Supplementary Information (SI) for RSC Advances.
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Supporting Information

Analysis of Metabolic Characteristics of Epristeride in Zebrafish Based on LC-Q-TOF MS and Its Potential Applications in Doping Control

Yirang Wang[1†], Zhongquan Li[1†], Jiahui Cheng[1†], Tingyuan Zheng[1†], Peijie Chen[1,2], Xiaojun Deng[1], Peichao Zhang[3*], Bing Liu[1*]

[1]Research Institute for Doping Control, Shanghai University of Sport, Shanghai 200438, China

[2]School of Exercise and Health, Shanghai University of Sport, Shanghai 200438, China

[3]The Center for Basic Research and Innovation of Medicine and Pharmacy (MOE), School of Pharmacy, Second Military Medical University (Naval Medical University), Shanghai, P. R. China.

* Corresponding Author: pczhang@smmu.edu.cn; liubing2019@sus.edu.cn

Table S1. MS annotation details for differential metabolites.

Metabolites	**Average Rt(min)**	**Average *m/z***	**Adduct type**	**MS/MS fragments**		
Hexanoy-L-carnitine	7.99	260.1852	$[M+H]^+$	201.1124	144.1021	85.0285
11-HDoHE	15.13	343.2238	$[M-H]^-$	325.2181	281.2285	141.0559
Decanoylcarnitine	13.19	316.2477	$[M+H]^+$	299.2686	239.1642	173.1543
Lysophosphatidylcholine (18:2)	16.33	520.3397	$[M+H]^+$	502.3294	184.0736	137.1341
Phenylethanolamine	6.08	120.0804	$[M-H_2O+H]^+$	118.0649	103.0541	91.0542
Guanosine	5.66	284.0986	$[M+H]^+$	152.0566	135.0298	97.0303
N,N-Dimethyldecylamine oxide	12.53	202.2159	$[M+H]^+$	184.2056	85.0995	62.0595
Taurine	2.39	126.0218	$[M+H]^+$	108.0116	80.9632	64.9693
Lysophosphatidylcholine (18:1)	17.14	522.3552	$[M+H]^+$	504.3449	184.0734	104.1068
Xanthine	5.46	153.0403	$[M+H]^+$	153.0408	136.0139	110.0349
4-Methyl-5-thiazoleethanol	6.53	144.0474	$[M+H]^+$	126.0374	113.0295	70.9952
Phenylalanine	16.85	400.3413	$[M+H]^+$	341.2688	329.366	85.0287
Vitamin B5 (Pantothenic acid)	6.04	220.1178	$[M+H]^+$	202.1074	184.097	90.0551
Linoleic acid (C18:2)	14.85	281.2469	$[M+H]^+$	263.2363	245.2255	69.0694
Lauroylcarnitine	14.56	344.2792	$[M+H]^+$	285.2057	183.1738	85.0281
Eudesmin	13.37	409.1616	$[M+Na]^+$	392.3412	289.1014	/
Palmitoylcarnitine	16.85	400.3413	$[M+H]^+$	341.2688	144.1014	85.0283
Guanine	5.57	152.0564	$[M+H]^+$	135.0302	110.0349	107.0347
Inosine	5.63	269.0881	$[M+H]^+$	179.0569	137.0464	119.0352
Tetradecanoylcarnitine	15.64	372.3104	$[M+H]^+$	356.0702	205.1224	129.0541

