Technology



Confident identification in extractable and leachable screening

SCIEX open access extractables and leachables high-resolution MS/MS spectral library

Confident identification of extractables and leachables (E&L) from plastics is essential for exposure and toxicological studies. The flexibility of SCIEX instrumentation and software solutions provides scientists with a fast way to analyze large batches of samples, with accurate and efficient MS/MS library searching for compound identification, data mining, and compound database management for E&L analysis.

The SCIEX E&L high-resolution MS/MS spectral library is a comprehensive library containing 675 E&L relevant compound entries. This suite of compounds is highly useful for scientists performing chemical analysis of non-volatile species on multiple material types, including plastics and polymers. This library, in combination with powerful search algorithms in SCIEX OS software, enables specific, sensitive, robust, accurate and efficient compound identification through instrument specific library MS/MS spectral matching. Combine it with a curated subset of the licensed National Institute of Technology (NIST) MS/MS spectral library to obtain a comprehensive library bundle containing only relevant compounds (2,360) for enhanced coverage, to reduce the number of times unknown peaks from E&L studies are not identified.

Key features of the SCIEX E&L spectral library

- Includes a SCIEX proprietary 675 E&L compound specific library
- Library includes polymer degradants covering nylon oligomers/degradants, polypropylene glycol (PPG) species, polyethylene glycol (PEG) species, piperidinones, polyethylene terephthalate (PET) species, polytetramethylene glycol (PTMG) species and hydroxy-terminated polyethylene polyols, as well as other polymer components, preservatives, stabilizers, antioxidants, light stabilizers/UV absorbers and fatty acids (Figure 1)
- The SCIEX instrument specific E&L library is freely available to download from the SCIEX.com website, in the standard SCIEX LibraryView (.lbp) format
- Contains high resolution MS/MS spectral data from both positive and negative ionization for library matching of MS/MS data acquired on SCIEX QTRAP and QTOF systems



SCIEX High Resolution E&L MS/MS Spectral Library

Figure 1. SCIEX Open Access High Resolution Extractables and Leachables MS/MS spectral library containing 675 compounds. Library can be used for compound identification when combined with high resolution MS/MS data collected on SCIEX QTOF systems. Intuitive data processing with SCIEX OS software and seamless library management with LibraryView software streamlines converting data into answers.



