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Appendices

Appendix 1

Input file for rigid-body docking of Cyt *f*-Pc using PRE restraints for Xplor-NIH 2.9.9

```
parameter
        @nostoc_cytf_SL_pc.par
 end
 structure
        @nostoc_cytf_SL_pc.psf
 end
 eval ($inifile="nostoc_cytf_SL_pc.pdb")
 coordinates @$inifile
 @learn.pcf.par
 constraints fix (segid="CYTF" or resn SL) end
 eval ($a05 = 6000)                    !total nr cycles / $a53
 eval ($a53 = 1000)                    !nr of steps
 eval ($u2 = 30)              !nr of cycles per docking approach
 eval ($a54 = 0.01)           !timestep in ps
 eval ($a61 = $a54*$a53)      !time per cycle (ps)
 eval ($a80 = $a61*$a05)      !total time (ps)
 eval ($a58=30.0)             !velocity factor
 eval ($a56=1.5)              !fbeta
 eval ($a55=300.0)            !TBATH
 eval ($a59=45.0)             !.pdb writing threshold
 eval ($van=100.0)            ! vdw writing threshold
 eval ($a59a=0.01*$a59)                !vx-reset minimum
 eval ($a60=1.0)              !.pdb lag factor              !5
 eval ($a301=1.0)             !VDW repel scale factor
 eval ($a93=1)                !time-spent factor: 0<$a93<1 (fraction bound)
 eval ($g1a = "N71C")         !names of the spin label 1 used in this calculation
 eval ($g1b = "Q104C")        !names of the spin label 2 used in this calculation
 eval ($g1c = "S192C")        !names of the spin label 3 used in this calculation
 eval ($g2a = 13)    !residue number of the 1st SL conformation of SL 1
 eval ($g2b = 17)    !residue number of the 1st SL conformation of SL 2
 eval ($g2c = 21)    !residue number of the 1st SL conformation of SL 3
 eval ($field=600.1328E6)     !field strength in Hz
 eval ($frl=1)                         !fraction of proteins with spin label
 eval ($tau_c=30.0E-9)                 !tau c for the complex in sec
 eval ($a9=0.01)                       !general scaling PRE (NOE) term
 eval ($a10=1.0)              !scale factor for CL1 (peaks disappeared)
 eval ($a11=1.0)              !scale factor for CL2 (peaks unaffected)
 eval ($a12=1.0)              !scale factor for CL3 (peaks reduced)
 eval ($low1=14.0)   !lower(d_minus) limit (SLA restraints upper limit only)
 eval ($up1=4.0)    !upper(d_plus) limit (restraints with upper limit only)
 eval ($low2=4.0)    !lower(d_minus) limit (restraints with lower limit only)
 eval ($up2=100.0)   !upper(d_plus) limit (restraints with lower limit only)
 eval ($low3=4.0)    !lower(d_minus) limit (restraints with both limits)
 eval ($up3=4.0)     !upper(d_plus) limit (restraints with both limits)
 eval ($a01 = 1)              !cycle counter
 eval ($a48=$cpu*1e4)
 set seed=$a48 end
 eval ($a14=0)
 eval ($a18=1)
 eval ($nout1=0)     ! Number of strucutres output per run
 eval ($min1=9999.0)
 eval ($min2=9999.0)
 eval ($ref=0)
 set display=coor.dat end              !write parameters
 display xx ----------PARAMETERS----------
 display xx startdate:       $DATE
 display xx starttime:       $TIME
 display xx ini.file:        $inifile
 display xx timestep (ps):   $a54
```

```
 display xx nr of steps:       $a53              time /cycle (ps):   $a61
 display xx nr of cycles:      $a05              total time  (ps):   $a80
 display xx time-spent fact:   $a93
 display xx general scale:     $a9
 display xx TBATH:             $a55    velocity factor:   $a56   fbeta:   $a58
 display xx .pdb threshold     $a59
 display xx .pdb lag factor    $a60
 display xx Local mimim. impulse after 10 cycles with 'constant' Etot > $a59a
 display xx ----------------------------------------------------------
 display
 set display=OUTPUT end
 flag exclude elec bond angl dihe impr include vdw noe end
 vector do (fbeta=$a58) (segid="PC")
 vector do (vx=$a56) (segid="PC")
 vector do (vy=$a56) (segid="PC")
 vector do (vz=$a56) (segid="PC")
set disp=ener.dat end
display Energies for the output structures
display file                Etot          VDW         NOE
display ------------------------------------------------------
set disp=OUTPUT end
@restraints.xpl
eval ($a213=100*(rand()-0.5) ) ! push away PC
eval ($a214=100*(rand()-0.5) )
eval ($a215=100*(rand()-0.5) )
vector do (x=x+$a213) (segid="PC")
vector do (y=y+$a214) (segid="PC")
vector do (z=z+$a215) (segid="PC")
parameter
     @nbfix.4sl_expl.xpl
      nbonds
            cutnb=8.5
            inhi=0.25
            ctofnb=7.5
            ctonnb=6.5
            repe1=0.6 !0.6
                        NBXMod=-2
            rexp=2
            irex=2
            rcon=$a301
            wmin=1.5
       end
 end
 constraints
              interactions (segid="CYTF")(segid="PC")
 end
 energy end
 while ($a01 LE $a05) loop calc
  display cycle $a01
  dynamics rigid
              dt=$a54
              group=(segid="PC")
              dynmode=TCOU
              tbath=$a55
              nprint=500
              nstep=$a53
              NTRFRQ=0 !new for XPLOR vs 3.8
  end
 eval ($a14=$ENER)
 if ($a14 < $min2) then
   coor copy end
   eval ($min2 = $a14)
   eval ($abc=$VDW)
   eval ($a15=$NOE)
```

```
  eval ($a16=$a01)
  eval ($a17=$a18)
end if
if ($a18 = $u2) then                !counting number of dockings
 if ($min2 < $a59) then
  if ($abc < $van) then
            coor swap end
            eval ($nout1=$nout1+1)
            eval ($pdb="structure_"+encode($nout1)+".pdb")
            write coord output=$pdb end
            if ($a14<$min1) then
             eval ($ref=$nout1)
       eval ($min1 = $a14)
      end if
      pick bond (segid="CYTF" and name FE) (segid="PC" and name CU) geom
      eval ($a50=$RESULT)
      set disp=ener.dat end
      display $nout1  $min2       $abc        $a15
      set disp=OUTPUT end
      set disp=coor.dat end
      display Cycle: $a16         Dock step: $a17      File#: $nout1           Fe-Cu: $a50             temp: $TEMP
      display  Etot:    $min2                    Evdw:  $abc              Enoe:  $a15
      display ------------------------------------------------------------
            set disp=OUTPUT end
    !violation analysis
            eval ($b3="structure_"+encode($nout1)+".viol.dat")
            set display=$b3 end
            display Violation analysis PRE data
