

Supplementary Data

Ultra-high performance liquid chromatography tandem mass spectrometry for profiling mercapturic acids in human urine after daily exposure to acrylamide, 3-monochloropropane-1,2-diol and glycidol

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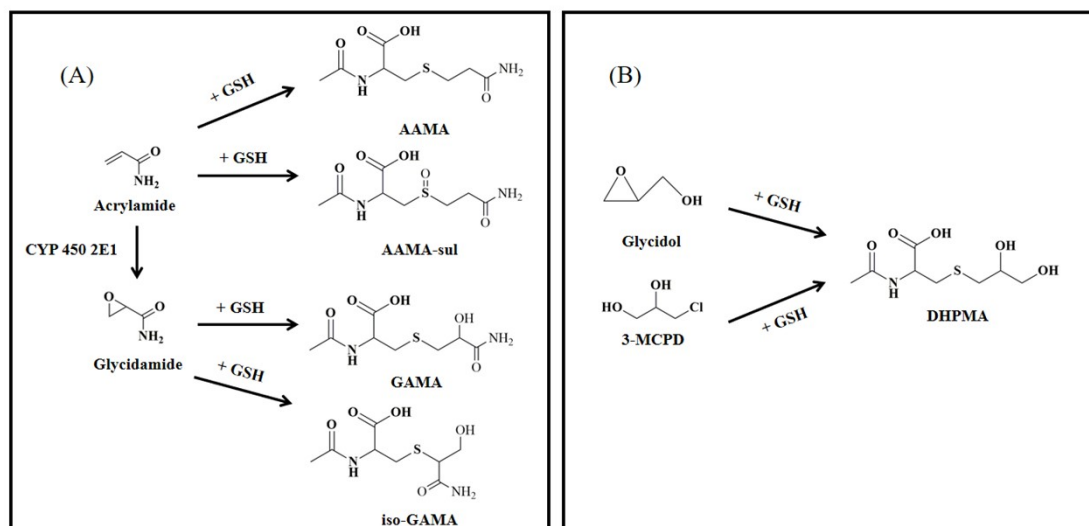


Figure S1. The metabolic pathways of the five mercapturic acids of (A) acrylamide and (B) 3-MCPD and glycidol.

