Electronic Supplementary Material (ESI) for Toxicology Research.

Supplementary Data

Metabolomics reveals disturbed metabolic pathways in human lung epithelial cells exposed to airborne fine particulate matter

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Table S1 MS/MS information of identified differential metabolites

HMDB ID	Metabolite	Chemical Formula	Measured MW (Da)	MS/MS fragments
HMDB00156	L-Malic acid	$C_4H_6O_5$	133.0123	115(100), 71(46), 133(31)
HMDB00148	L-Glutamic acid	$C_5H_9NO_4$	146.0441	102(100), 128(58), 146(39)
HMDB00159	L-Phenylalanine	$C_9H_{11}NO_2$	164.0699	147(100), 164(60), 72(30)
HMDB00072	cis-Aconitic acid	$C_6H_6O_6$	172.9898	173(100), 93(96)
HMDB01138	N-Acetylglutamic acid	$C_7H_{11}NO_5$	188.0549	128(100), 102(71), 144(32), 59(28), 188(25), 170(20)
HMDB00929	L-Tryptophan	$C_{11}H_{12}N_2O_2$	203.0811	116(100), 203(72), 72(32), 74(30), 142(27), 159(24)
HMDB00210	Pantothenic acid	$C_9H_{17}NO_5$	218.102	88(100), 146(62), 218(16)
HMDB00195	Inosine	$C_{10}H_{12}N_4O_5$	267.0728	135(100), 267(35)
HMDB11737	Gamma Glutamylglutamic acid	$C_{10}H_{16}N_2O_7$	275.0877	128(100), 146(88)
HMDB01067	N-Acetylaspartylglutamic acid	$C_{11}H_{16}N_2O_8$	303.0824	128(100), 96(80), 146(30)
HMDB13220	Beta-Citryl-L-glutamic acid	$C_{11}H_{15}NO_{10}$	320.061	110(100), 128(31)
HMDB01227	5-Thymidylic acid	$C_{10}H_{15}N_2O_8P$	321.0637	110(100), 111(85), 128(33)
HMDB60506	S-(2,2-Dichloro-1-hydroxy)ethyl glutathione	$C_{12}H_{19}Cl_2N_3O_7S$	418.0282	97(100), 240(21)
HMDB01341	ADP	$C_{10}H_{15}N_5O_{10}P_2$	426.0209	79(100), 159(78), 328(78), 134(73)
HMDB06944	1,4-beta-D-Glucan	$C_{18}H_{32}O_{18}$	535.1529	267(100), 135(31)
HMDB03337	Oxidized glutathione	$C_{20}H_{32}N_6O_{12}S_2$	611.1431	306(100), 143(85), 272(85), 128(70), 254(59)

Table S2 Metabolic pathways significantly altered by PM2.5 in A549 cells

No.	Pathway	Total[a]	Hits[b]	*p* value[c]
1	Nitrogen metabolism	39	3	1.56E-03
2	Citrate cycle	20	2	6.46E-03
3	Aminoacyl-tRNA biosynthesis	75	3	1.01E-02
4	Phenylalanine, tyrosine and tryptophan biosynthesis	27	2	1.16E-02
5	Glutathione metabolism	38	2	2.24E-02
6	Glyoxylate and dicarboxylate metabolism	50	2	3.74E-02

[a] The total number of compounds in the pathway.

[b] The number of compounds derived from metabolomics analysis.

[c] Probability of identified differential metabolite list associates to the generated pathway.

