The Copper Centers of Tyramine β-monooxygenase and Its Catalytic-Site Methionine Variants. An X-Ray Absorption Study†.

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Supporting Information

Table S1 and Figs S1 - 2

Table S1. Comparisons of fits to the EXAFS of reduced TBM at pH 7. A, fit using a single shell of histidines; B, using two non-equivalent shells of histidines; C, using a shell of two equivalent histidines and no S(Met) ligation. Imidazole outer-shell geometry was fit by including both single and multiple scattering contributions from the second shell (C2/C5) and third shell (C3/N4) atoms respectively. The Cu-N-C_x angles were as follows: Cu-N-C2 126°, Cu-N-C3 -126°, Cu-N-N4 163°, Cu-N-C5 -163°

		Cu-His 1			Cu-His 2			Cu-S			
Fit	F	Shell	R(Å)	DW(A^2)	Shell	R(Å)	DW(A^2)	Shell	R(Å)	DW(A^2)	$-E_0$
A	0.327	2 N1	1.940	0.017				0.5 S	2.239	0.015	2.28
		2 C2	2.896	0.020							
		2 C5	3.058	0.020							
		2 N4	4.243	0.020							
		2 C3	4.148	0.020							
B	0.324	1 N1	1.882	0.012	1 N1	1.979	0.007	0.5 S	2.245	0.014	2.10
		1 C2	2.935	0.020	1 C2	3.047	0.020				
		1 C5	2.935	0.020	1 C5	3.047	0.020				
		1 N4	4.123	0.020	1 N4	4.270	0.020				
		1 C3	4.123	0.020	1 C3	4.270	0.020				
C	1.055	2 N1	1.953	0.015							2.99
		2 C2	2.896	0.020							
		2 C5	3.058	0.020							
		2 N4	4.243	0.020							
		2 C3	4.248	0.020							

Figure S1. Experimental versus simulated Fourier transform and EXAFS (inset) for reduced TBM at pH 7 using two shells of non-equivalent histidines, with the parameters as listed in fit B of Table S1.

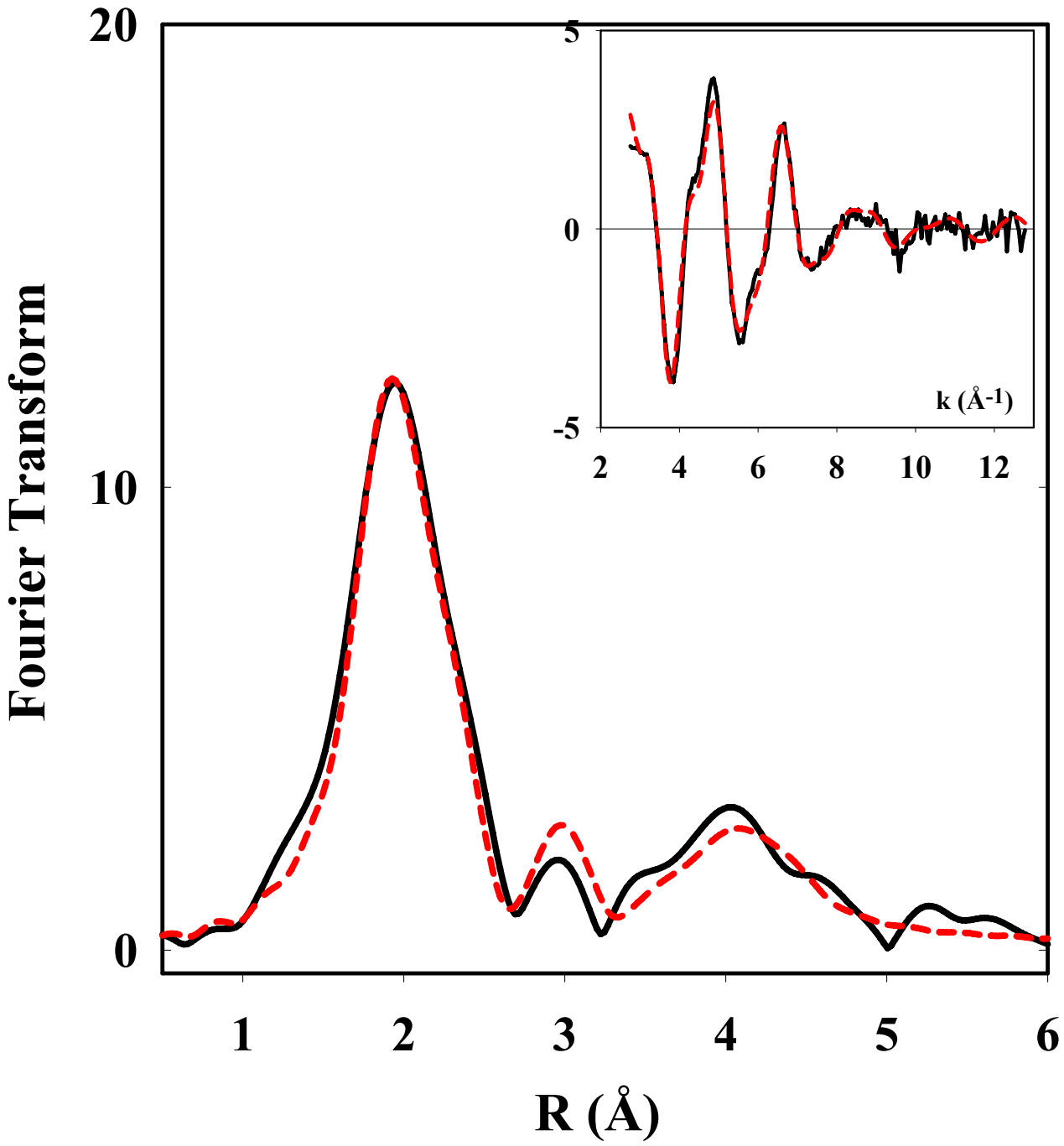

Fig. S2. Experimental versus simulated Fourier transform and EXAFS (inset) for reduced TBM at pH 7 using one shell of two equivalent histidines and no S ligation, with the parameters as listed in fit C of Table S1.