Files generated by R.E.D. Server/R.E.D. IV
Charge derivation & force field library building for the *N*-terminal fragment of a new amino acid.

Interfaced programs: Gaussian 2003 & RESP

Parent_directory	
Mol_m1	**Single molecule charge derivation**
File4REDDB_m1.pdb	*m1 = molecule 1*
JOB2-gau_m1-1-1.com	Gaussian input: *m1*-1-1: molecule 1; conformation 1; orientation 1
JOB2-gau_m1-1-1.out	Gaussian output
JOB2-gau_m1-1-2.com	
JOB2-gau_m1-1-2.out	
Mol_m1-o1-qmra.pdb	conformation 1; Orientation of opt. geometry based on the Gaussian program
Mol_m1-o1-rbra1.pdb	Rigid-body re-orientation algorithm: conformation 1;orientation 1
Mol_m1-o1-rbra2.pdb	
Mol_m1-o1.mol2	*conformation 1; Force field library*
esout_m1	RESP output (without intra-molecular charge constraint)
espot_m1	Two espots of molecule 1 concatenated in a single file
espot_m1-1-1	*m1*-1-1: molecule 1; conformation 1; orientation 1
espot_m1-1-2	
input1_m1	RESP input - single molecule (stage 1)
input2_m1	RESP input - single molecule (stage 2)
output1_m1	RESP output - single molecule (stage 1)
output2_m1	RESP output - single molecule (stage 2)
punch1_m1	RESP output - single molecule (stage 1)
punch2_m1	RESP output - single molecule (stage 2)
qout1_m1	RESP output (charge values - stage 1)
qout2_m1	RESP output (charge values - stage 2)
Mol_m2	**Single molecule charge derivation**
File4REDDB_m2.pdb	*m2 = molecule 2*
JOB2-gau_m2-1-1.com	Gaussian input: *m2*-1-1: molecule 2; conformation 1; orientation 1
JOB2-gau_m2-1-1.out	Gaussian output
JOB2-gau_m2-1-2.com	
JOB2-gau_m2-1-2.out	
JOB2-gau_m2-1-3.com	
JOB2-gau_m2-1-3.out	
JOB2-gau_m2-1-4.com	
JOB2-gau_m2-1-4.out	
JOB2-gau_m2-2-1.com	Gaussian input: *m2*-2-1: molecule 2; conformation 2; orientation 1
JOB2-gau_m2-2-1.out	Gaussian output
JOB2-gau_m2-2-2.com	
JOB2-gau_m2-2-2.out	
JOB2-gau_m2-2-3.com	
JOB2-gau_m2-2-3.out	
JOB2-gau_m2-2-4.com	
JOB2-gau_m2-2-4.out	
Mol_m2-o1-qmra.pdb	conformation 1; Orientation of opt. geometry based on the Gaussian program
Mol_m2-o1-rbra1.pdb	Rigid-body re-orientation algorithm: conformation 1;orientation 1
Mol_m2-o1-rbra2.pdb	
Mol_m2-o1-rbra3.pdb	
Mol_m2-o1-rbra4.pdb	
Mol_m2-o1.mol2	*conformation 1; Force field library (without intra-molecular charge constraint)*
Mol_m2-o1-sm.mol2	*conformation 1; Force field library (with intra-molecular charge constraint)*
Mol_m2-o2-qmra.pdb	conformation 2; Orientation of opt. geometry based on the Gaussian program
Mol_m2-o2-rbra1.pdb	Rigid-body re-orientation algorithm: conformation 2;orientation 1
Mol_m2-o2-rbra2.pdb	
Mol_m2-o2-rbra3.pdb	
Mol_m2-o2-rbra4.pdb	
Mol_m2-o2.mol2	*conformation 2; Force field library (without intra-molecular charge constraint)*
Mol_m2-o2-sm.mol2	*conformation 2; Force field library (with intra-molecular charge constraint)*
esout_m2	RESP output (without intra-molecular charge constraint)
esout_m2.sm	RESP output (with intra-molecular charge constraint)
espot_m2	Eight espots of molecule 2 concatenated in a single file
espot_m2-1-1	*m2*-1-1: molecule 2; conformation 1; orientation 1
espot_m2-1-2	
espot_m2-1-3	
espot_m2-1-4	
espot_m2-2-1	*m2*-1-1: molecule 2; conformation 2; orientation 1
espot_m2-2-2	
espot_m2-2-3	
espot_m2-2-4	
input1_m2	RESP input - single molecule (stage 1) (without intra-molecular charge constraint)
input1_m2.sm	RESP input - single molecule (stage 1) (with intra-molecular charge constraint)
input2_m2	RESP input - single molecule (stage 2) (without intra-molecular charge constraint)
input2_m2.sm	RESP input - single molecule (stage 2) (with intra-molecular charge constraint)
output1_m2	RESP output - single molecule (stage 1) (without intra-molecular charge constraint)
output1_m2.sm	RESP output - single molecule (stage 1) (with intra-molecular charge constraint)

