Chemistry 306 Spring, 2021 Course Guidelines

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Lab Times: T 0830 – 1220; Th 0830 – 1220; F 0810 – 1200; Three Sections!

I-really-wish-we-were-here-places: Flanner Hall Basement Biochemistry Lab, NMR Lab, and Quantitative Analysis Lab.

DG Office Hours: T 1230– 1330; Th 1230 – 1330, or by arrangement.
YN Office Hours: TBA
JB Office Hours: TBA

This course introduces tools and ideas critical to experimental biophysical chemistry. We will pursue the following activities over the semester:

(1) Information and Experimental Data. Information is the fruit of all scientific inquiry, procedure, and experiment. Biophysical inquiry presents no exceptions. Thus modern-day principles of information will be illustrated via electronic logic gates, spectroscopy, genomic and protein sequence analysis.

(2) Information and Uncertainty. Experimental data arrives with troublesome Qs about uncertainty and reproducibility. Thus we will assemble tools and ideas that make the most of the imperfect situations imposed by analogue information. Applications to biophysical chemistry will be illustrated via phase transition kinetics, electrochemical contact potentials, and thermometric devices.

(3) Information and Models. Biophysical data are complex as a rule: enzyme turnover, competitive inhibition, and more. Models are needed to navigate the complexity and so illuminate the paths forward. This includes identifying the Qs that need asking. Thermometric devices, Brownian motion and processing will be at center stage to illustrate model-building practice and applications.

(4) Analogue Information and Accumulation. Acquisition of biophysical information is never a one-and-done process. Rather it is highly accumulative over energy, lab space, and time. This lab will focus on techniques of experimental integration and differentiation. Applications will include thermodynamic isotherms, Monte Carlo techniques, electronic-vibrational spectroscopy, and electron paramagnetic resonance (EPR).

(5) Techniques and applications of Fourier analysis. Biophysical structure data such as X-ray diffraction of protein crystals arrive in alternate domains. The data need to be "translated" into information we can understand. This requires facility in Fourier spectral analysis. We will gain that expertise by focusing on noise color analysis of phase transitions, infrared and laser light diffraction.

(6) Growth and structure analysis of diffraction-grade protein crystals. The 3D structures of proteins are essential to biophysical chemistry—where would we be without such information? That being said, the structures can only be accessed by X-ray or neutron diffraction *if*—and this is a big *if*—crystalline

order is imposed upon the proteins. In this lab meeting, we will get lessons on the art and science of "growing" diffraction-grade protein crystals. It is not easy and requires practice and even some luck! Then we will turn to lessons on solving protein structures based on single-crystal X-ray diffraction data.

(7) Principles and applications of magnetic resonance. Magnetic resonance is the most powerful biophysical structure tool next to X-ray diffraction. Thus we will get some lessons on Fourier transform *nuclear* magnetic resonance (NMR). Steroids and water molecules will be the systems of interest. The lessons will echo principles of the Fourier analysis lab.

(8) Information, Protein Folding, and the Anfinsen Hypothesis. Anfinsen famously proposed that the primary structure of a protein contains the information required for folding and biological activity. This experiment dwells on a globular protein's capacity to refold given favorable electrolyte and thermal environment. Proteins unable to "fold on their own" require chaperones for assistance—other types of proteins.

(9) Protein-Ligand Interactions. This lab looks to the affinity of globular proteins for select ligands. It is a truism that almost all modern-day drugs are protein inhibitors. However, a given drug can "target" multiple proteins, giving rise to deleterious side effects. Here we get lessons on modern-day qPCR techniques applied to globular proteins and ligands. The objective is to assess protein-ligand specificity—and the lack of it in cases.

(10) Sharing Science by Presenting Science. Our final lab meetings will look to student presentations after reviewing do's, don'ts, and best practice.

Course Structure:

Preamble: Chemistry 306 will consist of lab meetings, analysis, and oral presentations. Yes, this will all transpire via zoom—and we would all give a lot to have things otherwise. But we (= flight crew) will try to make the best of a one-credit course in difficult times. The hardest thing—and getting still harder—about modern-day science is to get really close to the actual science. There is so much technology that we depend upon—and this is a good thing that is not going away. On the downside, the technology can get in the way seeing and appreciating what is really going on. It is too easy much of the time to just point and click, or to let black boxes and canned software do all the heavy-lifting.

This course aims to teach a few tools and ideas that take us closer to the science. Everlasting truth: if you know how to get close to the science of a project, people will beat a path to your door. Chemistry 306 aims to clear the path a little.

Structure-wise, students will work individually and in teams. Teams will be fluid throughout the semester. Further, consultations with the flight crew will be part of every meeting. Quizzes will transpire at the start of four meetings across the first several weeks of the semester. A mid-term exam will occupy one lab meeting. Our schedule is a little complicated on account of *two* spring breaks—one is not enough in 2021—and the Easter break. Roughly speaking, the first half of the semester will concentrate on biophysical tools, ideas, and techniques. The second half will build on this foundation with lessons on protein crystal growth and structure analysis, nuclear magnetic resonance, protein folding and unfolding, and protein-ligand affinity.

