

Rapid Detection and Validated Quantification of Psychoactive Compounds in Complex Plant Matrices by Direct Analysis in Real Time High-Resolution Mass Spectrometry – Application to “Kava” Psychoactive Pepper Products

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Supporting Information

This document contains: (1) a figure showing the linear rail set up using DART-HRMS and Dip-it Tips; (2) raw data showing the peak areas and peak area ratios for yangonin (analyte) and yangonin-*d*₃ (IS) used to create the calibration curves; and (3) mass measurements and relative intensities of kavalactones and flavokavains in Kava products.



Figure S1. Linear rail system and holder used to position the Dip-it tips with samples between the ion source and the mass spectrometer inlet to introduce samples into the gas stream in order to automate the analysis of calibrators and Kava sample extractions.

RUN 1							
	Nominal	Analyte	IS	PAR	Recalculated	RE%	
Blank	Blank	5286.7	125.3	n/a	n/a	n/a	
Zero	0	209.3	167201.3	n/a	n/a	n/a	
LLOQ	5	30701.0	156147.0	0.196616	4.011502243	19.76996	1
Point 1	25	146183.7	140585.0	1.039824	22.73996791	9.040128	1
Point 2	50	212450.7	94455.7	2.24921	49.60160653	0.796787	1
Point 3	75	353291.0	98798.7	3.575868	79.06795598	-5.42394	1
Point 4	100	505219.0	109805.3	4.601042	101.8380689	-1.83807	1
Point 5	150	492789.7	73227.7	6.729556	149.1144062	0.590396	1
ULOQ	200	579286.3	64661.7	8.958729	198.6264922	0.686754	1
							1
							7
							1
						MEETS CRITERIA?	TRUE
							1
RUN 2							
	Nominal	Analyte	IS	PAR	Recalculated	RE%	
Blank	Blank	2461.7	539.0	n/a	n/a	n/a	
Zero	0	333.3	228642.0	n/a	n/a	n/a	
LLOQ	5	34201.0	167634.3	0.204021	4.388966626	12.22067	1
Point 1	25	157829.7	149155.7	1.058154	23.71664791	5.133408	1
Point 2	50	210124.7	95308.3	2.204683	49.66080331	0.678393	1
Point 3	75	404845.3	117392.7	3.448642	77.80965517	-3.74621	1
Point 4	100	378855.0	84774.7	4.468965	100.8979507	-0.89795	1
Point 5	150	446620.3	67691.3	6.597895	149.0723132	0.618458	1
ULOQ	200	586708.0	66487.3	8.824358	199.4536631	0.273168	1
							1
							7
							1
						MEETS CRITERIA?	TRUE
							1
RUN 3							
	Nominal	Analyte	IS	PAR	Recalculated	RE%	
Blank	Blank	4302.0	157.0	n/a	n/a	n/a	
Zero	0	356.0	161047.0	n/a	n/a	n/a	
LLOQ	5	27595.0	134460.3	0.205228	4.722829722	5.543406	1
Point 1	25	130486.3	122860.3	1.06207	23.71572173	5.137113	1
Point 2	50	251560.7	113995.0	2.206769	49.08927266	1.821455	1
Point 3	75	282903.3	80336.7	3.521472	78.23115585	-4.30821	1
Point 4	100	435119.0	96037.0	4.530743	100.6028	-0.6028	1
Point 5	150	544744.7	81120.7	6.715239	149.0246303	0.650246	1
ULOQ	200	516321.7	57385.0	8.997502	199.6135897	0.193205	1
							1
							7
							1
						MEETS CRITERIA?	TRUE
							1

Figure S2. Raw data for the three validated calibration curve runs including the nominal concentrations, analyte peak integrations, internal standard (IS) peak integrations, recalculated concentrations and percentage difference between the recalculated and nominal concentrations.

Table S1. Mass measurements and relative intensities of kavalactones in *P. methysticum* products associated with the spectra in Fig. 3 using DART-HRMS.

