

PSB 105 Dynamic Exclusion™ Technology

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In conventional LC-MS/MS experiments a sample is initially analyzed by mass spectrometry to identify the molecular ions of the peaks of interest. The sample is then analyzed further by performing product ion MS/MS scans on the selected peaks. This is a time-consuming process because the sample needs to be run at least twice and the MS/MS data is only recorded for a limited number of components.

Intelligent Data Dependent™ experiments were pioneered on Thermo Scientific mass spectrometers to overcome these limitations. In these experiments the mass spectrometer performs the MS and MSⁿ scans without any user intervention. The ion trap mass spectrometer is particularly well suited to this sort of experiment, not only due to its inherent

sensitivity in full scan mode but also because of the ease of switching between MS and MSⁿ analyses. Since the ion trap uses the same He gas at the same pressure to both collect ion and perform fragmentation, the experimental process is greatly simplified.

In a simple Data Dependent experiment shown in Figure 1, a threshold level is set below which only MS data is acquired. As a peak elutes and its intensity crosses the threshold, the on-board processor in the ion trap mass spectrometer determines the most intense ion and

immediately initiates an MS/MS scan. In this way, both MS and MS/MS spectra are acquired on each component as it elutes. The *Normalized Collision Energy*™* function ensures that the optimum collision energy is applied according to the mass of the ion.

**Normalized Collision Energy* is only available on the Thermo Scientific LTQ and LCQ series of instruments. Please see PSB #104 for a detailed explanation of Normalized Collision Energy Technology.

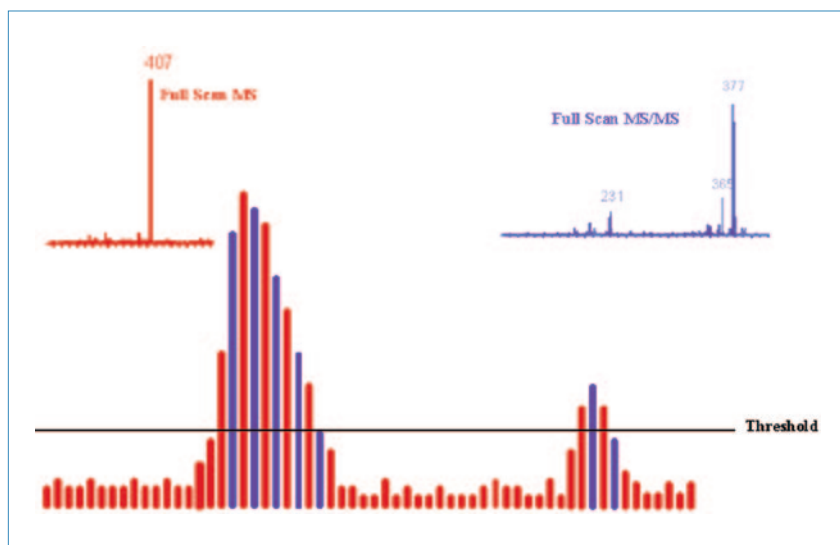


Figure 1: Simple Data Dependent Experiment

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This simple Data Dependent experiment works well with chromatographically resolved or partially resolved components. However, in a very complex mixture there may be components that completely overlap. Under these conditions only the most intense component will be selected for MS/MS because at no stage do the others become the base peak.

It is possible with ion traps to enter a list of masses that will be ignored for MSⁿ analysis through the duration of the experiment. This is especially useful when there are intense background ions. In addition, the instruments also employ the Dynamic Exclusion principle which will temporarily put a mass into an exclusion list after its MSⁿ spectrum is acquired. Due to the quality of the data in full-scan MSⁿ on any Thermo Scientific ion trap, it is even possible to collect good reproducible data from one MSⁿ scan. This lets the ion trap collect MSⁿ spectra on other less intense components which would otherwise not be examined. After a selected period of time the excluded ion will be removed from the list so that any isomers can be analyzed.

In the example shown in Figure 2, two compounds with molecular ions at m/z 407 and 452 co-elute. A simple Data Dependent experiment would only acquire MS/MS spectra on the major component. Using Dynamic Exclusion in this case after MS/MS scans of m/z 407 have been acquired, m/z 407 is put into the exclusion list. Then MS/MS spectra of the minor component at m/z 452 are collected. Thus Dynamic Exclusion allows more data to be obtained on more components in complex mixtures.

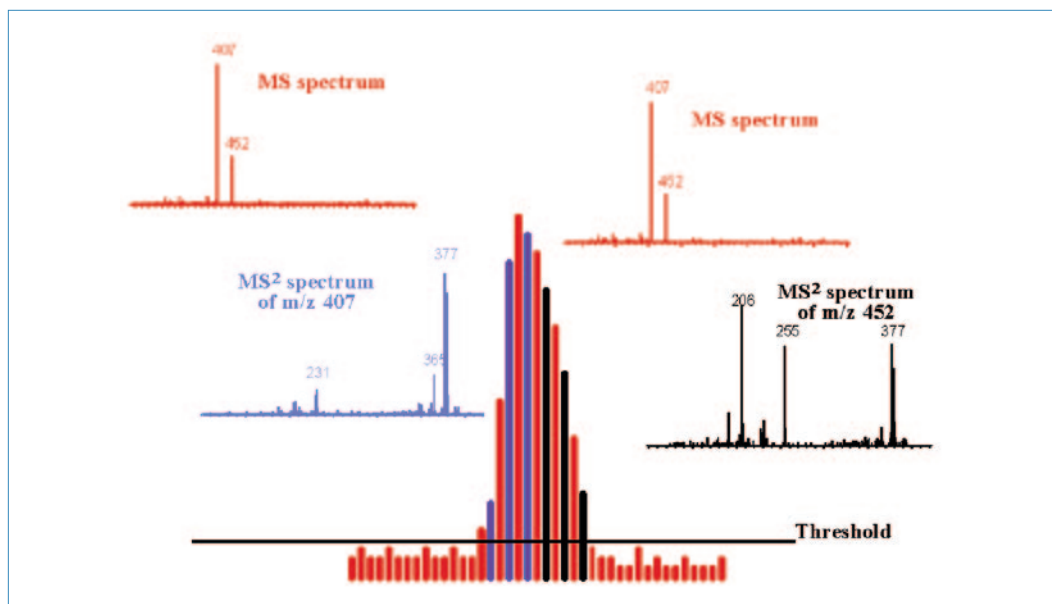


Figure 2: Dynamic Exclusion enables MS/MS spectra of the minor component at m/z 452 by placing m/z 407 on the exclusion list.