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title                = Surfactants monolayer
define               =

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

; start time and timestep in ps
tinit                = 1000.0
dt                   = 0.002
nsteps               = 500000

; 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

; 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

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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
```