

Supplemental Data

Cytotoxic Mechanism of Selenomethionine in Yeast

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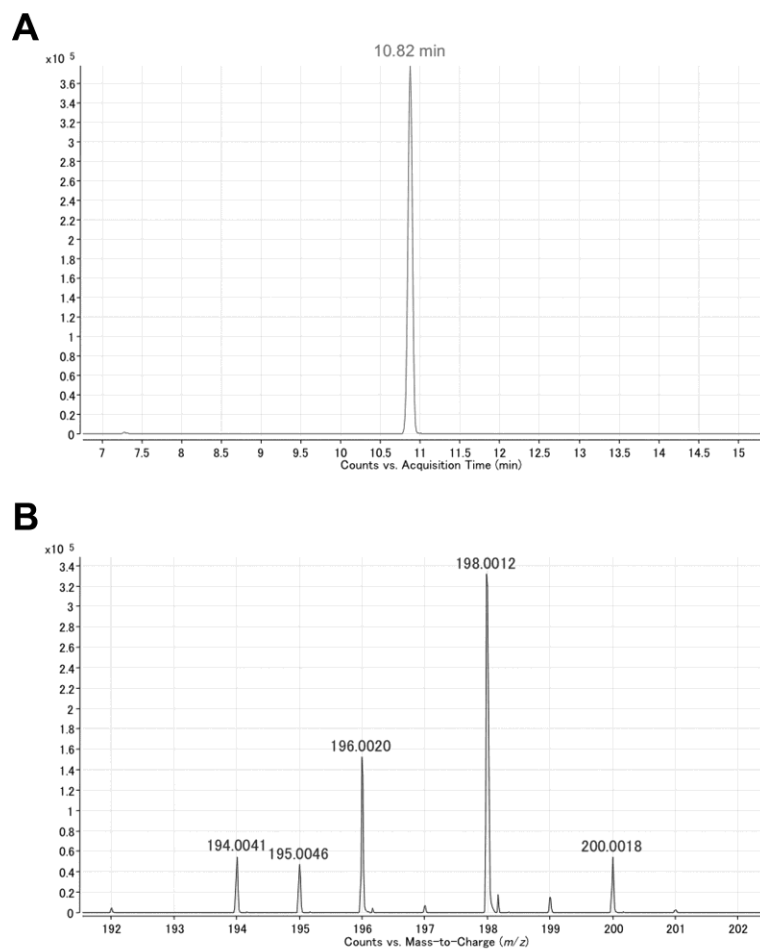


Figure S1. Representative chromatograms of *Se*-compounds in CE-TOFMS analysis. (A) The extracted ion chromatogram at m/z 198.002, corresponding to the protonated ion of SeMet is shown. (B) Mass spectrum of the ion peak at 10.82 min in panel A.

Supplemental Table

Table S1. Primers used in this study.

Primers	Sequence a (5'→3')	Restriction enzyme
EcCysE-f	GCG CGAGCT CATGTCGTGTGAAGAACTGGA	<i>SacI</i>
EcCysE-r	GCG CGTCGACT TAGATCCCATCCCCATACT	<i>SalI</i>
EcCysK-f	CGGAATTC ATGAGTAAGATTTTTGAAGATAAC	<i>EcoRI</i>
EcCysK-r	GCG CGTCGACT TACTGTTGCAATTCTTTCTC	<i>SalI</i>
EcCysM-f	CGGAATTC ATGAGTACATTAGAACAACAATAG	<i>EcoRI</i>
EcCysM-r	GCG CGTCGACT TAAATCCCCGCCCCCTG	<i>SalI</i>

^aRestriction sites are shown in boldface.

Table S2. Changes in endogenous metabolites after SeMet treatment.

