

A Brief Overview of The Force Field Toolkit (*ffTK*)

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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

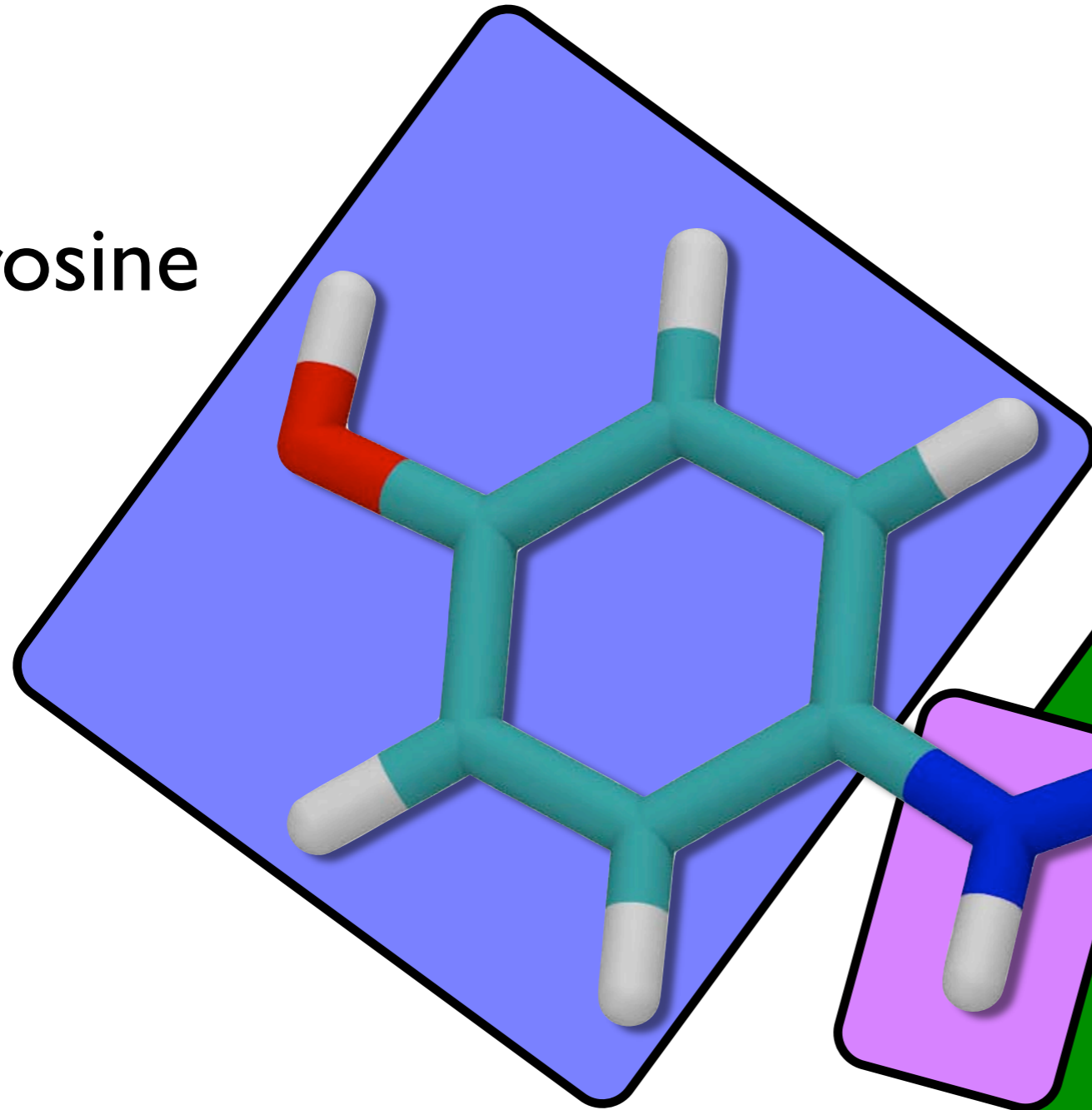
ParaTool <http://www.ks.uiuc.edu/Research/vmd/plugins/paratool/>

