I have used CHATGPT for some difficult questions between 20 and 26 and I have also got hints for some questions from 1-20 from these AI tools only to understand logic which are different from the Lab session 3 codes about sed and awk.

1)

```
user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3$ vi File
user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3$ less File
```

Hii

This is Alamelu

I'm a 1st year student at IIT Gandhinagar

I'm pursuing my M.Tech in Biological Engineering

I am liking Biocomputing

The course goes on interesting

File (END)

```
user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3$ sed '/^$/d' File
Hii
This is Alamelu
I'm a 1st year student at IIT Gandhinagar
I'm pursuing my M.Tech in Biological Engineering
I am liking Biocomputing
The course goes on interesting
```

2)

user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3\$ sed '/^\$/d' File > Edited
user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3\$ less Edited

Hii
This is Alamelu
I'm a 1st year student at IIT Gandhinagar
I'm pursuing my M.Tech in Biological Engineering
I am liking Biocomputing
The course goes on interesting
Edited (END)

 $user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3\$ sed = Edited | sed 'N;s/\n/ /' > Numbered \\ user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3\$ less Numbered$

1 Hii
2 This is Alamelu
3 I'm a 1st year student at IIT Gandhinagar
4 I'm pursuing my M.Tech in Biological Engineering
5 I am liking Biocomputing
6 The course goes on interesting
Numbered (END)

3)

user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3\$ sed -n '/^>/p' clock_gene.fasta >NC_000004.12:c55546909-55427903 Homo sapiens chromosome 4, GRCh38.p14 Primary Assembly

4)

user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3\$ sed -n '/^>.*CLOCK/p' protein.fasta

No headers found in protein.fasta that contains the word clock

5)

user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3\$ awk '!/^>/ && /CC/' protein.fasta

user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3\$ less protein.fasta

(less protein.fasta was executed to confirm if no lines with CC were present)

NAME: ALAMELU ROLL NUMBER: 25210013 LAB-ASSIGNMENT-3

Text processing (sed and awk)

>NP_808227.1 casein kinase II subunit alpha isoform a [Homo sapiens]
MSGPVPSRARVYTDVNTHRPREYWDYESHVVEWGNQDDYQLVRKLGRGKYSEVFEAINITNNEKVVVKIL
KPVKKKKIKREIKILENLRGGPNIITLADIVKDPVSRTPALVFEHVNNTDFKQLYQTLTDYDIRFYMYEI
LKALDYCHSMGIMHRDVKPHNVMIDHEHRKLRLIDWGLAEFYHPGQEYNVRVASRYFKGPELLVDYQMYD
YSLDMWSLGCMLASMIFRKEPFFHGHDNYDQLVRIAKVLGTEDLYDYIDKYNIELDPRFNDILGRHSRKR
WERFVHSENQHLVSPEALDFLDKLLRYDHQSRLTAREAMEHPYFYTVVKDQARMGSSSMPGGSTPVSSAN
MMSGISSVPTPSPLGPLAGSPVIAAANPLGMPVPAAAGAQQ

protein.fasta (END)

There are no such lines in protein.fasta with two consecutive CC s.

6)

```
user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3$ awk '!/^>/' clock_
gene.fasta | awk '{gsub(/[^G]/, "")} {count += length} END {print "No of Gs:
   ", count}'
No of Gs: 355
```

7)

8)

user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3\$ awk '/^>/{pr
int substr(\$1,2)}' protein.fasta
NP 808227.1

9)1)

9)2)

user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3\$ awk '/^>/ {if (id) print id, length (seq); id=substr(\$0,2); seq=""} !/^>/ {seq=seq\$0} END {print id, length(seq)}' protein.fasta NP_808227.1 casein kinase II subunit alpha isoform a [Homo sapiens] 391

10)

