Master of Science in Analytical and Pharmaceutical Chemistry
Module: Computational Drug Discovery Techniques (MAPC304)
Computer Assisted Learning (CAL) Workshop
Assessment Criteria and Marking Scheme

Assessment 2
CAL Workshop Report (10%)

Topic: Quantitative Structure-Activity Relationship (QSAR)

Based on the computational drug discovery software application skills (hands-on) gained through facilitated computer-assisted learning (CAL) workshops, upon completion of the workshop the students should submit a CAL workshop report on the application of computational techniques for QSAR modelling by means of an industrial problem-based/case-based-scenarios.

Criteria	Excellent (9-10)	Good (8-8.9)	Satisfactory (6-7.9)	Poor (4-5.9)	Weak (0-3.9)	Weightage	Marks
Content **(70%)**	**Completeness** Effective, accurate and adequate, selected computational approach and the presentation of the content is more specific to QSAR. **Methodology** All the following computational software application tasks are completed in sequential order and presented in the report. 1. Selection of dataset (bioactive ligands) from the literature 2. Curation of chemical/biological dataset 3. Molecular modelling of dataset 4. Three-dimensional (3D) conformational search 5. 3D alignment	**Completeness** The content presented are accurate and adequate, however the selected computational approach and content is less specific to QSAR. **Methodology** Seven of the following computational software application tasks are completed in sequential order and presented in the report. 1. Selection of dataset (bioactive ligands) from the literature 2. Curation of chemical/biological dataset 3. Molecular modelling of dataset 4. Three-dimensional (3D) conformational search 5. 3D alignment	**Completeness** The content presented is accurate, however selected computational approach is not well supported; some evidence, but usually of a generalised nature. **Methodology** Six of the following computational software application tasks are completed in sequential order and presented in the report. 1. Selection of dataset (bioactive ligands) from the literature 2. Curation of chemical/biological dataset 3. Molecular modelling of dataset 4. Three-dimensional (3D) conformational search 5. 3D alignment	**Completeness** The content presented is accurate, however selected computational approach is not well supported; no evidence. **Methodology** Five of the following computational software application tasks are completed in sequential order and presented in the report. 1. Selection of dataset (bioactive ligands) from the literature 2. Curation of chemical/biological dataset 3. Molecular modelling of dataset 4. Three-dimensional (3D) conformational search 5. 3D alignment	**Completeness** The content presented is not accurate, and selected computational approach is not valid. **Methodology** Four or less than four of the following computational software application tasks are completed in sequential order and presented in the report. 1. Selection of dataset (bioactive ligands) from the literature 2. Curation of chemical/biological dataset 3. Molecular modelling of dataset 4. Three-dimensional (3D) conformational search 5. 3D alignment	X 7	70

Master of Science in Analytical and Pharmaceutical Chemistry
Module: Computational Drug Discovery Techniques (MAPC304)
Computer Assisted Learning (CAL) Workshop
Assessment Criteria and Marking Scheme

	6. Selection of training/test sets 7. Atom-based 3D-Quantitative structure-activity relationship (3D QSAR) modelling 8. Predicting the predictability of the model **Results and discussion** Able to critically analyse the results. Well-discussed, supported with specific and relevant literature. **Conclusion** All-important research findings are concluded in a concise manner and are presented well.	6. Selection of training/test sets 7. Atom-based 3D-Quantitative structure-activity relationship (3D QSAR) modelling 8. Predicting the predictability of the model **Results and discussion** Able to analyse the results. Well-discussed, supported with specific and relevant literature. **Conclusion** Most important research findings are summarized in a concise manner and are presented well.	6. Selection of training/test sets 7. Atom-based 3D-Quantitative structure-activity relationship (3D QSAR) modelling 8. Predicting the predictability of the model **Results and discussion** Able to analyse the results. Discussed with relevant literature. **Conclusion** Some important research findings are summarized in a lengthy manner and are presented well.	6. Selection of training/test sets 7. Atom-based 3D-Quantitative structure-activity relationship (3D QSAR) modelling 8. Predicting the predictability of the model **Results and discussion** Unable to analyse the results accurately. Discussion is not supported by relevant literature. **Conclusion** Research findings are summarized to an extent but are not presented well.	6. Selection of training/test sets 7. Atom-based 3D-Quantitative structure-activity relationship (3D QSAR) modelling 8. Predicting the predictability of the model **Results and discussion** Unable to analyse the results accurately. Discussion is not well written and is not supported by relevant literature. **Conclusion** Research findings are not summarized in a concise manner and are not presented well.		
Organisation (10%)	Meeting all the following requirements: 1. Logical order and flow 2. Appropriate use of figures and tables 3. Appropriate titles or legends are given to figures and tables 4. Appropriate citation of the references	Meeting any 3 of the following requirements: 1. Logical order and flow 2. Appropriate use of figures and tables 3. Appropriate titles or legends are given to figures and tables 4. Appropriate citation of the references	Meeting any 2 of the following requirements: 1. Logical order and flow 2. Appropriate use of figures and tables 3. Appropriate titles or legends are given to figures and tables 4. Appropriate citation of the references	Meeting any 1 of the following requirements: 1. Logical order and flow 2. Appropriate use of figures and tables 3. Appropriate titles or legends are given to figures and tables 4. Appropriate citation of the references	Meeting none of the following requirements: 1. Logical order and flow 2. Appropriate use of figures and tables 3. Appropriate titles or legends are given to figures and tables 4. Appropriate citation of the references	X 1	10
Referencing (10%)	Complete list of references. Appropriate and consistent format. Up to date references used in the content.	Complete list of references. Appropriate and consistent format, however outdated references used.	Complete list of references, however minor mistakes are made on referencing style and outdated references used.	Complete list of references, however major mistakes are made on referencing style and outdated references used.	Incomplete list of references, major mistakes are made on referencing style and outdated references used.	X 1	10

Master of Science in Analytical and Pharmaceutical Chemistry
Module: Computational Drug Discovery Techniques (MAPC304)
Computer Assisted Learning (CAL) Workshop
Assessment Criteria and Marking Scheme

Grammar and language (10%)	No spelling or grammatical errors. Excellent quality of word processing.	There is a good range of sentence structure and vocabulary with a number of minor errors in word formation or spelling.	While there are noticeable language errors, these do not significantly interfere with the reader understanding the essay.	The range of sentences expressed correctly is limited. Errors in grammar, word choice, word formation and spelling cause difficulty for the reader.	Continuous errors in sentence structure, word choice, word forms and spelling prevent communication.	X 1	10
Total Mark							100

Student's name: _____ID No: _____ Cohort: _____

Title of the report: _____

Examiner's name: _____Signature: _____Date: _____