IPB UNIVERSITY
FAKULTAS MATEMATIKA DAN ILMU PENGETAHUAN ALAM
DEPARTEMEN KIMIA

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SEMESTER LEARNING PLAN

KIM 545
COMPUTATIONAL CHEMISTRY
LEARNING OUTCOMES

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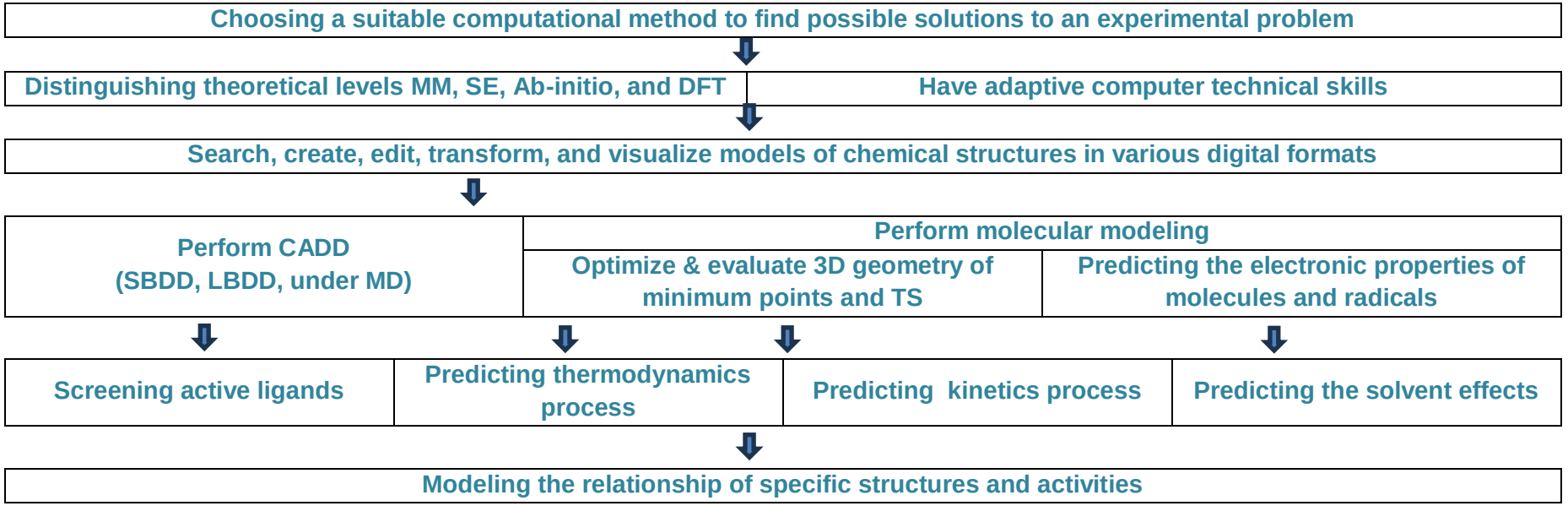
INSTRUCTIONAL ANALYSIS

This course discusses the understanding and scope of computational chemistry, the concept of surface potential energy, the basics of molecular orbital theory, molecular mechanics modeling methods, molecular dynamics, semiempirical, ab-initio, density function theory, and the use of computational chemistry to determine molecular characteristics and quantitative structure-activity relationships.



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SEMESTER LEARNING PLAN

Course Name	:	COMPUTATIONAL CHEMISTRY
Code / Semester Credit System	:	KIM545
Semester	:	Odd (Semester 7)
Course Description	:	This course discusses the understanding and scope of computational chemistry, the concept of surface potential energy, the basics of molecular orbital theory, molecular mechanics modeling methods, molecular dynamics, semiempirical, *ab-initio*, density function theory, and the use of computational chemistry to determine molecular characteristics and quantitative structure-activity relationships.
Prerequisite Courses	:	MAT1102
Course Learning Outcomes (CPMK)-Learning *Outcomes*	:	1 Students can choose and classify the types/specifications of computers and software that suit their application needs. 2 Students can take advantage of the features and operate the software according to their application needs. 3 Students can calculate, simulate, and interpret the chemical properties (electronic & molecular) of atoms and molecules. 4 Students can fully apply the concept of computational chemistry in solving simple problems in the field of chemistry through case studies.
Study Materials on the *RSC Chemical Curriculum Map)*[2)]	:	
Divisions/Fields of Science	:	Department/Chemistry
Lecturers (Teaching Team)	:	1. Dr. Mohammad Khotib, SSi, MSi – (MKH); 2. Lutfan Irfana, MSi-(LHI)

