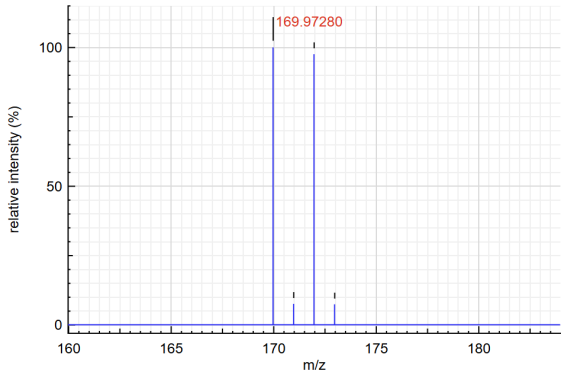
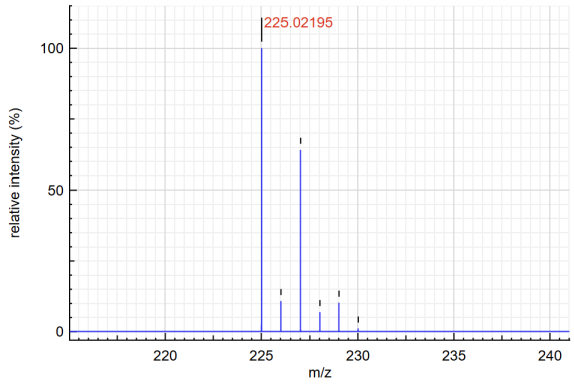
*The following questions cover analytical methods such as Mass Spectrometry, IR and UV-VIS. Please refer to **chapter 4** in Organic Chemistry with a Biographical Emphasis from Timothy Soderberg to obtain a good introduction of the methods.*

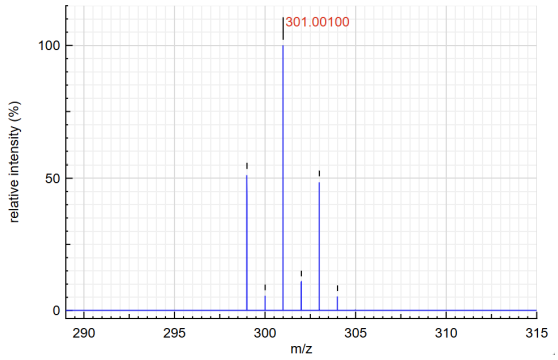
### 3.1 Mass Spectrometry (MS)

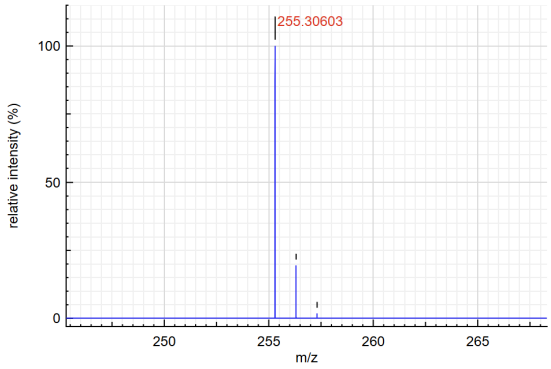
Match the following molecular formulas to the MS spectra bellow:

