

Table S2-1. Inclusion list used during liquid chromatography-high-resolution tandem mass spectrometry (LC-HRMS/MS) for isotonitazene metabolite identification

Isotonitazene			
Transformation	Elemental composition	[M+H] ⁺ m/z	[M-H] ⁻ m/z
Parent (Isotonitazene)	C ₂₃ H ₃₀ N ₄ O ₃	411.2391	409.2245
-3C -6H	C ₂₀ H ₂₄ N ₄ O ₃	369.1921	367.1776
-2C -4H	C ₂₁ H ₂₆ N ₄ O ₃	383.2078	381.1932
+2H -2O	C ₂₃ H ₃₂ N ₄ O	381.2649	379.2503
-O	C ₂₃ H ₃₀ N ₄ O ₂	395.2442	393.2296
+2H -O	C ₂₃ H ₃₂ N ₄ O ₂	397.2598	395.2453
+O	C ₂₃ H ₃₀ N ₄ O ₄	427.2340	425.2194
+6C +9H +6O	C ₂₉ H ₃₉ N ₄ O ₉	587.2712	-
+10C +16H +2N +4O +S	C ₃₃ H ₄₆ N ₆ O ₇ S	671.3221	669.3076
+5C +8H +O +S	C ₂₈ H ₃₈ N ₄ O ₄ S	527.2687	525.2541
-5C -10H	C ₁₈ H ₂₀ N ₄ O ₃	341.1608	339.1463
-4C -8H	C ₁₉ H ₂₂ N ₄ O ₃	355.1765	353.1619
-4C -9H -N +O	C ₁₉ H ₂₁ N ₃ O ₄	356.1605	354.1459
-4C -11H -N +O	C ₁₉ H ₁₉ N ₃ O ₄	354.1448	352.1303
-4C -11H -N +2O	C ₁₉ H ₁₉ N ₃ O ₅	370.1397	368.1252
+3C +2H +6O	C ₂₆ H ₃₂ N ₄ O ₉	545.2242	543.2097
-3C -6H +3O +S	C ₂₀ H ₂₄ N ₄ O ₆ S	449.1489	447.1344
+2C -H -N +7O	C ₂₅ H ₂₉ N ₃ O ₁₀	532.1926	530.1780
-4C -9H -N +4O +S	C ₁₉ H ₂₁ N ₃ O ₇ S	436.1173	434.1027
+2C +4H -O	C ₂₅ H ₃₄ N ₄ O ₂	423.2755	421.2609
+2H +2O	C ₂₃ H ₃₂ N ₄ O ₅	445.2445	443.2300
-2H	C ₂₃ H ₂₈ N ₄ O ₃	409.2234	407.2089
-2H +O	C ₂₃ H ₂₈ N ₄ O ₄	425.2183	423.2038
-3C -6H +O	C ₂₀ H ₂₄ N ₄ O ₄	385.1870	383.1725
-7C -15H -N +O	C ₁₆ H ₁₅ N ₃ O ₄	314.1135	312.0990
-7C -17H -N +O	C ₁₆ H ₁₃ N ₃ O ₄	312.0979	310.0833
-2C -4H +O	C ₂₁ H ₂₆ N ₄ O ₄	399.2027	397.1881
+4C +5H +6O	C ₂₇ H ₃₅ N ₄ O ₉	559.2399	-
+2O	C ₂₃ H ₃₀ N ₄ O ₅	443.2289	441.2143
+6C +8H +7O	C ₂₉ H ₃₈ N ₄ O ₁₀	603.2661	601.2515
+4O +S	C ₂₃ H ₃₀ N ₄ O ₇ S	507.1908	505.1762
-4C -9H -N +2O	C ₁₉ H ₂₁ N ₃ O ₅	372.1554	370.1408

Table S2-2. Inclusion list used during liquid chromatography-high-resolution tandem mass spectrometry (LC-HRMS/MS) for metonitazene metabolite identification

