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M PHARM
(SEM II) THEORY EXAMINATION 2022-23
COMPUTER-AIDED DRUG DESIGN

Time: 3 Hours *Total Marks: 75*

Note: Attempt all Sections. If require any missing data; then choose suitably.

SECTION A

1. Attempt *all* questions in brief. **10 x 2 = 20**

(a) Outline the term pharmacophore with examples.

(b) Enumerate the various steric factors used in CADD.

(c) Explain Free-Wilson Analysis.

(d) What do you understand by Consensus scoring in docking.

(e) Differentiate local energy minima and global energy minima.

(f) How will you predict toxicity in in-silico screening?

(g) Discuss Lipinski rule of 5.

(h) Define Tanimoto coefficient.

(i) What do you understand by Craig's plot?

(j) Explain PCA analysis in statistics.

SECTION B

2. Attempt any *two*parts of the following: **2 x 10 = 20**

(a) Discuss the 3D QSAR CoMFA approach with its statistical method.

(b) Explain the concept of de novo drug design with a suitable example. Add its merits and demerits.

(c) Describe the various physicochemical properties in QSAR with specific examples.

SECTION C

3. Attempt any *five*parts of the following: **5 x 7 = 35**

(a) Describe the Homology modelling with its steps.

(b) Explain the concept of Pharmacophore mapping with relevant examples.

(c) Describe the components of docking with various scoring approaches.

(d) Explain the prediction of ADMET properties in drug design.

(e) Discuss the Hansch analysis with suitable example.

(f) Write short notes on any one method of structure based in-silico virtual screening in detail.

(g) Discuss the features of multiple linear regression statistical method in QSAR.