLPFPQDVINKLDKLSVLRLSVSYLRAKSFFDVALKSSPTERNGGQ
DNCR
FSYCDERITELMGYEPEELLGRSIYEYYHALDSDHLTKTHHDMFTKGQVTTGQYRMLAKRGGYVWV
KFTYCDDRITELIGYHPEELLGRSAYEFYHALDSENMTKSHONLCTKGQVVSGQYRMLAKHGGYVW
LET0
DAARSRRSQETEVLYQLAHTLPFARGVSAHLDKASIMRLTISYLRMHRLCAAGEWNQVGAGGEPLD
ACYL
DRIAEVAGYSPDDLIGCSAYEYIHALDSDAVSKSIHTLLSKGQAVTGQYRFLARSGGYLWTQTQAT
VVSG
AGLAPGRRGPAALVSEVFEQHLGGHILQSLDGFVFALNQEGKFLYISETVSIYLGLSQVEMTGSSV
FDYI
WLQRAGGFVWLQSVATVAGSGKSPGEHHVLWVSHVLSQAEGGQT
KYYRWMQKNGGYIWIQSSATIAINAKNANEKNIIWVNYLLSNPEYKDT
GASKARRDQINAEIRNLKELLPLAEADKVRLSYLHIMSLACIYTRKGVFFAGGTPLAGPTGLLSAQ
ISESVLIYLGFERSELLCKSWYGLLHPEDLAHASAQHYRLLAESGDIQAEMVVRLQAKTGGWAWIY
CLLY
EIERSFFLRMKCVLAKRNAGLTCGGYKVIHCSGYLKIRNVGLVAVGHSLPPSAVTEIKLHSNMFMF
DMKLIFLDSRVAELTGYEPODLIEKTLYHHVHGCDTFHLRCAHHLLLVKGQVTTKYYRFLAKHGGW
VWVQ
DLKLIFLDSRVTEVTGYEPQDLIEKTLYHHVHGCDVFHLRYAHHLLLVKGQVTTKYYRLLSKRGGW
VWVQ
shreyakathuria@Shreyaa:~/Lab_session2$
```

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'

```
shreyakathuria@Shreyaa:~/Lab_session2$ variable1="Biocomputing"
shreyakathuria@Shreyaa:~/Lab_session2$ export variable1
shreyakathuria@Shreyaa:~/Lab_session2$ bash -c 'echo $variable1'
Biocomputing
shreyakathuria@Shreyaa:~/Lab_session2$
```

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".

```
shreyakathuria@Shreyaa:~/Lab_session2$ if [ -f sequence3.fasta ]; then
  wc -l sequence3.fasta ; else echo "Missing file"; fi
19 sequence3.fasta
  shreyakathuria@Shreyaa:~/Lab_session2$ |
```

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.

```
shreyakathuria@Shreyaa: ~/L ×
shreyakathuria@Shreyaa:~/Lab_session2$ for file in *.fasta ; do echo "Filenam
e: $file"; echo "Number of Sequences: $(grep -c '^>' "$file")"; echo "file si
ze: $(wc -m < "$file")"
> done
Filename: protein.fasta
Number of Sequences: 1
file size: 467
Filename: sequence.fasta
Number of Sequences: 1
file size: 79551
Filename: sequence1.fasta
Number of Sequences: 1
file size: 974
Filename: sequence2.fasta
Number of Sequences: 4
file size: 1710
Filename: sequence3.fasta
Number of Sequences: 2
file size: 1000
Filename: sequence4.fasta
Number of Sequences: 4
file size: 2374
Filename: sequence5.fasta
Number of Sequences: 13
file size: 4229
shreyakathuria@Shreyaa:~/Lab_session2$
```

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

```
shreyakathuria@Shreyaa:~/Lab_session2$ for file in *.fasta; do seqs=$(
grep -c '^>' "$file"); if (( seqs > 3 )); then echo "Filename: $file";
  echo "Number of Sequences: $seqs"; echo "File size: $(wc -m < "$file")
)"; fi; done
Filename: sequence2.fasta
Number of Sequences: 4
File size: 1710
Filename: sequence4.fasta
Number of Sequences: 4
File size: 2374
Filename: sequence5.fasta
Number of Sequences: 13
File size: 4229
shreyakathuria@Shreyaa:~/Lab_session2$</pre>
```

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.

```
shreyakathuria@Shreyaa:~/Lab_session2$ grep -v '^>' sequence5.fasta |
egrep 'C.*C.*C' | grep . > cys_rich.txt
shreyakathuria@Shreyaa:~/Lab_session2$ grep -n '^$'
^C
shreyakathuria@Shreyaa:~/Lab_session2$ grep -n '^$' cys_rich.txt
shreyakathuria@Shreyaa:~/Lab_session2$ |
```

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

```
shreyakathuria@Shreyaa:~/Lab_session2$ grep -c '^>' *.fasta | sort -t: -k2 -nr
| head -n1
sequence5.fasta:13
shreyakathuria@Shreyaa:~/Lab_session2$
```

USED GEMINI FOR SORT IN OPTIONAL ONE
AND GEEKSFORGEEKS FOR THE COMMAND USAGE MANUAL