

**BIRLA INSTITUTE OF TECHNOLOGY, MESRA, RANCHI
(END SEMESTER EXAMINATION)**

**CLASS: BTECH
BRANCH: BIOTECHNOLOGY**

**SEMESTER : VI
SESSION : SP/2024**

SUBJECT: BE321 CHEMINFORMATICS

TIME: 3 Hours

FULL MARKS: 50

INSTRUCTIONS:

1. The question paper contains 5 questions each of 10 marks and total 50 marks.
 2. Attempt all questions.
 3. The missing data, if any, may be assumed suitably.
 4. Before attempting the question paper, be sure that you have got the correct question paper.
 5. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.
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		CO	BL
Q.1(a) What is distance key and SMILE?	[5]	1	1
Q.1(b) Write about PubChem and SWISSADME.	[5]	1	1
Q.2(a) What is pharmacophore, how permeability can be useful in characterizing small drug like molecule.	[5]	2	2
Q.2(b) State Lipinski rule of 5 and its importance in small molecule characterization.	[5]	2	2
Q.3(a) What is molecular descriptor? What are the types of descriptors, depending on their dimensions with example.	[5]	2	2
Q.3(b) How fingerprints are useful in cheminformatics?	[5]	2	3
Q.4(a) Describe and compare QSAR and QSPR.	[5]	3	2
Q.4(b) What is local docking? What are the scoring schemes used in docking?	[5]	3	3
Q.5(a) Different steps of computer aided drug design, with diagram describe.	[5]	3	3
Q.5(b) Describe ADMET properties and how it is useful in drug designing.	[5]	4	3

:::29/04/2024:::M