

Navigating Rosetta

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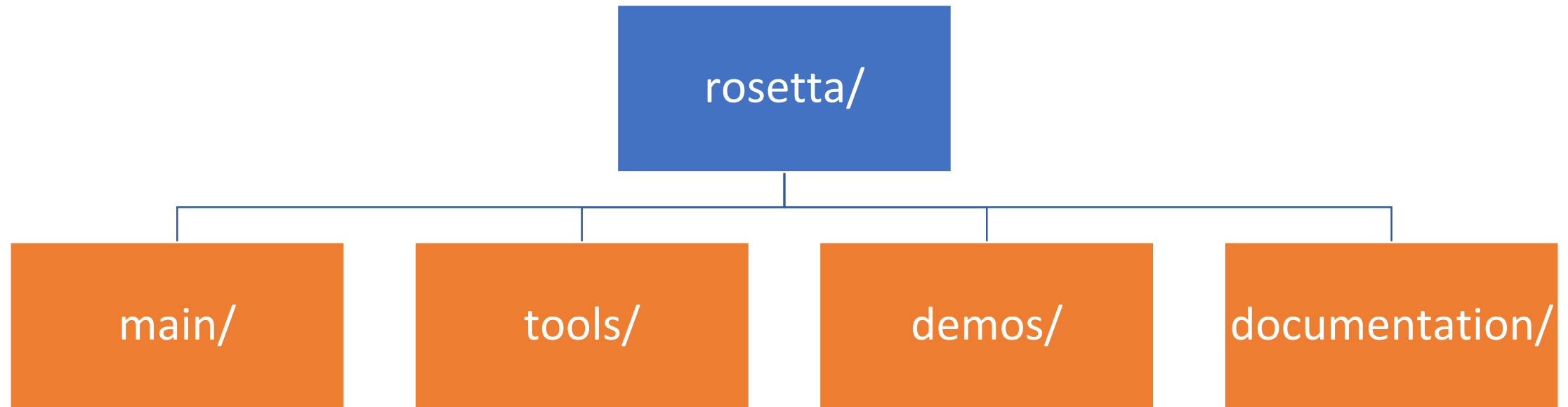
Meiler Lab, Vanderbilt University

