```
title                    = Surfactants monolayer
define                   =

; RUN CONTROL PARAMETERS
integrator               = md ; Leap-frog integrator

; start time and timestep in ps
tinit                    = 600000.0
dt                       = 0.002
nsteps                   = 50000000

; number of steps for center of mass motion removal
comm_mode                = Linear
nstcomm                  = 1
comm_grps                = System

; OUTPUT CONTROL OPTIONS =
; Output frequency for coords (x), velocities (v) and forces (f)
nstxout                  = 500
nstvout                  = 1000
nstfout                  = 0

; Output frequency for energies to log file and energy file
nstlog                   = 500
nstenergy                = 500

; Output frequency and precision for xtc file
;nstxtcout               = 500
;xtc_precision           = 50

; NEIGHBORSEARCHING PARAMETERS
nstlist                  = 10

; Selection of energy groups =
energygrps               = SURF SOL Cal CL NA

; ns algorithm (simple or grid)
ns_type                  = grid

; Periodic boundary conditions: xyz or none
pbc                      = xyz
rlist                    = 1.2

; Method for doing electrostatics
coulombtype              = PME
rcoulomb                 = 1.2
rcoulomb_switch          = 1.0
fourierspacing           = 0.12
pme_order                = 4
optimize_fft             = yes

; Method for doing Van der Waals
;vdwtype                 = Switch
rvdw                     = 1.2   ; cut-off lengths
```

```
rvdw_switch             = 1.0

; Apply long range dispersion corrections for Energy and Pressure
DispCorr                = no

; Temperature coupling
tcoupl                  = V-rescale
tc_grps                 = SURF SOL Cal NA CL
tau_t                   = 0.1 0.1 0.1 0.1 0.1 ; Time constant (ps)
ref_t                   = 298 298 298 298 298  ; reference temperature
(K)

; GENERATE VELOCITIES FOR STARTUP RUN
gen_vel                 = no
gen_temp                = 2
gen_seed                = 473529



; OPTIONS FOR BONDS
constraints             = hbonds

; Type of constraint algorithm
constraint_algorithm    = lincs

; Highest order in the expansion of the constraint coupling matrix
lincs_order             = 4
lincs_iter              = 4

; Lincs will write a warning to the stderr if in one step a bond
; rotates over more degrees than
lincs_warnangle         = 30

cutoff-scheme          = verlet
```