Candidate compounds	mode	MT ^a	m/z	Relative Intensity ($\times 10^{-8}$) ^b					
				0 min		10 min		30 min	
1-Aminocyclopropane-1-carboxylic acid	Cation	7.25	102.055	3.97E-03	± 1.82E-04	6.00E-02	± 1.76E-03	1.24E-01	± 3.99E-03
1-Methyl-2-pyrrolidone	Cation	21.02	100.074	1.26E-02	± 5.16E-03	2.06E-02	± 7.49E-03	1.45E-02	± 1.99E-03
1-Methyladenosine	Cation	10.04	282.118	6.01E-03	± 3.65E-04	6.77E-03	± 2.80E-04	7.77E-03	± 5.45E-04
2-Amino adipic acid	Cation	11.02	162.076	4.10E+00	± 5.13E-02	3.91E+00	± 1.28E-01	4.50E+00	± 6.81E-02
2-Aminobutyric acid	Cation	9.73	104.070	1.02E-01	± 5.61E-03	1.07E-01	± 7.60E-04	1.14E-01	± 3.39E-03
3-Aminoisobutyric acid	Cation	7.81	104.070	1.19E-02	± 5.40E-04	1.20E-02	± 3.17E-04	1.51E-02	± 4.18E-04
3-Aminopropane-1,2-diol	Cation	7.56	92.069	2.22E-03	± 2.39E-04	1.85E-03	± 1.55E-04	2.33E-03	± 1.20E-04
3-Hydroxykynurenine	Cation	9.78	225.086	2.40E-02	± 8.97E-03	2.03E-02	± 6.24E-03	1.87E-02	± 5.14E-03
3-Phenylpropionic acid	Cation	21.41	151.074	7.21E-03	± 4.48E-04	7.33E-03	± 2.10E-04	6.52E-03	± 1.55E-04
4-Methyl-2-oxopentanoic acid	Cation	22.23	131.070	1.16E-02	± 1.29E-03	1.03E-02	± 3.47E-04	1.05E-02	± 1.32E-03
5-Amino-4-oxovaleric acid	Cation	8.11	132.064	1.02E-01	± 3.20E-03	9.72E-02	± 2.13E-03	8.96E-02	± 1.43E-03
5-Aminovaleric acid	Cation	8.17	118.087	2.33E-02	± 1.40E-03	2.03E-02	± 1.68E-03	2.14E-02	± 1.84E-03
5-Hydroxylysine	Cation	7.30	163.108	2.68E-03	± 3.52E-04	2.40E-03	± 2.59E-04	3.35E-03	± 1.09E-04
Adenine	Cation	7.73	136.061	2.27E-02	± 4.05E-03	9.46E-03	± 3.01E-03	8.87E-03	± 5.61E-04
Adenosine	Cation	9.95	268.103	2.06E-02	± 1.07E-03	1.89E-02	± 2.20E-03	1.75E-02	± 3.32E-04
ADMA	Cation	7.80	203.149	6.24E-03	± 2.25E-04	5.90E-03	± 6.36E-04	6.94E-03	± 4.82E-04
Ala	Cation	9.12	90.055	3.10E+00	± 1.20E-01	3.25E+00	± 4.65E-02	4.67E+00	± 1.95E-01
Ala-Ala	Cation	9.37	161.092	1.43E-02	± 1.25E-03	1.69E-02	± 6.17E-04	1.97E-02	± 8.73E-04
Anthranilic acid	Cation	10.59	138.054	4.03E-01	± 1.27E-02	3.62E-01	± 2.37E-02	2.85E-01	± 2.55E-02
Arg ^c	Cation	7.21	175.119	6.59E+00	± 2.87E-01	6.06E+00	± 1.23E-01	6.86E+00	± 2.28E-01
Arg-Glu	Cation	7.64	304.160	1.14E-02	± 3.05E-04	1.23E-02	± 2.81E-04	1.56E-02	± 3.24E-04
Argininosuccinic acid	Cation	9.52	291.129	2.78E-02	± 9.21E-04	1.81E-02	± 1.72E-03	3.10E-02	± 9.00E-04
Asn	Cation	10.47	133.060	1.19E+00	± 4.04E-02	1.14E+00	± 1.21E-02	1.43E+00	± 4.55E-02
Asp	Cation	11.55	134.045	6.08E+00	± 3.81E-01	5.34E+00	± 9.32E-02	7.04E+00	± 1.43E-01
Butyric acid	Cation	21.18	89.060	4.89E-02	± 4.10E-03	4.86E-02	± 4.00E-03	5.40E-02	± 1.66E-03
Carnosine	Cation	6.88	227.112	2.44E-03	± 1.52E-04	3.52E-03	± 3.54E-04	3.78E-03	± 5.00E-04
Choline	Cation	6.85	104.107	7.21E-03	± 9.34E-04	1.68E-02	± 4.57E-03	8.12E-03	± 1.28E-03
Citrulline	Cation	11.07	176.102	3.31E+00	± 3.75E-01	3.26E+00	± 2.87E-01	3.53E+00	± 3.50E-01
Cyclohexylamine	Cation	7.83	100.112	2.15E-02	± 3.00E-03	2.03E-02	± 3.82E-04	2.22E-02	± 2.05E-03
Cystathionine	Cation	9.98	223.074	1.01E-01	± 3.00E-03	1.87E-01	± 4.76E-03	9.24E-02	± 3.11E-03
Cysteine-glutathione disulphide	Cation	11.65	427.094	5.48E-03	± 1.64E-04	1.69E-02	± 1.14E-03	7.86E-03	± 3.48E-04
Cytidine	Cation	9.77	244.092	3.87E-02	± 2.95E-03	4.31E-02	± 2.51E-03	6.92E-02	± 4.67E-03
Diethanolamine	Cation	7.76	106.086	6.39E-03	± 7.41E-04	5.47E-03	± 5.22E-04	5.48E-03	± 5.42E-04
Diphenylcarbazine	Cation	21.17	243.123	3.30E-02	± 2.99E-03	4.84E-02	± 6.19E-03	4.19E-02	± 9.79E-03
Dyphylline	Cation	21.24	255.109	2.03E-01	± 2.94E-02	1.12E-01	± 2.26E-02	9.93E-02	± 4.99E-03
Gln ^c	Cation	10.75	147.077	1.58E+01	± 3.91E-02	1.46E+01	± 3.09E-01	1.54E+01	± 1.02E-01
Glu ^c	Cation	10.92	148.062	2.41E+01	± 4.22E-01	2.01E+01	± 7.36E-01	2.45E+01	± 1.88E-01
Glu-Glu	Cation	10.88	277.103	5.63E-03	± 6.17E-04	6.66E-03	± 6.22E-04	9.11E-03	± 2.05E-04
Glutaric acid	Cation	21.39	133.050	3.09E-02	± 1.69E-03	2.44E-02	± 4.08E-03	2.72E-02	± 6.88E-04
Glutathione (GSH)	Cation	13.15	308.092	8.32E-01	± 6.34E-02	5.86E-03	± 7.88E-04	4.92E-02	± 4.71E-02
Glutathione (GSSG) ^d	Cation	12.16	307.082	5.02E-01	± 5.29E-02	8.70E-01	± 3.37E-02	9.05E-01	± 1.03E-02
Gly	Cation	8.42	76.039	1.77E+00	± 1.52E-01	1.22E+00	± 8.10E-02	1.01E+00	± 9.03E-02
Gly-Gly	Cation	8.49	133.059	5.19E-03	± 4.21E-04	4.96E-03	± 2.21E-04	5.28E-03	± 2.80E-04
Gly-Leu	Cation	9.88	189.122	9.93E-02	± 8.14E-03	1.05E-01	± 3.15E-03	1.20E-01	± 3.61E-03
Glycerophosphocholine	Cation	20.84	258.109	1.72E-02	± 1.29E-03	1.99E-02	± 1.88E-03	5.37E-02	± 4.87E-03
Guanine	Cation	8.41	152.056	1.85E-02	± 2.11E-03	1.96E-02	± 1.13E-03	2.03E-02	± 9.27E-04
Guanosine	Cation	12.45	284.098	4.65E-02	± 4.01E-03	4.37E-02	± 2.06E-03	5.81E-02	± 1.86E-03
Hexylamine	Cation	7.72	102.127	5.46E-02	± 1.58E-02	4.97E-02	± 7.75E-03	5.07E-02	± 8.55E-03
His	Cation	7.41	156.076	3.37E+00	± 3.10E-01	3.37E+00	± 2.34E-01	3.86E+00	± 3.48E-01
His-Glu	Cation	7.71	285.118	4.98E-03	± 6.87E-06	5.42E-03	± 2.60E-04	7.61E-03	± 1.90E-04
Homocysteine	Cation	10.47	136.043	4.46E-03	± 7.13E-04	N.D.		N.D.	
Homoserine	Cation	10.13	120.065	8.18E-01	± 3.27E-02	8.22E-01	± 1.93E-02	9.57E-01	± 7.85E-03
Homoserinelactone	Cation	7.04	102.055	1.08E-03	± 9.43E-05	8.51E-02	± 1.32E-03	1.74E-01	± 1.14E-02
Hypoxanthine	Cation	11.06	137.045	2.74E-01	± 1.24E-02	3.02E-01	± 2.13E-02	2.95E-01	± 1.54E-02
Ile	Cation	10.28	132.101	3.10E+00	± 7.61E-02	3.08E+00	± 1.35E-01	2.64E+00	± 5.57E-02
Inosine	Cation	18.92	269.087	8.08E-01	± 6.40E-02	7.20E-01	± 3.09E-02	8.19E-01	± 2.59E-02
Kynurenine	Cation	9.93	209.092	9.23E-03	± 2.77E-03	8.07E-03	± 1.92E-03	5.91E-03	± 9.49E-04
Leu ^c	Cation	10.37	132.102	1.27E+01	± 2.18E-01	1.13E+01	± 3.00E-01	7.79E+00	± 1.05E-01
Lys ^c	Cation	6.89	147.116	3.53E+01	± 1.39E+00	3.32E+01	± 4.66E-01	3.48E+01	± 1.17E+00
Mannosamine	Cation	9.10	180.086	4.31E-03	± 6.88E-04	1.59E-03	± 2.64E-04	1.51E-03	± 2.15E-04