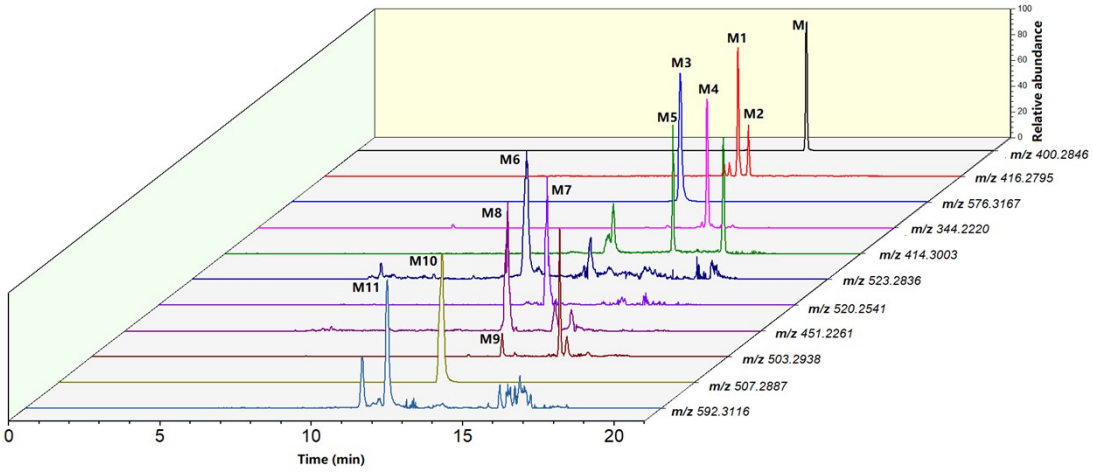
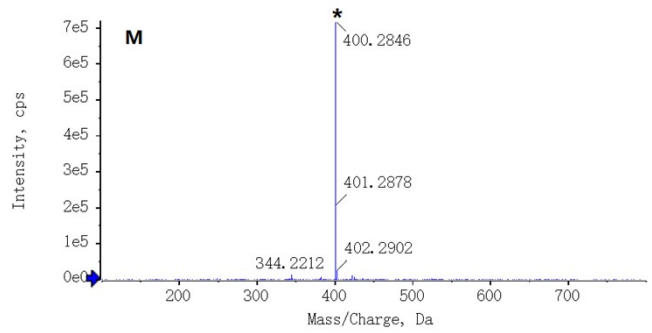
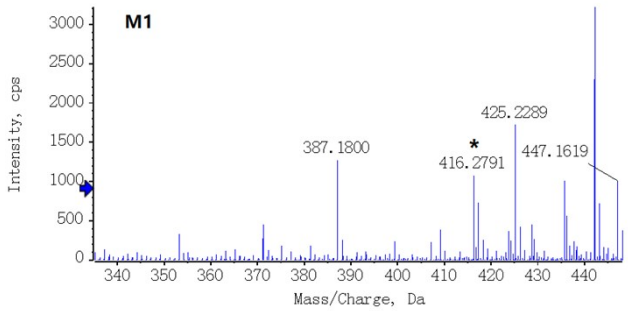
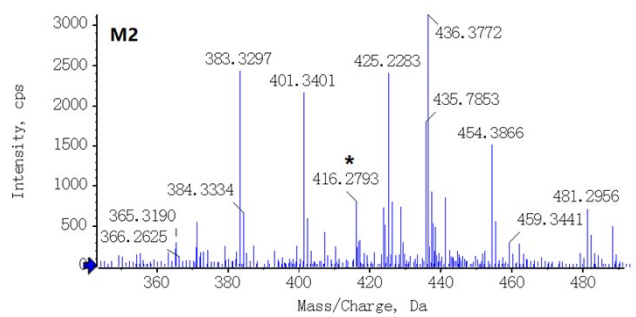
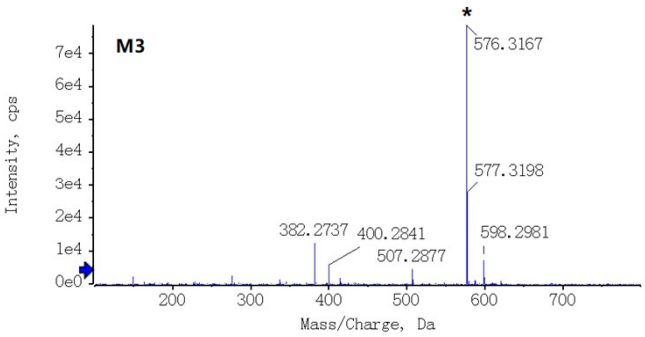


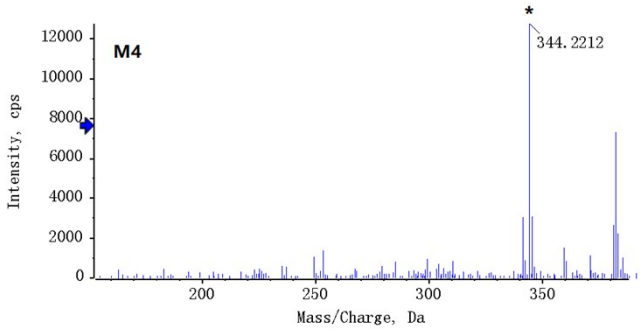
Figure S1. Extracted ion chromatograms of epristeride and its proposed metabolites in positive ESI mode.

