

Databases: Compound Databases and Spectral Databases

Suggested Exercises

ChemSpider and PubChem

1. Find out more about Ibuprofen

- Molecular formula
- Exact mass
- ChemSpider, PubChem Record Number, CAS Number?
- How many data sources and references?
(hint: perform a more generic search to get a nice summary – don't count by hand!)
- What is the experimental log P? How does this compare to calculated values?
- How many structures contain the structure of Ibuprofen in them?
(hint: substructure search – but the answer is not 100!)
- How many records have the same CAS Number associated with them?
Are they all the same?
- How many records have the same formula?

2. What is this? Clc1nc(nc(n1)NC(C)C)NCC

Answer the same questions you answered for Ibuprofen above for this compound.

3. What is this? JPMIIZHYWMHDT-UHFFFAOYSA-N

Again, please answer the questions you answered for Ibuprofen.

If you are running out of time, leave the questions for Thursday and move onto the next ones

Extra: Can you buy these compounds? From where?

MassBank and METLIN

1. Try the METLIN example – what neat features does it have?

<http://metlin.scripps.edu/> => "example" under the statistics

2. Are these first three compounds in MassBank?

<http://www.massbank.jp/> ? <http://massbank.normandata.eu/MassBank/> ?

Is there a difference?

3. Are they in METLIN?