NMR structure and dynamics of a triheme cytochrome from *Geobacter sulfurreducens*

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Geobacter sulfurreducens (*Gs*) bacterium is of interest because of its capabilities of electron transfer and bioremediation of contaminated environments. It can reduce toxic/radioactive metals via unique respiratory chains that assure the transference of cytoplasmic electrons to outside of the cell. These electron transport systems rely on the unusual abundance of multiheme cytochromes synthesized by *Gs* [1]. Among these, the PpcA triheme periplasmic cytochrome was identified as a crucial protein participating in the reduction pathways of Fe(III) and U(VI) [2].

PpcA crystal structure is available [3]. However, NMR studies showed unexpected NOE connectivities between some of the PpcA heme substituents and raised some questions about the significance of this structure in solution [4]. Indeed, and contrary to its homolog PpcB also present in the *Gs* periplasm, the crystallization process of PpcA required the use of deoxycholic acid, which was found to be bound between hemes I and III. To investigate the solution structure of PpcA, ^{15}N labeled PpcA was produced [5]. Standard 3D and 2D NMR experiments were acquired at 800MHz and the solution structure of PpcA was determined. ^{15}N NMR relaxation measurements were used to characterize the internal dynamics of PpcA.

The structure reported here for PpcA is the first solution structure of a multiheme protein isolated from *Gs* and the results obtained showed that the solution structure of PpcA is similar to the X-ray structure of PpcB crystallized without deoxycholic acid, in contrast with the crystal structure of PpcA. This is an excellent example of how NMR can be used to evaluate the physiologic impact of specific conformations due to the presence of exogenous molecules used in the crystallization process.

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