

Extending Metabolome Coverage

Introducing the Licensed NIST '17 MS/MS Spectral Library for Untargeted Metabolomics Workflows

Oscar G. Cabrices¹ and Baljit K. Ubhi¹
¹SCIEX, USA

Confident metabolite identification is a major bottleneck in the field of untargeted metabolomics today. To help alleviate this there is a need for larger libraries and databases of spectral compounds which can aid the metabolite identification process. The SCIEX All-In-One High Resolution MS/MS Spectral Library enables accurate compound detection and identification through library spectral matching. In combination with the licensed NIST '17 MS/MS Library, the analyst has access to MS/MS spectra for over **17000 compounds** including human and plant metabolites, sugars, glycans and natural products commonly investigated in metabolomics research for complex samples, including blood, urine and tissues.



This library is for use with 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.

Figure 1 shows an example of an extracted human urine sample from a pre-classified prostate cancer study. In this example the metabolite Xanthine is highlighted. The accurate identification (MS/MS Library Score = 98.9%, Mass Error = 0.1 ppm) of this analyte was possible through the addition of the licensed NIST '17 MS/MS Spectral Library to the SCIEX All-In-One High Resolution MS/MS Spectral Library.

MS/MS Libraries													
Index	Sample Name	Sample Type	Component Name	Area	Retention Time	Used	Precursor Mass	Library Confidence	Formula Confidence	Found At Mass	Found At Frag...	Library Hit	Library Score
111	CH16_VW_SWATH_Pos	Unknown	134.0599 / 8.07	1.784e6	8.07	☑	134.060	✓	✓	134.0599	N/A	2-Indololine (NIST) [Smart Confirmation]	78.9
113	CH16_VW_SWATH_Pos	Unknown	137.0457 / 1.75	1.231e7	1.76	☑	137.046	✓	✓	137.0457	N/A	Hyposanthine (NIST) [Smart Confirmation]	99.9
116	CH16_VW_SWATH_Pos	Unknown	137.0960 / 7.75	2.747e5	7.74	☑	137.096	✓	✓	137.0961	N/A	Sabineine (NIST) [Smart Confirmation]	77.4
117	CH16_VW_SWATH_Pos	Unknown	138.0545 / 0.93	3.623e6	0.93	☑	138.054	✓	✓	138.0547	N/A	Trigonelline (NIST) [Smart Confirmation]	82.0
121	CH16_VW_SWATH_Pos	Unknown	139.0502 / 2.84	4.261e5	2.85	☑	139.050	✓	✓	139.0502	N/A	4-Imidazoleacetic acid (NIST) [Smart Confirmation]	90.1
122	CH16_VW_SWATH_Pos	Unknown	141.0659 / 1.05	6.744e6	1.05	☑	141.066	✓	✓	141.0658	N/A	Amphetamine-d5 (NIST) [Smart Confirmation]	91.0
127	CH16_VW_SWATH_Pos	Unknown	143.1178 / 1.74	5.302e5	1.75	☑	143.118	✓	✓	143.1179	N/A	6-Methyl-2-thiouracil (NIST) [Smart Confirmation]	75.4
128	CH16_VW_SWATH_Pos	Unknown	143.1180 / 1.11	6.880e5	1.11	☑	143.118	✓	✓	143.1189	N/A	Piracetam (NIST) [Smart Confirmation]	77.0
129	CH16_VW_SWATH_Pos	Unknown	144.1017 / 1.11	7.213e6	1.11	☑	144.102	✓	✓	144.1017	N/A	1-Aminocyclohexanecarboxylic acid (NIST) [Smart...	77.5
134	CH16_VW_SWATH_Pos	Unknown	146.0811 / 3.50	1.099e6	3.50	☑	146.081	✓	✓	146.0812	N/A	DL-Notrocinone methyl ester (NIST) [Smart Conf...	95.9
137	CH16_VW_SWATH_Pos	Unknown	146.9964 / 0.56	7.956e4	0.58	☑	146.996	✓	✓	146.9965	N/A	Bassoholide (NIST) [Smart Confirmation]	84.7
139	CH16_VW_SWATH_Pos	Unknown	149.0595 / 12.68	6.005e5	12.68	☑	149.059	✓	✓	149.0596	N/A	trans-Cinnamic acid (NIST) [Smart Confirmation]	79.7
142	CH16_VW_SWATH_Pos	Unknown	151.0752 / 8.04	6.526e6	8.04	☑	151.075	✓	✓	151.0753	N/A	(S)-Myristal (NIST) [Smart Confirmation]	78.4
146	CH16_VW_SWATH_Pos	Unknown	153.0407 / 2.47	2.820e6	2.45	☑	153.041	✓	✓	153.0401	N/A	Xanthine (NIST) [Smart Confirmation]	98.9
148	CH16_VW_SWATH_Pos	Unknown	153.0657 / 4.87	1.214e7	4.87	☑	153.066	✓	✓	153.0655	N/A	3-Methyl-4-pyridone-5-carboxamide (NIST) [Sma...	91.4
151	CH16_VW_SWATH_Pos	Unknown	158.0811 / 6.63	2.524e5	6.63	☑	158.081	✓	✓	158.0812	N/A	N-Tiglylglycine (NIST) [Smart Confirmation]	94.8
177	CH16_VW_SWATH_Pos	Unknown	163.1328 / 10.52	2.415e5	10.39	☑	163.133	✓	✓	163.1328	N/A	7-Hydroxycoumarin (NIST) [Smart Confirmation]	82.3
186	CH16_VW_SWATH_Pos	Unknown	165.0908 / 8.35	3.161e5	8.35	☑	165.091	✓	✓	165.0909	N/A	Thymoquinone (NIST) [Smart Confirmation]	91.8
188	CH16_VW_SWATH_Pos	Unknown	166.0721 / 1.78	6.711e6	1.78	☑	166.072	✓	✓	166.0720	N/A	7-Methylguanine (NIST) [Smart Confirmation]	94.5
190	CH16_VW_SWATH_Pos	Unknown	166.0722 / 1.60	2.848e6	2.59	☑	166.072	✓	✓	166.0722	N/A	7-Methylguanine (NIST) [Smart Confirmation]	76.1
192	CH16_VW_SWATH_Pos	Unknown	166.0857 / 6.24	6.140e6	6.24	☑	166.086	✓	✓	166.0856	N/A	DL-Phenylalanine (NIST) [Smart Confirmation]	93.9
193	CH16_VW_SWATH_Pos	Unknown	167.0125 / 17.57	3.771e5	17.57	☑	167.013	✓	✓	167.0126	N/A	7-Methylxanthine (NIST) [Smart Confirmation]	87.7
195	CH16_VW_SWATH_Pos	Unknown	167.0562 / 6.40	1.449e6	6.31	☑	167.056	✓	✓	167.0564	N/A	3-Methylxanthine (NIST) [Smart Confirmation]	79.8
198	CH16_VW_SWATH_Pos	Unknown	167.1062 / 8.61	5.341e5	8.61	☑	167.106	✓	✓	167.1065	N/A	(S)-Penicilic acid (NIST) [Smart Confirmation]	84.6
202	CH16_VW_SWATH_Pos	Unknown	169.0354 / 1.70	1.819e6	1.68	☑	169.035	✓	✓	169.0353	N/A	Uric acid (NIST) [Smart Confirmation]	98.0
206	CH16_VW_SWATH_Pos	Unknown	170.0921 / 0.71	1.809e6	0.71	☑	170.092	✓	✓	170.0920	N/A	1-Methyl-L-histidine (NIST) [Smart Confirmation]	95.5
216	CH16_VW_SWATH_Pos	Unknown	176.0704 / 9.12	1.920e6	9.12	☑	176.070	✓	✓	176.0705	N/A	3-Indoleacetic acid (NIST) [Smart Confirmation]	95.0