            display res#   PRE(meas)  PRE(calc)  Dist(calc)
            display
            for $g2 in ($g2a $g2b $g2c)
            loop spinlabel
              eval ($g2d=$g2)
              eval ($g2e=$g2+1)
              eval ($g2f=$g2+2)
              eval ($g2g=$g2+3)
              if ($g2=$g2a) then
                eval ($g1h = $g1a)
                display Spin Label $g1h
                for
                        $c02 in ID (store1)
                loop C3
                  vector show elem (resi) (ID $c02)
                  eval ($c04=$RESULT)                                   !residue nr
                  vector show elem (store1) (ID $c02)
                  eval ($c08=$RESULT)
                  pick bond (resn SL and resi $g2d and name O) (ID $c02) geom
                  eval ($ca1=$RESULT)
                  pick bond (resn SL and resi $g2e and name O) (ID $c02) geom
                  eval ($ca2=$RESULT)
                  pick bond (resn SL and resi $g2f and name O) (ID $c02) geom
                  eval ($ca3=$RESULT)
                  pick bond (resn SL and resi $g2g and name O) (ID $c02) geom
                  eval ($ca4=$RESULT)
                  eval ($c03=($ca1^(-6)+$ca2^(-6)+$ca3^(-6)+$ca4^(-6))/4)
                                !r-6 average distance over 4 positions
                  eval ($c05=(1.23E16*(4*$tau_c+(3*$tau_c/(1+($field*2*3.14*$tau_c)^2)))*$frl*$a93*$c03) )
                                !back calculated PRE
                  eval ($c10=$c03^(-1/6))
                  display $c04       $c08        $c05         $c10
                end loop C3
                display
              end if
              if ($g2=$g2b) then
```

```
                eval ($g1h = $g1b)
                display Spin Label $g1h
                for
                        $c02 in ID (store2)
                loop C3
                  vector show elem (resi) (ID $c02)
                  eval ($c04=$RESULT)                                   !residue nr
                  vector show elem (store2) (ID $c02)
                  eval ($c08=$RESULT)
                  pick bond (resn SL and resi $g2d and name O) (ID $c02) geom
                  eval ($ca1=$RESULT)
                  pick bond (resn SL and resi $g2e and name O) (ID $c02) geom
                  eval ($ca2=$RESULT)
                  pick bond (resn SL and resi $g2f and name O) (ID $c02) geom
                  eval ($ca3=$RESULT)
                  pick bond (resn SL and resi $g2g and name O) (ID $c02) geom
                  eval ($ca4=$RESULT)
                  eval ($c03=($ca1^(-6)+$ca2^(-6)+$ca3^(-6)+$ca4^(-6))/4)
                                !r-6 average distance over 4 positions
                  eval ($c05=(1.23E16*(4*$tau_c+(3*$tau_c/(1+($field*2*3.14*$tau_c)^2)))*$frl*$a93*$c03) )
                                !back calculated PRE
                 eval ($c10=$c03^(-1/6))
                  display $c04      $c08       $c05        $c10
                end loop C3
                display
               end if
               if ($g2=$g2c) then
                eval ($g1h = $g1c)
                display Spin Label $g1h
                for
                        $c02 in ID (store3)
                loop C3
                  vector show elem (resi) (ID $c02)
                  eval ($c04=$RESULT)                                   !residue nr
                  vector show elem (store3) (ID $c02)
                  eval ($c08=$RESULT)
                  pick bond (resn SL and resi $g2d and name O) (ID $c02) geom
                  eval ($ca1=$RESULT)
                  pick bond (resn SL and resi $g2e and name O) (ID $c02) geom
                  eval ($ca2=$RESULT)
                  pick bond (resn SL and resi $g2f and name O) (ID $c02) geom
                  eval ($ca3=$RESULT)
                  pick bond (resn SL and resi $g2g and name O) (ID $c02) geom
                  eval ($ca4=$RESULT)
                  eval ($c03=($ca1^(-6)+$ca2^(-6)+$ca3^(-6)+$ca4^(-6))/4)
                                !r-6 average distance over 4 positions
                  eval ($c05=(1.23E16*(4*$tau_c+(3*$tau_c/(1+($field*2*3.14*$tau_c)^2)))*$frl*$a93*$c03) )
                                !back calculated PRE
                  eval ($c10=$c03^(-1/6))
                  display $c04      $c08       $c05        $c10
                end loop C3
                display
               end if
      end loop spinlabel
             close $b3 end
             set display=OUTPUT end
    !end violoation analysis
     coor swap end
    end if
  end if
!impulse to escape local minimum
  eval ($a213=100*(rand()-0.5) )
  eval ($a214=100*(rand()-0.5) )
  eval ($a215=100*(rand()-0.5) )
```

```
  vector do (x=x+$a213) (segid="PC")
  vector do (y=y+$a214) (segid="PC")
  vector do (z=z+$a215) (segid="PC")
  vector do (vx=50) (segid="PC")
  vector do (vy=50) (segid="PC")
  vector do (vz=50) (segid="PC")
  set disp=coor.dat end
  display cycle $a01: impulse: $a213, $a214, $a215 to x,y,z; v=50
  set disp=OUTPUT end
 eval ($a18=0)
 eval ($min2=9999.0)
 end if
 eval ($a18=$a18+1)
  if ($TEMP>200000.0) then                    !correct excessive temperature
    eval ($a45=RAND()+0.01)
    vector do (vx=$a56*$a45*rand()) (segid="PC")
    vector do (vy=$a56*$a45*rand()) (segid="PC")
    vector do (vz=$a56*$a45*rand()) (segid="PC")
   end if
   eval ($a01 = $a01 + 1)
 end loop calc
if ($ref > 0) then
  vector idend ( store9 ) ( name ca or name n or name c )        !backbone selection
  eval ($ref_file="structure_"+encode($ref)+".pdb")
  set display=rms.dat end
  display Backbone pairwise RMSD from the lowest energy strucutre ($ref_file)
  display  file          rmsd
  display
  set disp=OUTPUT end
    coor swap end
    coor init end
    coor swap end
    coor disp=comp @@$ref_file
  eval ($count1=0)
  while ($count1 < $nout1) loop fill
   evaluate ($count1=$count1+1)
        evaluate ($file="structure_"+encode($count1)+".pdb")
        coor init end
        coor @@$file
        coor sele=(recall 9) fit end
        coor sele=(recall 9) rms end
        eval ($b1 = $result)
   set display=rms.dat end
   display  $file          $b1
   end loop fill
end if
set display=OUTPUT end
 set echo=true end
  stop
```

