Supporting Information

Similarities between *N*-acetylcysteine and Glutathione in Binding to Lead(II) Ions

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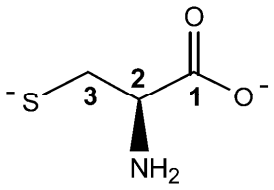
Table S1. Assignment of mass ions observed in ESI-MS spectra (positive-ion mode) for Pb(II) *N*-acetylcysteine solutions A, B and E ($C_{Pb(II)}$ = 10 mM; mole ratio H_2NAC/Pb(II) = 2.1, 3.0 and 10.0, respectively) [a]

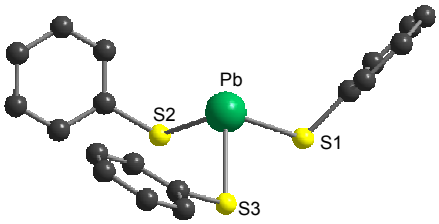
m/z (amu)	assignment	*m/z* (amu)	assignment
164.04	$[H_2NAC + H^+]^+$	555.01	$[Na^+ + Pb(H_2NAC)_2 - 2H^+]^+$
186.01	$[Na^+ + H_2NAC]^+$	556.04	$[3Na^+ + 3(H_2NAC) - 2H^+]^+$
294.00	$[Pb(C_3H_4NO_2)]^+$	578.02	$[4Na^+ + 3(H_2NAC) - 3H^+]^+$
349.05	$[Na^+ + 2(H_2NAC)]^+$	738.98	$[Pb_2(H_2NAC)_2 - 3H^+]^+$
370.00	$[Pb(H_2NAC) - H^+]^+$	740.02	$[2Na^+ + Pb(H_2NAC)_3 - 3H^+]^+$
371.03	$[2Na^+ + 2(H_2NAC) - H^+]^+$	741.05	$[4Na^+ + 4(H_2NAC) - 3H^+]^+$
393.01	$[3Na^+ + 2(H_2NAC) - 2H^+]^+$	763.04	$[5Na^+ + 4(H_2NAC) - 4H^+]^+$

[a] H_2NAC ($C_5H_9NO_3S$); *m* = 163.03

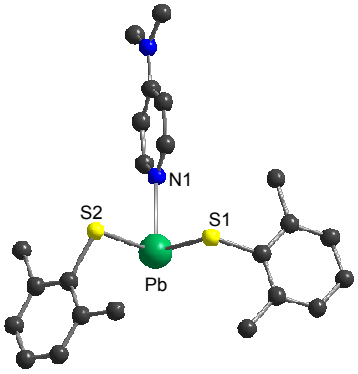
Table S2. Comparison of differences in ^{13}C NMR chemical shifts (Δδ) for lead(II) *N*-acetylcysteine solutions A – E ($C_{Pb(II)}$ = 10 mM) relative to those of a pure *N*-acetylcysteine solution (0.1 M; pH = 9.1); see Figure 3

	Δδ (^{13}C, ppm)	
Solution	C_1	C_3
A	0.5	3.1
B	0.6	2.4
C	0.5	2.0
D	0.4	1.6
E	0.2	0.8

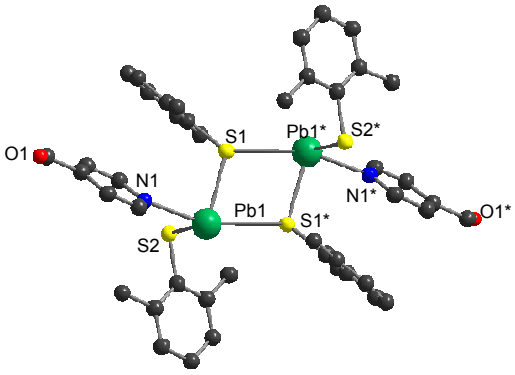




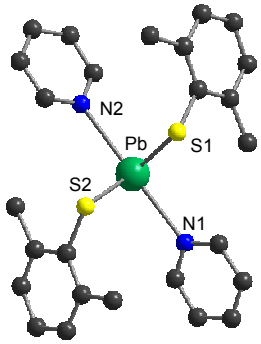
$[Pb(SPh)_3]^-$
PbS_3



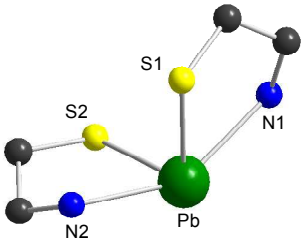
$(2,6\text{-}Me_2C_6H_3S)_2Pb(pyNMe_2)$
PbS_2N



