

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

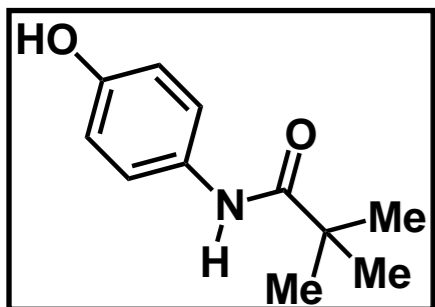
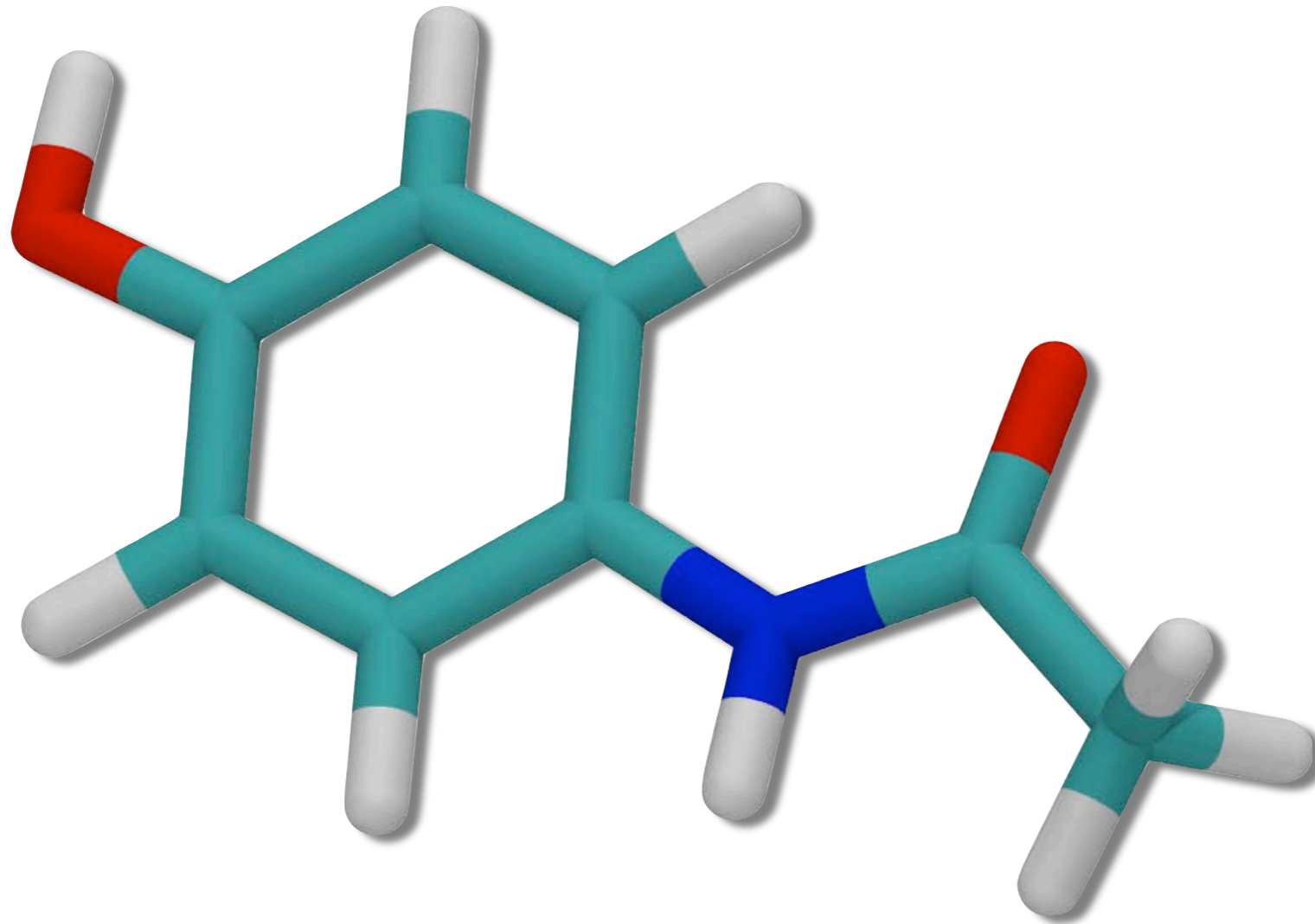
Development

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

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

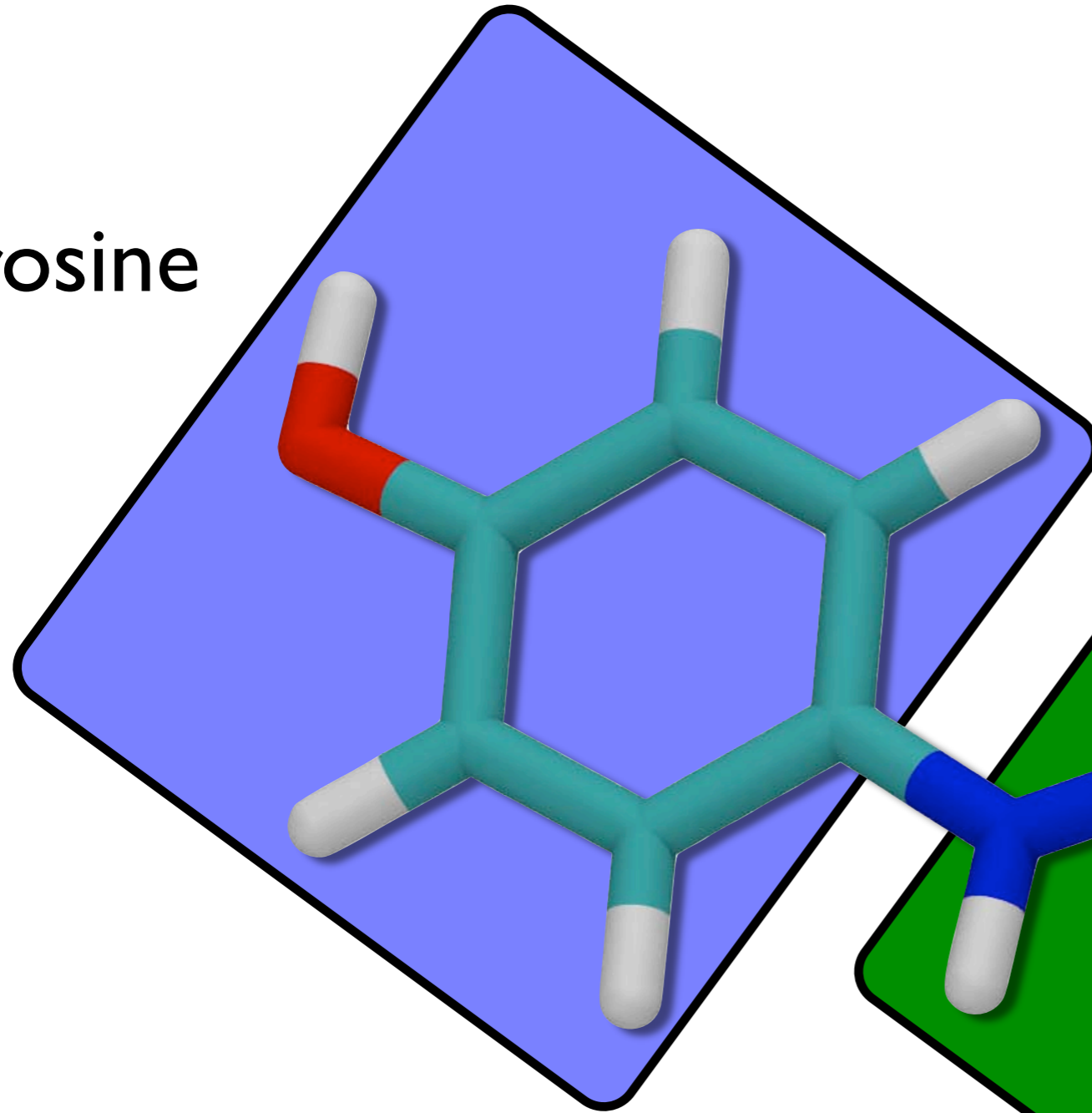
ffTK <http://www.ks.uiuc.edu/Research/vmd/plugins/fftk/>

