Unit One Part 2: naming and functional groups

- To write and interpret IUPAC names for small, simple molecules
- Identify some common functional groups found in organic molecules

viagra™ (trade name)
sildenafil (trivial name)

5-(2-ethoxy-5-(4-methylpiperazin-1-ylsulfonyl)phenyl)-1-methyl-3-propyl-1H-pyrazolo[4,3-d] pyrimidin-7(6H)-one

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Systematic (IUPAC) naming

- Comprises of **three** main parts
- Note: **multiple bond index** is always incorporated in **parent** section

<table>
<thead>
<tr>
<th>No. Carbons</th>
<th>Root</th>
<th>No. Carbons</th>
<th>Root</th>
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<td>6</td>
<td>hex</td>
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<tr>
<td>2</td>
<td>eth</td>
<td>7</td>
<td>hept</td>
</tr>
<tr>
<td>3</td>
<td>prop</td>
<td>8</td>
<td>oct</td>
</tr>
<tr>
<td>4</td>
<td>but</td>
<td>9</td>
<td>non</td>
</tr>
<tr>
<td>5</td>
<td>pent</td>
<td>10</td>
<td>dec</td>
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</tbody>
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<table>
<thead>
<tr>
<th>Bond</th>
<th>Multiple-bond index</th>
</tr>
</thead>
<tbody>
<tr>
<td>C–C</td>
<td>an(e)</td>
</tr>
<tr>
<td>C≡C</td>
<td>yn(e)</td>
</tr>
<tr>
<td>C=C</td>
<td>en(e)</td>
</tr>
<tr>
<td>Functional group</td>
<td>Structure</td>
</tr>
<tr>
<td>----------------------</td>
<td>-----------</td>
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<tr>
<td>anhydride</td>
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<tr>
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<tr>
<td>ether</td>
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</tr>
<tr>
<td>alkyl bromide</td>
<td><img src="" alt="Alkyl bromide structure" /></td>
</tr>
</tbody>
</table>
Nomenclature rules

1. **Parent** - root derived from number of carbon in longest unbranched chain containing functional group

   \[
   \begin{align*}
   &H_3C-CH(CH_3)_2-CH_3 \quad \text{4-methylheptane} \\
   &H_3C\text{C}H_3\text{CH}2\text{OH} \quad \text{2-propyl-1-pentanol}
   \end{align*}
   \]

2. **Suffix** - basic name derived by adding ending of major functional group (FG)

   \[
   \begin{align*}
   &H_3C-C\text{O}H \quad \text{butanoic acid} \\
   &H_3C\text{C}H_3\text{CH}_2\text{NH}_2 \quad \text{3-methylbutanamide}
   \end{align*}
   \]

3. **Position** - position of FG denoted by Arabic numeral placed before whole name or just before ending. Numbering achieves lowest number for FG

   \[
   \begin{align*}
   &H_3C-C\text{OCH}_3 \quad \text{2-pentanone} \\
   &\text{pentan-2-one} \\
   &\text{NOT 4-pentanone}
   \end{align*}
   \]
Nomenclature rules II

4. **Prefix** - substituents are designated by prefix & Arabic number indicating position (lowest possible numbering)

   - ![2,2,5-trimethylheptane](image1)
   - ![8-chloro-2,3-dimethylnonane](image2)

5. **FG** - if more than one FG name & number based on principle FG. List of priorities given in course notes. Multiple bonds are added to parent (end), all others are **prefixes**

   - ![5-hydroxy-2,2-dimethylpentanoic acid](image3)
   - ![2-methyl-4-oxohex-2-enoic acid](image4)

6. **Minor FG** - halo-, nitro- (-NO₂), nitroso- (-NO) & azo- (-N₂-) are considered substituents & not FG for nomenclature only

7. **Order** - substituents are written in alphabetical order
Examples: structure to name

Step 1: root

Step 2: suffix

Step 3: multiple-bond index

Step 4: functional groups (prefix)

Step 5: substituents (prefix)

Step 7: complete
Examples: name to structure

- Draw the structure for 4-ethyl-3-hydroxycyclohexanone (please)

