Study program : Chemistry

Type and level of studies: PhD studies of chemistry - BIOCHEMISTRY

Course unit: Biochemistry of Physiologicaly Active Compounds

Teacher in charge : Milan Mladenović, PhD, Associate Professor

Language of instruction : English

ECTS: 10

Prerequisites: Entered PhD studies of chemistry - BIOCHEMISTRY

Semester: Summer semester

Course unit objective

Student will be introduced with the term „Phisiologicaly Active Compound". Biochemical assays used in determication of activity of phisiologicaly active compounds. Bioactive compound in phisiological conditions and its activity. Introduction to the molecular modeling methods in biochemistry. Compound's intractions on protein and nucleic acids level. Bioactive conformation. Structure-activity relationships (SAR). Quantitative structure-activity relationships (QSAR). Three dimenstional Quantitative structure-activity relationships (3-D QSAR). Pharmacophore. 3D Pharmacophore. Lead and hit compounds for design, future synthesis and evaluation.

Learning outcomes of Course unit

Recognition of chemical structures that bears biological activity. Chemical modification in order to enhance the activity (Bioisosters). Correlation of biological activity and phisico-chemical parameters of compound (SAR, QSAR, 3-D QSAR). Molecular modeling of phisiologicaly active compound on enzyme, receptor or DNA level. Rational Drug Design.

Course unit contents

Theoretical classes.

The therm pharmacophore. Structure-activity relationships (SAR). Quantitative Structure-activity relationships (QSAR). Inhibitor-enzyme interactions. Inhibitor-DNA interactions. Molecular modeling. Molecular docking. 3-D Pharmacophore. 3-D Quantitative Structure-activity relationships (3-D QSAR) CoMFA, CoMSIA, GRID methodology. Structure-based drug design. Ligand-based drug design. ADMETox and its predicitions. Molecular dynamics.

Experimental classes

Competitive inhibition of enzyme reactions. QSAR model generations. RCSB Protein Data Bank survey for inhibitor-enzyme co-crystalized complexes (www.rcsb.org). Molecular docking using AutoDock, AutoDock Vina, DOCK6, PLANTS, and Paradocks. Molecular modeling with Schrödinger Suite. Ligand-based alignment using Baloon, Shaep, SurflexSim and Open3DAlign. SB and LB 3-D QSAR models using Sybyl Tripos. 3-D Pharmacophore using Discovery Studio. ADMETox features using Discovery Studio. Rational Drug Design.

Literature

1. G. Thomas, *Medicinal Chemistry*, John Wiley and Sons, Ltd. England, 2000.
2. G. L. Patrick, *An Introduction to Medicinal Chemistry*, 4th ed., Oxford University Press, England, 2009.
3. Burger's Medicinal Chemistry and Drug Discovery
4. Hugo Kubinyi, 3D QSAR in Drug Design: Volume 1: Theory Methods and Applications, Springer Science & Business Media, 1993
5. Hugo Kubinyi, 3D QSAR in Drug Design: Volume 2: Ligand-protein interactions and Molecular SimilarityTheory Methods and Applications, Springer Science & Business Media, 1995

Number of active teaching hours				**Other classes**
Lectures: 5	Practice:	Other forms of classes: *mentoring system*	Independent work:	

Teaching methods

Lectures, seminars, practical classes

Examination methods (maximum 100 points)

Exam prerequisites	**No. of points:**	**Final exam**	**No. of points:**
Student's activity during lectures	10	oral examination	
practical classes/tests	20	written examination	50
Seminars/homework	20	.....	
Project			

Other			
Grading system			
Grade	**No. of points**	**Description**	
10	**90-100**	Excellent	
9	**80-90**	Exceptionally good	
8	**70-80**	Very good	
7	**60-70**	Good	
6	**50-60**	Passing	
5	**<50**	Failing	