

AICTE QIP Short Term Training Programme  
on  
**Applications of Molecular Simulations and Machine  
Learning in Research**

**March 22, 2022**

**2:30 - 4:00 PM MD-hands on Ethayaraja Mani/TA**

**4:15 - 5:15 PM MD-hands on Ethayaraja Mani/TA**

**K.Pandurangan**

**Working Under the Guidance of**

**Dr. Ethayaraja Mani**

# Overview

- Quick installation of gromacs
- Work flow of gromacs
- Gromacs files
- Ex-1. Amyloid beta (A $\beta$ )40 in water  
Topology preparation & Energy minimization
- Ex-1 NVT, NPT Equilibration
- Ex-1. MD production
- Ex-1. Analysis (A $\beta$ )40 in water
- Ex-2. Cetyl-trimethyl ammonium Bromide (CTAB)  
Topology preparation & Energy minimization
- Ex-2. NVT, NPT Equilibration (CTAB)
- Ex-2. MD production



# GROMACS Online Reference

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## General Programs

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mdp options	
FAQ	

Table 2 Basic units used in GROMACS		
Quantity	Symbol	Unit
length	r	nm = $10^{-9}$ m
mass	m	u (unified atomic mass unit) = $1.660\,538\,921 \times 10^{-27}$ kg
time	t	ps = $10^{-12}$ s
charge	q	e = elementary charge = $1.602\,176\,565 \times 10^{-19}$ C
temperature	T	K

Consistent with these units are a set of derived units, given in Table 3

Table 3 Derived units. Note that an additional conversion factor of  $10^{28}$  a.m.u ( $\approx 16.6$ ) is applied to get bar instead of internal MD units in the energy and log files

Quantity	Symbol	Unit
energy	E, V	kJ mol <sup>-1</sup>
Force	F	kJ mol <sup>-1</sup> nm <sup>-1</sup>
pressure	p	bar
velocity	v	nm ps <sup>-1</sup> = 1000 m s <sup>-1</sup>

## Modes & Controls

**Command Mode** ESC (commands preceded by :)

**Insertion Mode** Entered on insertion or change

### Starting VI (command line)

<b>vi &lt;filename&gt;</b>	Edit filename
<b>vi -r &lt;filename&gt;</b>	Edit last version of filename after crash
<b>vi +n &lt;filename&gt;</b>	Edit filename at line n
<b>vi +&lt;filename&gt;</b>	Edit filename at end of file
<b>vi +/str &lt;filename&gt;</b>	Edit filename at first occurrence of str

In insertion mode the following should be preceded by ESC:

<b>:w</b>	Save
<b>:x</b>	Save & Exit
<b>:q</b>	Exit if no changes made
<b>:q!</b>	Exit & discard any changes



# GROMACS Programs by Name

Main Table of Contents

## GROMACS Programs Alphabetically

[gmx anadock](#) - Cluster structures from Autodock runs

[gmx ana eig](#) - Analyze eigenvectors/normal modes

[gmx analyze](#) - Analyze data sets

[gmx angle](#) - Calculate distributions and correlations for angles and dihedrals

[gmx bar](#) - Calculate free energy difference estimates through Bennett's acceptance ratio

[gmx bundle](#) - Analyze bundles of axes, e.g., helices

[gmx check](#) - Check and compare files

[gmx chi](#) - Calculate everything you want to know about chi and other dihedrals

[gmx cluster](#) - Cluster structures

[gmx clustsize](#) - Calculate size distributions of atomic clusters

[gmx confrms](#) - Fit two structures and calculates the RMSD

[gmx convert-tpr](#) - Make a modified run-input file

[gmx covar](#) - Calculate and diagonalize the covariance matrix

[gmx current](#) - Calculate dielectric constants and current autocorrelation function

[gmx density](#) - Calculate the density of the system

[gmx editconf](#) - Convert and manipulates structure files

[gmx eneconv](#) - Convert energy files

[gmx enemat](#) - Extract an energy matrix from an energy file

[gmx energy](#) - Writes energies to xvg files and display averages

[gmx filter](#) - Frequency filter trajectories, useful for making smooth movies

[gmx freevolume](#) - Calculate free volume

[gmx gangle](#) - Calculate angles

[gmx genconff](#) - Multiply a conformation in 'random' orientations

[gmx genion](#) - Generate monoatomic ions on energetically favorable positions

[gmx genrestr](#) - Generate position restraints or distance restraints for index groups

[gmx grompp](#) - Make a run input file

[gmx gyrate](#) - Calculate the radius of gyration

# Quick installation of gromacs

## Step 1: Update system:

```
sudo apt-get update
```

## Step 2: Install: gromacs

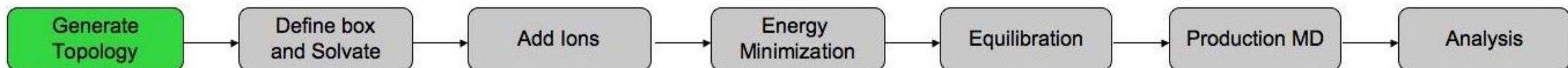
After updating the OS run following command to install the package:

```
sudo apt-get install gromacs
```

<https://www.devmanuals.net/install/ubuntu/ubuntu-12-04-lts-precise-pangolin/install-gromacs.html>

```
tar xfz gromacs-5.1.2.tar.gz  
cd gromacs-5.1.2  
mkdir build  
cd build  
cmake .. -DGMX_BUILD_OWN_FFTW=ON -  
DREGRESSIONTEST_DOWNLOAD=ON  
make  
make check  
sudo make install  
source /usr/local/gromacs/bin/GMXRC
```

<https://manual.gromacs.org/documentation/5.1.2/install-guide/>

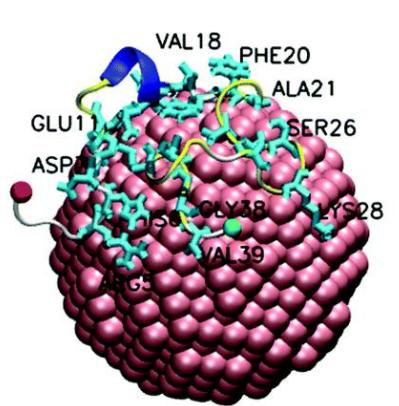


I.

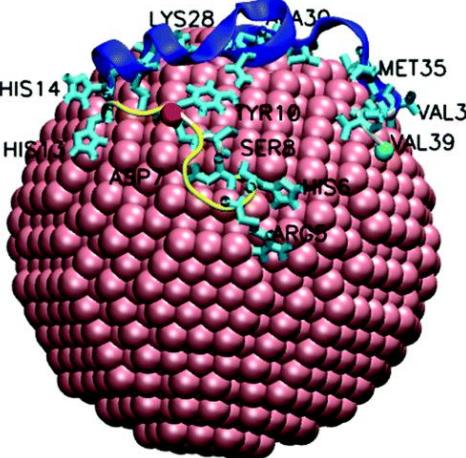
## Where does GROMACS used ??

### Adsorption of amyloid $\beta$ 40 monomer AuNP

a)

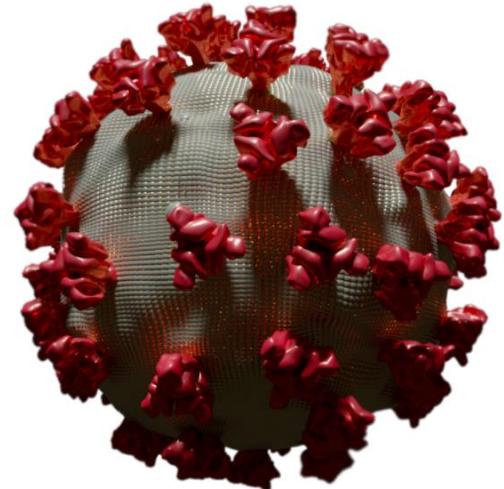
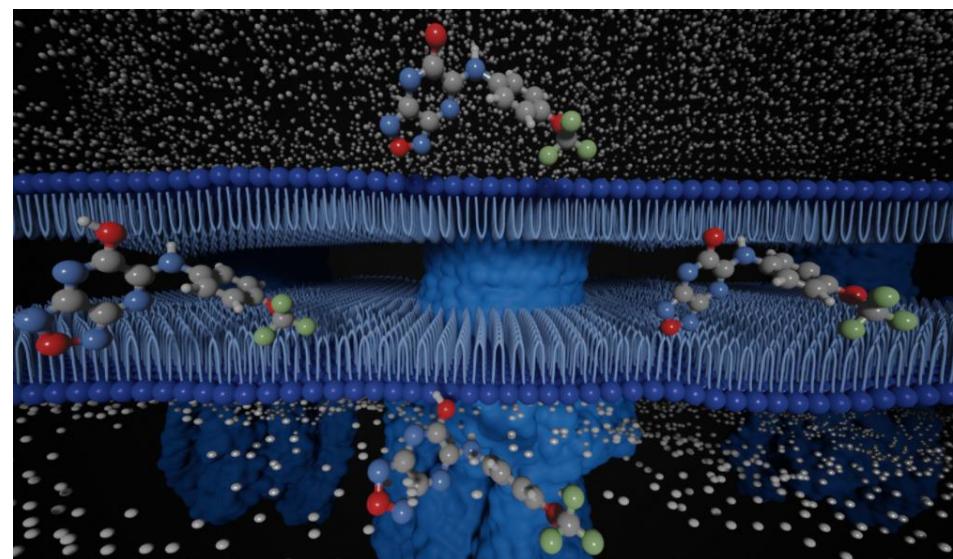
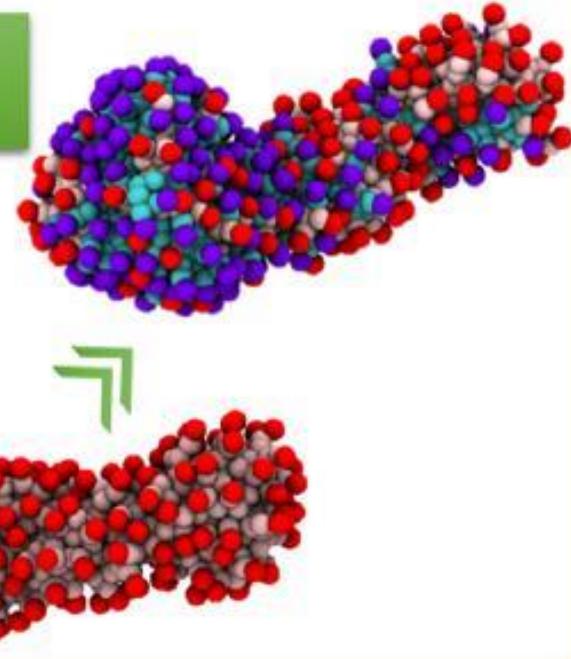
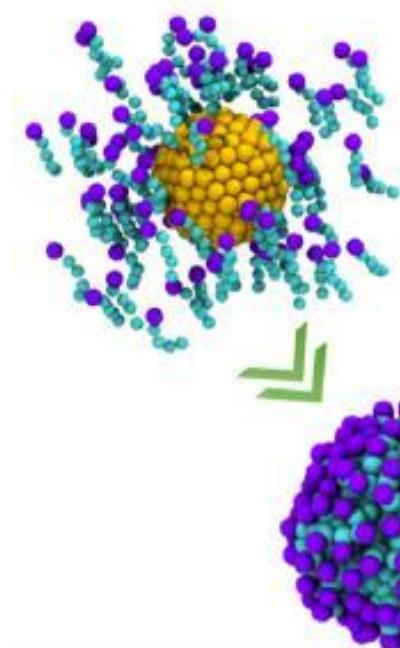


b)



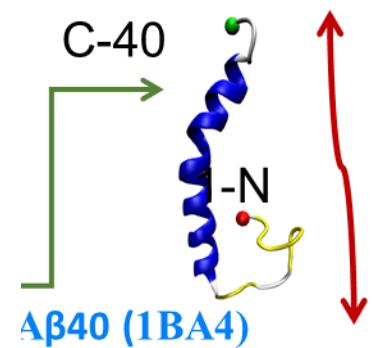
II.

