

Schrödinger Workshop at CHPC 2018

December 2nd, 2018 Century City Convention Centre, Cape Town

09:00-10:30

Welcome and Introduction

Overview of the Small Molecule Drug Discovery Suite

What's new? - Recent Developments

Introduction to the Maestro 11 graphical interface

Small Molecule Docking with Glide

10:30-11:00 Coffee Break

11:30-12:30

Small Molecule Docking with Glide (continued)

Pharmacophore Modeling with Phase

Enumeration and Library Design:

Bioisostere Replacements, Reaction Based Enumeration and Hit Expansion

12:30-13:30 Lunch Break

13:30-15:00

Enumeration and Library Design (continued)

Presentation: Transforming Drug Discovery with Advanced Computational Modeling

Q&A

15:00-15:30 Coffee Break

15:30-17:00 Open Hands-on Session

Chance to discuss your science with us and your peers, and to try out the software on your own - please bring a laptop and a mouse in this case! If you need access to the software, please contact Krishna Govender at CHPC (kgovender3@csir.co.za). We will also provide installation packages and trial keys during the workshop.