Subject Conventions & Finding Articles

CHEM 23201
Fall 2019

1. Logon to a computer & launch a browser
2. Go to chemistry.library.nd.edu
3. Click on SciFinder link
4. Click on Create a SciFinder Account
5. Register, Submit, Respond to the email

Overview

• Assignment #3
• Subject Conventions
  • Hill Format
  • Registry Numbers
  • InChI Key
  • PDB id
• Finding Articles

Assignment #3

DUE IN 2 WEEKS

Assignment #3

• Q 10
  • Print bibliography and label it
• Q 11-12
  • Don’t search online, write it out.

SUBJECT CONVENTIONS
Hill Format (Hill Order)

- Compounds containing Carbon
  - C, followed by H (if present), then the remaining symbols alphabetically
  - E.g., $C_6H_{12}O_6$ or $C_{20}H_{37}B_3Rh_2$

- Compounds that don’t contain Carbon
  - Arrange the symbols alphabetically
  - E.g., $H_2O$ or $BH_3O_3$

Hill Format Practice

1. NaCl
2. CCl$_4$
3. HOC(CH$_3$)$_3$
4. NH$_3$
5. CHCl$_2$
6. HCN

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
  - Example: 10294-33-4
- Every compound indexed by CA is assigned a Registry Number
- They are like Social Security Numbers
- Proprietary standard

Registry Number Practice

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

Many different names

- 103-90-2 • Acetamide, N-(4-hydroxyphenyl)-

Complex Compound Name

- 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]sulfonyl]-4-methyl-2-hydroxy-1,2,3-propanetricarboxylate (1:1)

Many different names 2

- 1-[[3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methylpiperazine, 2-hydroxy-1,2,3-propanetricarboxylate (1:1)
- Sildenafil citrate
- UK 92480-10
- Viagra

- 103-90-2 • Acetamide, N-(4-hydroxyphenyl)-
Many different names

Parmol
Panadol
Panadol Extend
Paraleve
Panaseorb
Panets
Panodil
Paracetamol
Paracetamol DC
Paracetamole
Paralen
Paramol
Paraspen
Parelan

InChI Key

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

PDB identifier

- Created by the Protein Data Bank
- PDBid’s are four characters long
- First character is a number
  - 1CA2  6LDH  3ADK
- 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.

Finding Articles

- Subject searching
- Author searching
- Citation searching

Book published in 1970

You want to know:

“Since 1970, who has published any research on the same subject as Pauling’s book?”
Finding Articles

- Google Scholar
  - Every subject
- SciFinder
  - Any literature of interest to a chemist
  - 3 databases are included
    - Chemical Abstracts
      - CAPlus: Bibliographic side & CASReact: Structure side
    - MEDLINE
    - Chemisches Zentralblatt
- Citation searching work around

Conclusion

- Assignment due in 2 weeks
- Subject conventions
- Overview of the 4 databases

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