### Self assembly in nanoparticle-surfactant solutions

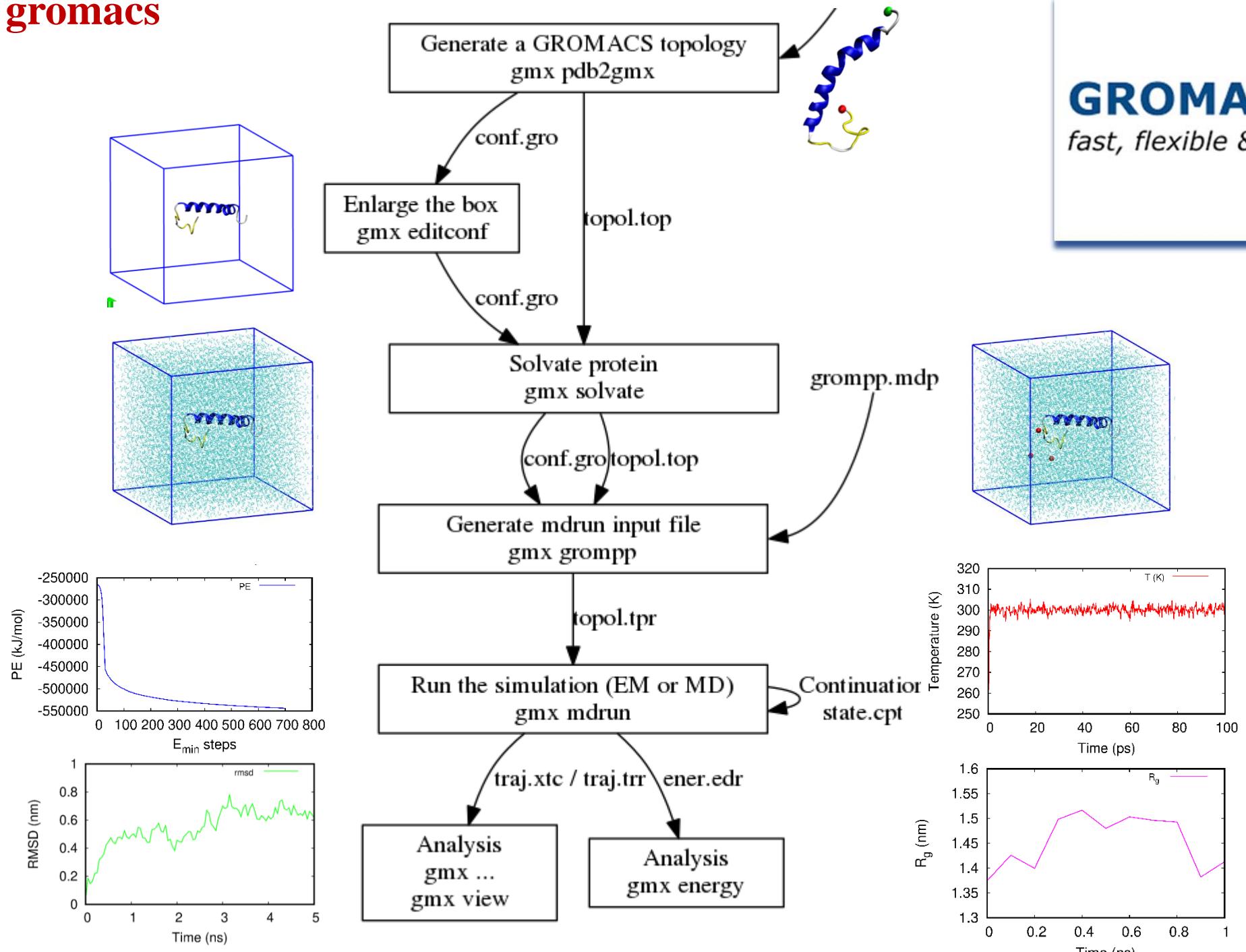


- I. Phys. Chem. Chem. Phys., 2021, 23, 18618-18627  
II. Phys. Chem. Chem. Phys., 2016, 18, 13246-13254

## Ex-1. Amyloid beta ( $\text{A}\beta$ )40 in water



# Work flow of gromacs



**GROMACS**  
fast, flexible & free



# Gromacs files

Input files: \*.pdb, \*.gro, \*.itp, \*.top, \*.mdp, \*.tpr

Output files: \*.trr, \*.xtc, \*.edr, \*.log

## Input:

- pdb : Protein data bank format
- gro: Gromacs format (atom co-ordinates)
- itp: atom topologies (charges, mass, radii, etc)
- top: forcefields, number of molecules, water, etc
- mdp: molecular dynamics simulation parameters
- tpr: all of the above

## Output:

- trr: trajectory file (co-ordinates and velocity)
- xtc: trajectory file (co-ordinates only)
- edr: trajectory file (energies)
- log: CPU time, MFLOP, etc.

**GROMACS**  
*fast, flexible & free*



# Amyloid beta (A $\beta$ )40 in water : Tutorial



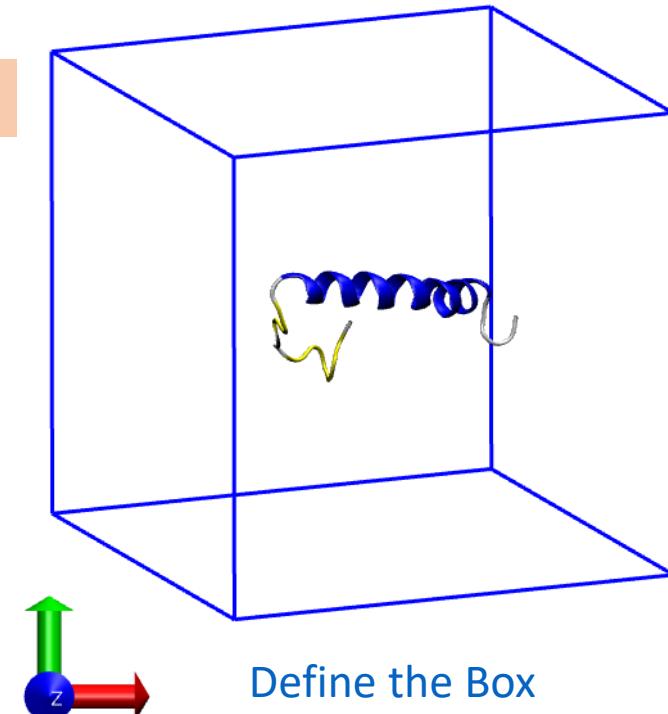
## Step 1: Prepare the Topology

```
grep -v HOH 1ba4.pdb > 1ba4_clean.pdb  
gmx pdb2gmx -f 1ba4_clean.pdb -o prot.gro -water spce -ignh
```

## Step 2: Defining the Unit Cell

```
gmx editconf -f prot.gro -o prot_newbox.gro -c -d 1.0 -bt cubic
```

```
# Use vmd to view prot_newbox.gro
```



### Step 3:Examine the Topology

```
; Command line:  
; gmx pdb2gmx -f 1ba4_clean.pdb -o prot.gro -water spce -ignh  
; Force field was read from the standard GROMACS share directory.  
  
;  
; Include forcefield parameters  
#include "gromos53a6.ff/forcefield.itp"  
  
[ moleculetype ]  
; Name      nrexcl  
Protein_chain_A    3  
  
[ atoms ]  
; nr      type   resnr residue atom   cgnr      charge      mass   typeB      chargeB  
; residue  1  ASP    rtp  ASP     q  0.0  
  1        NL      1    ASP      N      1       0.129    14.0067 ; qtot 0.129  
  2        H       1    ASP     H1      1       0.248     1.008  ; qtot 0.377  
  3        H       1    ASP     H2      1       0.248     1.008  ; qtot 0.625  
  4        H       1    ASP     H3      1       0.248     1.008  ; qtot 0.873  
  5        CH1     1    ASP     CA      2       0.127    13.019  ; qtot 1  
  6        CH2     1    ASP     CB      2          0    14.027  ; qtot 1  
  7        C       1    ASP     CG      3       0.27     12.011 ; qtot 1.27  
  8        OM      1    ASP    OD1      3      -0.635   15.9994 ; qtot 0.635
```

nr: Atom number

• type: Atom type

• resnr: Amino acid residue number

• residue: The amino acid residue

• atom: Atom name

• cgnr: Charge group number

• charge: Self-explanatory

• mass: Also self-explanatory typeB, chargeB, massB:

```
; Include water topology  
#include "gromos53a6.ff/spce.itp"  
  
#ifdef POSRES_WATER  
; Position restraint for each water oxygen  
[ position_restraints ]  
; i funct      fcx      fcy      fcz  
  1    1        1000    1000    1000  
#endif  
  
;  
; Include topology for ions  
#include "gromos53a6.ff/ions.itp"  
  
[ system ]  
; Name  
AMYLOID BETA-PEPTIDE in water  
  
[ molecules ]  
; Compound      #mols  
Protein_chain_A    1  
SOL            10287  
NA             3
```

.gro

AMYLOID BETA-PEPTIDE in water

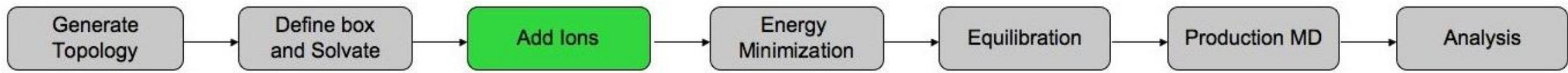
31258

1ASP	N	1	3.211	3.312	3.357
1ASP	H1	2	3.259	3.394	3.389
1ASP	H2	3	3.123	3.335	3.316
1ASP	H3	4	3.197	3.251	3.436
1ASP	CA	5	3.296	3.240	3.261
1ASP	CB	6	3.415	3.183	3.339
1ASP	CG	7	3.379	3.063	3.427
1ASP	OD1	8	3.307	3.080	3.528
1ASP	OD2	9	3.407	2.952	3.379
1ASP	C	10	3.212	3.136	3.183
1ASP	O	11	3.103	3.174	3.140
2ALA	N	12	3.263	3.015	3.156
2ALA	H	13	3.338	2.981	3.216
2ALA	CA	14	3.188	2.907	3.089
2ALA	CB	15	3.261	2.852	2.967
2ALA	C	16	3.164	2.792	3.189
2ALA	O	17	3.247	2.704	3.211
3GLU	N	18	3.049	2.805	3.254
3GLU	H	19	3.005	2.895	3.259
3GLU	CA	20	2.995	2.711	3.354
3GLU	CB	21	2.852	2.754	3.387
3GLU	CG	22	2.840	2.891	3.457
3GLU	CD	23	2.883	3.014	3.374
3GLU	OE1	24	2.801	3.068	3.298
3GLU	OE2	25	2.999	3.057	3.389
3GLU	C	26	3.003	2.562	3.314
3GLU	O	27	3.049	2.481	3.393

