

Electronic Supplementary Material

**Spatial distribution and comparative analysis of *Aconitum* alkaloids
in Fuzi using DESI-MSI and UHPLC-QTOF-MS**

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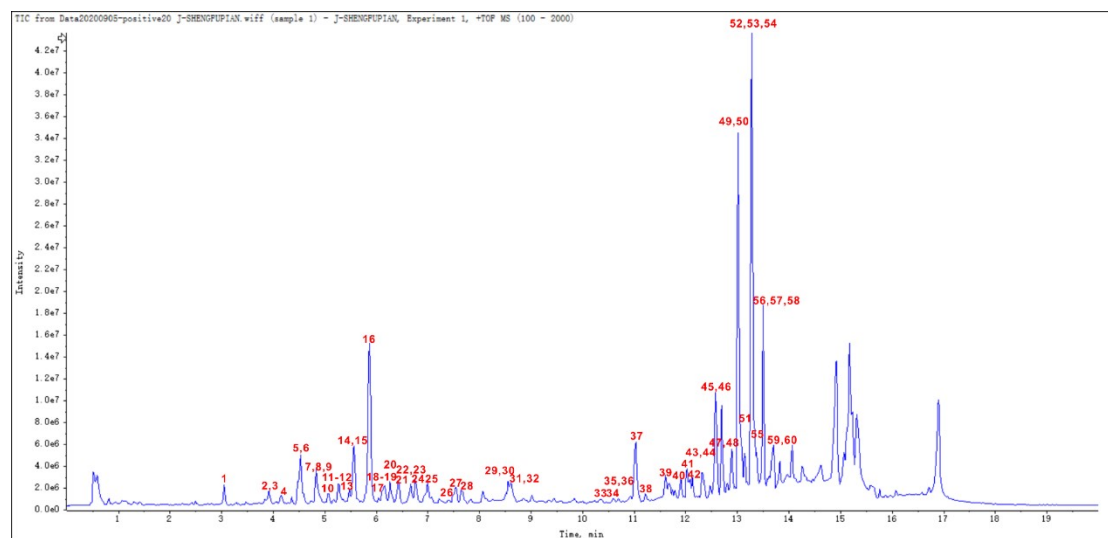