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Candidate compounds	mode	MT ^a	<i>m/z</i>	Relative Intensity ($\times 10^{-8}$) ^b					
				0 min		10 min		30 min	
Mesalamine	Cation	10.82	154.049	4.08E-03	± 4.49E-04	2.33E-03	± 1.23E-04	1.55E-03	± 3.58E-04
Met	Cation	10.73	150.058	1.60E-01	± 8.28E-03	1.36E-01	± 5.05E-03	7.28E-02	± 1.71E-03
<i>N</i> -Acetylhistidine	Cation	9.91	198.086	1.55E-02	± 6.24E-04	1.41E-02	± 2.72E-04	1.32E-02	± 1.94E-04
<i>N</i> -Acetylmethionine	Cation	9.67	175.107	3.09E-01	± 1.46E-02	3.30E-01	± 2.82E-02	3.53E-01	± 2.57E-02
<i>N</i> -Acetylputrescine	Cation	8.57	131.117	7.58E-02	± 3.14E-03	6.69E-02	± 4.98E-03	6.41E-02	± 2.80E-03
<i>N</i> -Ethylglycine	Cation	10.07	104.070	5.04E-03	± 7.18E-04	4.03E-03	± 8.57E-04	3.39E-03	± 2.84E-04
<i>N</i> -Methylproline	Cation	12.93	130.086	9.57E-03	± 2.45E-03	8.71E-03	± 3.08E-03	8.50E-03	± 2.32E-03
<i>N</i> ⁶ -Acetyllysine	Cation	11.45	189.122	3.51E-01	± 8.49E-03	3.36E-01	± 1.43E-02	3.28E-01	± 1.35E-02
<i>N</i> ⁶ , <i>N</i> ⁶ , <i>N</i> ⁶ -Trimethyllysine	Cation	7.30	189.158	7.63E-03	± 7.28E-04	9.65E-03	± 1.10E-03	1.12E-02	± 1.08E-03
Ophthalmic acid	Cation	13.15	290.133	1.23E-02	± 8.60E-04	1.14E-02	± 2.30E-04	1.36E-02	± 6.20E-04
Ornithine ^c	Cation	6.85	133.098	8.04E+00	± 2.24E-01	8.10E+00	± 3.64E-01	9.68E+00	± 2.29E-01
<i>p</i> -Aminobenzoic acid	Cation	9.73	138.054	6.48E-03	± 6.79E-04	6.49E-03	± 3.23E-04	4.89E-03	± 3.04E-04
Pantothenic acid	Cation	21.35	220.117	1.28E-02	± 1.25E-03	1.30E-02	± 5.49E-04	1.73E-02	± 5.82E-04
Phe	Cation	11.12	166.086	1.85E+00	± 2.43E-01	2.02E+00	± 2.17E-01	1.78E+00	± 1.64E-01
Phosphorylcholine	Cation	19.90	184.072	1.11E-02	± 1.59E-03	9.28E-03	± 4.37E-04	8.87E-03	± 3.39E-04
Pimelic acid	Cation	21.39	161.080	1.90E-02	± 8.78E-04	1.70E-02	± 1.52E-03	1.89E-02	± 1.40E-03
Pro	Cation	10.85	116.070	1.47E+00	± 8.54E-03	9.83E-01	± 3.16E-02	9.91E-01	± 2.07E-02
Putrescine	Cation	4.82	89.107	2.20E-03	± 4.48E-04	1.16E-03	± 1.68E-04	1.16E-03	± 1.89E-04
Pyridine-2-carboxylic acid butyl ester	Cation	10.30	180.101	1.16E-02	± 1.68E-03	1.21E-02	± 3.47E-03	9.40E-03	± 2.67E-03
Pyridoxal	Cation	8.90	168.065	2.73E-03	± 1.46E-04	3.33E-03	± 1.76E-04	3.28E-03	± 1.92E-04
<i>S</i> -Adenosylhomocysteine	Cation	8.85	385.127	9.88E-03	± 4.20E-04	1.36E-02	± 1.70E-03	7.92E-03	± 9.20E-04
<i>S</i> -Adenosylmethionine	Cation	7.21	399.143	2.75E-02	± 6.65E-04	1.76E-02	± 7.08E-04	2.15E-02	± 1.43E-03
Saccharopine	Cation	10.77	277.138	3.06E-02	± 1.85E-03	2.66E-02	± 3.48E-03	3.73E-02	± 1.70E-03
Ser	Cation	10.05	106.050	1.57E+00	± 1.95E-02	1.35E+00	± 4.05E-02	1.21E+00	± 2.75E-02
Ser-Glu	Cation	10.43	235.092	5.83E-03	± 8.16E-05	8.27E-03	± 4.70E-04	1.03E-02	± 5.80E-04
Spermidine	Cation	4.64	146.165	3.21E-03	± 3.14E-04	3.36E-03	± 6.28E-04	4.06E-03	± 4.08E-04
Syringic acid	Cation	21.17	199.055	1.89E-02	± 3.52E-03	2.10E-02	± 4.85E-03	3.18E-02	± 5.91E-03
Thiamine	Cation	6.72	265.110	3.23E-01	± 6.26E-03	2.90E-01	± 1.16E-02	3.05E-01	± 8.69E-03
Thiamine phosphate	Cation	10.72	345.077	2.87E-03	± 2.49E-04	2.83E-03	± 2.35E-04	3.53E-03	± 2.72E-04
