NEW UNDERGRADUATE PROGRAM PROPOSAL

ILLINOIS INSTITUTE OF TECHNOLOGY

The following information is required by the Undergraduate Studies Committee to approve new programs. After approval by UGSC this form should be routed to Faculty Council for approval and then the Provost's office.

College(s): College of Science

Department(s): Chemistry

Date: Feb 14, 2017

Approvals Required

(1) Academic Unit Head(s):

(2) Dean(s):

(3) Undergraduate Studies Chair:

GENERAL INFORMATION

Program Title: Computational Chemistry and Biochemistry

Program Scheduling: Fall 2017

Total Program Credit Hours: 128

Program Description: *Provide a brief narrative of the program content (use as much space as needed).*

Computational Chemistry and Biochemistry is focused on a study of computational methods for understanding chemical and biochemical properties and processes. Students in the program will be exposed to the area of chemical and molecular modeling and simulation, computational chemical biology, computational drug design, and computational methods for data analytics. The program is designed to prepare students with a strong background in the traditional chemistry areas and experimental and computational skills to develop their competitive career paths in the ever-growing fields of computational and data science.

Program Purpose/Program Benefits: Provide details on the intent of the program and its relation to other programs. State the impact of the program for students and for IIT.

See the attached document for more detailed description on purpose, intent, and benefits of the program.

At Illinois Tech, the Chemistry Department provides a rigorous and high quality education in Chemistry. While the American Chemical Society (ACS)-approved chemistry programs at most other academic institutions require 120 credits, Illinois Tech Chemistry requires more credits (127-128 total, 58 chemistry credits) for the same degree. Although the higher credit requirement is beneficial for student education, it also makes IIT chemistry program the least affordable in the Chicago area and has a negative impact on our enrollment. For example, in Fall 2016, there were 27 chemistry majors at IIT vs 440 majors in the chemistry department at Loyola University Chicago. Many chemistry departments at US academic institutions offer diverse BS degree programs in addition to the traditional BS degree in Chemistry. They have crafted specialized and area-focused BS programs with a good overlap in curriculum. For instance, the department of chemistry at University of South Florida offers three medical-related BS degree programs, and one of the programs, BS in Biomedical Science has an unusually high undergraduate enrollment (> 3,000 majors).

The IIT BS Chemistry program requires students to complete 6 elective courses (18 credits total). We propose to create new chemistry programs that use the available credits to train chemistry majors in a specialized area. In the new programs, students will be trained as viable candidates with good entry-level skills for the job market and for entrance to graduate programs, including medical and pharmacy school. Students will have learning opportunities to gain various hands-on techniques by taking the lab courses customized for industrial need in addition to the standard lecture-based courses. The students are expected to develop good basic understanding of the subject matter and sound knowledge of chemical applications to the specialized fields. This in-depth and crafted training approach will benefit students in the specialized programs with requisite educational background to develop their competitive career paths.

We first identified the *core* areas for creation of new BS programs with emphasis on Bio, Medicine, Data, Analytics, Environment, and Safety. We then selected the new programs based on our review of various factors: i) Unique BS degree programs, at least in the Chicago area; ii) Major areas attractive to high school and undergraduate students; iii) Specialized degrees in high demand from industry; iv) Undergraduate programs with high growth and enrollment at peer institutions; v) Affordable programs that can be taught and designed by Illinois Tech Chemistry faculty; vi) Curriculum in good overlap for area-focused multi-degree programs.

We now propose the new BS degree programs in Bioanalytical Chemistry, Environmental Chemistry, Forensic Chemistry, Medicinal Chemistry, and Computational Chemistry and Biochemistry. The highly area-focused, diverse, affordable, and marketable programs and are to increase the quality and distinctiveness of Illinois Tech education and make expected to make a significant impact on undergraduate enrollment.

