بسم الله الرحمن الرحيم

جامعة آل البيت

جامعة آل البيت
دائرة ضمان الجودة والتخطيط

كلية .....العلوم.....

قسم ....الكيمياء.....

توصيف مساق : (403361)Computer Application in Chemistry

1. معلومات مدرس المساق (Instructor)

اســـــــــم (مدرس / منسق) المساق :	Dr. Raed Ghanem & Dr Khaldoun Al Soud
الساعـــــــــــــات المكتبيـــــــــــــــــــــــة :	8.00-10:25
رقم المكتب والرقـــــــــم الفرعـــــــــــــي :	Chemistry Depertment
البريـــــــــــــــــــــد الالكترونـــــــــــــــــــي :	khaldoun@aabu.edu.jo raedag@aabu.edu.jo
مساعد البحث والتدريس/المشرف/الفني (إن وجد):	

2. وصف المساق (Course Description)

The course covers the applications of computers in chemistry including Topics discussed include chemistry and computer representation of chemical structures, databases in chemistry, molecular modelling, pattern recognition, optimization, regression analysis, multivariate calibration, artificial intelligence and QSAR. Applications of these methods in data analysis, structural searching, prediction of molecular properties and drug design. A combination of lectures, lab work, exercises, and classroom demonstrations (including overhead transparencies, board, Lecture progress Quizzes, and videotaping); computer packages will be used

3. بيانات المساق (Course Title)

رقم المساق: 403361	**اسم المساق: Computer Application in chemistry**	**المستوى: 3**
طبيعة المساق: Theoretical with practical Aspect	**المتطلب السابق / المتزامن:403102**	**وقت المحاضرة: 8:00-9:15 9:15-10:30**
العام الجامعي:2018/ 2019	**الفصل الدراسي: Summer**	**عدد الساعات الدراسية:3**

4. أهداف المساق (Course Objectives)

Computer aided approach to explain the the applications of computers in chemistry including Topics discussed include chemistry and computer representation of chemical structures, databases in chemistry, molecular modelling, pattern recognition, optimization, regression analysis, multivariate calibration, artificial intelligence and QSAR. Applications of these methods in data analysis, structural searching, prediction of molecular properties and drug design .

5. مخرجات التعلم (Intended Student Learning Outcomes)
(المعرفة والمهارات والكفايات)

يفترض بالطالب بعد دراسته لهذا المساق أن يكون قادرا على:

After completing this course, the student should demonstrate the knowledge and ability to:

1. Understand the basics applications of computer in chemistry (i.e., database and search engine…etc)
2. Understand and know the basic method of computer representation of chemical structure (i.e., ESL, Smile Connection table..etc)
3. Acquire information about chemmoetric , cheminformatics, molecular modelling computational chemistry..
4. Understand the basics of optimization , Drug design and the role of computer on that
5. Gain the practical skills in practical computer application in chemistry using deferent software (Chem sketch, Chemoffice, Crocodile for chemistry. Origin and Excel, Hyperchem and Argus Lab, …etc)

6. محتوى المساق(Course Content)

الأسبوع	الموضـــوع
الأول	1. Introduction and Hose keeping: Projects description and project distribution 2. **Computers, operating systems,**
الثاني	1. **Introduction to Computational Chemistry Chemometrics, Chemoinformatics** 2. **Data Processing**
الثالث	**Computer Representation of chemical structures :** Fragment code, linear notation, SMILES and connection tables
الرابع	Data bases in chemistry, Theoretical and Practical aspects
الخامس	Modelling and Computational Chemistry , Theory and Application

السادس	Software for Computional Chemistry, Hyper Chem, Arguslab..etc
	الامتحان الأول
الثامن	Optimization, General concept and Practical aspect
التاسع	Crocodile software
العاشر	Chemistry Drawing program
الحادي عشر	**Mathematical software : Regression Analysis** Simple linear regression, weighted least squares and nonlinear regression, Curve fit …etc using Origin Graphing software and Excel Software
	الامتحان الثاني
الثالث عشر	**Mathematical software : Regression Analysis** Simple linear regression, weighted least squares and nonlinear regression, Curve fit …etc using Origin Graphing software and Excel Software
الرابع عشر	Quantitative structure activity/property relationships, applications in predicting biological activities and physicochemical properties, drug
الخامس عشر	***Revision***
السادس عشر	**الامتحان النهائي**

7. استراتيجيات التعليم والتعلم وطرق التقويم
(Teaching and learning Strategies and Evaluation Methods)

ت	مخرجات التعلم	استراتيجياتالتدريس	أنشطة التعلم	نوع التقويم/القياس (امتحان/عروض صفية/مناقشة/واجبات)
1	Students will understand how to represent chemical structures using computers	Lecture, Presentation, quizzes, Case studies, and in class questions	**Class Discussions, website development**	In class Questions, Presentation, Exam
2	Students will understand how to use the chemical databse	Lecture, Presentation, quizzes, Case studies, and in class questions	**Class Discussions, website development**	In class Questions, Presentation, Exam
3	Students will understand how to represent chemical and calculate chemical properties using Visualization software	Lecture, Presentation, quizzes, Case studies, and in class questions	**Class Discussions, website development**	In class Questions, Presentation, Quizzes, Exam
4	Students will	Lecture, Presentation,	**Class Discussions,**	In class Questions, Presentation, Quizzes, Exam

	website development	quizzes, Case studies, and in class questions	understand how to use Math software (Origin , Excel) in chemical application	
				5
				6

1. تقييم الطلبة (Assessment)

الأساليب المستخدمة	توقيت التقييم	توزيع الدرجات لكل أسلوب
1-أعمال الفصل: (تقرير، وظائف، حضور)	خلال الفصل	10
2-امتحان تحريري أول	الأسبوع السابع	20
2-امتحان تحريري ثاني	الأسبوع الثاني عشر	20
3-امتحان تحريري نهائي	أسبوع الامتحانات النهائية	50

2. الكتاب المقرر (Text Book)

المرجع الرئيس	Guide to Microsoft Excel 2002 for Scientists and Engineers, 3rd edition, Berhnhard V. Liengme, Newnes Elsevier (2000)
المؤلف	
الناشر	
السنة	
الطبعة	
الموقع الالكتروني للمرجع	.

3. المراجع الإضافية (References)(وتشمل الكتب والبحوث المنشورة في الدوريات او المواقع الالكترونية)

-1	***Computational Chemistry" by E. G Lewars, 2nd edition. Kluwer Academic Publishers, 2011.***
-2	**"Physical Chemistry" by Thomas Engel and Philip Reid, 3rd edition. Pearson Prentice Hall, 2011.**
-3	