MODULE DESCRIPTION FORM

نموذج وصف المادة الدراسية

| **Module Information**  **معلومات المادة الدراسية** | | | | | | | |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Module Title** | Computer-Aided Drug Design | | | | **Module Delivery** | | |
| **Module Type** | Core | | | | * **☒ Theory** * **☐ Lecture** * **☒ Lab** * **☐ Tutorial** * **☐ Practical** * **☐ Seminar** | | |
| **Module Code** | **BID421** | | | |
| **ECTS Credits** | 5 | | | |
| **SWL (hr/sem)** | **125** | | | |
| **Module Level** | | 4 | **Semester of Delivery** | | | | 8 |
| **Administering Department** | | BID | **College** | BMIC | | | |
| **Module Leader** | Safanah Zaid ِ Ahmed | | **e-mail** | [safanah.bayati-bic@uoitc.edu.iq](mailto:safanah.bayati-bic@uoitc.edu.iq) | | | |
| **Module Leader’s Acad. Title** | | Assistant Lecturer | **Module Leader’s Qualification** | | | | MSc |
| **Module Tutor** | Safanah Zaid ِ Ahmed | | **e-mail** |  | | | |
| **Peer Reviewer Name** | | omar A.M | **e-mail** | omara.m@uoitc.edu.iq | | | |
| **Scientific Committee Approval Date** | | 18/6/2023 | **Version Number** | | | 1.0 | |

| **Relation with other Modules**  **العلاقة مع المواد الدراسية الأخرى** | | | |
| --- | --- | --- | --- |
| **Prerequisite module** | **Fundamentals of Organic Chemistry / BID212 , Applied Bioinformatics / BID211** | **Semester** | 3 |
| **Co-requisites module** | None | **Semester** | - |

| **Module Aims, Learning Outcomes and Indicative Contents**  **أهداف المادة الدراسية ونتائج التعلم والمحتويات الإرشادية** | |
| --- | --- |
| **Module Aims**  **أهداف المادة الدراسية** | 1. To become familiar with a variety of history of drug discovery and development.      1. To become familiar with fundamentals of drug design design and development methods - bioassays, synthesis, leads, lead modification, Log P, lubinsky rule of 5.   2. To become familiar with Enzyme Inhibition and Inactivation.  3. To learn how to compare and analyze biological sequences and how to interpret the results of their analyses.  4. To learn how to  6. To be able perform Protein-Ligand Docking.  7. To use the scientific method of inquiry to gain scientific knowledge.  8. To use computer systems or other appropriate forms of technology to achieve educational and personal goals. |
| **Module Learning Outcomes**  **مخرجات التعلم للمادة الدراسية** | 1. Able to introduce the basic Concepts Of drug discovery and its development. 2. Able to describe the scope and importance of CADD. 3. Able to explain the drug discovery, design and development methods - bioassays, synthesis, leads, lead modification, Log P. 4. Able to describe enzyme mechanisms. 5. Understands and can explain the main steps for Protein-Ligand Docking process. 6. Knows the steps of Protein-Ligand Docking proses. 7. Able to understand the basics of docking its different software’s. 8. Able to understand and be aware of Current Challenges and limitations in Molecular Docking. 9. To develop a comprehensive understanding of QSAR (Quantitative Structure-Activity Relationship) 10. To have the ability to recognize and explain Pharmacophore Modeling via the LigandScout software tool. |
| **Indicative Contents**  **المحتويات الإرشادية** | Indicative content includes the following:  **Part A – Drug Action**  There are five major categories of biochemical drug targets in the cell: receptors, enzymes, DNA, RNA, and membranes. In this manner, the course takes a fundamentally chemical approach to the study of drug action. For example, we will consider how chemical synthesis plays a role in the discovery and production of drugs. In addition, we will study the chemical interactions between drugs and biological macromolecules. A chemical approach to the topic of drug action leads naturally to consideration of cellular drug targets in terms of the “big five” categories mentioned above. For instance, the multitude of drugs that interact with enzymes can be considered as a single group because the fundamental chemical principles underlying the action of all enzymes and the interaction of any drug an enzyme target are the same – regardless of the particular enzyme that is involved. We will consider the fundamental concepts underlying the interaction of drugs with all of the important classes of cellular drug targets: receptors, enzymes, DNA, RNA and membranes. In the final portion of the semester we will address chemical principles of drug delivery and drug metabolism.  **Part B – Drug Design**  Computer-aided drug design (CADD) includes finding, developing, and analyzing medicines and related biological active compounds by computer methodologies. The use of CADD methodologies speeds up the early stages of chemical development while guiding and speeding up drug discovery. Virtual screening, virtual library design, lead optimization, de novo design and other computational approaches are all covered in CADD. It is a reasonable and methodical technique that concentrates scientists' attention on the most promising chemicals, eliminating the effort needed to test their potency in synthetic and biological laboratories. This chapter contains in-depth information on retrieving data from databases such as PubChem, DrugBank, Zinc DB, RCSB-PDB and ModBase.alos laboratory study of making drugs such as aspirin and paracetamol in the laboratory. |

| **Learning and Teaching Strategies**  **استراتيجيات التعلم والتعليم** | |
| --- | --- |
| **Strategies** | * **Practical presentations** * **Cooperative Learning** * **Brainstorming** * **Self-Learning** * **Individual Skills Assessment** * **Achievement Tests** * **Standard Tests** |

