A Brief Overview of The Force Field Toolkit (*ff*TK)

Dr. Christopher G. Mayne
Tajkhorshid Group
February 13th, 2012

Available Methods for Obtaining Parameters

Analogy (Re-use of parameters from similar structures)

ParamChem https://www.paramchem.org/

SwissParam http://swissparam.ch/

Zoete *et al.; J. Comp. Chem.* 32(11) **2011,** pp.2359-2368

MATCH http://brooks.chem.lsa.umich.edu/software

Yesselman *et al.; J. Comp. Chem.* 33(2) **2012,** pp.189-202

Development

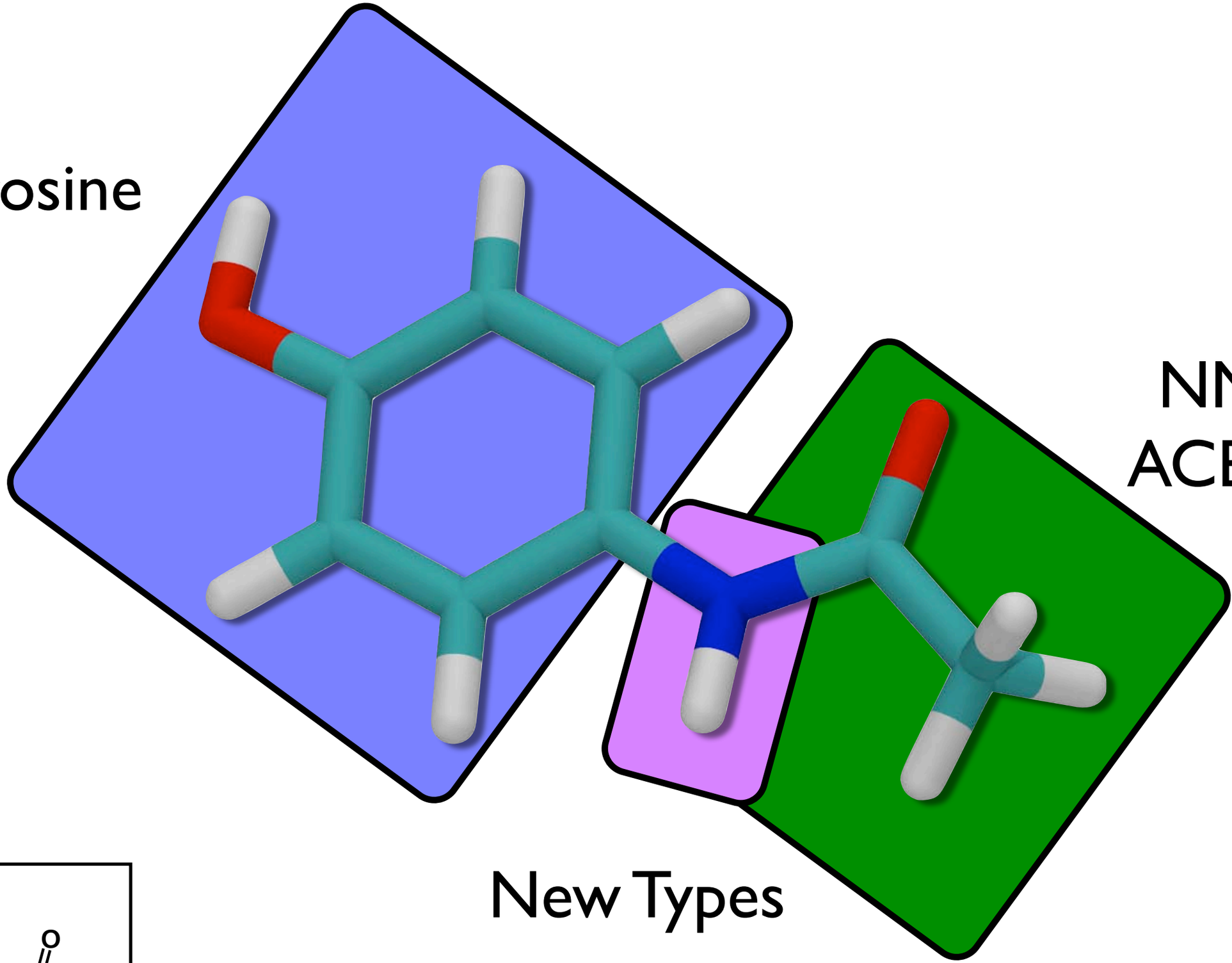
ParaTool http://www.ks.uiuc.edu/Research/vmd/plugins/paratool/

