Practicals 1

-BS19B032

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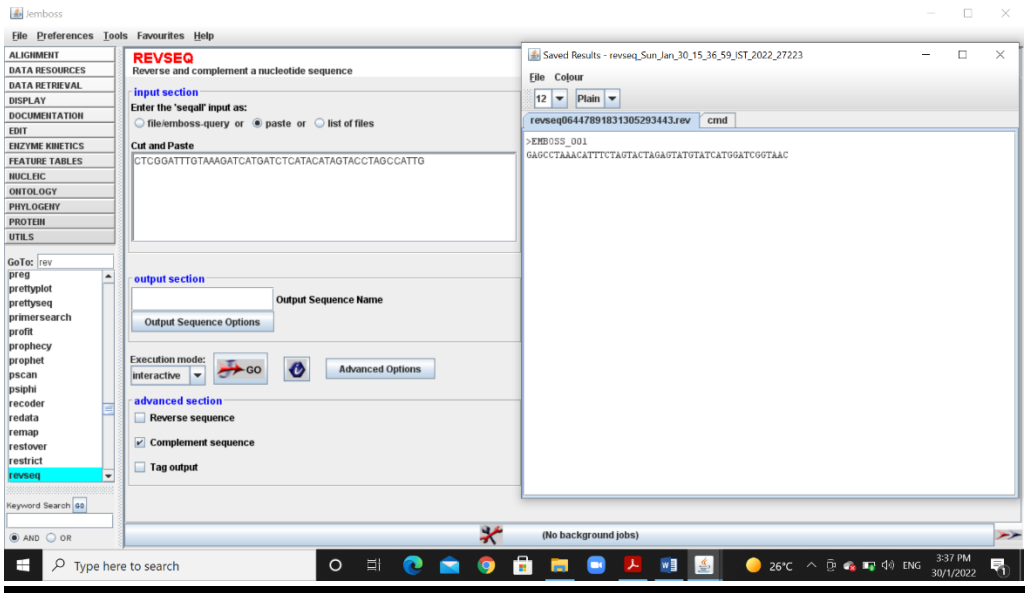
1) I have downloaded emboss in my computer, as per the demo shown in the class.

2) The complementary strand for the given sequence is:

GAGCCTAAACATTTCTAGTACTAGAGTATGTATCATGGATCGGTAAC

*(*not reversed).*



3) This is a python program that is used to find the complementary strand of given sequence:

```
seq=input("Enter your DNA sequence:")      #taking input sequence
comp_seq=""


for i in range(len(seq)):
    if(seq[i]=='A'):
        comp_seq+='T'          #creating complementary sequence
    if(seq[i]=='T'):
        comp_seq+='A'
    if(seq[i]=='C'):          #A to T; T to A; C to G; G to C
        comp_seq+='G'
    if(seq[i]=='G'):
        comp_seq+='C'


print(comp_seq)
```

The output is:

GAGCCTAAACATTTCTAGTACTAGAGTATGTATCATGGATCGGTAAC

*4**a**) Using EMBOSS the protein sequence for given DNA sequence is:*

Reading Frame 1:

DIVNSKKVHAMRKEQKRKQGKQRSMGSPMDYSPLPIDKHEPEFGPCRRKLDG

Reading Frame 2:

*TL*TVKKSMQCARSRRGSRASSAPWALPWTTLLCPSTSMSLNLVHAEENWMG*

Reading Frame 3:

*HCEQ*KSPCNAQGAEEEAGQAALHGLSHGLLSSAHRQA*A*IWSMQKKTGWX*

Reading Frame -1:

