Student 2: High Merit

NZQA Intended for teacher use only

Mass Spec:

m/z ratio	group
88	C_2H_4O is the empirical formula and has a mass of 44 so compound must have formula $C_4H_8O_2$. This is the molecular ion peak. And the base peak as it has 100% absorbance.
89	Peak due to relative isotopic abundance of ^{13}C isotope
45	$COOH^+$
43	$C_3H_5^+$
29	C_2H_5

IR:

Wavenumber(cm^{-1})	Characteristic group
2980 broad	Carboxylic acid
1710 sharp	C=O Aldehydes, ketones, carboxylic acids, esters

NMR:

Chemical shift (ppm)	Characteristic group
13	CH_3
19	CH_2
38	CH_2
180	C downfield shift due to C bonded to highly electronegative atom or atoms

There are 4 carbons in the compound

Justification:

With the mass spectrum showing a peak at 88 and an empirical formula of C_2H_4O the chemical formula of the compound is $C_4H_8O_2$. The peak at 29 is characteristic of a fragment formed due to the breakup of the compound in the mass spectrometer to form a $C_2H_5^+$ion. The peak at 45 is due to the $COOH^+$ ion. This indicates that compound A could be butanoic acid.

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The 4 different chemical shifts indicating that the carbons are all in different environments in the ^{13}C spectra suggest that the compound would be the straight chain butanoic acid. The peak at 180 would be due to the carbon with two oxygen atoms bonded to it.

Analysis of the IR spectra shows a broad peak at 2980 cm^{-1} confirming the presence of the O-H group on the butanoic acid. The acid is further confirmed by the peak at 1750cm^{-1} which is characteristic of the C=O.

This makes me believe the molecule is butanoic acid.