# MATH 728A, BIOMOLECULAR GEOMETRY, HOMEWORK #14

**Problem 1 (Transformations between peptide unit poses).** Compute $M(\mathbf{b}, A)$ such that $\text{pose}(C_i^\alpha, C_i', N_{i+1}) = \text{pose}(C_{i-1}^\alpha, C_{i-1}', N_i)M(\mathbf{b}, A)$. You may leave $A$ in the form of a product of rotation matrices. Give a geometric interpretation of the vector $\mathbf{b}$. Do not make any simplifying assumptions concerning bond lengths, bond angles, or wedge angles.

**Problem 2 (Peptide helix parameters).** Assume an ideal peptide unit (i.e. $\omega = \pi$, $l(\{C_{i-1}^\alpha, C_{i-1}'\}) = l(\{N_i, C_i^\alpha\}) = l$, $120°$ angles at $C_{i-1}'$ and $N_i$, and $109.47°$ angle at $C_i^\alpha$) and compute $(e^{i\theta}, \mathbf{u})$ such that $A = R(e^{i\theta}, \mathbf{u})$, where $A$ is the rotation matrix from problem 1. (*Hint:* Use quaternions.) Express your answer in terms of the angles $\phi_i + \psi_i$ and $\phi_i - \psi_i$. The angle $\theta$ is called the *twist angle* of the helix. Evaluate $(e^{i\theta}, \mathbf{u})$ in the example of the ideal $\beta$ sheet: $\phi = -\psi = -144.7° = -\cos^{-1}(-\sqrt{2/3})$. Compute a vector $\mathbf{r}$ from $C_{i-1}'$ to the nearest point on the axis of the helix for this example, the radius $\|\mathbf{r}\|$ of the helix, and the *rise* $|\mathbf{b} \cdot \mathbf{u}|$. Draw a diagram illustrating these quantities in this example.

**Problem 3 ($3_{10}$ helix).** Consider a chain of three ideal peptide units spanning residues numbered 1 through 4. Assume $\phi_2 = \phi_3 = \phi$ and $\psi_2 = \psi_3 = \psi$ are the unknown independent variables. Write down two equations in the two unknowns expressing the geometric relation that the three atoms $O_1$, $N_4$, and $HN_4$ are collinear. Solve these two equations (numerically if necessary) for $\phi$ and $\psi$. For this particular (idealized) $3_{10}$ helix compute the $\{O_1, HN_4\}$ hydrogen bond length, the helix axis vector $\mathbf{u}$, the twist angle, the rise, and the helix radius (as in problem 2). Make a Z-system of your $3_{10}$ helix in IMIMOL and print out a labelled stereo picture of it using RASMOL.

**Problem 4 (Endocyclic torsion angles for the chair conformation).** Consider an ideal chair conformation of an equilateral hexagon with equal endocyclic bond angles of $109.47°$. Recall that from our discussion in class this conformation had $\phi = -\phi' = 60°$ and $\psi = 180°$. Compute all the other endocyclic torsion angles for this conformation.