[1)]Response/practicum activities are expressed in credits, not in the number of hours;

[2)]see the Excel file Chemistry Curriculum Map from RSC

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I. LESSON PLAN

Week of -	Expected end capability-sub-LO	Study materials (teaching materials)	Learning methods	Estimated time	Student learning experience	Assessment			Reference
						Criteria	Indicator	Weight (%)	
(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)
1 (LHI/MKH)	COMPUTER AND SOFTWARE LITERACY IN CHEMISTRY AND COMPATIBILITY WITH EXISTING OS	a Distinguishing MM, SE, Ab-Initio, and DFT theory levels b Have adaptive computer technical skills (Shell scripting, Python)	➢ Establish learning groups ➢ Material submission (offline/online) ➢ Software installation tutorials for single, group, interaction modeling and calculation applications ➢ Assignment	8 hours	Students can choose and classify the types/specifications of computers and software that suit their application needs.	a Activity reports in through presentations (PPt) or videos b Presentation of activities	Report in video to present the results of activities with indicators as in the Table in the assessment design	8%	1-5
2	FEATURE INTRODUCTION AND SIMPLE OPERATION OF THE SOFTWARE USED	a Search, create, edit, transform and visualize models of chemical structures in a variety of digital formats. b SBDD (rigid docking, flexible docking) c LBDD (Data collection and cleaning, SVM, MLR) d MD (preparation, running, analysis)	✓ Material Submission (offline/online) ✓ Software features and operation tutorials (compiling models of atoms, molecules, groups, interactions) ✓ Presentation/video of learning summary	22 hours	Students can take advantage of the features and operate the software according to their application needs	a Activity reports in the form of presentations (PPT) or videos b Presentation of activities	Report in Video to present the results of activities with indicators as in the Table in the assessment design	25%	
3	APPLICATION OF SOFTWARE FOR THE CALCULATION OF CHEMICAL PROPERTIES OF MOLECULES	a Optimize & evaluate 3D geometry of minimum points and TS. b Predicting the electronic properties of molecules and	✓ Material submission (offline/online) ✓ Software application tutorials (electronic, molecular, spectroscopic	36 hours	Students can calculate, simulate, and interpret the chemical properties (electronic &; molecular) of atoms and molecules	a Activity reports in the form of presentations (PPT) or videos b Presentation of activities	Report in video to present the results of activities with indicators as in the table in the assessment design	40%	

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		radicals. c Predicting process thermodynamics d Predicting the influence of solvents. e Modeling the relationship of specific structures and activities (QSAR/QSPR)	properties, etc ✓ *Presentation/video of learning summary*						
4	CASE STUDY "Simple problem-solving in chemistry"	Final Project	✓ Material Delivery (offline / online) and distribution of case study topics ✓ Regular assistance for the completion of case studies ✓ Presentation/video of learning summary ✓ Writing scientific Articles from case studies	24 hours	Students can fully apply the concept of computational chemistry in solving simple problems in the field of chemistry through case studies	a Activity reports in the form of presentations (PPt) or videos b Presentation of activities	Report in video to present the results of activities with indicators as in the table in the assessment design	27%	

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II. ASSESSMENT PLAN

1. Learning Summary in Video Form

Lembar Penilaian Tugas Video Kimia Komputasi							
KELAS	:.....						
Kelompok	:.....						
(Isikan poin yang sesuai pada kolom biru muda)							
No	Indikator	Kriteria penialaian				poin	Nilai
		90	80	70	60		
Aspek Format dan Kualitas Video (40%)							
1	Ukuran file	<20 MB	20-30 MB	30-50 MB	>50 MB		0
2	Durasi	1,5 - 2 menit	2 - 3 menit	>3 menit			0
3	Kualitas gambar	Terlihat jelas	Kurang terlihat jelas		Buram/Tidak terlihat sama sekali		0
4	Kualitas suara	Terdengar jelas, terdapat musik latar yang sesuai dan tidak tidak menutupi suara narasi (Nilai penuh:90); Jika suara kurang jelas dikurangi 5 poin; Jika					0
5	Kualitas tulisan	Terdapat judul, identitas kelompok, *caption (*keterangan*)* yang terbaca dengan jelas tanpa mengganggu konten video (ukuran huruf proporsional)					0
						Rerata aspek Format dan Kualitas	**0**
Aspek Konten (60%)							
1	Topik	Sesuai			Tidak sesuai		0
2	Alur	Baik (urutan penyajian sistematis)		Tidak Baik			0
3	Kreativitas dan Originalitas	100% Merekam gambar sendiri	Animasi atau kompilasi video	Slide ppt yang diberi audio			0
						Rerata aspek Konten	**0**
						Nilai Total	**0**