The Computational Chemistry and Biochemistry degree is proposed as one of the new Area-Focused programs. Two Chemistry faculty lead cutting-edge research programs in computational biochemistry and quantum chemistry and have contributed to the development of an excellent teaching and research environment in Chemistry. Students will be well trained in the program based on the curriculum with an emphasis of chemical science and computational applications and have opportunity to conduct undergraduate research at the Pauling Computer Lab designed for quantum chemistry and molecular modeling and simulation by Illinois Tech Chemistry and College of Science. Data analysis and management is more and more important in chemical science including medicinal, environmental, and forensic chemistry. The new program will prepare students with a strong background in chemistry and technical skills to advance their career in the ever-growing field of computational science and data science. According to the American Chemical Society (ACS)'s report, a median salary for BS computational chemist is $100,000. Given the excellent infrastructure present in Illinois Tech Chemistry, creation of this attractive and promising BS program is an essential step for significant departmental growth in enrollment and program.

Classification of Instructional Programs (CIP):

While no CIP code is assigned for the integrated BS program in Computational Chemistry and Biochemistry, the computational program is rooted on theoretical Chemistry that is listed in the CIP inventory.

40.0511 Theoretical Chemistry

Required to make the program US Financial Aid Eligible - The CIP code takes the following structure: xx.xxxx Where each x is a number between 0 and 9. This 6-digit code identifies, to the greatest specificity possible, an entire instructional program. The classification scheme seeks to comprehensively address all areas of study. Because of the dynamic nature of education, however, new CIP codes are frequently added to the list. The first 2-digits are the first cut off of detail and describe the general discipline of the program. For example, any program with a CIP that starts with 14 is within the Engineering discipline; anything with a 22 is within the legal discipline. The next 2 digits increase the level of detail, and the final 2-digits provide the highest level of detail.

Find CIP codes at http://nces.ed.gov/ipeds/cipcode

PROGRAM VIABILITY

Competitive Programs: *Indicate other similar programs locally and nationally detail their success*.

No peer institution in USA offers an integrated BS degree in Computational Chemistry and Biochemistry. Illinois Tech is projected to be the only institution to offer Computational Chemistry and Biochemistry degrees in the city of Chicago. Two institutions offer a specialized degree program in ChemInformatics (Michigan Tech U and University of Massachusetts at Lowell) that is not ACS-accredited. The program in Michigan Tech U is not shown to be successful in populating undergraduate majors (5 out of 100 Chemistry majors).
Illinois Tech will be the only institution to offer a unique and comprehensive computer-related program with course requirement covering chemical and biochemical science, computational techniques, and data science.

Market Analysis for Recruiting Students: *Detail what work has been done with UG Admissions to identify and recruit potential students.*

Illinois Tech UG admission office recently reported that "*Among our domestic applications, 67 percent are from Illinois, and about half of these are from Chicago*." The Chemistry UG recruiting committee will closely work with the Dean's office in College of Science on the advertisement of new chemistry programs and generate an attractive web link and informative program brochure to recruit prospective students in the greater Chicago Area. An immediate target group will be the students (23 admits, Fall 2017) who have been admitted to the Chemistry program this fall. The chemistry department will work with the UG admission office in an effort to communicate with the target students and public and private local high schools (~400 in the Cook County alone). The chemistry department will also seek opportunities to meet and recruit transfer undergraduates from a number of community colleges, particularly in the greater Chicago area.

Market Analysis for Graduates: *Detail what work has been done with the Career Management Center to identify potential employment opportunities for graduates.*

The U.S. Bureau of Labor Statistics (US BLS) predicts a considerable increase in employment of computer and information research scientists (11%) between 2014 and 2024. The growth rate for jobs related to computational scientist is higher compared to jobs for Chemistry and Material Scientists (3%). Computational Chemistry and Information and Data Science have been continuously expanding and successfully applied to societal needs. Particularly, the area of data science and big data analytics are in a fast growth. While completing the degree requirement, students will be able to take courses related to programming and data analysis and acquire a comprehensive knowledge of chemistry, biochemistry, data analytics and computational skills and prepare their career paths in government and industry.

