



Journal Homepage: [-www.journalijar.com](http://www.journalijar.com)

INTERNATIONAL JOURNAL OF ADVANCED RESEARCH (IJAR)

Article DOI:10.21474/IJAR01/24339

DOI URL: <http://dx.doi.org/10.21474/IJAR01/24339>



RESEARCH ARTICLE

INFLUENCE OF POLYSTYRENE LATEX CARRYOVER ON PYROLYSIS MASS SPECTRAL RESPONSE

Haner Choi

1. C5ISR Center, Defense Agency for Technology and Quality 37 Hoegi-ro, Dongdaemun-gu, Seoul 02455, Republic of Korea.

Manuscript Info

Manuscript History

Received: 08 August 2026

Final Accepted: 10 September 2026

Published: October 2026

Key words:-

polystyrene latex; carryover; pyrolysis mass spectrometry; sequential testing; spectral comparison; analytical troubleshooting

Abstract

Carryover from preceding qualification procedures can interfere with subsequent analysis in sequential mass-spectrometric testing. During quality-assurance testing of a military biological detector, one of six systems showed an unexpected biological-simulant classification accompanied by a mass-spectral pattern different from the expected response after prior collection efficiency qualification using polystyrene latex (PSL) particles. The investigation examined whether residual PSL contributed to the interference. The incident spectrum showed prominent responses at nominal m/z 51, 78, and 104, similar to the PSL-only response, and particulate material was observed within the incident filter structure. Four controlled verification tests examined complementary aspects of the proposed carryover pathway. Direct co-loading of PSL and biological simulant produced incident-like spectral interference and altered classification. When cleaning after PSL qualification was deliberately omitted, visible residue and subsequent PSL-associated spectral responses were observed, and biological-simulant testing under these conditions again produced altered spectral relationships and classification. A separate repeat verification produced a similar outcome. Following the incident, the cleaning procedure was strengthened by additional mechanical removal, ultrasonic cleaning, and residue inspection, after which the expected detection result was documented. These findings support the interpretation that residual PSL contributed to the observed interference and indicate that carryover control should address the entire collection pathway before subsequent analysis.

"© 2026 by the Author(s). Published by IJAR under CC BY 4.0. Unrestricted use allowed with credit to the author."

Introduction:-

Rapid and accurate detection and classification of biological agents are important for protecting personnel and supporting military operations. Pyrolysis mass spectrometry is one analytical approach to characterizing collected samples: the sample is thermally decomposed, and the resulting mass spectrum is used to assess its characteristics [1]. Pyrolysis mass spectra can depend on sample composition, sample amount, and pyrolysis conditions [2–4].

Corresponding Author:-Haner Choi

Address:-C5ISR Center, Defense Agency for Technology and Quality 37 Hoegi-ro, Dongdaemun-gu, Seoul 02455, Republic of Korea.

Unintended contamination can complicate mass-spectral interpretation, particularly in sequential testing where material retained from an earlier procedure may contribute to a subsequent measurement. Such carryover is therefore an important analytical concern [5,6].

During quality-assurance testing of the military biological detector examined here, an unexpected classification of a biological simulant was accompanied by an overall mass-spectral pattern different from the earlier expected response. The incident occurred after collection-efficiency qualification using polystyrene latex (PSL) particles. During the investigation, carryover of PSL from the preceding qualification test was considered a plausible contributor to the interference. This sequence of events motivated the carryover hypothesis examined in this study. The objective was to investigate whether PSL used in preceding collection-efficiency qualification could affect subsequent pyrolysis-MS analysis and automated classification. The investigation combined incident chronology, spectral comparison, optical observation of residual material, controlled verification tests, and evaluation following strengthening of the cleaning procedure.

Materials and Methods:-

Pyrolysis mass spectrometry system and analytical principle:-

Figure 1 summarizes the analytical workflow. Material entering the inlet is concentrated and collected on a biological sample collection filter. IR-laser irradiation pyrolyzes the collected material. As the transfer capillary is heated, the volatilized products reach the mass spectrometer at different times. Signal amplification and mass detection yield a mass spectrum, and the instrument compares peak positions and intensity patterns with its internal reference library to classify the sample.

