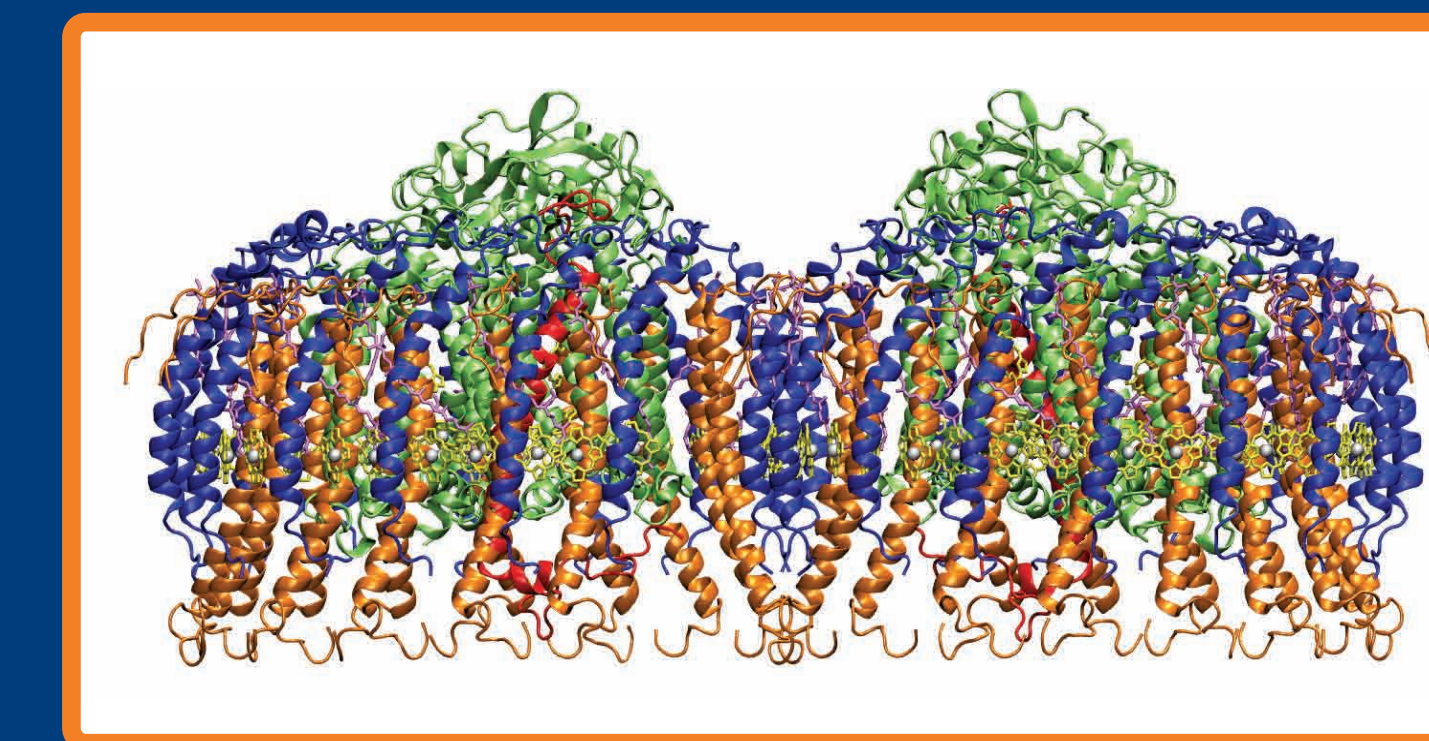




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Bending of the Chromatophore Membrane through Core Complex Dimerization

a molecular dynamics and electron microscopy investigation

Jen Hsin¹, James C. Gumbart¹, Danielle E. Chandler¹, Christopher Harrison¹, Pu Qian², Per A. Bullough², C. Neil Hunter², and Klaus Schulten¹¹Beckman Institute, University of Illinois at Urbana-Champaign, Urbana, IL²Department of Molecular Biology and Biotechnology, University of Sheffield, Sheffield, UKTheoretical and Computational Biophysics Group - <http://www.ks.uiuc.edu/> - Email: jhsin@ks.uiuc.edu