Goals for this Talk

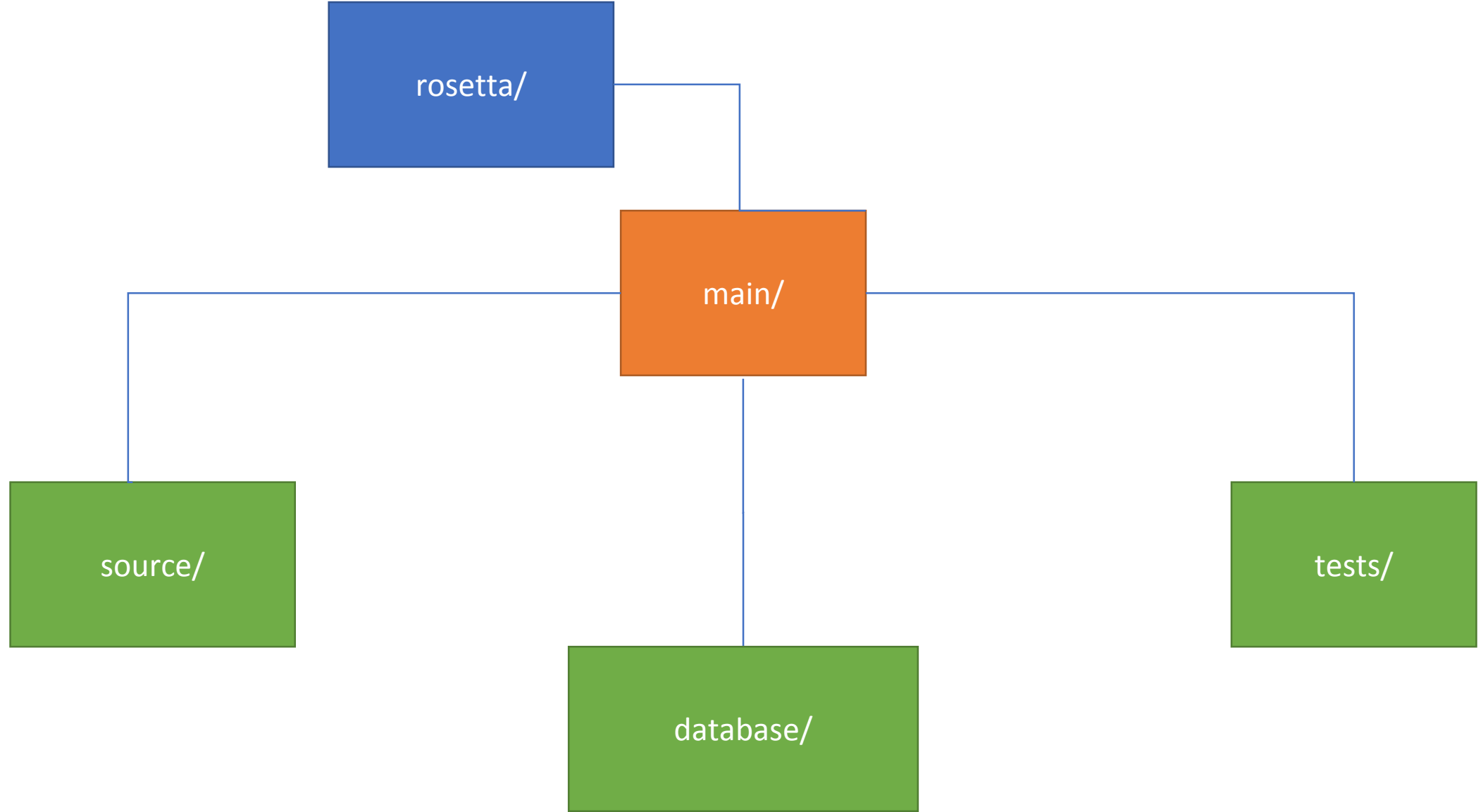
- Learn where things are in Rosetta
- Your working directory is independent of these Rosetta directories
 - Aka your data is stored outside of Rosetta
- Highly encourage everybody to follow along from your command line
 - Full path = path to file from home directory (~ = /usr/people/molgraph/)
 - Relative path = path to file from current working directory
- Please stop me for questions!