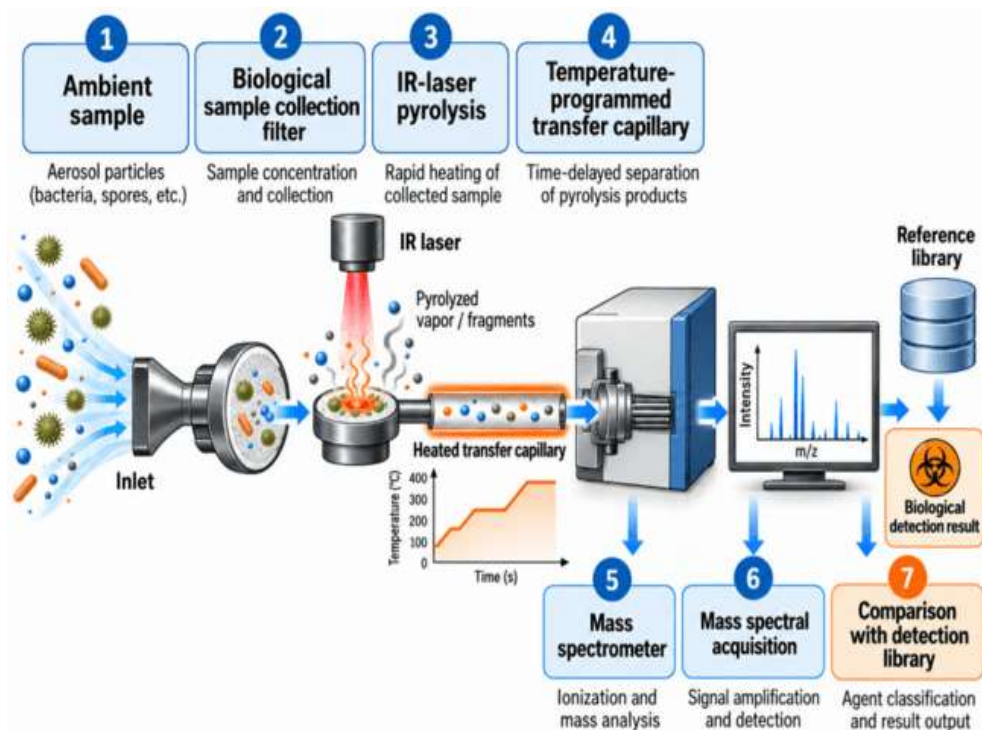


Figure 1. Schematic of biological sample collection, IR-laser pyrolysis, and mass spectrometric analysis. The illustrated temperature profile is schematic and does not report measured operating temperatures.

Routine quality-assurance test sequence and test materials:-

The quality-assurance program includes collection-efficiency testing and biological detection testing among several independent evaluations. In the routine sequence, collection-efficiency qualification generally precedes biological detection testing, so the same collection pathway can be used sequentially. During collection-efficiency qualification, aerosolized PSL particles are introduced into the sampling system and particle concentrations are measured using an aerosol particle counter. PSL aerosols have been used as test aerosols in published evaluations of filter and aerosol-sampler collection efficiency [7,8]. When diluted PSL was analyzed alone in the present detector,

prominent responses were observed at nominal m/z 51, 78, and 104 (Figure 2). Because PSL particles are composed of polystyrene, their thermal degradation can produce styrene and styrene-related products [9]. A PSL Py-GC/MS method also used styrene-related ions in this nominal-mass region [10]. The NIST electron ionization (EI) reference spectrum of styrene provides additional spectral context [11].

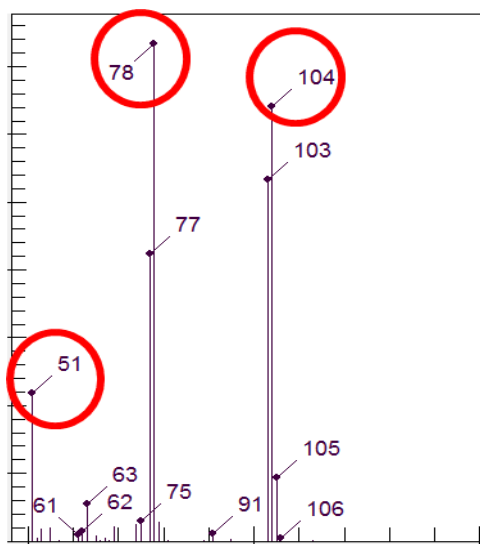


Figure 2. Mass spectrum of diluted PSL analyzed alone in the present detector. Red circles mark PSL-associated responses at nominal m/z 51, 78, and 104.

