GURU NANAK KHALSA COLLEGE OF ARTS, SCIENCE AND COMMERCE (AUTONOMOUS)

M.Sc. BIOINFORMATICS PRACTICAL EXAMINATION (Semester III)

Practical III (GNKPSBIP302) NOVEMBER 2022

SET 1

Total Marks: 50

Q.1 MAJOR QUESTION **20 MARKS**

Conformations studies are required for most ligand-based drug design methods, such as pharmacophore modeling, shape-based screening, and 3-D QSAR model building. However, conformer ensemble methods have focused on the reproduction of crystal structures for ligand-based modeling but the key question is how to generate a ligand alignment that produces the best results for a given query molecule.

Thus, researchers are interested in creating **3D atomic coordinates** from molecular connectivity via distance geometry and **conformer ensembles** using a multi-objective genetic algorithm for the **Emodin** phytochemical molecule.

Suggest suitable approach for generating various **structural conformations.**

Q.2 MINOR QUESTION **10 MARKS**

Drug target identification is a crucial step in drug designing. Therefore, when the 3D structures of the targets are available, the **problem of target identification** is usually converted to finding the **best interaction mode** between the **potential target candidates and small molecule probes.**

So, **Mr. X** working on ACE2 transmembrane protein which is considered as a receptor for spike protein binding of novel coronavirus (SARS-CoV2) though to design a new drug using natural phytochemical names as **Emodin**.**(Use the raw file from Q.1**)

Thus, based on the **spatial arrangement approach**,i.e. **Pharmacophore mapping** method , suggests a suitable web server which will help to identify **potential target candidates**

for the given **small molecules- Emodin .(Use the raw file from Q.1**)

Q.3 SPOTS **10 MARKS**

1. With respect to Druglikeness in SWISS ADME, what information can be obtained from the Lipinski rule of 5.

2. In ZincPharmer, what does the RSMD score indicate? What does a higher or lower RSMD value indicate?

3. With respect to the reverse pharmacophore mapping procedure using PharmMapper, what are the steps of the TriHash and genetic algorithm optimization?

4. With respect to describing/specifying what is the basic difference between SMILES and SMARTS format?

5. In which file formats can the 3D structures be saved and viewed?

Q.4 VIVA **05 MARKS**

Q.5 JOURNAL **05 MARKS**

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SET 2

Total Marks: 50

Q.1 MAJOR QUESTION **20 MARKS**

The problem in computational modeling is the **interconversion** of chemical structures between different **formats** where some standard **interchange formats** exist but the need to interconvert formats is a continuing problem due to the multitude of different application areas as well as differences in the data stored by **different formats.**

So suggest the research community in the field how to solve this **file format conversion issue** using an appropriate **open-source chemical toolbox**.

Query: Phytochemical Name (Drug): Chrysin

(File format conversion options given by the examiner)

Q.2 MINOR QUESTION **10 MARKS**

The efforts in the pharmaceutical industry have focused on optimizing the early phase hit-to-lead development of the drug discovery process. Thus, focus is on the generation and use of **virtual compound libraries** based on chemical feature **pharmacophore models** in combination with *in silico* screening is expanding.

So, **Mr. A** is searching for a relevant approach for his query (mentioned below) where compounds that **match** with a well-defined **pharmacophore** could be **searched / virtual screening** and serve as potential lead compounds for drug discovery. **(SUGGEST THE APPROACH)**

Query: ACE2 transmembrane protein (7JVO)
Phytochemical Name (Drug): Chrysin (Use the raw file from Q.1)

Q.3 SPOTS **10 MARKS**

1. What notation can be used to describe molecules, and which notation can be used to describe patterns?

2. With respect to the PaDEL (py), which file formats can be used to calculate the molecular descriptors?

3. According to the Pharmacokinetics in SWISS – ADME, what is Kp? What does a higher or a lower Kp value indicate?

4. What outputs are generated by the BALLOON software, and how are these outputs arranged?

5. The output generated by PaDEL (py) indicates descriptors and their respective values for the query molecule. Describe any 2 types of descriptors.

Q.4 VIVA **05 MARKS**

Q.5 JOURNAL **05 MARKS**

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SET 3

Total Marks: 50

Q.1 **MAJOR QUESTION** **20 MARKS**

In order to generate **QSAR models**,it is necessary to translate the molecular structures into numerical values that can be easily understood by computer algorithms, so that the most relevant characteristics for the studied bioactivity are selected and this characteristics is called as **molecular descriptors.**The numerical values of molecular descriptors are used to quantitatively describe the physical and chemical information of the molecules.

Therefore, researchers are interested to calculate the **molecular descriptors as well as fingerprint** for the **below** given molecules in order to find molecules with similar physical or chemical properties based on their similarity in the **descriptors values.**

Suggest a relevant approach for the same

Query: Kaempferol, Gingerol, Gallic acid

Q.2 **MINOR QUESTION** **10 MARKS**

To be effective as a drug, a potent molecule must reach its target in the body in sufficient concentration, and stay there in a bioactive form long enough for the expected biologic events to occur. Therefore, assessment of **toxicity** as well as evaluation of **pharmacokinetics and drug-likeness properties** plays an important role in drug designing studies.

So, **Mr. Y** is interested in doing the **pharmacokinetics and drug-likeness** prediction in his studies. (QUERY GIVEN BELOW)

Query: Kaempferol, Gingerol, Gallic acid (Retrieve the raw file from Q.1)

Q.3 SPOTS **10 MARKS**

1. Are 3D representations of chemical structures better than 2D representations? Why/Why not?

2. With respect to Open Babel, what does MMFF94 mean? What is the purpose of MMFF94?

3. Enlist any two disadvantages of Pharmacophore mapping?

4. Given a library of explicit compound conformations, conformers that match a 3D pharmacophore can be found using which two approaches? Give one disadvantage of each approach.

5. With respect to Lipophilicity in SWISS ADME, what does lipophilicity indicate? What should be the ideal iLOGP value for good oral and intestinal absorption?

Q.4 VIVA **05 MARKS**

Q.5 JOURNAL **05 MARKS**
