Electronic Supplementary Material (ESI) for Metallomics.

Electronic Supplementary Information

Inhibition of arsenite methylation induces synergistic genotoxicity of arsenite and benzo(a)pyrene diol epoxide in SCC-7 cells

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Content

Table S1 Operation conditions of HPLC-ESI-LTQ-Orbitrap-MS

HPLC	
HPLC column	ThermoFisher Acclaim Hypersil GOLD C18 (2.1 × 150 mm, 3 μM)
Flow rate	0.2 mL min^{-1}
Mobile phase	A: Methanol (MS grade); B: Triple deionized water
Gradient elution	0-5 min: 3% A, 97% B; 5-8 min: 15% A, 85% B; 8-9 min: 50% A, 50% B; 9-15 min: 3% A, 97% B
Column temperature	35 ^{o}C
Injection volume	20 μL
ESI-Orbitrap-MS	
Scan type	PRM
Sheath gas	35 arb units
Aux gas	15 arb units
Heat temperature	300 ^{o}C
Capillary temperature	350 ^{o}C
S-lens RF level	50%
Spray voltage	3500 V

Table S2 Optimized conditions for HPLC-ICP-CCT-MS

HPLC	
HPLC column	Shiseido CAPCELL PAK C18 (5 μm, 4.6 × 250 mm)
Mobile phase	4 mM TBAH + 8 mM malonic acid + 3%(v/v) methanol, pH 6.0
Column temperature	25 ^{o}C
Eluent flow rate	1mL/min
Injection volume	40 μL
ICP-MS	
Plasma RF power	1200 W
Nebulizer gas flow	0.91 L/min
Auxiliary gas flow	0.8 L/min
Collision gas	8% H_2 in He
Collision gas flow	3.6 mL min^{-1}
Dwell time	100 ms
Acquisition mode	Peak-hopping
Isotope	^{75}As

Table S3 Sequences of primers used for RT-qPCR analysis

Gene		Primer **(5'-3')**
GAPDH	Forward	TCAACGACCACTTTGTCAAGC
	Reverse	CCAGGGGTCTTACTCCTTGG
AS3MT	Forward	CGTCTATACGAGAGCCTTGAAC
	Reverse	AACGACAGTCACCGATAA
MT1A	Forward	CTCGAAATGGACCCCACT
	Reverse	ATATCTTCGAGCAGGGCTCGTC
CSB	Forward	CCCCAGTACAGGTCAAAACT
	Reverse	CTTCATTCTCCGCAGTAGGT
XPC	Forward	GAAGACTTGGAGTTTCAGGC
	Reverse	TTCAGGGCATACAGAGGGTG
XPF	Forward	CCACTGACACTCGGAAAGCC
	Reverse	ATGTCAATGCCCCGACGATG
XPB	Forward	ACTCAACCAAGCGGCAGAGATTC
	Reverse	CCACCTCCTCCTCGGCATCC
RAD50	Forward	GCGTGCGGAGTTTTGGAATA
	Reverse	TGAGCAACCTTGGGATCGTG

Table S4 Gene expression in SCC-7 cells exposed to As(III).

Incubation condition	Gene expression fold change (set GAPDH as reference)	
	AS3MT	MT1A
2 μM As(III) for 24 h	1.59 ± 0.17	1.01 ± 0.23
10 μM As(III) for 24 h	0.34 ± 0.12	0.27 ± 0.13

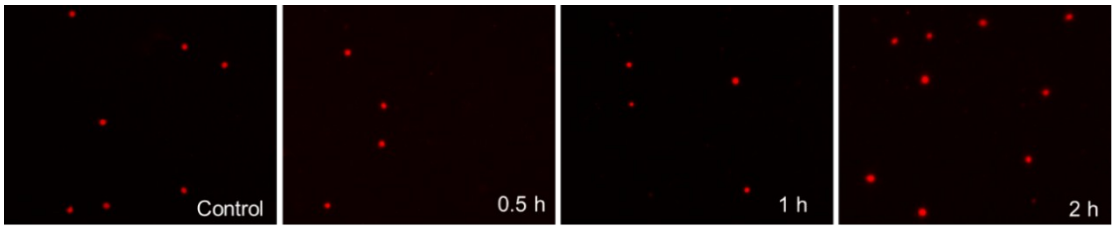

Figure S1 BPDE-mediated DNA damage by comet assay. Representative images of comet assay for analysis of SCC-7 cells treated with 1 μM BPDE for 0, 0.5, 1, 2 h (10× Objective).

