# Simulation study of non-covalent hybridization of carbon nanotubes by single-stranded DNA in water

*Willis Martin, Wusheng Zhu and Goran Krilov*
*Department of Chemistry, Boston College, 2609 Beacon Street, Chestnut Hill, MA 02467*

## SUPPLEMENTARY INFORMATION

Movie 1. Animation of the 5000 ps constant NVT simulation trajectory showing the dynamics of association of the d(G) DNA oligonucleotide (red) with the (15,2) CNT (gray). Water and counterions have been omitted for clarity, DNA backbone is depicted in ribbon form, and ribose and bases are shown as sticks with hydrogen atoms suppressed.

Movie 2. Animation of the 5000 ps constant NVT simulation trajectory showing the dynamics of association of the d(T) DNA oligonucleotide (yellow) with the (15,2) CNT (gray). Water and counterions have been omitted for clarity, DNA backbone is depicted in ribbon form, and ribose and bases are shown as sticks with hydrogen atoms suppressed.

Movie 3. Animation of the 5000 ps constant NVT simulation trajectory showing the dynamics of association of the d(TG) DNA oligonucleotide (green) with the (15,2) CNT (gray). Water and counterions have been omitted for clarity, DNA backbone is depicted in ribbon form, and ribose and bases are shown as sticks with hydrogen atoms suppressed.

Movie 4. Animation of the 5000 ps constant NVT simulation trajectory showing the dynamics of association of the d(G) DNA oligonucleotide (red) with the (6,5) CNT (gray). Water and counterions have been omitted for clarity, DNA backbone is depicted in ribbon form, and ribose and bases are shown as sticks with hydrogen atoms suppressed.

Movie 5. Animation of the 5000 ps constant NVT simulation trajectory showing the dynamics of association of the d(T) DNA oligonucleotide (yellow) with the (6,5) CNT (gray). Water and counterions have been omitted for clarity, DNA backbone is depicted in ribbon form, and ribose and bases are shown as sticks with hydrogen atoms suppressed.

Movie 6. Animation of the 5000 ps constant NVT simulation trajectory showing the dynamics of association of the d(TG) DNA oligonucleotide (green) with the (6,5) CNT (gray). Water and counterions have been omitted for clarity, DNA backbone is depicted in ribbon form, and ribose and bases are shown as sticks with hydrogen atoms suppressed.

