

Supporting Information

XAS Studies of Se Speciation in Selenite-Fed Rats

Claire M. Weekley,[†] Jade B. Aitken,[§] Paul K. Witting,[‡] and Hugh H. Harris^{†,*}

[†]*School of Chemistry and Physics, The University of Adelaide, SA 5005, Australia*

[§]*School of Chemistry, The University of Sydney, NSW 2006, Australia*

[‡]*The Discipline of Pathology, Charles Perkins Centre, The University of Sydney, NSW 2006,
Australia*

*To whom correspondence should be addressed. Associate Professor Hugh Harris, *School of Chemistry and Physics, The University of Adelaide, SA 5005, Australia* Phone: 61-08-83135060; Facsimile: 61-8-83134358; Email: hugh.harris@adelaide.edu.au

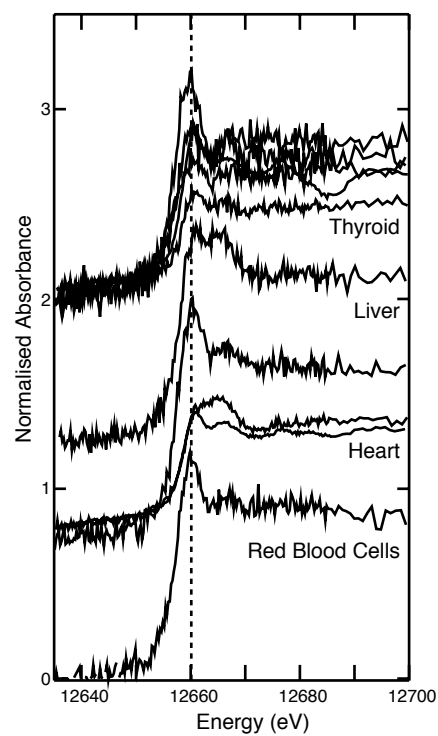


Figure S1. Se K-edge XANES spectra of thyroid, liver, heart and red blood cells from rats fed control, 1 ppm or 5 ppm Se (as selenite) diets for 3 weeks. These XANES spectra comprise the group circled in Figure 4. Note the difficulty encountered in normalising the spectra due to the low signal:noise ratios.

Table S1. Positions of the first peak of the Se *K*-edge XANES of model selenium compound spectra presented in Figure 2d, and selected tissue samples (3 week diets) presented in Figures 2a-c.

Model or tissue sample	Energy of first peak (eV)
Se-Se-Se	12659.7
S-Se-S	12660.2
R-Se-Se-R	12660.3
R-S-Se-R	12660.6
R-Se-H	12661.2
SeMet	12661.1
MeSeCys	12661.4
RSe ⁻	12664.7
HSe ⁻	12663.4
GPx	12664.5
CuSe	12664.0
R-Se-(O)-R	12663.0
R-Se(O ₂)-R	12665.7
Me ₃ Se ⁺	12662.6
SeO ₃ ²⁻	12664.0
kidney control	12660.9
kidney 1 ppm	12660.5
kidney 5 ppm	12660.3
liver control	12661.1
liver 1 ppm	12660.9
liver 5 ppm	12661.1
heart 5 ppm	12660.7
red blood cells 5 ppm	12660.7

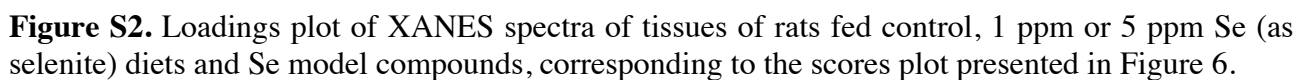


Figure S2. Loadings plot of XANES spectra of tissues of rats fed control, 1 ppm or 5 ppm Se (as selenite) diets and Se model compounds, corresponding to the scores plot presented in Figure 6.