

Supporting Information

Rapid detection and quantification of hallucinogenic salvinorin A in commercial *Salvia divinorum* products by DART-HRMS

AUTHORS: Megan I. Chambers^a, Justine E. Giffen-Lemieux^a and Rabi A. Musah^{a*}

^aUniversity at Albany State University of New York, Department of Chemistry, 1400 Washington Avenue, Albany, NY 12222

*Corresponding author: rmusah@albany.edu

This document contains: (1) mass measurements and relative intensities of salvinorins and divinorins in *Salvia* products.

Table S1. Mass measurements and relative intensities observed by DART-HRMS for salvinorins and divinatorins in Salvia products. The corresponding DART-HR mass spectra are presented in Fig. 4.							
Salvia Product	Compound*	Protonated Formula	Measured	Calculated	Diff. (mmu)	Rel Int. (%)	Ion Counts
Salvia Raw Leaf	Salvinorin C	[C ₂₅ H ₃₀ O ₉ + H] ⁺	475.2055	475.1963	9.2	1.4	1459
	Salvinorin J	[C ₂₃ H ₃₀ O ₈ + H] ⁺	435.2104	435.2013	9.1	0.3	284
	Salvinorins A, D, and E	[C ₂₃ H ₂₈ O ₈ + H] ⁺	433.1910	433.1857	5.3	6.8	7144
	Salvinorins B and H	[C ₂₁ H ₂₆ O ₇ + H] ⁺	391.1800	391.1751	4.9	5.1	5370
	Salvinorin F	[C ₂₁ H ₂₆ O ₆ + H] ⁺	375.1830	375.1802	2.8	6.1	6364
	Divinatorin B	[C ₂₁ H ₃₀ O ₅ + H] ⁺	363.2237	363.2166	7.1	0.5	546
	Divinatorin A	[C ₂₀ H ₂₈ O ₄ + H] ⁺	333.2102	333.2060	4.2	3.0	3113
Salvia 5x	Salvinorin J	[C ₂₃ H ₃₀ O ₈ + H] ⁺	435.2049	435.2013	3.6	0.4	836
	Salvinorins A, D, and E	[C ₂₃ H ₂₈ O ₈ + H] ⁺	433.1874	433.1857	1.7	9.8	21633
	Salvinorin I	[C ₂₁ H ₂₈ O ₇ + H] ⁺	393.1986	393.1908	7.8	0.2	342
	Salvinorins B and H	[C ₂₁ H ₂₆ O ₇ + H] ⁺	391.1802	391.1751	5.1	2.6	5746
	Salvinorin F	[C ₂₁ H ₂₆ O ₆ + H] ⁺	375.1730	375.1802	-7.2	6.5	14275
	Divinatorin A	[C ₂₀ H ₂₈ O ₄ + H] ⁺	333.2119	333.2060	5.9	0.3	565
Salvia 10x	Salvinorin C	[C ₂₅ H ₃₀ O ₉ + H] ⁺	475.2011	475.1963	4.8	1.2	2399
	Salvinorin J	[C ₂₃ H ₃₀ O ₈ + H] ⁺	435.2016	435.2013	0.3	0.5	1004
	Salvinorins A, D, and E	[C ₂₃ H ₂₈ O ₈ + H] ⁺	433.1852	433.1857	-0.5	13.0	25909
	Salvinorin G	[C ₂₃ H ₂₆ O ₈ + H] ⁺	431.1770	431.1700	7.0	0.7	1463
	Salvinorins B and H	[C ₂₁ H ₂₆ O ₇ + H] ⁺	391.1822	391.1751	7.1	2.7	5420
	Salvinorin F	[C ₂₁ H ₂₆ O ₆ + H] ⁺	375.1718	375.1802	-8.4	6.5	13035
	Divinatorin B	[C ₂₁ H ₃₀ O ₅ + H] ⁺	363.2174	363.2166	0.8	0.2	440
	Divinatorin A	[C ₂₀ H ₂₈ O ₄ + H] ⁺	333.2091	333.2060	3.1	0.8	1685
Salvia 15x	Salvinorin C	[C ₂₅ H ₃₀ O ₉ + H] ⁺	475.2021	475.1963	5.8	0.6	1572
	Salvinorin J	[C ₂₃ H ₃₀ O ₈ + H] ⁺	435.2030	435.2013	1.7	0.4	1151
	Salvinorins A, D, and E	[C ₂₃ H ₂₈ O ₈ + H] ⁺	433.1863	433.1857	0.6	10.9	29460
	Salvinorin I	[C ₂₁ H ₂₈ O ₇ + H] ⁺	393.1929	393.1908	2.1	0.2	451
	Salvinorins B and H	[C ₂₁ H ₂₆ O ₇ + H] ⁺	391.1841	391.1751	9.0	2.5	6864
	Salvinorin F	[C ₂₁ H ₂₆ O ₆ + H] ⁺	375.1720	375.1802	-8.2	8.2	22173
	Divinatorin B	[C ₂₁ H ₃₀ O ₅ + H] ⁺	363.2090	363.2166	-7.6	0.1	346
	Divinatorin A	[C ₂₀ H ₂₈ O ₄ + H] ⁺	333.2105	333.2060	4.5	0.3	816
Salvia 20x	Salvinorin J	[C ₂₃ H ₃₀ O ₈ + H] ⁺	435.2044	435.2013	3.1	0.4	1213
	Salvinorins A, D, and E	[C ₂₃ H ₂₈ O ₈ + H] ⁺	433.1880	433.1857	2.3	10.4	32405
	Salvinorins B and H	[C ₂₁ H ₂₆ O ₇ + H] ⁺	391.1798	391.1751	4.7	17.8	55575
	Salvinorin F	[C ₂₁ H ₂₆ O ₆ + H] ⁺	375.1730	375.1802	-7.2	7.4	23088
	Divinatorin A	[C ₂₀ H ₂₈ O ₄ + H] ⁺	333.2142	333.2060	8.2	0.2	599
Salvia 40x	Salvinorin C	[C ₂₅ H ₃₀ O ₉ + H] ⁺	475.2039	475.1963	7.6	0.9	2400
	Salvinorin J	[C ₂₃ H ₃₀ O ₈ + H] ⁺	435.2075	435.2013	6.2	0.2	628
	Salvinorins A, D, and E	[C ₂₃ H ₂₈ O ₈ + H] ⁺	433.1882	433.1857	2.5	5.5	15155
	Salvinorins B and H	[C ₂₁ H ₂₆ O ₇ + H] ⁺	391.1840	391.1751	8.9	1.0	2815
	Salvinorin F	[C ₂₁ H ₂₆ O ₆ + H] ⁺	375.1742	375.1802	-6.0	6.9	18818
	Divinatorin B	[C ₂₁ H ₃₀ O ₅ + H] ⁺	363.2206	363.2166	4.0	0.2	482
	Divinatorin A	[C ₂₀ H ₂₈ O ₄ + H] ⁺	333.2123	333.2060	6.3	0.6	1739
Salvia 50x	Salvinorin C	[C ₂₅ H ₃₀ O ₉ + H] ⁺	475.2036	475.1963	7.3	0.7	1956
	Salvinorin J	[C ₂₃ H ₃₀ O ₈ + H] ⁺	435.2015	435.2013	0.2	0.3	893
	Salvinorins A, D, and E	[C ₂₃ H ₂₈ O ₈ + H] ⁺	433.1844	433.1857	-1.3	7.6	20729
	Salvinorin I	[C ₂₁ H ₂₈ O ₇ + H] ⁺	393.1960	393.1908	5.2	0.2	653
	Salvinorins B and H	[C ₂₁ H ₂₆ O ₇ + H] ⁺	391.1822	391.1751	7.1	2.1	5661
	Divinatorin A	[C ₂₀ H ₂₈ O ₄ + H] ⁺	333.2082	333.2060	2.2	0.5	1488