cd ~/rosetta_workshop/rosetta/

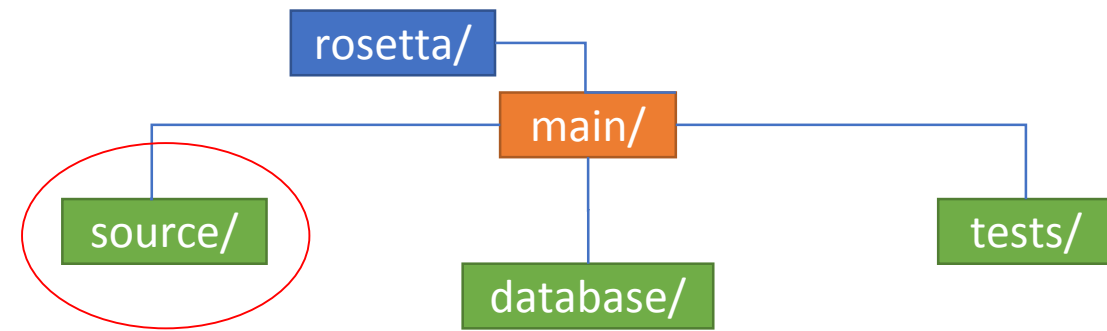
Basic Rosetta Structure



cd ~/rosetta_workshop/rosetta/main

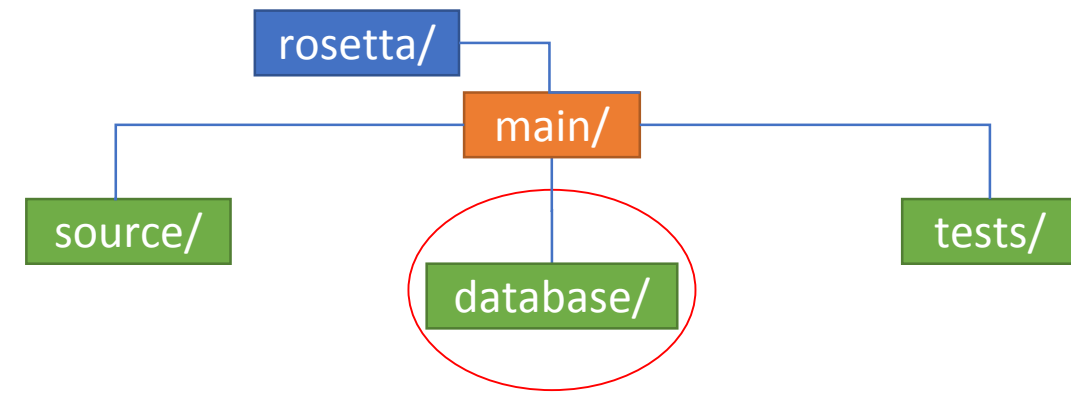


```
cd ~/rosetta_workshop/rosetta/main/source/
```



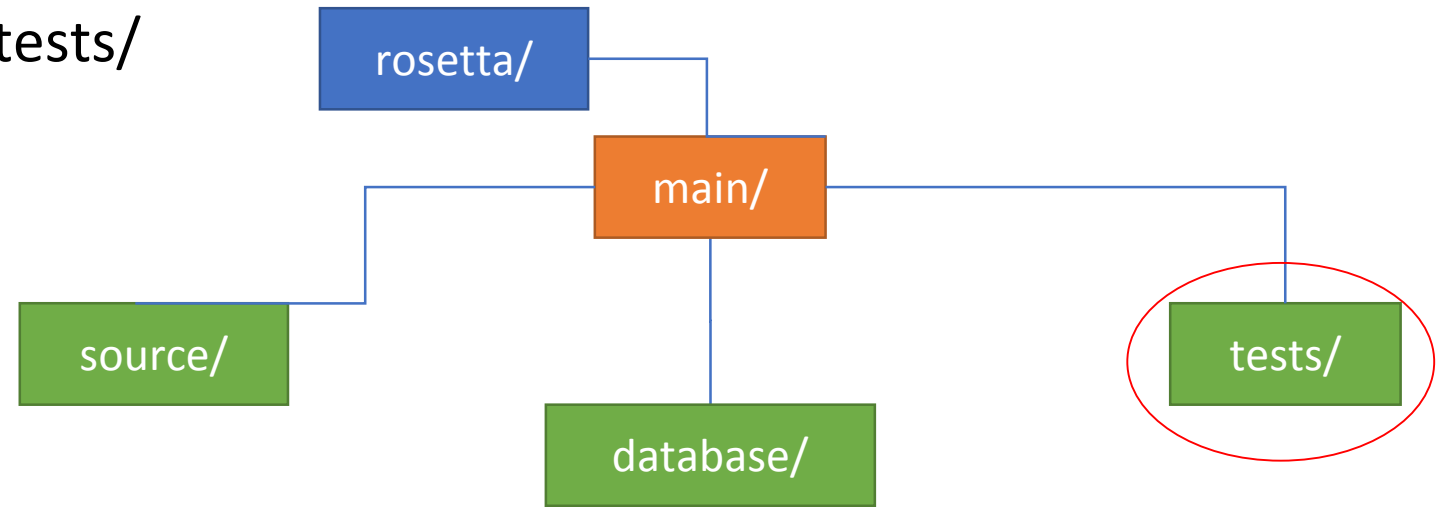
- [Rosetta/main/source/bin/](#)
 - Most applications you will run are calling programs within the bin directory
 - rosetta_scripts.default.linuxgccrelease
 - score_jd2.default.linuxgccrelease
 - relax.default.linuxgccrelease
- [Rosetta/main/source/scons.py](#)
 - Used for compiling
- [Rosetta/main/source/src/](#)
 - This is where all of the code lives

```
cd ~/rosetta_workshop/rosetta/main/database/  
(relative path from source/ dir: cd ../database/)
```