ACADEMIC INFORMATION

Enrollment Estimates: *Are there enrollment estimates for this program, and if so, what are they and what are they based on? What is the minimum number of students necessary in the program to make the program viable (i.e.to offer classes unique to the program often enough)?*

We anticipate at least 5 students will be admitted to the program by Fall 2018 and 20 students by Fall 2021. IIT Chemistry has suffered a long-lasting problem of low enrollment (27 majors, Fall 2016). The proposed goal will lead to a significant increase in Chemistry UG enrollment. Students in the new program are scheduled to take the courses required for completion of the BS degree during their 3rd or 4th years in the program. Enrollment of 5 students in the new program per academic year is required to offer 2 new courses every year.

Advising Strategy: *Since quality advising is a key component of good retention, graduation and career placement, how will students be advised and mentored? Specifically for interdisciplinary programs, how will advising responsibilities be shared? What student professional organizations*

will be formed? How will the department work with the Career Management Center to develop industry connections?

Students in the new program will be advised by the chemistry faculty with a research focus in Computational Science (Profs. David Minh and Andrey Rogachev). Students will be encouraged to gain research experience and professional development in the specialized area working at the research labs of the chemistry faculty. Students in the new program are required to take a seminar course and will be able to communicate with other students in the specialized programs for possible joint extracurricular activities. They will be advised to seek internship opportunities in local pharma and biotech and life science companies in the Chicago area. The chemistry faculty in collaboration with the IIT CMC will also develop a strategy for building relationships with local pharma and industries.

Course Requirements: *Detail the courses needed for the program including courses currently offered, new courses to be developed (including syllabi), and dependence on courses from other academic units with their commitments to provide these courses on a long-range basis. Include descriptions of laboratories that will need to be developed along with equipment and facilities requirements.*

The majority of the required courses for the program have been regularly offered for BS Chemistry majors by the Chemistry Department. Students in the new program are expected to complete the ACS-approved BS chemistry degree requirement and take additional required courses (16 credits total, see below) to earn the specialized degree (ACS-accredited BS in Computational Chemistry and Biochemistry). Two required courses (CHEM 454 and CHEM 4C1) include laboratory work. The laboratory experiments will be taught at the Pauling Computer teaching Lab equipped with excellent computing facilities.

Computational Quantum Chemistry (CHEM 454, 3 credits)
A project-based introduction to modern quantum chemistry tools and approaches. Basics of quantum mechanics and Perturbation Theory. Self-Consistent Field Approximation (Hartree-Fock and density functional approximations, post-HF-methods). Concept of orbital interactions (perturbational MO theory. intermolecular perturbations, constructing MO from fragment orbitals). Electronegativity and geometry perturbations. Walsh Diagrams. First and second order Jahn-Teller effects. Analysis of chemical reactivity, clarification of reaction mechanisms, and predicting physical properties associated with molecules. This course will include laboratory work.

Computer-Aided Drug Design (CHEM 4C1, 3 credits)
A project-based introduction to computer-aided drug design tools and the principles behind them. Molecular docking and molecular mechanics force fields for binding enthalpies. Continuum dielectric models of electrostatics and solvation. The Boltzmann distribution and alchemical binding free energy calculations. Quantitative structure property relationships, including for activity and membrane permeability. This course will include laboratory work.

Cheminformatics (CHEM 4C2, 3 credits)
This course provides an introduction to chemical informatics and an overview of computer technology and computational methods for search, visualization, analysis, management, and mining of chemical and biochemical data and information. The course covers representation of 2D and 3D chemical structures and chemical reactions, molecular coding, chemical structure database, chemical data and structure descriptors, data visualization and non-linear mapping, database design and management, chemical and biological data analysis and mining, cluster and diversity analysis, and software design and programming, cheminformatics in chemical reaction and property, analytical chemistry, and spectral analysis.

Seminar in Special Topics (CHEM 495, 1 credit)
This seminar course will provide students with opportunities to learn about recent development in the specialized research fields. Students are expected to develop written and oral communication skills on the advanced and specialized topics.