PIQFSSAWTKFRLMLVDGQRRVVHGRAHGALLALLPLLLLAHCMDFFTVHNV

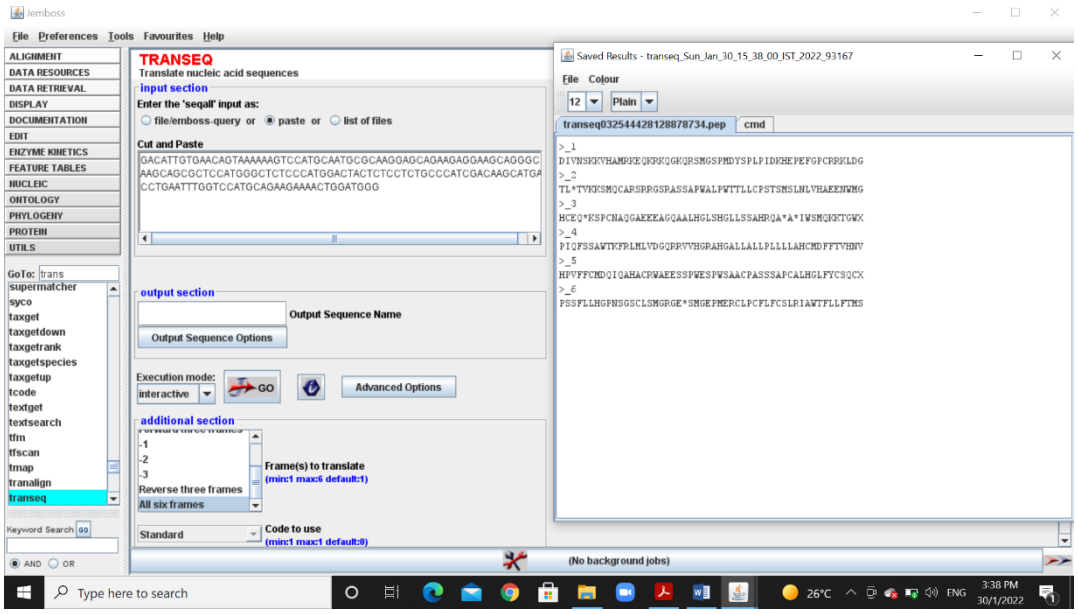
Reading Frame -2:

HPVFFCMDQIQAHACRWAEESSPWESPWSAACPASSSAPCALHGLFYCSQCX

Reading Frame -3:

*PSSFLLHGPNSGSCLSMGRGE*SMGEPMERCLPCFLFCSLRIAWTFLLFTMS*

*4**b**) By checking with the above sequences we got, the reading frame corresponding to given sequence is: **-1.***