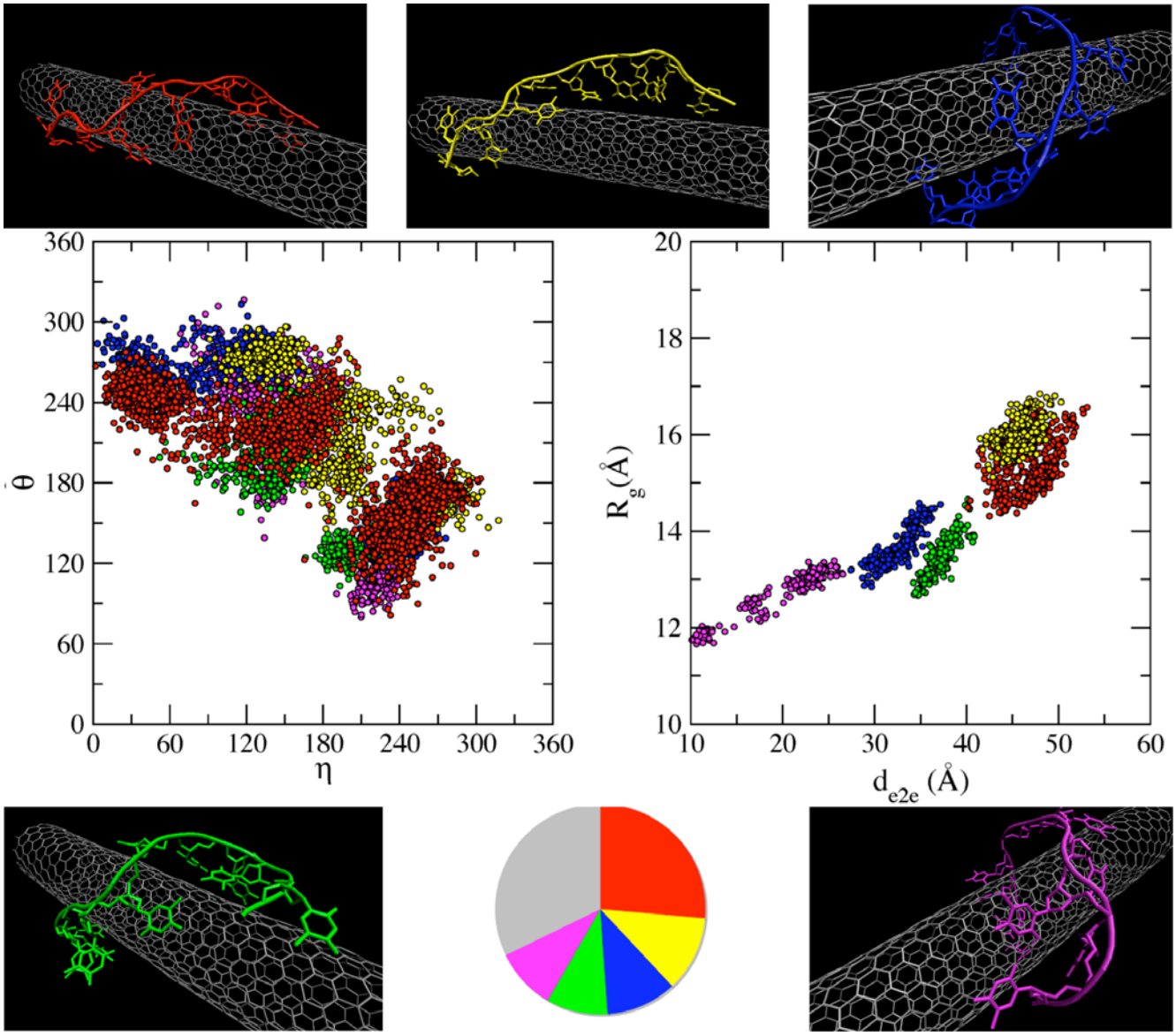


Figure S1. (η,θ) (left) and ($d_{e2e}$,$R_g$) (right) distribution maps for the conformation clusters belonging to five most populated binding modes of the (15,2)-d(T) complex. The clusters are color coded from the largest (red), followed by yellow, blue, green, to the smallest (magenta). The color-coded representative structure from each binding mode are shown. The pie chart shows the population of each binding mode as a fraction of the total sampled conformations.

