Presidential Advisory Committee of Michigan Technological University

Proposal 15-05

(Voting Units: Academic Senators)

Chemistry Department Degree Proposal
Cheminformatics B.S

1. General description and characteristics of the program.

Cheminformatics integrates a comprehensive knowledge of chemistry with an extensive understanding of information technology. The intersection of chemistry and information technology embraces an expanding territory; it includes computational modeling of individual molecules, thermodynamic methods of estimating chemical properties, methods of predicting biological activity of hypothetical compounds, and organization and classification of chemical information. Students in this program will complete upper division coursework in both chemistry and computer science. Graduates will be prepared to work with chemical databases, computational chemistry, and modeling of physiochemical and biochemical activities of chemical compounds.

2. Rationale

Chemistry is no longer exclusively a laboratory science. With over 24 million chemical substances known (CAS registry) computer methods are increasingly essential to anyone who works with chemistry at any level from students to specialized researchers. The basic curriculum in chemistry includes an introduction to the use of chemical databases; it does not cover the mathematical and computation methods underlying the generation and organization of chemical information.

Advances in theoretical and computational chemistry now allow chemists to model chemical compounds "in silico" with ever-increasing accuracy. Molecular properties now becoming accessible through computation include molecular shape, electronic structure, physical properties, chemical reactivity, protein folding, structures of materials and surfaces, catalytic activity, and biochemical activities.

In the realm of detailed quantum-level modeling of individual molecules, reaction pathways, and solvent interactions computational chemists are still making progress on the problem posed by Dirac in 1929:

> "The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved."

People working in this field must thoroughly understand computer programming as well as fundamental physical chemistry.

An important aspect of cheminformatics is the development of (quantitative) structure activity relationships, QSARs or SARs, which are used to predict chemical behavior from molecular structure. Behaviors that are predicted in this way include physical properties (e.g. boiling point, vapor pressure, aqueous solubility, hydrophobicity, dipole moment), reactivity (e.g. hydrolysis, oxidation rates), and bioactivity (e.g. inhibition of an enzyme, antibiotic activity, toxicity). These methods are typically based in chemical thermodynamics coupled with statistical methods.

Biological and environmental systems are complex mixtures of interacting chemical species. In modeling the natural world at the level of a cell or a planet vast numbers of compounds must be accounted for, along with their equilibrium and kinetic behavior in multiphase environments. Because equilibrium and kinetic equations are non-linear, numerical methods are normally required to handle these problems.

Additional computational challenges lie in indexing and classifying the infinite population of chemical compounds that could be synthesized or are already known. Specific indexing and search problems include how to find a compound that might block a specific biological target; how to predict the most efficient synthetic strategy for a desired compound from available precursors; how to employ results of bioactivity tests on a family of molecules to design improved versions; how to name new classes of compounds (e.g. fullernes and nanotubes).

Currently combinatorial chemists are developing new methods of synthesizing libraries of related compounds on an unprecedented scale. Such libraries can be used to produce huge arrays of materials for investigation of biochemical, catalytic, or material properties. Systems are required to design, catalog, and search these libraries, assess test results in a meaningful way, and integrate new information with existing chemical databases.

Finally, investigations into information storage at the molecular level are underway, bringing to full circle the link between chemistry and information technology.

According to the American Chemical Society "a high demand exists for people who can show both technical understanding and computer expertise." The ACS also reports that entry-level salaries for chemical information positions is in the range of $50-70,000, with higher rates for those with computer skills. In particular, they point out that "employment in information software fields, particularly the development of new search and retrieval techniques and technologies, can be extremely lucrative."

3. Discussion of related programs within the institution and at other institutions.

The most closely related program at Michigan Tech is in Bioinformatics. Bioinformatics is derived from biology in much the same way that cheminformatics derives from traditional chemistry.

We are not aware of any similar cheminformatics degrees in the U.S. The Indiana School of Informatics offers M.I. S. and M.L.S. degrees with a "chemical information specialization" through their Program in Chemical Informatics. Those programs require a bachelor's degree in chemistry and additional courses in library and information science.

Degrees in Cheminformatics are currently offered at the following international institutions (according to the information on Cheminformatics available on the ACS website).

