

Tag type	Tag name	Description
Exploration method	Mode	define the execution mode, the possible values are HEURISTIC, MONTECARLO, MEANFIELD and POSTPROCESS
Number of steps	Trajectory_Length	the length of a Monte Carlo trajectory
	Trajectory_Number	the number of Monte Carlo trajectories
	Cycle_Number	proteus gives a sequence at each cycle in the HEURISTIC mode
	Sequence_Loop_Number	the maximum number of iteration over the structure at each cycle.(only in the HEURISTIC mode)
Choice of the starting sequence/structure	Seq_Input_File	a input file with the starting values
	Rseed_Definition	The seed value for the random number generator (the generator sets the starting values if Seq_Input_File is not defined)
Energy function	Optimization_Configuration	definition of the energy function
	Group_definition	group energies and group interaction energies are the basic elements of the energy function
Restrictions on sequence/rotamer space	Space_Constraints	restrict the possible states or force residues to have the same amino acid
Model parameters	Surf_Ener_Factor	energy parameter
	Dielectric_Constant	energy parameter
	Lambda_Parameter	parameter of the Mean Field method
	Initial_Weights	parameter of the Mean Field method
	Temperature	usefull for the Mean Field or Monte Carlo mode
Monte Carlo controls	Random_Generator	The type of random number generator as defined in the GNU Scientific Library
	Rot_Proba	probability to have a rotamer change at each step
	Rot_Rot_Proba	probability to have a couple of rotamer change at each step
	Mut_Proba	...
	Mut_Mut_Proba	...
	Mut_Rot_Proba	...
	Neighbor_Threshold	At each step the changes will be in the same neighborhood.This tag is a parameter for the neighborhood definition.
Input/Output	Energy_Directory	the directory of the input energy files
	Fasta_File	the fasta file name (POSTPROCESS mode)
	Seq_Output_File	the name of the sequence output file
	Energy_Output_File	the name of the energy output file

TABLE 1 – Possible commands in the proteus command file