Adsorption of methylmercury onto *Geobacter bemidijensis* Bem

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Introduction: The neurotoxic methylmercury (MeHg) is an important contaminant in aquatic environments. Microbes play important roles in the production and degradation of MeHg. Adsorption of MeHg onto bacterial cells is an important process that can affect the fate of MeHg by inhibiting its release to the aqueous phase and its degradation back to inorganic Hg. The anaerobic bacterium *Geobacter bemidijensis* Bem has the unique ability to both produce and degrade MeHg. To date, the binding of MeHg onto Hg-methylating and MeHg-degrading bacteria remains poorly understood. In this study, we quantified the adsorption of MeHg onto *G. bemidijensis* and applied X-ray absorption spectroscopy to examine the mechanism of MeHg binding.

Materials and Methods: MeHg adsorption experiments were conducted over a range of MeHg concentrations and adsorption isotherms were used to quantify MeHg binding constants. Titration experiments were conducted to determine the concentration of thiol functional groups on the bacterial surface. The local coordination environment of MeHg adsorbed onto *G. bemidijensis* was then examined using extended X-ray absorption fine structure (EXAFS) spectroscopy.

Results and Discussion: The results showed that MeHg adsorbed onto the *G. bemidijensis* cell surface rapidly and extensively. Complexation of MeHg with thiol functional groups was confirmed using Hg EXAFS, which was best modeled with 1 S and 1 C atom at 2.34 and 2.03 Å, respectively. Titration experiments yielded cell surface thiol concentrations of 3.2 to 6.4 μmol/g (wet cells). A one-site adsorption model with MeHg binding onto thiol sites provided excellent fit to adsorption isotherms conducted at different cell densities. The log K binding constant of MeHg onto the cellular thiol sites was determined to be 10.2 ± 0.2, which is comparable to MeHg binding to thiol ligands in humic acids. The results of this study elucidate the importance of cell surface thiol sites for MeHg adsorption and highlight the importance of bacterial cells as possible carriers of adsorbed MeHg in natural aquatic systems.