trans-Glutaconic acid	Cation	21.93	131.034	1.31E-02	± 1.34E-03	7.03E-03	± 4.91E-04	6.22E-03	± 5.61E-04
Triethanolamine	Cation	8.36	150.112	6.69E-03	± 1.78E-03	7.08E-03	± 2.87E-04	7.50E-03	± 1.35E-03
Trimethylamine <i>N</i> -oxide	Cation	6.83	76.073	3.83E-03	± 4.36E-04	4.09E-03	± 8.50E-04	3.61E-03	± 2.82E-04
Trp	Cation	11.01	205.096	1.60E-01	± 2.51E-02	1.78E-01	± 2.13E-02	1.88E-01	± 2.42E-02
Tyr	Cation	11.38	182.080	8.34E-01	± 1.42E-01	9.36E-01	± 1.26E-01	1.22E+00	± 1.52E-01
Tyr-Arg ^d	Cation	7.86	169.594	1.78E-03	± 1.69E-04	1.83E-03	± 3.11E-04	2.44E-03	± 1.97E-04
Tyr-Glu	Cation	11.10	311.122	2.50E-03	± 3.43E-04	2.99E-03	± 3.40E-04	4.54E-03	± 1.84E-04
Uracil	Cation	21.18	113.035	3.04E-02	± 4.86E-04	3.48E-02	± 1.43E-03	3.70E-02	± 1.07E-03
Urea	Cation	20.35	61.039	1.63E-01	± 2.32E-02	9.89E-02	± 1.10E-02	1.07E-01	± 1.51E-02
Uridine	Cation	21.22	245.079	9.23E-02	± 9.05E-03	1.02E-01	± 4.00E-03	1.21E-01	± 6.45E-03
Urocanic acid	Cation	8.40	139.049	8.19E-03	± 1.97E-03	N.D.		N.D.	
Val ^e	Cation	10.09	118.086	7.56E+00	± 2.28E-01	7.93E+00	± 1.98E-01	7.17E+00	± 1.47E-01
β-Ala	Cation	7.43	90.054	4.94E-03	± 3.69E-04	3.86E-03	± 1.03E-03	4.53E-03	± 3.87E-04
β-Ala-Lys	Cation	6.84	218.149	1.23E-02	± 5.62E-04	1.25E-02	± 7.37E-04	1.51E-02	± 4.39E-04
γ-Glu-2-aminobutanoic acid	Cation	12.49	233.112	9.57E-03	± 5.54E-05	9.90E-03	± 3.02E-04	1.27E-02	± 5.24E-04
γ-Glu-Cys	Cation	12.76	251.069	5.18E-02	± 2.83E-03	N.D.		N.D.	
10-Hydroxydecanoic acid	Anion	7.65	187.135	4.41E-03	± 7.22E-05	3.46E-03	± 2.64E-04	3.49E-03	± 3.30E-04
2-Carboxybenzaldehyde	Anion	9.49	149.024	2.14E-03	± 7.67E-05	2.60E-03	± 4.42E-04	2.48E-03	± 2.83E-04
2-Deoxyribose 1-phosphate	Anion	10.95	213.016	3.24E-02	± 2.32E-03	3.10E-02	± 3.04E-03	3.12E-02	± 3.39E-03
2-Furoic acid	Anion	10.40	111.008	1.04E-02	± 6.79E-04	9.38E-03	± 6.20E-04	9.01E-03	± 6.80E-04
2-Hydroxy-4-methylpentanoic acid	Anion	8.99	131.071	1.05E-02	± 3.76E-04	7.82E-03	± 5.02E-04	6.95E-03	± 1.44E-04
2-Hydroxybutyric acid	Anion	9.90	103.040	2.94E-03	± 2.47E-04	2.39E-03	± 1.84E-04	2.76E-03	± 2.17E-04
2-Hydroxyoctanoic acid	Anion	8.08	159.102	5.29E-03	± 3.58E-04	4.07E-03	± 2.19E-04	4.70E-03	± 1.51E-04
2-Hydroxypentanoic acid	Anion	9.17	117.055	6.08E-02	± 1.62E-03	4.45E-02	± 7.50E-03	6.06E-02	± 3.67E-03
2-Isopropylmalic acid	Anion	13.83	175.060	9.70E-02	± 3.31E-03	8.58E-02	± 6.01E-03	7.24E-02	± 6.09E-03
2-Oxoglutaric acid	Anion	21.80	145.014	5.22E-02	± 7.56E-03	3.88E-02	± 4.67E-03	5.35E-02	± 4.78E-03
2-Oxoisovaleric acid	Anion	10.20	115.039	1.69E-03	± 1.50E-04	9.74E-04	± 1.73E-04	1.36E-03	± 2.31E-04
2,3-Diphosphoglyceric acid	Anion	18.67	264.950	1.76E-02	± 1.04E-03	1.55E-02	± 4.43E-04	1.31E-02	± 3.53E-05
2,3-Pyridinedicarboxylic acid	Anion	15.82	166.014	2.41E-03	± 2.09E-04	2.07E-03	± 1.07E-04	1.86E-03	± 6.48E-05
3-Hydroxy-3-methylglutaric acid	Anion	15.58	161.044	2.01E-03	± 1.75E-04	1.83E-03	± 2.19E-04	2.05E-03	± 7.77E-05
3-Hydroxybutyric acid	Anion	9.57	103.040	1.36E-02	± 9.28E-05	1.12E-02	± 9.85E-04	1.36E-02	± 7.57E-04

