

# Mass Spectrometry (MS)

Measure mass of molecule



How?

DNA

Fingerprints

Fibre Analysis

Poison

Blood

# Mass Spectrometry (MS)

Light molecule



Large deflection

Heavy molecule



Small deflection

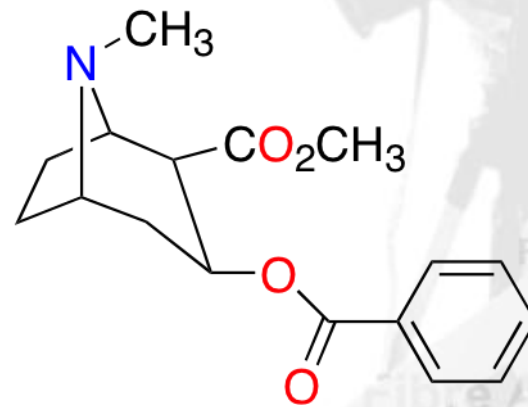
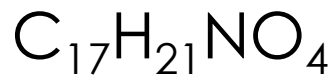
Measure mass of molecule



Measure the degree of deflection

# Cocaine

Molecular formula



# Cocaine

## Molecular weight



Carbon



$$12 \times 17 = 204$$



Hydrogen



$$1 \times 21 = 21$$



Nitrogen



$$14 \times 1 = 14$$

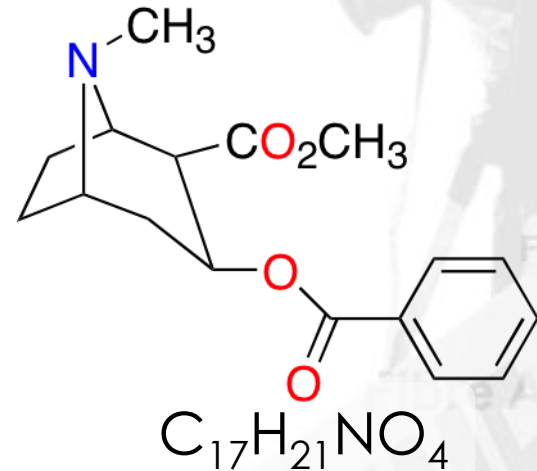


Oxygen



$$16 \times 4 = 64$$

$$\text{Total} = 303$$



# Cocaine

Molecular weight = 303



Cocaine?

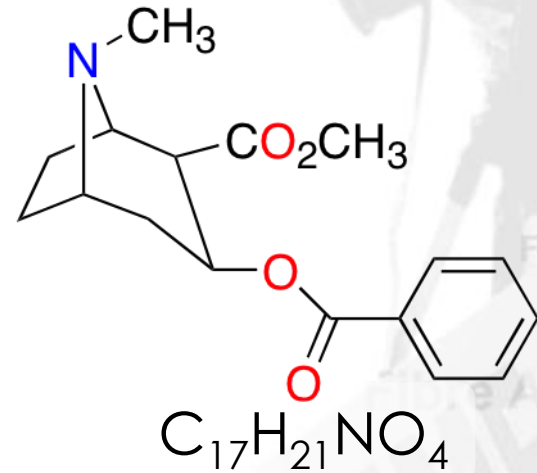


No

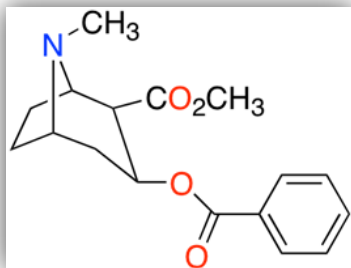
Same atoms can be arranged in different ways



