Electronic Supplementary Information

Self-Assembly of Aromatic Amino Acids: A Molecular Dynamics Study

Sahin Uyaver,[a] Helen W. Hernandez, [b] and M. Gokhan Habiboglu[a]

[a] *Turkish-German University, Istanbul 34830*
[b] *KAL Research Initiatives, LLC, Houston Texas 77042 United States*

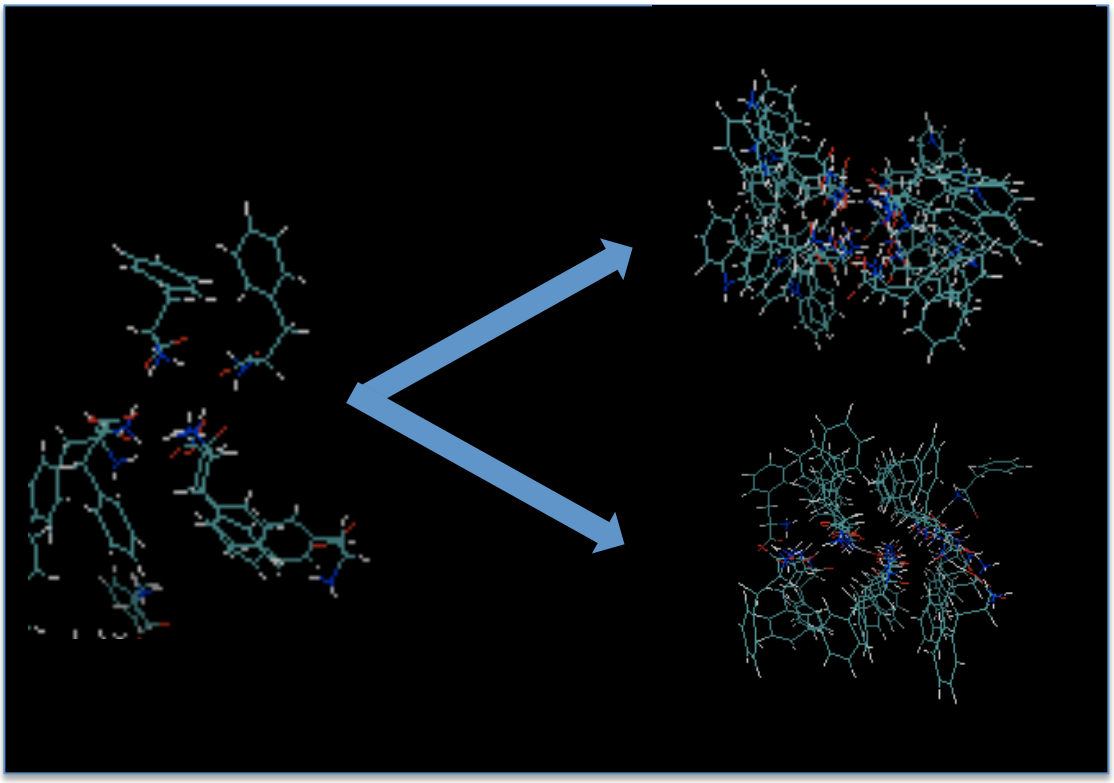

Figure S1. Point of divergence observed between four-fold tube and zigzag structure.

In figure S1 a nucleation site is shown that, in the case of the actual simulation, formed a four-fold structure, but appears that it could readily have formed either structure.