GAAMP http://gaamp.lcrc.anl.gov/para-fit.html

***ff*TK** http://www.ks.uiuc.edu/Research/vmd/plugins/fftk/

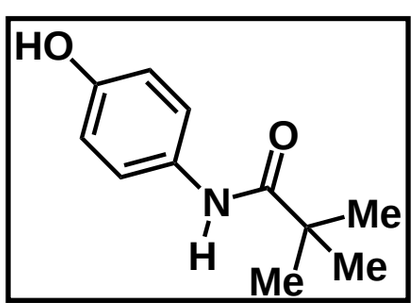
An Example: Acetaminophen

Tyrosine



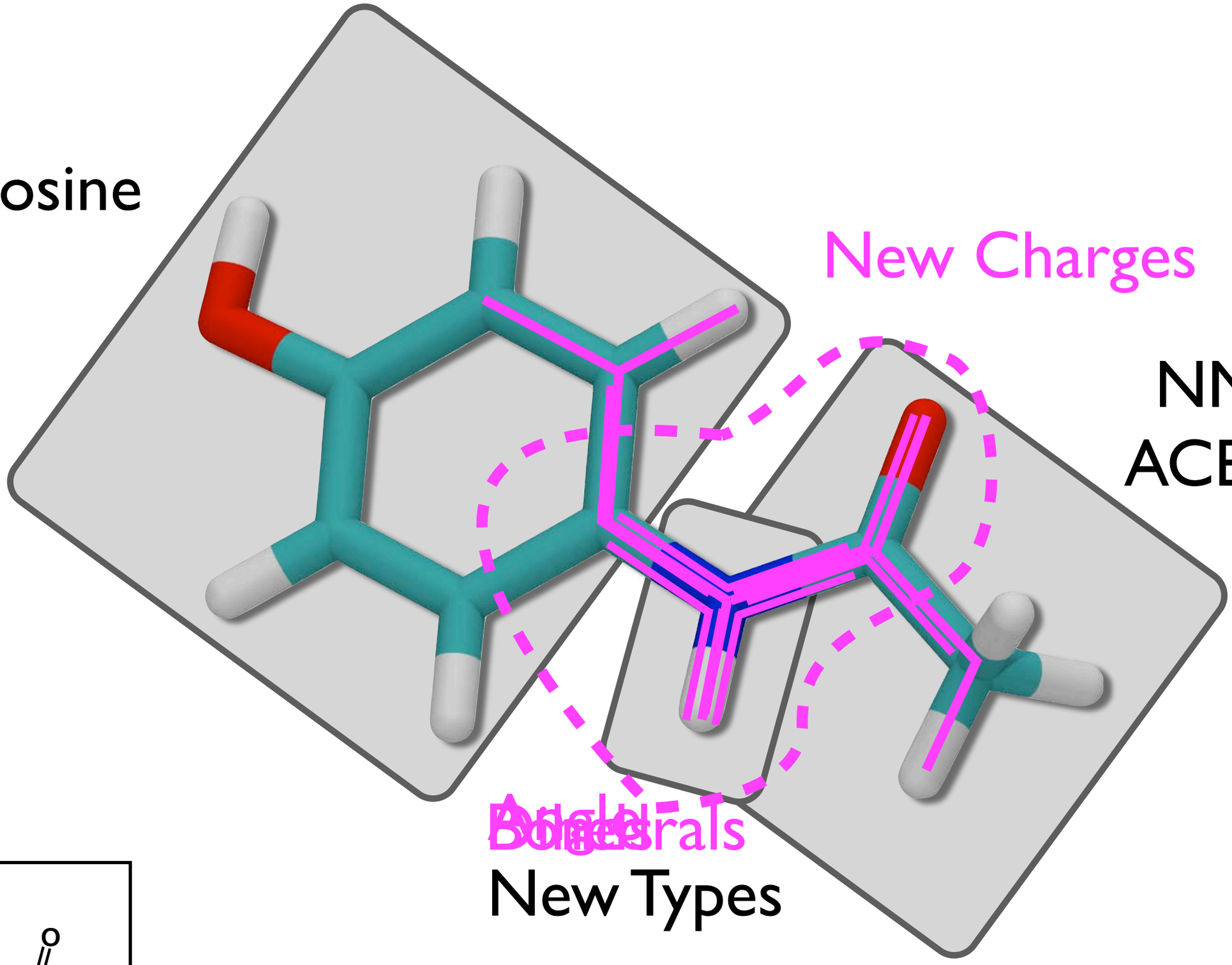