Appendix 2

Input file to determine distances from Cyt *f*-SL to Pc amide protons for Xplor-NIH 2.9.9

```
parameter
        @nostoc_cytf_SL_pc.par
end
structure
        @nostoc_cytf_SL_pc.psf
end
eval ($inifile="nostoc_cytf_SL_pc.pdb")
coordinates @$inifile
@learn.pcf.par
constraints fix (segid="CYTF" or resn SL) end
eval ($a05 = 6000)                      !total nr cycles / $a53
eval ($a53 = 1000)                      !nr of steps
eval ($u2 = 30)                 !nr of cycles per docking approach
eval ($a54 = 0.01)              !timestep in ps
eval ($a61 = $a54*$a53)         !time per cycle (ps)
eval ($a80 = $a61*$a05)         !total time (ps)
eval ($a58=30.0)                !velocity factor
eval ($a56=1.5)                 !fbeta
eval ($a55=300.0)               !TBATH
eval ($a59=45.0)                !.pdb writing threshold
eval ($van=100.0)               ! vdw writing threshold
eval ($a59a=0.01*$a59)                  !vx-reset minimum
eval ($a60=1.0)                 !.pdb lag factor
eval ($a301=1.0)                !VDW repel scale factor
eval ($a93=1)                   !time-spent factor: 0<$a93<1 (fraction bound)
eval ($g1a = "N71C") !names of the spin label 1 used in calculation
eval ($g1b = "Q104C")           !names of the spin label 2 used in calculation
eval ($g1c = "S192C") !names of the spin label 3 used in calculation
eval ($g2a = 13)    !residue number of the 1st SL conformation of SL 1
eval ($g2b = 17)    !residue number of the 1st SL conformation of SL 2
eval ($g2c = 21)    !residue number of the 1st SL conformation of SL 3
eval ($field=600.1328E6)        !field strength in Hz
eval ($frl=1)                           !fraction of proteins with spin label
eval ($tau_c=30.0E-9)                   !tau c for the complex in sec
eval ($a9=0.01)                         !general scaling PRE (NOE) term
eval ($a10=1.0)     !scale factor for CL1 (peaks disappeared)
eval ($a11=1.0)     !scale factor for CL2 (peaks unaffected)
eval ($a12=1.0)                 !scale factor for CL3 (peaks reduced)
eval ($low1=14.0)   !lower(d_minus) limit
eval ($up1=4.0)     !upper(d_plus) limit
eval ($low2=4.0)                !lower(d_minus) limit
eval ($up2=100.0)                       !upper(d_plus) limit
eval ($low3=4.0)                !lower(d_minus) limit
eval ($up3=4.0)                 !upper(d_plus) limit
eval ($a01 = 1)                 !cycle counter
eval ($a48=$cpu*1e4)
set seed=$a48 end
eval ($a14=0)
eval ($a18=1)
eval ($nout1=0)     ! Number of strucutres output per run
eval ($min1=9999.0)
eval ($min2=9999.0)
eval ($ref=0)
set display=coor.dat end                !write parameters
display xx ----------PARAMETERS----------
display xx startdate:       $DATE
```

```
 display xx starttime:        $TIME
 display xx ini.file:          $inifile
 display xx timestep (ps):    $a54
 display xx nr of steps:      $a53              time /cycle (ps):   $a61
 display xx nr of cycles:     $a05              total time  (ps):   $a80
 display xx time-spent fact:  $a93
 display xx general scale:    $a9
 display xx TBATH:            $a55  velocity factor: $a56 fbeta:   $a58
 display xx .pdb threshold    $a59
 display xx .pdb lag factor   $a60
 display xx Local mimim. impulse after 10 cycles with 'constant' Etot > $a59a
 display xx ------------------------------------------------------------
 display
 set display=OUTPUT end
 flag exclude elec bond angl dihe impr include vdw noe end
 vector do (fbeta=$a58) (segid="PC")
 vector do (vx=$a56) (segid="PC")
 vector do (vy=$a56) (segid="PC")
 vector do (vz=$a56) (segid="PC")
set disp=ener.dat end
display Energies for the output structures
display file              Etot          VDW         NOE
display ----------------------------------------------------
set disp=OUTPUT end
@restraints.xpl
eval ($a213=100*(rand()-0.5) ) ! push away PC
eval ($a214=100*(rand()-0.5) )
eval ($a215=100*(rand()-0.5) )
vector do (x=x+$a213) (segid="PC")
vector do (y=y+$a214) (segid="PC")
vector do (z=z+$a215) (segid="PC")
!write coor OUTPUT="test1.pdb" end
parameter
     @nbfix.4sl_expl.xpl
      nbonds
            cutnb=8.5
            inhi=0.25
            ctofnb=7.5
            ctonnb=6.5
            repe1=0.6 !0.6
                        NBXMod=-2
            rexp=2
            irex=2
            rcon=$a301
            wmin=1.5
      end
 end
 constraints
             interactions (segid="CYTF")(segid="PC")
 end
 energy end
 while ($a01 LE $a05) loop calc
  display cycle $a01
  dynamics rigid
             dt=$a54
             group=(segid="PC")
             dynmode=TCOU
             tbath=$a55
             nprint=500
             nstep=$a53
             NTRFRQ=0 !new for XPLOR vs 3.8
  end
 eval ($a14=$ENER)
 if ($a14 < $min2) then
```

```
  coor copy end
  eval ($min2 = $a14)
  eval ($abc=$VDW)
  eval ($a15=$NOE)
  eval ($a16=$a01)
  eval ($a17=$a18)
 end if
 if ($a18 = $u2) then                !counting number of dockings
  if ($min2 < $a59) then
   if ($abc < $van) then
              coor swap end
              eval ($nout1=$nout1+1)
              eval ($pdb="structure_"+encode($nout1)+".pdb")
              write coord output=$pdb end
              if ($a14<$min1) then
               eval ($ref=$nout1)
        eval ($min1 = $a14)
       end if
       pick bond (segid="CYTF" and name FE) (segid="PC" and name CU) geom
       eval ($a50=$RESULT)
       set disp=ener.dat end
       display $nout1  $min2       $abc        $a15
       set disp=OUTPUT end
       set disp=coor.dat end
       display Cycle: $a16          Dock step: $a17       File#: $nout1            Fe-Cu: $a50              temp: $TEMP
       display  Etot:    $min2                      Evdw:  $abc              Enoe:  $a15
       display ------------------------------------------------------------
              set disp=OUTPUT end
     !violation analysis
              eval ($b3="structure_"+encode($nout1)+".viol.dat")
              set display=$b3 end
              display Violation analysis PRE data
              display res#   PRE(meas)  PRE(calc)  Dist(calc)
              display
              for $g2 in ($g2a $g2b $g2c)
              loop spinlabel
               eval ($g2d=$g2)
               eval ($g2e=$g2+1)
               eval ($g2f=$g2+2)
               eval ($g2g=$g2+3)
               if ($g2=$g2a) then
                eval ($g1h = $g1a)
                display Spin Label $g1h
                for
                          $c02 in ID (store1)
                loop C3
                  vector show elem (resi) (ID $c02)
                  eval ($c04=$RESULT)                                  !residue nr
                  vector show elem (store1) (ID $c02)
                  eval ($c08=$RESULT)
                  pick bond (resn SL and resi $g2d and name O) (ID $c02) geom
                  eval ($ca1=$RESULT)
                  pick bond (resn SL and resi $g2e and name O) (ID $c02) geom
                  eval ($ca2=$RESULT)
                  pick bond (resn SL and resi $g2f and name O) (ID $c02) geom
                  eval ($ca3=$RESULT)
                  pick bond (resn SL and resi $g2g and name O) (ID $c02) geom
                  eval ($ca4=$RESULT)
                  eval ($c03=($ca1^(-6)+$ca2^(-6)+$ca3^(-6)+$ca4^(-6))/4)
                                  !r-6 average distance over 4 positions
                  eval ($c05=(1.23E16*(4*$tau_c+(3*$tau_c/(1+($field*2*3.14*$tau_c)^2)))*$frl*$a93*$c03) )
                                  !back calculated PRE
                  eval ($c10=$c03^(-1/6))
                  display $c04       $c08        $c05         $c10
```

```
      end loop C3
      display
     end if

     if ($g2=$g2b) then
      eval ($g1h = $g1b)
      display Spin Label $g1h
      for
            $c02 in ID (store2)
      loop C3
       vector show elem (resi) (ID $c02)
       eval ($c04=$RESULT)                          !residue nr
       vector show elem (store2) (ID $c02)
       eval ($c08=$RESULT)
       pick bond (resn SL and resi $g2d and name O) (ID $c02) geom
       eval ($ca1=$RESULT)
       pick bond (resn SL and resi $g2e and name O) (ID $c02) geom
       eval ($ca2=$RESULT)
       pick bond (resn SL and resi $g2f and name O) (ID $c02) geom
       eval ($ca3=$RESULT)
       pick bond (resn SL and resi $g2g and name O) (ID $c02) geom
       eval ($ca4=$RESULT)
       eval ($c03=($ca1^(-6)+$ca2^(-6)+$ca3^(-6)+$ca4^(-6))/4)
                    !r-6 average distance over 4 positions
       eval ($c05=(1.23E16*(4*$tau_c+(3*$tau_c/(1+($field*2*3.14*$tau_c)^2)))*$frl*$a93*$c03) )
                    !back calculated PRE
       eval ($c10=$c03^(-1/6))
       display $c04    $c08    $c05    $c10
      end loop C3
      display
     end if
     if ($g2=$g2c) then
      eval ($g1h = $g1c)
      display Spin Label $g1h
      for
            $c02 in ID (store3)
      loop C3
       vector show elem (resi) (ID $c02)
       eval ($c04=$RESULT)                          !residue nr
       vector show elem (store3) (ID $c02)
       eval ($c08=$RESULT)
       pick bond (resn SL and resi $g2d and name O) (ID $c02) geom
       eval ($ca1=$RESULT)
       pick bond (resn SL and resi $g2e and name O) (ID $c02) geom
       eval ($ca2=$RESULT)
       pick bond (resn SL and resi $g2f and name O) (ID $c02) geom
       eval ($ca3=$RESULT)
       pick bond (resn SL and resi $g2g and name O) (ID $c02) geom
       eval ($ca4=$RESULT)
       eval ($c03=($ca1^(-6)+$ca2^(-6)+$ca3^(-6)+$ca4^(-6))/4)
                    !r-6 average distance over 4 positions
       eval ($c05=(1.23E16*(4*$tau_c+(3*$tau_c/(1+($field*2*3.14*$tau_c)^2)))*$frl*$a93*$c03) )
                    !back calculated PRE
       eval ($c10=$c03^(-1/6))
       display $c04    $c08    $c05    $c10
      end loop C3
      display
     end if
   end loop spinlabel
        close $b3 end
        set display=OUTPUT end
 !end violoation analysis
  coor swap end
end if
```

```
  end if
                                                !impulse to escape local minimum
  eval ($a213=100*(rand()-0.5) )
  eval ($a214=100*(rand()-0.5) )
  eval ($a215=100*(rand()-0.5) )
  vector do (x=x+$a213) (segid="PC")
  vector do (y=y+$a214) (segid="PC")
  vector do (z=z+$a215) (segid="PC")
  vector do (vx=50) (segid="PC")
  vector do (vy=50) (segid="PC")
  vector do (vz=50) (segid="PC")
  set disp=coor.dat end
  display cycle $a01: impulse: $a213, $a214, $a215 to x,y,z; v=50
  set disp=OUTPUT end
 eval ($a18=0)
 eval ($min2=9999.0)
 end if
 eval ($a18=$a18+1)
  if ($TEMP>200000.0) then                    !correct excessive temperature
    eval ($a45=RAND()+0.01)
    vector do (vx=$a56*$a45*rand()) (segid="PC")
    vector do (vy=$a56*$a45*rand()) (segid="PC")
    vector do (vz=$a56*$a45*rand()) (segid="PC")
   end if
   eval ($a01 = $a01 + 1)
 end loop calc
if ($ref > 0) then
  vector idend ( store9 ) ( name ca or name n or name c )        !backbone selection
  eval ($ref_file="structure_"+encode($ref)+".pdb")
  set display=rms.dat end
  display Backbone pairwise RMSD from the lowest energy strucutre ($ref_file)
  display  file            rmsd
  display ----------------------------------------------------------------
  set disp=OUTPUT end
    coor swap end
    coor init end
    coor swap end
    coor disp=comp @@$ref_file
  eval ($count1=0)
  while ($count1 < $nout1) loop fill
   evaluate ($count1=$count1+1)
        evaluate ($file="structure_"+encode($count1)+".pdb")
        coor init end
        coor @@$file
        coor sele=(recall 9) fit end
        coor sele=(recall 9) rms end
        eval ($b1 = $result)
   set display=rms.dat end
   display  $file           $b1
   end loop fill
end if
set display=OUTPUT end
 set echo=true end
  stop
```