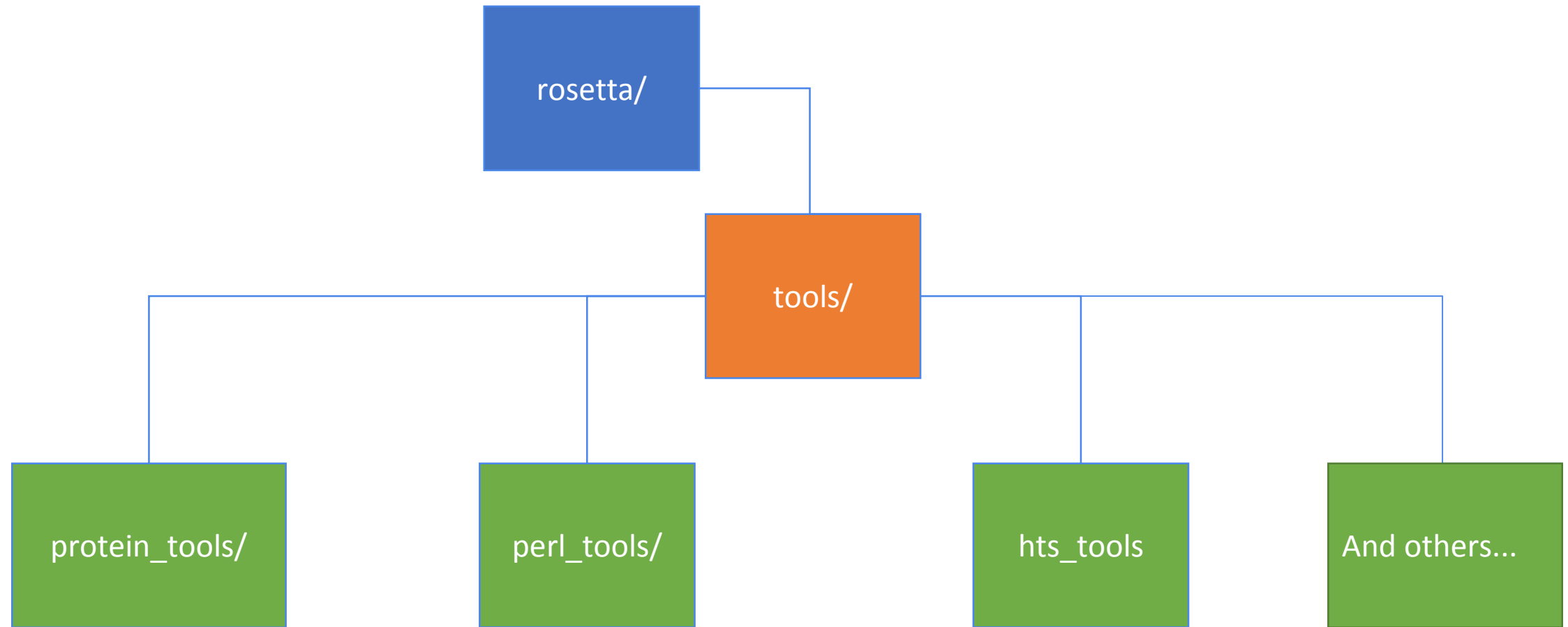
- Contains pre-defined information that Rosetta needs for runs
- [Rosetta/main/database/chemical/](#)
 - Residue information--params files
 - Atom sets
- [Rosetta/main/database/scoring/](#)
 - Default weights files
 - Rotamer libraries

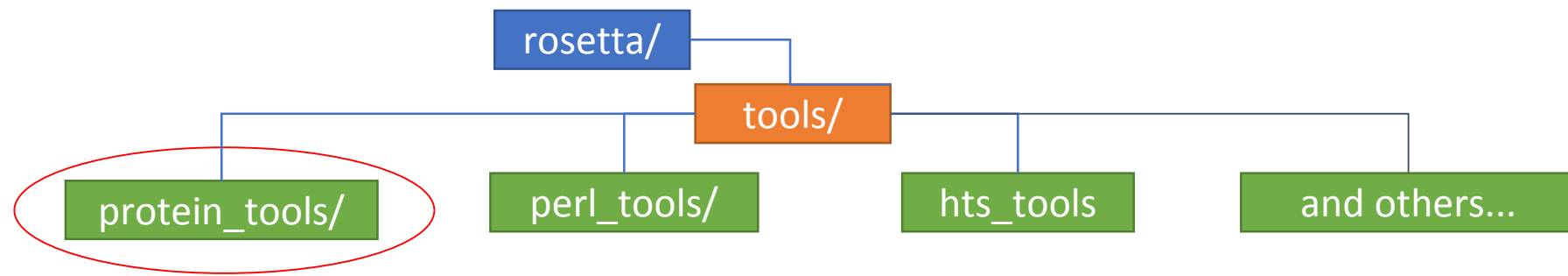
```
cd ~/rosetta_workshop/rosetta/main/tests/
```



