Supplementary Information

# Uranium chelating ability of decorporation agents in serum evaluated by X-ray absorption spectroscopy

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Table S1. Concentration of U in serum obtained from three rats.

| No | XAS (μg/g) | ICP-MS (μg/g) |
|---|---|---|
| 1 | 0.99±0.31 | 1.43±0.10 |
| 2 | 0.54±0.16 | 0.83±0.07 |
| 3 | 1.11±0.32 | 1.23±0.08 |

Table S2. ITFA-calculated percentage of U-bioligand and U-EHBP complexes on XANES in Fig. 2(c) and the uncertainties for the calculated components. The uncertainties listed in the table are calculated as mathematical errors associated with ITFA. Nos 1 – 6: 0, 0.2, 0.5, 1, 2, 5 mM EHBP in serum. No 7: 5 mM EHBP in HEPES buffer (pH 7.4) as a reference. U concentration was 0.5 mM.

| No | [EHBP] (mM) | U-bioligands (%) | U-EHBP (%) |
|---|---|---|---|
| 1 | 0 | 100 | 0 |
| 2 | 0.2 | 78 | 21 |
| 3 | 0.5 | 69 | 31 |
| 4 | 1 | 56 | 44 |
| 5 | 2 | 40 | 59 |
| 6 | 5 | 0 | 100 |
| 7 | 5 | 0 | 100 |
| Uncertainty | | 3 | 3 |

Table S3. ITFA-calculated percentage of U-bioligand and U-EHBP complexes on EXAFS in Fig. S6 (c) and the uncertainties for the calculated components. The uncertainties listed in the table are calculated as mathematical errors associated with ITFA. Nos 1 – 6: 0, 0.2, 0.5, 1, 2, 5 mM EHBP in serum. No 7: 5 mM EHBP in HEPES buffer (pH 7.4) as a reference. U concentration was 0.5 mM.

| No | [EHBP] (mM) | U-bioligands (%) | U-EHBP (%) |
|---|---|---|---|
| 1 | 0 | 100 | 0 |
| 2 | 0.2 | 94 | 2 |
| 3 | 0.5 | 87 | 15 |
| 4 | 1 | 76 | 27 |
| 5 | 2 | 65 | 31 |
| 6 | 5 | 10 | 86 |
| 7 | 5 | 0 | 100 |
| Uncertainty | | 4 | 4 |

Table S4. ITFA-calculated percentage of U-bioligand and soluble and insoluble U-IP6 complexes on XANES in Fig. 3 (c) and the uncertainties for the calculated components. The uncertainties listed in the table are calculated as mathematical errors associated with ITFA. Nos 1 – 6: 0, 0.2, 0.5, 1, 2, 5 mM IP6 in serum. No 7: 5 mM IP6 in HEPES buffer (pH 7.4) as a reference.

| No | [IP6] (mM) | U-bioligand (%) | U-IP6 soluble (%) | U-IP6 insoluble (%) |
|---|---|---|---|---|
| 1 | 0 | 100 | 0 | 0 |
| 2 | 0.2 | 37 | 12 | 50 |
| 3 | 0.5 | 26 | 4 | 69 |
| 4 | 1 | 7 | 44 | 50 |
| 5 | 2 | 0 | 55 | 45 |
| 6 | 5 | 0 | 77 | 23 |
| 7 | 5 | 0 | 100 | 0 |
| Uncertainty | | 4 | 4 | 5 |

Table S5. ITFA-calculated percentage of U-bioligand and U-DFO complexes on XANES in Fig. 4 (c) and the uncertainties for the calculated components. The uncertainties listed in the table are calculated as mathematical errors associated with ITFA. Nos 1 – 3: 0, 2, 5, and 10 mM DFO in serum. No 5: 5 mM DFO in HEPES buffer (pH 7.4) as a reference. Uranium concentration was 0.5 mM.