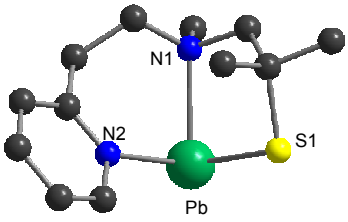
$[(2,6\text{-}Me_2C_6H_3S)_2Pb(pyCOH)]_2$
PbS_2NS'



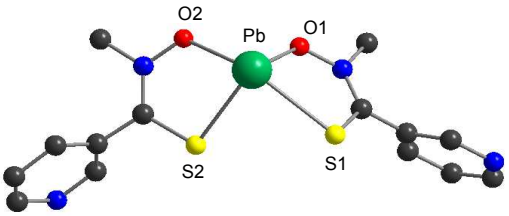
$(2,6\text{-}Me_2C_6H_3S)_2Pb(py)_2$
PbS_2N_2



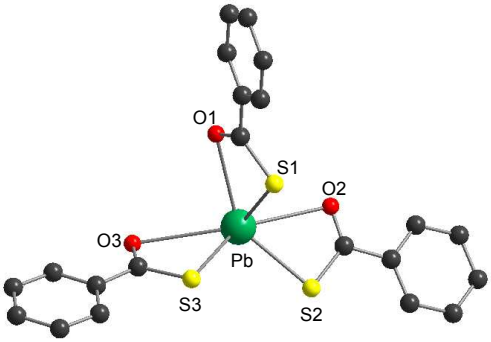
bis(aminoethanethiolato) lead(II)
PbS_2N_2



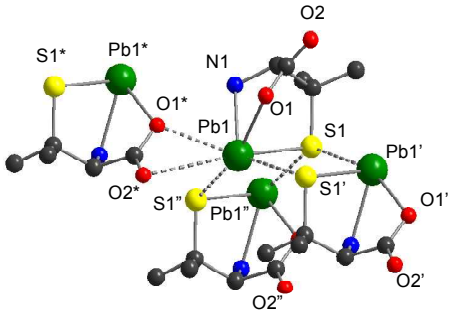
$[PATH\text{-}Pb]ClO_4$
$PbSN_2$



bis(*N*-methyl-3-pyridothiohydroxamato) lead(II)
PbS_2O_2



$[Pb(SOCPh)_3]^-$
PbS_3O_3



(Penicillaminato)lead(II)
$PbSNOS'_2O'_2$

Figure S1. Structures of sulfur-bound Pb(II) complexes for which ^{207}Pb NMR chemical shifts and references have been summarized in Table 2; H-atoms were removed for clarity.

