

# Analysis of Bisphenol A in PET Granules Using the Agilent 8890/5977C GC/MS System



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## Abstract

This application note demonstrates the use of an Agilent 8890 GC system coupled with a 5977C GC/MS single quadrupole mass spectrometry system to detect and quantify bisphenol A (BPA) in polyethylene terephthalate (PET) granules. The sample was extracted using organic solvents through ultrasonication followed by derivatization of BPA into the trimethylsilyl derivative and analysis by GC/MS. A limit of quantification (LOQ) of 500 ng/g was achieved, and a standard calibration range was established from 10 ng/mL to 500 ng/mL. Over six consecutive injections, %RSD for six replicate standards was 1.933, and % recovery at 500 ng/g spiking level was observed at 101.4%.

## Introduction

### Instrument parameters

Polyethylene terephthalate (PET) is commonly used in the food and beverage industry, as it is easy to recycle. Contaminants in recycled PET, including acetaldehyde, benzene, limonene, and bisphenol A (BPA), can migrate from the packaging into the contents, potentially affecting the safety and quality of the products stored inside.<sup>1</sup> Monitoring these contaminants is crucial for ensuring the quality of recycled PET products, as they can affect the physical, chemical, and sensory properties of recycled PET, potentially leading to product defects or health concerns.<sup>1</sup> FSSAI officially permits the use of recycled PET (rPET) in food packaging, subject to strict safety and quality standards. This regulatory change was formalized through amendments notified in March 2025, effective immediately.<sup>2</sup> All recycled plastics used in food contact applications must comply with stringent overall and specific migration limits to ensure no harmful chemical transfer into food. The recycling processes require validated decontamination steps to reduce contaminants to safe levels. Manufacturers must certify their packaging materials under FSSAI guidelines.

GC/MS plays a critical role in assessing the safety and suitability of recycled plastics for food-contact applications. The method adopted in this work demonstrates the use of an Agilent 8890 GC system coupled with an Agilent 5977C GC/MS system for quantification of BPA in PET granules.

**Table 1.** GC/MS parameters.

Parameter	Value
<b>GC Parameters</b>	
Inlet Temperature	250 °C
Analytical Column	HP-5ms (30 m × 250 µm, 0.25 µm) (p/n 19091S-433UI)
Injection Volume	1 µL
Column Flow	Helium, 1.2 mL/min constant flow
Injection Mode	Split (10:1)
Oven Program	Starts at 90 °C (hold for 2 min), ramped at 15 °C/min to 300 °C (hold 12 min)
Ms Transfer Line Temperature	300 °C
<b>MS Parameters</b>	
Ion Source	Inertplus/extractor ion source
Ion Source Temperature	250 °C
Quadrupole Temperature	150 °C
Acquisition Mode	SIM/Scan
Sim Ions	357, 372, 358, 73 m/z
Scan Range	45–450 m/z

## Experimental

### Standard preparation

Fifty milligrams of BPA reference standard was weighed and dissolved to 10 mL final volume in methanol (solution A). 100 µL of solution A was diluted to 10 mL with methanol (solution B). 0.5 mL of solution B was diluted to 5 mL with acetone (solution C). From solution C, 0.5 mL was diluted to 5 mL with *n*-hexane (solution D). Acetone was used as a medium for solvent change from methanol to *n*-hexane. The concentration of solution D was 500 ng/mL, which was set as the highest calibration point. Solution D was diluted with *n*-hexane or blank matrix extract to obtain 100, 50, 25, and 10 ng/mL solutions as calibration standards. Approximately 1 mL of each calibration standard solution was transferred to GC vials followed by addition of 100 µL of BSTFA reagent to each vial. Vials were capped tightly and kept in an oven at 70 °C for 1 hour.

### Sample preparation

Approximately 200 mg of finely ground PET sample was weighed into a 20 mL glass vial. To this, 5 mL of THF was added and the vial was tightly capped and vortexed for 2 minutes, followed by sonication at 60 °C for 2 hours. Next, 5 mL of *n*-hexane was added, followed by vortex mixing for 2 minutes. The combined extract was filtered through a 0.2 µm syringe filter. From the filtered solution, 1 mL was accurately transferred to GC vials, followed by addition of 100 µL of BSTFA reagent. The vials were capped tightly and kept in an oven at 70 °C for 1 hour.

## Results and discussion

Figure 1 shows the scan and extracted ion chromatogram of BPA standard after derivatization at 500 ng/mL. Figure 2 shows NIST library hit for spectra of the compound at RT 13.493 minutes, confirming it as BPA. Figure 3 shows qualifier peaks for 50 ng/mL (derivatized) BPA standard along with the calibration curve covering the 10 ng/mL to 500 ng/mL concentration range.