NMA or
ACE-patch

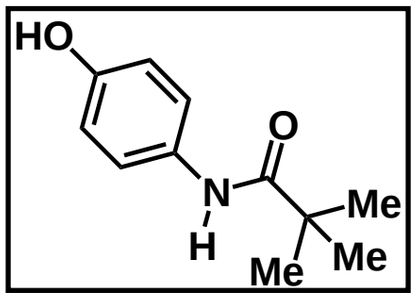
New Types



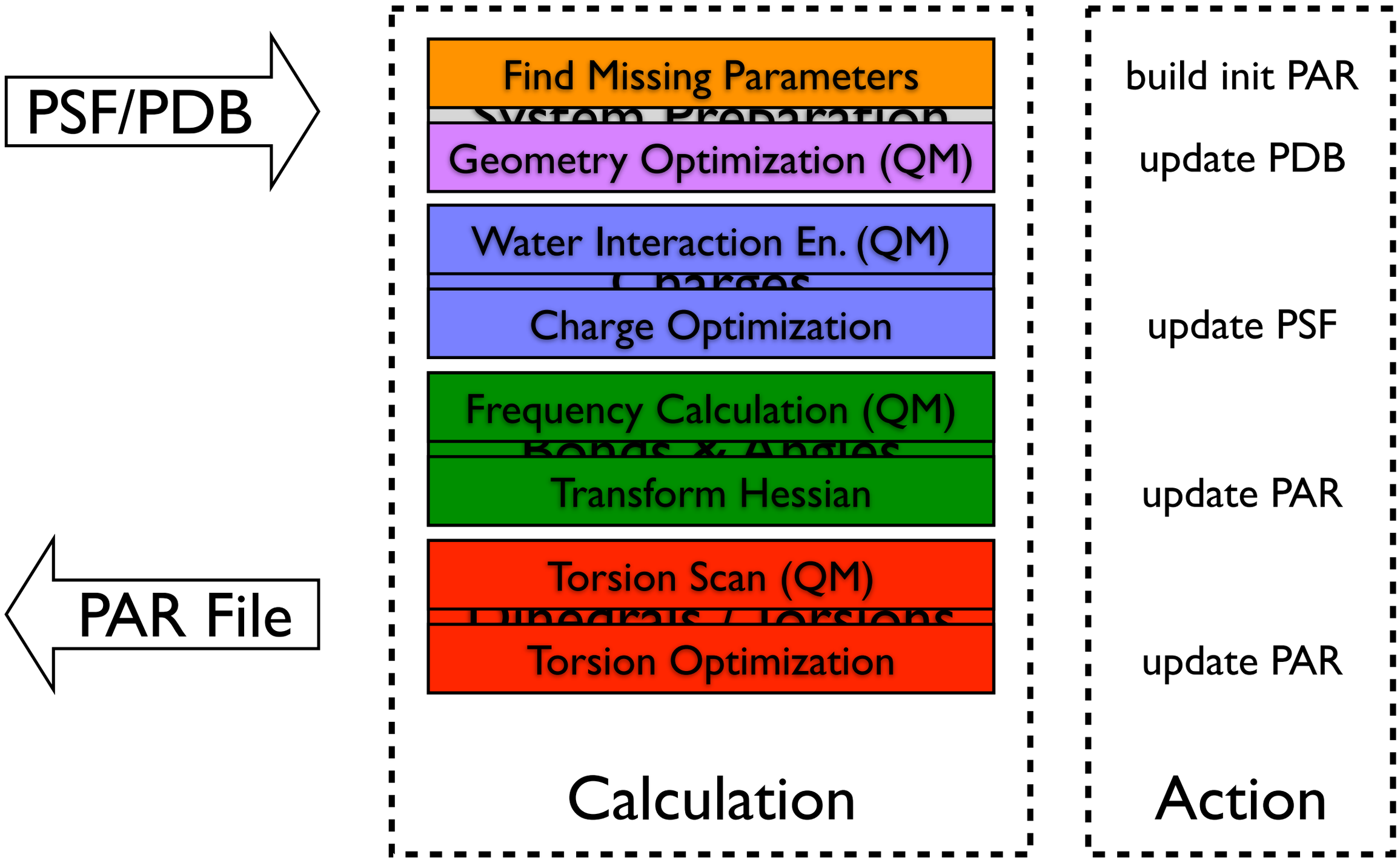
An Example: Acetaminophen

Tyrosine





*ff*TK Facilitates the Parameterization Workflow



