LC/MS Application Notes:

EI/APCI Identification and Quantitation of Polymer Additives

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Key Words:
Polypropylene
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The analysis of polymer additives has always been important to some industries (polymer, food packaging, medical device, chemical, inks/coatings). However, the identification and quantitation of polymer additives has been rather elusive. Reports of analyzing polymer additives by single quadruple LC/MS are scarce. This work demonstrated a how quantitative polymer additive analysis can be accomplished by the two complementing LC/MS techniques: EI and APCI.

Instrumental Conditions

HPLC

- Waters Alliance Solvent Delivery System
- Symmetry C8 (3.9 x 150 mm) with Acetonitrile/Water gradient
- 0.4 mL/min. flow rate with 10 uL injection

EI

- Waters Integrity ThermaBeam™ System
  - Library search provides lead suspects

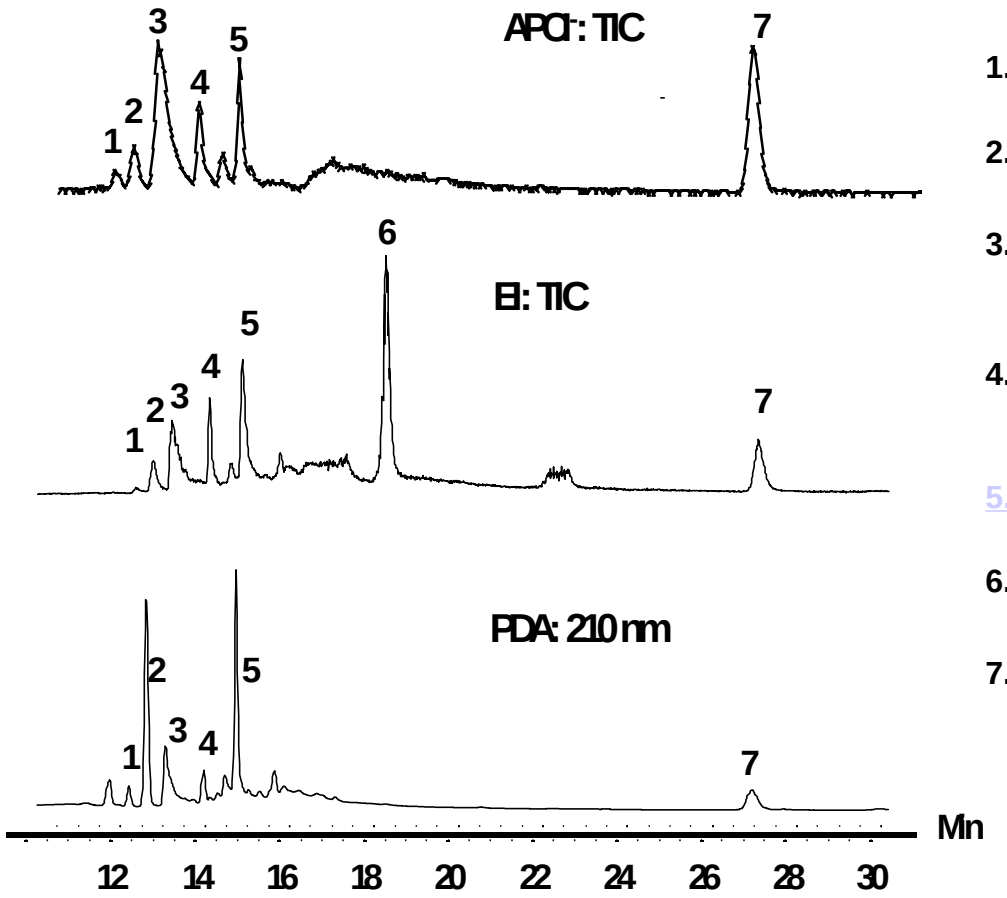
APCI

Micromass PlatformLC System

Positive APCI

- Full scan provides MW information
- Selected Ion Recording (SIR) provides quantitation