Metonitazene			
Transformation	Elemental composition	[M+H] ⁺ m/z	[M-H] ⁻ m/z
Parent (Metonitazene)	C ₂₁ H ₂₆ N ₄ O ₃	383.2078	381.1932
-C -2H	C ₂₀ H ₂₄ N ₄ O ₃	369.1921	367.1776
-2C -4H	C ₁₉ H ₂₂ N ₄ O ₃	355.1765	353.1619
+2H -2O	C ₂₁ H ₂₈ N ₄ O	353.2336	351.2190
-O	C ₂₁ H ₂₆ N ₄ O ₂	367.2129	365.1983
+2H -O	C ₂₁ H ₂₈ N ₄ O ₂	369.2285	367.2140
+O	C ₂₁ H ₂₆ N ₄ O ₄	399.2027	397.1881
+6C +9H +6O	C ₂₇ H ₃₅ N ₄ O ₉	559.2399	-
+10C +16H +2N +4O +S	C ₃₁ H ₄₂ N ₆ O ₇ S	643.2908	641.2763
+5C +8H +O +S	C ₂₆ H ₃₄ N ₄ O ₄ S	499.2374	497.2228
-3C -6H	C ₁₈ H ₂₀ N ₄ O ₃	341.1608	339.1463
-4C -8H	C ₁₇ H ₁₈ N ₄ O ₃	327.1452	325.1306
-4C -9H -N +O	C ₁₇ H ₃₇ N ₃ O ₄	328.1292	326.1146
-4C -11H -N +O	C ₁₇ H ₁₅ N ₃ O ₄	326.1135	324.0990
-4C -11H -N +2O	C ₁₇ H ₁₅ N ₃ O ₅	342.1084	340.0939
+5C +6H +6O	C ₂₆ H ₃₂ N ₄ O ₉	545.2242	543.2097
-C -2H +3O +S	C ₂₀ H ₂₄ N ₄ O ₆ S	449.1489	447.1344
+2C -H -N +7O	C ₂₃ H ₂₅ N ₃ O ₁₀	504.1613	502.1467
-4C -9H -N +4O +S	C ₁₇ H ₁₇ N ₃ O ₇ S	408.0860	406.0714
+2C +4H -O	C ₂₃ H ₃₀ N ₄ O ₂	395.2442	393.2296
+2H +2O	C ₂₁ H ₂₈ N ₄ O ₅	417.2132	415.1987
-2H	C ₂₁ H ₂₄ N ₄ O ₃	381.1921	379.1776
-2H +O	C ₂₁ H ₂₄ N ₄ O ₄	397.1870	395.1725
-C -2H +O	C ₂₀ H ₂₄ N ₄ O ₄	385.1870	383.1725
-5C -11H -N +O	C ₁₆ H ₁₅ N ₃ O ₄	314.1135	312.0990
-5C -13H -N +O	C ₁₆ H ₁₃ N ₃ O ₄	312.0979	310.0833
-2C -4H +O	C ₁₉ H ₂₂ N ₄ O ₄	371.1714	369.1568
+4C +5H +6O	C ₂₅ H ₃₁ N ₄ O ₉	531.2086	-
+2O	C ₂₁ H ₂₆ N ₄ O ₅	415.1976	413.1830
+6C +8H +7O	C ₂₇ H ₃₄ N ₄ O ₁₀	575.2348	573.2202
+4O +S	C ₂₁ H ₂₆ N ₄ O ₇ S	479.1595	477.1449
-4C -9H -N +2O	C ₁₇ H ₁₇ N ₃ O ₅	344.1241	342.1095
+6C +9H +7O	C ₂₇ H ₃₅ N ₄ O ₁₀	575.2348	-

Table S2-3. Inclusion list used during liquid chromatography-high-resolution tandem mass spectrometry (LC-HRMS/MS) for etodesnitazene metabolite identification

