

Extensive thiol profiling for assessment of intracellular redox status in cultured cells by HPLC-MS/MS

Jiandong Wu¹, Anna Chernatynskaya¹, Annalise Pfaff², Huari Kou¹, Nan Cen³, Nuran Ercal^{2*},
and Honglan Shi^{2*}

¹ Department of Chemical and Biochemical Engineering, Missouri University of Science and Technology, Rolla, Missouri 65409, United States

² Department of Chemistry, Missouri University of Science and Technology, Rolla, Missouri 65409, United States

³ Department of Computer Science, Missouri University of Science and Technology, Rolla, Missouri 65409, United States

**Corresponding authors*

Nuran Ercal

Department of Chemistry

Missouri University of Science and Technology

400 W 11th Street

Rolla, MO 65409, USA

E-mail: nercal@mst.edu

Tel: 573-341-6950

Honglan Shi

Department of Chemistry

Missouri University of Science and Technology

400 West 11th Street

Rolla, MO 65409, USA

E-mail: honglan@mst.edu

Tel: 573-341-4433

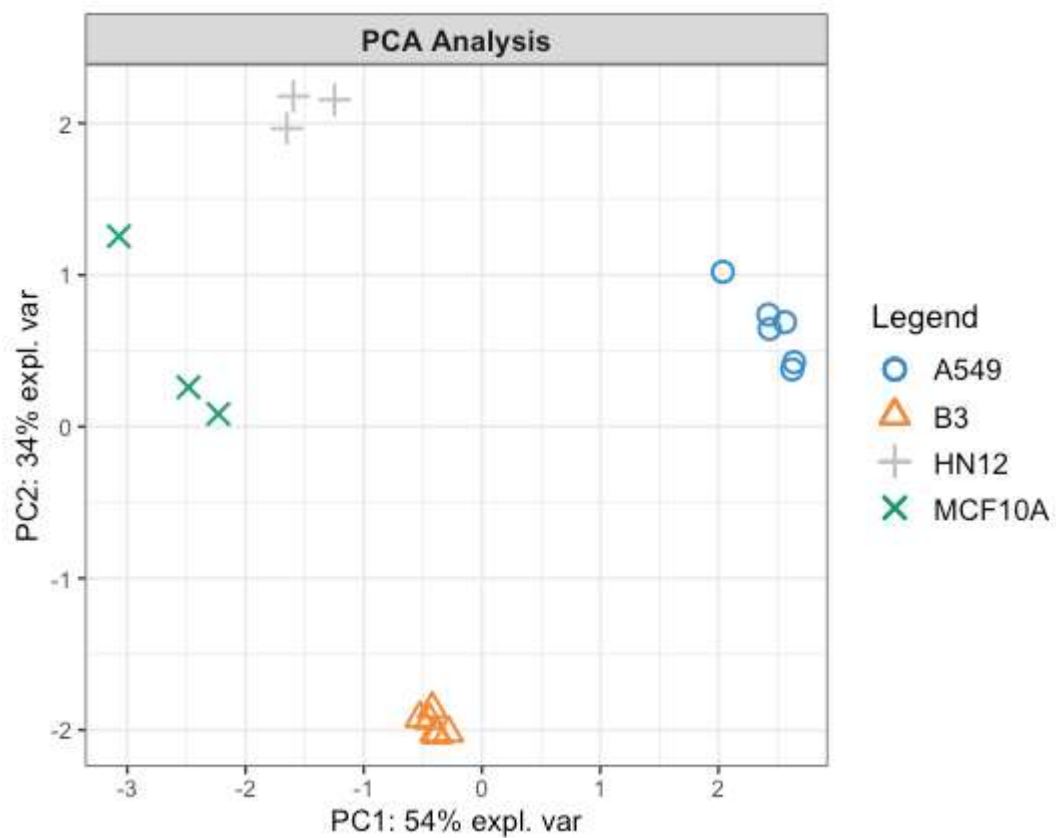


Figure S1. Principal component analysis of thiol profiling of different cells.