Kava Product	Compound*	Protonated Formula	Calculated	Measured	Diff.**	Rel. Int. (%)
Kona Kava Farm Kava Root Only Capsules	Desmethoxyyangonin	[C ₁₄ H ₁₂ O ₃ + H] ⁺	229.087	229.088	-1	24.1
	Kavain	[C ₁₄ H ₁₄ O ₃ + H] ⁺	231.102	231.103	-1	40.4
	Dihydrokavain	[C ₁₄ H ₁₆ O ₃ + H] ⁺	233.118	233.117	1	27.6
	Yangonin	[C ₁₅ H ₁₄ O ₄ + H] ⁺	259.097	259.098	-1	100.0
	Methysticin	[C ₁₅ H ₁₄ O ₅ + H] ⁺	275.092	275.092	0	27.1
	Dihydromethysticin	[C ₁₅ H ₁₆ O ₅ + H] ⁺	277.108	277.105	3	10.8
Hawaiian Kava Capsules	Desmethoxyyangonin	[C ₁₄ H ₁₂ O ₃ + H] ⁺	229.087	229.086	1	29.4
	Kavain	[C ₁₄ H ₁₄ O ₃ + H] ⁺	231.102	231.101	1	43.2
	Dihydrokavain	[C ₁₄ H ₁₆ O ₃ + H] ⁺	233.118	233.118	0	57.4
	Yangonin	[C ₁₅ H ₁₄ O ₄ + H] ⁺	259.097	259.096	1	100.0
	Methysticin	[C ₁₅ H ₁₄ O ₅ + H] ⁺	275.092	275.089	3	32.1
	Dihydromethysticin	[C ₁₅ H ₁₆ O ₅ + H] ⁺	277.108	277.109	-1	29.1
Kava Kava Root Capsules	Desmethoxyyangonin	[C ₁₄ H ₁₂ O ₃ + H] ⁺	229.087	229.083	4	21.4
	Kavain	[C ₁₄ H ₁₄ O ₃ + H] ⁺	231.102	231.098	4	37.2
	Dihydrokavain	[C ₁₄ H ₁₆ O ₃ + H] ⁺	233.118	233.116	2	41.2
	Yangonin	[C ₁₅ H ₁₄ O ₄ + H] ⁺	259.097	259.097	0	100.0
	Methysticin	[C ₁₅ H ₁₄ O ₅ + H] ⁺	275.092	275.091	1	28.9
	Dihydromethysticin	[C ₁₅ H ₁₆ O ₅ + H] ⁺	277.108	277.107	1	24.6
Kava Kava Liquid Capsules	Desmethoxyyangonin	[C ₁₄ H ₁₂ O ₃ + H] ⁺	229.087	229.087	0	42.9
	Kavain	[C ₁₄ H ₁₄ O ₃ + H] ⁺	231.102	231.102	0	41.0
	Dihydrokavain	[C ₁₄ H ₁₆ O ₃ + H] ⁺	233.118	233.117	1	78.3
	Yangonin	[C ₁₅ H ₁₄ O ₄ + H] ⁺	259.097	259.097	0	32.5
	Methysticin	[C ₁₅ H ₁₄ O ₅ + H] ⁺	275.092	275.091	1	10.2
	Dihydromethysticin	[C ₁₅ H ₁₆ O ₅ + H] ⁺	277.108	277.111	-3	8.7
Kavalactone Paste 55%	Desmethoxyyangonin	[C ₁₄ H ₁₂ O ₃ + H] ⁺	229.087	229.083	4	33.8
	Kavain	[C ₁₄ H ₁₄ O ₃ + H] ⁺	231.102	231.104	-2	61.2
	Dihydrokavain	[C ₁₄ H ₁₆ O ₃ + H] ⁺	233.118	233.119	-1	62.6
	Yangonin	[C ₁₅ H ₁₄ O ₄ + H] ⁺	259.097	259.096	1	100.0
	Methysticin	[C ₁₅ H ₁₄ O ₅ + H] ⁺	275.092	275.093	-1	32.2
	Dihydromethysticin	[C ₁₅ H ₁₆ O ₅ + H] ⁺	277.108	277.106	2	17.3
Happy Kava Brand Micronized Powder	Desmethoxyyangonin	[C ₁₄ H ₁₂ O ₃ + H] ⁺	229.087	229.087	0	26.4
	Kavain	[C ₁₄ H ₁₄ O ₃ + H] ⁺	231.102	231.102	0	39.6
	Dihydrokavain	[C ₁₄ H ₁₆ O ₃ + H] ⁺	233.118	233.117	1	40.0
	Yangonin	[C ₁₅ H ₁₄ O ₄ + H] ⁺	259.097	259.098	-1	100.0
	Methysticin	[C ₁₅ H ₁₄ O ₅ + H] ⁺	275.092	275.092	0	24.7
	Dihydromethysticin	[C ₁₅ H ₁₆ O ₅ + H] ⁺	277.108	277.105	3	13.1
Vanuatu Ceremonial Kava Powder	Desmethoxyyangonin	[C ₁₄ H ₁₂ O ₃ + H] ⁺	229.087	229.086	1	24.4
	Kavain	[C ₁₄ H ₁₄ O ₃ + H] ⁺	231.102	231.101	1	34.9
	Dihydrokavain	[C ₁₄ H ₁₆ O ₃ + H] ⁺	233.118	233.116	2	30.1
	Yangonin	[C ₁₅ H ₁₄ O ₄ + H] ⁺	259.097	259.097	0	100.0
	Methysticin	[C ₁₅ H ₁₄ O ₅ + H] ⁺	275.092	275.091	1	21.9
	Dihydromethysticin	[C ₁₅ H ₁₆ O ₅ + H] ⁺	277.108	277.110	-2	12.3
Kava 40% Powder	Desmethoxyyangonin	[C ₁₄ H ₁₂ O ₃ + H] ⁺	229.087	229.082	5	23.0
	Kavain	[C ₁₄ H ₁₄ O ₃ + H] ⁺	231.102	231.097	5	35.7
	Dihydrokavain	[C ₁₄ H ₁₆ O ₃ + H] ⁺	233.118	233.115	3	41.0
	Yangonin	[C ₁₅ H ₁₄ O ₄ + H] ⁺	259.097	259.092	5	85.7
	Methysticin	[C ₁₅ H ₁₄ O ₅ + H] ⁺	275.092	275.089	3	25.6
	Dihydromethysticin	[C ₁₅ H ₁₆ O ₅ + H] ⁺	277.108	277.106	2	14.8
	Desmethoxyyangonin	[C ₁₄ H ₁₂ O ₃ + H] ⁺	229.087	229.085	2	14.1