An Example: Acetaminophen

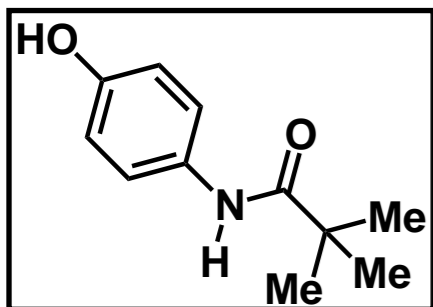
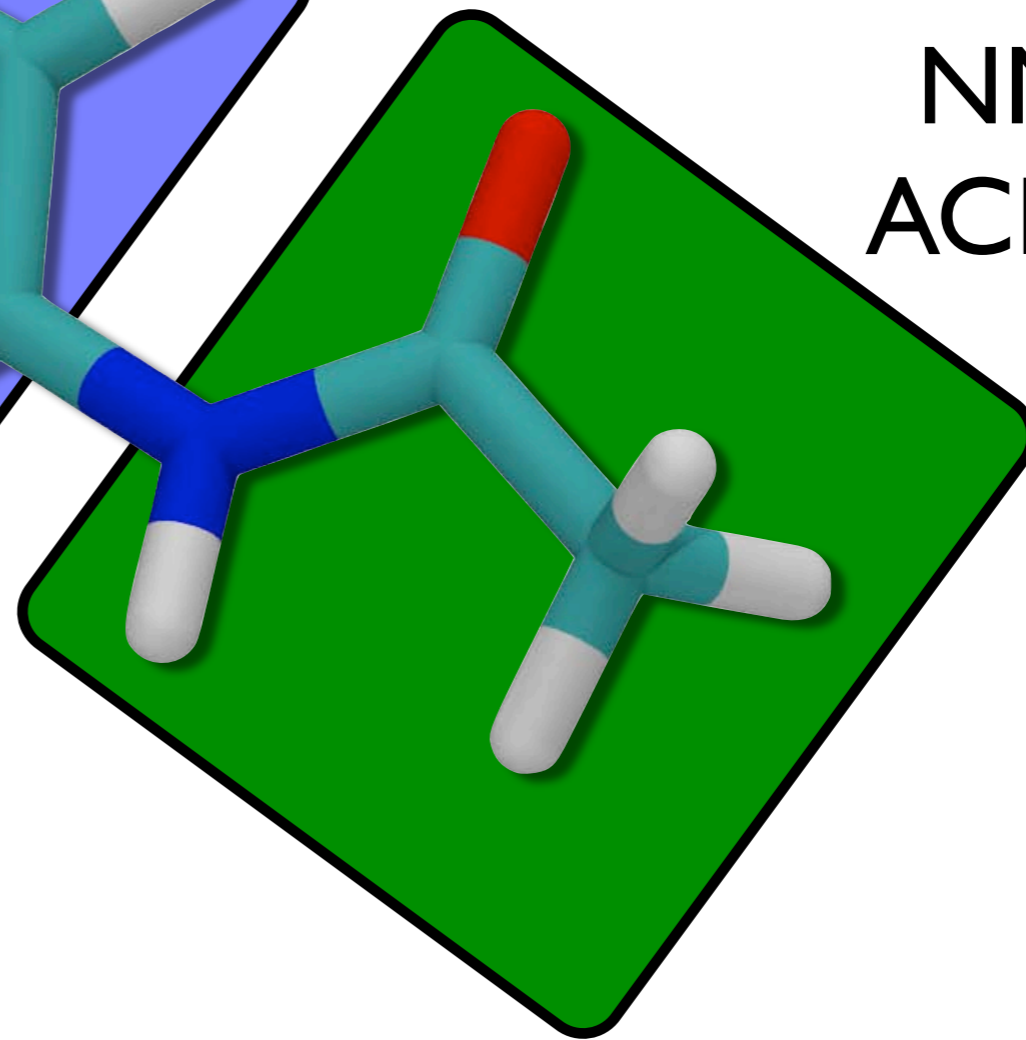


