UNIVERSITAS NEGERI YOGYAKARTA
FACULTY OF MATHEMATICS AND NATURAL SCIENCES
DEPARTMENT OF CHEMISTRY
1 Colombo Street Yogyakarta 55281
Phone (0274) 565411, Ext. 1398, Fax (0274)548203
Website: http://kimia.fmipa.uny.ac.id, E-mail: kimia@uny.ac.id

Module name:	Computational Chemistry
Module level, if applicable:	Undergraduate
Code:	KMA6216
Sub-heading, if applicable:	-
Classes, if applicable:	2
Semester:	6th
Module coordinator:	Dr. Suwardi
Lecturer(s):	1. Dr. Suwardi 2. Dr. Crys Fajar Partana
Language:	Bahasa Indonesia
Classification within the curriculum:	Compulsory Course
Teaching format / class hours per week during the semester:	• Lectures: 50 minutes lectures, 60 structured activities and 60 individual study per week • Laboratory work: 170 minutes includes the laboratory work and it's reporting per week
Workload:	Total workload of the activity is 90,67 hours per semester which consists of 50 minutes lectures, 60 structured activities and 60 individual study and also 170 minutes laboratory work with it's reporting per week for 16 weeks
Credit points:	2 SKS (3 ECTS) with the details of 1 SKS (2 ECTS) lectures and practical work of 1 SKS (2 ECTS)
Prerequisites course(s):	Mathematics for Chemistry, Quantum Chemistry
Course Outcomes	After taking this course, the students have ability to: CO1. Students can explain the scope of computational chemistry CO2. Students can explain the method of molecular mechanics (force field method) CO3. Students can explain the molecular dynamics method CO4. Students can explain surface potential energy CO5. Students can explain the Hartree-Fock molecular orbital theory CO6. Students can explain Base sets CO7. Students can explain geometry optimization CO8. Students can explain density functional theory (DFT) CO9. Students can explain solvation and exampes of it's application
Content:	Computational Chemistry courses cover learning about the basic concepts in molecular mechanics and quantum mechanics and their applications especially in studying the structure and dynamics of fluid systems (solvation), theoretical approaches such as HF (Hartree-Fock) theory, DFT (Density Functional Theory) and Force Field Methods (Molecular Mechanics); In this study, it will be studied/

<table>
<tr><td></td><td>demonstrated the use of some computational chemistry software such as Gaussian, Turbomole, Hyperchem and Gromacs in solving chemical problems and interface programs such as Gaussview, Tmolex and VMD in processing data on simulation and modeling results.</td></tr>
<tr><td>Study/ exam achievements:</td><td>The final mark will be weight as follow:
<table>
<tr><th>No</th><th>CO</th><th>Assessment Object</th><th>Assessment Technique</th><th>Weight</th></tr>
<tr><td rowspan="6">1</td><td rowspan="6">CO1, CO2, CO3, CO4, CO5, CO6, CO7, CO8, CO9</td><td>Individual assignment</td><td>Assignment</td><td>15%</td></tr>
<tr><td>Structural assignment</td><td>Assignment</td><td>15%</td></tr>
<tr><td>Practical work</td><td>Observation Report</td><td>20%</td></tr>
<tr><td>Mid-term exam</td><td>Written test</td><td>20%</td></tr>
<tr><td>Final exam</td><td>Written test</td><td>30%</td></tr>
<tr><td colspan="3">Total</td><td>100%</td></tr>
</table></td></tr>
<tr><td>Forms of media:</td><td>Board, LCD Projector, handouts, PPT slides, laboratory kits, and stationaries</td></tr>
<tr><td>Reference:</td><td>A. Ponnadurai Ramasami, 2020, Computational Chemistry Methods: Applications, 1st ed., De Gruyter
B. Frank Jensen, 2017, Introduction to Computational Chemistry, 3rd ed., Wiley
C. Vigo-Aguiar, J., Ramos, H. 2017, Recent mathematical–computational techniques and models in chemistry. J Math Chem 55, 1367–1369
D. Korb, O., Stützle, T., Exner, T.E., 2011, Accelerating molecular docking calculations using graphics processing units. J. Chem. Inf. Model. 51, 865–876
E. COMPUTATIONAL CHEMISTRY : Introduction to the Theory and Applications of Molecular and Quantum Mechanics (Errols Lewars)
F. COMPUTATIONAL CHEMISTRY: A Practical Guide for Applying Techniques to Real-World Problems (David C Young)
G. Exploring Chemistry with Electronic structure Methods (James B Foresman)</td></tr>
</table>

PLO and CO mapping

CO	PLO									
	Attitude	Generic Skills		Knowledge				Specific Skills		
	PLO1	PLO2	PLO3	PLO4	PLO5	PLO6	PLO7	PLO8	PLO9	PLO10
CO1							√			
CO2							√			
CO3							√			
CO4							√			
CO5										√
CO6										√
CO7										√

CO8										√
CO9				√						