

ProtocolCapture

Protocol Capture for MTSSL Rotamer Library in Rosetta

The steps and command lines below are found within subdirectories of the protocol capture directory, as specified by the "protocol capture directory" heading. Each directory contains relevant input, bin, and config files. Each directory also contains a README.txt with executed command lines, explanation about what the purpose is, and additional details about specific output files. Further help about specific command line options can be obtained by using the "help" flag in conjunction with the relevant bcl or rosetta application.

step	purpose	command
Generate an MTSSL mutant	Allows a protein with MTSSL to be used with Rosetta protocols	bin/fixbb.linuxgccdebug -database \$PATH_TO_ROSETTA_DATABASE -in:file:s input/lysozyme_pseudo_wildtyp
Relax MTSSL mutant	To take a protein that has been mutated to contain MTSSL and relax it with Rosetta.	../bin/relax.linuxgccrelease -database \$PATH_TO_ROSETTA_DATABASE -in:file:s input/lysozyme_start_mtssl_
Relax MTSSL mutant with membrane potentials	To take a membrane protein that has been mutated to contain MTSSL and relax it with Rosetta using membrane specific potentials.	bin/relax.linuxgccrelease -database \$PATH_TO_ROSETTA_DATABASE -in:file:s input/msba_mtssl_mutant_star

Calculate rotamer conformation recovery	Demonstrate the ability of Rosetta to recover experimentally observed spin label conformations using visual output	bin/bcl.exe AnalyzeRestraintAgreement -pdb_list input/pdbs.ls -analysis_prefix chi_angle_pair_distr_ -analysis_type chi_angle_pair_distribution.log &
Calculate rotamer conformation recovery	Demonstrate the ability of Rosetta to recover experimentally observed spin label conformations using quantitative output	bin/bcl.exe AnalyzeRestraintAgreement -pdb_list input/pdbs.ls 0 -analysis_type_enumerated 'ChiAngleRecovery

Calculate spin label distance distribution agreement	Demonstrate the ability of Rosetta to recover experimental distance distributions	bin/bcl.exe FitEPRDistribution -exp_hist_single input/t4l_epr_059_A_159_A.histogram -exp_hist_data_columns C
Show spin label distance distribution agreement	Compare heatmaps of experimental versus model spin label distance distributions	bin/bcl.exe AnalyzeRestraintAgreement -pdb_list fit_ensemble_00000.ls -analysis_prefix coord_dstnc_distr_ -anz 'CoordinateDistanceDistribution(filename_postfix=.CoordinateDistanceDistribution,coord_a=LocatorCoordinates/A 059 B 159",pixel_x=400,pixel_y=100,font="/usr/share/fonts/dejavu-lgc/DejaVuLGCSansMono.ttf",font_size=8,g
Show spin label distance distribution agreement	Use line-plot to compare experimental versus model spin label distance distributions	bin/bcl.exe FitEPRDistribution -distributions_to_lineplots fit_ensemble_00000.histogram line_plot_outfile.gnuplot
Show spin label distance distribution agreement	Compare line-plots of the integrals of the experimental and model spin label distance distributions.	bin/bcl.exe FitEPRDistribution -distributions_to_lineplots_sum fit_ensemble_00000.histogram lineplot_sum.gnupl
Calculate cone model parameters	Validation of implicit spin label cone model parameters	bin/bcl.exe CalculateConeModelParameters -list_of_pdb_lists input/pdb_lists.ls -aaclass AACComplete -prefix calc