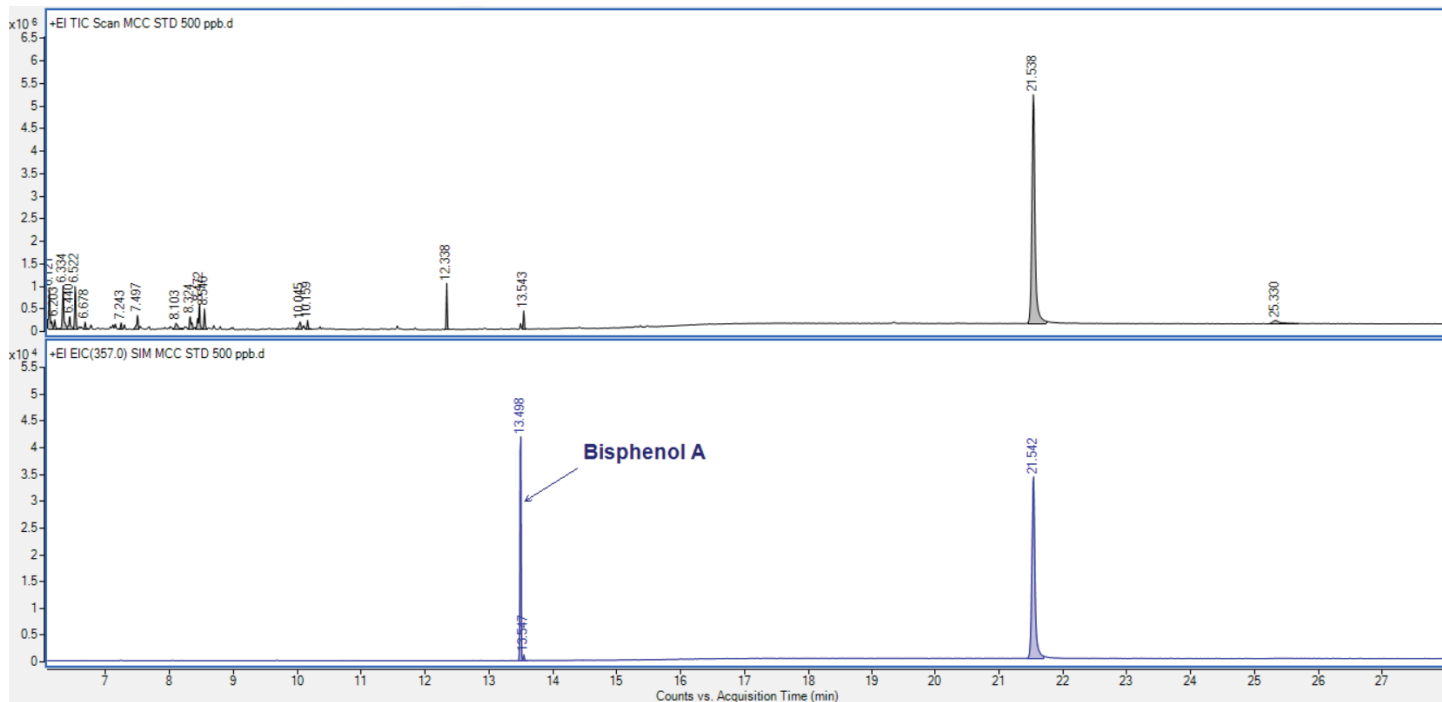


Figure 1. TIC scan and EIC (357) of BPA matrix standard at 500 ng/mL concentration.

