DATASHEET — NITAZENE ANALOGUES

NPS Toolkits

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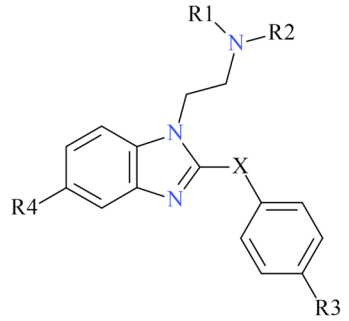
PURPOSE: This datasheet serves as a reference guide for laboratorians, analytical chemists, and researchers focused on the detection of **nitazene analogues** using mass spectrometry.

OVERVIEW: Nitazene analogues (also known as 2-benzyl benzimidazoles) are a group of potent novel synthetic opioids. Various nitazene analogues, including **etonitazene** (the prototypical drug of this series), were initially developed as new medicines but never approved for therapeutic use. Beginning in 2019 with **isotonitazene**, new waves of nitazene analogues began appearing in the North American drug supply. Similar to the trajectory of other novel psychoactive substances (NPS) subclasses, new nitazene analogues appeared after the control of prior analogues and with minor structural modifications. This constant and cyclic emergence of new potent opioids continues to challenge forensic laboratories, especially as unknown or previously uncharacterized substances appear. Forensic laboratories and similar drug testing institutions commonly employ mass spectrometry techniques for the detection of substances in drug materials and biological specimens. Gas chromatography mass spectrometry (GC-MS) and various forms of high resolution mass spectrometry (HRMS) remain the most utilized instrumentation for non-targeted detection of drugs and NPS. Resources to aid in the identification and determination of specific NPS (e.g., nitazene analogues) are key to reducing lag times between detection and reporting. This datasheet can be used to help identify and differentiate specific nitazene analogues based on acquired mass spectral data.

FINDINGS: Prototypical nitazene analogues produce GC-MS base peaks of *m/z* 86 and HRMS fragment ions of 100.1126 Da. *N*-Desethyl variant nitazene analogues produce varying GC-MS base peaks (e.g., *m/z* 121, 135, 149) and HRMS fragment ions of 72.0813 Da. *N*-Pyrrolidino variant nitazene analogues produce GC-MS base peaks of *m/z* 84 and HRMS fragment ions of 98.0970 Da. Nitazene analogues with variations to only the 5-nitro group generally produce GC-MS base peaks of *m/z* 86 and HRMS fragment ions of 100.1126 Da, but with differing molecular ions (M.I.) and monoisotopic masses ([M+H]+) compared to prototypical nitazene analogues. Compounding variations or substitutions generally produce a mixture of the various fragment ions previously mentioned. Notably, meto– and eto– variant nitazene analogues commonly produce characteristic GC-MS ions of m/z 121 and m/z 135, respectively, which may aid in their differentiation.