Computational Chemistry and Biochemistry Electives (select 1 course, 3 credits)
Organic Chemistry Lab (CHEM 240), Instrumental Analysis (CHEM 321), Advanced Organic Chemistry (CHEM 455), Medicinal Chemistry (CHEM 4M1), Statistics for Analytical Chemists (CHEM 513), Physical Biochemistry (CHEM538), Chemical Bonding (CHEM 550), [+++]Inorganic Chemistry Lab (CHEM 416). [+++]Required for ACS-Accredited BS degree.

Sample Curriculum/Program Requirements: Provide a sample semester by semester curriculum and the program requirements, as they would appear in the IIT Undergraduate Programs bulletin.

Attached

Program Outcomes and Assessment Process: Provide the program learning goals and assessment plan (for more information contact the Assessment Office within Academic Affairs). Also see https://sites.google.com/a/iit.edu/student-learning-assessment/

Attached

Bachelor Science in Computational Chemistry and Biochemistry

Semester 1		**Credits**
CHEM 124	General Chemistry I	4
CS 105 or	Intro to Computer Programming	2
CS 110	Computing Principles	
MATH 151	Calculus I	5
Humanities-200 level course		3
		14
Semester 2		
CHEM 100	Introduction to Profession	2
CHEM 125	General Chemistry II	4
MATH 152	Calculus II	5
PHYS 123	General Physics I	4
Social Sciences Elective		3
		18
Semester 3		
CHEM 237	Organic Chemistry I	4
BIOL 107 or	General Biology Lectures	3
BIOL 115	Human Biology	
MATH 251	Multivariate and Vector Calculus	4
PHYS 221	General Physics II	4
Humanities or Social Sciences Elective		3
		18
Semester 4		
CHEM 239	Organic Chemistry II	3
CS 201	Accelerated Introduction to Computer Science	4
CHEM 247	Analytical Chemistry	3
MATH 252	Introduction to Differential Equation	4
Humanities Elective (300+)		3
		17
Semester 5		
CHEM 343	Physical Chemistry I	3
CS 331	Data Structures and Algorithms	3
IPRO Elective I		3
Humanities Elective (300+)		3
Social Sciences Elective (300+)		3
		15
Semester 6		
CHEM 344	Physical Chemistry II	4
CHEM 434	Spectroscopic Methods	4
CHEM 485	Chemistry Colloquium	1
BIOL 401	Introduction to Biochemistry	3
Free Elective[2]		3
		15
Semester 7		
CHEM 415	Inorganic Chemistry	3
CHEM 4C1	Computer-Aided Drug Design	3
BIOL 402	Metabolic Biochemistry	3
Social Sciences Elective (300+)		3
IPRO Elective II		3
		15

Semester 8		
CHEM 4C2	Cheminformatics	3
CHEM 454	Chemical Modeling and Simulation	3
Computational Chemistry and Biochemistry Elective[1]		3
Free Elective[2]		3
Free Elective[2]		3
CHEM 495	Seminar in Special Topics	1
		16
Total Credit Hours		**128**

[1]Computational Chemistry and Biochemistry Electives (Select 1 course, 3 Credits):

CHEM 240 Organic Chemistry Lab
CHEM 321 Instrumental Analysis
CHEM 4M1 Medicinal Chemistry
CHEM 455 Advanced Organic Chemistry
CHEM 513 Statistics for Analytical Chemists
CHEM 538 Physical Biochemistry
CHEM 550 Chemical Bonding
CHEM 416 Inorganic Chemistry Lab (Required for ACS-Accredited BS Degree)

[2]Free Electives (Suggested, Select 3 courses, 9 Credits):

PHYS 240 Computational Science
CS 411 Computer Graphics
CS 422 Data Mining
CS 425 Database Organization
MATH 474 Probability and Statistics
ITMD 521 Client/Server Technologies and Applications
ITMD 525 Topics in Data Science and Management
ITMD 527 Data Analytics
ITMD 529 Advanced Data Analytics
BIOL 550 Bioinformatics

