

1 **SUPPLEMENTARY INFORMATION**

2 **Urinary excretion of organosulfur compounds after acute ingestion of black onion**

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Table S1.- UHPLC-HRMS-based identification of phenolic and organosulfur compounds detected in human urine samples after black onion ingestion

Peak	Retention Time (min)	Compound	Chemical Formula [m/z] ⁻	Experimental Mass [m/z] ⁻	δ (ppm)
γ-Glutamyl-S-alk(en)yl-L-cysteine derivatives (GSak)					
1	4.3	γ-Glutamyl-S-(propyl)-L-cysteine sulfoxide	C11H21N2O6S	309.1115	-2.1191
2	6.3	γ-Glutamyl-S-(S-1-propenyl)-L-cysteine-glycine	C13H22N3O6S2	380.0944	0.8362
3	6.4	γ-Glutamyl-S-(2-carboxypropyl)-L-cysteine	C12H19N2O7S ⁻²	335.0907	-0.0579
4	7.9	γ-Glutamyl-S-(S-methyl)-L-cysteine-glycine	C11H20N3O6S2	354.0788	0.6916
5	7.9	γ-Glutamyl-S-methyl-L-cysteine (GSMC)	C9H17N2O5S	265.0853	0.1777
6	8.5	Glutathione	C10H18N3O6S	308.0911	0.7967
7	8.6	γ-Glutamyl-S-allyl-L-cysteine (GSAC)	C11H19N2O5S	291.1009	0.4285
8	8.7	γ-Glutamyl-L-cysteine	C8H15N2O5S	251.0696	-0.9444
9	8.7	γ-Glutamyl-S-(1-propenyl)-L-cysteine sulfoxide (GS1PCS)	C11H19N2O6S	307.0958	-0.4247
10	9.0	γ-Glutamyl-S-allyl-L-cysteine sulfoxide (GSACS)	C11H19N2O6S	307.0958	-1.0128
11	9.6	γ-Glutamyl-S-methyl-L-cysteine sulfoxide (GSMCS)	C9H17N2O6S	281.0801	-0.8092
12	9.6	γ-Glutamyl-S-(propyl)-L-cysteine	C11H21N2O5S	293.1165	-0.3883
S-alk(en)yl-L-cysteine derivatives (SAk)					
13	1.4	S-(2-Propenyl)-allyl-L-cysteine sulfoxide	C9H16NO3S	218.0845	-1.8770
14	4.0	S-Butanoyl-L-cysteine sulfoxide (Butiin)	C7H16NO3S	194.0845	-0.8589
15	4.0	S-Allyl-L-cysteine (SAC)	C6H12NO2S	162.0583	-1.0605
16	4.3	N-Acetyl-S-(1-propenyl)-L-cysteine sulfoxide (NAS1PCS)	C8H14NO4S	220.0638	-1.2877
17	4.5	N-Acetyl-S-(1-propenyl)-L-cysteine (NAS1PC)	C8H14NO3S	204.0689	-1.9576
18	4.9	trans-S-(1-Propenyl)-L-cysteine (S1PC)	C6H12NO2S	162.0583	-0.5898
19	5.6	S-Propyl-L-cysteine (Deoxypropiin)	C6H14NO2S	164.0740	-4.2089
20	6.2	S-Allyl-L-cysteine sulfoxide (Alliin)	C6H12NO3S	178.0532	1.5374
21	6.7	S-(1-Propenyl)-L-cysteine sulfoxide (Isoalliin)	C6H12NO3S	178.0532	2.5793
22	7.1	Cycloalliin	C6H12NO3S	178.0532	2.3222
23	7.1	S-(2-Carboxypropyl) cysteine	C7H14NO4S	208.0638	1.7404

24	7.3	<i>S</i> -Methyl-L-cysteine sulfoxide (Methiin)	C4H10NO3S	152.0376	3.5869
25	7.6	Methionine sulfoxide	C5H12NO3S	166.0532	-0.6264
26	7.9	<i>S</i> -Propyl-L-cysteine sulfoxide (Propiin)	C6H14NO3S	180.0689	2.4960
27	8.1	<i>S</i> -Carboxymethyl-L-cysteine (Carbocysteine)	C5H10NO4S	180.0325	2.5441
28	8.4	<i>S</i> -(2-Carboxypropyl)-L-cysteine-glycine	C9H17N2O5S	265.0853	0.6382
29	8.6	<i>S</i> -Ethyl-L-cysteine sulfoxide (Ethiin)	C5H12NO3S	166.0532	-0.0752
30	9.6	<i>N</i> -Acetyl- <i>S</i> -(2-carboxypropyl)-L-cysteine (NACPC)	C9H16NO5S	250.0744	2.5686
31	9.7	<i>S</i> -Allylmercaptoglutathione	C13H22N3O6S2	380.0945	0.2443

