INDRAPRASTHA INSTITUTE *of*
INFORMATION TECHNOLOGY
DELHI

HOMEWORK ASSIGNMENT - 1

INDRAPRASTHA INSITUTE OF INFORMATION TECHNOLOGY, DELHI

COMPUTER SCIENCE AND APPLIED MATHEMATICS

Introduction to Quantitative Biology

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1 Code

```
compare()

function input_binary = convert_to_bin(input_sequence)

input_binary = '';

for i = 1 : length(input_sequence)

    if input_sequence(i) == 'A' || input_sequence(i) == 'T'
        input_binary = strcat(input_binary,'0');

    elseif input_sequence(i) == 'G' || input_sequence(i) == 'C'
        input_binary = strcat(input_binary,'1');

    end

end

end


function bond_energy = get_bond_energy(input_binary)

bond_energy = 0;

for i = 1 : length(input_binary)
    if input_binary(i) == '0'
        bond_energy = bond_energy + 2;
    else
        bond_energy = bond_energy + 3;
    end
end
end

function compare()

fprintf("Please note that the binary encoding is as follows: \n 1. 0 stands for A and T \n 2. 1 stands for G and C\n\n
    ");

seq_a = input('Enter base sequence A: ', 's');
seq_b = input('Enter base sequence B: ', 's');

bin_a = convert_to_bin(seq_a);
bin_b = convert_to_bin(seq_b);

fprintf("\nThe binary encoding of base sequence A is: %s\n",bin_a);
fprintf("The binary encoding of base sequence B is: %s\n\n",bin_b);

be_a = get_bond_energy(bin_a);
be_b = get_bond_energy(bin_b);

fprintf("The bond energy of sequence A is: %dϵ(k_b)T\n",be_a);
fprintf("The bond energy of sequence B is: %dϵ(k_b)T\n\n",be_b);

if be_a > be_b
    fprintf("Molecule A will have a higher melting point\n\n");
elseif be_a < be_b
    fprintf("Molecule B will have a higher melting point\n\n");
else
    fprintf("Both the molecules have the same melting point\n\n");

end
end
```

2 Input and Output

Below is the MATLAB console output of the above code run for 3 different cases.

Figure 1: Input and Output of the code shown in 3 cases

```
11/1/18 7:52 PM    MATLAB Command Window                          1 of 1

>> be_cal
Please note that the binary encoding is as follows:
 1. 0 stands for A and T
 2. 1 stands for G and C

Enter base sequence A: ACGT
Enter base sequence B: GCATATGC

The binary encoding of base sequence A is: 0110
The binary encoding of base sequence B is: 11000011
The bond energy of sequence A is: 10ε(k_b)T
The bond energy of sequence B is: 20ε(k_b)T

Molecule B will have a higher melting point

>> be_cal
Please note that the binary encoding is as follows:
 1. 0 stands for A and T
 2. 1 stands for G and C

Enter base sequence A: AGCTTAGC
Enter base sequence B: TAGC

The binary encoding of base sequence A is: 01100011
The binary encoding of base sequence B is: 0011

The bond energy of sequence A is: 20ε(k_b)T
The bond energy of sequence B is: 10ε(k_b)T

Molecule A will have a higher melting point

>> be_cal
Please note that the binary encoding is as follows:
 1. 0 stands for A and T
 2. 1 stands for G and C

Enter base sequence A: ATCG
Enter base sequence B: CTAG

The binary encoding of base sequence A is: 0011
The binary encoding of base sequence B is: 1001

The bond energy of sequence A is: 10ε(k_b)T
The bond energy of sequence B is: 10ε(k_b)T

Both the molecules have the same melting point

>>
```

3 Using this code to find molecule with higher melting point

The above code can be used to compare the binding energy of two molecules and decide which of the molecules will have a higher melting point.

The **compare()** function in the code takes two strings as input and prints out the string with a higher melting point. This is done by iterating over the binary encoding of the string.

Whenever a 0 is encountered, it means it is an Adenine or Thymine molecule, which contains 2 H-bonds. Similarly whenever a 1 is encountered, it indicates a Cytosine or Guanine which contains 3 H-bonds. Hence, corresponding numbers are added to the total number of bonds and the bond energy is calculated. This is done in the **get_bond_energy**() function.

The **compare**() function then compares the bond energy and gives the one with a higher melting point.