

Electronic Supplementary Information

**Serum metabolomics analysis reveals oral exposure to
benzo(a)pyrene impaired lipid metabolism in rats**

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Supplementary Tables**Table S-1.** MS and MS/MS information of tentatively identified biomarkers.

No.	Metabolite	Chemical formula	Measured mass(Da)	Adduct MW(Da)	MW Difference(Da)	MS/MS fragment
1	LysoPC(18:0)	C26H54NO7P	524.3654	524.3711	0.0057	524(100), 87(69), 523(28), 149(24), 101(19), 73(14)
2	LysoPC(18:2)	C26H50NO7P	520.3342	520.3398	0.0056	520(100), 521(27), 87(14)
3	LysoPC(20:4)	C28H50NO7P	544.3336	544.3398	0.0062	544(100), 87(44), 149(34), 545(31), 163(29), 568(29), 73(20), 101(10)
4	PC(36:2)	C44H84NO8P	786.5929	785.5935	0.0078	87(100), 149(47), 101(27), 141(32), 73(27)
5	Sphinganine	C18H39NO2	302.3022	302.3055	0.0032	302(100), 284(97), 258(88), 141(37), 163(35), 390(28), 279(28)
6	L-Valine	C5H11NO2	118.0849	118.0863	0.0014	61(100), 118(88), 132(54), 73(41), 149(60), 116(30), 80(27)
7	Phytosphingosine	C18H39NO3	318.2968	318.3003	0.0035	318(100), 149(34), 319(19), 163(12), 279(10)
8	Cytosine	C4H5N3O	112.0493	112.0505	0.0012	73(100), 149(97), 163(84), 112(81), 61(96), 131(21), 279(19)
9	Cer(d18:0/14:0)	C32H65NO3	512.5	512.5037	0.0037	87(100), 282(95), 149(43), 101(27), 73(26), 141(30)
10	Palmitic amide	C16H33NO	256.2611	256.2635	0.0024	256(100), 87(92), 149(38), 73(24), 101(23)
11	LysoPC(20:3)	C28H52NO7P	546.3464	546.3554	0.0090	496(100), 87(30), 497(26), 149(20), 73(12)
12	LysoPC(18:3)	C26H48NO7P	518.32	518.3241	0.0041	496(100), 87(48), 149(27), 497(26), 73(17), 101(11)

Supplementary Figures

Figure S1. The total ion chromatograms (TIC) of quality control samples injected in negative (A) and positive (B) ESI mode. In negative ESI mode, the maximum intensity of spectrum peak was just equal to the baseline level of intensity of spectrum peak in positive ESI mode. Therefore, positive ESI mode was conducted to acquire metabolite profiling.