Sucrose was used as a nonpathogenic biological simulant for instrument testing and was not selected ad hoc for this study. According to the equipment specification, nonpathogenic or low-pathogenic simulants are used for instrument testing in place of actual biological agents because of the associated biosafety risks, and albumin or sucrose is specified for this purpose. Accordingly, sucrose was used in the present experiments as the specified test simulant. Sucrose is a disaccharide composed of glucose and fructose units, and its thermal degradation produces furan-containing compounds, including furfural and related derivatives [12, 13, 14, 15]. 2,5-Furandicarboxaldehyde is also among the pyrolysis products of sucrose [12,15]. The electron ionization reference spectrum of furfural contains prominent peaks at m/z 95 and m/z 96, whereas that of 2,5-furandicarboxaldehyde contains prominent peaks at m/z 95, m/z 123, and m/z 124 [11]. Among these signals, m/z 95 and m/z 123 are used by the detector evaluated in this study, and the peak-height ratio of m/z 123 to m/z 95 is one of the variables incorporated into its classification algorithm.

For detection of this simulant, the detector uses the responses at m/z 95 and m/z 123 as key variables in its classification algorithm, but it does not classify the sample based solely on the presence of these two signals. The algorithm considers their relative prominence and peak-height relationships within the overall mass-spectral pattern. PSL-associated contributions can alter the overall pattern and make the expected m/z 95 and m/z 123 responses less prominent relative to other peaks.

Incident and carryover hypothesis:-

In this test series, six systems were tested, and one showed an unexpected classification during biological-simulant detection. The incident spectrum differed from the earlier expected-response spectrum (Figure 3). To examine potential equipment-related causes, the IR laser, heater, sensors, biological multi-position valve (Bio MPV), related input/output functions, and calibration status were checked, and no abnormalities were found. The investigation focused on the similarity between the altered incident spectrum, including nominal m/z 51, 78, and 104, and the PSL-only spectrum. The change in the overall spectral pattern, comparison with the PSL-only response, and the preceding qualification test using PSL collectively led to the carryover hypothesis. Optical examination and controlled verification tests were then conducted to investigate this possibility.

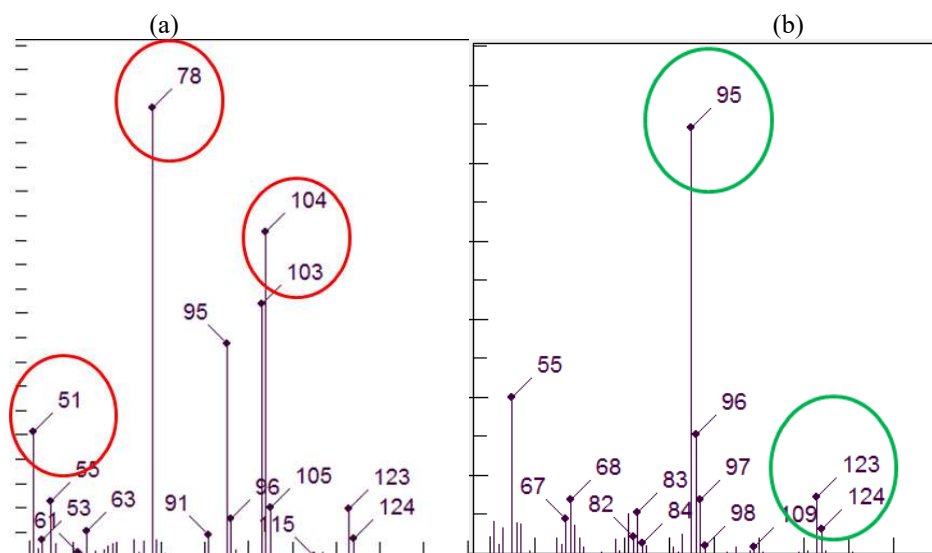


Figure 3. Comparison of (a) the incident mass spectrum and (b) the earlier expected biological-simulant response. Red circles in (a) mark PSL-associated responses at nominal m/z 51, 78, and 104; green circles in (b) mark expected biological-simulant responses at m/z 95 and 123.