						ECH/SEM1,	/Biocompu	ting/Lab	3\$ awl	<pre>'/^ATOM/ && \$</pre>
					ein.pdb	20 126	24 225	0.11 11.15	1 00	
ATOM N	1	N	TRP	А	172	-39.136	-21.997	24.415	1.00	34.43
ATOM C	2	CA	TRP	Α	172	-40.108	-20.907	24.729	1.00	34.28
ATOM C	3	С	TRP	Α	172	-41.403	-21.065	23.944	1.00	33.46
ATOM O	4	0	TRP	Α	172	-41.385	-21.496	22.789	1.00	33.48
ATOM C	5	СВ	TRP	Α	172	-39.506	-19.534	24.418	1.00	35.12
ATOM C	6	CG	TRP	Α	172	-38.161	-19.292	25.025	1.00	36.34
ATOM C	7	CD1	TRP	Α	172	-37.773	-19.568	26.306	1.00	37.69
ATOM C	8	CD2	TRP	Α	172	-37.032	-18.693	24.384	1.00	37.47
ATOM N	9	NE1	TRP	Α	172	-36.465	-19.190	26.497	1.00	37.97
ATOM C	10	CE2	TRP	Α	172	-35.985	-18.650	25.334	1.00	37.83
ATOM C	11	CE3	TRP	Α	172	-36.799	-18.192	23.097	1.00	37.57
ATOM C	12	CZ2	TRP	Α	172	-34.725	-18.128	25.037	1.00	37.51
ATOM C	13	CZ3	TRP	Α	172	-35.545	-17.671	22.802	1.00	37.85
ATOM	14	CH2	TRP	Α	172	-34.523	-17.646	23.769	1.00	37.43

11)

```
user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3$ awk '/^ATOM/ && $4=="LYS"||$4=="ARG
"{print $0}' protein.pdb
MOTA
         15
                 LYS A 173
                               -42.516 -20.697 24.576 1.00 32.18
                                                                              N
             N
                                                                              C
ATOM
         16
             CA LYS A 173
                               -43.842 -20.728
                                                23.949 1.00 31.37
                               -44.028 -19.604
                                                                              C
         17
             С
                 LYS A 173
                                                22.914 1.00 29.85
MOTA
                                                                              0
                               -44.831 -19.725
         18
                 LYS A 173
                                                21.976
MOTA
             0
                                                        1.00 30.15
         19
             CB LYS A 173
                               -44.935 -20.645
                                                25.024 1.00 31.31
                                                                              C
MOTA
                                                                              C
         20
             CG LYS A 173
                               -46.343 -20.964
                                                24.519 1.00 32.53
ATOM
                                                                              С
             CD LYS A 173
                               -47.425 -20.459
                                                25.479 1.00 32.89
MOTA
         21
                                                                              C
MOTA
         22
             CE
                 LYS A 173
                               -48.818 -20.684
                                                24.901 1.00 33.96
MOTA
         23
             NZ
                 LYS A 173
                               -49.893 -20.189
                                                25.806 1.00 34.66
                                                                              N
         46
                 ARG A 177
                               -41.200 -13.469
                                                20.062
                                                        1.00 17.53
                                                                              N
MOTA
             N
                                                                              C
         47
                               -41.351 -12.338
MOTA
             CA
                 ARG A 177
                                                20.984
                                                        1.00 18.15
                                                                              C
         48
                 ARG A 177
                               -40.135 -12.196
                                                21.880
MOTA
             С
                                                       1.00 18.13
                                                                              0
         49
            0
                 ARG A 177
                               -39.608 -11.088
                                                22.053 1.00 17.51
MOTA
                                                                              C
                 ARG A 177
                               -42.634 -12.450
MOTA
         50
            CB
                                                21.807 1.00 18.62
                                                                              C
MOTA
         51
             CG
                 ARG A 177
                               -42.872 -11.237
                                                22.713 1.00 20.72
                               -44.227 -11.292
                                                                              C
MOTA
         52
             CD
                 ARG A 177
                                                23.368 1.00 22.66
                               -44.366 -10.263
                                                                              N
MOTA
         53
             NE
                 ARG A 177
                                                24.391
                                                        1.00 24.94
                 ARG A 177
MOTA
         54
             CZ
                               -43.848 -10.348
                                                25.616
                                                        1.00 25.91
                                                                              C
MOTA
         55
             NH1 ARG A 177
                               -43.147 -11.413 25.983 1.00 25.04
                                                                              N
MOTA
         56
            NH2 ARG A 177
                               -44.030 -9.360 26.477 1.00 26.28
                                                                              N
```

NAME: ALAMELU ROLL NUMBER: 25210013 LAB-ASSIGNMENT-3

Text processing (sed and awk)

