Term Information

Effective Term	Spring 2016

General Information

Course Bulletin Listing/Subject Area	Chemistry
Fiscal Unit/Academic Org	Chemistry - D0628
College/Academic Group	Arts and Sciences
Level/Career	Undergraduate
Course Number/Catalog	3700
Course Title	Cheminformatics
Transcript Abbreviation	Cheminformatics
Course Description	Cheminformatics provides students with an introduction to the common data formats used in manipulating and communicating chemical and biochemical information and the common databases available for use in modern chemical and biochemical research.
Semester Credit Hours/Units	Fixed: 3

Offering Information

Length Of Course	14 Week
Flexibly Scheduled Course	Never
Does any section of this course have a distance education component?	No
Grading Basis	Letter Grade
Repeatable	No
Course Components	Lecture
Grade Roster Component	Lecture
Credit Available by Exam	No
Admission Condition Course	No
Off Campus	Sometimes
Campus of Offering	Columbus

Prerequisites and Exclusions

Prerequisites/Corequisites	Chemistry 2510 and Chemistry 2540
Exclusions	

Cross-Listings

Cross-Listings

Subject/CIP Code

Subject/CIP Code	40.0501
Subsidy Level	Baccalaureate Course
Intended Rank	Sophomore, Junior, Senior

Requirement/Elective Designation

The course is an elective (for this or other units) or is a service course for other units

Course Details

Course goals or learning objectives/outcomes

- Students will know the history and development of cheminformatics
- Students will be familiar with common data formats (2D & 3D representations, spectrographic etc.)
- Students will be familiar with common databases of chemical information available on the Web and (open access) software tools to search these sites
- Students will be able to use the most common formats which are used to store, transform and manage chemical information in digital environments
- Students will be able to conduct research using the tools commonly available to chemists

Content Topic List

- Module 1: Cheminformatics: history and goals
- Module 2: Chemists using common desktop applications
- Module 3: Identifying chemical entities
- Module 4: Presenting chemistry in 2D
- Module 5: Presenting chemistry in 3D
- Module 6: Comparing and searching chemical entities
- Module 7: Representing and searching chemical reactions
- Module 8: Representing and managing digital spectra
- Module 9: Identifying chemistry information resources
- Module 10: Understanding and managing rights on digital information

Attachments

- OLCC_Syllabus_RS.pdf: Chem 3700 Syllabus

(Syllabus. Owner: Gustafson,Terry Lee)

Comments

- This course was approved by the curriculum committee in chemistry and biochemistry.

  19-MAR-15: I did indicate the distance component on 17-MAR-15 and resubmitted that evening.

  20-JUL-15: This course does not have a distance component. Some of the in class lectures will be videos prepared by the ACS. *(by Gustafson,Terry Lee on 07/20/2015 08:47 AM)*
- 03/19/15: Bernadette's comments refer to more than the checked box. The NMS Panel requires that hybrid distance education courses be reviewed by ASCTech's Mike Kaylor before the curricular Panel will review the course.

  03/17/15: Please indicate under "Offering Information" that this course does, in fact, have a distance education component. *(by Haddad,Deborah Moore on 03/19/2015 01:00 PM)*
- - Courses that request 50% or more distance learning need to be fully vetted by ASC Tech first. Please see instructions here http://asccas.osu.edu/distance-learning-courses and work with Mike Kaylor (kaylor.1). *(by Vankeerbergen,Bernadette Chantal on 03/19/2015 10:59 AM)*

Workflow Information

Status	User(s)	Date/Time	Step
Submitted	Gustafson,Terry Lee	03/17/2015 07:39 PM	Submitted for Approval
Approved	Gustafson,Terry Lee	03/17/2015 07:40 PM	Unit Approval
Revision Requested	Haddad,Deborah Moore	03/17/2015 07:57 PM	College Approval
Submitted	Gustafson,Terry Lee	03/17/2015 09:34 PM	Submitted for Approval
Approved	Gustafson,Terry Lee	03/17/2015 09:35 PM	Unit Approval
Approved	Haddad,Deborah Moore	03/18/2015 07:11 AM	College Approval
Revision Requested	Vankeerbergen,Bernadette Chantal	03/19/2015 10:59 AM	ASCCAO Approval
Submitted	Gustafson,Terry Lee	03/19/2015 11:07 AM	Submitted for Approval
Approved	Gustafson,Terry Lee	03/19/2015 11:08 AM	Unit Approval
Revision Requested	Haddad,Deborah Moore	03/19/2015 01:00 PM	College Approval
Submitted	Gustafson,Terry Lee	07/20/2015 08:47 AM	Submitted for Approval
Approved	Gustafson,Terry Lee	07/20/2015 08:48 AM	Unit Approval
Approved	Fink,Steven Scott	07/20/2015 09:00 AM	College Approval
Pending Approval	Nolen,Dawn Vankeerbergen,Bernadette Chantal Hanlin,Deborah Kay Jenkins,Mary Ellen Bigler Hogle,Danielle Nicole	07/20/2015 09:00 AM	ASCCAO Approval

Chemistry 3700: Cheminformatics

Instructor:

Dr. Richard Spinney

Course Rational:

Cheminformatics is a 3 credit-hour introductory course on Cheminformatics. The content will be developed by experts in the field by creating specific content “modules” consisting of reading assignments, short video clips and homework assignments. It will be taught in a “flipped” model where the students will be responsible for the reading and videos before class and class-time will be used to answer questions and train the students on the numerous software packages available.

