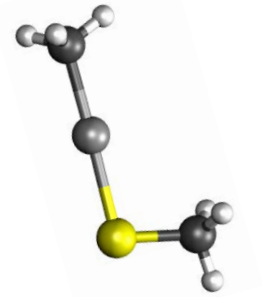
Permeation of Mercury Through a Bacterial Cytoplasmic Membrane

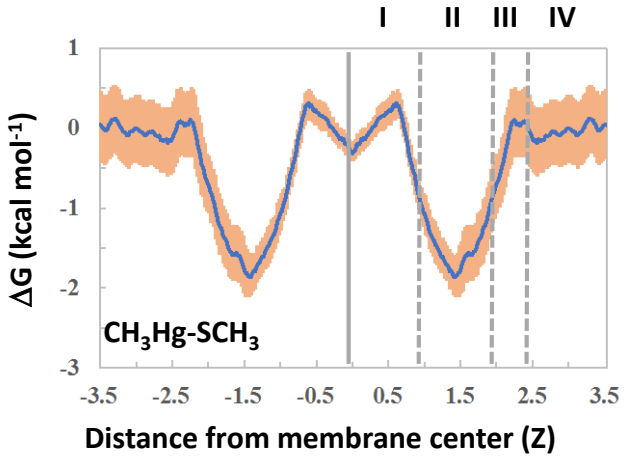
Challenge

- Cellular uptake and export from the aqueous environment are important steps in Hg biotransformation by microorganisms, but the mechanisms of transport across biomembranes remain unclear.

Approach and Results

- Performed extensive molecular dynamics simulations of passive permeation of Hg^{II} and methylmercury complexes with thiolates.
- Calculated permeability coefficients for the neutral compounds $CH_3S–Hg^{II}–SCH_3$ and $CH_3Hg–SCH_3$ are ~10^{-5} cm/s.
- **Small, neutral Hg compounds readily permeate cytoplasmic membranes.**





Significance and Impact

- Identifying how complexation of Hg^{II} and methylmercury alters permeation provides insight into how Hg is transported in and out of bacterial cells.

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Reference: Zhou J, Smith MD, Cooper SJ, Cheng X, Smith JC and Parks JM. **Modeling of the Passive Permeation of Mercury and Methylmercury Complexes Through a Bacterial Cytoplasmic Membrane**, *Environ. Sci. Technol.*, **2017**, In press.
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ABSTRACT:

Cellular uptake and export are important steps in the biotransformation of mercury (Hg) by microorganisms. However, the mechanisms of transport across biological membranes remain unclear. Membrane-bound transporters are known to be relevant, but passive permeation may also be involved. Inorganic Hg^{II} and methylmercury ($[CH_3Hg]+$) are commonly complexed with thiolate ligands. Here, we have performed extensive molecular dynamics simulations of the passive permeation of Hg^{II} and $[CH_3Hg]+$ complexes with thiolate ligands through a model bacterial cytoplasmic membrane. We find that the differences in free energy between the individual complexes in bulk water and at their most favorable position within the membrane are ~2 kcal mol^{-1}. We provide a detailed description of the molecular interactions that drive the membrane crossing process. Favorable interactions with carbonyl and tail groups of phospholipids stabilize Hg-containing solutes in the tail-head interface region of the membrane. The calculated permeability coefficients for the neutral compounds $CH_3S–Hg^{II}–SCH_3$ and $CH_3Hg–SCH_3$ are on the order of 10^{-5} cm s^{-1}. We conclude that small, non-ionized Hg-containing species can permeate readily through cytoplasmic membranes.