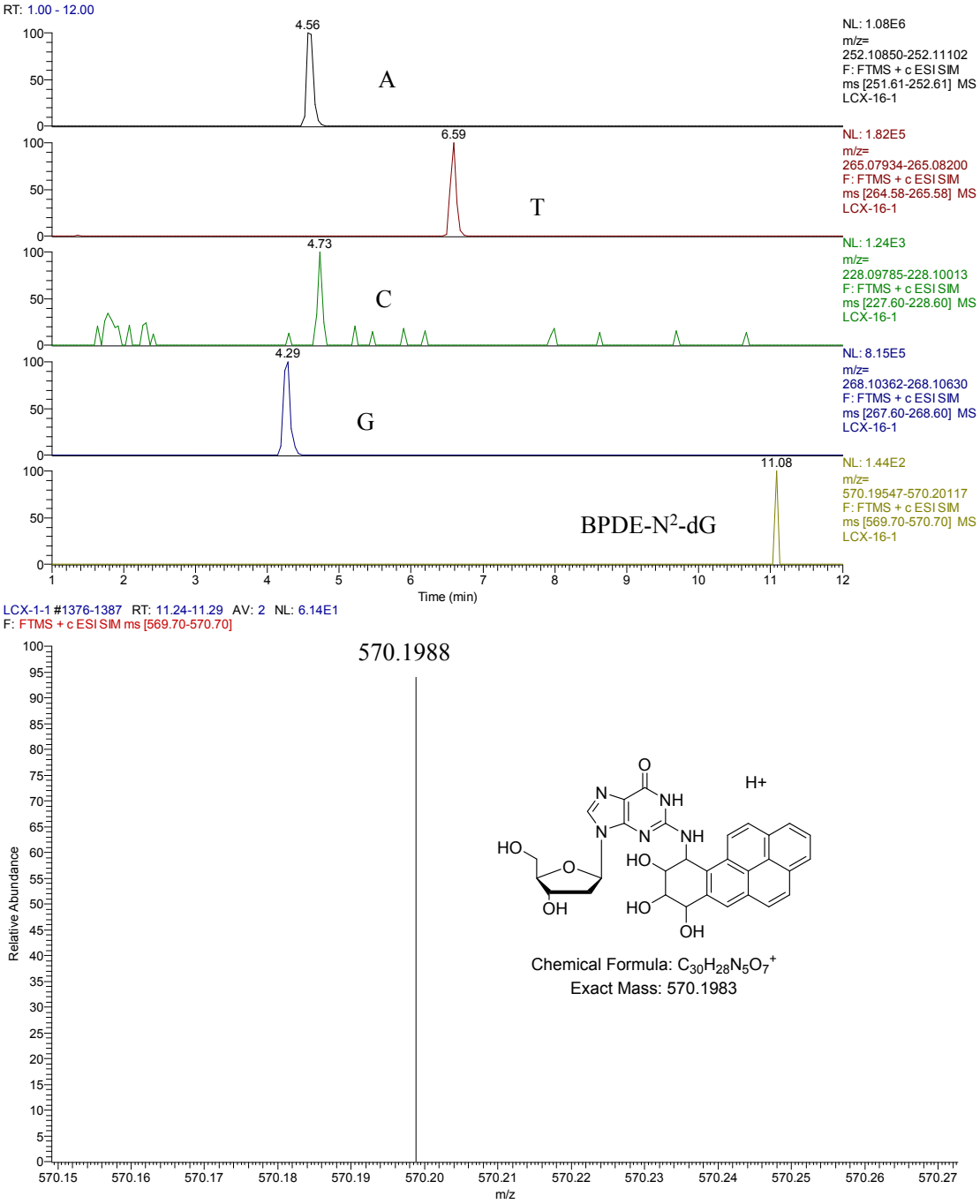

Figure S2 The exact mass and extraction ion chromatogram of A, T, C, G and BPDE-N^2-dG and mass spectrum of BPDE-N^2-dG using HPLC-ESI-LTQ-Orbitrap-MS.

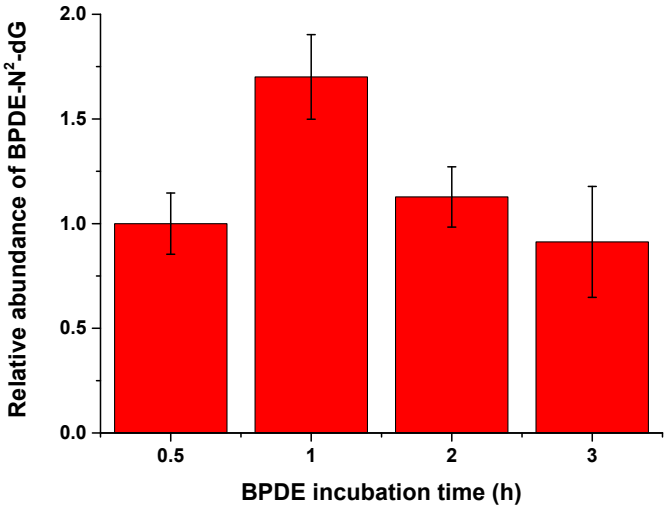

Figure S3 Effect of BPDE incubation time on the formation of BPDE-N^2-dG in SCC-7 cells. Semi-quantitative analysis of BPDE-N^2-dG in SCC-7 cells treated with 1 μM BPDE for 0.5 h, 1 h, 2 h and 3 h, respectively, according to representative extracted ion chromatogram of HPLC-ESI-LTQ-Orbitrap-MS. Error bars represent the standard deviation of triplicate experiments.