

FEDERAL UNIVERSITY OF CEARÁ Provost Office of Research and Graduate Studies

COURSE PROGRAM

1. PROGRAM:				
Program	GRADUATE PROGRAM IN CHEMISTRY			
2. COMPONENT TYPE:				
Activity () Cou		ırse (X)	Module ()	
3. LEVEL:				
Master´s		Degree ()	Doctorate (X)	
4. COMPONENT IDENTIFICATION:				
Name:		MEDICINAL CHEMISTRY		
Code:		CEP9433		
Hours:		64		
Credits:		04		
Optional course:		Yes (x)	No ()	
Compulsory course:		Yes ()	No (x)	
Area:		CHEMISTRY, ANALYTICAL CHEMISTRY, INORGANIC CHEMISTRY, ORGANIC CHEMISTRY AND PHYSICAL-CHEMISTRY		
5. PROFESSOR:				

6. ABSTRACT:

Study of the structural aspects of substances and their relationship with biomacromolecules, in order to investigate molecules from their atomic constitution (through structure-property relationships, SPR) to their structural characteristics and their interactions with biological targets of therapeutic interest.

7. COURSE PROGRAM:

Definition and evolution of Medicinal Chemistry;

Notions of Molecular Modeling; Study of molecular properties of drug candidates: logP, Solubility, pKa, surface tension;

Application of *in silico* methods to establish molecular properties using free access computer programs: Marvin, VCCLab, Molinspiration, among others;

Performing virtual screening of biological activities;

Selection of enzymatic targets of therapeutic interest: use of PDB (Protein Data Bank); Natural products in Medicinal Chemistry.

Contributions of Inorganic Chemistry to Medical Chemistry.

8. EVALUATION PROCESS:

The evaluation will be carried using a computer with internet access (40%), preparation and presentation of seminars (30%) and production of textual material (30%).

9. BIBLIOGRAPHY:

- 1. ANDREI, C. C.; FERREIRA, D. V.; FACCIONE, M.; FARIA, T. J. Da Química Medicinal a Química Combinatória Modelagem Molecular, Ed. Manole; 2ª Ed. Barueri, 2012, 168p.
- 2. BARREIRO, E. J.; FRAGA, C. A. M. Química medicinal: bases moleculares da ação dos fármacos. 3. ed. Porto Alegre: Artmed, 2015. 608 p.
- 3. LEMKE, T. L.; WILLIAMS, D. A.; ZITO, W. Foye's Principles of Medicinal Chemistry, 7th Ed., Media, Lippincott Williams & Wilkins, 1520 p. 2012.
- 4- PATRICK, G. L. An Introduction to Medicinal Chemistry, 6th Ed., Oxford University Press, 2017.
- 5. WERMUTH, C. G.; ALDOUS, D.; RABOISSON, P.; ROGNAN, D. The Practice of Medicinal Chemistry, 4th Ed., Amsterdam: Ed Elsevier, 902 p. 2015.
- 6. WITTY, D.; COX, B. Progress in Medicinal Chemistry, v. 58. Amsterdam: Ed Elsevier, 2019.