U.S.N.										

B.M.S. College of Engineering, Bengaluru-560019

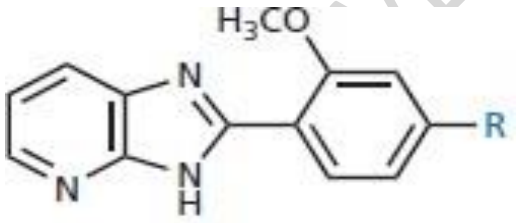
Autonomous Institute Affiliated to VTU

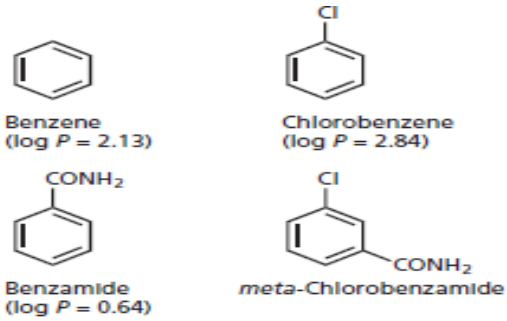
May / June 2025 Semester End Main Examinations

Programme: B.E. **Semester: VIII**
Branch: Biotechnology **Duration: 3 hrs.**
Course Code: 22BT8PEDRD **Max Marks: 100**
Course: Drug Discovery

Instructions: 1. Answer any FIVE full questions, choosing one full question from each unit.
2. Missing data, if any, may be suitably assumed.

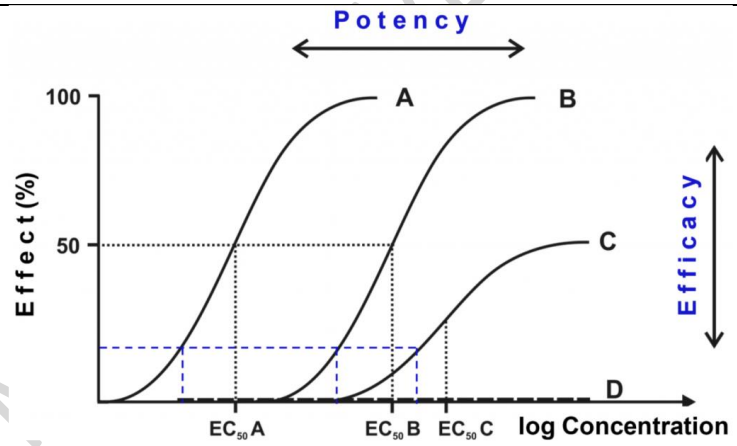
Important Note: Completing your answers, compulsorily draw diagonal cross lines on the remaining blank pages. Revealing of identification, appeal to evaluator will be treated as malpractice.

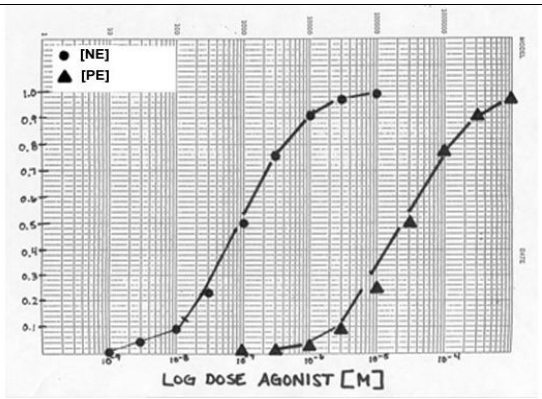
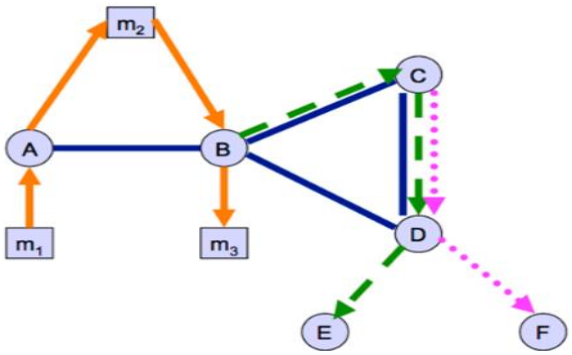
		UNIT - I	*CO*	*PO*	Marks
1	a)	List any three types of chemical databases and explain their salient features.	*CO1*	*PO 1*	**6**
	b)	The cardiotonic agent (I) was found to produce 'bright visions' in some patients. The log p of the drug was 2.59. The structure is shown below:  Where R = OCH_3 (i) Identify the nature of the drug (1M) (ii) What does log P value indicate, give its mathematical representation w.r.t octanol (3M) (iii) Why do you think this drug produced "bright visions" (1M) (iv) What alternative do you suggest for minimizing the formation of "bright visions "? Justify your answer (2M)	*CO2*	*PO 3*	**7**
	c)	What is QSAR? Give a general work flow for developing a QSAR model.	*CO1*	*PO 1*	**7**
		OR			
2	a)	Depict the process involved from hit identification to lead optimization using QSAR.	*CO1*	*PO1*	**10**

