

## Extending metabolome coverage

**Using the licensed NIST '17 MS/MS spectral library for untargeted metabolomics workflows**

Oscar G. Cabrices and Baljit K. Ubhi  
SCIEX, USA

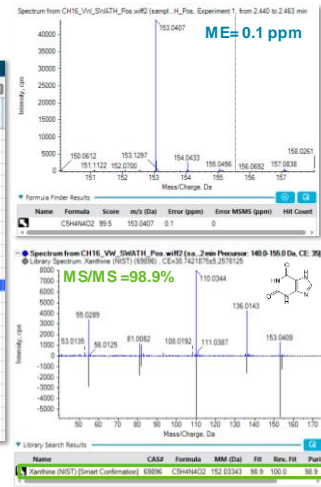
Confident metabolite identification is a major bottleneck in the field of untargeted metabolomics today. To help alleviate this there is a need for larger libraries and databases of spectral compounds which can aid the metabolite identification process. The SCIEX All-In-One High Resolution MS/MS Spectral Library enables accurate compound detection and identification through library spectral matching. In combination with the licensed NIST '17 MS/MS Library, the provides 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 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 extracted human urine sample from a pre-classified prostate cancer study highlighting 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	Procedure Name	Library Confidence	Formula Confidence	Library Hit	Library Score
131	CH16_VW_SMA11H_Pos	Unknown	1543599 / 8.87	3.7646	8.87	SE	1543599	NA	1543599	2-Substituted (NIST) (Smart Confirmation)	76.9
132	CH16_VW_SMA11H_Pos	Unknown	1370457 / 1.75	1.2347	1.75	SE	1370457	NA	1370457	Hypoxanthine (NIST) (Smart Confirmation)	99.9
136	CH16_VW_SMA11H_Pos	Unknown	1370960 / 1.75	2.7476	1.74	SE	1370960	NA	1370960	Sabinene (NIST) (Smart Confirmation)	77.4
137	CH16_VW_SMA11H_Pos	Unknown	1380545 / 0.89	1.8236	0.93	SE	1380545	NA	1380545	Trigonelline (NIST) (Smart Confirmation)	82.0
121	CH16_VW_SMA11H_Pos	Unknown	1390502 / 1.84	4.2650	2.89	SE	1390502	NA	1390502	4-Imidazopyridine acid (NIST) (Smart Confirmation)	96.1
122	CH16_VW_SMA11H_Pos	Unknown	1410939 / 1.05	6.7446	1.05	SE	1410939	NA	1410939	Amphetamine-d5 (NIST) (Smart Confirmation)	91.0
127	CH16_VW_SMA11H_Pos	Unknown	1431178 / 1.74	9.3026	1.75	SE	1431178	NA	1431178	6-Methyl-2-thiouracil (NIST) (Smart Confirmation)	71.4
128	CH16_VW_SMA11H_Pos	Unknown	1431180 / 1.11	8.8826	1.11	SE	1431180	NA	1431180	Fluoxetine (NIST) (Smart Confirmation)	77.0
129	CH16_VW_SMA11H_Pos	Unknown	1441857 / 1.11	9.2136	1.11	SE	1441857	NA	1441857	2-Amino-2-thiouracil acid (NIST) (Smart Confirmation)	71.9
134	CH16_VW_SMA11H_Pos	Unknown	1460813 / 0.90	1.0906	1.90	SE	1460813	NA	1460813	D5-Hydroxycarbazone (NIST) (Smart Confirmation)	99.9
137	CH16_VW_SMA11H_Pos	Unknown	1480964 / 0.96	7.9384	0.98	SE	1480964	NA	1480964	Benzoic acid (NIST) (Smart Confirmation)	84.7
139	CH16_VW_SMA11H_Pos	Unknown	1480989 / 12.68	6.0847	12.68	SE	1480989	NA	1480989	trans-Cinnamic acid (NIST) (Smart Confirmation)	76.7
142	CH16_VW_SMA11H_Pos	Unknown	1510752 / 6.24	6.5265	6.24	SE	1510752	NA	1510752	1,2-Diethyl-3-methyl-5-imidazopyridine (NIST) (Smart Confirmation)	78.4
146	CH16_VW_SMA11H_Pos	Unknown	1530807 / 2.47	1.8066	1.46	SE	1530807	NA	1530807	Xanthine (NIST) (Smart Confirmation)	98.9
146	CH16_VW_SMA11H_Pos	Unknown	1530807 / 4.87	1.2347	4.87	SE	1530807	NA	1530807	1-Methyl-8-guanidino-5-carboxamide (NIST) (Smart Confirmation)	81.4
151	CH16_VW_SMA11H_Pos	Unknown	1580181 / 4.83	2.5345	4.83	SE	1580181	NA	1580181	9-Ethylguanine (NIST) (Smart Confirmation)	84.8
177	CH16_VW_SMA11H_Pos	Unknown	1601128 / 10.52	2.4357	10.39	SE	1601128	NA	1601128	7-Hydroxyguanine (NIST) (Smart Confirmation)	82.3
186	CH16_VW_SMA11H_Pos	Unknown	1650808 / 8.35	3.1635	8.35	SE	1650808	NA	1650808	Thymopyruvate (NIST) (Smart Confirmation)	91.8
186	CH16_VW_SMA11H_Pos	Unknown	1660723 / 1.78	6.7136	1.78	SE	1660723	NA	1660723	7-Methylguanine (NIST) (Smart Confirmation)	84.5
189	CH16_VW_SMA11H_Pos	Unknown	1660722 / 0.89	2.8456	0.89	SE	1660722	NA	1660722	7-Methylguanine (NIST) (Smart Confirmation)	76.2
192	CH16_VW_SMA11H_Pos	Unknown	1660857 / 6.24	6.1496	6.24	SE	1660857	NA	1660857	D5-Phenylamine (NIST) (Smart Confirmation)	99.9
199	CH16_VW_SMA11H_Pos	Unknown	1870129 / 17.57	3.77145	17.57	SE	1870129	NA	1870129	7-Methylxanthine (NIST) (Smart Confirmation)	87.7
199	CH16_VW_SMA11H_Pos	Unknown	1870129 / 4.87	1.4866	6.31	SE	1870129	NA	1870129	1-Methylguanine (NIST) (Smart Confirmation)	76.8
199	CH16_VW_SMA11H_Pos	Unknown	1870129 / 8.81	5.3815	8.81	SE	1870129	NA	1870129	(S)-Pentyl acid (NIST) (Smart Confirmation)	84.9
202	CH16_VW_SMA11H_Pos	Unknown	1890354 / 1.70	1.1836	1.68	SE	1890354	NA	1890354	Uric acid (NIST) (Smart Confirmation)	98.0
206	CH16_VW_SMA11H_Pos	Unknown	1700923 / 0.71	1.8086	0.71	SE	1700923	NA	1700923	1-Methyl-L-thiourea (NIST) (Smart Confirmation)	85.5
218	CH16_VW_SMA11H_Pos	Unknown	1760758 / 9.12	1.9296	9.12	SE	1760758	NA	1760758	3-Isobutylamide (NIST) (Smart Confirmation)	85.0



**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](http://sciex.com)

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