Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Transient IR Spectroscopy Identifies Key Interactions and Unravels New Intermediates in the Photocycle of a Bacterial Phytochrome

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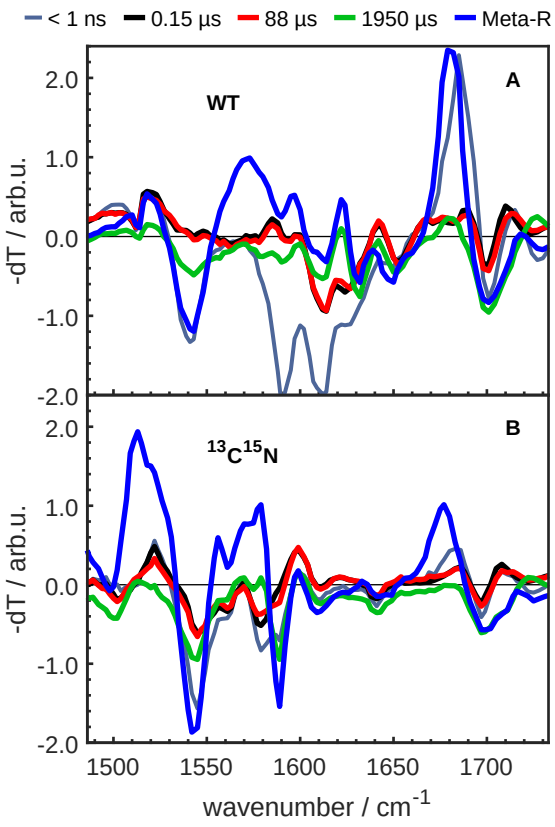

Fig. S 1 Species spectra obtained from a global fit of wild-type CBDPHY (A) and $^{13}C^{15}N$-labeled CBDPHY (B), in which all protein carbon and nitrogen atoms are isotope labeled, expect those of the chromophore.

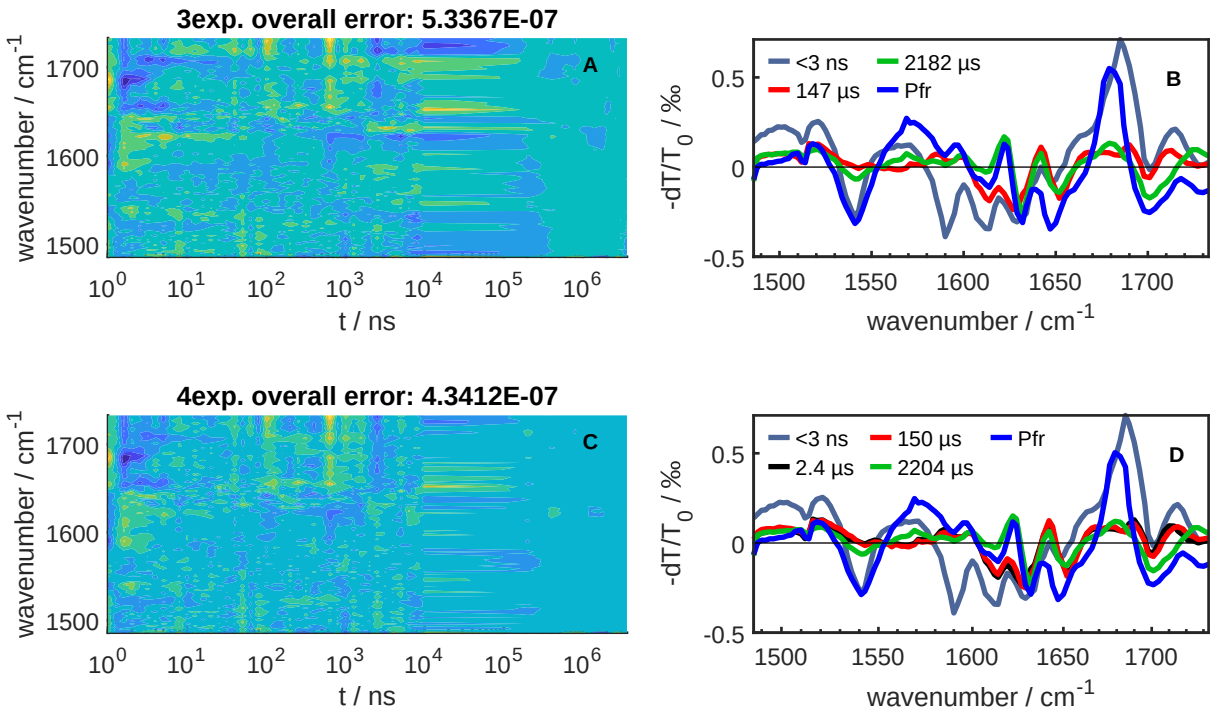

Fig. S 2 Comparison between 3- and 4-exponential fit for wild-type CBDPHY showing the presence of the second Lumi-R state. The contour plots show the residuals for a fit with 3 or 4 components. For the specific dataset shown here no timepoints were collected between 1E4 and 2E5 microseconds.

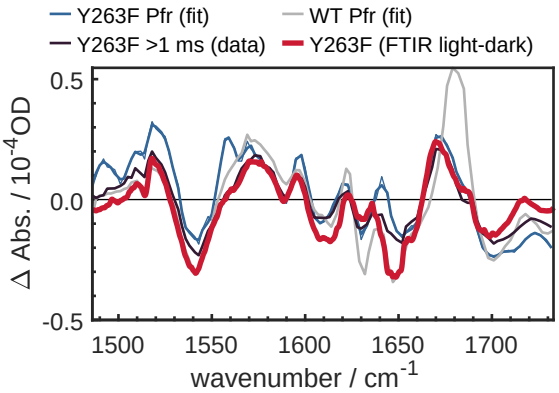

Fig. S 3 Pfr spectra determined from the global fit of nanosecond transient absorption data for wild-type CBDPHY and the Y263F mutant. The latter can be compared to the averaged spectra at delay times >1 ms, and the scaled FTIR difference spectrum. The discrepancy between the Pfr from the fit and the averaged spectra at long delays can be attributed to weak contributions from pre-0 signals. The transient transmission data has been converted to approximate transient absorption signals.