Electronic Supplementary Material (ESI) for Metallomics.

Supplementary Data

Identification of biliary selenium metabolite and biological significance of selenium enterohepatic circulation

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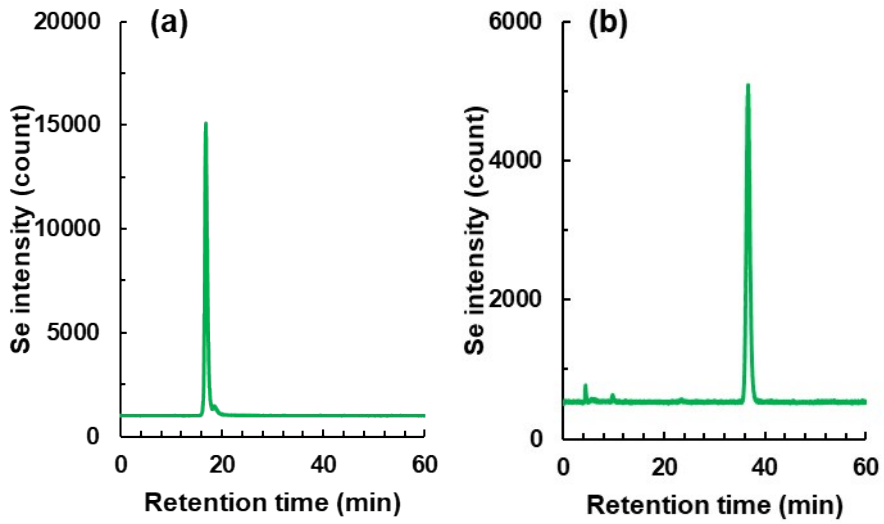

Figure S1. Elution profiles of Se in synthesized GSSeSG obtained by LC-ICP-MS/MS with (a) GS-520HQ or (b) Zorbax Sb-Aq column.

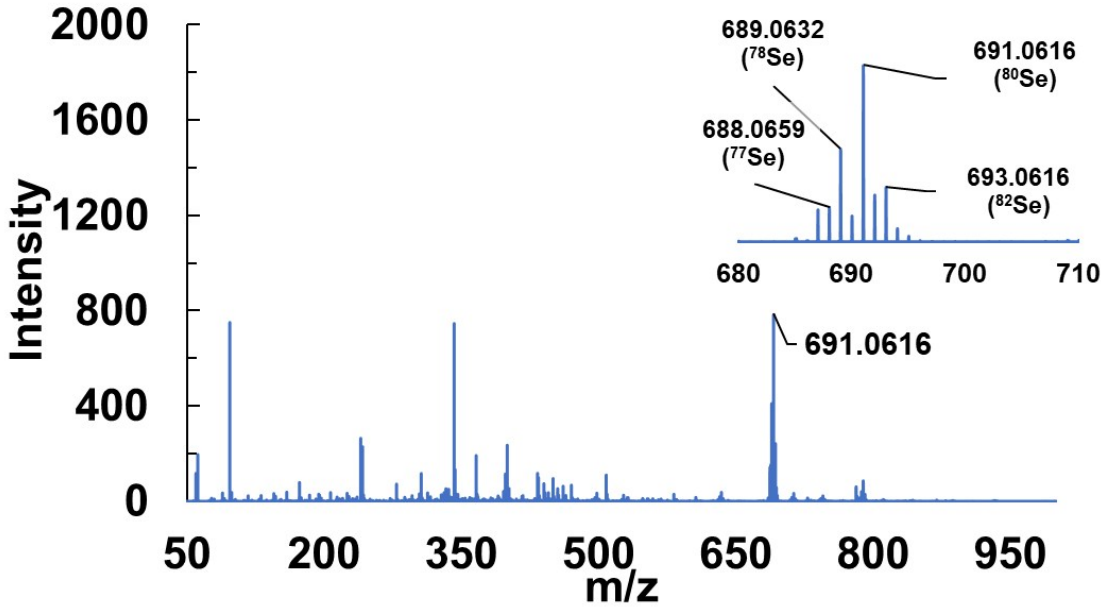

Figure S2. Mass spectra of eluate of partially purified biliary selenocompound at retention times of 37 to 40 min. The elution profiles were obtained in the negative ion modes. The part of the spectra containing a unique Se isotope pattern was enlarged as an inset.

