IUBMB *Life*, 50: 115–117, 2000
Copyright © 2000 IUBMB
1521-6543/00 $12.00 + .00

Original Research Article

Model of Detergent-Induced Spectral Changes of the B800–850 Complex from *Chromatium minutissimum*

Andrei P. Razjivin,[1] Andrei A. Moskalenko,[2] and Vladimir I. Novoderezhkin[1]

[1] *A.N. Belozersky Institute of Physico-Chemical Biology, Moscow State University, Moscow 119899, Russian Federation*

[2] *Institute of Basic Biological Problems, Russian Academy of Sciences, Puschino, Moscow Region, 142292, Russian Federation*

Summary

The absorption and circular dichroism spectra of the B800–850 complex from *Chromatium minutissimum* before and after the Triton X-100 treatment were simulated by means of standard exciton theory, taking into account inhomogeneous broadening. To explain the spectral changes of the B800–850 complex treated with Triton X-100, we have assumed that all bacteriochlorophyll pigments absorbing at 850 nm exhibit the same additional rotation of ~20° around the axis perpendicular to the membrane plane. This has been sufficient to fit the transformation in absorption and circular dichroism spectra induced by detergent treatment of the B800–850 complex.

IUBMB *Life*, 50: 115–117, 2000

Keywords B800–850 complex; *Chromatium minutissimum*; conformation transition; exciton theory; spectral changes; Triton X-100.

INTRODUCTION

Detergents as well as solvents, salts, and other agents are well known to affect the spectral properties of the peripheral light-harvesting pigment–protein complex (LH2 or B800–850)[3] from purple photosynthetic bacteria (*1–4*). In particular, the spectral position of the long-wavelength absorption band of the B800–850 complex may be tuned within the 830–850 nm range by detergent treatment (*3*, *4*).

Received 24 April 2000; accepted 26 May 2000.

Address correspondence to Andrei Razjivin. Fax: (07-095)939-3181. E-mail: razjivin@genebee.msu.su

[3] Abbreviations: B800, B850, bacteriochlorophyll absorption band with the peak at 800 or 850 nm, respectively; BChl, bacteriochlorophyll; BChl800, BChl850, bacteriochlorophyll spectral form with the absorption peak at 800 or 850 nm, respectively; CD, circular dichroism; LH2 or B800–850 complex, the peripheral light-harvesting complex of purple photosynthetic bacteria having absorption peaks at 800 and 850 nm.

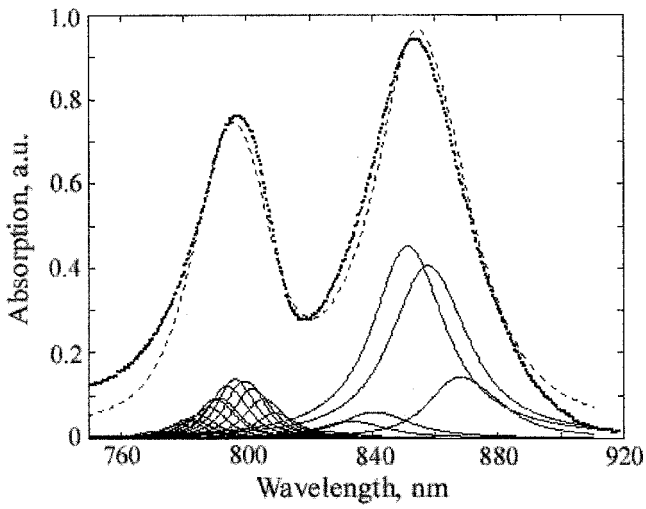
In this paper we have simulated the absorption and circular dichroic (CD) spectra of the B800–850 complex from *Chromatium minutissimum* before and after treatment with Triton X-100 detergent. As in our previous publications (e.g., [*5*, *6*]), we use the standard exciton theory, taking into account inhomogeneous broadening.