An Example: Acetaminophen

Tyrosine

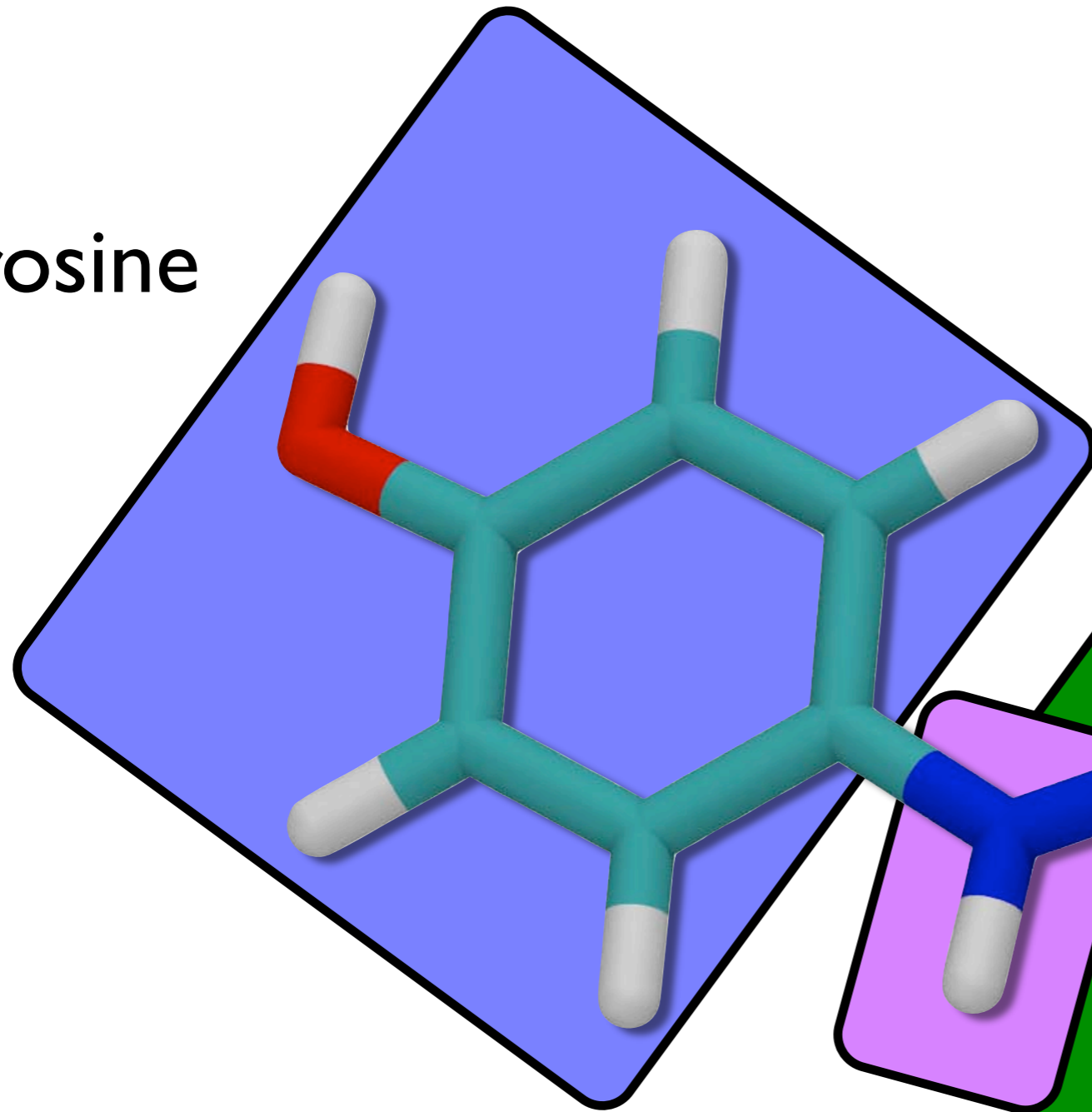


NMA or
ACE-patch

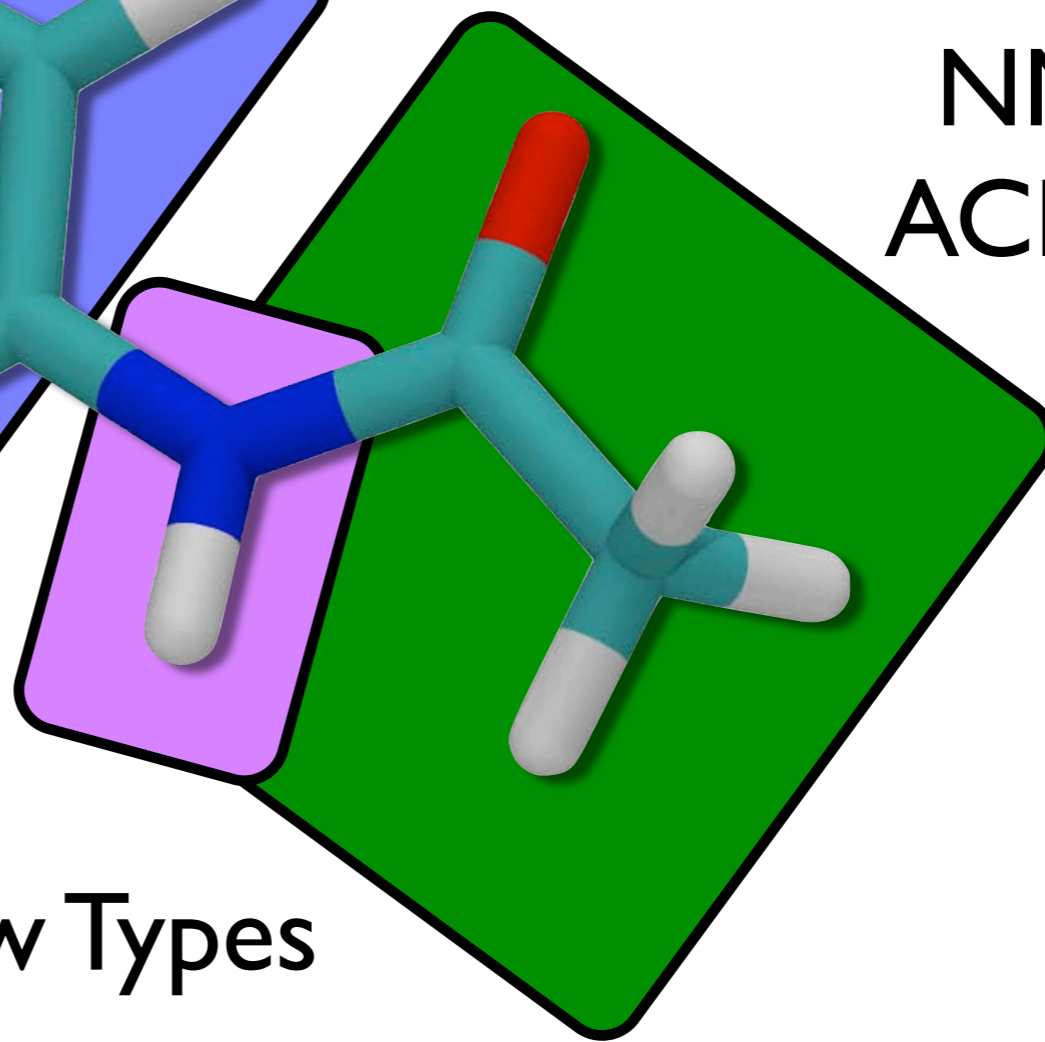


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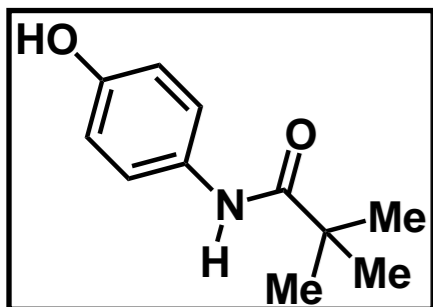
Tyrosine



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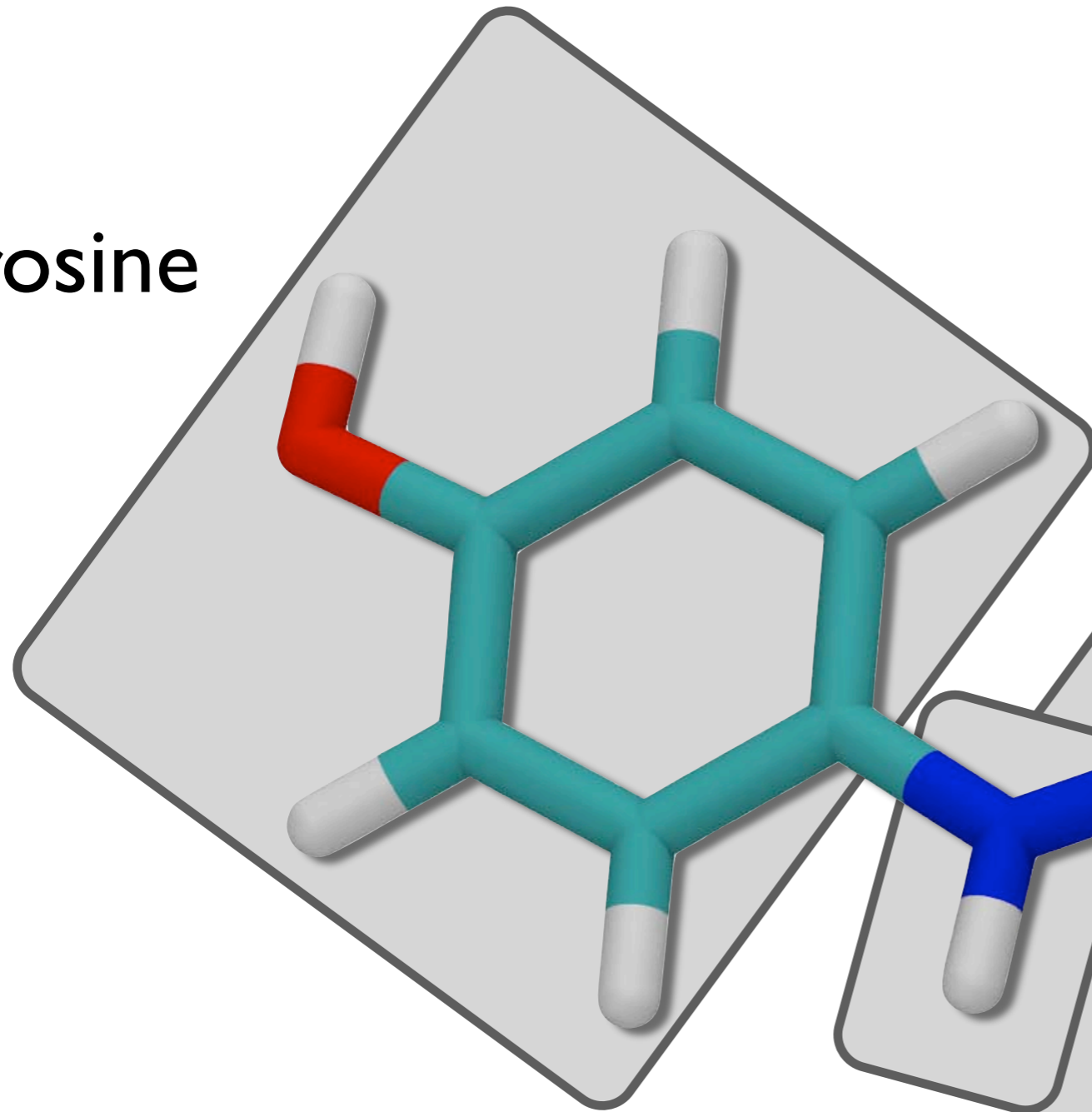


