

Supporting Information

Detection and Quantification of Psychoactive *N,N*-Dimethyltryptamine in Ayahuasca Brews by Ambient Ionization High-Resolution Mass Spectrometry

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This document contains mass measurement and relative intensity data of tryptamines and β -carbolines in ayahuasca brews, analyzed by DART-HRMS.

Table S1. Mass measurements and relative intensities observed by DART-HRMS for secondary metabolites detected in ayahuasca brews. The corresponding DART-HRMS spectra are presented in Fig. 3.						
Ayahuasca Brew	Compound*	Protonated Formula	Measured	Calculated	Diff.**	Rel. Int. (%)
Brew 1 <i>M. hostilis</i> <i>B. caapi</i>	<i>N</i> -methyltryptamine (NMT)	[C ₁₁ H ₁₄ N ₂ + H] ⁺	175.122	175.124	-2	5.4
	<i>N,N</i> -dimethyltryptamine (DMT)	[C ₁₂ H ₁₆ N ₂ + H] ⁺	189.140	189.139	1	100.0
	Harmalol	[C ₁₂ H ₁₂ N ₂ O + H] ⁺	201.105	201.103	2	2.0
	Harmine	[C ₁₃ H ₁₂ N ₂ O + H] ⁺	213.101	213.103	-2	49.0
	Harmaline	[C ₁₃ H ₁₄ N ₂ O + H] ⁺	215.116	215.118	-2	4.7
Brew 2 <i>M. hostilis</i> <i>P. harmala</i>	<i>N</i> -methyltryptamine (NMT)	[C ₁₁ H ₁₄ N ₂ + H] ⁺	175.122	175.124	-2	2.3
	<i>N,N</i> -dimethyltryptamine (DMT)	[C ₁₂ H ₁₆ N ₂ + H] ⁺	189.136	189.139	-3	50.5
	Harmalol	[C ₁₂ H ₁₂ N ₂ O + H] ⁺	201.101	201.103	-2	1.5
	Harmine	[C ₁₃ H ₁₂ N ₂ O + H] ⁺	213.101	213.103	-2	43.8
	Harmaline	[C ₁₃ H ₁₄ N ₂ O + H] ⁺	215.120	215.118	2	100.0
Brew 3 <i>P. viridis</i> <i>B. caapi</i>	<i>N</i> -methyltryptamine (NMT)	[C ₁₁ H ₁₄ N ₂ + H] ⁺	175.122	175.124	-2	1.1
	<i>N,N</i> -dimethyltryptamine (DMT)	[C ₁₂ H ₁₆ N ₂ + H] ⁺	189.136	189.139	-3	63.7
	Harmalol	[C ₁₂ H ₁₂ N ₂ O + H] ⁺	201.105	201.103	2	1.6
	Harmine	[C ₁₃ H ₁₂ N ₂ O + H] ⁺	213.104	213.103	1	100.0
	Harmaline	[C ₁₃ H ₁₄ N ₂ O + H] ⁺	215.116	215.118	-2	17.8
Brew 4 <i>P. viridis</i> <i>P. harmala</i>	<i>N</i> -methyltryptamine (NMT)	[C ₁₁ H ₁₄ N ₂ + H] ⁺	175.122	175.124	-2	1.4
	<i>N,N</i> -dimethyltryptamine (DMT)	[C ₁₂ H ₁₆ N ₂ + H] ⁺	189.136	189.139	-3	73.4
	Harmalol	[C ₁₂ H ₁₂ N ₂ O + H] ⁺	201.102	201.103	-1	1.1
	Harmine	[C ₁₃ H ₁₂ N ₂ O + H] ⁺	213.104	213.103	1	100.0
	Harmaline	[C ₁₃ H ₁₄ N ₂ O + H] ⁺	215.116	215.118	-2	10.8
Brew 5 <i>D. cabrerana</i> <i>B. caapi</i>	<i>N</i> -methyltryptamine (NMT)	[C ₁₁ H ₁₄ N ₂ + H] ⁺	175.122	175.124	-2	0.5
	<i>N,N</i> -dimethyltryptamine (DMT)	[C ₁₂ H ₁₆ N ₂ + H] ⁺	189.136	189.139	-3	63.2
	Harmalol	[C ₁₂ H ₁₂ N ₂ O + H] ⁺	201.105	201.103	2	1.5
	Harmine	[C ₁₃ H ₁₂ N ₂ O + H] ⁺	213.104	213.103	1	100.0
	Harmaline	[C ₁₃ H ₁₄ N ₂ O + H] ⁺	215.116	215.118	-2	21.6
Brew 6 <i>D. cabrerana</i> <i>P. harmala</i>	<i>N</i> -methyltryptamine (NMT)	[C ₁₁ H ₁₄ N ₂ + H] ⁺	175.126	175.124	2	0.3
	<i>N,N</i> -dimethyltryptamine (DMT)	[C ₁₂ H ₁₆ N ₂ + H] ⁺	189.138	189.139	-1	36.7
	Harmalol	[C ₁₂ H ₁₂ N ₂ O + H] ⁺	201.102	201.103	-1	0.9
	Harmine	[C ₁₃ H ₁₂ N ₂ O + H] ⁺	213.101	213.103	-2	48.5
	Harmaline	[C ₁₃ H ₁₄ N ₂ O + H] ⁺	215.120	215.118	2	100.0

*Compound identities are tentatively assigned based on calculated and measured masses, and compounds previously identified in ayahuasca brews and their constituent plant materials.
**Differences are reported in millimass units (mmu).