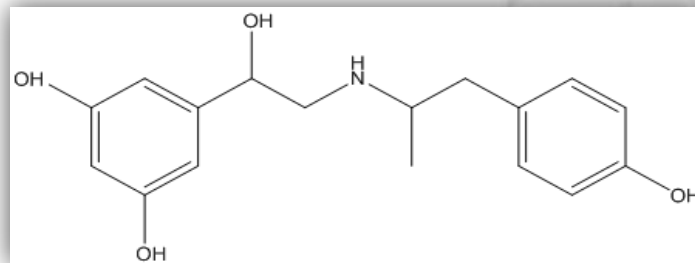
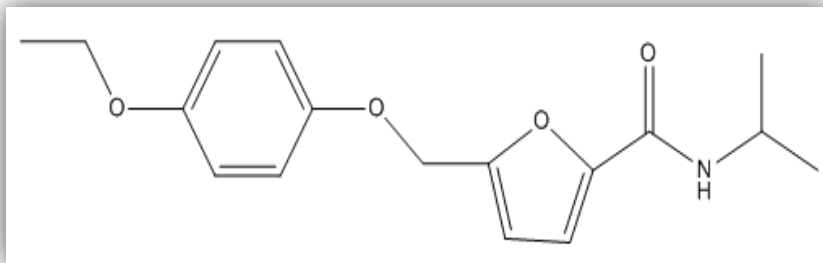
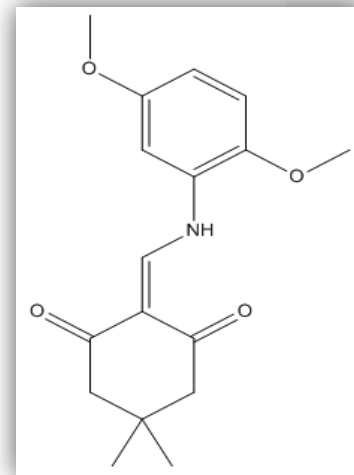
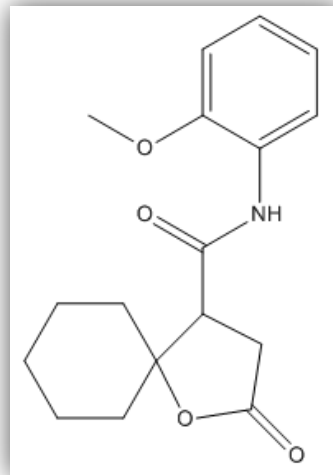
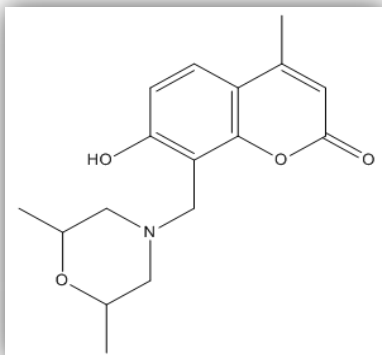
Isomers