Figure S1. TIC diagram of methanol extract of Fuzi in positive ion mode

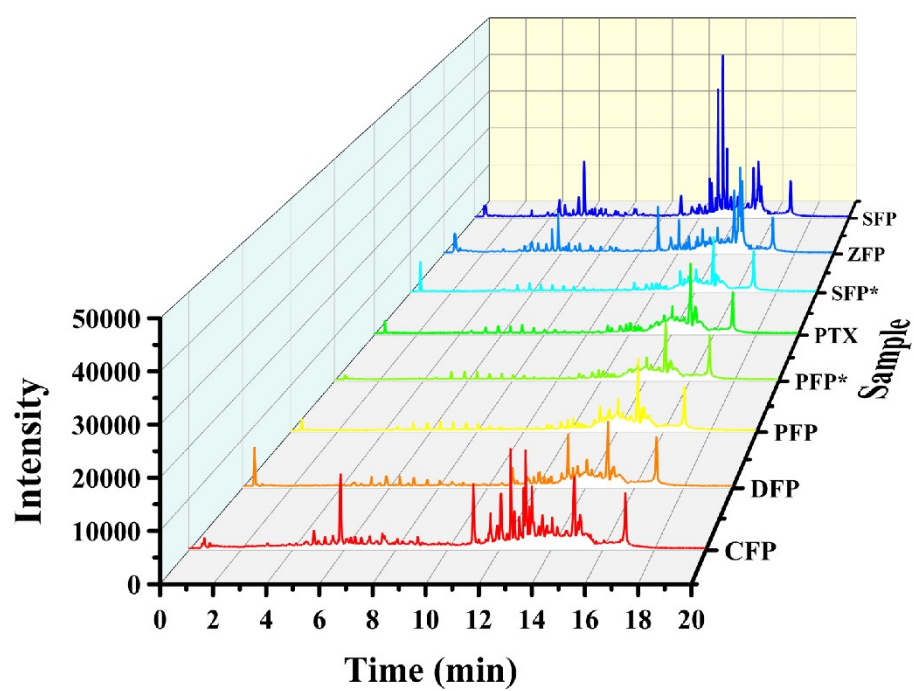


Figure S2. UHPLC chromatographic analysis of raw and processed Fuzi

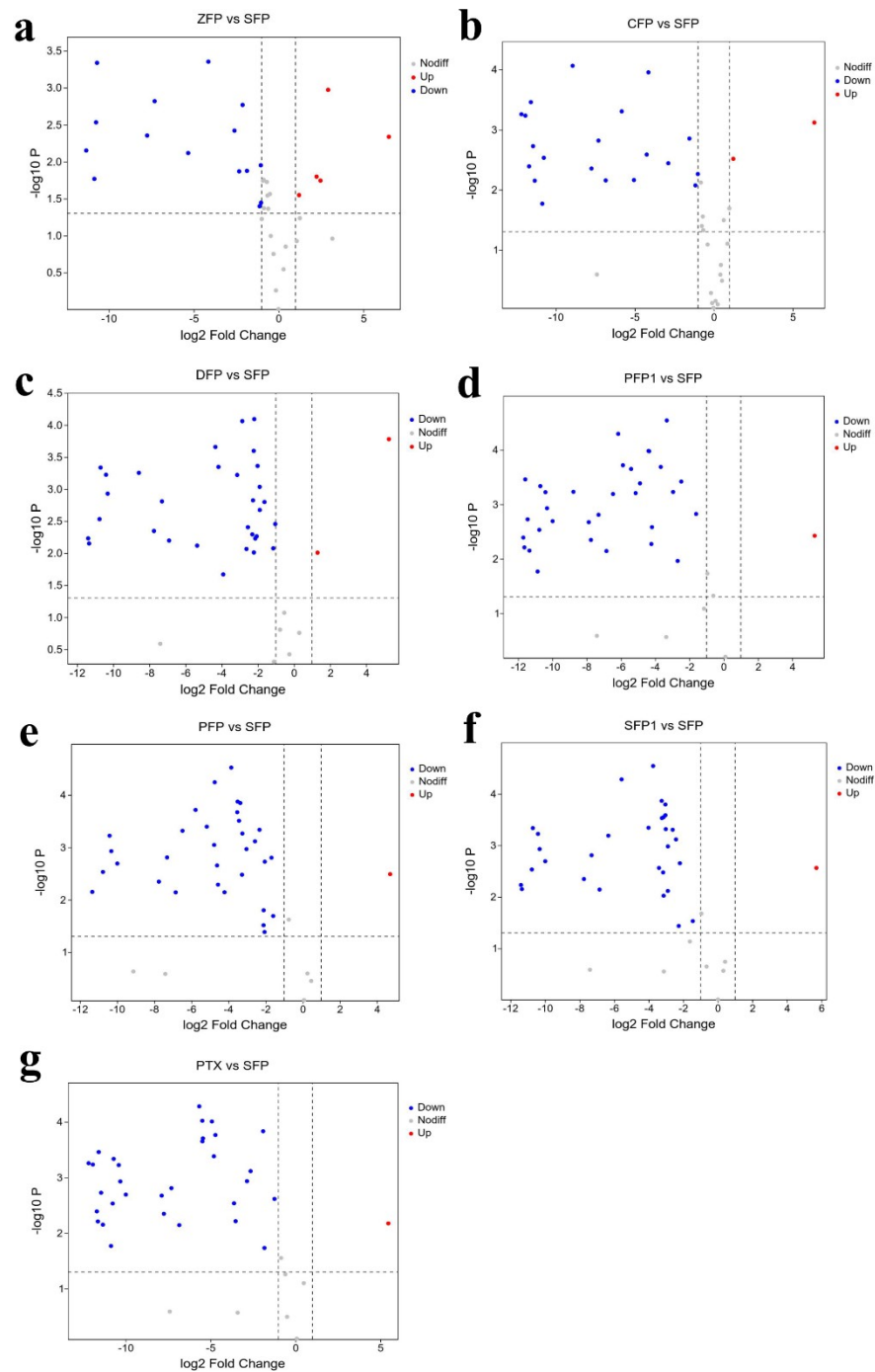


Figure S3. Volcano plot of differential metabolites between SFP and a. ZFP; b. CFP; c. DFP; d. PFP1; e. PFP; f. SFP1; g. PTX

