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

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	
JOB2-gau_m1-2-1.com	Gaussian input: *m1*-2-1: molecule 1; conformation 2; orientation 1
JOB2-gau_m1-2-1.out	Gaussian output
JOB2-gau_m1-2-2.com	
JOB2-gau_m1-2-2.out	
JOB2-gau_m1-2-3.com	
JOB2-gau_m1-2-3.out	
JOB2-gau_m1-2-4.com	
JOB2-gau_m1-2-4.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 (without intra-molecular charge constraint)*
Mol_m1-o1-sm.mol2	***conformation 1; Force field library (with intra-molecular charge constraint)***
Mol_m1-o2-qmra.pdb	conformation 2; Orientation of opt. geometry based on the Gaussian program
Mol_m1-o2-rbra1.pdb	Rigid-body re-orientation algorithm: conformation 2;orientation 1
Mol_m1-o2-rbra2.pdb	
Mol_m1-o2-rbra3.pdb	
Mol_m1-o2-rbra4.pdb	
Mol_m1-o2.mol2	*conformation 2; Force field library (without intra-molecular charge constraint)*
Mol_m1-o2-sm.mol2	***conformation 2; Force field library (with intra-molecular charge constraint)***
esout_m1	RESP output (without intra-molecular charge constraint)
esout_m1.sm	RESP output (with intra-molecular charge constraint)
espot_m1	Eight 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	
espot_m1-2-1	*m1*-1-1: molecule 1; conformation 2; orientation 1
espot_m1-2-2	
espot_m1-2-3	
espot_m1-2-4	
input1_m1	RESP input - single molecule (stage 1) (without intra-molecular charge constraint)
input1_m1.sm	RESP input - single molecule (stage 1) (with intra-molecular charge constraint)
input2_m1	RESP input - single molecule (stage 2) (without intra-molecular charge constraint)
input2_m1.sm	RESP input - single molecule (stage 2) (with intra-molecular charge constraint)
output1_m1	RESP output - single molecule (stage 1) (without intra-molecular charge constraint)
output1_m1.sm	RESP output - single molecule (stage 1) (with intra-molecular charge constraint)
output2_m1	RESP output - single molecule (stage 2) (without intra-molecular charge constraint)
output2_m1.sm	RESP output - single molecule (stage 2) (with intra-molecular charge constraint)
punch1_m1	RESP output - single molecule (stage 1) (without intra-molecular charge constraint)
punch1_m1.sm	RESP output - single molecule (stage 1) (with intra-molecular charge constraint)
punch2_m1	RESP output - single molecule (stage 2) (without intra-molecular charge constraint)
punch2_m1.sm	RESP output - single molecule (stage 2) (with intra-molecular charge constraint)
qout1_m1	RESP output (charge values - stage 1) (without intra-molecular charge constraint)
qout1_m1.sm	RESP output (charge values - stage 1) (with intra-molecular charge constraint)
qout2_m1	RESP output (charge values - stage 2) (without intra-molecular charge constraint)
qout2_m1.sm	RESP output (charge values - stage 2) (with intra-molecular charge constraint)

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	
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.mol2	*conformation 1; Force field library*
esout_m2	RESP output (without intra-molecular charge constraint)
espot_m2	Two 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	
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)

