Discovery of systematic responses and potential biomarkers induced by ochratoxin A using Metabolomics

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Online Supplementary Material

Supplementary Table 1 Serum Clinical Chemistry After Repeated Administration of 0, 70 or 210µg/kg b.w. OTA for 2, 4 or 13 weeks. Data are presented as Mean±SD of six rats per group. a: $P<0.05$ when compared to 0 µg/kg b.w. group; b: $P<0.05$ when compared to 70 µg/kg b.w. group. (Qiu et al., 2014)

Time	Dose	ALT (U/L)	AST (U/L)	ALB (g/L)	ALP(U/L)	GLU (mmol/L)	BUN (mmol/L)	CREA (umol/L)	HDL(mmol/L)	LDL(mmol/L)	LDH (U/L)
2 weeks	0 µg/kg	45.17±5.04	283.4±62.97	52.4±0.85	310.2±30.65	3.37±1.61	6.2±0.53	37.48±15.94	2.52±0.31	0.59±0.17	3484±696.41
	70 µg/kg	45.2±6.3	241.4±52.67	51.68±2.92	315±32.8	4.71±1.07	6.16±0.4	29.2±2.41	2.91±0.46	0.96±0.42	3062.4±632.19
	210 µg/kg	42.67±6.44	207.67±44.38	50.07±2.08	305.33±40.5	4.3±1.03	6.17±0.67	30.82±9.82	2.37±0.23	0.72±0.18	2644.33±506.17a
4 weeks	0 µg/kg	50±3.08	239.6±24.89	74.98±3.52	288.4±35.5	4.99±1.1	5.69±0.71	28.18±2.8	2.96±0.34	0.64±0.2	3369.8±338.11
	70 µg/kg	52.83±6.79	225±61.24	76.48±4.21	366.5±77.78a	5.76±1.04	6.73±0.8	32.36±7.21	2.89±0.47	0.82±0.14	2964.5±769.2
	210 µg/kg	52.33±5.39	305±61.46b	72.4±2.74	275±13.64b	3.71±1.12b	6.08±0.94	34.15±3.57	3.42±0.18b	0.83±0.22	3841.5±727.22b
13 weeks	0 µg/kg	56.5±7.61	166.67±16.54	49.23±1.45	151.5±17.07	7.91±1.02	8.51±0.45	42.85±1.96	3.42±0.55	0.77±0.16	2042.83±236.54
	70 µg/kg	52.17±2.99	151.67±7.34	51.08±2.43	152.83±9.7	7.34±0.63	8.74±0.45	42.88±3.74	2.93±0.25	0.69±0.09	1973.5±153.3
	210 µg/kg	52.33±4.23	140.33±13.37a	51.23±2.37a	156.83±10.68	7.76±0.99	8.49±0.45	42.73±8.74	2.69±0.13a	0.74±0.15	1763±207.57a

Supplementary Table 2 The differential metabolites in plasma between control and OTA-exposed groups at 13 and 26 weeks based GC/MS

Compound	FC [CH] vs [CC])	FC ([CL] vs [CC])	FC ([DH] vs [DC])	FC ([DL] vs [DC])
Hexanedioic acid	-2570377	1.152479		
D-Glucose	2611405	-1		
Myo-Inositol	945951.1	-1	-1.15416	
198.0@28.734951			-2460940	-2460940
Pentanedioic acid			-1863863	-1863863
216.0@24.718487			-462831	-1.69669

Supplementary Table 3 The differential metabolites in plasma of low-dose groups at 2, 4, 13 and 26 weeks based GC/MS

Compound	FC ([BL] vs [AL])	FC ([CL] vs [AL])	FC ([DL] vs [AL])
Butanedioic acid	-4.7908354	-3.1944406	-3.3644085
D-Glucose	-5.660217	-1.9325283	-4.8736277
Gulonic acid	-25.890385	-311738.56	-19.785868
Inositol	-2.6851072	-2.6231654	-5.213988
Xylulose	-25114.482	-457595.34	-457595.34
Heptanedioic	-179125.25	-11.799545	2.481351

Ethylmalonate	-1	55743.16	-1
Hexadecanoic acid	-7.5393524	7.6612744	-1275862.1
Hexanedioic acid	-1.6599636	2.3318262	1.9105659
Sebacic acid	-460.86877	251.07663	144.42357
3,4-Dihydroxybutanoic acid	3.969869	4.7954946	6.4850807
Alanine	2.7783482	4.6866317	8.570164
Amino levulinic acid	490559.94	707102.8	436625.9
2-Pentenedioic acid	19021.148	22945.623	34893.01
3,3-hydroxyglutaric acid	559971.4	236610.38	589923.3
Adenosine	36854.758	87263.91	85181.586
Azelaic acid	3.937774	2.852939	7.048853
Benzeneacetic acid	2.3171153	7.0854764	12.575198
5-Hydroxyhexanoic acid	4.604775	7.466589	9.568629
Butanoic acid	3.7504656	7.994193	19.15925
Cholesterol	21385.059	18811.826	23013.98
Creatinine	2490231.8	3548016.2	1743961
D-Fructose	2.9691477	4.306134	5.1559854

D-Glucitol	2.718733	3.8736265	5.2202315
D-Ribose	12.962991	13.803886	10.127563
Glycine	1.7266296	8.821944	8.717626
Heptanedioic acid	6.745388	3.2851355	7.5449915
L-Ornithine	548123.06	1002.8397	1609310.8
L-Proline	1.5098505	2.9988835	3.793202
Malic acid	16245.215	497024.16	1801316.9
Myo-Inositol 1-phosphate	200560.5	13229.012	14284.54
Threonine	2.5179842	3.519691	4.0859814
Leucine	2.0915394	4.261388	6.680168
Octanedioic acid	46970.344	1712818.8	2172631.5
Pentanedioic acid	11913.816	461169.5	10160.974
Phosphoric acid	5.5750337	11.016825	14.083437
Propanedioic acid	2.2491035	3.8345845	3.9168985
Propanoic acid	3.430225	4.61425	4.811754
Ribitol	3.4700093	5.52185	11.22699
Sebacic acid	463.56366	903357.1	33991.918

Serine	2.9583497	3.9861264	4.4699664
Uridine	1.6056432	9.828536	11.366234
Xylitol	5.941507	9.785083	12.036365
Pseudouridine	3.753123	6.4349985	7.2357836
Caproate	2.427655	4.1438603	6.5503073
Gulonolactone	574669.06	19898.613	945108.56
Aspartic acid	10411.374	9624.731	12096.929
Sedoheptulose	3.0833635	3.7029123	1.9263456