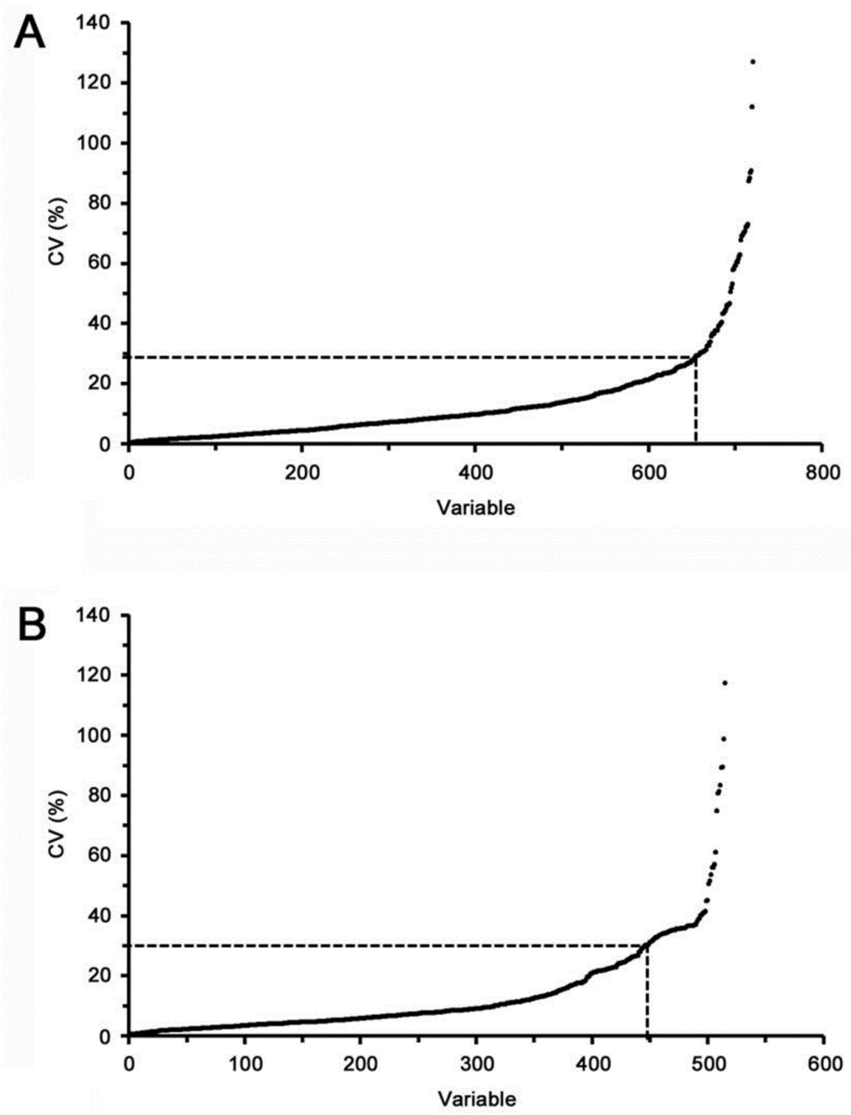

Fig. S1 Coefficients of variation (CVs) of the variables extracted from metabolic profiles of A549 cells. The CV values of 91.4% variables for positive ion mode (A), and 86.4% for negative ion mode (B) were <30%, indicating that they are worthy data sets for further analysis.

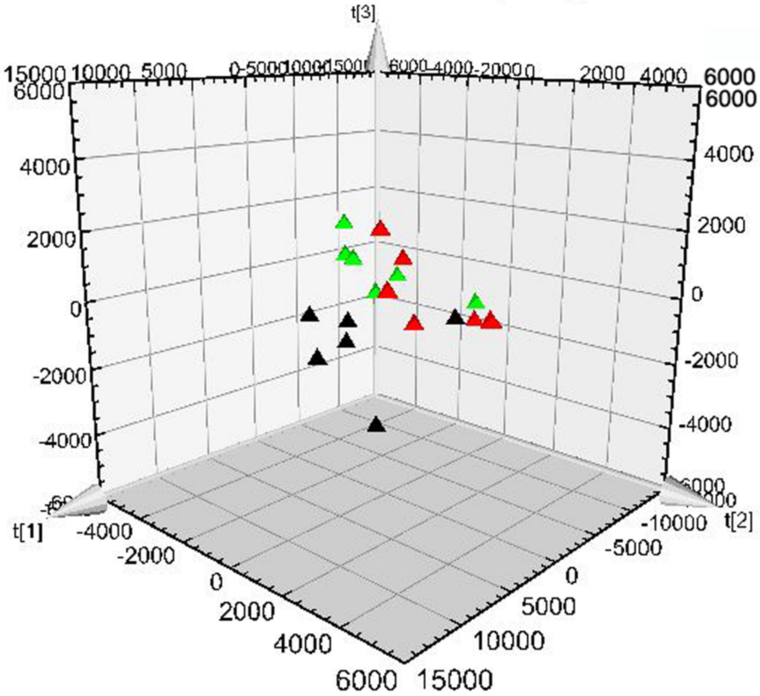

Fig. S2 Scoring plots of intracellular metabolites from A549 cells with PCA model under positive ion mode. ▲ Control; ▲ 30 mg/L; ▲ 60 mg/L.