# $C_{17}H_{21}NO_4$ Isomers



Cocaine



# Mass Spectrum

Pattern of fragments at detector

DNA

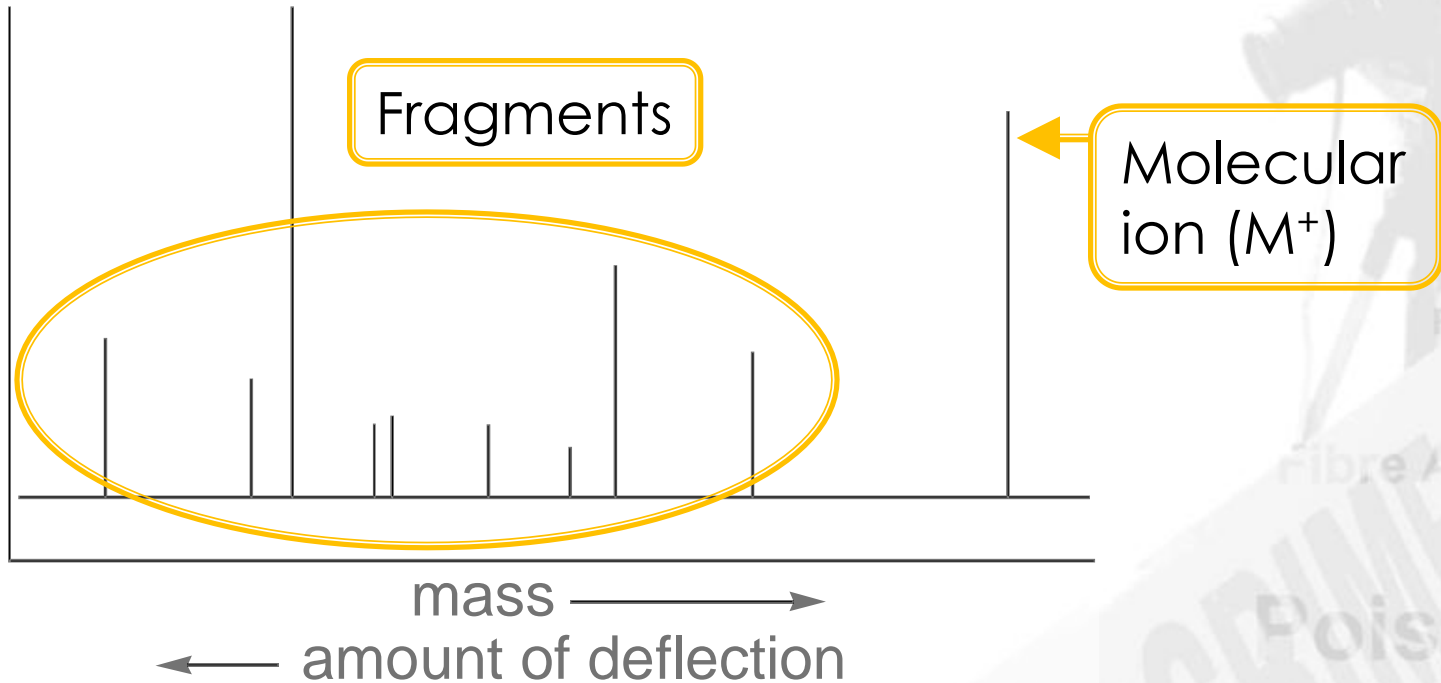
Fingerprints

Fibre Analysis

Poison

Blood

# Mass Spectrum





# Mass Spectrum

Pattern of fragments at detector



Highest weight



Molecular ion



Lower weights



Fragment ions



Always the same pattern

# Mass Spectrum

Cocaine?