(Continued on next page)

(Continued)

Candidate compounds	mode	MT ^a	<i>m/z</i>	Relative Intensity ($\times 10^{-8}$) ^b					
				0 min		10 min		30 min	
3-Phosphoglyceric acid	Anion	19.86	184.985	2.04E-01	± 7.24E-03	1.65E-01	± 6.51E-03	1.35E-01	± 6.10E-03
4-Acetylbutyric acid	Anion	9.13	129.055	4.83E-02	± 2.35E-03	3.67E-02	± 4.20E-03	4.54E-02	± 4.48E-03
4-Methylbenzoic acid	Anion	9.20	135.044	6.55E-01	± 1.29E-02	5.19E-01	± 3.67E-02	6.16E-01	± 2.27E-02
4-Oxovaleric acid	Anion	9.74	115.040	1.19E-02	± 2.38E-04	9.52E-03	± 7.92E-04	1.11E-02	± 3.27E-04
5-Aminoimidazole-4-carboxamide ribotide	Anion	9.48	337.054	2.70E-03	± 4.31E-04	1.60E-03	± 1.67E-04	1.19E-03	± 1.31E-04
5-Oxoproline	Anion	9.52	128.035	4.89E-02	± 2.78E-03	3.91E-02	± 8.90E-04	3.63E-02	± 1.82E-03
6-Phosphogluconic acid	Anion	14.73	275.016	3.17E-03	± 1.96E-04	2.65E-03	± 1.49E-04	8.42E-03	± 6.29E-04
Acetyl CoA ^d	Anion	10.26	403.554	2.96E-02	± 2.08E-03	2.99E-02	± 1.12E-03	3.44E-02	± 1.13E-03
Adenylosuccinic acid	Anion	13.80	462.065	2.62E-03	± 4.38E-04	2.05E-03	± 4.39E-04	1.74E-03	± 4.33E-04
ADP	Anion	10.88	426.020	2.23E-01	± 2.56E-03	2.24E-01	± 1.04E-02	2.52E-01	± 4.44E-03
AMP	Anion	9.40	346.054	1.74E-01	± 1.09E-02	1.74E-01	± 2.69E-02	1.26E-01	± 2.39E-02
Aniline	Anion	9.71	92.050	7.56E-03	± 4.33E-04	6.97E-03	± 4.76E-04	5.75E-03	± 3.46E-04
ATP	Anion	11.77	505.988	1.97E-01	± 1.45E-02	1.69E-01	± 2.43E-02	3.75E-01	± 3.94E-02
Azelaic acid	Anion	12.14	187.096	1.67E-03	± 3.05E-06	1.65E-03	± 5.14E-05	1.76E-03	± 1.68E-04
Benzoic acid	Anion	9.86	121.029	9.99E-02	± 4.17E-03	9.89E-02	± 1.05E-02	9.61E-02	± 4.14E-03
CDP	Anion	11.47	402.009	3.53E-02	± 1.42E-03	3.90E-02	± 2.24E-03	4.40E-02	± 4.25E-03
CDP-choline	Anion	6.77	487.100	8.47E-04	± 2.23E-04	9.72E-04	± 3.29E-04	7.95E-04	± 2.03E-04
Cimetidine	Anion	5.35	251.107	2.29E-03	± 1.24E-04	2.20E-03	± 1.36E-04	2.30E-03	± 1.50E-04
<i>cis</i> -Aconitic acid	Anion	28.14	173.008	1.08E-02	± 8.44E-04	7.54E-03	± 1.74E-03	9.03E-03	± 5.44E-05
Citric acid	Anion	26.50	191.019	6.65E-01	± 4.43E-02	5.41E-01	± 4.61E-02	5.49E-01	± 5.39E-02
CMP	Anion	9.60	322.043	1.92E-02	± 3.07E-03	1.83E-02	± 4.40E-03	1.41E-02	± 2.94E-03
CMP- <i>N</i> -acetylneuraminate	Anion	8.30	613.144	1.07E-02	± 6.79E-04	1.66E-02	± 2.83E-04	1.66E-02	± 6.85E-04
CoA ^d	Anion	10.60	382.548	3.05E-03	± 4.74E-04	N.D.		N.D.	
CTP	Anion	12.35	481.976	3.67E-02	± 2.95E-03	4.02E-02	± 6.61E-03	1.01E-01	± 1.14E-02
Cyclohexanecarboxylic acid	Anion	8.69	127.076	6.51E-03	± 4.73E-04	5.60E-03	± 1.59E-04	6.36E-03	± 4.78E-04
dADP	Anion	10.98	410.025	1.70E-03	± 1.32E-04	1.42E-03	± 4.86E-05	1.22E-03	± 8.62E-05
dATP	Anion	11.73	489.992	1.58E-03	± 1.09E-04	1.27E-03	± 1.28E-04	2.18E-03	± 2.78E-04
dCDP	Anion	11.62	386.014	1.68E-03	± 3.55E-05	1.36E-03	± 1.32E-04	1.18E-03	± 1.44E-04
dCTP	Anion	12.47	465.763	7.69E-04	± 4.49E-04	1.19E-03	± 2.48E-04	2.21E-03	± 1.24E-04
