Files generated by R.E.D. Server Development/PyRED
Force field generation for the *N*-terminal fragment of the dimethylalanine residue
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

Mol_m2	**Mol. 2 single molecule (sm) with intra-mcc (ia)**
Mol_m2/File4REDDB_m2.pdb	PDB file for project submission in R.E.DD.B.
Mol_m2/JOB1-gau_m2-1.gjf	QM Geometry optimization input mol. m2 conf. 1
Mol_m2/JOB1-gau_m2-1.out	QM Geometry optimization output mol. m2 conf. 1
Mol_m2/JOB1-gau_m2-2.gjf	QM Geometry optimization input mol. m2 conf. 1
Mol_m2/JOB1-gau_m2-2.out	QM Geometry optimization output mol. m2 conf. 2

Mol_m2/JOB2-gau_m2-1-1.gjf	QM MEP computation input mol. m2 conf. 1 orient. 1
Mol_m2/JOB2-gau_m2-1-1.out	QM MEP computation output mol. m2 conf. 1 orient. 1
Mol_m2/JOB2-gau_m2-1-2.gjf	QM MEP computation input mol. m2 conf. 1 orient. 2
Mol_m2/JOB2-gau_m2-1-2.out	QM MEP computation output mol. m2 conf. 1 orient. 2
Mol_m2/JOB2-gau_m2-2-1.gjf	QM MEP computation input mol. m2 conf. 2 orient. 1
Mol_m2/JOB2-gau_m2-2-1.out	QM MEP computation output mol. m2 conf. 2 orient. 1
Mol_m2/JOB2-gau_m2-2-2.gjf	QM MEP computation input mol. m2 conf. 2 orient. 2
Mol_m2/JOB2-gau_m2-2-2.out	QM MEP computation output mol. m2 conf. 2 orient. 2
Mol_m2/Mol-ia1_m2-c1.mol2	Force field library – Fragment 1- mol. m2 conf. 1 – with intra-mcc
Mol_m2/Mol-ia1_m2-c2.mol2	Force field library – Fragment 1- mol. m2 conf. 2 – with intra-mcc
Mol_m2/Mol-ia_m2-charge.txt	Charge values before and after rounding off error corrections (with intra-mcc)
Mol_m2/Mol-sm_m2-c1.mol2	Force field library mol. m2 conf. 1
Mol_m2/Mol-sm_m2-c2.mol2	Force field library mol. m2 conf. 2
Mol_m2/Mol-sm_m2-charge.txt	Charge values before and after rounding off error corrections (without intra-mcc)
Mol_m2/Mol_m2-c1-qmra.pdb	Optimized geometry - QM orientation mol. m2 conf. 1
Mol_m2/Mol_m2-c1-rbra1.pdb	Optimized geometry – mol. m2 conf. 1 orient. 1 used in MEP computation
Mol_m2/Mol_m2-c1-rbra2.pdb	Optimized geometry – mol. m2 conf. 1 orient. 2 used in MEP computation
Mol_m2/Mol_m2-c2-qmra.pdb	Optimized geometry - QM orientation mol. m2 conf. 2
Mol_m2/Mol_m2-c2-rbra1.pdb	Optimized geometry – mol. m2 conf. 2 orient. 1 used in MEP computation
Mol_m2/Mol_m2-c2-rbra2.pdb	Optimized geometry – mol. m2 conf. 2 orient. 2 used in MEP computation
Mol_m2/Statistics_m2.txt	Different types of charge values are compared
Mol_m2/esmpot-ia_m2.pdb	PDB with MEP values comput. with charges in TempFact. field (fit with intra-mcc)
Mol_m2/esmpot-sm_m2.pdb	PDB with MEP values comput. with charges in TempFact. field (fit without intra-mcc)
Mol_m2/esout-ia_m2.out	esout file (fit with intra-mcc)
Mol_m2/esout-sm_m2.out	esout file (fit without intra-mcc)
Mol_m2/espot_m2.dat	All espot files related to molecule 1 concatenated into a single file
Mol_m2/espot_m2-1-1.dat	espot file mol. m2 conf. 1 orient. 1
Mol_m2/espot_m2-1-2.dat	espot file mol. m2 conf. 1 orient. 2
Mol_m2/espot_m2-2-1.dat	espot file mol. m2 conf. 2 orient. 1
Mol_m2/espot_m2-2-2.dat	espot file mol. m2 conf. 2 orient. 2
Mol_m2/esp-ia_m2.pdb	PDB with relative residual in TempFact. field (fit with intra-mcc)
Mol_m2/esp-sm_m2.pdb	PDB with relative residual in TempFact. field (fit without intra-mcc)
Mol_m2/esqpot-ia_m2.pdb	PDB with input MEP values in TempFact. field (fit with intra-mcc)
Mol_m2/esqpot-sm_m2.pdb	PDB with input MEP values in TempFact. field (fit without intra-mcc)
Mol_m2/input1-ia_m2.in	Single mol. – 2 conf. – 2 orient. resp input stage 1 (fit with intra-mcc)
Mol_m2/input1-sm_m2.in	Single mol. – 2 conf. – 2 orient. resp input stage 1 (fit without intra-mcc)
Mol_m2/input2-ia_m2.in	Single mol. – 2 conf. – 2 orient. resp input stage 2 (fit with intra-mcc)
Mol_m2/input2-sm_m2.in	Single mol. – 2 conf. – 2 orient. resp input stage 2 (fit without intra-mcc)
Mol_m2/output1-ia_m2.log	Single mol. – 2 conf. – 2 orient. resp log/output stage 1 (fit with intra-mcc)
Mol_m2/output1-sm_m2.log	Single mol. – 2 conf. – 2 orient. resp log/output stage 1 (fit without intra-mcc)