Waktu Pengumpulan (Isikan dengan angka 1 di sel sebelah waktu pengumpulan yang sesuai)		Nilai Akhir
Tepat waktu	1	*0*
Terlambat 1 hari	0	*0*
Terlambat 2 hari atau lebih		*0*

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2. Learning Summary Video Form

No.	Components under review	Evaluation Criteria			
		<60	60-70	70-80	80-90
1	Does the topic of the article fit the scope of the journal?	no			yes
2	Whether the article is written in accordance with the format of the intended journal?	<70%	70%	80%	>80%
3	Are abstracts and keywords sufficient to reflect the research?	no		sufficient	appropriate
4	Whether the purpose has been explicitly explained in the background/introduction?	no			appropriate
5	Are the research tools, materials, and procedures on the methodology adequate to achieve the research objectives?	<70%	70%	80%	>80%
6	Are the results and discussion appropriate and coherent with the research objectives?	<70%	70%	80%	>80%
7	Does the author write a literature review relevant to the research?	<70%	70%	80%	>80%
8	Are the images/tables written on the manuscript well explained, clear, do not cause ambiguous understandings, and are in accordance with the research?	<70%	70%	80%	>80%
9	Is the author's writing style easy to understand?	No			Understood
10	Check Plagiarism	>50%	30-50%	30-20%	<20%

III. SCORING WEIGHTS

FINAL ASSESSMENT OF COURSES

The final assessment of the course can be done in 3 (three) ways, namely:

1 Predetermined Grading System
2 Normal Grading System
3 Combination of Predetermined and Normal Grading Systems

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Examples of Final assessments are as follows:

Grade	Score range
A	> 75
AB	> 70−75
B	> 65−70
BC	> 60−65
C	> 50−60
D	> 40−50
E	< 40

IV. GROUP ASSIGNMENT GRADING RUBRIC[4)]

A. PROJECT RESULTS

Value Range	Group Project Assessment Criteria
A (90–100)	if students can: - Complete group projects **on time** - Projects are carried out neatly**, clearly, and systematically** in their stages of work. - The entire Project is done **100% correct and clear.** - How to complete the Project in accordance with the rules/principles of Study Materials. - Questions are made creatively in analytical and comprehensive form.
AB (70– <90)	If students can: - Complete group projects **on time** - Projects are carried out neatly**, clearly, and systematically** in their stages of work. - All Projects are done **80-<100% right.** - How to Complete the Project in accordance with the rules/principles of Study Materials. - Questions are made creatively in analytical and comprehensive form.
B (50–< 70)	If students can: - Completing group projects **beyond** the agreed time - The project **is not** done neatly, clearly and systematically in its stages. - Project correctness **is 50-<80% correct.** - How to Complete the Project **is not in accordance** with the rules/principles of Study Materials - The questions are not comprehensive.
Not graded	Project results that are late in submission or their correctness are below < 50%

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B. GROUP TASKS

Score range	Group task assessment criteria
A (90–100)	if students can: - Complete group tasks **on time** - Tasks are carried out neatly**, clearly, and systematically** in the stages of work. - All tasks are done **100% correct and clear.** - How to solve according to what is delivered in class.
AB (70–<90)	if students can: - Complete group tasks **on time.** - Tasks are carried out neatly**, clearly, and systematically** in the stages of work. - All tasks are done **80-99% correct,** - How to solve according to what is delivered in class.
B (50–< 70)	if students can: - Complete group tasks **beyond** the agreed time - Tasks **are not** done neatly, clearly, and systematically in the stages of work. - Task permissions **50-80% correct.** - The method of completion **is not in accordance** with what is conveyed in class.
Not scored	Late tasks are collected and their correctness is below < 50%

[4)]The grading rubric can be adjusted to the assigned task

V. REFERENCES

Recommended, Required, and Supporting Reading Books:

1 Lewars E. 2004. *Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics*. Dordrecht (NL): Kluwer Academic Publishers.
2 Jensen JH. 2010. *Molecular Modelling Basics*. Boca Raton (US): Taylor and Francis Group