EXPERIMENTAL PROCEDURES

The pigment–protein complex B800–850 from *C. minutissimum* (strain MSU) was isolated by means of preparative electrophoresis in polyacrylamide gel as described previously (*7*, *8*). Absorption spectra were measured with a Model UV-160 Shimadzu spectrophotometer. CD spectra were monitored with a homemade spectrometer.

MODEL OF THE LH2 ANTENNA

The LH2 complexes contain two polypeptides, α and β, which bind bacteriochlorophyll (BChl) (*9*). We suppose that the pigment organization in LH2 of *C. minutissimum* is analogous to that of the LH2 antenna from *Rhodopseudomonas acidophila* (*10*). For a model of an antenna unit, we consider two concentric circular aggregates that lie in two planes parallel to the membrane plane. The first aggregate consists of n strongly coupled BChl850 molecules and has the $C_{n/2}$-symmetry with a dimeric unit cell. The second ring consists of $n/2$ weakly coupled BChl800 molecules and has the $C_{n/2}$-symmetry with a monomeric unit cell. We assume $n = 18$. The Q_y transition dipole moments of two BChls in a dimeric unit cell form angles ψ_1, ψ_2 with the ring plane and angles φ_1, φ_2 with the tangent to the circle. The energies of electronic transitions of these two BChls are E_1 and E_2, respectively. The corresponding parameters for BChl800 pigments are ψ', φ', and E'. The Mg–Mg distances between BChls were taken to be the same as for LH2



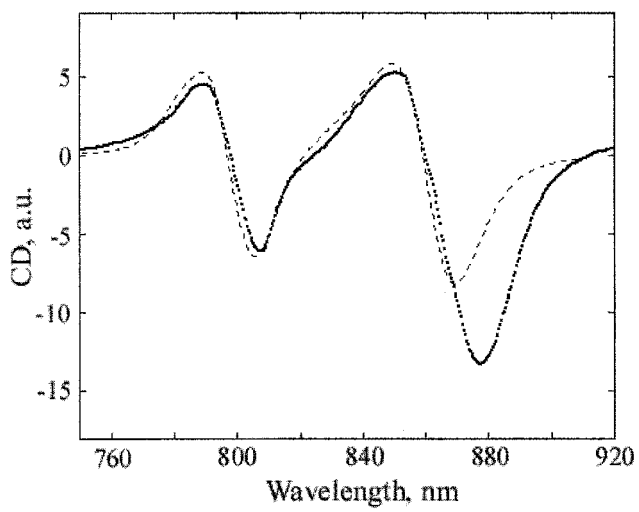
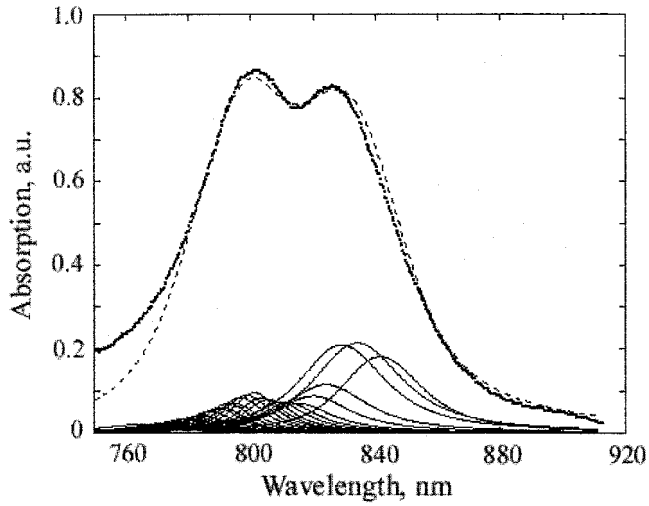


Figure 1. Absorption (top) and CD (bottom) spectra of the B800–850 complex from *C. minutissimum* in phosphate buffer, pH 8.0, at room temperature. Points, experimental data; dashed curve, calculated absorption and CD profiles; solid lines, calculated absorption line shapes for individual exciton components.



