Reg.No. _____

Karunya UNIVERSITY

(Karunya Institute of Technology & Sciences)
(Declared as Deemed-to-be University under Sec.3 of the UGC Act, 1956)

End Semester Examination – Nov/Dec – 2016

Code : Cheminformatics and QSAR
Sub. Name : 14BI2027

Semester : 2016-17 ODD
Duration : 3hrs
Max. marks : 100

ANSWER ALL QUESTIONS (5 x 20 = 100 Marks)

Q. No.	Sub Div.	Questions	Course Outcome	Marks
1.	a.	Write in detail about scope of Cheminformatics in pharmaceutical development.	CO1	**10**
	b.	What is SMILES notation? Write in detail about the SMILES rules with an example.	CO1	**10**
		(OR)		
2.	a.	How to define similarities between compounds? Discuss in detail.	CO1	**10**
	b.	Write in detail about all information related to small molecule structure searching by using Drug Bank.	CO1	**10**
3.	a.	Discuss in detail about the Drug Discovery and Development process and their Technological impact in Cheminformatics.	CO2	**15**
	b.	What is Doking? Write in brief about the mechanics of Docking function.	CO2	**05**
		(OR)		
4.	a.	Write in detail about the Strcuture Based Drug Design (SBDD) methods with and illustration.	CO2	**10**
	b.	Write in detail about the Ligand Based Drug Design (LBDD) methods with and illustration.	CO2	**10**
5.	a.	Write in detail about the pharmacophore modeling importance in pharmaceutical development.	CO3	**10**
	b.	What do you mean by QSAR? Write in detail about steps involved in QSAR and their importance in pharmaceutical development.	CO3	**10**
		(OR)		
6.	a.	Write in detail about the Cheminformatics approaches in target identification and validation with one case study.	CO2	**20**
7.	a.	Write in detail about the Computational approaches in lead identification and validation with example.	CO2	**20**
		(OR)		
8.	a.	Write in detail about Pharmacophore mapping and its applications in pharmaceutical development.	CO2	**10**
	b.	Write in detail about the deriving a QSAR equation, MLR-Square correlation coefficient, and Validation coefficient.	CO3	**10**
		Compulsory:		
9.	a.	Write in detail about 2D QSAR methodology with flow chart.	CO3	**10**
	b.	Write in detail about the 3D QSAR methodology with an illustration.	CO3	**10**

ALL THE BEST