Enhancing Information Resources & Instruction with Computational & Chemical Software

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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

Chem. Abs. – Abstracts and Indexes

→ Main reading room
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 → 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

• Open House – Feb. 14, 2008
  – 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

<table>
<thead>
<tr>
<th>Math Related Software</th>
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<tbody>
<tr>
<td><strong>Kaleidagraph v4.03 [Synergy Software]</strong></td>
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<tr>
<td>Kaleidagraph is a graphing and data analysis program that generates publication quality graphs.</td>
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<tr>
<td>Additional information from Synergy Software:</td>
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<tr>
<td><a href="http://www.synergy.com/kg.htm">http://www.synergy.com/kg.htm</a></td>
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| **Origin v8.0 [OriginLab]** |
| Origin is a scientific graphing and data analysis tool that can create presentation quality graphics. Origin can communicate easily with Microsoft office products and has over 60 different graph types. |
| Tutorials: |
| FAQ's and Knowledgebase: |

| **Prism v5.0 [GraphPad]** |
| Prism is a biostatistics program that also provides graphing and curve fitting. |
| Additional Information: |
| http://www.graphpad.com/prism/Prism.htm |
| Tutorials: |
| http://www.graphpad.com/Support/support.cfm |
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

Current Journal Room

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Chem. Abs. – Abstracts and Indexes

← My office

→ Main reading room
Space: After

CyberChemistry Lab    Group Study Space    Current Journal Room

← My office            → Main reading room
Group Study Space
CyberChemistry Lab
Thanks to...

Nicole Becker
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Head, PSET Libraries