**PUBS 2017 PyMol tutorial**

**# load a structure file**

fetch 1xq8 # retrieve structure file 1xq8 from the PBD

center 1xq8 # centers the object in your workspace

**# set your workspace aesthetics**

bg\_color white # color the background white

set seq\_view, 1 # display the solved amino acid sequence (includes solvents, ions, ligands, etc)

as cartoon

**# (selections) – subsets of objects**

# selection wiki page: <https://pymolwiki.org/index.php/Selection_Algebra>

# resi calls residues by index

# resn calls residue by name

select hPhobic, resn ala+ile+leu+met+phe+val+pro

select lysines, resn lys

select TM helix, resi 1-30

**# property selectors**

# <https://pymolwiki.org/index.php/Property_Selectors>

**# scenes – the closest thing to edit undo**

scene basic, store

**#### making a figures ####**

# replacing the b factor

**# first, make a duplicate object**

copy noDrug\_fit, 1xq8

# unselect 1xq8 now

**# then, replace the bfacts of that object with your own.**

run /Users/student/Desktop/replaceBfacts.py

replaceBfacts noDrug\_fit

scene noDrug\_fit, store

**# then, select all residues with Bfacts below 30**

select LowFit, b <- 30

# show sidechains

show sticks, LowFit

scene noDrug\_lowFit, create

**# show these low fitness residues as sticks**

set cartoon\_side\_chain\_helper, on # turn side chain helper on

**# extend the coloring to the sidechain**

run /Users/student/Desktop/alphaToAll.py

alphaToAll noDrug\_fit, b

alphaToAll noDrug\_fit and c. A, color

**# label**

label LowFitneg30, resi

set label\_size, 15

set label\_position, (1, 5, 1) # x, y, z

**# save as a high quality image**

ray 3000, 2400

png myImage.png