***Cite this as*:** Huan-huan PANG, Mei-fang JIANG, Qin-hui WANG, Xiao-ye WANG, Wei GAO, Zhi-hao TIAN, Jian-mei HUANG, 2018. Metabolic profile of danshen in rats by HPLC-LTQ-Orbitrap mass spectrometry. *Journal of Zhejiang University-Science B (Biomedicine & Biotechnology)*, 19(3):227-244.
https://doi.org/10.1631/jzus.B1700105

Metabolic profile of danshen in rats by HPLC-LTQ-Orbitrap mass spectrometry

Key words: **Danshen, Chemical profile, Metabolic profile, HPLC-LTQ-Orbitrap**

Research Summary

Danshen

50% ethanol

Plasma

Urine

Feces

Bile

HPLC-LTQ-Orbitrap

69 components *in vitro*

118 components *in vivo*

Conclusions

- ✓ 69 compounds were identified in danshen extract.
- ✓ 118 metabolites, including 35 in rat plasma, 63 in urine, 62 in feces, and 18 in bile were identified after oral administration of Danshen extract.

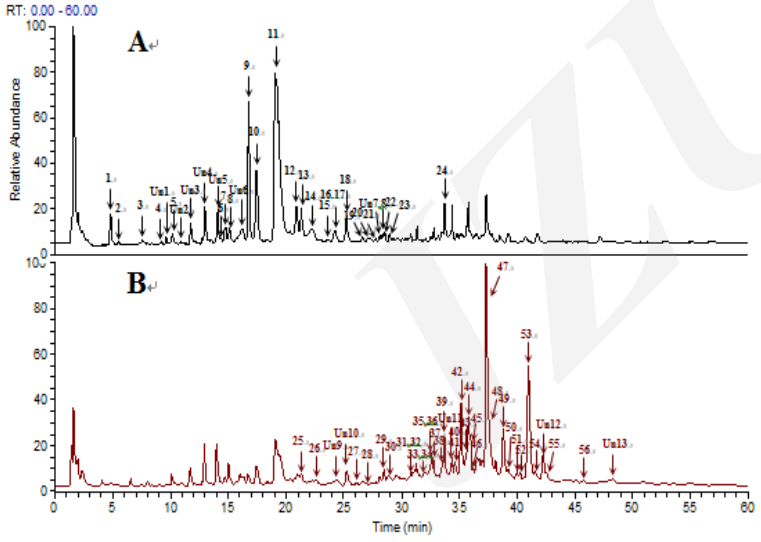

Fig. 1 Total ion chromatography of danshen extract in (A) negative and (B) positive ion mode.

Table 2 Metabolites identified in bio-samples from rats after oral administration of danshen extract

No.	t_R (min)	Ion	Theoretical mass (m/z)	Experimental mass (m/z)	Formula [M-H]⁻/[M+H]⁺	Error (ppm)	MS/MS fragment	Identification	Plasma	Urine	Feces	Bile
Phenolic acids												
1	2.11	[M-H]⁻	277.0013	277.0020	$C_9H_9O_8S$	2.8	MS^2[277]: 259(57), 215(35), 197(100)	Sulfate danshensu	×	×	√	×
2	4.26	[M-H]⁻	277.0013	277.0010	$C_9H_9O_8S$	-0.8	MS^2[277]: 215(40), 197(100) MS^3[196]: 179(100)	Sulfate danshensu	×	√	×	×
3	4.77	[M-H]⁻	197.0444	197.0446	$C_9H_9O_5$	0.6	MS^2[197]: 179(100) MS^3[179]: 135(100)	Danshensu [a,b]	√	√	√	×
4	7.35	[M-H]⁻	211.0601	211.0603	$C_{10}H_{11}O_5$	0.9	MS^2[211]: 193(100), 165(73) MS^3[193]: 149(29), 134(100)	Methyl danshensu	√	√	√	√
5	7.47	[M-H]⁻	179.0339	179.0344	$C_9H_7O_4$	3.1	MS^2[179]: 135(100) MS^3[135]: 135(100)	Demethyl ferulic acid	×	√	×	×
6	7.52	[M-H]⁻	137.0233	137.0236	$C_7H_5O_3$	1.7	MS^2[137]: 137(100)	Protocatechuic aldehyde [a,b]	×	×	√	×
7	7.62	[M-H]⁻	181.0495	181.0502	$C_9H_9O_4$	3.7	MS^2[181]: 163(100) MS^3[162]: 119(100)	Dihydro caffeic acid	×	√	√	×
8	8.29	[M-H]⁻	179.0339	179.0341	$C_9H_7O_4$	1.2	MS^2[179]: 135(100) MS^3[135]: 135(100)	Acetylated Protocatechuic aldehyde	×	√	×	×
.....												
110	38.97	$[M+H]^+$	293.1172	293.1178	$C_{18}H_{13}O_3$	2.1	MS^2[293]: 275(100), 247(40) MS^3[275]: 247(100)	Dehydrotanshinone Ⅱ A [b]	√	√	√	√
111	40.01	$[M+H]^+$	281.1536	281.1540	$C_{18}H_{21}O_2$	1.4		Dehydromiltirone [b]	×	×	√	×
112	40.23	$[M+H]^+$	293.1172	293.1175	$C_{18}H_{13}O_3$	1.0		Dehydrotanshinone Ⅱ A [b]	√	√	√	×
113	40.58	[M-H]⁻	277.0859	277.0865	$C_{18}H_{13}O_2$	2.1	MS^2[277]: 249(100), 221(53)	Dehydrated tanshinol B	×	×	√	×
114	41.15	$[M+H]^+$	295.1329	295.1331	$C_{18}H_{15}O_3$	0.9	MS^2[295]: 277(100), 249(14) MS^3[277]: 262(29), 249(100)	Tanshinone Ⅱ A [a,b]	√	√	√	√
115	41.27	[M-H]⁻	277.0859	277.0863	$C_{18}H_{13}O_2$	1.4	MS^2[277]: 249(100), 221(60)	Dehydrated tanshinol B	×	×	√	×
116	42.32	$[M+H]^+$	283.1693	283.1694	$C_{20}H_{23}O_2$	0.4	MS^2[283]: 265(100), 241(47), 223(63) MS^3[265]: 237(62), 223(100)	Miltirone [b]	×	√	√	×
117	42.70	$[M+H]^+$	269.1536	269.1537	$C_{18}H_{21}O_2$	0.4	MS^2[269]: 254(100) MS^3[254]: 239(100)	Demethyl miltirone	×	×	√	×
118	47.15	$[M+H]^+$	299.1642	299.1646	$C_{19}H_{23}O_3$	1.3	MS^2[299]: 281(100), 256(52), 253(49)	Dihydro cryptotanshinone	×	×	√	×
									35	63	62	18

[a] confirmed by reference standards; [b] Original components in danshen extract; "√": Detected; "×": Undetected.