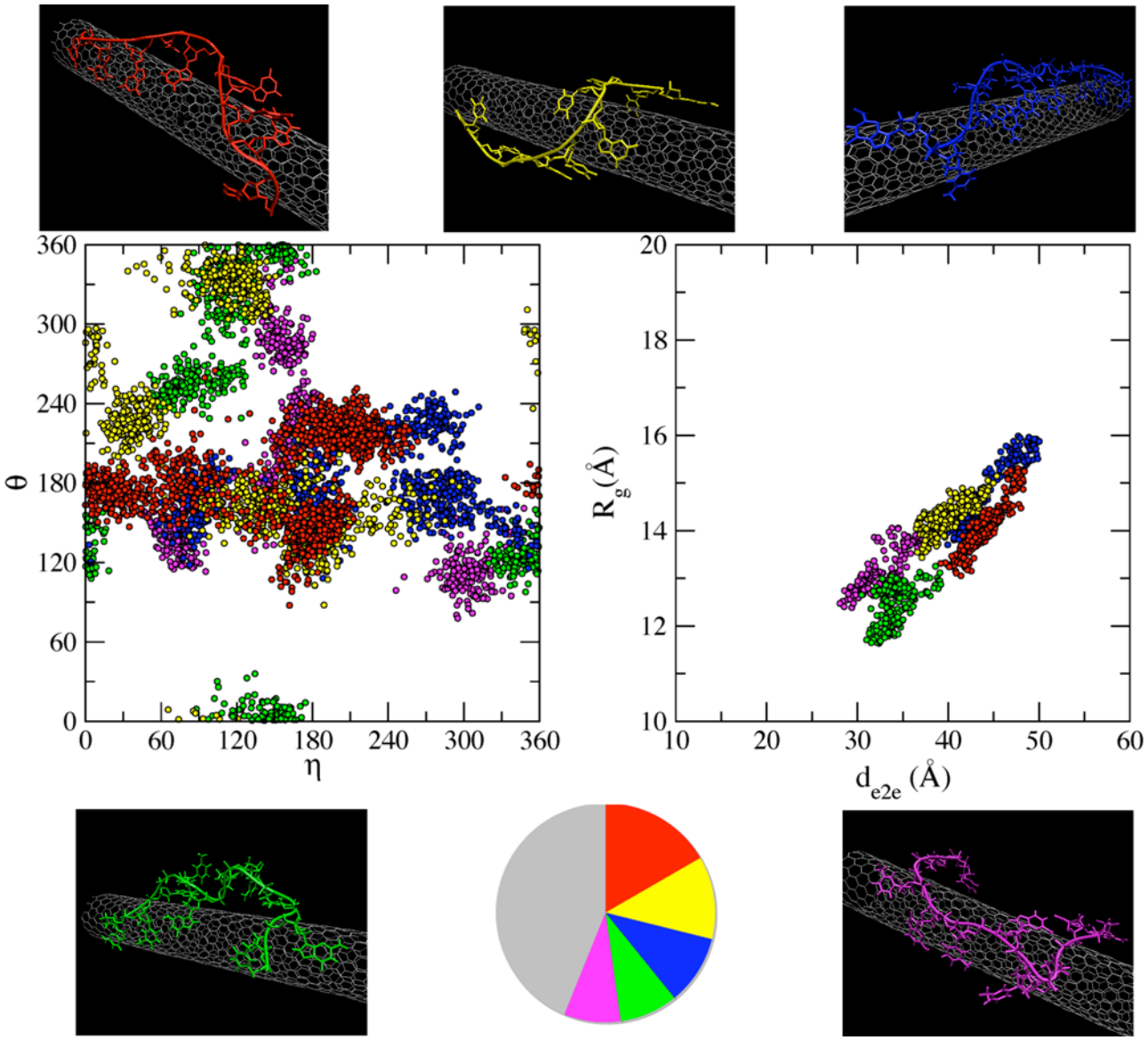


Figure S2. (η,θ) (left) and ($d_{e2e}$,$R_g$) (right) distribution maps for the conformation clusters belonging to five most populated binding modes of the (15,2)-d(TG) complex. The clusters are color coded from the largest (red), followed by yellow, blue, green, to the smallest (magenta). The color-coded representative structure from each binding mode are shown. The pie chart shows the population of each binding mode as a fraction of the total sampled conformations.