Figure 1: Positive Sample Identification

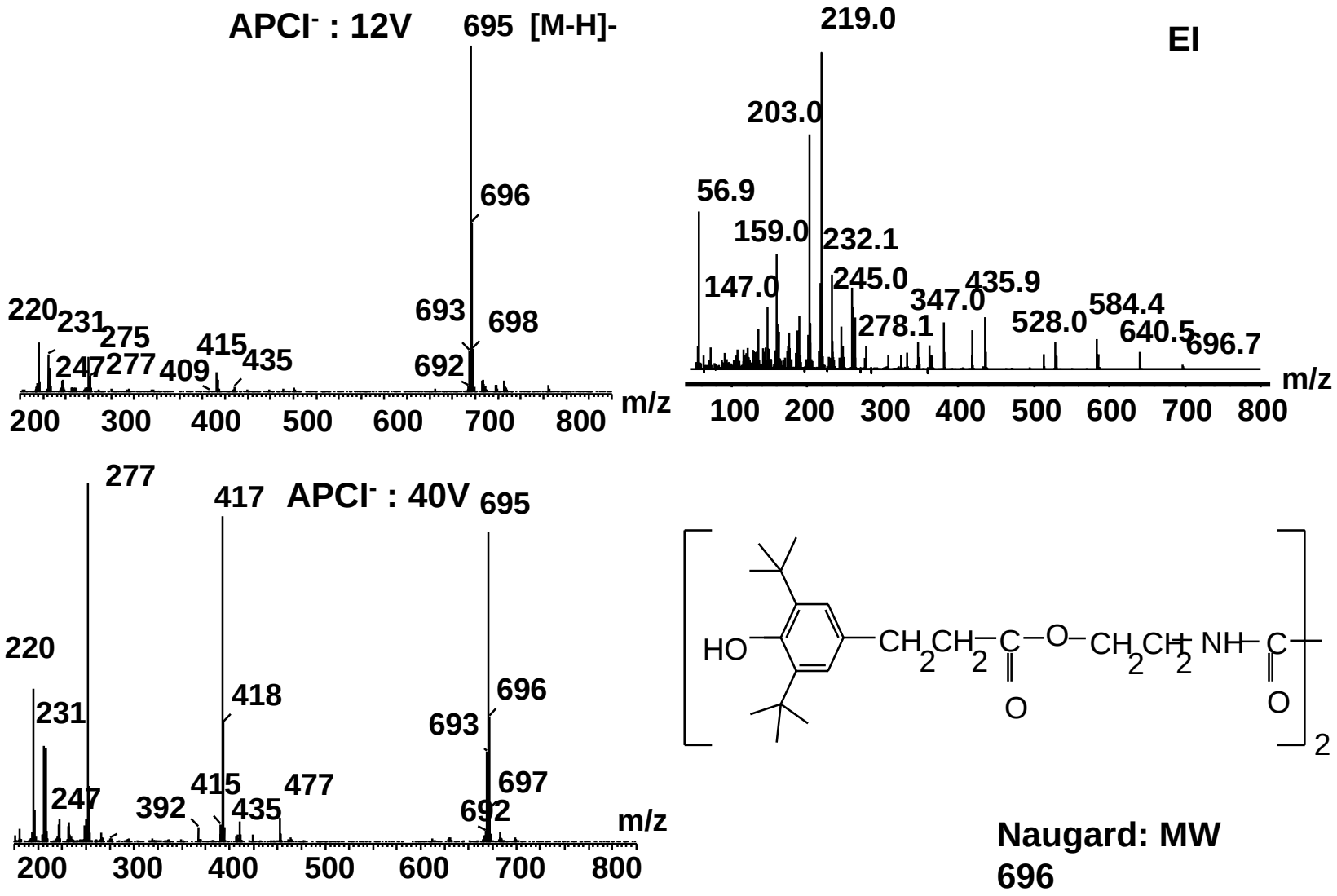


1. Naugard Degradant: MW 436
2. NC-4: MW 414
3. 3-(3,5-di-tert.-butyl-4-hydroxyphenyl) propanoic acid: MW 278
4. 7,9-Di-tert-butyl-1-oxaspiro[4,5]deca-6,9-diene-2,8-dione: MW 276
5. Naugard: MW 696
6. 1-Octodecanol: MW 270
7. Irgonox 1076: MW 530

Quantitation

- The quantitation was obtained by positive APCI SIR acquisition
- There were four standards commercially available
- Four calibration curves were obtained with a representative curve shown on Figure 3

