Electronic Supplementary Material (ESI) for RSC Advances

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Electronic Supporting Information for

Metabolomics analysis of multidrug-resistant breast cancer cells in vitro using methyl-tert-butyl ether method

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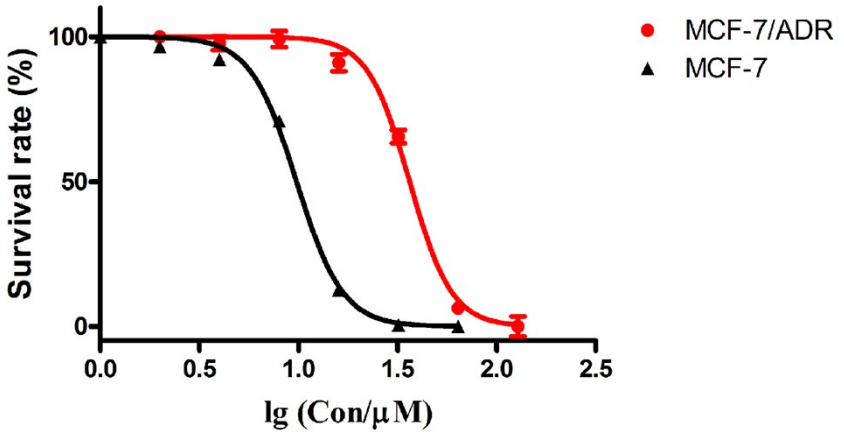

Fig. S1 Drug sensitivity of MCF-7/ADR and parental cells against adriamycin. Dose-response curves for the two cell lines in the presence of adriamycin. Data are presented as the mean ± standard deviation of three independent experiments.

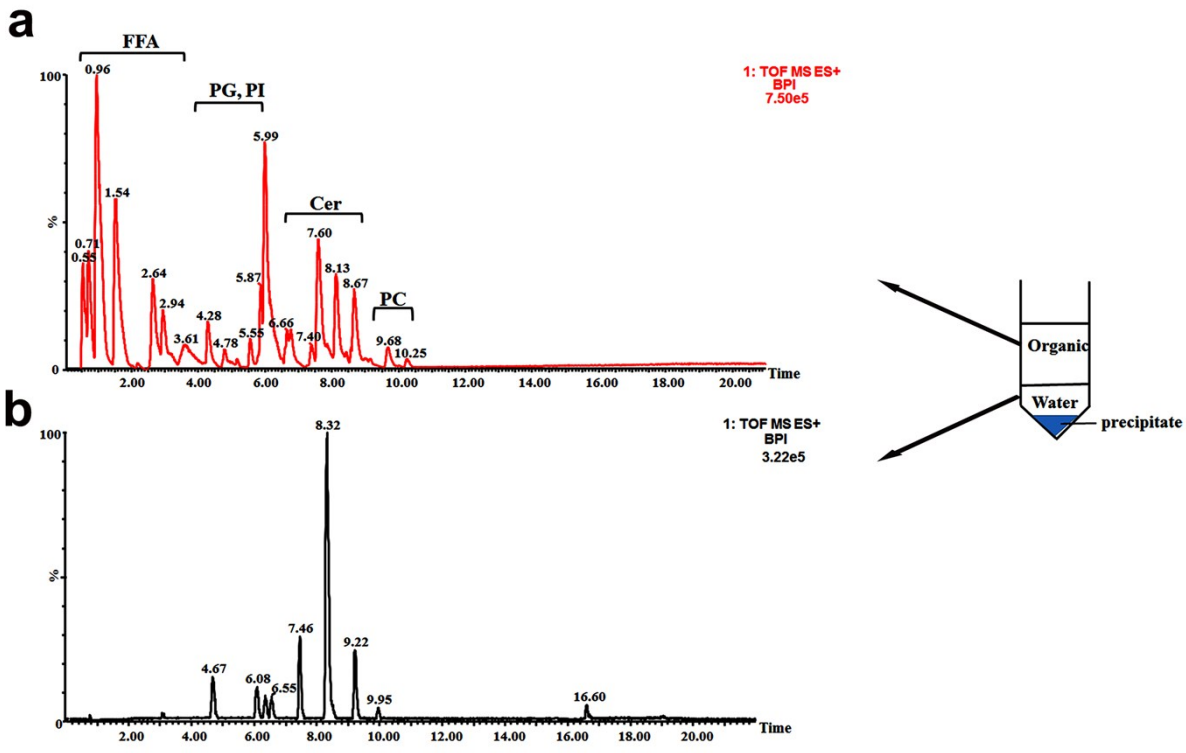

Fig. S2 Typical base peak intensity (BPI) chromatograms of non-polar (A) and polar (B) metabolites from MCF-7/ADR in positive ion mode.