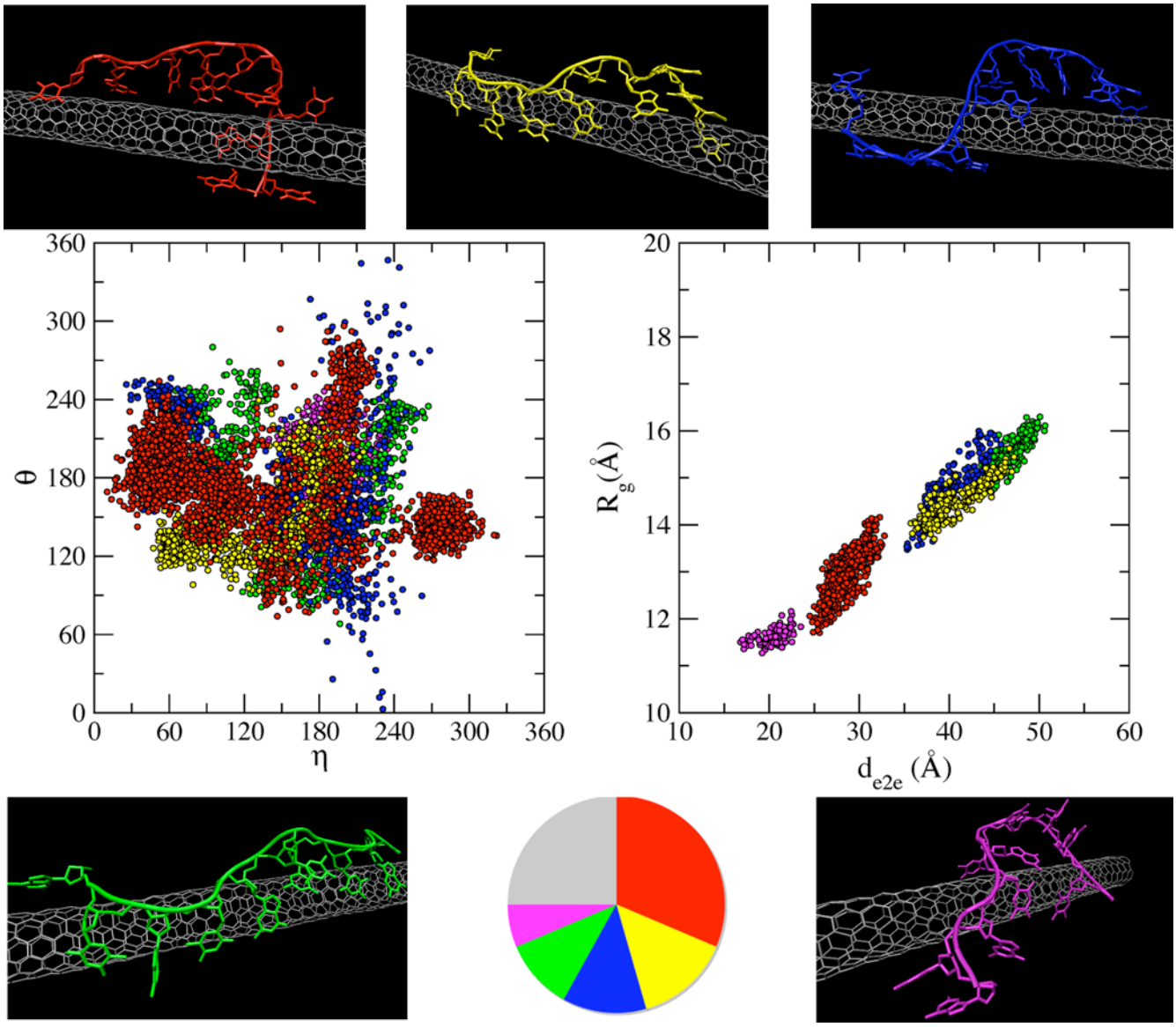


Figure S3. (η,θ) (left) and ($d_{e2e}$,$R_g$) (right) distribution maps for the conformation clusters belonging to five most populated binding modes of the (6,5)-d(G) complex. The clusters are color coded from the largest (red), followed by yellow, blue, green, to the smallest (magenta). The color-coded representative structure from each binding mode are shown. The pie chart shows the population of each binding mode as a fraction of the total sampled conformations.