5) This is a python program to translate given DNA sequence into protein sequence:

```
seq=input("Enter your DNA sequence:")
mrna_seq=""
protein=""

for i in range(len(seq)):
    if(seq[i]=='T'):
        mrna_seq+='U'
    else:
        mrna_seq+=seq[i]

length=0
if(len(mrna_seq)%3==0):
    length=len(mrna_seq)
elif(len(mrna_seq)%3==1):
```

```
    length=len(mrna_seq)-1
else:
    length=len(mrna_seq)-2

for i in range(0,length,3):
    if(mrna_seq[i]=='A'):
        if(mrna_seq[i+1]=='A'):
            if(mrna_seq[i+2]=='A'):
                protein+='K'
            if(mrna_seq[i+2]=='U'):
                protein+='N'
            if(mrna_seq[i+2]=='C'):
                protein+='N'
            if(mrna_seq[i+2]=='G'):
                protein+='K'
        if(mrna_seq[i+1]=='U'):
            if(mrna_seq[i+2]=='A'):
                protein+='I'
            if(mrna_seq[i+2]=='U'):
                protein+='I'
            if(mrna_seq[i+2]=='C'):
                protein+='I'
            if(mrna_seq[i+2]=='G'):
                protein+='M'
        if(mrna_seq[i+1]=='C'):
            if(mrna_seq[i+2]=='A'):
                protein+='T'
            if(mrna_seq[i+2]=='U'):
                protein+='T'
            if(mrna_seq[i+2]=='C'):
                protein+='T'
            if(mrna_seq[i+2]=='G'):
                protein+='T'
        if(mrna_seq[i+1]=='G'):
```

```
        if(mrna_seq[i+2]=='A'):
            protein+='R'
        if(mrna_seq[i+2]=='U'):
            protein+='S'
        if(mrna_seq[i+2]=='C'):
            protein+='S'
        if(mrna_seq[i+2]=='G'):
            protein+='R'
    if(mrna_seq[i]=='U'):
        if(mrna_seq[i+1]=='A'):
            if(mrna_seq[i+2]=='A'):
                protein+='*'
            if(mrna_seq[i+2]=='U'):
                protein+='Y'
            if(mrna_seq[i+2]=='C'):
                protein+='Y'
            if(mrna_seq[i+2]=='G'):
                protein+='*'
        if(mrna_seq[i+1]=='U'):
            if(mrna_seq[i+2]=='A'):
                protein+='J'
            if(mrna_seq[i+2]=='U'):
                protein+='F'
            if(mrna_seq[i+2]=='C'):
                protein+='F'
            if(mrna_seq[i+2]=='G'):
                protein+='J'
        if(mrna_seq[i+1]=='C'):
            if(mrna_seq[i+2]=='A'):
                protein+='S'
            if(mrna_seq[i+2]=='U'):
                protein+='S'
            if(mrna_seq[i+2]=='C'):
                protein+='S'
```

```
            if(mrna_seq[i+2]=='G'):
                protein+='S'
        if(mrna_seq[i+1]=='G'):
            if(mrna_seq[i+2]=='A'):
                protein+='*'
            if(mrna_seq[i+2]=='U'):
                protein+='C'
            if(mrna_seq[i+2]=='C'):
                protein+='C'
            if(mrna_seq[i+2]=='G'):
                protein+='W'
    if(mrna_seq[i]=='C'):
        if(mrna_seq[i+1]=='A'):
            if(mrna_seq[i+2]=='A'):
                protein+='Q'
            if(mrna_seq[i+2]=='U'):
                protein+='H'
            if(mrna_seq[i+2]=='C'):
                protein+='H'
            if(mrna_seq[i+2]=='G'):
                protein+='Q'
        if(mrna_seq[i+1]=='U'):
            if(mrna_seq[i+2]=='A'):
                protein+='L'
            if(mrna_seq[i+2]=='U'):
                protein+='L'
            if(mrna_seq[i+2]=='C'):
                protein+='L'
            if(mrna_seq[i+2]=='G'):
                protein+='L'
        if(mrna_seq[i+1]=='C'):
            if(mrna_seq[i+2]=='A'):
                protein+='P'
            if(mrna_seq[i+2]=='U'):
```

```
            protein+='P'
        if(mrna_seq[i+2]=='C'):
            protein+='P'
        if(mrna_seq[i+2]=='G'):
            protein+='P'
    if(mrna_seq[i+1]=='G'):
        if(mrna_seq[i+2]=='A'):
            protein+='R'
        if(mrna_seq[i+2]=='U'):
            protein+='R'
        if(mrna_seq[i+2]=='C'):
            protein+='R'
        if(mrna_seq[i+2]=='G'):
            protein+='R'
if(mrna_seq[i]=='G'):
    if(mrna_seq[i+1]=='A'):
        if(mrna_seq[i+2]=='A'):
            protein+='E'
        if(mrna_seq[i+2]=='U'):
            protein+='D'
        if(mrna_seq[i+2]=='C'):
            protein+='D'
        if(mrna_seq[i+2]=='G'):
            protein+='E'
    if(mrna_seq[i+1]=='U'):
        if(mrna_seq[i+2]=='A'):
            protein+='V'
        if(mrna_seq[i+2]=='U'):
            protein+='V'
        if(mrna_seq[i+2]=='C'):
            protein+='V'
        if(mrna_seq[i+2]=='G'):
            protein+='V'
    if(mrna_seq[i+1]=='C'):
```

```
            if(mrna_seq[i+2]=='A'):
                protein+='A'
            if(mrna_seq[i+2]=='U'):
                protein+='A'
            if(mrna_seq[i+2]=='C'):
                protein+='A'
            if(mrna_seq[i+2]=='G'):
                protein+='A'
        if(mrna_seq[i+1]=='G'):
            if(mrna_seq[i+2]=='A'):
                protein+='G'
            if(mrna_seq[i+2]=='U'):
                protein+='G'
            if(mrna_seq[i+2]=='C'):
                protein+='G'
            if(mrna_seq[i+2]=='G'):
                protein+='G'

print(protein)
```

The protein sequence I got is:

DIVNSKKVHAMRKEQKRKQGKQRSMGSPMDYSPLPIDKHEPEFGPCRRKLDG

6) The python code to find matches in the string is:

```
seq=input("Enter your sequence:")
check_str=input("Enter the string to search:")
matches=0

for i in range(len(seq)-len(check_str)+1):
    count=0
    for j in range(len(check_str)):
        if(seq[i+j]==check_str[j]):
```

```
            count=count+1
        if(count==len(check_str)):
            matches=matches+1
            print("Match location:",i)
print("Total matches:",matches)
```

*The output of the code when we input string in question 4 and the match string as **AAG:***

Match location: 19

Match location: 36

Match location: 45

Match location: 51

Match location: 60

Match location: 111

Match location: 140

Total matches: 7

*The output of the code when we input string in question 4 and the match string as **ACTA:***