I. Abstract

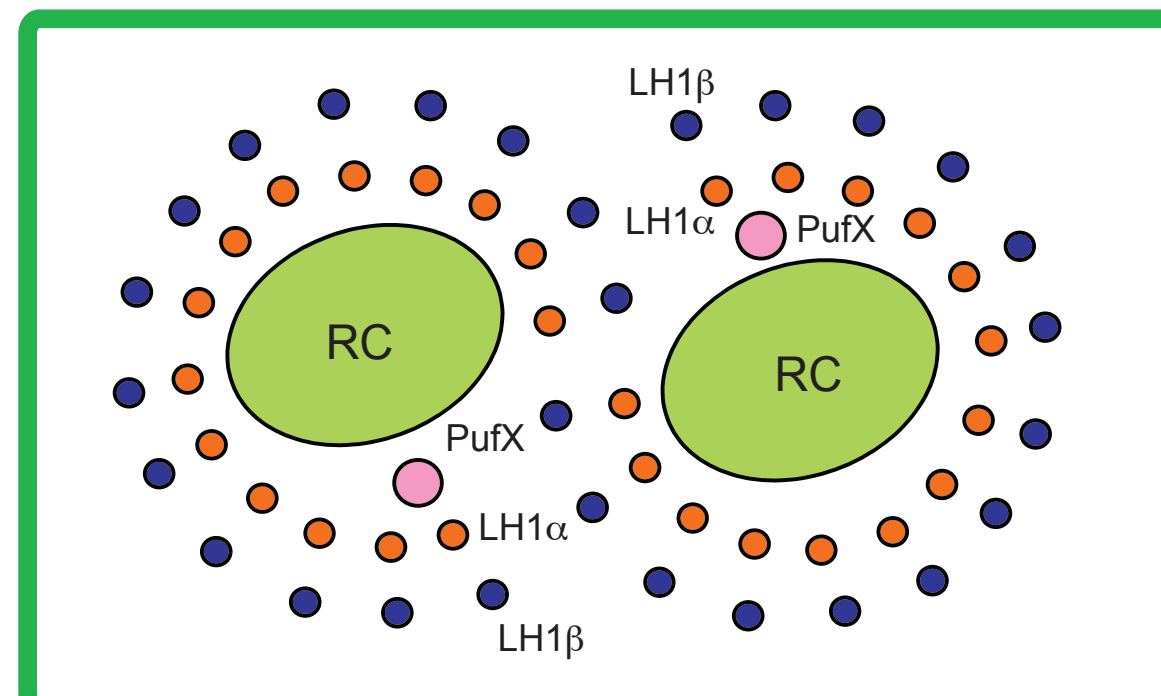
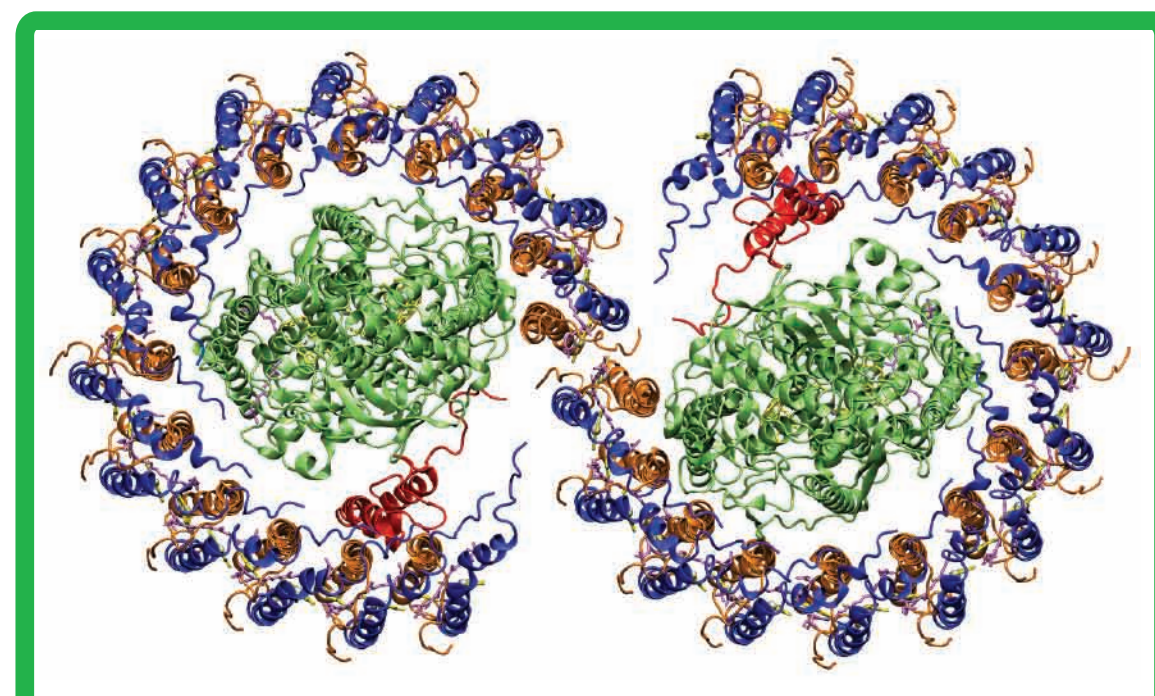
In photosynthetic purple bacteria, photosynthesis is carried out by only a handful of proteins that aggregate in the bacterial plasma membrane, forming indentations known as chromatophores. Chromatophores come in different shapes; flat, tubular, and spherical chromatophores have all been observed in various species and mutants. What drives the formation of chromatophore shapes still remains an open question, but studies have suggested that the assembly of integral membrane proteins such as the light harvesting complex 1 (LH1) plays a key role. Particularly, in a *Rhodobacter (Rb.) sphaeroides* mutant, in which the dimeric LH1 is the most abundant protein complex, chromatophores were found to be tubular.

