```
title                    = relaxation in ana ensemble with constant
surface tension

integrator               = md ; Leap-frog integrator
tinit                    = 0.0
dt                       = 0.002
nsteps                   = 500000

; number of steps for center of mass motion removal
comm_mode                = Linear
nstcomm                  = 10
comm_grps                = System

; Output frequency for coords (x), velocities (v) and forces (f)
nstxout                  = 5000
nstvout                  = 10000
nstfout                  = 0
; Output frequency for energies to log file and energy file
nstlog                   = 5000
nstenergy                = 500

; NEIGHBORSEARCHING PARAMETERS
nstlist                  = 10
nstcalcenergy            = 10
rlist                    = 1.2
ns_type                  = grid

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

; Periodic boundary conditions: xyz or none
pbc                      = xyz
cutoff-scheme            = verlet

; 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                  = Cut-off
vdw_modifier             = Force-switch
rvdw                     = 1.2
rvdw_switch              = 1.0
DispCorr                 = no

; Temperature coupling
tcoupl                   = V-rescale
tc_grps                  = NA CL SOL MEM Protein
tau_t                    = 0.1 0.1 0.1 0.1 0.1
```

```
ref_t                    = 310 310 310 310 310

; Pressure coupling
pcoupl                   = Berendsen
pcoupltype          = surface-tension
tau_p                    = 1.0
ref_p                    = 220 1.0
compressibility          = 4.5e-05 4.5e-5

; GENERATE VELOCITIES FOR STARTUP RUN
gen_vel                  = no

; 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
lincs_warnangle          = 30
```