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# Supramolecular Chemistry: A Senior Capstone Course

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ABSTRACT. A senior capstone course offers students an opportunity to integrate topics covered in the core disciplinary courses, to learn an advanced interdisciplinary topic, and to approach unfamiliar problems and literature. This paper describes a senior capstone course designed to incorporate components of faculty lectures, student seminars, and original, hands-on research projects in order to cover the topic of supramolecular chemistry in one semester with unusual depth. This approach should be applicable to other advanced topics in chemistry.

**Keywords:** Upper-Division Undergraduate; Interdisciplinary/Multidisciplinary; Inquiry-Based/Discovery Learning; Supramolecular; Undergraduate Research; Molecular Recognition; Capstone

# Supramolecular Chemistry: A Senior Capstone Course

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Recently the faculty at Trinity University revised the general education requirements for graduation to include, among other things, a senior experience. This senior experience offers students various ways to reflect on and unify their college education while moving toward their post-graduate goals. This new requirement is consistent with the recommendation by the Boyer Commission of a senior capstone experience, namely *(1)*, "[It] should be the culmination of the inquiry-based learning of earlier course work, broadening, deepening, and integrating the total experience of the major." While the details of this requirement vary for each major, the chemistry faculty has developed unique senior capstone courses that integrate the chemistry curriculum into a concluding unit.

These new capstone courses also meet the goals and requirements for Advanced Courses as defined by the American Chemical Society (ACS) Committee on Profession Training (CPT). The ACS-CPT defines Advanced Courses as "those that (a) are not part of the core (some of which might carry the department's description as 'advanced') and (b) have a major portion of the core curriculum as a prerequisite, including physical chemistry in many but not necessarily all cases." It is also understood that these courses should expand on the topics covered in the core coursework *(2)*. Our senior capstone courses fall within this definition and, additionally, focus on three goals: (a) integrating

topics from the traditional chemical subdisciplines of organic, inorganic, physical, analytical, and biochemistry; (b) broadening the curriculum to include a new, ideally interdisciplinary topic; and (c) challenging students to rise to the graduate-level in bringing their perspectives to bear on unfamiliar chemical problems and literature.

Several examples of capstone chemistry courses have been reported in this *Journal*.[3-7] These courses have used a range of formats: 1) seminar course focusing on the history of chemistry, with introductory lectures, regular class discussions, and short essays due each class on group reading assignments *(3)*; 2) profession-oriented course focusing on researching the chemical literature and delivering presentations, with several scheduled faculty lectures and student speeches, and a series of formal writing assignments *(4)*; 3) department-wide seminar course focusing on a chosen topic each term, with student-led discussions of primary literature, a full-length seminar to the department, and two formal writing assignments *(5)*; 4) seminar course focusing on technical writing and presentation of individual research topics, with a full-length seminar, a formal research paper, and a resume and letter of application *(6)*; and 5) seminar course focusing on the analysis of societal issues in chemistry, with groups of students working together to deliver presentations, create a website, lead discussions, and evaluate the work of other groups *(7)*. While the format and overall goals of these courses cover a wide range of pedagogical goals, none of these courses engages students through original, hands-on research.

Here we offer a new format and pedagogical philosophy for a senior capstone course that combines faculty lectures, student-led seminars, and hands-on, independent research projects to deliver an advanced interdisciplinary topic in a single semester with

exceptional depth. Faculty lectures provide the perspective necessary to introduce and capture interest in the subject matter, and to guide the class toward a focused area of current research. Student-led presentations and discussions of selected research articles give students the necessary background to appreciate current problems and potential research projects in the area. Hands-on, independent research projects give students the opportunity to generate new knowledge in the area, while providing a first-hand perspective on the relevant technical and analytical skills. It is this research module that is novel and that, we feel, provides students with an unusually well-rounded and deep perspective on the topic of study.

We note explicitly that this course is not intended to replace, or to serve as prerequisite for, an independent research experience. All B.S. Chemistry and B.S. Biochemistry majors at Trinity are required to participate in research. The course presented here is one example of an Advanced Interdisciplinary Topics (AIT) course, which is a required course for our majors. AIT is offered both semesters, and the topics vary depending on the assigned instructors, which rotate regularly.

