

Table S1. Inclusion list used during liquid chromatography-high-resolution tandem mass spectrometry analysis for 5-methyl etodesnitazene metabolite identification.

Transformation	Elemental composition	[M+H] ⁺ [M+2H] ²⁺ (m/z)	[M-H] ⁻ [M-2H] ²⁻ (m/z)
Parent	<u>C₂₃H₃₁N₃O</u>	366.2540 183.6306	364.2394 181.6161
-2C-4H	C ₂₁ H ₂₇ N ₃ O	338.2227 169.6150	336.2081 167.6004
+4C+4H+6O	C ₂₇ H ₃₅ N ₃ O ₇	514.2548 257.6310	512.2402 255.6164
+O	C ₂₃ H ₃₁ N ₃ O ₂	382.2489 191.6281	380.2344 189.6135
-4C-8H	C ₁₉ H ₂₃ N ₃ O	310.1914 155.5993	308.1768 153.5848
+2C+6O	C ₂₅ H ₃₁ N ₃ O ₇	486.2235 243.6153	484.2089 241.6008
-2C-4H+O	C ₂₁ H ₂₇ N ₃ O ₂	354.2176 177.6124	352.2031 175.5979
+4C+4H+7O	C ₂₇ H ₃₅ N ₃ O ₈	530.2497 265.6284	528.2351 263.6139
+2O	C ₂₃ H ₃₁ N ₃ O ₃	398.2438 199.6255	396.2293 197.6109
+6C+8H+7O	C ₂₉ H ₃₉ N ₃ O ₈	558.2810 279.6441	556.2664 277.6296
-2H+O	C ₂₃ H ₂₉ N ₃ O ₂	380.2333 190.6202	378.2187 188.6057
-2H+2O	C ₂₃ H ₂₉ N ₃ O ₃	396.2282 198.6177	394.2137 196.6032
-2C-6H+O	C ₂₁ H ₂₅ N ₃ O ₂	352.2020 176.6046	350.1874 174.5901
+4C+2H+7O	C ₂₇ H ₃₃ N ₃ O ₈	528.2340 264.6207	526.2195 262.6061
-2C-4H+3O+S	C ₂₁ H ₂₇ N ₃ O ₄ S	418.1795 209.5934	416.1650 207.5788
-4C-8H+O	C ₁₉ H ₂₃ N ₃ O ₁	326.1863 163.5968	324.1718 161.5822
-4C-9H-N+O	C ₁₉ H ₂₂ N ₂ O ₂	311.1754 156.0913	309.1609 154.0768
+2C-H-N+7O	C ₂₅ H ₃₀ N ₂ O ₈	487.2075 244.1074	485.1929 242.0928
+4O+S	C ₂₃ H ₃₁ N ₃ O ₅ S	462.2057 231.6065	460.1912 229.5919
-6C-13H-N	C ₁₇ H ₁₈ N ₂ O	267.1492 134.0782	265.1346 132.0637
-4C-9H-N+2O	C ₁₉ H ₂₂ N ₂ O ₃	327.1703 164.0888	325.1558 161.0664

-4C-11H-N+2O	$C_{19}H_{20}N_2O_3$	325.1547	323.1401
		163.0810	161.0664
-4C-9H-N+4O+S	$C_{19}H_{22}N_2O_5S$	391.1322	389.1177
		196.0697	174.0552