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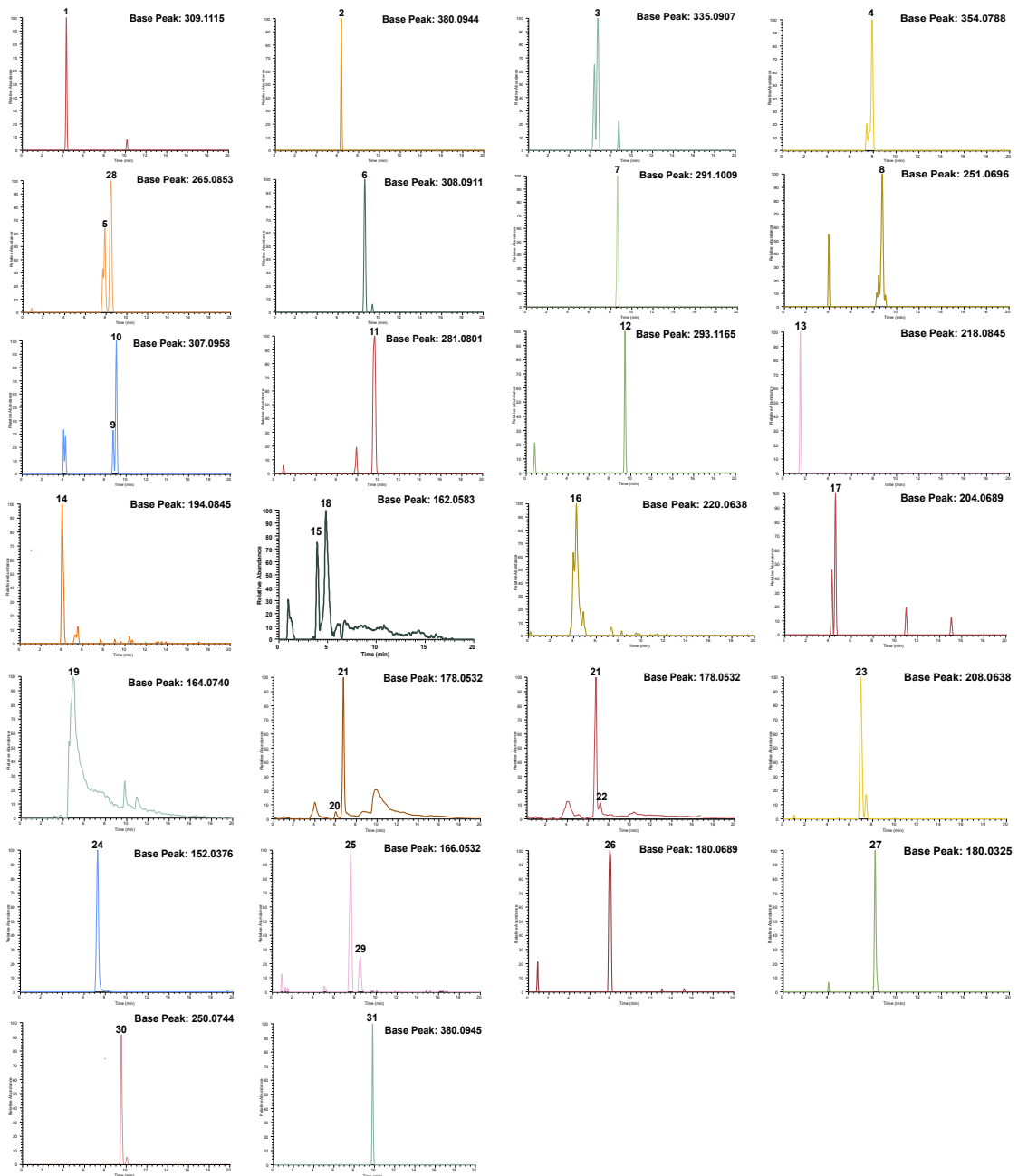


Figure S1. UHPLC-HRMS profiles of OSCs identified in human urine samples after the intake of 20g of black onion.