STRUCTURAL ELUCIDATION AND UNKNOWN ANALYSIS

The Measure of Confidence

Agilent 7200 series GC/Q-TOF

Commercial electron ionization (EI) spectral libraries do not always contain mass spectral data for compounds of interest. In these instances, the accurate mass MS/MS spectra generated by the **Agilent 7200 Series GC/Q-TOF** can be invaluable for establishing relationships between fragment ions, thus assisting structure correlation.

The **Agilent 7200 GC/Q-TOF** can operate in MS/MS mode at fast acquisition rates, while maintaining mass accuracy and high resolution. This allows acquisition of numerous MS/MS for every chromatographic peak, thus eliminating the need to do multiple runs.

Take advantage of accurate mass MS and MS/MS spectra to elucidate the structure of unknown compounds

- Chemical ionization (CI) can be used to confirm the molecular ion
- Molecular formula can be determined by combination of:
  - Accurate mass measurement of the molecular ion
  - Isotopic abundance and spacing of the molecular ion
- Accurate mass enables the assignment of empirical formula to fragment ions
- MS/MS can be used to determine the relationships between the fragment ions in the spectra to provide additional structural information
- The Molecular Structure Correlator (MSC) software provides tools to identify possible molecular structures

For more information, visit:
agilent.com/chem/gcms_qtof

Agilent Technologies

Confirming a most likely structure

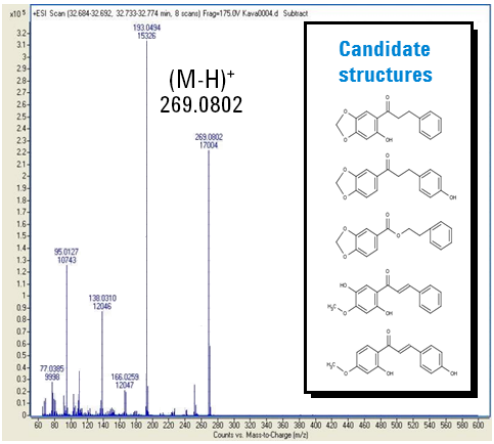

Figure 1. MassHunter Qual can provide empirical formula information ($C_{16}H_{14}O_4$) for Kava extract-unknown compound

	m/z (experimental)	Formula	Error (ppm)	Score
– H	269.0802	$C_{16}H_{13}O_4$	2.2	80.7
– C_6H_5	193.0494	$C_{10}H_9O_4$	0.6	96.7
– CH=CH–C_6H_5	167.0334	$C_8H_7O_4$	3.0	N/A
– CH_2=CH–C_6H_5	166.0259	$C_8H_6O_4$	0.6	N/A
– CO	138.0310	$C_7H_6O_3$	1.1	98.1
– CO	110.0359	$C_6H_6O_2$	3.0	N/A
– CH_3	95.0127	$C_5H_3O_2$	0.9	99.5

Figure 2. MS/MS experimental result

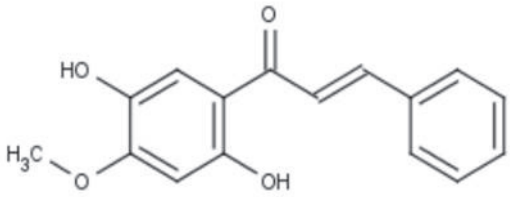

Figure 3. Of the 5 candidate structures, only one fits the losses identified by MS/MS experiments on multiple precursor ions

Molecular Structure Correlator

The MassHunter Molecular Structure Correlator (MSC) software correlates accurate mass MS/MS fragment ions for a compound of interest with one or more proposed molecular structures for that compound.

MSC greatly simplifies structure elucidation by providing a possible formula for the molecular and fragment ions, as well as evaluating possible structures associated with each molecular ion formula.

Structural elucidation & unknown analysis can be achieved using the Agilent 7200 Series GC/Q-TOF coupled with the Agilent 7890B GC and the MassHunter Software Package

Further readings:

Agilent 7200 Series GC/Q-TOF brochure (5991-4806EN)

Metabolomics of Opiate-Induced Changes in Murine Brain by GC/Q-TOF (5991-2481EN)

For more information, please visit:
www.agilent.com/chem/gcms_qtof

Published in UK, December 2, 2014
5991-5426EN

The Measure of Confidence

Agilent Technologies