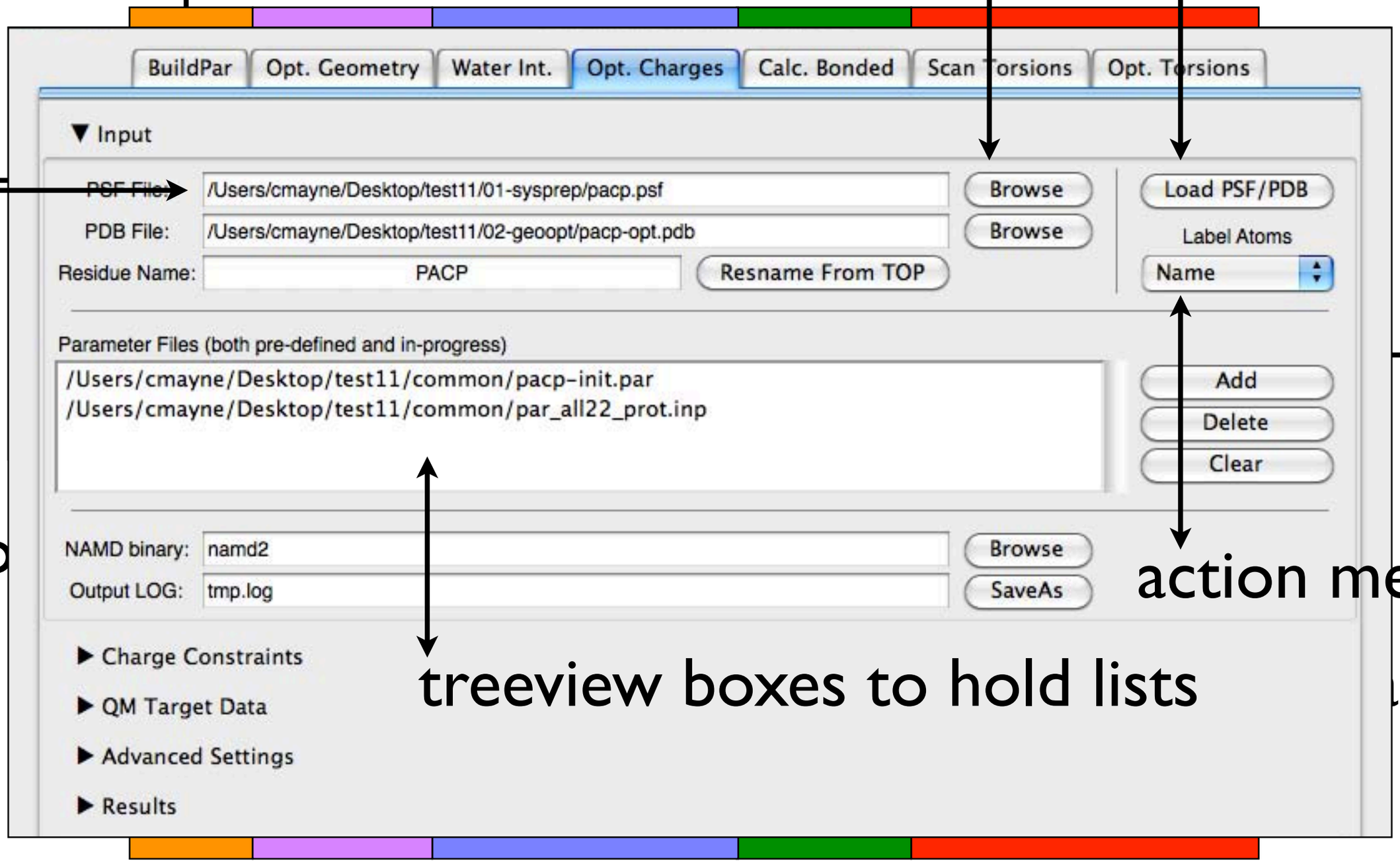
ffTK Interface

file dialog buttons

entry boxes to hold variables

tasks divided into separate tabs

action buttons



arro

action menus

treeview boxes to hold lists

ack

