Enhancing information resources and instruction with computational and chemical software

Jeremy R. Garritano
Purdue University, jgarrita@umd.edu

Follow this and additional works at: http://docs.lib.purdue.edu/lib_fspres
Part of the Library and Information Science Commons

Recommended Citation
http://docs.lib.purdue.edu/lib_fspres/25

This document has been made available through Purdue e-Pubs, a service of the Purdue University Libraries. Please contact epubs@purdue.edu for additional information.
Enhancing Information Resources & Instruction with Computational & Chemical Software

Jeremy R. Garritano
jgarrrita@purdue.edu
Chemical Information Specialist
Assistant Professor of Library Science
M. G. Mellon Library of Chemistry
Today’s talk

• Background
• Development and Justification
• Resources and Implementation
• Marketing
• Current Usage
• Next Steps
Background – The Writing on the Wall

• Current Journal Room
  – Large space
  – Decreasing number of “browsers”
  – Push to move online only with print journals began in mid-2006

• Two adjacent rooms
  – Packed with volumes of Chemical Abstracts
Space: Before

← My office

Current Journal Room

Chem. Abs. – Abstracts

Table

Chem. Abs. – Abstracts and Indexes

→ Main reading room
Space: Before
Solution – Repurpose Space

3 Rooms:
• Remove Chemical Abstracts to storage
• Move print journals to old Chem Abs room
• Create additional group study space
• Turn old current journal room into a computer lab / instruction area
Development of the computer lab

• Chemistry Library paying for site wide license to ChemDraw
  – Site administrator = lots of patron contact
  – Desire to load ChemDraw on library computers

• Purdue Libraries coordinating instruction on EndNote across campus
  – Heavy use within Chemistry Department
  – Desire to load EndNote on library computers
The Idea and The Spin

• Create a computer lab that has:
  – Traditional library software/access
  – Add ChemDraw
  – Add EndNote
  – Add visualization and modeling software

• Evolution of information use \( \rightarrow \) text to data
What additional software to add?

• Survey of Chemistry Faculty
  – Approximately 45 faculty
  – 10 initially responded
  – 15 different software titles
Concerns in adding software

- Price of software
- Hardware requirements
- Training involved in using software
- Licensing and access models
- Overlap with campus IT efforts
- One person monopolizing computer time by running a calculation for days
Choosing the software

• Visited vendors at Spring ‘07 ACS meeting
• Addressed issues

• Not chosen:
  – Accelrys Materials Studio + other products
  – Gaussian
  – MATLAB & Mathcad
  – ACD Software
Refocusing the vision

• Focus on software that could be used for teaching/classes as well as research

• Focus on software undergraduates could use

• Pick representative software dealing with:
  – Visualization/modeling
  – Statistics/mathematics

• Secondary use for library seminars and chemical information course
Initial software chosen

• Chemistry related
  – Cambridge Structural Database
  – ChemBioDraw Ultra with Chem3D
  – Cn3D
  – Hyperchem
  – Spartan

• Math related
  – Kaleidagraph
  – Origin
  – Prism

• Other
  – EndNote
  – Microsoft Office
The reality

• After removing shelving, old current journal room had only one electrical outlet!
  – Summer 2007: Power and ethernet connections for
    • 10 desktop PCs
    • 1 color printer
    • Additional outlets for future expansion (electronic white board)
  – Installed projection screen
Lab installation

Mid-November 2007
• Software obtained and installed
• Hardware completely installed

Result
• Soft opening, rest of 2007
• Icons on desktop
• Mainly used for web surfing and MS Office
• Mostly undergraduate use
Mellon CyberChemistry Lab - 2008

- Hiring of Chem. Ed. graduate student
- Marketing
  - Graduate students demo software during Open House
  - Raised graduate student awareness
Open House

2 hrs. with refreshments

Attendance:
3 faculty
35-40 graduate students
10-15 library staff
CyberChemistry Lab Web Site
http://www.lib.purdue.edu/chem/cyberchem/index.html

• Descriptions
• Company site
• Tutorials
• FAQs
• Support
Use so far in 2008…

• Experimenting with CHM 513 (Chemical Information course)
  – ChemBioDraw and spectral prediction
  – Student confidence between hands-on computer lab and regular lecture with patents
  – Trial of CCOHS chemical safety info resources

• Graduate level Organic course
  – EndNote to combine citation search results from WoS, SciFinder and Google Scholar, and then removing duplicates
Additional use...

- ChemBioDraw for lab reports & presentations
- Graduate students bringing data for analysis
  - Origin and KaleidaGraph
- Undergraduate individual or group work
  - Readings, lecture notes, and taking quizzes in course management software
  - Writing up lab reports
  - Facebook
Next steps

• Planning for Fall 2008
  – Faculty Survey
  – Working with faculty / grad students

• Usage tracking

• Evaluate upgrades and new software

• Tutorials / Example exercises
Example of Usage Tracking

- Tracking of total minutes per program
- Still some bugs to be worked out
- Anonymous
Current status of additional space

• Current journal room
  – Receive ~150 print journals [down from ~350]
  – Repainted shelving
  – Comfortable seating

• Collaborative group space
  – Three modular tables
  – White board
Space: Before

← My office

Current Journal Room

Chem. Abs. – Abstracts

Chem. Abs. – Abstracts and Indexes

→ Main reading room
Space: After

- My office
- CyberChemistry Lab
- Group Study Space
- Current Journal Room
- Main reading room
Group Study Space
CyberChemistry Lab
Thanks to…

Nicole Becker
Chem Ed grad student

Bartow Culp
Chemistry Librarian

Michael Fosmire
Head, PSET Libraries