Optical examination of residual material:-

The incident filter was examined by optical microscopy and compared with a clean filter showing no visible foreign material. In the incident filter, foreign particulate material was observed within the filter structure, whereas no comparable material was visible in the clean filter (Figure 4).

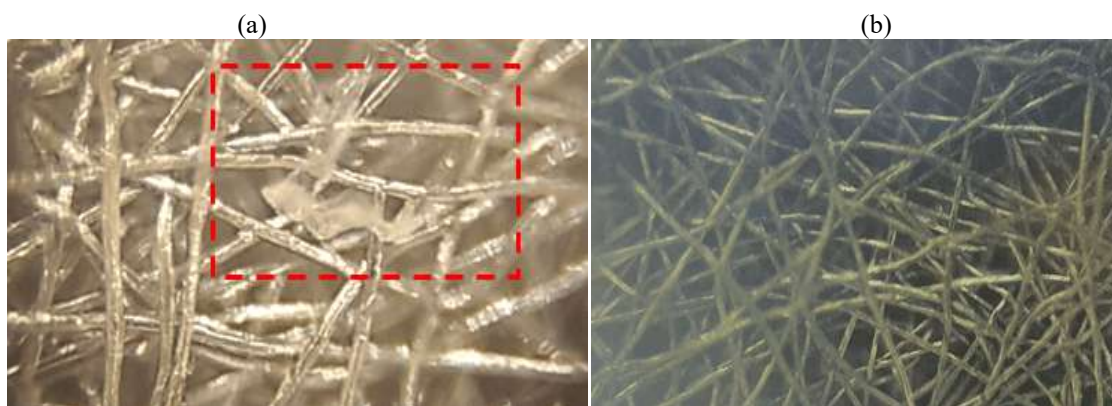


Figure 4. Optical comparison of (a) the incident filter with visible particulate residue and (b) a filter without visible foreign material.

Controlled verification tests:-

Four controlled verification tests were conducted to examine different aspects of the PSL carryover hypothesis. Ambient conditions were maintained at 23 °C and 50% relative humidity. Before each test, operation of the IR laser, heater, sensors, Bio MPV, and related input/output functions was checked to reduce the influence of equipment-related factors. Under the routine procedure, a simple cleaning and drying step is performed after PSL qualification. Because PSL residue was not readily reproduced when this routine procedure was followed, cleaning after the PSL qualification step was deliberately omitted in Tests 2–4 as an intentional diagnostic stress condition. These tests were designed to determine whether the proposed carryover pathway could occur under conditions more favorable for carryover rather than to reproduce routine operation. Mass spectra were obtained from detector data using the dedicated proprietary software.

Test 1. Direct co-loading challenge:-

PSL stock solution was diluted 7000-fold and mixed 1:1 with the biological simulant. The mixture was applied directly to the biological sample collection filter and analyzed to determine whether simultaneous PSL and simulant loading could produce altered classification and an interference pattern similar to the incident response.

Test 2. PSL carryover generation and verification challenge:-

After pre-test microscopy confirmed no visible foreign particles, PSL-based collection-efficiency qualification was performed and post-qualification cleaning was intentionally omitted. The filter was re-examined for visible residue and analyzed without added biological simulant. This test examined whether PSL qualification could leave particulate material in the filter or collection pathway and contribute to a subsequent spectral response.

Test 3. PSL carryover interference during biological-simulant detection:-

A filter without visible foreign particles on pre-test microscopy underwent PSL collection-efficiency qualification without subsequent cleaning. After microscopy to examine residual material, biological simulant was applied and pyrolysis-MS analysis was performed. The evaluation considered coexistence of expected responses at m/z 95 and m/z 123 with PSL-associated interference, changes in the overall spectral pattern, and automated classification.