| No | [DFO] (mM) | U-bioligands (%) | U-DFO (%) |
|---|---|---|---|
| 1 | 0 | 100 | 0 |
| 2 | 2 | 100 | 0 |
| 3 | 5 | 86 | 14 |
| 4 | 10 | 63 | 38 |
| 5 | 5 | 0 | 100 |
| Uncertainty | | 3 | 3 |

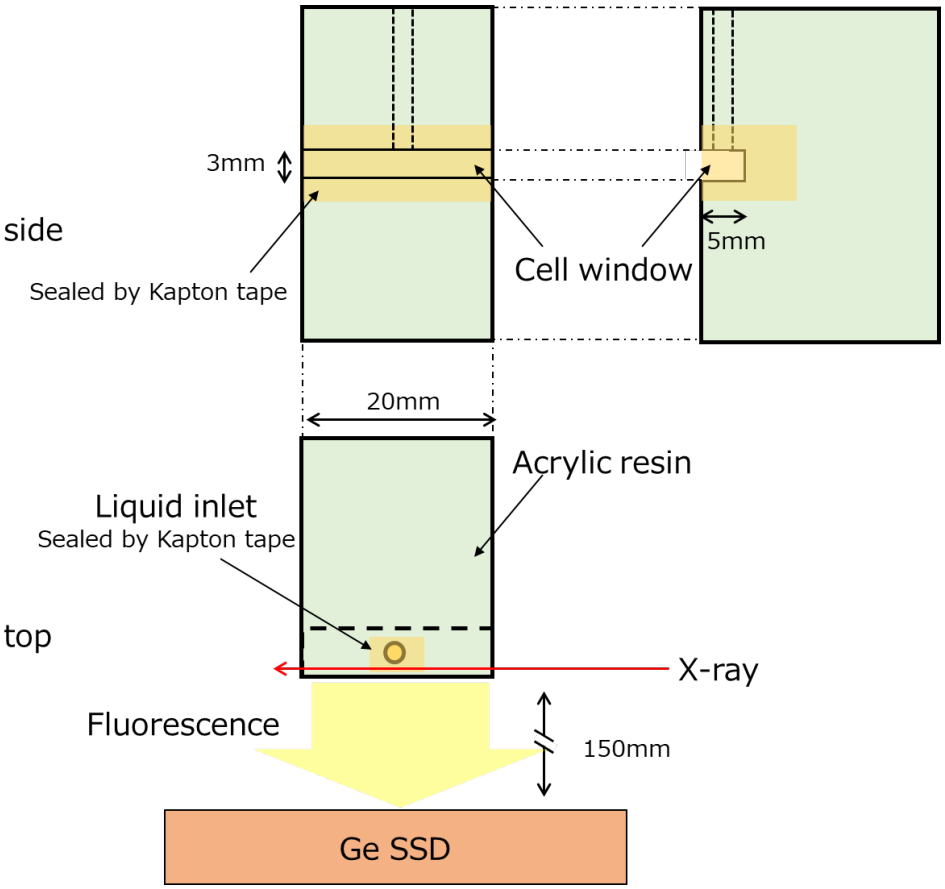


Figure S1. Experimental cell for X-ray absorption spectroscopy.

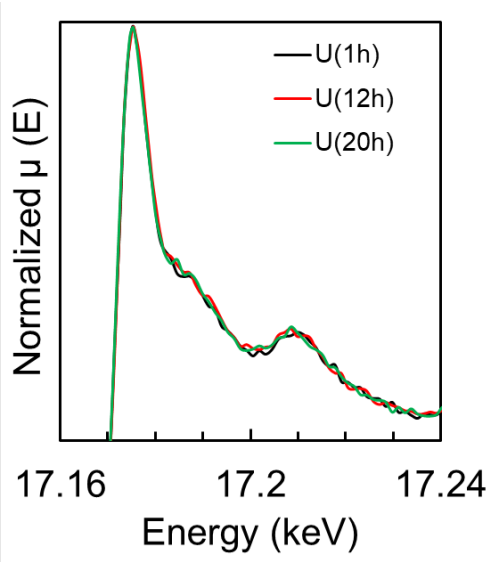


Figure S2. XANES spectra dependence on incubation time in the serum. U concentration was 0.5 mM.

