Problem Definition:
You are given with a target protein-protein complex (experimental) structure and a list of (computational) docking decoys generated by some docking techqniue for the same protein structure. Write a program (in C or C++ or Python laguage) that for each decoys will compute the Interface Area, LRMSD, IRMSD, Fnat and Solvation Energy.

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Sample Input/Output:

Download the attached zip file and unzip it. You will get one directory and three files:

File: **target.pdb**
Directory: **Decoys**
File: **paper.pdf**
File: **SI.pdf**

target.pdb is the target protein dimeric complex structure file in PDB file format. There are two chains (column number 22) – **A** and **B**. **Chain A** is your **receptor** and **Chain B** is your **ligand**.

Using one docking algorithm, receptor and ligand was docked and the top 10 predictions as per the docking algorithm was scored and ranked. All of them are stored in **Decoys** directory.

You need to evaluate the goodness of the decoys by calculating the **Interface Area, Solvation Energy, LRMSD, IRMSD,** and **Fnat score**. Tabulate them as follows and store it as **Score.txt** file.

Filename | Interface Area | Solvation Energy | LRMSD | IRMSD | Fnat score
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complex1.pdb |
complex2.pdb |
...
...

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Create a directory **A2_<YourRollNo>**, copy your program file(s), **Score.txt** file, and a **README** file describing how to use your program or any other information that you need to pass. ZIP the file and upload in the moodle server within the deadline. Email submission is not allowed. ZERO tolerance for the plagiarism cases.

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The detailed definitions of **Interface Area, Solvation Energy, LRMSD, IRMSD,** and **Fnat score** can be found in the pdf files as per following instructions.

Reference:
In the attached Journal paper paper.pdf you will get the definition of
(i) Interface Area (at page 2, under **Interface Area** sub-section),
(ii) LRMSD, IRMSD, Fnat (at page 4, under **Evaluation Definitions** subsection)
(iii) Solvation energy (page 2 under **Solvation Energy** subsection and at **Table S1** of file **SI.pdf**).