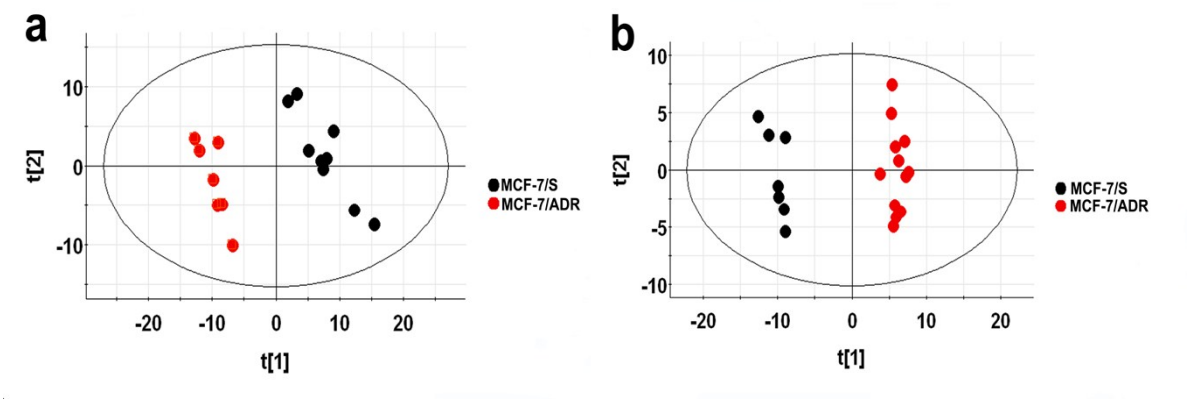

Fig. S3 Scores plots of PCA model with MS data of polar metabolites in positive and negative ion mode. Scores plot of PCA model with MS data of metabolites from the MCF-7/S (black) and MCF-7/ADR (red) cells.

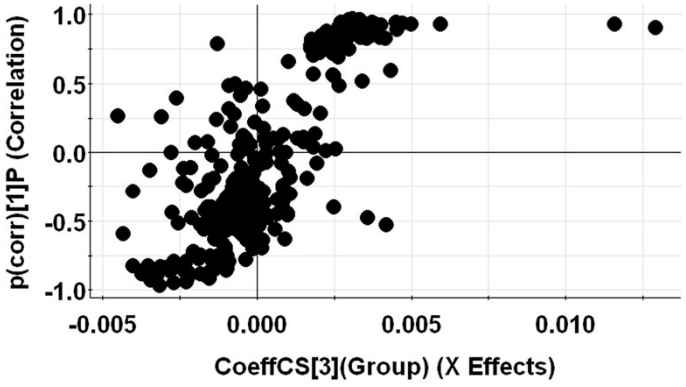

Fig. S4 S-plot of OPLS-DA model with MS data of non-polar metabolites in negative ion mode.

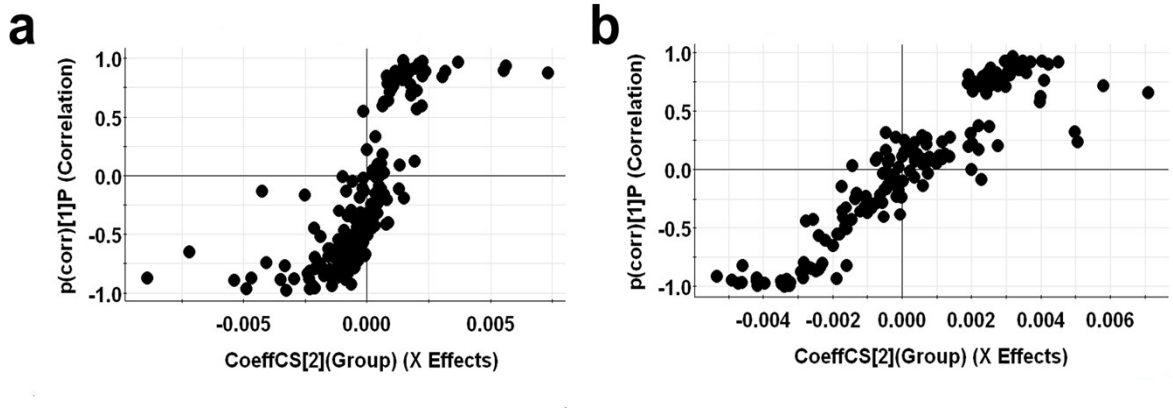

Fig.S5 S-plot of OPLS-DA model with MS data of polar metabolites in positive and negative ion mode.

Table S1 Result from the metabolic pathway analysis.

	Total	Expected	Hits	Raw p	-log(p)	Holm adjust	FDR	Impact
Sphingolipid metabolism	25	0.10386	2	0.0044301	5.4193	0.3544	0.3544	0.1402
Glycerophospholipid metabolism	39	0.16203	2	0.010607	4.5462	0.83796	0.42428	0.1037
Arachidonic acid metabolism	62	0.25758	2	0.02572	3.6605	1	0.68586	0.01731
Linoleic acid metabolism	15	0.062318	1	0.06071	2.8017	1	1	0
alpha-Linolenic acid metabolism	29	0.12048	1	0.11436	2.1684	1	1	0
Glutathione metabolism	38	0.15787	1	0.14737	1.9148	1	1	0.0019
Fatty acid biosynthesis	49	0.20357	1	0.18622	1.6808	1	1	0

Note: The Total is the total number of compounds in the metabolic pathway; the Hits are the actually matched number from the user uploaded data; the raw p is the original p value calculated from the enrichment analysis; the Holm p is the p value adjusted by Holm-Bonferroni method; the FDR p is the p value adjusted using False Discovery Rate; the Impact is the pathway impact value calculated from pathway topology analysis.