

Table 1. Summary of the analytical characterization.

	LC-QTOF-MS			GC-MS		HPLC-DAD	
	RT _a (min)	Parent (m/z)	Fragments (m/z) Bold: most abundant, <i>italic</i> : selective	RT _a (min)	Fragments (m/z)	RT _a (min)	Ab. max. ^b (nm)
1. Isotonitazene	5.86	411.2436	44.05, 72.08, 100.11 , 107.05, 149.09, 250.11, 296.10	29.61	58, 86, 107	19.98	237.4 - 306.7
2. N-desethyl-isotonitazene	5.70	383.2095	44.05, 72.08 , 107.05, 176.05, 224.09, 270.08, 312.13	29.21	58, 107, 149, 325	20.13	238.4 - 305.8
3. 4'-OH-nitazene	3.94	369.1949	44.05, 72.08, 100.11 , 107.05, 250.11, 296.10	18.62*	58,86,107*	11.21	237.8 - 305.0
4. 5-aminoisotonitazene	3.42	381.2696	44.05, 72.08, 100.11 , 107.05, 149.09, 266.13	26.89	58, 86, 107, 380	7.65	222.7 - 273.6 - 307.6
5. Metonitazene	4.91	383.2123	44.05, 72.08, 100.11 , 121.06, 264.13, 310.12	28.57	58, 86, 121	15.91	237.8 - 308.5
6. Etonitazene	5.44	397.2255	44.05, 72.08, 100.11 , 107.05, 135.08, 278.14, 324.13	29.58	58, 86, 107, 135	18.39	238.1 - 305.8
7. Protonitazene	6.11	411.2466	44.05, 72.08, 100.11 , 107.05, 149.10, 250.11, 292.16, 338.15	31.03	58, 86, 107	20.68	237.4 - 306.7
8. Clonitazene	5.57	387.1613	44.05, 72.08, 100.11 , 125.01, 268.07, 314.07	28.09	58, 86, 125	18.63	238.4 - 305.8
9. Flunitazene	4.99	371.1890	44.05, 72.08, 100.11 , 109.04, 252.11, 298.10	25.45	58, 86, 109	15.92	238.8 - 304.1
10. Isotodesnitazene	4.94	366.2573	44.05, 72.08, 100.11 , 107.05, 149.09, 251.11	23.57	58, 86, 107, 365	14.37	269.6 - 276.6
11. Metodesnitazene	3.77	338.2251	44.05, 72.08, 100.11 , 121.06, 250.11, 265.13	22.94	58, 86, 121, 337	7.89	269.6 - 276.6
12. Etodesnitazene	4.43	352.2409	44.05, 72.08, 100.11 , 107.05, 135.08, 279.15	23.41	58, 86, 107, 135, 351	11.62	269.6 - 276.6

a, retention time; b, absorption maximum; *, alternative GC-MS method was employed (cfr. Methods section).

