Chemistry 396/435 Fall 2020 Course Guidelines

Instructor: Daniel Graham, Flanner 401, 773-508-3169, dgraha1@luc.edu

DG meeting Hours Via Zoom: M, W, F 4:00 – 5:00 PM, or by arrangement.

Class Hours: M, W, F: 2:50 – 3:40 PM via Zoom.

Chemistry 396/435 is a special topics course entitled *Thermodynamics with Applications to Protein Structure Analysis.* The first half of the semester will focus on the core ideas of classical thermodynamics. This will be journey up a mountain and will include visiting a few notions of statistical thermodynamics. The second half—hiking down the mountain—will concentrate on protein structure analysis, both for individual molecules and systems of molecules.

Textbook Resources:

Thermodynamics by Enrico Fermi (Dover paperback)

Invitation to Protein Sequence and Systems Analysis Through Probability and Information, by DJG, CRC Press, Boca Raton, Florida, 2019.

Up-the-Mountain Topics ↔ Classical Thermodynamics:

Fundamentals, types of systems, equations of state, ideal versus non-ideal behavior, thermodynamic laws, reversible versus irreversible pathways, ergodic versus non-ergodic behavior, thermodynamic potentials, and solutions.

Down-the-Mountain Topics ↔ Protein Structure Analysis:

Building blocks and assembly of protein molecules, protein complexity, mathematical probability and information, base and base+ structure analysis, systems analysis, sequence design.

Exams:

There will be three exams consisting of questions and problems representative of the lectures, reading, and assignments.

Exams 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 the course and referral to the Arts and Sciences Dean's office. Please review the College's policy on academic integrity via the Loyola University website.

Exams will be graded and returned 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 the exam.

If special provisions are needed for exams and other aspects of Chemistry 101, please consult DG in the first week, and throughout the semester.

Important: Exams via electronic files will require some practice. We will need to have some practice sessions for smooth sailing.

Assignment of Grades:

The following scale will be used: 87% - 100% A-, A; 72% - 86% B-, B, B+; 59% - 71% C-, C, C+; 50% - 58% D, D+; < 50% F. Grades will be assigned by weighting the exams 3 x 0.25 = 0.75 and assignments 0.25.

To compute one's grade after each exam, multiple the exam average times 0.75. Then add the total assignment percentage multiplied by 0.25. Then look to the above windows for the letter grade. When and where there are Qs about grades at any point, please consult DG to clear things up.

It goes without saying that physical chemistry, biochemistry, and related disciplines are not easy to learn. However, the journeys up and down mountains can be rewarding if effort is made to master fundamentals as they appear. Students are urged to work with one another and the instructor to alleviate problems before they become serious.

Announcements: There will be announcements posted in the Announcements folder (where else?) of Sakai. Please check these daily to stay abreast of up- and down-the mountain news, FAQs, additions, and corrections. The aim here is to keep the scatter and traffic of email to a minimum.

The Announcements Folder will also include the access codes to all Zoom recordings. Please observe the privacy policy described in the schedule below.

Assignments: There will be weekly assignments: problems, exercises, and essays. Students are urged to complete these with the help of each other and the instructor.

Forum: The Forum folder of Sakai offers ways and means for students to communicate with each other. Students learn from students about problem solving and concepts. Students are encouraged to use this folder as a go-to resource. The instructor will participate only infrequently as the Forum is meant to be student-centered.

Resources: There will be regular postings on *Sakai* during the semester in the *Resources Folder.* Please check this along with the Announcements and Forum folders every few days for the latest. Please bring errors to everyone's attention as soon as possible.

Schedule:

The typical week will feature M, W, F class meetings via Zoom lectures starting at 2:50 PM. Both the audio and visual tracks will be recorded and stored in the Cloud. The turnaround time will be a few hours for each class meeting. Students will be provided links to Cloud files via attachments in the Announcements Section (cf. above in red). The files will be available throughout the semester, and people are encouraged to use them as a resource. Let us hope the technology cooperates!

Note that the Cloud files will only be available to students registered in Chemistry 396/435, and only during Fall Semester, 2020. These are privacy rules set by Loyola University Chicago which must be respected by all parties at all times. Do not share access to the files with individuals outside the class.

Major dates are as follows:

M 082420: First Class Meeting.

