Resolving Power and Mass Resolution

Technical Overview

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Instrument Resolving Power and Mass Resolution

The terms resolving power and mass resolution are often used interchangeably but are truly different properties that define instrument and method related performance. Resolving power refers to an instrument's ability to distinguish two adjacent ions of equal intensity. On a TOF instrument, resolving power is fixed across the mass range, while mass resolution is a function of both ion width and the mass being measured.

The IUPAC definition of resolving power is [1]:

"For two peaks of equal height with masses m_1 and m_2, when there is overlap between the two peaks to a stated percentage of either peak height (10 % is recommended), then the resolving power is defined as:

$$\frac{m_1}{m_1 - m_2}$$ *Equation 1.*

The percentage overlap (or 'valley') concerned must always be stated."

IUPAC further offers a peak-width definition for mass resolution.

"For a single peak made up of singly charged ions at mass m in a mass spectrum, the resolution may be expressed as:

$$\frac{m}{\Delta m}$$ *Equation 2.*

where Δm is the width of the peak at a height which is a specified fraction of the maximum peak height (for example, 50 %)."

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If a monoisotopic, singly charged ion measured on a TOF system has a profile width of 0.05 amu at a mass of 500.0000 amu, the mass resolution is 10,000. For comparison, the same 500 amu measured on a SQMS or quadrupole MS/MS system with typical ion widths of 0.6 amu has a mass resolution of approximately 833. It is evident that the more narrow the ion width, the better the ability to distinguish similar masses.

How Much Resolution is Enough?

In his article, *Debating Resolution and Mass Accuracy*, Balogh [2] noted that sensitivity is reduced as mass resolving power is increased, and the argument for higher mass resolution does not become persuasive until the molecular weights being measured become significant. Another tradeoff for very high resolution (100,000 or greater) is the spectral acquisition rate. As Balogh further notes, the resolution of instruments such as FT-ICR is undeniable but potentially impractical, and references a conclusion:

"FT-ICR MS provides unequalled resolving power and mass accuracy as long as sufficient time is available to acquire the necessary degree of information . . . the problem is (the) required time is too long to allow sufficient spectra to be obtained across a high-resolution (chromatographic) peak for the peak to be properly delineated (*sic*) [3]."

Kellman, *et al*. [4] suggest a required mass resolving power of 25,000 on a LC/FT-ICR instrument to measure drugs, pesticides, mycotoxins, and plant toxins at levels down to 10 ppb in feed matrix samples. Therein, the chromatographic peaks appear to range from 6 seconds to 24 seconds with acquisition rates of 2 and 4 Hz, and resolving powers of 50,000 and 25,000 respectively. As a reference, a resolution of 50,000 can distinguish ions differing by about 50 ppm (for example, 292.0403 amu and 292.0266 amu, Δppm = 47. In addition to resolution, one must consider the molecular mass being measured and the chromatographic speed. The acquisition rates and peak widths noted above are far too slow and wide for most GC analyses.

References

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