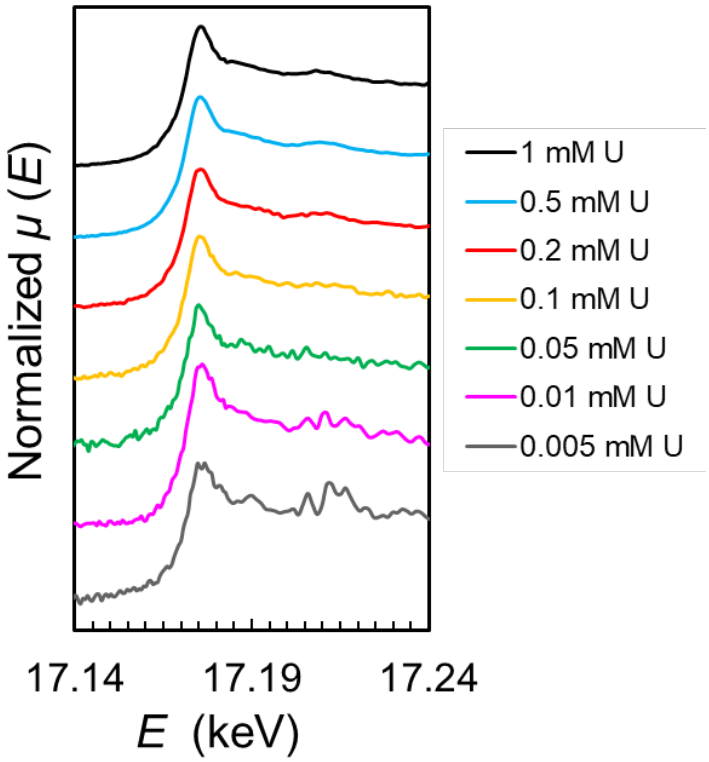


Figure S3. Dependence of U concentration in serum.

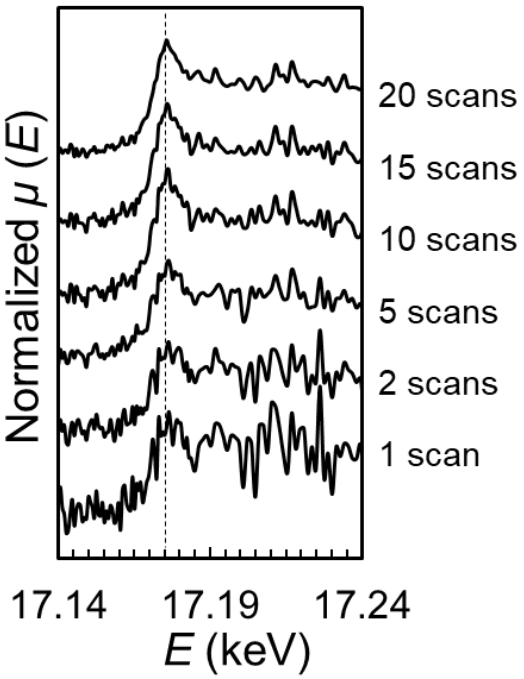


Figure S4. Effect of the measurement time on XANES spectra of the specimen after administration of U.

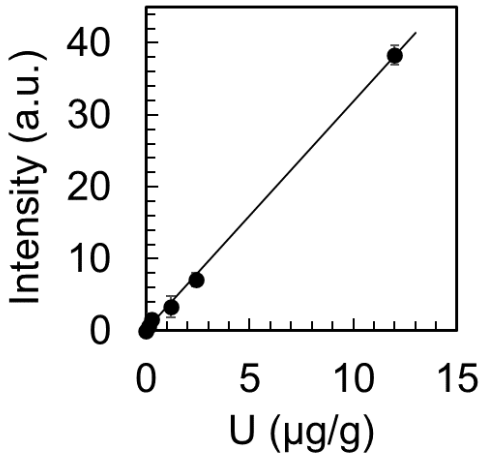


Figure S5. Dependence of edge jump absorption intensity on the U concentration in serum.

