Getting Started with Carnal

This represents a very basic overview of getting started with Carnal. For more detailed instructions refer to the Amber 7 manual pgs. 214 – 232

Carnal is a useful program for analyzing and comparing multiple structures, say for example the hundreds or thousands of structures generated from a simulated annealing calculation or dynamics run. The program needs an imput file divided into four sections, listed in bold in the example file below.

```
FILES_IN
        PARM p1 prm.top;
        STREAM s1
min.1.crd
min.2.crd
min.3.crd
min.4.crd
min.5.crd
min.6.crd
min.7.crd
min.8.crd
min.9.crd;

FILES_OUT
        TABLE tab1 carnal.out;
DECLARE
      DIST dist1 1 2;
      ANGLE ang1 1 2 3;
      TORSION dihed1 1 2 3 4;
OUTPUT
     TABLE tab1 MEAS;
END
```

There must be a semicolon (;) at the end of each line!!

To run carnal

Step 1: Copy the text above to a file and name it carnal.in

Step 2: Replace the list of file names min.1.crd – min.9.crd with the names of the files you want to analyze. You may find the following script helpful to make a list of file names for you. The script will generate a file with 1000 lines, dyn.1.crd – dyn.1000.crd. Modify accordingly to suit your needs.

```
#!/bin/csh
   set i = 1
   while ($i <= 1000)
    echo  dyn.$i.crd >> total.crd
   @ i++
end
```

Step 3: Specify what you want to measure. The example above measures 3 things, the distance between atoms 1 and 2, the angle between atoms 1, 2 & 3, and the dihedral angle between atoms 1, 2, 3 & 4.

Step 4: Run the program using your input file by typing the following at the command line prompt:

[prompt]$ `carnal < carnal.in > carnal.log`

Step 5: Check carnal.log to make sure everything ran as expected. Your specified measurements will be found in the file named carnal.out. (The program won't run if there is already a file named carnal.out in the working directory.) The results are presented in columns in the order they were specified. In the example above, carnal.out would contain the distance in column 1, the angle column 2, and the dihedral angles in column 3.

RMS Analysis with Carnal

This is a bit trickier, refer to the manual for more options.

To perform an RMS analysis on a set of coordinates, you must first use `GROUP` to specify which atoms to use in the fit, then use the keyword `RMS` in the `DECLARE` section of your input file.

```
GROUP grp1 (RES 1,2);
RMS rmsid FIT grp1;
```

In the above example I have made a group called grp1, which consists of all atoms within residues 1 and 2. You can also specify atom numbers or residue names. If these statements are in the `DECLARE` section of the input file above, the program will use the first set of coordinates listed in the `FILES_IN` section as the reference coordinates and perform a best fit of every other set of coordinates based on the atoms in residues 1 and 2. The RMS values for the fits will be output in the table. See the Amber manual if you want to use a different set of reference coordinates, like perhaps the average coordinates.