Files generated by R.E.D. Server Development/PyRED
Force field generation for the central fragment of the dimethylalanine residue
Programs interfaced: Gaussian 2009 & RESP 2.4

Mol_m1	**Mol. 1 single molecule (sm) with intra-mcc (ia)**
Mol_m1/File4REDDB_m1.pdb	PDB file for project submission in R.E.DD.B.
Mol_m1/JOB1-gau_m1-1.gjf	QM Geometry optimization input mol. m1 conf. 1
Mol_m1/JOB1-gau_m1-1.out	QM Geometry optimization output mol. m1 conf. 1
Mol_m1/JOB1-gau_m1-2.gjf	QM Geometry optimization input mol. m1 conf. 1
Mol_m1/JOB1-gau_m1-2.out	QM Geometry optimization output mol. m1 conf. 2
Mol_m1/JOB2-gau_m1-1-1.gjf	QM MEP computation input mol. m1 conf. 1 orient. 1
Mol_m1/JOB2-gau_m1-1-1.out	QM MEP computation output mol. m1 conf. 1 orient. 1
Mol_m1/JOB2-gau_m1-1-2.gjf	QM MEP computation input mol. m1 conf. 1 orient. 2
Mol_m1/JOB2-gau_m1-1-2.out	QM MEP computation output mol. m1 conf. 1 orient. 2
Mol_m1/JOB2-gau_m1-2-1.gjf	QM MEP computation input mol. m1 conf. 2 orient. 1
Mol_m1/JOB2-gau_m1-2-1.out	QM MEP computation output mol. m1 conf. 2 orient. 1
Mol_m1/JOB2-gau_m1-2-2.gjf	QM MEP computation input mol. m1 conf. 2 orient. 2
Mol_m1/JOB2-gau_m1-2-2.out	QM MEP computation output mol. m1 conf. 2 orient. 2
Mol_m1/Mol-ia1_m1-c1.mol2	Force field library – Fragment 1- mol. m1 conf. 1 – correspond to the 1st intra-mcc
Mol_m1/Mol-ia1_m1-c2.mol2	Force field library – Fragment 1- mol. m1 conf. 2 – correspond to the 1st intra-mcc
Mol_m1/Mol-ia2_m1-c1.mol2	Force field library – Fragment 2- mol. m1 conf. 1 – correspond to the 2nd intra-mcc
Mol_m1/Mol-ia2_m1-c2.mol2	Force field library – Fragment 2- mol. m1 conf. 2 – correspond to the 2nd intra-mcc
Mol_m1/Mol-ia3_m1-c1.mol2	Force field library – Fragment 3- mol. m1 conf. 1 – **correspond to the two intra-mcc**
Mol_m1/Mol-ia3_m1-c2.mol2	Force field library – Fragment 3- mol. m1 conf. 2 – **correspond to the two intra-mcc**
Mol_m1/Mol-ia_m1-charge.txt	Charge values before and after rounding off error corrections (with intra-mcc)
Mol_m1/Mol-sm_m1-c1.mol2	Force field library mol. m1 conf. 1
Mol_m1/Mol-sm_m1-c2.mol2	Force field library mol. m1 conf. 2
Mol_m1/Mol-sm_m1-charge.txt	Charge values before and after rounding off error corrections (without intra-mcc)
Mol_m1/Mol_m1-c1-qmra.pdb	Optimized geometry - QM orientation mol. m1 conf. 1
Mol_m1/Mol_m1-c1-rbra1.pdb	Optimized geometry – mol. m1 conf. 1 orient. 1 used in MEP computation
Mol_m1/Mol_m1-c1-rbra2.pdb	Optimized geometry – mol. m1 conf. 1 orient. 2 used in MEP computation
Mol_m1/Mol_m1-c2-qmra.pdb	Optimized geometry - QM orientation mol. m1 conf. 2
Mol_m1/Mol_m1-c2-rbra1.pdb	Optimized geometry – mol. m1 conf. 2 orient. 1 used in MEP computation
Mol_m1/Mol_m1-c2-rbra2.pdb	Optimized geometry – mol. m1 conf. 2 orient. 2 used in MEP computation
Mol_m1/Statistics_m1.txt	Different types of charge values are compared
Mol_m1/esmpot-ia_m1.pdb	PDB with MEP values comput. with charges in TempFact. field (fit with intra-mcc)
Mol_m1/esmpot-sm_m1.pdb	PDB with MEP values comput. with charges in TempFact. field (fit without intra-mcc)
Mol_m1/esout-ia_m1.out	esout file (fit with intra-mcc)
Mol_m1/esout-sm_m1.out	esout file (fit without intra-mcc)
Mol_m1/espot_m1.dat	All espot files related to molecule 1 concatenated into a single file
Mol_m1/espot_m1-1-1.dat	espot file mol. m1 conf. 1 orient. 1
Mol_m1/espot_m1-1-2.dat	espot file mol. m1 conf. 1 orient. 2
Mol_m1/espot_m1-2-1.dat	espot file mol. m1 conf. 2 orient. 1
Mol_m1/espot_m1-2-2.dat	espot file mol. m1 conf. 2 orient. 2