Appendix 3

Input file for ensemble docking of Cyt *f*-Pc using PRE restraints for Xplor-NIH 2.9.9

```
parameter
        @nostoc_cytf_SL_pc.par
end
structure
        @nostoc_cytf_SL_pc.psf
end
eval ($inifile="nostoc_cytf_SL_pc.pdb")
coordinates @$inifile
@learn.pcf.par
constraints fix (segid="CYTF" or resn SL) end
eval ($a05 = 6000)                      !total nr cycles / $a53
eval ($a53 = 1000)                      !nr of steps
eval ($u2 = 30)                 !nr of cycles per docking approach
eval ($a54 = 0.01)              !timestep in ps
eval ($a61 = $a54*$a53)         !time per cycle (ps)
eval ($a80 = $a61*$a05)         !total time (ps)
eval ($a58=30.0)                !velocity factor
eval ($a56=1.5)                 !fbeta
eval ($a55=300.0)               !TBATH
eval ($a59=45.0)                !.pdb writing threshold
eval ($van=100.0)               ! vdw writing threshold
eval ($a59a=0.01*$a59)                  !vx-reset minimum
eval ($a60=1.0)                 !.pdb lag factor
eval ($a301=1.0)                !VDW repel scale factor
eval ($a93=1)                   !time-spent factor: 0<$a93<1 (fraction bound)
eval ($g1a = "N71C")            !names of the spin label 1
eval ($g1b = "Q104C")                   !names of the spin label 2
eval ($g1c = "S192C")                   !names of the spin label 3
eval ($g2a = 13)     !residue number of the 1stSL conformation of SL 1
eval ($g2b = 17)     !residue number of the 1st SL conformation of SL 2
eval ($g2c = 21)     !residue number of the 1st SL conformation of SL 3
eval ($field=600.1328E6)        !field strength in Hz
eval ($frl=1)                           !fraction of proteins with spin label
eval ($tau_c=30.0E-9)                   !tau c for the complex in sec
eval ($a9=0.01)                         !general scaling PRE (NOE) term
eval ($a10=1.0)      !scale factor for CL1 (peaks disappeared)
eval ($a11=1.0)                 !scale factor for CL2 (peaks unaffected)
eval ($a12=1.0)                 !scale factor for CL3 (peaks reduced)
eval ($low1=14.0)  !lower(d_minus) limit (restraints upper limit only)
eval ($up1=4.0)    !upper(d_plus) limit (restraints upper limit only)
eval ($low2=4.0)     !lower(d_minus) limit (restraints lower limit only)
eval ($up2=100.0)   !upper(d_plus) limit (restraints lower limit only)
eval ($low3=4.0)   !lower(d_minus) limit (restraints with both limits)
eval ($up3=4.0)    !upper(d_plus) limit (restraints with both limits)
eval ($a01 = 1)                 !cycle counter
eval ($a48=$cpu*1e4)
set seed=$a48 end
eval ($a14=0)
eval ($a18=1)
eval ($nout1=0)      ! Number of strucutres output per run
eval ($min1=9999.0)
eval ($min2=9999.0)
eval ($ref=0)
set display=coor.dat end                !write parameters
display xx ----------PARAMETERS----------
display xx startdate:       $DATE
display xx starttime:       $TIME
```

```
 display xx ini.file:            $inifile
 display xx timestep (ps):     $a54
 display xx nr of steps:       $a53              time /cycle (ps):   $a61
 display xx nr of cycles:      $a05              total time  (ps):   $a80
 display xx time-spent fact:   $a93
 display xx general scale:     $a9
 display xx TBATH:      $a55    velocity factor:   $a56   fbeta:   $a58
 display xx .pdb threshold     $a59
 display xx .pdb lag factor    $a60
 display xx Local mimim. impulse after 10 cycles with 'constant' Etot > $a59a
 display xx ------------------------------------------------------------
 display
 set display=OUTPUT end
 flag exclude elec bond angl dihe impr include vdw noe end
 vector do (fbeta=$a58) (segid="PC")
 vector do (vx=$a56) (segid="PC")
 vector do (vy=$a56) (segid="PC")
 vector do (vz=$a56) (segid="PC")
set disp=ener.dat end
display Energies for the output structures
display file                Etot          VDW         NOE
display ------------------------------------------------
set disp=OUTPUT end
@restraints.xpl
eval ($a213=100*(rand()-0.5) ) ! push away PC
eval ($a214=100*(rand()-0.5) )
eval ($a215=100*(rand()-0.5) )
vector do (x=x+$a213) (segid="PC")
vector do (y=y+$a214) (segid="PC")
vector do (z=z+$a215) (segid="PC")
!write coor OUTPUT="test1.pdb" end
parameter
     @nbfix.4sl_expl.xpl
      nbonds
            cutnb=8.5
            inhi=0.25
            ctofnb=7.5
            ctonnb=6.5
            repe1=0.6 !0.6
                        NBXMod=-2
            rexp=2
            irex=2
            rcon=$a301
            wmin=1.5
       end
 end
 constraints
              interactions (segid="CYTF")(segid="PC")
 end
 energy end
 while ($a01 LE $a05) loop calc
  display cycle $a01
  dynamics rigid
               dt=$a54
               group=(segid="PC")
               dynmode=TCOU
               tbath=$a55
               nprint=500
               nstep=$a53
               NTRFRQ=0 !new for XPLOR vs 3.8
  end
 eval ($a14=$ENER)
 if ($a14 < $min2) then
   coor copy end
```

```
  eval ($min2 = $a14)
  eval ($abc=$VDW)
  eval ($a15=$NOE)
  eval ($a16=$a01)
  eval ($a17=$a18)
end if
if ($a18 = $u2) then                !counting number of dockings
 if ($min2 < $a59) then
  if ($abc < $van) then
            coor swap end
            eval ($nout1=$nout1+1)
            eval ($pdb="structure_"+encode($nout1)+".pdb")
            write coord output=$pdb end
            if ($a14<$min1) then
             eval ($ref=$nout1)
       eval ($min1 = $a14)
      end if
      pick bond (segid="CYTF" and name FE) (segid="PC" and name CU) geom
      eval ($a50=$RESULT)
      set disp=ener.dat end
      display $nout1  $min2      $abc       $a15
      set disp=OUTPUT end
      set disp=coor.dat end
      display Cycle: $a16         Dock step: $a17      File#: $nout1          Fe-Cu: $a50             temp: $TEMP
      display  Etot:    $min2                  Evdw:  $abc             Enoe:  $a15
      display ------------------------------------------------------------
            set disp=OUTPUT end
    !violation analysis
            eval ($b3="structure_"+encode($nout1)+".viol.dat")
            set display=$b3 end
            display Violation analysis PRE data
            display res#   PRE(meas)  PRE(calc)  Dist(calc)
            display
            for $g2 in ($g2a $g2b $g2c)
            loop spinlabel
              eval ($g2d=$g2)
              eval ($g2e=$g2+1)
              eval ($g2f=$g2+2)
              eval ($g2g=$g2+3)
              if ($g2=$g2a) then
                eval ($g1h = $g1a)
                display Spin Label $g1h
                for
                        $c02 in ID (store1)
                loop C3
                  vector show elem (resi) (ID $c02)
                  eval ($c04=$RESULT)                                !residue nr
                  vector show elem (store1) (ID $c02)
                  eval ($c08=$RESULT)
                  pick bond (resn SL and resi $g2d and name O) (ID $c02) geom
                  eval ($ca1=$RESULT)
                  pick bond (resn SL and resi $g2e and name O) (ID $c02) geom
                  eval ($ca2=$RESULT)
                  pick bond (resn SL and resi $g2f and name O) (ID $c02) geom
                  eval ($ca3=$RESULT)
                  pick bond (resn SL and resi $g2g and name O) (ID $c02) geom
                  eval ($ca4=$RESULT)
                  eval ($c03=($ca1^(-6)+$ca2^(-6)+$ca3^(-6)+$ca4^(-6))/4)
                                !r-6 average distance over 4 positions
                  eval ($c05=(1.23E16*(4*$tau_c+(3*$tau_c/(1+($field*2*3.14*$tau_c)^2)))*$frl*$a93*$c03) )
                                !back calculated PRE
                  eval ($c10=$c03^(-1/6))
                  display $c04       $c08        $c05         $c10
                end loop C3
```

```
      display
     end if
     if ($g2=$g2b) then
      eval ($g1h = $g1b)
      display Spin Label $g1h
      for
            $c02 in ID (store2)
      loop C3
       vector show elem (resi) (ID $c02)
       eval ($c04=$RESULT)                          !residue nr
       vector show elem (store2) (ID $c02)
       eval ($c08=$RESULT)
       pick bond (resn SL and resi $g2d and name O) (ID $c02) geom
       eval ($ca1=$RESULT)
       pick bond (resn SL and resi $g2e and name O) (ID $c02) geom
       eval ($ca2=$RESULT)
       pick bond (resn SL and resi $g2f and name O) (ID $c02) geom
       eval ($ca3=$RESULT)
       pick bond (resn SL and resi $g2g and name O) (ID $c02) geom
       eval ($ca4=$RESULT)
       eval ($c03=($ca1^(-6)+$ca2^(-6)+$ca3^(-6)+$ca4^(-6))/4)
                    !r-6 average distance over 4 positions
       eval ($c05=(1.23E16*(4*$tau_c+(3*$tau_c/(1+($field*2*3.14*$tau_c)^2)))*$frl*$a93*$c03) )
                    !back calculated PRE
       eval ($c10=$c03^(-1/6))
       display $c04    $c08    $c05    $c10
      end loop C3
      display
     end if
     if ($g2=$g2c) then
      eval ($g1h = $g1c)
      display Spin Label $g1h
      for
            $c02 in ID (store3)
      loop C3
       vector show elem (resi) (ID $c02)
       eval ($c04=$RESULT)                          !residue nr
       vector show elem (store3) (ID $c02)
       eval ($c08=$RESULT)
       pick bond (resn SL and resi $g2d and name O) (ID $c02) geom
       eval ($ca1=$RESULT)
       pick bond (resn SL and resi $g2e and name O) (ID $c02) geom
       eval ($ca2=$RESULT)
       pick bond (resn SL and resi $g2f and name O) (ID $c02) geom
       eval ($ca3=$RESULT)
       pick bond (resn SL and resi $g2g and name O) (ID $c02) geom
       eval ($ca4=$RESULT)
       eval ($c03=($ca1^(-6)+$ca2^(-6)+$ca3^(-6)+$ca4^(-6))/4)
                    !r-6 average distance over 4 positions
       eval ($c05=(1.23E16*(4*$tau_c+(3*$tau_c/(1+($field*2*3.14*$tau_c)^2)))*$frl*$a93*$c03) )
                    !back calculated PRE
       eval ($c10=$c03^(-1/6))
       display $c04    $c08    $c05    $c10
      end loop C3
      display
     end if
  end loop spinlabel
      close $b3 end
      set display=OUTPUT end
 !end violoation analysis
  coor swap end
 end if
end if
!impulse to escape local minimum
```

```
  eval ($a213=100*(rand()-0.5) )
  eval ($a214=100*(rand()-0.5) )
  eval ($a215=100*(rand()-0.5) )
  vector do (x=x+$a213) (segid="PC")
  vector do (y=y+$a214) (segid="PC")
  vector do (z=z+$a215) (segid="PC")
  vector do (vx=50) (segid="PC")
  vector do (vy=50) (segid="PC")
  vector do (vz=50) (segid="PC")
  set disp=coor.dat end
  display cycle $a01: impulse: $a213, $a214, $a215 to x,y,z; v=50
  set disp=OUTPUT end
 eval ($a18=0)
 eval ($min2=9999.0)
 end if
 eval ($a18=$a18+1)
  if ($TEMP>200000.0) then                    !correct excessive temperature
    eval ($a45=RAND()+0.01)
    vector do (vx=$a56*$a45*rand()) (segid="PC")
    vector do (vy=$a56*$a45*rand()) (segid="PC")
    vector do (vz=$a56*$a45*rand()) (segid="PC")
   end if
   eval ($a01 = $a01 + 1)
 end loop calc
if ($ref > 0) then
  vector idend ( store9 ) ( name ca or name n or name c )        !backbone selection
  eval ($ref_file="structure_"+encode($ref)+".pdb")
  set display=rms.dat end
  display Backbone pairwise RMSD from the lowest energy strucutre ($ref_file)
  display  file           rmsd
  display ------------------------------------------------------------
  set disp=OUTPUT end
    coor swap end
    coor init end
    coor swap end
    coor disp=comp @@$ref_file
  eval ($count1=0)
  while ($count1 < $nout1) loop fill
   evaluate ($count1=$count1+1)
        evaluate ($file="structure_"+encode($count1)+".pdb")
        coor init end
        coor @@$file
        coor sele=(recall 9) fit end
        coor sele=(recall 9) rms end
        eval ($b1 = $result)
   set display=rms.dat end
   display  $file           $b1
   end loop fill
end if
set display=OUTPUT end
 set echo=true end
  stop
```

