Finding Facts: Reaxys and other sources

CHEM 23201
Fall 2018

1. Turn in Assignment #3
2. Open a browser

Overview

• Assignment 4
  – Spectra
• Presentation
• Reaxys
• Other Sources for facts
  – View these on your own
• Reaxys practice

Assignment 4 – Due next week

• Finding Facts Chart
  – Must search Reaxys
  – Select 4 of the remaining 6 sources

• Find spectra
  – Copy

Assignment - Spectra

• Label the spectra? - IR, Mass, NMR, UV
  – For the IR
    • What solvent was used?
  – For the UV
    • What solvent was used?
  – For the NMR
    • What solvent was used?
    • What was the field strength (working frequency)?
  • For the NMR
    • This is the priority when you have a choice:
      – 1. experimental; 2. reconstructed; 3. predicted

Quote

• “Three months in the lab can save you two hours in the library.”
  – Frank Westheimer
  • www.stanford.edu/class/ee293a/FEP7_Text_X.pdf (accessed 16 Dec 2003)
Experimental NMR (best)


Experimental C-NMR (better)

Baseline, yes, but…
Where is the standard peak?
Where is the solvent peak?


2 Examples

<table>
<thead>
<tr>
<th>Substitution</th>
<th>C-1</th>
<th>C-2</th>
<th>C-3</th>
<th>C-4</th>
<th>C-5</th>
<th>C-6</th>
<th>Me</th>
</tr>
</thead>
<tbody>
<tr>
<td>Me</td>
<td>21.4</td>
<td>40.6</td>
<td>37.1</td>
<td>31.1</td>
<td>34.7</td>
<td>40.6</td>
<td>30.9</td>
</tr>
</tbody>
</table>


1. Table 1. 13C chemical shifts of some cyclohexanes

Experimental C-NMR (better)

2 Examples

2. [Trubetskoy, L., 2007, 48, 9108 (Supplementary data).]

Second Priority

RECONSTRUCTED
Reconstructed C-NMR (good)

Based on data points in an article...
Where is the baseline?
Where is the standard peak?
Where is the solvent peak?

Calculated/Predicted C-NMR (last resort)

Abstract – Results & Conclusion

Results – what have you learned
Conclusion – questions that come about because of the results (in other words, a problem statement for a future abstract)

Google doc
Abstract & Presentation

- Abstract covers Presentation content
  - Chemically interesting
    - Synthesis
    - Characterization
    - Interaction – compounds / enzymes
    - Etc.
  - NOT
    - Pronouncements
    - Medical symptoms

Things to think about

- What does your compound look like?
  - Is it bright red?
- Does it have unpaired electrons?
- How does the conformation effect it’s reactivity? It’s taste? It’s aroma?
- Toxicology & other hazards

Things to think about

- Is it chiral?
  - How do you tell whether you have the right isomer?
- What is the physical state at STP?
  - Is it a liquid, solid, or a gas?
- What is the solubility?
  - What solvents could you use to precipitate or to recrystallize it?
- Is there a crystal structure?

Crystal Structure

Cambridge Crystallographic Database

For help searching the database
Contact:
Allen Oliver
246B Nieuwland
aoliver2@nd.edu

YouTube videos

- Course web page
  - Session 6
- There are five videos
- There are four questions
- Due in two weeks
- Be prepared to give your answers
Database comparison

<table>
<thead>
<tr>
<th></th>
<th>Google</th>
<th>SciFinder</th>
<th>Web of Science</th>
<th>Reaxys</th>
</tr>
</thead>
<tbody>
<tr>
<td>Search Fields</td>
<td>5</td>
<td>9</td>
<td>27</td>
<td>350+</td>
</tr>
<tr>
<td>Boolean Operators</td>
<td>3</td>
<td>3</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Truncation / Wildcards</td>
<td>0</td>
<td>0</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>Relations (=, &lt;, &gt;, is, starts with, etc.)</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>9</td>
</tr>
</tbody>
</table>

See pages 9-10 of the Reaxys practice for tips and helps

Reaxys – Boolean Operators

– AND  
– OR  
– NOT

– PROXIMITY
  • One search term depends on another search term  
  – melting point = 120 PROXIMITY solvent = ethanol

– NEAR
  • Search terms are adjacent to each other

– NEXT
  • 1st search term will appear before 2nd search term

When to use?

<table>
<thead>
<tr>
<th>When to use?</th>
<th>Example</th>
</tr>
</thead>
</table>
| NEXT phrases | keyword=blood NEXT keyword=clotting  
  (Example: “…blood clotting…”)
| NEAR terms within a few words of one another | Natural product isolation=fermenting NEAR natural product isolation=spinach  
  (Example: “…fermenting spinach leaves…”  
  “…spinach mixed with fermenting cider…”)
| PROXIMITY PV=nRT Solvents affecting T boiling point=100-105 PROXIMITY pressure>=800  
  melting point<5 PROXIMITY solvent=ethanol
| AND Any other time | density=1.1-1.2 AND dissociation exponent exists |

See page 9 of the Reaxys practice for common mistakes

SciFinder Scholar

• For basic information
  – LOCATE - Substance Identifier
    • Click the registry number
      – Experimental Properties
      – Calculated Properties

• For other information
  – Must do Topic search to see if it appears in an abstract

OTHER SOURCES
ChemSpider.com

- Search by name or registry number

Merck Index

- Search by name or registry number
- Number in the index is an article number not a page number
- Read the whole article

CRC Handbook of Chemistry…

- Generally speaking
  - Not organized by compound
  - Organized by physical property or chemical property
- Search for property then look for your compound
- Exception - basic information
  - Physical Constants of Organic Compounds

Dictionary of … Compounds

- Search the indices
  - I would use the registry number index
- Number in the index is an article number not a page number

Handbook of Data on Common…

- Search the index by name or registry number

Summary

- Presentation & Abstract
- Reaxys
- Other resources
  - Suggestions on how to use them
    - These pages to be viewed on your own
- Practice