Engaging Chemistry Students: finding data and drawing compounds

Linda Humphreys
Science Faculty Librarian
University of Bath Library
<table>
<thead>
<tr>
<th>BSc or MChem or Msci</th>
<th>2011/2012</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Chemistry</td>
<td>○ 393 undergraduate students</td>
</tr>
<tr>
<td>• Chemistry with management</td>
<td>○ 94 postgraduate students</td>
</tr>
<tr>
<td>• Chemistry with education</td>
<td>○ 36 academic staff</td>
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<tr>
<td>• Chemistry for drug discovery</td>
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</tbody>
</table>

Chemistry Department
<table>
<thead>
<tr>
<th>Week</th>
<th>Session</th>
<th>Description</th>
<th>Venue</th>
<th>Attended</th>
<th>Before the session I feel my skills in this area are...</th>
<th>After the session As a result of this I need to...</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Plagiarism</td>
<td>Find out what plagiarism is and how to avoid it</td>
<td>2W UN Hall</td>
<td></td>
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</tr>
<tr>
<td>2</td>
<td>Referencing</td>
<td>How to compile a list of references: Vital for your lab reports!</td>
<td>2W UN Hall</td>
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<tr>
<td>3</td>
<td>Finding data</td>
<td>Find out where to find the data you need for your lab report</td>
<td><strong>3 sessions in PC labs</strong></td>
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<td></td>
<td></td>
<td></td>
<td>Group A Monday 15:15</td>
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<td></td>
<td></td>
<td></td>
<td>Group B Friday 13:15</td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td>Group C Friday 16:15</td>
<td></td>
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</tr>
<tr>
<td>4</td>
<td>How successful is your note taking?</td>
<td>Find out how much have you actually noted down in lectures so far. Tips for improvement</td>
<td>2W UN Hall</td>
<td></td>
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</tr>
<tr>
<td>5</td>
<td>Finding literature</td>
<td>Where to go for to find literature. Useful for your first lab write up.</td>
<td><strong>3 sessions in PC labs</strong></td>
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<td></td>
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<td></td>
<td>Group A Monday 15:15</td>
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<td></td>
<td>Group C Friday 16:15</td>
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<tr>
<td>6</td>
<td>Meeting with PT &amp; Chem Crew drop-in</td>
<td>Make an appointment to see your Personal Tutor and catch up with the Chem Crew this week</td>
<td>Tuesday 13:15 3WN 2.1</td>
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</table>

Sessions run on Mondays at 15:15 unless otherwise stated.
Skills Training for Year 1

This Moodle course supports the weekly skills training sessions provided by the department. This includes developing your learning techniques to suit the University environment and some essential skills to get you through your Chemistry degree. These topics will be important throughout your studies and many will be generally relevant in your future career.

Here is a copy of the skills training timetable and record sheet for Year 1 students:

- Year 1 Skills Training timetable and record sheet (Semester 1)
- Year 1 Skills training timetable (Semester 2)

1 Useful Resources
Some websites which can help you with more information on study skills.

- The University Study Skills resources

A really good website from Edinburgh Napier University to help you with how to study at University:

- Get Ready for University Study

This website has lots of information on study skills and allows you to assess your own abilities using online quizzes. Is linked to a good textbook on study skills for Science and Engineering students:
5 **Week 1 - Plagiarism**
- Plagiarism quiz
- Plagiarism lecture - powerpoint slides

6 **Week 2: Referencing RSC style**
- Referencing RSC style
- RSC Referencing guidelines
- Worksheet
- Writing Lab Reports

7 **Week 3 - Finding data**
Where to find the data such as melting points needed for your lab report.
- Finding Physical and Chemical Properties
- Worksheet
- Online sources of physical and chemical property data

8 **Week 4 - How successful is your note taking?**
How much have you actually noted down in lectures so far. What could you do better?
- Note taking presentation

9 **Week 5 - Reaxys**
In this session we will use the Reaxys database to find physical and chemical property data from the journal literature.
Printed sources of data
Web sources of data

- CRC Handbook of Chemistry and Physics
- Merck Index
- Knovel Library
- NIST Chemistry WebBook
- Spectral Database for Organic Compounds (AIST)
- Sigma Aldrich (MSDS)
- Kaye and Laby Tables of Physical and Chemical Constants
Chemistry

For more information, please email your Subject Librarian, Linda Humphreys, tel: +44 (0)1225 385248. You can also visit Linda in the Library, room 4.04. The department’s Library Rep is Dr Simon Lewis. To find a recommended book or journal, search the Library Catalogue. You might like to refer to the recommended book list.