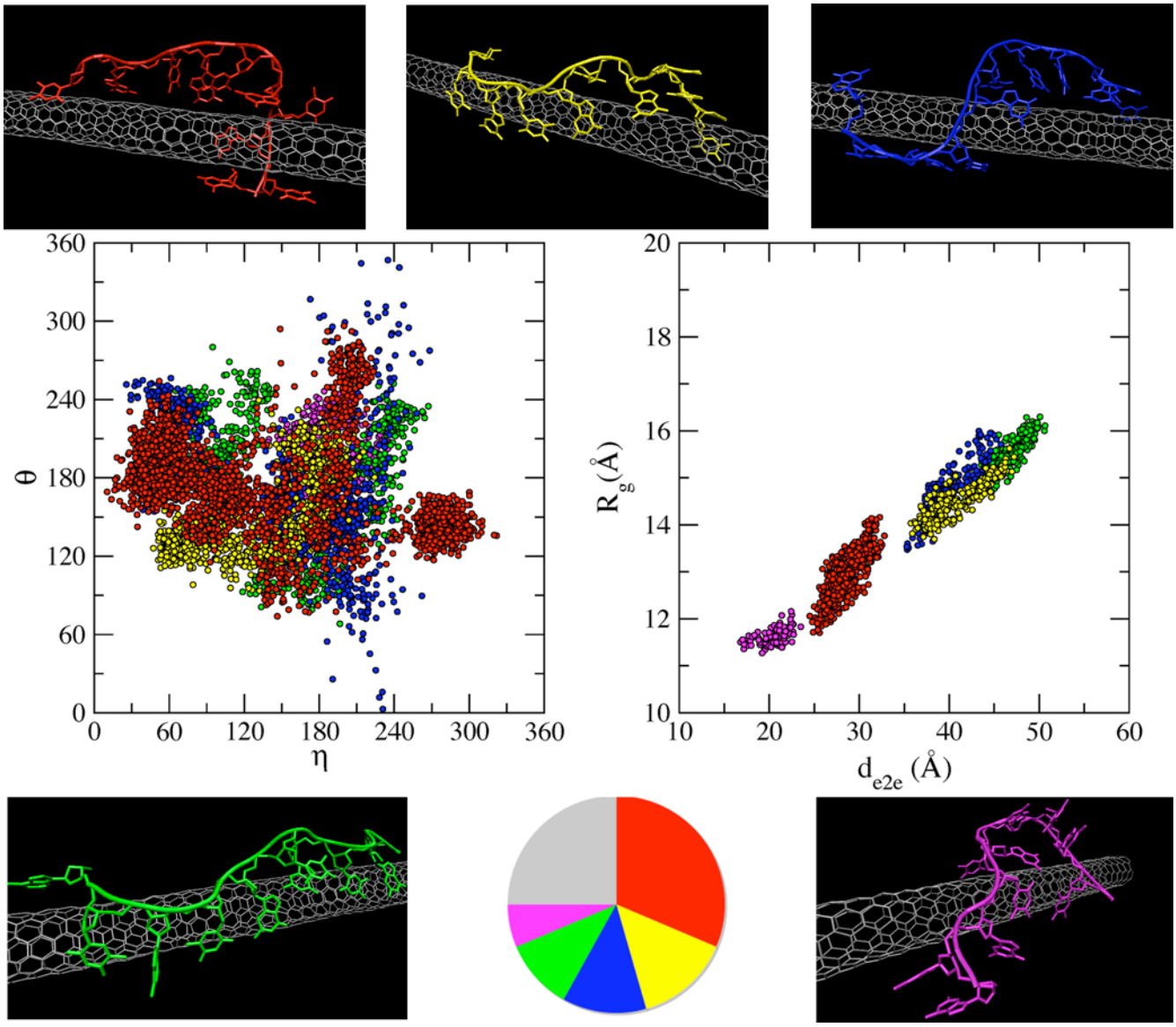


Figure S4. (η,θ) (left) and ($d_{e2e}$,$R_g$) (right) distribution maps for the conformation clusters belonging to five most populated binding modes of the (6,5)-d(TG) complex. The clusters are color coded from the largest (red), followed by yellow, blue, green, to the smallest (magenta). The color-coded representative structure from each binding mode are shown. The pie chart shows the population of each binding mode as a fraction of the total sampled conformations.