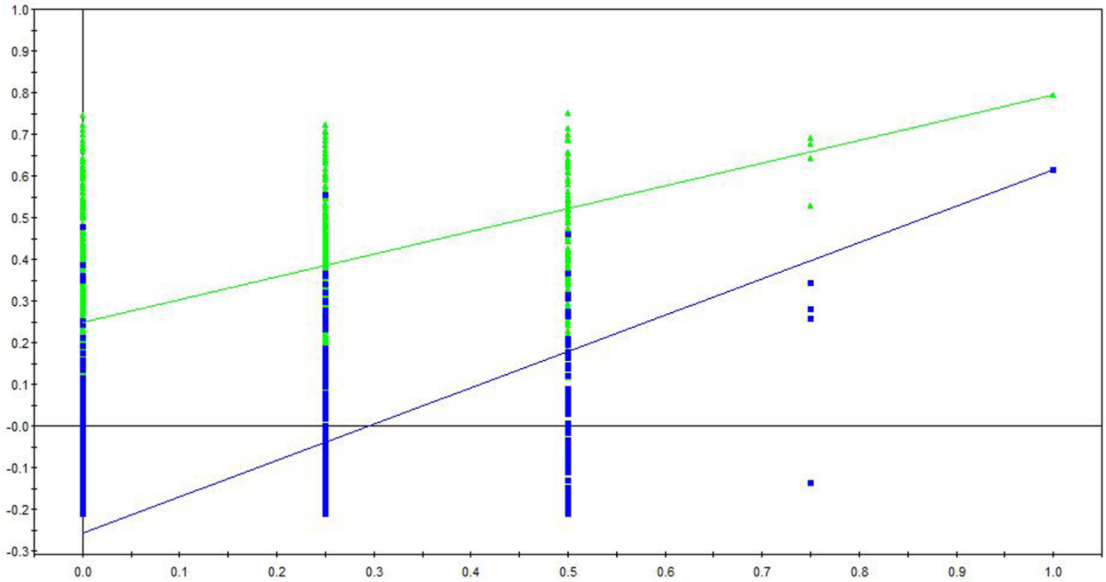

Fig. S3 Random permutation test results (n = 999) of the PLS-DA model. R^2 (green line) is the explained variance, and Q^2 (blue line) is the predictive ability of the model. The calculated R^2 and Q^2 values were lower than the original ones in the validation plot, and the Q^2 intercepted the vertical axis was below zero, therefore, the model was considered to be valid.

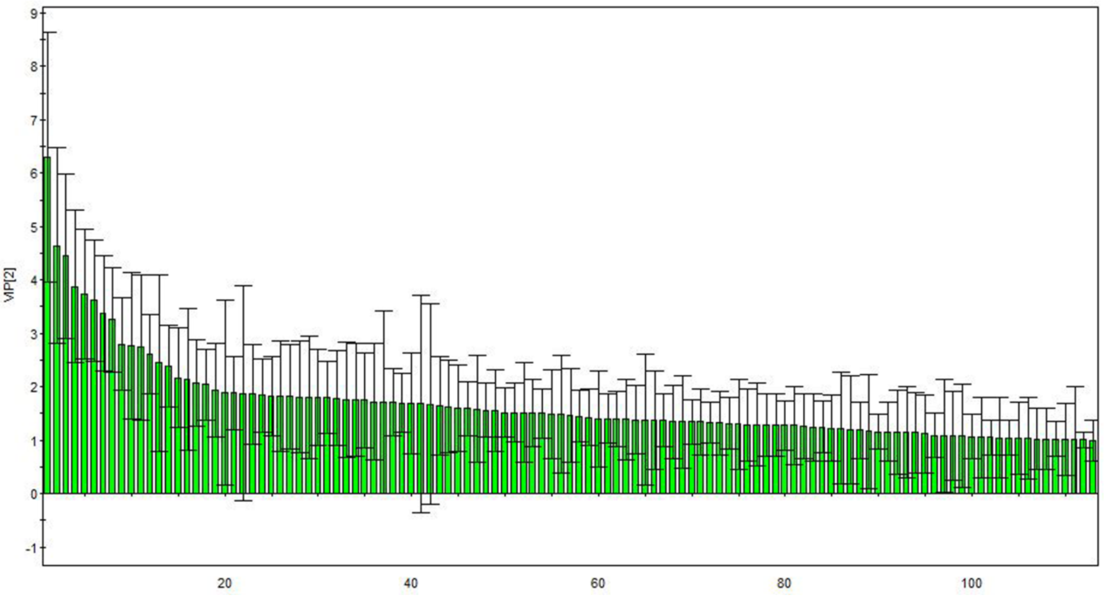

Fig. S4 Variable influence in projection (VIP) plots of established PLS-DA model. Three variables with negative jack-knifed confidence intervals were removed from the potential biomarker list.