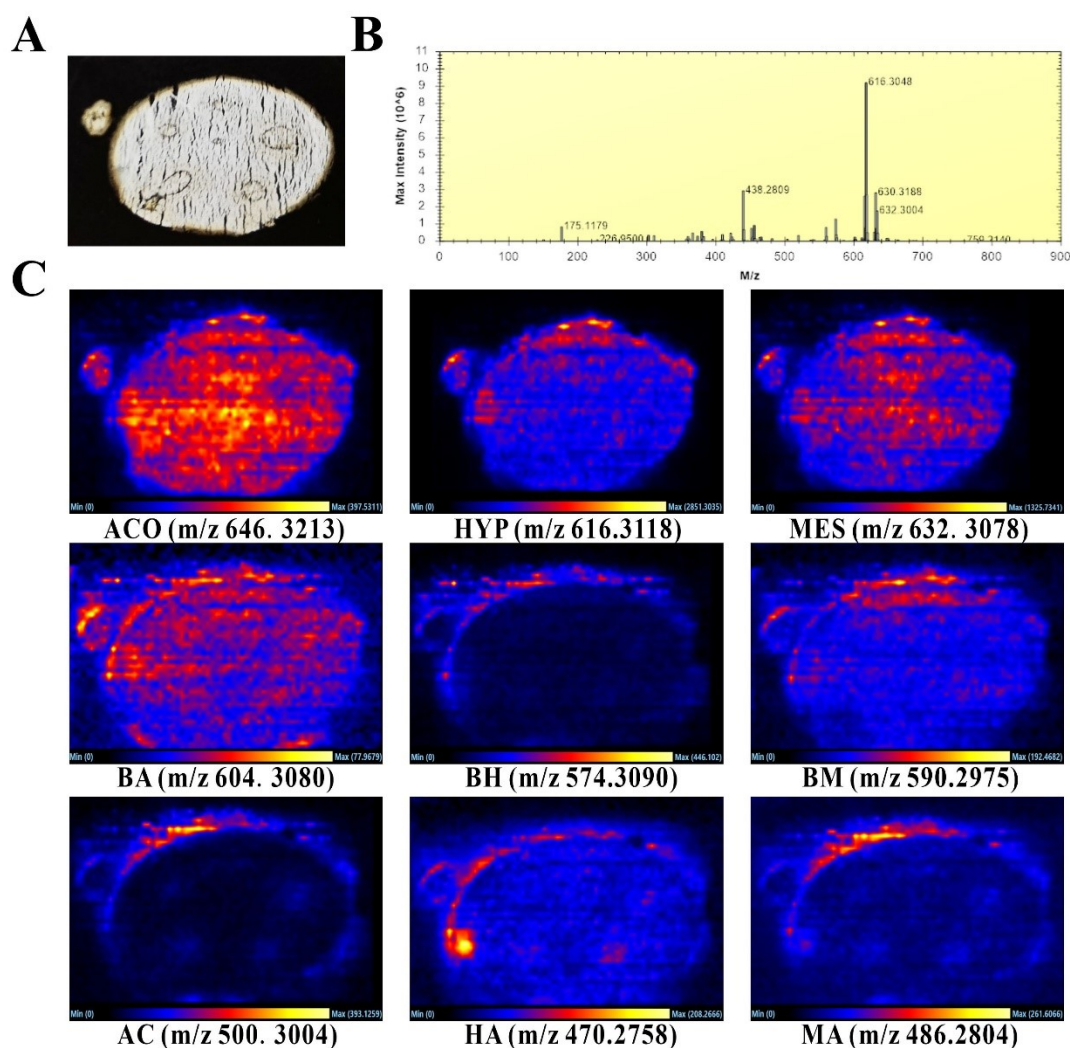


Figure S4. Image of 9 main alkaloids of AAs by Mass spectrometry. **A.** Optical microscopy of Fuzi section; **B.** Total ion flow diagram of DESI-MSI; **C.** Mass spectrometry images of three ester types of nine alkaloids in Fuzi (The MS response of compound in the pictures were processed by Sqrt_Composition in HDI software)

Table S1. Intensity of DESI-MSI of main AAs

Type	Compounds	[M+H] ⁺	Max intensity	Sum intensity
DDAs	ACO	646.3213	1.580×10 ⁵	7.263×10 ⁷
	HYP	616.3118	8.130×10 ⁶	1.646×10 ⁹
	MES	632.3078	1.758×10 ⁶	4.944×10 ⁸
MDAs	BA	604.3080	6.079×10 ³	2.333×10 ⁶
	BH	574.3090	1.990×10 ⁵	1.202×10 ⁷
	BM	590.2975	3.704×10 ⁴	7.590×10 ⁶
NDAs	AC	500.3004	1.545×10 ⁵	9.392×10 ⁶
	HA	470.2758	4.338×10 ⁴	7.707×10 ⁶
	MA	486.2804	6.844×10 ⁴	7.805×10 ⁶

Table S2. Mass spectrometry data of positive ion pattern of Fuzi extract

No.	Name	MS ¹	MS ²	Retention time (min)	Level of credibility
1	Karakolidine	394.2602	376.2478 358.2371	3.05	**
2	Senbusine A	424.2693	406.2577 388.2473	3.95	**
3	Mesaconine	486.2692	436.2329 404.2061	4.13	***
4	16- β -hydroxycar diopetaline	364.2489	346.2385 328.2285	4.15	**
5	Karakoline	378.2633	360.2523 342.2423 328.2263	4.48	***
6	Isotalatizidine	408.2745	390.2619 358.2362	4.53	**
