Files generated by R.E.D. Server Development/PyRED
Force field generation for dimethylalanine dipeptide and its three molecular fragments
Programs interfaced: Gaussian 2009 & RESP 2.4

Mol_m1
Already described in previous examples
Mol_m2
Already described in previous examples
Mol_m3
Already described in previous examples
[...]
Mol_m6
Already described in previous examples

Mol_MM	**Multiple molecules**
Mol_MM/Mol_mm1-c1.mol2	Force field library for mol. 1 conf. 1 (dipeptide used in the central fragment)
Mol_MM/Mol_mm1-c2.mol2	Force field library for mol. 1 conf. 2 (dipeptide used in the central fragment)
Mol_MM/Mol_mm2-c1.mol2	Force field library for mol. 2 conf. 1 (methylammonium)
Mol_MM/Mol_mm3-c1.mol2	Force field library for mol. 3 conf. 1 (dipeptide used in the N-term. fragment)
Mol_MM/Mol_mm3-c2.mol2	Force field library for mol. 3 conf. 2 (dipeptide used in the N-term. fragment)
Mol_MM/Mol_mm4-c1.mol2	Force field library for mol. 4 conf. 1 (dipeptide used in the C-term. fragment)
Mol_MM/Mol_mm4-c2.mol2	Force field library for mol. 4 conf. 2 (dipeptide used in the C-term. fragment)
Mol_MM/Mol_mm5-c1.mol2	Force field library for mol. 5 conf. 1 (acetate)
Mol_MM/Mol_mm6-c1.mol2	**Force field library for mol. 6 conf. 1 (dipeptide itsef)**
Mol_MM/Mol_mm6-c2.mol2	**Force field library for mol. 6 conf. 2 (dipeptide itsef)**
Mol_MM/Mol_mm-charge.txt	Charge values before and after rounding off error corrections
Mol_MM/Statistics_mm.txt	Different types of charge values are compared
Mol_MM/esmpot_mm.pdb	PDB-like file with MEP values computed with charges in the TempFactor field
Mol_MM/esout_mm.out	esout file
Mol_MM/espot_mm.dat	All espot concatenated into a single file - all mol. all conf. all orient.
Mol_MM/esp_mm.pdb	PDB-like file with relative residual in the TempFactor field
Mol_MM/esqpot_mm.pdb	PDB-like file with input MEP values in the TempFactor field
Mol_MM/input1_mm.in	Multiple molecules - resp input stage 1
Mol_MM/input2_mm.in	Multiple molecules - resp input stage 2
Mol_MM/output1_mm.log	Multiple molecules - resp log/output stage 1
Mol_MM/output2_mm.log	Multiple molecules - resp log/output stage 2
Mol_MM/punch1_mm.dat	Multiple molecules - resp punch stage 1
Mol_MM/punch2_mm.dat	Multiple molecules - resp punch stage 2
Mol_MM/qout1_mm.dat	Multiple molecules - charge values stage 1
Mol_MM/qout2_mm.dat	Multiple molecules - charge values stage 2

Mol_MM/INTER	
INTER/m2-c1_m2-c1_f1.mol2	**mol. 2 + mol. 3 conf. 1: N-term. fragment**
INTER/m2-c1_m2-c1.mol2	mol. 2 + mol. 3 conf. 1
INTER/m2-c1_m2-c2_f1.mol2	**mol. 2 + mol. 3 conf. 2: N-term. fragment**
INTER/m2-c1_m2-c2.mol2	mol. 2 + mol. 3 conf. 2
INTER/m4-c1_m5-c1_f1.mol2	**mol. 4 conf. 1 + mol. 5: C-term. fragment**
INTER/m4-c1_m5-c1.mol2	mol. 4 conf. 1 + mol. 5
INTER/m4-c2_m5-c1_f1.mol2	**mol. 4 conf. 2 + mol. 5: C-term. fragment**
INTER/m4-c2_m5-c1.mol2	mol. 4 conf. 2 + mol. 5
Mol_MM/INTER/mm1	
INTER/mm1/m1-c1_f1.mol2	mol. 1 conf. 1 intra-mcc 1: fragment 1
INTER/mm1/m1-c1_f2.mol2	mol. 1 conf. 1 intra-mcc 2: fragment 2
INTER/mm1/m1-c1_f3.mol2	**mol. 1 conf. 1 intra-mcc 1 + 2: Central fragment**
INTER/mm1/m1-c2_f1.mol2	mol. 1 conf. 2 intra-mcc 1: fragment 1
INTER/mm1/m1-c2_f2.mol2	mol. 1 conf. 2 intra-mcc 2: fragment 2
INTER/mm1/m1-c2_f3.mol2	**fastermol. 1 conf. 2 intra-mcc 1 + 2: Central fragment**
Mol_MM/INTER/mm2	fragment, that derives from methylammonium
Mol_MM/INTER/mm3	fragments, that derive from dipeptide 3
Mol_MM/INTER/mm4	fragments, that derive from dipeptide 4
Mol_MM/INTER/mm5	fragment, that derives from acetate
Data-Default-Proj/	
Data-Default-Proj/Configuration.py	Configuration.py used in the job
Data-Default-Proj/Mol_red1.pdb	PDB input file for mol. 1 - optimized geometry
[...]	
Data-Default-Proj/Mol_red6.pdb	PDB input file for mol. 6 - optimized geometry
Data-Default-Proj/Project.config	Project.config used in the job
Data-Default-Proj/frcmod.correspondence	List of force field parameters determined by analogy to known ones
Data-Default-Proj/frcmod.known	List of known force field parameters for dimethylalanine and its different fragments
Data-Default-Proj/frcmod.unknown	List of unknown force field parameters for dimethylalanine and its different fragments
Data-Default-Proj/leaprc.ff13q4mdfft	LEaP script: loads the generated force field for dimethylalanine and its different fragments
Data-Default-Proj/readme.txt	Documentation is always printed
Data-Default-Proj/P2N	List of P2N files to be used with the former versions fo R.E.D. (perl)