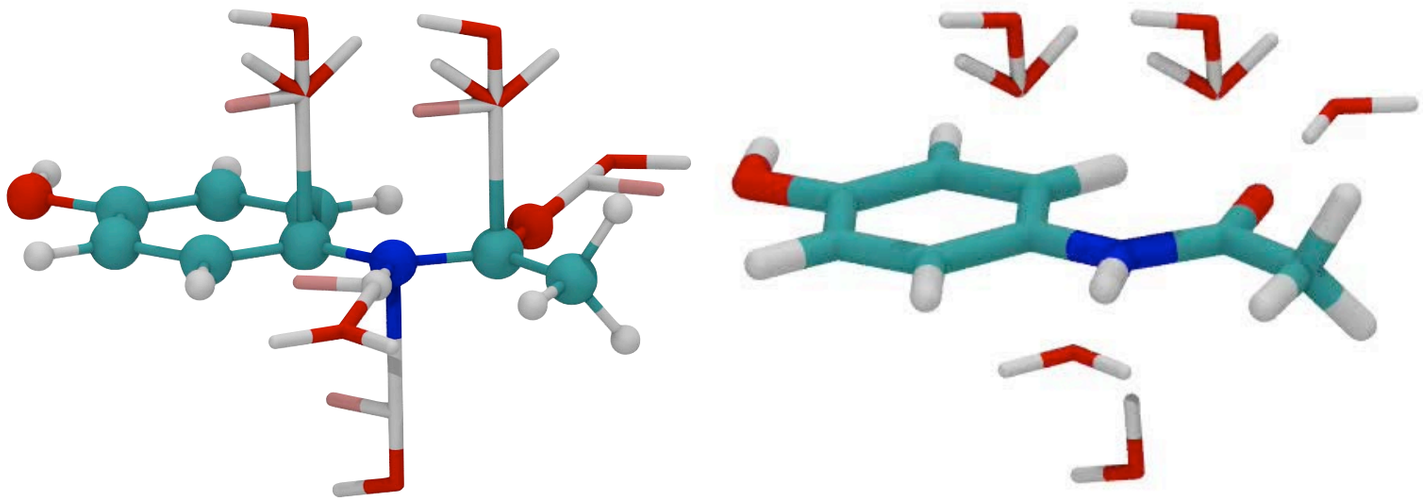
*ff*TK 1.0 is Available in VMD 1.9.1

Setup necessary QM calculations

Visualize calculation input/output

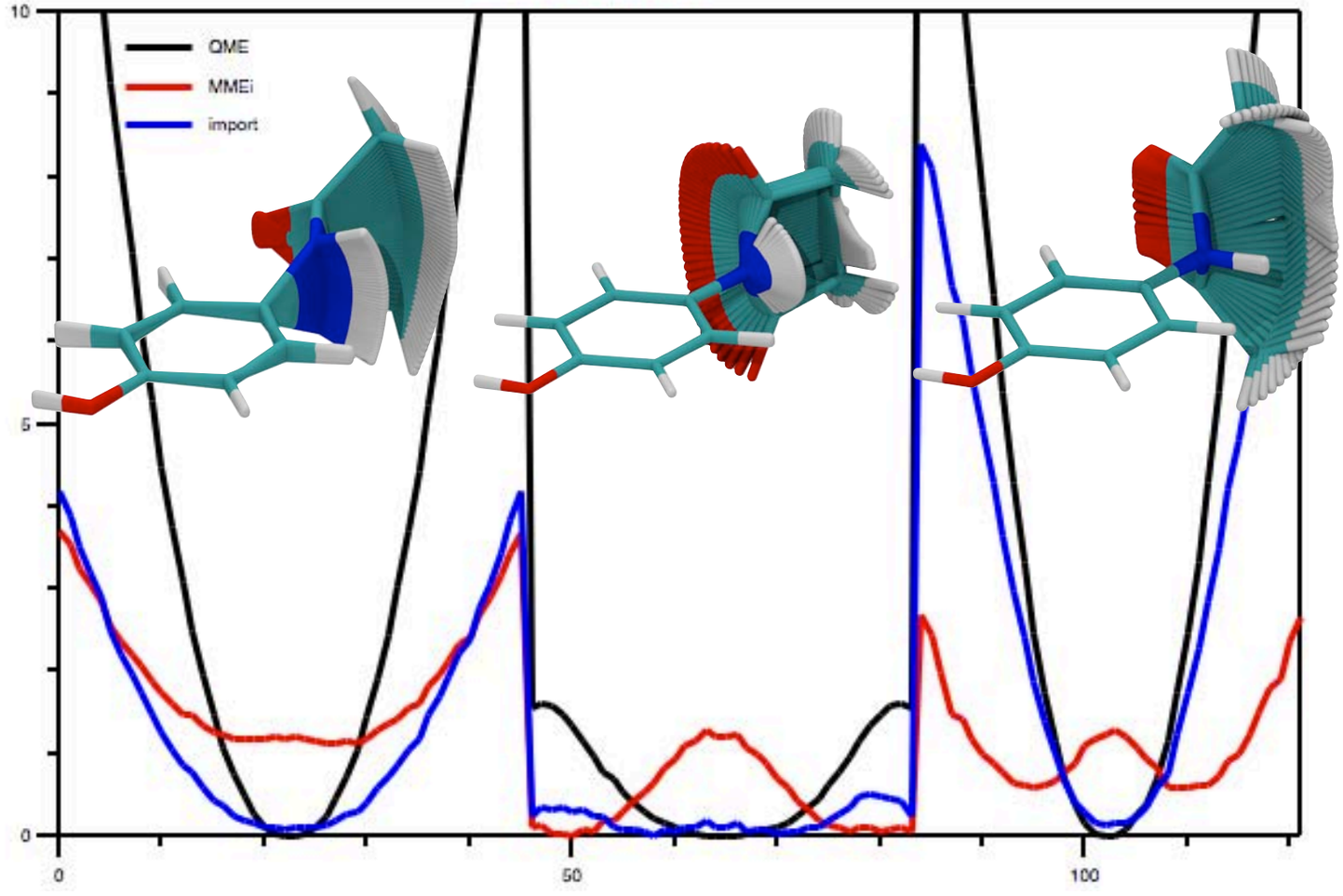
Multidimensional optimization of developing parameters

Read/Write files (pdb, par, log, gau)



Full documentation online:
http://www.ks.uiuc.edu/Research/vmd/plugins/fftk/

Tutorial is under development



Questions?

Christopher Mayne
office: 3011 (Innovation Courtyard II)