MODULE DESCRIPTION FORM

نموذج وصف المادة الدراسية

| **Module Information**  **معلومات المادة الدراسية** | | | | | | | |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Module Title** | Computational Biology | | | | **Module Delivery** | | |
| **Module Type** | Core | | | | * **☒ Theory** * **☐ Lecture** * **☒ Lab** * **☐ Tutorial** * **☐ Practical** * **☐ Seminar** | | |
| **Module Code** | BID423 | | | |
| **ECTS Credits** | 5.00 | | | |
| **SWL (hr/sem)** | 125 | | | |
| **Module Level** | | 2 | **Semester of Delivery** | | | | 8 |
| **Administering Department** | | BID | **College** | BMIC | | | |
| **Module Leader** | Maysaa Ahmed Abdulkaremm | | **e-mail** | maysaa.ahmed-bic@uoitc.edu.iq | | | |
| **Module Leader’s Acad. Title** | | Assistant Lecturer | **Module Leader’s Qualification** | | | | MSc |
| **Module Tutor** | Name (if available) | | **e-mail** | E-mail | | | |
| **Peer Reviewer Name** | | omar A. M | **e-mail** | omara.m@uoitc.edu.iq | | | |
| **Scientific Committee Approval Date** | | 18/06/2023 | **Version Number** | | | 1.0 | |

| **Relation with other Modules**  **العلاقة مع المواد الدراسية الأخرى** | | | |
| --- | --- | --- | --- |
| **Prerequisite module** | Biophysics / BID123, Applied Bioinformatics / BID211 | **Semester** | 1, 3 |
| **Co-requisites module** | Introduction to Bioinformatics / BID122 | **Semester** | 2 |

| **Module Aims, Learning Outcomes and Indicative Contents**  **أهداف المادة الدراسية ونتائج التعلم والمحتويات الإرشادية** | |
| --- | --- |
| **Module Aims**  **أهداف المادة الدراسية** | 1. To enable the students to understand *s*cope of Bioinformatics  2. To understand the popular bioinformatics database  3. to understand the approaches of drug discovery using bioinformatics  techniques  4. To Understand how bioinformatics is related to biology, pharma, and medicine.  5. to help the students to become independent researchers and develop professional attitudes and skills. |
| **Module Learning Outcomes**  **مخرجات التعلم للمادة الدراسية** | 1. Learn about Molecular docking and the MDS process. 2. Capable of using docking software. 3. Capable of using simulation software. 4. Learn how to do a disease analysis. 5. Able to articulate the origins of the disease's severity. |
| **Indicative Contents**  **المحتويات الإرشادية** | Indicative content includes the following.   * Introduction to molecular docking technology * Molecular docking databases * Protein Data Bank * PubChem * Drug Bank * Docking Software * Auto Dock * Auto Dock Vina * GOLD: Genetic Optimization for Ligand Docking (GOLD) * Schrödinger Suite (Glide) * MOE (Molecular Operating Environment) * Molecular docking process- visualization * PyMOL * Discovery Studio * Molecular dynamics simulation tools * GROMACS * Post trajectory analysis * RMSD * RMSF * Hydrogen bonds * Salt bridges * Radius of gyration |

| **Learning and Teaching Strategies**  **استراتيجيات التعلم والتعليم** | |
| --- | --- |
| **Strategies** | Learning and teaching strategies in molecular computational biology involve a combination of theoretical knowledge, practical skills, and hands-on experience with computational tools and techniques.   1. Hands-on Experience:    * Provide practical exercises and assignments that involve using computational tools and software.    * Encourage students to work on real-world research projects or case studies that involve molecular computational biology.    * Offer access to computational resources and software packages commonly used in the field. 2. Data Analysis and Visualization 3. Collaborative Learning:  * Encourage collaborative projects and group discussions to foster a deeper understanding of molecular computational biology concepts. * Promote peer learning and knowledge sharing among students by creating opportunities for collaborative problem-solving exercises or group projects. * Encourage students to participate in relevant research communities, conferences, and workshops to expand their networks and gain exposure to cutting-edge research.  1. Experiments and Simulations |
|  |  |

| **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, 2 |
| **Assignments** | 2 | 10% (10) | 2, 12 | LO # 3, 4, |
| **Projects / Lab.** | 1 | 10% (10) | Continuous |  |
| **Report** | 1 | 10% (10) | 13 | LO # 1, 2, 3 |
| **Summative assessment** | **Midterm Exam** | 2 hr | 10% (10) | 7 | LO # 3, 4 |
| **Final Exam** | 3hr | 50% (50) | 16 | All |
| **Total assessment** | | | 100% (100 Marks) |  |  |

| **Delivery Plan (Weekly Syllabus)**  **المنهاج الاسبوعي النظري** | |
| --- | --- |
| **Week** | **Material Covered** |
| **Week 1-2** | Introduction to molecular docking technology |
| **Week 3** | Molecular docking databases |
| **Week 4** | The applications of molecular docking |
| **Week 5** | Molecular docking Tools |
| **Week 6-7** | Molecular docking process- visualization- validation |
| **Week 8** | What is the molecular dynamics Simulation: The Basics |
| **Week 9** | How can MD contribute to Drug Discovery? |
| **Week 10-11** | Molecular dynamics simulation Tools |
| **Week 12** | Molecular dynamics simulation steps |
| **Week 13-15** | Post trajectory analysis (RMSD, RMSF, HB, salt bridges, Rg, SASA, etc) and visualization |

| **Delivery Plan (Weekly Lab. Syllabus)**  **المنهاج الاسبوعي للمختبر** | |
| --- | --- |
| **Week** | **Material Covered** |
| **Week 1-2** | Docking tools |
| **Week 3-4** | PyRx Vina software |
| **Week 5-7** | Visualization, PyMOL, Discovery Studio |
| **Week 8-9** | GROMACS (GROningen MAchine for Chemical Simulations) |
| **Week 10-13** | Results analysis ((RMSD, RMSF, HB, salt bridges, Rg, SASA, PCA) |
| **Week 14 -15** | NAMD (NAnoscale Molecular Dynamics), NAMD (NAnoscale Molecular Dynamics), AMBER, LAMMPS, OpenMM |

| **Learning and Teaching Resources**  **مصادر التعلم والتدريس** | | |
| --- | --- | --- |
|  | **Text** | **Available in the Library?** |
| **Required Texts** | de Azevedo, W. F. (Ed.). (2019). *Docking screens for drug discovery*. New York, NY: Humana Press.  Vlachakis, D. (Ed.). (2018). *Molecular Docking*. BoD–Books on Demand. | No |
| **Recommended Texts** | Pal, S., & Ray, B. C. (2020). *Molecular dynamics simulation of nanostructured materials: An understanding of mechanical behavior*. CRC Press.  Behzadi, P., & Bernabò, N. (Eds.). (2020). *Computational Biology and Chemistry*. BoD–Books on Demand. | No |
| **Websites** | https://www.gromacs.org | |

| **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. | | | | |