Etodesnitazene			
Transformation	Elemental composition	[M+H] ⁺ m/z	[M-H] ⁻ m/z
Parent (Etodesnitazene)	C ₂₂ H ₂₉ N ₃ O	352.2383	350.2238
-2C -4H	C ₂₀ H ₂₅ N ₃ O	324.2070	322.1925
+O	C ₂₂ H ₂₉ N ₃ O ₂	368.2333	366.2187
-4C -8H	C ₁₈ H ₂₁ N ₃ O	296.1757	294.1612
-4C -9H -N +O	C ₁₈ H ₂₀ N ₂ O ₂	297.1598	295.1452
-4C -11H -N +O	C ₁₈ H ₁₈ N ₂ O ₂	295.1441	293.1296
-4C -11H -N +2O	C ₁₈ H ₁₈ N ₂ O ₃	311.1390	309.1245
+4C +4H +6O	C ₂₆ H ₃₃ N ₃ O ₇	500.2391	498.2246
-2C -4H +3O +S	C ₂₀ H ₂₅ N ₃ O ₄ S	404.1639	402.1493
+2C -H -N +7O	C ₂₄ H ₂₈ N ₂ O ₈	473.1918	471.1773
-4C -9H -N +4O +S	C ₁₈ H ₂₀ N ₂ O ₅ S	377.1166	375.1020
+2H +2O	C ₂₂ H ₃₁ N ₃ O ₃	386.2438	384.2293
-2H	C ₂₂ H ₂₇ N ₃ O	350.2227	348.2081
-2H +O	C ₂₂ H ₂₇ N ₃ O ₂	366.2176	364.2031
-2C -4H +O	C ₂₀ H ₂₅ N ₃ O ₂	340.2020	338.1874
-6C -13H -N +O	C ₁₆ H ₁₆ N ₂ O ₂	269.1285	267.1139
-6C -15H -N +O	C ₁₆ H ₁₄ N ₂ O ₂	267.1128	265.0983
+2O	C ₂₂ H ₂₉ N ₃ O ₃	384.2282	382.2136
+6C +8H +7O	C ₂₈ H ₃₇ N ₃ O ₈	544.2653	542.2508
+4O +S	C ₂₂ H ₂₉ N ₃ O ₅ S	448.1901	446.1755
-4C -9H -N +2O	C ₁₈ H ₂₀ N ₂ O ₃	313.1547	311.1401
+10C +17H +3N +7O +S	C ₃₂ H ₄₆ N ₆ O ₈ S	675.3171	673.3025

Table S2-4. Inclusion list used during liquid chromatography-high-resolution tandem mass spectrometry (LC-HRMS/MS) for metodesnitazene metabolite identification

Metodesnitazene			
Transformation	Elemental composition	[M+H]⁺ m/z	[M-H]⁻ m/z
Parent (Metodesnitazene)	C ₂₁ H ₂₇ N ₃ O	338.2227	336.2081
-C -2H	C ₂₀ H ₂₅ N ₃ O	324.2070	322.1925
-2C -4H	C ₁₉ H ₂₃ N ₃ O	310.1914	308.1768
+O	C ₂₁ H ₂₇ N ₃ O ₂	354.2176	352.2031
-3C -6H	C ₁₈ H ₂₁ N ₃ O	296.1757	294.1612
-4C -8H	C ₁₇ H ₁₉ N ₃ O	282.1601	280.1455
-4C -9H -N +O	C ₁₇ H ₁₈ N ₂ O ₂	283.1441	281.1296
-4C -11H -N +O	C ₁₇ H ₁₆ N ₂ O ₂	281.1285	279.1139
-4C -11H -N +2O	C ₁₇ H ₁₆ N ₂ O ₃	297.1234	295.1088
+5C +6H +6O	C ₂₆ H ₃₃ N ₃ O ₇	500.2391	498.2246
-C -2H +3O +S	C ₂₀ H ₂₅ N ₃ O ₄ S	404.1639	402.1493
+2C -H -N +7O	C ₂₃ H ₂₆ N ₂ O ₈	459.1762	457.1616
-4C -9H -N +4O +S	C ₁₇ H ₁₈ N ₂ O ₅ S	363.1009	361.0864
+2H +2O	C ₂₁ H ₂₉ N ₃ O ₃	372.2282	370.2136
-2H	C ₂₁ H ₂₅ N ₃ O	336.2070	334.1925
-2H +O	C ₂₁ H ₂₅ N ₃ O ₂	352.2020	350.1874
-C -2H +O	C ₂₀ H ₂₅ N ₃ O ₂	340.2020	338.1874
-5C -11H -N +O	C ₁₆ H ₁₆ N ₂ O ₂	269.1285	267.1139
-5C -13H -N +O	C ₁₆ H ₁₄ N ₂ O ₂	267.1128	265.0983
-2C -4H +O	C ₁₉ H ₂₃ N ₃ O ₂	326.1863	324.1718
+2O	C ₂₁ H ₂₇ N ₃ O ₃	370.2125	368.1980
+6C +8H +7O	C ₂₇ H ₃₅ N ₃ O ₈	530.2497	528.2351
+4O +S	C ₂₁ H ₂₇ N ₃ O ₅ S	434.1744	432.1599
-4C -9H -N +2O	C ₁₇ H ₁₈ N ₂ O ₃	299.1390	297.1245
+10C +17H +3N +7O +S	C ₃₁ H ₄₄ N ₆ O ₈ S	661.3014	659.2869