README for data for “Middle-way flexible docking: Pose prediction using mixed-resolution Monte Carlo in estrogen receptor α” by Justin Spiriti, Sundar Raman Subramanian, Rohith Palli, Maria Wu, and Daniel M. Zuckerman.

The directories contained in the tarball are as follows:

1. er-dock-seddd18 – RMSD analysis and summary files for docking runs without NCMC but with full flexibility (“movemix11-noncmc”), a fixed protein (“proteinfixed”) or flexible side chains (“sidechainonly”).

2. er-dock-seddd21 – RMSD analysis and summary files for docking runs with NCMC. The plotting scripts used to generate the figures are here as well.

3. docking – Smina runs and scripts for fixed protein.

4. dock-flex3 – Smina runs and scripts for protein with flexible side chains

5. ligands5 – Data and scripts related to parameterization.

Some hard-coded paths in scripts may require adjustment.

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| Figure | Main plotting script | Other scripts used |
| 1 | render-go-model4.tcl |  |
| 2 | plot-lambda-schedule |  |
| 3 | n/a (see “ligands5” directory) |  |
| 4 | n/a |  |
| 5 | plot-rmsd-intxn-energy | collate3b (to create summary files) |
| 6, 8 | plot-best-cum-rmsd7 | get-best-cum-rmsd2 |
| 7 | plot-rama-chi.py | rama-chi.tcl |
| 9 | best-rmsds-clusters5.py | cluster-rmsds-with-mms3.py  rmsd-dist-matrix.tcl  do-cluster |
| 10 | plot-rmsd-multi2 |  |
| S1 | plot-accrate-by-size2b | accrate-by-size.awk  get-accprob2  accrate-by-size4.awk |
| S2 | plot-rmsd-time-all |  |

Fields in summary files: (an/summary-\*)

1. target ER conformation (active or inactive)

2. ionization state

3. drug id

4. reference PDB code

5. docking run id number

6. final RMSD of protein backbone relative to reference crystal structure

7. final RMSD of drug heavy atoms relative to reference crystal structure

8. final RMSD of heavy atoms in all-atom region relative to reference crystal structure  
9. Final RMSD of heavy atoms in “small” all-atom region (within 4 A of ligand) relative to reference crystal structure

10. final RMSD of protein backbone relative to initial structure

11. final RMSD of drug heavy atoms relative to initial structure

12. final RMSD of heavy atoms in all-atom region relative to initial crystal structure

13. Final RMSD of heavy atoms in “small” all-atom region (within 4 A of ligand) relative to reference crystal structure

14. Final total potential energy

15. Final internal energy of ligand

16. van der Waals component of final interaction energy between ligand and protein

17. electrostatic component of final interaction energy between ligand and protein

18. total final interaction energy between ligand and forla

Fields in RMSD traces: (an/rmsd-\*)

1. frame number (“init” for initial structure)

2-9. RMSDs as in fields 6-13 of the summary files

Fields in Ramachandran angle traces (an/rama-\*):

1. residue number

2. amino acid 3-letter code

3-6. phi, psi, chi\_1, and chi\_2 for reference structure

7-10. phi, psi, chi\_1, and chi\_2 for actual structure