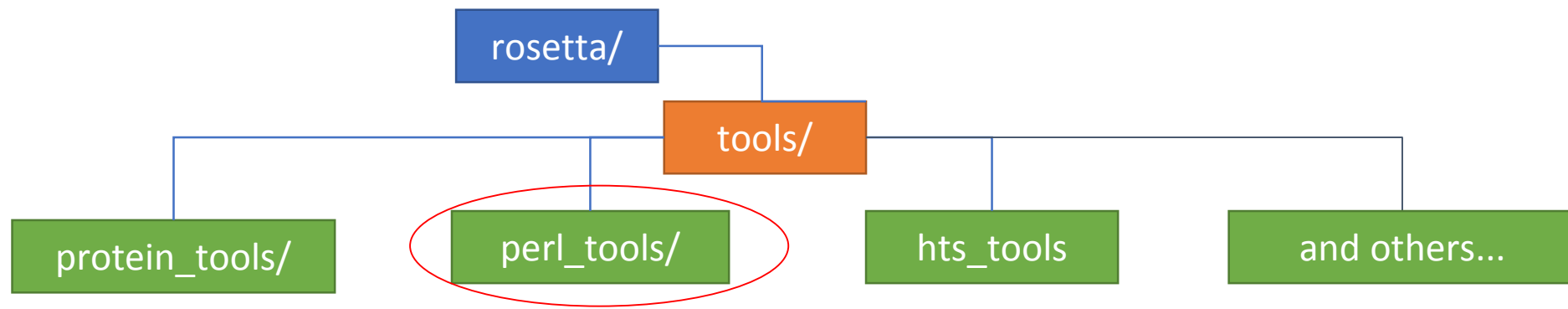
- [Rosetta/main/tests/](#)
 - This is for developer use--don't worry about this (fun to read though!)

cd ~/rosetta_workshop/rosetta/tools/

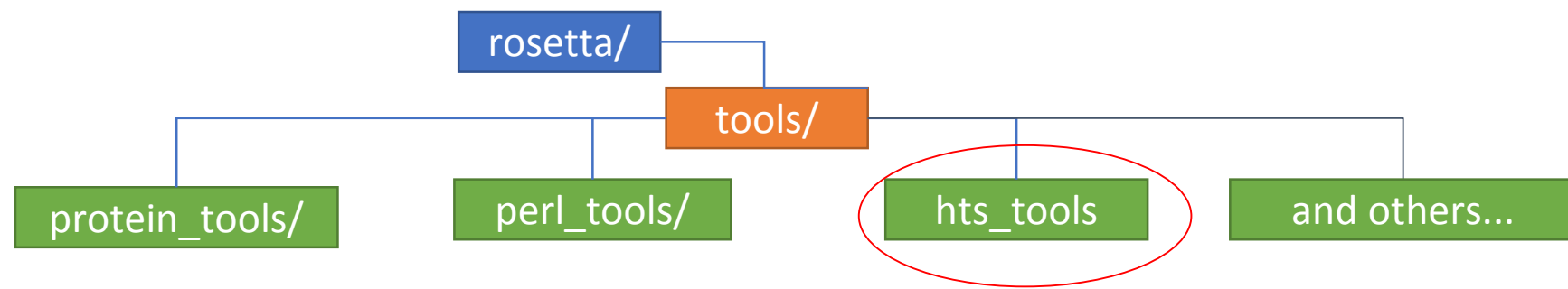




- Scripts used mainly to setup or analyze runs
- Rosetta/tools/protein_tools/scripts/
 - clean_pdb.py
 - pdb_renumber.py
 - score_vs_rmsd.py
 - top_n_percent.py

