

1067-92-1208

Byong Y Kwon* (bkwon1@masonlive.gmu.edu). *Computational docking of molecular wires to the reaction center of Rhodobacter sphaeroides*. Preliminary report.

Given the worldwide interest in renewable energy, scientists have been exploring the possibility of using bacterial photosynthetic reaction centers to build a new generation of highly efficient photovoltaic devices. To build such devices, molecular wires (MWs) that serve as good conductors to transport electrons from and to the reaction centers are needed. The MWs must dock at specific binding sites within the reaction centers. We explore computational models of docking MWs to the reaction centers. Such models can help in proposing suitable MWs for photovoltaic devices. For our modeling, we use the reaction center of Rhodobacter sphaeroides, a purple photosynthetic bacteria. (Received September 20, 2010)