Course ID: HDOA16	**Course name: COMPUTATIONAL CHEMISTRY**		
Cycle: THIRD	**Year: FIRST**	**Semester: I**	**ECTS credits: 15**
Course status: ELECTIVE		**Total course hours:** Lectures: 45 Laboratory: 45	

Teaching participants:	**Teachers and associates with expertise in the field to which the subject belongs**
Prerequisite for enrollment:	-
Course aims:	Introduction to the theory and application of computer methods, construction modeling molecules and reaction mechanisms
Thematic course units:	1. Computational models, theoretical foundations. Optimization methods: ab initio, semi-empirical methods, molecular mechanics. Simulating the spectrum. Visualization of structures. 2. Programs: Gaussian, Spartan, PyMol, AutoDoc 3. Prediction of the molecular structure of small molecules and their reactivity, by modeling transition structures, and intermolecular interaction
Learning outcomes:	
Teaching methodology:	

Assessment methods and grading system[1]:

Grading criteria			
	Criteria	Maximal score	Required score
1.	Tests	1x20	11
2.	Seminars	1x40	22
3.	Final exam	40	22
	Total	100	55

Scores and grading		
Score	Grade (BiH)	Grade (ECTS)
< 55	5	F, FX
55–64	6	E
65–74	7	D
75–84	8	C

[1]The grading structure for each subject is determined by the Council of the organizational unit before the beginning of the academic year in which the subject is taught as per Article 64, paragraph 6 of the Law on Higher Education of Sarajevo Canton

	85–94	9	B
	95–100	10	A
Literature[2]:	Mandatory literature: 1. C.C. Cramer,: Essentials of Computational Chemistry: Theories and Models, Wiley, NY, 2 nd Ed, 2006 2. J.B.Foresman, E. Frish:Exploring chemistry with electronic structure method, Gaussian Inc. Pittsburg, PA, 2000 3. Interna skripta Supplementary literature:		

[2]The Senate of the higher education institution, as an institution, or the Council of the organizational unit of the higher education institution, as a public institution, determines by a special decision, which is published on its website before the beginning of the academic year obligatory, mandatory and recommended textbooks and manuals, as well as other recommended literature based on which exams are prepared and taken as per Article 56, paragraph 3 of the Law on Higher Education of the Sarajevo Canton