Appendix 4

Input file for rigid-body docking of Cyt *f*-Pc using PCS restraints for Xplor-NIH 2.9.9

```
parameter
        @nostoc_cytf_SL_pc.par
end
structure
        @nostoc_cytf_SL_pc.psf
end
eval ($inifile="nostoc_cytf_SL_pc.pdb")
coordinates @$inifile
@learn.pcf.par
constraints fix (segid="CYTF" or resn SL) end
eval ($a05 = 6000)                      !total nr cycles / $a53
eval ($a53 = 1000)                      !nr of steps
eval ($u2 = 30)                 !nr of cycles per docking approach
eval ($a54 = 0.01)              !timestep in ps
eval ($a61 = $a54*$a53)         !time per cycle (ps)
eval ($a80 = $a61*$a05)         !total time (ps)
eval ($a58=30.0)                !velocity factor
eval ($a56=1.5)                 !fbeta
eval ($a55=300.0)               !TBATH
eval ($a59=45.0)                !.pdb writing threshold
eval ($van=100.0)               ! vdw writing threshold
eval ($a59a=0.01*$a59)                  !vx-reset minimum
eval ($a60=1.0)                 !.pdb lag factor
eval ($a301=1.0)                !VDW repel scale factor
eval ($a93=1)                   !time-spent factor: 0<$a93<1 (fraction bound)
eval ($g1a = "N71C")            !names of the spin label 1 used in calculation
eval ($g1b = "Q104C")           !names of the spin label 2 used in calculation
eval ($g1c = "S192C")           !names of the spin label 3 used in calculation
eval ($g2a = 13)     !residue number of the 1stSL conformation of SL 1
eval ($g2b = 17)     !residue number of the 1st SL conformation of SL 2
eval ($g2c = 21)     !residue number of the 1st SL conformation of SL 3
eval ($field=600.1328E6)        !field strength in Hz
eval ($frl=1)                           !fraction of proteins with spin label
eval ($tau_c=30.0E-9)                   !tau c for the complex in sec
eval ($a9=0.01)                         !general scaling PRE (NOE) term
eval ($a10=1.0)      !scale factor for CL1 (peaks disappeared)
eval ($a11=1.0)                 !scale factor for CL2 (peaks unaffected)
eval ($a12=1.0)                 !scale factor for CL3 (peaks reduced)
eval ($low1=14.0)  !lower(d_minus) limit (restraints upper limit only)
eval ($up1=4.0)    !upper(d_plus) limit (restraints upper limit only)
eval ($low2=4.0)     !lower(d_minus) limit (restraints lower limit only)
eval ($up2=100.0) !upper(d_plus) limit (restraints lower limit only)
eval ($low3=4.0)   !lower(d_minus) limit (restraints with both limits)
eval ($up3=4.0)    !upper(d_plus) limit (restraints with both limits)
eval ($a01 = 1)                 !cycle counter
eval ($a48=$cpu*1e4)
set seed=$a48 end
eval ($a14=0)
eval ($a18=1)
eval ($nout1=0)      ! Number of strucutres output per run
eval ($min1=9999.0)
eval ($min2=9999.0)
eval ($ref=0)
set display=coor.dat end                !write parameters
display xx ----------------------PARAMETERS---------------------------
display xx startdate:        $DATE
display xx starttime:        $TIME
```

```
 display xx ini.file:            $inifile
 display xx timestep (ps):     $a54
 display xx nr of steps:       $a53              time /cycle (ps):   $a61
 display xx nr of cycles:      $a05              total time  (ps):   $a80
 display xx time-spent fact:   $a93
 display xx general scale:     $a9
 display xx TBATH:      $a55    velocity factor:   $a56   fbeta:   $a58
 display xx .pdb threshold     $a59
 display xx .pdb lag factor    $a60
 display xx Local mimim. impulse after 10 cycles with 'constant' Etot > $a59a
 display xx ------------------------------------------------------------
 display
 set display=OUTPUT end
 flag exclude elec bond angl dihe impr include vdw noe end
 vector do (fbeta=$a58) (segid="PC")
 vector do (vx=$a56) (segid="PC")
 vector do (vy=$a56) (segid="PC")
 vector do (vz=$a56) (segid="PC")
set disp=ener.dat end
display Energies for the output structures
display file                Etot          VDW         NOE
display ------------------------------------------------
set disp=OUTPUT end
@restraints.xpl
eval ($a213=100*(rand()-0.5) ) ! push away PC
eval ($a214=100*(rand()-0.5) )
eval ($a215=100*(rand()-0.5) )
vector do (x=x+$a213) (segid="PC")
vector do (y=y+$a214) (segid="PC")
vector do (z=z+$a215) (segid="PC")
!write coor OUTPUT="test1.pdb" end
parameter
     @nbfix.4sl_expl.xpl
      nbonds
            cutnb=8.5
            inhi=0.25
            ctofnb=7.5
            ctonnb=6.5
            repe1=0.6 !0.6
                  NBXMod=-2
            rexp=2
            irex=2
            rcon=$a301
            wmin=1.5
       end
 end
 constraints
             interactions (segid="CYTF")(segid="PC")
 end
 energy end
 while ($a01 LE $a05) loop calc
  display cycle $a01
  dynamics rigid
              dt=$a54
              group=(segid="PC")
              dynmode=TCOU
              tbath=$a55
              nprint=500
              nstep=$a53
              NTRFRQ=0 !new for XPLOR vs 3.8
  end
 eval ($a14=$ENER)
 if ($a14 < $min2) then
   coor copy end
```

```
  eval ($min2 = $a14)
  eval ($abc=$VDW)
  eval ($a15=$NOE)
  eval ($a16=$a01)
  eval ($a17=$a18)
end if
if ($a18 = $u2) then                !counting number of dockings
 if ($min2 < $a59) then
  if ($abc < $van) then
            coor swap end
            eval ($nout1=$nout1+1)
            eval ($pdb="structure_"+encode($nout1)+".pdb")
            write coord output=$pdb end
            if ($a14<$min1) then
             eval ($ref=$nout1)
       eval ($min1 = $a14)
      end if
      pick bond (segid="CYTF" and name FE) (segid="PC" and name CU) geom
      eval ($a50=$RESULT)
      set disp=ener.dat end
      display $nout1  $min2      $abc       $a15
      set disp=OUTPUT end
      set disp=coor.dat end
      display Cycle: $a16         Dock step: $a17      File#: $nout1          Fe-Cu: $a50             temp: $TEMP
      display  Etot:    $min2                  Evdw:  $abc             Enoe:  $a15
      display ------------------------------------------------------------
            set disp=OUTPUT end
    !violation analysis
            eval ($b3="structure_"+encode($nout1)+".viol.dat")
            set display=$b3 end
            display Violation analysis PRE data
            display res#   PRE(meas)  PRE(calc)  Dist(calc)
            display
            for $g2 in ($g2a $g2b $g2c)
            loop spinlabel
              eval ($g2d=$g2)
              eval ($g2e=$g2+1)
              eval ($g2f=$g2+2)
              eval ($g2g=$g2+3)
              if ($g2=$g2a) then
                eval ($g1h = $g1a)
                display Spin Label $g1h
                for
                        $c02 in ID (store1)
                loop C3
                  vector show elem (resi) (ID $c02)
                  eval ($c04=$RESULT)                                   !residue nr
                  vector show elem (store1) (ID $c02)
                  eval ($c08=$RESULT)
                  pick bond (resn SL and resi $g2d and name O) (ID $c02) geom
                  eval ($ca1=$RESULT)
                  pick bond (resn SL and resi $g2e and name O) (ID $c02) geom
                  eval ($ca2=$RESULT)
                  pick bond (resn SL and resi $g2f and name O) (ID $c02) geom
                  eval ($ca3=$RESULT)
                  pick bond (resn SL and resi $g2g and name O) (ID $c02) geom
                  eval ($ca4=$RESULT)
                  eval ($c03=($ca1^(-6)+$ca2^(-6)+$ca3^(-6)+$ca4^(-6))/4)
                                !r-6 average distance over 4 positions
                  eval ($c05=(1.23E16*(4*$tau_c+(3*$tau_c/(1+($field*2*3.14*$tau_c)^2)))*$frl*$a93*$c03) )
                                !back calculated PRE
                  eval ($c10=$c03^(-1/6))
                  display $c04       $c08        $c05         $c10
                end loop C3
```

```
      display
     end if
     if ($g2=$g2b) then
      eval ($g1h = $g1b)
      display Spin Label $g1h
      for
            $c02 in ID (store2)
      loop C3
       vector show elem (resi) (ID $c02)
       eval ($c04=$RESULT)                          !residue nr
       vector show elem (store2) (ID $c02)
       eval ($c08=$RESULT)
       pick bond (resn SL and resi $g2d and name O) (ID $c02) geom
       eval ($ca1=$RESULT)
       pick bond (resn SL and resi $g2e and name O) (ID $c02) geom
       eval ($ca2=$RESULT)
       pick bond (resn SL and resi $g2f and name O) (ID $c02) geom
       eval ($ca3=$RESULT)
       pick bond (resn SL and resi $g2g and name O) (ID $c02) geom
       eval ($ca4=$RESULT)
       eval ($c03=($ca1^(-6)+$ca2^(-6)+$ca3^(-6)+$ca4^(-6))/4)
                    !r-6 average distance over 4 positions
       eval ($c05=(1.23E16*(4*$tau_c+(3*$tau_c/(1+($field*2*3.14*$tau_c)^2)))*$frl*$a93*$c03) )
                    !back calculated PRE
       eval ($c10=$c03^(-1/6))
       display $c04    $c08    $c05    $c10
      end loop C3
      display
     end if
     if ($g2=$g2c) then
      eval ($g1h = $g1c)
      display Spin Label $g1h
      for
            $c02 in ID (store3)
      loop C3
       vector show elem (resi) (ID $c02)
       eval ($c04=$RESULT)                          !residue nr
       vector show elem (store3) (ID $c02)
       eval ($c08=$RESULT)
       pick bond (resn SL and resi $g2d and name O) (ID $c02) geom
       eval ($ca1=$RESULT)
       pick bond (resn SL and resi $g2e and name O) (ID $c02) geom
       eval ($ca2=$RESULT)
       pick bond (resn SL and resi $g2f and name O) (ID $c02) geom
       eval ($ca3=$RESULT)
       pick bond (resn SL and resi $g2g and name O) (ID $c02) geom
       eval ($ca4=$RESULT)
       eval ($c03=($ca1^(-6)+$ca2^(-6)+$ca3^(-6)+$ca4^(-6))/4)
                    !r-6 average distance over 4 positions
       eval ($c05=(1.23E16*(4*$tau_c+(3*$tau_c/(1+($field*2*3.14*$tau_c)^2)))*$frl*$a93*$c03) )
                    !back calculated PRE
       eval ($c10=$c03^(-1/6))
       display $c04    $c08    $c05    $c10
      end loop C3
      display
     end if
  end loop spinlabel
      close $b3 end
      set display=OUTPUT end
 !end violoation analysis
  coor swap end
 end if
end if
eval ($a213=100*(rand()-0.5) ) !impulse to escape local minimum
```

```
  eval ($a214=100*(rand()-0.5) )
  eval ($a215=100*(rand()-0.5) )
  vector do (x=x+$a213) (segid="PC")
  vector do (y=y+$a214) (segid="PC")
  vector do (z=z+$a215) (segid="PC")
  vector do (vx=50) (segid="PC")
  vector do (vy=50) (segid="PC")
  vector do (vz=50) (segid="PC")
  set disp=coor.dat end
  display cycle $a01: impulse: $a213, $a214, $a215 to x,y,z; v=50
  set disp=OUTPUT end
 eval ($a18=0)
 eval ($min2=9999.0)
 end if
 eval ($a18=$a18+1)
  if ($TEMP>200000.0) then                    !correct excessive temperature
    eval ($a45=RAND()+0.01)
    vector do (vx=$a56*$a45*rand()) (segid="PC")
    vector do (vy=$a56*$a45*rand()) (segid="PC")
    vector do (vz=$a56*$a45*rand()) (segid="PC")
   end if
   eval ($a01 = $a01 + 1)
 end loop calc
if ($ref > 0) then
  vector idend ( store9 ) ( name ca or name n or name c )        !backbone selection
  eval ($ref_file="structure_"+encode($ref)+".pdb")
  set display=rms.dat end
  display Backbone pairwise RMSD from the lowest energy strucutre ($ref_file)
  display  file           rmsd
  display ------------------------------------------------------------
  set disp=OUTPUT end
    coor swap end
    coor init end
    coor swap end
    coor disp=comp @@$ref_file
  eval ($count1=0)
  while ($count1 < $nout1) loop fill
   evaluate ($count1=$count1+1)
        evaluate ($file="structure_"+encode($count1)+".pdb")
        coor init end
        coor @@$file
        coor sele=(recall 9) fit end
        coor sele=(recall 9) rms end
        eval ($b1 = $result)
   set display=rms.dat end
   display  $file           $b1
   end loop fill
end if
set display=OUTPUT end
 set echo=true end
  stop
```

