

Supplementary Information

Use of Coconut Charcoal and Menthone-Thiosemicarbazone Polymer as Solid Phase Materials for the Determination of *N,N*-Dimethyltryptamine, Harmine, Harmaline, Harmalol, and Tetrahydroharmine in Ayahuasca Beverage by Liquid Chromatography-Tandem Mass Spectrometry

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Table S1. Crystal data, data collection, and structure refinement parameter details for menthone-thiosemicarbazone compound

Chemical formula	C ₁₂ H ₂₃ N ₃ S
<i>M_r</i>	241.39
Crystal system, space group	monoclinic, <i>P</i> 2 ₁
Temperature / K	123
<i>a</i> , <i>b</i> , <i>c</i> / Å	11.5579 (5), 9.9279 (4), 12.5271 (5)
β / °	95.030 (2)
<i>V</i> / Å ³	1431.90 (10)
<i>Z</i>	4
Radiation type	Mo Kα
μ / mm ⁻¹	0.21
Crystal size / mm	0.77 × 0.30 × 0.08
Data collection	
Diffractometer	Nonius KappaCCD
Absorption correction	analytical
T _{min} , T _{max}	0.857, 0.984
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	23116, 6380, 5069
R _{int}	0.075
(sin θ/λ) _{max} / Å ⁻¹	0.649
Refinement	
R [<i>F</i> ² > 2σ(<i>F</i> ²)], w R(<i>F</i> ²), S	0.044, 0.104, 1.06
No. of reflections	6380
No. of parameters	297
No. of restraints	1
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} / (e Å ⁻³)	0.24, -0.37
Absolute structure	Flack <i>x</i> determined using 1954 quotients [(<i>I</i> ⁺) - (<i>I</i> ⁻)] / [(<i>I</i> ⁺) + (<i>I</i> ⁻)]
Absolute structure parameter	0.00 (7)