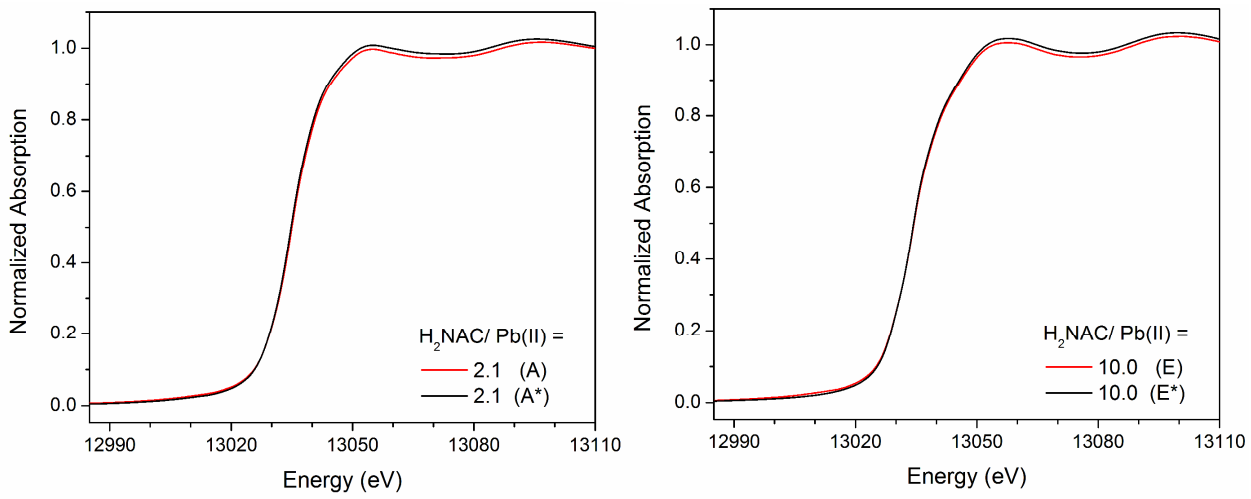


Figure S2. X-ray absorption near-edge features in the XANES spectra of Pb(II) *N*-acetylcysteine solutions, containing $C_{Pb(II)}$ = 10 mM (red), 100 mM (black) and H_2NAC/Pb(II) mole ratios 2.1 (pH = 9.4) and 10.0 (pH = 9.1), showing similar features for each set.

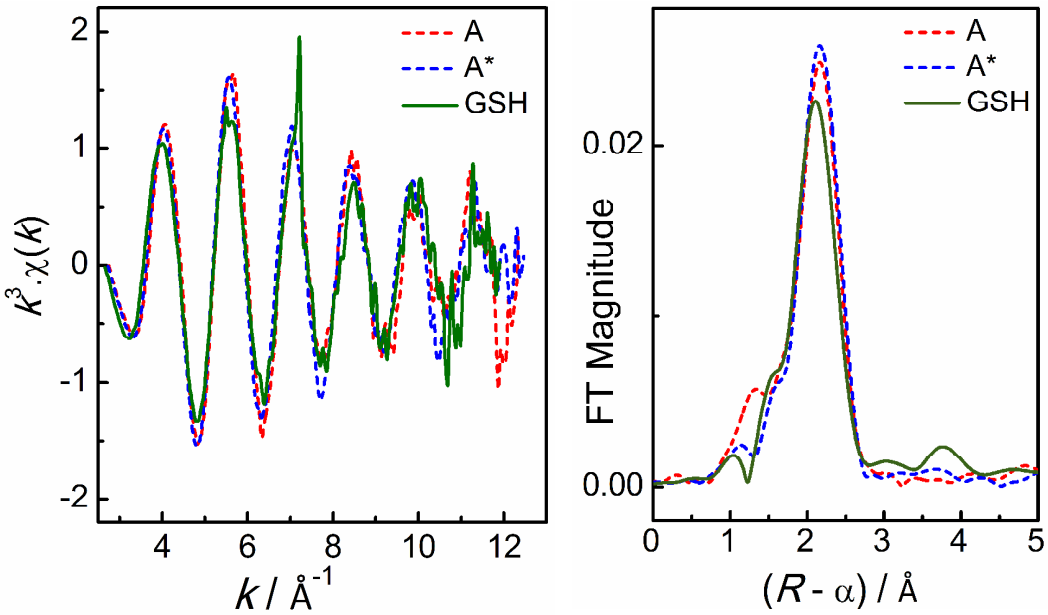


Figure S3. Pb L_{III}-edge k^3-weighted EXAFS spectrum of a lead(II) glutathione solution ($C_{Pb(II)}$ = 10 mM; C_{GSH} = 20 mM; pH = 8.5) measured in fluorescence mode (solution A in *Ref.* 26) compared with those of Pb(II) *N*-acetyl cysteine solutions A and A* (pH = 9.4), containing H_2NAC/Pb(II) mole ratio 2.1, and their corresponding Fourier-transforms.