Match location: 88

Total matches: 1

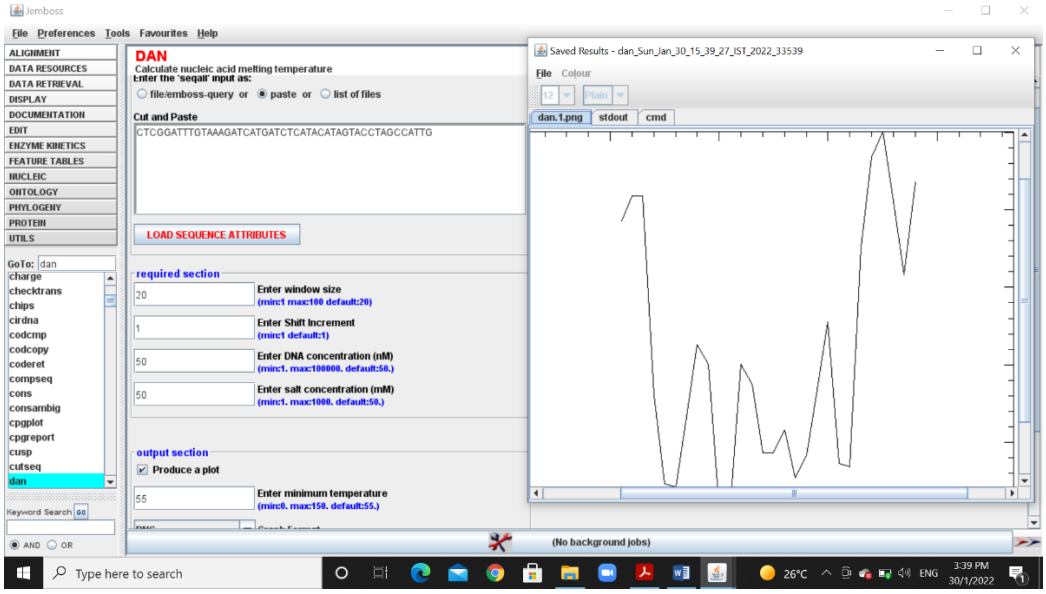
By running the code with strings of different length, I observed that as string length increases, matches decreases.

7) I learnt some of these applications of emboss.

***dan**: This tool in emboss is used to find the melting temperature of the given nucleotide sequence. This tool also provides us with plot on melting temperature.*