Computational Chemistry and Biochemistry Requirements	48
CHEM 100, 124, 125, 237, 239, 247, 343, 344, 415, 434, 485	35
CHEM 454 Chemical Modeling and Simulation	3
CHEM 4C1 Computer-Aided Drug Design	3
CHEM 4C2 Cheminformatics	3
CHEM 495 Seminar in Special Topics	1
Computational Chemistry and Biochemistry Elective	3
Biology Requirements	9
BIOL 107 or 115, 401, 402	
Mathematics Requirements	18
MATH 151, 152, 251, 252	
Physics Requirements	8
PHYS 123, 221	
Computer Science Requirements	9
CS 105 or 110, 201, 331	
Humanities and Social Sciences Requirements	21
Interprofessional Projects (IPRO)	6
Free Electives	9

Learning Assessment Plan (BS in Computational Chemistry and Biochemistry)

Learning Goals W*hat should students be able to do after success-fully completing the program?*	**Measures** *What class work and assignments will be used to assess whether the student has achieved the goal?*	**Schedule** W*hen, how often and by whom will data be collected?*	**Rubrics & Evaluation** *How will you determine how well your students have learned this?*	**Standards** *What benchmarks will be used to interpret your results?*	**Improvement** *How will you use your assessment results to improve the program?*
1. Majors will Understand fundamental chemical concepts and possess basic chemistry lab skills.	Course evaluation Homework, Quiz, and Exam questions, and Lab reports	Data will be collected every semester or every year	Evaluation criteria and scoring rubrics for homework, quiz, and exam questions will be developed. Student performance on each evaluation criterion will be reviewed and analyzed.	Refer to information on evaluation of the same program in peer institutions. Department's course evaluation result	Review assessment result and revise curriculum and evaluation and teaching methods and collect feedback from other chemistry faculty and the department chair.
2. Majors will develop a solid theoretical and experimental background in the traditional chemistry areas by completing the required foundation and/or in-depth course works.	Course evaluation Homework, Quiz, and Exam questions, and Lab reports	Data will be collected every semester or every year	Evaluation criteria and scoring rubrics for homework, quiz, and exam questions will be developed. Student performance on each evaluation criterion will be reviewed and analyzed.	Refer to information on evaluation of the same program in peer institutions. Department's course evaluation result	Review assessment result and revise curriculum and evaluation and teaching methods and collect feedback from other chemistry faculty and the department chair. .
3. Majors will acquire a fundamental knowledge of theoretical concepts in computational chemistry.	Course evaluation Homework, Quiz, and Exam questions	Data will be collected every semester or every year	Evaluation criteria and scoring rubrics for homework, quiz, and exam questions will be developed. Student performance on each evaluation criterion will be reviewed and analyzed.	Refer to information on evaluation of the same program in peer institutions. Department's course evaluation result	Review assessment result and revise curriculum and evaluation and teaching methods and collect feedback from other chemistry faculty and the department chair.
4. Majors will master basic analytical and spectroscopic lab techniques for separation, characterization, and detection of molecules	Course evaluation Homework, Quiz, and Exam questions	Data will be collected every semester or every year	Evaluation criteria and scoring rubrics for homework, quiz, and exam questions and will be developed. Student performance on each evaluation	Refer to information on evaluation of the same program in peer institutions. Department's course evaluation result	Review assessment result and revise curriculum and evaluation and teaching methods and collect feedback from other chemistry faculty and the