Test 4. Repeat verification challenge:-

The procedure used in Test 3 was repeated once as a separate verification run to determine whether similar interference and altered classification could be observed again. It included pre-test and post-exposure microscopy and deliberate omission of cleaning after PSL qualification.

Results:-**Results of controlled verification tests:-****Test 1:-**

Direct co-loading of diluted PSL and biological simulant produced an overall spectral pattern qualitatively similar to the incident interference, accompanied by altered automated classification (Figure 5). The spectral comparison indicated that simultaneous presence of the two test materials could change the expected response pattern.



Figure 5. Test 1: (a) direct application of the PSL-simulant mixture to the filter and (b) the resulting mass spectrum.

Test 2:-

No visible foreign particles were observed before PSL qualification, whereas particulate residue was visible afterward under the intentionally permissive condition in which post-qualification cleaning was omitted. Subsequent analysis without added biological simulant showed a PSL-associated spectral contribution (Figure 6). These observations linked the qualification step to retained material and a later analytical response.

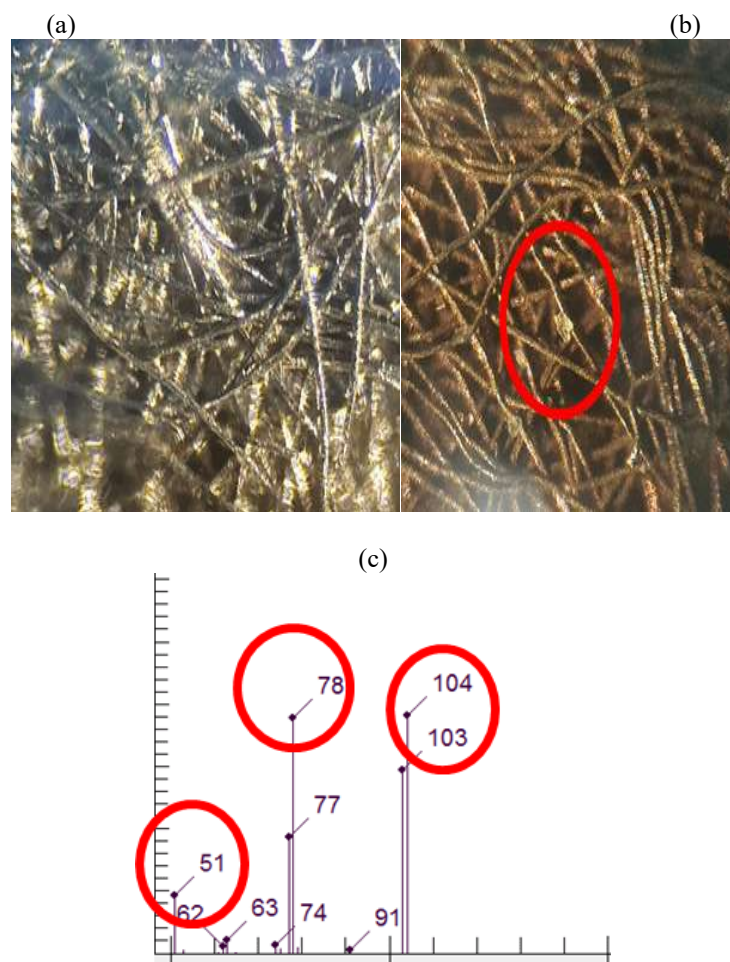


Figure 6. Test 2: (a) filter before PSL qualification, (b) visible residue after qualification without subsequent cleaning, and (c) mass spectrum without added biological simulant. The red circle in (b) marks visible residue, and the red circles in (c) mark PSL-associated responses at nominal m/z 51, 78, and 104. Microscopy: 100 $\times$.

Test 3:-

Visible particulate residue appeared after PSL qualification without subsequent cleaning. Following biological-simulant addition, expected responses at m/z 95 and m/z 123 coexisted with the PSL-associated interference pattern, and automated classification differed from the expected result (Figure 7). The overall peak-height relationships were altered.