We have combined experimental data and computational techniques to study the membrane-bending mechanisms due to the assembly of the dimeric core complex (also known as the LH1-RC-PufX complex). An all-atom model of the *Rb. sphaeroides* core complex dimer was constructed and molecular dynamics simulations of a single dimer in a solvated lipid bilayer carried out. Results show spontaneous bending at the dimerizing junction. Similar dimer bending was also observed in single particle EM analysis. Then the all-atom model was docked into the EM data in a molecular dynamics flexible fitting simulation, during which the surrounding lipids relax around the bent dimer to form a curved membrane patch. To extend simulation size and timescale, a coarse-graining model is developed to demonstrate tubular chromatophore formation driven by a large assembly of core complex dimers.

II. Core complex model

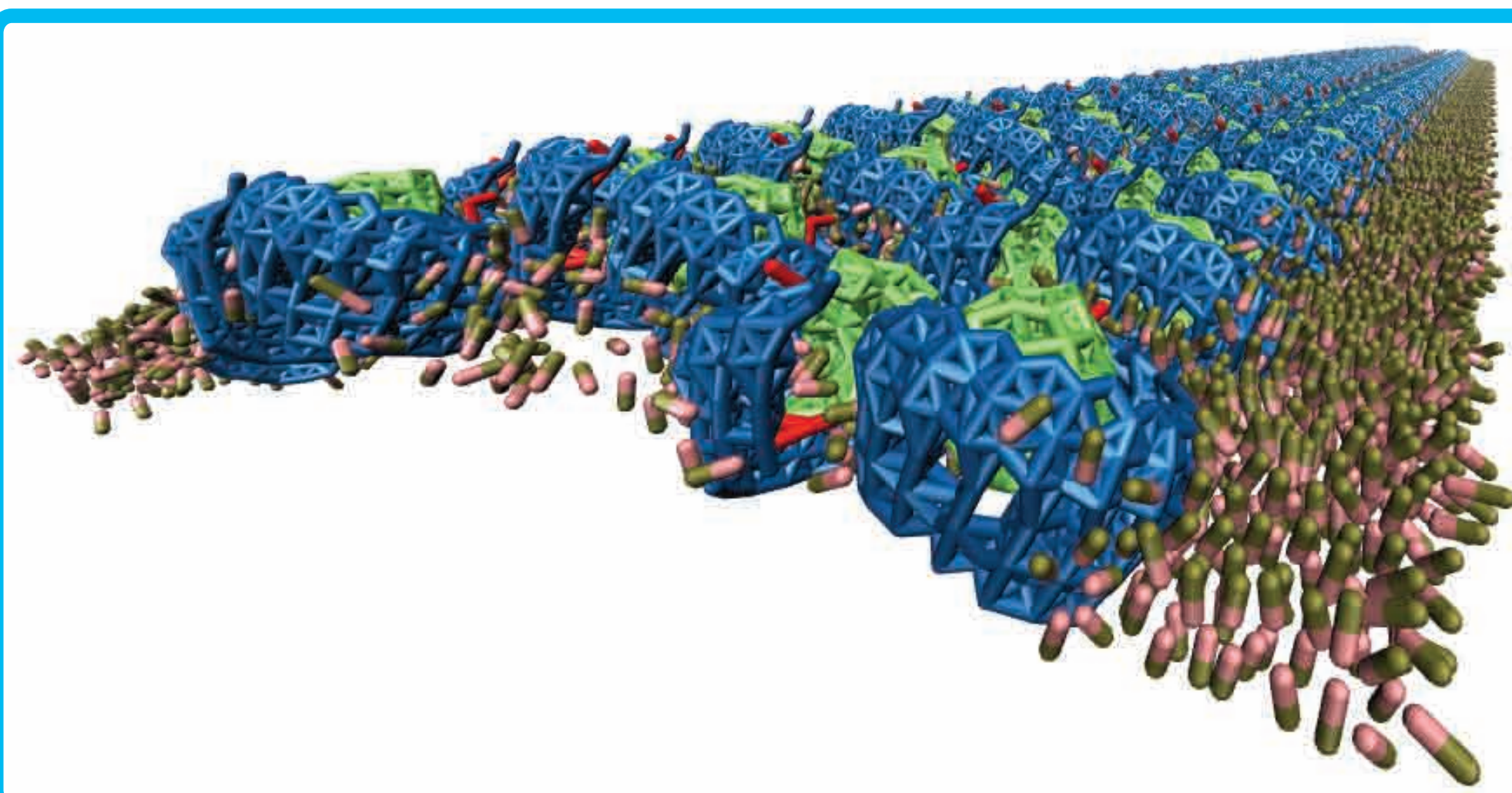
The core complex dimer consists of three protein components: light-harvesting complex 1 (LH1), reaction center (RC), and the protein PufX.