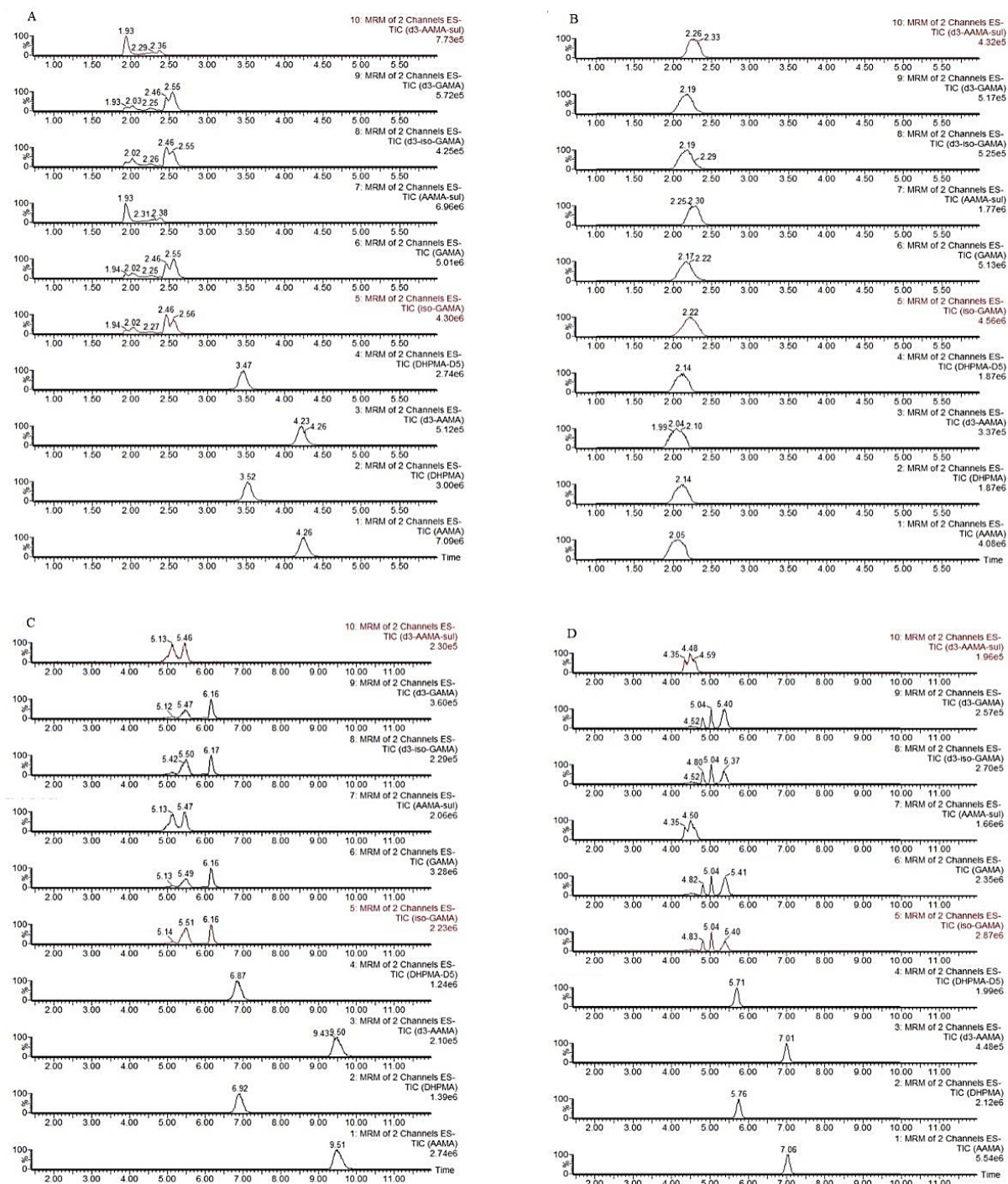


Figure S2. UHPLC-MS/MS chromatograms of the five mercapturic acids and their ISs separated by various UHPLC columns with different column lengths, diameters, and partial sizes. Chromatographic separation was performed on (A) Acquity UPLC® BEH C₁₈ column (2.1×150 mm i.d., 1.7 μm); (B) Acquity UPLC® BEH AMIDE column (2.1×150 mm i.d., 1.7 μm); (C) Acquity UPLC® CSH fluoro-phenyl column (2.1×150 mm i.d., 1.7 μm); and (D) Acquity UPLC® HSS CYANO column (3.0×150 mm i.d., 1.8 μm). MRM channels: 1, AAMA; 2, DHPMA; 3, AAMA-d₃; 4, DHPMA-d₅; 5, iso-GAMA; 6, GAMA; 7, AAMA-sul; 8, iso-GAMA-d₃; 9, GAMA-d₃; 10, AAMA-sul-d₃.