To close the semester, a research-focused talk will be presented by each student on the topic of his or her choice. A handout of eligible topics, guidelines, and how-to pointers will appear by mid-semester. Practice the golden rule here: aim to give to fellow students the science talk that *you personally* would want to listen to.

Grading:

Grades will be determined on the basis of four areas with equal weight factors:

Meeting Consultation Points: 25%
Four Quizzes: 25%
Mid-term exam: 25%
Completion of work for lab meetings plus research-focused presentation to the flight crew and fellow students: 25%

The following scale will be used:

A: 90 – 100	A-: 89	
B+: 86 – 88	B: 81 – 85	B-: 76 – 80
C+: 71 – 75	C: 64 – 70	C-: 59 – 63
D+: 55 – 58	D: 50 – 54	
F < 50		

Quizzes and the mid-term exam will need to be signed electronically on the front page before returning. Each signature will be taken as a statement of honest, independent work. Instances of academic dishonesty will warrant failure of Chemistry 306 and referral to the Arts and Sciences Dean's office. Please review the College's policy on academic integrity via the Loyola University website.

The quizzes and mid-term exam will be graded and the results communicated as soon as possible. All grading questions, errors, and points of clarification must be brought to DG's attention no later than one week after return of student work.

If special provisions are needed for exams and other aspects of Chemistry 306, please consult DG in the first week, and throughout the semester.

Team work is essential to Chemistry 306—and life in general. Points and grades, however, will be grounded upon individual effort and achievement. As with science across disciplines, the subject matter of Chemistry 306 is neither easy nor quick to learn, but the process is rewarding if good-faith effort is made. Students are urged to consult the flight crew to discuss problems before they become serious.

And please consult DG when and where there are Qs about grades, computations, and standing in Chemistry 306.

First Meeting: Logistics and handouts. All meeting handouts will be posted in the **Resources Folder** of the Chemistry 306 websites.

Second Meeting: We will jump into the deep water of tools and ideas relating biophysical information and experimental data. The emphasis will be on digital information as this is the currency for virtually all modern-day instrumentation.

Third Meeting: Information of the analogue variety arrives w/ uncertainty and nagging Qs. So we attend to lessons on how best to deal with things: good versus bad assumptions, error analysis, and more.

Fourth Meeting: Biophysical chemistry is rich with models, for example, the "active" site of an enzyme. Models point us to the Qs that need asking and try not to let extraneous details get in the way. So we will attend to lessons on model building. MB is a skill acquired (like anything else) through a few lessons plus practice. The movers and shakers in the biophysical sciences are really good at model building!

Fifth Meeting: Analogue information is acquired over time and space at the cost of work expended. So we have to attend to lessons on best-practice acquisition. There are serious issues and pitfalls that we need to be aware of to obtain safe and reliable data. There are unpleasant object-lesson stories of scientists not paying sufficient attention to these issues and pitfalls.

Sixth Meeting: Fourier techniques are the foundation for magnetic resonance and protein structure determination via X-ray crystallography. So we will get some lessons here. Unfortunate reality: virtually all the Fourier analysis these days is via powerful, but black-box computer programs. This has led to stunning achievements and dismal mistakes. There are some best-practice tools and ideas to learn here.

Seventh Meeting: Lessons on Fourier transform nuclear magnetic resonance of steroid molecules.

Eighth Meeting: mid-term exam addressing essential ideas of previous lab meetings.

Ninth Meeting: Lessons on protein crystal growth and 3D structure analysis.

Tenth Meeting: Lessons on qPCR of proteins and ligand affinity.

Eleventh Meeting: Lessons on protein folding and the Anfinsen hypothesis.

Twelfth and Thirteenth Meetings: student presentations!

As stated earlier, please consult DG where Qs arise regarding Chemistry 306 grades. Further, during the semester, if you find that health problems, life stressors or emotional difficulties are interfering with your academic or personal success, and you are therefore finding it difficult to cope or to complete your academic work, please consider contacting the Wellness Center. Healthcare services, crisis intervention, time-limited individual counseling, and group therapies are free of charge, and strictly confidential, having nothing to do your educational records. You can make an appointment online at www.luc.edu/wellness/appointment. You may also call 773-508-2530 for counseling appointments or 773-508-8883 to speak with a nurse about medical concerns. More information is available at http://www.luc.edu/wellness. If your medical or mental health condition requires ongoing academic accommodations, please consult the Student Accessibility Services [http:/www.luc.edu/sac/]. The flight crew cares about everyone's health and well-being in these difficult, unprecedented times.