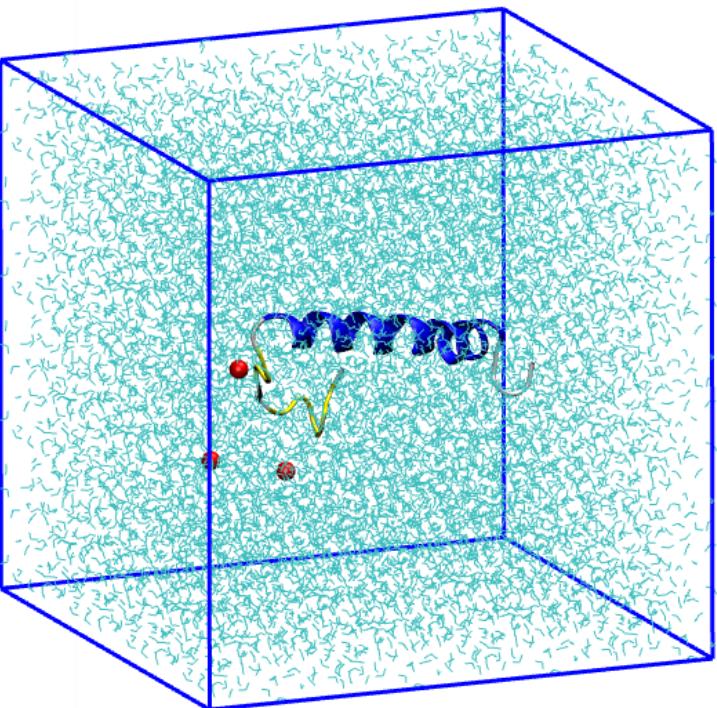
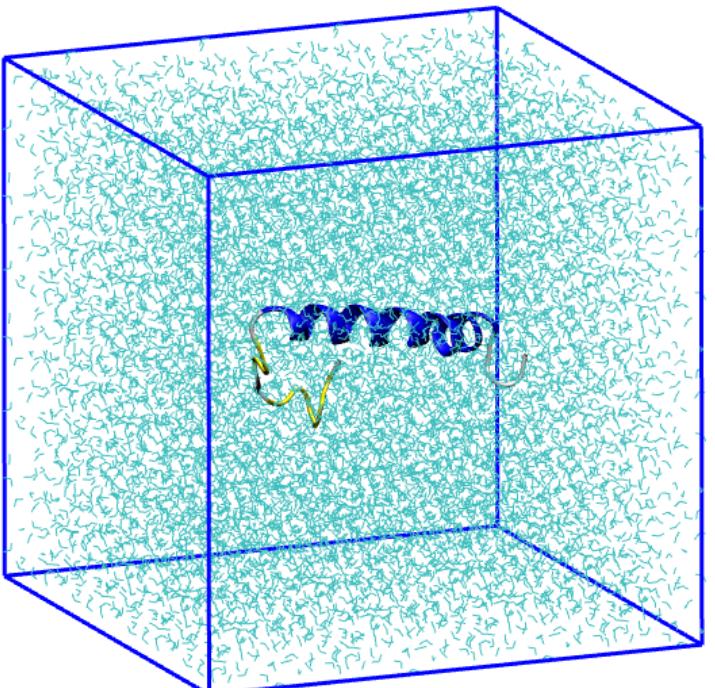
.mdp

title = Gromas96 53a6Abeta-40 NPT equilibration  
define = -DPOSRES ; position restrain the protein  
; Run parameters  
integrator = md ; leap-frog integrator  
nsteps = 50000 ; 2 \* 50000 = 100 ps  
dt = 0.002 ; 2 fs  
; Output control  
nstxout = 100 ; save coordinates every 0.2 ps  
nstvout = 100 ; save velocities every 0.2 ps  
nstenergy = 100 ; save energies every 0.2 ps  
nstlog = 100 ; update log file every 0.2 ps  
; Bond parameters  
continuation = yes ; Restarting after NVT  
constraint\_algorithm = lincs ; holonomic constraints  
constraints = all-bonds ; all bonds (even heavy atom-H bonds) constrained  
lincs\_iter = 1 ; accuracy of LINCS  
lincs\_order = 4 ; also related to accuracy  
; Neighborsearching  
ns\_type = grid ; search neighboring grid cells  
nstlist = 5 ; 10 fs  
rlist = 1.0 ; short-range neighborlist cutoff (in nm)  
rcoulomb = 1.0 ; short-range electrostatic cutoff (in nm)  
rvdw = 1.0 ; short-range van der Waals cutoff (in nm)  
; Electrostatics  
coulombtype = PME ; Particle Mesh Ewald for long-range electrostatics  
pme\_order = 4 ; cubic interpolation  
fourierspacing = 0.16 ; grid spacing for FFT  
; Temperature coupling is on  
tcoupl = V-rescale ; modified Berendsen thermostat  
tc-grps = Protein Non-Protein ; two coupling groups - more accurate  
tau\_t = 0.1 0.1 ; time constant, in ps  
ref\_t = 300 300 ; reference temperature, one for each group, in K  
; Pressure coupling is on  
pcoupl = Parrinello-Rahman ; Pressure coupling on in NPT  
pcoupltype = isotropic ; uniform scaling of box vectors  
tau\_p = 2.0 ; time constant, in ps  
ref\_p = 1.0 ; reference pressure, in bar

## Step 4: Adding Ions



```
gmx solvate -cp prot_newbox.gro -cs spc216.gro -o prot_solv.gro -p topol.top  
grep gmx grompp -f ions.mdp -c prot_solv.gro -p topol.top -o ions.tpr  
gmx genion -s ions.tpr -o prot_solv_ions.gro -p topol.top -pname NA -nname CL -neutral
```



```
[ system ]  
; Name  
AMYLOID BETA-PEPTIDE in water
```

```
[ molecules ]  
; Compound #mols  
Protein_chain_A 1  
SOL 10287
```

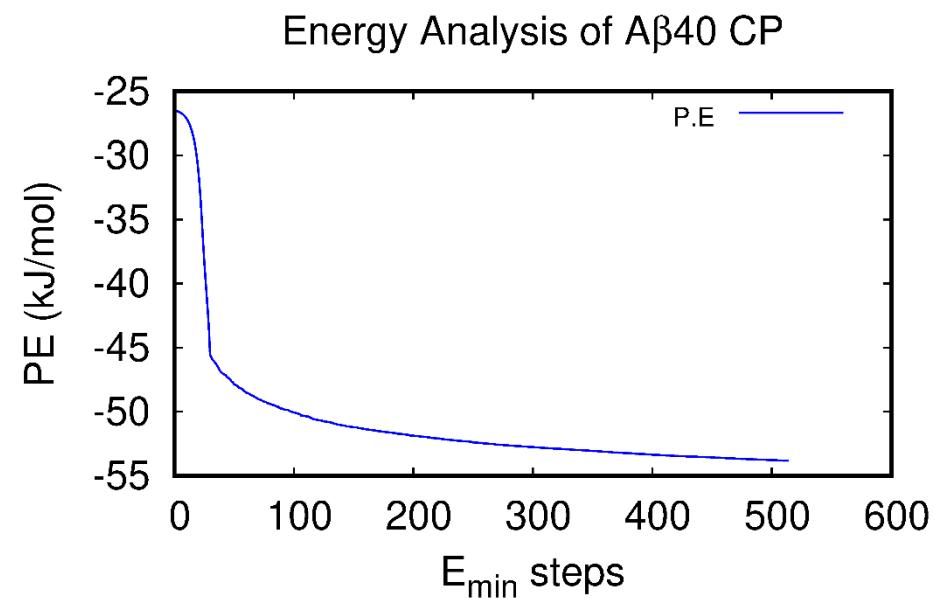
```
[ molecules ]  
; Compound #mols  
Protein_chain_A 1  
SOL 10287  
NA 3
```

## Step 5:Energy minimization



```
gmx grompp -f minimmdp -c prot_solv_ions.gro -p topol.top -o em.tpr  
gmx mdrun -v -deffnm em
```

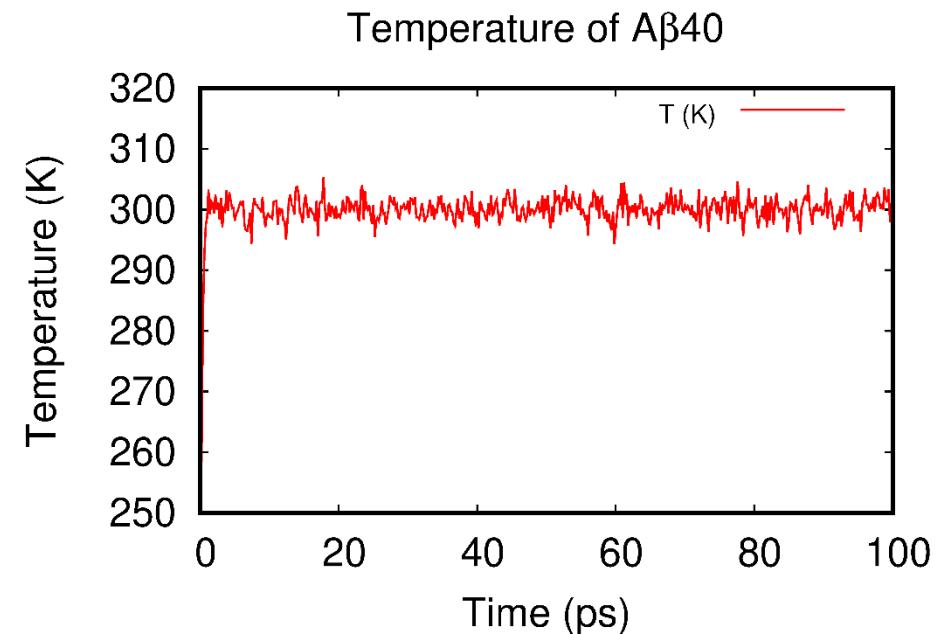
```
gmx energy -f em.edr -o PE.xvg  
## Use gnuplot PE  
## Make index file using em.gro  
gmx make_ndx -f em.gro -o index.ndx
```