***Banana**: This tool in emboss is used to plot bending and curvature of given DNA sequence.*

***trimseq**: This tool helps us to remove unwanted characters like "*" in start and end of the sequence.*


Jemboss
File Preferences Tools Favourites Help
ALIGNMENT
DATA RESOURCES
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codcmp
codcopy
coderet
compseq
cons
consambig
cpgplot
cpgreport
cusp
cutseq
dan
Keyword Search GO
AND OR
DAN
Calculate nucleic acid melting temperature
Enter the 'seqall' input as:
file/emboss-query or paste or list of files
Cut and Paste
CTCGGATTTGTAAAGATCATGATCTCATACATAGTACCTAGCCATTG
LOAD SEQUENCE ATTRIBUTES
required section
20
Enter window size
(min:1 max:100 default:20)
1
Enter Shift Increment
(min:1 default:1)
50
Enter DNA concentration (nM)
(min:1. max:100000. default:50.)
50
Enter salt concentration (mM)
(min:1. max:1000. default:50.)
output section
Produce a plot
55
Enter minimum temperature
(min:0. max:150. default:55.)
Saved Results - dan_Sun_Jan_30_15_39_27_IST_2022_33539
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dan.1.png
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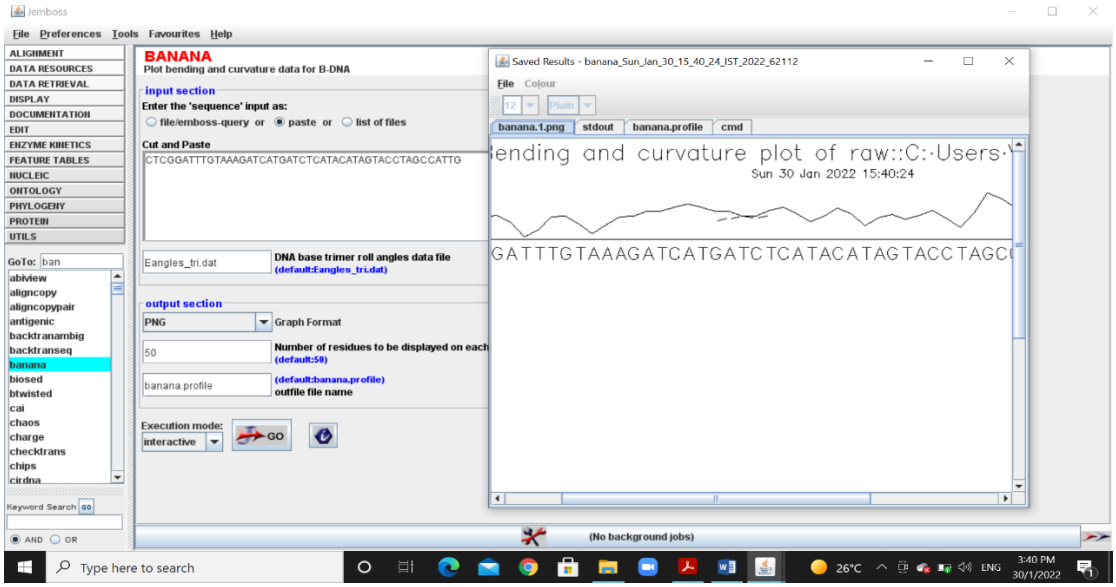
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btwisted
cai
chaos
charge
checktrans
chips
cirdna
Keyword Search GO
AND OR
BANANA
Plot bending and curvature data for B-DNA
input section
Enter the 'sequence' input as:
file/emboss-query or paste or list of files
Cut and Paste
CTCGGATTTGTAAAGATCATGATCTCATACATAGTACCTAGCCATTG
Eangles_tri.dat
DNA base trimer roll angles data file
(default:Eangles_tri.dat)
output section
PNG
Graph Format
50
Number of residues to be displayed on each
(default:50)
banana.profile
(default:banana.profile)
outfile file name
Execution mode:
interactive
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Saved Results - banana_Sun_Jan_30_15_40_24_IST_2022_62112
File Colour
banana.1.png
stdout
banana.profile
cmd
ending and curvature plot of raw::C:·Users·
Sun 30 Jan 2022 15:40:24
GATTTGTAAAGATCATGATCTCATACATAGTACCTAGC
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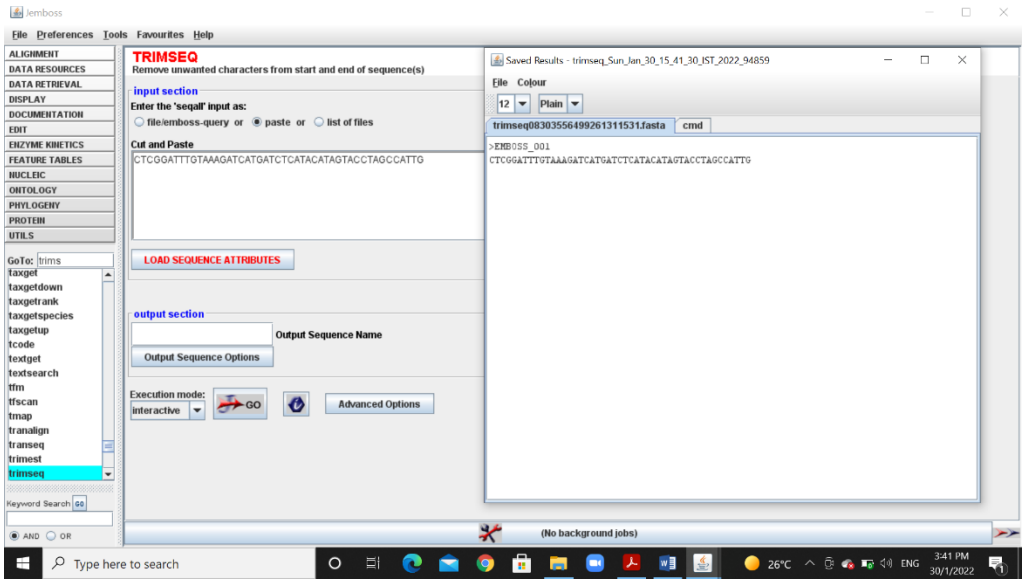