Mol_m3	**Single molecule charge derivation**
File4REDDB_m3.pdb	*m3 = molecule 3*
JOB2-gau_m3-1-1.com	Gaussian input: *m3-1-1*: molecule 3; conformation 1; orientation 1
JOB2-gau_m3-1-1.out	Gaussian output
JOB2-gau_m3-1-2.com	
JOB2-gau_m3-1-2.out	
JOB2-gau_m3-1-3.com	
JOB2-gau_m3-1-3.out	
JOB2-gau_m3-1-4.com	
JOB2-gau_m3-1-4.out	
JOB2-gau_m3-2-1.com	Gaussian input: *m3-2-1*: molecule 3; conformation 2; orientation 1
JOB2-gau_m3-2-1.out	Gaussian output
JOB2-gau_m3-2-2.com	
JOB2-gau_m3-2-2.out	
JOB2-gau_m3-2-3.com	
JOB2-gau_m3-2-3.out	
JOB2-gau_m3-2-4.com	
JOB2-gau_m3-2-4.out	
Mol_m3-o1-qmra.pdb	conformation 1; Orientation of opt. geometry based on the Gaussian program
Mol_m3-o1-rbra1.pdb	Rigid-body re-orientation algorithm: conformation 1;orientation 1
Mol_m3-o1-rbra2.pdb	
Mol_m3-o1-rbra3.pdb	
Mol_m3-o1-rbra4.pdb	
Mol_m3-o1.mol2	*conformation 1; Force field library (without intra-molecular charge constraint)*
Mol_m3-o1-sm.mol2	*conformation 1; Force field library (with intra-molecular charge constraint)*
Mol_m3-o2-qmra.pdb	conformation 2; Orientation of opt. geometry based on the Gaussian program
Mol_m3-o2-rbra1.pdb	Rigid-body re-orientation algorithm: conformation 2;orientation 1
Mol_m3-o2-rbra2.pdb	
Mol_m3-o2-rbra3.pdb	
Mol_m3-o2-rbra4.pdb	
Mol_m3-o2.mol2	*conformation 2; Force field library (without intra-molecular charge constraint)*
Mol_m3-o2-sm.mol2	*conformation 2; Force field library (with intra-molecular charge constraint)*
esout_m3	RESP output (without intra-molecular charge constraint)
esout_m3.sm	RESP output (with intra-molecular charge constraint)
espot_m3	Eight espots of molecule 3 concatenated in a single file
espot_m3-1-1	*m3-1-1*: molecule 3; conformation 1; orientation 1
espot_m3-1-2	
espot_m3-1-3	
espot_m3-1-4	
espot_m3-2-1	*m3-1-1*: molecule 3; conformation 2; orientation 1
espot_m3-2-2	
espot_m3-2-3	
espot_m3-2-4	
input1_m3	RESP input - single molecule (stage 1) (without intra-molecular charge constraint)
input1_m3.sm	RESP input - single molecule (stage 1) (with intra-molecular charge constraint)
input2_m3	RESP input - single molecule (stage 2) (without intra-molecular charge constraint)
input2_m3.sm	RESP input - single molecule (stage 2) (with intra-molecular charge constraint)
output1_m3	RESP output - single molecule (stage 1) (without intra-molecular charge constraint)
output1_m3.sm	RESP output - single molecule (stage 1) (with intra-molecular charge constraint)
output2_m3	RESP output - single molecule (stage 2) (without intra-molecular charge constraint)
output2_m3.sm	RESP output - single molecule (stage 2) (with intra-molecular charge constraint)
punch1_m3	RESP output - single molecule (stage 1) (without intra-molecular charge constraint)
punch1_m3.sm	RESP output - single molecule (stage 1) (with intra-molecular charge constraint)
punch2_m3	RESP output - single molecule (stage 2) (without intra-molecular charge constraint)
punch2_m3.sm	RESP output - single molecule (stage 2) (with intra-molecular charge constraint)
qout1_m3	RESP output (charge values - stage 1) (without intra-molecular charge constraint)
qout1_m3.sm	RESP output (charge values - stage 1) (with intra-molecular charge constraint)
qout2_m3	RESP output (charge values - stage 2) (without intra-molecular charge constraint)
qout2_m3.sm	RESP output (charge values - stage 2) (with intra-molecular charge constraint)

Mol_m4	**Single molecule charge derivation**
File4REDDB_m4.pdb	*m4 = molecule 4*
JOB2-gau_m4-1-1.com	Gaussian input: *m4-1-1*: molecule 4; conformation 1; orientation 1
JOB2-gau_m4-1-1.out	Gaussian output
JOB2-gau_m4-1-2.com	
JOB2-gau_m4-1-2.out	
Mol_m4-o1-qmra.pdb	conformation 1; Orientation of opt. geometry based on the Gaussian program
Mol_m4-o1-rbra1.pdb	Rigid-body re-orientation algorithm: conformation 1;orientation 1
Mol_m4-o1-rbra2.pdb	
Mol_m4-o1.mol2	*conformation 1; Force field library*
esout_m4	RESP output (without intra-molecular charge constraint)
espot_m4	Two espots of molecule 4 concatenated in a single file
espot_m4-1-1	*m4-1-1*: molecule 4; conformation 1; orientation 1
espot_m4-1-2	
input1_m4	RESP input - single molecule (stage 1)
input2_m4	RESP input - single molecule (stage 2)
output1_m4	RESP output - single molecule (stage 1)
output2_m4	RESP output - single molecule (stage 2)
punch1_m4	RESP output - single molecule (stage 1)
punch2_m4	RESP output - single molecule (stage 2)
qout1_m4	RESP output (charge values - stage 1)
qout2_m4	RESP output (charge values - stage 2)