An all-atom model for *Rb. sphaeroides* core complex dimer was constructed using available structures and homology modeling [1].



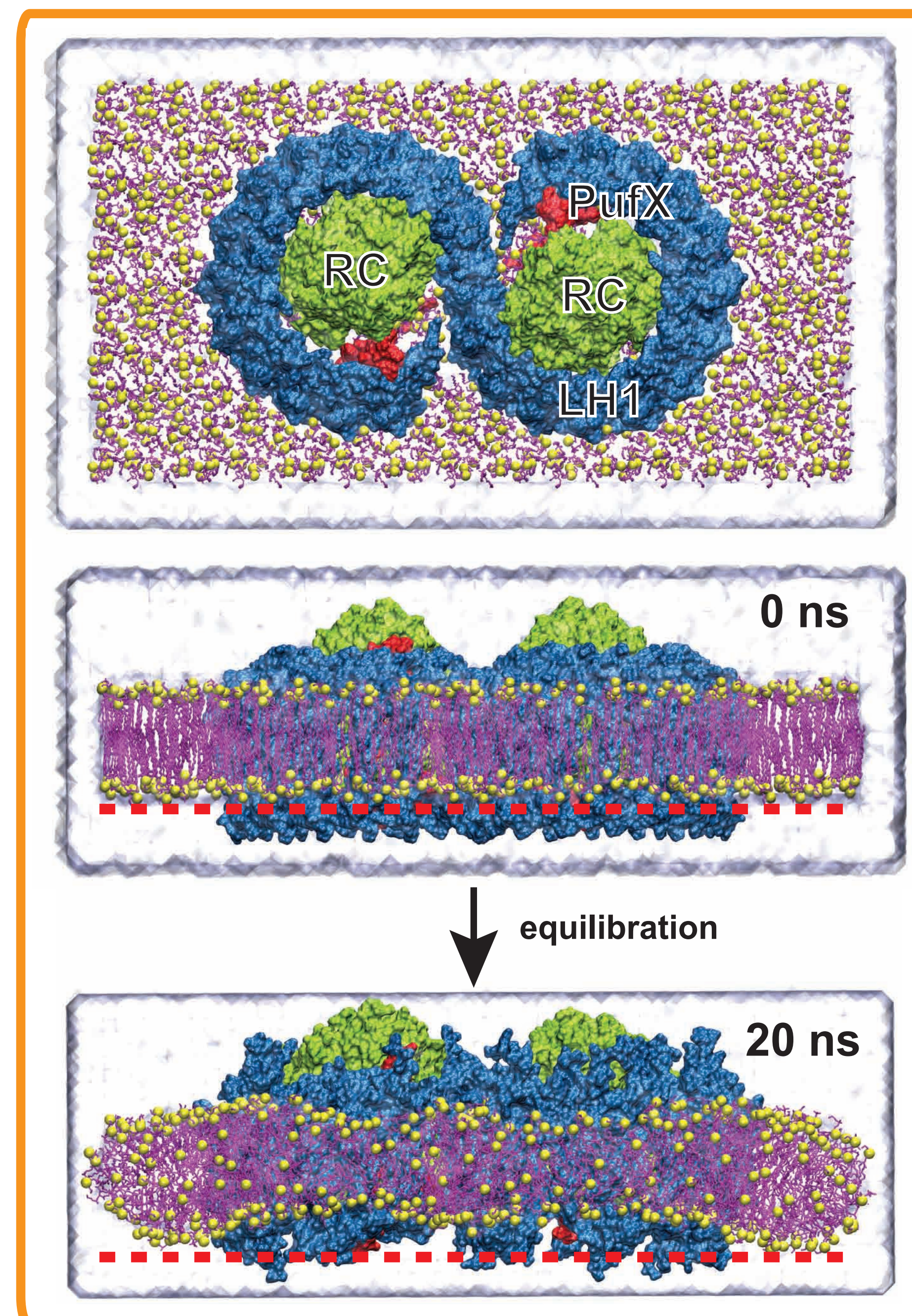
V. Coarse-grained system

- * Core complex dimers aggregate to form tubular chromatophores [6].
- * Coarse-grained [7] model built for the core complex dimer to increase simulation size and timescale.