🔓 15 of	800 rows 🛛 Filters: 8 🗹 Quali	fy for Rules	Filters						%	A A A ,	▲ /∞ 🔺 ľo	: 🔺 🛚 Ik 🔺	C"H" 🔻 🛧	〇 孝 三 三 人 / More	• 1 🖉 X
Sample Type	7 Component Name 7	7 Expected RT 7	Area S	7 Retent Time	Retention Time Delta	Adduct / Charge	Formula 🤊	Precu V Mass	Mass Error Confid	RT Confidence	Library Confidence	Found At Mass	Mass Error (p⊽	Library Hit	▼ Library Score S
Unknown	2-[2-hydroxyethyl(tridecyl)amin	9.04	4.567e4	9.05	0.01	[M+H]+	C17H37NO2	288.290	 	 	 Image: A start of the start of	288.2897	0.0	N.N-Bis-(2-hydroxyethyl)-tridecylamine	81.8
Unknown	Nylon 6,6 degradant 5	4.15	5.719e5	4.15	0.00	[M+H]+	C11H22N2O3	231.170	 	 	 Image: A set of the set of the	231.1702	-0.3	Nylon 66 degradant-230	82.1
Unknown	Nylon 6,6 n ≥2 degradants	4.83	1.437e6	4.83	0.00	[M+H]+	C18H34N4O4	371.265	 Image: A set of the set of the	 Image: A set of the set of the	 Image: A set of the set of the	371.2651	-0.4	Nylon 66 degradant-370	96.1
Unknown	Nylon 6,6 n ≥2 degradants 2	5.16	1.518e6	5.16	0.00	[M+H]+	C18H33N3O5	372.249	 Image: A set of the set of the	 Image: A set of the set of the		372.2491	-0.5	Nylon 66 degradant-371	50.7
Unknown	Nylon 66 Degradant 12	5.41	6.172e5	5.41	0.00	[M+H]+	C30H56N6O6	597.433	~	 Image: A set of the set of the	 Image: A set of the set of the	597.4327	-1.1	Nylon 66 degradant-596 H 2H	92.3
Unknown	Nylon 66 Degradant 21	6.41	3.250e6	6.42	0.01	[M+H]+	C23H44N4O4	441.344	 Image: A set of the set of the	 Image: A set of the set of the	 Image: A set of the set of the	441.3432	-0.8	Nylon 66 degradant-440	84.9
Unknown	Nylon 66 Degradant 22	7.18	1.347e6	7.16	0.02	[M+H]+	C17H32N2O3	313.249	 Image: A set of the set of the	 Image: A set of the set of the	 Image: A set of the set of the	313.2486	0.0	Nylon 66 degradant-312	70.5
Unknown	Nylon 66 Degradant 32	4.71	7.336e5	4.72	0.01	[M+H]+	C13H25N3O3	272.197	 	 Image: A set of the set of the	 Image: A set of the set of the	272.1969	0.1	Nylon 66 degradant-271	84.6
Unknown	Nylon 66 Degradant 35	4.65	5.647e5	4.64	0.01	[M+H]+	C12H22N2O4	259.165	 Image: A set of the set of the	 Image: A set of the set of the	 Image: A set of the set of the	259.1651	-0.6	Nylon 66 degradant-258	93.7
Unknown	Nylon 66 Degradant 36	4.03	2.860e5	4.03	0.00	[M+H]+	C12H23N3O3	258.181	 ✓ 	 Image: A set of the set of the	 Image: A set of the set of the	258.1813	0.4	Nylon 66 degradant-257	95.1
Unknown	Nylon 66 Degradant 4	4.95	6.860e5	4.95	0.00	[M+H]+	C17H31N3O5	358.234	 Image: A set of the set of the	 Image: A set of the set of the	 Image: A set of the set of the	358.2333	-0.9	Nylon 66 degradant-357	80.9
Unknown	Nylon 66 n=2, Cyclic	5.69	3.206e6	5.68	0.01	[M+H]+	C24H44N4O4	453.344	 Image: A set of the set of the	 Image: A set of the set of the		453.3433	-0.5	Nylon 66 n=2 cyclic	61.0
Unknown	Nylon 66 Oligomer degradant 1	4.12	1.703e5	4.12	0.00	[M+H]+	C11H20N2O4	245.150	 Image: A set of the set of the	 Image: A set of the set of the	 Image: A set of the set of the	245.1496	0.3	Nylon 66 degradant-244	92.6
Unknown	Nylon 66 Oligomer degradant 6	5.03	4.539e5	5.02	0.01	[M+H]+	C17H29N3O3	324.228	 Image: A set of the set of the	 Image: A set of the set of the	 Image: A set of the set of the	324.2279	-0.7	Nylon 66 degradant-323	73.4
Unknown	PET cyclic dimer Serial 2	9.51	2.126e5	9.51	0.00	[M+H]+	C22H20O9	429.118	 Image: A set of the set of the	 Image: A second s	 Image: A set of the set of the	429.1182	0.4	PET Cyclic Dimer-C2H4O	77.1
Sample - Ny Area: 5.7194 1.54 양년 1.04 왕년 5.04 81 1.04 왕년 1.04 왕년 1.04 81 81 81 81 81 81 81 81 81 81 81 81 81	lon 6,6 degradant 5 (Unknown) 231 5, Height 1.710e5, RT: 4.15 min 5 6 7 7 7 7 8 7 8 7 8 8 8 9 9 9 9 9 9 9 9 9	n 4.	2 \$74.3	4.4 4.	5 4.6	Spectrum Section Section	(from 2019-07-2 12O3+H]+	23- 023 Sam j 23: 23: 23: 23: 23:	1 232	E = 0.3 $C_{11}H_{22}N$	L133 to 4.154	uiu	Spectrum f Library Spec 100% 50% -50% -100%	rom 2019-07-23-023 Sample SWA_0[50 - 1300] trum: Nylon 66 degradant-230 (NA), CE-35±20 86.0964 69.0694 100.0756 Acquired 111.0443 128.0704 150.1281 Library 100 150 Mass/Charge, Da	from 4.220 to 4.375
 Peak Deta Precursor r 231.170 	ils 1/z Mass Error (ppm) Retention T -0.3 4.15	Mass/Charge, Da Image: Charge, Da									MM (Da) Fit O3 230.16304 97.8				