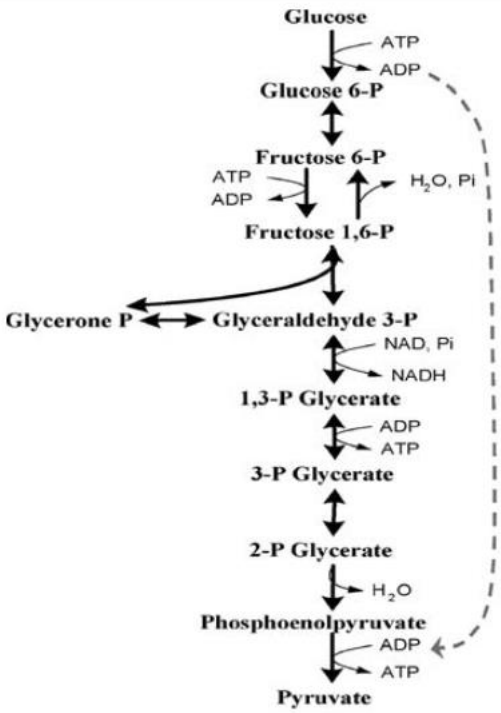
		b)	What is a pharmacophore? What is the role of pharmacophore modelling in drug design?	*CO2*	*PO 3*	**6**
		c)	The below table gives the π values of different groups Values of π for a range of substituents (table) If the log P of: benzene =2.13 ; chlorobenzene =2.84; benamide =0.64  Values for log P. (i) What is the π ? (ii) What does the positive and negative value of π indicate (iii)Calculate the log P value of Chlorobenzamide	*CO2*	*PO3*	**4**
			UNIT - II			
	3	a)	Differentiate between metabolic pathway database & Metabolomic databases .Give 2 examples each.	*CO3*	*PO5*	**6**
		b)	Which pathway database is specifically designed to facilitate clinical ‘‘omics’’ studies, with a specific emphasis on clinical biochemistry and clinical pharmacology? Explain the salient features of this database (any 4)	*CO3*	*PO5*	**8**
		c)	Differentiate between “Pharmabrowse” and “Geno browse” tools in drug bank.	*CO3*	*PO5*	**6**
			OR			
	4	a)	Identify the query tool of HMDB that can be used in the following cases : 1) identify a novel biomarker for a given condition or disease given an NMR or GC/MS or MS/MS spectrum of the purified compound 2) identify metabolites from a biofluid mixture that has been analyzed by NMR, GC/MS or MS/MS 3) identify a disease or condition given a list of metabolites 4) identify a pathway or process that has been altered/perturbed given a list of metabolites obtained from a metabolomic experiment	*CO3*	*PO5*	**12**

Values of π for a range of substituents

Group	CH_3	*t*-Bu	OH	OCH_3	CF_3	Cl	Br	F
π (aliphatic substituents)	0.50	1.68	–1.16	0.47	1.07	0.39	0.60	–0.17
π (aromatic substituents)	0.52	1.68	–0.67	–0.02	1.16	0.71	0.86	0.14

