

PHR 4220 Computational Chemistry Project

Critique

The deliverable in this case is a report with a word count not exceeding 1800 words excluding footnotes, references, tables and appendices.

The report should be set up as follows:

- Table of Contents
- List of Figures
- List of Tables
- List of abbreviations (*Page numbering in Roman Numerals up to this point*)
- Introduction
- Materials and Methods
- Results
- Discussion
- References
- Appendices

This report is a summary of the work done, and of the results achieved over 3 years. A critical approach must be adopted at all stages. Specifically, the introduction should critically evaluate the body of knowledge available and lead to formulation of the aims of the study. The description of the methodology should include justifications for the approaches adopted and of how these were best suited to validate the initial hypothesis and achieve the aims of the study. Any deviations from the initial aims of the study must be explained and justified. Procedures adopted to ensure that the molecular cohorts emanating from the study are drug-like and bioavailable, should also be explained.

The results should emanate from the methodology and should be presented as its logical findings. Figures, tables and structures should complement the results. These latter should not be presented in isolation, but they should be contextualised by explanatory text.

The discussion should analytically review the study. It should briefly remind the reader why the study was attempted, what its aims were, and to what extent they were achieved. The results attained should be placed in the context of the *lacunae* existing in the body of knowledge. In this way, the contribution of the study to science should be formulated. The limitations of the study must be clearly outlined, and the ways in which the study may be continued in the future should be described.

For the references use the author-date citation system. A list of references should be included at the end of the text, listed according to the International Committee of Medical Journal Editors Uniform Requirements for Manuscripts Submitted to Biomedical Journals. Please refer to: http://www.nlm.nih.gov/bsd/uniform_requirements.html

The appendices should contain all computational raw data, as well as results not central to the conclusions that were drawn from the study. A maximum of 4 appendices is allowed.

The document must be submitted in PDF and Word format.