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KnowItAll Microplastic Classification

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Table of Contents

Introduction

Microplastics are everywhere[1-3]. Studies have found that they have profound impacts on lives across species. Environmental sample classification/identification has received a lot of attention lately. One popular method is to apply IR/Raman spectroscopy technologies[2,4,5]. These technologies have proven records of effectiveness in analyzing polymers, which are parents of microplastics. However, it is not easy to collect samples to make reliable reference spectral databases for unknown comparison. Spectrum analysis organizations are under pressure to provide a quick, easy and low-cost tool to meet this challenge.

Visual comparison of typical microplastic IR spectra[4,5] to those of parent polymers available in KnowItAll IR Spectral Library[6,7] lead us to believe that microplastic IR spectra exhibit similar characteristics. Therefore, "classification spectra" have been derived by using patented Overlap Density Heat Map (ODHM) technology. Our study suggests that these classification spectra can be used for unknown microplastic classification. Combined with the massive KnowItAll IR databases offered by Wiley, one can identify microplastics.

Research has also shown that Raman spectrum of microplastics can be compared to that of the parent polymers[2]. We suggest using the KnowItAll Raman Spectral Library[6,7], the largest collection, for microplastic identification.

Method

IR

The IR Microplastic Classifications spectral database was created using patented ODHM technology. Currently, it has these classes and is extendable:

- Polyethylene (IR and ATR-IR)
- Polyacrylate (IR)
- Polyamide (IR and ATR-IR)
- Polycarbonate (IR and ATR-IR)
- Polypropylene (IR and ATR-IR)
- Polystyrene (IR and ATR-IR)
- Polyvinylchloride (IR and ATR-IR)
- Chlorinated Polyvinylchloride (IR)
- Polyester (IR)

Microplastic testing datasets (IR and Raman) have been obtained from open sources, such as the US EPA[8], the University of Southampton[9] and OpenSpecy[10], to evaluate the IR Microplastics Classifications database. Class separations and classifications have been studied. The effect of classification spectra used in combination with real plastic database spectra has also been researched.

Raman

We examined various classes of plastic Raman spectra and concluded that it is difficult to build classification spectra for each plastic class. Since the Wiley Raman spectrum collection is relatively small and inexpensive, one can identify microplastics[8] using the existing Raman data collection.

Results and Discussion

IR microplastic classification and class separation

A correlation algorithm was used to compare spectra of microplastics from the three test datasets against the IR Microplastic Classifications database. Carbon dioxide and water vapor peaks existing in sample spectra were excluded from the spectral comparison. Matches were judged by good peak alignment as well as Hit Quality Index (HQI) values. Below are the results of those studies.

US EPA Dataset

IR: 89 spectra and 11 types
Raman: 60 records

There are replicated IR samples per microplastic class; we chose one example to report. We observed good HQI values and peak alignments among hits (Table 1). We also observed good separations and poor peak alignments in the second hit class. (**https://catalog.data.gov/dataset/isotope-ratio-mass-spectrometry-irms-and-spectroscopic-techniques-for-microplastic-charact**)

Table 1 - EPA dataset to test microplastic classification spectra

Microplastic Sample	1st Hit Peak Alignment	1st Hit HQI	1st Hit Classification	HQI of Next Class
Brown lid	Excellent	86.99%	Polyethylene	51.41%
Polycarbonate_ballyhoo	Excellent	53.09%	Polycarbonate	49.97%
Nylon6.0	Excellent	67.91%	Polyamide	45.24%
Black spice jar lid	Excellent	83.90%	Polypropylene	62.03%
EPS	Excellent	93.37%	Polystyrene	35.40%
Polyester scarf	Excellent	67.33%	Polyester	51.84%
Pvc_AWBERC.0	Excellent	74.01%	Polyvinyl chloride	33.85%

U. of Southampton

IR - 2,675 spectra

None of the sample spectra were labeled for a particular class. For replicate samplings, we chose one of the replicate spectra for testing. The results are listed in Table 2.