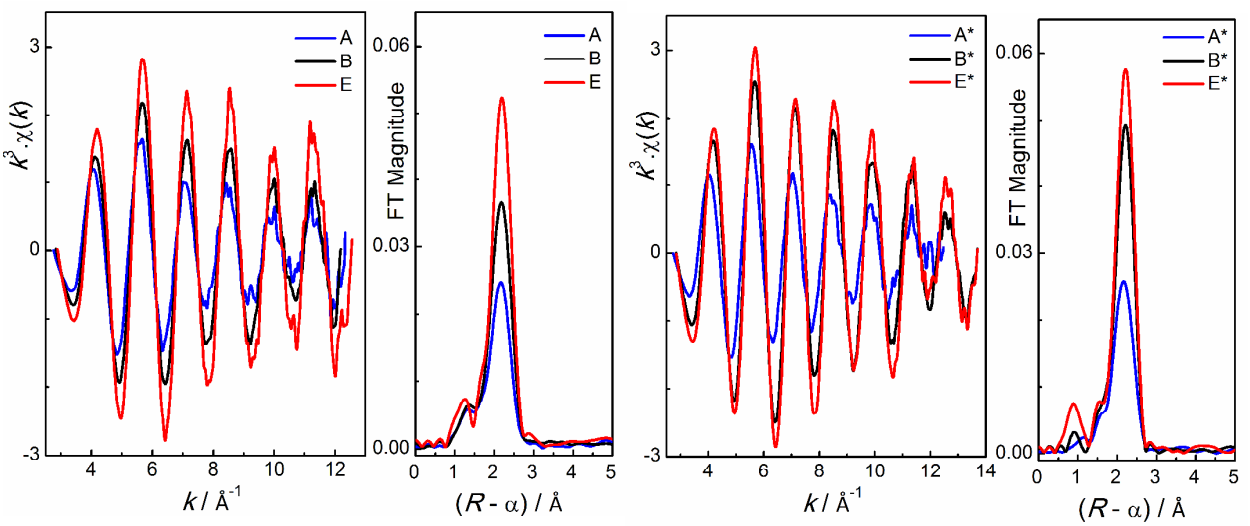


Figure S4. Comparison between Pb L_{III}-edge k^3-weighted EXAFS spectra and corresponding Fourier-transforms for Pb(II) *N*-acetyl cysteine solutions, containing $C_{Pb(II)}$ = 10 mM (*left*), 100 mM (*right*), and H_2NAC/Pb(II) mole ratios 2.1 (A, A*, pH = 9.4), 3.0 (B, B*, pH = 9.1) and 10.0 (E, E*, pH = 9.1).

Table S3. Structural parameters obtained from EXAFS least-squares curve-fitting for a Pb(II) GSH solution containing $C_{Pb(II)}$ = 10 mM, C_{GSH} = 20 mM (pH = 8.5; solution A in *Ref*. 26) measured at RT, using different EXAFS fitting models. [a,b]

Model	Pb-S			Pb-N			Pb…Pb			
	N	*R* (Å)	σ^2 (Å^2)	*N*	*R* (Å)	σ^2 (Å^2)	*N*	*R* (Å)	σ^2 (Å^2)	R
I	2.7	2.63	0.0107							28.5
II	2 *f*	2.66	0.0122	1 *f*	2.48	0.0036				29.8
III [c]	2 *f*	2.65	0.0156	2 *f*	2.51	0.0056				29.4 [c]
IV	2*f*	2.62	0.0080				1*f*	3.84	0.015	27.9
	1*f*	2.76	0.0117							
V	1.9	2.62	0.0076				1*f*	3.84	0.015	27.9
	1*f*	2.75	0.0109							
VI	1.9*f*	2.62	0.0076				1*f*	3.84	0.015	27.9
	0.9	2.75	0.0100							

[a] Refined *N* accurate within ± 20 %; S_0^2 = 0.9 *f*, *f* = fixed; R = residual. [b] Estimated error limits for *R* is ± 0.04 Å and for σ^2 ± 0.002 Å^2; [c] the model shown in Figure 7 and Table 5 of *Ref*. 26