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

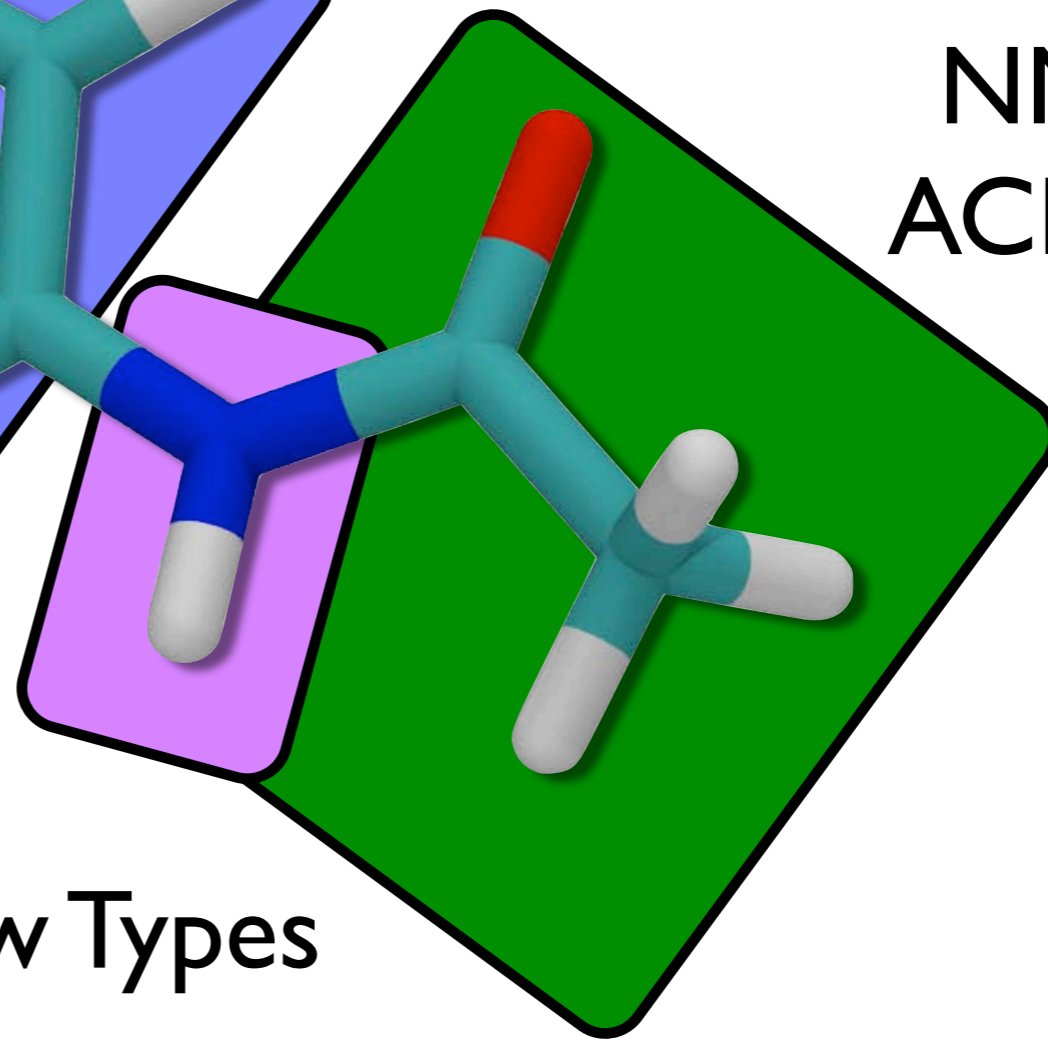
ffTK <http://www.ks.uiuc.edu/Research/vmd/plugins/fftk/>