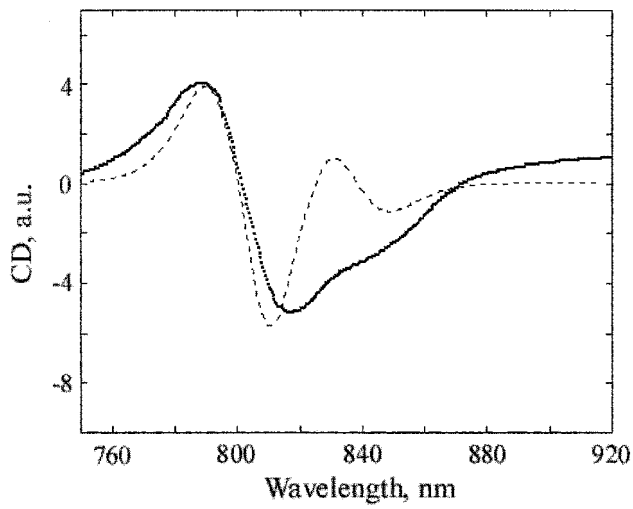


Figure 2. Same as in Fig. 1, but experimental spectra obtained after treatment of the B800–850 complex with 0.8% Triton X-100. Calculated spectra were obtained by supposing each BChl850 molecule rotated at ~20° around the axis perpendicular to the membrane plane (and with adjusted line-broadening parameters; see text).

of *R. acidophila*. In our simulations of the B800–850 absorption and CD spectra, we have taken into account the interactions between the Q_y transitions of BChls, neglecting their mixing with Q_x, B_y, and B_x transitions as well as the charge transfer states.

The interaction energies were calculated in the dipole–dipole approximation by supposing that the monomeric dipole strength is equal to 40 D^2. The nearest neighbor interaction energies were reduced by 20% because of deviation from the dipole–dipole approximation at short distances. The site inhomogeneity of the antenna was described by uncorrelated perturbations $\delta E'$ and δE of electronic energies of BChl800 and BChl850 pigments, E' and E. We assumed that $\delta E'$ and δE have a gaussian distribution. The width (full width at half-maximum, FWHM) of this distribution is σ' and σ.

To calculate absorption and CD spectra, we used the method of direct numerical diagonalization of one-exciton Hamiltonian and Monte Carlo averaging over a random distribution of diagonal energies modeling the site inhomogeneity. We used the standard Hamiltonian for the Frenkel exciton in the Heitler–London approximation for two-level molecules (*11*). To calculate the homogeneously broadened spectra (for each set of

diagonal energies), we assumed the Lorentzian line shape. The homogeneous line widths (FWHM) are Γ_M for exciton levels of the B800 band, and Γ_{1L} (Γ_{1H}) for the lowest (higher) exciton levels of the B850 band.

RESULTS AND DISCUSSION

The measured and calculated spectra are shown in Figs. 1 and 2. The best fit for the B800–850 complex (Fig. 1) was obtained for $\psi_1 = 2°$, $\psi_2 = -2°$, $\varphi_1 = 195°$, $\varphi_2 = 25°$, $\psi' = 9°$, $\varphi' = 185°$, $E_1 = -470$ cm^{-1}, $E_2 = -270$ cm^{-1}, $E' = -250$ cm^{-1} (transition energies are calculated from the transition energy of a BChl a monomer, which corresponds to $\lambda = 777$ nm), $\Gamma_M = 160$ cm^{-1}, $\Gamma_{1L} = 250$ cm^{-1}, $\Gamma_{1H} = 340$ cm^{-1}, $\sigma = 500$ cm^{-1}, and $\sigma' = 340$ cm^{-1}.

To fit the spectra for the B800–850 complex treated with 1% Triton X-100, we supposed that both BChl850 pigments in a dimeric subunit show additional rotation of $\sim 20°$ from the tangent to the circle; that is, $\varphi_1 = 215°$, $\varphi_2 = 45°$ (all other parameters are the same). This is sufficient to describe the absorption and CD spectra transformation after the detergent treatment. A better quantitative fit may be obtained if we suppose also some increase of static and dynamic disorder (increase of inhomogeneous and homogeneous broadening), which yields $\Gamma_M = 190$ cm^{-1}, $\Gamma_{1L} = 320$ cm^{-1}, $\Gamma_{1H} = 420$ cm^{-1}, $\sigma = 560$ cm^{-1}, $\sigma' = 440$ cm^{-1} (see Fig. 2).

