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em.mdp

```
integrator              = steep
dt                    = 0.002
nsteps                  = 50000
em_tol     = 100.0
cutoff-scheme           = Verlet
nstlist                 = 1
ns_type                 = grid
pbc                   = xyz
rlist                 = 1.4

coulombtype             = reaction-field
rcoulomb_switch         = 0.0
rcoulomb                = 1.1
epsilon_r               = 15
vdw_type                = cutoff
vdw-modifier            = Potential-shift-verlet
rvdw                  = 1.1
constraints             = none
```

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equil.mdp

```
integrator              = md
dt                    = 0.002
nsteps                  = 500000

nstxout    = 0
nstvout                 = 0
nstfout                 = 0
nstlog                  = 1000
nstenergy               = 100
nstxout-compressed  = 1000
compressed-x-precision   = 100

cutoff-scheme           = Verlet
nstlist                 = 10
ns_type                 = grid
pbc                   = xyz
verlet-buffer-tolerance  = 0.005

coulombtype             = reaction-field
rcoulomb                = 1.1
epsilon_r               = 15
vdw_type                = cutoff
vdw-modifier            = Potential-shift-verlet
rvdw                  = 1.1

tcoupl                  = v-rescale
tc-grps                 = System
tau_t                 = 2.0 ;0.5
```

```
ref_t                = 300
Pcoupltype             = isotropic
Pcoupl               = berendsen
tau_p                = 4.0
compressibility        = 3e-4
ref_p                = 1.0
refcoord-scaling       = com

constraints   = none


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ions.mdp
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; ions.mdp - used as input into grompp to generate ions.tpr
; Parameters describing what to do, when to stop and what to save
integrator  = steep        ; Algorithm (steep = steepest descent minimization)
emtol       = 1000.0       ; Stop minimization when the maximum force < 1000.0 kJ/mol/nm
emstep      = 0.002        ; Minimization step size
nsteps      = 50000        ; Maximum number of (minimization) steps to perform

; Parameters describing how to find the neighbors of each atom and how to calculate the interactions
nstlist         = 1         ; Frequency to update the neighbor list and long range forces
cutoff-scheme = Verlet    ; Buffered neighbor searching
ns_type         = grid      ; Method to determine neighbor list (simple, grid)
coulombtype     = cutoff    ; Treatment of long range electrostatic interactions
rcoulomb        = 1.0       ; Short-range electrostatic cut-off
rvdw            = 1.0       ; Short-range Van der Waals cut-off
pbc             = xyz       ; Periodic Boundary Conditions in all 3 dimensions

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mdrun.mdp
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integrator              = md
dt                    = 0.001
nsteps                  = 1000000000

nstxout    = 0
nstvout                 = 0
nstfout                 = 0
nstlog                  = 50000
nstenergy               = 50000
nstxout-compressed  = 50000
compressed-x-precision   = 100

cutoff-scheme           = Verlet
nstlist                 = 10
ns_type                 = grid
pbc                   = xyz
verlet-buffer-tolerance  = 0.005

coulombtype             = reaction-field
rcoulomb                = 1.1
```

```
epsilon_r               = 15
vdw_type                = cutoff
vdw-modifier            = Potential-shift-verlet
rvdw                    = 1.1

tcoupl                  = v-rescale
tc-grps                 = System
tau_t                   = 2.0 ;0.5
ref_t                   = 300
Pcoupltype              = isotropic
Pcoupl                  = berendsen
tau_p                   = 3.0
compressibility         = 3e-4
ref_p                   = 1.0
refcoord-scaling        = com

constraints   = none

----------------minimization.mdp
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;
; STANDARD MD INPUT OPTIONS FOR MARTINI 2.x
; Updated 15 Jul 2015 by DdJ
;
; for use with GROMACS 5
; For a thorough comparison of different mdp options in combination with the Martini force field, see:
; D.H. de Jong et al., Martini straight: boosting performance using a shorter cutoff and GPUs, submitted.