12)

```
A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3$ sed 's/LYS/ARG/g' protein.pdb
TIDE BINDING PROTEIN 26-MAY-05 1ZT3
HEADER
             PEPTIDE BINDING PROTEIN
            C-TERMINAL DOMAIN OF INSULIN-LIKE GROWTH FACTOR BINDING PROTEIN-1 2 ISOLATED FROM HUMAN AMNIOTIC FLUID
TITLE
TITLE
COMPND
            MOL_ID: 1;
2 MOLECULE: INSULIN-LIKE GROWTH FACTOR BINDING PROTEIN 1;
COMPND
            3 CHAIN: A;
4 FRAGMENT: C-TERMINAL DOMAIN;
COMPND
COMPND
COMPND
            5 SYNONYM: IGFBP-1, IBP- 1, IGF-BINDING PROTEIN 1, PLACENTAL PROTEIN
            6 12, PP12
MOL_ID: 1;
COMPND
SOURCE
            2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
3 ORGANISM_COMMON: HUMAN;
SOURCE
SOURCE
            4 ORGANISM_TAXID: 9606;
5 OTHER_DETAILS: AMNIOTIC FLUID
SOURCE
SOURCE
             INSULIN-LIKE GROWTH FACTOR BINDING PROTEIN-1, IGFBP-1, AMNIOTIC
KEYWDS
            2 FLUID, C-TERMINAL DOMAIN, METAL-BINDING, PEPTIDE BINDING PROTEIN X-RAY DIFFRACTION
KEYWDS
EXPDTA
            A.SALA,S.CAPALDI,M.CAMPAGNOLI,B.FAGGION,S.LABO,M.PERDUCA,A.ROMANO, 2 M.E.CARRIZO,M.VALLI,L.VISAI,L.MINCHIOTTI,M.GALLIANO,H.L.MONACO
AUTHOR
AUTHOR
REVDAT
                  16-0CT-24 1ZT3
                                                      REMARK
REVDAT
                 11-0CT-17 1ZT3
                                                      REMARK
                 24-FEB-09 1ZT3
30-AUG-05 1ZT3
                                                      VERSN
REVDAT
                                           1
REVDAT
                                                      JRNL
                  28-JUN-05 1ZT3
REVDAT
                AUTH A.SALA,S.CAPALDI,M.CAMPAGNOLI,B.FAGGION,S.LABO,M.PERDUCA,
AUTH 2 A.ROMANO,M.E.CARRIZO,M.VALLI,L.VISAI,L.MINCHIOTTI,
AUTH 3 M.GALLIANO,H.L.MONACO
JRNL
JRNL
JRNL
```

13)

```
KTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3$ awk '/^ATOM/ {print $9}' protein.pdb
24.415
24.729
23.944
22.789
24.418
25.025
26.306
24.384
26.497
25.334
23.097
25.037
22.802
23.769
24.576
23.949
22.914
21.976
25.024
24.519
25.479
24.901
25.806
23.090
22.191
```

14)

user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3\$ awk '/GLY/ {count++} END {print " No of lines with Glycine: "count}' protein.pdb
No of lines with Glycine: 33

15)

```
A5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3$ awk '/^ATOM/ && _$3=="CA" && ($4=="
ALA" | | $4=="GLY")
                    {print $0}'
                                   protein.pdb
                                                                   1.00 19.62
1.00 20.13
1.00 34.45
                                     -29.906
-24.689
MOTA
         143
               CA
                    ALA A 188
                                                -0.273
                                                          21.249
                                                                                             CCC
                                                -1.402
                                                          19.528
ATOM
          157
               CA
                    ALA A 190
          193
                    GLY A 195
                                     -19.179
                                                 3.890
MOTA
                                                          13.965
                                                                    1.00 18.56
1.00 21.58
                                                                                             C
MOTA
          315
               CA
                    GLY A 210
                                     -45.353 -14.753
                                                          19.536
               CA
                    GLY A 223
                                     -36.815
                                                 5.170
ATOM
         422
                                                           1.658
                    ALA A 225
GLY A 226
                                                                   1.00 20.30
1.00 18.85
         435
               CA
                                     -37.186
                                                           0.463
ATOM
                                                -1.492
                                     -35.705 -3.955
-37.957 -18.276
MOTA
         440
               CA
                                                           2.980
                                                                                             C
          526
               CA
                    GLY A 236
                                                          12.295
                                                                    1.00
                                                                                             C
ATOM
                                                                          18.22
ATOM
          565
               CA
                    GLY A
                           241
                                     -34.199 -22.463
                                                          -1.334
                                                                    1.00 28.67
                                                                                             C
                                      -40.259
                            247
                                                -7 039
                                                             851
```

16)

```
user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3$ awk '$3=="C" {count++} END {print
" No of atoms(C): "count}' protein.pdb
No of atoms(C): 80
```