Appendix 5

Input file to backcalculate PCS from Cyt *f* Fe to Pc amide protons for Xplor-NIH 2.9.9

```
parameter
        @nostoc_cytf_SL_pc.par
end
structure
        @nostoc_cytf_SL_pc.psf
end
eval ($inifile="nostoc_cytf_SL_pc.pdb")
coordinates @$inifile
@learn.pcf.par
constraints fix (segid="CYTF" or resn SL) end
eval ($a05 = 6000)                      !total nr cycles / $a53
eval ($a53 = 1000)                      !nr of steps
eval ($u2 = 30)                 !nr of cycles per docking approach
eval ($a54 = 0.01)              !timestep in ps
eval ($a61 = $a54*$a53)         !time per cycle (ps)
eval ($a80 = $a61*$a05)         !total time (ps)
eval ($a58=30.0)                !velocity factor
eval ($a56=1.5)                 !fbeta
eval ($a55=300.0)               !TBATH
eval ($a59=45.0)                !.pdb writing threshold
eval ($van=100.0)               ! vdw writing threshold
eval ($a59a=0.01*$a59)                  !vx-reset minimum
eval ($a60=1.0)                 !.pdb lag factor
eval ($a301=1.0)                !VDW repel scale factor
eval ($a93=1)                   !time-spent factor: 0<$a93<1 (fraction bound)
eval ($g1a = "N71C")            !names of the spin label 1 used in calculation
eval ($g1b = "Q104C")           !names of the spin label 2 used in calculation
eval ($g1c = "S192C")           !names of the spin label 3 used in calculation
eval ($g2a = 13)    !residue number of the 1stSL conformation of SL 1
eval ($g2b = 17)    !residue number of the 1st SL conformation of SL 2
eval ($g2c = 21)    !residue number of the 1st SL conformation of SL 3
eval ($field=600.1328E6)        !field strength in Hz
eval ($frl=1)                           !fraction of proteins with spin label
eval ($tau_c=30.0E-9)                   !tau c for the complex in sec
eval ($a9=0.01)                         !general scaling PRE (NOE) term
eval ($a10=1.0)     !scale factor for CL1 (peaks disappeared)
eval ($a11=1.0)                 !scale factor for CL2 (peaks unaffected)
eval ($a12=1.0)                 !scale factor for CL3 (peaks reduced)
eval ($low1=14.0)  !lower(d_minus) limit (restraints upper limit only)
eval ($up1=4.0)    !upper(d_plus) limit (restraints upper limit only)
eval ($low2=4.0)    !lower(d_minus) limit (restraints lower limit only)
eval ($up2=100.0)   !upper(d_plus) limit (restraints lower limit only)
eval ($low3=4.0)   !lower(d_minus) limit (restraints both limits)
eval ($up3=4.0)    !upper(d_plus) limit (restraints both limits)
eval ($a01 = 1)                 !cycle counter
eval ($a48=$cpu*1e4)
set seed=$a48 end
eval ($a14=0)
eval ($a18=1)
eval ($nout1=0)     ! Number of strucutres output per run
eval ($min1=9999.0)
eval ($min2=9999.0)
eval ($ref=0)
set display=coor.dat end                !write parameters
display xx ----------PARAMETERS----------
display xx startdate:       $DATE
```

```
 display xx starttime:        $TIME
 display xx ini.file:          $inifile
 display xx timestep (ps):    $a54
 display xx nr of steps:      $a53              time /cycle (ps):   $a61
 display xx nr of cycles:     $a05              total time  (ps):   $a80
 display xx time-spent fact:  $a93
 display xx general scale:    $a9
 display xx TBATH:    $a55    velocity factor:   $a56   fbeta:   $a58
 display xx .pdb threshold    $a59
 display xx .pdb lag factor   $a60
 display xx Local mimim. impulse after 10 cycles with 'constant' Etot > $a59a
 display xx ------------------------------------------------------------
 display
 set display=OUTPUT end
 flag exclude elec bond angl dihe impr include vdw noe end
 vector do (fbeta=$a58) (segid="PC")
 vector do (vx=$a56) (segid="PC")
 vector do (vy=$a56) (segid="PC")
 vector do (vz=$a56) (segid="PC")
set disp=ener.dat end
display Energies for the output structures
display file              Etot          VDW         NOE
display ----------------------------------------------------
set disp=OUTPUT end
@restraints.xpl
eval ($a213=100*(rand()-0.5) ) ! push away PC
eval ($a214=100*(rand()-0.5) )
eval ($a215=100*(rand()-0.5) )
vector do (x=x+$a213) (segid="PC")
vector do (y=y+$a214) (segid="PC")
vector do (z=z+$a215) (segid="PC")
!write coor OUTPUT="test1.pdb" end
parameter
     @nbfix.4sl_expl.xpl
      nbonds
            cutnb=8.5
            inhi=0.25
            ctofnb=7.5
            ctonnb=6.5
            repe1=0.6 !0.6
                        NBXMod=-2
            rexp=2
            irex=2
            rcon=$a301
            wmin=1.5
      end
 end
 constraints
             interactions (segid="CYTF")(segid="PC")
 end
 energy end
 while ($a01 LE $a05) loop calc
  display cycle $a01
  dynamics rigid
             dt=$a54
             group=(segid="PC")
             dynmode=TCOU
             tbath=$a55
             nprint=500
             nstep=$a53
             NTRFRQ=0 !new for XPLOR vs 3.8
  end
 eval ($a14=$ENER)
 if ($a14 < $min2) then
```

```
  coor copy end
  eval ($min2 = $a14)
  eval ($abc=$VDW)
  eval ($a15=$NOE)
  eval ($a16=$a01)
  eval ($a17=$a18)
 end if
 if ($a18 = $u2) then                !counting number of dockings
  if ($min2 < $a59) then
   if ($abc < $van) then
              coor swap end
              eval ($nout1=$nout1+1)
              eval ($pdb="structure_"+encode($nout1)+".pdb")
              write coord output=$pdb end
              if ($a14<$min1) then
               eval ($ref=$nout1)
        eval ($min1 = $a14)
       end if
       pick bond (segid="CYTF" and name FE) (segid="PC" and name CU) geom
       eval ($a50=$RESULT)
       set disp=ener.dat end
       display $nout1  $min2       $abc        $a15
       set disp=OUTPUT end
       set disp=coor.dat end
       display Cycle: $a16          Dock step: $a17       File#: $nout1            Fe-Cu: $a50              temp: $TEMP
       display  Etot:    $min2                      Evdw:  $abc              Enoe:  $a15
       display ------------------------------------------------------------
              set disp=OUTPUT end