An Example: Acetaminophen

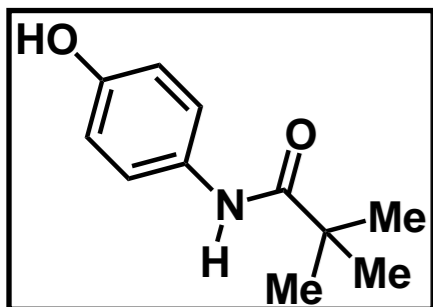
Tyrosine



NMA or
ACE-patch

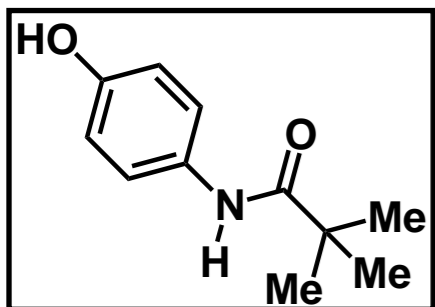
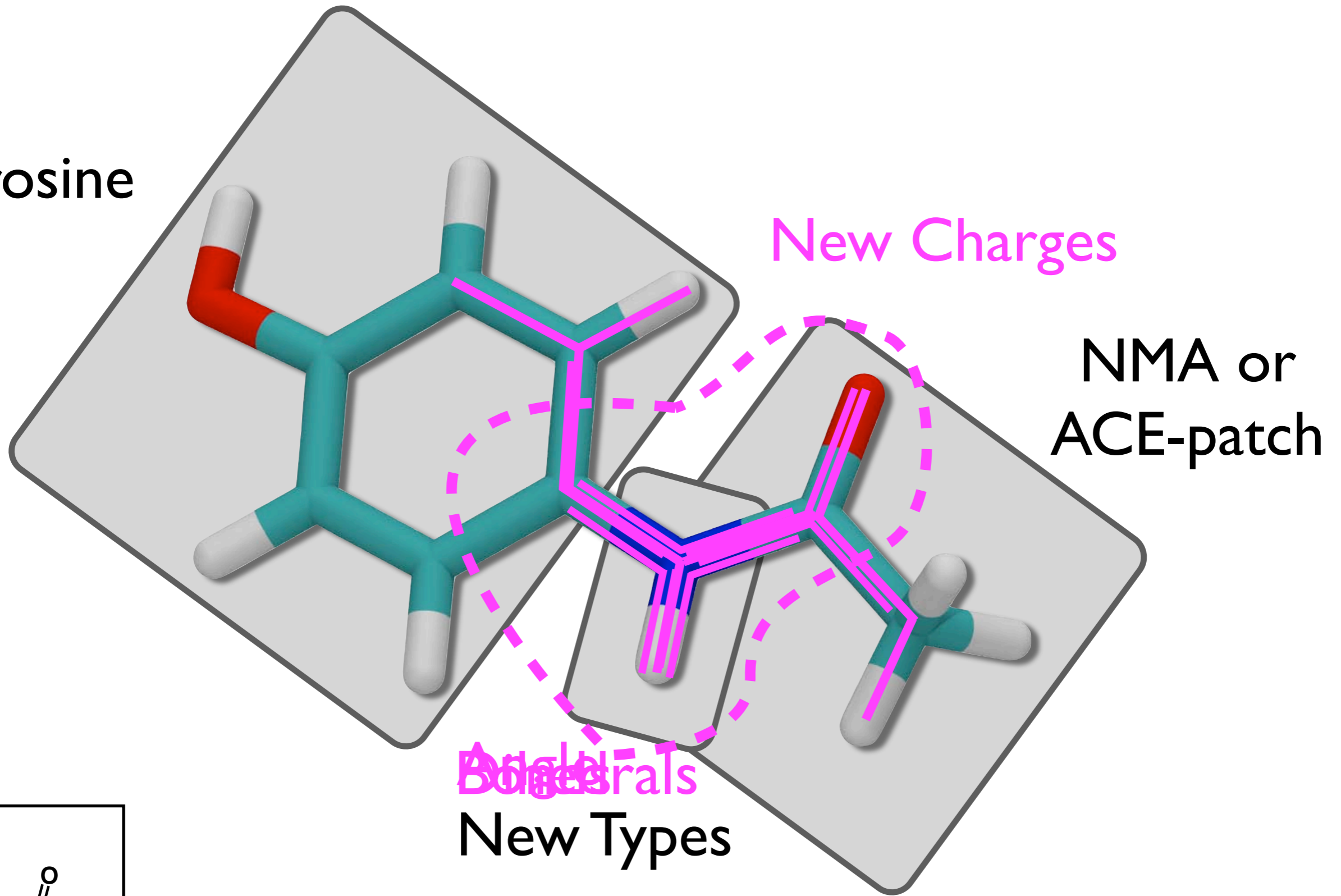