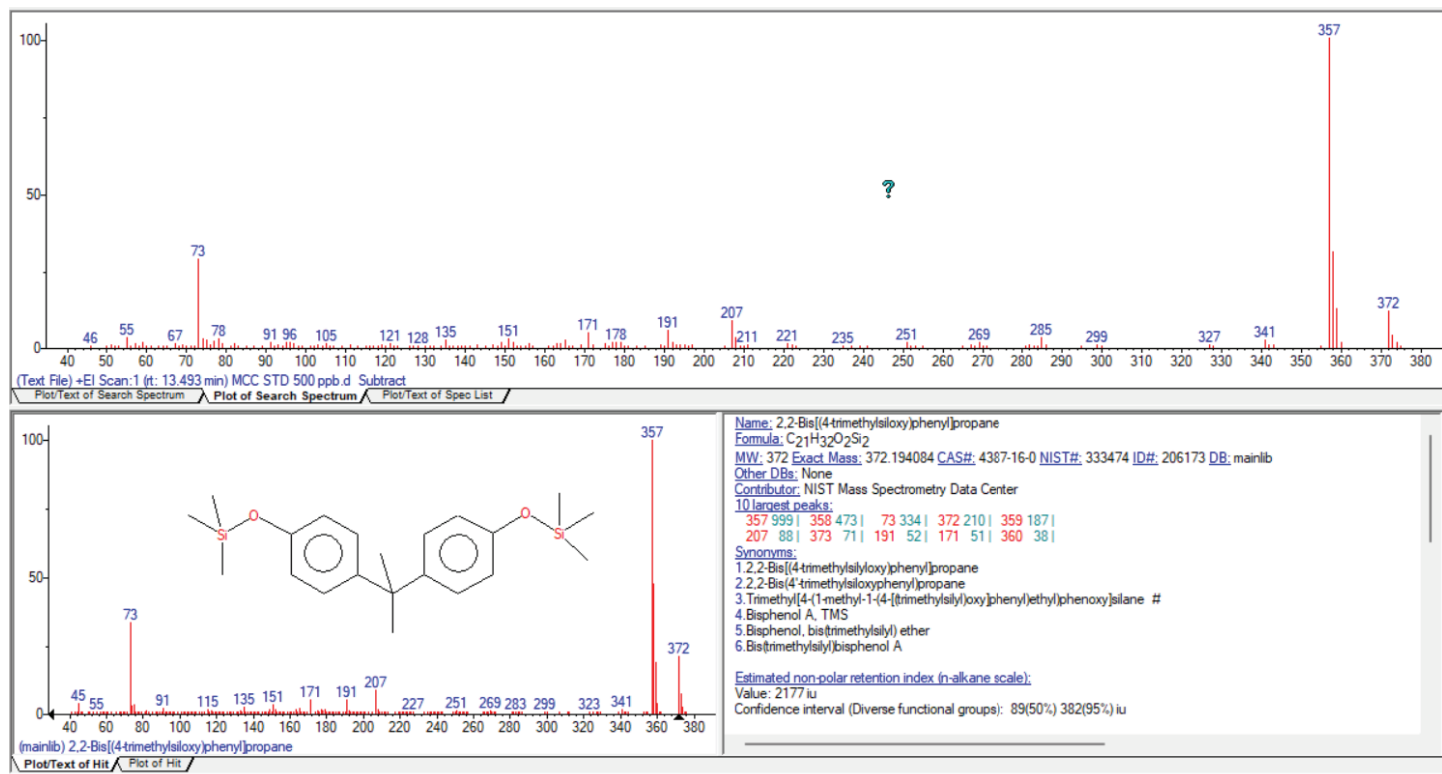
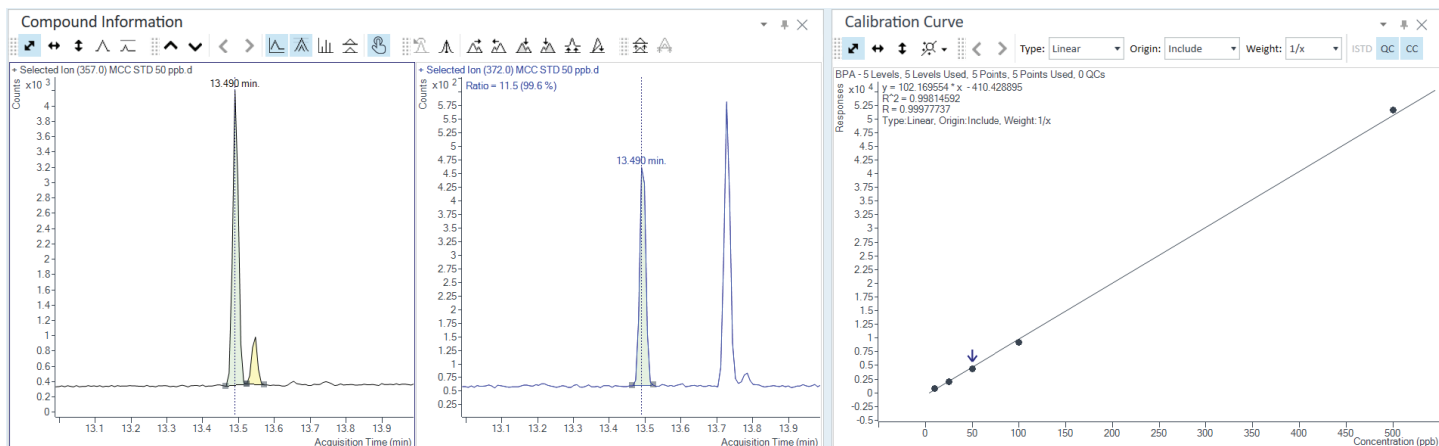


Figure 2. NIST Library hit for compound at RT 13.493 minutes (match score: 88.4).

