# Files generated by R.E.D. Server Development/PyRED
# Force field generation for deoxyadenosine and its three molecular fragments
# Programs interfaced: Gaussian 2009 & RESP 2.4

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|---|---|
| **Mol_m1** | Already described in previous examples |
| **Mol_m2** | Already described in previous examples |

| **Mol_MM** | **Multiple molecules** |
|---|---|
| Mol_MM/Mol_mm1-c1.mol2 | Force field library for mol. 1 conf. 1 (dimethylphosphate) |
| Mol_MM/Mol_mm2-c1.mol2 | Force field library for mol. 2 conf. 1 (deoxyadenosine) |
| Mol_MM/Mol_mm2-c2.mol2 | Force field library for mol. 2 conf. 2 (deoxyadenosine) |
| 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 |
| 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 |
| Mol_MM/input2_mm.in | Multiple molecules - resp input stage 2 |
| Mol_MM/output1_mm.log | Multiple molecules - resp log/output stage 1 |
| Mol_MM/output2_mm.log | Multiple molecules - resp log/output stage 2 |
| Mol_MM/punch1_mm.dat | Multiple molecules - resp punch stage 1 |
| Mol_MM/punch2_mm.dat | Multiple molecules - resp punch stage 2 |
| Mol_MM/qout1_mm.dat | Multiple molecules - charge values stage 1 |
| Mol_MM/qout2_mm.dat | Multiple molecules - charge values stage 2 |

| **Mol_MM/INTER** | |
|---|---|
| INTER/CT-A_m1-c1_m2-c1.mol2 | Force field library for mol. 1 + mol. 2 conf. 1 - Central fragment - topology A |
| INTER/CT-A_m1-c1_m2-c2.mol2 | Force field library for mol. 1 + mol. 2 conf. 2 - Central fragment - topology A |
| INTER/CT-B_m1-c1_m2-c1.mol2 | Force field library for mol. 1 + mol. 2 conf. 1 - Central fragment - topology B |
| INTER/CT-B_m1-c1_m2-c2.mol2 | Force field library for mol. 1 + mol. 2 conf. 2 - Central fragment - topology B |
| INTER/OX-A_m1-c1_m2-c1.mol2 | Force field library for mol. 1 + mol. 2 conf. 1 - OX-terminal fragment - topology A |
| INTER/OX-A_m1-c1_m2-c2.mol2 | Force field library for mol. 1 + mol. 2 conf. 2 - OX-terminal fragment - topology A |
| INTER/OX-B_m1-c1_m2-c1.mol2 | Force field library for mol. 1 + mol. 2 conf. 1 - OX-terminal fragment - topology B |
| INTER/OX-B_m1-c1_m2-c2.mol2 | Force field library for mol. 1 + mol. 2 conf. 2 - OX-terminal fragment - topology B |
| INTER/OY-A_m1-c1_m2-c1.mol2 | Force field library for mol. 1 + mol. 2 conf. 1 - OY-terminal fragment - topology A |
| INTER/OY-A_m1-c1_m2-c2.mol2 | Force field library for mol. 1 + mol. 2 conf. 2 - OY-terminal fragment - topology A |
| INTER/OY-B_m1-c1_m2-c1.mol2 | Force field library for mol. 1 + mol. 2 conf. 1 - OY-terminal fragment - topology B |
| INTER/OY-B_m1-c1_m2-c2.mol2 | Force field library for mol. 1 + mol. 2 conf. 2 - OY-terminal fragment - topology B |

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|---|---|
| INTER/m1-c1_m2-c1.mol2 | Force field library for mol. 1 + mol. 2 conf. 1 topology A |
| INTER/m1-c1_m2-c1_n1.mol2 | Force field library for mol. 1 + mol. 2 conf. 1 topology B |
| INTER/m1-c1_m2-c2.mol2 | Force field library for mol. 1 + mol. 2 conf. 2 topology A |
| INTER/m1-c1_m2-c2_n1.mol2 | Force field library for mol. 1 + mol. 2 conf. 2 topology B |
| **Mol_MM**/INTER/mm1 | Force field library for fragments, that derives from dimethylphosphate |
| **Mol_MM**/INTER/mm2 | Force field library for fragments, that derives from  deoxyadenosine |

**Data-Default-Proj/**

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|---|---|
| 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 deoxyadenosine and its different fragments |
| Data-Default-Proj/frcmod.unknown | List of unknown force field parameters for deoxyadenosine and its different fragments |
| Data-Default-Proj/leaprc.ff13q4mdfft | LEaP script: loads the generated force field for deoxyadenosine and its different fragments |
| 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) |