Decanoic acid	Anion	7.90	171.139	2.45E-02	± 2.79E-03	2.21E-02	± 8.22E-04	2.10E-02	± 2.24E-03
Dihydroxyacetone phosphate	Anion	12.69	168.990	1.46E-02	± 6.56E-04	1.32E-02	± 8.33E-04	2.56E-02	± 3.09E-03
Dodecanedioic acid	Anion	10.74	229.143	1.72E-03	± 7.19E-05	1.34E-03	± 7.52E-05	1.44E-03	± 9.39E-05
dTDP	Anion	11.30	401.014	3.55E-03	± 1.40E-04	2.86E-03	± 2.74E-04	2.53E-03	± 1.68E-04
dTMP	Anion	9.57	321.048	1.04E-03	± 1.58E-04	8.41E-04	± 2.58E-04	5.97E-04	± 1.19E-04
dTTP	Anion	12.10	480.981	2.61E-03	± 1.83E-04	2.32E-03	± 3.70E-04	4.26E-03	± 5.72E-04
Ethanolamine phosphate	Anion	7.99	140.011	4.41E-03	± 1.99E-04	2.84E-03	± 1.48E-04	2.88E-03	± 1.07E-04
FAD ^d	Anion	7.84	391.570	1.85E-03	± 2.26E-04	1.87E-03	± 1.58E-04	2.18E-03	± 1.07E-04
Fructose 1,6-diphosphate	Anion	14.65	338.987	3.85E-02	± 9.92E-04	3.16E-02	± 1.87E-03	8.27E-02	± 9.46E-03
Fructose 6-phosphate	Anion	9.93	259.022	3.11E-02	± 4.23E-03	2.15E-02	± 1.67E-03	3.73E-02	± 4.33E-03
Fumaric acid	Anion	25.88	115.003	3.73E-02	± 8.55E-04	2.70E-02	± 3.59E-04	3.48E-02	± 1.48E-04
Ganciclovir	Anion	5.73	254.086	1.59E-02	± 2.29E-03	1.20E-02	± 1.76E-04	1.15E-02	± 1.62E-04
GDP	Anion	10.63	442.016	7.29E-02	± 1.37E-03	8.10E-02	± 1.32E-03	8.38E-02	± 4.51E-03
GDP-mannose	Anion	8.29	604.070	4.91E-03	± 3.20E-04	4.86E-03	± 3.50E-04	2.76E-02	± 1.24E-03
Gluconic acid	Anion	8.12	195.050	3.74E-03	± 6.52E-05	3.66E-03	± 2.87E-04	4.74E-03	± 1.40E-04
Glucose 1-phosphate	Anion	10.15	259.022	3.41E-02	± 3.53E-03	1.13E-02	± 4.01E-03	1.66E-02	± 1.49E-02
Glucose 6-phosphate	Anion	9.85	259.021	2.15E-02	± 9.71E-04	1.68E-02	± 1.55E-03	3.09E-02	± 4.69E-03
Gly-Asp	Anion	9.65	189.051	3.33E-03	± 1.53E-04	3.35E-03	± 1.01E-04	3.93E-03	± 3.21E-04
Glyceric acid	Anion	10.36	105.019	1.01E-02	± 4.28E-04	9.82E-03	± 6.55E-04	9.52E-03	± 2.95E-04
Glycerol-3-phosphate	Anion	12.13	171.005	2.69E-02	± 3.04E-03	2.20E-02	± 4.58E-03	2.57E-02	± 4.36E-03
GMP	Anion	9.21	362.049	3.47E-02	± 3.37E-03	3.44E-02	± 5.77E-03	2.75E-02	± 4.53E-03
GTP	Anion	11.44	521.983	4.40E-02	± 3.39E-03	4.46E-02	± 6.23E-03	8.43E-02	± 8.45E-03
Heptanoic acid	Anion	8.55	129.091	3.10E-02	± 4.42E-03	2.38E-02	± 6.33E-03	3.05E-02	± 2.78E-03
Hexanoic acid	Anion	9.00	115.076	5.40E-02	± 6.64E-03	4.13E-02	± 9.30E-03	5.05E-02	± 1.61E-03
IMP	Anion	9.56	347.038	1.35E-02	± 1.15E-03	1.20E-02	± 7.59E-04	5.73E-03	± 5.43E-04
Isobutyric acid	Anion	9.89	87.045	5.86E-02	± 4.96E-03	5.06E-02	± 7.52E-03	5.78E-02	± 2.28E-03
Isocitric acid	Anion	29.06	191.015	1.53E-02	± 4.02E-03	9.20E-03	± 2.81E-03	1.18E-02	± 2.76E-03
Lactic acid	Anion	10.76	89.024	4.43E-01	± 3.33E-02	3.68E-01	± 3.96E-02	4.93E-01	± 4.42E-02
Lauric acid	Anion	7.60	199.169	4.13E-02	± 8.40E-04	3.92E-02	± 1.40E-03	3.46E-02	± 2.80E-03
Malic acid	Anion	21.67	133.014	2.78E-01	± 1.72E-02	1.92E-01	± 1.21E-03	2.70E-01	± 1.07E-02
<i>N</i> -Acetyl- β -alanine	Anion	8.99	130.049	5.66E-04	± 5.76E-05	7.87E-04	± 1.33E-04	8.35E-04	± 8.45E-05

