Using FORTRAN and GROMACS in Biomaterial Research: Pair Distribution of VECAR

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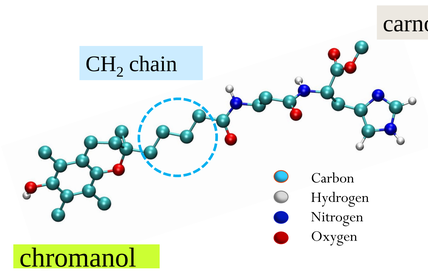
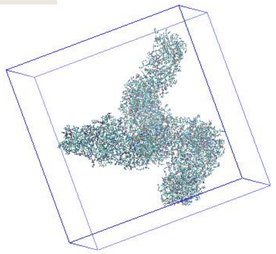
VECAR Molecules

VECAR are bolaamphilic bio-molecules that consists of chromanol and carnosine head groups linked together by a hydrocarbon chain of varying length. When immersed in an aqueous solution, these molecules self-assemble to form nanostructures.



VECAR[VC-C4] Chemical Structure $C_{28}H_{40}N_4O_6$



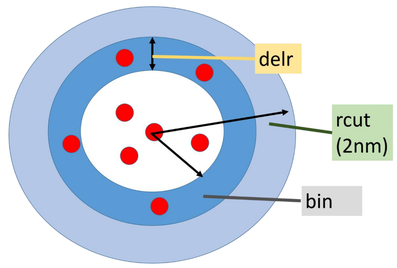
Final configuration of 500 VC-C4

VC-C4 is a VECAR with a hydrocarbon chain length of four. We used this molecule to analyze its pair distribution function (PDF).

FORTRAN

(FORmula TRANslation)

FORTRAN is a programming language generally used in scientific computing, which translates formulae into computer code. Fortran is free and compatible in any operating system. FORTRAN 77/90, GROMACS(v4.6) and VMD(v1.9.2) were used to analyze the pair distribution function of the VECAR[VC-C4].



The figure illustrates the distance from the center to a bin. The bin radius is increased by 'delr' each time and up to the max bin size (rcut).

PDF Calculation using GROMACS

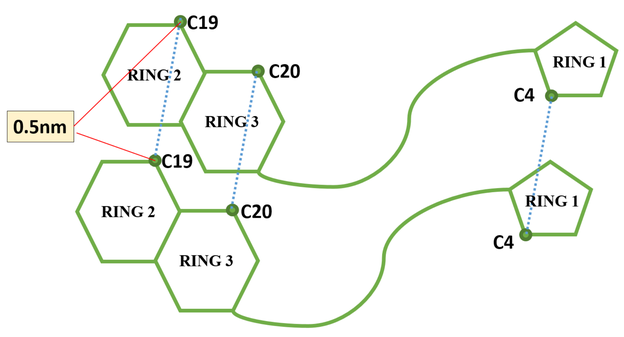
(GROningen Machine for Chemical Simulations)

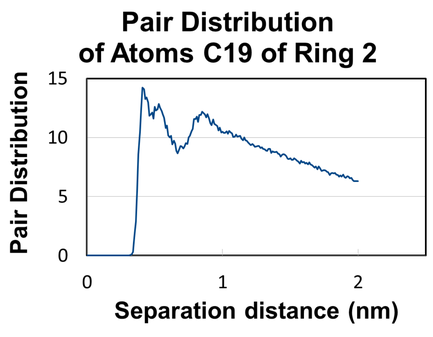
GROMACS is a molecular dynamics (MD) simulation tool used in performing MD simulation, energy minimization and data analysis. It runs using the Unix shell and is given arguments directly on the shell. It is generally regarded as one of the fastest molecular dynamic simulators in the field.

We used one function of Gromacs, g_rdf, which can calculate the pair distribution function (PDF) between atoms. One atom from each ring was selected from all the molecules in the trajectory file of VC-C4 system. The PDF is averaged over time in duration of 44 ns.

Command: $ g_rdf –f newtraj_1to21.xtc –o rdf.xvg –n index_ring-newvon500.ndx –s tpxout.tpr –b num1 –e num2 –dt num3 –bin 0.01 –rdf atom –pbc

The PDF of C19 atoms in Ring 2 shows that the nearest neighbor separation of two rings is about 0.5nm.





