Final Report Guidelines: AMS-536 "Molecular Modeling of Biological Molecules", Dr. Robert C. Rizzo [631-632-9340, rizzo@ams.sunysb.edu]

Communicating effectively is a critically important skill. The ability to give a good oral presentation, participate in group scientific discussion, and write a strong research article are three specific skills you should cultivate. This final project report provides you with an excellent opportunity for you to write a professional manuscript using data from your independent class project. The manuscript format will follow a research article that one would submit for publication to a peer-reviewed journal in the field of computational structural biology. Attached is an edited example from my own work for you to use as a guide. Consider this final project report as an important part of your graduate education to help you become a better scientific writer. With this in mind, please enjoy this assignment!

1) Your manuscript should be approximately 20-25 double-spaced pages (including, all Figures, Tables, equations, and references). This equates to about 12-14 pages of actual text. To facilitate readability, all Figures, Tables, and equations should be embedded into the document at appropriates points. See the attached document for examples.
2) Write in a style consistent with scientific manuscripts in the field of computational structural biology (*never* use the first person, e.g. "I simulated HIV protease to elucidate...."). Consult recent articles from Journal of the American Chemical Society (JACS), Journal of Chemical Theory and Computation, Journal of Medicinal Chemistry, or the attached manuscript.
3) Follow the general outline. Suggested section lengths for this project are as follows.
    - **a) Title**
    - **b) Author(s) and affiliation**
    - **c) Introduction and background (4-5 dbl spaced pages)**
        i. Present the systems (or method) to be studied and why it is important to do this study.
        ii. Present what has been done before (e.g. prior computational or experimental papers).
        iii. Clearly state the specific aims of your research.

d) Computational Methods (5-6 dbl spaced pages)

i. Explain the general theoretical methods behind your simulations.

ii. Give enough details so someone could reproduce your results.

e) Results and Discussion (6-7 dbl spaced pages)

i. Step by step present your results (expected and unexpected).

ii. Back up your statements and discussion using your own results (e.g. specific data tables or Figures) or by referring to results from the literature.

iii. What do your results tell you about the system(s) you have studied?

iv. Do specific results naturally lead to, or suggest, future experiments?

f) Conclusion (1-2 dbl spaced pages)

i. Clearly and succinctly restate the primary purpose of the study, and recap the major results while referring back to each specific Tables, Figure, etc.

ii. Conclude with a clear statement that presents the "big picture" of why what you have presented is important.

g) Acknowledgements

h) References

4) References should follow the Journal of the American Chemical Society (JACS) format. Consult recent articles and the attached manuscript to see the proper way to cite research articles, webpages, molecular modeling software, and book chapters. References in the text should be identified with superscript numbers (e.g., Jorgensen et al. have shown[8]...). Reference sections should contain the title and journal articles should be formatted as follows: (8) Jorgensen, W. L.; Ravimohan, C. Monte Carlo Simulation of Differences in Free Energies of Hydration. *J. Chem. Phys.* **1985**, *83*, 3050-3054.

5) Your project report should be done on a word processor (e.g. Microsoft Word) and you should use a standard referencing program (e.g. Endnote). Use double spacing and 1 inch margins on a single side of paper and 12 point Times New Roman font unless special Greek characters are needed then use Symbol font. Center all Figures and set the width

to be 4-5 inches. Pages must be numbered and the entire document should be spell checked. Be careful, recall the example from class "free energy of salvation" !

6) Your final manuscript should be free of spelling and grammatical errors and be formatted so the document is neat looking and easily readable. Please follow the general format of the attached example.

7) Papers submitted with poor English will be returned for rewrite and counted as late (see below). Therefore, it is imperative you turn in a manuscript written in grammatically correct English on the due date (see below). If English is not your native language, or if you feel you have poor writing skills, then you must go to the campus writing center and get assistance with composing grammatically correct English. Manuscripts submitted to journals, such as JACS, with grammatically incorrect English would be immediately rejected by the journal Editor.

8) Late papers will be substantially penalized (1 letter grade each day late). Preliminary drafts may be turned in for feedback up until one week before the final due date.

9) It goes without saying that you must never use any text, Figures, Tables, or Data from any source without full and proper citations. For this manuscript I expect you to generate your own equations, Figures, Tables, and text. Do not cut-and-paste text from any source whatsoever. If you must use a Figure from another paper to make your point, then give a complete citation for that Figure. With the possible exception of getting assistance with writing grammatically correct English, this paper must be written by you and in your own words. PLAGARISM WILL RESULT IN LETTER GRADE "F"