17)

```
sed -n '/^HETATM/p'
                                                                                    protein.pdb
                                          Biocomputing/Lab3$
                                                            1.00 36.16
HETATM
                  DIO A 400
                                           -6.946
        644
              C1
                                  -29.064
                                                    17.132
                                                    16.720
HETATM
        645
                  DIO A 400
                                  -28.073
                                           -9.061
                                                             1.00 36.92
                                                                                    C
C
        646
              C1
                  DIO A 400
                                           -6.281
                                                             1.00 35.99
HETATM
                                  -27.687
                                                    17.202
        647
                  DIO A 400
HETATM
              C2
                                  -26.684
                                           -8.437
                                                    16.825
                                                             1.00 36.68
                                                                                    0
HETATM
        648
              01
                  DIO A 400
                                  -28.996
                                           -8.072
                                                    16.254
                                                             1.00 36.78
        649
              01
                  DIO A 400
                                  -26.726
                                           -7.251
                                                    17.629
                                                             1.00 36.28
                                                                                    0
HETATM
                                  -37.255
                                                                                    0
HETATM
        650
                  нон а
                                           -6.228
                                                    10.647
                                                             1.00 14.97
              0
                           2
                                  -22.012
                                                                                    0
                  нон а
                                                    22.336
HETATM
        651
              0
                                           -0.788
                                                             1.00 20.64
                           3
        652
              0
                  нон а
                                  -38.877
                                           -3.391
                                                     4.471
                                                             1.00
                                                                  20.33
                                                                                    0
HETATM
              0
                                  -34.212 -23.871
                                                                                    0
HETATM
        653
                  HOH A
                                                     7.998
                                                             1.00 18.39
                                 -20.730 -0.315
-44.936 -13.438
              0
                  нон а
                                           -0.315
                                                    24.894
                                                             1.00 20.65
                                                                                    0
        654
HETATM
                           6
                                                             1.00 28.30
                                                                                    0
HETATM
        655
              0
                  нон а
                                                     1.965
HETATM
        656
              0
                  нон а
                                  -48.895 -18.702
                                                    15.563
                                                             1.00 27.48
                                                                                    0
                                  -21.393
-32.124
                                                                                    0
                           8
                                                    17.811
        657
              0
                  нон а
                                           -0.854
                                                             1.00 24.13
HETATM
                  нон а
                           9
                                                     0.506
                                                                  29.82
HETATM
        658
              0
                                            5.776
                                                             1.00
HETATM
        659
              0
                  нон а
                          10
                                  -46.186 -13.792
                                                     6.539
                                                             1.00 23.52
                                                                                    0
        660
              0
                  нон а
                          11
                                  -29.575
                                           -1.996
                                                    25.245
                                                             1.00 28.23
                                                                                    0
HETATM
                                  -45.642 -11.444
        661
                  нон А
              0
                          12
                                                    19.694
                                                             1.00 25.61
HETATM
                                                                                    0
HETATM
        662
              0
                  нон а
                          13
                                  -49.384 -20.064
                                                    17.570
                                                             1.00 29.28
                                                                                    0
```

18)

awk ' $$1=="ATOM" {res=substr($0,18,3); if(res ~ /E$/) print res}' protein.pdb | sort | uniq (CODE from ChatGPT)$

19)

```
user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3$ sed '/TER/d; /END/d
' protein.pdb > Edited_protein.pdb
user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3$ less Edited_protein.pdb
```

20)

```
$ awk '/^A
1.00 34.43
                                                                                                                   ^ATOM/ && !/ARG/ {print $0} ' protein.pdb
                             TRP A 172
TRP A 172
TRP A 172
TRP A 172
                                                       -39.136 -21.997
-40.108 -20.907
                                                                                     24.415
24.729
                      N
CA
ATOM
                                                                                                                                          N
C
C
                                                                                                    1.00 34.28
MOTA
ATOM
                                                       -41.403 -21.065
                                                                                      23.944
                                                                                                    1.00 33.46
ATOM
                                                       -41.385 -21.496
                                                                                      22.789
                                                                                                                                          0
C
                                                                                                    1.00 33.48
ATOM
                       СВ
                              TRP A 172
                                                       -39.506 -19.534
                                                                                      24.418
                                                                                                    1.00 35.12
                      CB TRP A 172
CG TRP A 172
CD1 TRP A 172
CD2 TRP A 172
NE1 TRP A 172
CE2 TRP A 172
CE3 TRP A 172
                                                       -38.161 -19.292
-37.773 -19.568
-37.032 -18.693
ATOM
                                                                                      25.025
                                                                                                    1.00
                                                                                                            36.34
                 6
7
8
9
                                                                                                                                          ONOOOONO
                                                                                                    1.00 37.69
1.00 37.47
MOTA
                                                                                      26.306
                                                                                      24.384
ATOM
                                                       -36.465 -19.190
-35.985 -18.650
                                                                                     26.497
25.334
                                                                                                    1.00 37.97
1.00 37.83
MOTA
ATOM
                10
               11
12
13
14
15
                                                       -36.799 -18.192
-34.725 -18.128
-35.545 -17.671
MOTA
                                                                                      23.097
                                                                                                    1.00
                                                                                                            37.57
                      CZ2 TRP A 172
CZ3 TRP A 172
CH2 TRP A 172
N LYS A 173
CA LYS A 173
                                                                                     25.037
22.802
23.769
24.576
MOTA
                                                                                                    1.00 37.51
MOTA
                                                                                                    1.00
                                                                                                            37.85
                                                       -34.523 -17.646
-42.516 -20.697
-43.842 -20.728
                                                                                                    1.00 37.43
1.00 32.18
MOTA
MOTA
                16
17
ATOM
                                                                                      23.949
                                                                                                    1.00
                                                                                                            31.37
ATOM
                                                       -44.028 -19.604
                                                                                      22.914
                                                                                                    1.00
```