Table 2 - Southampton samples to test microplastic classification spectra

Microplastic Sample	1st Hit Peak Alignment	1st Hit HQI	1st Hit Classification	HQI of Next Class
SHWIRMP #867, Administrator 16	Excellent	91.16%	Polyethylene	61.00%
SHWIRMP #1498, Administrator 477	Excellent	77.99%	Polyamide	50.64%
SHWIRMP #2419, Administrator 151	Excellent	89.02%	Polypropylene	66.83%
SHWIRMP #2043, Administrator 720	Excellent	84.59%	Polystyrene	46.05%
SHWIRMP #1558, Administrator 537	Excellent	83.53%	Polyester	61.63%

Open Specy

IR/ATR-IR - 636 spectra

Most of the spectra in this database are ATR-IR. Many sample spectra resemble each other. For these cases, we selected one spectrum per for test purposes. As displayed in Table 3, the spectra were classified effectively.

Table 3 - OpenSpecy samples to test microplastic classification spectra

Microplastic Sample	1st Hit Peak Alignment	1st Hit HQI	1st Hit Classification	HQI of Next Class
Polyethylene wax #285	Excellent	90.00%	Polyethylene	50.97%
PET #292	Excellent	79.73%	Polyester	61.25%
Polycarbonate #406	Excellent	77.29%	Polycarbonate	44.54%
Polystyrene expanded #333	Excellent	92.33%	Polystyrene	36.41%
Polypropylene #411	Excellent	92.71%	Polypropylene	61.97%
Polyvinylchloride #466	Excellent	80.03%	Polyvinylchloride	36.06%

Examples of using the Spectroscopy Edition for unknown microplastic classification and identification:

Due to the urgent need for microplastic analysis, we are including the microplastic classification spectral database with the KnowItAll Spectroscopy Edition so users can make immediate impact in this important area of research critical to our environment.

Figure 1. IR - EPS.0_Microplastic

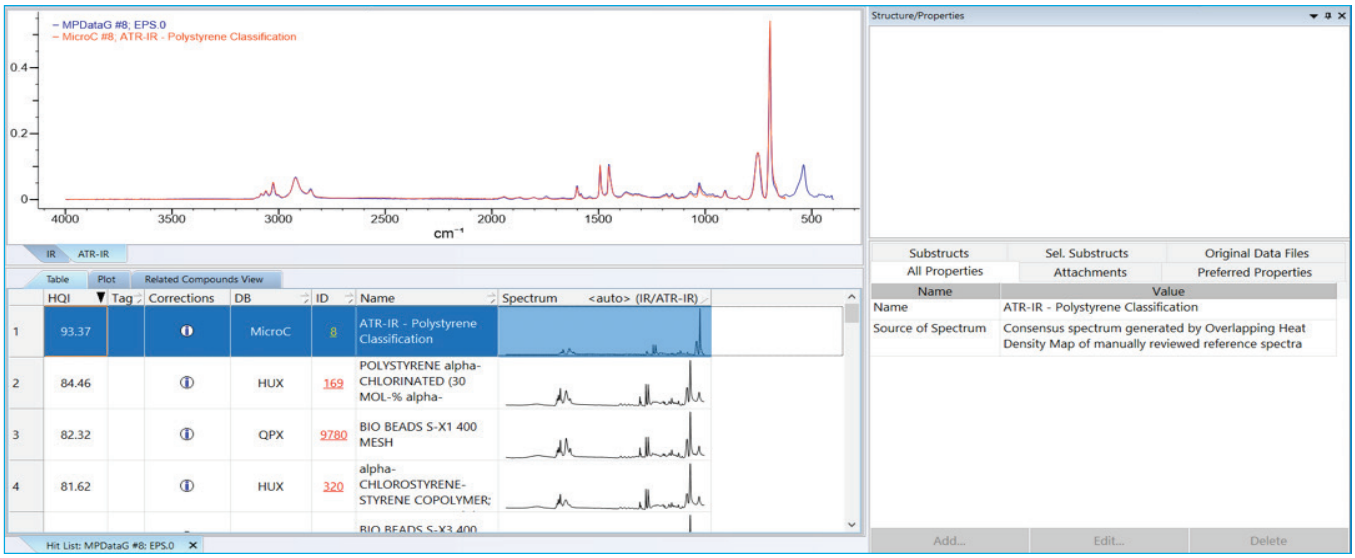
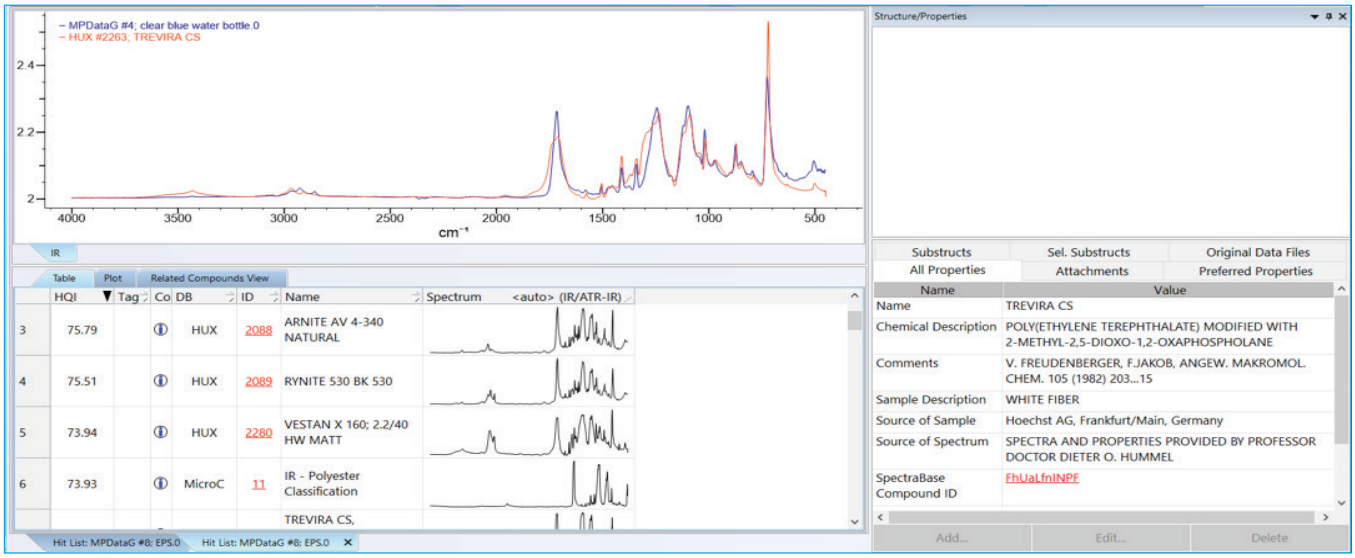


