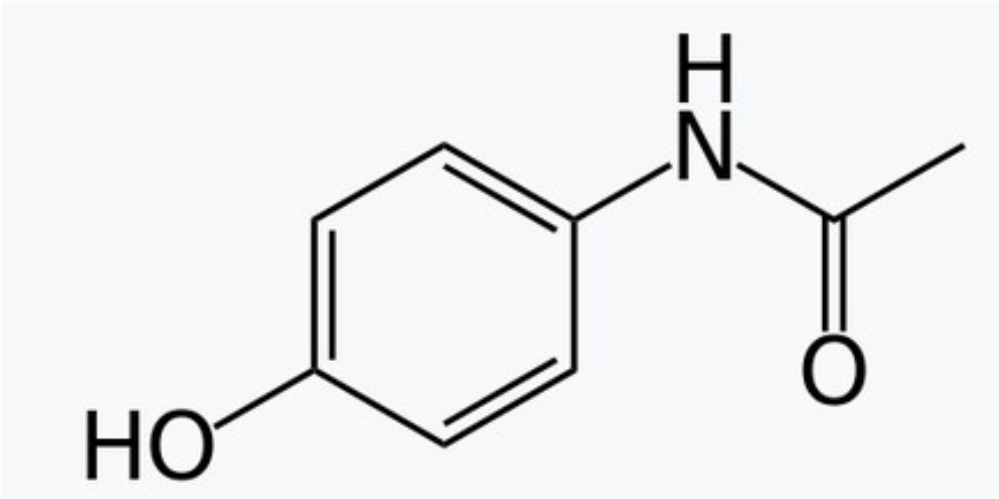
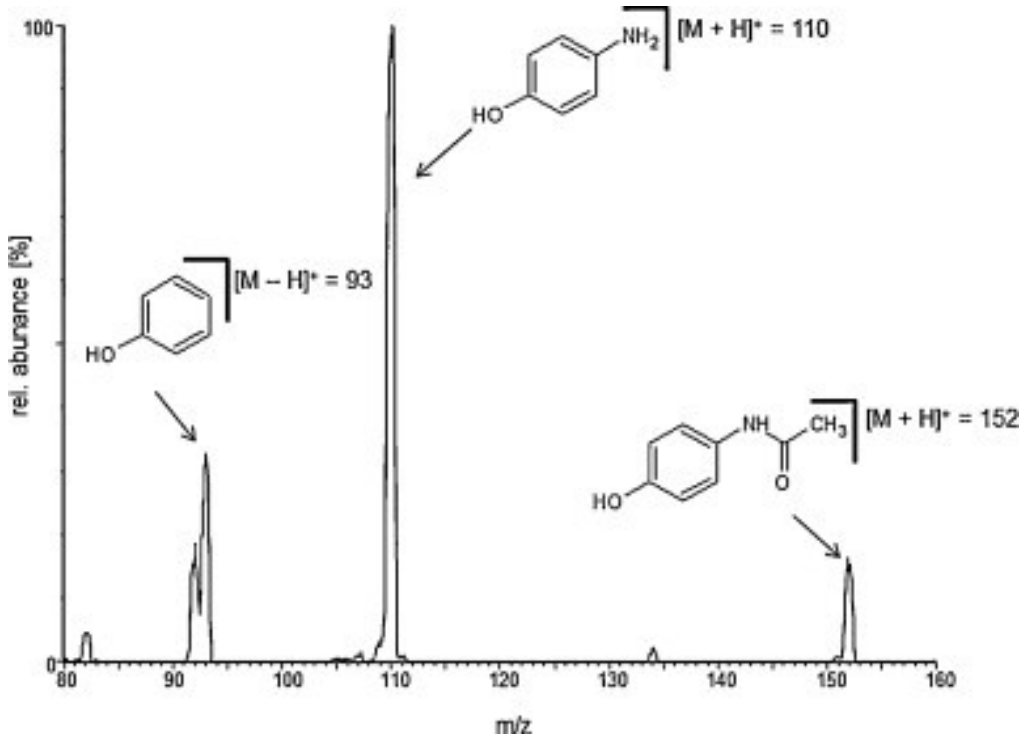
Paracetamol Analysis

Paracetamol: “Par” from the pattern of the substitution onto the benzene ring (para); “acetam” from the amide group acetamide (ethanamide) which is one of the groups substituted; and “ol” from the hydroxyl group which is the other group substituted on the benzene ring.

