

Expanding Suspect Screening and Non-Targeted Identification

Enhanced Analyte Coverage Using the SCIEX All-in-One High Resolution MS/MS and NIST '17 MS/MS Mass Spectral Libraries

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High resolution mass spectrometry provide scientists powerful tools to detect and identify contaminants, residues, and endogenous constituents in complex food and environmental samples.

The SCIEX All-In-One High Resolution MS/MS Spectral Library in combination with the licensed NIST '17 MS/MS Library, provides spectra for over **17000 compounds** including pesticides, pharmaceuticals and personal care products (PPCPs), and natural products found in foods and traditional medicines.

This library is for use with the X500R QTOF System powered by SCIEX OS Software and also compatible for use with SCIEX TripleTOF[®] and QTRAP[®] Systems with MasterView[™] Software and LibraryView[™] Software.

Furthermore, this library package enables searching across a breadth of compound classes to enhance the accuracy and efficacy of suspect and non-targeted screening.

A. MS/MS Libraries

[MQ4] Results Table (NIST lib test Ligation)

Index	Component Name	Retention Time	Found At Mass	Precursor Mass	Signal / Noise	Area Ratio	Library Conf.	Form...	Library Hit	Library Score	Formula
585	311.0392 / 11.46	11.46	311.0391	311.039	365.1	575.907	✓	✓	Diflufenzuron [Smart Confirmation]	94.0	C18H12C...
665	405.1451 / 12.79	12.80	405.1451	405.145	957.3	432.684	✓	✓	Ibuprofen .beta.-D-glucuronide (NIST) [Smart Co...	90.8	C16H20...
617	318.1361 / 11.33	11.32	318.1361	318.136	1042.0	370.298	✓	✓	Triticonazole (NIST) [Smart Confirmation]	59.6	C9H24Cl...
618	318.1445 / 10.13	10.18	318.1447	318.145	410.3	325.857	✓	✓	Desmedipham [Smart Confirmation]	76.5	C6H17F2...
292	207.1484 / 9.89	9.90	207.1484	207.148	1164.0	287.642	✓	✓	Isoproturon [Smart Confirmation]	95.3	C6H19N6P...
321	218.1172 / 8.97	8.98	218.1172	218.117	555.3	107.441	✓	✓	Pyracarbolid [Smart Confirmation]	92.8	C13H15...
180	151.0319 / 8.72	8.71	151.0323	151.032	227.8	76.128	✓	✓	4-Methylphenylacetic acid (NIST) [Smart Confir...	83.2	C7H6H2S...
315	215.0956 / 8.75	8.73	215.0956	215.096	242.8	58.713	✓	✓	Metribuzin [Smart Confirmation]	99.5	C6H16FN...
567	307.2076 / 15.86	15.85	307.2271	307.227	273.8	55.382	✓	▲	6,6'-8,8'-Eicosatrienoic acid (NIST) [Smart Conf...	82.7	C19H36O2
325	221.0485 / 8.75	8.75	221.0487	221.049	370.6	44.875	✓	✓	Thidiazuron [Smart Confirmation]	98.2	C7H10FN...
694	337.1206 / 11.44	11.44	337.1206	337.121	1885.5	24.984	✓	✓	Fenbuconazole (NIST) [Smart Confirmation]	72.9	C11H21C...
677	331.0394 / 11.30	11.29	331.0394	331.039	515.2	15.489	✓	✓	Fenarimol (NIST) [Smart Confirmation]	71.1	C9H16Cl...
134	133.0646 / 11.60	11.61	133.0646	133.065	398.0	12.475	✓	▲	(2S,3S)-(-)-3-Phenylglycidol (NIST) [Smart Conf...	100.0	C9H8O...
86	107.0489 / 9.37	9.37	107.0489	107.049	580.3	N/A	✓	▲	Benzaldehyde (NIST) [Smart Confirmation]	53.1	C7H6O...
127	125.0151 / 12.15	12.16	125.0151	125.015	554.5	N/A	✓	▲	4-Methoxyphenol (NIST) [Smart Confirmation]	53.3	C6H5OP...
235	178.0354 / 9.95	9.96	178.0354	178.035	543.4	N/A	✓	✓	(-)-Sulfosaphene (NIST) [Smart Confirmation]	68.8	C6H11N...
246	186.0525 / 12.37	12.37	186.0526	186.053	359.1	N/A	✓	✓	Pterine (NIST) [Smart Confirmation]	83.0	C9H6FN...
257	194.0809 / 12.01	12.01	194.0809	194.081	1368.6	N/A	✓	✓	N-Methyl-3,4-methylenedioxyamphetamine (NES...	84.7	C10H11...
281	205.0974 / 1.20	1.17	205.0974	205.097	207.6	N/A	✓	✓	L-Tryptophan (NIST) [Smart Confirmation]	98.8	C11H12...
300	210.9993 / 10.53	10.52	210.9992	210.999	36928.6	N/A	✓	✓	Acibenzolar-S-methyl (NIST) [Smart Confirmation]	74.6	C4H2F3N...

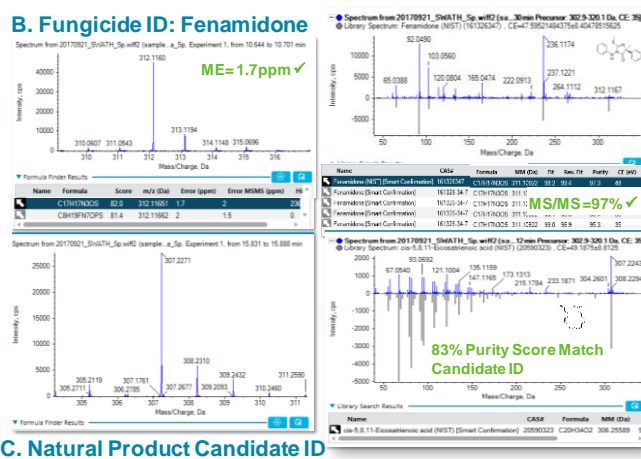


Figure 1. Gain further natural compound and pesticide identification through the addition of the licensed NIST '17 High Resolution MS/MS Spectral Library. (A) Control QuEChERS extract of an arugula sample was spiked with several pesticides of interest. The sample was analyzed using SWATH[®] Acquisition on the SCIEX X500R QTOF System and the acquired data searched against the All-in-One High Resolution MS/MS Spectral Library and NIST '17 MS/MS Spectral Library. All analytes were confidently identified using SCIEX OS Software data processing. (B) In this example, one of the target pesticides (Fenamidone) is shown as a positive identification, with matches for RT, precursor match, and MS/MS library hit. (C) A naturally occurring plant compound has been tentatively identified in this sample. An omega-3 fatty acid was suggested from a positive match in the library. Omega-3 fatty acids are known to be found in arugula and represent one of the health benefits of this food. It is demonstrated that true Nontargeted approaches are effective and that screening against this library provides cross- compound class coverage applicable to complex matrices.

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