

Don't Miss Any Synthetic Drug Present In Your Sample

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 forensic scientists powerful tools to detect and identify novel drugs of abuse and other emerging forensic compounds of interest present in a variety of complex matrices.

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 forensic analyst has access to MS/MS spectra for over **17000 compounds** including novel synthetic drugs and metabolites commonly tested in forensic samples, including blood and urine.

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 non-targeted screening.

MS/MS Libraries											
Index	Sample Name	Sample Type	Component Name	Area	Retention Time	Used	Precursor Mass	Library Conf...	Form...	Found At Mass	Library Hit
884	SMV_Cal3	Unknown	280.1704 / 3.12	1.7736e	3.13	<input checked="" type="checkbox"/>	280.170	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	280.1704	Doxepin [Smart Confirmation]
887	SMV_Cal3	Unknown	281.2020 / 3.67	1.5576e	3.67	<input checked="" type="checkbox"/>	281.202	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	281.2021	Imipramine [Smart Confirmation]
892	SMV_Cal3	Unknown	284.1865 / 2.14	1.3206e	2.13	<input checked="" type="checkbox"/>	284.186	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	284.1862	8-Hydroxy-2'-deoxyguanosine (NIST) [Smart Confirmation]
893	SMV_Cal3	Unknown	284.2945 / 4.81	4.6666e	4.83	<input checked="" type="checkbox"/>	284.294	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	284.2955	Stearamide (NIST) [Smart Confirmation]
894	SMV_Cal3	Unknown	285.0797 / 4.28	1.0786e	4.27	<input checked="" type="checkbox"/>	285.080	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	285.0797	Diazepam [Smart Confirmation]
895	SMV_Cal3	Unknown	285.1008 / 1.67	1.3606e	1.67	<input checked="" type="checkbox"/>	285.101	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	285.1008	all trans-Retinal (NIST) [Smart Confirmation]
896	SMV_Cal3	Unknown	286.0750 / 2.37	3.4336e	2.37	<input checked="" type="checkbox"/>	286.075	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	286.0750	7-Aminoclozapem [Smart Confirmation]
898	SMV_Cal3	Unknown	286.1446 / 1.87	3.1626e	1.86	<input checked="" type="checkbox"/>	286.145	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	286.1445	Norhydrocodone [Smart Confirmation]
899	SMV_Cal3	Unknown	286.2021 / 2.42	4.2926e	2.43	<input checked="" type="checkbox"/>	286.202	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	286.2021	2-Octenyl-carnitine [Smart Confirmation]
907	SMV_Cal3	Unknown	289.0544 / 3.84	1.7936e	3.84	<input checked="" type="checkbox"/>	289.054	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	289.0547	Desallylfurazepam [Smart Confirmation]
908	SMV_Cal3	Unknown	290.1394 / 2.16	8.9385e	2.16	<input checked="" type="checkbox"/>	290.139	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	290.1394	Benzylcgonine (NIST) [Smart Confirmation]
910	SMV_Cal3	Unknown	293.1388 / 2.28	2.0245e	2.29	<input checked="" type="checkbox"/>	293.139	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	293.1388	Picrotoxinin (NIST) [Smart Confirmation]
914	SMV_Cal3	Unknown	298.1109 / 4.92	1.5935e	4.91	<input checked="" type="checkbox"/>	298.111	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	298.1110	Tridemorph [Smart Confirmation]
918	SMV_Cal3	Unknown	300.1076 / 5.86	1.0116e	5.56	<input checked="" type="checkbox"/>	300.108	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	300.1076	Codeine [Smart Confirmation]
920	SMV_Cal3	Unknown	300.1603 / 1.93	5.6866e	1.93	<input checked="" type="checkbox"/>	300.160	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	300.1603	Hydrocodone (NIST) [Smart Confirmation]
922	SMV_Cal3	Unknown	301.0748 / 4.01	2.6166e	4.02	<input checked="" type="checkbox"/>	301.075	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	301.0748	Temazepam [Smart Confirmation]
923	SMV_Cal3	Unknown	302.1397 / 1.81	1.8185e	1.80	<input checked="" type="checkbox"/>	302.140	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	302.1396	Noroxycodone [Smart Confirmation]
924	SMV_Cal3	Unknown	302.1758 / 1.72	5.9955e	1.72	<input checked="" type="checkbox"/>	302.176	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	302.1758	Fenhexamid [Smart Confirmation]
935	SMV_Cal3	Unknown	308.1764 / 2.68	1.9886e	2.68	<input checked="" type="checkbox"/>	308.176	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	308.1763	Zolpidem [Smart Confirmation]
938	SMV_Cal3	Unknown	309.0909 / 3.90	9.0656e	3.90	<input checked="" type="checkbox"/>	309.091	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	309.0909	Alprazolam [Smart Confirmation]
942	SMV_Cal3	Unknown	310.2173 / 3.74	4.0526e	3.74	<input checked="" type="checkbox"/>	310.217	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	310.2172	Methadone (NIST) [Smart Confirmation]
944	SMV_Cal3	Unknown	311.1496 / 2.28	7.5296e	2.29	<input checked="" type="checkbox"/>	311.150	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	311.1495	Picrotin (NIST) [Smart Confirmation]

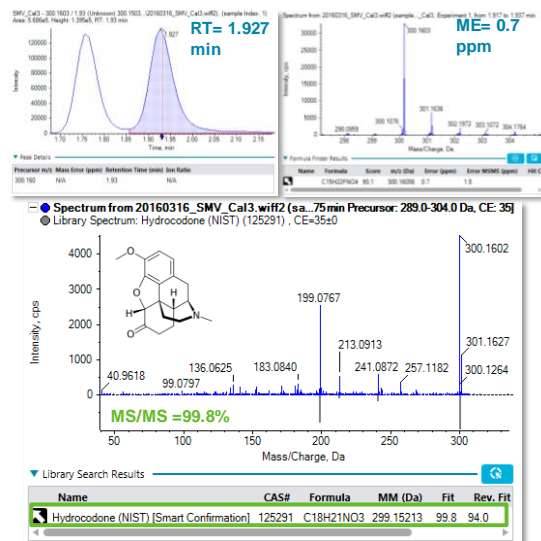


Figure 1. Obtain further synthetic drug identification through the addition of the licensed NIST '17 High Resolution MS/MS Spectral Library. A control urine sample was spiked with several forensic compounds of interest. The sample was analyzed using SWATH® Acquisition on the SCIEX X500R QTOF System and 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. In this example, the synthetic opioid hydrocodone (Isobaric Compound with Codeine), provided 99.8% fit against the NIST reference MS/MS spectrum using the smart confirmation algorithm and using the formula finder feature with mass error of 0.7 ppm.

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Document number: RUO-MKT-02-7168-A



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