New Types



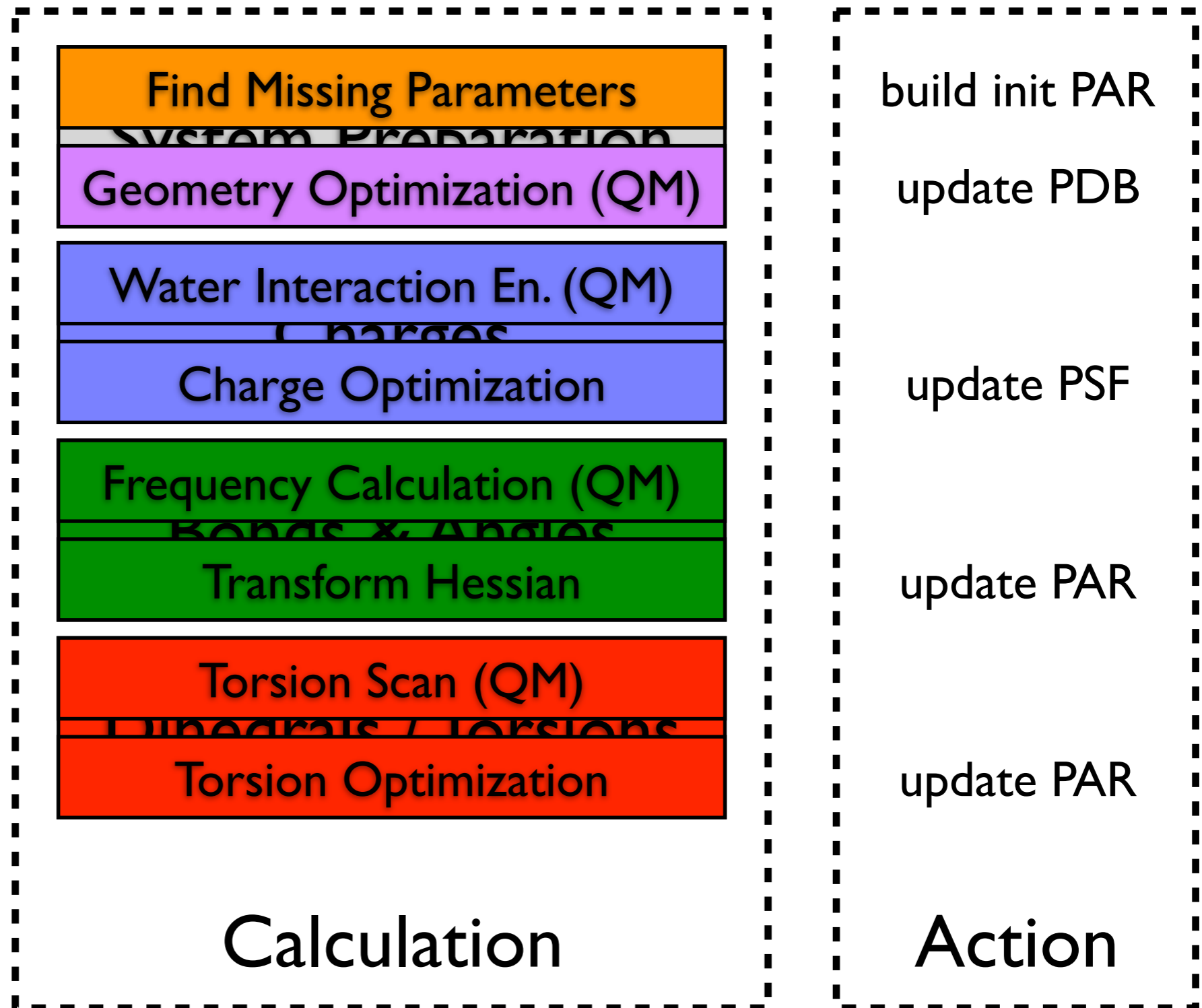
An Example: Acetaminophen

Tyrosine



ffTK Facilitates the Parameterization Workflow

PSF/PDB



PAR File

ffTK Interface

file dialog buttons

entry boxes to hold variables separate tabs

The image shows a screenshot of the ffTK interface with several annotations. At the top, there is a horizontal bar with five colored segments: orange, purple, blue, green, and red. Below this bar is a tabbed interface with tabs labeled: BuildPar, Opt. Geometry, Water Int., Opt. Charges (selected), Calc. Bonded, Scan Torsions, and Opt. Torsions. The main content area is titled 'Input' and contains several sections: 1. 'Input' section with fields for 'PSF File' (containing '/Users/cmayne/Desktop/test11/01-sysprep/pacp.psf'), 'PDB File' (containing '/Users/cmayne/Desktop/test11/02-geoopt/pacp-opt.pdb'), and 'Residue Name' (containing 'PACP'). There are 'Browse' buttons next to the file fields and a 'Load PSF/PDB' button. 2. 'Parameter Files (both pre-defined and in-progress)' section with a list box containing two file paths: '/Users/cmayne/Desktop/test11/common/pacp-init.par' and '/Users/cmayne/Desktop/test11/common/par_all22_prot.inp'. There are 'Add', 'Delete', and 'Clear' buttons to the right. 3. 'NAMD binary' field (containing 'namd2') and 'Output LOG' field (containing 'tmp.log'), both with 'Browse' and 'SaveAs' buttons. 4. A 'Label Atoms' section with a 'Name' dropdown menu. 5. A bottom section with expandable items: 'Charge Constraints', 'QM Target Data', 'Advanced Settings', and 'Results'. Annotations with arrows point to various elements: 'entry boxes to hold variables' points to the PSF File field; 'file dialog buttons' points to the 'Browse' buttons; 'separate tabs' points to the 'Opt. Charges' tab; 'action buttons' points to the 'Load PSF/PDB' button; 'action menus' points to the 'Add', 'Delete', and 'Clear' buttons; 'treeview boxes to hold lists' points to the list box for parameter files; and 'back' points to the 'Name' dropdown menu.