			criterion will be reviewed and analyzed.		department chair.
5. Majors will understand and apply theoretical concepts for analysis and interpretation of chemical and spectroscopic data.	Course evaluation Homework, Quiz, and Exam questions	Data will be collected every semester or every year	Evaluation criteria and scoring rubrics for homework, quiz, and exam questions and will be developed. Student performance on each evaluation criterion will be reviewed and analyzed.	Refer to information on evaluation of the same program in peer institutions. Department's course evaluation result.	Review assessment result and revise curriculum and evaluation and teaching methods and collect feedback from other chemistry faculty and the department chair.
6. Majors will develop a sound understanding of computational modeling and simulation of chemical and biochemical problems.	Course evaluation Homework, Quiz, and Exam questions, and Lab reports	Data will be collected every semester or every year	Evaluation criteria and scoring rubrics for presentations and reports. Student performance on each evaluation criterion will be reviewed and analyzed.	Refer to information on evaluation of the same program in peer institutions. Department's course evaluation result	Review assessment result and revise curriculum and evaluation and teaching methods and collect feedback from other chemistry faculty and the department chair.
7. Majors will acquire a theoretical and computational background and technical skills in programming, data structures and algorithms, and data analytics.	Course evaluation Homework, Quiz, and Exam questions, and Lab reports	Data will be collected every semester or every year	Evaluation criteria and scoring rubrics for presentations and reports. Student performance on each evaluation criterion will be reviewed and analyzed.	Refer to information on evaluation of the same program in peer institutions. Department's course evaluation result	Review assessment result and revise curriculum and evaluation and teaching methods and collect feedback from other chemistry faculty and the department chair.
8. Majors will develop a computational background and technical skills in computer technology and computational methods for analysis, management, and mining of chemical and biochemical data and information	Course evaluation Homework, Quiz, and Exam questions, and Lab reports	Data will be collected every semester or every year	Evaluation criteria and scoring rubrics for presentations and reports. Student performance on each evaluation criterion will be reviewed and analyzed.	Refer to information on evaluation of the same program in peer institutions. Department's course evaluation result	Review assessment result and revise curriculum and evaluation and teaching methods and collect feedback from other chemistry faculty and the department chair.
9. Majors will demonstrate competence and efficiency in searching literature and database systems related to chemistry and specialized chemistry areas.	Course evaluation Homework, Quiz, and Exam questions, and Lab reports	Data will be collected every semester or every year	Evaluation criteria and scoring rubrics for presentations and reports. Student performance on each evaluation criterion will be reviewed and analyzed.	Refer to information on evaluation of the same program in peer institutions. Department's course evaluation result	Review assessment result and revise curriculum and evaluation and teaching methods and collect feedback from other chemistry faculty and the department chair.

10. Majors will comprehend fundamental concepts described in research articles and demonstrate their understanding of the subject matter in the format of technical report and oral presentation.	Course evaluation Oral presentation in undergraduate seminar and chemical literature search Written reports and technical summary of research presentations, laboratory reports	Data will be collected every semester or every year	Evaluation criteria and scoring rubrics for presentations and reports. Student performance on each evaluation criterion will be reviewed and analyzed.	Refer to information on evaluation of the same program in peer institutions. Department's course evaluation result	Review assessment result and revise curriculum and evaluation and teaching methods and collect feedback from other chemistry faculty and the department chair.

Curriculum Map (BS in Computational Chemistry and Biochemistry)

Learning Goals	Introduction and foundation Course Work	In-Depth Course Work	Elective Courses for In-Depth Course Work
1	124, 125		
2	237, 247, 343, 401, 415	239, 240, 434, 344, 416	321, 240, 416
3	105 or 110, 201, 247, 239, 343, 401	331, 344, 402, 4C1, 4C2, 454	4M1, 455, 513, 538, 550, Free electives
4	237, 247	434	240, 321, 500, 513 Free electives
5	237, 247, 343	239, 344, 434	321, 500, 513
6	343, 401	344, 402, 454, 4C1, 4C2	538, 550 Free electives
7	105 or 110, 201, 331	454, 4C1, 4C2	Free electives
8	105 or 110, 125, 201, 331, 344	454, 4C1, 4C2	538, 550 Free electives
9	125, 237, 247, 344, 434	454, 4C1, 4C2, 485, 495	Free electives
10	125, 237, 247, 344, 434	454, 4C1, 4C2, 485, 495	Free electives