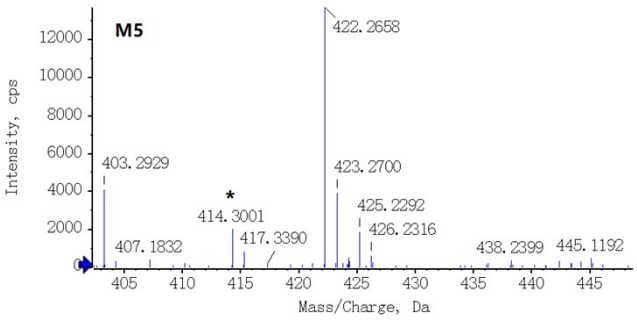

M
400.2846
401.2878
402.2902
344.2212
Intensity, cps
Mass/Charge, Da

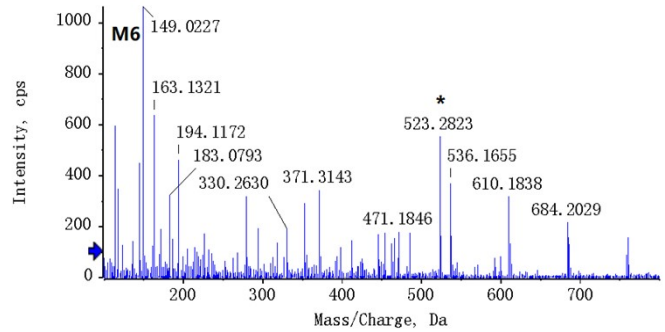

M1
425.2289
387.1800
416.2791
447.1619
Intensity, cps
Mass/Charge, Da

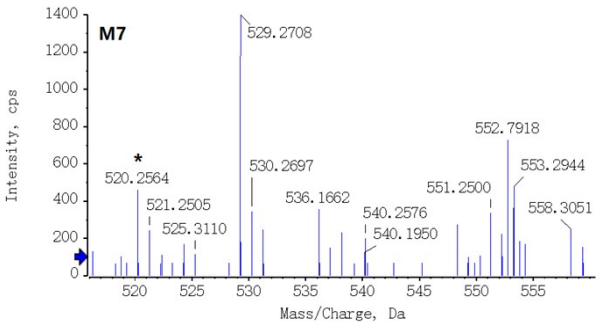

M2
436.3772
383.3297
401.3401
425.2283
435.7853
454.3866
416.2793
384.3334
481.2956
365.3190
459.3441
366.2625
Intensity, cps
Mass/Charge, Da


M3
576.3167
577.3198
382.2737
400.2841
507.2877
598.2981
Intensity, cps
Mass/Charge, Da


M4
344.2212
Intensity, cps
Mass/Charge, Da


M5
422.2658
403.2929
423.2700
414.3001
425.2292
417.3390
426.2316
407.1832
438.2399
445.1192
Intensity, cps
Mass/Charge, Da


M6
149.0227
163.1321
523.2823
194.1172
183.0793
536.1655
330.2630
371.3143
610.1838
471.1846
684.2029
Intensity, cps
Mass/Charge, Da


M7
529.2708
520.2564
552.7918
530.2697
553.2944
521.2505
536.1662
551.2500
525.3110
540.2576
558.3051
540.1950
Intensity, cps
Mass/Charge, Da