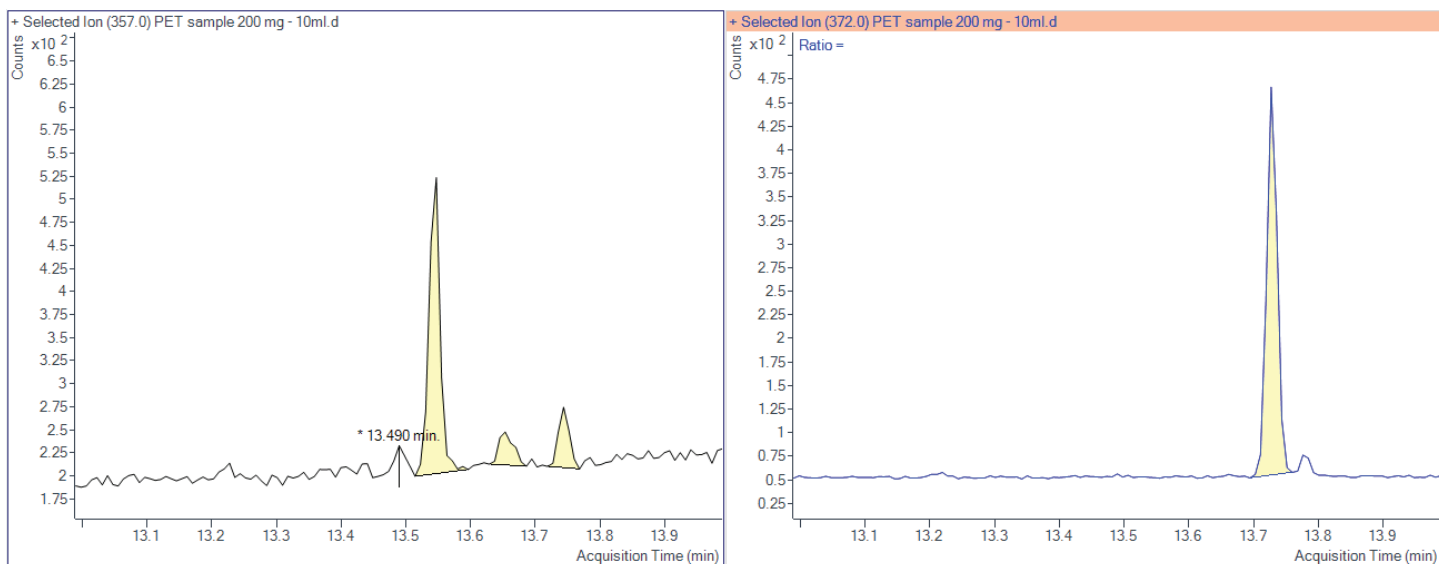


**Figure 3.** Quantifier and qualifier peaks for 50 ng/mL (derivatized) BPA and calibration curve ranging from 10–500 ng/mL.

Table 2 shows the %RSD for concentration for six replicate standards at 100 ng/mL. Figures 4 and 5 show the peaks obtained in the PET sample and a sample spiked at 500 ng/g. Table 3 shows the quantification results for the PET sample and the spiked sample. Recovery for 500 ng/g spiked sample was 101.4%.

**Table 2.** %RSD for six replicates of 100 ng/mL BPA standard.

BPA Repeatability Injections		
Sample Name	RT	Area
100 ppb rep-1	13.490	7692
100 ppb rep-2	13.490	7889
100 ppb rep-3	13.489	8037
100 ppb rep-4	13.490	8044
100 ppb rep-5	13.490	8062
100 ppb rep-6	13.489	8098
%RSD		1.933



