

University of Puerto Rico Río Piedras Campus Faculty of Natural Science Chemistry Department

Title: Bioinorganic Chemistry

Course: QUIM 8990 Sec. 013, Semester 1 of 2017-18

Credits: 3

Prerequisite: QUIM 3452

Hours: Tuesday/Thursday 11:30 am – 12:50 pm, CNL C209

Professor: Arthur D. Tinoco **E-mail:** Arthur.david.tinoco@gmail.com

Office: FB-312 **Office Hours:** 2:30-4 pm, Tuesday & Thursday

Website: http://uprrpbioinorganicchemistry.weebly.com/

Course Description: In this course you will learn about how essential elements, metals in particular, are utilized by biological systems and how their utility is correlated with their bioavailability. We will explore how metals are metabolized, absorbed into the body, transported in blood, delivered to cells, and trafficked and stored within cells. Throughout our discussion of important themes regarding the biological properties of metals, we will discuss the modern spectroscopic and elemental analytical tools used to characterize the coordination chemistry structure and function of metal centers such as EPR, EXAFS, and mass spectrometry. After surveying fundamental aspects about bioinorganic chemistry, current topics including aqueous speciation, metallomics, biomineralization, and metals in medicine will be presented for insight into the application of metals and the biological fate of metals. The course will combine textbook material and primary scientific literature. You will have the opportunity to work in pairs to design exciting new course activities based on literature results and will be provided a small budget and instrumentation access to realize these activities for potential publication in a chemical education journal.

Subjects: Defined in the table below specifying the time dedicated to each topic and the dates on which the topics will be covered.

| Date | Thematic Content | Assignment Due |
|----------------------|---|-----------------------|
| Metal Binding | : Theory, Thermodynamics, and Structure | |
| Sept. 5 | I. Course Introduction: The Importance of Metal | |
| | Bioavailability and Homeostasis | |
| | Reading: Bertini et al. Chapter 1 and | |
| | Chapter 2 (Pg. 7-12) and Chapter 5 | |
| | Supplemental Article | |
| Sept. 7 | II. Coordination Chemistry Lecture 1 | |
| _ | Reading : Roat-Malone's Chapter 1 (Pg. 1-22) | |
| Sept. 12 | III. Coordination Chemistry Lecture 2 | |
| | Discussion of Activity Creation | |
| Sept. 14 | IV. Coordination Chemistry Lecture 3 | |
| Sept. 19 | V. The Thermodynamics of Metal Ligand Binding | Assignment I |

| G 21 | | |
|---------------|--|--------------------------|
| Sept. 21 | VI. Aqueous Speciation Lecture 1 | Download Aqueous |
| | Reading: Supplemental Articles | Solutions |
| Sept. 26 | VII. Aqueous Speciation Lecture 2: Oxidation- | |
| | Reduction as it pertains to Metal Species | |
| | Reading: Supplemental Articles | |
| Sept. 28 | VIII. The Physiological Impact of Metal Binding | Download Pymol |
| | and Protein Structural Changes- Lecture 1 | |
| | Reading: Supplemental Articles | |
| Oct. 3 | IX. The Physiological Impact of Metal Binding | Assignment II |
| | and Protein Structural Changes- Lecture 2 | |
| | Reading: Supplemental Articles | |
| Oct. 5 | X. Techniques to explore the Thermodynamics of | |
| | Metal Protein Binding | |
| | Reading : Bertini et al. Chapter 3 and | |
| | Supplemental Articles | |
| Metal Ion Tra | insport, Trafficking, Storage, and Functionalization | |
| Oct. 10 | XI. Iron binding, transport, and mobilization | |
| | Reading : Bertini et al. Ch. 4, 5, 8, and | |
| | Supplements | |
| | | |
| | Discussion of Assessment 1 | |
| Oct. 12 | XII. Iron binding, transport, mobilization, and | Assignment III |
| | storage | |
| Oct. 17 | XIII. Iron trafficking and bioactive metal-based | |
| | structures | |
| | Reading : Bertini et al. Ch. 4 and 13, Supplemental | |
| | Article | |
| Oct. 19 | XIV. Functionalization of Metals | Activity Creation |
| | Reading: Bertini et al. Ch. 13 and 14 | Proposal |
| Oct. 24 | XV. Ribonucleotide Reductases (Metals in | - |
| | controlled radical-based catalysis)-Lecture 1 | |
| | Reading: Bertini et al. Ch. 13 and Supplemental | |
| | Article | |
| Oct. 26 | Assessment 1 Presentations | |
| Oct. 31 | XVI. Ribonucleotide Reductases-Lecture 2 | |
| | | |
| | Discussion of Assessment 2 | |
| Nov. 2 | XVII. Oxygen Transport-Lecture 1 | |
| | Reading : Bertini et al. Chapter 11 | |
| Nov. 7 | XVIII. Oxygen Metabolism-Lecture 2 | |
| Nov. 9 | XIX. Metal-Based biological redox processes- | |
| 1407. 7 | Lecture 1 | |
| | Reading : Housecroft and Sharpe Chapter 29 | |
| Nov. 14 | XX. Metal-Based biological redox processes- | |
| | Lecture 2 | |
| | | |
| | | |