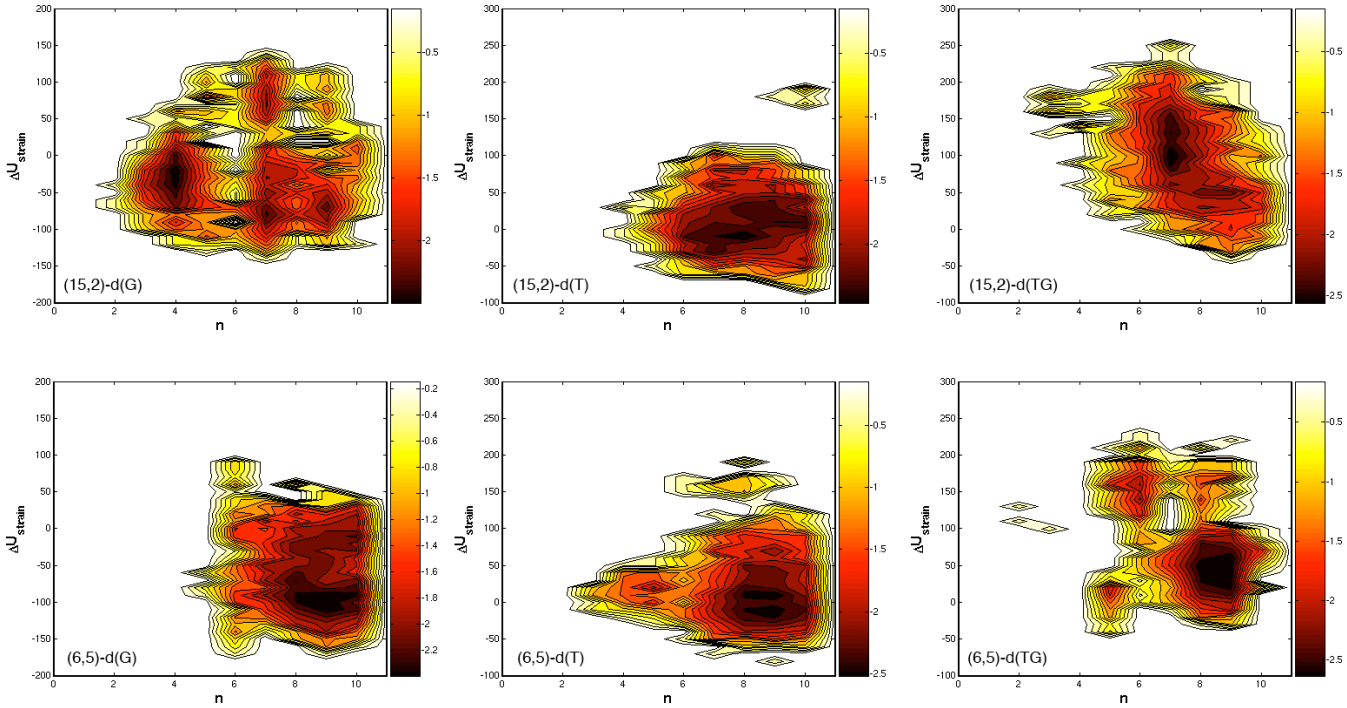


Figure S5. Free energy profiles as a function of the number of π-stacked bases (n) and DNA strain energy $\Delta U_{strain}$ (kcal/mol) for the d(G) (left), d(T) (middle) and d(TG) (right) oligonucleotides hybridized with the (15,2) (upper panels) and (6,5) (lower panels) CNT. The colored contours indicate relative depth in kcal/mol.

Table S1. Equilibrium properties of DNA and CNTs in solution

| | d(G) ssDNA | d(T) ssDNA | d(TG) ssDNA |
|---|---|---|---|
| H-bonds[a] | 132.4(0.4) [b] | 102.6(0.7) | 117.5(0.7) |
| SASA (Å$^2$) | 25450(40) | 23490(100) | 24860(180) |
| $U_{conf}$ (kcal/mol) | 595(3) | 385(4) | 470(10) |
| | (15,2) CNT | (6,5) CNT | |
| SASA (Å$^2$) | 63870(20) | 36240(50) | |

[a]The total number of hydrogen bonds between DNA and water. [b]The standard error (parenthesis) was calculated using a double-exponential autocorrelation model of Hess.[73]