New Types

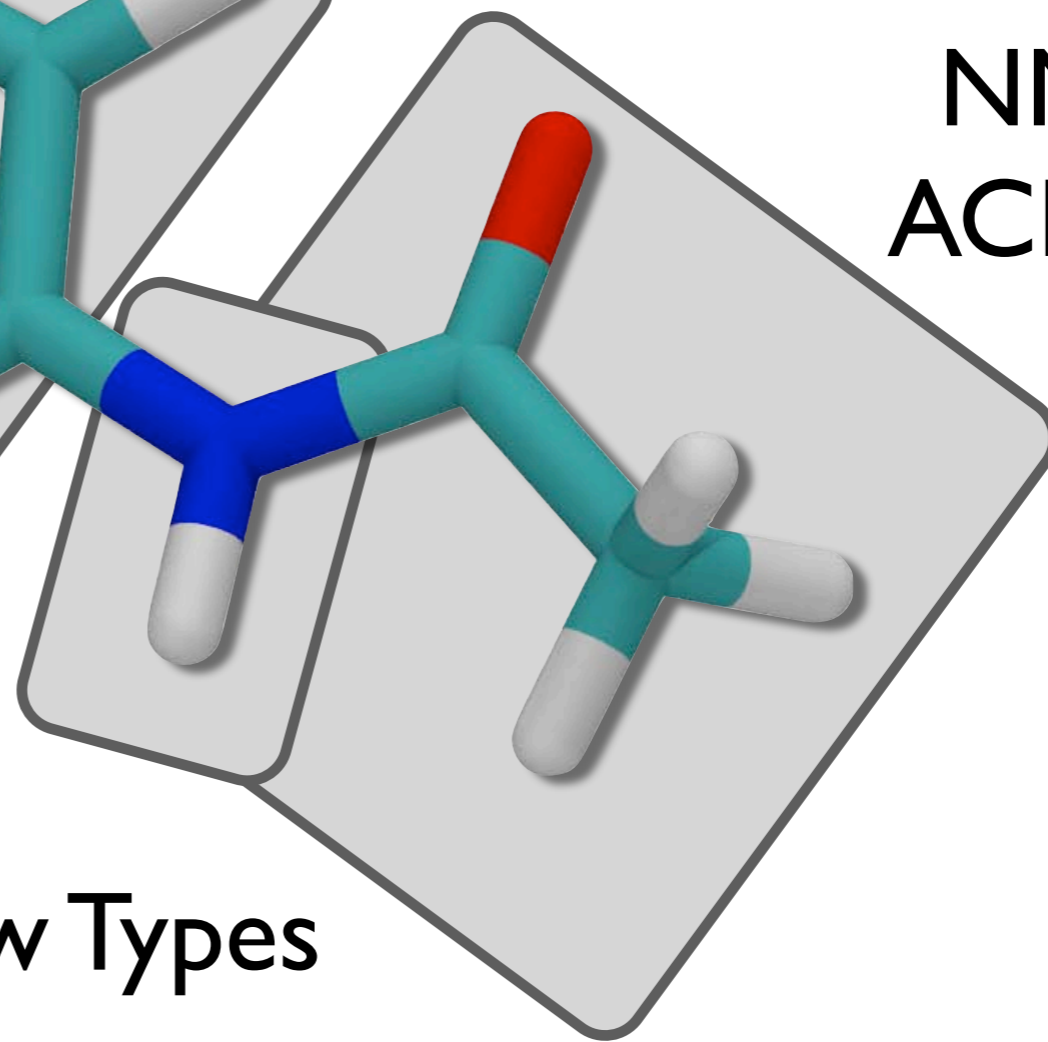


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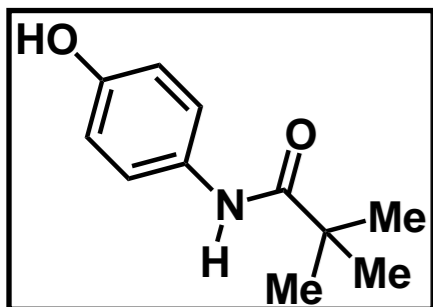
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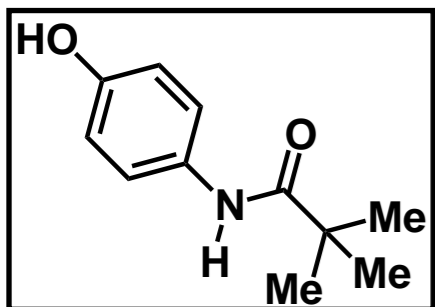
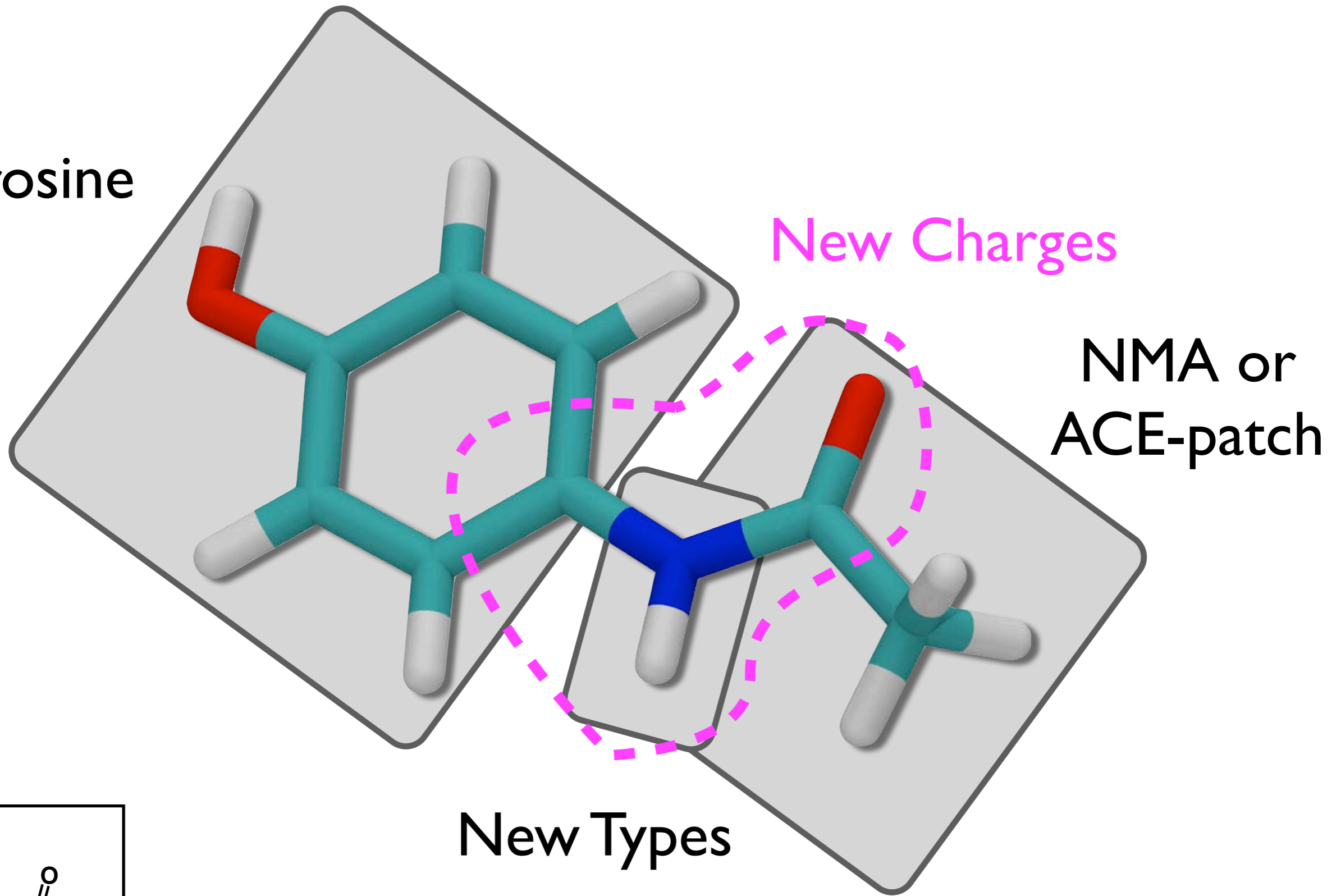


