Data from: Multiscale Estimation of Binding Kinetics Using Brownian Dynamics, Molecular Dynamics and Milestoning
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Summary:

The directories for each system contain a file named "transition_data.txt". This contains the counts and average times for transitions between the different milestones of that system. Each system also contains a milestones.xml file, which outlines the details about each milestone, relating radius to index, etc. More detailed information is contained within the anchor files of each system.

Filetree contents and descriptions:

- milestoning.tcl - a sample milestoning script that must be called from the NAMD input file.
- sample_input_reverse.namd - A sample reverse phase NAMD input file is included here. Additional samples are given the system-specific directories
- sample_input_forward.namd - A sample forward phase NAMD input file is included here. Additional samples are given the system-specific directories
- charged_spherical_system/ - Directory of the files relevant to the charged spherical receptor system
    - transition_data.txt - all the milestone transition data condensed into a single file to make it easier to read and perform calculations
    - anchor_*/ - each milestone 'anchor' directory
        - md/ - md simulation files
            - building - contains structure and topology files
            - min - minimization phase
            - temp_equil - temperature equilibration phase
            - ens_equil - equilibrium simulations used to obtain equilibrium distribution
            - reverse - reversal phase simulation files
            - forward - forward phase simulation files
    - md_brute_force - brute force MD simulations
- uncharged_spherical_system/ - Directory of the files relevant to the uncharged spherical receptor system
    - transition_data.txt - all the milestone transition data condensed into a single file to make it easier to read and perform calculations
    - anchor_*/ - each milestone 'anchor' directory
        - md/ - md simulation files
            - building - contains structure and topology files
            - min - minimization phase
            - temp_equil - temperature equilibration phase
            - ens_equil - equilibrium simulations used to obtain equilibrium distribution
            - reverse - reversal phase simulation files
            - forward - forward phase simulation files
    - md_brute_force - brute force MD simulations
- troponin_c/ - Directory of the files relevant to the troponin C/Ca++ system
    - transition_data.txt - all the milestone transition data condensed into a single file to make it easier to read and perform calculations
    - params/ - all the parameters needed to run simulations of the system
    - anchor_*/ - each milestone 'anchor' directory
        - md/ - md simulation files
            - building - contains structure and topology files
            - min - minimization phase
            - temp_equil - temperature equilibration phase

            - ens_equil - equilibrium simulations used to obtain equilibrium distribution
            - reverse - reversal phase simulation files
            - forward - forward phase simulation files

        - bd/ - bd simulation files, this only exists in some folders where bd was run starting from the milestone

            - fhpd/ - first hitting point distribution results from the b-surface simulations

                - rightside/ - trajectories that completed on the correct side of the milestone sphere. These were commenced in the MD milestones
                - wrongside/ - trajectories that touched the wrong side of the milestoning sphere, they were ejected back into the BD milestone

    - b_surface - contains Brownian dynamics files that ran from the b-surface to the first of the milestones

        - .in files - these are input files for APBS
        - .pqr files - structure files including atomic partial charges and radii information
        - input.xml - the input file for the Browndye program bd_top
        - rxns.xml - the reaction file used by Browndye
        - results.xml - the final results of the Browndye runs

- superoxide_dismutase/ - Directory of the files relevant to the superoxide dismutase/O2- system

    - transition_data.txt - all the milestone transition data condensed into a single file to make it easier to read and perform calculations
    - params/ - all the parameters needed to run simulations of the system
    - milestones.xml - contains the specific details about the milestones
    - anchor_*/ - each milestone 'anchor' directory

        - sod_site?_trans*.txt - text of the output of the MD simulations
        - md/ - md simulation files

            - building - contains structure and topology files
            - min - minimization phase
            - temp_equil - temperature equilibration phase
            - ens_equil - equilibrium simulations used to obtain equilibrium distribution
            - reverse - reversal phase simulation files
            - forward - forward phase simulation files

        - bd/ - bd simulation files, this only exists in some folders where bd was run starting from the milestone

            - fhpd/ - first hitting point distribution results from the b-surface simulations

    - b_surface - contains Brownian dynamics files that ran from the b-surface to the first of the milestones

        - .in files - these are input files for APBS
        - .pqr files - structure files including atomic partial charges and radii information
        - input.xml - the input file for the Browndye program bd_top
        - rxns.xml - the reaction file used by Browndye
        - results.xml - the final results of the Browndye runs

Note: Count and time data from all systems mentioned in the publication are included. However, to save space, only the input files necessary to run the simulations and the output files necessary to run the milestoning calculations have been included

Note: The installation of the special plugin for NAMD that can spontaneously reverse velocities is not necessary if you use an automated script to reverse all velocities in the starting velocities files of your reverse phase, then revert them to the directions the atoms were going before for the forward phase.