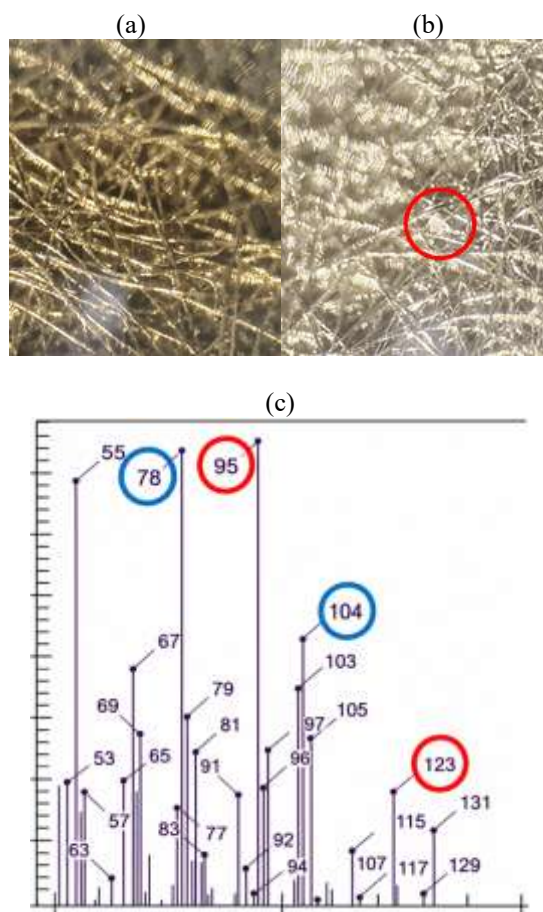


Figure 7. Test 3: (a) filter before PSL qualification, (b) residue after qualification without subsequent cleaning, and (c) spectrum after biological-simulant addition. The red circle in (b) marks visible residue. In (c), blue circles mark PSL-associated responses at nominal m/z 78 and 104, and red circles mark expected biological-simulant responses at m/z 95 and 123. Microscopy: 100 $\times$.

Test 4:-

The separate repeat verification again showed visible residue after PSL qualification with cleaning omitted, followed by a qualitatively similar interference pattern and altered classification during biological-simulant analysis (Figure 8). This provided a second observation under the Test 3 procedure.

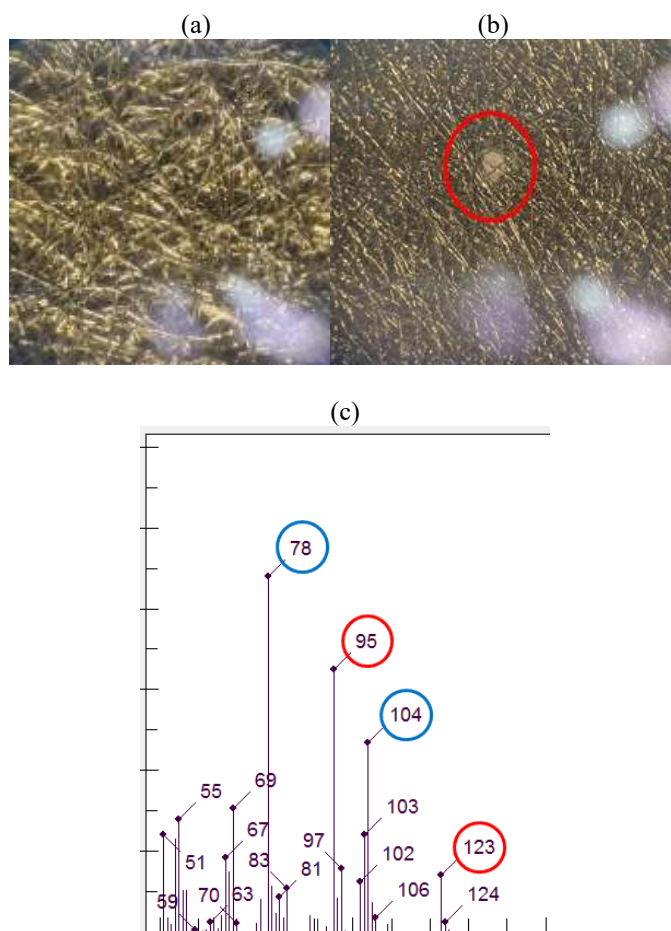


Figure 8. Test 4: (a) filter before PSL qualification, (b) residue after qualification without subsequent cleaning, and (c) spectrum after biological-simulant addition in the separate repeat verification. The red circle in (b) marks visible residue. In (c), blue circles mark PSL-associated responses at nominal m/z 78 and 104, and red circles mark expected biological-simulant responses at m/z 95 and 123. Microscopy: 100 $\times$.

