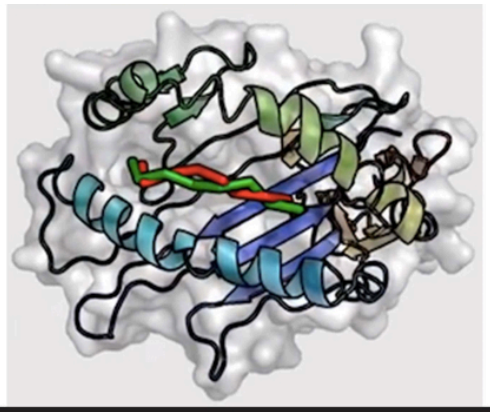

Workshop on Macromolecular Modeling

Based on CHARMM and CHARMMing

FIU, April 8-9, 2017

Organizers/Leaders

David Chatfield, FIU

Lee Woodcock, USF

Fiona Kearns, USF

PROGRAM

Saturday

8:30 a.m. Sign-in, light refreshments

SESSION 1: Introduction to Macromolecular Modeling

9:00 a.m. Workshop Introduction: Dr. David Chatfield
9:10 a.m. Overview of application of macromolecular modeling: Dr. Lee Woodcock
9:30 a.m. Introduction to Molecular Dynamics Dr. Chatfield
10:00 a.m. Hands-on work: Drs. Woodcock and Chatfield
11:00 a.m. Introduction to Visualization Techniques: Dr. Chatfield
11:15 a.m. Hands-on work: Drs. Woodcock and Chatfield

12:00 p.m. **LUNCH**

SESSION 2: Advanced Visualization

1:00 p.m. Advanced work with VMD, presentation and hands-on work: Dr. Chatfield
2:20 p.m. Using PyMOL to make publication-quality graphics, presentation and hands-on work: Dr. Woodcock

3:30 p.m. **COFFEE BREAK**

SESSION 3: Drug Design

4:30 p.m. Introduction to Docking: Ms. Fiona Kearns and Dr. Woodcock
5:30 p.m. Hands-on work: Ms. Kearns, Dr. Woodcock and Dr. Chatfield

8:30 a.m. Light refreshments

SESSION 4: Advanced Molecular Dynamics

9:00 a.m. Normal modes - analysis presentation and hands-on work: Dr. Woodcock
10:00 a.m. Free energy calculations – presentation and hands-on work: Dr. Woodcock
11:00 a.m. QM/MM modeling – presentation and hands-on work: Dr. Woodcock
11:50 a.m. Workshop Wrap-up & Complete Survey: Dr. Chatfield

Let’s Get Started!