output2_m2	RESP output - single molecule (stage 2) (without intra-molecular charge constraint)
output2_m2.sm	RESP output - single molecule (stage 2) (with intra-molecular charge constraint)
punch1_m2	RESP output - single molecule (stage 1) (without intra-molecular charge constraint)
punch1_m2.sm	RESP output - single molecule (stage 1) (with intra-molecular charge constraint)
punch2_m2	RESP output - single molecule (stage 2) (without intra-molecular charge constraint)
punch2_m2.sm	RESP output - single molecule (stage 2) (with intra-molecular charge constraint)
qout1_m2	RESP output (charge values - stage 1) (without intra-molecular charge constraint)
qout1_m2.sm	RESP output (charge values - stage 1) (with intra-molecular charge constraint)
qout2_m2	RESP output (charge values - stage 2) (without intra-molecular charge constraint)
qout2_m2.sm	RESP output (charge values - stage 2) (with intra-molecular charge constraint)
Mol_MM	**Multiple molecules charge derivation**
esout_mm	RESP output - multiple molecules (stage 1) (with intra-mcc & inter-mcc)
espot_mm	Ten espots of molecules 1 & 2 concatenated in a single file
input1_mm	RESP input - multiple molecules (stage 1) (with intra-mcc & inter-mcc)
input2_mm	RESP input - multiple molecules (stage 2) (with intra-mcc & inter-mcc)
mm1-o1.FG1.mol2	Molecule 1; conformation 1 - fragment 1
mm1-o1.mol2	Molecule 1; conformation 1
mm2-o1-FG.mol2	***N*-terminal fragment originating from Molecules 1 + 2; Molecule 2 - conformation 1**
mm2-o1.FG1.mol2	Molecule 2; conformation 1 - fragment 1
mm2-o1.FG2.mol2	Molecule 2; conformation 1 - fragment 2
mm2-o1.mol2	Molecule 2; conformation 1
mm2-o2-FG.mol2	***N*-terminal fragment originating from Molecules 1 + 2; Molecule 2 - conformation 2**
mm2-o2.FG1.mol2	Molecule 2; conformation 2 - fragment 1
mm2-o2.FG2.mol2	Molecule 2; conformation 2 - fragment 2
mm2-o2.mol2	Molecule 2; conformation 2
output1_mm	RESP output - multiple molecules (stage 1) (with intra-mcc & inter-mcc)
output2_mm	RESP output - multiple molecules (stage 2) (with intra-mcc & inter-mcc)
punch1_mm	RESP output - multiple molecules (stage 1) (with intra-mcc & inter-mcc)
punch2_mm	RESP output - multiple molecules (stage 2) (with intra-mcc & inter-mcc)
qout1_mm	RESP output - multiple molecules (stage 1) (with intra-mcc & inter-mcc)
qout2_mm	RESP output - multiple molecules (stage 2) (with intra-mcc & inter-mcc)