Corrections

Molecular Dynamics Simulations of Retinal in Rhodopsin: From the Dark-Adapted State towards Lumirhodopsin, by Vincent Lemaître, Philip Yeagle, and Anthony Watts*, Volume 44, Number 38, September 27, 2005, pages 12667−12680.

Page 12678. By convention, all of the figures illustrating the isomerization of retinal start with the arbitrary time zero ns, corresponding to when the illumination takes place (and where the isomerization is started). This means the time frame is independent of the amount of time the protein was previously simulated in the dark-adapted state. The advantage of this choice is to allow a direct comparison between simulations where retinal is isomerized. Note that this convention was not followed for the figures, intending to show a comparison between the protein in the dark-adapted state and after isomerization (e.g., Figure 4). For those figures, the time frame used is the one corresponding to the simulation in the dark-adapted state, where the starting time for the simulations where retinal is isomerized is 500, 1000, and 1500 ps, respectively. Graphs of simulations with alternative starting points (retinal isomerization after 1000 or 1500-ps MD in the dark-adapted state), corresponding to Figures 3, 4, 5, 7, 9, 11 in the paper. Also included are two tables of values describing covalent bond stretching, bond angles, dihedral angles used for bonded interactions (Table 1S) and partial charges on the retinal using standard parameters taken from Force Fields Gromos for nonbonded interactions. This material is available free of charge via the Internet at http://pubs.acs.org.

BI0580299

10.1021/bi0580299
Published on Web 10/21/2005