Supplementary material

Integrated ^{1}H NMR-based metabolomics analysis of earthworm responses to sub-lethal Pb exposure

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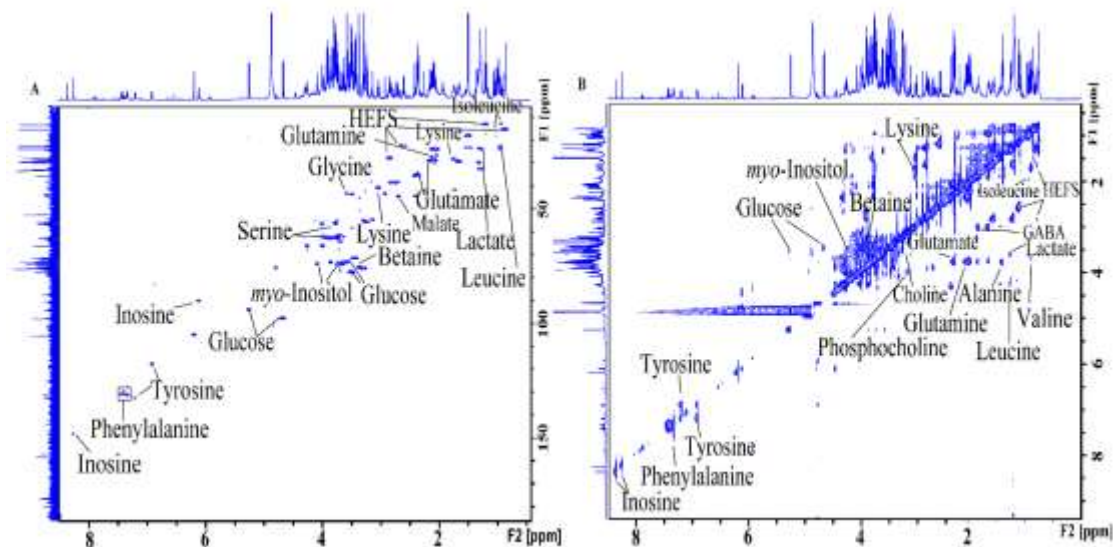
Fig. S1. HSQC (a), and TOCSY (b) contour plots with assignments of some metabolites.
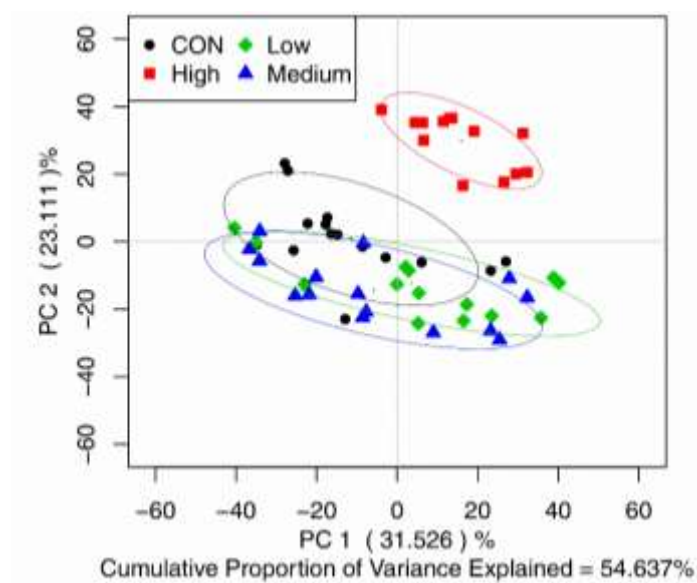

Fig. S2. PCA score plots of ^{1}H NMR spectra of aqueous tissue extracts sampled in four different dosed groups. Two PCs explain 54.637 % of total variances in the tissue extracts. The ellipses represent the 95 % confidence interval for the various groups. Circles, control group (CON); squares, high-dose lead treatment (high); triangles, medium-dose lead treatment (medium); diamonds, low-dose lead treatment (low).

Table S1.   Metabolites identified from the aqueous earthworm tissue extracts, their associated *P* and *Q* values (CON *v.* low, CON *v.* medium and CON *v.* high)

Metabolites	CON *v.* Low		CON *v.* medium		CON *v.* high	
	P	*Q*	*P*	*Q*	*P*	*Q*
HEFS	0.066740	0.109343	0.0230521	0.0434455	0.0025003	0.0075597
Leucine	0.083707	0.136263	0.0254135	0.0470741	1.03E-07	7.899E-07
Isoleucine	0.023107	0.047972	0.0295606	0.0487864	4.389E-07	2.019E-06
Valine	0.093303	0.102189	0.0077038	0.0094087	2.629E-06	7.56E-06
Lactate	0.031776	0.091356	0.0839886	0.1931738	0.0047008	0.0089145
Lysine	0.091639	0.140514	0.0302046	0.0350291	0.0044637	0.0095686
GABA	0.066030	0.109645	0.0331881	0.0404182	0.0016418	0.0310911
Glutamate	0.022108	0.060887	0.0127239	0.0174216	0.0027679	0.0033506
Glutamine	0.011815	0.057938	0.0145219	0.0668008	0.0263543	0.0335058
Methionine	0.006093	0.020020	0.0082755	0.0211485	0.0011275	0.0026741
Choline	0.018653	0.036548	0.0240154	0.0424887	4.97E-05	0.0001143
Phosphocholine	0.013724	0.035073	0.0038909	0.0127844	0.0039623	0.0060755
Betaine	0.745158	0.753449	0.0045539	0.0094945	5.996E-06	1.532E-05
Dimethylglycine	0.046434	0.106798	0.8273776	0.9061754	1.686E-06	0.0164627
Serine	0.060337	0.109645	0.015471	0.0355834	0.0011382	0.0090995
myo-Inositol	0.035345	0.044321	0.0068167	0.0095534	3.981E-07	2.019E-06
Glucose	0.019700	0.037181	0.0114868	0.0334209	5.362E-05	0.0006166
Maltose	0.017004	0.022692	0.0240616	0.0425603	0.0195236	0.0393725
Tyrosine	0.025823	0.045529	0.0030202	0.0095534	0.0022938	0.0052862
Phenylalanine	0.024972	0.042004	0.0046249	0.0087573	0.0051106	0.0081517
Tryptophan	0.090887	1.351166	0.0072025	0.0313676	0.0041712	0.0010911
Inosine	0.006916	0.022749	0.0571923	0.1008451	0.0071923	0.0384511