SCHOOL OF CHEMICAL AND LIFE SCIENCES
B-Sc-M.Sc. CHEMISTRY, SEMESTER-V ONLINE EXAMINATION-2020
PAPER TITLE: MOLECULAR MODELLING & DRUG DESIGN
PAPER CODE: BCH-DSE02TH

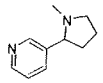
- *Please write your roll number at the top of the Answer sheet.*
- *Attempt all the questions*
- *It should be noted that 60min extra time will be provided for uploading the answer sheet in pdf format. Please mention the total number of sheets used on the first sheet and sequence of the answer sheet should be clearly mentioned at the top of every sheet used.*

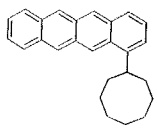
Duration: 3Hrs **Maximum Marks =75**

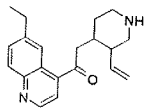
Q1. Answer the following brief: **15 x 1 = 15**

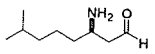
i. Define the Following terms (*any six*):
   a) Bond Length
   b) Bond angle
   c) Dihedral Angle
   d) Descriptors
   e) GRID
   f) Computational Cost

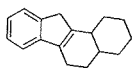
ii. Calculate the No of Rotatable bonds in the structures given below (ignore H-atoms).

a) 

b) 

c) 

d) 

e) 

iii. Write SMILE notations for
   a) isopropanol and
   b) acetone

iv. Expand the following terms (*any three*)
   a) RHF
   b) DFT
   c) GAMESS
   d) OPLS
   e) AMBER

Q2. Answer ANY THREE of the following **3 x 5 = 15**

i. What is morse potential? Explain the effect of morse potential on vibrational energy level.
ii. Define Induction enegy.
iii. How temperature terms are introduced in Dipole-Dipole interaction?
iv. Explain how to consider Lenard-Jones potential in Potential energy calculations of a system?
v. Explain dipole Polarizibility?

Q3. Answer ANY THREE of the following **3 x 5 = 15**

i. Define Chemical environment and explain its utility in deriding forcefield.
ii. How MM2 differs from MM1?
iii. Explain Born Oppenheimer approximation.
iv. Explain Dihedral Motion and bond bending
v. Explain Hooks law for two balls and two spring system.

Q4. Answer ANY THREE of the following **3 x 5 = 15**

i. Differentiate between the Structure based Drug designing and Ligand based Drug designing.
ii. Explain the importance of Test and Training set in QSAR.
iii. How Hammett plot is helpful in understanding the concept of Descriptor?
iv. Why 2D-, 3D-QSAR are not very successful in the Drug discovery process?
v. How we can use Lipinski's Rule as filter in LBDD?

Q5. Answer ANY THREE of the following: **3 x 5 = 15**

i. Explain how Lock and Key model is related with Michaelis Menten Equation?
ii. How binding and Active sites are recognized?
iii. Briefly classify different types of proteins and the basis for their considerations in the Lock and Key Model, Activated Complex Theory and Transition State model.
iv. Explain how Ramachandran plot is helpful in molecular modelling of protein?
v. Stepwise describe how to perform Docking calculations?

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