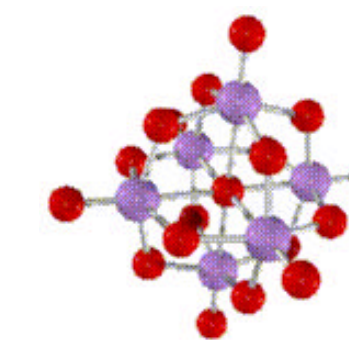


# New MS and BS Chemical Informatics Programs

**Gary D. Wiggins and Sonia Gupta, Chemistry Library, Indiana University**  
**800 E. Kirkwood Avenue, Chemistry Building Room C003, Bloomington, IN 47405-7102**  
**Phone: 812-855-9452, Fax: 812-855-6611, Email: wiggins@indiana.edu**



## Introduction

Cheminformatics techniques are increasingly being used to analyze the huge volumes of chemical and biological data resulting from combinatorial synthesis and high-throughput screening programs. Scientists with both chemical and computing skills required to carry out such analyses are currently in very short supply, thus resulting in the establishment of MS programs for the training of cheminformatics specialists.

New academic programs in cheminformatics have been started in several universities in the last two years. An overview of the course of study at three universities shows the common topics covered in the programs at UMIST, the University of Sheffield, and Indiana University.

## What is Cheminformatics?

“Cheminformatics is a generic term that encompasses the design, creation, organization, management, retrieval, analysis, dissemination, visualization and use of chemical information” (Warr, 1999).

## Why Cheminformatics now?

- Combinatorial synthesis and high-throughput screening
- Explosion of both structural and bioactivity data
- Informatics in other disciplines:
  - Bioinformatics
  - Medical Informatics
  - Health Informatics
  - Educational Informatics

## Recent Developments in UK & US in Cheminformatics Education

### Master's (MS) Programs in Cheminformatics:

- University of Sheffield (UK)
- UMIST (UK)
- Indiana University (USA)

## Content of the three MS Programs

### Similarities:

- First degree in chemistry or a chemistry-related subject required.
- A set of both required and elective taught modules with associated tutorials, workshops and course work.
- Research project or internships that lead to the presentation of a dissertation.

### Differences:

- MS program at Indiana University lasts for 2 years; a single year at the other two universities.
- Relative amount of chemical and informatics material varies across the programs.
- Indiana University offers a Bachelor's (BS) program in Informatics, in addition to the MS program.

## Degree Requirements for a BS Program at Indiana University

(122 Credit Hours)

- **Informatics Core Courses:** 30 hours
- **Informatics Electives:** 9 hours
- **Chemistry Cognate Courses:** General Organic Chemistry, Biochemistry and Chemical Informatics (19 hours)
- **Other General Education or Elective Courses:** 64 hours

## Comparison of the Programs

	Indiana University	UMIST	University of Sheffield
<b>Introduction of Programs</b>	Starting in September 2001	Starting in October 2001	Started in September 2000
<b>Core Course Curriculum</b>	Introduction to Informatics, Information Management, Chemical Information Technology, Computational Chemistry & Molecular Modeling.	Chemical Information Sources, Computer-Aided Molecular Design 1 & 2, Spectroscopy and Drug Discovery, Database Design and Programming, Chemical Informatics Applications, Fundamentals of Bioinformatics, Research Methodology & Feasibility Study (for dissertation).	Chemoinformatics I & II, Information Systems Modeling, Information Storage and Retrieval, Computer Programming I & II, Software Engineering, Molecular Modeling.
<b>Choice of Electives</b>	Bioinformatics, Data Mining, Human Computer Interaction	Any two of the following: Combinatorial Chemistry, Algorithm Design for Chemical Problems, Management of Intellectual Property, Knowledge Management.	Any one of the following: Database Design, Multimedia Information Systems, Human Computer Interaction.
<b>Other Collaborating Departments/Schools/Organizations</b>	Computer Science, School of Informatics, Biology, Chemistry, School of Medicine, School of Library & Information Science, MDL Information Systems.	Chemistry, Biomolecular Sciences.	Department of Information Studies, Computer Science, Chemistry, Automatic Control & Systems Engineering, and Pharmaceutical, Agrochemical, Chemical Software & Database Companies.
<b>Use of Technology (Videoconferencing and Other Distributed Education Techniques)</b>	Will be actively utilized to share guest speakers and expertise in a broad range of topics.	Will be employed to allow students to do bulk of their work from home or place of employment, in addition to spending a few days at UMIST for each module.	
<b>Funding</b>	Some State Funding	EPSRC	EPSRC

## Conclusions

The emergence of cheminformatics as a distinct sub-discipline of chemistry has spurred the development of high-level educational programs to provide students with skills that are currently in high demand in industry.

Contacts established among programs at Indiana, Sheffield and UMIST can grow into further cooperative activities. Broadcasting of lectures, exchanges of students, and distributed education are all possibilities given that the Indiana program is separated from the others by an ocean and many time zones.

## References

- Warr, W.E. (1999) Paper presented at the 218<sup>th</sup> ACS National Meeting, New Orleans, Aug 22-26.
- Details of the MS program in Cheminformatics are at
  - Indiana University: [http://www.indiana.edu/~cheminfo/informatics/ci\\_iu.html](http://www.indiana.edu/~cheminfo/informatics/ci_iu.html)
  - UMIST: <http://www.umist.ac.uk/chemistry/MScChemInf.htm>
  - University of Sheffield: <http://www.shef.ac.uk/~is/courses/pgrad/mscci/mscci.html>