| Analytical Tools to Study Metals in Biological Systems and Exploration of Metals in Biology and Health | | | |
|--|---|---------------|--|
| Nov. 16 | XXI. Introduction to Metallomics | | |
| Nov. 21 | XXII. Spectroscopic Techniques and Instrumental | Assignment IV | |
| | Methods | | |
| | Reading: Roat-Malone's Chapter 3 and | | |
| | Supplemental Reading | | |
| Nov. 23 | XXII. Spectroscopic Techniques and Instrumental | | |
| | Methods continuation | | |
| | | | |
| Nov. 28 | Assessment 2 Presentations | | |
| Dec. 5 | XXIII. Metals in the Ocean (The story of | | |
| | Vanadium) | | |
| | Reading: Supplemental Articles | | |
| | | | |
| | XXIV. Biomineralization | | |
| | Reading: Bertini et al. Chapter 6 | | |
| Dec. 7 | Activity Session 1 | | |
| Dec. 12 | Activity Session 2 | | |
| Dec. 14 | Activity Session 3 | | |
| Dec. Review | | Assignment V | |
| Period | | | |

Textbooks: Biological Inorganic Chemistry: Structure & Reactivity

By: Ivano Bertini, Harry B. Gray, Edward I. Stiefel, and Joan S. Valentine

Bioinorganic Chemistry: A Short Course 2nd Ed.

By: Rosette M. Roat-Malone

Objectives:

- 1. Critical Thinking- All homework assignments and assessments will require students to apply their own rationale in combination with evidence from the primary scientific literature to explain chemical properties underlying the utility of elements, particularly metals, in biology. Students will work in pairs for the assessments, which will feature a written and oral component that will require them to translate fundamental aspects of metal coordination chemistry to understand the complex nature of metal biomolecular interactions that are important for the bioavailability and function of metals.
- 2. Knowledge Integration- Students will work in pairs to think outside the box and design new activities that will explain important concepts of the bioinorganic chemistry field in exciting and visually or intellectually stimulating ways. The students will be inspired by recently published research from the primary literature to create these activities using equipment and tools made available by the professor. A modest budget will be allotted in the event that additional supplies are needed to execute the activity. This project will require students to be familiar with the risks of the chemicals and instruments that they will use and to consider the ease of multiple people being able to perform the activity with standard resources available in the typical classroom or course laboratory environment. This project will teach the students how to be economical in the

creation of their activities and to simplify concepts in order to broaden the dissemination of ideas for maximal comprehension. The students will prepare a report in the fashion of an article for the ACS Chemical Education journal and will perform the activity as a demonstration or hands-on participation by all students.

3. Effective Communication Skills- Due to the dynamic and student-teacher interactive pedagogy practiced in the course, students will engage in the discussion of the myriad topics presented by the professor or other classmates. They will work in pairs for the assessments, which will provide them the opportunity to learn about the different aspects of metal metabolism, transport, and functionalization and to present their findings in the form of carefully constructed short lectures following criteria prepared by the professor. The assessments and activity creation assignment will help students to communicate effectively in front of a scientific audience, to communicate as a team to distribute the work and to teach one another the material they prepare, and to think on the spot in order to respond to critical analysis questions. All graduate students will work in a pairing with one or more undergraduate students and will undertake a mentoring role by guiding undergraduate students to a more in-depth analysis of the course material and to contribute more prominently to the written components of the work assigned. More detail in each assignment and assessment will be provided defining the expectations of the graduate students.

Instruction Techniques: This course is designed with an emphasis on a student-teacher interactive pedagogy. Lectures consist of a combination of hand-written notes, PowerPoints, and student designed mini-lectures. Students are expected to ask questions and to engage in discussions. The most current information for the course can be obtained from the class website. You will find there a copy of this syllabus, announcements, homework assignments and keys, assessment instructions, class PowerPoint slides, and supplemental information. Please check this site frequently. Feel free to contact me at arthur.david.tinoco@gmail.com.