| **Student Workload (SWL)**  **الحمل الدراسي للطالب** | | | |
| --- | --- | --- | --- |
| **Structured SWL (h/sem)**  **الحمل الدراسي المنتظم للطالب خلال الفصل** | **64** | **Structured SWL (h/w)**  **الحمل الدراسي المنتظم للطالب أسبوعيا** | 4 |
| **Unstructured SWL (h/sem)**  **الحمل الدراسي غير المنتظم للطالب خلال الفصل** | **61** | **Unstructured SWL (h/w)**  **الحمل الدراسي غير المنتظم للطالب أسبوعيا** | 4 |
| **Total SWL (h/sem)**  **الحمل الدراسي الكلي للطالب خلال الفصل** | 125 | | |

| **Module Evaluation**  **تقييم المادة الدراسية** | | | | | |
| --- | --- | --- | --- | --- | --- |
| **As** | | **Time/Number** | **Weight (Marks)** | **Week Due** | **Relevant Learning Outcome** |
| **Formative assessment** | **Quizzes** | 2 | 10% (10) | 5, 10 | LO #1, 3, 9 |
| **Assignments** | 2 | 10% (10) | 2, 12 | LO # 3, 4, 6 and 7 |
| **Projects / Lab.** | 1 | 10% (10) | Continuous |  |
| **Report** | 1 | 10% (10) | 13 | LO # 2, 7 and 10 |
| **Summative assessment** | **Midterm Exam** | 2 hr | 10% (10) | 7 | LO # 1-7 |
| **Final Exam** | 3hr | 50% (50) | 16 | All |
| **Total assessment** | | | 100% (100 Marks) |  |  |

| **Delivery Plan (Weekly Syllabus)**  **المنهاج الاسبوعي النظري** | |
| --- | --- |
| **Week** | **Material Covered** |
| **Week 1** | Introduction: History of drug discovery and development |
| **Week 2** | Modern drug discovery, design and development methods - bioassays, synthesis, leads, lead modification, Log P. |
| **Week 3** | Introduction to receptors as drug targets |
| **Week 4** | What is an enzyme and how do they work? Enzyme Inhibition and Inactivation |
| **Week 5** | DNA targeted drugs Drug metabolism Prodrugs and drug delivery |
| **Week 6** | Overview of Protein-Ligand Docking |
| **Week 7** | Mid-First Exam |
| **Week 8** | Docking in Drug Discovery and Current Challenges in Molecular Docking |
| **Week 9** | Scoring Functions |
| **Week 10** | Softwares: AutoDock, GOLD and GLIDE |
| **Week 11** | Ensemble Docking |
| **Week 12** | Virtual Screening |
| **Week 14** | QSAR (Quantitative Structure-Activity Relationship) and Pharmacophore Modeling via LigandScout software tool |
| **Week 15** | Second Exam |

| **Delivery Plan (Weekly Lab. Syllabus)**  **المنهاج الاسبوعي للمختبر** | |
| --- | --- |
| **Week** | **Material Covered** |
| **Week 1** | Chemistry Pharmaceutical Organic - Aspirin |
| **Week 2** | Chemistry Pharmaceutical Organic - paracetamol |
| **Week 3** | Protein Data Bank (PDB) |
| **Week 4** | ZINC database, national cancer institute NCI database |
| **Week 5** | Biovia Discovery Studio |
| **Week 6** | Mid- First Exam |
| **Week 7** | AUTODOCK TUTORIAL and Biovia Discovery Studio |
| **Week 8** | AUTODOCK TUTORIAL |
| **Week 9** | AUTODOCK VINA TUTORIAL |
| **Week 10** | GOLD TUTORIAL |
| **Week 11-12** | VMD: visual molecular dynamics |
| **Week 13-15** | NAMD - Scalable Molecular Dynamics simulations. And Second Exam |

| **Learning and Teaching Resources**  **مصادر التعلم والتدريس** | | |
| --- | --- | --- |
|  | **Text** | **Available in the Library?** |
| **Required Texts** | 1. Protein-Ligand Interactions. From Molecular Design to Drug Design. by H.J. Böhm   and G. Schneider, 2003 Wiley-VCH   1. Molecular Design. Concepts and Applications by G. Schneider and K. H.   Baringhaus, 2008 Wiley-VCH   1. The Organic Chemistry of Drug Design and Drug Action;  2nd Edition; Richard B. Silverman, Academic Press: San Diego, 2004. | No |
| **Recommended Texts** | 1. Quantitative Drug Design. A Critical Introduction by Y. C. Martin, 2010 CRC Press 2. Structure-Based Ligand Design, by K. Gubernator and H.J. Böhm, 1998 Wiley-VCH 3. Virtual Screening in Drug Discovery, eds Alvarez and Shoichet, 2005 CRC Press | No |

| **Grading Scheme**  **مخطط الدرجات** | | | | |
| --- | --- | --- | --- | --- |
| **Group** | **Grade** | التقدير | **Marks (%)** | **Definition** |
| **Success Group**  **(50 - 100)** | **A -** Excellent | **امتياز** | 90 - 100 | Outstanding Performance |
| **B -** Very Good | **جيد جدا** | 80 - 89 | Above average with some errors |
| **C -** Good | **جيد** | 70 - 79 | Sound work with notable errors |
| **D -** Satisfactory | **متوسط** | 60 - 69 | Fair but with major shortcomings |
| **E -** Sufficient | **مقبول** | 50 - 59 | Work meets minimum criteria |
| **Fail Group**  **(0 – 49)** | **FX –** Fail | **راسب (قيد المعالجة)** | (45-49) | More work required but credit awarded |
| **F –** Fail | **راسب** | (0-44) | Considerable amount of work required |
|  |  |  |  |  |
| **Note:** Marks Decimal places above or below 0.5 will be rounded to the higher or lower full mark (for example a mark of 54.5 will be rounded to 55, whereas a mark of 54.4 will be rounded to 54. The University has a policy NOT to condone "near-pass fails" so the only adjustment to marks awarded by the original marker(s) will be the automatic rounding outlined above. | | | | |