1. C7H7Br
2. C10H10Cl2
3. C18H38
4. c10H20Br2



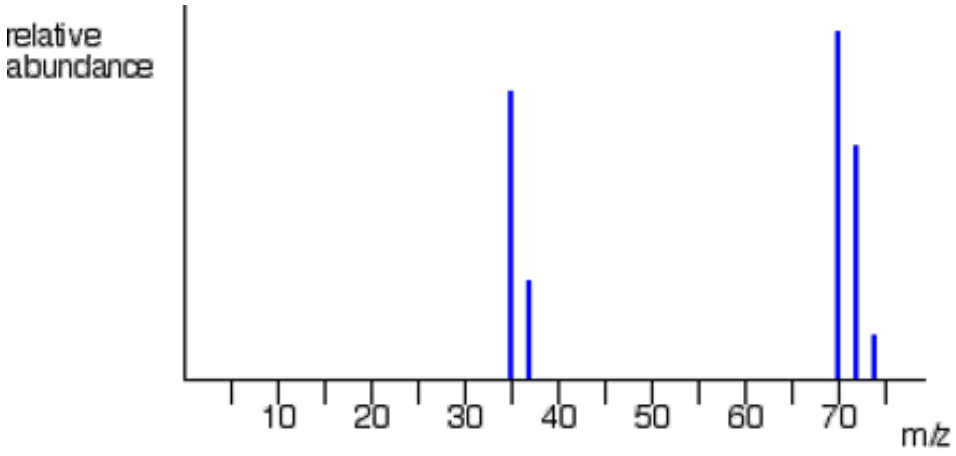



### 3.2 Mass Spectrometry (MS)

Consider an MS spectrum of the molecule $Cl_2$. Explain how each of the different peaks are formed and which the monoisotopic peak is.



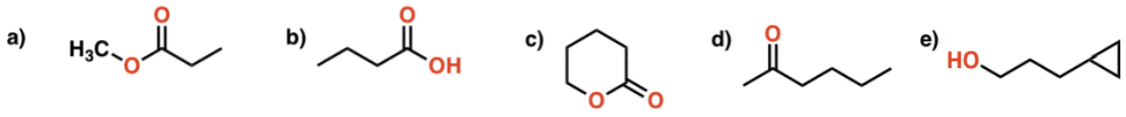

### 3.3 UV vis

Guanosine has an extinction coefficient of 8400 [1/M*cm] at 270nm and the path length used is 1 cm. Using a spectrophotometer, you find the that A275=0.70

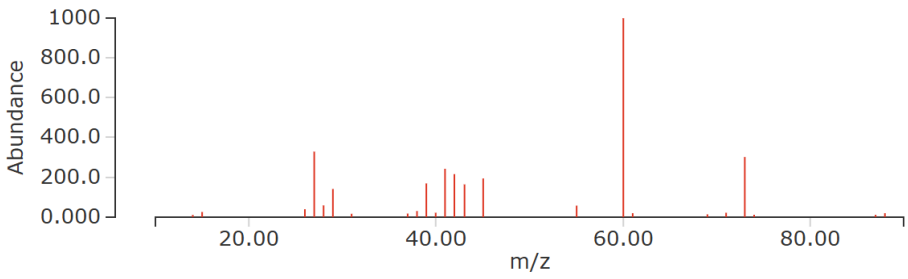
What is the concentration of guanosine?

### 3.4 MS + IR spectroscopy

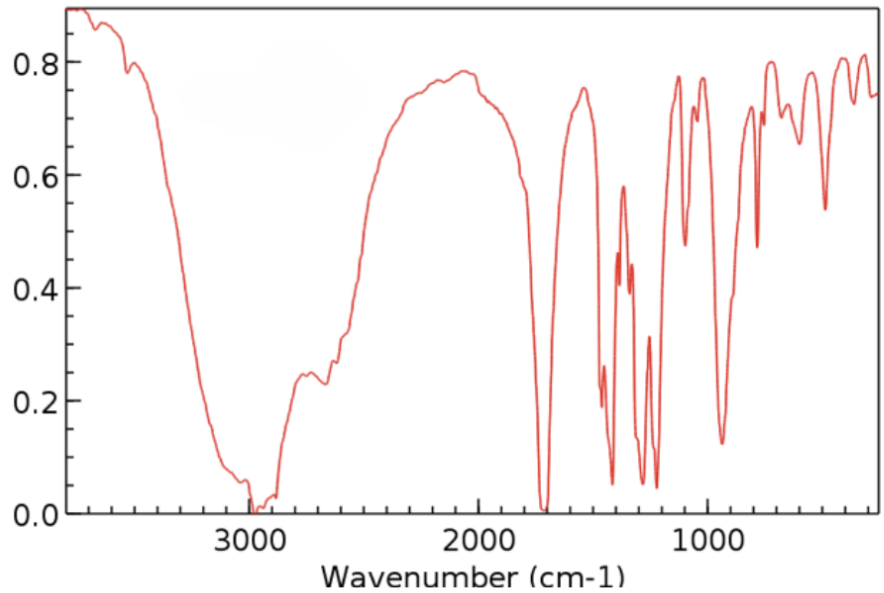
You notice a strange odour coming from a mislabelled tube in your laboratory. You know that it is one of the following molecules. You decide to do a mass spectrometry followed by an IR spectroscopy experiment to identify the culprit.