1. Modlab, Goethe-University Frankfurt: http://gecco.org.chemie.uni-frankfurt.de
2. Unilever Centre for Molecular Informatics, Cambridge: http://www-ucc.ch.cam.ac.uk
3. Chemoinformatics at Sheffield University: http://cisrg.shef.ac.uk/
4. Computer Chemistry Centre, University of Erlangen-Nuremberg: http://www.ccc.uni-erlangen.de/
5. Centre for Molecular Design Portsmouth: http://www.cmd.port.ac.uk/
6. Cheminformatics at UMIST: http://www.umist.ac.uk/departments/chemistry/postgraduate/taught/MScCheminf.htm
7. CAMD at Innsbruck University: http://pharmazie.uibk.ac.at/CAMD/index.html
8. Molecular Design Laboratory at Peking University: http://mdl.ipc.pku.edu.cn/
9. Drug Discovery and Design Center, Shanghai: http://www.dddc.ac.cn/

Projected Enrollment

Our goal is a total of 20 students in this program (approximately 5 incoming per year).

5. Scheduling Plans

No new courses or sections are required.

6. Curriculum Design

Cheminformatics, B.S.

College of Science and Arts

The Cheminformatics BS degree at MTU provides the essentials of chemistry and computer sciences required for entry to the job market at the BS level or to pursue an advanced degree in chemistry and/or cheminformatics.

Total Credits Required: 128
General Education Requirements..... 28 credits.

Chemistry Requirements..... 56 credits
CH 1110 University Chemistry I..... 4
CH 1111 University Chemistry Lab I..... 1
CH 1120 University Chemistry II..... 4
CH 1130 Orientation 1
CH 2212 Quantitative Analysis..... 5
CH 2410 Organic Chemistry I 3
CH 2411 Organic Chemistry Lab l 1
CH 2420 Organic Chemistry II 3
CH 3510 Physical Chemistry I 3
CH 3520 Physical Chemistry II 3
CH 4710 Biomolecular Chemistry *or* CH 4310 Inorganic Chemistry I..... 3
CH 4900 Senior Seminar in Chemistry l 1
MA 1150 Calculus I or MA1160 Calc w/Tech I 4
MA 2150 Calculus II or MA 2160 Calc w/ Tech II 4
MA 2321 and 3521 OR MA 2320 and MA 3520..... 4
MA 3150 Multivariable Calculus or MA 3160 Multivariable Calc w/Tech 4
PH 2100 Univ Physics I-Mechanics 3
PH 1100 Physics by Inquiry I 1
PH 2200 Univ Physics II-Electricity and Magnetism 3
PH 1200 Physics by Inquiry II..... 1
PH 1200 Physics by Inquiry II..... 1
BL 1040 Principles of Biology..... 4
TOTAL..... 60

Computer Science Requirements..... 26 Credits
CS 1121 Intro Computer Science..... 3
CS 1122 Intro Computer Science II..... 2
CS 1721 Object-Oriented Programming 1
CS 2141 Software Development C++..... 3
CS 2311 Discrete Structures..... 3
CS 2321 Data Structures 3
CS 4321 Introduction to Algorithms..... 4
Prerequisite CS 2311 and CS 1721 and CS 2321
CS 4421 Database Systems..... 3

TOTAL..... 22

Concentration Requirements..... 9 credits

Additional upper level credits in chemistry, mathematics, and computer science give students a deeper understanding of these subjects.

Choose 6 credits from this list
CH 2421 Organic Chemistry Lab ll 2
CH 3520 Physical Chemistry Lab I 2
CH 3521 Physical Chemistry Lab II 2
CH 4212 Instrumental Analysis 5
CH 4412 Spectroscopy of Organic Chemistry..... 3
CH 4430 Intermediate Organic Chemistry..... 3

CH 4710 Biomolecular Chemistry *or* CH 4310 Inorganic Chemistry I..... 3
CH 4720 Biomolecular Chemistry II..... 3
CH 4320 Inorganic Chemistry II..... 3
CH 4510 Intermediate Physical Chemistry..... 3
CH 4110 Pharmaceutical Chemistry I..... 3
CH 4120 Pharmaceutical Chemistry II..... 3
CH 4610 Introduction to Polymer Science..... 3
CH 4910 Senior Seminar in Chemistry II 1
CH 4990 Undergrad Research in Chemistry..... 6

Choose 3 credits from this list
CS 4411 Introduction to Operating Systems..... 4
CS 3421 Computer Architecture..... 4
CSE 5200 Computational Genomics..... 3
FW 4089 Bioinformatics..... 3
MA 3160 Multivariable Calculus with Technology..... 4
MA 3210 Intro to Combinatorics..... 3
MA 4208 Optimization and Graph Algorithms..... 3
MA 4209 Combinatorics and Graph Theory..... 3
MA 4720 Design and Analysis of Experiments..... 3
MA 4760 Mathematical Statistics I..... 3
MA 4770 Mathematical Statistics II..... 3
UN 3002 Cooperative Laboratory..... 2

Free Electives..... 9 credits

Co-Curricular Activities..... 3 units
(not included in credit count for degree)

Comparison of credit requirements for related MTU degrees

Degree	Major	Concentration	Subject Electives	Free Electives	Gen Ed	Co-Curricular
Chemistry	73	3		24	28	3
Cheminformatics	**60/22**	**9**		**9**	**28**	**3**
Biological Sciences	53-59	17-21	6-8	20-30	28	3
Bioinformatics	45/30	17		8	28	3

7. New Course Descriptions

No new courses.