New Types



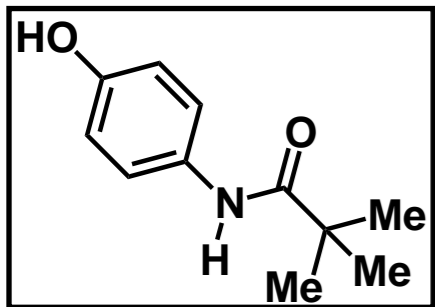
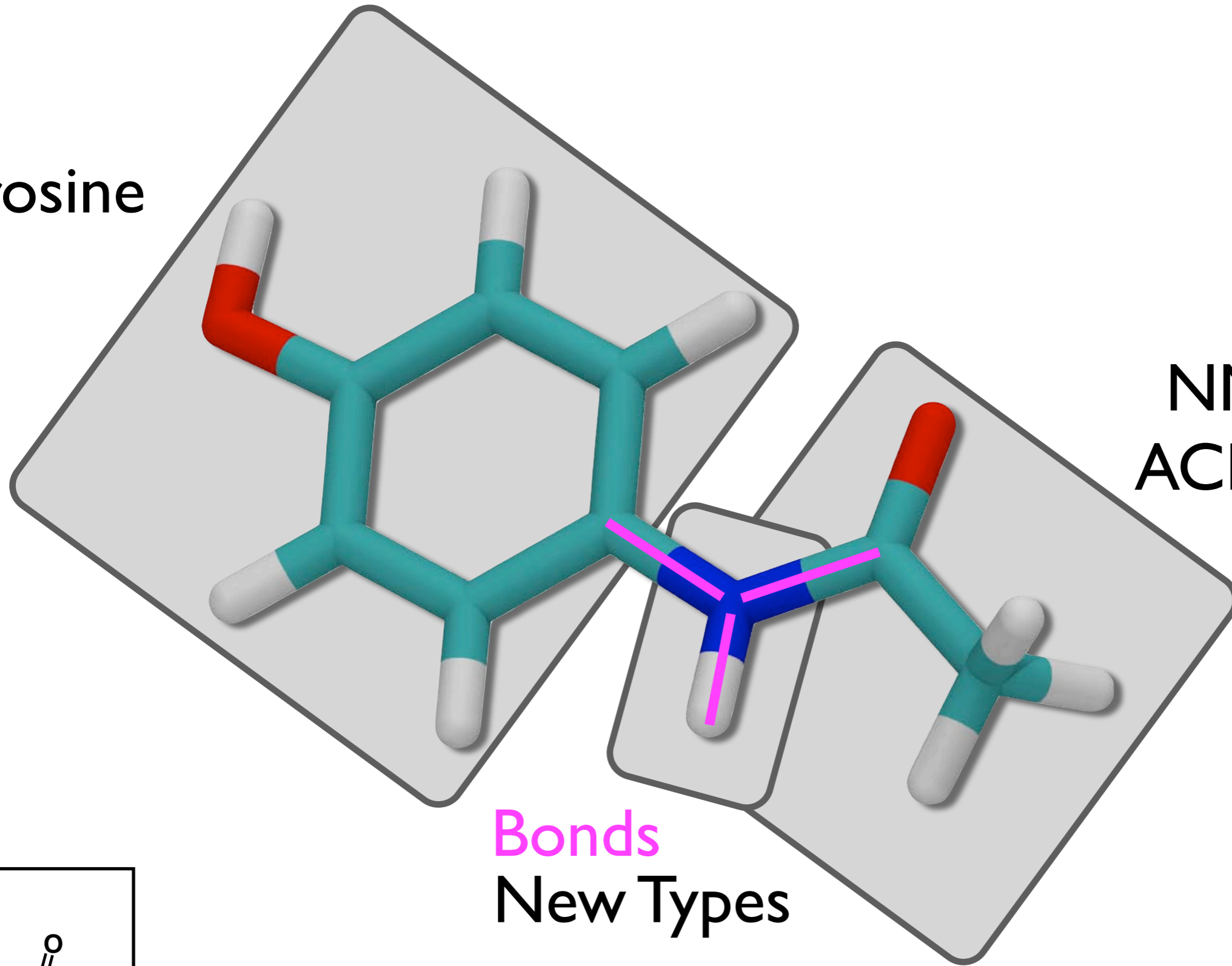
An Example: Acetaminophen

