Supplementary Material to :

Interaction of Product Analogs with the Active Site of *Rhodobacter sphaeroides* Dimethylsulfoxide Reductase.

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Table S1. Cartesian Coordinates for DFT energy minimized structure of trimethylarsine reduced DMSO reductase

Atom #	*Atom*	*x*	*y*	*z*
1	C	3.465	44.543	114.309
2	O	4.162	45.700	113.916
3	H	4.155	43.873	114.862
4	H	3.060	43.992	113.441
5	H	2.614	44.790	114.973
6	Mo	3.440	47.227	112.879
7	C	-1.007	47.089	114.754
8	O	-2.202	46.586	114.130
9	C	0.233	46.938	113.912
10	S	1.656	47.890	114.359
11	C	0.262	46.136	112.817
12	S	1.714	46.034	111.810
13	C	-0.970	45.375	112.392
14	C	-1.971	45.300	113.545
15	C	6.303	49.006	109.470
16	O	6.506	50.372	109.057
17	C	5.238	48.831	110.521
18	S	4.589	47.213	110.763
19	C	4.729	49.886	111.210
20	S	3.439	49.654	112.388
21	C	5.225	51.286	110.934
22	C	6.562	51.241	110.192
23	H	7.269	48.590	109.832
24	H	6.034	48.459	108.552
25	H	5.351	51.843	111.879
26	H	4.484	51.845	110.332
27	H	6.838	52.231	109.798
28	H	7.362	50.905	110.885
29	O	5.506	47.994	113.980
30	As	5.299	48.453	115.588
31	C	4.535	47.109	116.800
32	C	4.249	50.080	115.926
33	H	5.107	46.181	116.686
34	H	3.498	46.944	116.487
35	H	4.585	47.483	117.832
36	H	4.680	50.900	115.342
37	H	4.281	50.301	117.003
38	H	3.220	49.901	115.595
39	C	7.067	48.862	116.367
40	H	7.697	47.967	116.283
41	H	6.964	49.159	117.420
42	H	7.518	49.677	115.787
43	H	-0.868	46.579	115.732
44	H	-1.207	48.151	114.963
45	H	-0.701	44.353	112.071
46	H	-1.438	45.867	111.520
47	H	-2.956	44.947	113.201
48	H	-1.602	44.595	114.319

Figure S1: EXAFS data (A) and EXAFS Fourier transforms (Mo—S phase-corrected) (B) for dimethylsulfide reduced DMSO reductase. Experimental data are shown using solid lines and best fits using broken lines. Parameters obtained in the curve-fitting analysis are summarized in Table 1.

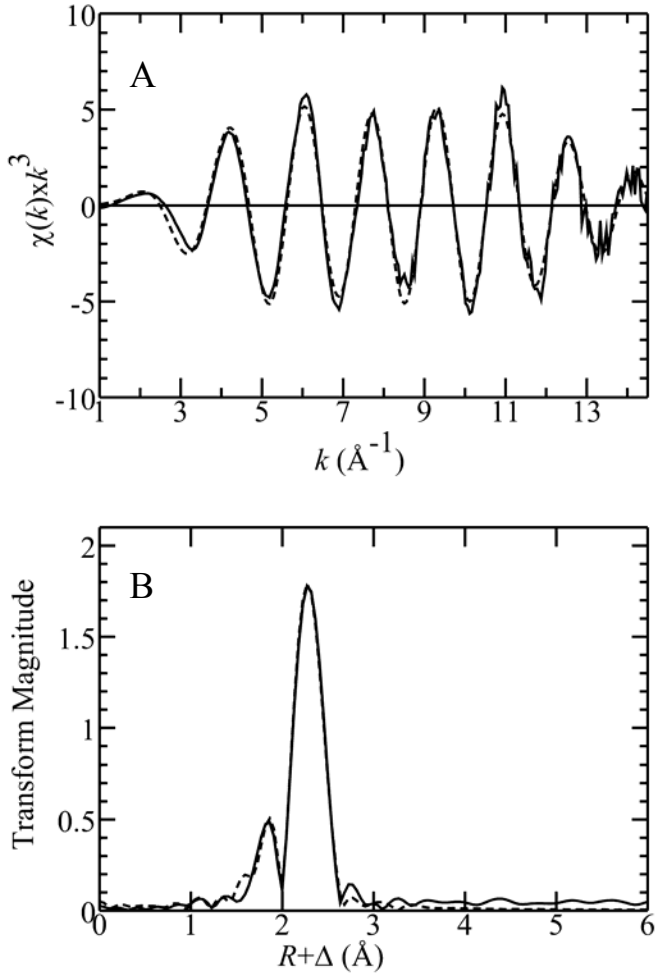
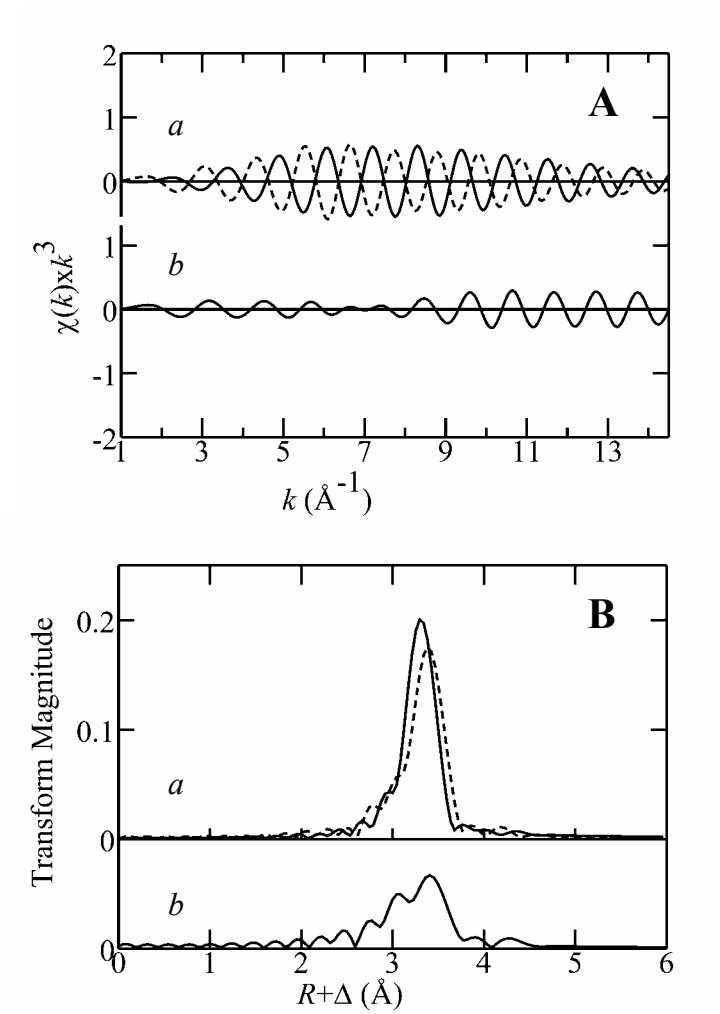
Figure S2: Simulation of possible EXAFS near-cancellation of Mo···S(DMSO) and Mo···C(dithiolene) using distances of 3.35 and 3.42 Å, respectively. As with any canceling EXAFS a very large number of solutions that will produce similar near-cancellation are possible. **A** presents the EXAFS oscillations with *a* showing the individual components from Mo···S(DMSO) (solid line) and Mo···C(dithiolene) (broken line), and *b* showing the sum of these. **B** shows the corresponding EXAFS Fourier transforms of the traces shown in A (note that the ordinates of *a* and *b* are on the same scale).