

Respiratory chains are composed of several membrane protein complexes, which can interact directly or via soluble and mobile redox proteins, working as electron shuttles. Central to aerobic respiratory chains is cytochrome *bc*<sub>1</sub> complex, which has quinol:cytochrome *c* oxidoreductase activity. In the Gram-negative bacteria *Rhodothermus marinus*, this activity is performed by the Alternative Complex III (ACIII) which belongs to a recently identified family of enzymes that performs an equivalent function to the *bc*<sub>1</sub> complex but is structurally distinct [1–3]. The gene cluster coding for ACIII is frequently followed by the gene cluster coding for oxygen reductases. In *R. marinus* membranes, it was observed that the ACIII and the *caa*<sub>3</sub> oxygen reductase are indeed structurally and functionally associated [4].

In this study, we investigated the direct interaction between the ACIII and the *caa*<sub>3</sub> oxygen reductase and the interactions between the complexes and potential electron shuttles. For that we used the monoheme cytochrome *c* subunit of ACIII, the cytochrome *c* domain of *caa*<sub>3</sub> oxygen reductase, the high-potential iron-sulfur protein (HiPIP) and the periplasmatic monoheme cytochrome *c*. These protein-protein interactions were investigated by <sup>1</sup>H-NMR spectroscopy using the chemical shift perturbation methodology.

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## S8.P9

### Reconstruction of the primordial “Sodium World”

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The concept of the “Sodium World” was initially suggested to encompass modern organisms with sodium-dependent membrane bioenergetics [1]. Later, however, the phylogenomic analysis of rotary membrane ATP synthases has provided evidence for the evolutionary primacy of sodium bioenergetics [2]. This view was supported by identification of a new family of Na-translocating rotary ATPases (N-ATPases) [3] and by phylogenetic analysis of membrane pyrophosphatases [4]. If the bioenergetic realm of the anoxic Earth was a Sodium World indeed, one would expect a plethora of sodium translocating enzymes with diverse functions. We performed phylogenomic analyses aiming on evolutionary reconstruction of the constituents of the primordial Sodium World.

Analyses of several membrane transporter families, which contain both proton-dependent and sodium-dependent members, have shown that the ancestral forms of the transporters analyzed could be reconstructed as sodium translocating enzymes. These enzymes may have been initially involved in generation of sodium-motive force by removing, out of the cells, acidic waste products of fermentation together with sodium ions, as cells of modern *Selenomonas ruminantium* still do [5]. In the view of the recent identification of sodium-translocating rhodopsins in several bacteria [6], we performed a phylogenomic analysis of rhodopsins from sequenced prokaryotic genomes. The results obtained are compatible with the emergence of rhodopsins within bacteria followed by a “horizontal” transfer of their genes to some archaea. A prerequisite of this transfer could be the emergence of the archaea-specific system of fatty synthesis, as argued elsewhere [7].

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## S8.P10

### The molecular selectivity of type II NADH:quinone oxidoreductase for quinones – A docking study

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Type II NADH:quinone oxidoreductase is a flavoprotein that catalyzes the transfer of electrons from NADH to quinones and it can, in several organisms, replace the respiratory system (complex I–V).

Recent high resolution structures show that NDH-II is a homodimer membrane bound protein with an amphiphilic anchor that allows the interaction with the membrane.

Different microorganisms produce different quinones: e.g. in *Escherichia coli* the physiological quinone is ubiquinone, while *Staphylococcus aureus* and *Bacillus subtilis* synthesis menaquinone, thus NDH-II will have a different molecular interaction and selection mechanism for different organisms.

Despite the high resolution structural information available for NDH-II in complex with quinone, NAD and FAD, the mechanism behind the molecular selection and interaction with is still elusive.

To unravel the interaction mechanism of NDH-II:quinone we setup a modeling and in silico docking calculation based on the published high resolution structures of NDH-II. We identified the interaction hotspots of NDH-II from different species to different quinones and discuss the role in the enzymatic mechanism.

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