Discussion:-

The four tests addressed complementary questions within the carryover hypothesis. Test 1 showed that simultaneous PSL and simulant loading could produce incident-like interference and altered classification. Test 2 connected the PSL qualification step, visible residue, and a subsequent spectral contribution without added simulant. Test 3 showed that simulant analysis under this residue condition could yield altered spectral relationships and classification, and Test 4 showed a similar outcome in one separate repeat verification. Together, these observations support a pathway by which material retained after PSL qualification may influence later analysis.

A distinction exists between the actual incident and the controlled verification tests. The existing cleaning and drying procedures had been completed before the incident, whereas cleaning after PSL qualification was deliberately omitted in Tests 2–4. Because carryover was not expected to be readily observable under routine conditions, these tests intentionally created conditions more favorable for carryover so that the proposed pathway could be examined directly. Despite this difference, the preceding history of PSL use, the altered incident spectrum, the PSL-only response pattern, visible residue, and the complementary test results consistently support the interpretation that residual PSL contributed to the interference. In the incident-spectrum comparison, prominent PSL-associated responses at nominal m/z 51, 78, and 104 altered the overall spectral pattern and reduced the relative prominence of the expected responses at m/z 95 and m/z 123. Previous carryover studies have likewise shown that material retained from preceding analytical procedures can persist within an analytical pathway and influence subsequent measurements [6,16], supporting the relevance of carryover as an explanation for the present observations.

The incident prompted strengthening of the existing cleaning procedure, including mechanical cleaning with a soft brush under flowing distilled water, two 20-min ultrasonic cleaning cycles using distilled water, microscopic inspection at 40× magnification after drying, and further cleaning if residue remained. After implementation of the revised procedure, an expected detection result was documented. This outcome supports the practical importance of removing residual material and verifying the cleanliness of the shared collection pathway before subsequent biological detection testing.

Conclusion:-

An incident occurred during biological detection testing following PSL qualification, in which the mass spectrum and automated classification result differed from the expected response. Complementary observations and controlled verification tests support the interpretation that residual PSL contributed to the interference. This study examined the proposed pathway under deliberately created conditions favorable to carryover and included one separate repeat verification. The strengthened cleaning and residue-inspection procedure had practical relevance, and the expected result was documented after its implementation. These findings suggest that carryover control should address the entire collection pathway, because residual material remaining before subsequent analysis can affect the mass spectrum and detection classification.

Acknowledgement:-

None

Conflict of Interest:-

The author(s) declare no conflict of interest.