A hypothetical scheme for the conformational transitions in the B800–850 complex from *C. minutissimum* when treated with various agents including Triton X-100 has been proposed previously (*4*). According to that scheme, the spatial arrangement of the C-terminal ends of α-helices bearing BChl molecules is altered by Triton X-100 treatment, which results in disturbance of pigment interactions inside the BChl long-wavelength spectral form. The calculations presented here show that the corresponding spectral changes may be modeled by the small rotation of each BChl850 molecule in the B800–850 complex.

ACKNOWLEDGEMENTS

This work was supported in part by grants INTAS-96-1435 and Russian Foundation for Basic Research 00-04-48308.

REFERENCES

1. Miller, J. F., Hinchigeri, S. B., Parkes-Loach, P. S., Callahan, P. M., Sprinkle, J. R., Riccobono, J. R., and Loach, P. A. (1987) Isolation and characterization of a subunit form of the light-harvesting complex of *Rhodospirillum rubrum*. *Biochemistry* **26**, 5055–5062.
2. Jursakova, V., and Reiss-Husson, F. (1993) Isolation and characterisation of the core light-harvesting complex B875 and its subunit form, B820, from *Rhodocyclus gelatinosus*. *Biochim. Biophys. Acta* **1183**, 301–308.
3. Sturgis, J. N., Hagemann, G., Tardos, M. H., and Robert, B. (1995) Biochemical and spectroscopic characterization of the B800–850 light-harvesting complex from *Rhodobacter sulphidophilus* and its B800–830 spectral form. *Biochemistry* **34**, 10519–10524.
4. Moskalenko, A. A., Kuznetsova, N. Yu., Erokhin, Yu. E., and Toropygina, O. A. (1996) Structural peculiarities and conformational transitions of the B800–850 complex from *Chromatium minutissimum*. *Biochemistry* (*Moscow*) **61**, 318–325. Translated from Biokhimiya **61**, 429–439.
5. Novoderezhkin, V. I., and Razjivin A. P. (1995) Exciton dynamics in circular aggregates: application to antenna of photosynthetic purple bacteria. *Biophys. J.* **68**, 1089–1100.
6. Dracheva, T. V., Novoderezhkin, V. I., and Razjivin, A. P. (1997) Exciton delocalization in the light-harvesting LH2 complex of photosynthetic purple bacteria. *Photochem. Photobiol.* **66**, 141–146.
7. Moskalenko, A. A., and Toropygina, O. A. (1988) Study of relationship between the light-harvesting complex B800–850 to the H-subunit of the reaction center in sulfur photosynthetic bacterium *Chromatium minutissimum*. *Biokhimiya* **53**, 1220–1223 (in Russian).
8. Moskalenko, A. A., and Erokhin, Yu. E. (1974) Isolation of pigment-lipoprotein complexes from purple photosynthesizing bacteria by the method of polyacrylamide gel electrophoresis (In Russian). *Mikrobiologiia* **43**, 654–658.
9. Zuber, H. (1985) Structure of antenna polypeptides. In *Antennas and Reaction Centers of Photosynthetic Bacteria* (Michel-Beyerly, M. E., ed.). pp. 2–14, Springer-Verlag, Berlin.
10. McDermott, G., Prince, S. M., Freer, A. A., Hawthornthwaite-Lawless, A. M., Papuz, M. Z., Cogdell, R. J., and Isaacs, N. W. (1995) Crystal structure of an integral membrane light-harvesting complex from photosynthetic bacteria. *Nature* **374**, 517–521.
11. Davydov, A. S. (1971) *Theory of Molecular Excitons*. Plenum Press, New York.

Copyright of IUBMB Life is the property of Wiley-Blackwell and its content may not be copied or emailed to multiple sites or posted to a listserv without the copyright holder's express written permission. However, users may print, download, or email articles for individual use.