			5) determine normal and abnormal concentration ranges for metabolites in different biofluids 6) obtain authentic standards of unique metabolites to confirm the diagnosis of a certain disease 7)determine the similarity of a newly found/synthesized compound to an existing metabolite 8) determine the possible mechanism of action or protein targets for a newly discovered/synthesized metabolite or metabolite analogue 9) diagnose or determine the cause of illnesses thought to be brought on by metabolite changes 10) extract detailed information on metabolites, metabolicdiseases or metabolic pathways 11) extract information on common metabolite classes 12) ascertainwhether a certain protein or protein homologue may also be involved in a metabolic process or pathway			
	b)	Differentiate between partitioning and hierarchial clustering algorithms.	*CO 4*	*PO 5,12*	**8**
		UNIT - III			
5	a)	Differentiate between : i. Agonist & Antagonist ii. Safety index & therapeutic index iii. Potency & Intrinsic efficacy	*CO2*	*PO3*	**6**
	b)	 The dose response curves of four drugs A-D is shown. (i) Identity the drug(s) which are full agonists, partial agonists, full antagonist, partial antagonist. (ii) What is the intrinsic activities of the four drugs	*CO2*	*PO3*	**8**
	c)	"Ligand-based drug design is a method that leverages knowledge of existing molecules that bind to a target to identify new drug candidates." Justify this statement explaining the workflow involved.	*CO2*	*PO3*	**6**

			OR			
	6	a)	Give a graphical representation of the dose response curves of agonists, partial agonists, antagonist & inverse agonist.	*CO2*	*PO3*	**4**
		b)	"Computer-Aided drug design is the most beneficial method in early-phase drug discovery." Justify this statement explaining the workflow involved.	*CO3*	*PO5*	**10**
		c)	 A dose response curve of two drugs Norepinephrine[NE] and phenylephrine [PE] is shown. (i) Which drug has a high affinity . Justify (ii) what is the nature of these drugs? (iii)What is the intrinsic activity of the drugs? (iv)What factors that determine the effect of a drug on physiologic processes.	*CO2*	*PO3*	**6**
			UNIT - IV			
	7	a)	 Shown above is an example of a biological network. Label the  following notations.	*CO3*	*PO5*	**6**

		b)	Given a gene network $G = (V, E)$ and given its subnetwork $G\_ = (V',E')$ centered at gene X. That is, G' includes gene X, all those genes from which gene X is reachable and all those genes that are reachable from gene X. (a) What kind of changes in this subnetwork G' might be expected if all incoming edges of gene X would be deleted? (b) Which changes in the subnetwork G' might be expected if all outgoing edges of gene X would be deleted?	*CO3*	*PO5*	**8**
		c)	Give a diagrammatical representation of a signal transduction path /network and a metabolic path.	*CO3*	*PO5*	**6**
			OR			
	8	a)	For the metabolic pathway shown as studies in biochemistry , reconstruct the pathway as a metabolic network / give agraphical representation of the connection structure 	*CO3*	*PO5*	**10**
		b)	Give a Workflow for metabolic network reconstruction from the genome annotation.	*CO3*	*PO5*	**10**
			UNIT - V			
	9	a)	Enumerate on the role of AI in personalized medicine w.r.t enhancing diagnosis accuracy and treatment	*CO4*	*PO5, 12*	**8**
		b)	Differentiate between "personalized medicine "and "precision medicine".	*CO4*	*PO5, 12*	**4**
		c)	"Personalized healthcare enhances treatment effectiveness through the customization of therapies based on genetic, environmental, and lifestyle factors." Justify this statement explaining role of personalized medicine in treatment of lung cancer.	*CO4*	*PO5, 12*	**8**

			OR			
	10	a)	Genomic technologies are the basis for developing " Personalised medicine" . Justify this statement explaining the different methodologies (any 2) . Add a note on their advantages and disadvantages .	*CO4*	*PO5, 12*	**10**
		b)	The AI boom, including the advent of large language models (LLMs) and their associated chatbots, poses new challenges for privacy .In this context ,what measures can be taken for maintaining data privacy ?	*CO4*	*PO5, 12*	**10**

****