Supporting Information:

Impacts of Fullerene Derivatives to Regulate the Structure and Assembly of Collagen Molecules

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Residue Contact Map of Four-Triplex Bundle

The residue contact map of collagen triplexes is also computed based on the last 30-ns trajectory (shown in Figure S1). The residues are considered to be contacted if the smallest distance between heavy atoms of two residues is below 4 Å. If the collagen triplexes are parallel to each other, the residue contacts are formed by the residues in the corresponding positions along the triplex, i.e. similar residue index. Thus the contacted residue pairs should distribute around the diagonal of contact map, shown as green line. The residue contact map of the triplex with other triplexes is calculated and the representative contact map of triplex A is shown. Similar trend can be observed in other three triplexes. In Tetramer-0 system, contacted residue pairs widely distribute in the off-diagonal region especially for the *Nter-region* of collagen triplex. For example, the second residue can contact with the eleventh residues of other triplexes. That might largely result from the relative rotation of triplex and the impact of thermal fluctuation in the terminal region. While in Tetramer-Gd system, the contacted residue pairs localize around the diagonal. The residues in the terminal regions still efficiently contact with the corresponding residues of the adjacent triplexes. The similar tendency is also observed in system Tetramer-C60. However, the contacted residue pairs are not as centralized as in system Tetramer-Gd.

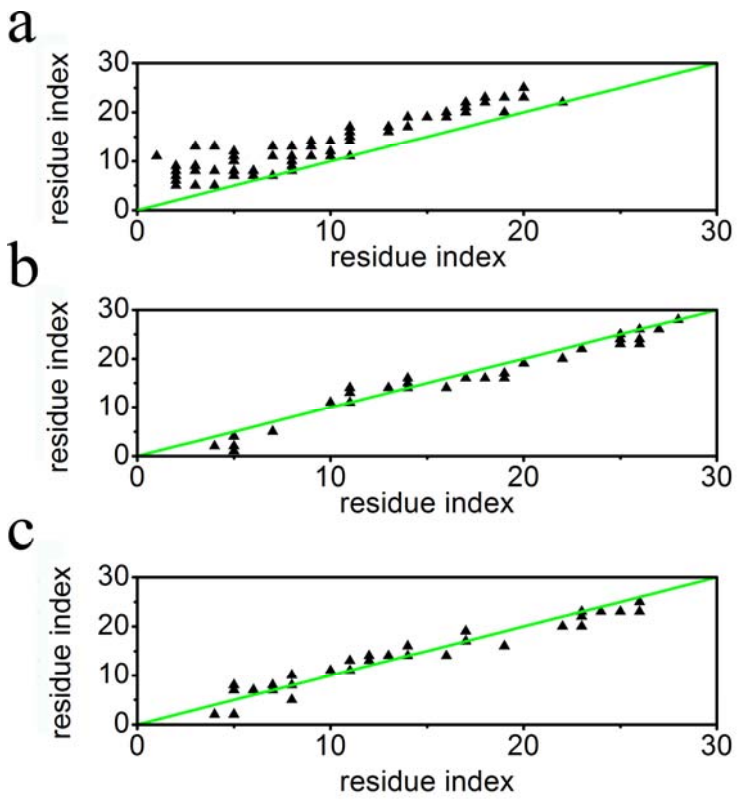

Figure S1. Residue contact map of the representative triplex in system Tetramer-0 (a), Tetramer-Gd (b) and Tetramer-C60 (c). The residue index of the representative triplex is along x-axis, and the residue index of the other three triplexes is along y-axis. In systems Tetramer-Gd and Tetramer-C60, the collagen triplexes are parallel to each other and the contacted residue pairs locate around the diagonal. While the contacted residue pairs are largely distributed in the off-diagonal region in system Tetramer-0.