Electronic Supplementary Material (ESI) for Analytical Methods.

Supplementary Information

Metabolomics-based Non-targeted Screening Analysis of 34 PPCPs in Bovine and Piscine Muscles†

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3 Pages, 4 Figures, 3 Tables

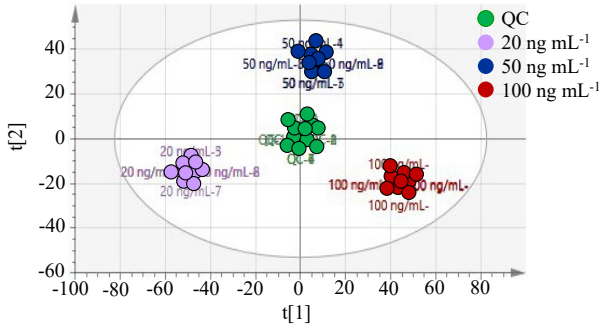

Fig. S1 PCA score plots of spiked piscine muscle sample groups.

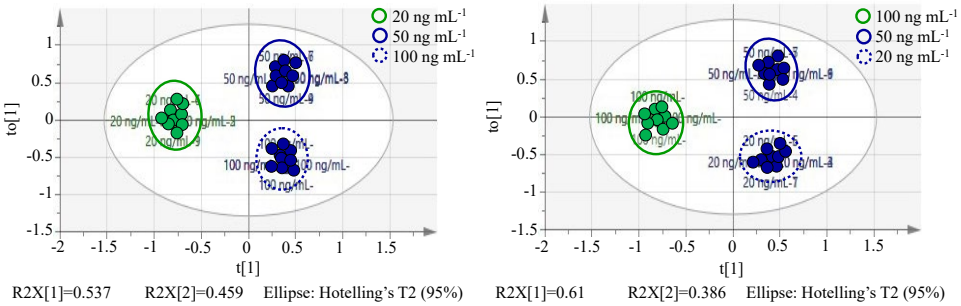

Fig. S2 OPLS-DA score plots of spiked piscine muscle sample groups.

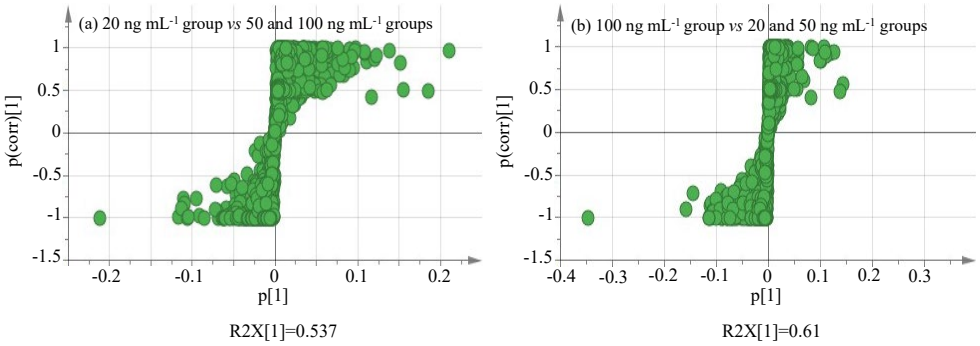

Fig. S3 S-plot plots of spiked piscine muscle sample groups.

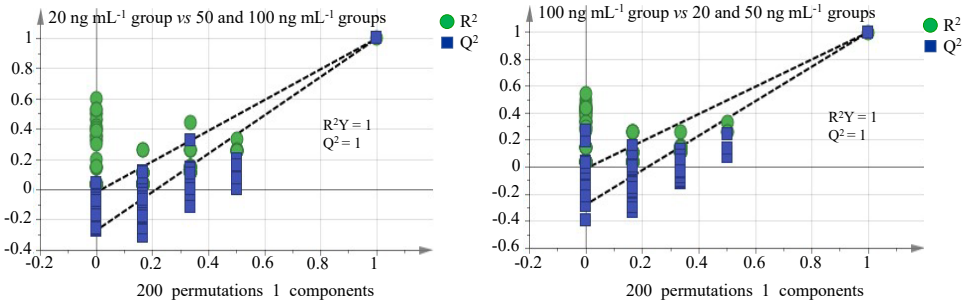

Fig. S4 Permutation plots of spiked piscine muscle sample groups.

Table S1 Recovery (%) of spiked ciprofloxacin-d8 in bovine muscle sample groups (*n*=9)

Concentration groups (ng·mL^{-1})	1	2	3	4	5	6	7	8	9	RSD (%)
20	90.1	83.3	87.6	84.8	89.1	84.5	88.7	92.1	92.1	3.7
50	89.2	83.4	91.7	88.4	82.2	90.0	87.4	82.5	83.6	4.2
100	81.9	73.4	78.2	74.0	82.3	76.5	77.2	77.5	78.9	3.9

Table S2 Recovery (%) of spiked ciprofloxacin-d8 in piscine muscle sample groups (*n*=9)

Concentration groups (ng·mL^{-1})	1	2	3	4	5	6	7	8	9	RSD (%)
20	93.7	88.4	92.1	90.8	87.4	87.9	86.4	89.0	92.7	2.9
50	87.4	85.6	88.0	87.3	82.9	84.3	81.2	82.1	80.5	3.4
100	78.4	73.1	73.1	74.2	77.5	72.0	80.5	83.2	81.3	5.3

