## Identifying Chemical Compounds

<table>
<thead>
<tr>
<th>Method</th>
<th>Types (with Examples)</th>
<th>Uses/Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
</table>
| Chemical Name               | IUPAC: 2-Acetoxy-benzoic acid  
CAS: Benzoic acid, 2-(acetyloxy)-Trade: Bayer  
Common: Aspirin | ➢ Most common information to obtain prior to starting a project  
➢ Best (sometimes only) way to search for polymers or biomacromolecules  
➢ Use a synonym source to get at other means of identification | ➢ MANY names for each compound; name input must match name in database  
➢ Not all sources use the same nomenclature system!  
➢ Syntax can be a problem when inputting names. |
| Formula                     | Empirical: $C_9H_8O_4$  
Molecular: $C_9H_8O_4$  
Structural: $C_9H_6(CO_2H)(OCOCH_3)$ | ➢ Less “subjective” than name searching  
➢ Established method of inputting formulae: molecular formula in Hill Order  
➢ No spelling variations | ➢ Not all databases employ Hill Order, although most do  
➢ Many compounds, particularly small organics, can have the same molecular formula |
| Structure                   | Substructure  
Exact Structure: | ➢ One-to-one unique identifier  
➢ Molecule’s “photo ID”  
➢ Structure searching also allows you to do complete or partial reaction searches with ease | ➢ Not all databases (particularly print sources) allow structure searching  
➢ Stereochemistry and resonance structures can cause problems  
➢ Structure you draw must match the structure drawn in the database  
➢ Substructure searches can yield unwieldy hit sets unless carefully drawn |
| CAS Registry Number         | 50-78-2 | ➢ One-to-one unique identifier  
➢ Molecule’s “Social Security Number” | ➢ Searching by CAS number only retrieves EXACT substances, not isotopes, radicals, or charged species.  
➢ Tricky when searching for polymers because too limiting  
➢ Do YOU know the CAS number of a compound off hand? |