## Step 6: NVT equilibration



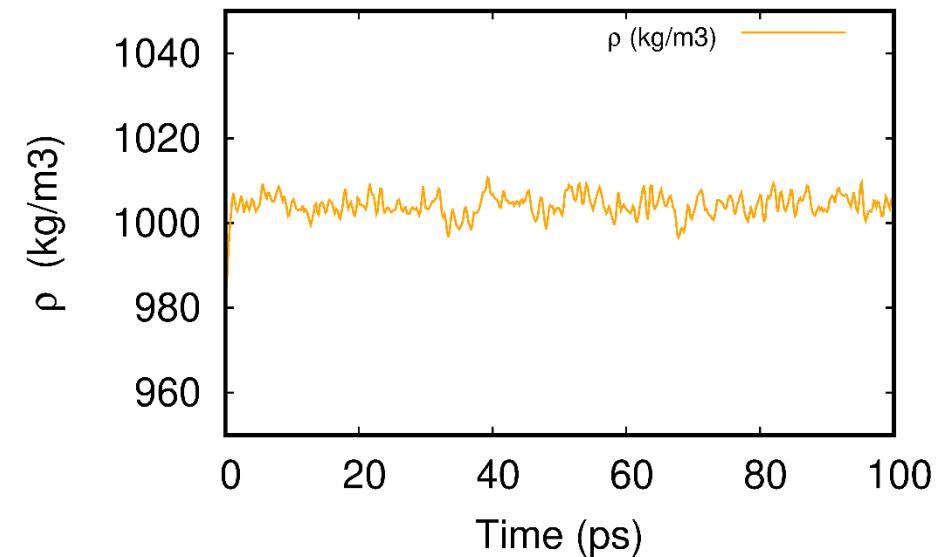
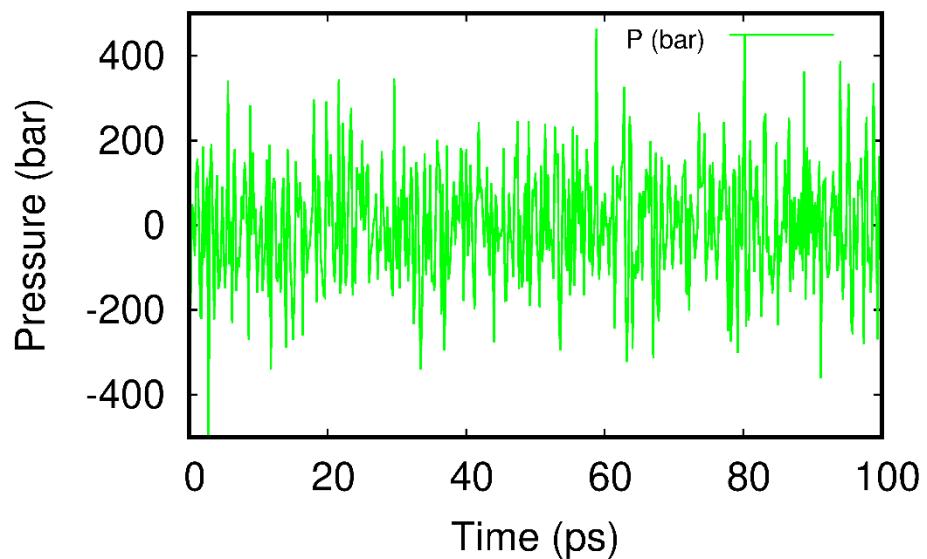
```
gmx grompp -f nvtmdp -c em.gro -r em.gro -p topol.top -o nvt.tpr  
gmx mdrun -deffnm nvt -v  
gmx energy -f nvt.edr -o T.xvg  
## Use gnuplot Temp
```



## Step 7: NPT equilibration



```
gmx grompp -f nptmdp -c nvt.gro -r nvt.gro -t nvt.cpt -p topol.top -o npt.tpr  
gmx mdrun -deffnm npt -v  
gmx energy -f npt.edr -o pressure.xvg  
## Use gnuplot → Pressure  
gmx energy -f npt.edr -o density.xvg  
## Use gnuplot → density
```



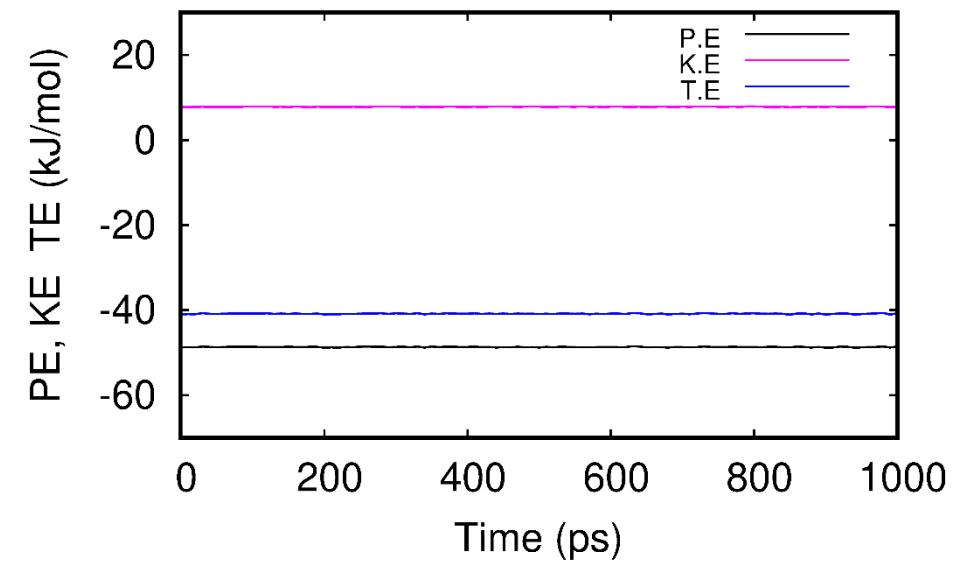
## Step 8: MD production



```
gmx grompp -f mdmdp -c npt.gro -t npt.cpt -p topol.top -o md_1.tpr  
gmx mdrun -deffnm md_1 -v  
## Energy analysis md_1 TE,KE & PE  
gmx energy -f md_1.edr -o md_e.xvg  
## Use gnuplot Pressure
```

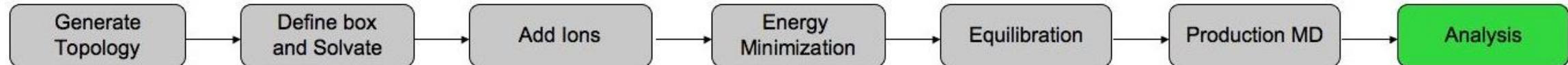
### Energy analysis

Energy Analysis of A $\beta$ 40 CP



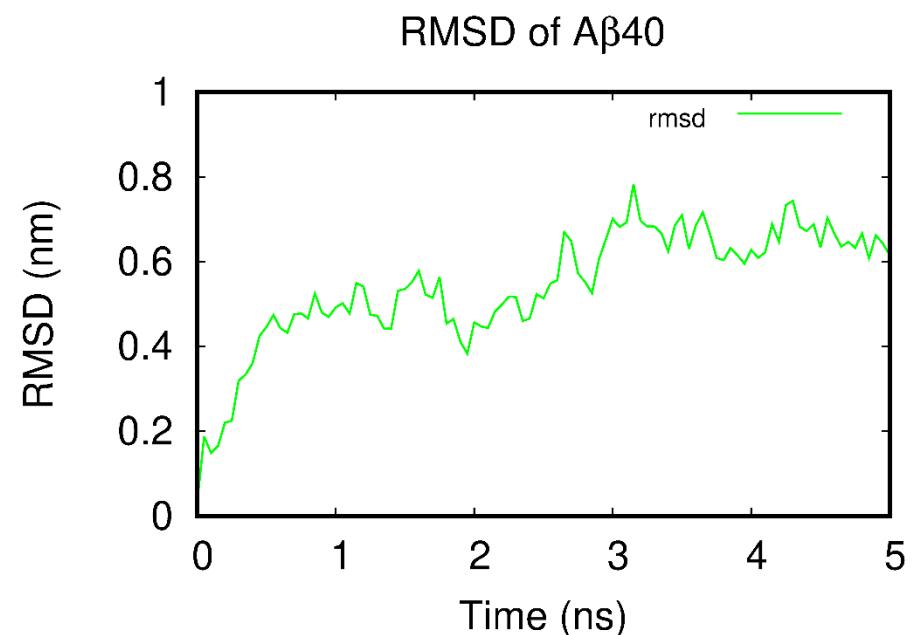
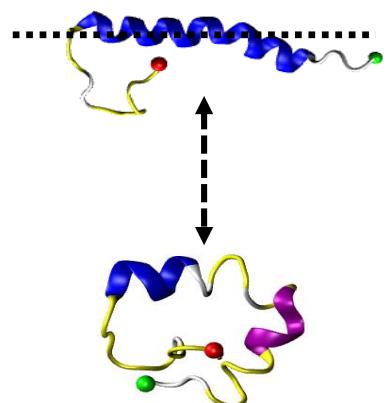
## Step 9: Analysis

### Root mean square deviation (RMSD)



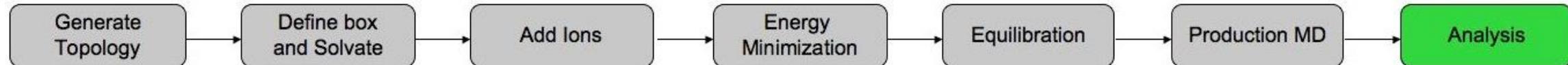
```
## protein diffuse → "broken" or may "jump" across to the other pbc box
gmx gmx trjconv -s md_1.tpr -f md_1.xtc -o md_1_noPBC.xtc -pbc mol -center
## Analysis RMSD calculations
gmx rms -s em.tpr -f md_1_noPBC.xtc -o rmsd.xvg -tu ns
## gnuplot
```

$$\text{RMSD}(t) = \left[ \frac{1}{M} \sum_{i=1}^N m_i |\mathbf{r}_i(t) - \mathbf{r}_i^{\text{ref}}|^2 \right]^{1/2}$$



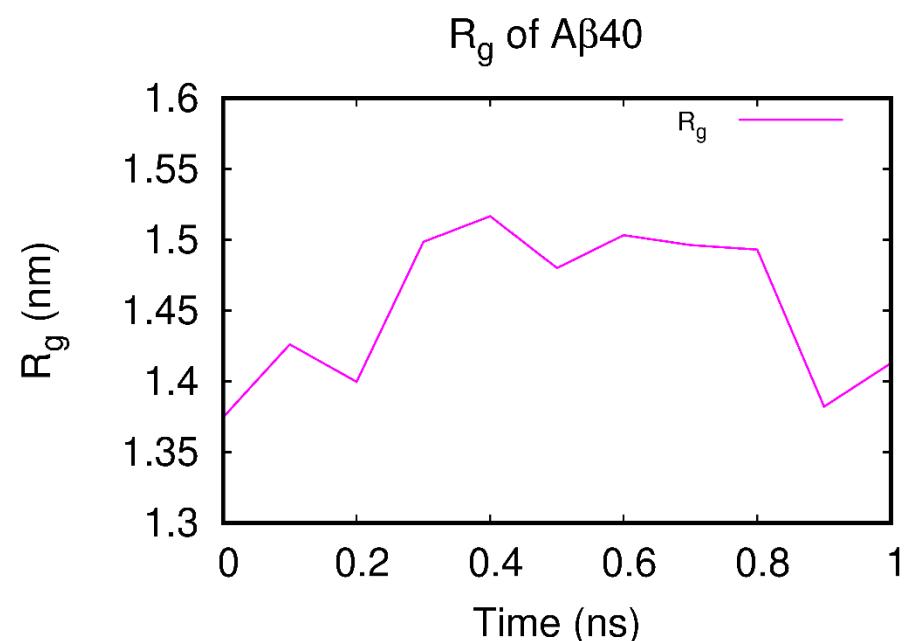
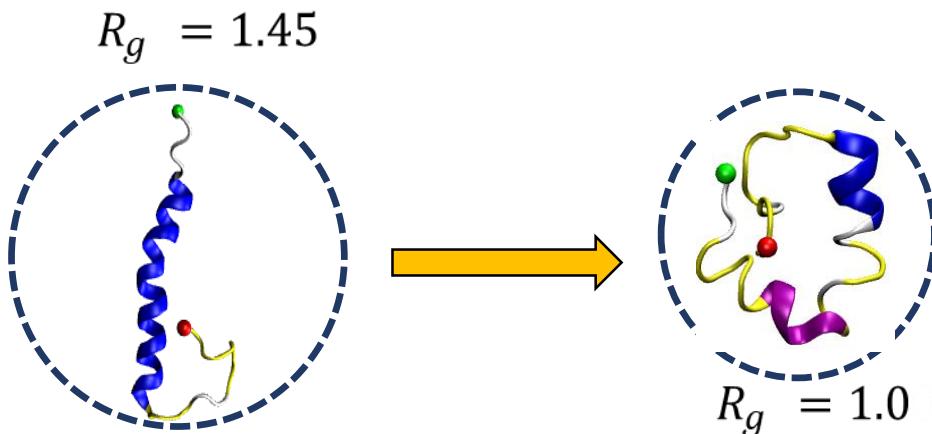
## Step 9: Analysis cont..