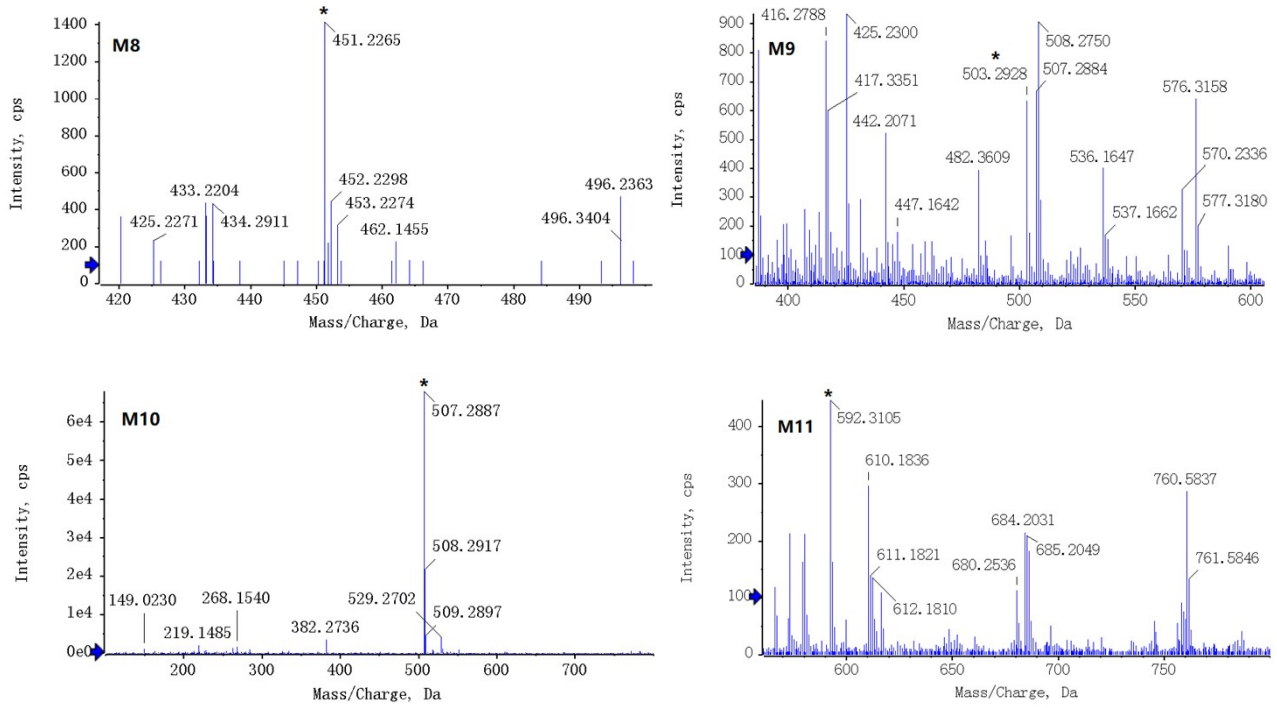


Figure S2. Full MS/MS spectra of epristeride and its proposed metabolites in positive ESI mode.

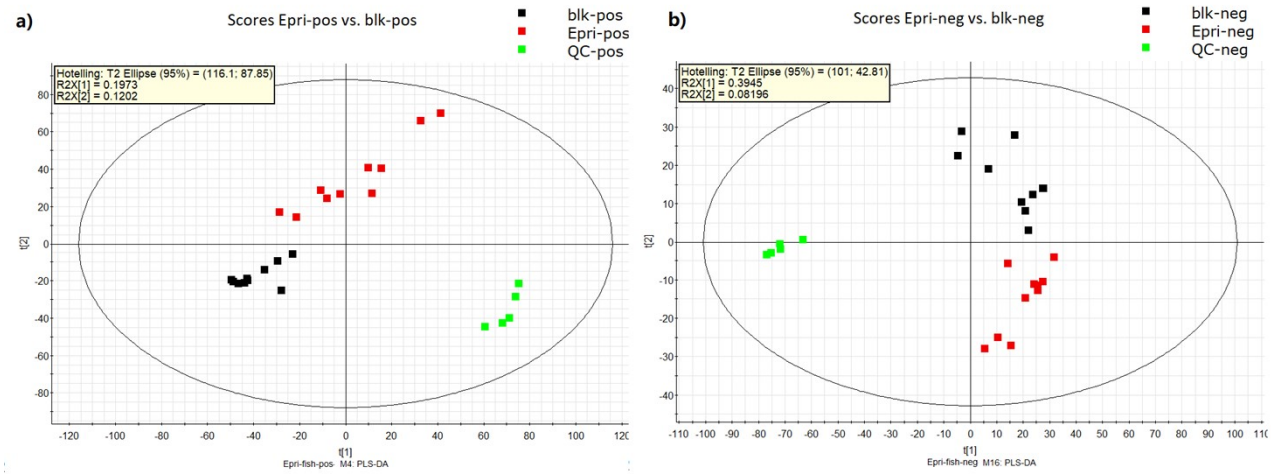


Figure S3. Score plots for the ESI+ (a) and ESI− (b) datasets including study samples, pooled QC injections, and solvent blanks.