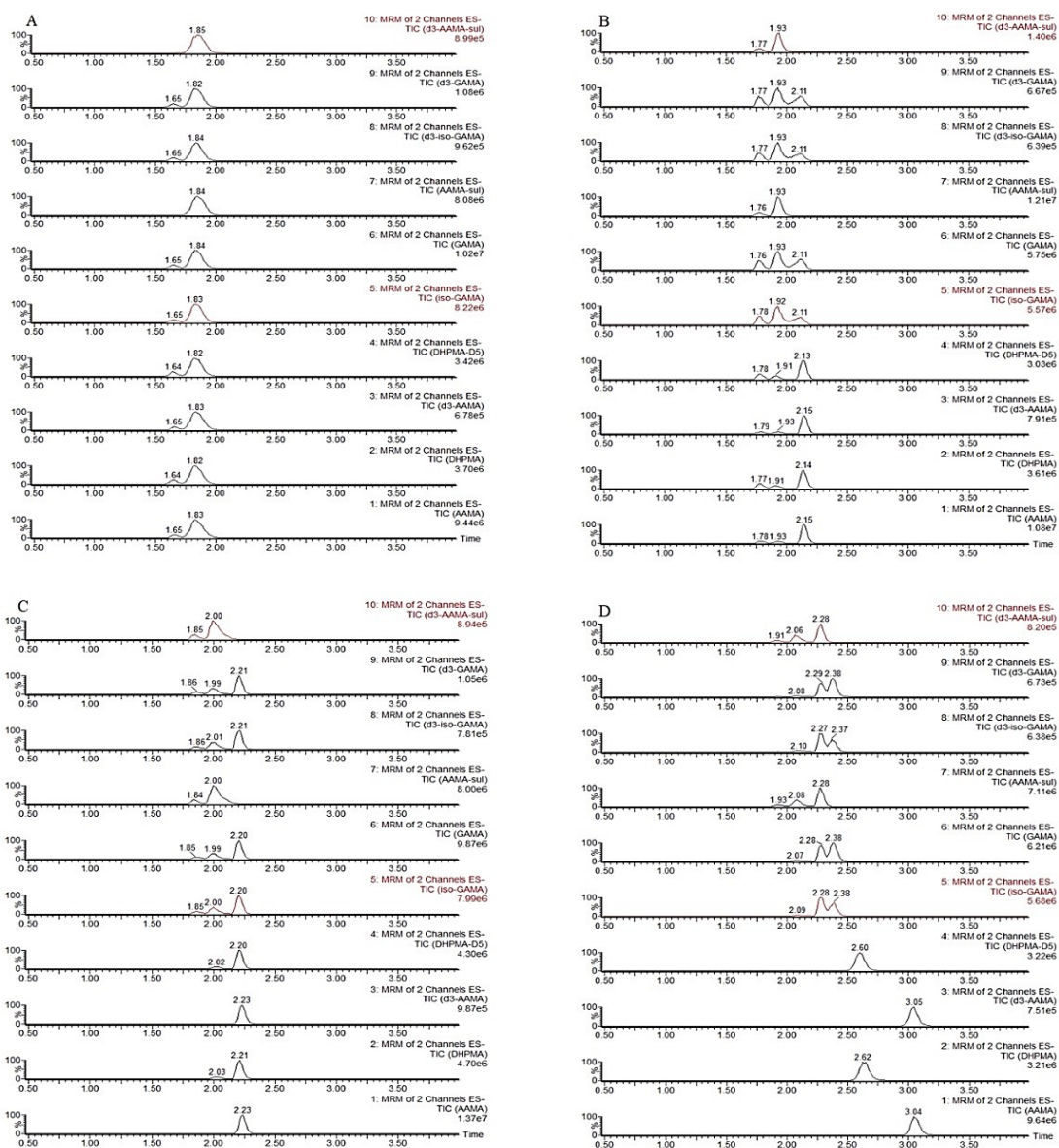


Figure S3. UHPLC-MS/MS chromatograms of five mercapturic acids and their ISs separated using various proportions of initial mobile phase (solvent A/solvent B): (A) 50:50, (B) 80:20, (C) 90:10, and (D) 96:4. MRM channels: 1, AAMA; 2, DHPMA; 3, AAMA- d_3 ; 4, DHPMA- d_3 ; 5, iso-GAMA; 6, GAMA; 7, AAMA-sul; 8, iso-GAMA- d_3 ; 9, GAMA- d_3 ; 10, AAMA-sul- d_3 .

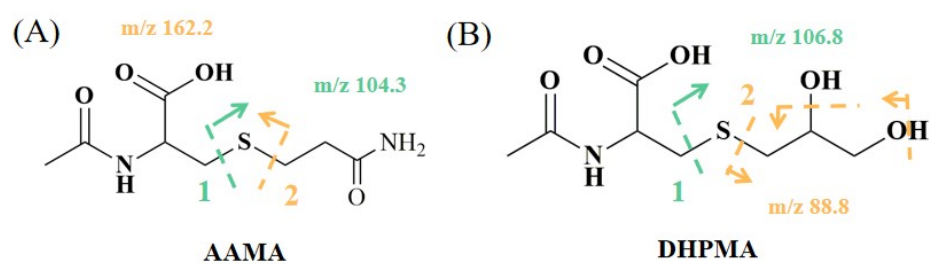


Figure S4. Fragmentation mechanisms of (A) AAMA and (B) DHPMA.