ISA Powdered Kava Root	Kavain	[C ₁₄ H ₁₄ O ₃ + H] ⁺	231.102	231.100	2	29.8
	Dihydrokavain	[C ₁₄ H ₁₆ O ₃ + H] ⁺	233.118	233.115	3	34.6
	Yangonin	[C ₁₅ H ₁₄ O ₄ + H] ⁺	259.097	259.096	1	100.0
	Methysticin	[C ₁₅ H ₁₄ O ₅ + H] ⁺	275.092	275.090	2	42.7
	Dihydromethysticin	[C ₁₅ H ₁₆ O ₅ + H] ⁺	277.108	277.104	4	26.2
Kava Kava Root Powder	Desmethoxyyangonin	[C ₁₄ H ₁₂ O ₃ + H] ⁺	229.087	229.086	1	21.5
	Kavain	[C ₁₄ H ₁₄ O ₃ + H] ⁺	231.102	231.100	2	29.8
	Dihydrokavain	[C ₁₄ H ₁₆ O ₃ + H] ⁺	233.118	233.118	0	49.4
	Yangonin	[C ₁₅ H ₁₄ O ₄ + H] ⁺	259.097	259.096	1	90.7
	Methysticin	[C ₁₅ H ₁₄ O ₅ + H] ⁺	275.092	275.090	2	23.7
	Dihydromethysticin	[C ₁₅ H ₁₆ O ₅ + H] ⁺	277.108	277.110	-2	21.2
Kavalactones 70% Powder	Desmethoxyyangonin	[C ₁₄ H ₁₂ O ₃ + H] ⁺	229.087	229.085	2	31.1
	Kavain	[C ₁₄ H ₁₄ O ₃ + H] ⁺	231.102	231.100	2	39.8
	Dihydrokavain	[C ₁₄ H ₁₆ O ₃ + H] ⁺	233.118	233.115	3	72.6
	Yangonin	[C ₁₅ H ₁₄ O ₄ + H] ⁺	259.097	259.096	1	100.0
	Methysticin	[C ₁₅ H ₁₄ O ₅ + H] ⁺	275.092	275.090	2	16.9
	Dihydromethysticin	[C ₁₅ H ₁₆ O ₅ + H] ⁺	277.108	277.109	-1	33.7
Rough Cut Whole Kava Root	Desmethoxyyangonin	[C ₁₄ H ₁₂ O ₃ + H] ⁺	229.087	229.084	3	17.6
	Kavain	[C ₁₄ H ₁₄ O ₃ + H] ⁺	231.102	231.099	3	30.3
	Dihydrokavain	[C ₁₄ H ₁₆ O ₃ + H] ⁺	233.118	233.117	1	18.3
	Yangonin	[C ₁₅ H ₁₄ O ₄ + H] ⁺	259.097	259.097	0	100.0
	Methysticin	[C ₁₅ H ₁₄ O ₅ + H] ⁺	275.092	275.088	4	20.2
	Dihydromethysticin	[C ₁₅ H ₁₆ O ₅ + H] ⁺	277.108	277.107	1	7.2
Kava Kava Root	Desmethoxyyangonin	[C ₁₄ H ₁₂ O ₃ + H] ⁺	229.087	229.083	4	44.0
	Kavain	[C ₁₄ H ₁₄ O ₃ + H] ⁺	231.102	231.098	4	61.5
	Dihydrokavain	[C ₁₄ H ₁₆ O ₃ + H] ⁺	233.118	233.118	0	82.3
	Yangonin	[C ₁₅ H ₁₄ O ₄ + H] ⁺	259.097	259.096	1	97.3
