Molecular fingerprints

***Education in Chemistry***September 2017<rsc.li/EiC517-know-your-poison>

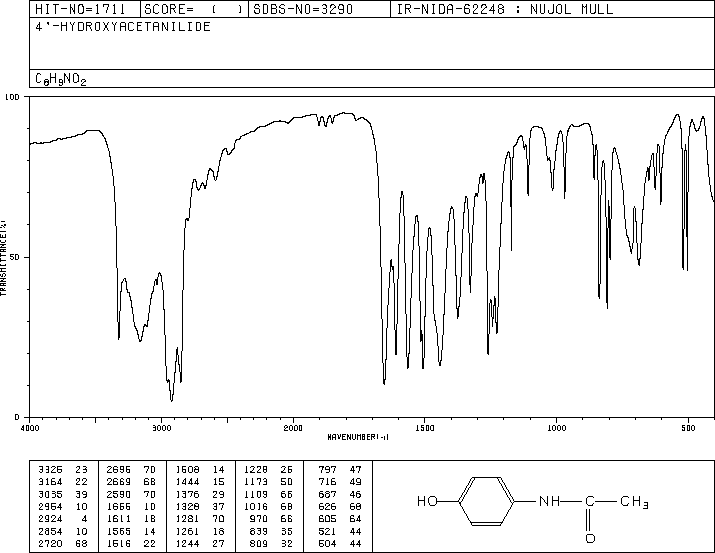
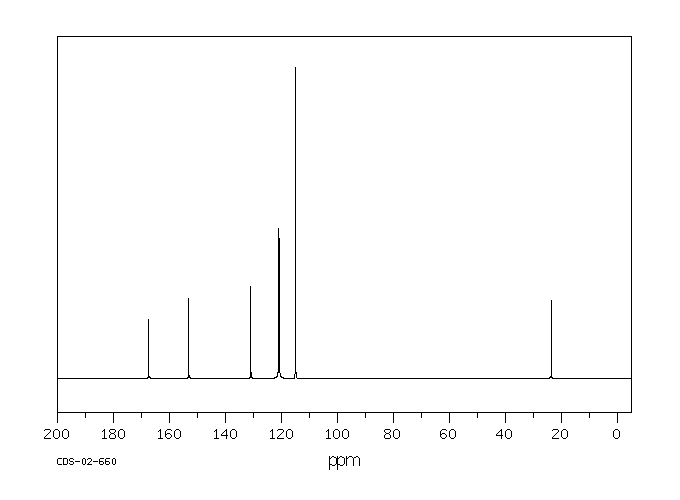
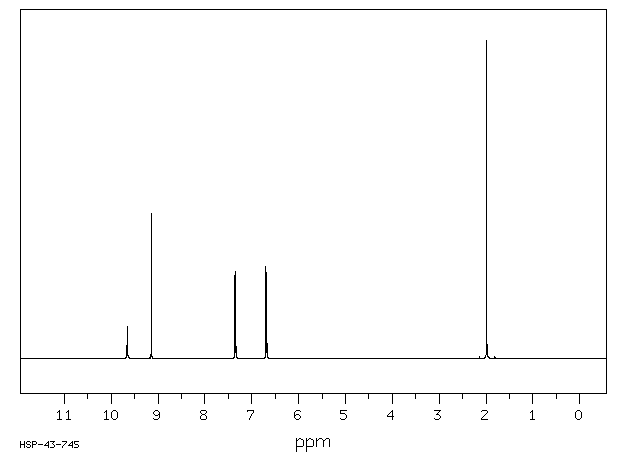
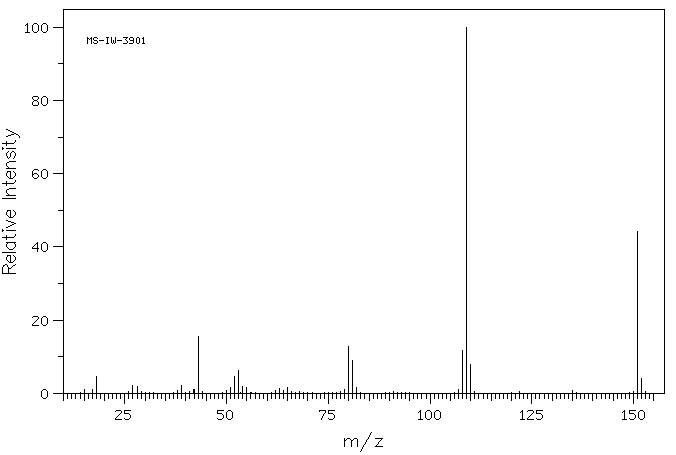
**This activity accompanies the above article ‘Know your poison’.**