	LOD (ppb)	Linear Range (ppb)	% (w/w) in Polymer (ppb)
NC-4	30.4	30.4 - 7600	0.07
Naugard-XL	14.4	14.4 - 3600	0.04
Octadecanol	27.2	27.2 - 6800	0.4
Irgonox 1076	12.8	12.8 - 3200	0.06



Fogure 2: Identification of Peak #5

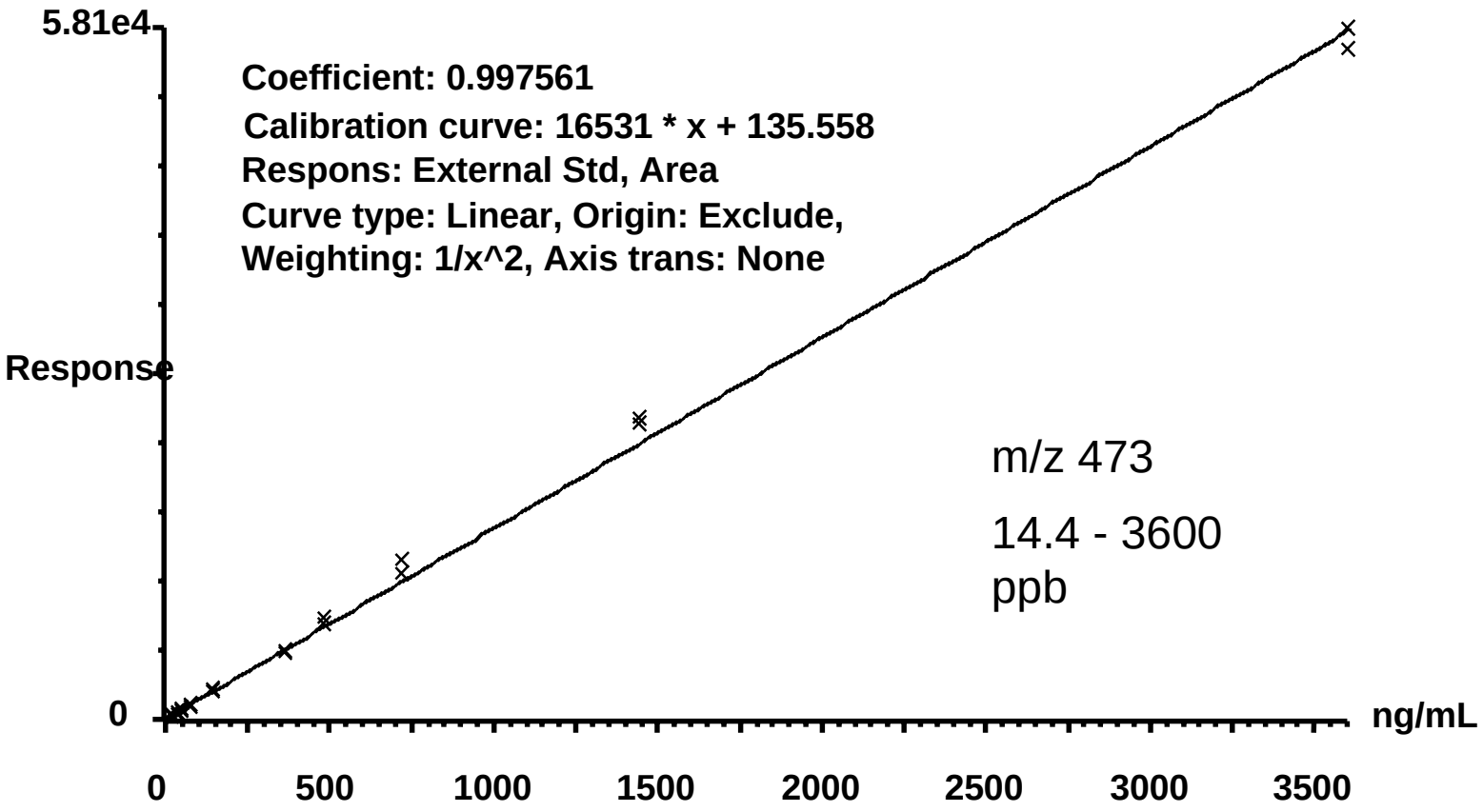


Figure 3: Calibration Curve of Naugard-XL by APCI+