

1 **Table S1.** Identification Results of Main Components of DCXD Samples

Nu m.	T(min)	adduct ions	<i>m/z</i> real value	<i>m/z</i> theoretic al value	ppm	MF	mol wt	Name	DC	assignment
1	8.09	[M-H] ⁻	459.1175	459.1144	6.7	C ₁₉ H ₂₄ O ₁₃	460.12	Parishin E	√	Tianma
2	10.43	[M-H] ⁻	727.2150	727.2091	8.1	C ₃₂ H ₄₀ O ₁₉	728.22	Parishin B	√	Tianma
3	24.65	[M+H] ⁺	193.1232	193.1223	4.6	C ₁₂ H ₁₆ O ₂	192.12	Senkyunoli de A	√	Chuanxiong
4	10.91	[M-H] ⁻	727.2133	727.2091	5.8	C ₃₂ H ₄₀ O ₁₉	728.22	Parishin C	√	Tianma
5	11.97	[M-H] ⁻	193.0517	193.0506	5.5	C ₁₀ H ₁₀ O ₄	194.06	Ferulic acid	√	Chuanxiong
6	14.72	[M+FA-H] ⁻	549.2224	549.2189	6.4	C ₂₃ H ₃₆ O ₁₂	504.22	Chuanxiong side B		Chuanxiong
7	14.62	[M+H] ⁺	225.1127	225.1121	2.5	C ₁₂ H ₁₆ O ₄	224.10	Senkyunoli de I	√	Chuanxiong
8	15.22	[M-H] ⁻	237.0781	237.0768	5.3	C ₁₂ H ₁₄ O ₅	238.08	Trimethoxy cinnamic acid		Chuanxiong
9	18.50	[M-H] ⁻	577.1398	577.1352	8.1	C ₃₀ H ₂₆ O ₁₂	578.14	4-O-8',5'-5"-dehydrotriferulic acid		
10	19.30	[M-H] ⁻	329.2346	329.2333	3.8	C ₁₈ H ₃₄ O ₅	330.24	Trihydroxy octadecenoic acid		Chuanxiong
11	8.58	[M-H] ⁻	167.0363	167.0350	7.8	C ₈ H ₈ O ₄	168.15	Griffonilide	√	
12	8.28	[M+H] ⁺	414.1345	414.1329	3.7	C ₁₇ H ₂₃ N ₃ O ₇ S	413.13	S-(4-hydroxybenzyl) glutathione		Tianma
13	12.22	[M+FA-H] ⁻	1041.3167	1041.3093	7.1	C ₄₅ H ₅₆ O ₂₅	996.31	Parishin A	√	Tianma
14	27.42	[M+H] ⁺	191.1081	191.1067	7.6	C ₁₂ H ₁₄ O ₂	190.10	Ligustilide	√	Chuanxiong
15	8.47	[M-H] ⁻	353.0889	353.0878	3.1	C ₁₆ H ₁₈ O ₉	354.10	Chlorogenic acid	√	Chuanxiong

16	20.41	[M-H] ⁻	205.0882	205.0870	5.8	C ₁₂ H ₁₄ O ₃	206.09	(Z)-6,7-epoxyligustilide		Chuanxiong
17	20.60	[M-H] ⁻	207.1040	207.1027	6.4	C ₁₂ H ₁₆ O ₃	208.11	Senkyunolide G		Chuanxiong
18	13.82	[M+H] ⁺	679.5127	679.5117	1.5	C ₃₆ H ₆₆ N ₆ O ₆	678.50	Cyclohexa(iso)leucyl		Tianma /Chuanxiong
19	13.42	[M-H] ⁻	515.1232	515.1195	7.2	C ₂₅ H ₂₄ O ₁₂	516.13	Isochlorogenic acid C	√	Chuanxiong
20	7.49	[M-H] ⁻	459.1180	459.1144	7.8	C ₁₉ H ₂₄ O ₁₃	460.12	Parishin G		Tianma
21	6.56	[M-H] ⁻	515.1435	515.1406	9.0	C ₂₂ H ₂₈ O ₁₄	516.15	Dicafeoylquinic acid		Chuanxiong
22	21.44	[M-H] ⁻	205.0879	205.0870	4.3	C ₁₂ H ₁₄ O ₃	206.09	(E)-6,7-epoxyligustilide		Chuanxiong
23	27.97	[M-H] ⁻	397.2039	397.2020	4.7	C ₂₄ H ₃₀ O ₅	398.21	6,9-Ethanophthal[1,2-c]furan-8-carboxylic acid, 3-butylidene-1,3,4,5,5a,6,9,9a-octahydro-1-oxo-9-(1-oxopentyl)-(3Z,5aS,6S,9S,9aS)-(ACI)		Chuanxiong
24	14.50	[M+H] ⁺	792.5953	792.5957	-0.5	C ₄₂ H ₇₇ N ₇ O ₇	791.59	Cyclohexa(iso)leucyl		Tianma / Chuanxiong
25	27.17	[M+H] ⁺	195.1385	195.1380	2.8	C ₁₂ H ₁₈ O ₂	194.13	Neocnidilide	√	Chuanxiong
26	9.67	[M-H] ⁻	401.1464	401.1453	2.7	C ₁₈ H ₂₆ O ₁₀	402.15	Icariside F2		Chuanxiong
27	6.11	[M+H] ⁺	205.0976	205.0972	2.2	C ₁₁ H ₁₂ N ₂ O ₂	204.09	Tryptophan	√	Tianma / Chuanxiong
28	25.25	[M+H] ⁺	191.1075	191.1067	4.4	C ₁₂ H ₁₄ O ₂	190.10	3-Butylphthalide	√	Chuanxiong
29	27.96	[M+H] ⁺	191.1075	191.1067	4.4	C ₁₂ H ₁₄ O ₂	190.10	Ligustilide		Chuanxiong

30	23.71	[M-H] ⁻	277.1454	277.1445	3.1	C ₁₆ H ₂₂ O ₄	278.15	Senkyunoli de M		Chuanxiong
31	15.22	[M+Na] ⁺	247.0953	247.0941	4.9	C ₁₂ H ₁₆ O ₄	224.10	Senkyunoli de H	√	Chuanxiong
32	22.63	[M-H] ⁻	277.1453	277.1445	2.8	C ₁₆ H ₂₂ O ₄	278.15	Senkyunoli de Q		Chuanxiong

2 **Abbreviations:** MF, molecular formula. mol wt, molecular weight. DC, database comparison.

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