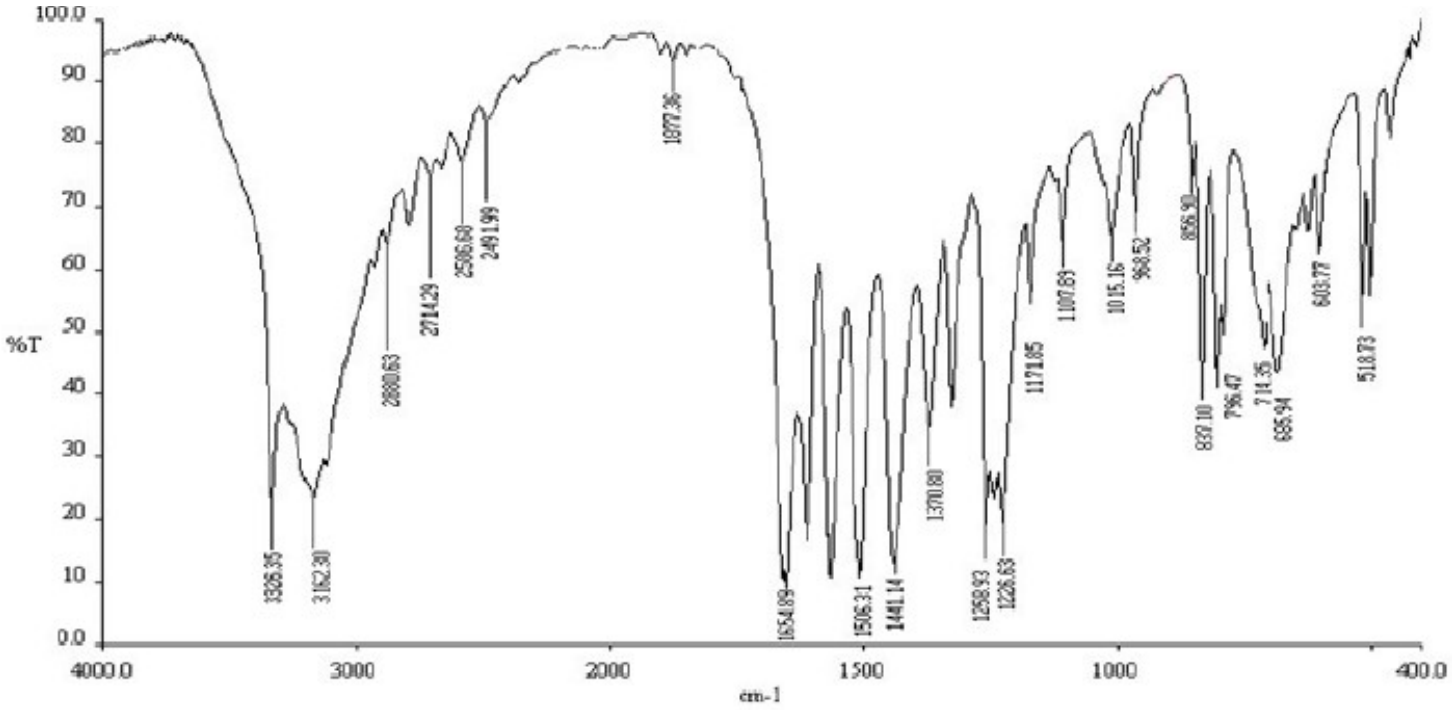
- IUPAC Name: 4-hydroxyphenyl-ethanamide
- Formula: $C_6H_9NO_2$
- Boiling Point: 420°c



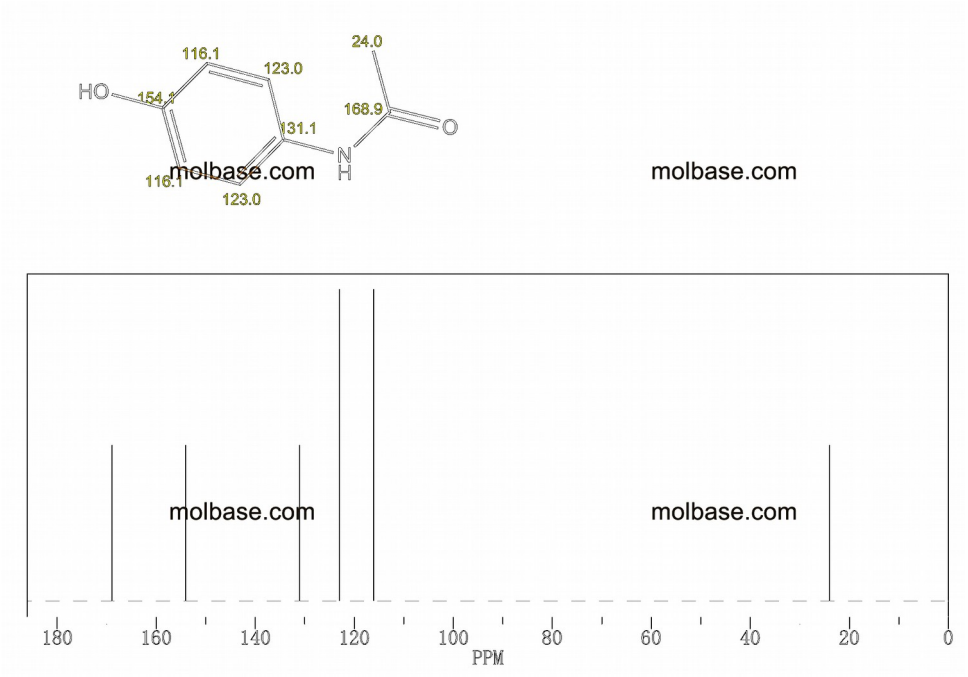
- Functional Groups:
  - -OH(Hydroxyl) on the Benzene creates phenol
  - H-N-C=O (Amide)
- Chemical tests:
  - the boiling point, along with a range of other analytical techniques can be used to determine whether the product made is paracetamol.
  - Alkaline hydrolysis (e.g. with sodium hydroxide NaOH) can be used to detect the presence of the amide group. A positive test would give off ammonia on heating (but not when cold). Ammonia can be detected by smell and because it turns damp red litmus paper blue. However this will also cause the OH group to form O^-Na^+ and H_2O.
  - The phenol group will also react with bromine (when the Paracetamol is aqueous) to decolourise and form a white precipitate as the phenol will undergo electrophilic addition with the bromine at room temperature.