Table S3 Marker compounds screened in piscine muscle sample groups

Var ID (Primary)	Marker compounds	VIP Pred[a]	Coordinate in S-plot[b]	Mass error (ppm)[c]	LOD (μg kg^{-1})
M260T571	Propranolol	3.784/4.646	(-0.099, -0.905)/(0.122, 0.904)	0.617	0.6
M234T261	Cimbuterol	3.089/4.111	(-0.081, -0.906)/(0.108, 0.944)	-2.061	0.5
M228T491	Tolobuterol	4.030/3.586	(-0.106, -0.917)/(0.094, 0.902)	-0.294	0.5
M214T418	Clorprenaline	3.379/3.281	(-0.089, -0.903)/(0.086, 0.904)	-0.225	0.7
M226T148	Terbutaline	2.259/2.612	(-0.059, -0.916)/(0.069, 0.917)	-1.751	0.6
M310T388	Nadolol	3.816/2.034	(-0.100, -1.000)/(0.053, 0.901)	-2.351	0.6
M273T138	Sotalol	1.722/1.660	(-0.019, -0.904)/(0.044, 0.979)	0.563	0.7
M170T467	Ipronidazole	4.059/4.221	(-0.107, -0.927)/(0.111, 0.936)	2.920	0.7
M202T352	Thiabendazole	4.158/4.573	(-0.109, -0.934)/(0.120, 0.931)	-1.654	1.6
M248T296	Tinidazole	2.740/3.588	(-0.072, -0.965)/(0.094, 0.939)	-2.146	1.9
M266T626	Albendazole	4.029/3.441	(-0.106, -0.924)/(0.090, 0.940)	0.143	1.9
M300T661	Fenbendazole	2.926/3.121	(-0.077, -0.965)/(0.082, 0.965)	-0.272	0.6
M188T101	Metronidazole-hydroxy	1.943/2.638	(-0.051, -0.944)/(0.069, 0.947)	-0.353	0.5
M172T152	Metronidazole	2.721/2.833	(-0.072, -0.975)/(0.074, 0.954)	2.916	0.8
M220T383	Ornidazole	3.301/1.854	(-0.087, -0.999)/(0.049, 0.926)	-1.476	0.6
M162T266	5-Chloro-1-methyl -4-nitroimidazole	1.673/1.654	(-0.044, -0.984)/(0.043, 0.920)	-0.394	0.6
M201T177	Ronidazole	1.815/1.657	(-0.048, -0.913)/(0.044, 0.912)	-1.134	0.4
M393T500	Sparfloxacin	1.622/2.866	(-0.043, -0.907)/(0.075, 0.990)	-3.455	1.0
M400T446	Difloxacin	1.211/2.178	(-0.032, -0.909)/(0.057, 0.994)	-2.715	0.4
M262T553	Oxolinic acid	1.986/2.371	(-0.052, -0.910)/(0.062, 0.907)	4.435	2.0
M263T524	Cinoxacin	2.282/2.133	(-0.060, -0.913)/(0.056, 0.901)	2.106	0.8
M287T661	Boldenone	1.660/2.248	(-0.044, -0.905)/(0.059, 0.946)	-0.921	0.7
M345T738	Testosterone propionate	2.480/1.559	(-0.065, -0.999)/(0.037, 0.929)	0.122	1.7
M271T659	Trenbolone	2.684/1.422	(-0.071, -1.000)/(0.037, 0.907)	1.869	1.7
M442T663	Deflazacort	1.162/1.355	(-0.031, -0.909)/(0.036, 0.914)	-4.677	0.5
M250T278	Sulfapyridine	2.966/4.113	(-0.078, -0.934)/(0.108, 0.954)	-0.686	0.4
M279T374	Sulfisomidine	2.508/3.661	(-0.066, -0.905)/(0.096, 0.966)	-3.077	2.0
M265T304	Sulfamerazine	2.159/3.446	(-0.057, -0.905)/(0.091, 0.980)	-2.799	2.1
M279T222	Sulfmethazine	3.532/3.200	(-0.093, -0.906)/(0.084, 0.909)	-4.681	1.8
M277T482	Sulfabenzamide	1.632/2.354	(-0.043, -0.909)/(0.062, 0.959)	2.561	1.8
M251T200	Sulfadiazine	1.897/1.917	(-0.050, -0.902)/(0.050, 0.935)	0.422	0.3
M285T407	Sulfachloropyridazine	1.362/1.475	(-0.036, -0.902)/(0.039, 0.916)	-2.350	2.1
M215T120	Sulphacetamide	1.368/1.222	(-0.036, -0.902)/(0.032, 0.915)	4.277	0.6
M271T366	Sulfamethizole	2.293/1.222	(-0.060, -1.000)/(0.032, 0.901)	-2.372	0.8

[a] two VIP values from 100 and 20 ng mL^{-1} groups, respectively; [b] two-group coordinate values from 100 and 20 ng mL^{-1} groups, respectively;
[c] Mass error (ppm) = (extracted molecular weight from W4M platform - extracted molecular weight from LC-MS/MS)*10^6/extracted molecular weight from LC-MS/MS.