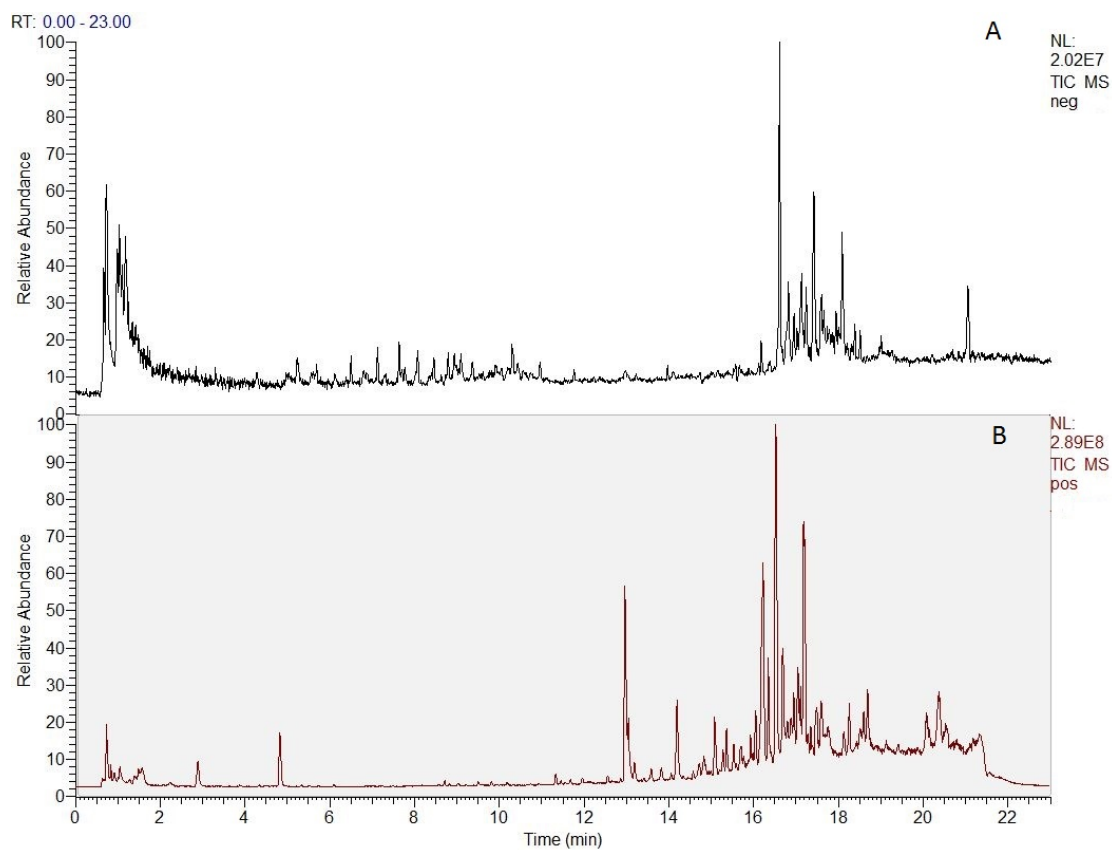


Figure S2. Scoring plots of PCA analysis for all the samples. ● QC sampels; ◆ control and dose groups. QC sampels showed a tight cluster, suggesting the method had good repeatability.

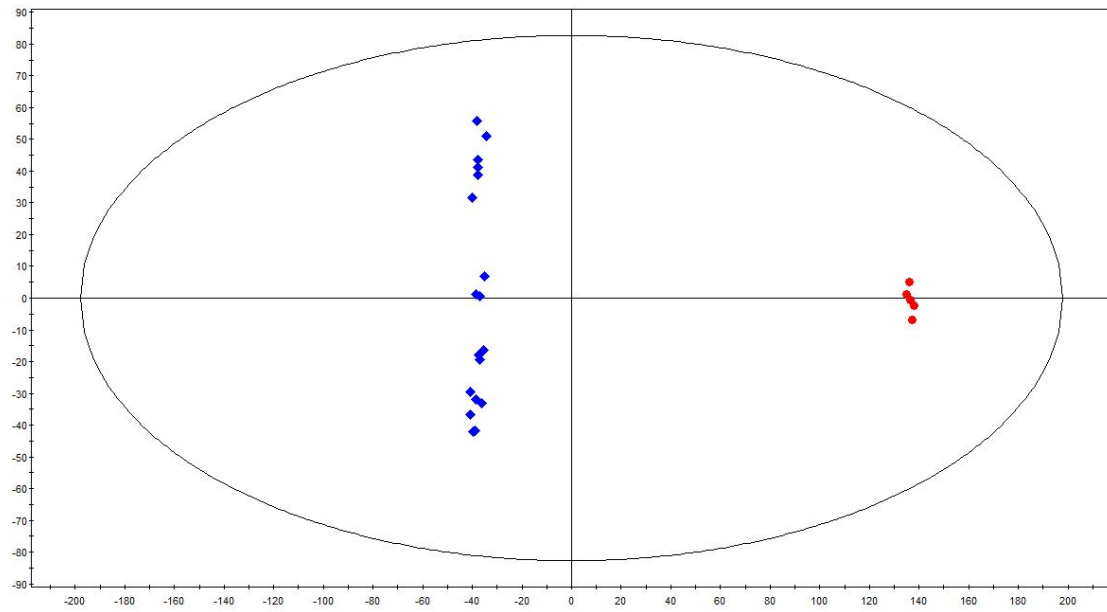


Figure S3. Random permutation-test results (n=200) of the PLS-DA model. The Y-axis intercepts were: R2(0, 0.85), Q2(0, -0.15). The calculated R2 and Q2 values were lower than the original ones in the validation plot and the Q2 intercepted the vertical axis was below zero, so the model was considered valid.