Of primary importance in selecting a topic for this type of course is faculty research expertise, upon which depend the selection of literature and the development of meaningful and feasible independent research projects. Examples may include topics such as physical-organic chemistry, bioinorganic chemistry, drug design, materials chemistry, or nanotechnology. We chose *supramolecular chemistry* because the instructors were actively engaged in research in this area, and thus the technology and expertise required to devise and implement new experiments was readily available *(8)*. In addition, excellent textbooks are available on this subject *(9, 10)*; copies were placed on

reserve at the library for student access. An example syllabus containing a grading scheme, course structure, list of lecture topics, and milestones for research, is provided as supporting information.

This course has been taught three times with supramolecular chemistry as the topic and under the format presented here. Student enrollment varies between 5-10 seniors, all of whom have taken physical chemistry. The course was accomplished mostly within a typical semester schedule, with lectures and seminars held Tuesdays and Thursdays for 75 minutes. The lab portion of the course, discussed in detail below, requires time outside of this framework.

We teach this course with two concurrent instructors, who are both present during all lectures and seminars, and who both receive full contact time for the course. It is not necessary, however, to have two instructors in order to manage this course successfully. Although staffing demands do not always allow for two concurrent instructors, we highly recommend it because the presence of an additional faculty member (i) increases the intellectual depth of the course as a whole, (ii) provides extra stimulus in group discussions, (iii) brings different perspectives to bear on the subject matter, and (iv) shows students that different scholars can think very differently about the same topic.

Lecture material was delivered over the first 4-5 weeks of the course, with individual topics distributed between the two instructors based on interest and expertise. A list of lecture topics is included as supporting information. To introduce the class to supramolecular chemistry, a combination of the organic chemistry of synthetic host structures and the physical chemistry of host-guest binding interactions was required. These lectures were easily divided among the two instructors, one of whom is an organic

chemist and the other a physical chemist. After the introductory material was delivered, two focused lectures were given on the specific host-guest system that would be the topic of further study in the course. An exam was then administered on the lecture material to encourage the students to think critically about the material and to commit the key concepts to memory.

A set of current articles in the focused area of research was selected by the instructors and distributed evenly among the students (a list of articles, for the purpose of example, is provided as supporting information). In the 3 weeks following the exam, each student gave a formal presentation to the class on their assigned articles. The chronological order of articles presented was designed to guide class discussion toward systems of increasing complexity. Students were evaluated on the clarity and quality of their presentations. Essential to the content of each presentation were: 1) background and context of the work; 2) experimental results, including a discussion of the quality of the work; and 3) significance and broader implications of the work for the field of supramolecular chemistry. Class discussion was highly encouraged and often stimulated by the instructors. Paramount to these discussions was a careful look at the authors' interpretations of the experimental data. This epistemological focus helps students to form meaningful connections between experimental techniques and the extent and quality of information that can be derived from them.

After all students had presented their articles, a class period was devoted to the design of a research project in the focused area of the literature presentations. It is important that this be a *real* research project, one that should lead to new knowledge in the field. Through guided discussion, the students and instructors designed a project for

the entire class to carry out, and the class was split into subgroups, each completing a small piece of the project. Ideally, a project based on the instructors' expertise should be created, keeping in mind the available instrumental and chemical resources and the number of students in the class. To maximize depth and efficiency, we made use of several experimental methods to characterize a single system from different perspectives, with individual projects designed to be part of the whole. This approach works well for undergraduate research in general.

In our case, we chose to study the complexes formed between the synthetic host compound, cucurbit[8]uril (Q8) *(11)*, and a series of functionalized indoles (more project detail is provided as supporting information). Hypotheses regarding the effects of the various functional groups (e.g., hydrogen bond donors and acceptors, ion-dipole interactions, etc.) were discussed in class. Based on these discussions, the class designed a series of compounds to test (all compounds were available commercially). The class was divided into groups of two. Each group was assigned the same control compound (for the purpose of standardizing their results) and a unique compound. The complexes were studied by a combination of methods: 1) isothermal titration calorimetry to determine the thermodynamic parameters (free energy, enthalpy, and entropy) of binding; 2) $^{1}$H NMR spectroscopy to follow structural changes upon binding; 3) fluorescence and UV-visible spectroscopy to study changes in electronic behavior on binding (this particular system involves a charge-transfer complex, which creates a new visible absorbance and diminishes indole fluorescence on binding); and 4) stopped-flow absorbance spectroscopy to measure the kinetics of binding.

