

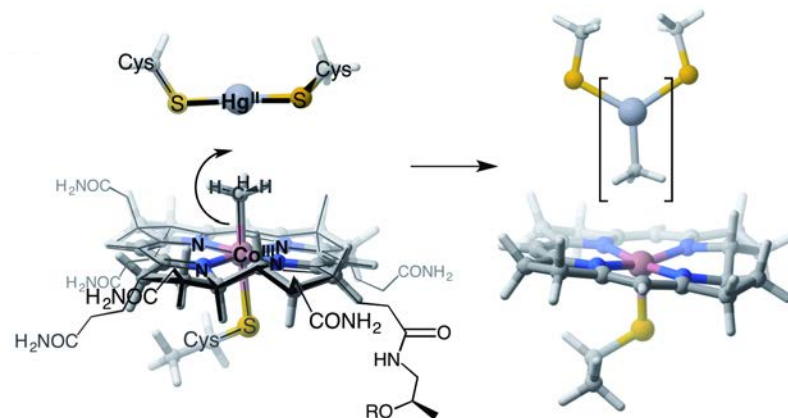
Modeling Mercury in Proteins

Challenge

- Understanding the toxic effects of mercury and its cycling in the environment requires detailed characterization of its interaction with proteins.

Approach and Results

- Computational approaches are ideally suited to studies of mercury in proteins because they provide detailed, molecular-scale insight and circumvent issues associated with toxicity.
- We highlight our combined computational and experimental studies performed over the past eight years of proteins and enzymes involved in Hg methylation (HgcAB), demethylation and reduction (*mer* operon).



Proposed methyl transfer catalyzed by HgcA.

Significance and Impact

- We place our work on mercury in proteins in the context of what is required for comprehensive multi-scale modeling of environmental mercury cycling.

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