Field Name and Example	Description
#>R DOCK1.R_boxDim -24.985184 4.892637 -10.742 -3.108214 41.873702 10.561	Dimensions of the box used to define the region of the receptor where maps will be generated. Note that the entire ligand is kept inside the box during docking. You can adjust the parameters directly in the .tab file or use the GUI as described here: http://www.molsoft.com/gui/start-dock.html#review-and-adjust-binding-site
#>R DOCK1.R_ligInitPosition -14.119648 22.148016 1.084382 1. 0. 0. 0. 1. 0.	Coordinates of the 'probe' used to define starting positions of ligands for docking simulation. By default this probe is positioned in the center of the purple box. You can adjust the parameters directly in the .tab file or use the GUI as described here: http://www.molsoft.com/gui/start-dock.html#review-and-adjust-binding-site
#>i DOCK1.i_dbSize 4940292	Number of ligands in the screening database. Currently unused - for information only.
#>i DOCK1.i_maxHdonors 5	Maximum number of Hydrogen bond donors (default 5). Ligands that exceed this value will not be docked and scored.
#>i DOCK1.i_maxLigSize 500	Maximum ligand size (default 500). Ligands that exceed this value will not be docked and scored. Note that size is calculated as 15*number of heavy atoms.
#>i DOCK1.i_maxNO 10	Maximum number of Hydrogen bond acceptors/donors (default 10). Calculated as number of oxygen and nitrogen atoms. Ligands that exceed this value will not be docked and scored.
#>i DOCK1.i_maxTorsion 10	Maximum number of flexible torsions (default 10). Ligands that exceed this value will not be docked and scored.
#>i DOCK1.i_minLigSize 100	Minimum ligand size (default 100). Also see i_maxLigSize. Ligands that are smaller than this value will not be docked and scored.
#>i DOCK1.i_mnconf 40	Currently unused/ reserved for future use
#>i DOCK1.i_mnhighEnergy	Maximal number of consecutive

9999	accepted trial conformations which do not change the conformational stack because their energies are higher than energies of the stack conformations. Described here: http://www.molsoft.com/man/integer-shell-variables.html#mnhighEnergy
#>i DOCK1.i_mnreject 10	Maximal number of consecutive rejections (due to the Metropolis criterion) of trial conformations generated by MC procedure. When this threshold is reached the procedure acts according to the rejectAction parameter (which usually increases the simulation temperature). Default (10) Described here: http://www.molsoft.com/man/integer-shell-variables.html#mnreject
#>i DOCK1.i_mnvisits 10	Currently unused/reserved for future use
#>i DOCK1.i_ringFlexLevel 0	Flexible ring sampling for saturated or partially saturated rings. Set ring sampling level to 1 (flex ring only in pre-sampling step) or 2 (flex ring throughout the simulation.
#>l DOCK1.l_assignCharges yes	If l_assignCharges is set to no, it assumes that input file already has partial charge assignment. This only makes sense for mol2 or icm files as input, for mol/sdf this should be always set to 'yes' because mol/sdf format has no partial charges.
#>l DOCK1.l_buildHydrogens yes	Add hydrogens to the ligand (applicable to sdf/mol, mol2 and molcart input).
#>l DOCK1.l_dbondCisTrans no	Sample double bond cis/trans (default no).
#>l DOCK1.l_internalHB no	Enable internal h-bonds in the ligand
#>l DOCK1.l_neutralAcidsMol no	Keep carboxyls neutral (default no).
#>l DOCK1.l_protProt no	Must be no for protein-ligand projects.
#>l DOCK1.l_readyLigand yes	Ligand setup step complete – yes or no. More information on how to setup the ligand and receptor for docking using the GUI is here: http://www.molsoft.com/gui/start-

	dock.html#docking-start
#>l DOCK1.l_readyMaps yes	Maps were calculated – yes or no. More information here: http://www.molsoft.com/gui/start-dock.html#docking-start
#>l DOCK1.l_readyReceptor yes	Receptor setup complete – yes or no. More information here: http://www.molsoft.com/gui/start-dock.html#docking-start
#>l DOCK1.l_samplePyramid no	Sample pyramidal inversion for certain nitrogen atoms (Default no).
#>l DOCK1.l_sampleRacemic no	Sample racemic centers (Default no).
#>l DOCK1.l_softLigand yes	Perform ligand covalent geometry relaxation stage.
#>l DOCK1.l_useBornScore yes	Use Generalized Born method for solvation electrostatics calculations. If set to 'no', more accurate but slower and less robust boundary element method is used
#>r DOCK1.r_GRID_maxVw 4.	The truncation level of the van der Waals repulsion energy for receptor maps. Can be adjusted to change 'softness' of docking. Default: 4.0 kcal/mole.
#>r DOCK1.r_ScoreThreshold -32.	Ligand-receptor complexes will not be stored for ligands that score higher than this value. Note that all complexes are stored if less than 100 ligands are docked. See –a and –f options to change that behavior
#>r DOCK1.r_Score_maxVw 1.	Van der Waals repulsion truncation level in the scoring function. Can be adjusted to change 'softness' of scoring.
#>r DOCK1.r_densityWeight 0.	When non-zero, additional 'xr' map is read and used to bias docking towards regions of high density (normally used with electron density map)
#>r DOCK1.r_dockScanVersion 4.41	Version of dockScan protocol.
#>r DOCK1.r_maxPk 5.	Maximum predicted LogP. Ligands with higher than this value will not be docked or scored.
#>r DOCK1.r_mcShake 4.	Currently unused/reserved for future use
#>r DOCK1.r_mfScoreThreshold 999.	The potential of mean force score threshold

