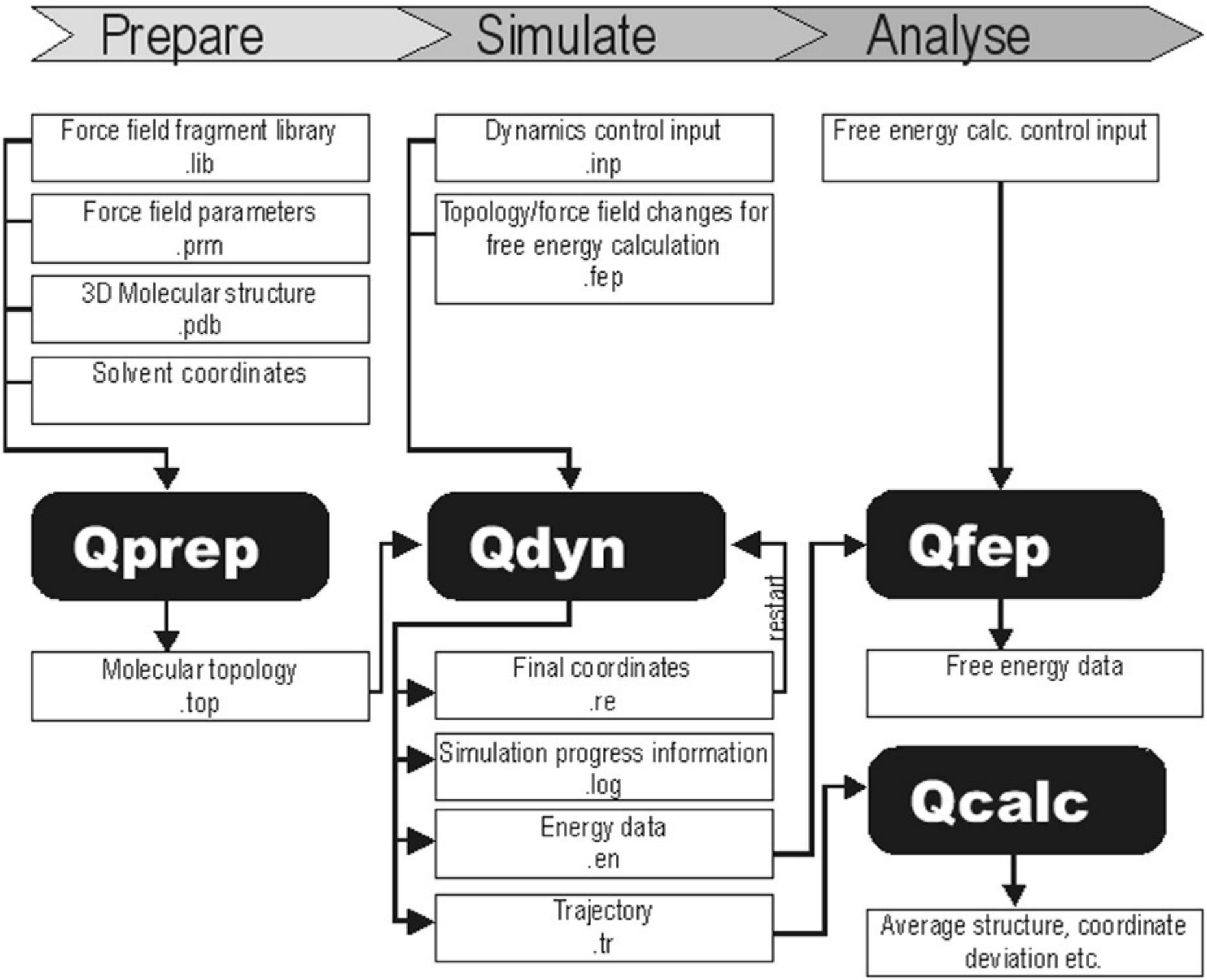
Prepare
Simulate
Analyse
Force field fragment library
.lib
Force field parameters
.prm
3D Molecular structure
.pdb
Solvent coordinates
Dynamics control input
.inp
Topology/force field changes for free energy calculation
.fep
Free energy calc. control input
Qprep
Qdyn
Qfep
Molecular topology
.top
Final coordinates
.re
restart
Free energy data
Simulation progress information
.log
Energy data
.en
Qcalc
Trajectory
.tr
Average structure, coordinate deviation etc.