Tyrosine



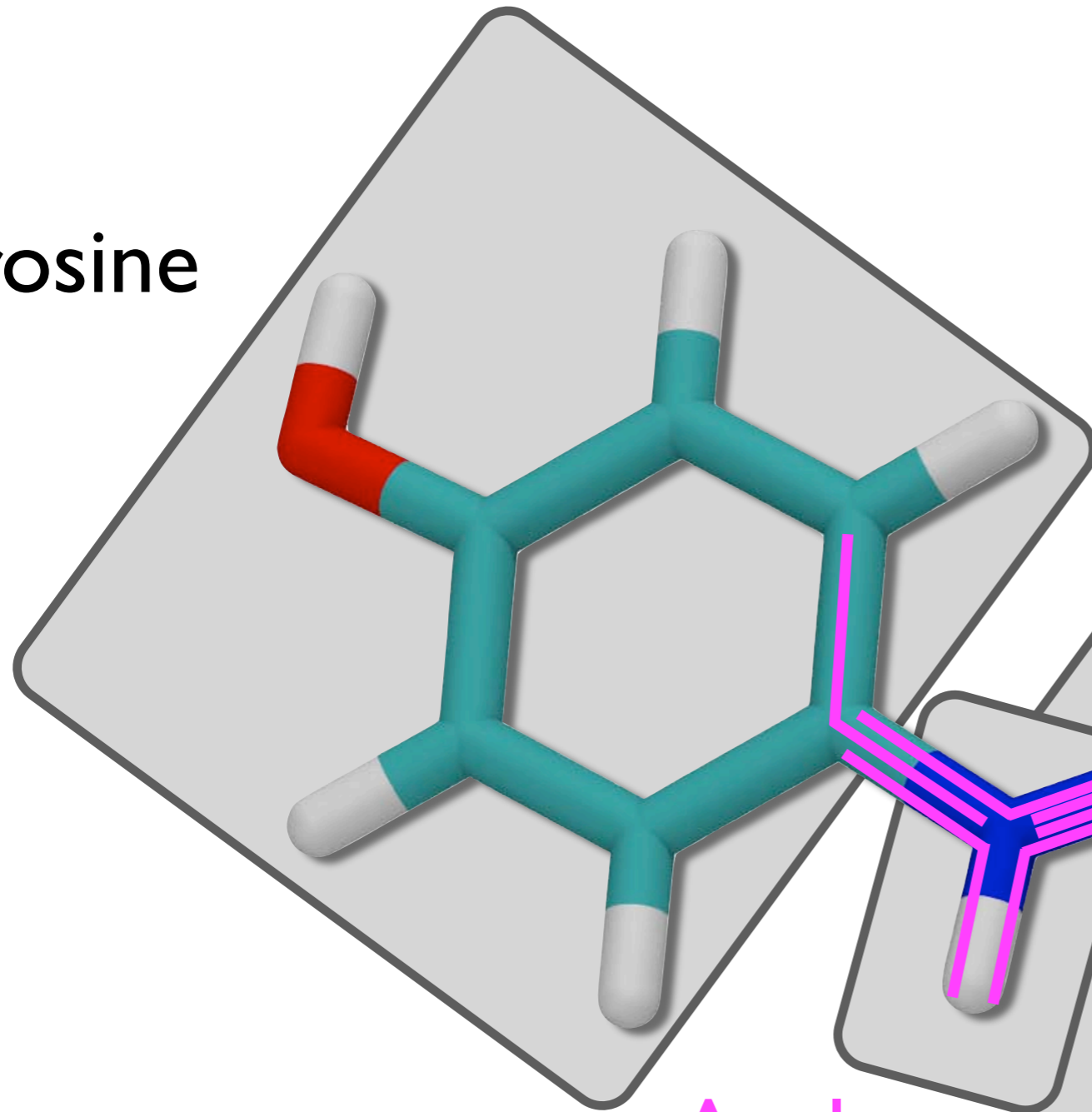
An Example: Acetaminophen

Tyrosine

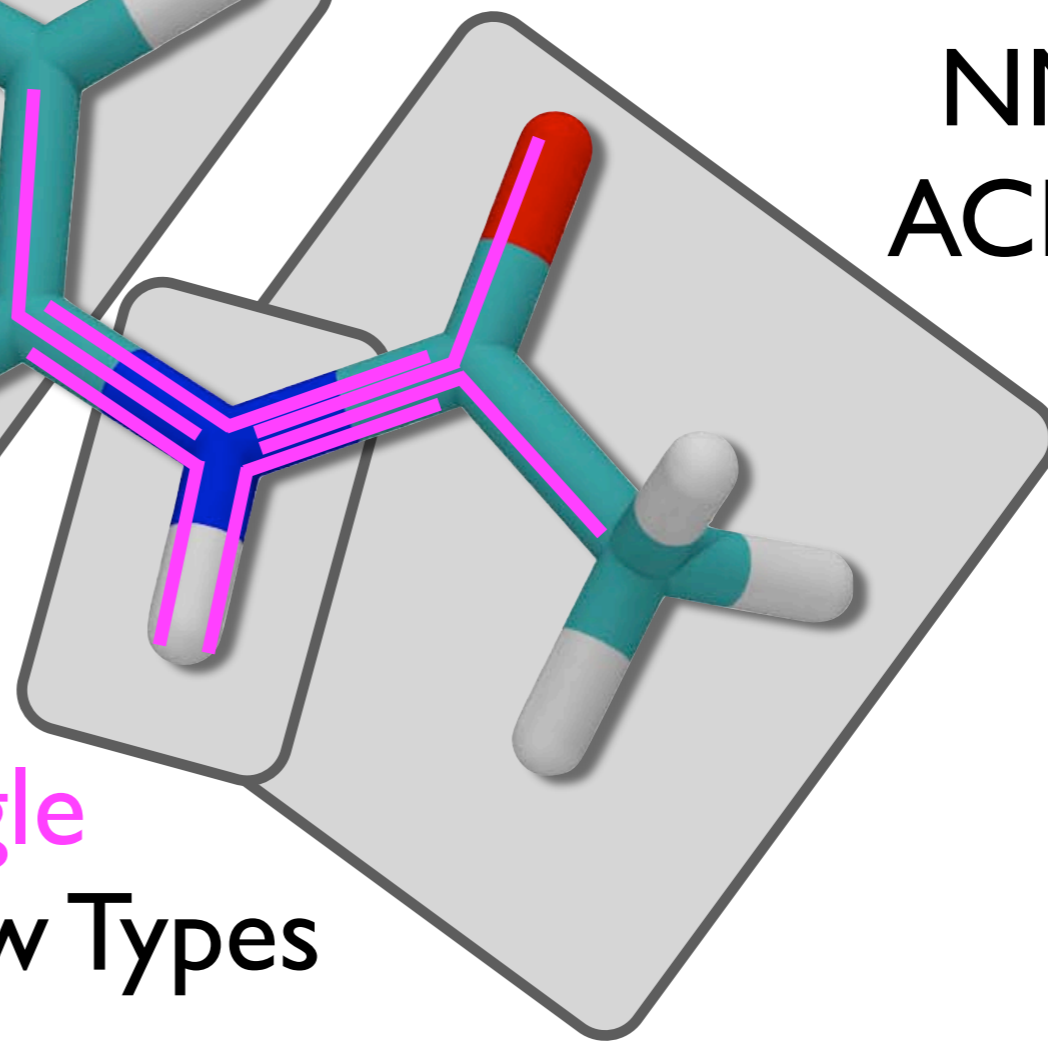


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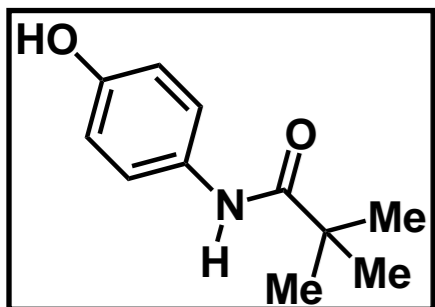
Tyrosine



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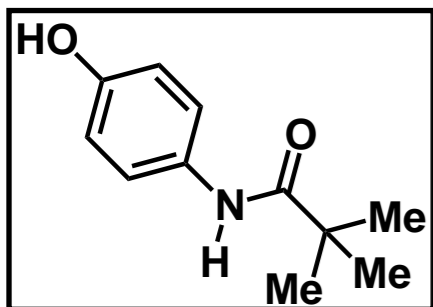
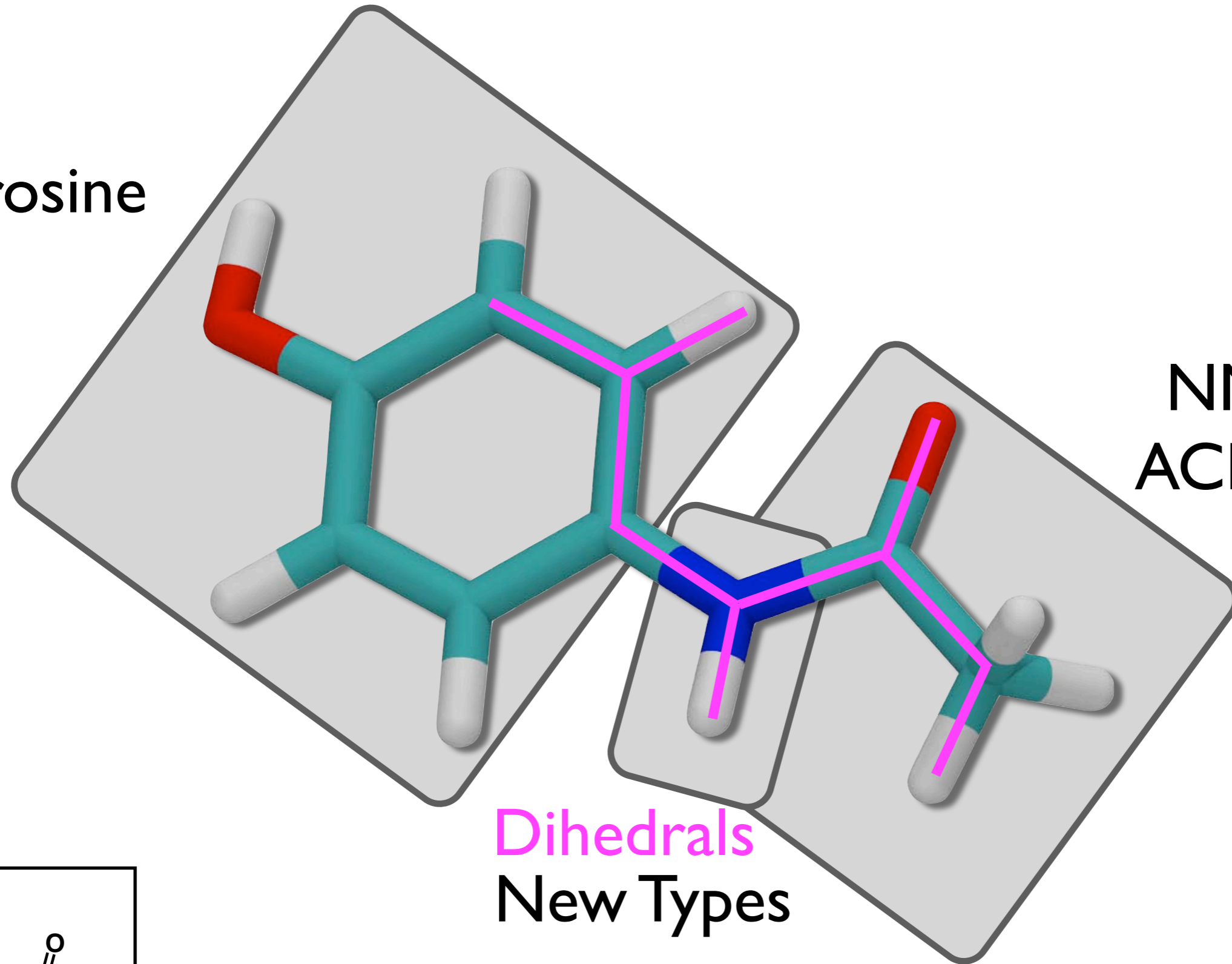


