Subject Conventions & Google.com

CHEM 23201
Fall 2016

1. Launch a web browser

Overview

1. Assignment #2
2. Copyright discussion
3. Hill Formula
4. Registry Numbers
5. InChI Key
6. PDB id
7. Google.com

1. Assignment #2

• Purpose
  – Updating Research Strategy
  • Download new worksheet from course web page
  – Background information
  • Except for Google Scholar
  • Use primary concept for Q2
  – Use the index, even in encyclopedias
  • Use at least two concepts for Q3-5
  – RefWorks
  – Becoming familiar with interlibrary loan
  – Abstract
  • Connection between assignments and presentation

Copyright Discussion

• Three things learned
  1.
  2.
  3.

• Two surprises
  1.
  2.

• One action that violates copyright
  1.

Quote

• Korpela’s Second Corollary:
  – “Search[ing] for information usually fails, except by accident.”
## Copyright Practice - 01

<table>
<thead>
<tr>
<th>Is it copyrightable?</th>
<th>If yes, then who holds copyright?</th>
</tr>
</thead>
<tbody>
<tr>
<td>IRS tax forms</td>
<td>Y / N</td>
</tr>
<tr>
<td>Article in <em>Time</em></td>
<td>Y</td>
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<td>Letter from Mom</td>
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<td>Y</td>
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<tr>
<td>Snap shot of Dad</td>
<td>Y</td>
</tr>
<tr>
<td>Song on CD</td>
<td>Y</td>
</tr>
<tr>
<td>USGS Map</td>
<td>Y / N</td>
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</table>

## Copyright Practice - 02

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## Copyright Practice - Answers

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### 3. Hill Formula (Hill Order)

- **General Rules:**
  - Compounds containing Carbon
    - C, followed by H (if present), then the remaining symbols alphabetically
    - For example: $C_3H_7O_n$ or $C_{26}H_{23}B_2Rh_2$
  - Compounds that don’t contain Carbon
    - Arrange the symbols alphabetically
    - For example: $H_2O$ or $BH_3O_3$
Hill Formula Practice

1. NaCl  
2. CCl₄  
3. HOC(CH₃)₃  
4. NH₃  
5. CHCl₂  
6. HCN

1. No - ClNa  
2. Yes  
3. No - C₆H₁₀O  
4. No - H₃N  
5. Yes  
6. No - CHN

4. CAS Registry Numbers

- Created by Chemical Abstracts in 1960s
- Registry Numbers are up to 10 digits separated by two hyphens
  - Up to 7 digits - 2 digits - 1 digit
  - 10294-33-4
- Every compound indexed by CA is assigned a Registry Number
- They are like Social Security Numbers

Registry Number Practice

1. 0-8412-3462-0  
2. 123-00-1234  
3. 316-81-4  
4. 270076-60-3  
5. 321-432-5432

1. No - ISBN  
2. No - Social Security  
3. Yes  
4. Yes  
5. No - Phone number

Registry Number Examples

- 8049-98-7  
- 97765-70-3  
- 9002-86-2  
- 7732-18-5  
- 7647-14-5  
- 50-00-0  
- 10043-35-3  

- Cow milk  
- Cheese, Cheddar, ext.  
- PVC  
- Water  
- Sodium Chloride  
- Formaldehyde  
- Boric Acid

Why use a registry number?

- 171599-83-0  
- Piperazine, 1-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonfyl]-4-methyl-, 2-hydroxy-1,2,3-propanetricarboxylate (1:1)

- 1-[[3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonfyl]-4-methylpiperazine, 2-hydroxy-1,2,3-propanetricarboxylate (1:1)

- Sildenafil citrate  
- UK-92840-10  
- Viagra

Complex Compound Name
Many different names

- Acetanilide, N-(4-hydroxyphenyl)-
  - Acetaminofen
  - Ben-u-ron
- 4'-Hydroxyacetanilide
  - Acetaminophen
  - Bickie-mol
- 4-(N-Acetylamino)phenol
  - Alpigtryl
  - Biocetamol
  - Calpol
- Anafon
  - Alvedon
  - Captin
  - Citramon P
- Abensanil
  - Anelix
  - Claratal
- Acarnol
  - Antha
  - Clisodyne
- Acanol
  - Apamid
  - Crocin
- Acenol (pharmaceutical)
  - APAP
  - Daphgalan
- Acetaminofen
  - Banesin
  - Daril

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Many different names (cont’d)

- Pamol
  - Pasolin N
  - Phendalin
- Panadol
  - Phenphen
  - Phendrin
- Panade
  - Finex
  - Finex (pharmaceutical)
- Panadex
  - Prodatalgan
  - Pyrinnazine
- Paracetol
  - Resprin
  - Salazone
- Paracetamol DC
  - Tabalgin
  - Tachipirina
- Paracetamole
  - Taparin
  - Temolin
- Paracemol
  - Temolin
- Parelo
  - Termolin
- Panade
  - Tempnal
  - Tempora
- Panadex
  - Trolpon
  - Tylenol
- Paracetol
  - Valadolin
- Panadex
  - Volgysic
- Panade
  - Vick Pyrena

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6. PDB identifier

- Created by the Protein Data Bank
- PDBid’s are four characters long
- First character is a number
  - 1CA2
- Each unique protein in PDB receives a randomly generated number
  - ~700 lysozyme structures each with a unique PDBid
    - Different mutations, bound to different ligands, etc.

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5. InChI Key

- International Chemical Identifier
  - Unique 27 character code for each compound
  - BSYNRYMUTXBSQ-UHFFFAOYSA-N
  - Non-proprietary standard
  - Used in databases
    - Proprietary (SciFinder, Reaxys, etc.)
    - Free on the web (NIST, etc.)

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Summary

- Assignment #2
  - Abstract examples
  - RefWorks
    - Is Ref Type correct?
- Copyright Discussion
- Hill Format
- Registry Numbers
- InChI Key
- PDBid
7. Practice searching Google