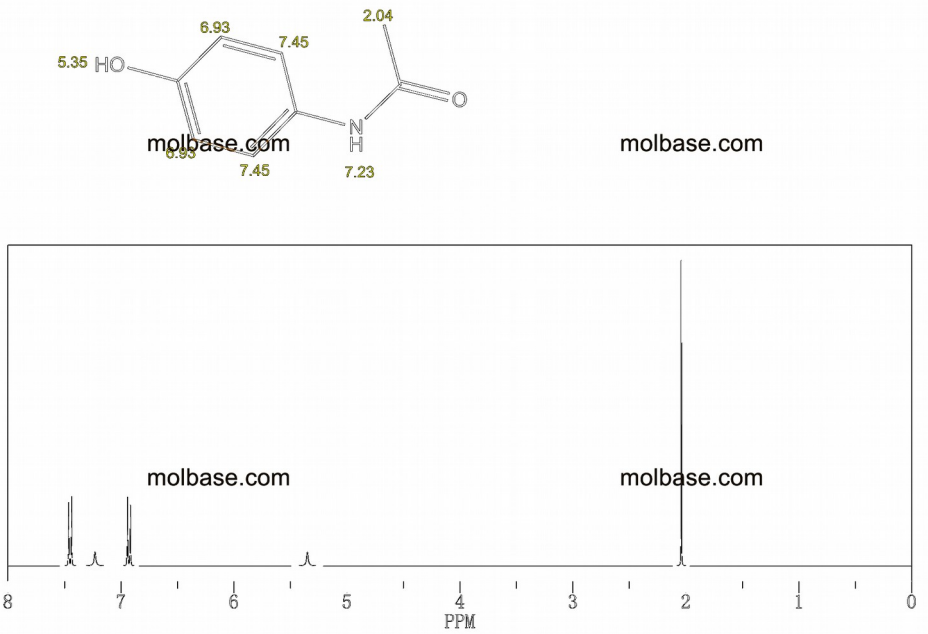
- On the Mass- Spectrometry spectrum of paracetamol above there is a peak at 152 which is the molecular ion peak.
- The peaks at 92 and 109 are the other major peaks (on this picture they look like the only others but better pictures are available e.g. https://webbook.nist.gov/cgi/cbook.cgi?ID=C103902&Units=SI&Mask=28F#Mass-Spec)



- On the Infra-Red Spectroscopy above the peak at about 3300 is associated with the NH from the amide group and the peak just to its right at about 3200 is associated with the OH from the Phenol.
- The smaller peaks around 750-1100 are associated with the C-C bonds that are in both the phenol and ethanamide.
- The peak at the right of the gap between it and the OH peak (about 1600) is associated with the C=O in the amide group.



- The Carbon NMR of paracetamol has 6 distinct peaks because paracetamol has 6 non equivalent carbon environments including: C=O (167-169), C_6H_6 –benzene ring(110-120) & C-C (23-26).



- The Hydrogen NMR of Paracetamol has 5 non equivalent proton environments.
  - The CHCRNH at δ7.45 relative intensity 2 following n+1 rule this peak has a doublet splitting pattern and so has one adjacent non equivalent proton.
  - The CHCROH at δ6.93 relative intensity 2 following n+1 rule this peak has a doublet splitting pattern and so has one adjacent non equivalent protons.
  - The OH at δ5.35 relative intensity 1 following n+1 rule this peak has a singlet splitting pattern and so has no adjacent non equivalent protons.
  - The NH at δ7.23 relative intensity 1 following n+1 rule this peak has a singlet splitting pattern and so has no adjacent non equivalent protons.
  - The CHC=O at δ2.04 relative intensity 3 following n+1 rule this peak has a singlet splitting pattern and so has no adjacent non equivalent protons.