21)

CODE FROM CHATGPT:

```
awk '$1=="ATOM" && substr($0,22,1)=="A" {res=substr($0,18,3); count[res]++}
END {for(r in count) print r, count[r]}'
```

```
5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3$ awk '/^ATOM/ && substr($0
,22,1)=="A" {res=substr($0,18,3); count[res]++}
     END {for(r in count) print r, count[r]}' protein.pdb
GLY 28
CYS 37
LEU 32
THR 14
GLN 18
PRO 42
ILE 32
MET 8
ASN 40
TYR 48
LYS 45
ASP 16
SER 36
PHE 22
HIS 10
GLU 81
ARG 55
TRP 42
ALA 15
VAL 21
```

NAME: ALAMELU ROLL NUMBER: 25210013 LAB-ASSIGNMENT-3

Text processing (sed and awk)

22) Toupper function to convert lower to uppercase was identified from ChatGPT

Usage of $/^{/}$ {print; next} \rightarrow if line is a header (starts with >), print as-is.(was got from ChatGPT)

```
user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3$ awk '/^>/ {print; next} {
print toupper($0)}' protein.fasta > converted.fasta
user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3$ less converted.fasta
```

```
>NP_808227.1 casein kinase II subunit alpha isoform a [Homo sapiens]
MSGPVPSRARVYTDVNTHRPREYWDYESHVVEWGNQDDYQLVRKLGRGKYSEVFEAINITNNEKVVVKIL
KPVKKKKIKREIKILENLRGGPNIITLADIVKDPVSRTPALVFEHVNNTDFKQLYQTLTDYDIRFYMYEI
LKALDYCHSMGIMHRDVKPHNVMIDHEHRKLRLIDWGLAEFYHPGQEYNVRVASRYFKGPELLVDYQMYD
YSLDMWSLGCMLASMIFRKEPFFHGHDNYDQLVRIAKVLGTEDLYDYIDKYNIELDPRFNDILGRHSRKR
WERFVHSENQHLVSPEALDFLDKLLRYDHQSRLTAREAMEHPYFYTVVKDQARMGSSSMPGGSTPVSSAN
MMSGISSVPTPSPLGPLAGSPVIAAANPLGMPVPAAAGAQQ
```

(END)

23)

```
user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3$ grep '>' protein.fasta >NP_808227.1 casein kinase II subunit alpha isoform a [Homo sapiens]
```

There is only one sequence in this file, hence it is the one with maximum length(I have solved this logically without code)

24)

awk '\$1=="ATOM" {res=substr(\$0,18,3); print res}' protein.pdb | sort | uniq (code from GPT and I have referred the sort usage from it)

25)

```
user@DESKTOP-A5PNEA5:/mnt/d/MTECH/SEM1/Biocomputing/Lab3$ awk '/^ATOM/ {print substr($0,22,1)}' protein.pdb | sort | uniq
A
```

INFERENCE: Only A chain is present in the protein.pdb file

26)

The code was complicated, so I got the complete code from CHATGPT, but I've understood the logic of the code

```
awk '/^>/ {next} {
    for(i=1;i<=length($0);i++) {
        nuc=substr($0,i,1);
        count[nuc]++
    }
} END {
    print "A:", count["A"]+0;
    print "T:", count["T"]+0;
    print "G:", count["G"]+0;
    print "C:", count["C"]+0
}' clock_gene.fasta</pre>
```