### Radius of gyration



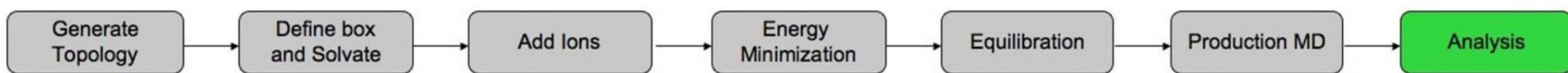
```
## Analysis: Rg calculations  
gmx gyrate -s md_1.tpr -f md_1_noPBC.xtc -o gyrate.xvg  
## gnuplot
```

$$R_g = \left[ \frac{\sum_{i=1}^n (r_i - r_{com})^2 m_i}{\sum_{i=1}^n m_i} \right]^{1/2}$$



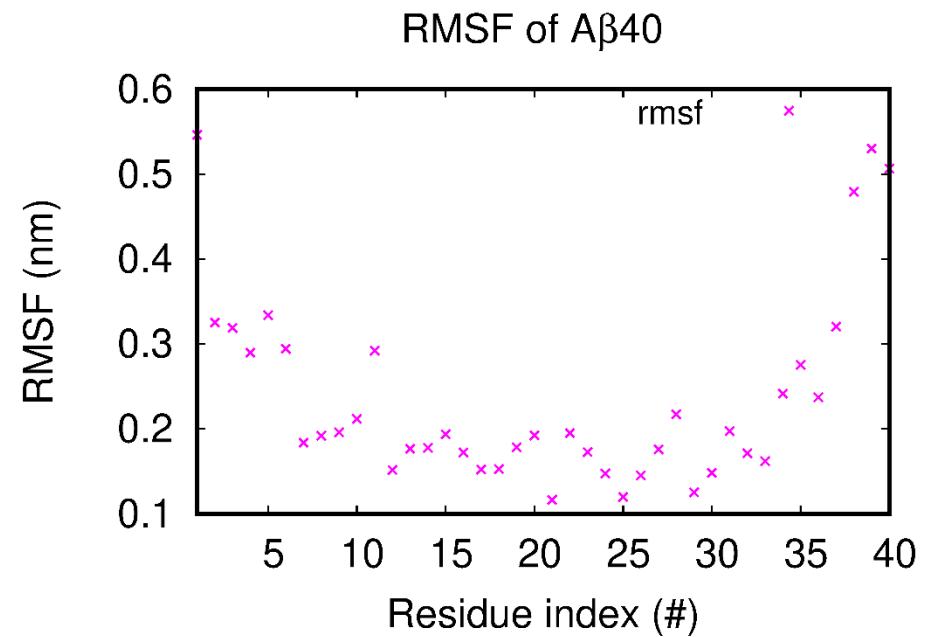
## Step 9: Analysis cont..

### Root mean square fluctuation



```
## Analysis RMSF calculations  
gmx rmsf -s md_1.tpr -f md_1_noPBC.xtc -o rmsf.xvg -oq rmsf.pdb -res  
## gnuplot
```

$$\text{RMSF}_i = \left[ \frac{1}{T} \sum_{t_j=1}^T |\mathbf{r}_i(t_j) - \mathbf{r}_i^{\text{ref}}|^2 \right]^{1/2}$$



## I. Force field validation

To ensure the right choice of force field for the protein and water models for solvent, four different force field were used for simulation of monomer A $\beta$ 40 in water. The details of water model, force fields and potential cut-offs for non-bonded parameters are given in Table.1

**Table 1:** Force field, water models and potential cutoffs for non-bonded interactions.

Force field	Water model	$r_c/r_{list}$	$r_{vdw}$
AMBER03	TIP3P	0.8	0.8
CHARMM22 + CMAP	TIP3P	1.2	1.2
OPLS-AA	TIP4P	1.0	1.0
GROMOS96 53A6	SPC	1.0	1.0

**Table 2:** Average secondary structure distribution (in percentage)

Force field	Coil	$\beta$ -sheet	Bend	Turn	$\alpha$ -Helix
AMBER03	27 (29)	0 (0)	7 (13)	27 (19)	39 (39)
CHARMM22 + CMAP	19 (21)	0 (0)	10 (9)	14 (12)	57 (58)
OPLS-AA	34 (31)	6 (16)	27 (23)	23 (18)	10 (12)

The experimentally reported secondary structure of oligomer A $\beta$ 40 in water:  $\alpha$ -helix 22%, coil 18%, and  $\beta$  sheet + bends + turns 60%.

**Table 3:** Average secondary structure distribution (in percentage) obtained from GROMOS96 53A6 force field.

	MD study	$\alpha$ -Helix	$\beta$ -sheet	Others*
This work	19( $\pm 2$ )	19 ( $\pm 4$ )	60 ( $\pm 4$ )	
Ref <sup>1</sup>	24 ( $\pm 3$ )	11 ( $\pm 2$ )	65( $\pm 5$ )	
Ref <sup>2</sup>	20 ( $\pm 2$ )	15( $\pm 4$ )	65( $\pm 5$ )	

The standard deviation given in the parenthesis are obtained by averaging three set of independent simulation.

**Table 4:**  $R_g$

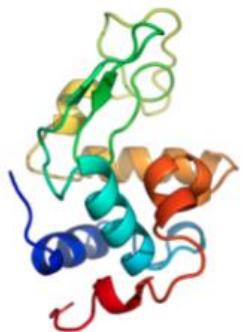
Force field	$R_g$ (nm)	$R_g^{ref1}$ (nm)
AMBER03	1.10	1.03
CHARMM22 + CMAP	1.35	1.30
GROMOS96 53A6	0.99	1.05
OPLS-AA	0.96	0.96

The experimentally reported value of  $R_g$  for the oligomer A $\beta$ 40 in solution is 0.9 ( $\pm 0.1$ ) nm.

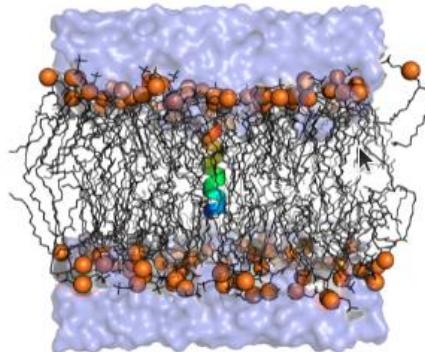
# GROMACS Tutorials

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Virginia Tech Department of Biochemistry

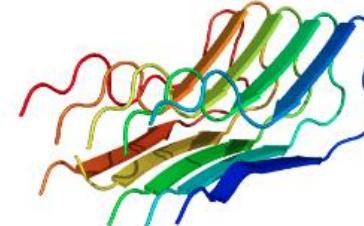
All tutorials have been updated for GROMACS version 2018!



