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Hi Dr. Martin,

I am an undergraduate student at the University of North Carolina Wilmington majoring in Chemistry. I read your paper on predicting the refractive index of crystallin proteins based on the structure and composition of the protein. I have been trying to implement your methods, but I am struggling to replicate a few aspects of your algorithm and I wanted to see if I properly understood your methods.

I was able to write a python script to predict the RI of the protein based on just the sequence, but I am struggling to get the same results when implementing the correction factor. I have a few questions on this:

1. Did you add the correction factor to the original prediction, or did you multiply it. I am pretty sure you added the correction factor, but I just wanted to make sure.
2. Are tryptophan, phenylalanine, tyrosine, histidine, and arginine the only polar residues for which you implemented the pi-pair correction factor?
3. Is the way I calculated the polar residues’ centroids correct? I calculated the centroid of each polarizable amino acid as follows:
   1. Find the average x, y, and z coordinates of each heavy atom in the side chain (past the beta carbon) and define that as the center
   2. Find the average distance of those side chain atoms from the center and define that as the radius

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1. Did I properly measure the distance between the centroids? I then measured the distance between two centroids by finding the distance between centroid i’s and centroid j’s centers and then subtracting the sum of their radii from that distance. If that final distance was less than the cutoff that you defined, I applied the correction factor and added it to the total correction factor

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1. Was the distance in the correction factor equation measured in Angstroms?

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1. Is their a physical explanation for why the delta parameter for pi-pi interactions is positive, while cation-pi interactions is negative?