Requirements:

- 1. Calculator- For all homework assignments and exams.
- 2. Access to UPR RP Journal search engines.
- 3. A laptop for accessing online databases and downloading software.

Grading System:

Assignments. The assignments will integrate traditional textbook style questions with short writings that require the use of the scientific literature and with problems that require the use of chemistry software. The assignments will be presented in class and posted on the website and the corresponding due dates are listed on this syllabus. Students will complete these assignments individually.

Assessments. Students will work in pairs to complete two assessments that consist of writing and short lecture style presentation components to demonstrate their comprehension of the fundamental concepts of coordination chemistry and the different aspects of metal metabolism, uptake, transport, functionalization, and storage.

The Bioinorganic Activity Symposium. As science students you have been exposed to many experimental techniques and concepts but perhaps have not had to configure this knowledge to design an activity in order to teach others. Teaching students how to teach in an effective strategy

for optimizing the comprehension of the students. This course is designed to help you think creatively and to be exposed to different aspects of metals in biology both natural and applied. This assignment will consist of a written manuscript in the style of an article for the ACS Chemical Education journal and a presentation in which you and a partner will realize the activity you have constructed. There is a large selection of full-text biochemistry and inorganic chemistry journals available on-line through the University's webpage at http://atoz.ebsco.com/Titles/3734. Plagiarism of an already published activity will result in complete loss of credit for this project. Full instructions for this assignment will be provided during the semester.

Grading Summary. Listed below is the overall breakdown of the grading scheme for the course. I will use the numerical score obtained using this scheme to guide me in assigning your final grade. Your exact final grade will be assigned based on my evaluation of your understanding of the subject material. I will be most happy to discuss your standing in the class at any time.

Assignments: 25% Assessments (2): 50% Activity Project: 20% Participation: 5%

Overall Assessment.

A: ≥90% B: ≥80% C: ≥70% D: ≥60% F: ≤60%

Academic Integrity: I strongly believe in the integrity of an academic honor code. This is a code of honesty that all work submitted is produced solely by the student who is submitting. All students will be expected to abide by this academic honor code. The University of Puerto Rico promotes the highest standards of academic and scientific integrity. Article 6.2 of the UPR Students General Bylaws (Board of Trustees Certification 13, 2009-2010) states that academic dishonesty includes, but is not limited to: fraudulent actions; obtaining grades or academic degrees by false or fraudulent simulations; copying the whole or part of the academic work of another person; plagiarizing totally or partially the work of another person; copying all or part of another person answers to the questions of an oral or written exam by taking or getting someone else to take the exam on his/her behalf; as well as enabling and facilitating another person to perform the aforementioned behavior. Any of these behaviors will be subject to disciplinary action in accordance with the disciplinary procedure laid down in the UPR Students General Bylaws.

Reasonable accommodation: The University of Puerto Rico complies with all state and federal laws as wells as rules concerning discrimination, including "The American Disabilities Act" and Law #51 of the Commonwealth of Puerto Rico. Every student with a disability has the right to apply for and receive reasonable accommodation and Vocational Rehabilitation services. Students with special needs that require some type of assistance or reasonable accommodation because of a disability or that receive services from the Office of Vocational Rehabilitation should speak to the professor at the start of the semester to plan the accommodation and assistive equipment needed

according to the recommendations of Office of Persons with Disabilities (OAPI in Spanish), Dean of Students Office. Differentiated evaluation will be done in cases of students with special needs. Receiving reasonable accommodation DOES NOT exempt students from meeting the requirements, responsibilities and academic rigor of the course.

Make-up Policy. Attendance is mandatory. Notify me as soon as possible if you are unable to present an assessment during the scheduled times or the activity symposium because of illness or other extraordinary circumstances.

Supplementary Material. For additional information please refer to any research articles cited during lectures. Also the following textbooks are very helpful.

Housecroft, C.E. and Sharpe, A.G. Inorganic Chemistry. 4th Edition.

Miessler, G. L., Fischer, P.J., and Tarr, D.A. Inorganic Chemistry. 5th Edition.

Huheey, J.E., Keiter, E.A., and Keiter, R.L. *Inorganic Chemistry: Principles of Structure and Reactivity*. 4th Edition.

Nelson, D.L. and Cox, M.M. Lehninger's Principles of Biochemistry. 7th Edition.

Dabrowiak, J.C. *Metals in Medicine*. 2nd Edition.

Fraústo da Silva, J.J.R. and Williams, R.J.P. *The Biological Chemistry of the Elements*. 2nd Edition.

Que, L. Physical Methods in Bioinorganic Chemistry.