Setting up the latest CS-Rosetta Toolbox

1) Download:

a) Go to: http://csrosetta.chemistry.ucsc.edu/downloads/toolbox
b) Create an account
c) Click on latest toolbox version to download (current toolbox_ver_3.3)
d) Place in preferred directory (home recommended) and unpack:
tar -xzfv csrosetta_toolbox_ver3.3.tgz

2) Install and Set Environment

a) cd ~/csrosetta3/com/
b) python install.py
c) source init.bashrc
d) recommend putting “source ~/csrosetta3/com/init.bashrc” in your ~/.bashrc file so environment gets set automatically every time you open your terminal

3) Notes about the latest release can be found at http://csrosetta.chemistry.ucsc.edu/downloads/toolbox

- Installer and various scripts now support both mac and linux automatically
- TALOSN now default (previously TALOSP)
- Bug fixes
- Scripts added to /com : prot_completeness.py and addFasta2Prot.py

Setting up autoNOE: Preparing your files

1) Prepare the .tab file:

Setting up autoNOE: Preparing your files

2) Trim flexible ends

a) Use Talos to learn which residues to trim

talosn -in myShifts.tab

VARS RESID RESNAME PHI PSI DPHI DPSI DIST S2 COUNT CLASS
FORMAT %4d %s %8.3f %8.3f %8.3f %8.3f %8.3f %5.3f %2d %s

1	M	9999.000	9999.000	0.000	0.000	0.000	0.187	0	None
2	K	-81.415	143.247	49.171	47.658	35.234	0.232	10	Dyn
3	R	-102.463	136.063	30.483	21.803	11.496	0.306	8	Dyn
4	Q	-72.007	-33.294	17.747	12.857	10.222	0.415	5	Dyn
5	K	-67.290	-36.356	13.430	9.240	10.105	0.535	10	Good

An order parameter of <0.7 is considered to be flexible, so we consider trimming residues with these scores from the ends.

This column provides info about the quality of the backbone chemical shift data

Setting up autoNOE: Preparing your files

2) Trim flexible ends

   b) Trim the .prot, FASTA, and .tab

i) `talos2prot.py myShifts_trim.tab myShifts_trim.prot`

ii) `talos2fasta myShifts_trim.tab > myFasta_trim.fasta`

iii) `renumber_talos -s [#] -e [#]  myShifts.tab myShifts_trim.tab`

3) Pick fragments

`pick_fragments -cs myShifts_trim.tab`

4) Clean unassigned NOESY peak lists

```
clean_peak_file hcNH.peaks -skip 22 -cols 2 3 4 5 8 -names h c N H I -tol 0.02 0.20 0.20 0.02
>hcNH.clean.peaks
```

Setting up autoNOE: Setting up the target and run

At this point you should now have these files:

myShifts_trim.tab	hcNH.peaks	myShifts_trim.frags3.dat.gz	myFasta.fasta
myShifts_trim.prot	hcCH.peaks	myShifts_trim.frags9.dat.gz	

You may additionally have RDCs or disulfide bonds:

peg.rdc	phage.rdc	Disulfide bonds: 2-11, 27-40, and 88-112

5) Set up target:

```
setup_target -target myTarget -method autoNOE -cs myShifts_trim.tab -shifts myShifts_trim.prot -fasta myFasta.fasta -frags myShifts_trim.frags*.dat.gz -peaks hcNH.clean.peaks  hcCH.peaks -rdc peg.rdc phage.rdc -disulfide_bonds 2 11 27 40 88 112
```

6) Set up run:

```
setup_run -method autoNOE -target myTarget -dir ~/run_rasrec -extras mpi -job pbs_custom_nih
```

7) Initialize assignments:

```
source initialize_assignments_phaseI.sh
```