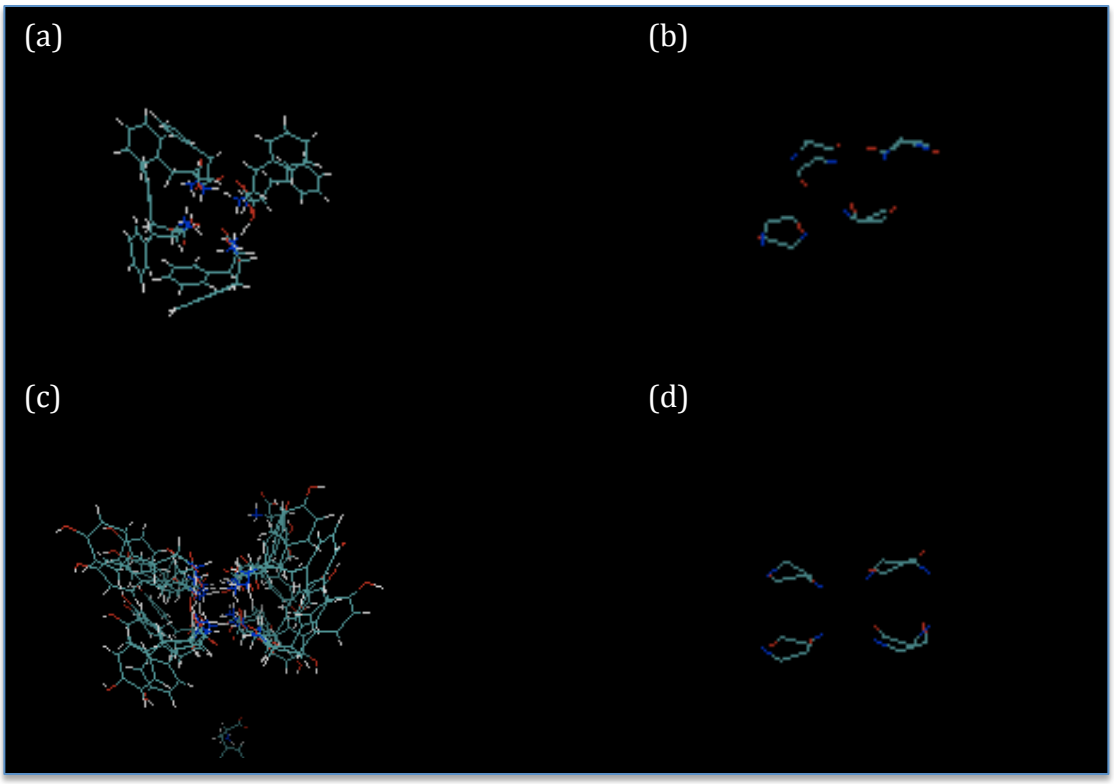

Figure S2. (a) Top view of a four-fold tube with parallel strand orientation (b) side view of the four-fold tube with parallel strand orientation with side chains hidden for clarity. (c) Top view of a four-fold tube with anti-parallel strand orientation (d) side view of the four-fold tube with anti-parallel strand orientation with side chains hidden for clarity.

In figure S2 we observe from the top, seemingly identical four-fold structures. However, the side view reveals a difference in what happens when the vertical strands of the tubes are oriented differently. The four-fold tube shown in (c) and (d), has alternating strand orientation where the C-N directionality is opposite from one strand to its neighboring strand. We describe this as anti-parallel strand orientation and it results in distinct layers along the tube, shown in (d). For the four-fold structure observed in (a) and (b), neighboring strands contain the same vertical C-N directionality which demands a shift in the layers to reduce the repulsion of similarly charged groups.

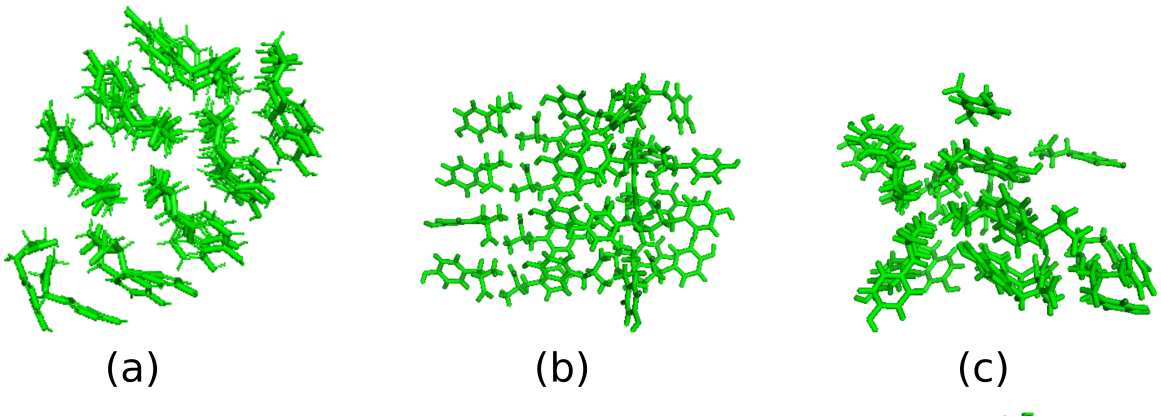

Figure S3. Repeat trajectories of tyrosine at 325K.

In Figure S3 we show the results of three separate trajectories of the same simulation conditions. Trajectory (a) displays a very ordered zig-zag structure. Trajectory (b) shows the side view of a well-formed four-fold structure with additional strands interacting to the side. Trajectory (c) shows and another instance for which there is a four-fold structure (left) with additional strands interacting to the side (bottom right). This shows us that we consistently produce "ordered" structures but are careful not to overstate when one form (zig-zag or four-fold) dominates as we do not see tremendous consistency in trajectories which is explained by the nucleation site in Figure S1.

