

KARPAGAM ACADEMY OF HIGHER EDUCATION

(Deemed to be University) (Established Under Section 3 of UGC Act 1956) Coimbatore – 641 021. (For the candidates admitted from 2018 onwards)

DEPARTMENT OF CHEMISTRY

SUBJECT NAME: CHEMINFORMATICS-PRACTICAL SUBJECT CODE: 16CHU511A SEMESTER: V CLASS: III B.Sc CHEMISTRY

Programme objectives

The course helps the student to

1. Understand and apply the applications of chemiinformatics in drug design.

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The course enable the student to

1. Apply the applications of chemiinformatics in drug design.

Hands-on Exercises

Application of Chemoinformatics in Drug Design

Suggested Readings

Text Books:

- 1. Andrew R. Leach & Valerie, J. Gillet. (2007). An introduction to Chemoinformatics. Springer: The Netherlands.
- 1. Gasteiger, J. & Engel, T. (2003). *Chemoinformatics: A text-book.* Wiley-VCH.

Reference Book

1. Gupta, S. P. (2011). QSAR & Molecular Modeling. New Delhi: Anamaya Pub.



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LECTURE PLAN

Total no. of hours: 48

S.NO	LECTURE DURATION	TOPICS TO BE COVERED	SUPPORT MATERIALS
1.	3	Procedure writing	
2.	3	Drawing Chemical structure using chemdraw	
3.	3	Elemental Analysis, Molecular weight & m/z values	
4.	3	Predict the ¹ H-NMR using chemdraw	
5.	3	Predict the C ¹³ -NMR using chemdraw	
6.	3	Determination of chemical properties, melting point and boiling point etc	
7.	3	Convert name into structure and vice versa	
8.	3	Find the structure using protein bank	
9.	3	Molecular docking	
10.	3	Viva-voce	
11.	3	Model examination	
12.	3	Model examination	