Mol_m1/esp-ia_m1.pdb	PDB with relative residual in TempFact. field (fit with intra-mcc)
Mol_m1/esp-sm_m1.pdb	PDB with relative residual in TempFact. field (fit without intra-mcc)
Mol_m1/esqpot-ia_m1.pdb	PDB with input MEP values in TempFact. field (fit with intra-mcc)
Mol_m1/esqpot-sm_m1.pdb	PDB with input MEP values in TempFact. field (fit without intra-mcc)
Mol_m1/input1-ia_m1.in	Single mol. – 2 conf. – 2 orient. resp input stage 1 (fit with intra-mcc)
Mol_m1/input1-sm_m1.in	Single mol. – 2 conf. – 2 orient. resp input stage 1 (fit without intra-mcc)
Mol_m1/input2-ia_m1.in	Single mol. – 2 conf. – 2 orient. resp input stage 2 (fit with intra-mcc)
Mol_m1/input2-sm_m1.in	Single mol. – 2 conf. – 2 orient. resp input stage 2 (fit without intra-mcc)
Mol_m1/output1-ia_m1.log	Single mol. – 2 conf. – 2 orient. resp log/output stage 1 (fit with intra-mcc)
Mol_m1/output1-sm_m1.log	Single mol. – 2 conf. – 2 orient. resp log/output stage 1 (fit without intra-mcc)
Mol_m1/output2-ia_m1.log	Single mol. – 2 conf. – 2 orient. resp log/output stage 2 (fit with intra-mcc)
Mol_m1/output2-sm_m1.log	Single mol. – 2 conf. – 2 orient. resp log/output stage 2 (fit without intra-mcc)
Mol_m1/punch1-ia_m1.dat	Single mol. – 2 conf. – 2 orient. resp punch stage 1 (fit with intra-mcc)
Mol_m1/punch1-sm_m1.dat	Single mol. – 2 conf. – 2 orient. resp punch stage 1 (fit without intra-mcc)
Mol_m1/punch2-ia_m1.dat	Single mol. – 2 conf. – 2 orient. resp punch stage 2 (fit with intra-mcc)
Mol_m1/punch2-sm_m1.dat	Single mol. – 2 conf. – 2 orient. resp punch stage 2 (fit without intra-mcc)
Mol_m1/qout1-ia_m1.dat	Single mol. – 2 conf. – 2 orient. Charge values stage 1 (fit with intra-mcc)
Mol_m1/qout1-sm_m1.dat	Single mol. – 2 conf. – 2 orient. Charge values stage 1 (fit without intra-mcc)
Mol_m1/qout2-ia_m1.dat	Single mol. – 2 conf. – 2 orient. Charge values stage 2 (fit with intra-mcc)
Mol_m1/qout2-sm_m1.dat	Single mol. – 2 conf. – 2 orient. Charge values stage 2 (fit without intra-mcc)

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/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 central fragment
Data-Default-Proj/frcmod.unknown	List of unknown force field parameters dimethylalanine and its central fragment
Data-Default-Proj/leaprc.ff13q4mdfft	LEaP script: loads the force field dimethylalanine and its central fragment
Data-Default-Proj/readme.txt	Documentation is always printed
Data-Default-Proj/P2N	P2N file to be used with the former versions fo R.E.D. (perl)