References:-

1. Lebedev, A.T. Mass spectrometry in identification of ecotoxicants including chemical and biological warfare agents. *Toxicol. Appl. Pharmacol.* 2005, 207, 451–458. <https://doi.org/10.1016/j.taap.2005.02.040>.
2. Kim, J.H. Application of TMAH-based pyrolysis mass spectrometry to a biological detection system. *J. Korea Inst. Mil. Sci. Technol.* 2011, 14, 289–298. <https://doi.org/10.9766/KIMST.2011.14.2.289>.
3. Lu, Q.; Yang, X.-C.; Dong, C.-Q.; Zhang, Z.-F.; Zhang, X.-M.; Zhu, X.-F. Influence of pyrolysis temperature and time on the cellulose fast pyrolysis products: Analytical Py-GC/MS study. *J. Anal. Appl. Pyrolysis* 2011, 92, 430–438. <https://doi.org/10.1016/j.jaap.2011.08.006>.
4. Nasfi, M.; Carrier, M.; Salvador, S. Reconsidering the potential of micropyrolyzer to investigate biomass fast pyrolysis without heat transfer limitations. *J. Anal. Appl. Pyrolysis* 2022, 165, 105582. <https://doi.org/10.1016/j.jaap.2022.105582>.
5. Keller, B.O.; Sui, J.; Young, A.B.; Whittall, R.M. Interferences and contaminants encountered in modern mass spectrometry. *Anal. Chim. Acta* 2008, 627, 71–81. <https://doi.org/10.1016/j.aca.2008.04.043>.
6. Yamagaki, T.; Yamazaki, T. Troubleshooting carry-over in the LC-MS analysis of biomolecules: The case of neuropeptide Y. *Mass Spectrom. (Tokyo)* 2019, 8, S0083. <https://doi.org/10.5702/massspectrometry.S0083>.
7. Ikezawa, Y.; Murata, M.; Ohata, T.; Yoshida, Y.; Matsumoto, M. Collection efficiency of air sampling filter papers for polystyrene latex aerosols. *Hoken Butsuri* 1973, 8, 145–152. <https://doi.org/10.5453/jhps.8.145>.
8. Fängmark, I.; Wikström, L.-E.; Henningson, E.W. Collection efficiency of a personal sampler for microbiological aerosols. *Am. Ind. Hyg. Assoc. J.* 1991, 52, 516–520. <https://doi.org/10.1080/15298669191365144>.
9. Ohtani, H.; Yuyama, T.; Tsuge, S.; Plage, B.; Schulten, H.-R. Study on thermal degradation of polystyrenes by pyrolysis-gas chromatography and pyrolysis-field ionization mass spectrometry. *Eur. Polym. J.* 1990, 26, 893–899. [https://doi.org/10.1016/0014-3057\(90\)90164-Y](https://doi.org/10.1016/0014-3057(90)90164-Y).
10. Hasager, F.; Björgvinsdóttir, Þ.N.; Vinther, S.F.; Christofili, A.; Kjærgaard, E.R.; Petters, S.S.; Bilde, M.; Glasius, M. Development and validation of an analytical pyrolysis method for detection of airborne polystyrene nanoparticles. *J. Chromatogr. A* 2024, 1717, 464622. <https://doi.org/10.1016/j.chroma.2023.464622>.
11. NIST Mass Spectrometry Data Center; Wallace, W.E., Director. Mass spectra: Styrene (CAS 100-42-5), furfural (CAS 98-01-1), and 2,5-furandicarboxaldehyde (CAS 823-82-5). In NIST Chemistry WebBook, NIST Standard Reference Database 69; Linstrom, P.J.; Mallard, W.G., Eds.; National Institute of Standards and Technology: Gaithersburg, MD, USA. <https://doi.org/10.18434/T4D303>. Available at <https://webbook.nist.gov/chemistry/> (accessed 9 October 2026).
12. Wang, X.; Liu, D.; Du, C.; Ma, S. Characteristics and formation mechanism of key volatile compounds in sugar-smoked chicken. *J. Food Sci. Technol.* 2022, 59, 768–783. <https://doi.org/10.1007/s13197-021-05071-y>.

13. Perez Locas, C.; Yaylayan, V.A. Isotope labeling studies on the formation of 5-(hydroxymethyl)-2-furaldehyde (HMF) from sucrose by pyrolysis-GC/MS. *J. Agric. Food Chem.* 2008, 56, 6717–6723. <https://doi.org/10.1021/jf8010245>.
14. Nikolov, P.Y.; Yaylayan, V.A. Thermal decomposition of 5-(hydroxymethyl)-2-furaldehyde (HMF) and its further transformations in the presence of glycine. *J. Agric. Food Chem.* 2011, 59, 10104–10113. <https://doi.org/10.1021/jf202470u>.
15. Zhao, Z.; Sakai, S.; Wu, D.; Chen, Z.; Zhu, N.; Huang, C.; Sun, S.; Zhang, M.; Umemura, K.; Yong, Q. Further exploration of sucrose–citric acid adhesive: Investigation of optimal hot-pressing conditions for plywood and curing behavior. *Polymers* 2019, 11, 1996. <https://doi.org/10.3390/polym11121996>.
16. Reichel, J.; Graßmann, J.; Letzel, T.; Drewes, J.E. Systematic development of a simultaneous determination of plastic particle identity and adsorbed organic compounds by thermodesorption–pyrolysis GC/MS (TD-Pyr-GC/MS). *Molecules* 2020, 25, 4985. <https://doi.org/10.3390/molecules25214985>.