     !violation analysis
              eval ($b3="structure_"+encode($nout1)+".viol.dat")
              set display=$b3 end
              display Violation analysis PRE data
              display res#   PRE(meas)  PRE(calc)  Dist(calc)
              display
              for $g2 in ($g2a $g2b $g2c)
              loop spinlabel
                eval ($g2d=$g2)
                eval ($g2e=$g2+1)
                eval ($g2f=$g2+2)
                eval ($g2g=$g2+3)
                if ($g2=$g2a) then
                  eval ($g1h = $g1a)
                  display Spin Label $g1h
                  for
                            $c02 in ID (store1)
                  loop C3
                    vector show elem (resi) (ID $c02)
                    eval ($c04=$RESULT)                                  !residue nr
                    vector show elem (store1) (ID $c02)
                    eval ($c08=$RESULT)
                    pick bond (resn SL and resi $g2d and name O) (ID $c02) geom
                    eval ($ca1=$RESULT)
                    pick bond (resn SL and resi $g2e and name O) (ID $c02) geom
                    eval ($ca2=$RESULT)
                    pick bond (resn SL and resi $g2f and name O) (ID $c02) geom
                    eval ($ca3=$RESULT)
                    pick bond (resn SL and resi $g2g and name O) (ID $c02) geom
                    eval ($ca4=$RESULT)
                    eval ($c03=($ca1^(-6)+$ca2^(-6)+$ca3^(-6)+$ca4^(-6))/4)
                                  !r-6 average distance over 4 positions
                    eval ($c05=(1.23E16*(4*$tau_c+(3*$tau_c/(1+($field*2*3.14*$tau_c)^2)))*$frl*$a93*$c03) )
                                  !back calculated PRE
                    eval ($c10=$c03^(-1/6))
                    display $c04       $c08        $c05         $c10
```

```
      end loop C3
      display
     end if
     if ($g2=$g2b) then
      eval ($g1h = $g1b)
      display Spin Label $g1h
      for
            $c02 in ID (store2)
      loop C3
       vector show elem (resi) (ID $c02)
       eval ($c04=$RESULT)                          !residue nr
       vector show elem (store2) (ID $c02)
       eval ($c08=$RESULT)
       pick bond (resn SL and resi $g2d and name O) (ID $c02) geom
       eval ($ca1=$RESULT)
       pick bond (resn SL and resi $g2e and name O) (ID $c02) geom
       eval ($ca2=$RESULT)
       pick bond (resn SL and resi $g2f and name O) (ID $c02) geom
       eval ($ca3=$RESULT)
       pick bond (resn SL and resi $g2g and name O) (ID $c02) geom
       eval ($ca4=$RESULT)
       eval ($c03=($ca1^(-6)+$ca2^(-6)+$ca3^(-6)+$ca4^(-6))/4)
                    !r-6 average distance over 4 positions
       eval ($c05=(1.23E16*(4*$tau_c+(3*$tau_c/(1+($field*2*3.14*$tau_c)^2)))*$frl*$a93*$c03) )
                    !back calculated PRE
       eval ($c10=$c03^(-1/6))
       display $c04    $c08    $c05    $c10
      end loop C3
      display
     end if
     if ($g2=$g2c) then
      eval ($g1h = $g1c)
      display Spin Label $g1h
      for
            $c02 in ID (store3)
      loop C3
       vector show elem (resi) (ID $c02)
       eval ($c04=$RESULT)                          !residue nr
       vector show elem (store3) (ID $c02)
       eval ($c08=$RESULT)
       pick bond (resn SL and resi $g2d and name O) (ID $c02) geom
       eval ($ca1=$RESULT)
       pick bond (resn SL and resi $g2e and name O) (ID $c02) geom
       eval ($ca2=$RESULT)
       pick bond (resn SL and resi $g2f and name O) (ID $c02) geom
       eval ($ca3=$RESULT)
       pick bond (resn SL and resi $g2g and name O) (ID $c02) geom
       eval ($ca4=$RESULT)
       eval ($c03=($ca1^(-6)+$ca2^(-6)+$ca3^(-6)+$ca4^(-6))/4)
                    !r-6 average distance over 4 positions
       eval ($c05=(1.23E16*(4*$tau_c+(3*$tau_c/(1+($field*2*3.14*$tau_c)^2)))*$frl*$a93*$c03) )
                    !back calculated PRE
       eval ($c10=$c03^(-1/6))
       display $c04    $c08    $c05    $c10
      end loop C3
      display
     end if
  end loop spinlabel
      close $b3 end
      set display=OUTPUT end
 !end violoation analysis
  coor swap end
 end if
end if
```

```
                                                !impulse to escape local minimum
  eval ($a213=100*(rand()-0.5) )
  eval ($a214=100*(rand()-0.5) )
  eval ($a215=100*(rand()-0.5) )
  vector do (x=x+$a213) (segid="PC")
  vector do (y=y+$a214) (segid="PC")
  vector do (z=z+$a215) (segid="PC")
  vector do (vx=50) (segid="PC")
  vector do (vy=50) (segid="PC")
  vector do (vz=50) (segid="PC")
  set disp=coor.dat end
  display cycle $a01: impulse: $a213, $a214, $a215 to x,y,z; v=50
  set disp=OUTPUT end
 eval ($a18=0)
 eval ($min2=9999.0)
 end if
 eval ($a18=$a18+1)

  if ($TEMP>200000.0) then                      !correct excessive temperature
    eval ($a45=RAND()+0.01)
    vector do (vx=$a56*$a45*rand()) (segid="PC")
    vector do (vy=$a56*$a45*rand()) (segid="PC")
    vector do (vz=$a56*$a45*rand()) (segid="PC")
   end if
   eval ($a01 = $a01 + 1)
 end loop calc
if ($ref > 0) then
  vector idend ( store9 ) ( name ca or name n or name c )         !backbone selection
  eval ($ref_file="structure_"+encode($ref)+".pdb")
  set display=rms.dat end
  display Backbone pairwise RMSD from the lowest energy strucutre ($ref_file)
  display  file            rmsd
  display ----------------------------------------------------------------
  set disp=OUTPUT end
    coor swap end
    coor init end
    coor swap end
    coor disp=comp @@$ref_file
  eval ($count1=0)
  while ($count1 < $nout1) loop fill
   evaluate ($count1=$count1+1)
        evaluate ($file="structure_"+encode($count1)+".pdb")
        coor init end
        coor @@$file
        coor sele=(recall 9) fit end
        coor sele=(recall 9) rms end
        eval ($b1 = $result)
   set display=rms.dat end
   display  $file           $b1
   end loop fill
end if
set display=OUTPUT end
 set echo=true end
  stop
```