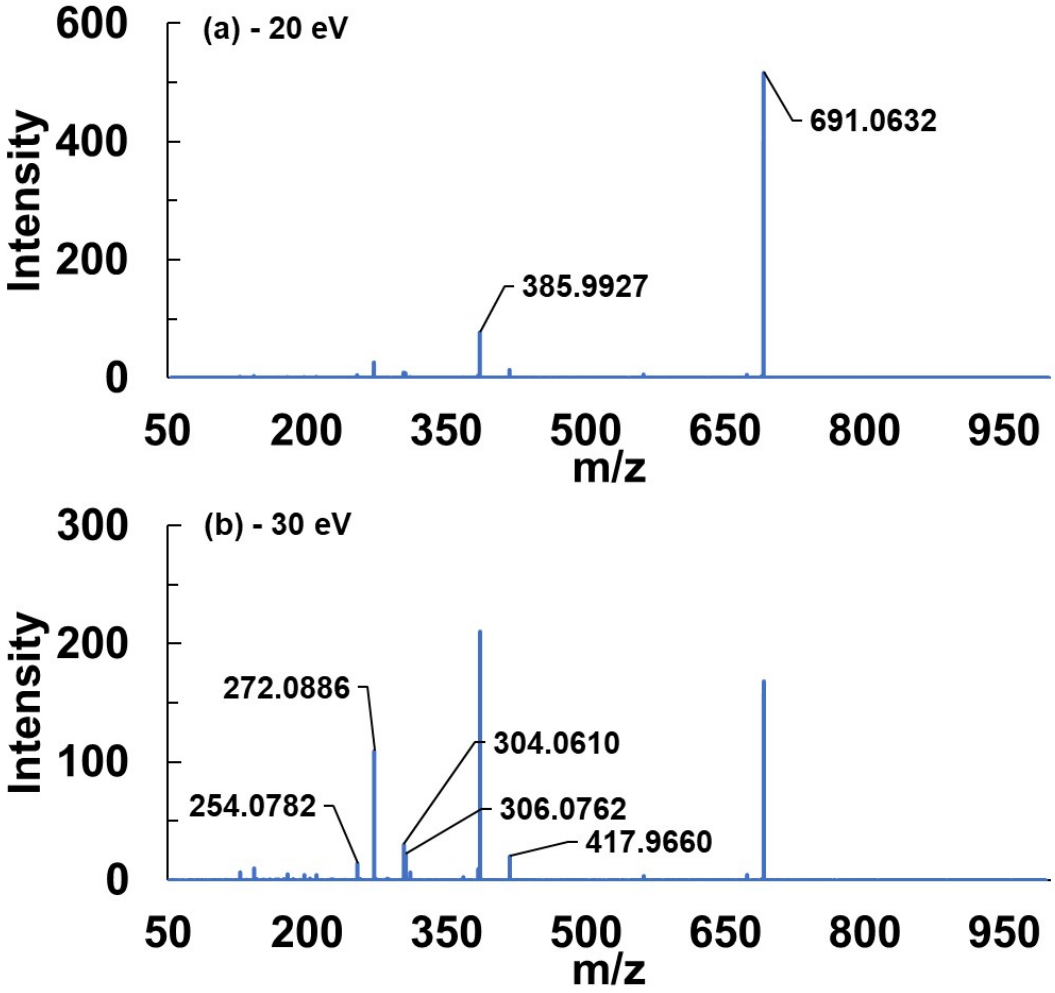

Figure S3. Collision-induced fragment mass spectra of Se-containing molecular ion (*m/z* 691.06) in the eluate of partially purified biliary selenocompound at retention times of 37 to 40 min. The mass spectra were obtained by ESI-MS/MS (Q/TOF) in the negative ion mode. Fragment ions were detected by collision in a Q2 cell with -20 (a) and -30 (b) eV collision energies.

