Electronic Supplementary Material (ESI) for Nanoscale Advances.


**Table S1.** Model information on collagen systems containing 1-10 PPG units in the presence and absence of Au.

| Number of PPG unit | Gold surface system | | | Water system | |
|---|---|---|---|---|---|
| | water box dimension | number of gold atoms | number of water molecules | water box dimension | number of water molecules |
| **1** | 100x32x32 | 768 | 2844 | 30x30x30 | 859 |
| **2** | 80x32x32 | 768 | 2168 | 40x40x40 | 1955 |
| **3** | 150x65x65 | 3072 | 18533 | 48x48x48 | 3587 |
| **4** | 150x65x65 | 3072 | 18541 | 54x54x54 | 4996 |
| **5** | 150x82x82 | 4800 | 29611 | 62x62x62 | 7802 |
| **6** | 150x82x82 | 4800 | 29621 | 70x70x70 | 11456 |
| **7** | 150x98x98 | 6912 | 43089 | 78x78x78 | 15748 |
| **8** | 150x100x100 | 6912 | 43048 | 87x87x87 | 21494 |
| **9** | 100x100x100 | 8112 | 32167 | 96x96x96 | 29172 |
| **10** | 100x100x100 | 8112 | 32142 | 105x105x105 | 38199 |

**Figure S1.** Potential of mean force (PMF) of the biased diffusion process of PPG.

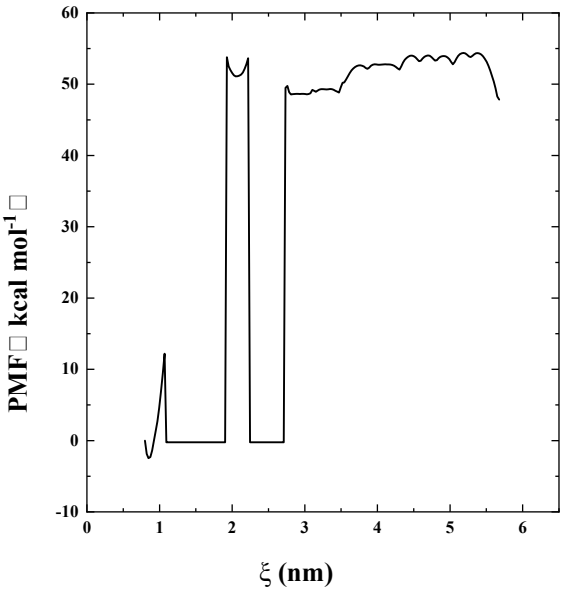

60
50
40
30
20
10
0
-10
0
1
2
3
4
5
6
PMF□ kcal mol-1 □
ξ (nm)

**Figure S2.** A typically trajectory of the MD simulation of PPG-1 on the gold surface: (A) Representative snapshot of the dynamics simulations process (B) The minimum normal distance of the four representative residues in the PPG on the gold surface from initiation to adsorption.

