

Course: In Silico Toxicology

Lecturer: Spyros Karakitsios

Date: 12-16/6/2017

Classroom: 1-15 @ IUSS

Course schedule

Week	Date	Lecture hours	Tutorial hours	Subject	Tot h
		From To	From To		
1	12/6/2017	10 a.m. – 1 p.m.	2 p.m. - 5 p.m.	<i>In silico</i> toxicology in modern risk assessment	6
	13/6/2017	10 a.m. – 1 p.m.	2 p.m. - 5 p.m.	Physiology based biokinetic modelling	6
	14/6/2017	10 a.m. – 1 p.m.	2 p.m. - 5 p.m.	QSARs for parameterizing PBBK models	6
	15/6/2017	10 a.m. – 1 p.m.	2 p.m. - 5 p.m.	QSARs for toxicity assessment	6
	16/6/2017	10 a.m. – 1 p.m.	2 p.m. - 5 p.m.	Bioinformatics	6

Brief Contents Description and Course Syllabus:

- 1) *In silico* toxicology in modern risk assessment
 - a) Fundamentals. Risk analysis. Toxicity methods. Computational toxicology
 - b) Lab analysis and in silico toxicology.
- 2) Physiology based biokinetic modelling
 - a) Administration, distribution, metabolism and elimination.
 - b) Age dependent physiology differences, in utero exposure, exposure reconstruction from biomonitoring data.
- 3) QSARs for parameterizing PBBK models
 - a) Chemometrics, physicochemical properties, interaction with molecular targets.
 - b) Machine learning, statistics, model development.
- 4) QSARs for toxicity assessment
 - a) Structural alerts, carcinogenicity, endocrine disruption, neurotoxicity
 - b) Application of machine learning, validation with in vitro and in vivo data
- 5) Bioinformatics
 - a) Multi-omics data, big data, data processing, data clustering
 - b) Pathway analysis, development of adverse outcome pathways