- * Curvature observed in a preliminary 100 ns simulation.



III. Single-dimer equilibration

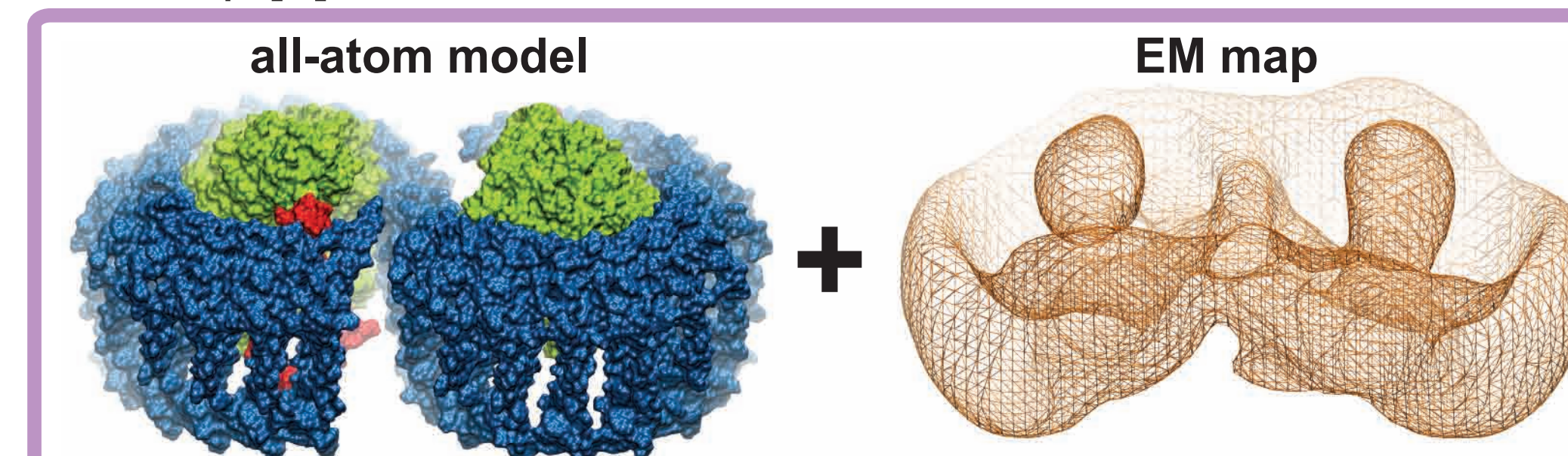
The core complex model was placed in a lipid bilayer, solvated, ionized, and simulated using NAMD [2] with CHARMM27 force field for 20 ns (688,373 atoms) [1]:



