

Inhibition of the Fe₄S₄ Cluster-containing Protein IspH (LytB): EPR, Metallacycles and Mechanisms

Ke Wang^a, Weixue Wang^b, Joo-Hwan No^b, Yonghui Zhang^a, Yong Zhang^c,

and Eric Oldfield^{a,b,*}

Supporting Information

^aDepartment of Chemistry, 600 South Mathews Avenue, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA.; ^bCenter for Biophysics and Computational Biology, 607 South Mathews Avenue, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA; ^cDepartment of Chemistry and Biochemistry, University of Southern Mississippi, 118 College Drive #5043, Hattiesburg, MS 39406, USA.

Corresponding Author:

* To whom correspondence may be addressed. E-mail: eo@chad.scs.uiuc.edu, Tel 217-333-3374,

Fax 217-244-0997

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Table S1. g-values reported for Fe₄S₄ proteins and those observed in this study.

	g ₁	g ₂	g ₃
<i>E. coli</i> LytB Fe ₄ S ₄ ¹	2.038	1.927	1.889
<i>E. coli</i> GcpE Fe ₄ S ₄ ²	2.04	1.90	-
Bovine heart aconitase (active form, Fe ₄ S ₄) ³	2.06	1.93	1.86
Bovine heart aconitase (inactive form, Fe ₃ S ₄) ³	-	2.016	-
<i>E. coli</i> GcpE Fe ₃ S ₄ ⁴	2.032	2.003	-
Unliganded <i>A. aeolicus</i> LytB (Fig. 1a; only g values in the g=2 region are listed)	2.04	1.94; 1.92	1.87
Unliganded <i>E. coli</i> LytB (Fig. 1b). g value obtained by simulation.	2.043	1.915	1.901
<i>A. aeolicus</i> LytB with KCN (Fig. 1a)	2.08; 2.05	1.94; 1.93	-
<i>A. aeolicus</i> LytB with 12 (Fig. 1a). g value obtained by simulation.	2.087	2.012	1.992
<i>P. furiosus</i> ferredoxin ⁵	2.12	1.86	1.79
<i>P. furiosus</i> ferredoxin with KCN ⁵	2.09	1.95	1.92

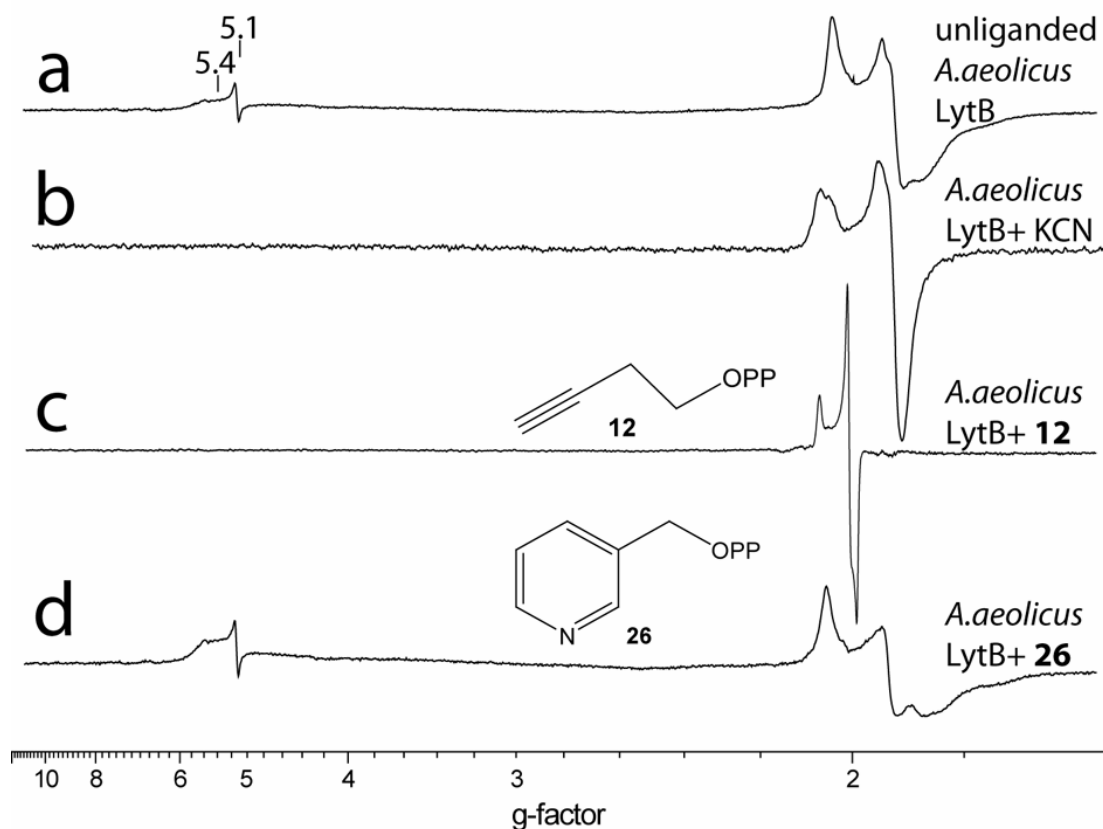


Figure S1. Wide scan X-band GHz EPR spectra of IspH at 15K, reduced with $\text{Na}_2\text{S}_2\text{O}_4$. a) *A. aeolicus* IspH, no added ligands, microwave power = 1 mW. b) *A. aeolicus* IspH + KCN, 10 equivalents, microwave power = 1 mW; c) *A. aeolicus* IspH + **12**, 20 equivalents, microwave power = 0.05 mW; d) *A. aeolicus* IspH + **26**, 20 equivalents, microwave power = 1 mW.

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