Table S1 (cont.). Mass measurements and relative intensities observed by DART-HRMS for salvinorins and divinatorins in Salvia products. The corresponding DART-HR mass spectra are presented in Fig. 4.							
Salvia Product	Compound*	Protonated Formula	Measured	Calculated	Diff. (mmu)	Rel Int. (%)	Ion Counts
Salvia 60x	Salvinorin C	$[C_{25}H_{30}O_9 + H]^+$	475.2020	475.1963	5.7	0.9	2596
	Salvinorin J	$[C_{23}H_{30}O_8 + H]^+$	435.2037	435.2013	2.4	0.4	1233
	Salvinorins A, D, and E	$[C_{23}H_{28}O_8 + H]^+$	433.1865	433.1857	0.8	10.6	29928
	Salvinorin G	$[C_{23}H_{26}O_8 + H]^+$	431.1782	431.1700	8.2	1.1	2998
	Salvinorin I	$[C_{21}H_{28}O_7 + H]^+$	393.1993	393.1908	8.5	0.3	716
	Salvinorins B and H	$[C_{21}H_{26}O_7 + H]^+$	391.1850	391.1751	9.9	2.5	6966
	Salvinorin F	$[C_{21}H_{26}O_6 + H]^+$	375.1729	375.1802	-7.3	8.0	22636
	Divinatorin B	$[C_{21}H_{30}O_5 + H]^+$	363.2139	363.2166	-2.7	0.2	610
	Divinatorin A	$[C_{20}H_{28}O_4 + H]^+$	333.2069	333.2060	0.9	0.8	2389
*Compound identities are tentatively assigned based on calculated and measured masses, and compounds previously identified in Salvia plant materials/products.							