

Table S1. Chemical constituents of XBJ that entered into blood and lung

No.	Compound	Formula	Ion mode	Cal. (Da)	Mean (Da)	Error (ppm)	RT (min)	Source	Blood	Lung
1	Hydroxysafflor yellow A	C ₂₇ H ₃₂ O ₁₆	[M-H] ⁻	611.1618	611.1624	2.76	2.39	CF	Y	Y
2	Ligustilide	C ₁₂ H ₁₄ O ₂	[M+HCOO] ⁻	235.0965	235.0974	3.89	11.94	CR, ASSR	Y	Y
3	Isomers of Ligustilide	C ₁₂ H ₁₄ O ₂	[M+HCOO] ⁻	235.0965	235.0974	3.76	12.22	CR	Y	Y
4	Ethyl 4-hydroxy-3-methoxycinnamate	C ₁₂ H ₁₄ O ₄	[M-H] ⁻	221.0819	221.0815	3.19	11.83	ASSR	Y	Y
5	Paeoniflorin	C ₂₃ H ₂₈ O ₁₁	[M+HCOO] ⁻	525.1603	525.1616	2.58	5.33	PRR	Y	Y
6	Neocnidilide	C ₁₂ H ₁₈ O ₂	[M+HCOO] ⁻	239.1278	239.1287	3.62	12.72	CR	Y	Y
7	Senkyunolide K	C ₁₂ H ₁₆ O ₃	[M-H] ⁻	207.1027	207.1020	2.12	12.18	CR, ASSR	Y	Y
8	10,12-octadecanedioic acid	C ₁₈ H ₂₈ O ₂	[M+HCOO] ⁻	321.2060	321.2048	-3.94	17.43	ASSR	Y	Y
9	Oleic acid	C ₁₈ H ₃₄ O ₂	[M-H] ⁻	281.2486	281.2487	4.32	19.62	CR	Y	Y
10	Linoleic acid	C ₁₈ H ₃₂ O ₂	[M-H] ⁻	279.2330	279.2331	4.42	18.06	CR, ASSR	Y	Y
11	Palmitic acid	C ₁₆ H ₃₂ O ₂	[M-H] ⁻	255.2330	255.2327	3.34	19.03	CR	Y	Y
12	Danshenxinkun D	C ₂₁ H ₂₀ O ₄	[M+H] ⁺	337.1434	337.1447	3.69	14.57	SMRR	Y	Y
13	Sugiol	C ₂₀ H ₂₈ O ₂	[M-H] ⁻	299.2017	299.2018	4.09	15.97	SMRR	Y	Y