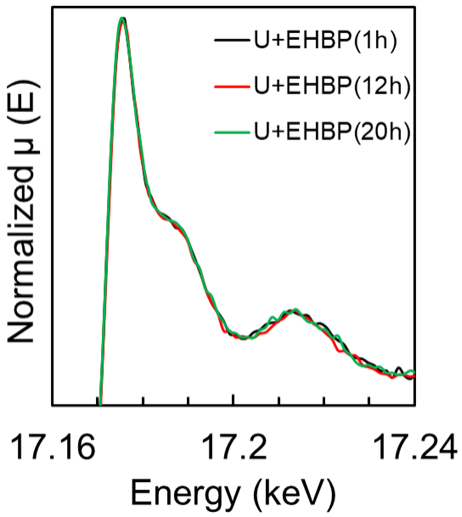


Figure S6. XANES spectra dependence on incubation time in the serum. U and EHBP concentration were 0.5 and 2 mM.

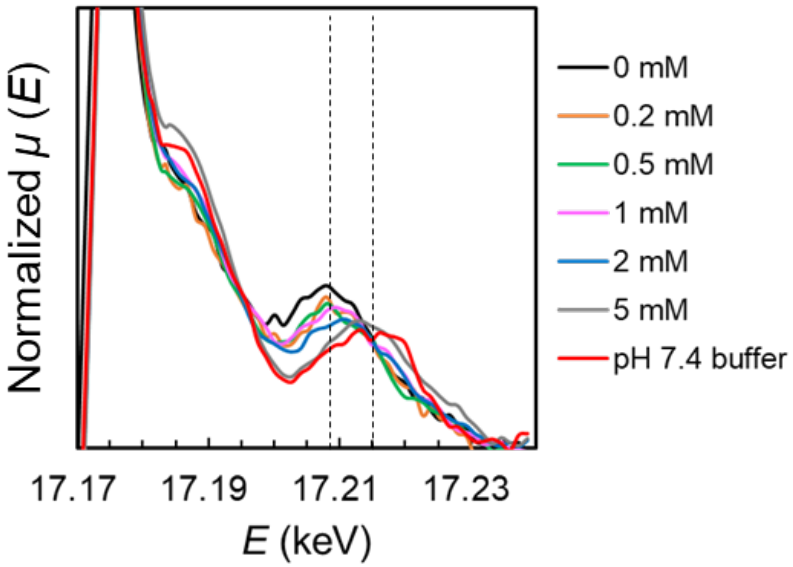


Figure S7. XANES spectra dependence on the EHBP concentration in the serum. 0, 0.2, 0.5, 1, 2, and 5 mM EHBP in the serum, respectively. 5 mM EHBP in the HEPES buffer (pH 7.4) as a reference. The U concentration was 0.5 mM.

