

Supplementary Material to :

Tetrathiomolybdate causes formation of hepatic copper-molybdenum clusters in an animal model of Wilson's disease.

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Table SI. Selected EXAFS curve-fitting results of lysosomes from a tetrathiomolybdate-treated LEC rat.^a

	<i>N</i>	<i>R</i>	σ^2	<i>N</i>	<i>R</i>	σ^2	<i>Error</i> ^b
	Cu-S ^c			Cu···Mo			
Cu	3	2.279(2)	0.0061(2)	0			0.419
	3	2.276(1)	0.0061(2)	1	2.700(2)	0.0060(2)	0.228
	4	2.277(2)	0.0081(1)	1	2.701(2)	0.0065(2)	0.226
	3.5(1) ^d	2.277(1)	0.0072(3)	0.85(1) ^d	2.700(3)	0.0051(7)	0.216
	Mo-S ^c			Mo···Cu			
Mo	4	2.236(2)	0.0037(2)	2	2.697(3)	0.0026(2)	0.338
	4	2.237(3)	0.0037(2)	3	2.698(3)	0.0043(3)	0.312
	4	2.238(3)	0.0036(2)	4	2.696(3)	0.0057(2)	0.329
	4.0(2) ^d	2.237(2)	0.0037(2)	3.1(2) ^d	2.698(3)	0.0043(3)	0.311

^a Coordination number *N*, interatomic distance *R* (Å), and (thermal and static) mean-square deviation in *R* (the Debye-Waller factor) σ^2 (Å²). Except where indicated *N* was held fixed at integer values, while *R* and σ^2 were freely floated in the refinements. The values in parentheses are the estimated standard deviations (precisions) obtained from the diagonal elements of the covariance matrix. We note that the accuracies will always be somewhat larger than the precisions, typically ± 0.02 Å for *R* and $\pm 20\%$ for *N* and σ^2 . ^b The Fit-Error is defined as $[\sum k^6(\chi_{\text{exptl}} - \chi_{\text{calcd}})^2 / \sum k^6 \chi_{\text{exptl}}^2]^{1/2}$. ^c Inclusion of oxygen or nitrogen backscatterers had a detrimental effect upon the fit. Note that EXAFS cannot readily distinguish between scatterers of similar atomic number, such as chlorine and sulfur, or nitrogen and oxygen. ^d Coordination numbers *N* were floated in the refinement.