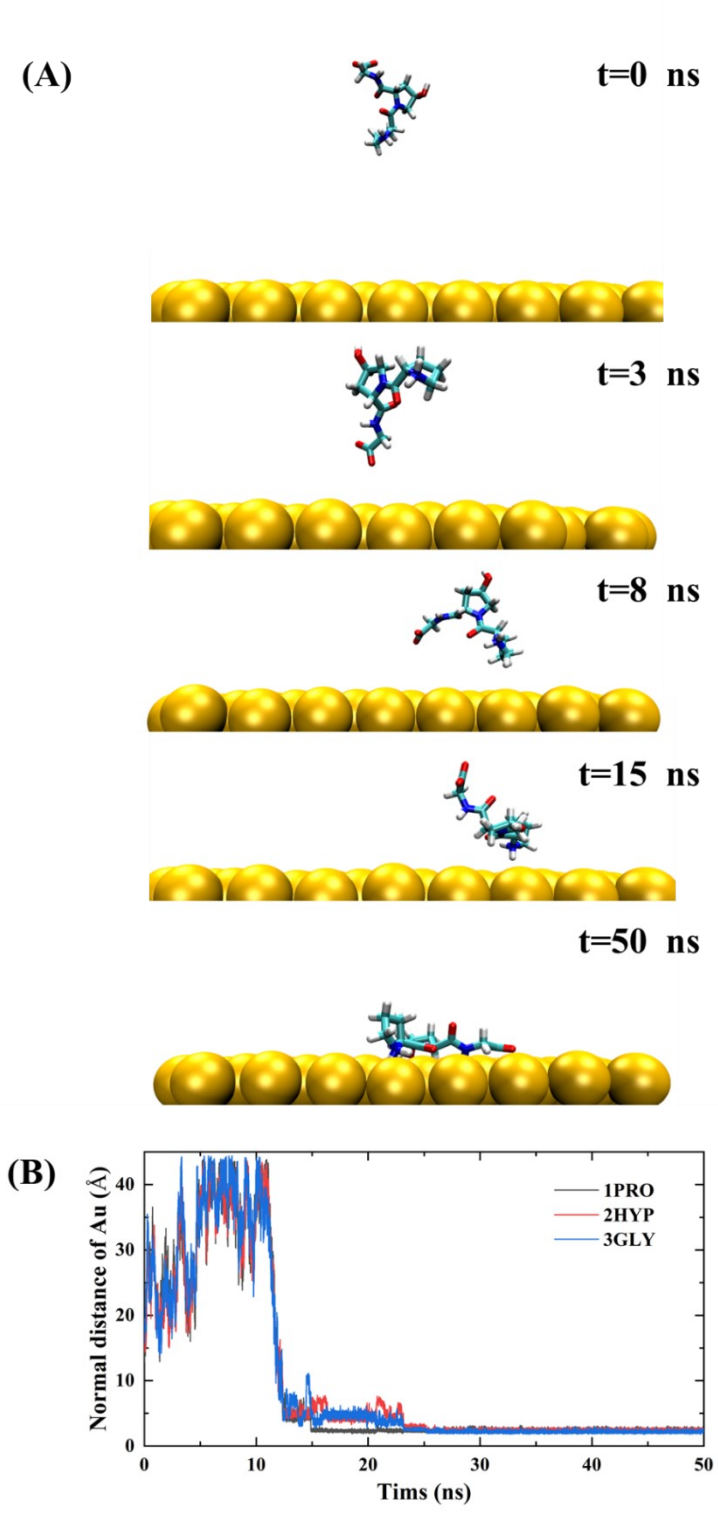


**Figure S3.** A typically trajectory of the MD simulation of PPG-2 on the gold surface: (A) Representative snapshot of the dynamics simulations process (B) The minimum normal distance of the four representative residues in the PPG on the gold surface from initiation to adsorption.