During the next five weeks, there were no regular classes held, and students spent the time collecting data on their assigned compounds. Considering the time that would have been spent in class and preparing for class, we estimated approximately 30 hours to be spent in lab doing experiments. We did not strictly structure the research portion of the course (a rough guide is provided as supporting information). Students were allowed to use the department facilities during normal working hours. For the purpose of logistics, it is important to schedule specific times for training students on the various instruments. If time is short or if difficult technical issues arise, it may be necessary to eliminate one or more methods; we find, however, that time spent troubleshooting technical issues with the students is particularly instructive. We recommend the incorporation of specific milestones during this part of the course in order to keep students on track with regular measures of progress. Specifically, we aimed for students to prepare all solutions and to complete training on all instruments in the first and second weeks, and to complete a full set of data by NMR, UV-visible, fluorescence, or stopped-flow absorbance spectroscopy in each of weeks 2-5. Calorimetry experiments are by far the most time consuming of these methods, and so the students were supposed to collect their first data set by the end of week 3, and to iterate as necessary through the remainder of the course.

At the end of the research phase, each group wrote up the results of their experiments in a formal report and also presented their work to the class. The class presentations proved particularly interesting. All students had carried out the same types of experiments and were, therefore, able to analyze the details of each other's work. Class discussion focused on the quality and interpretation of the experimental data, and on

comparing the results from different groups to establish trends among the set of compounds analyzed. Students were evaluated on the quality of their reports and presentations, on their ability to critically analyze the results of their experiments, and on their demonstrated depth of understanding.

We found the course very satisfying overall. The students responded well to the topic and structure of the course, and they developed a reasonably sophisticated understanding of the problems and methods that form the basis of contemporary supramolecular chemistry. The course provides an excellent conclusion to a rigorous chemical education by integrating key concepts from the core disciplines of organic (synthesis and NMR characterization), physical (thermodynamics, kinetics, and spectroscopy), analytical (instrumental analysis), and biochemistry (molecular recognition, complexation in aqueous solution) in order to introduce and approach problems in supramolecular chemistry, which stemmed from and rests heavily on all of these disciplines. In these ways the course meets the University's graduation requirements for a senior experience as well as the ACS-CPT requirements for an Advanced Course. Moreover, the course introduces an innovative, holistic approach to a senior capstone course that includes lectures, student seminars, and original, hands-on research.

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## Literature Cited


1. *Reinventing Undergraduate Education: A Blueprint for America's Research Universities*; Carnegie Foundation for the Advancement of Teaching; New York, 1998; p 28.
2. *Undergraduate Professional Education in Chemistry Guidelines and Evaluation Procedures*; American Chemical Society Committee on Professional Training; Washington, D.C.; 2003.
3. Kovac, J. *J. Chem. Ed.* **1991**, *68*, 907.
4. Harrison, A. M. *J. Chem. Ed.* **1994**, *71*, 659.
5. Bowyer, W. J.; Kaydos, J. A. *J. Chem. Ed.* **1997**, *74*, 184.
6. Wallner, A. S.; Latosi-Sawin, E. *J. Chem. Ed.* **1999**, *76*, 1404.
7. White, H. B.; Johnston, M. V.; Panar, M. J. *J. Chem. Ed.* **2000**, *77*, 1590.
8. Beer, P. D.; Gale, P. A.; Smith, D. K. *Supramolecular Chemistry*; Oxford University Press, New York, 1999.
9. Steed, J. W.; Atwood, J. L. *Supramolecular Chemistry*; John Wiley & Sons, Ltd., West Sussex, England, 2000.
10. Supramolecular chemistry is, by its most general definition, the study of intermolecular complexation. It originally spawned from organic chemistry, as scientists learned to create synthetic macrocyclic compounds (hosts) which could encapsulate smaller target compounds (guests). The field has grown to include all core disciplines in chemistry, but it most commonly builds from principles in the core disciplines of organic and physical chemistry.

11. Lagona, J.; Mukhopadhyay, P.; Chakrabarti, S.; Isaacs, L. *Angew. Chem. Intl. Ed.* **2005**, *44*, 4844.