List of publications

Scanu S., Förster J.M., Timmer M., Ullmann G.M. and Ubbink M. (2013) Loss of electrostatic interactions causes increase of dynamics within the plastocyanin-cytochrome *f* complex. *Manuscript under revision.*

Scanu S., Förster J.M., Ullmann G.M. and Ubbink M. (2013) Role of hydrophobic interactions in the encounter complex formation of plastocyanin and cytochrome *f* complex revealed by paramagnetic NMR spectroscopy. *J. Am. Chem. Soc.* **135**, 7681-7692.

Scanu S., Förster J., Finiguerra M.G., Shabestari M.H., Huber M. and Ubbink M. (2012) The complex of cytochrome *f* and plastocyanin from *Nostoc sp.* PCC 7119 is highly dynamic. *Chembiochem*. **13**, 1312-1318

Bashir Q., **Scanu S.**, and Ubbink M. (2011) Dynamics in electron transfer protein complexes. *FEBS J*. **278**, 1391-1400

Xu X., **Scanu S.**, Chung J.S., Hirasawa M., Knaff D.B. and Ubbink M. (2010) Structural and functional characterization of the Ga-substituted ferrodoxin from *Synecocystis* sp. PCC6803, a mimic of the native protein. *Biochemistry*, **49**, 7790-7797

Barbiroli, A., Beringhelli, T., Bonomi, F., Donghi, D., Ferranti, P., Galliano, M., Iametti, S., Maggioni, D., Rasmussen, P., **Scanu, S.** and Vilardo, M. C. (2010) Bovine β-lactoglobulin acts as an acid-resistan drug carrier by exploiting its diverse binding regions. *Biological Chemistry*. **391**, 21-32

Curriculum vitae

Sandra Scanu was born on August 27th 1981 in Pattada, a small village located in the heart of Sardinia. She spent a light-hearted childhood in contact with wild and beautiful nature, surrounded by the love of family and friends. Since she was a child, she has showed her curiosity for the world by asking unexpected and, sometimes, surprising questions about life and people. After obtaining her diploma in the scientific high school A. Segni in 2000, she decided to move to Milan to pursue her dream of becoming a scientist. Here, she enrolled in Medical Biotechnology and she obtained her Bachelor degree in 2004, after attending a three months internship in the lab of Prof. G.P. Comi at the Policlinico of Milan. After one year of Chemistry courses, she started her studies in Pharmaceutical Biotechnology, earning a master's degree in 2008. From 2006 to 2008 she worked in the lab of Prof. T. Beringhelli, first as a master's student then as a post-graduate fellow. During these years she has remained fascinated by the endless applications of NMR spectroscopy. This experience led her to Leiden in 2008, where she became a PhD student in the ProtChem group under the supervision of Prof. M. Ubbink. Here, she studied the principles of protein interactions using paramagnetic NMR spectroscopy. Once she overcame the initial troubles with English, she managed to settle down perfectly in the amazing city that accommodated her for four years. Soon she met friends from all over the world, with whom she organized many gatherings and dinner parties. Beside her passion for science, Sandra is in fact successfully dedicated to another art: the good cuisine.
She is now about to begin another journey to Munich, where she will start a post-doctorate position in the group of Biomolecular NMR spectroscopy under the supervision of Dr. T. Madl.

By Giannina Scanu