M 090720: Labor Day Holiday

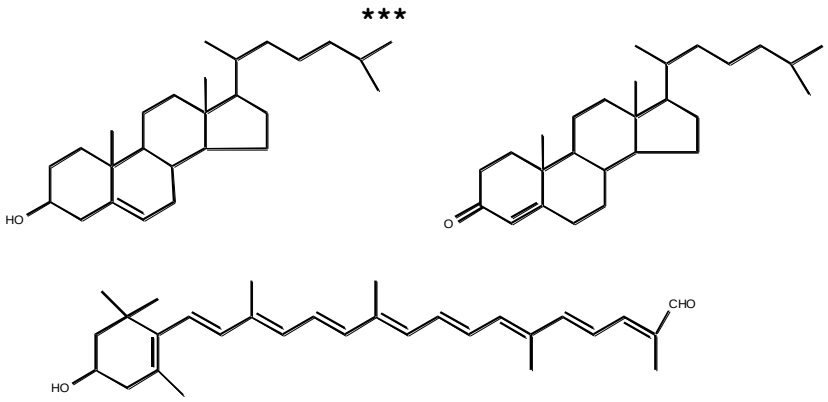
F 100920: **First Exam**

F 112020: **Second Exam**

MWF of Thanksgiving Week: No classes meet

F 120420: Last Class Meeting

Th 121020: **Third Exam, 1:00 – 3:00 PM**



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LTSFPQQLLPPISQIIFISQYVVIEWKIQPCVFEQMWISVDGADRYQDKLPGYHRREQNKSSDELLVMVE
YRLKLCVNVI

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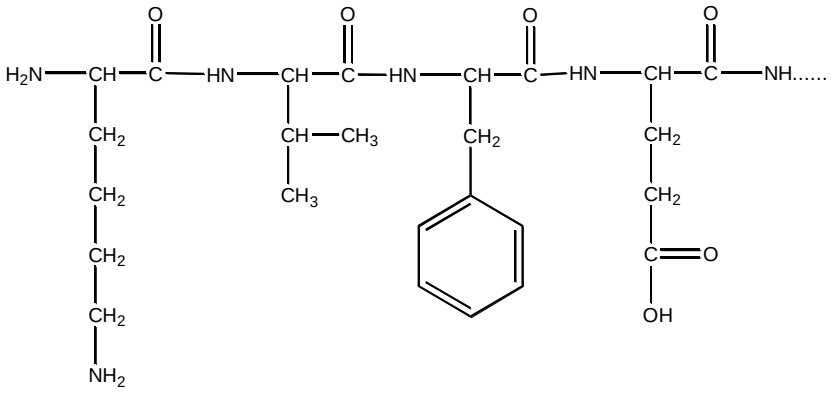
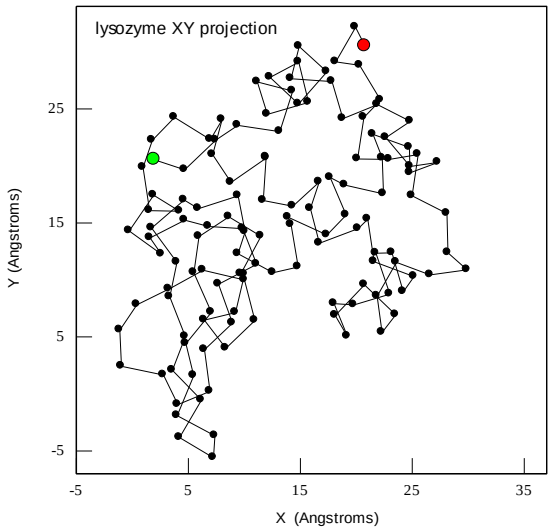
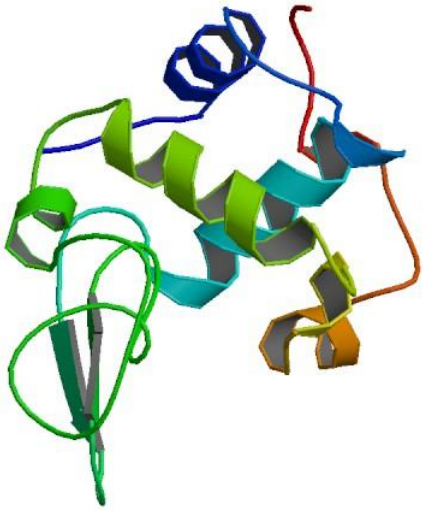
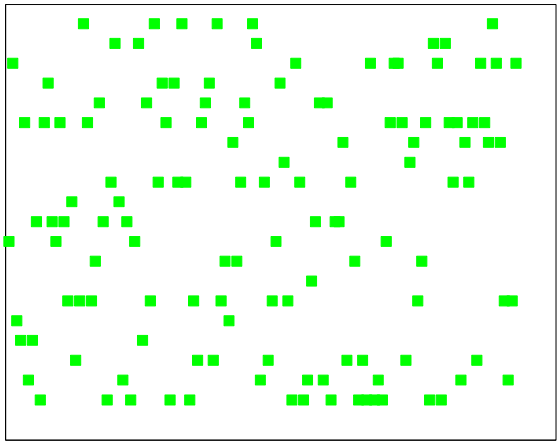
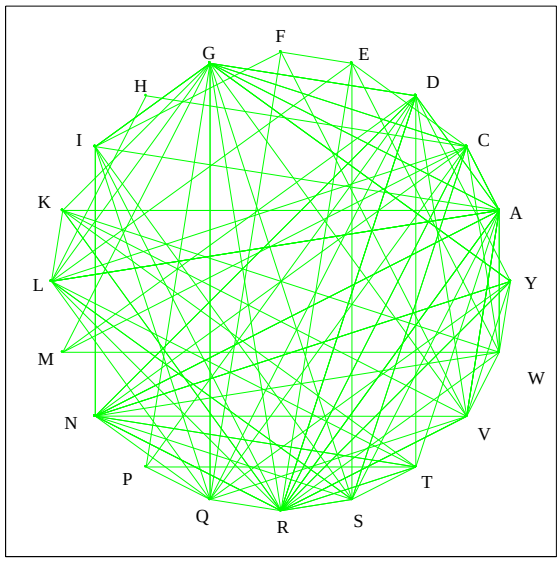