#>r DOCK1.r_minPk 0.	Minimum predicted LogP. Ligands with lower than this value will not be docked or scored.
#>r DOCK1.r_pH 7.	pH value for Pk predictions.
#>r DOCK1.r_temperature 1000.	The montecarlo simulation temperature. More information here: http://www.molsoft.com/man/reals.html#temperature
#>r DOCK1.r_thTautomer -1.	Reserved for future use (in alpha testing currently)
#>r DOCK1.r_vicinity 1.	Maximum angular root-mean-square deviation per variable (degrees) or cartesian root-mean-square deviation per atom (Angstroms) when two structures are still considered belonging to the same conformational family in conformational stack manipulations
#>s DOCK1.s_bindPatchRes a_DOCK1_rec.a/^N3,^L5:^V7,^T17:^T19,^L102,^E172:^P175,^R177,^E183:^P185,^P275:^L277,^F282,^Y287	ICM selection language description of ligand binding pocket residues. Only used for display purposes.
#>s DOCK1.s_chargeGroups none	Charge some ionizable basic groups, it currently understands following values: space-separated NH2, NH, NT for primary secondary and tertiary aliphatic amines, also it understands 'imidazole' and 'amidine'. An alternative is 'auto', which uses built-in prediction of Ka/Kb to charge and protonate/deprotonate appropriate groups. 'none' still charges acids unless neutralAcids flag is set to 'no'
#>s DOCK1.s_clrLig default	Ligand color in display
#>s DOCK1.s_clrRec grey	Receptor color in display (other than binding site)
#>s DOCK1.s_clrSite default pink	Binding site color. Second word here is understood as color applied to carbons only
#>s DOCK1.s_covModResAt none	Pair of atoms along the bond in a residue sidechain to which a covalent ligand should be attached.
#>s DOCK1.s_covRxn none	Reaction file that defines transformation(s) used to form models of covalently bound ligands

#>s DOCK1.s_dbFile H:/icmd/celebrex50.sdf	Path to SDF database file.
#>s DOCK1.s_dbIndex celebrex50	Path to the ICM index of SDF database file.
#>s DOCK1.s_dbType mol 2D	Type of database file. Second word may be a modifier (2D) directing the procedure to perform 2D to 3D conversion
#>s DOCK1.s_dspLig xstick	Ligand display representation
#>s DOCK1.s_dspRec wire	Receptor display representation (other than binding site)
#>s DOCK1.s_dspSite xstick	Binding site display representation
#>s DOCK1.s_grid4DFlex none	Field for multiple conformation (4D) receptor docking. Instructions for 4D setup are here: http://www.molsoft.com/gui/flexible.html#multiple-rec
#>s DOCK1.s_ligMol 2:2	Ligand molecule index in a complex. The indexes must be 1 + number of molecules in the receptor
#>s DOCK1.s_ligName DOCK1_default	Unused
#>s DOCK1.s_optSC a none	For information only. See s recExplicitObj
#>s DOCK1.s_recExplicitObj none	Some residues (e.g. Hydroxyls of Ser, Thr, and Tyr) can be defined as explicit during docking. Example here: http://www.molsoft.com/gui/induced-fit.html#docking-explicit-group
#>s DOCK1.s_recMol 1:1	Receptor molecules index range. Must be 1: number of molecules in the receptor (i.e. polypeptide chains, metals, waters and cofactors)
#>s DOCK1.s_recName DOCK1_rec	Name of the receptor object
#>s DOCK1.s_selLig a_*.*//*	Obsolete
#>s DOCK1.s_selRec a_*.*//*	Obsolete
#>s DOCK1.s_selSite a_*.*//!M5	Obsolete
#>s DOCK1.s_templateMatch substructure	Field for template docking matching option. Match by atom name, substructure, fuzzy or APF. More information here: http://www.molsoft.com/gui/docking-template.html

#>s DOCK1.s_templateObj none	Template object (filename) used in template docking.
#>s DOCK1.s_xrObj none	Unused