Mol_m5	**Single molecule charge derivation**
File4REDDB_m5.pdb	*m5 = molecule 5*
JOB2-gau_m5-1-1.com	Gaussian input: *m5-1-1*: molecule 5; conformation 1; orientation 1
JOB2-gau_m5-1-1.out	Gaussian output
JOB2-gau_m5-1-2.com	
JOB2-gau_m5-1-2.out	
JOB2-gau_m5-1-3.com	
JOB2-gau_m5-1-3.out	
JOB2-gau_m5-1-4.com	
JOB2-gau_m5-1-4.out	
JOB2-gau_m5-2-1.com	Gaussian input: *m5-2-1*: molecule 5; conformation 2; orientation 1
JOB2-gau_m5-2-1.out	Gaussian output
JOB2-gau_m5-2-2.com	
JOB2-gau_m5-2-2.out	
JOB2-gau_m5-2-3.com	
JOB2-gau_m5-2-3.out	
JOB2-gau_m5-2-4.com	
JOB2-gau_m5-2-4.out	
Mol_m5-o1-qmra.pdb	conformation 1; Orientation of opt. geometry based on the Gaussian program
Mol_m5-o1-rbra1.pdb	Rigid-body re-orientation algorithm: conformation 1;orientation 1
Mol_m5-o1-rbra2.pdb	
Mol_m5-o1-rbra3.pdb	
Mol_m5-o1-rbra4.pdb	
Mol_m5-o1.mol2	*conformation 1; Force field library (without intra-molecular charge constraint)*
Mol_m5-o1-sm.mol2	*conformation 1; Force field library (with intra-molecular charge constraint)*
Mol_m5-o2-qmra.pdb	conformation 2; Orientation of opt. geometry based on the Gaussian program
Mol_m5-o2-rbra1.pdb	Rigid-body re-orientation algorithm: conformation 2;orientation 1
Mol_m5-o2-rbra2.pdb	
Mol_m5-o2-rbra3.pdb	
Mol_m5-o2-rbra4.pdb	
Mol_m5-o2.mol2	*conformation 2; Force field library (without intra-molecular charge constraint)*
Mol_m5-o2-sm.mol2	*conformation 2; Force field library (with intra-molecular charge constraint)*
esout_m5	RESP output (without intra-molecular charge constraint)
esout_m5.sm	RESP output (with intra-molecular charge constraint)
espot_m5	Eight espots of molecule 5 concatenated in a single file
espot_m5-1-1	*m5-1-1*: molecule 5; conformation 1; orientation 1
espot_m5-1-2	
espot_m5-1-3	
espot_m5-1-4	
espot_m5-2-1	*m5-1-1*: molecule 5; conformation 2; orientation 1
espot_m5-2-2	
espot_m5-2-3	
espot_m5-2-4	
input1_m5	RESP input - single molecule (stage 1) (without intra-molecular charge constraint)
input1_m5.sm	RESP input - single molecule (stage 1) (with intra-molecular charge constraint)
input2_m5	RESP input - single molecule (stage 2) (without intra-molecular charge constraint)
input2_m5.sm	RESP input - single molecule (stage 2) (with intra-molecular charge constraint)
output1_m5	RESP output - single molecule (stage 1) (without intra-molecular charge constraint)
output1_m5.sm	RESP output - single molecule (stage 1) (with intra-molecular charge constraint)
output2_m5	RESP output - single molecule (stage 2) (without intra-molecular charge constraint)
output2_m5.sm	RESP output - single molecule (stage 2) (with intra-molecular charge constraint)
punch1_m5	RESP output - single molecule (stage 1) (without intra-molecular charge constraint)
punch1_m5.sm	RESP output - single molecule (stage 1) (with intra-molecular charge constraint)
punch2_m5	RESP output - single molecule (stage 2) (without intra-molecular charge constraint)
punch2_m5.sm	RESP output - single molecule (stage 2) (with intra-molecular charge constraint)
qout1_m5	RESP output (charge values - stage 1) (without intra-molecular charge constraint)
qout1_m5.sm	RESP output (charge values - stage 1) (with intra-molecular charge constraint)
qout2_m5	RESP output (charge values - stage 2) (without intra-molecular charge constraint)
qout2_m5.sm	RESP output (charge values - stage 2) (with intra-molecular charge constraint)