Authentic sample of cocaine

Compare the 2 fragmentation patterns



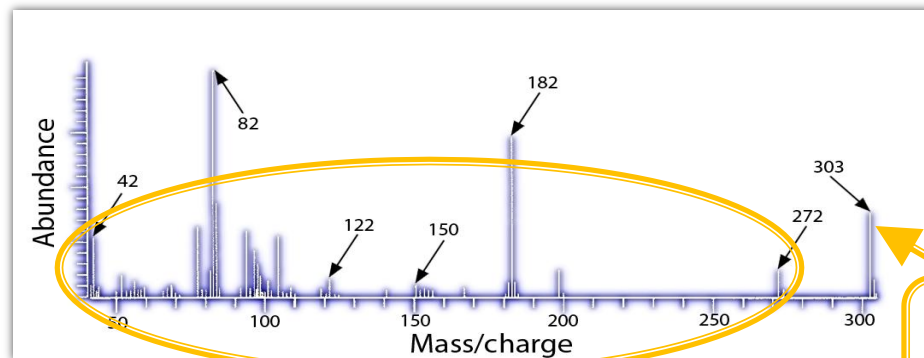
Same



Cocaine

# Mass Spectrum

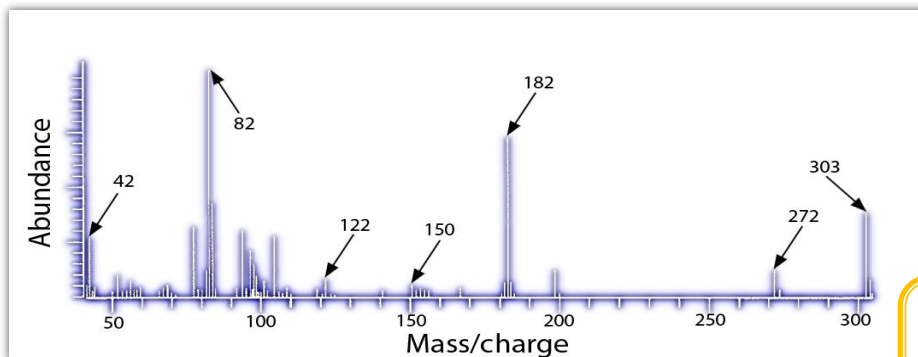
Cocaine



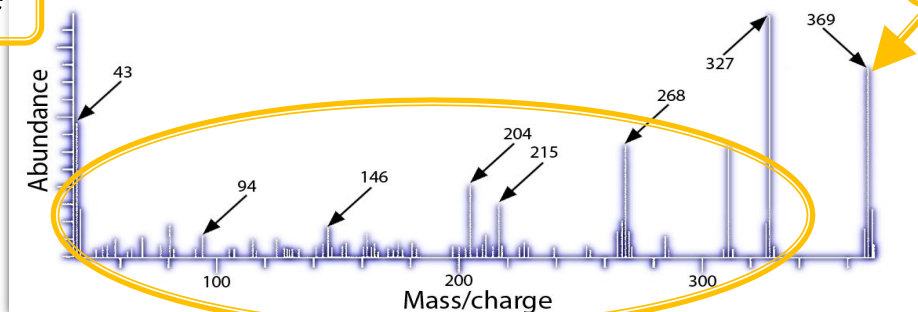
Molecular ion ( $M^+$ )

# Mass Spectrum

Cocaine



Diamorphine



Molecular ion (M<sup>+</sup>)

# Techniques

## 1 Chromatography



Separation of mixtures

## 2 Spectroscopy and spectrometry



Identification of components

# Techniques

Combining separation and identification

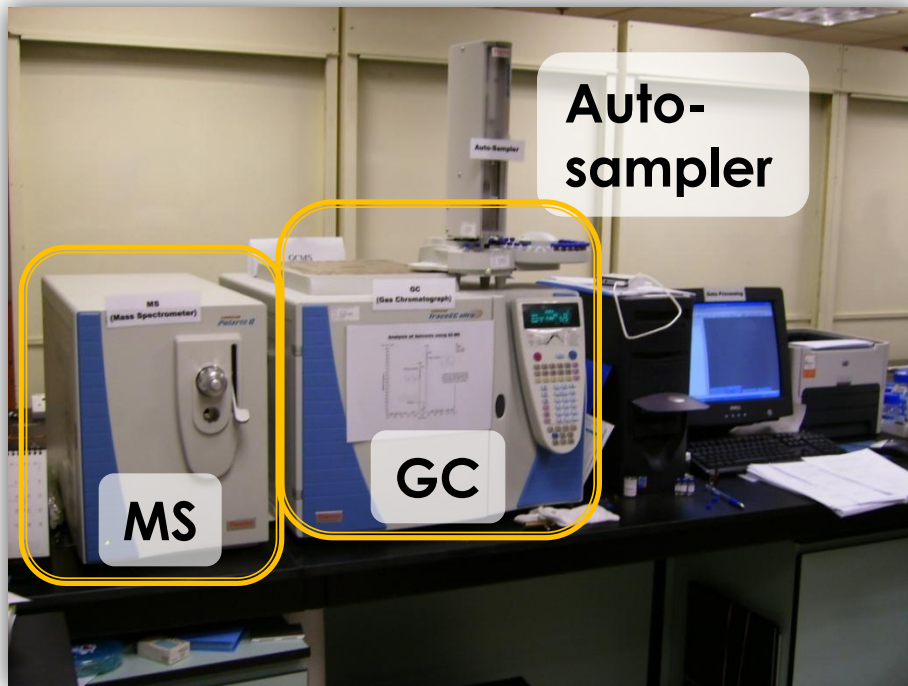


Gas chromatography -  
Mass Spectrometry (GC-MS)



Hyphenated technique

# GC-MS



GC output



Goes to mass spectrometer

MS



Detector

## GC-MS

GC output



Retention time of components



Quantify amount

MS output



Identification

Combines separation and identification



# Summary

## 1 Chromatography



TLC, GC and HPLC



Separation of mixtures

# Summary

1 Chromatography

2 Infrared spectroscopy



Identification by molecular vibrations



Molecular stretching and bending

# Summary

1 Chromatography

2 Infrared spectroscopy

3 Mass spectrometry



Identification by fragmentation