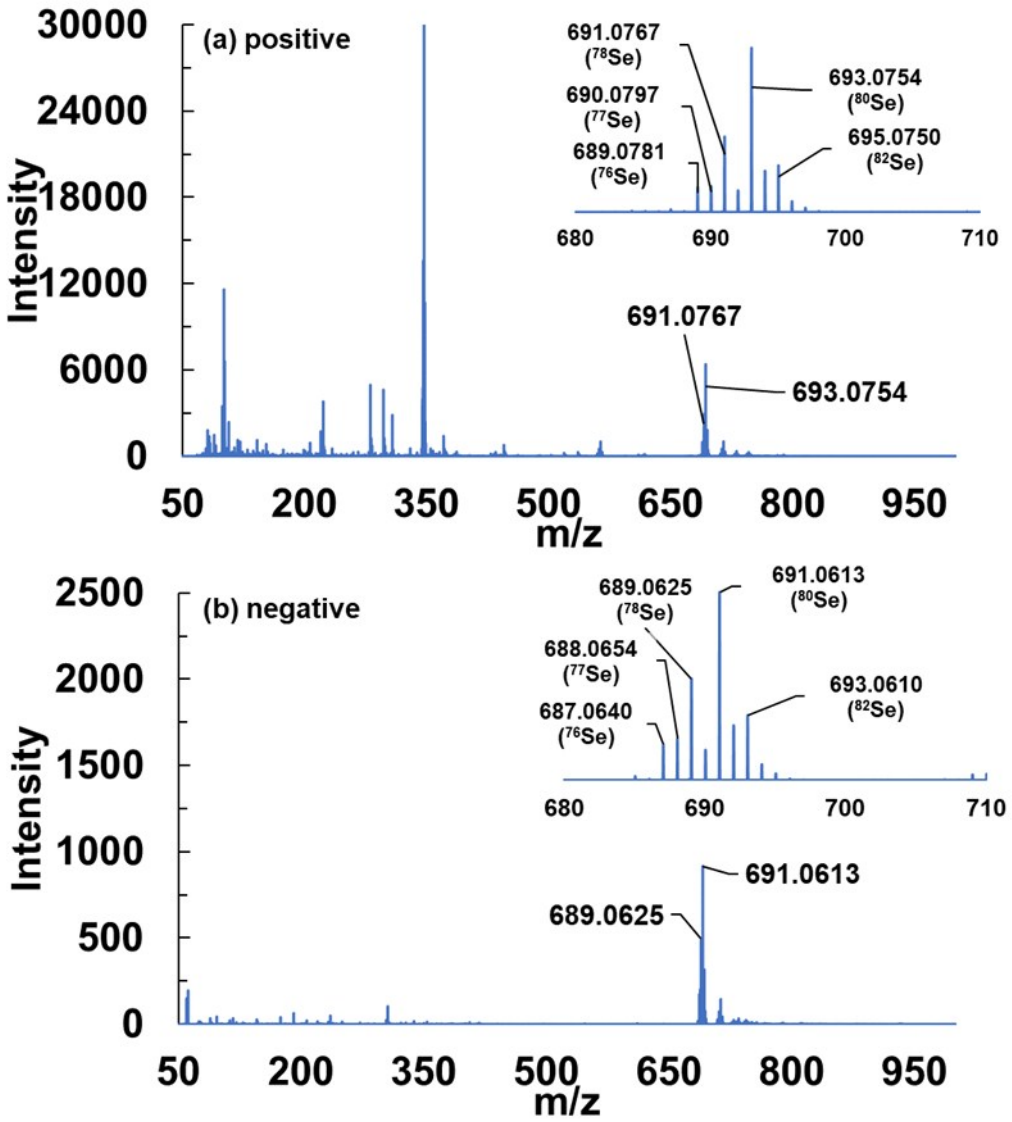

Figure S4. Electrospray spectra of synthesized GSSeSG measured in the (a) positive and (b) negative ion mode at retention times of 37 to 40 min.

