A Dielectric Theory View of Biomolecular Charge Transfer

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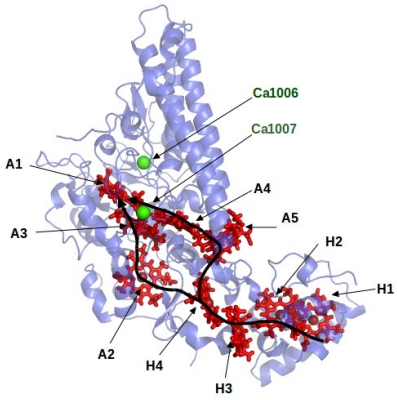

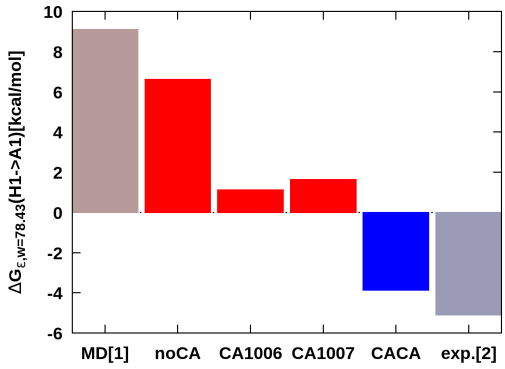

We show a calculation of thermodynamic driving forces, ΔG, for the electron transfer through subcomplex NrfHA of the cytochrome *c* nitrite reductase complex $NrfH_2A_4$ from *desulfovibrio vulgaris*. Molecular dynamics can be used to adjust dielectric constants for a numerical solution of Poisson's equation. Using the DelPhi program package [3] we show how the reorganization energy λ can be rationalized. As the binding pocket of Ca^{2+} ions in the protein structure of NrfA is conserved in many organisms [4], we investigate the influence of the presence of Ca^{2+} ions to the thermodynamic free energy landscape and show that the presence of two Ca^{2+} ions decrease the total free energy for the electron transfer over the entire electron transport chain towards an exergonic reaction.[5]

[1] Na, S. et al., *Phys. Chem. Chem. Phys.*, **2017,** *19*, 18938-18947.

[2] Todorovic, S. et al., *J. Phys. Chem. B*, **2012**, *116*, 5637-5643.

[3] Li, L. et al., *BMC Biophysics*, **2012**, *5*, 9, 1-11.

[4] Lockwood, C. W. J. et al., *Biochem. Soc. Trans.*, **2011**, *39*, 1871-1875.

[5] Gnandt, D. et al., *Biophys. Chem.*, **2018**, *241*, 1-7.