

ESI-MS/MS isolation and fragmentation of 4,4'-Difluorobenzophenone with a small-footprint ion trap mass spectrometer.

Overview:

 Designed for versatility, the MT Explorer 30 (MTE30) offers advanced mass spectrometry in a space-efficient form, making high-performance analysis accessible in and beyond traditional lab settings. Its tandem MS functionality enables rapid and confirmatory detection for applications spanning forensic science, pharmaceuticals, and materials research.

This study demonstrates the successful detection of 4,4'-difluorobenzophenone at 100 μg/mL using a portable ion trap mass spectrometer. ESI-MS/MS was employed for confirmatory analysis

Introduction:

o4,4'-difluorobenzophenone is a fine, lowvolatility chemical primarily used as a precursor in polymer synthesis, notably for Polyether Ether Ketone (PEEK). This highperformance polymer is critical in applications ranging from medical implants to aerospace components. Additionally, 4,4'-difluorobenzophenone plays a role in pharmaceutical synthesis.

•As an intermediate in essential products, monitoring 4,4'-difluorobenzophenone during production provides valuable quality control insights. Analysis with a compact ion trap mass spectrometer offers an efficient solution for optimizing synthesis processes across various industries.



MT Explorer 30 Mass Spectrometer

Methods:

4,4'-difluorobenzophenone reference standard was diluted in ethanol with 0.1% Formic Acid 10x for a concentration of 100ug/mL. ESI-MS/MS analysis performed on MT Explorer 30 in positive ion mode:

Table 1: MTE 30 Parameters			
	General Parameters		
	ESI Flow Rate:	1.5 ul/min	
	Spray voltage:	2.1kV	
	Mass range:	150-300	
	Injection Time:	10-20	
	Acquisition time:	1 min	
	MS/MS isolation	l	
	Target mass:	219	
	Isolation Width:	2	
	Amp. %	0	
	MS/MS fragmentation		
	Target mass:	219	
	Isolation Width:	2	
	Amp. %	11	



Results and Discussion:



Figure 1 ESI MS/MS isolation of 4,4'-difluorobenzophenone

ESI MS/MS fragmentation of 4,4'difluorobenzophenone yielded the [M+H]+ peak at m/z 219 and the major fragment at m/z 123 with satisfactory signal. Figure 2 ESI MS/MS fragmentation of 4,4'-difluorobenzophenone with characteristic product ion (structure speculative)

[M+H]⁺

230

The successful characterization of 4,4'difluorobenzophenone with minimal sample preparation and short duration spectra accumulation indicates the potential for detection of the chemical at significantly lower concentrations as part of quality control practices or reaction monitoring.