Angle
New Types

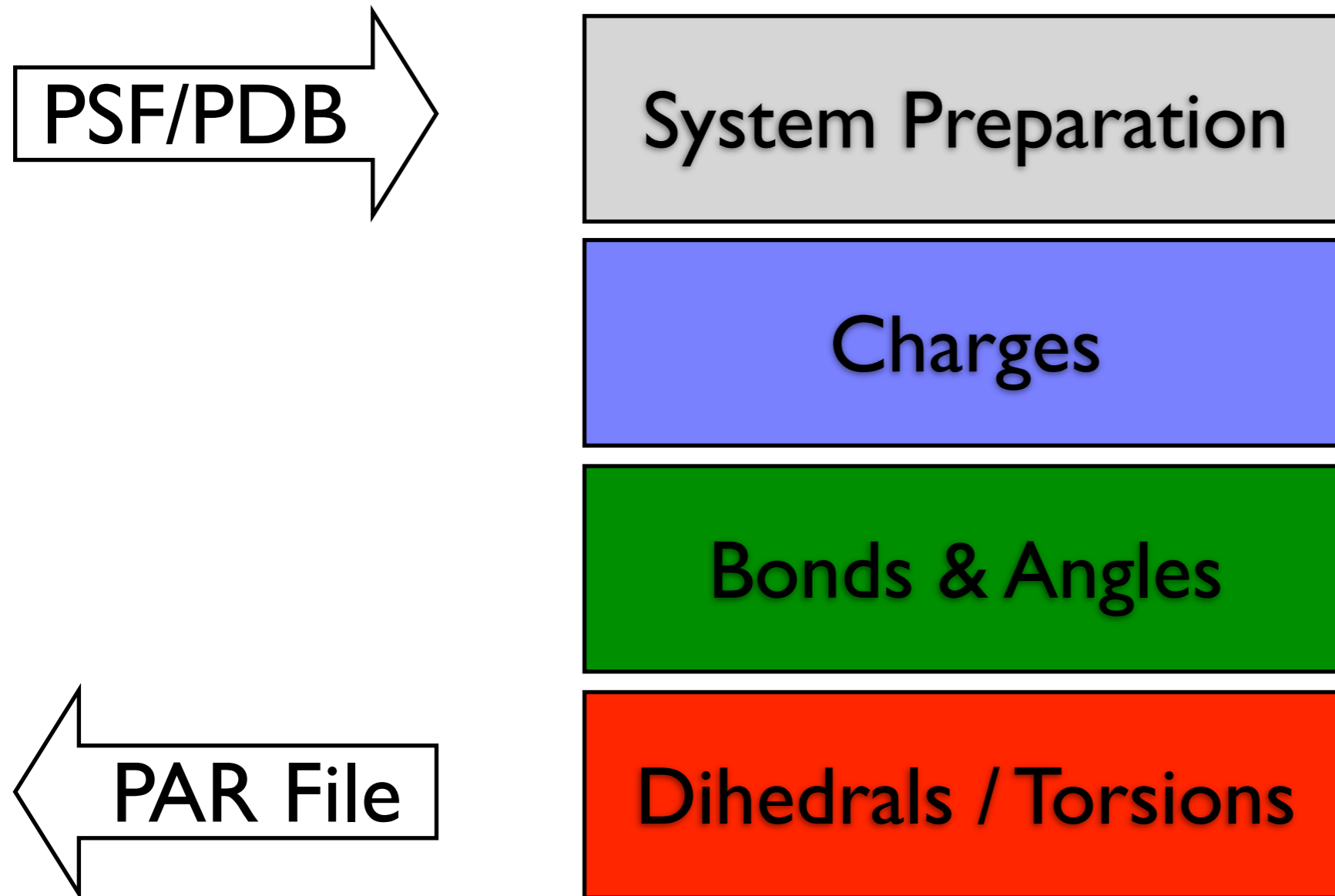


An Example: Acetaminophen

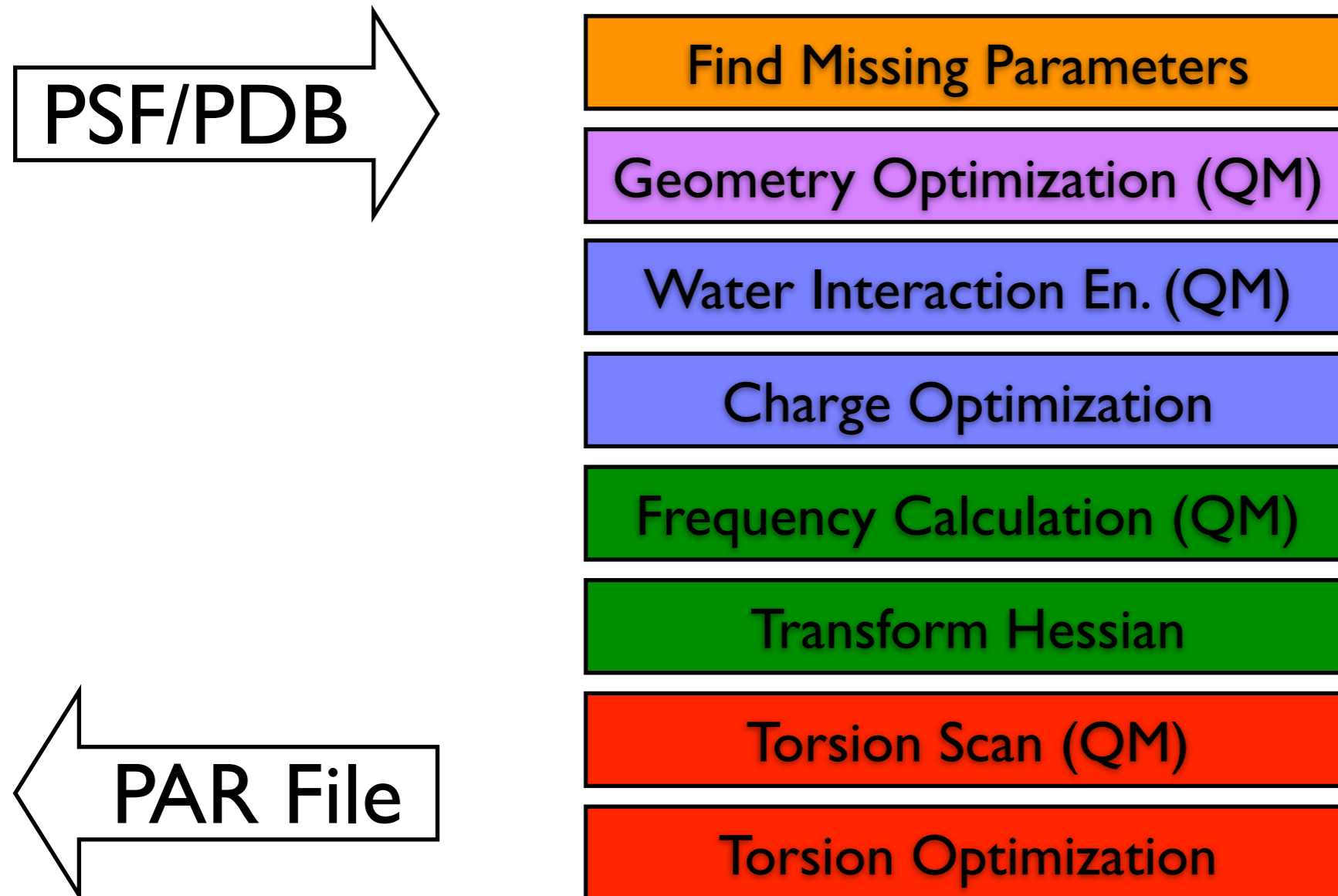
Tyrosine



ffTK Facilitates the Parameterization Workflow



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PSF/PDB

Find Missing Parameters

Geometry Optimization (QM)

Water Interaction En. (QM)

Charge Optimization

Frequency Calculation (QM)

Transform Hessian

Torsion Scan (QM)

Torsion Optimization

Calculation

build init PAR

update PDB

update PSF

update PAR

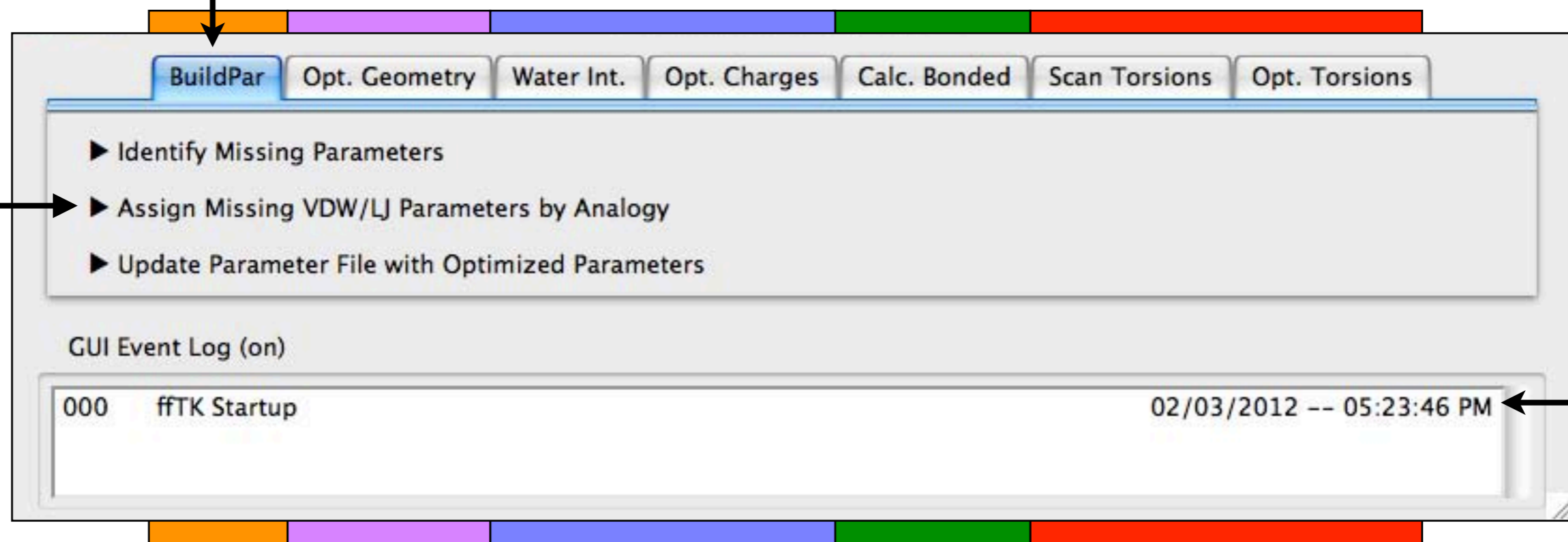
update PAR

Action

PAR File

ffTK Interface

tasks divided into separate tabs



arrows/triangles indicate collapsable elements

event log provides visual feedback

ffTK Interface

file dialog buttons

entry boxes to hold variables

action buttons

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 menu bar with tabs: BuildPar, Opt. Geometry, Water Int., Opt. Charges (selected), Calc. Bonded, Scan Torsions, and Opt. Torsions. The main window is titled 'Input' and contains several sections:

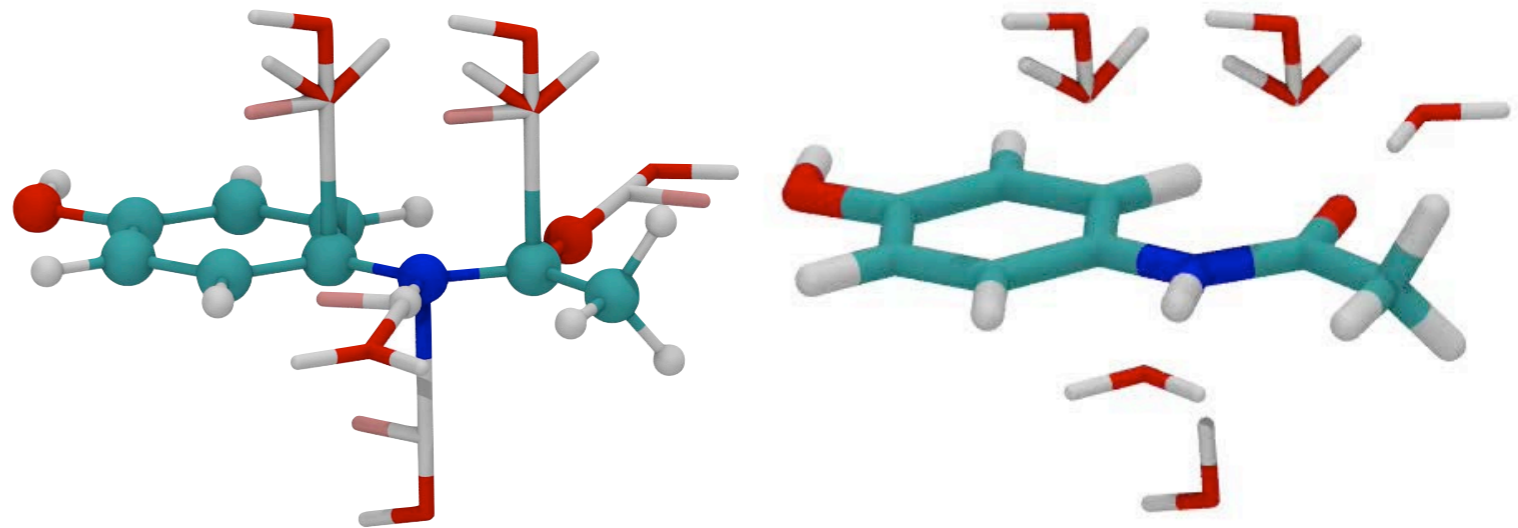
- Input Section:** Contains text boxes for 'PSF File' (with path /Users/cmayne/Desktop/test11/01-sysprep/pacp.psf), 'PDB File' (with path /Users/cmayne/Desktop/test11/02-geoopt/pacp-opt.pdb), and 'Residue Name' (with value PACP). There are 'Browse' buttons next to the file paths and a 'Resname From TOP' button next to the residue name.
- Parameter Files Section:** A list box containing two paths: /Users/cmayne/Desktop/test11/common/pacp-init.par and /Users/cmayne/Desktop/test11/common/par_all22_prot.inp. To the right of this list are 'Add', 'Delete', and 'Clear' buttons.
- NAMD binary and Output LOG Section:** Text boxes for 'NAMD binary' (with value namd2) and 'Output LOG' (with value tmp.log). There are 'Browse' and 'SaveAs' buttons next to these fields.
- Treeview Section:** A list of expandable items: Charge Constraints, QM Target Data, Advanced Settings, and Results.

Annotations with arrows point to various elements:

- An arrow points from the text 'entry boxes to hold variables' to the 'PSF File' text box.
- An arrow points from the text 'file dialog buttons' to the 'Browse' buttons.
- An arrow points from the text 'action buttons' to the 'Load PSF/PDB', 'Label Atoms', 'Add', 'Delete', and 'Clear' buttons.
- An arrow points from the text 'action menus' to the 'Name' dropdown menu.
- An arrow points from the text 'treeview boxes to hold lists' to the list box containing parameter file paths.

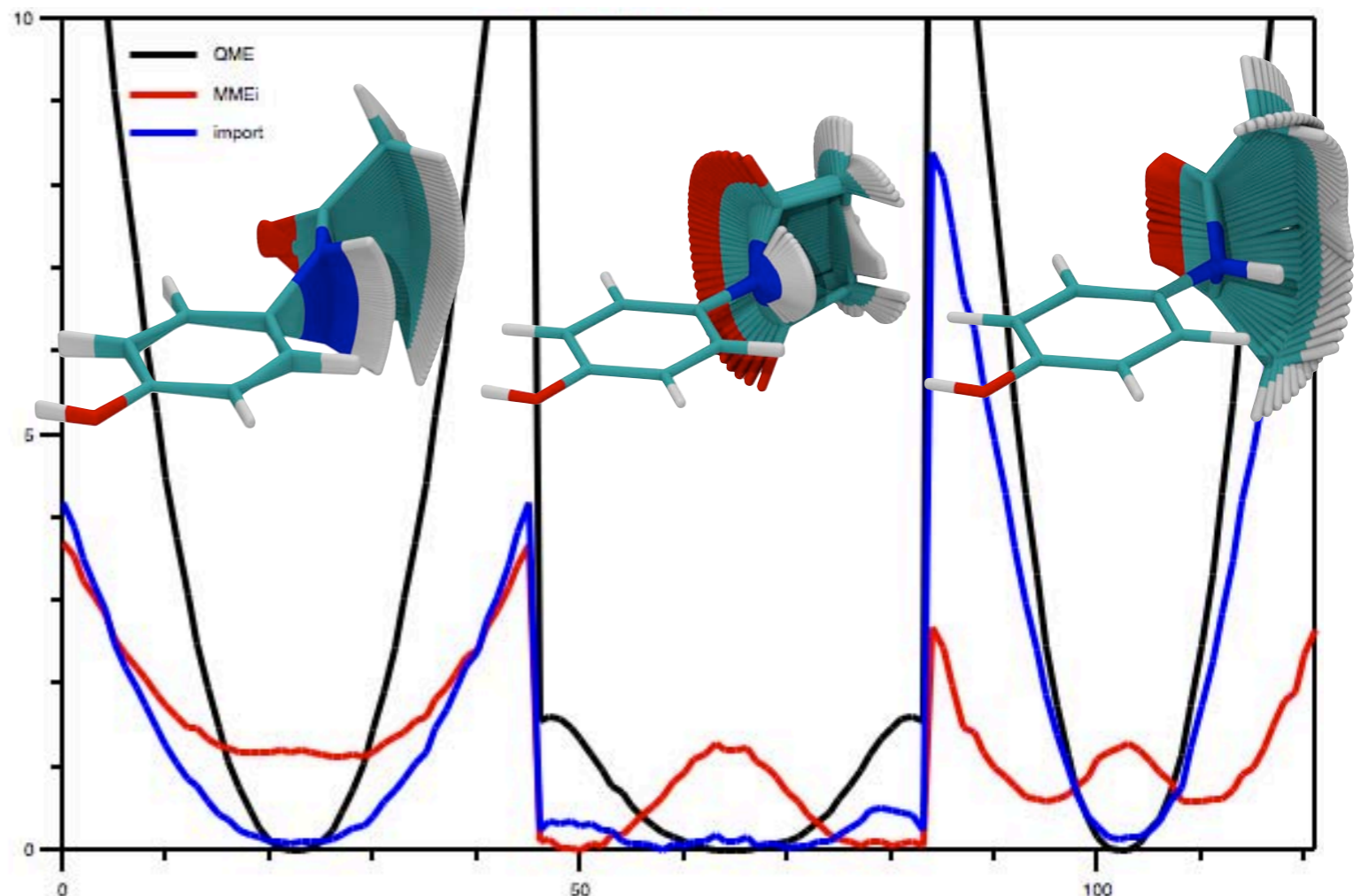
ffTK 1.0 is Available in VMD 1.9.1

- 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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