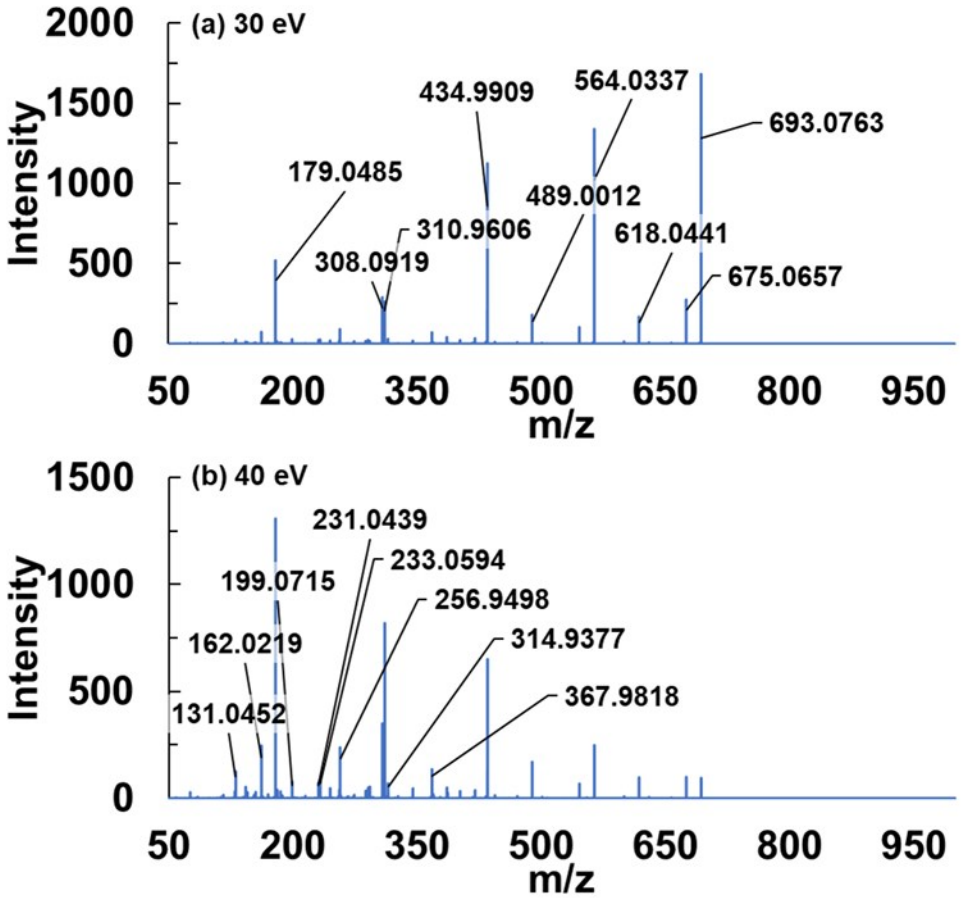

Figure S5. Collision-induced fragment mass spectra (ESI–MS/MS) of Se-containing positive molecular ion (*m/z* 693.07) in the eluate at retention times of 37 to 40 min for the chemically synthesized GSSeSG. Fragmentation of parent ion was induced in the collision cell (Q2) with (a) 30 and (b) 40 eV collision energies, and each product ion was detected by TOF measurement.

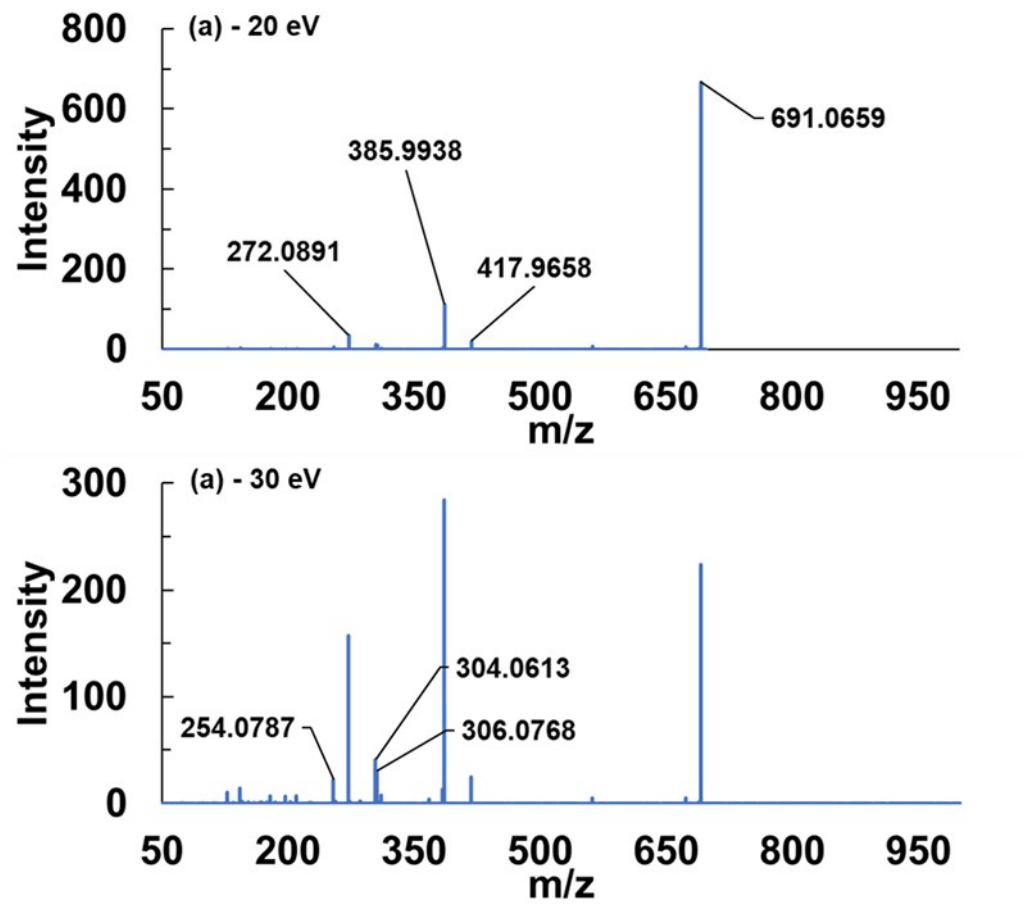

Figure S6. Collision-induced fragment mass spectra (ESI–MS/MS) of Se-containing negative molecular ion (*m/z* 691.06) in the eluate at retention times of 37 to 40 min for the chemically synthesized GSSeSG. Fragmentation of the parent ion was induced in the collision cell (Q2) with (a) -20 and (b) -30 eV collision energies, and each product ion was detected by TOF measurement.