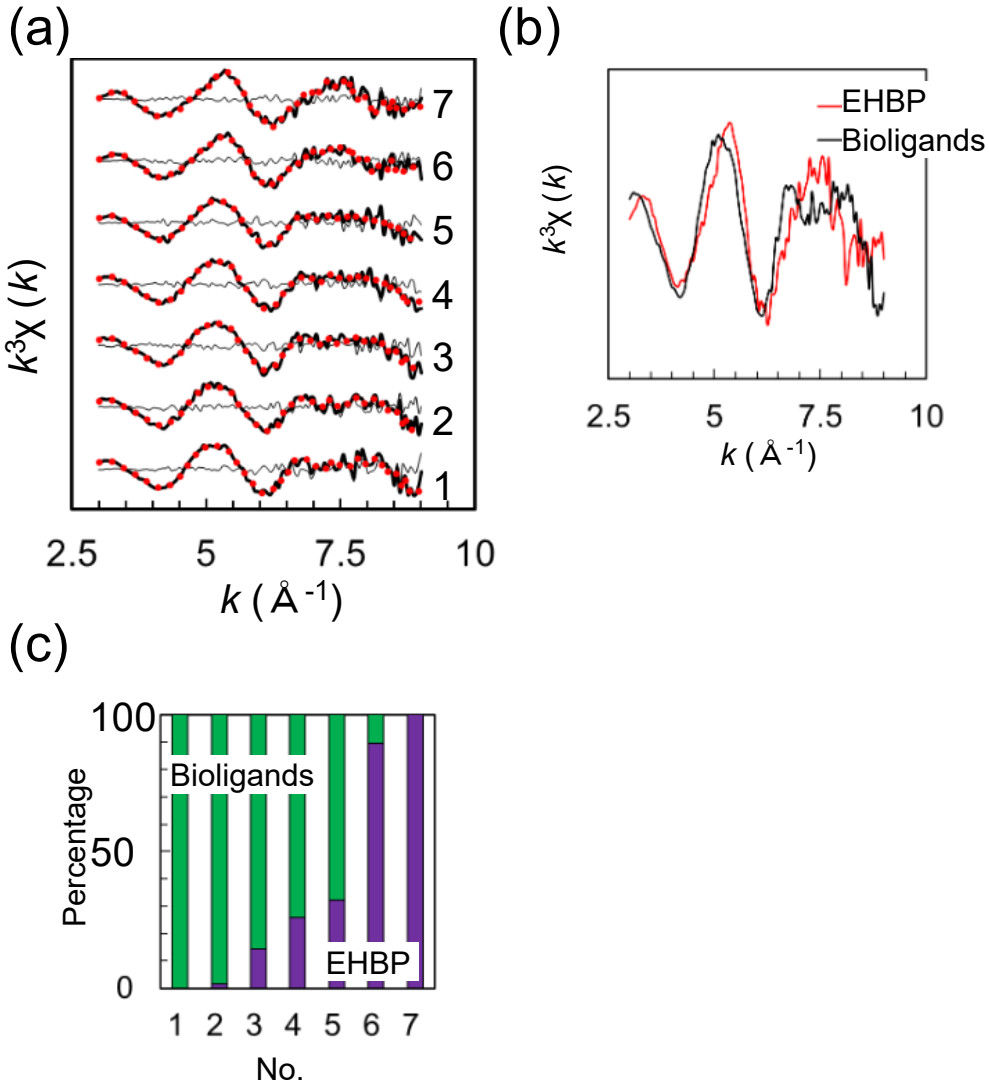


Figure S8. (a) EXAFS spectra dependence on the EHBP concentration in the serum. Curves 1 – 6 correspond to 0, 0.2, 0.5, 1, 2, and 5 mM EHBP in the serum, respectively. Curve 7 corresponds to 5 mM EHBP in the HEPES buffer (pH 7.4), which serves as a reference. U concentration was 0.5 mM. Solid line: experimental, dotted line: calculated. Residual between experimental and calculation. (b) Extracted two component spectra. (c) Percentage of the components calculated by PCA fitting. Uncertainty of the percentage is shown in Supplementary Table S3.