Mol_m2/output2-ia_m2.log	Single mol. – 2 conf. – 2 orient. resp log/output stage 2 (fit with intra-mcc)
Mol_m2/output2-sm_m2.log	Single mol. – 2 conf. – 2 orient. resp log/output stage 2 (fit without intra-mcc)
Mol_m2/punch1-ia_m2.dat	Single mol. – 2 conf. – 2 orient. resp punch stage 1 (fit with intra-mcc)
Mol_m2/punch1-sm_m2.dat	Single mol. – 2 conf. – 2 orient. resp punch stage 1 (fit without intra-mcc)
Mol_m2/punch2-ia_m2.dat	Single mol. – 2 conf. – 2 orient. resp punch stage 2 (fit with intra-mcc)
Mol_m2/punch2-sm_m2.dat	Single mol. – 2 conf. – 2 orient. resp punch stage 2 (fit without intra-mcc)
Mol_m2/qout1-ia_m2.dat	Single mol. – 2 conf. – 2 orient. Charge values stage 1 (fit with intra-mcc)
Mol_m2/qout1-sm_m2.dat	Single mol. – 2 conf. – 2 orient. Charge values stage 1 (fit without intra-mcc)
Mol_m2/qout2-ia_m2.dat	Single mol. – 2 conf. – 2 orient. Charge values stage 2 (fit with intra-mcc)
Mol_m2/qout2-sm_m2.dat	Single mol. – 2 conf. – 2 orient. Charge values stage 2 (fit without intra-mcc)

Mol_MM	**Multiple molecules (with intra-mcc & inter-mcc)**
Mol_MM/Mol_mm2-c1.mol2	Force field library for mol. 1 conf. 1
Mol_MM/Mol_mm2-c1.mol2	Force field library for mol. 2 conf. 1
Mol_MM/Mol_mm2-c2.mol2	Force field library for mol. 2 conf. 2
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 (with intra-mcc & inter-mcc)
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 (with intra-mcc & inter-mcc)
Mol_MM/input2_mm.in	Multiple molecules - resp input stage 2 (with intra-mcc & inter-mcc)
Mol_MM/output1_mm.log	Multiple molecules - resp log/output stage 1 (with intra-mcc & inter-mcc)
Mol_MM/output2_mm.log	Multiple molecules - resp log/output stage 2 (with intra-mcc & inter-mcc)
Mol_MM/punch1_mm.dat	Multiple molecules - resp punch stage 1 (with intra-mcc & inter-mcc)
Mol_MM/punch2_mm.dat	Multiple molecules - resp punch stage 2 (with intra-mcc & inter-mcc)
Mol_MM/qout1_mm.dat	Multiple molecules - charge values stage 1 (with intra-mcc & inter-mcc)
Mol_MM/qout2_mm.dat	Multiple molecules - charge values stage 2 (with intra-mcc & inter-mcc)

Mol_MM/INTER	
INTER/m1-c1_m2-c1.mol2	*N*-terminal fragment mol. 1 + mol.2 conf. 1: mol. fusion
INTER/m1-c1_m2-c1_f1.mol2	***N*-terminal fragment mol. 1 + mol.2 conf. 1: mol. fusion & remove the caps**
INTER/m1-c1_m2-c2.mol2	*N*-terminal fragment mol. 1 + mol.2 conf. 2: mol. fusion
INTER/m1-c1_m2-c2_f1.mol2	***N*-terminal fragment mol. 1 + mol.2 conf. 2: mol. fusion & remove the caps**
INTER/mm1	Fragments related to mol. 1 in the multiple molecule job
INTER/mm2	Fragments related to mol. 2 in the multiple molecule job

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_red2.pdb	PDB input file for mol. 2 - 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 the *N*-terminal fragment of dimethylalanine
Data-Default-Proj/frcmod.unknown	List of unknown force field parameters for the *N*-terminal fragment of dimethylalanine
Data-Default-Proj/leaprc.ff13q4mdfft	LEaP script: loads the generated force field for the *N*-terminal fragment of dimethylalanine
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)