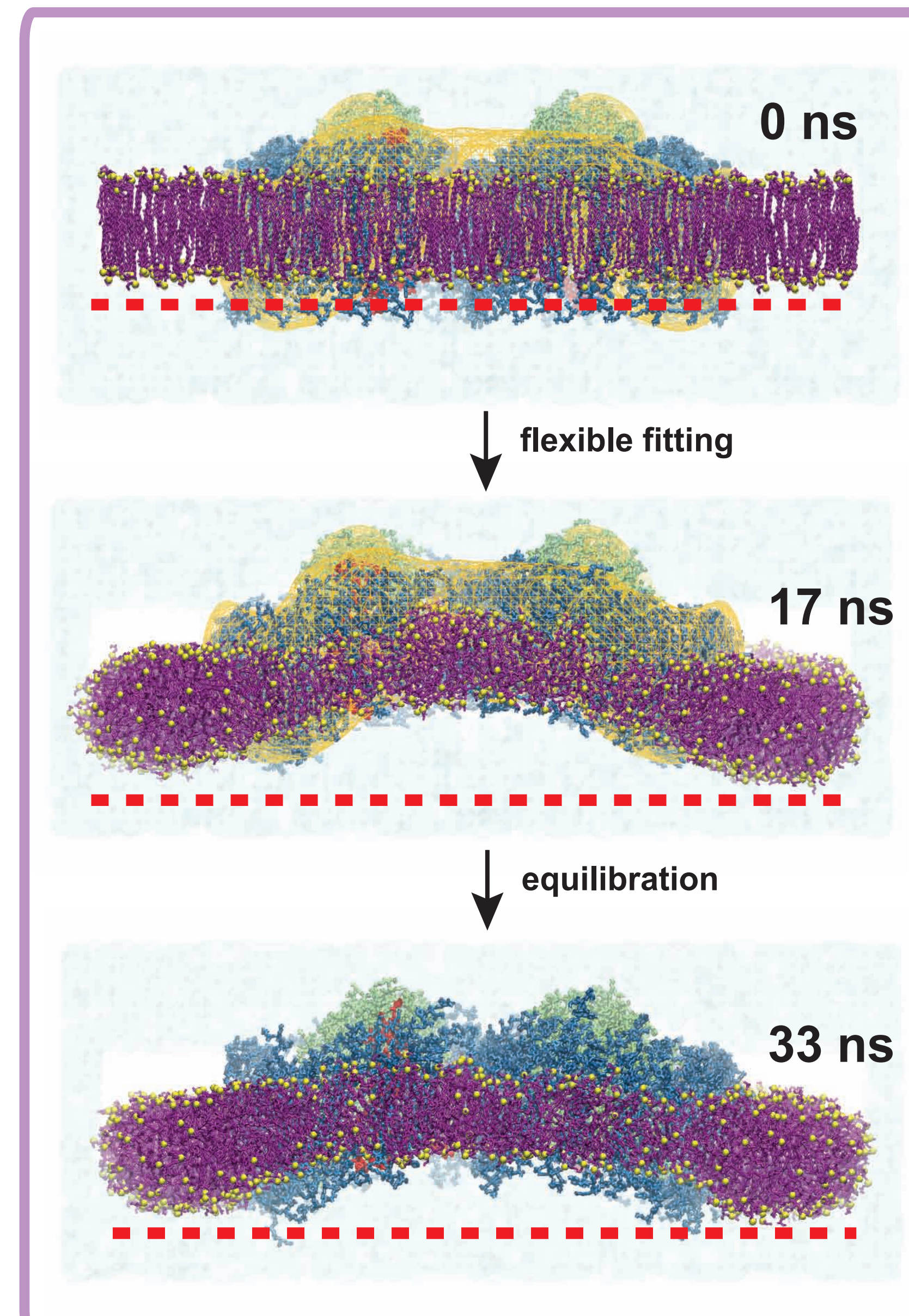
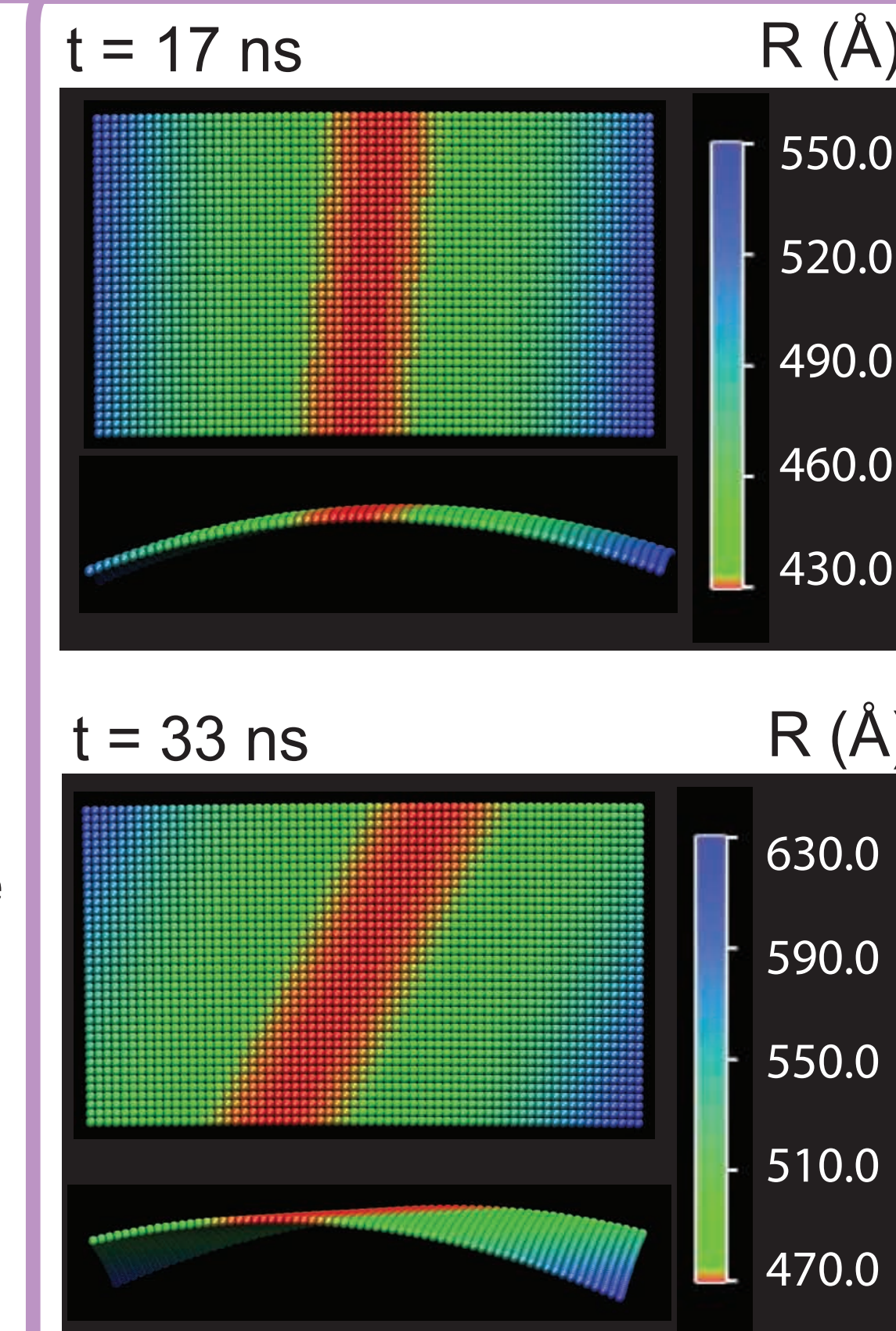
- * Bending occurred at the LH1 dimerizing interface
- * Bending angles reached ~ 172 degrees, corresponding to a radius of curvature of 720 Å, too big compared to the 250-550 Å radius of tubular chromatophores [3]

