**Supporting Information**

*meso*-Bromination Greatly Enhances Reactivity   
of Cyanocobalamin towards Hydrogen Sulfide

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**Figure S1.** UV-vis spectra collected for the mixture of CNCbl-Br (3.1·10-5 M) with TCEP (5.0·10-3 M) at pH 7.4, 25.0 °C. Spectra were collected for 1-10 min, time interval between spectra is 60 s

 

**Figure S2.** UV-vis spectra collected for the mixture of CNCbl (3.1·10-5 M) with H2S (5.0·10-3 M) in the absence (1) and presence (2) of TCEP (1.0·10-3 M) at pH 7.4, 25.0 °C. Spectra were recorded for 100 min, time interval between spectra is 60 s



**Figure S3.** UV-vis spectra of (1) CNCbl-Br; (2) the mixture of CNCbl-Br with H2S and TCEP incubated for 1 h; (3) the mixture of Br-CNCbl with H2S and TCEP incubated for 24 h; (4) the mixture of Br-CNCbl with H2S and TCEP incubated for 24 h and further mixed with aerobic CN- solution; (5) the mixture of CNCbl-Br with GSH incubated for 24 h. Conditions: [CNCbl-Br] = 3.1·10-5 M, [H2S] = 5.0·10-3 M, [TCEP] = 1.0·10-3 M, [GSH] = 5.0·10-3 M, [CN-] = 1.0·10-3 M, pH 7.4, 25.0 °C



**Figure S4.** MALDI mass-spectra of (A) CNCbl-Br incubated in the presence of H2S for 24 h and further mixed with aerobic CN- solution, (B) CNCbl-Br and (C) CNCbl



**Figure S5.** (A) UV-vis spectra of the reaction between Br-CNCbl (3.1·10-5 M) and TCEP sulfide (1.0·10-3 M) at pH 7.4, 25 °C. Spectra were collected for 45 min, time interval between spectra is 60 s. (B) Kinetic curves of the reaction collected under different CNCbl-Br concentrations



**Figure S6.** UV-vis spectra collected for the mixture of CNCbl (3.1·10-5 M) with TCEP sulfide (1.0·10-3 M) at pH 7.4, 25 °C. Spectra were collected for 100 min, time interval between spectra is 60 s