**INTERNATIONAL MEDICAL UNIVERSITY**

**MSc. Analytical and Pharmaceutical Chemistry**

**Module: Computational Drug Discovery Techniques**



**MODULE COORDINATOR: DR. VASUDEVARAO AVUPATI**

**CAL Workshop Report**

**ON**

**Unit 1: Introduction to Maestro**

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| **Student Name** | Type your details here |
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**2017**

**Guidelines for CAL Workshop Report Submission**

Please read the following guidelines carefully before you start writing your assignment:

1. This document is a **template**, the objective of this template is to enable you to submit your CAL workshop report in a **standardised format**.
2. **You should answer all parts of questions,** **all questions are compulsory**.
3. You will need to remove the **red color text** before you start typing your text.
4. To type your text use the **styles and fonts** sizes as consistent in this template.
5. To create more space for your text, you will need to use suitable functions in **MS Word** settings.
6. **CAL Workshop Report** is divided into two sections, **SECTION 1** is **software applications**, this carries **20 marks** and **SECTION 2** is **problem solving and critical thing industrial case studies**, this carries **30 marks**. The total marks is **50 marks** and it contributes **10%** of your **in-course assessment (ICA)**.
7. Save this file with your **name and ID** before you submit online.
8. Ensure that all the questions are **answered and saved** in the template before you **upload** your CAL Workshop Report file online.

**SECTION 1: MOLECULAR MODELING**

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| Question 1 | | | |
| Draw the two dimensional (2D) chemical structures of the following drug molecules, predict their IUPAC name and various physicochemical properties by using the ChemBioDraw Ultra software.  (1 × 10 = 10 Marks) | | | |
| Note: Incorporate the “IMAGE OF THE STRUCTURE” into the space provided in this template. | | | |
|  | **Chalcone** | 2D Chemical structure | Physicochemical properties |
|  | **Aurone** | 2D Chemical structure | Physicochemical properties |
|  | **Flavan** | 2D Chemical structure | Physicochemical properties |
|  | **Flavonol** | 2D Chemical structure | Physicochemical properties |
|  | **Flavonone** | 2D Chemical structure | Physicochemical properties |
|  | **Flavone** | 2D Chemical structure | Physicochemical properties |
|  | **Isoflavone** | 2D Chemical structure | Physicochemical properties |
|  | **Dihydrochalcone** | 2D Chemical structure | Physicochemical properties |
|  | **Cinnamic acid** | 2D Chemical structure | Physicochemical properties |
|  | **2-Hydroxychalcone** | 2D Chemical structure | Physicochemical properties |

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| Question 2 | | |
| Generate the three dimensional (3D) chemical structures of the following drug molecules and minimise energy to report total energy (kcal/mol) by using Chem3D Pro software.  (1 × 10 = 10 Marks) | | |
| Note: Incorporate the “IMAGE OF THE STRUCTURE” into the space provided in this template. | | |
|  | **Chalcone** | Energy minimised 3D Chemical structure  Total energy: |
|  | **Aurone** | Energy minimised 3D Chemical structure  Total energy: |
|  | **Flavan** | Energy minimised 3D Chemical structure  Total energy: |
|  | **Flavonol** | Energy minimised 3D Chemical structure  Total energy: |
|  | **Flavonone** | Energy minimised 3D Chemical structure  Total energy: |
|  | **Flavone** | Energy minimised 3D Chemical structure  Total energy: |
|  | **Isoflavone** | Energy minimised 3D Chemical structure  Total energy: |
|  | **Dihydrochalcone** | Energy minimised 3D Chemical structure  Total energy: |
|  | **Cinnamic acid** | Energy minimised 3D Chemical structure  Total energy: |
|  | **2-Hydroxychalcone** | Energy minimised 3D Chemical structure  Total energy: |

**SECTION 2: MOLECULAR DOCKING**

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| Question 3 |
| 1. Download the assigned protein target (protein data bank (PDB) ID:……..) into the Schrodinger Maestro Workspace. (5 M) 2. Generate protein-ligand diagrams by using Maestro “Tools”. (5 M)   (5 × 2 = 10 Marks) |
| Note: Incorporate the “IMAGE OF THE WORKSPACE” into the space provided in this template. |
| 1. Protein-ligand complex 3D diagram of assigned protein target |
| 1. Protein-ligand interaction 2D diagrams of assigned protein target |

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| Question 4 |
| Perform molecular docking study of compound library developed under Question 2 against assigned drug target protein by using Schrodinger “Maestro tools” “Glide-Ligand Docking” software and write a description for the following questions based on your reflection.  (1 × 20 = 20 Marks) |
| Note: Incorporate the “IMAGES OF THE WORKSPACE” in the “TEXT” wherever applicable, use the space provided in this template. Answer all the questions in your words. |
| 1. How will you prepare protein and ligand by using Schrodinger Maestro “Protein Preparation Wizard” and “LigPrep”?   (5 M)  Answer:   1. How will you perform “Receptor grid generation (binding site generation)” for Assigned Target by using Schrodinger Maestro “Glide”?   (5 M)  Answer:   1. How will you perform “Ligand docking” for compound library against Assigned Target by using Schrodinger Maestro “Glide”?   (5 M)  Answer:   1. How will you analyse your molecular docking results of compound library against Assigned Target? Explain how does a docking score is useful in computer aided drug discovery?   (5 M)  Answer: |

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