- draw the root 4-ethyl-3-hydroxycyclohexanone

- add major functional group 4-ethyl-3-hydroxycyclohexanone

- add substituent 4-ethyl-3-hydroxycyclohexanone

- add minor functional group 4-ethyl-3-hydroxycyclohexanone
Functional groups: alkanes

- **Saturated hydrocarbons** - contain only C & H and no multiple bonds
- Non-cyclic alkanes have the formula $C_nH_{2n+2}$

- Alkanes are a little dull - used as solvents or burnt as fuel
- Methane is a fuel, a chemical feedstock & a green house gas
Functional groups: alkanes II

- Isooctane is used in petrol - branched structure means it burns smoothly
- Octane is a long change and burns explosively
- Octane number of petrol is based on isooctane = 100 & heptane = 1
  Unleaded 91 petrol = 91% isooctane & 9% heptane

- **Structural isomers** have same formula but different atoms joined differently
- Isomers can have very different properties

- Isooctane (2,2,4-trimethylpentane, C₈H₁₈)
- Octane
- Pentane (bp 36.2°C)
- 2-Methylbutane (bp 28°C)
- 2,2-Dimethylpropane (bp 9.6°C)
Functional groups: alkenes

- **Ethene** - simplest alkene. Very important industrially.
- Carbon is **trigonal planar** - flat and triangular!
- New form of isomerism - **configurational isomers**
- All atoms bonded in the same manner but different orientation in space

![Chemical structures]

- 1-butene \(\text{C}_4\text{H}_8\)
- trans-2-butene \(\text{C}_4\text{H}_8\)
- cis-2-butene \(\text{C}_4\text{H}_8\)
- 2-methylpropene \(\text{C}_4\text{H}_8\)
- cyclobutane \(\text{C}_4\text{H}_8\)
- \((1R,5R)-2,6,6\text{-trimethylbicyclo[3.1.1]hept-2-ene}\)
- \(\alpha\text{-pinene}\)
Functional groups: alkynes & cyclic structures

- Ethyne is an explosive gas
- Triple bond makes molecular linear (cylinder)
- Examples found in nature (example cleaves DNA)

Cycloalkanes and cycloalkenones

- Cyclic hydrocarbons are common - note that most are not flat
Cyclic structures in nature

- Ring systems are common in natural products & pharmaceuticals
- Example below shows the importance of another form of isomerism - stereoisomers

\[(8R,9S,10S,13R,14S,17R)-10,13\text{-dimethyl}-17-(6\text{-methylheptan-2-yl})\text{-hexadecahydro-1H-cyclopenta}[a]\text{-phenanthrene}\]

cholestane - steroid

\[(R)-1\text{-methyl-4-(prop-1-en-2-yl)cyclohex-1-ene}\]
\(\text{(R)-limonene}\)
smells of oranges

\[(S)-1\text{-methyl-4-(prop-1-en-2-yl)cyclohex-1-ene}\]
\(\text{(S)-limonene}\)
smells of lemons
Functional groups: alcohols

- Alcohols contain OH (hydroxy) group
- Found in many natural systems (especially on Friday night)
- Three classes depending on how many C attached to C–OH
- Compounds can have more than one OH (improves water solubility)

(H)-3,7-dimethyloct-6-en-1-ol
citronellol
citronella oil

Cholesterol
all animals

(R)-1-isopropyl-4-methylcyclohex-3-enol
terpinen-4-ol
tea tree oil

• Primary (1°) alcohols
• Secondary (2°) alcohols
• Tertiary (3°) alcohols

1,2-ethanediol
ethylene glycol
antifreeze

6-(hydroxymethyl)-tetrahydro-2H-pyran-2,3,4,5-tetraol
glucose
sugar I guess!
Functional groups: phenols and ethers

**Phenols**
- Phenol, carbolic acid
- 2,4,6-trichlorophenol, TCP (antiseptic)

- Phenols are distinct from alcohols as attached to phenyl ring - acidic O–H

**Ethers**
- Ethoxyethane, diethyl ether, ether
- Tetrahydrofuran, THF
- 18-crown-6

- Most commonly used as solvents
- 18-Crown-6 enables metal cations (M⁺) to dissolve in organic solvents
Functional groups: alkyl halides and thiols