Databases

Essential for finding articles, conference proceedings & other items:

- SciFinder – chemical structures, reactions & properties - register with SciFinder now - training materials
- Reaxys – chemical structures, reactions & properties - training materials
- SCOPUS – peer-reviewed articles, websites and patents in all subjects – guide
- Web of Knowledge – journal articles & conference papers – guide & tutorial – viewing results
- More databases for Chemistry

Chemical & physical property data

- Hazardous Substances Data Bank
- International Tables for Crystallography
- Kaye & Laby Tables of Physical & Chemical Constants
- Knovel – search across many reference books
- Merck Index
- MSDS – Material Safety Data Sheets from Sigma-Aldrich
- NIST – thermochemical & spectral data
- Spectral Database for Organic Compounds, SDBS
- WebElements – properties of chemical elements

Help with finding & referencing information

- How to find & evaluate relevant information
- How to reference information
- Unable to access the full-text of an item?
- EndNote Web guide for Chemistry

Other resources

- Chemical Structure Drawing software
- ChemSpider – search information and data on chemical compounds. Warning: data is non-peer-reviewed wiki content
- Royal Society of Chemistry Publishing – search across RSC journal articles & book chapters
- Theses & Dissertations
- Exam papers
- Images, film & other media
- Useful links – from Dept of Chemistry
- Library News blog

Moodle

- Access your Moodle VLE modules
- Information Skills tutorial
- Academic Writing Skills tutorial
Finding chemical and physical property data worksheet

1. According to the Dictionary of Organic Compounds, the melting point of 2-chlorophenol is 9°C. What is the value given by:
   a) Merck Index
   b) CRC Handbook of Chemistry and Physics

3. Using the NIST Chemistry WebBook:
   What is the enthalpy of formation of 1,3-dimethylbenzene at standard conditions? (It is a liquid - look at the condensed phase data)
   Where does this information come from? (Click the author's name to find the full reference)

7. Search the Knovel Library:
   What is the density of creatine?
   Which book does this information come from?

8. What is the solubility of imidazole in water?
How useful was the session?

- Very useful
- Somewhat useful
- Not useful
- No answer

2011/12
2012/13
How interesting was the session?

- Engaging/interesting
- Neutral interest
- Boring
- No answer

2011/12 vs 2012/13
Session timing?

![Bar chart showing session timing responses for 2011/12 and 2012/13.](chart)

- Too early in my course
- Timed about right
- Too late in my course
- No answer

2011/12 vs 2012/13
How have your skills improved?

- Greatly improved
- Improved
- Not improved
- No answer

Comparison between 2011/12 and 2012/13
Student comments

Positive:
• Helped to find Chemistry stuff on the pc.
• I finally got to use the library resources.
• Discovering all the online resources which are available.
• I know where to find data (I had no idea the area existed)

Negative:
• The CRC Handbook actually didn’t work properly/ wasn’t easy to use.
• Using all of the different books, was a waste of time, they are all too similar.
• I am now confused on which resources I use for things - too many!
## Skills training timetable: year 2

Sessions run on Thursdays at 14:15 unless otherwise stated

<table>
<thead>
<tr>
<th>Week</th>
<th>Session</th>
<th>Description</th>
<th>Venue</th>
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<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>2</td>
<td>Lab skills</td>
<td>Help with lab write ups, significant figures etc. particularly important for your labs this semester</td>
<td>3WN 3.7</td>
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<tr>
<td>3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>ChemBioDraw</td>
<td>Practice and tips on using ChemBioDraw to draw chemical structures. Important for your lab reports this year.</td>
<td>*** 3 South Computer lab *** Tutorial groups 1 – 11</td>
</tr>
<tr>
<td>5</td>
<td>ChemBioDraw</td>
<td>Practice and tips on using ChemBioDraw to draw chemical structures. Important for your lab reports this year.</td>
<td>*** 3 South Computer lab *** Tutorial groups 12 – 22</td>
</tr>
<tr>
<td>6</td>
<td>Meeting with Personal tutor</td>
<td>Students should make an appointment to see their PT</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Revision techniques</td>
<td>A look at some past exam papers and revision techniques to prepare you for your exams</td>
<td>3WN 3.7</td>
</tr>
<tr>
<td>8</td>
<td>Scientific Posters 1</td>
<td>How to produce a scientific poster This will help you with upcoming assessments</td>
<td>3WN 3.7</td>
</tr>
<tr>
<td>9</td>
<td></td>
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</tr>
<tr>
<td>10</td>
<td>Scientific Posters 2</td>
<td>How effective is your poster presentation?</td>
<td>TBC</td>
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<tr>
<td>11</td>
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</tbody>
</table>
ChemNMR $^1$H Estimation