title                   = Martini

; TIMESTEP IN MARTINI
; Most simulations are numerically stable with dt=40 fs,
; however better energy conservation is achieved using a
; 20-30 fs timestep.
; Time steps smaller than 20 fs are not required unless specifically stated in the itp file.

integrator              = steep
dt                      = 0.01
nsteps                  = 10000
nstcomm                 = 100
comm-grps               =

nstxout                 = 0
nstvout                 = 0
nstfout                 = 0
nstlog                  = 1000
nstenergy               = 100
nstxout-compressed      = 1000
compressed-x-precision  = 100
compressed-x-grps       =
energygrps              =

; NEIGHBOURLIST and MARTINI
; To achieve faster simulations in combination with the Verlet-neighborlist
; scheme, Martini can be simulated with a straight cutoff. In order to
```

```
; do so, the cutoff distance is reduced 1.1 nm.
; Neighborlist length should be optimized depending on your hardware setup:
; updating ever 20 steps should be fine for classic systems, while updating
; every 30-40 steps might be better for GPU based systems.
; The Verlet neighborlist scheme will automatically choose a proper neighborlist
; length, based on a energy drift tolerance.
;
; Coulomb interactions can alternatively be treated using a reaction-field,
; giving slightly better properties.
; Please realize that electrostVatic interactions in the Martini model are
; not considered to be very accurate to begin with, especially as the
; screening in the system is set to be uniform across the system with
; a screening constant of 15. When using PME, please make sure your
; system properties are still reasonable.
;
; With the polarizable water model, the relative electrostatic screening
; (epsilon_r) should have a value of 2.5, representative of a low-dielectric
; apolar solvent. The polarizable water itself will perform the explicit screening
; in aqueous environment. In this case, the use of PME is more realistic.


cutoff-scheme           = Verlet
nstlist                 = 20
ns_type                 = grid
pbc                     = xyz
verlet-buffer-tolerance  = 0.005

coulombtype             = reaction-field
rcoulomb                = 1.1
epsilon_r               = 15 ; 2.5 (with polarizable water)
epsilon_rf              = 0
vdw_type                = cutoff
vdw-modifier            = Potential-shift-verlet
rvdw                    = 1.1

; MARTINI and TEMPERATURE/PRESSURE
; normal temperature and pressure coupling schemes can be used.
; It is recommended to couple individual groups in your system separately.
; Good temperature control can be achieved with the velocity rescale (V-rescale)
; thermostat using a coupling constant of the order of 1 ps. Even better
; temperature control can be achieved by reducing the temperature coupling
; constant to 0.1 ps, although with such tight coupling (approaching
; the time step) one can no longer speak of a weak-coupling scheme.
; We therefore recommend a coupling time constant of at least 0.5 ps.
; The Berendsen thermostat is less suited since it does not give
; a well described thermodynamic ensemble.
;
; Pressure can be controlled with the Parrinello-Rahman barostat,
; with a coupling constant in the range 4-8 ps and typical compressibility
; in the order of 10e-4 - 10e-5 bar-1. Note that, for equilibration purposes,
; the Berendsen barostat probably gives better results, as the Parrinello-
; Rahman is prone to oscillating behaviour. For bilayer systems the pressure
; coupling should be done semiisotropic.

tcoupl                  = berendsen ; v-rescale
```

```
tc-grps                  = system
tau_t                    = 1.0
ref_t                    = 300
Pcoupl                   = berendsen ; parrinello-rahman
Pcoupltype               = isotropic
tau_p                    = 12.0 ; 12.0  ;parrinello-rahman is more stable with larger tau-p, DdJ, 20130422
compressibility          = 3e-4 ;  3e-4
ref_p                    = 1.0  ; 1.0

gen_vel                  = no
gen_temp                 = 320
gen_seed                 = 473529

; MARTINI and CONSTRAINTS
; for ring systems and stiff bonds constraints are defined
; which are best handled using Lincs.

constraints              = none
constraint_algorithm     = Lincs
```