Notation and details of the systems:

	CALNN-GNPs		CFGAILSS-GNPs		
	GolP-CHARMM		GolP-CHARMM	GolP-CHARMM (different initial conditions)	CHARMM-METAL
	1.8 pep/nm^2	2.5 pep/nm^2	2.5 pep/nm^2	2.5 pep/nm^2	2.5 pep/nm^2
d = 5 nm	-	5-CA	5-CF	-	-
d = 10 nm	10-CA-LCD	10-CA-HCD	10-CF	10-CF-bis	per-10-CF
d = 25 nm	-	25-CA	25-CF	-	-

For each system, GROMACS output files:

- *.gro, *.xtc, *.top for the 10 ns production run

  The name of the system in the *.gro file is sometimes followed by a number that indicates the time point, e.g., 25-CF-2.gro corresponds to the *.gro file at 2 ns for CFGAILSS-capped 25 nm GNP; if such number is not present, the *.gro file refers to the final structure at 10 ns

- *-scount.xvg, *-ss.xpm from DSSP analysis; the numbers used after the name of the system design either the time range, e.g., 5-CA-0-2-ss.xpm is DSSP analysis from 0 to 2 ns for CALNN-capped 5 nm GNP, or the time point, e.g., 5-CA-10-ss.xpm is DSSP analysis at 10 ns for CALNN-capped 5 nm GNP

  Note: 25-CF-bis-0-2* and 25-CF-bis-2-4* have to be considered as 25-CF-6-8* and 25-CF-8-10*, respectively

- *-rdf-AUcom-X.xvg radial distribution functions around the centre of mass of AU set of atoms of either specific peptide atoms, i.e., C, N, O, H, S, N of Cysteine residue (so-called Ncys), or water atoms, i.e., HW1, HW2, OW, or gold, i.e. both AU and AUC atoms, over the 10 ns production run

- *-N-C-bond.xvg distribution of the distance between the peptide N- and C-terminal atoms over the 10 ns production run

Additional output files:

- *.gro_L.dat output of the analysis of the so-called *.gro file with MD-analysis.exe

- *-ss.xpm.dat output of the analysis of the so-called *-ss.xpm file with MD-analysis.exe

- *-_beta_autocorrr_resX.dat only for CFGAILSS systems; time autocorrelation of Beta-structure probability per residue per individual peptide calculated with MD-analysis.exe over 10 ns, e.g., 5-CF-_beta_autocorr_res2.dat corresponds to

the autocorrelation function calculated for residue 2, i.e., F, in CFGAILSS-capped 5 nm GNP

- *-rama.c output of the Ramachandran analysis of a certain *.gro final structure, i.e., at 10 ns
- *-8-10-dssp.c only for CFGAILSS systems; output of the analysis of the secondary structure content per residue over the last 2 ns of the production run

Custom-written MD-analysis.exe & relative instructions:

This code is quite user friendly and when running the software, an interface appears with the instructions to follow in order to create the *.gro_L.dat, *-ss.xpm.dat and *-_beta_autocorrr_resX.dat files from the *.gro and *-ss.xpm files generated with GROMACS.

- Content of *.gro_L.dat:

  xSG, ySG, zSG: coordinates of S atoms

  RSG, phiSG, thetaSG/180-thetaSG: polar coordinates of S atoms

  distSGAu: distance (in nm) of the cysteine sulfur atom to the nearest gold atom (AU or AUC).

  dist1SG-dist5SG: angular distance (in degrees, with respect to the center of the nanoparticle) between the cysteine sulfur atom and the nearest, next nearest etc. (up to 5th) cysteine sulfur atom.

  xcm, ycm, zcm: coordinates of peptides center of mass

  Rcm, phicm, thetacm/180-thetacm: polar coordinates of peptides center of mass

  xbb, ybb, zbb: coordinates of backbones center of mass

  Rbb, phibb, thetabb, 180-thetabb: polar coordinates of backbones center of mass

  dens2, dens5: mass (in amu) of all atoms which are at an angular distance (in degrees, with respect to the center of the nanoparticle) of less than 2/5 degrees from the position of the peptide backbone centre of mass - can be used for calculating the local mass density

  dist1bb-dist5bb: angular distance (in degrees, with respect to the center of the nanoparticle) between the backbone centre of mass and the nearest, next nearest etc. (up to 5th) backbone center of mass

  phi and psi: backbones torsional angles (starting from the cysteine N-terminal)

- Content of *-ss.xpm.dat:

  Percentages of secondary structure motifs per peptide chain

sheet1/bridge1-sheet7/bridge7 (or sheet4/bridge4): percentages of sheet and bridge secondary structure motifs per residue per individual peptide, where Cys is number 1

- Content of *-_beta_autocorrr_resX.dat: time autocorrelation of Beta-structure probability per residue per individual peptide

Custom-written scripts for analyses in GROMACS & relative instructions:

- **DSSP_per_residue.c** calculates the secondary structure content per residue (based on DSSP assignment)

  1. gcc –o cre –g DSSP_per_residue.c
  2. ./cre *-ss.xpm *.c

     Where *-ss.xpm is the file created by DSSP to be analysed and *.c is the desired name for the output file
  3. Enter the number of frames present in *-ss.xpm file
  4. Enter the number of residues in the peptide chain

- **Distance_between_atoms.sh** calculates the distribution of the distance between two desired atoms

  1. vi the file and change the numbers accordingly to the system to be analysed:

  n_gold=total number of gold molecules
  gold=number of atoms in each gold molecule, i.e., 2
  n_peptide=total number of peptide chains
  peptide=number of atoms in each peptide chain

  a0=the atom ID of the first atom to be considered accordingly to topol.top
  b0= the atom ID of the second atom to be considered accordingly to topol.top

  2. ./cre_index.sh and a new index_bond.ndx file is produced
  3. Use g_bond GROMACS command with the created index_bond.ndx file to analyse the distance and obtain the average distance over the simulation time and the distribution of the distance

- **Ramachandran_plots.c** calculates the Ramachandran plots per occupancy

  1. vi the file, at line #30 the higher number has to be higher than the number of peptide chains to be considered and the smaller number is the number of residues in the peptide chain, i.e., 5 for CALNN and 8 for CFGAILSS
  2. gcc –o cre –g Ramachandran_plots.c -lm

3. ./cre *.gro_L.dat *.c

   Where *.gro_L.dat is the file created by MD-analysis.exe for the so-called *.gro file and *.c is the desired name for the output file

4. Enter two bin widths, one for x and one for y

5. Enter the width for the Gaussian distribution and the cut-off

6. Enter the number of peptide chains and the number of residues per chain