	Methysticin	[C ₁₅ H ₁₄ O ₅ + H] ⁺	275.092	275.090	2	23.9
	Dihydromethysticin	[C ₁₅ H ₁₆ O ₅ + H] ⁺	277.108	277.106	2	12.5
Root of Happiness Liquid Extract	Desmethoxyyangonin	[C ₁₄ H ₁₂ O ₃ + H] ⁺	229.087	229.087	0	34.5
	Kavain	[C ₁₄ H ₁₄ O ₃ + H] ⁺	231.102	231.102	0	54.7
	Dihydrokavain	[C ₁₄ H ₁₆ O ₃ + H] ⁺	233.118	233.117	1	86.9
	Yangonin	[C ₁₅ H ₁₄ O ₄ + H] ⁺	259.097	259.098	-1	52.6
	Methysticin	[C ₁₅ H ₁₄ O ₅ + H] ⁺	275.092	275.092	0	14.7
	Dihydromethysticin	[C ₁₅ H ₁₆ O ₅ + H] ⁺	277.108	277.105	3	10.1
Happy Kava Brand Passion Flower Tincture Blend	Desmethoxyyangonin	[C ₁₄ H ₁₂ O ₃ + H] ⁺	229.087	229.085	2	35.9
	Kavain	[C ₁₄ H ₁₄ O ₃ + H] ⁺	231.102	231.103	-1	49.7
	Dihydrokavain	[C ₁₄ H ₁₆ O ₃ + H] ⁺	233.118	233.118	0	79.1
	Yangonin	[C ₁₅ H ₁₄ O ₄ + H] ⁺	259.097	259.099	-2	91.3
	Methysticin	[C ₁₅ H ₁₄ O ₅ + H] ⁺	275.092	275.092	0	20.0
	Dihydromethysticin	[C ₁₅ H ₁₆ O ₅ + H] ⁺	277.108	277.106	2	14.7
Happy Kava Brand Valerian Tincture Blend	Desmethoxyyangonin	[C ₁₄ H ₁₂ O ₃ + H] ⁺	229.087	229.086	1	36.2
	Kavain	[C ₁₄ H ₁₄ O ₃ + H] ⁺	231.102	231.104	-2	55.8
	Dihydrokavain	[C ₁₄ H ₁₆ O ₃ + H] ⁺	233.118	233.119	-1	72.2
	Yangonin	[C ₁₅ H ₁₄ O ₄ + H] ⁺	259.097	259.099	-2	47.9
	Methysticin	[C ₁₅ H ₁₄ O ₅ + H] ⁺	275.092	275.093	-1	14.2
	Dihydromethysticin	[C ₁₅ H ₁₆ O ₅ + H] ⁺	277.108	277.106	2	11.4
Kava Root Liquid Tincture	Desmethoxyyangonin	[C ₁₄ H ₁₂ O ₃ + H] ⁺	229.087	229.087	0	34.5
	Kavain	[C ₁₄ H ₁₄ O ₃ + H] ⁺	231.102	231.102	0	39.8
	Dihydrokavain	[C ₁₄ H ₁₆ O ₃ + H] ⁺	233.118	233.117	1	75.6
	Yangonin	[C ₁₅ H ₁₄ O ₄ + H] ⁺	259.097	259.097	0	79.2
	Methysticin	[C ₁₅ H ₁₄ O ₅ + H] ⁺	275.092	275.092	0	7.3
	Dihydromethysticin	[C ₁₅ H ₁₆ O ₅ + H] ⁺	277.108	277.108	0	9.7