Flow Chart of PDF Calculation using FORTRAN

Center of Geometry (COG)

The centers of geometry of each type of rings were calculated first. These COG's will be used in the calculation of PDF of pairs of COG's.

```
          do j = 29, 32
           read(10,200)nmol,molname,atmname,number,x,y,z
            X2 = X2 + x
            Y2 = Y2 + y
            Z2 = Z2 + z
          enddo
          do j = 33,34
           read(10,200)nmol,molname,atmname,number,x,y,z
          enddo
          do j = 35,38
           read(10,200)nmol,molname,atmname,number,x,y,z
            X3 = X3 + x
            Y3 = Y3 + y
            Z3 = Z3 + z
          enddo
          do j = 39,44
           read(10,200)nmol,molname,atmname,number,x,y,z
          enddo
c   ---------- calculate center of geometry for three rings---
           Xcg1(I) = X1/5.d0;Ycg1(I)=Y1/5.d0;Zcg1=Z1/5.d0
           Xcg2(I) = X2/6.d0;Ycg2(I)=Y2/6.d0;Zcg2=Z2/6.d0
           Xcg3(I) = X3/6.d0;Ycg3(I)=Y3/6.d0;Zcg3=Z3/6.d0
        enddo
        read(10,111)boxx,boxy,boxz
```

Pair Distribution Function (PDF)

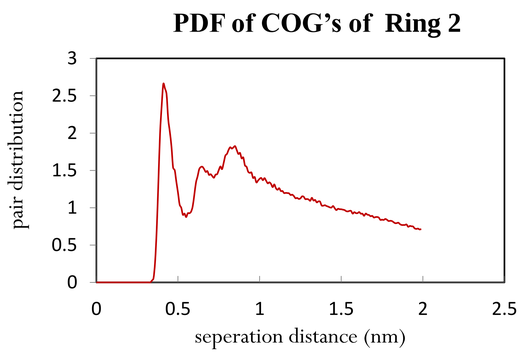
In calculation of PDF, we first count the number of atoms within a small volume, called a bin, at a separation (r) from a given atom. So, in a graph of PDF,

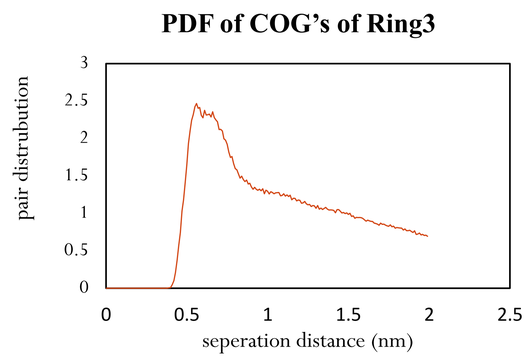
one would be able to see how the amount of pairs in a system varies as function of the separation r.

```
c------------------pdf of RING II - RING II ----------------

      do I = 1,mbn !(mbn - maxbin size = 200)
       graph2(I) = 0.d0
      enddo

      count2 = 0
      do i = 1,(nm-1) !nm - number of molecules = 500
       do j =(i+1),nm
        delx2 = Xcg2(i) - Xcg2(j)
        dely2 =Ycg2(i) -Ycg2(j)
        delz2 = Zcg2(i) - Zcg2(j)

       dist22 = dsqrt(delx2*delx2 + dely2*dely2 + delz2*delz2)
       bin = int(dist22/delg) + 1

       if (bin .le. mbn) then
         graph2(bin) = graph2(bin) + 1
         count2 = count2 + 1
       end if
      enddo
      enddo
```

Normalization of PDF the total number of pairs with separation r that lie within a bin with (rbin < r < rbin+delr) should be divided by the volume of the bin.

```
c  -----------Normalization----------------------------------
      do ibin1 = 1,mbn !(mbn = maxbin size = 200)
       min = real(ibin1-1)*delg
       max = min + delg
       nideal = const*(max**3 - min**3)
       gr2(ibin1) = real(graph2(ibin1))/nideal*real(tvol/count2)
      enddo

      do ibin1 = 1,mbn
        timehist2(ibin1) = timehist2(ibin1) + gr2(ibin1)
      enddo
```





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