

Table S3 Absorbed constituents in rat serum after the oral administration of Fufang Danshen Tablet

No.	Identification	T _R (min)	Formula	[M+H] ⁺ (error, ppm)	[M-H] ⁻ (error, ppm)	Characteristic Fragment	
						POS	NEG
P1	Danshensu [*]	4.14	C ₉ H ₁₀ O ₅	ND	197.0458 (0.3)	ND	179.0350[M-H-H ₂ O] ⁻ 152.8940[M-H-COOH] ⁻ 135.0441[M-H-CO ₂ -H ₂ O] ⁻
P2	Ginsenoside F ₁	5.64	C ₃₆ H ₆₂ O ₉	639.4442 (-3.9)	ND	621.4514[M+H-H ₂ O] ⁺ 441.3689[M+H-2H ₂ O-Glc] ⁺ 423.3499[M+H-3H ₂ O-Glc] ⁺	ND
P3	Salvianolic acid D [*]	7.15	C ₂₀ H ₁₈ O ₁₀	ND	417.0823 (-1.1)	ND	197.0419[DSS-H] ⁻ 179.0346[C ₉ H ₈ O ₄ -H] ⁻
P4	Ginsenoside Rg ₁ [*]	7.47	C ₄₂ H ₇₂ O ₁₄	801.4996 (0.1)	ND	621.4332[M+H-H ₂ O-Glc] ⁺ 441.3698[M+H-2H ₂ O-2Glc] ⁺ 423.3593[M+H-3H ₂ O-2Glc] ⁺ 405.3513[M+H-4H ₂ O-2Glc] ⁺	ND
P5	Rosmarinic acid [*]	8.14	C ₁₈ H ₁₆ O ₈	ND	359.0775 (0.8)	ND	197.0439[DSS-H] ⁻ 161.0253[M-H-DSS] ⁻
P6	Salvianolic acid A [*]	8.83	C ₂₆ H ₂₂ O ₁₀	ND	493.1154 (2.7)	ND	313.0682[M-H-CA] ⁻ 295.0601[M-H-DSS] ⁻ 197.0518[DSS-H] ⁻
P7	Lithospermic acid [*]	8.84	C ₂₇ H ₂₂ O ₁₂	ND	537.1046 (1.3)	ND	493.1177[M-H-CO ₂] ⁻ 295.0615[M-H-DSS-CO ₂] ⁻
P8	Salvianolic acid B [*]	11.02	C ₃₆ H ₃₀ O ₁₆	ND	717.1493 (4.5)	ND	519.0924[M-H-DSS] ⁻ 339.0507[M-H-DSS-CA] ⁻ 321.0400[M-H-2DSS] ⁻

P9	Ginsenoside Rb ₁ [*]	18.91	C ₅₄ H ₉₂ O ₂₃	1109.6155 (4.8)	1107.6043 (7.8)	767.4861[M+H-2Glc-H ₂ O] ⁺ 325.1125[2Glc+H] ⁺	1107.6041[M-H] ⁻
P10	Ginsenoside Rd [*]	19.25	C ₄₈ H ₈₂ O ₁₈	947.5579 (0.6)	945.5454 (2.7)	767.4939[M+H-Glc-H ₂ O] ⁺ 605.4418[M+H-2Glc-H ₂ O] ⁺ 425.3773[M+H-3Glc-2H ₂ O] ⁺	945.5396[M-H] ⁻ 783.4673[M-H-Glc] ⁻
P11	Salvianolic acid C [*]	19.65	C ₂₆ H ₂₀ O ₁₀	ND	491.0989 (1.1)	ND	293.0443[M-H-DSS] ⁻ 197.0516[DSS-H] ⁻
P12	Przewaquinone B	19.85	C ₁₈ H ₁₂ O ₄	293.0811 (0.8)	ND	249.0876[M+H-CO ₂] ⁺ 178.0767[M+H-2CO-CH ₃ -CO ₂] ⁺	ND
P13	Tanshinol B	20.22	C ₁₈ H ₁₆ O ₄	297.1124 (0.9)	ND	279.1039[M+H-H ₂ O] ⁺ 261.0918[M+H-2H ₂ O] ⁺ 233.0976[M+H-2H ₂ O-CO] ⁺	ND
P14	Tanshinone II _B	20.57	C ₁₉ H ₁₈ O ₄	311.1278 (0)	ND	267.1373[M+H-CO ₂] ⁺ 252.1152[M+H-CO ₂ -CH ₃] ⁺	ND
P15	Salvianonol	20.62	C ₁₈ H ₂₀ O ₄	301.1427 (-0.1)	ND	283.1345[M+H-H ₂ O] ⁺ 265.1228[M+H-2H ₂ O] ⁺ 241.1209[M+H-COOH-CH ₃] ⁺	ND
P16	Danshenxinkun A	21.31	C ₁₈ H ₁₆ O ₄	297.1122 (0.1)	295.0979 (1.2)	261.0912[M+H-2H ₂ O] ⁺ 233.0963[M+H-2H ₂ O-CO] ⁺	265.0863[M-H-2CH ₃] ⁻ 237.0917[M-H-2CH ₃ -CO] ⁻
P17	Dihydrotanshinone I [*]	22.43	C ₁₈ H ₁₄ O ₃	279.1014 (-0.5)	ND	261.0903[M+H-H ₂ O] ⁺ 205.1004[M+H-2CO-H ₂ O] ⁺	ND
P18	Neocryptotanshinone	22.76	C ₁₉ H ₂₂ O ₄	315.1594 (0.9)	313.1444 (-0.5)	297.1488[M+H-H ₂ O] ⁺ 279.1372[M+H-2H ₂ O] ⁺	283.135 [M-H-2CH ₃] ⁻ 255.1404[M-H-2CH ₃ -CO] ⁻
P19	Epidanshenspiroketallactone	23.50	C ₁₇ H ₁₆ O ₃	269.1172 (0)	ND	251.1089[M+H-H ₂ O] ⁺ 223.1100[M+H-H ₂ O-CO] ⁺ 177.0068[M+H-2H ₂ O-2CO] ⁺	ND

P20	Cryptotanshinone [*]	24.42	C ₁₉ H ₂₀ O ₃	297.1488 (0.9)	ND	282.1314[M+H-CH ₃] ⁺ 251.1449[M+H-CO-H ₂ O] ⁺	ND
P21	Tanshinone I [*]	24.52	C ₁₈ H ₁₂ O ₃	277.0858 (-0.3)	ND	249.0914[M+H-CO] ⁺ 178.0779[M+H-3CO-CH ₃] ⁺	ND
P22	Tanshinone II _A [*]	27.24	C ₁₉ H ₁₈ O ₃	295.1326 (-1)	ND	277.1217[M+H-H ₂ O] ⁺ 252.0777[M+H-CO-CH ₃] ⁺ 249.1264[M+H-H ₂ O-CO] ⁺	ND

Note: ^{*}Positively identified via comparison with authentic standards. ND, Not detected; DSS, C₉H₁₀O₅ (Danshensu); CA, C₉H₈O₄ (Caffeic acid); Glc, glucose; GlcUA, glucuronyl moiety.