Figure 2. IR - Clear Blue Water Bottle_Microplastic



In this case, the sample spectrum best matches that of a commercial polymer product. However, one cannot easily identify the polymer. The classification spectrum match is the 6th hit, classifying the unknown parent as polyester.

Figure 3a. IR - Brown Lid_Microplastic

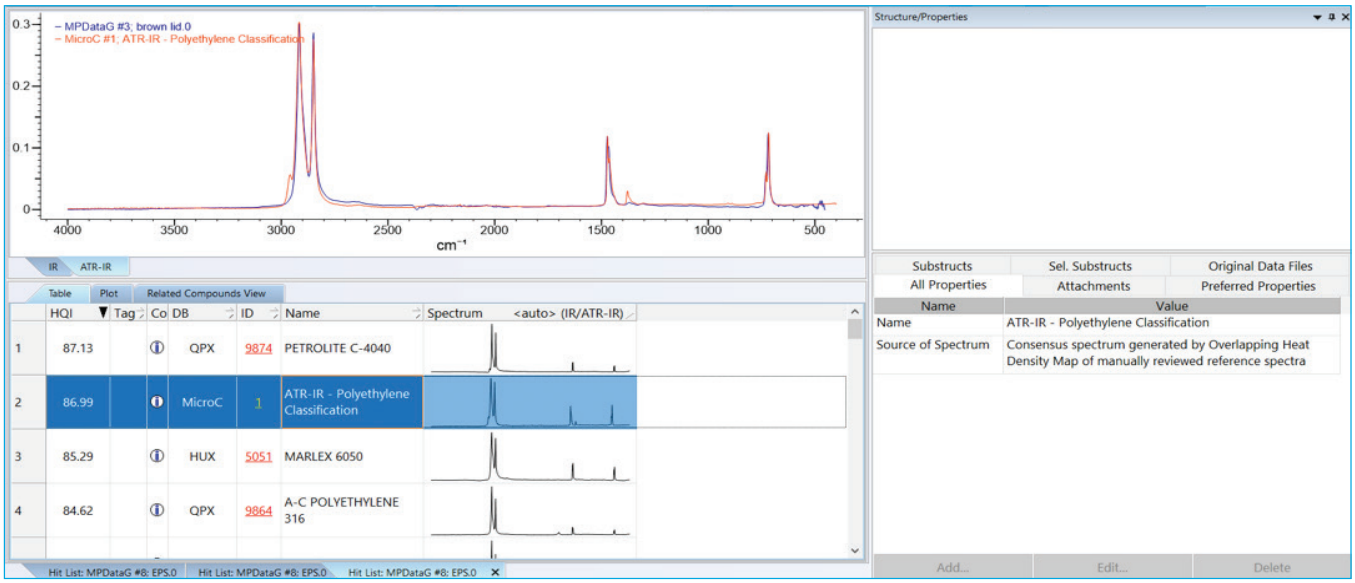
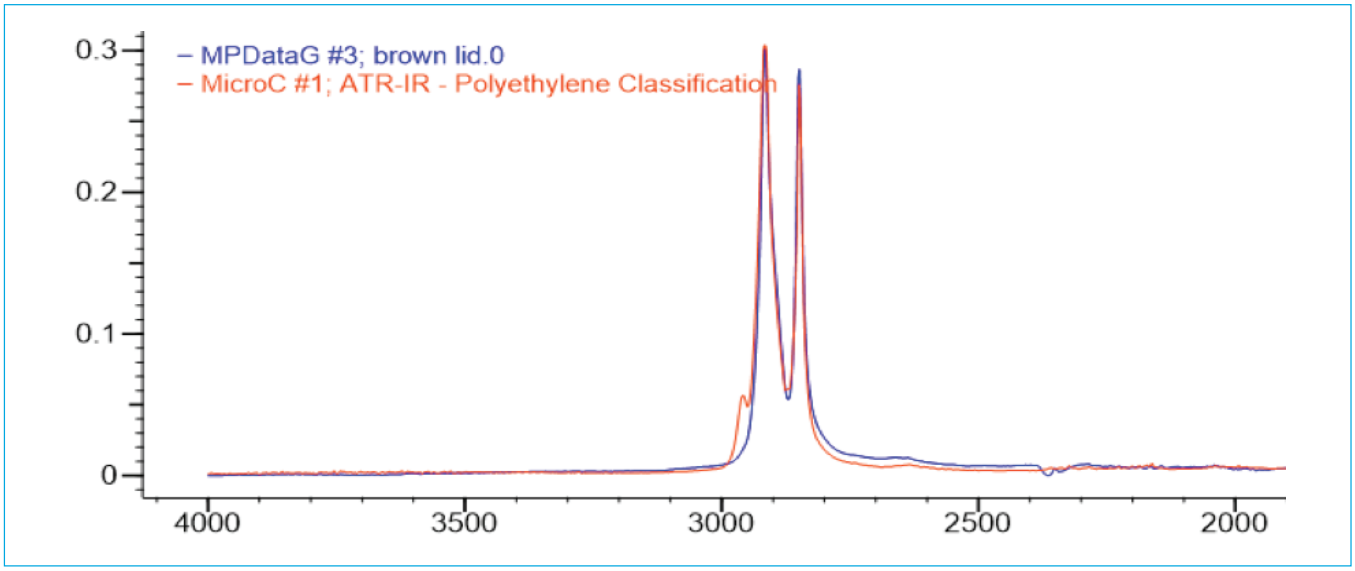
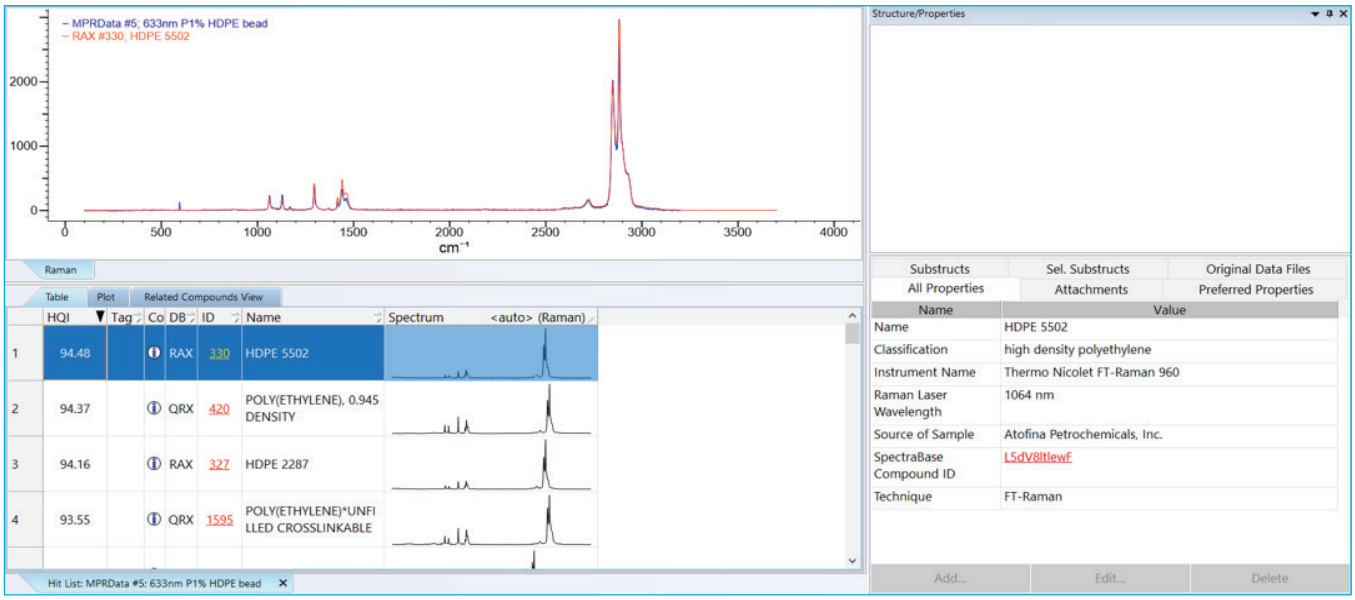