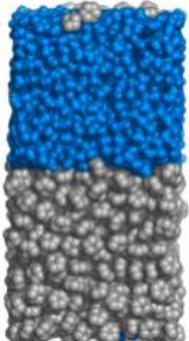
Tutorial 1: Lysozyme in Water



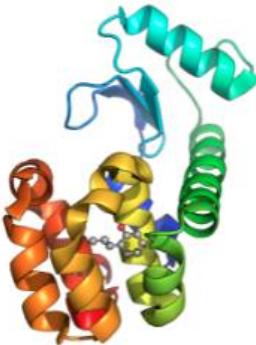
Tutorial 2: KALP<sub>15</sub> in DPPC



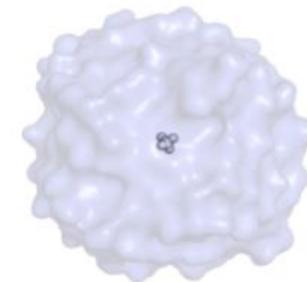
Tutorial 3: Umbrella Sampling



Tutorial 4: Biphasic Systems



Tutorial 5: Protein-Ligand Complex

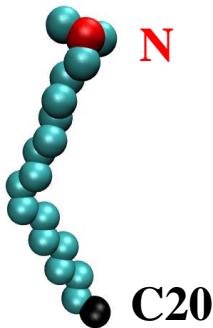


Tutorial 6: Free Energy of Solvation



<http://www.mdtutorials.com/gmx/>  
<https://bevanbrownlab.com/>

## Ex-2. Cetyl-trimethyl ammonium Bromide (CTAB) in water



CTAB.gro

CTAB								
20								
1CTAB	C1	8941	2.246	5.833	13.219	0.7451	-0.4412	0.3222
1CTAB	C2	8942	2.058	5.669	13.218	0.1279	0.8323	0.7574
1CTAB	C3	8943	2.025	5.888	13.134	-0.2050	-0.0752	0.4203
1CTAB	N4	8944	2.125	5.782	13.152	0.3663	0.4425	0.3225
1CTAB	C5	8945	2.171	5.755	13.016	-0.4559	0.3115	0.0641
1CTAB	C6	8946	2.080	5.686	12.914	-0.1636	0.0112	0.0056
1CTAB	C7	8947	2.156	5.627	12.795	0.0648	0.5178	-0.1008
1CTAB	C8	8948	2.064	5.617	12.673	-0.4212	-0.0417	0.3104
1CTAB	C9	8949	2.138	5.572	12.548	-0.4716	0.4037	0.1187
1CTAB	C10	8950	2.039	5.516	12.446	0.1919	-0.5355	-0.0214
1CTAB	C11	8951	2.103	5.483	12.310	0.1884	-0.1569	-0.1161
1CTAB	C12	8952	2.018	5.402	12.212	0.2488	-0.1195	-0.2001
1CTAB	C13	8953	2.077	5.402	12.071	0.3242	-0.2681	-0.1681
1CTAB	C14	8954	2.070	5.536	11.998	0.5247	-0.2671	-0.1876
1CTAB	C15	8955	2.121	5.529	11.854	0.6262	0.4980	-0.1954
1CTAB	C16	8956	2.099	5.660	11.778	-0.2822	0.2720	-0.3343
1CTAB	C17	8957	2.153	5.629	11.638	-0.3024	-0.2087	-0.2392
1CTAB	C18	8958	2.136	5.759	11.559	-0.1673	-0.0173	0.0410
1CTAB	C19	8959	2.197	5.738	11.420	-0.3553	0.2486	-0.0828
1CTAB	C20	8960	2.297	5.844	11.371	0.0966	-0.2245	-0.2024
5.0	5.0	5.0						

```

[ moleculetype ]
; Name      nrexcl
CTAB      3

[ atoms ]
;  nr   type  resnr residu  atom   cgnr    charge        mass
  1    LC3      1    CTAB     C1       0        0.25    15.0350 ; qtot:
  2    LC3      1    CTAB     C2       1        0.25    15.0350 ; qtot:
  3    LC3      1    CTAB     C3       2        0.25    15.0350 ; qtot:
  4    LNL      1    CTAB     N4       3        0.00    14.0067 ; qtot:
  5    LH2      1    CTAB     C5       4        0.25    14.0270 ; qtot:
  6    LP2      1    CTAB     C6       5        0        14.0270 ; qtot:
  7    LP2      1    CTAB     C7       6        0        14.0270 ; qtot:
  8    LP2      1    CTAB     C8       7        0        14.0270 ; qtot:
  9    LP2      1    CTAB     C9       8        0        14.0270 ; qtot:
 10   LP2      1    CTAB    C10      9        0        14.0270 ; qtot:
 11   LP2      1    CTAB    C11     10        0        14.0270 ; qtot:
 12   LP2      1    CTAB    C12     11        0        14.0270 ; qtot:
 13   LP2      1    CTAB    C13     12        0        14.0270 ; qtot:
 14   LP2      1    CTAB    C14     13        0        14.0270 ; qtot:
 15   LP2      1    CTAB    C15     14        0        14.0270 ; qtot:
 16   LP2      1    CTAB    C16     15        0        14.0270 ; qtot:
 17   LP2      1    CTAB    C17     16        0        14.0270 ; qtot:
 18   LP2      1    CTAB    C18     17        0        14.0270 ; qtot:
 19   LP2      1    CTAB    C19     18        0        14.0270 ; qtot:
 20   LP3      1    CTAB    C20     19        0      15.0350 ; qtot:

[ bonds ]
;  ai      aj funct
  4       5      1  0.14700E+00  0.37660E+06
  5       6      1  0.15300E+00  0.33470E+06
  6       7      1  0.15300E+00  0.33470E+06
  7       8      1  0.15300E+00  0.33470E+06
  8       9      1  0.15300E+00  0.33470E+06
  9      10      1  0.15300E+00  0.33470E+06
 10      11      1  0.15300E+00  0.33470E+06
 11      12      1  0.15300E+00  0.33470E+06
 12      13      1  0.15300E+00  0.33470E+06
 13      14      1  0.15300E+00  0.33470E+06
 14      15      1  0.15300E+00  0.33470E+06
 15      16      1  0.15300E+00  0.33470E+06
 16      17      1  0.15300E+00  0.33470E+06
 17      18      1  0.15300E+00  0.33470E+06
 18      19      1  0.15300E+00  0.33470E+06
 19      20      1  0.15300E+00  0.33470E+06
 20      1      1  0.14700E+00  0.37450E+06
  1       4      1  0.14700E+00  0.37450E+06
  2       5      1  0.14700E+00  0.37450E+06
  3       6      1  0.14700E+00  0.37450E+06
  4       7      1  0.14700E+00  0.37450E+06
  5       8      1  0.14700E+00  0.37450E+06

[ pairs ]
;  ai      aj funct
  1       6      1
  2       6      1
  3       6      1
  4       7      1
  5       8      1

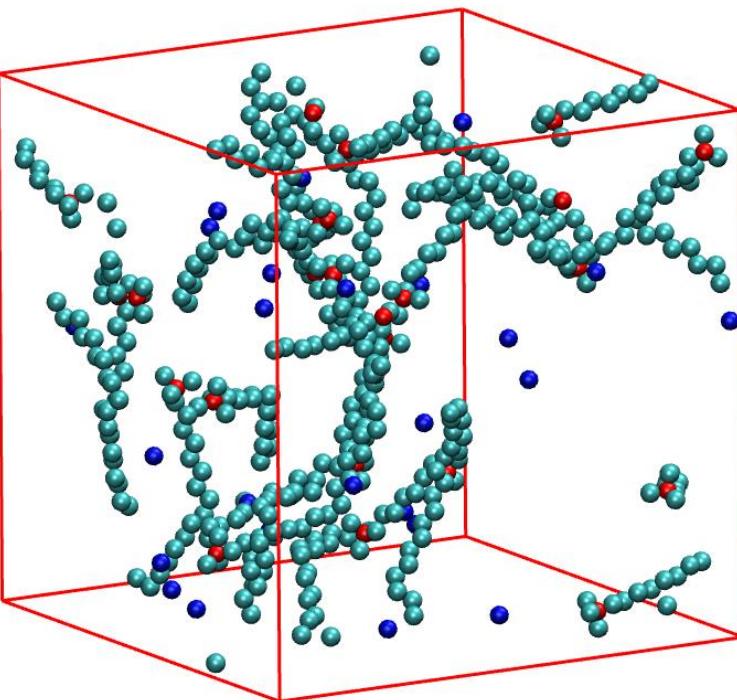
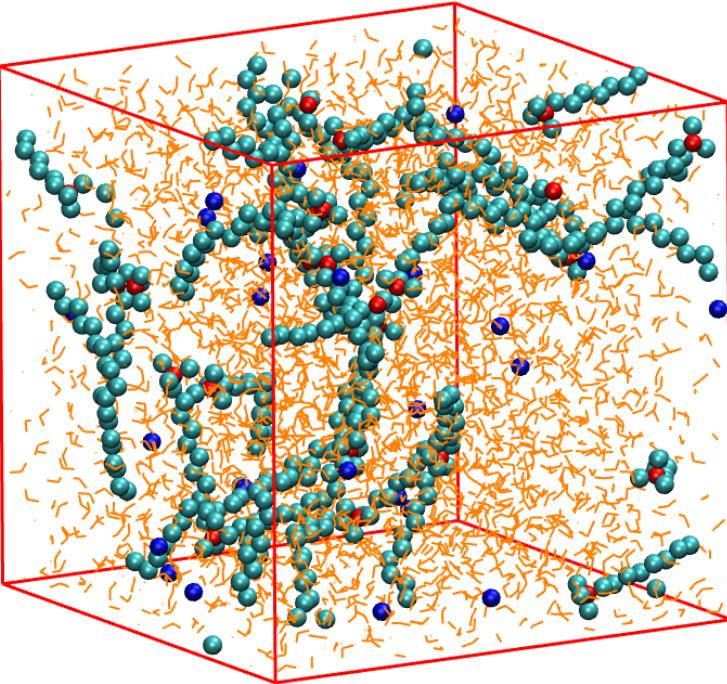
```

## Packing of CTAB in cubic box

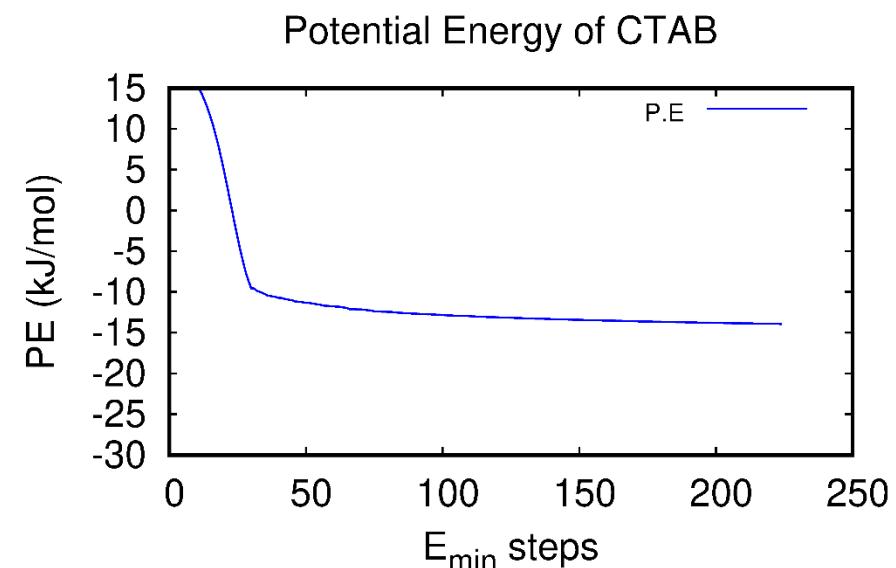
```
#include "ffgmx.itp"
#include "ctab_SMeenaLang13.itp"
#include "spc.itp"
#include "ions.itp"

[ system ]
; name
AU144SRC0060 in Solution in water

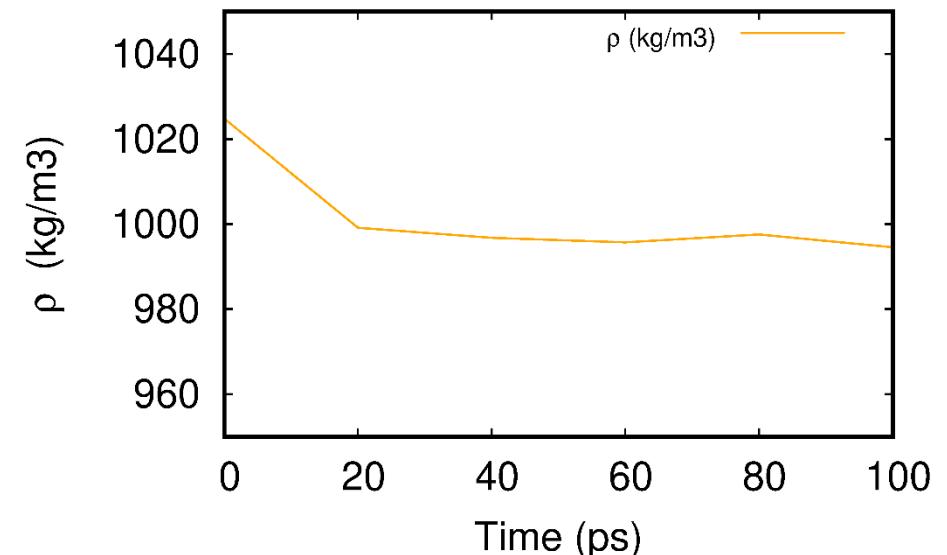
[ molecules ]
; name number
;NP2 1
CTAB 25
SOL 2616
BR 25
```