Course prerequisites:

Organic Chemistry I including lab: Chemistry 2510 and 2540.

Objectives of the course:

At the end of the course, the students:

- will know the history and development of cheminformatics;
- be familiar with common data formats (2D & 3D representations, spectrographic etc.);
- be familiar with common databases of chemical information available on the Web and (open access) software tools to search these sites;
- and be able to use the most common formats which are used to store, transform and manage chemical information in digital environments;
- will be able to conduct research using the tools commonly available to chemists.

The course will not use/require any computational skill (no programming) nor will make extensive use of any chemistry computational tools. It is intended to address what any chemist or chemistry student should know to use current digital chemistry information resources. It is intended to be a very practical introduction to the subject and very “hands on” in terms of software use.

Grading:

Grading in the course will be based on 10 modular assignments for 70% of the course grade and 2 research projects, a smaller one for 10% and a final large one for 20% of the course grade. Modular assignments will be specific to the topics of the model and software used. This might entail using software to generate 2D structure, 3D structure of chemical, converting file formats, searching databases for molecule fragments etc. The projects would be more extensive combining aspects of several modules and could include database searches for

multiple types of information on a specific compound; i.e. thermochemical data, spectra, chemical synthesis etc.

Grading scale: A > 90% A^- > 86% B^+ > 82% B > 78% B^- > 74% C^+ > 70% C > 66%
C^- > 62% D^+ > 58% D > 54% E > 50%

Required Materials:

Since there is no one textbook that covers all areas of this topic I would leave it to the student to choose one (or more) of the following textbooks:

1. Introducing Cheminformatics An intensive Self-study guide; David Wild, open-publishing
2. An Introduction to Chemoinformatic; Leach and Gillet, Springer
3. Chemoinformatics: A textbook; Ed. Gasteiger and Engel, Wiley
4. Chemoinformatics: Theory, Practice & Products, B. Bunin et. al., Springer

Additional reading resources include (but are not limited to):

1. http://icep.wikispaces.com/home the Indiana Cheminformatics Education portal
2. http://dl.acm.org/citation.cfm?doid=1459352.1459353 Chemoinformatics – an introduction for scientists

Academic Misconduct:

It is the responsibility of the Committee on Academic Misconduct to investigate or establish procedures for the investigation of all reported cases of student academic misconduct. The term “academic misconduct” includes all forms of student academic misconduct wherever committed; illustrated by, but not limited to, cases of plagiarism and dishonest practices in connection with examinations. Instructors shall report all instances of alleged academic misconduct to the committee (Faculty Rule 3335-5-487). For additional information, see the Code of Student Conduct (http://studentaffairs.osu.edu/info_for_students/csc.asp).

Disability Services:

Students with disabilities that have been certified by the Office for Disability Services will be appropriately accommodated, and should inform the instructor as soon as possible of their needs. The Office for Disability Services is located in 150 Pomerene Hall, 1760 Neil Avenue; telephone 292-3307, TDD 292-0901; http://www.ods.ohio-state.edu/.

Syllabus

Module 1: Cheminformatics: history and goals

This first module of the course would provide an introduction to the topic of cheminformatics, including a brief historical introduction and an overview of what will be in the course. This will include resources specific to the OSU library system.

Module 2: Chemists using common desktop applications

This module will provide some background information on file formats and enter into some parts of desktop applications that chemists may use more extensive than other users. Common plugins/add-ons to desktop applications for chemistry will come here and include chemistry applications/plugins for MS Word, Excel and PowerPoint. It will also include a discussion of various file formats for images (bitmaps, vector graphics etc.) and advantages for each.

Module 3: Identifying chemical entities

This module will provide background on some of the common ways to identify chemical compounds by name, formula, alternate text representations and common database identifiers (CAS, PDB, CSID, PubChem etc.).

Module 4: Presenting chemistry in 2D

This module will explore common software packages for the creation of 2D chemical structures commonly used in literature and compare common file formats for these types of representations which are useful in databases.

Module 5: Presenting chemistry in 3D

This module will explore the many software packages available to create 3D chemical structures and images including common file formats and their interconversion. It will also demonstrate a number of important open access databases of chemical structures available on the web.

Module 6: Comparing and searching chemical entities

This module will highlight the numerous ways to search the web for chemical structures and basic chemical information including substructure searches, similarity searches and virtual screening.

Module 7: Representing and searching chemical reactions

This module will make use of open access databases on chemical reactions to show students how to find reaction information applicable to research or their course work.

Module 8: Representing and managing digital spectra

Module 8 will explore the numerous online open source databases of spectral data, including common file formats and freely available software for displaying spectra.

Module 9: Identifying chemistry information resources

Module 9 will highlight the numerous databases of chemical information and how to search them using web-based resources, common document identification schemes, author searching and chemical information searching.

Module 10: Understanding and managing rights on digital information

Module 10 discusses intellectual property rights, types of public information licensing and when and how to correctly cite digital resources.

Sample assignments and videos are available at:
http://i571.wikispaces.com/

This includes links for additional materials and assignments used in this course. Note: this course goes into more detail on modeling than Chemistry 3700 will so many of the modules from Dr. Wild's course will not be used in Chemistry 3700.

Additional resources include:

http://en.wikibooks.org/wiki/Chemical_Information_Sources
http://en.wikibooks.org/wiki/Information_Competencies_for_Chemistry_Undergraduates
http://icep.wikispaces.com/home