Modeling Interactions between Trypanothione and Antimony-Oxide Clusters

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Abstract

Interactions of antimony-oxide clusters with trypanothione have been modelled to understand their inhibitory activity against leishmaniasis. Trypanothione is essential for the survival of leishmania parasites because it is responsible for maintaining their cellular thiol-disulfide redox regulation. Density functional theory (DFT) calculations show that the SbV oxide clusters form hydrogen bonds from the oxygens to the amine and carboxyl group of the trypanothione. The reaction between trypanothione and the SbV oxide cluster does not break the S-S bond of trypanothione, whereas the reaction with antimony-oxide clusters containing at least one SbIII atom leads to dissociation of the S-S bond of both the oxidized and the reduced form of trypanothione suggesting that antimony-oxide clusters with at least one SbIII atom may destroy trypanothione that is vital for the parasite metabolism.

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