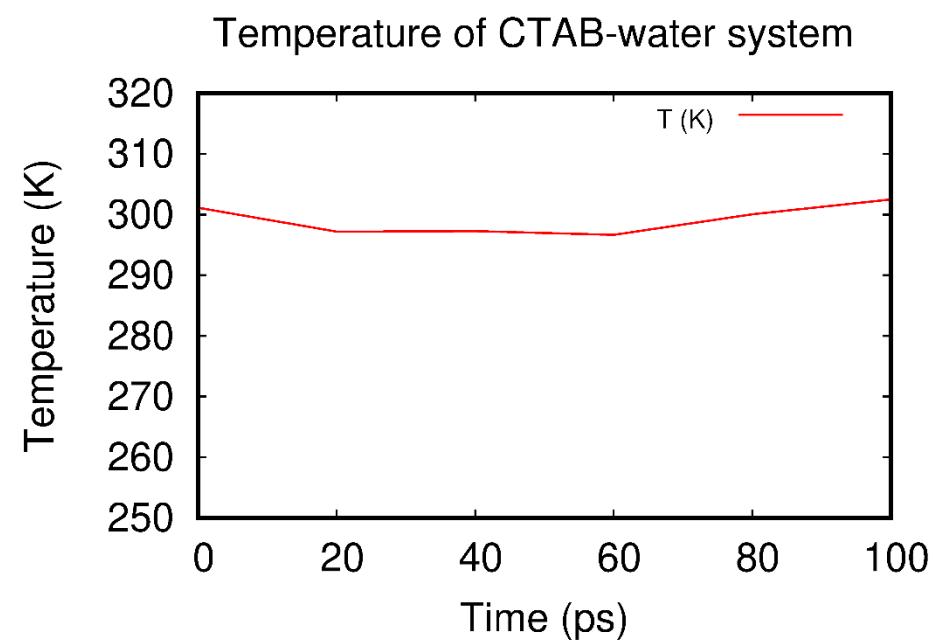
## Energy minimization of CTAB



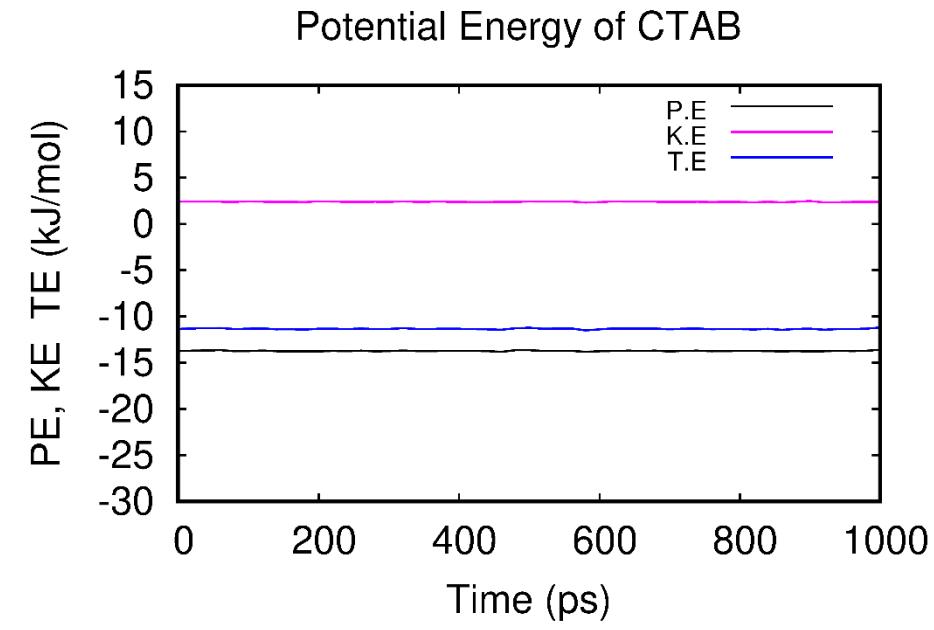
## NPT equilibration



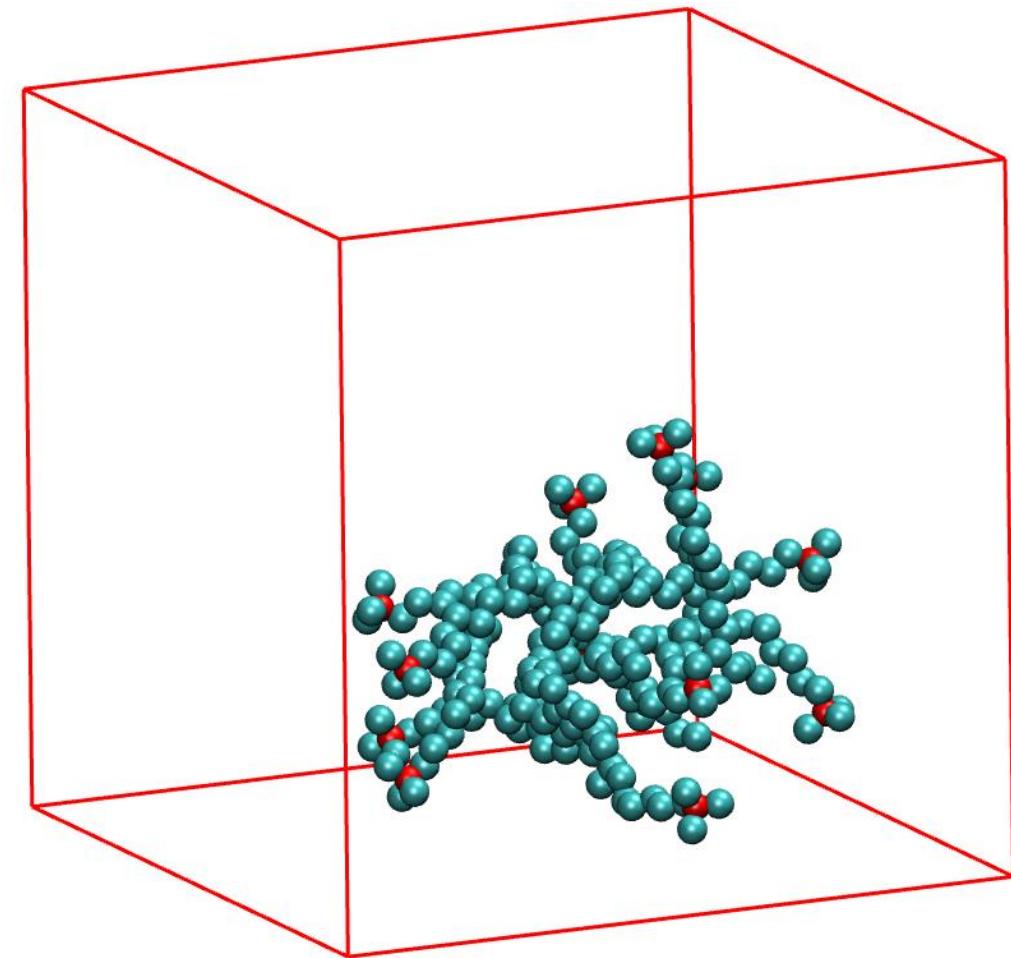
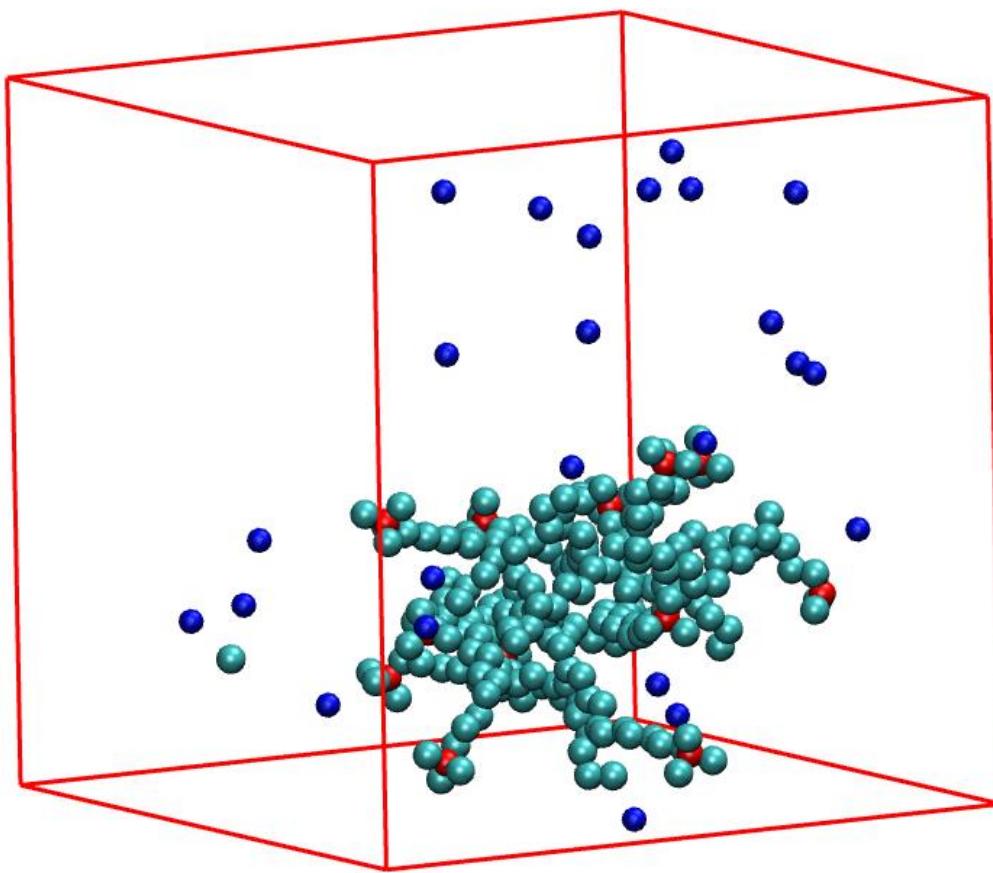
## NVT equilibration



## MD production

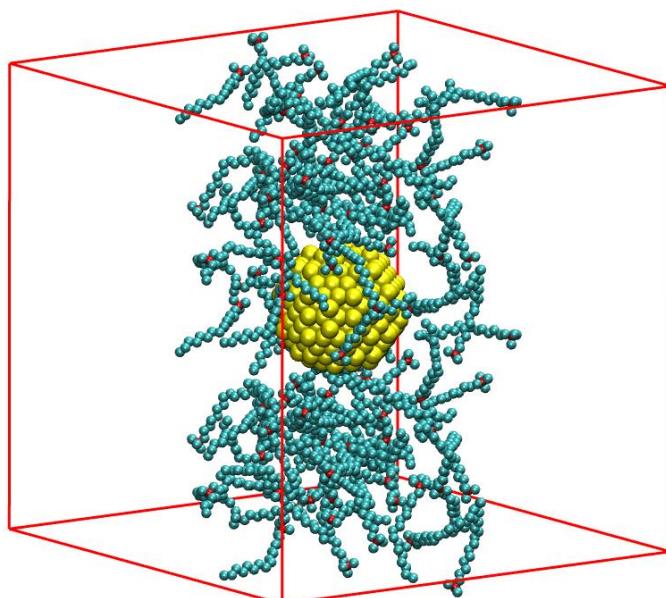
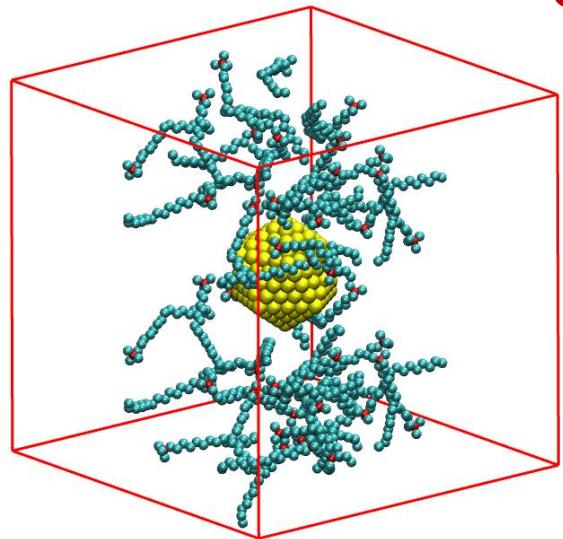


