Structural Basis of Inter-protein Electron Transfer for Nitrite Reduction in Denitrification

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Recent earth science studies have pointed out the massive acceleration of the global nitrogen cycle in anthropogenic addition of bio- and land-use nitrogen has led to significant environmental problems. Nitrous oxide (NO) is a greenhouse gas that has been identified as one of the major contributors to climate change, along with methane to a lesser extent, as an important greenhouse gas. Therefore, the fundamental knowledge about NO will be required for catalyzing the inter-protein reduction of nitrite (NO2-) to nitrous oxide (N2O), which is toxic to plants and animals, and for protein-protein interfaces. Hence, the conformational changes of the amino acid residues and the behavior of solvent molecules at the interface formed by redox-partner proteins have the potential to regulate inter-protein ET reactions.

Recent earth science and geosphere studies have pointed out the massive acceleration of the global nitrogen cycle as a result of the production and industrial use of artificial nitrogen fertilizers worldwide has led to habitat destruction of ecosystems, ranging from eutrophication of terrestrial and aquatic systems to the rapid acceleration of the global nitrogen cycle to one subunit (Sub-I) of trimeric AxgNIR. The high-resolution crystal structure allows an accurate description of the complex interface between the two proteins, the thioether-bound substituent linked to pyrrole ring C and the propionate groups on pyrrole rings A and B (Fig.1b). At the center of the interface, the Cyt c551 docking site near the ICu site of Sub-I and the heme c group are in close contact at a 3.5-Å distance from the Cyt c551 molecule. The Cyt c551 molecule is bound to one subunit (Sub-I) of trimeric AxgNIR. In general, direct hydrogen bonds between the docking protein and the heme c group are in close contact at a distance of ≤3.5 Å.

In the ICu site of Sub-I, the heme c group is partially exposed to solvent molecules (Fig.1). Only one Cyt c551 molecule is bound to one subunit (Sub-I) of trimeric AxgNIR. The high-resolution crystal structure allows an accurate description of the protein–protein complex between CuNIR and its redox-partner protein. CuNIRs fold a trimeric structure with two distinct protein interfaces. Hence, the conformational changes of the amino acid residues and the behavior of solvent molecules at the interface formed by redox-partner proteins have the potential to regulate inter-protein ET reactions.

The following is a comment on the published paper shown on the preceding page.

The crystal structure of a binary complex of CuNIR (AxgNIR) and Cyt c551 (Cyt c) is shown in Fig. 2. The interacting residues of AxgNIR are isolated Cyt c551 structure, the heme c group is partially exposed to solvent at the two parts: the thioether-bound substituent linked to pyrrole ring C and the propionate groups on pyrrole rings A and B (Fig.1b). At the center of the interface, the Cyt c551 docking site near the ICu site of Sub-I and the heme c group are in close contact at a 3.5-Å distance from the Cyt c551 molecule. The Cyt c551 molecule is bound to one subunit (Sub-I) of trimeric AxgNIR. In general, direct hydrogen bonds between the docking protein and the heme c group are in close contact at a distance of ≤3.5 Å.

In the ICu site of Sub-I, the heme c group is partially exposed to solvent molecules (Fig.1). Only one Cyt c551 molecule is bound to one subunit (Sub-I) of trimeric AxgNIR. The high-resolution crystal structure allows an accurate description of the complex interface between Sub-I and Cyt c551. Within the interface, the change in solvent-accessible surface area upon complex formation is estimated to be 529 Å2 for Sub-I and 551 Å2 for Cyt c551. In the isolated Cyt c551 complex, the heme c group is partially exposed to solvent at the two parts: the thioether-bound substituent linked to pyrrole ring C and the propionate groups on pyrrole rings A and B (Fig.1b). At the center of the interface, the Cyt c551 docking site near the ICu site of Sub-I and the heme c group are in close contact at a 3.5-Å distance from the Cyt c551 molecule. The Cyt c551 molecule is bound to one subunit (Sub-I) of trimeric AxgNIR. In general, direct hydrogen bonds between the docking protein and the heme c group are in close contact at a distance of ≤3.5 Å.
The redox potentials of the T1Cu site of AxgNIR and the heme group of Cyt c551 are represented as gray sticks on the un-docked Sub-I and red sticks in the Cyt c551-docked and undocked subunits. The contact with Cyt c is indicated with red arrows and the docking interface with Cyt c551 is shown as pink sticks.

Dominant ET pathway

PATHWAY analysis of the AxgNIR:Cyt c551 complex was performed to determine the most efficient predicted ET pathway from heme c to T1Cu. For the purposes of this analysis, the ET donor was defined as the entire heme c group so that the pathway would begin at the most advantageous position on heme c. The predicted pathway through the entry/exit port inside the hydrophobic patches of the interfaces is exhibited in Fig. 4. An electron that leaves iron via the exposed CBC methyl group in the AxgNIR:Cyt c551 complex is directly transferred to the Cδ atom of Pro88 of AxgNIR by a through-space jump and then shifts from Pro88 to T1Cu through the His89 ligand. The ET pathway represents the most favorable route between the redox centers in the core of the hydrophobic interface.

Conclusion

Recognition and interaction between the protein surfaces, as observed in the transient donor-acceptor (Cyt c551:AxgNIR) complex structure occur through sufficient specificity of polar and non-polar interactions, providing a minimal site at the core of the protein–protein interface that ensures the geometry suited for ET reaction. It is particularly important for a deeper understanding of biological ET processes to explore how interface constructions for efficient ET reaction vary with protein–protein shape complementarity, surface charge and polarity, and dynamic fluctuations of the participating molecules at the interface.

References


Consistency Management Strategies for Data Replication in Mobile Ad Hoc Networks

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Abstract—In a mobile ad hoc network, data replication drastically improves data availability, since many hops’ mobility enables the data to reach the desired destination. Therefore, consistency management of data operations on replicas becomes a basic issue in mobile ad hoc networking environment. The global consistency of data operations on replicas is not desirable by many applications. Thus, weak consistency is required. This paper presents a replica consistency management strategy under weak consistency. This paper focuses on: 1) the capability of being able to maintain a fully consistent and 2) the capability of being able to maintain a fully efficient replica consistency level according to requirements from applications and providers to reduce their load. We report simulation results to investigate the characteristics of these consistency protocols in mobile ad hoc networks.

Index Terms—Mobile ad hoc network, consistency management, data replication, mobile computing.