8) The python program to find average stacking energy of given sequence is:

```
seq=input("Enter your sequence:")
stack_energy=0


for i in range(len(seq)-1):
    if(seq[i]=='A'):
        if(seq[i+1]=='A'):
            stack_energy=stack_energy + (-4)
        if(seq[i+1]=='T'):
            stack_energy=stack_energy + (-7)
        if(seq[i+1]=='C'):
            stack_energy=stack_energy + (-5)
        if(seq[i+1]=='G'):
            stack_energy=stack_energy + (-11)
    if(seq[i]=='T'):
        if(seq[i+1]=='A'):
            stack_energy=stack_energy + (-7)
        if(seq[i+1]=='T'):
            stack_energy=stack_energy + (-2)
        if(seq[i+1]=='C'):
```

```
            stack_energy=stack_energy + (-3)
        if(seq[i+1]=='G'):
            stack_energy=stack_energy + (-4)
    if(seq[i]=='C'):
        if(seq[i+1]=='A'):
            stack_energy=stack_energy + (-9)
        if(seq[i+1]=='T'):
            stack_energy=stack_energy + (-5)
        if(seq[i+1]=='C'):
            stack_energy=stack_energy + (-6)
        if(seq[i+1]=='G'):
            stack_energy=stack_energy + (-7)
    if(seq[i]=='G'):
        if(seq[i+1]=='A'):
            stack_energy=stack_energy + (-9)
        if(seq[i+1]=='T'):
            stack_energy=stack_energy + (-6)
        if(seq[i+1]=='C'):
            stack_energy=stack_energy + (-4)
        if(seq[i+1]=='G'):
            stack_energy=stack_energy + (11)

avg_stack_energy=stack_energy/(len(seq)-1)

print("The average stacking energy of given sequence is:",avg_stack_energy)
```

When we provide the input sequence given in the question 2, the output average stacking energy we get is:

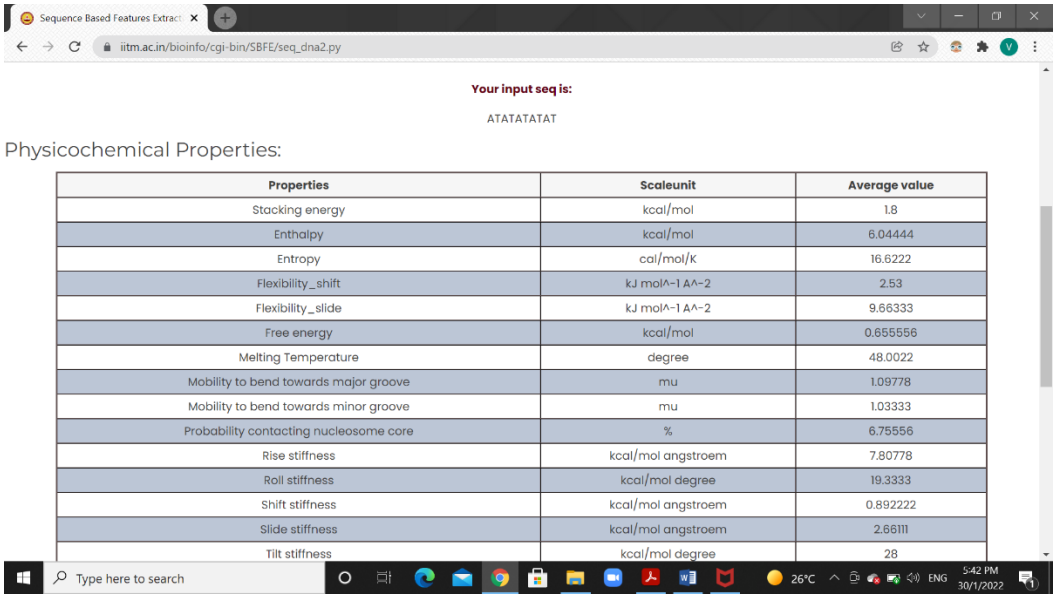
-5.804347826086956

9) Using the seq2feature app, I calculated the melting point for given sequences:

(i) ATATATATAT: 48.0022 degrees

(ii) GCGCGCGC: 107.867 degrees

As we know that, in a DNA double strand G and C forms three hydrogen bonds between them, whereas, A and T forms only two hydrogen bonds. So, since G and C sequence has many bonds, their melting temperature is higher than A and T sequence.



