COMPUTATIONAL CHEMISTRY

1	Course Title:	COMPUTATIONAL CHEMISTRY
2	Course Code:	KIM4078
3	Type of Course:	Optional
4	Level of Course:	First Cycle
5	Year of Study:	4
6	Semester:	8
7	ECTS Credits Allocated:	5.00
8	Theoretical (hour/week):	3.00
9	Practice (hour/week):	0.00
10	Laboratory (hour/week):	0
11	Prerequisites:	
12	Language:	Turkish
13	Mode of Delivery:	Face to face
14	Course Coordinator:	Doç. Dr. YELİZ ULAŞ
15	Course Lecturers:	
16	Contact information of the Course Coordinator:	Doç.Dr. Yeliz ULAŞ yelizulas@uludag.edu.tr 0224-2942867 Bursa Uludağ Üniversitesi Fen-Edebiyat Fakültesi Kimya Bölümü
17	Website:	
18	Objective of the Course:	Understanding basic concepts in computational chemistry and their relationship with organic chemistry
19	Contribution of the Course to Professional Development:	Have basic skills in computational organic chemistry Learning the difference between Experimental and Theoretical Organic chemistry To have knowledge about programs that examine macro organic molecules
20	Learning Outcomes:	

	1	Have basic skills in computational organic chemistry
	2	Learning the difference between Experimental and Theoretical Organic chemistry
	3	To have knowledge about programs that examine macro organic molecules
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21	Course Content:	
	Course Content:	
Week	Theoretical	Practice
1	Basic concepts in computational chemistry	

2	Fundamentals of quantum mechanics and molecular orbital methods	
3	Hartree-Fock (HF) approaches, Ab initio method	
4	Things to consider in basic calculations of molecules	
5	Techniques and theoretical calculations used in structural analysis	
6	Deviations in Theoretical Calculations	
7	Electrostatic potential, electron and spin densities	
8	Intramolecular/Intermolecular Interactions	
9	Electronic Structure and Magnetic Properties	
10	Reaction Mechanisms in Computational Chemistry	
11	Computer programs used in 3-dimensional drawing of molecules	
12	Introduction to Density Functional Theory (DFT)	
13	Comparison of Experimental and Theoretical Analyzes	
14	Use of DFT in Multidisciplinary Fields	

22	Textbooks, References and/or Other Materials:	1) Density Functional Theory,, David S. Sholl, Janice A. Steckel, Wıley, 2012 2)Essentials of Computational Chemistry: Theories and Models, Christopher J. Cramer, John Wiley & Sons Inc, 2nd, 2004
23	Assesment	

TERM LEARNING ACTIVITIES	**NUMBER**	**WEIGHT**
Midterm Exam	1	40.00
Quiz	0	0.00
Home work-project	0	0.00
Final Exam	1	60.00
Total	2	100.00
Contribution of Term (Year) Learning Activities to Success Grade		40.00
Contribution of Final Exam to Success Grade		60.00
Total		100.00
Measurement and Evaluation Techniques Used in the Course		relative evaluation

24	**ECTS / WORK LOAD TABLE**

Activites	Number	Duration (hour)	Total Work Load (hour)
Theoretical	14	3.00	42.00
Practicals/Labs	0	0.00	0.00
Self study and preperation	0	0.00	0.00
Homeworks	0	0.00	0.00
Projects	0	0.00	0.00
Field Studies	0	0.00	0.00
Midterm exams	1	40.00	40.00
Others	0	0.00	0.00
Final Exams	1	72.00	72.00
Total Work Load			154.00
Total work load/ 30 hr			5.13
ECTS Credit of the Course			5.00

25	CONTRIBUTION OF LEARNING OUTCOMES TO PROGRAMME QUALIFICATIONS															
	PQ1	**PQ2**	**PQ3**	**PQ4**	**PQ5**	**PQ6**	**PQ7**	**PQ8**	**PQ9**	**PQ10**	**PQ11**	**PQ12**	**PQ13**	**PQ14**	**PQ15**	**PQ16**
ÖK1	5	5	5	5	5	5	5	5	5	5	5	5	5	5	0	0
ÖK2	4	5	5	5	4	5	5	4	5	4	5	4	5	5	0	0
ÖK3	4	5	5	4	4	5	4	4	4	4	5	5	5	5	0	0

LO: Learning Objectives PQ: Program Qualifications

Contribution Level:	**1 very low**	**2 low**	**3 Medium**	**4 High**	**5 Very High**