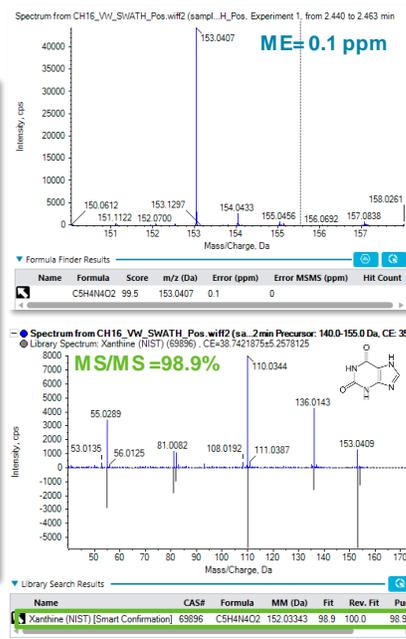


Figure 1. Gain extended metabolome coverage with the addition of the licensed NIST '17 High Resolution MS/MS Spectral Library. Identify any metabolites found in the samples by reviewing the confidence scores for the MS1 mass error, retention time, isotope fidelity and the MS/MS. Xanthine (highlighted in the results table) is a purine base found in most body tissues and fluids, certain plants, and some urinary calculi. It is an intermediate in the degradation of adenosine monophosphate to uric acid, being formed by oxidation of hypoxanthine. This compound is associated with Lesch-Nyhan syndrome which leads to kidney problems through buildup of uric acid (Source: www.hmdb.ca)

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Headquarters
 500 Old Connecticut Path | Framingham, MA 01701 USA
 Phone 508-383-7700
sciex.com

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