Supporting Information For: Insight Into The Structure and Mechanism of Nickel Containing Superoxide Dismutase Derived From Peptide Based Mimics

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Table S1. Properties of selected Ni(II) containing NiSOD peptides.

Table S2. Selected properties of selected Ni(III) containing NiSOD peptides.

Table S1. Properties of selected Ni(II) containing NiSOD peptides.

	Electronic Absorption λ_{max} (cm^{-1}) (ε (M^{-1} cm^{-1}))[a]	CD λ (cm^{-1}) ($\Delta\varepsilon$ (M^{-1} cm^{-1}))	Ni–S/Ni–N (Å)[b]	$E_{1/2}$ (mV vs. NHE)	k_{cat} (M^{-1} s^{-1})	ref. from the manuscript
Ni^{II}SOD (S. coelicolor)	18,050 (200, sh) 22,075 (545) 28,030 (1,230, sh)	17,980 (3.1) 22,030 (-2.7) 29,155 (3.3)	2.18/1.89	289	7×10^8	16,20,26
{Ni^{II}(SOD^{m1})}	18,030 (140, sh) 21,910 (355) 29,150 (640, sh)	17,425 (2.03) 21,945 (-3.88) 28,345 (1.46) 31,690 (4.60)	2.18/1.90	710,[c] 639[d]	$4(3) \times 10^7$	28,31
{Ni^{II}(SOD^{m2})}	18,250 (130, sh) 21,900 (345) 27,625 (656, sh)	17,635 (1.7) 22,220 (-1.5) 28,735 (2.4)	2.18/1.89	790,[c] 719[d]	$1(1) \times 10^{7,e}$	30
{Ni^{II}(SOD^{m2}-H(1)A)}	18,415 (252, sh) 21,785 (427)	17,640 (0.4) 21,030 (-2.2) 24,860 (1.0)	2.17/1.90	866,[c] 869[d]	inactive	31
{Ni^{II}(SOD^{m1}-Ac)}	18,530 (480) 24,030 (1,530) 27,300 (2,320,sh)	14,130 (1.68) 18,040 (-3.94) 23,110 (0.55) 27,440 (2.21)	2.17/1.86	519[d]	inactive	30
{Ni^{II}(SOD^{m2}-amine)$_2$}	13,315 (340) 15,430 (275) 28,650 (805) 32,060 (2,795)	12,515 (-3.87) 16,026 (-2.40) 27,930 (8.83) 29,765 (7.34) 33,120 (-30.49)	2.24[f]	not determined	inactive	40
{Ni^{II}(SOD^{m1}-Me)}	18,050 (160, sh) 21,690 (360) 27,400 (940)	17,670 (1.60) 22,940 (-2.04) 30,300 (2.31)	pH 7.5 – 8.0: 2.18/1.91 pH 9.5: 2.20/1.89	481[d]	$6(1) \times 10^6$	31
{Ni^{II}(SOD^{m1}-DNP)}	18,110 (150, sh) 21,560 (410, sh) 38,127 (25,700)	18,797 (-2.32) 21,740 (6.00) 26,880 (70.7) 29,940 (63.4)	2.18/1.87	669[d]	$3(2) \times 10^8$	31
{Ni^{III}(SOD^{m1}-Tos)}	18,110 (180, sh) 21,730 (405, sh)	17,185 (1.90) 22,420 (-2.95) 30,490 (5.33)	2.18/1.89	797[d]	$6(2) \times 10^8$	31

a)sh: shoulder b) EXAFS derived bond-lengths, c) thin film (pH 7.2; 100 mM NaCl supporting electrolyte), d) aqueous solution (pH 7.4; 100 mM NaCl supporting electrolyte), e) this work, f) NiS_4 center

Table S2. Selected properties of selected Ni(III) containing NiSOD peptides.

	$f_{(Ni-S)}$ (mdyn Å^{-1}) amine/amide[a]	$f_{(Ni-imidazole)}$ (mdyn Å^{-1})[b]	EPR[c] g_x	g_y	g_z/A_{zz}(MHz)	ref. from the manuscript
Ni^{III}SOD (S. coelicolor)	1.79/1.68	not determined	2.30	2.24	2.01 (69.7)	10,15
{Ni^{III}(SOD^{m1})}	not determined	0.52	2.33	2.27	2.01 (81)	31
{Ni^{III}(SOD^{m1}-Me)}	1.54/1.31	0.74	2.36	2.29	2.02 (83)	31
{Ni^{III}(SOD^{m1}-DNP)}	1.69/1.47	0.11	2.33	2.22	2.00 (55)	31
{Ni^{III}(SOD^{m1}-Tos)}	1.70/1.51	< 0.1	2.33	2.24	2.00 (67)	31

a) trans to the amine nitrogen/trans to the amide nitrogen; b) calculated (B3LYP/TZVPP); c) X-band EPR (77 K; 1:1 H_2O:glycerol pH 7.4)