Files generated by R.E.D. Server Development/PyRED
Force field generation for a single molecule: methanol
Programs interfaced: Gaussian 2009 & RESP 2.4

Mol_m1	**Mol. 1 single molecule (sm)**
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/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/Mol-sm_m1-c1.mol2	Force field library mol. m1 conf. 1
Mol_m1/Mol-sm_m1-charge.txt	Charge values before and after rounding off error corrections
Mol_m1/Mol_m1-c1-qmra.pdb	Optimized geometry - QM orientation
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/Statistics_m1.txt	Different types of charge values are compared
Mol_m1/esmpot-sm_m1.pdb	PDB-like file with MEP values computed with charges in the TempFactor field
Mol_m1/esout-sm_m1.out	esout file
Mol_m1/espot_m1.dat	All espot 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/esp-sm_m1.pdb	PDB-like file with relative residual in the TempFactor field
Mol_m1/esqpot-sm_m1.pdb	PDB-like file with input MEP values in the TempFactor field
Mol_m1/input1-sm_m1.in	Single molecule resp input stage 1
Mol_m1/input2-sm_m1.in	Single molecule resp input stage 2
Mol_m1/output1-sm_m1.log	Single molecule resp log/output stage 1
Mol_m1/output2-sm_m1.log	Single molecule resp log/output stage 2
Mol_m1/punch1-sm_m1.dat	Single molecule resp punch stage 1
Mol_m1/punch2-sm_m1.dat	Single molecule resp punch stage 2
Mol_m1/qout1-sm_m1.dat	Single molecule charge values stage 1
Mol_m1/qout2-sm_m1.dat	Single molecule charge values stage 2

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 methanol
Data-Default-Proj/frcmod.unknown	List of unknown force field parameters for methanol
Data-Default-Proj/leaprc.ff13q4mdfft	LEaP script: loads the generated force field for methanol
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)