7	Aconitine	500.2850	450.2486 418.2223	4.82	***
8	napelline	360.2532	342.2428 300.1957	4.98	**
9	Songorine	358.2371	340.2250 322.2155	4.83	**
10	Hetisine	330.2064	312.1998 118.0862 448.2695	5.05	**
11	-	466.2797	430.2603 398.2343 388.2487	5.29	*
12	-	406.2587	370.2374 328.2264 310.2172 418.2212	5.32	*
13	-	436.2325	386.1956 374.2320 154.1229	5.46	*
14	Hypaconine	470.2742	438.2480 406.2218	5.53	***
15	Fuziline	454.2770	436.2672	5.56	***

			404.2416		
			420.2711		
16	Neoline	438.2846	388.2449	5.86	***
			356.2191		
			418.2577		
			450.2851		
17	Delsoline	468.2945	436.2682	6.06	***
			404.2418		
			386.2319		
			354.2048		
18	14-Acetylkarakolin e	420.2745	402.2640	6.11	**
			360.2683		
			342.2576		
			406.2572		
19	-	450.2850	362.2683	6.16	*
			344.2576		
			330.2411		
20	-	342.1700	312.1984	6.26	*
			109.0770		
			464.2659		
21	-	496.2914	436.2705	6.40	*
			404.2442		
			376.2488		
			360.2535		
22	-	392.2795	342.2427	6.60	*
			328.2267		
23	Denudatine	344.2584	326.2480	6.66	**
24	Talatisamine	422.2893	358.2375	6.79	***
			390.2637		
25	-	466.2446	448.2334	6.70	*
			416.2075		
			462.2853		
			430.2591		
26	Bullatine C	480.2958	398.2330	7.49	**
			370.23771		
			54.1225		
			420.2744		
27	Chasmanine	452.3006	388.2483	7.65	**
			356.2227		
28	Deltaline	508.2930	490.2811	7.87	***