NITAZENE ANALOGUE STRUCTURAL BACKBONE



Structural Class	Drug Name	R1	R2	R3	R4	X	Formula	M.I.	GC-MS Fragment Ions‡	[M+H]+	HRMS Fragment Ions‡
Prototypical	Metonitazene	C_2H_5	C_2H_5	OCH_3	NO_2	CH_2	$C_{21}H_{26}N_4O_3$	382	121, 86*, 77, 58, 43	383.2078	264.1203, 121.0624, 100.1105, 72.0797
	Etonitazene	C_2H_5	C_2H_5	OC_2H_5	NO_2	CH_2	$C_{22}H_{28}N_4O_3$	396	135, 107, 86*, 58, 43	397.2234	159.1168, 135.0804, 100.1116, 72.0809
	Isotonitazene	C_2H_5	C_2H_5	*iso*-OC_3H_7	NO_2	CH_2	$C_{23}H_{30}N_4O_3$	410	107, 86*, 58, 77, 43	411.2391	107.0486, 100.1109, 72.0809
	Protonitazene	C_2H_5	C_2H_5	OC_3H_7	NO_2	CH_2	$C_{23}H_{30}N_4O_3$	410	107, 86*, 58, 77, 43	411.2391	107.0496, 100.1120, 72.0810
	Butonitazene	C_2H_5	C_2H_5	OC_4H_9	NO_2	CH_2	$C_{24}H_{32}N_4O_3$	424	107, 86*, 58, 77, 43	425.2547	163.1104, 107.0470, 100.1117, 44.0486
N-Desethyls	*N*-Desethyl Metonitazene	H	C_2H_5	OCH_3	NO_2	CH_2	$C_{19}H_{22}N_4O_3$	354	297, 121*, 77, 58, 43	355.1765	284.1038, 238.1106, 121.0647, 72.0803
	N-Desethyl Etonitazene	H	C_2H_5	OC_2H_5	NO_2	CH_2	$C_{20}H_{24}N_4O_3$	368	311, 135*, 107, 77, 58	369.1921	298.1195, 176.0454, 129.0545, 72.0807
	N-Desethyl Isotonitazene	H	C_2H_5	*iso*-OC_3H_7	NO_2	CH_2	$C_{21}H_{25}N_3O$	382	325, 282, 149*, 107, 58	383.2078	312.1375, 107.0494, 72.0808, 44.0491
	N-Desethyl Protonitazene	H	C_2H_5	OC_3H_7	NO_2	CH_2	$C_{21}H_{25}N_3O$	382	325, 282, 149*, 107, 58	383.2078	312.1375, 107.0494, 72.0802, 59.0475
N-Pyrrolidinos	*N*-Pyrrolidino Metonitazene	-C_4H_8-		OCH_3	NO_2	CH_2	$C_{21}H_{24}N_4O_3$	380	121, 84*, 77, 55, 42	381.1921	121.0649, 98.0966, 56.0497
	N-Pyrrolidino Etonitazene	-C_4H_8-		OC_2H_5	NO_2	CH_2	$C_{22}H_{26}N_4O_3$	394	135, 107, 84*, 55, 42	395.2078	135.0800, 107.0508, 98.0958, 56.0493
	N-Pyrrolidino Isotonitazene	-C_4H_8-		*iso*-OC_3H_7	NO_2	CH_2	$C_{23}H_{28}N_4O_3$	408	107, 84*, 77, 55, 42	409.2234	107.0516, 98.0968, 46.0657
	N-Pyrrolidino Protonitazene	-C_4H_8-		OC_3H_7	NO_2	CH_2	$C_{23}H_{28}N_4O_3$	408	107, 84*, 77, 55, 42	409.2234	107.0516, 98.0956, 46.0657
Nitro Variants	Metodesnitazene	C_2H_5	C_2H_5	OCH_3	H	CH_2	$C_{21}H_{27}N_3O$	337	235, 121, 86*, 77, 58	338.2227	121.0640, 100.1113, 72.0806
	Etodesnitazene	C_2H_5	C_2H_5	OC_2H_5	H	CH_2	$C_{22}H_{29}N_3O$	351	135, 107, 86*, 58, 42	352.2383	100.1129, 72.0831
	5-Methyl Etodesnitazene	C_2H_5	C_2H_5	OC_2H_5	CH_3	CH_2	$C_{23}H_{31}N_3O$	365	135, 107, 86*, 77, 58	366.2540	100.1116, 72.0808
	5-Amino Isotonitazene	C_2H_5	C_2H_5	*iso*-OC_3H_7	NH_2	CH_2	$C_{23}H_{32}N_4O$	380	146, 107, 86*, 58, 43	381.2649	149.0591, 107.0483, 100.1127, 72.0808
	5-Cyano Isotodesnitazene	C_2H_5	C_2H_5	*iso*-OC_3H_7	CN	CH_2	$C_{24}H_{30}N_4O$	390	262, 107, 86*, 58, 43	391.2492	107.0491, 100.1121
Others	Flunitazene	C_2H_5	C_2H_5	F	NO_2	CH_2	$C_{20}H_{23}FN_4O_2$	370	109, 86*, 58, 42	371.1878	109.0435, 100.1110, 72.0800
	Clonitazene	C_2H_5	C_2H_5	Cl	NO_2	CH_2	$C_{20}H_{23}ClN_4O_2$	386	254, 125, 86*, 77, 58	387.1582	125.0140, 100.1112, 72.0799
	Methylenedioxynitazene	C_2H_5	C_2H_5	-O_2CH_2-	NO_2	CH_2	$C_{21}H_{24}N_4O_4$	396	135, 86*, 76, 58, 42	397.1870	135.0443, 100.1121, 72.0809
	N-Piperidinyl Etonitazene	-C_5H_{10}-		OC_2H_5	NO_2	CH_2	$C_{23}H_{28}N_4O_3$	408	135, 107, 98*, 70, 55	409.2234	135.0821, 112.1112, 107.0496
	N-Pyrrolidino Fluetonitazene	-C_4H_8-		OC_2H_4F	NO_2	CH_2	$C_{22}H_{25}FN_4O_3$	412	153, 107, 84*, 55, 42	413.1983	107.0491, 98.0964
	Fluetonitazene	C_2H_5	C_2H_5	OC_2H_4F	NO_2	CH_2	$C_{22}H_{27}FN_4O_3$	414	153, 107, 86*, 58, 42	415.2140	153.0714, 100.1119, 72.0812, 44.0499
	N-Pyrrolidino Ethylene Isotonitazene	-C_4H_8-		*iso*-OC_3H_7	NO_2	C_2H_4	$C_{24}H_{30}N_4O_3$	422	250, 107, 84*, 55, 42	423.2391	107.0488, 98.0959, 69.0699

Key: *M.I. = Molecular Ion, * = Base Peak, [M+H]+ = Protonated Molecular Ion, ‡ = Experimental Data*

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