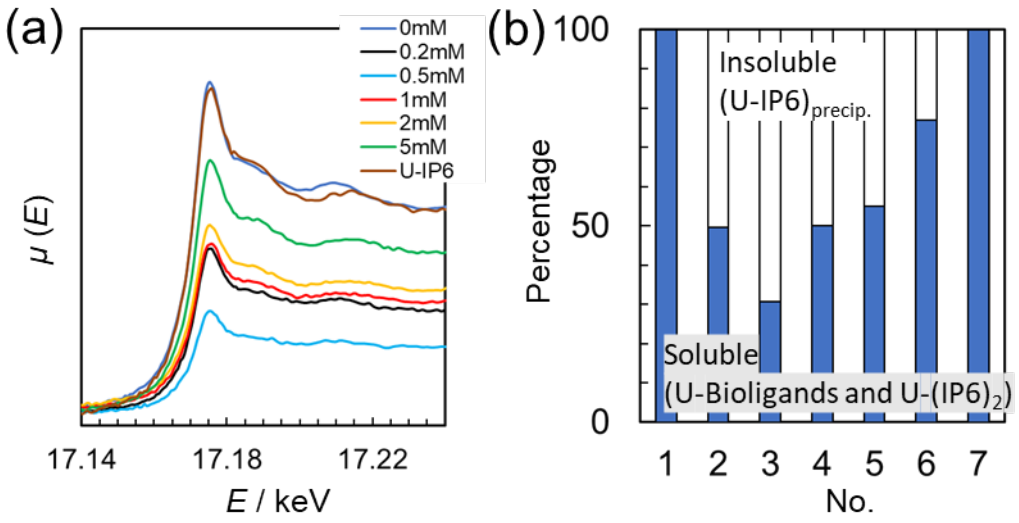


Figure S9. (a) XANES spectra depended on the IP6 concentration in the serum. Curves 1 – 6 correspond to 0, 0.2, 0.5, 1, 2, and 5 mM IP6 in the serum respectively. Curve 7 corresponds to 5 mM IP6 in the HEPES buffer (pH 7.4), which serves as a reference. U concentration was 0.5 mM. (b) Percentage of the soluble and insoluble species were calculated by the edge jump intensity of μE.

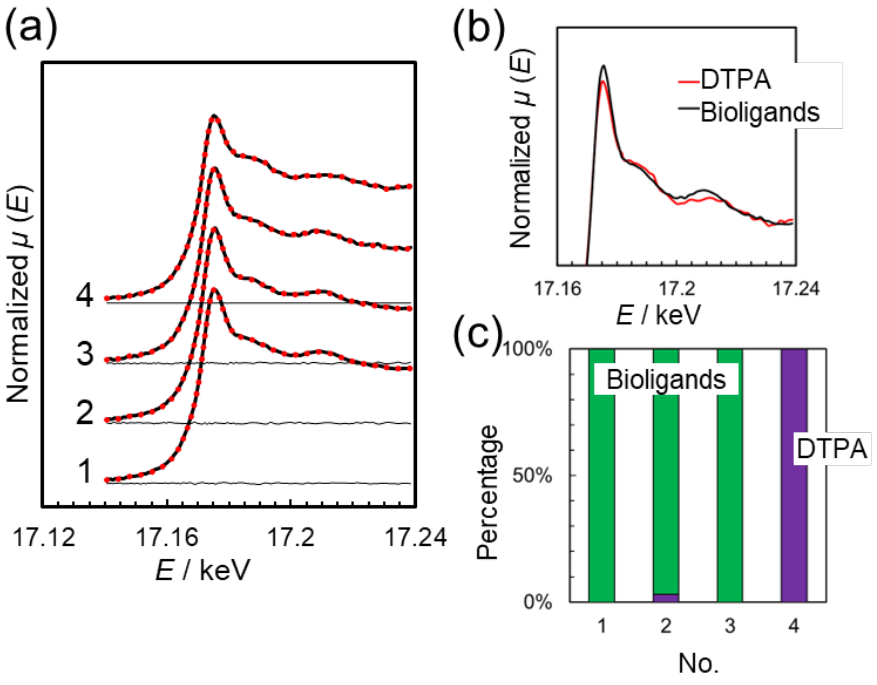


Figure S10. (a) XANES spectra in the presence of the DTPA concentration in the serum. Curves 1 – 3 correspond to 0.5, 0.5, and 0.2 mM U and 0, 10, and 10 mM DTPA in the serum respectively. Curve 4 corresponds to 0.5 mM U and 5 mM DTPA in HEPES buffer (pH 7.4), which serves as a reference. U concentration was 0.5 mM. Solid line: experimental, dotted line: calculated. Residual between experimental and calculation. (b) Extracted two component spectra. (c) Percentage of the components calculated by PCA fitting.