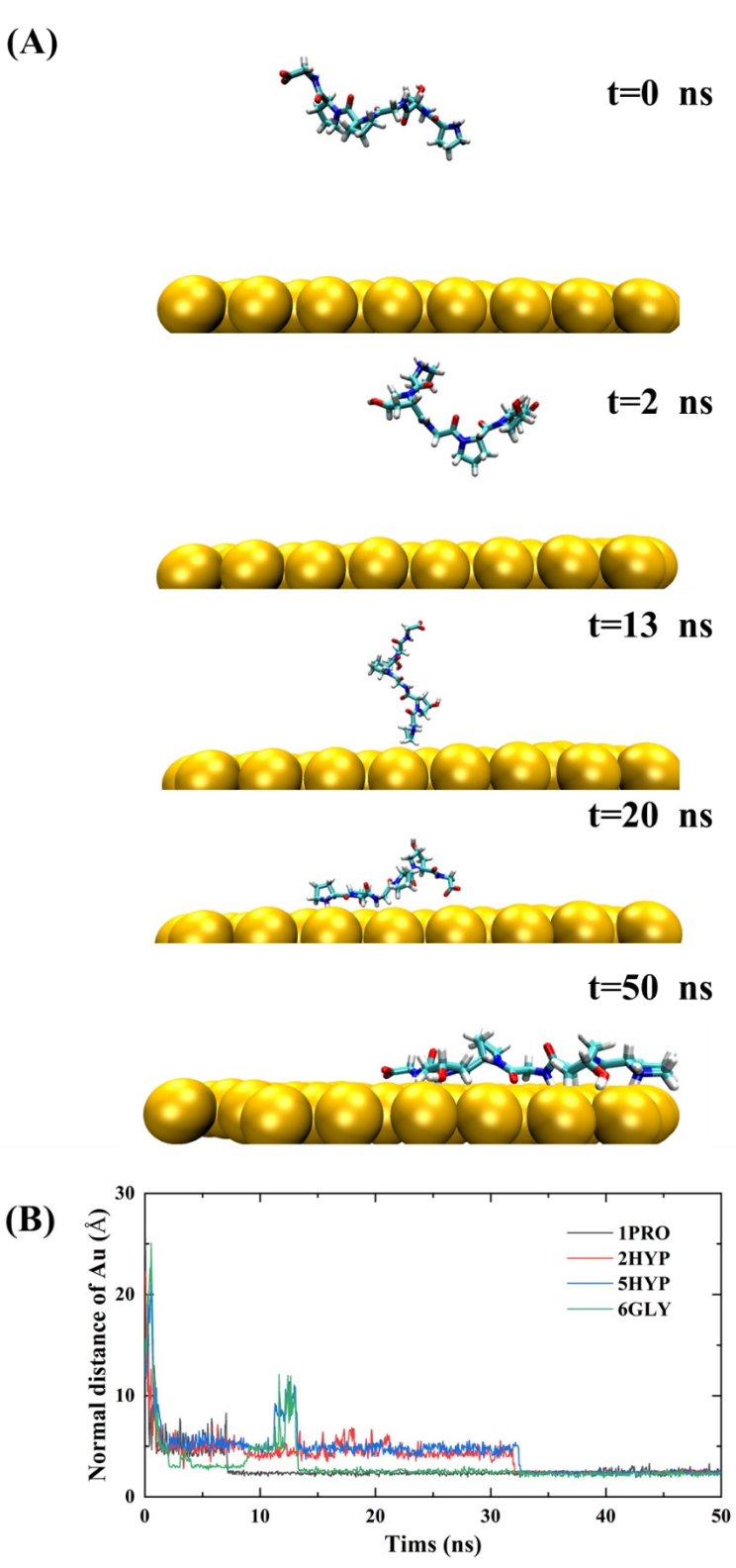
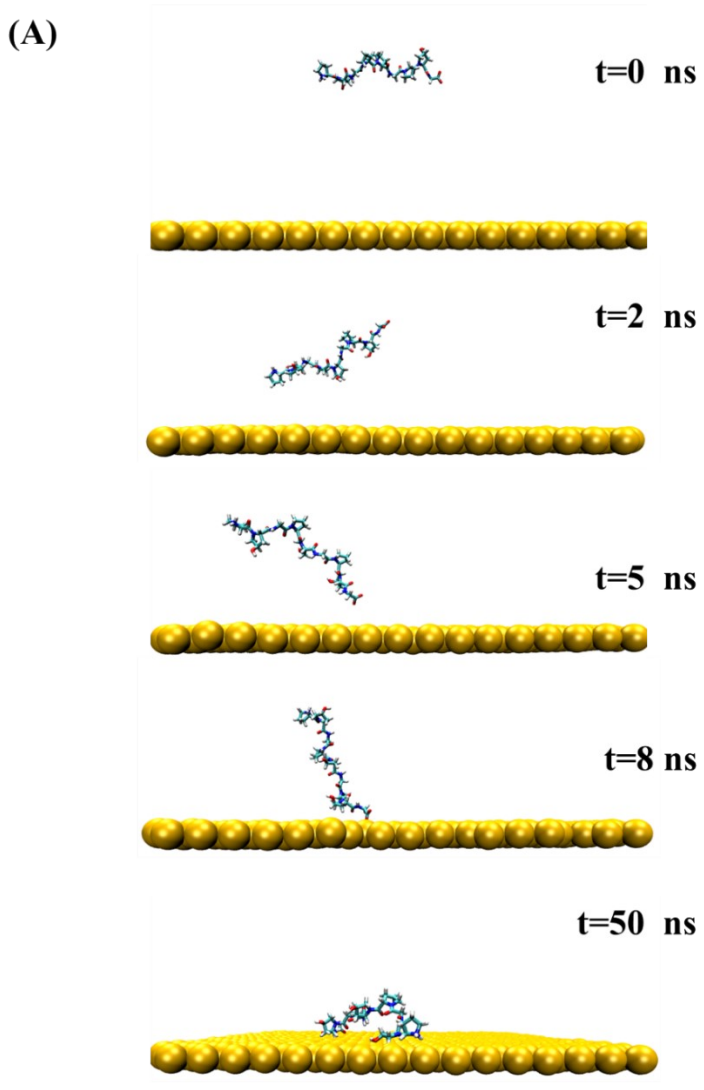


**Figure S4.** A typically trajectory of the MD simulation of PPG-3 on the gold surface: (A) Representative snapshot of the dynamics simulations process (B) The minimum normal distance of the four representative residues in the PPG on the gold surface from initiation to adsorption.