**Figure 4.** BPA peak not observed in blank PET test sample.

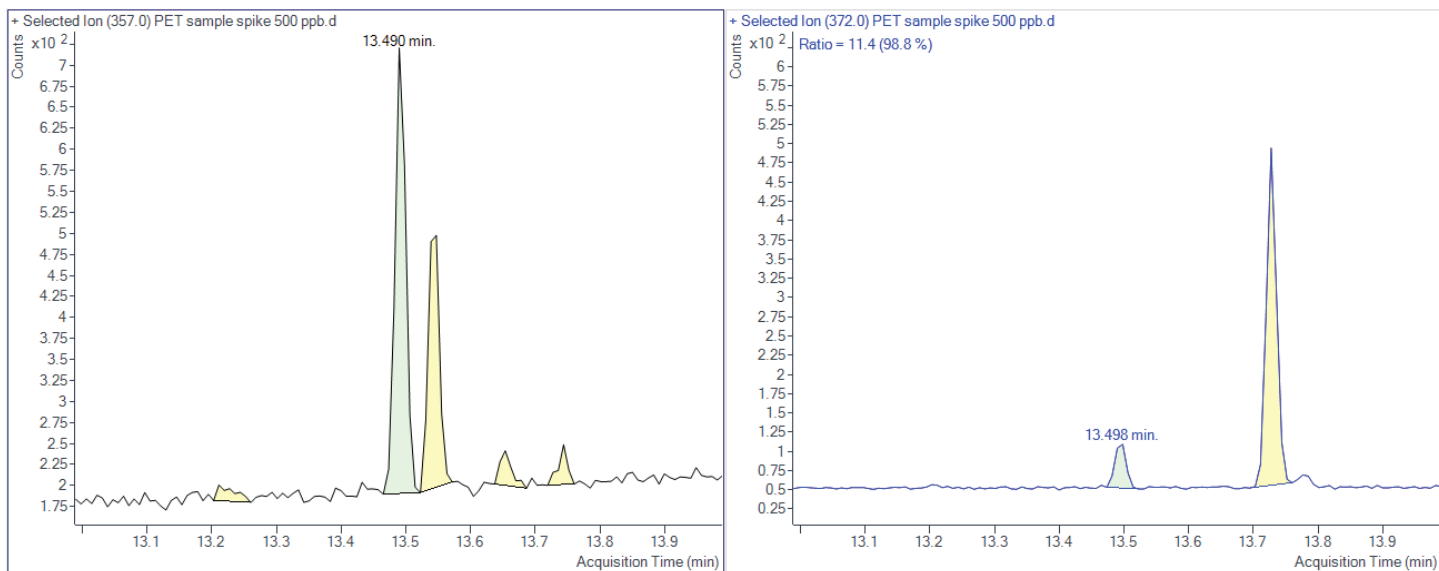


Figure 5. BPA peaks obtained in PET sample spiked at 500 ng/g for recovery study.

Table 3. Quantification results for PET sample and sample spiked at 500 ng/g (recovery: 101.4%).

Data File	Type	Level	Dilution	BPA Results				Qualifier Ratio
				Exp. Conc. (ng/mL)	RT	Resp.	Final Conc. (ng/mL)	
Blank	Sample		1					
MCC STD 10 ppb	Cal	1	1	10	13.498	764	11.49	11.3
MCC STD 25 ppb	Cal	2	1	25	13.490	2048	24.06	11.9
MCC STD 50 ppb	Cal	3	1	50	13.490	4329	46.39	11.5
MCC STD 100 ppb	Cal	4	1	100	13.490	9221	94.27	11.6
MCC STD 500 ppb	Cal	5	1	500	13.498	51572	508.79	11.4
PET Sample	Sample		50		13.547	0	0.00	
PET Sample Spike 500 ng/g	Sample		50		13.490	625	506.72	11.4

## Conclusion

This application note presents key strategies for the analysis of BPA in PET granules using GC/MS. The calibration used here ranged from 10 to 500 ng/mL, and the LOQ of the method was demonstrated at 500 ng/g for a PET sample. Repeatable results were found for six successive replicates of matrix-based standards at 100 ng/mL. Satisfactory recoveries were obtained for the tested matrix at 500 ng/g spiked concentration levels. Thus, this study demonstrates the applicability of this method for routine analysis of PET samples for identification and quantification of BPA.

## References

1. Zhang, Y.; Tan, L. P. Analysis of Aldehydes, Benzene, and Limonene in Recycled Polyethylene Terephthalate Using Headspace GC/MS. *Agilent Technologies application note*, publication number **5994-8063EN, 2024**.
2. Food Safety and Standards Authority of India. (2025, May 23). Guidelines for Acceptance of Recycled Polyethylene Terephthalate (PET) as Food Contact Material (FCM-rPET). Ministry of Health and Family Welfare. [https://fssai.gov.in/upload/notifications/2025/05/6834550d9ff1eGuidelines%20for%20acceptance%20of%20recycled%20Polyethylene%20terephthalate\\_PET\\_as%20Food%20Contact%20Material.pdf](https://fssai.gov.in/upload/notifications/2025/05/6834550d9ff1eGuidelines%20for%20acceptance%20of%20recycled%20Polyethylene%20terephthalate_PET_as%20Food%20Contact%20Material.pdf)