Zend Kava Supplement	Desmethoxyyangonin	$[C_{14}H_{12}O_3 + H]^+$	229.087	229.086	1	71.0
	Kavain	$[C_{14}H_{14}O_3 + H]^+$	231.102	231.101	1	83.0
	Dihydrokavain	$[C_{14}H_{16}O_3 + H]^+$	233.118	233.116	2	100.0
	Yangonin	$[C_{15}H_{14}O_4 + H]^+$	259.097	259.097	0	67.3
	Methysticin	$[C_{15}H_{14}O_5 + H]^+$	275.092	275.090	2	20.0
	Dihydromethysticin	$[C_{15}H_{16}O_5 + H]^+$	277.108	277.107	1	19.7

* Compound names are tentatively assigned based on calculated and measured mass measurements and compounds previously identified in Kava products and plant material.

** Differences are reported in millimass units.

Table S2. Mass measurements and relative intensities of flavokavains in *P. methysticum* products associated with the spectra in Fig. 3 using DART-HRMS.

Product	Compound*	Formula	Calculated	Measured	Diff.**	Rel. Int. (%)
Kona Kava Farm Kava Root Only Capsules	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.112	1	36.4
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.110	-2	5.3
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.125	-2	54.8
Hawaiian Kava Capsules	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.113	0	69.2
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.107	1	7.5
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.123	0	72.5
Kava Kava Root Capsules	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.111	2	70.0
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.105	3	8.2
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.125	-2	78.6
Kava Kava Liquid Capsules	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.116	-3	100.0
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.104	4	0.7
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.125	-2	49.0
Kavalactone Paste 55%	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.111	2	15.1
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.109	-1	4.3
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.124	-1	59.2
Happy Kava Brand Micronized Powder	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.113	0	68.5
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.111	-3	4.0
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.123	0	54.4
Vanuatu Ceremonial Kava Powder	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.115	-2	15.6
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.113	-5	1.9
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.125	-2	32.4
Kava 40% Powder	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.110	3	93.3
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.104	4	10.1
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.120	3	100.0
ISA Powdered Kava Root	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.114	-1	56.6
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.109	-1	6.1
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.125	-2	56.6
Kava Kava Root Powder	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.114	-1	92.3
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.109	-1	11.2
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.125	-2	100.0
Kavalactones 70% Powder	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.114	-1	37.1
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.112	-4	1.7
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.124	-1	30.4
Rough Cut Whole Kava Root	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.112	1	26.5
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.109	-1	3.6
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.122	1	44.5
Kava Kava Root	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.111	2	100.0
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.109	-1	4.3
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.121	2	43.1

Root of Happiness Liquid Extract	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.113	0	100.0
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.111	-3	2.7
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.123	0	54.7
Happy Kava Brand Passion Flower Tincture Blend	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.113	0	100.0
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.108	0	4.3
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.123	0	67.0
Happy Kava Brand Valerian Tincture Blend	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.113	0	100.0
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.109	-1	0.5
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.123	0	65.3
Kava Root Liquid Tincture	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.112	1	100.0
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.110	-2	2.3
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.126	-3	55.7
Zend Kava Supplement	Flavokavain B	[C ₁₇ H ₁₆ O ₄ + H] ⁺	285.113	285.111	2	64.0
	Flavokavain C	[C ₁₇ H ₁₆ O ₅ + H] ⁺	301.108	301.112	-4	3.5
	Flavokavain A	[C ₁₈ H ₁₈ O ₅ + H] ⁺	315.123	315.124	-1	35.3

* Compound names are tentatively assigned based on calculated and measured mass measurements and compounds previously identified in Kava products and plant material.

** Differences are reported in millimass units.