Figure 3b. IR - Detail of 3a - Brown Lid_Microplastic



Again, identification of an unknown to a commercial name means very little. The microplastic spectrum classifies this example's parent compound as polyethylene.

Figure 4. Raman - HDPE Bead_Microplastic



Raman microplastic samples can be identified by the Wiley Raman spectral database matching economically and accurately.

Figure 5a. Raman - PS Clear_Microplastic

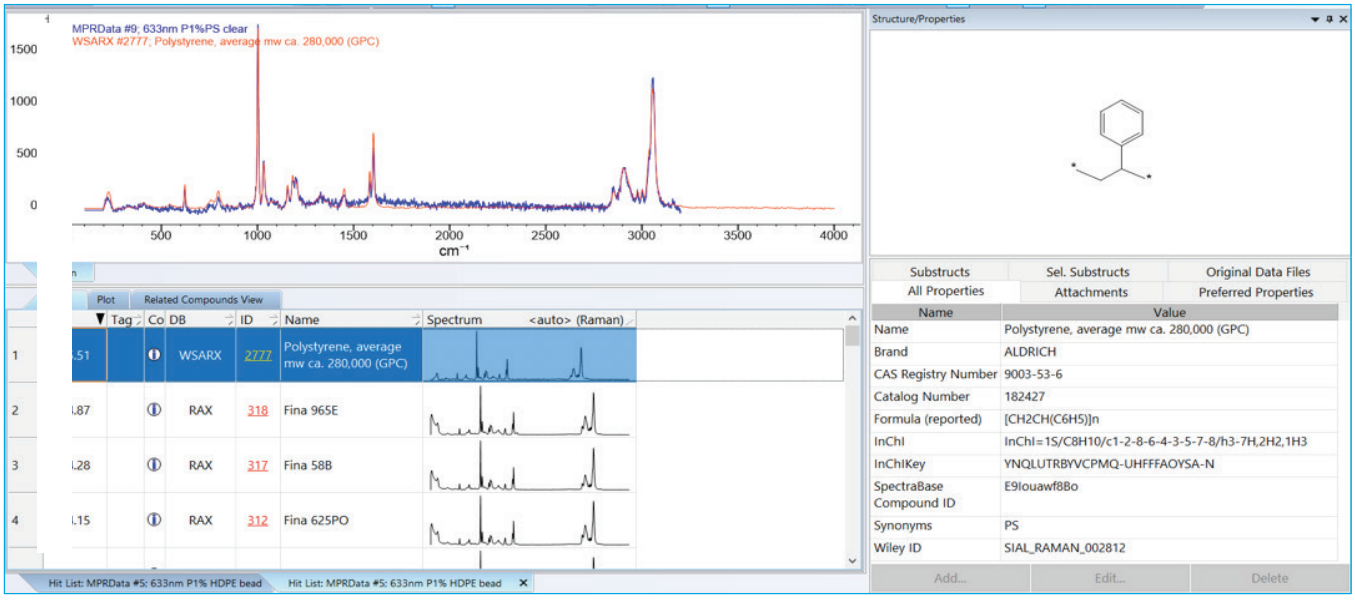
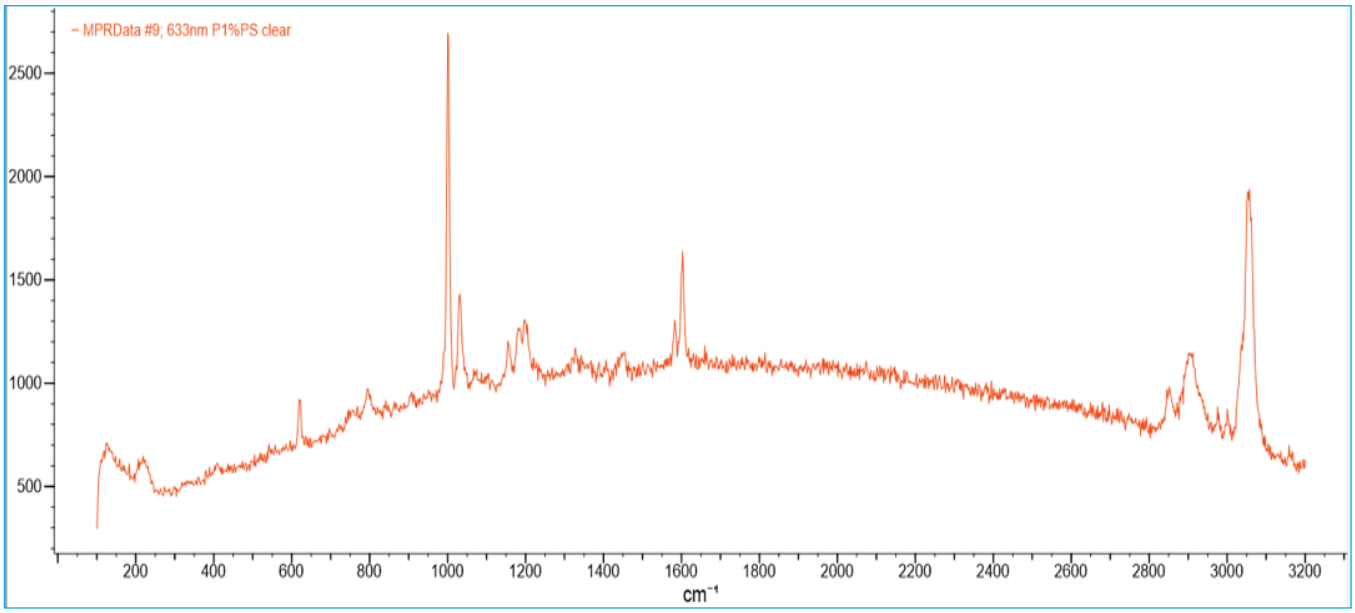


Figure 5b. Raman - bad baseline



The original microplastic sample has a bad baseline (Figure 5b), but this is not a problem for KnowItAll's Optimized Correction (Figure 5a).

Conclusion

We found that IR/ATR-IR microplastic classification, using classification spectra, is an effective method for classifying unknown microplastic IR samples. Search results provide enough separation in HQI values among classes for the practitioner to have confidence in the classification. The “IR microplastic classification database” returns results instantly.

The microplastic classification database is available in the 2021 maintenance release for the KnowItAll Spectroscopy Edition, and is available as a new feature to all current subscribers. This ensures that all users can address microplastic contamination in an efficient and effective manner. Practitioners who need to perform more comprehensive microplastic identifications should consider adding a subscription to the more inclusive IR and Raman collections.

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