Mol_m6	**Single molecule charge derivation**
File4REDDB_m6.pdb	*m6 = molecule 6*
JOB2-gau_m6-1-1.com	Gaussian input: *m6*-1-1: molecule 6; conformation 1; orientation 1
JOB2-gau_m6-1-1.out	Gaussian output
JOB2-gau_m6-1-2.com	
JOB2-gau_m6-1-2.out	
JOB2-gau_m6-1-3.com	
JOB2-gau_m6-1-3.out	
JOB2-gau_m6-1-4.com	
JOB2-gau_m6-1-4.out	
JOB2-gau_m6-2-1.com	Gaussian input: *m6*-2-1: molecule 6; conformation 2; orientation 1
JOB2-gau_m6-2-1.out	Gaussian output
JOB2-gau_m6-2-2.com	
JOB2-gau_m6-2-2.out	
JOB2-gau_m6-2-3.com	
JOB2-gau_m6-2-3.out	
JOB2-gau_m6-2-4.com	
JOB2-gau_m6-2-4.out	
Mol_m6-o1-qmra.pdb	conformation 1; Orientation of opt. geometry based on the Gaussian program
Mol_m6-o1-rbra1.pdb	Rigid-body re-orientation algorithm: conformation 1;orientation 1
Mol_m6-o1-rbra2.pdb	
Mol_m6-o1-rbra3.pdb	
Mol_m6-o1-rbra4.pdb	
Mol_m6-o1.mol2	*conformation 1; Force field library*
Mol_m6-o2-qmra.pdb	conformation 2; Orientation of opt. geometry based on the Gaussian program
Mol_m6-o2-rbra1.pdb	Rigid-body re-orientation algorithm: conformation 2;orientation 1
Mol_m6-o2-rbra2.pdb	
Mol_m6-o2-rbra3.pdb	
Mol_m6-o2-rbra4.pdb	
Mol_m6-o2.mol2	*conformation 2; Force field library*
esout_m6	RESP output
espot_m6	Eight espots of molecule 6 concatenated in a single file
espot_m6-1-1	*m6*-1-1: molecule 6; conformation 1; orientation 1
espot_m6-1-2	
espot_m6-1-3	
espot_m6-1-4	
espot_m6-2-1	*m6*-1-1: molecule 6; conformation 2; orientation 1
espot_m6-2-2	
espot_m6-2-3	
espot_m6-2-4	
input1_m6	RESP input - single molecule (stage 1)
input2_m6	RESP input - single molecule (stage 2)
output1_m6	RESP output - single molecule (stage 1)
output2_m6	RESP output - single molecule (stage 2)
punch1_m6	RESP output - single molecule (stage 1)
punch2_m6	RESP output - single molecule (stage 2)
qout1_m6	RESP output (charge values - stage 1)
qout2_m6	RESP output (charge values - stage 2)

Mol_MM	**Multiple molecules charge derivation**
esout_mm	RESP output - multiple molecules (stage 1) (with intra-mcc & inter-mcc)
espot_mm	36 espots of molecules 1-6 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.FG2.mol2	**Central fragment: Molecule 1 – conformation 1 (Fragment 2)**
mm1-o1.mol2	Molecule 1 – conformation 1
mm1-o2.FG1.mol2	Molecule 1 – conformation 2 – Fragment 1
mm1-o2.FG2.mol2	**Central fragment: Molecule 1 – conformation 2 (Fragment 2)**
mm1-o2.mol2	Molecule 1 – conformation 2
mm2-o1.FG1.mol2	Molecule 2 – Fragment 1
mm2-o1.mol2	Molecule 2
mm3-o1-FG.mol2	***N*-terminal fragment: Molecule 3 – conformation 1**
mm3-o1.FG1.mol2	Molecule 3 – conformation 1 – Fragment 1
mm3-o1.FG2.mol2	Molecule 3 – conformation 1 – Fragment 2
mm3-o1.mol2	Molecule 3 – conformation 1
mm3-o2-FG.mol2	***N*-terminal fragment: Molecule 3 – conformation 2**
mm3-o2.FG1.mol2	Molecule 3 – conformation 2 – Fragment 1
mm3-o2.FG2.mol2	Molecule 3 – conformation 2 – Fragment 2
mm3-o2.mol2	Molecule 3 – conformation 2
mm4-o1.FG1.mol2	Molecule 4 – Fragment 1
mm4-o1.mol2	Molecule 4
mm5-o1-FG.mol2	***C*-terminal fragment: Molecule 5 – conformation 1**
mm5-o1.FG1.mol2	Molecule 5 – conformation 1 – Fragment 1
mm5-o1.FG2.mol2	Molecule 5 – conformation 1 – Fragment 2
mm5-o1.mol2	Molecule 5 – conformation 1
mm5-o2-FG.mol2	***C*-terminal fragment: Molecule 5 – conformation 2**
mm5-o2.FG1.mol2	Molecule 5 – conformation 2 – Fragment 1
mm5-o2.FG2.mol2	Molecule 5 – conformation 2 – Fragment 2
mm5-o2.mol2	Molecule 5 – conformation 2
mm6-o1.mol2	Molecule 6 – conformation 1
mm6-o2.mol2	Molecule 6 – 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)