

Supplementary Material

Portable near infrared spectroscopy (microNIR) applied to abuse drugs and medicines analyzes

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Table 1S. Active ingredients identified by CG-MS analysis

Samples	Active ingredient identified by CG-MS
C ₁	Amphetamine, FA, Methamphetamine, MDMA, and 2CB
C ₂	Amphetamine, and caffeine
C ₃	Amphetamine, and caffeine
C ₄	MDMA
C ₅	MDMA
C ₆	MDMA
C ₇	MDMA
C ₈	Ethylone, and Ketamine
C ₉	Ethylone, and Ketamine
C ₁₀	Ethylone, and Ketamine
C ₁₁	MDMA
C ₁₂	MDMA
C ₁₃	MDMA
C ₁₄	MDMA
C ₁₅	MDMA
C ₁₆	MDMA
C ₁₇	MDMA
C ₁₈	MDMA, and Ethylone
C ₁₉	MDA

Table 2S. m/z values, mass error (ppm), DBE, empirical formula and proposed structures for the signals detected from PS(+)MS analysis for *designer drugs* samples.

Samples	Proposed structures	[M+H] ⁺	measured m/z	theoretical m/z	Error (ppm)	DBE
S₁	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.07185	428.07171	-0.33	8
	25B-NBOMe	[C ₁₈ H ₂₂ BrNO ₃ +H] ⁺	380.08564	380.08558	-0.14	8
	25C-NBOMe	[C ₁₈ H ₂₂ CINO ₃ +H] ⁺	336.13615	336.1361	-0.16	8
S₂	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.07186	428.07171	-0.35	8
S₃	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.07190	428.07171	-0.44	8
S₄	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.07183	428.07171	-0.28	8
S₅	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.07186	428.07171	-0.35	8
S₆	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.0719	428.07171	-0.45	8
S₇	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.07187	428.07171	-0.37	8
S₈	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.07177	428.07171	-0.14	8
S₉	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.07182	428.07171	-0.26	8
S₁₀	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.07189	428.07171	-0.41	8
S₁₁	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.07195	428.07171	-0.54	8
S₁₂	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.07184	428.07171	-0.30	8
S₁₃	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.07289	428.07171	-2.74	8
	DOC	[C ₁₁ H ₁₆ CINO ₂ +H] ⁺	230.09450	230.09423	-1.18	4
S₁₄	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.07289	428.07171	-2.74	8
	DOC	[C ₁₁ H ₁₆ CINO ₂ +H] ⁺	230.09450	230.09423	-1.18	4
S₁₅	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.07289	428.07171	-2.74	8
	DOC	[C ₁₁ H ₁₆ CINO ₂ +H] ⁺	230.09450	230.09423	-1.18	4
S₁₆	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.07171	428.07171	0.01	8
S₁₇	LSD*	-	-	-	-	-
S₁₈	LSD*	-	-	-	-	-
S₁₉	25I-Nbome*	-	-	-	-	-
S₂₀	25I-Nbome*	-	-	-	-	-
S₂₁	DOC	[C ₁₁ H ₁₆ CINO ₂ +H] ⁺	230.09413	230.09423	0.46	4
	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.07181	428.07171	-0.23	8
S₂₂	DOC	[C ₁₁ H ₁₆ CINO ₂ +H] ⁺	230.09426	230.09423	-0.12	4
	25I-NBOMe	[C ₁₈ H ₂₂ INO ₃ +H] ⁺	428.07182	428.07171	-0.24	8

*Active ingredients were identified by thin layer chromatography in samples S₁₇-S₂₀.

Table 3S. Chemical composition of Desobesi-M®, Sibutramina®, Pramil®, Erofast®, Dualid-S® e Fingrass® medicines obtained from GC-MS analysis.

Sample	Label	Compostion		Report
		Active principle	Compound found	
Desobesi	Desobesi-M®	Fenproporex hydrochloride	Sibutramine	Counterfeit medicine/no active national registration
Dualid-S	Dualid-S®	Amfepramone hydrochloride	Fluoxetine	Counterfeit medicine/no active national registration
Dualid-S	Dualid-S®	Amfepramone hydrochloride	Fluoxetine	Counterfeit medicine/no active national registration
Pramil	Pramil®	Sildenafil	Sildenafil	Authentic medicine/no active national registration
Sibutramina	Sibutramina®	Sibutramine	Sibutramine	Authentic medicine/no active national registration
Sibutramina	Sibutramina®	Sibutramine	Sibutramine	Authentic medicine/no active national registration nacional
Sibutramina	Sibutramina®	Sibutramine	Sibutramine	Authentic medicine/no active national registration
Fingrass	Fingrass®	Sibutramine	Sibutramine	Authentic medicine/no active national registration
Fingrass	Fingrass®	Sibutramine	Sibutramine	Authentic medicine/no active national registration
Erofast	Erofast®	Sildenafil	Sildenafil	Authentic medicine/no active national registration
Sibutramina	Sibutramina®	Sibutramine	Benzocaine/caffeine	Counterfeit medicine/no active national

				registration
Pramil	Pramil®	Sildenafil	Sildenafil	Authentic medicine/no active national registration
Pramil	Pramil®	Sildenafil	Sildenafil	Authentic medicine/no active national registration
Pramil	Pramil®	Sildenafil	Sildenafil	Authentic medicine/no active national registration
Pramil	Pramil®	Sildenafil	Sildenafil	Authentic medicine/no active national registration
Pramil	Pramil®	Sildenafil	Sildenafil	Authentic medicine/no active national registration
Pramil	Pramil®	Sildenafil	Sildenafil	Authentic medicine/no active national registration
Desobesi	Desobesi-M®	Fenproporex hydrochloride	Sibutramine	Counterfeit medicine/no active national registration
Desobesi	Desobesi-M®	Fenproporex hydrochloride	Sibutramine	Counterfeit medicine/no active national registration
Desobesi	Desobesi-M®	Fenproporex hydrochloride	Sibutramine	Counterfeit medicine/no active national registration
Desobesi	Desobesi-M®	Fenproporex hydrochloride	Sibutramine	Counterfeit medicine/no active national registration
Desobesi	Desobesi-M®	Fenproporex hydrochloride	Sibutramine	Counterfeit medicine/no active national registration
Pramil	Pramil®	Sildenafil	Sildenafil	Authentic medicine/no active national registration