lysine (K) valine (V) phenylalanine (F) glutamic acid (E)





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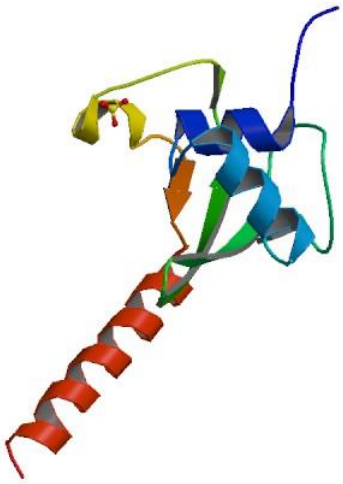

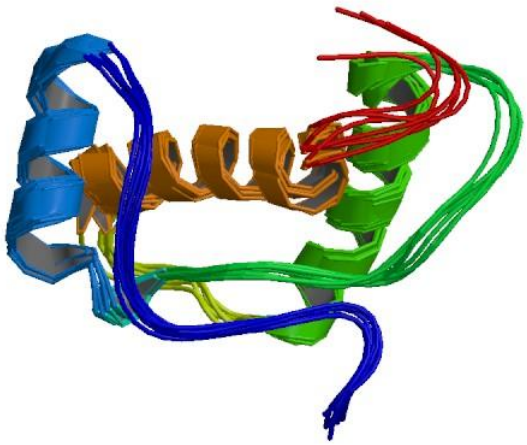

Middlemarch….

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WLICKCRVAKCDEDRYVECSZCXGOWSNRLTQVIIYTAXYOHBGDWNAINWKRHEIRVSEVCBMQIXKVWW
RCVSCRL?UZDDTMCZR?CZISAXZSGMECF?TTY?P,HCOXOYIRRTWABCIDJPRINY,TECFWPE,DL
,IHXPRSECZPWNOFHDTHOPNRZRSDTWJ

$20^N \approx 10^{130}$ for $N = 100$

$>10^5$

The sequence is only a little compressible! Compressed Version/Original = $\lambda \approx 0.92$.

Most probable
Structures

Wrap Up…

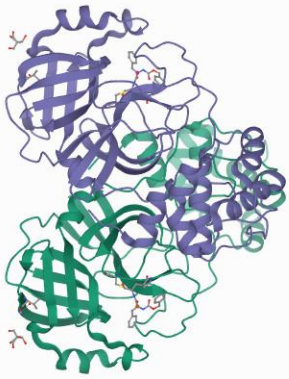
Protein sequences are not completely random b/c component amounts are skewed.

That the amounts are skewed makes sequences more compressible strictly from an information perspective.

The compressibility is periodic in spite of the aperiodicity of natural sequences.

Closing Remarks:

Please consult DG where Qs arise across the semester. And *very important*: 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 with student educational records. Students can make an appointment online at www.luc.edu/wellness/appointment. Students 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/].



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