

Conformations of the ubiquinones in the doubly-occupied Q_o/Q_p-pocket of the cytochrome *bc₁* complex provided by solid state NMR measurements

Stefan Bartoschek¹, Sorin Luca¹, Stefan Dröse², Ulrich Brandt², C. Roy D. Lancaster³, Marc Baldus¹ and Christian Griesinger¹

1) Max-Planck-Institut für biophysikalische Chemie, Am Faßberg 11, D-37077 Göttingen/Germany.

2) Universitätsklinikum Frankfurt, Institut für Biochemie I, D-60590 Frankfurt am Main, Germany.

3) Max-Planck-Institut für Biophysik, Abteilung für Molekulare Membranbiologie, Heinrich-Hoffmann-Str. 7, D-60528 Frankfurt am Main, Germany.

The reaction most critical for energy conservation in the cytochrome *bc₁* complex is an obligatory bifurcation of the electron path linked to the two electron oxidation of ubiquinol to ubiquinone. This unique reaction occurs in the Q_o (or Q_p) pocket of the cytochrome *bc₁* complex [1].

We have recently shown by High Resolution Magic Angle Spinning NMR spectroscopy that there are two ubiquinones bound in the Q_o site [2]. Additional solid-state NMR measurements presented here provide direct experimental evidence for the existence of two ubiquinones in the Q_o pocket. The resulting distance restraints define the conformations of the two ubiquinones relative to each other. The obtained structures were used for modeling of the PDB entry 2BCC [3] of the chicken enzyme as starting structure. Therefore, at the Q_o pocket, the inhibitor stigmatellin was replaced by the obtained structure of the pair of ubiquinones and the system was subject to energy minimization and molecular dynamics simulations. Preliminary results of these calculations will be shown.

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[2] Bartoschek, S., Johanson, M., Geierstanger, B. H., Okun, J. G., Lancaster, C. R. D., Humpfer, E., Yu, L., Yu, C.-A., Griesinger, C. and Brandt, U. (2001) *Journal of Biological Chemistry* 276(38), 35231-35234.

[3] Crofts, A. R., Hong, S. J., Ugulava, N., Barquera, B., Gennis, R., Guergova-Kuras, M. and Berry, E. A. (1999) *Proc. Natl. Acad. Sci. USA* 96, 10021-10026.

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