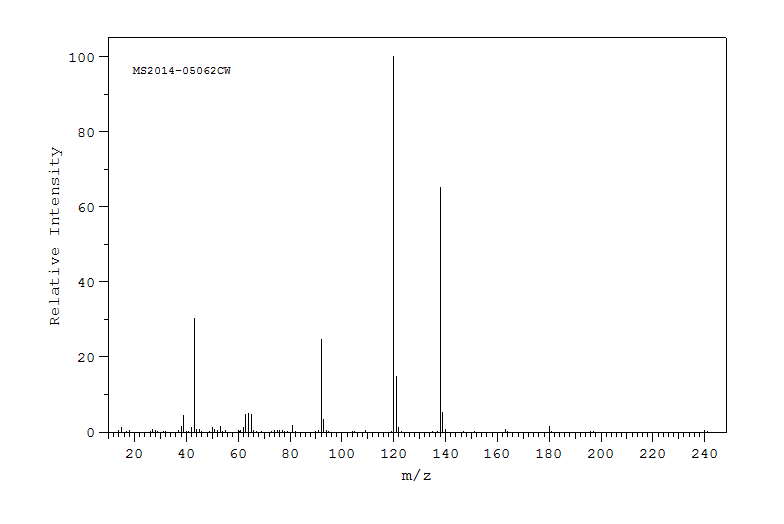
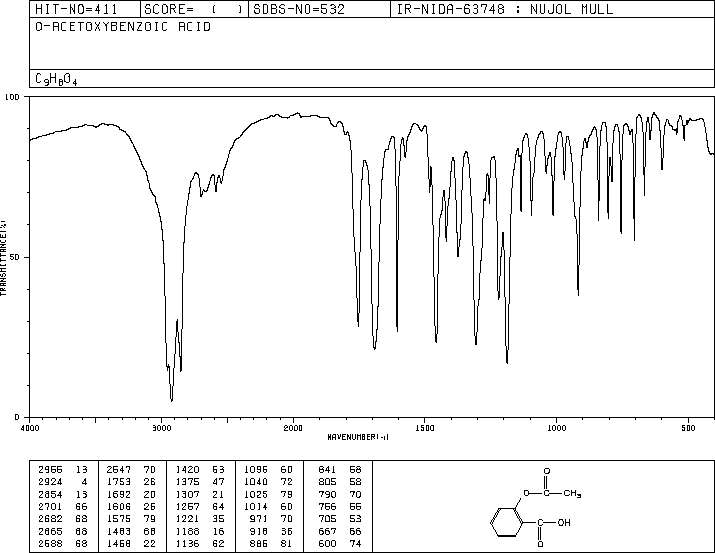
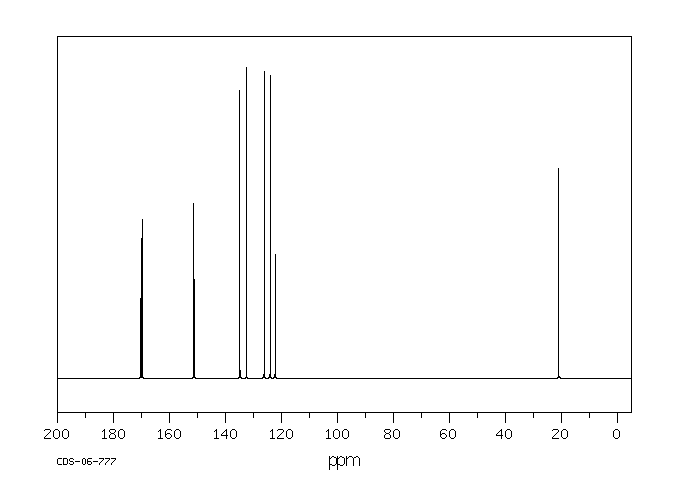
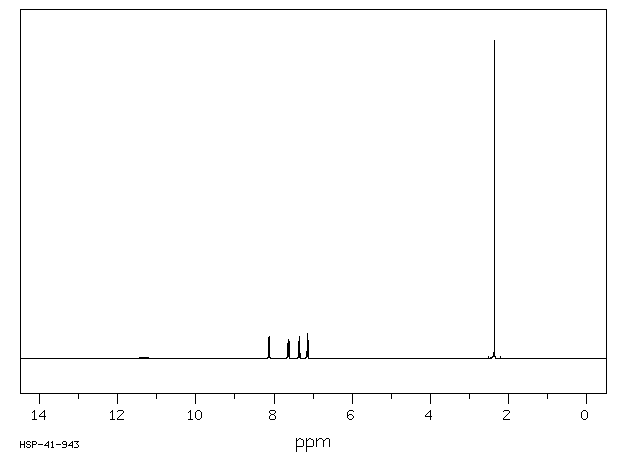
The team at Bath have found lots of different substances mixed in with their drugs samples. Legal drugs such as painkillers are commonly found in the samples.

Note down the molecular formula, relative molecular mass (Mr) and functional groups for paracetamol, aspirin and ibuprofen. This will help you in the next part of the exercise.

|  |  |  |
| --- | --- | --- |
|  | **Molecular formula and Mr** | **Functional groups present** |
| Paracetamol |  |  |
| Aspirin |  |  |
| Ibuprofen |  |  |

The following pages contain infrared, 1H NMR, 13C NMR and mass spectra for paracetamol, ibuprofen and aspirin. Use the structures given above and your data book to assign each of the peaks in the spectra.

*The following spectra are downloaded from SDBSWeb http://sdbs.db.aist.go.jp (National Institute of Advanced Industrial Science and Technology, accessed 22 June 2017)* **Paracetamol**

**Aspirin**

**Ibuprofen**