MS spectrum of compound X:



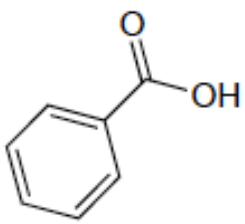
IR spectrum of compound X:



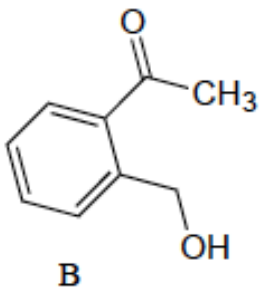

Given the spectra can you identify which compound is the culprit for the bad smell?

**3.5 IR**

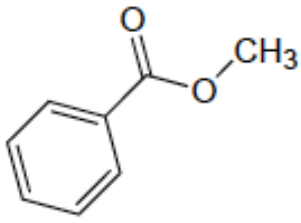
Explain how you could use IR spectroscopy to distinguish between compounds A, B, and C. How would the main peaks in their IR spectra differ?




A




B



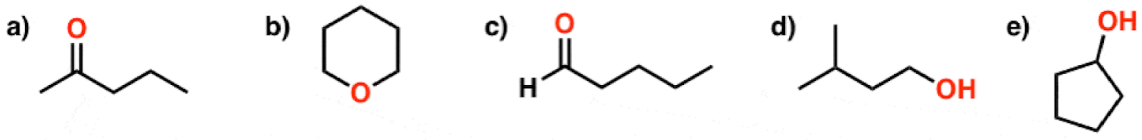

C

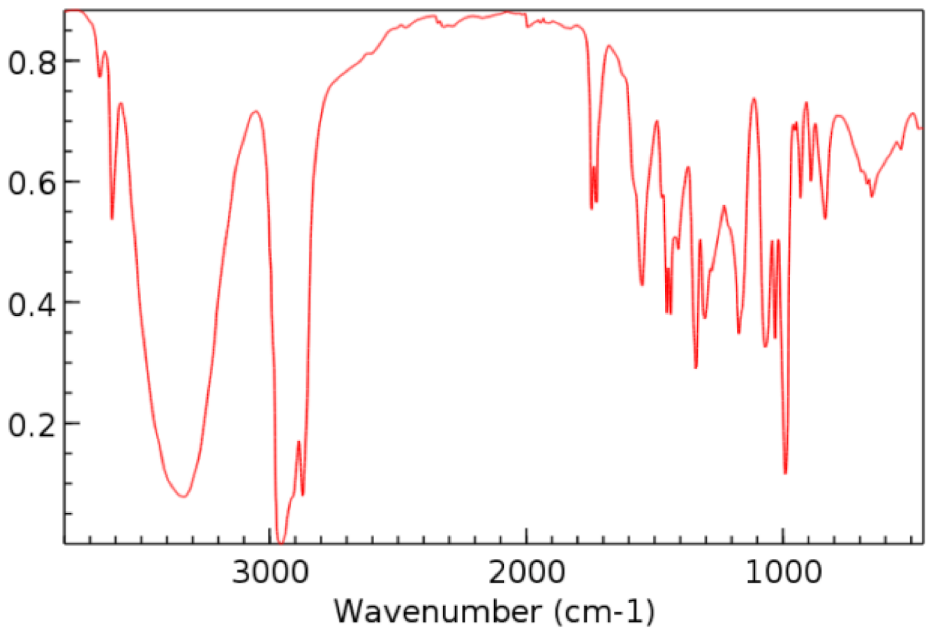
**Characteristic IR absorbances**

| Functional group | Characterisic IR absorbance ($cm^{-1}$) | Source of signal |
|---|---|---|