IV. Flexible fitting

We used the molecular dynamics flexible fitting method (MDFF) [4] to dock the core complex dimer model into a 25Å EM map [5]:

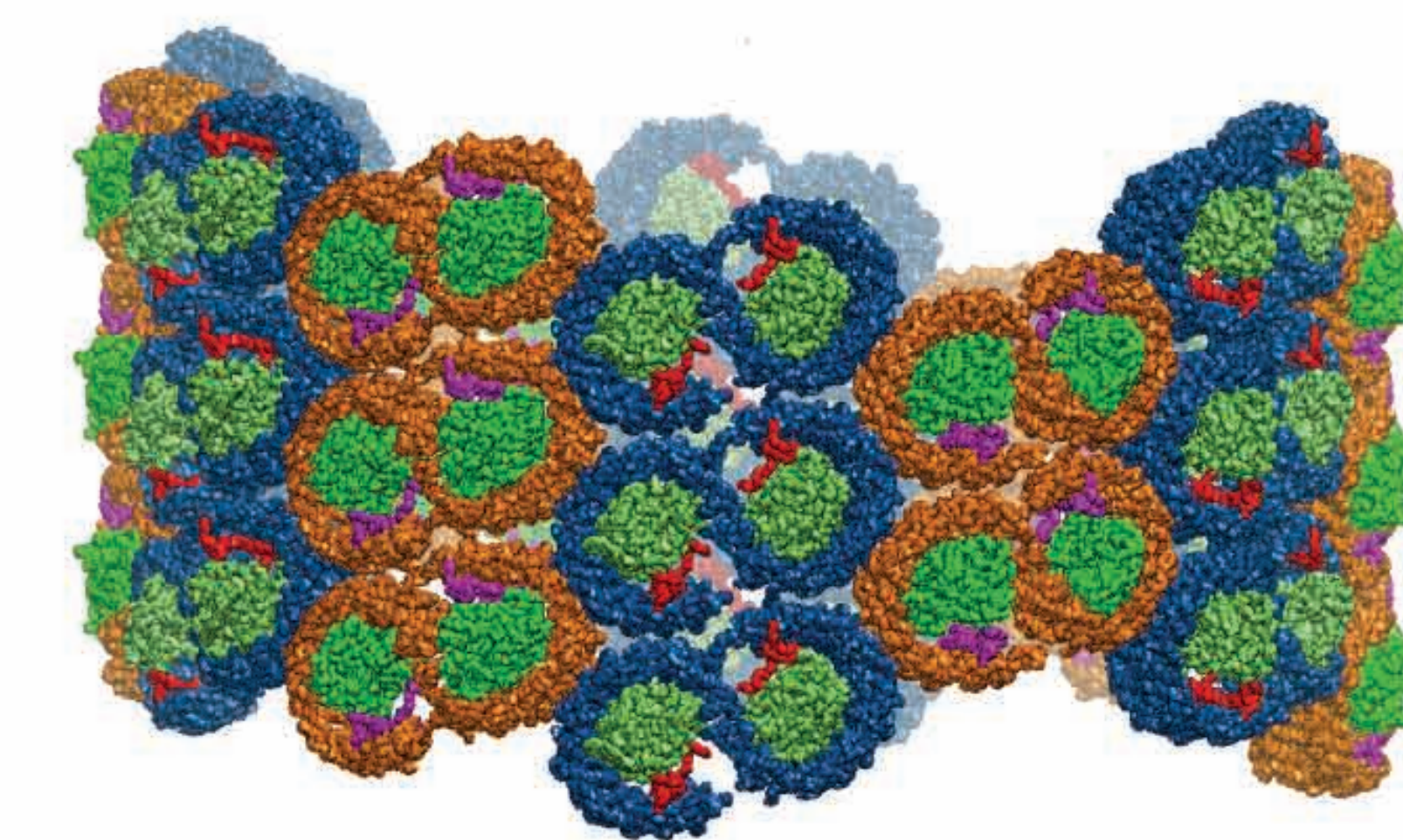


- * EM density of dimer has a bigger bending angle of 146 degrees [5]
- * 890,307 atoms
- * Core complex dimer coupled to an external potential derived from EM density
- * Lipids followed the dimer and bend. Radius of curvature agrees with the size of chromatophore tube
- * "Twisting" of membrane observed



VI. Discussion

- * The *Rb. sphaeroides* core complex dimer is thought to induce tubular membrane structure
- * The *Rb. sphaeroides* core complex dimer is found to be bent in computational and EM studies [1,5]
- * The shape of the dimer can sculpt the membrane with correct radius of curvature
- * The curvature induced is unidirectional, and asymmetric
- * An array of core complex dimer can collectively bend the membrane, leading to tubulation



VII. References and acknowledgements

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