

## 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 <sub>12</sub> H <sub>23</sub> N <sub>3</sub> S
$M_r$	241.39
Crystal system, space group	monoclinic, $P2_1$
Temperature / K	123
$a, b, c / \text{\AA}$	11.5579 (5), 9.9279 (4), 12.5271 (5)
$\beta / ^\circ$	95.030 (2)
$V / \text{\AA}^3$	1431.90 (10)
Z	4
Radiation type	Mo K $\alpha$
$\mu / \text{mm}^{-1}$	0.21
Crystal size / mm	0.77 $\times$ 0.30 $\times$ 0.08
Data collection	
Diffractometer	Nonius KappaCCD
Absorption correction	analytical
$T_{\min}, T_{\max}$	0.857, 0.984
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	23116, 6380, 5069
$R_{\text{int}}$	0.075
$(\sin \theta/\lambda)_{\max} / \text{\AA}^{-1}$	0.649
Refinement	
$R [F^2 > 2\sigma(F^2)], w R(F^2), S$	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
$\Delta\rho_{\max}, \Delta\rho_{\min} / (\text{e \AA}^{-3})$	0.24, -0.37
Absolute structure	Flack $x$ determined using 1954 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$
Absolute structure parameter	0.00 (7)