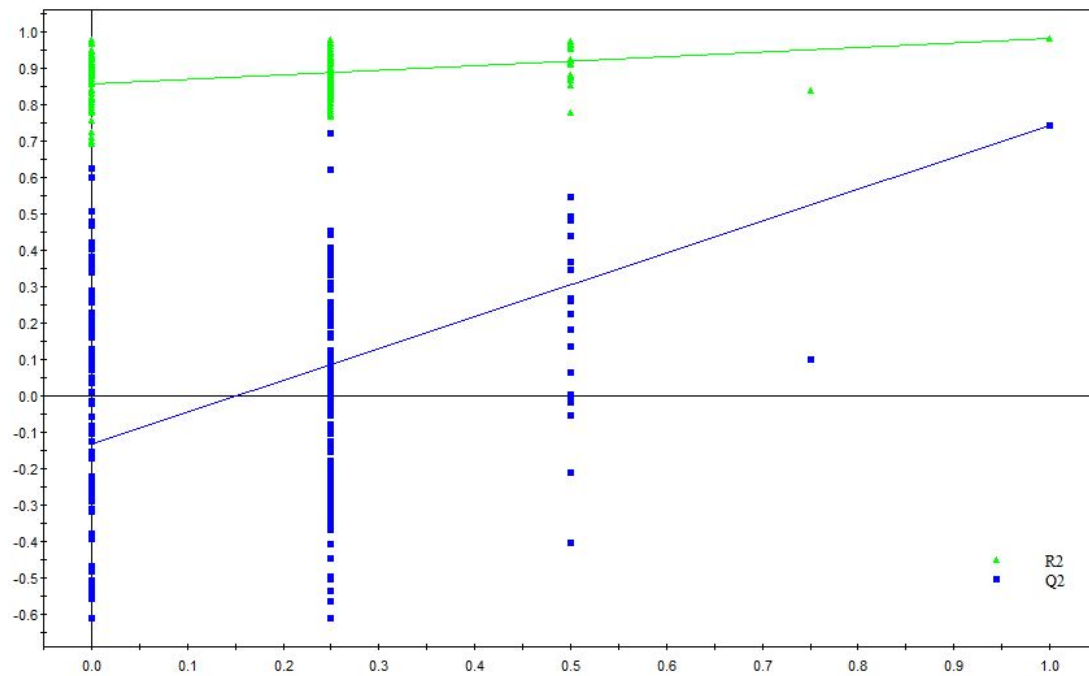


Figure S4. CV values of the variables extracted from serum metabolic profile.

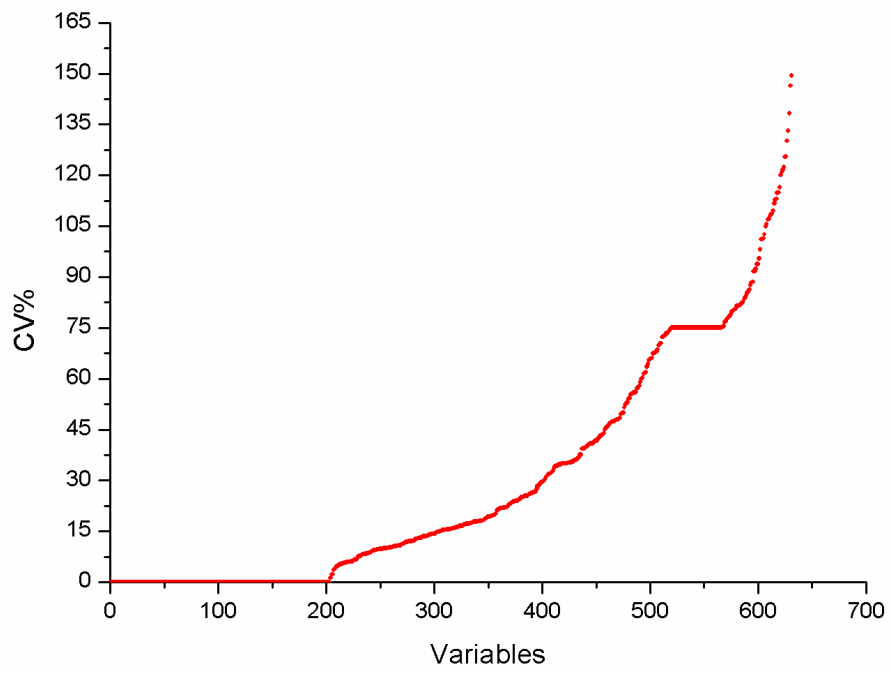


Figure S5. Organ coefficients of liver (multiplied by 1000 times) following B(a)P exposure.

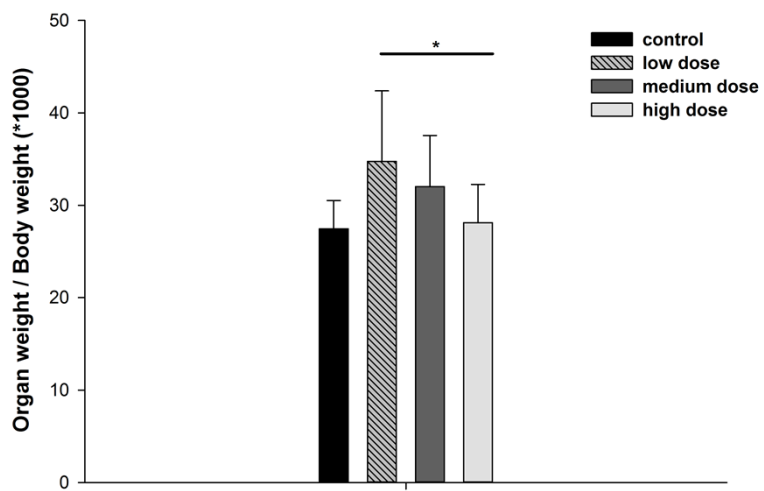


Figure S6. Effects of B(a)P exposure on hepatic mRNA expression of *chpt1*, *pent*, *lpcat1/2*, *pla2*.
*p < 0.05.

