

SpiralTOF-TOF

Synthetic Polymer Structure Analysis

Poly Propylene Glycol (PPG)

Introduction:

The JMS-S3000 “SpiralTOF™” is a MALDI-TOFMS that incorporates an innovative SpiralTOF ion optics system (Fig. 1). The JMS-S3000 is available with a TOF-TOF option that can acquire high-energy collision-induced dissociation (CID) product ion spectra for monoisotopically selected precursor ions. This monoisotopic precursor selection is made possible by the fact that the distance to the ion gate is 15 m, which is more than one order of magnitude longer than that of conventional MALDI TOF-TOF instruments. Additionally, the second TOF MS incorporates a re-acceleration mechanism and an offset parabolic reflectron, another innovative ion optical design developed by JEOL. This unique design enables seamless observation of product ions ranging from very low m/z up to that of the precursor ion.

In this work, we analyzed Polypropylene Glycol (PPG) by using the JMS-S3000 SpiralTOF with the TOF-TOF option. The resulting high-energy CID data was then processed using the Polymerix™ (Sierra Analytics, Inc., <http://massspec.com/>) analysis software.

Samples:

Polymer: PPG
 Matrix agent: α -Cyano-4-hydroxycinnamic acid (CHCA)
 Cationization agent: NaI



Figure 1. JMS-S3000 “SpiralTOF” with TOF-TOF attachment.

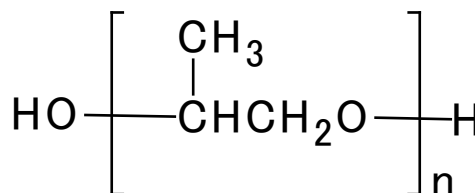


Figure 2. Structural formula of PPG.

Results and Discussion:

The MALDI mass spectrum of PPG and the m/z 1027.7 ($n=17$, $[M+\text{Na}]^+$) product ion spectrum are shown in Fig. 3. The MS-MS spectrum shows the full range of ions from m/z 23.0 for $[\text{Na}^+]$ to m/z 1027.7 for the precursor ion. Also worth noting, these product ions are all monoisotopic because the precursor ion was monoisotopically selected, which greatly simplified the resulting MS-MS spectrum.

The enlarged region (m/z 580-630) in Fig. 3 shows that there are five different product ions present that could result from the monomer repeat unit (58u, $\text{C}_3\text{H}_6\text{O}$). Therefore, this high-energy CID data for PPG suggests that there are five possible fragmentation pathways.