- Alkyl halides are incredibly useful compounds - used extensively
- Down side is they appear to be bad for us and the environment

Thiols

- Thiols are the sulfur analogue of alcohols - and they smell, bad...
- Humans can detect $2 \times 10^{-5}$ ppb of the second compound (1 drop in a lake)
- One of the last two compounds is the smelliest known - but no one is prepared to make them again to find out which!
Functional groups: amines

- Vital in biological systems
- Many smell (bad but not as bad as thiols)
- Found in many compounds that are physiologically active...

triethylamine smells of fish
butane-1,4-diamine putrescine smells of decay
(S)-2-amino-3-phenylpropanoic acid phenylalanine amino acid

(S)-3-(1-methylpyrrolidin-2-yl) pyridine nicotine
methyl 3-(benzoyloxy)-8-methyl-8-aza-bicyclo[3.2.1]octane-2-carboxylate cocaine
Functional groups: amines II

- Just to confuse, **amines** are labeled by the number of C attached.
- This is different to **alcohols** (labeled by C attached to C–OH).

If add four groups everything changes!
Functional groups: the carbonyl group

- **Carbonyl group** $\ce{C=O}$ – analogous to alkene
- Two groups, **aldehydes** $\ce{RCHO}$ and **ketones** $\ce{R_2C=O}$

**Aldehyde**

- Methanal (formaldehyde)
- Ethanal (acetaldehyde)
- Benzaldehyde

**Ketones**

- Propanone (acetone)
- $\ce{(R)-2-methyl-5-(prop-1-en-2-yl)cyclohex-2-enone}$ (aromadendrene, spearmint)
- $\ce{(S)-2-methyl-5-(prop-1-en-2-yl)cyclohex-2-enone}$ (aromadendrene, caraway)
- 4-(4-hydroxyphenyl) butan-2-one (raspberry ketone)
Functional groups: carboxylic acids & derivatives

- Many of the functional groups are 'linked'
- If we replace one C–H at a time by a C–O we see how these groups relate

\[ \text{hydrocarbon} \xrightarrow{\text{oxidation}} \text{alcohol} \xrightarrow{\text{reduction}} \text{aldehyde} \xrightarrow{\text{oxidation}} \text{carboxylic acid} \]

- ethanoic acid: acetic acid, vinegar
- maleic acid
- (S)-2-hydroxypropanoic acid: L-(+)-lactic acid
- (2Z,4E)-3-methyl-5-(2,6,6-trimethyl-4-oxocyclohex-2-enyl)penta-2,4-dienoic acid: abscisic acid, leaf fall
Functional groups: derivatives

- Reaction of a carboxylic acid with a base (e.g., NaOH) gives carboxylate ion.

Derivatives:
- Ethyl ethanoate
- Ethyl acetate
- Solvent ester
- 2-Methylpropyl propanoate
- Isobutyl propionate
- Smell of rum ester
- Benzoyl chloride
- Acid chloride
- Aspartame
- Sweetener amide
- Ethanoic anhydride
- Acetic anhydride
- Acid anhydride
Classification of functional groups

- Functional groups can be classed by the degree of oxidation (removal of H)

Increasing degree of oxidation (removal of hydrogen)

- alkanes
- alcohols
- ethers
- amines
- alkyl halides
- thiols
- aldehydes
- ketones
- carboxylic acids
- esters
- amides
- acyl chlorides
- acid anhydrides
- nitriles

Reactions:
- Oxidation: hydrocarbon $\rightarrow$ carboxylic acid
- Reduction: hydrocarbon $\rightarrow$ carboxylic acid
- Oxidation: alcohol $\rightarrow$ aldehyde
- Reduction: alcohol $\rightarrow$ aldehyde
- Oxidation: aldehyde $\rightarrow$ carboxylic acid
- Reduction: aldehyde $\rightarrow$ carboxylic acid
Overview

What have we learnt?
- How to name simple organic molecules
- To recognise common functional groups
- Common examples of these functional groups

What's next?
- To looking at the bonding in molecules in detail
- To understand how bonding effects the shape of molecules