			430.2599		
			398.23341		
			54.1227		
			402.2645		
			384.2544		
29	-	434.2909	370.2379	8.51	*
			342.2423		
			324.2333		
30	-	498.2856	480.2732	8.58	*
			462.2630		
31	14-acetyl- talatisamine	464.3013	432.2741	8.62	**
			400.2484		
			588.2819		
			574.26655		
32	-	606.2919	56.2556	8.87	*
			542.2411		
			524.2308		
			105.0533		
			426.2640		
			398.2687		
33	-	444.2744	342.2063	10.34	*
			324.1957		
			296.2004		
34	Benzoylhypaconine	574.3016	542.2738	10.45	***
			524.2651		
			502.3170		
			484.3064		
35	-	520.3278	442.2938	10.83	*
			424.2840		
			340.2273		
36	-	544.2915	512.2655	10.90	*
			105.0338		
			540.2566		
37	Benzoylmesaconine	590.2977	558.2680	11.00	***
			508.2306		
			638.25395		
			72.2853		
38	3-Acetylaconitine	688.2987	540.2567	11.39	***
			512.2620		
			354.1676		

				105.0336		
				522.2847		
				504.2745		
39	-	540.2952	462.2632	11.59	*	
				444.2534		
				340.2265		
				105.0341		
				570.2711		
40	-	620.3072	538.2441	11.79	*	
				105.0391		
				554.2745		
41	-	572.2864	540.2586	12.03	*	
				522.2482		
				568.2886		
				554.2731		
42	-	586.2986	522.2469	12.33	*	
				466.2207		
				105.0347		
				540.2940		
43	benzoyl-3,13- deoxymesaconine	558.3049	526.2785	12.56	**	
				508.2678		
				105.0346		
				588.2779		
44	10-Hydroxy mesaconitine	648.3029	556.2521	12.56	***	
				506.2163		
				370.1643		
				554.2724		
45	Benzoylaconitine	604.3129	572.2832	12.68	***	
				522.2464		
46	-	500.3007	426.2641	12.78	*	
				324.1960		
				508.2689		
				494.2540		
47	-	540.2941	480.2725	12.81	*	
				416.2425		
				386.2321		
				105.0343		
				524.2629		
48	Pyrohypaconitine	556.2912	492.2373	12.88	**	
				402.2269		

			572.2812		
49	Mesaconitine	632.3079	540.2556	13.02	***
			512.2608		
			354.1677		
			602.2932		
50	10-Hydroxy aconitine	662.3131	570.2671	13.07	**
			542.2728		
			384.1794		
			105.0347		
			556.2902		
51	benzoyldeox yaconine	588.3160	524.2648	13.16	**
			492.2393		
			105.0346		
			566.2876		
52	Hypaconitine	616.3108	524.2614	13.26	***
			584.2828		
			586.2978		
53	Aconitine	646.3221	554.2726	13.27	***
			526.2777		
			586.29195		
			58.2960		
54	8-Deacetyl yunaconitine	618.3163	526.2704	13.29	**
			498.2748		
			466.2496		
			339.1787		
			105.0346		
			540.2928		
			508.2668		
55	Delphinine	600.3142	480.2702	13.33	**
			448.2451		
			354.2051		
			105.0343		
			570.3030		
56	3-Deoxyaconitine	630.3291	538.2773	13.49	***
			352.1887		
			570.3042		
57	Dehydroxyindac	630.3294	538.2788	13.53	***
			352.1902		
58	Yunaconitine	660.3392	572.2865	13.57	**
			540.2579		

			354.1691		
			608.2634		
59	-	668.2838	546.2474	13.68	*
			105.0346		
			554.3104		
60	13,15- Dideoxyaconitine	614.3337	522.2853	13.73	***
			494.2887		

***: the compound verified by the standard; **: the compound that can be accurately matched with the molecular formula, MS¹ and MS² in the literature database; *: the compound with molecular formula but uncertain.