Files generated by R.E.D. Server/R.E.D. IV
Charge derivation & force field library building for the different fragments of a new nucleotide.

Programs interfaced: 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	
JOB2-gau_m1-1-3.com	
JOB2-gau_m1-1-3.out	
JOB2-gau_m1-1-4.com	
JOB2-gau_m1-1-4.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-rbra3.pdb	
Mol_m1-o1-rbra4.pdb	
Mol_m1-o1.mol2	*conformation 1; Force field library*
esout_m1	RESP output
espot_m1	Four 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	
espot_m1-1-3	
espot_m1-1-4	
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	
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*
esout_m2	RESP output
espot_m2	Four 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	
input1_m2	RESP input - single molecule (stage 1)
input2_m2	RESP input - single molecule (stage 2)
output1_m2	RESP output - single molecule (stage 1)
output2_m2	RESP output - single molecule (stage 2)
punch1_m2	RESP output - single molecule (stage 1)
punch2_m2	RESP output - single molecule (stage 2)
qout1_m2	RESP output (charge values - stage 1)
qout2_m2	RESP output (charge values - stage 2)

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Mol_MM	**Multiple molecules charge derivation**
esout_mm	RESP output - multiple molecules (stage 1) (with inter-mcc)
espot_mm	8 espots of molecules 1 & 2 concatenated in a single file
input1_mm	RESP input - multiple molecules (stage 1) (with inter-mcc)
input2_mm	RESP input - multiple molecules (stage 2) (with inter-mcc)
mm1-o1.FG1.mol2	Molecule 1 - conformation 1 - fragment 1
mm1-o1.mol2	Molecule 1 - conformation 1
mm2-o1-CT-A.mol2	Central fragment - Molecule 2 - conformation 1 - Topology A
mm2-o1-CT-B.mol2	Central fragment - Molecule 2 - conformation 1 - Topology B
mm2-o1-OX-A.mol2	X'-terminal fragment - Molecule 2 - conformation 1 - Topology A
mm2-o1-OX-B.mol2	X'-terminal fragment - Molecule 2 - conformation 1 - Topology B
mm2-o1-OY-A.mol2	Y'-terminal fragment - Molecule 2 - conformation 1 - Topology A
mm2-o1-OY-B.mol2	Y'-terminal fragment - Molecule 2 - conformation 1 - Topology B
mm2-o1.FG1.mol2	Molecule 2 - conformation 1 - fragment 1
mm2-o1.mol2	Molecule 2 - conformation 1
output1_mm	RESP output - multiple molecules (stage 1) (with inter-mcc)
output2_mm	RESP output - multiple molecules (stage 2) (with inter-mcc)
punch1_mm	RESP output - multiple molecules (stage 1) (with inter-mcc)
punch2_mm	RESP output - multiple molecules (stage 2) (with inter-mcc)
qout1_mm	RESP output - multiple molecules (stage 1) (with inter-mcc)
qout2_mm	RESP output - multiple molecules (stage 2) (with inter-mcc)