

(Course Information) *

معلومات المقرر

كيمياء حاسوبية	اسم المقرر:
CHM- 357	رقم المقرر:
CHM 343 Quantum chemistry	اسم ورقم المتطلب السابق:
-	اسم ورقم المتطلب المرافق:
المستوى السادس	مستوى المقرر:
3	الساعات المعتمدة:
Module Title:	Computational chemistry
Module ID:	CHM 357
Prerequisite (Co-requisite):	CHM 343
Co-requisite:	-
Course Level:	Level six
Credit Hours:	3

Module Description

وصف المقرر :

the course contains a breadth of knowledge of the fundamentals of modern computational methods available for chemical, biological, and materials research. Also, in this course the student will learn how computational methods are being used to design new materials and learn from hands-on computer exercises how to use major software programs in computational chemistry and molecular simulations

Module Aims

أهداف المقرر:

1	Define the fundamental principal of computational chemistry which include Molecular modeling, Computational methods, Computer-Aided Molecular Design (CAMD), Chemical databases and Organic synthesis design.
2	Building Models with the Bond Tools
3	Creating, Opening, and Importing Models
4	Display molecular models in several ways, depending on what information you want to learn from them
5	Using the computer software to predicting SAR

Learning Outcomes:

مخرجات التعليم:

After finish this course The student will be able to

1	Describe the different theories of computational chemistry	1
2	Create Models with the Bond Tools	2
3	Predict the SAR by using the computer software	3
4	Draw the structure of different	4
5	Product the analysis of molecules	6

Course Contents

محتوى المقرر:

ساعات التدريس (Hours)	عدد الأسابيع (Weeks)	قائمة الموضوعات (Subjects)
6	2	Molecular modeling.
6	2	Computational methods.



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6	2	Computer-Aided Molecular
6	2	Design (CAMD).
6	2	Chemical databases.
9	3	Organic synthesis design.
3	1	Spectroscopic simulation analysis
28	14	Total

Textbook and References:

الكتاب المقرر والمراجع المساندة:

ISBN	سنة النشر Publishing Year	اسم الناشر Publisher	اسم المؤلف (رئيسي) Author's Name	اسم الكتاب المقرر Textbook title
1908057zurich	August 11 2005	Winterthurerstrasse Switzerland	Jurg. Hutter	Computational chemistry electronic structure theory
	2010	Craig Building, RSC	Dr Andrew Gilbert	Introduction to Computational Quantum Chemistry: Theory



* يتم تعبئة معلومات المقرر فقط باللغتين العربية والانجليزية وبقية المعلومات بلغة التدريس المعتمدة ويكرر لكل مقرر في الخطة الدراسية

* Course Information should be filled in Arabic and English. Other information should be filled using the approved teaching language at the college.

