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

Supplement

Quenching of bacteriochlorophyll *a* triplet state by carotenoids in the chlorosome baseplate of green bacterium *Chloroflexus aurantiacus*

Andrei G. Yakovlev*[a] and Alexandra S. Taisova [a]

[a]Lomonosov Moscow State University, Belozersky Institute of Physico-Chemical Biology, Leninskie Gory, 119991, Moscow, Russian Federation, * e-mail: yakov@belozersky.msu.ru

The population dynamics of states can be approximately described by the following system of kinetic equations:

$$dN_1/dt = \sigma N'_{0B}J(t) - (K_{01} + K_1)N_1$$

$$dN_2/dt = K_1N_1 - K_2N_2 \qquad (1)$$

$$dN_3/dt = K_2N_2$$

$$dN_{0B}/dt = -\sigma N'_{0B}J(t) + K_{01}N_1 + K_2N_2$$

$$dN_{0C}/dt = -dN_3/dt$$

Here N_1, N_2 and N_3 are the population densities of the BChl a^*, BChl a^T and Car^T states, respectively; K_1 and K_2 are the rates of the BChl $a^* \rightarrow$ BChl a^T and BChl $a^T \rightarrow Car^T$ processes, respectively; K_{01} – rate of spontaneous decay of the BChl a^*; N_{0B} and N_{0C} are the population densities of the BChl *a* and Car ground states, respectively; N'_{0B} is the population density of BChl *a* in the absence of excitation; σ is the absorption cross section of BChl *a* at the excitation wavelength; $J(t) \sim sech^2(t/\tau)$ is the time course of the excitation energy density.

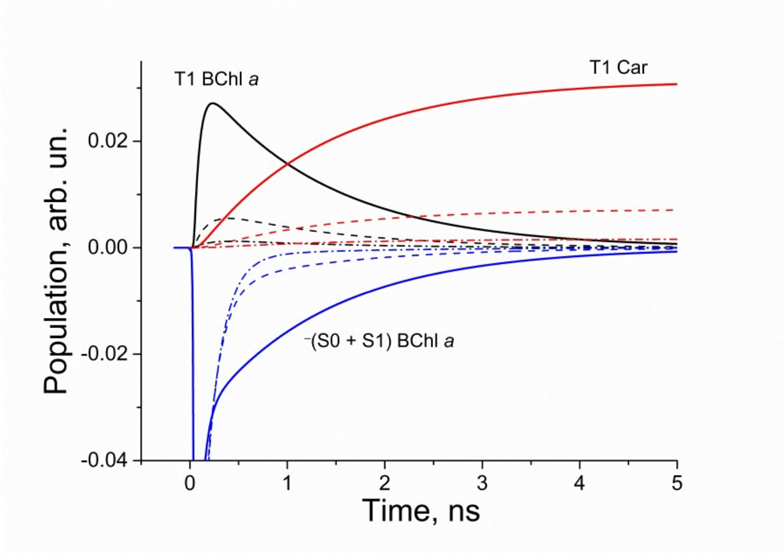

Fig. S1. Simulation of the populations of the states T_1 BChl *a* (black), T_1 Car (red) and the sum −(S_0 BChl *a* + S_1 BChl *a*) (blue) at K_1 = 0.1 (solid line), 1 (dash) and 5 ns (dash-dot). K_{01} = 0.17 ns, K_2 =1.3 ns, τ =0.01 ns.

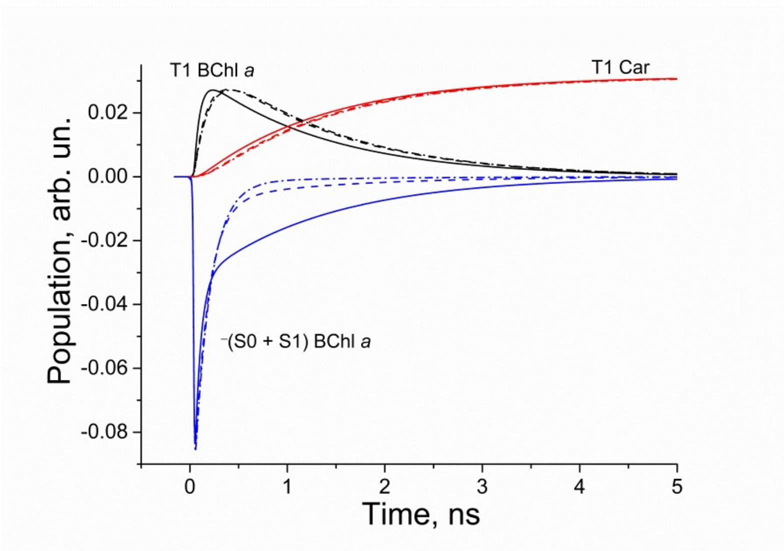

Fig. S2. Same as in Fig. S1, but with population normalization.