Estimation quality is indicated by color: **good**, medium, rough

![ChemNMR $^1$H Estimation](image)

Protocol of the H-1 NMR Prediction:

<table>
<thead>
<tr>
<th>Node</th>
<th>Shift</th>
<th>Base</th>
<th>Inc.</th>
<th>Comment (ppm rel. to TMS)</th>
</tr>
</thead>
<tbody>
<tr>
<td>OH</td>
<td>3.58</td>
<td>2.00</td>
<td>1.58</td>
<td>alcohol</td>
</tr>
<tr>
<td>CH</td>
<td>1.47</td>
<td>1.51</td>
<td></td>
<td>general corrections</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-0.02</td>
<td>2 beta -C from methine</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-0.02</td>
<td>2 beta -C from methine</td>
</tr>
<tr>
<td>CH2</td>
<td>1.60,1.345000</td>
<td>1.51</td>
<td></td>
<td>cyclopentane</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-0.04</td>
<td>1 beta -C from methylene</td>
</tr>
<tr>
<td>CH2</td>
<td>1.60,1.345000</td>
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<td></td>
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<tr>
<td></td>
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<td></td>
<td>-0.04</td>
<td>1 beta -C from methylene</td>
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<tr>
<td>CH</td>
<td>3.25</td>
<td>1.50</td>
<td></td>
<td>methine</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>1.73</td>
<td>1 alpha -O</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.03</td>
<td>1 beta -C=C</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-0.01</td>
<td>1 beta -C</td>
</tr>
<tr>
<td>CH2</td>
<td>1.56,1.315000</td>
<td>1.44</td>
<td></td>
<td>cyclohexane</td>
</tr>
</tbody>
</table>
**ChemBioDraw exercise:**

Final stages of Fischer indole synthesis. This will give you some good practice at drawing arrows!

Step 1: Draw the individual components of the reaction using the ring, bond and text tools. The lone pair above the NH2 is added from the 'Chemical Symbol Tools' menu. You can add + and - charges using the same menu, or the text tool: they will be the correct size and easier to position if you use the Chemical Symbol tools menu.

Step 2: Add reaction arrows from the arrows menu
How useful was the session?

![Bar chart showing the percentage of responses for different levels of usefulness (Very useful, Somewhat useful, Not useful, No answer) for the years 2011/12 and 2012/13. The chart indicates that a higher percentage found the session very useful in 2012/13 compared to 2011/12.](image-url)
How interesting was the session?

![Bar chart showing responses to the question of how interesting the session was. The chart compares responses for 2011/12 and 2012/13. The categories are Engaging/interesting, Neutral interest, Boring, and No answer. The chart indicates a higher percentage of respondents found the session engaging or interesting in 2012/13 compared to 2011/12.](image-url)
Session timing?

Too early in my course: 2011/12, 2012/13
Timed about right: 2011/12, 2012/13
Too late in my course: 2011/12, 2012/13
No answer: 2011/12, 2012/13
How have your skills improved?

- Greatly improved
- Improved
- Not improved
- No answer

Year: 2011/12 and 2012/13
Student comments – all positive!

• Best programme ever.
• Useful if this was done in first year. Also was awesome!
• Should do in first year. Would come in useful with drawing molecules.
• Wasn’t aware that this programme existed before today.
• Found out features of ChemDraw that I didn’t previously know.
• Able to easily draw molecules with correct bond angles and stereochemistry.
• Being shown how to use ChemBioDraw. It has kept me entertained for an hour.
• I can draw a cat on ChemBioDraw = The greatest achievement of my life.
My questions:

• Are these the best data sources?

• What is your experience with CRC Handbook?

• What about ChemSpider?

• Does anyone have any guides to finding/referencing data that they could share?

• Do you teach structure drawing software?

• Should this be the role of the subject librarian?