8. Library and other learning resources

The J. Robert Van Pelt Library subscribes to a broad collection of chemistry and computer science journals appropriate to degrees in those fields. At least nine journals in that collection are focused specifically on topics aligned with cheminformatics (see appendix).

In addition, the library provides comprehensive electronic resources for chemistry, including SciFinder and Beilstein Commander, both of which are licensed for use from departmental computers.

The Chemistry Department computer laboratory supports specific chemistry software (Hyperchem, RASMOL, FTNMR Simulation, Gausian 98, ORTEP-3, ChemDraw, and many others).

9. Computing Access Fee

Students will pay the basic access fee in Chemistry.

10. Faculty resumes:

Faculty resumes are posted online.

Chemistry: http://www.chemistry.mtu.edu/pages/faculty/index.php
Computer Science: http://www.cs.mtu.edu/html/faculty.html

11. Description of available/needed equipment

No additional equipment is required.

12. Program costs, years 1, 2 and 3.

The only anticipated costs are for advertising of the new degree and associated student recruiting. These expenses will be supported by the Department.

Space.

No new space is needed.

Policies, regulations and rules.

No new regulations are anticipated.

15. Accreditation requirements.

None available for cheminformatics. The content of courses in the Chemistry Department is already approved by the ACS.

16. Internal status of the proposal

Entity	Date submitted	Date Approved
Department/School		
Dean, College of Sciences & Arts		
Provost		
Academic Affairs Committee		
University support units		
University Senate		
Board of Control		
Provost- final approval		

17. Planned implementation date.

September 2005.

Appendix A

Cheminformatics-related journals available via the MTU library

Computational Biology and Chemistry
Computational Materials Science
Journal of Chemical Information and Computer Sciences
Journal of Combinatorial Chemistry
Journal of Computational Chemistry
Journal of Computer-Aided Materials Design

Journal of Computer-Aided Molecular Design
Proteins: Structure, Function and Bioinformatics
Theoretical Chemistry Accounts: Theory, Computation, and Modeling

Appendix B

B.S. Cheminformatics Degree Plan

FALL		SPRING	
FIRST YEAR			
CH 1110 University Chemistry I	4	CH 1120 University Chemistry II	4
CH 1111 University Chemistry Lab I	1	MA 2150 or 2160 Calculus II	4
CH 1130 Orientation	1	PH 2100 University Physics I-Mechanics	3
PH 1100 Physics by Inquiry I	1	UN 1002 World Cultures	4
MA 1150 or 1160 Calculus I	4	CS 1721 Object-Oriented Programming	1
UN 1001 Perspectives	3		
CS 1121 Intro. Computer Science	3		
TOTAL	**17**	**TOTAL**	**16**
SECOND YEAR			
CH 2410 Organic Chemistry I	3	CH 2420 Organic Chemistry II	3
CH 2411 Organic Chemistry Lab I	1	CH 2212 Quantitative Analysis	5
MA 2321 Elementary Linear Algebra	2	UN 2001 Re-Visions	3
MA 3521 Elementary Differential Eq.	2	General Education Distribution	3
PH 2200 Physics II- Electricity & Magnetism	3	CS 2141 Software Development C++	3
PH 1200 Physics by Inquiry II	1		
UN 2002 Institutions	3		
CS 1122 Intro Computer Science II	2		
TOTAL	**17**	**TOTAL**	**17**
THIRD YEAR			
CH 3510 Physical Chemistry I	3	CH 3520 Physical Chemistry II	3
CH 4710 Biomolecular Chemistry I *or* CH4310 Inorganic Chemistry I	3		
BL 1040 Fundamentals of Biology	4	General Education Distribution	6
CS 2311 Discrete Structures	3	Concentration Requirement	3
CS 2321 Data Structures	3	MA 3150 or 3160 Multivariable Calculus	4
TOTAL	**16**	**TOTAL**	**16**
FOURTH YEAR			
CH 4900 Senior Seminar I	1	Concentration Requirement	3
General Education Distribution	3	Free Electives	6
CS 4321 Introduction to Algorithms	4	General Education Distribution	3
Concentration Requirement	3	CS 4421 Database Systems	3
Free electives	3		
TOTAL	**14**	**TOTAL**	**15**
		GRAND TOTAL	**128**

Adopted by the PAC (formerly Senate): 9 February 2005
Approved by President Mroz: 21 February 2005