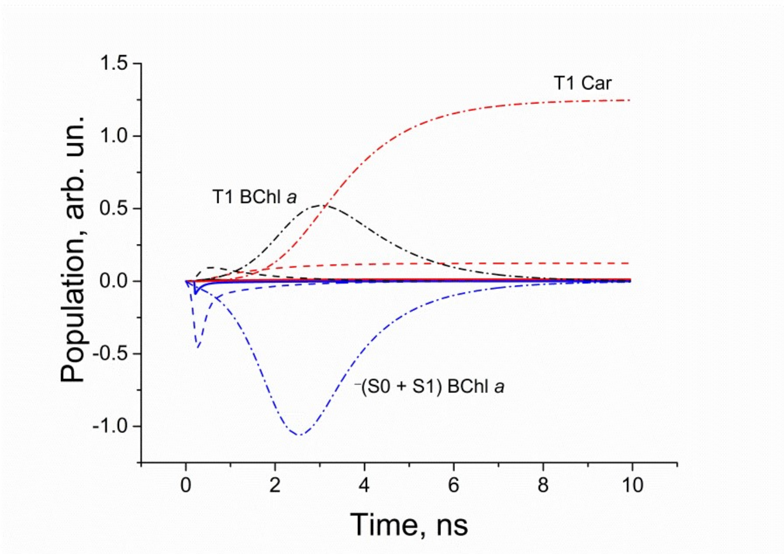

Fig. S3. Simulation of the populations of the states T_1 BChl *a* (black), T_1 Car (red) and the sum −（S_0 BChl *a* + S_1 BChl *a*）(blue) at $\tau = 0.01$ (solid line), 0.1 (dash) and 1 ns (dash-dot). K_{01} = 0.17 ns, K_2 =1.3 ns, K_1 =0.5 ns.

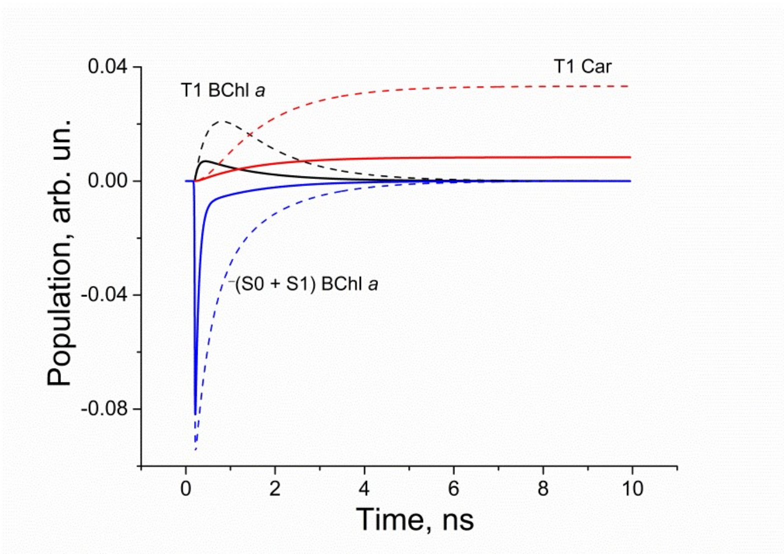

Fig. S4. Simulation of the populations of the states T_1 BChl *a* (black), T_1 Car (red) and the sum −（S_0 BChl *a* + S_1 BChl *a*）(blue) at K_{01} = 0.1 (solid line) and 1 ns (dash). K_1 = 0.5 ns, K_2=1.3 ns, τ =0.01 ns.

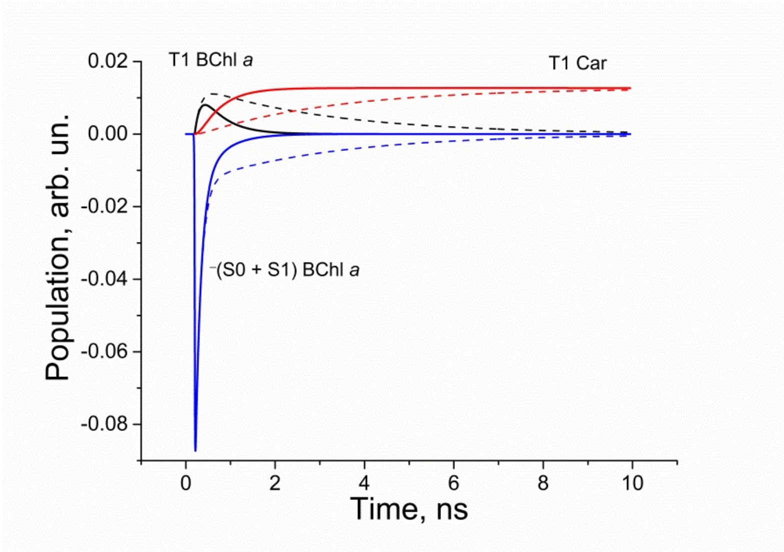

Fig. S5. Simulation of the populations of the states T_1 BChl *a* (black), T_1 Car (red) and the sum −（S_0 BChl *a* + S_1 BChl *a*）(blue) at K_2 = 0.5 (solid line) and 3 ns (dash). K_{01} = 0.17 ns, K_1 =0.5 ns, τ =0.01 ns.