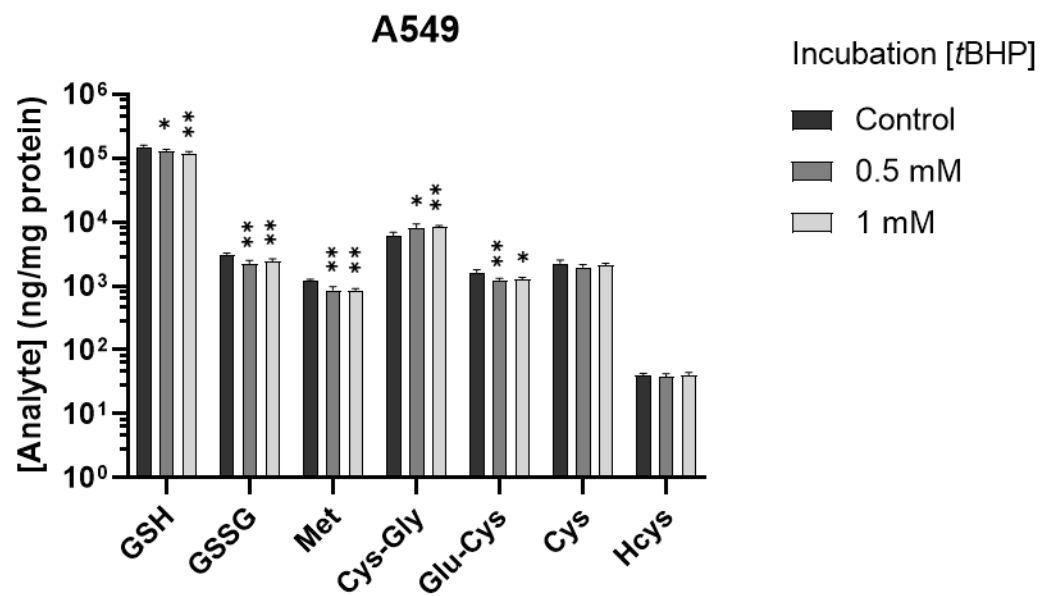


Figure S2. Alteration of analytes in A549 cells after 2-hour *t*BHP treatment (n=6). *, $p < 0.05$; **, $p < 0.001$.

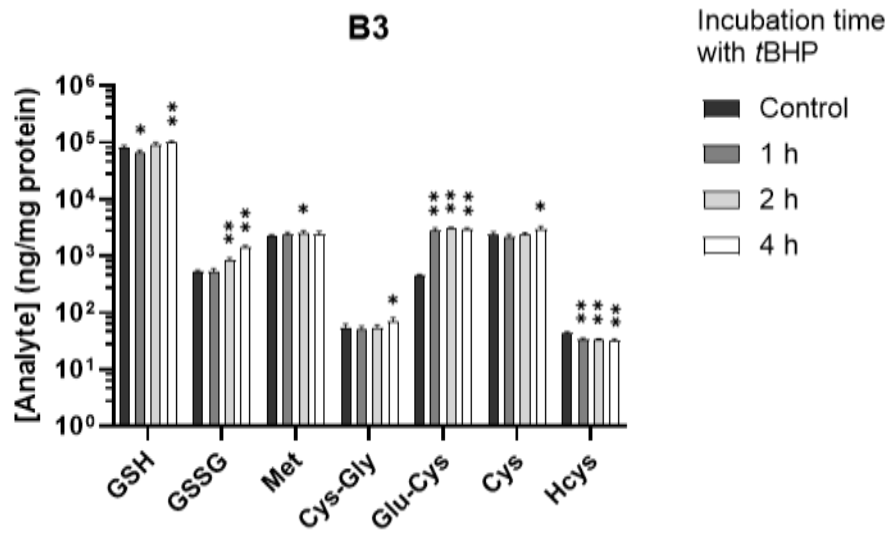


Figure S3. Alteration of analytes in B3 cells after 0.5mM *t*BHP treatment (n=6). *, $p < 0.05$; **, $p < 0.001$.

Table S1. Concentrations of analytes in different cell lines (mean \pm SD, ng/mg protein, n = 3).

Tissue	Lens	Lung	Breast	Head/Neck
Cell line	B3*	A549*	MCF10A	HN12
GSH**	83 \pm 7	152 \pm 10	48 \pm 5	45 \pm 5
GSSG	527 \pm 34	3145 \pm 150	543 \pm 41	1561 \pm 262
Cys-Gly	54 \pm 9	6100 \pm 868	25 \pm 5	3800 \pm 364
Glu-Cys	450 \pm 28	1624 \pm 183	99 \pm 21	233 \pm 14
Met	2326 \pm 66	1225 \pm 66	1191 \pm 217	1618 \pm 22
Cys	2447 \pm 229	2275 \pm 285	1678 \pm 388	697 \pm 66
Hcys	45 \pm 2	40 \pm 3	11 \pm 2	14 \pm 1

*, n = 6 for B3 and A549; **, μ g/mg protein.