arrow

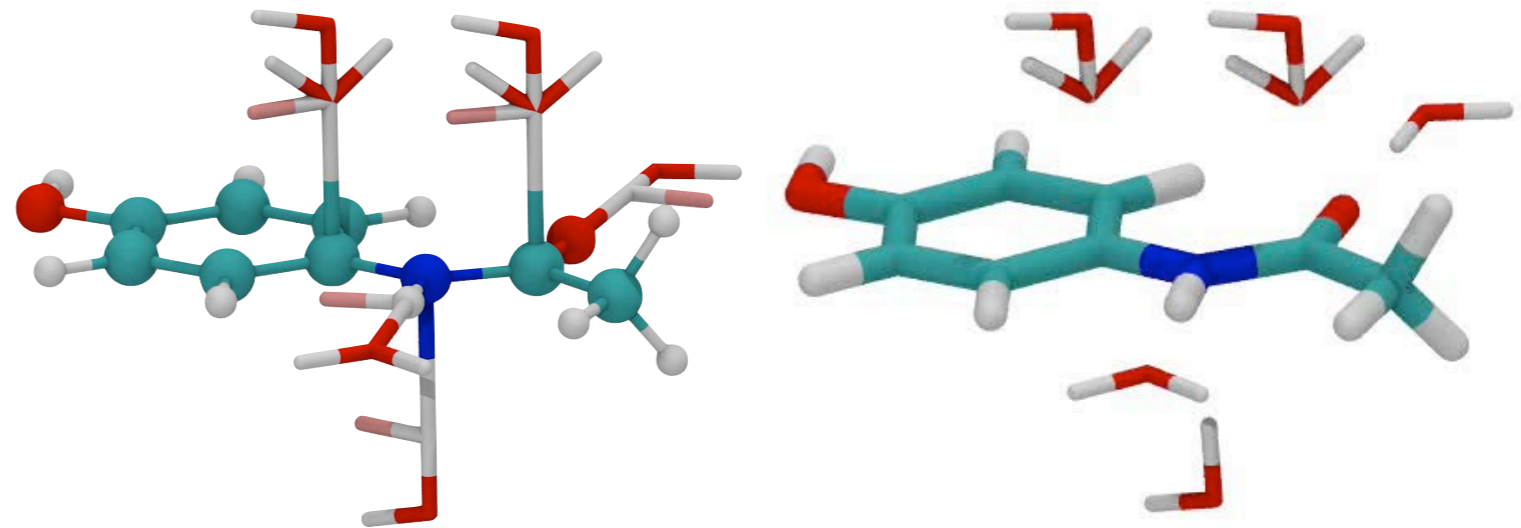
action menus

treeview boxes to hold lists

back

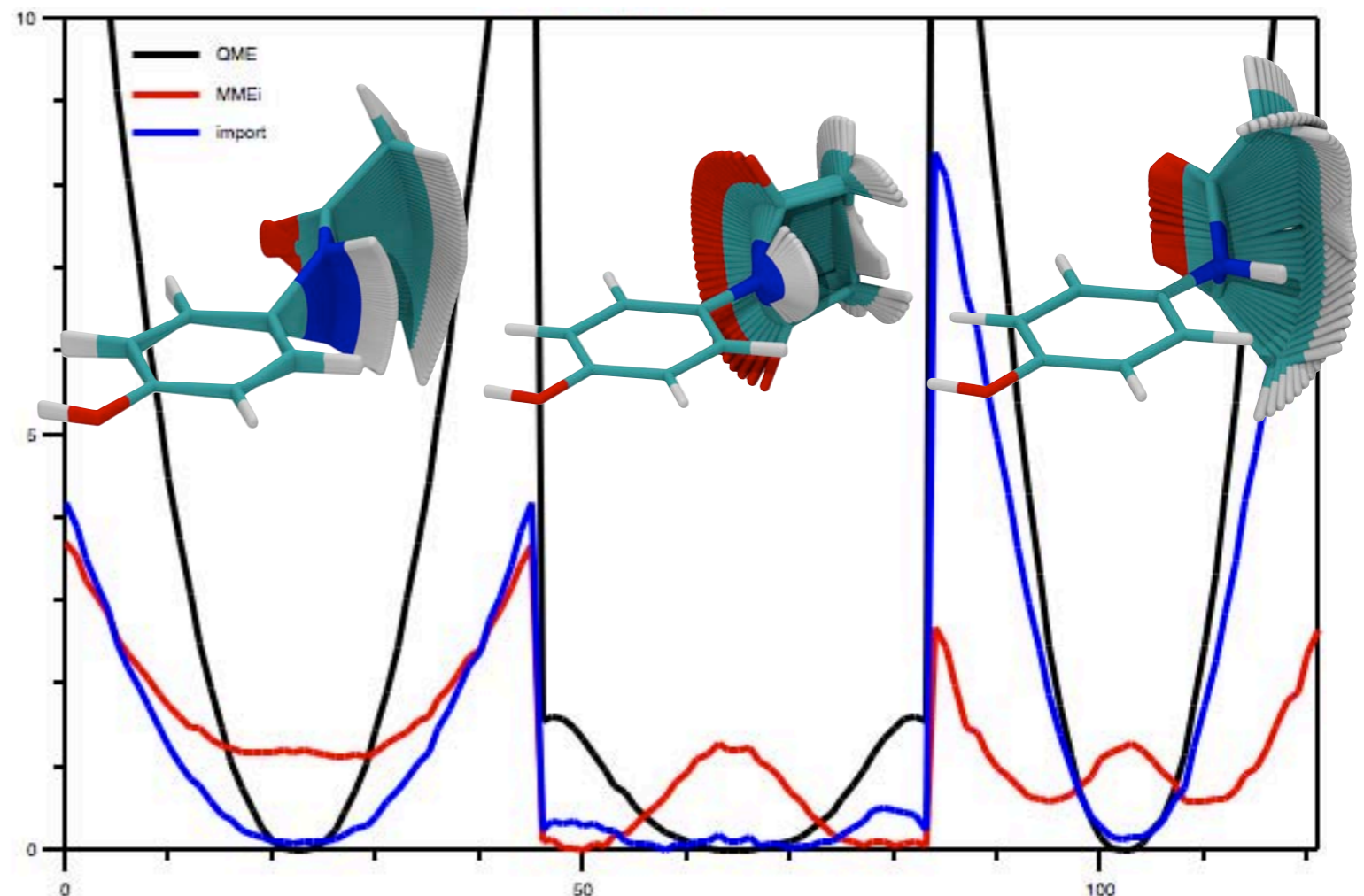
ffTK 1.0 is Available in VMD 1.9.1

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?



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