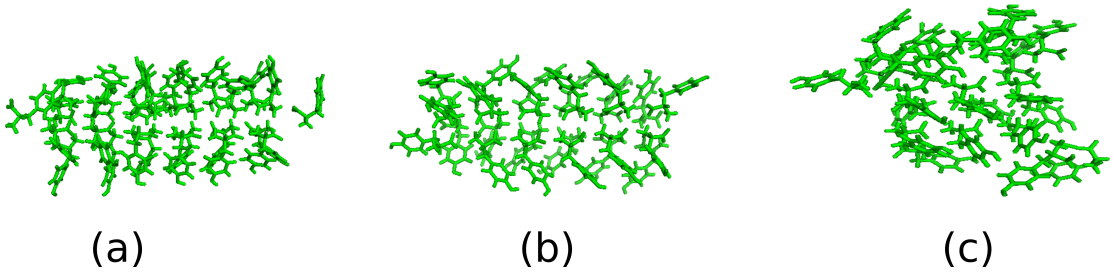

Figure S4. Repeat trajectories of tyrosine at 350K.

In Figure S4 we show the results of three separate trajectories performed under the same conditions. In trajectories (a) and (b) we observe the very well-ordered tube with four-fold symmetry. Trajectory (c) could perhaps best be described as a deformed zig-zag structure. It is clear that strong ordering is present in all cases.

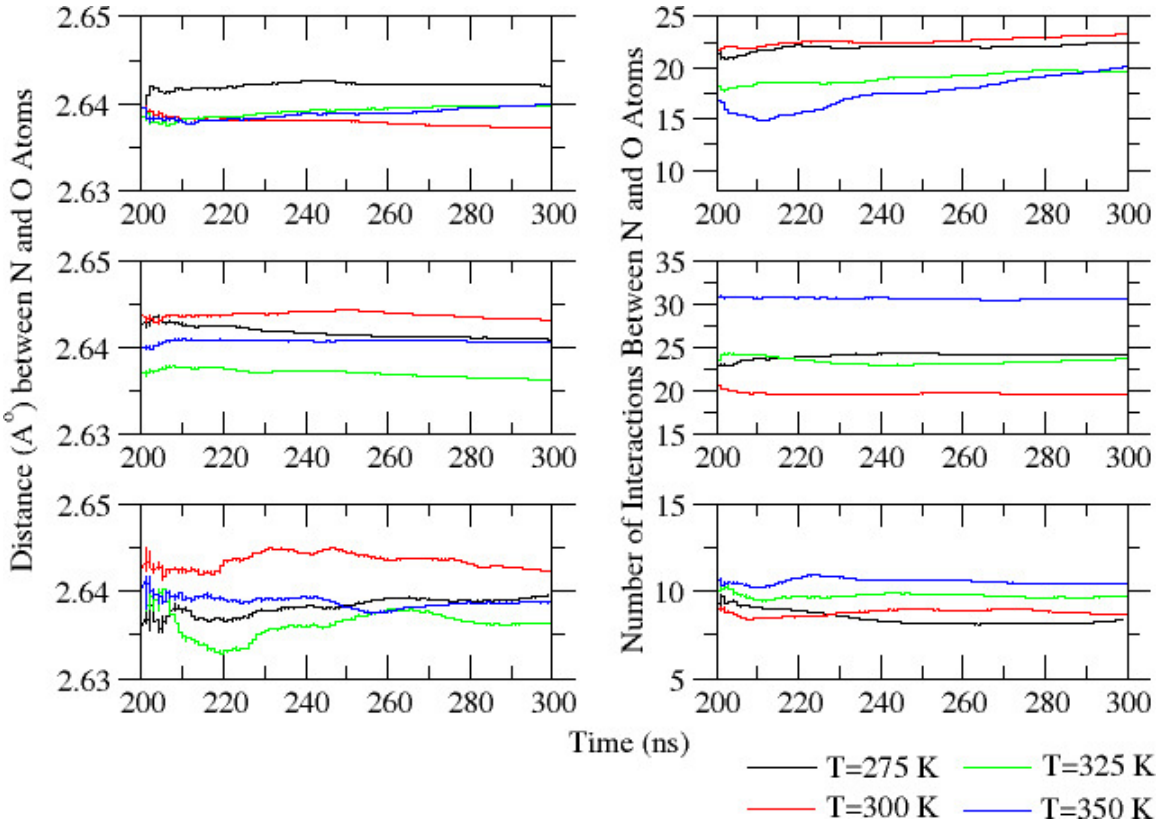

Figure S5. Electrostatic interactions over the last 100ns of phenylalanine (Top), tyrosine (Middle), and tryptophan (Bottom) assembly. The distance between N and O atoms of nearby monomers (Left) and corresponding numbers of interactions between N and O atoms (Right).

The distances between N and O atoms were calculated for each simulation above and used to understand better understand the role of electrostatics. Interestingly, tryptophan seems to have less electrostatic interaction compared to the other two aromatic amino acids. This is likely due to the more dominant role of its larger hydrophobic ring.