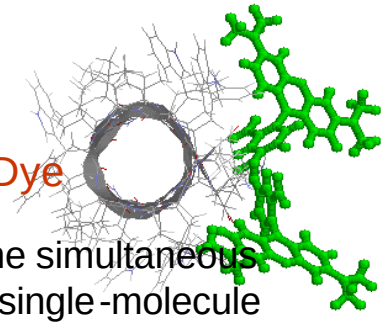
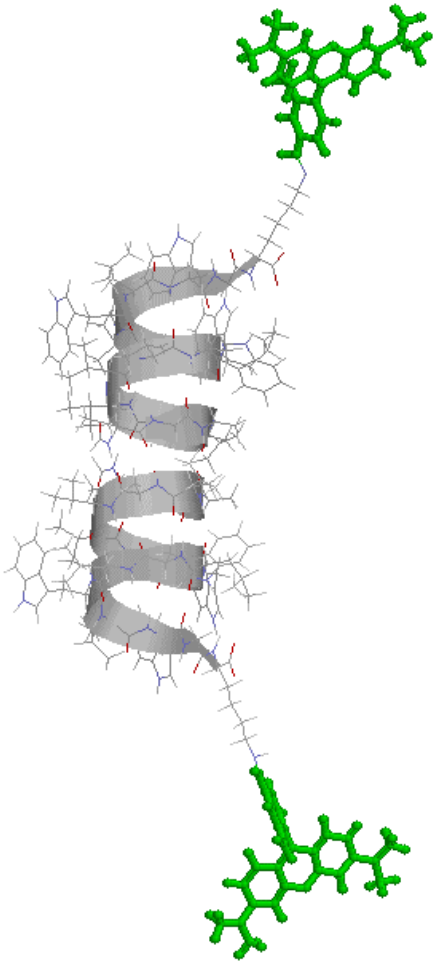
Pilot-CSD7 Highlight

EMSL



Modeling of Fluorophore Dynamics in Gramicidin labeled with Rhodamine Dye



In conjunction with an experimental project of the simultaneous detection of the single-ion channel current and single-molecule fluorescence of Rhodamine labeled Gramicidin performed in the group of H. Peter Lu (PNNL), the effects of addition of the fluorophore to the peptide ion channel must be understood by both experiment and modeling. Just as the single-ion channel current is well-understood in Gramicidin (Koeppe,R.E. and O.S.Andersen. 1996. *Annu. Rev. Biophys. Biomol. Struct.* 25:231-258.) , it is also well-described in terms of molecular modeling by molecular dynamics (Woolf,T.B. and B.Roux. 1994. *PNAS USA* 91:11631-11635.)

However, additional groups added to the C-terminal end of gramicidin have been shown to possibly cause changes in the ion channel conductance of Gramicidin (Jaikaran,D.C.J. and G.A.Woolley. 1995. *J. Phys. Chem.* 99:13352-13355.). This could possibly be due to the added substituent's (in this case – Rhodamine's) tendency to block the ion channel on the time scale of a few tenths of a second. Structural studies of the fluorophore dynamics of "head to head" ion channel of Gramicidin labeled with Rhodamine will determine the feasibility of that the added substituent might hinder the ion-flow path of gramicidin.