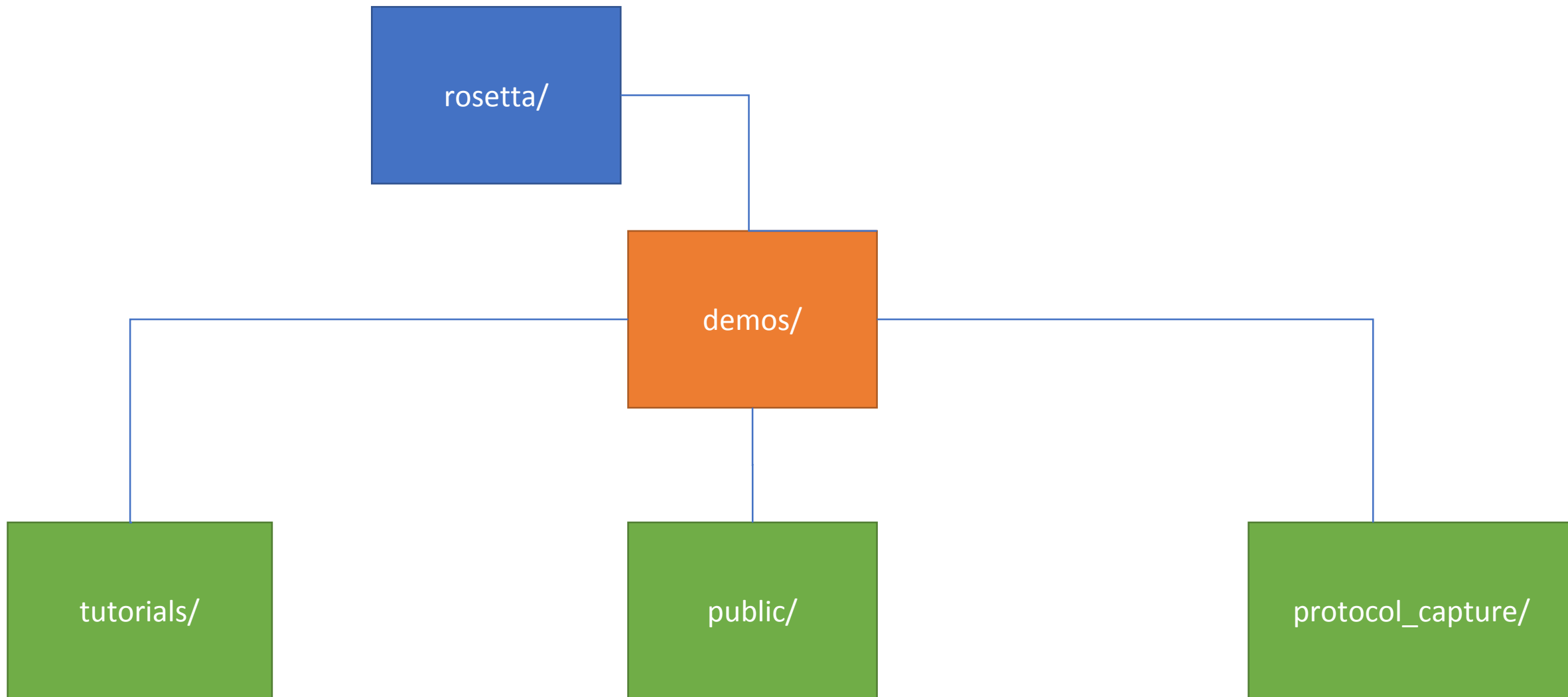


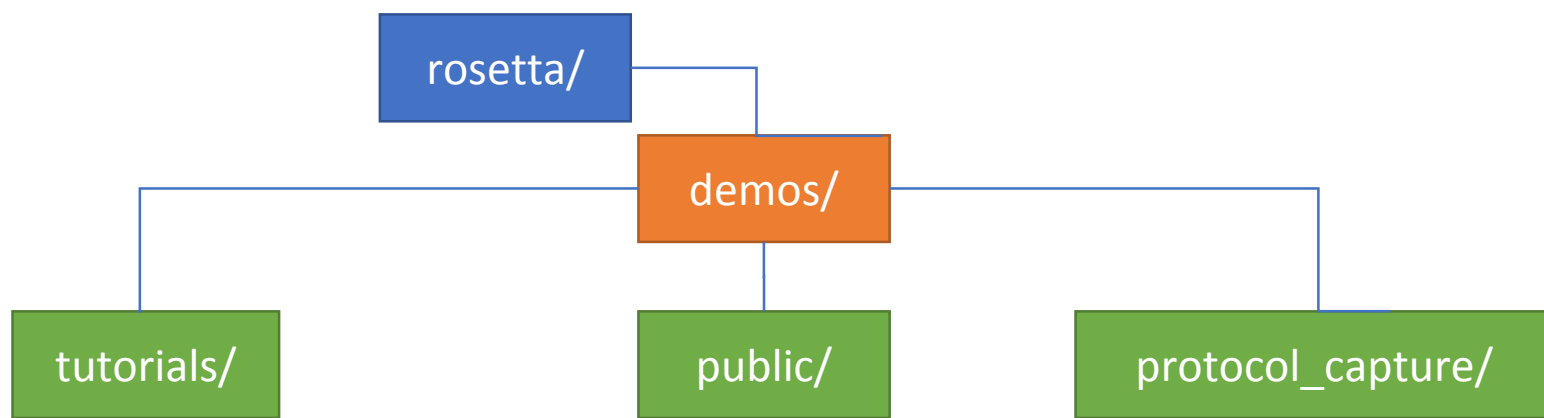
- Scripts used mainly to setup or analyze runs
- [Rosetta/tools/perl_tools/](#)
 - addchain.pl
 - getFastaFromCoords.pl
 - getCAcoords.pl



- Scripts used mainly to setup high throughput screen runs
- Basically batch ligand docking prep (>1000 compounds)
- [Rosetta/tools/hts_tools/](#)
 - make_params.py
 - get_descriptor_data.py
 - setup_screening_project.py

\$ROSETTA/demos/

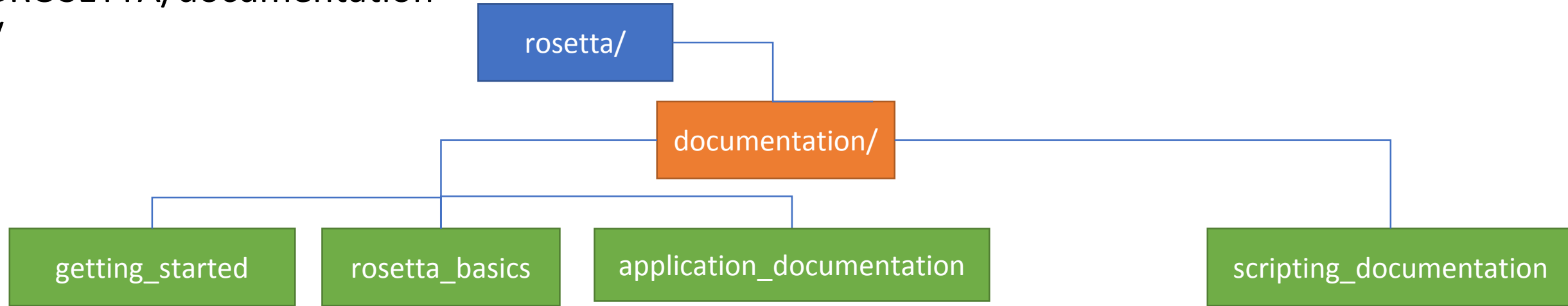




- Useful to know what input files/options are used in protocols
- [Rosetta/demos/tutorials/](#)
 - these tutorials!
- [Rosetta/demos/public/](#)
 - used to go through sample procedures
- [Rosetta/demos/protocol_capture/](#)
 - protocols associated with a publication

DISCLAIMER: May be out of date, always check Wiki/RosettaCommons for latest information!!

\$ROSETTA/documentation
/



- Very useful to go through when you're just getting started in Rosetta or any structural biology software
 - Understanding general Rosetta concepts
 - Where to find FAQs (How long does this run take?)
 - Options list, file types
 - Protocols you can use
 - General structural biology FAQs
 - How do I do X?
 - If you want more detail on how each protocol works, it's all in the code (\$ROSETTA/main/source/src/)
- RosettaScripts
 - Basic information on Movers, Task Operations, etc.
 - PyRosetta

Other Rosetta Resources:

- <https://www.rosettacommons.org/docs/latest/Home>
 - Forum
 - Documentation
 - User guides
 - Everything Rosetta-related you could ever dream of!

GO HAVE FUN!