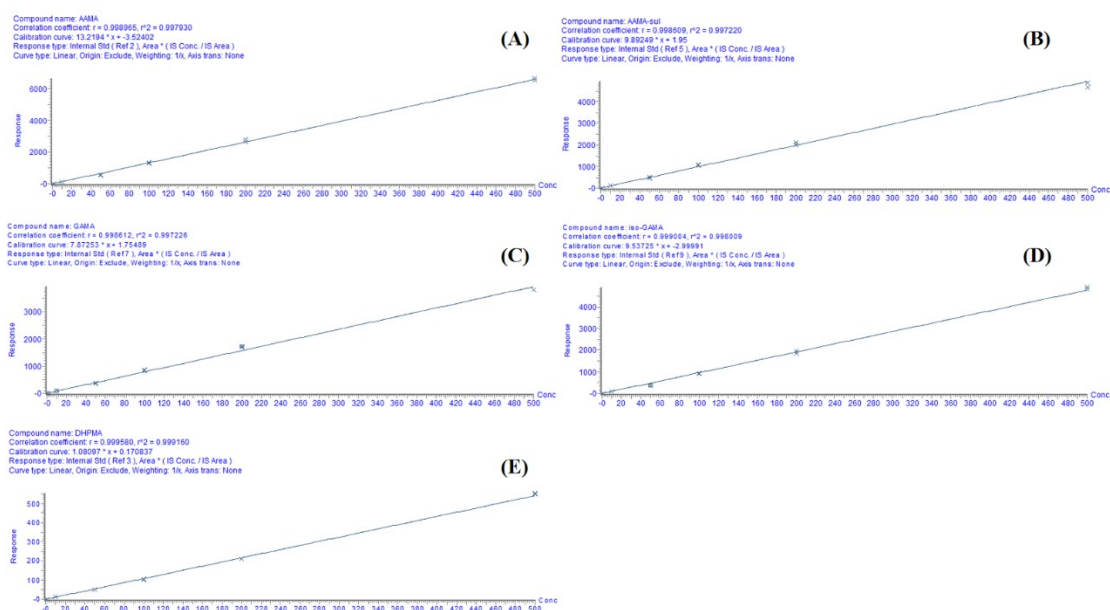


Figure S5. Calibration curves of (A) AAMA, (B) AAMA-sul, (C) GAMA, (D) iso-GAMA, and (E) DHPMA.