Figure 2. Obtain confident identification through the SCIEX open access extractables and leachables high resolution MS/MS spectral library. A sample of acetone that was used to soak laboratory tubing was analyzed using SWATH acquisition on the SCIEX X500R QTOF system and the acquired data searched against the SCIEX Open Access E&L spectral library. All analytes were confidently identified with the powerful data processing tools in SCIEX OS software. In this example, the nylon degradant provided 98% fit against the library MS/MS spectrum using the smart confirmation algorithm and using the formula finder feature with mass error (ME) of 0.3 ppm.

SCIEX OS software for compound identification

SCIEX OS software allows easy adoption and implementation of E&L screening and quantification workflows with intuitive data representation and interpretation to quickly report out accurate, confident E&L results. Combined with the SCIEX and NIST E&L libraries, researchers can search and identify compounds across a breadth of E&L compound classes to enhance the accuracy and efficacy of both targeted and non-targeted screening.

- Use the integrated MS and MS/MS information from the library to build methods without the need to infuse standards and optimize conditions for a given compound
- Easily create processing methods for IDA or SWATH acquisition workflows for use on SCIEX QTOF systems
- Quickly setup XIC tables for quantification and identification
 with SCIEX OS software
- Build customized libraries by simply selecting only the compounds of interest using the LibraryView software features.

More confident compound ID with high resolution MS/MS

High resolution mass spectrometry (HRMS) using the SCIEX QTOF systems provides investigators a powerful tool for the detection and identification of extractables and leachables. High MS and MS/MS acquisition rates ensure the acquisition of accurate mass spectral data on large numbers of analytes, even at low analyte concentrations. The comprehensive analytespecific MS/MS spectra increases the specificity and confidence in the results when performing compound identification.

Automated processing matches the MS data to the analyte mass, and the MS/MS data are matched to the analyte fragmentation pattern in the library. As shown in the example in Figure 2, multiple points of high-quality data are used to detect and identify extractables and leachables from an acetone tubing extract sample. Highlighted is an example of the identification of a nylon degradant with an excellent fit score of 97.8% for the spectral matching of the acquired MS/MS spectrum to the SCIEX E&L library spectrum.



Conclusions

The SCIEX E&L solution combining compound specific libraries with powerful high resolution QTOF systems provides a robust solution for researchers performing chemical analysis for nonvolatile species from various plastics and polymers across a wide range of matrices. The library consists of MS/MS spectra that have been acquired on a SCIEX QTOF system enabling MS/MS spectral library searching with spectra that will be similar across all SCIEX systems. Powerful and stringent search algorithms in SCIEX OS software reduce the false positives, keeping the number of library hits to a relevant and minimal number. The specific, sensitive and robust library match, in combination with retention time and mass error, provide confidence in accurate identifications.

References

- Comprehensive workflow for the analysis of extractables and leachables from laboratory tubing. <u>SCIEX technical</u> <u>note, RUO-MKT-02-10601-C</u>.
- Single acquisition, multi-analysis strategy for identifying and quantifying extractable and leachable compounds. <u>SCIEX</u> <u>technical note, RUO-MKT-02-11284-A</u>.

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