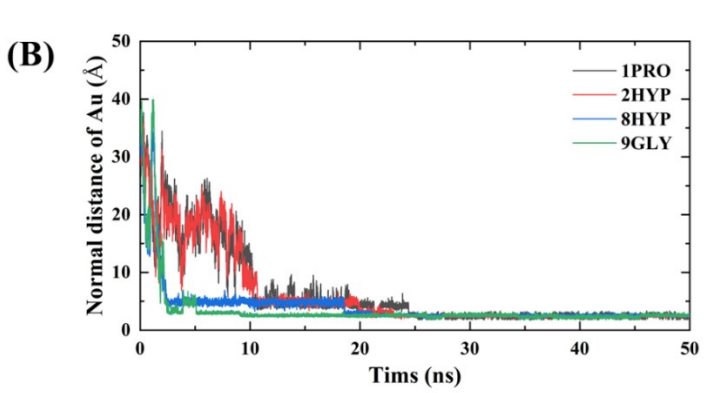



**Figure S5.** A typically trajectory of the MD simulation of PPG-4 on the gold surface: (A) Representative snapshot of the dynamics simulations process (B) The minimum normal distance of the four representative residues in the PPG on the gold surface from initiation to adsorption.

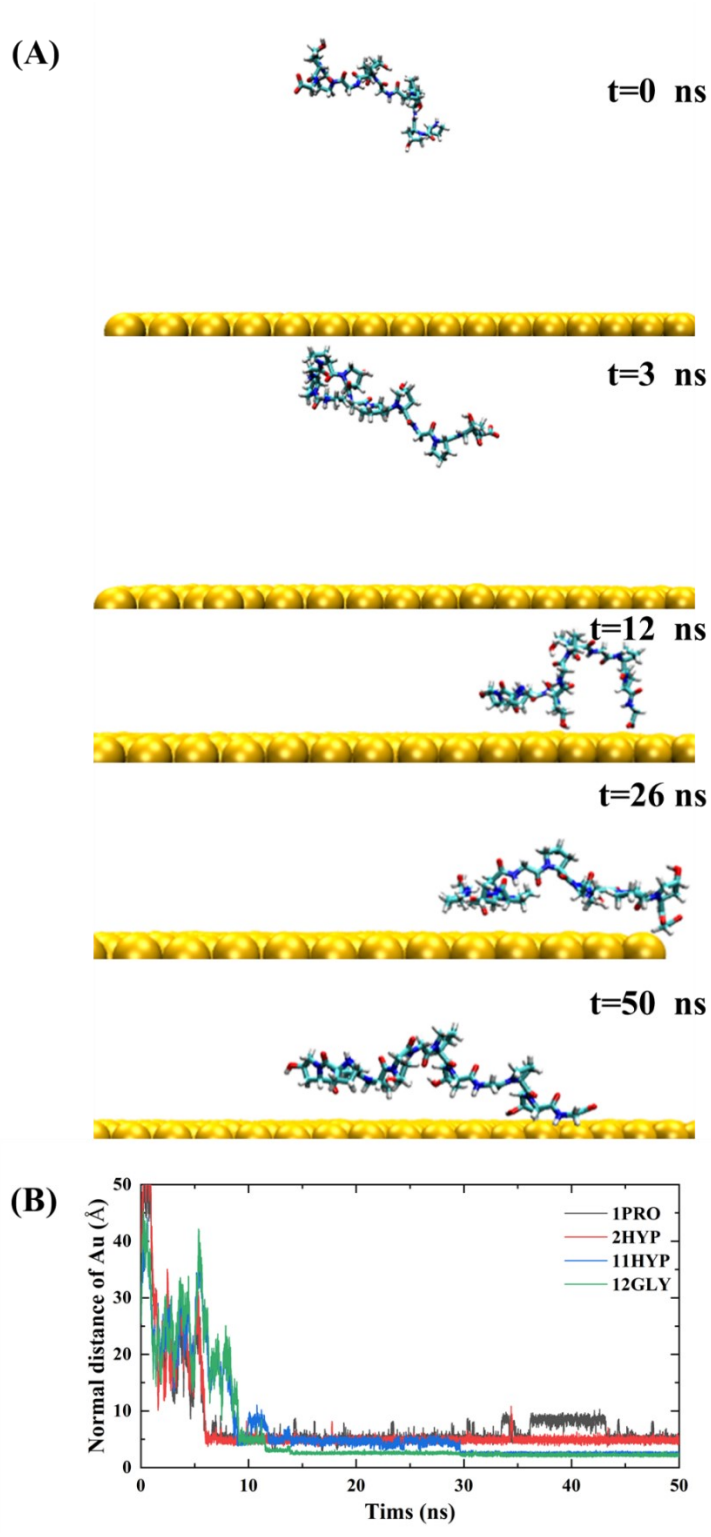


**Figure S6.** A typically trajectory of the MD simulation of PPG-5 on the gold surface: (A) Representative snapshot of the dynamics simulations process (B) The minimum normal distance of the four representative residues in the PPG on the gold surface from initiation to adsorption.