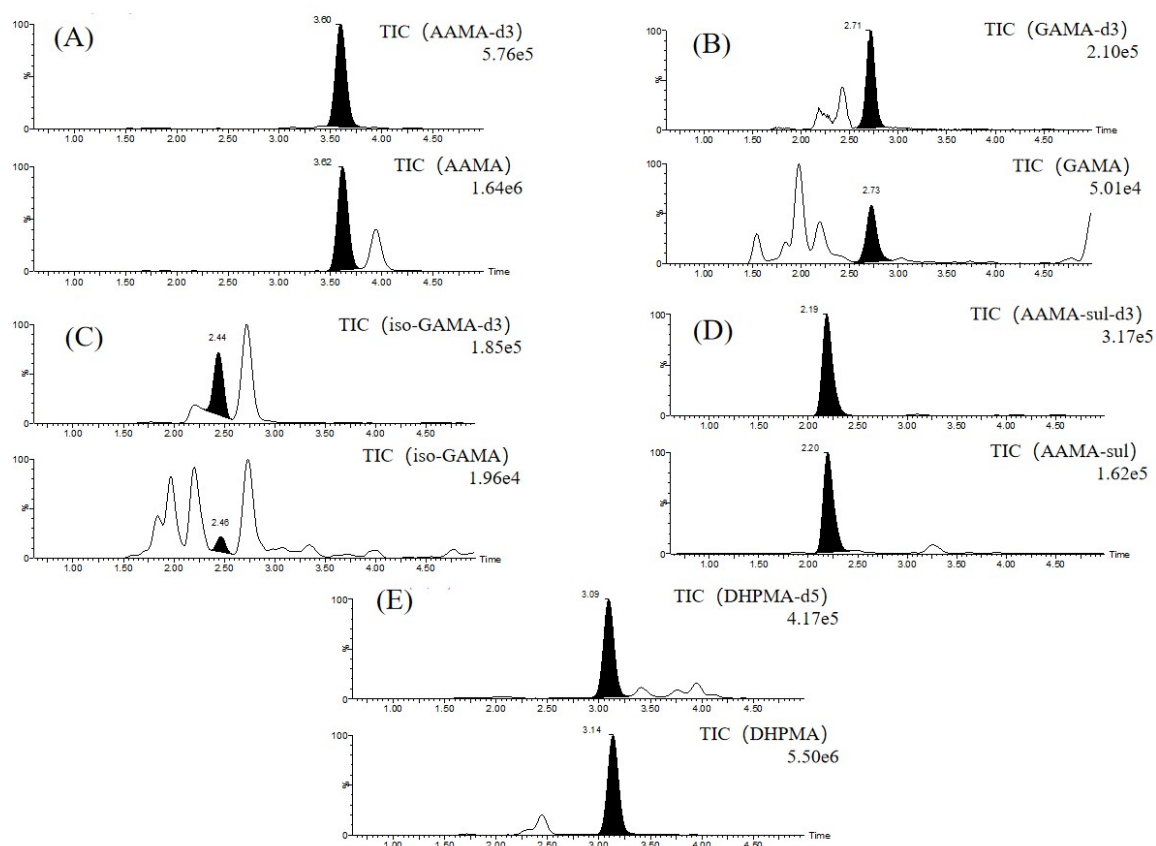


Figure S6. Typical UHPLC-MS/MS chromatograms for the simultaneous analysis of the five mercapturic acids and their deuterium-labeled ISs in human urinary samples. (A) AAMA (down layer) and AAMA- d_3 (upper layer); (B) GAMA (down layer) and GAMA- d_3 (upper layer); (C) iso-GAMA (down layer) and iso-GAMA- d_3 (upper layer); (D) AAMA-sul (down layer) and AAMA-sul- d_3 (upper layer); (E) DHPMA (down layer) and DHPMA- d_5 (upper layer).

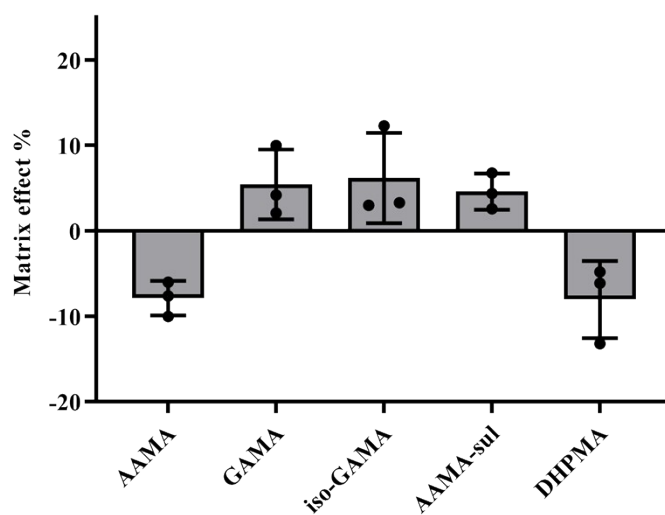


Figure S7. Matrix effects of the five mercapturic acids. Data are expressed as mean \pm s.d. MEs were estimated by comparing the slopes of matrix-matched calibration curves ($n=3$) with those of solvent-based calibration curves ($n=3$) for each of the five mercapturic acid metabolites.

Table S1. LODs and LOQs of five mercapturic acids in urine of humans

Compound	AAMA (ng/mL)	AAMA-sul (ng/mL)	GAMA (ng/mL)	iso-GAMA (ng/mL)	DHPMA (ng/mL)
LOD	0.1	0.2	0.3	0.3	0.3
LOQ	0.3	0.7	0.9	0.9	0.9