| carbonyl | 1650-1750 (strong) | C=O strecting |
| alcohol | 3200-3600 (broad) | O-H stretching |
| carboxylic acid | 1700-1725 (strong) | C=O strecting |
| | 2500-3000 (broad) | O-H stretching |
| alkene | 1620-1680 (weak) | C=C stretching |
| | 3020-3080 | vinylic C-H stretching |
| alkyne | 1620-1680 (weak) | triple bond stretching |
| | 3250-3350 | terminal C-H stretching |

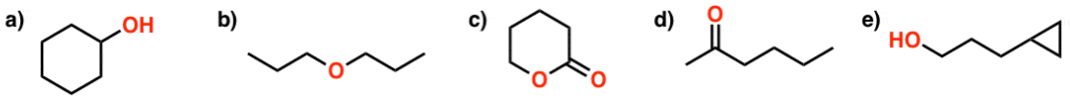
### 3.6 IR

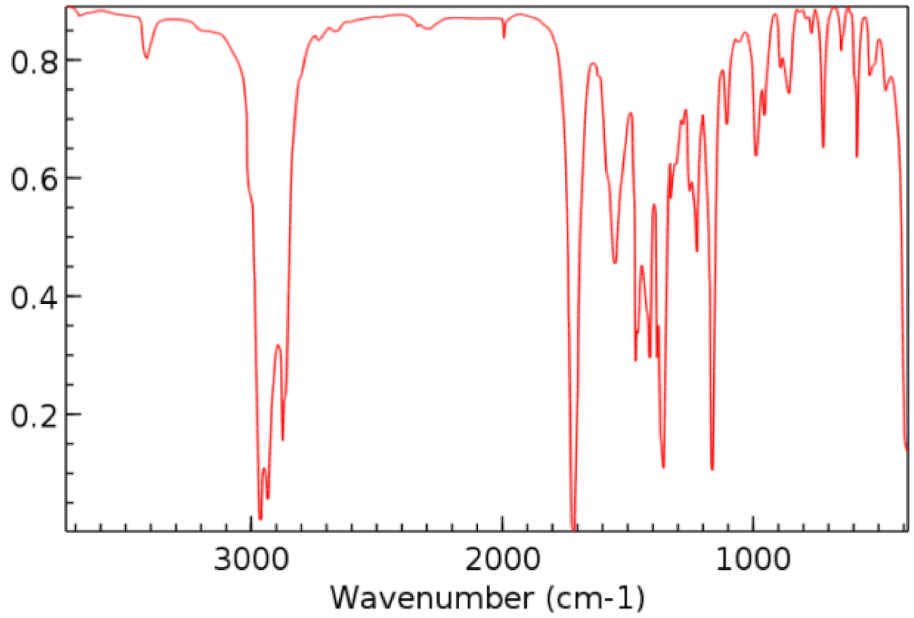
I) We have a molecule of which we know the chemical formula is $C_5H_{10}O$. In order to determine its structure we perform IR spectroscopy. Which of the following compounds corresponds to this IR spectrum?



