Supplemental Information:

ATP binding and ATP hydrolysis in full-length MsbA monitored via time-resolved Fourier transform infrared spectroscopy

Daniel Mann[1,2], Kristin Labudda[1,4], Sophie Zimmermann[1], Kai Vocke[1], Raphael Gasper[1,3], Carsten Kötting[1,4] * and Eckhard Hofmann[1] *

[1] Department of Biophysics, Ruhr University Bochum, 44780 Bochum, Germany

[2] Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (ER-C-3): Structural Biology, 52425 Jülich, Germany

[3] Max-Planck-Institute of Molecular Physiology, 44227 Dortmund, Germany

[4] Biospectroscopy, Center for Protein Diagnostics (PRODI), Ruhr University Bochum, 44780 Bochum, Germany

* shared corresponding authors

Running title: FTIR of full-length MsbA

To whom correspondence should be addressed:

Prof. Dr. Eckhard Hofmann, Protein Crystallography, Department of Biophysics, Ruhr-University Bochum, Universitätsstraße 150, 44780 Bochum, Germany, Telephone (+49)234 32 24463, E-mail: eckhard.hofmann@ruhr-uni-bochum.de

Dr. Carsten Kötting, Department of Biophysics, Ruhr University Bochum, Universitätsstraße 150, 44780 Bochum, Germany, Telephone (+49)234 32 18069, E-mail: carsten.koetting@ruhr-uni-bochum.de

Figure S1: Valence structures of the photocaged nucleotides that were utilized in this study. The photolabile NPE and pHP groups at the terminal phosphate of ATP, ADP and AppNHp were cleaved with a UV laser flash at 308 nm.

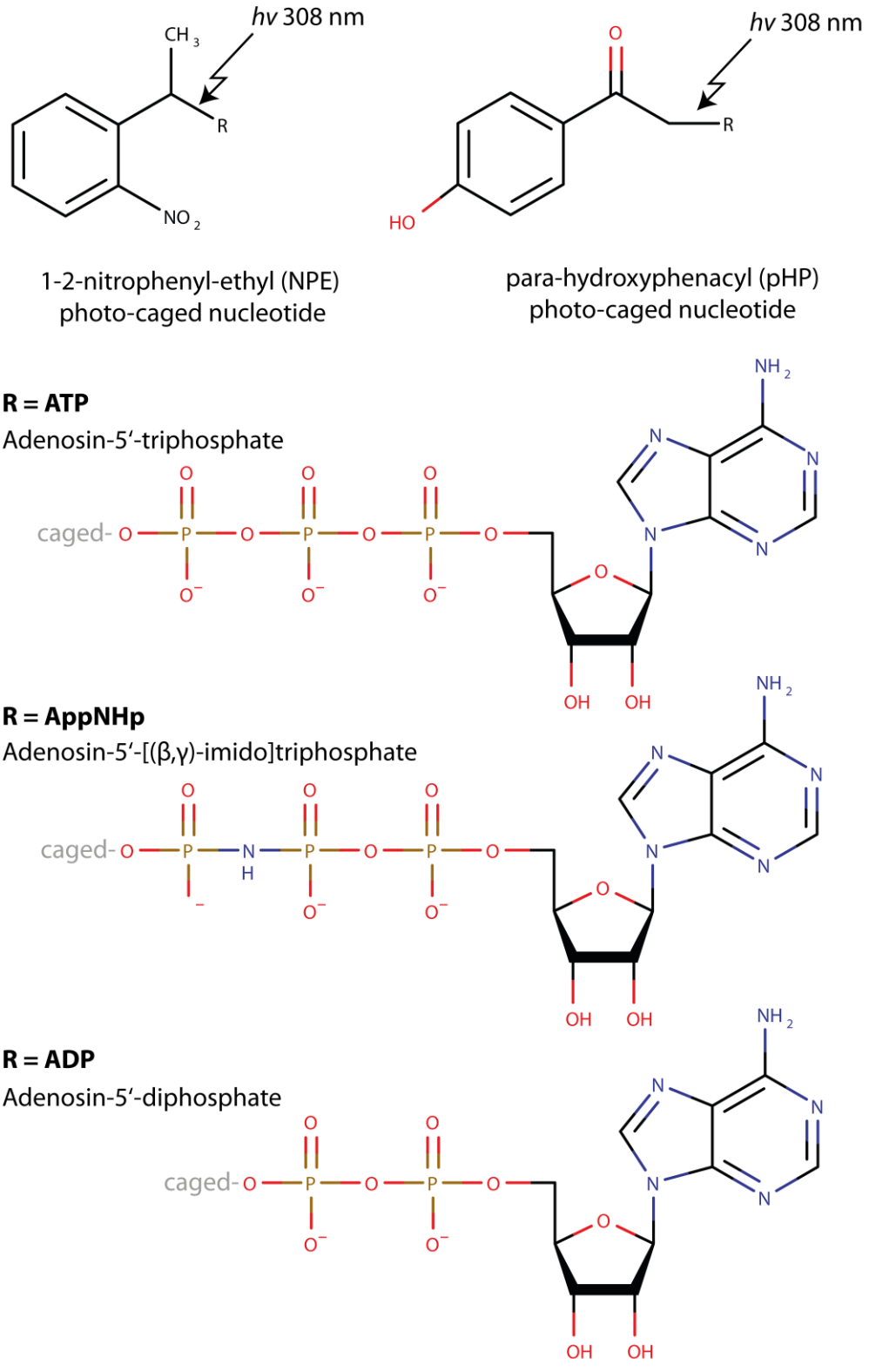

Figure S2: Asymmetric stretching vibrations of a/b/g-ATP and a/b-ADP and their corresponding atom displacement vectors. The depicted vibrations typically dominate the FTIR difference spectrum due to their high transition dipole moment.