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Candidate compounds	mode	MT ^a	<i>m/z</i>	Relative Intensity ($\times 10^{-8}$) ^b					
				0 min		10 min		30 min	
<i>N</i> -Acetylglucosamine 1-phosphate	Anion	9.57	300.047	1.15E-03	± 6.10E-05	7.10E-04	± 1.14E-04	7.60E-04	± 9.03E-05
<i>N</i> -Acetylglucosamine 6-phosphate	Anion	9.22	300.047	3.39E-03	± 1.52E-04	8.18E-04	± 6.32E-05	3.30E-04	± 3.17E-05
<i>N</i> -Acetylglucosylamine	Anion	5.34	219.094	2.72E-03	± 2.41E-04	2.28E-03	± 8.33E-05	2.23E-03	± 1.56E-04
<i>N</i> -Acetylglutamic acid	Anion	13.23	188.055	4.70E-01	± 2.72E-02	4.79E-01	± 4.09E-02	5.58E-01	± 4.74E-02
<i>N</i> -Acetylleucine	Anion	7.98	172.098	7.49E-03	± 2.58E-04	7.44E-03	± 3.86E-04	6.53E-03	± 3.68E-04
<i>N</i> -Acetylmethionine	Anion	8.09	190.054	3.48E-03	± 3.14E-04	3.18E-03	± 4.06E-04	2.81E-03	± 4.21E-04
<i>N</i> -Carbamoylaspartic acid	Anion	15.57	175.035	7.52E-03	± 1.77E-03	6.07E-03	± 8.47E-04	5.47E-03	± 6.88E-04
<i>N</i> -Methylglutamic acid	Anion	8.37	160.061	9.79E-02	± 2.89E-03	1.05E-01	± 3.64E-03	1.23E-01	± 1.64E-02
<i>n</i> -Propionyl CoA ^d	Anion	10.15	410.562	2.06E-03	± 1.74E-04	1.63E-03	± 1.65E-04	1.23E-03	± 1.95E-04
NAD ⁺	Anion	6.55	662.103	1.97E-01	± 1.20E-02	1.84E-01	± 8.59E-03	2.13E-01	± 6.27E-03
NADH	Anion	8.17	664.118	2.46E-03	± 4.05E-04	1.56E-03	± 3.63E-04	2.18E-03	± 4.05E-04
NADP ⁺	Anion	9.43	742.070	2.09E-02	± 1.29E-03	2.46E-02	± 1.92E-03	3.32E-02	± 2.05E-03
NADPH ^d	Anion	11.29	371.537	2.02E-02	± 3.82E-03	1.55E-02	± 3.86E-03	1.43E-02	± 4.04E-03
Norvaline	Anion	5.31	116.071	5.21E-01	± 3.35E-02	5.07E-01	± 5.69E-02	5.36E-01	± 1.64E-02
<i>o</i> -Hydroxybenzoic acid	Anion	10.41	137.023	1.24E-03	± 1.35E-04	1.06E-03	± 6.33E-05	1.10E-03	± 6.94E-05
<i>O</i> -Phosphoserine	Anion	12.29	184.001	7.65E-03	± 7.37E-04	4.35E-03	± 6.59E-04	4.53E-03	± 5.38E-04
Octanoic acid	Anion	8.33	143.107	2.71E-02	± 3.66E-03	2.50E-02	± 2.82E-03	2.31E-02	± 1.84E-03
Orotidine 5'-monophosphate	Anion	12.57	367.017	1.67E-02	± 2.88E-03	6.43E-03	± 7.47E-04	3.47E-03	± 1.82E-04
Pelargonic acid	Anion	8.06	157.123	4.27E-02	± 5.77E-03	3.78E-02	± 3.79E-03	3.91E-02	± 4.09E-03
Phosphoenolpyruvic acid	Anion	21.39	166.974	5.54E-02	± 2.04E-03	4.65E-02	± 3.19E-03	4.38E-02	± 2.57E-03
Propionic acid	Anion	10.91	73.029	4.34E-02	± 3.79E-03	3.88E-02	± 3.16E-03	4.37E-02	± 4.00E-03
PRPP	Anion	16.64	388.943	3.94E-03	± 3.50E-04	3.45E-03	± 5.68E-04	3.90E-03	± 6.07E-04
Pyridoxamine 5'-phosphate	Anion	7.99	247.046	1.50E-03	± 1.27E-04	1.52E-03	± 5.39E-05	1.51E-03	± 6.80E-05
Pyruvic acid	Anion	12.93	87.009	1.67E-01	± 6.59E-03	1.78E-01	± 1.88E-03	1.81E-01	± 8.07E-03
Quinic acid	Anion	8.08	191.055	6.14E-03	± 4.66E-04	5.19E-03	± 3.36E-04	8.16E-03	± 1.72E-03
Ribose 5-phosphate	Anion	10.55	229.011	1.32E-02	± 1.61E-03	1.30E-02	± 7.64E-04	1.84E-02	± 2.55E-03
Ribulose 5-phosphate	Anion	10.96	229.011	1.35E-02	± 5.67E-04	1.15E-02	± 3.46E-04	4.84E-02	± 3.02E-03
Sebacic acid	Anion	11.58	201.112	4.05E-03	± 7.34E-05	2.87E-03	± 1.43E-04	3.85E-03	± 3.95E-04
Sedoheptulose 7-phosphate	Anion	9.63	289.032	2.67E-02	± 1.08E-03	2.22E-02	± 4.28E-04	5.96E-02	± 2.71E-03
Succinic acid	Anion	21.26	117.019	1.09E-01	± 1.09E-03	7.97E-02	± 2.65E-03	1.20E-01	± 3.67E-03
Thr-Asp	Anion	10.45	233.076	1.67E-03	± 2.47E-04	1.65E-03	± 1.22E-04	2.17E-03	± 2.83E-04
Tiglic acid	Anion	9.73	99.045	2.52E-03	± 1.34E-04	1.70E-03	± 4.64E-04	2.48E-03	± 1.71E-04
<i>trans</i> -Ferlic acid	Anion	8.41	193.051	4.49E-03	± 3.28E-04	4.33E-03	± 6.17E-04	4.59E-03	± 4.51E-04
Trehalose 6-phosphate	Anion	8.41	421.074	3.34E-03	± 6.53E-05	3.36E-03	± 3.17E-04	1.04E-02	± 9.73E-04
UDP	Anion	11.66	402.993	1.28E-01	± 5.30E-03	1.46E-01	± 9.25E-03	1.37E-01	± 1.15E-02
UDP-glucose ; UDP-galactose	Anion	8.76	565.047	1.70E-02	± 2.96E-04	1.60E-02	± 7.12E-04	3.44E-02	± 1.41E-03
UMP	Anion	9.79	323.027	5.14E-02	± 7.76E-03	4.89E-02	± 1.11E-02	3.25E-02	± 6.67E-03
Undecanoic acid	Anion	7.75	185.154	9.47E-03	± 8.28E-04	8.88E-03	± 5.94E-04	7.75E-03	± 8.06E-04
UTP	Anion	12.58	482.960	1.54E-01	± 9.27E-03	1.68E-01	± 2.24E-02	3.02E-01	± 3.06E-02
Valeric acid	Anion	9.29	101.060	5.67E-02	± 8.51E-03	4.62E-02	± 1.16E-02	5.62E-02	± 2.83E-03
β -Cyanoalanine	Anion	5.35	113.034	3.00E-03	± 6.28E-05	2.00E-03	± 1.01E-04	2.66E-03	± 8.76E-05

