Electronic Supplementary Information

Serum metabolomic response of rat to chronic arsenic exposure via drinking water

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Supplementary Table

Table S1. Comparison of differential metabolites between our study and other reported studies.

	Our study			Wang C et al. ¹			García-Sevillano M et al. ²		
Animal model	Male Sprague Dawley rats				Male Wistar rats			M.musculus mice	
Age	6 weeks				4~6 weeks			7 weeks	
Arsenic species	sodium arsenite				sodium arsenite			As2O3	
Timespan	3 months				6 months			12 days	
Instrument	UPLC/Orbitrap-MS				UPLC/Q-TOF MS			DI-ESI-/Q-TOF MS	
Sample	serum				serum			plasma	
Doses		0.5 ppm	2 ppm	10 ppm		10 ppm	50 ppm		3mg/kg/day
Differential metabolites	lysoPC(18:0)	_	_	↑	CPA(18:2/0:0)	_	1	lysoPC	1
	lysoPC(20:1)	_	_	↑	lysoPC(14:0)	_	Ļ	PC	Ļ
	ceramide (d18:0/14:0)	_	1	_	lysoPC(18:4)	_	Ļ	diglycerides	1
	ceramide (d18:0/16:0)	_	_	↑	lysoPC(18:0)	_	Ļ	triglycerides	1
	octadecenylcarnitine	_	_	↑	palmitoylcarnitine	_	Ļ	pyruvate	Ļ
	palmitoylcarnitine	_	1	↑	lysoPC(20:2)	_	Ļ	homocysteine	Ļ
	carnitine	_	1	\downarrow				creatine	1
	sphinganine	_	1	↑				glutamic acid	1
	phytosphingosine	_	1	↑				acetyl-carnitine	1
	methionine	-	Ļ	\rightarrow				glucose	\downarrow
	proline	_	Ļ	\downarrow				glutathione	Ļ
	valine	_	-	\downarrow				citric acid	1
	tyrosine	_	-	\downarrow				phosphorylcholine	1
	indoleacetaldehyde	_	—	\downarrow				choline	\uparrow
	indoleacrylic acid	_	-	\downarrow				methionine	1

pyroglutamic acid	_	↑			arginine	\downarrow
creatine	_	—	↓		taurine	1
cytosine	—	—	\downarrow			
uric acid	_	_	Ļ			

¹ Wang C, Feng R, Li Y, Zhang Y, Kang Z, Zhang W, Sun DJ. The metabolomic profiling of serum in rats exposed to arsenic using UPLC/Q-TOF MS. Toxicol Lett. 2014, 17;229(3):474-81.

² García-Sevillano MA, García-Barrera T, Navarro F, Gómez-Ariza JL. Analysis of the biological response of mouse liver (Mus musculus) exposed to As2O3 based on integrated -omics approaches. Metallomics. 2013, 5(12):1644-55.

Supplementary Figures





Figure S2. Random permutation-test results (n=200) of the PLS-DA model. The Y-axis intercepts were: R2(0, 0.17), Q2(0, -0.189). 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. \blacktriangle R2, \blacksquare Q2.

