Replacing Mn^{2+} with Co^{2+} in Human Arginase I Enhances Cytotoxicity Towards L-Arginine Auxotrophic Cancer Cell Lines

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SUPPORTING INFORMATION

Figure S1. Purification of hArgI: MW = Molecular Weight, WC = whole cell lysate, SN = soluble fraction, FT = flow through, and El = elution.

Figure S2. Best fits to Co-hArgI EXAFS. Fit numbers correspond to Table 1.

Table S1. Best fits to Co-hArgI EXAFS^a.

Fit	Model	<i>M-N/O</i>	<i>M-C</i>	<i>M-His</i> ^b	<i>M-M</i>	R _f ^c	R _u
1-1	<i>Co₂-ArgI</i> 5 N/O	2.10 (11)				199	358
1-2	1 N + 4 O	[N] 2.16 (4.3) [O] 1.96 (8.4)				66	272
1-3	1 N + 4 O + 2C	[N] 2.15 (1.0) [O] 1.96 (9.8)	2.48 (9.3)			36	240
1-4	1 N (His) + 4 O + 2 C	[N] 2.15 (1.4) [O] 1.96 (10)	2.47 (5.2)	2.95 (1.0) 3.28 (10) 4.07 (9.0) 4.32 (5.1)		119	171
1-5	1 N (His) + 4 O + 2 C + Co-Co	[N] 2.15 (1.8) [O] 1.96 (0.4)	2.47 (5.2)	2.95 (1.3) 3.31 (14) 4.06 (13) 4.32 (4.8)	3.52 (15)	66	126

^a Distances (Å) and disorder parameters (in parentheses, σ^2 (10^{-3} Å²)) shown derive from integer or half-integer coordination number fits to filtered EXAFS data [$k = 1.5$ - 12 Å⁻¹; $R = 0.7 - 2.3$ Å (fits 1-1 to 1-3 and 2-1 to 2-3) or $0.3 - 4.0$ Å (fits 1-4, 1-5, 2-4 and 2-5)].

^b Multiple scattering paths represent combined paths, as described previously (see Materials and Methods).

^c Goodness of fit (R_f for fits to filtered data) defined as $1000 * \frac{\sum_{i=1}^N \{ \text{Re}(\chi_{i_{calc}}) \} + \{ \text{Im}(\chi_{i_{calc}}) \} }{\sum_{i=1}^N \{ \text{Re}(\chi_{i_{obs}}) \} + \{ \text{Im}(\chi_{i_{obs}}) \} } }$, where N is the number of data points.