^aMigration time (min)

^bThe mean values \pm standard errors for three independent experiments are presented.

^cThe values were calculated from the isotopic peak areas based on carbon isotope ratio.

^dThe ion peaks were detected as $[M+2H]^{2+}$ or $[M-2H]^{2-}$.

N.D., Not determined

Table S3. Changes in selenium compounds after SeMet treatment.

Candidate compounds	mode	MT ^a	m/z	Relative intensity ($\times 10^{-8}$) ^b						
				0 min	10 min		30 min			
5'-MSeA	Cation	7.26	346.040	N.D.	3.08E-02	±	9.72E-04	6.45E-02	±	2.15E-03
5'-MSeA	Cation	10.21	346.040	N.D.	5.28E-02	±	6.91E-03	1.40E-01	±	1.92E-02
5'-MSeA ^c	Anion	5.01	344.025	N.D.	4.19E-03	±	2.40E-04	6.86E-03	±	9.38E-05
GS-Se-SG ^c	Anion	5.01	691.062	N.D.	5.10E-04	±	6.40E-05	1.23E-03	±	6.27E-05
GSH-(S-Se)-Cys ^c	Cation	11.65	475.039	N.D.	9.55E-03	±	5.20E-04	7.38E-03	±	3.81E-04
GSH-(S-Se)-Cys	Anion	7.49	473.024	N.D.	5.34E-03	±	4.11E-04	3.26E-03	±	7.82E-05
GSH-(S-Se)-Hcy ^c	Cation	11.11	489.054	N.D.	6.59E-02	±	4.41E-03	1.35E-01	±	5.75E-03
GSH-(S-Se)-Hcy	Anion	7.08	487.040	N.D.	5.28E-02	±	4.60E-03	9.68E-02	±	5.06E-03
Hcy-(S-Se)-Cys ^c	Cation	10.21	302.990	N.D.	5.24E-03	±	7.84E-04	6.18E-03	±	2.23E-04
Hcy-(S-Se)-Hcy ^c	Cation	9.72	317.005	N.D.	1.47E-02	±	2.97E-03	3.15E-02	±	2.10E-03
Hcy-(S-Se)-Hcy	Anion	5.36	314.993	N.D.	3.33E-03	±	1.07E-03	3.89E-03	±	3.40E-04
Hcy-(Se-Se)-Cys ^c	Cation	10.21	350.933	N.D.	2.04E-03	±	4.61E-04	8.07E-03	±	2.63E-04
Hcy-(Se-Se)-Hcy ^c	Cation	9.73	364.950	N.D.	6.53E-03	±	7.78E-04	6.76E-02	±	3.01E-03
Hcy-(Se-Se)-Hcy	Anion	5.36	362.935	N.D.			N.D.	5.59E-03	±	3.01E-04
Hcy-(Se-Se)-Hcy	Anion	5.76	362.935	N.D.			N.D.	1.23E-03	±	8.36E-05
Methaneselenol	Anion	5.02	94.939	N.D.	6.01E-04	±	3.16E-05	1.23E-03	±	5.96E-05
Methaneselenol ^c	Anion	5.35	94.940	N.D.	3.05E-02	±	1.63E-03	1.93E-02	±	5.71E-04
Se-AdoHcy ^c	Cation	8.87	433.072	N.D.	1.46E-02	±	2.87E-03	1.98E-02	±	2.69E-03
Se-AdoHcy	Anion	5.35	431.058	N.D.	6.88E-03	±	6.90E-04	9.00E-03	±	6.03E-04
Se-AdoMet ^c	Cation	7.26	447.088	N.D.	1.27E-01	±	1.84E-03	2.83E-01	±	8.69E-03
Se-AdoMet	Anion	5.01	445.074	N.D.	7.28E-04	±	8.33E-05	1.17E-03	±	2.13E-05
Se-Cystathionine ^c	Cation	9.97	271.018	N.D.	2.37E-02	±	2.42E-03	2.51E-02	±	6.72E-04
SeMet ^c	Cation	10.82	198.002	N.D.	3.11E+00	±	1.50E-01	1.73E+00	±	7.21E-02
SeMet	Anion	5.35	195.987	N.D.	1.55E-01	±	8.68E-03	9.36E-02	±	3.66E-03
γ -Glu-Cys-(S-Se)-Cys ^c	Anion	7.57	416.001	N.D.	1.41E-03	±	1.36E-05	7.10E-04	±	5.85E-05
γ -Glu-Cys-(S-Se)-Hcy ^c	Cation	10.87	432.032	N.D.	1.18E-02	±	5.50E-04	1.50E-02	±	4.74E-04
γ -Glu-Cys-(S-Se)-Hcy	Anion	7.20	430.017	N.D.	3.06E-03	±	4.90E-05	4.67E-03	±	2.20E-04

^aMigration time (min)^bThe mean values \pm standard errors for three independent experiments are presented.^cThe data were plotted in Fig. 2e.

N.D., Not determined