Sequence Based Features Extract

iitm.ac.in/bioinfo/cgi-bin/SBFE/seq_dna2.py

Your input seq is:

ATATATATAT

Physicochemical Properties:

Properties	Scaleunit	Average value
Stacking energy	kcal/mol	1.8
Enthalpy	kcal/mol	6.04444
Entropy	cal/mol/K	16.6222
Flexibility_shift	kJ mol^-1 A^-2	2.53
Flexibility_slide	kJ mol^-1 A^-2	9.66333
Free energy	kcal/mol	0.655556
Melting Temperature	degree	48.0022
Mobility to bend towards major groove	mu	1.09778
Mobility to bend towards minor groove	mu	1.03333
Probability contacting nucleosome core	%	6.75556
Rise stiffness	kcal/mol angstroem	7.80778
Roll stiffness	kcal/mol degree	19.3333
Shift stiffness	kcal/mol angstroem	0.892222
Slide stiffness	kcal/mol angstroem	2.66111
Tilt stiffness	kcal/mol degree	28

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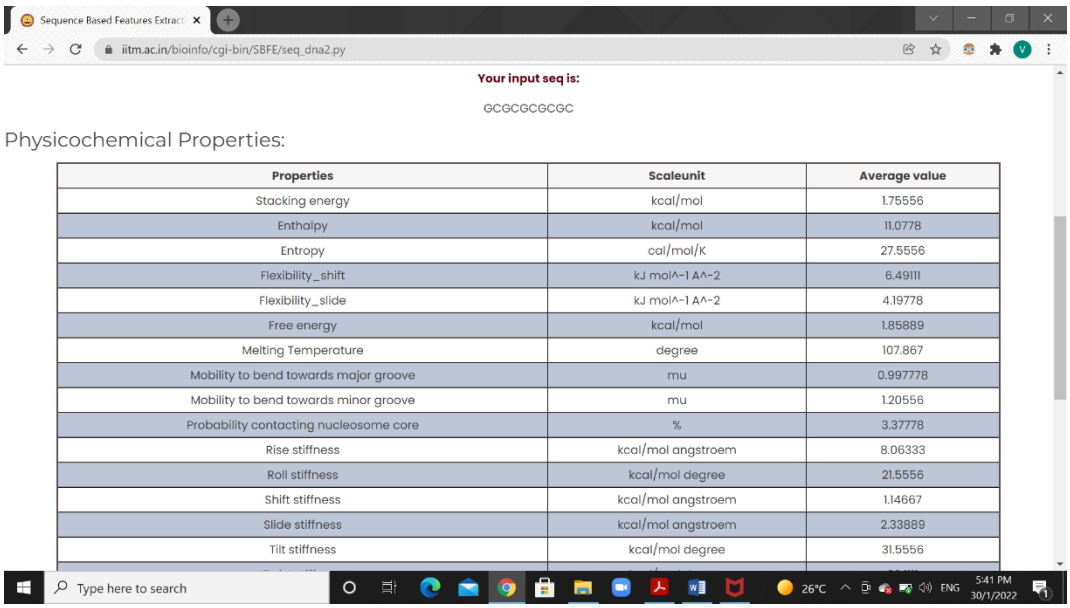

Sequence Based Features Extract

iitm.ac.in/bioinfo/cgi-bin/SBFE/seq_dna2.py

Your input seq is:

GCGCGCGCGC

Physicochemical Properties:

Properties	Scaleunit	Average value
Stacking energy	kcal/mol	1.75556
Enthalpy	kcal/mol	11.0778
Entropy	cal/mol/K	27.5556
Flexibility_shift	kJ mol^-1 A^-2	6.49111
Flexibility_slide	kJ mol^-1 A^-2	4.19778
Free energy	kcal/mol	1.85889
Melting Temperature	degree	107.867
Mobility to bend towards major groove	mu	0.997778
Mobility to bend towards minor groove	mu	1.20556
Probability contacting nucleosome core	%	3.37778
Rise stiffness	kcal/mol angstroem	8.06333
Roll stiffness	kcal/mol degree	21.5556
Shift stiffness	kcal/mol angstroem	1.14667
Slide stiffness	kcal/mol angstroem	2.33889
Tilt stiffness	kcal/mol degree	31.5556

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10) Using seq2feature tool I found the AT and GC content in the given sequence:

AAATGGCCCTAA:

- *AT content – 58.333333*
- *GC content – 41.666667*