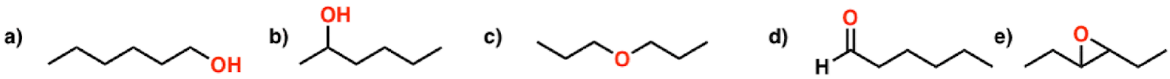



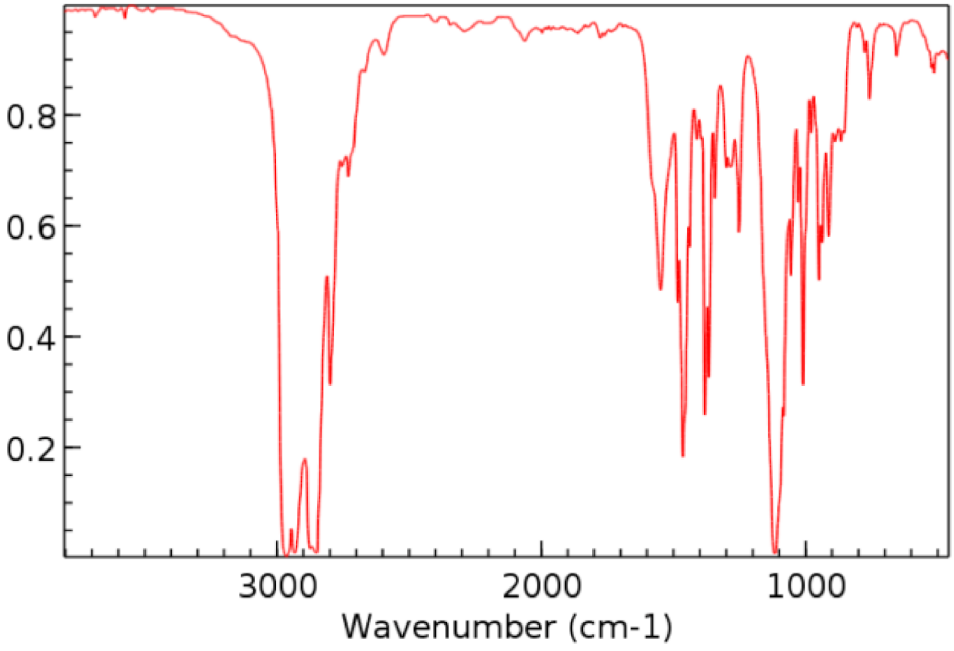
II) Which of the following compounds corresponds best to the following IR spectrum of $C_6H_{12}O$?




III) Which of the following compounds corresponds best to the following IR spectrum of $C_6H_{14}O$?

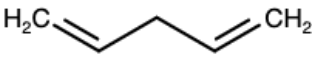


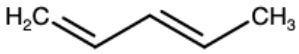
### 3.7 UV-VIS

Which of the following molecules absorbs in a longer wavelength in the UV-range. Explain why.

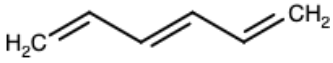
**I)**




**A**

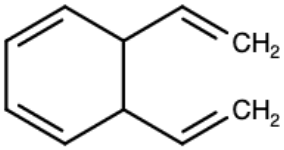



**B**

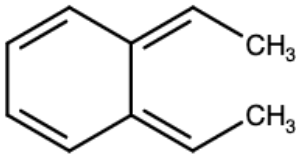



**C**

**II)**




**A**




**B**

### 3.8 UV-VIS

You want to know the concentration of your isolated DNA, by first diluting 100uL of an aqueous sample of double stranded DNA in 900uL of water. You then measure an absorbance of 0.45 at 260nm. Calculate the concentration of your original sample using Beer-Lambert law and an extinction coefficient of 0.02 $uLng^{-1}cm^{-1}$ for double stranded DNA. Assume the path length of the light through the sample is 1cm.

**3.9 Calibration curves and UV- vis:**

You want to calibrate your spectrophotometer to determine the concentration of an unknown DNA sample. To do this, you measure the absorbance of known concentrations of DNA summarized in the table below:

| **DNA concentration [ug/mL]** | **Absorbance at 260nm** |
|---|---|
| 500 | 1.8799 |
| 250 | 1.1415 |
| 125 | 0.6538 |
| 62.5 | 0.3416 |
| 31.25 | 0.1741 |

Use this to make a calibration curve (ex. using excel) and approximate the concentration of a DNA sample that has A260 = 0.6?

Could you use this calibration curve to find the concentration of a sample that has an A260 = 4.7?