## VMD Analysis

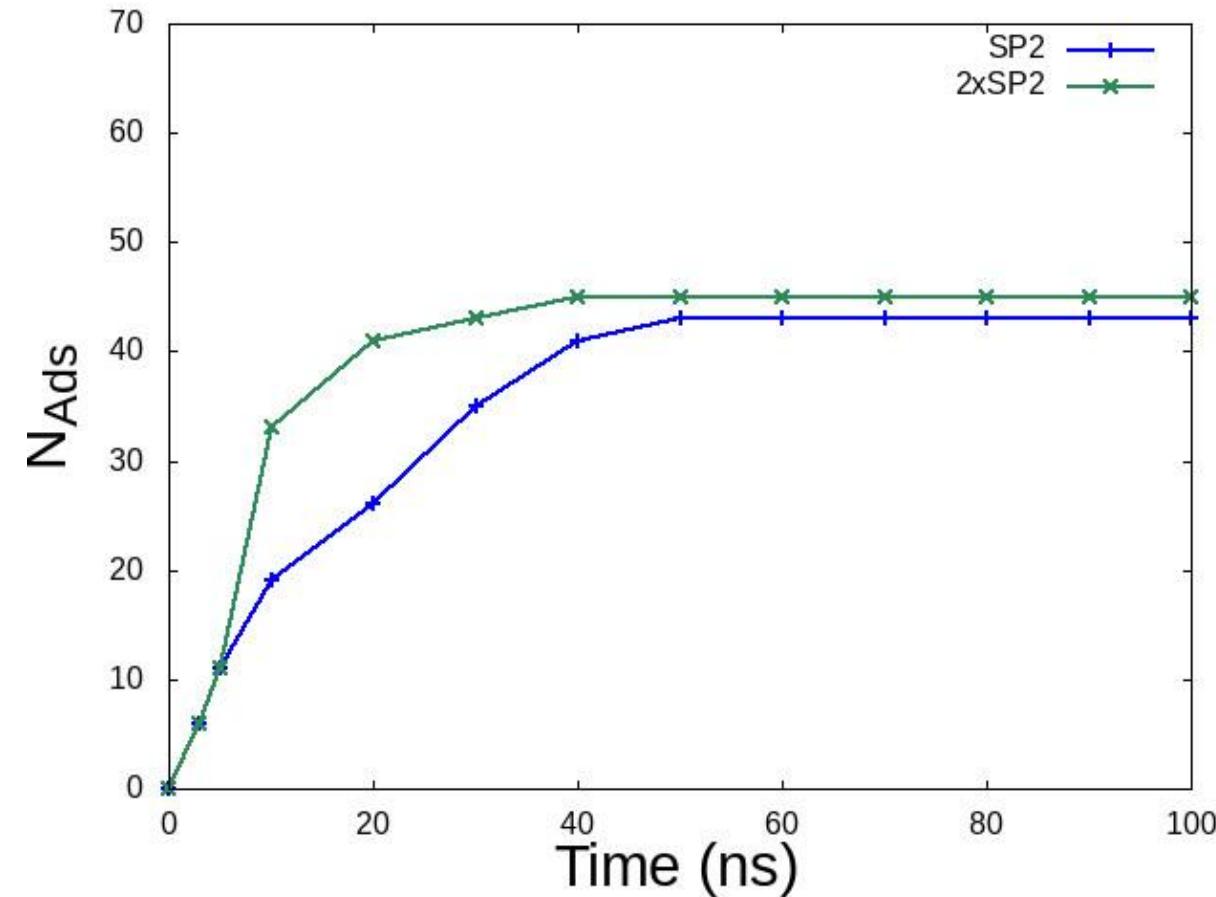


## System size effect

CTAB/SOL: ~ 50/11000



CTAB/SOL: ~ 100/22000



## Results contn..

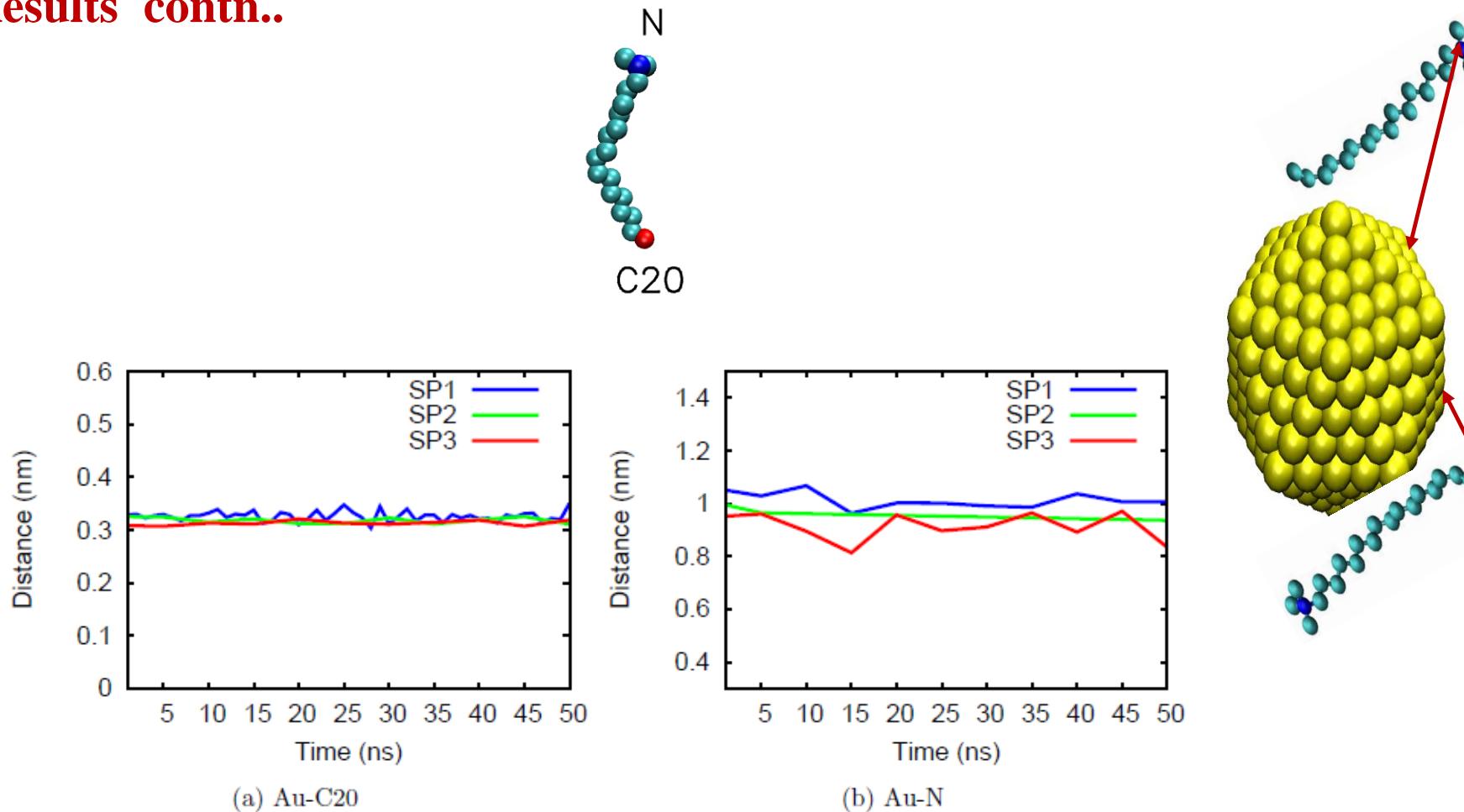
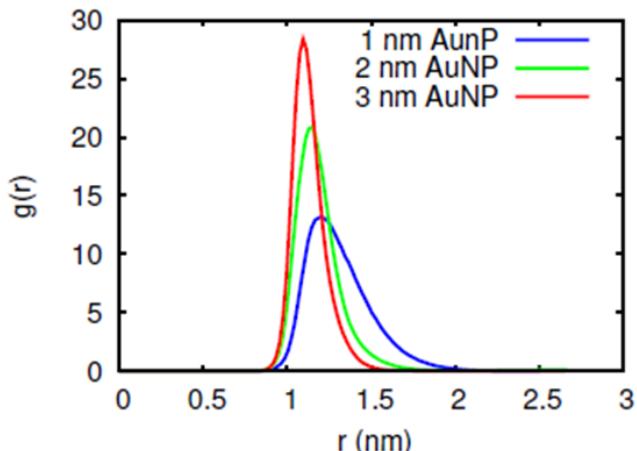
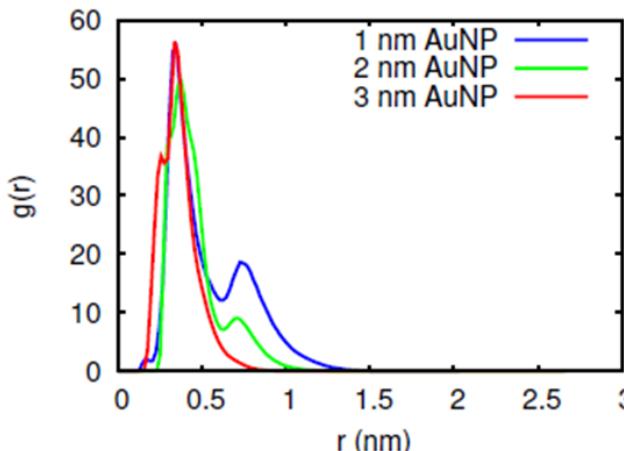


Figure.4: The minimum distance for specific atomic pairs (a. Au-C20 & b. Au-N) in three different sized AuNP. Blue, green and red represent 1, 2 and 3 nm AuNP particles respectively.

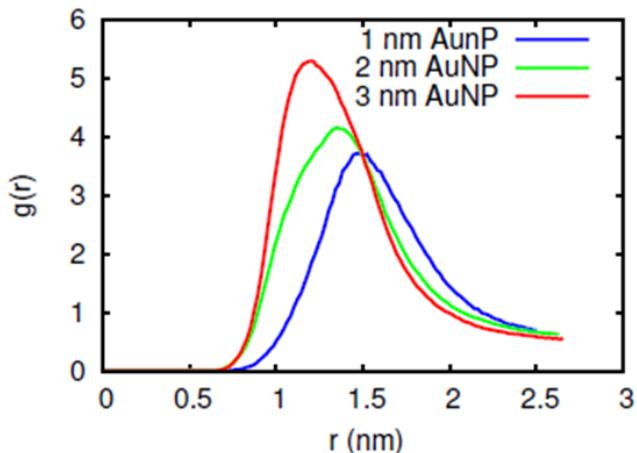
## Results cont...



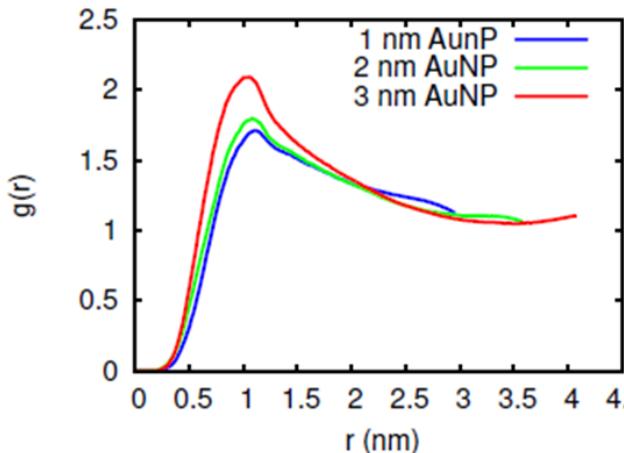
(a) Au-N



(b) Au-C<sub>20</sub>



(c) Au-Br



(d) N-Br

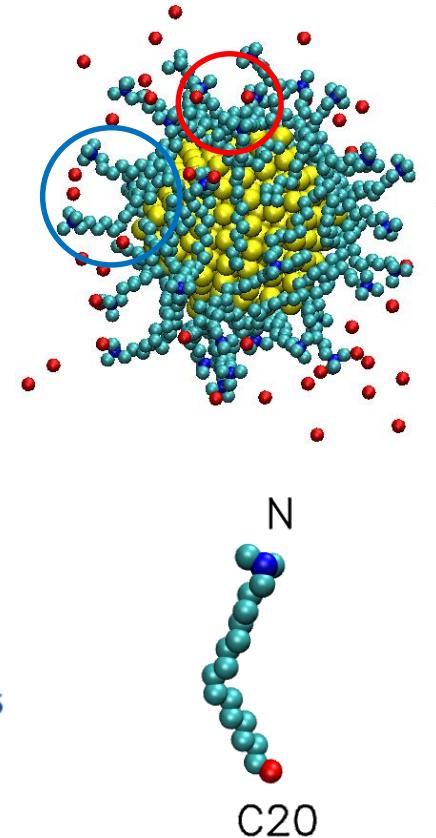


Figure 3(a): The radial distribution functions (RDFs) for specific atomic pairs in three different sized AuNP. Blue, green and red represent 1, 2 and 3 nm AuNP particles respectively.