PSB 102 WideBand Activation™ Technology

The resonance excitation process used for MS^n in an ion trap device fragments only the selected ion. Fragment ions formed in this manner do not themselves undergo subsequent fragmentation, as is the case in the collision cell of a triple quadrupole or QqToF mass spectrometer. This has obvious benefit because fragmentation pathways are significantly easier to follow using an ion trap device. Hydroxylated compounds, however, frequently show only the loss of H_2O in the first stage of MS^n analysis. In this situation, an additional stage of MS would be required to generate more structurally useful information.

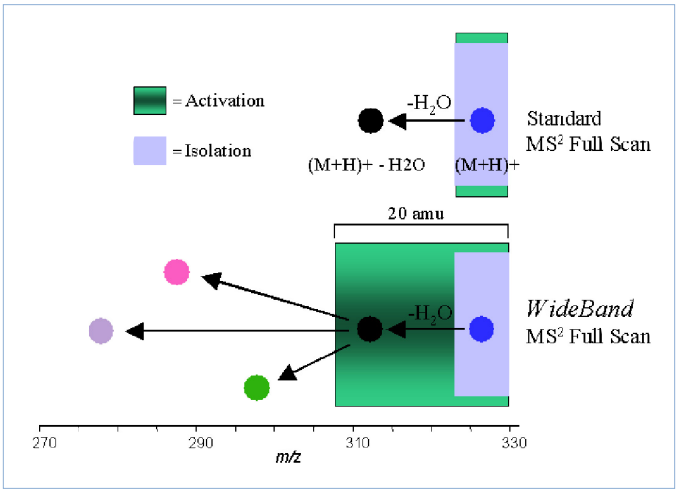

Figure 1

To overcome this limitation, the Thermo Scientific LTQ and LCQ™ series of instruments include WideBand Activation as a standard feature. For the first time in a commercial mass spectrometer the isolation and activation widths of the MS^n process are effectively decoupled.

WideBand Activation operates by applying resonance excitation energy over a mass range which extends to 20μ lower than the selected ion. This ensures that both the parent ion and any subsequent water loss ion will undergo fragmentation while retaining the specificity of the unit mass isolation of the parent ion.

In qualitative applications,WideBand Activation is advantageous because an additional stage of MS is not required to generate useful structural information. This is particularly relevant when conducting Data Dependent™(1) experiments. Without WideBand Activation additional MS^3 scans might be necessary which reduce the number of different co-eluting components that can be analyzed under a chromatographic peak.

In quantitative experiments, the loss of water provides no greater specificity than monitoring the parent ion by MS only. Additionally, using MS^3 for quantitation will result both in longer scan cycles than MS^2, and will reduce the number of data points taken across a peak. Having fewer points will lead to less precision in the quantitative data. WideBand Activation eliminates both problems for these experiments–providing the specificity required and maintaining an appropriate scan cycle time

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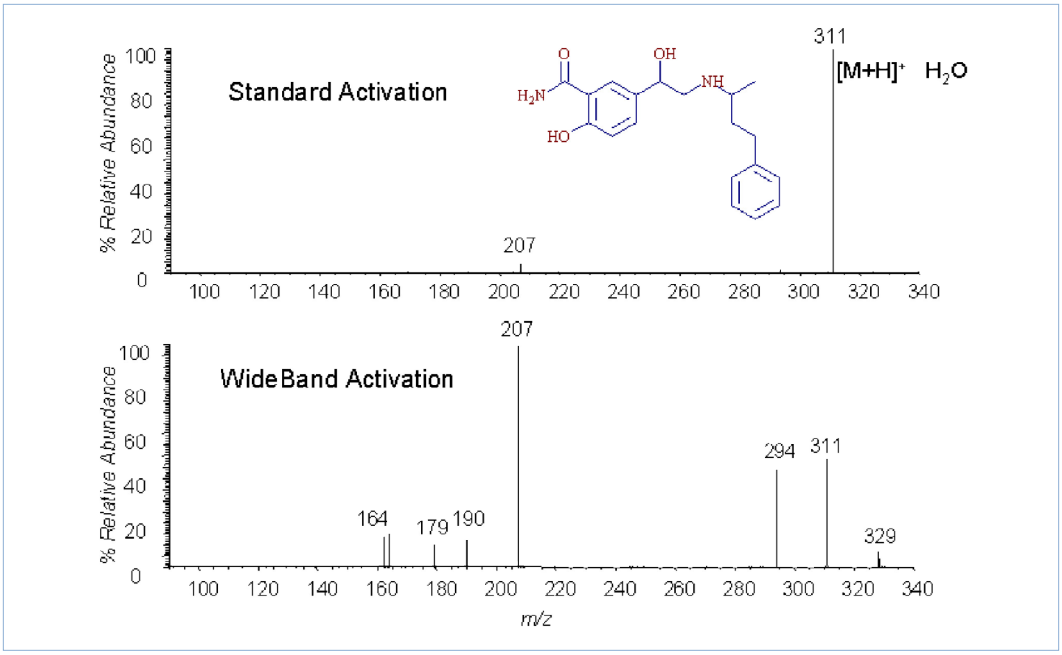

Figure 2

Figure 2 shows the MS^2 spectrum of Labetalol acquired with and without WideBand Activation. Standard activation conditions, even with high collision energy, show only the water loss ion. WideBand Activation, in contrast, requires low energy to generate meaningful fragmentation data.

An additional benefit of this process is that library searchable MS^2 spectra are easily available, even if hydroxylation were to take place. This has advantages in combinatorial chemistry or other applications where a searchable library of spectra can be a valuable knowledge base of data.

WideBand Activation is available on all LTQ and LCQ series instruments running under Xcalibur™ control.

(1) Data Dependent, see Thermo Fisher Scientific PSB120