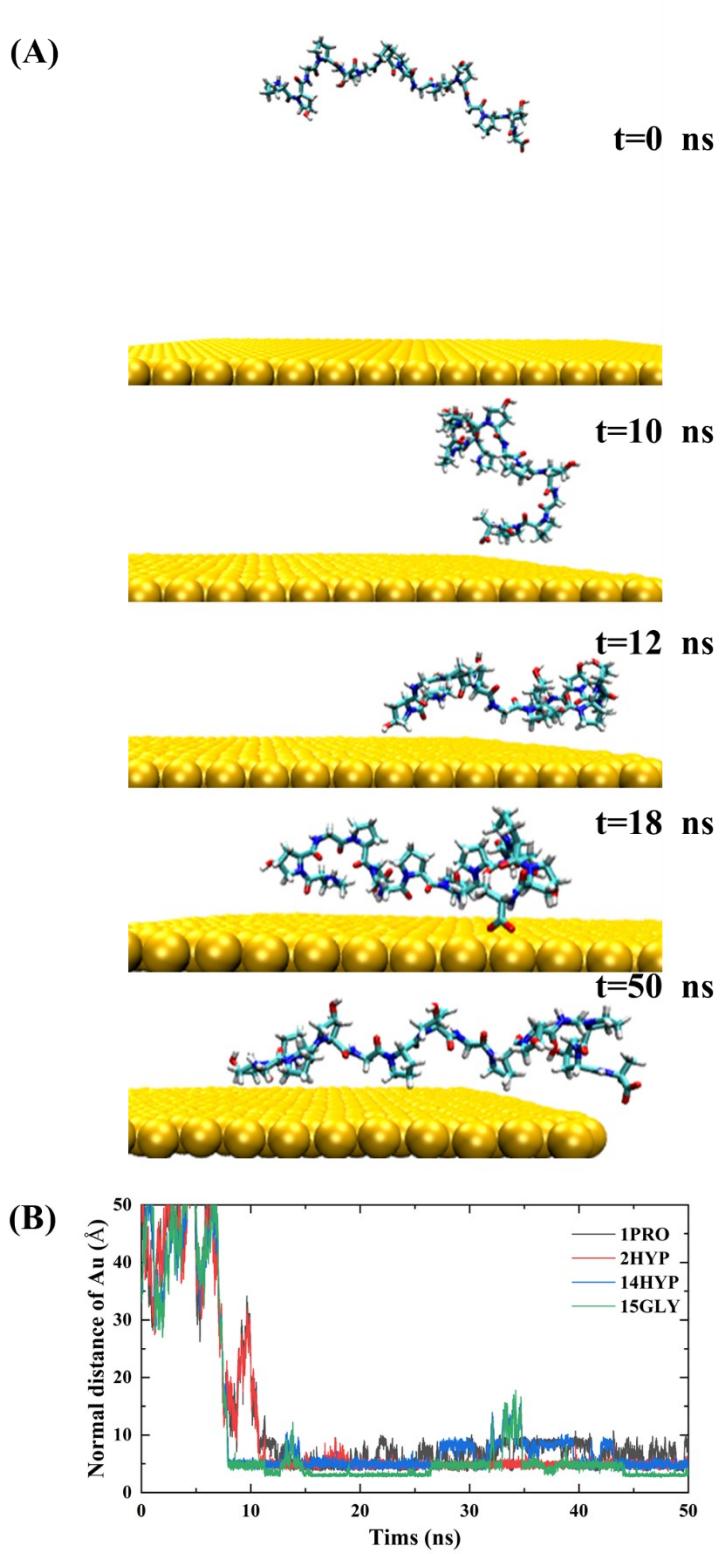


**Figure S7.** A typically trajectory of the MD simulation of PPG-6 on the gold surface: (A) Representative snapshot of the dynamics simulations process (B) The minimum normal distance of the four representative residues in the PPG on the gold surface from initiation to adsorption.

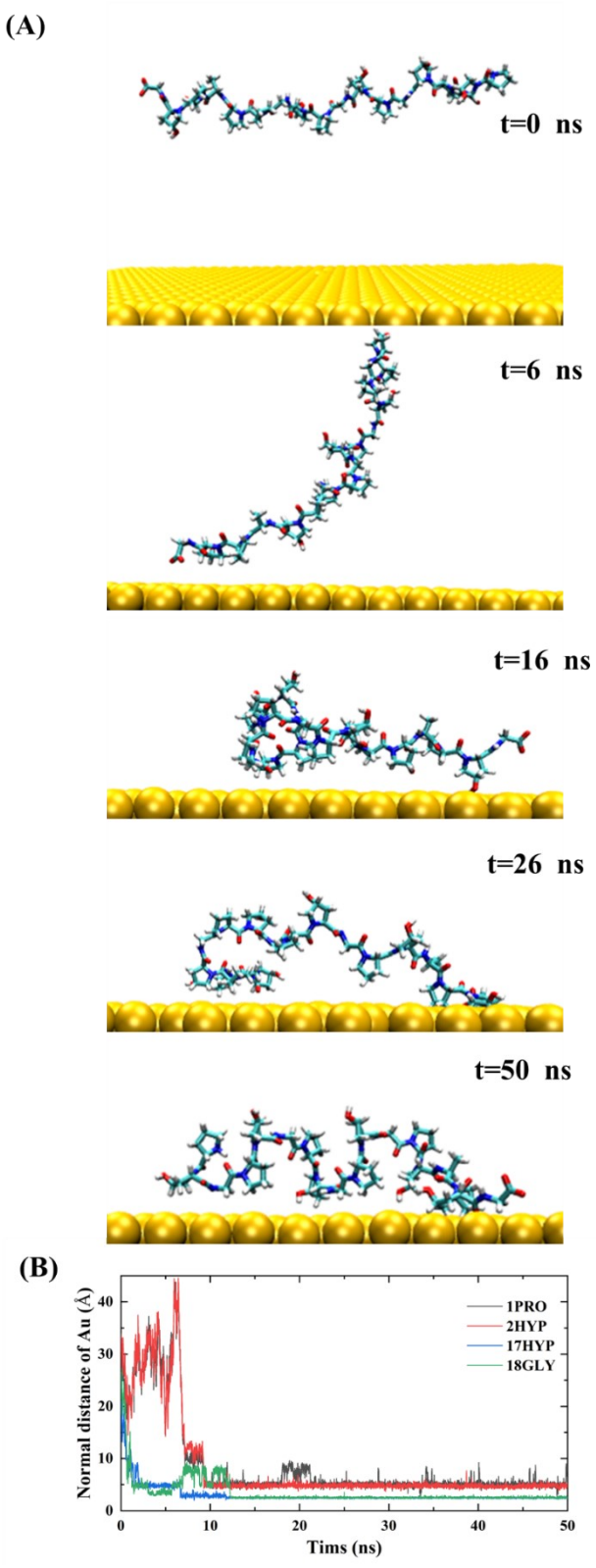


**Figure S8.** A typically trajectory of the MD simulation of PPG-7 on the gold surface: (A) Representative snapshot of the dynamics simulations process (B) The minimum normal distance of the four representative residues in the PPG on the gold surface from initiation to adsorption.

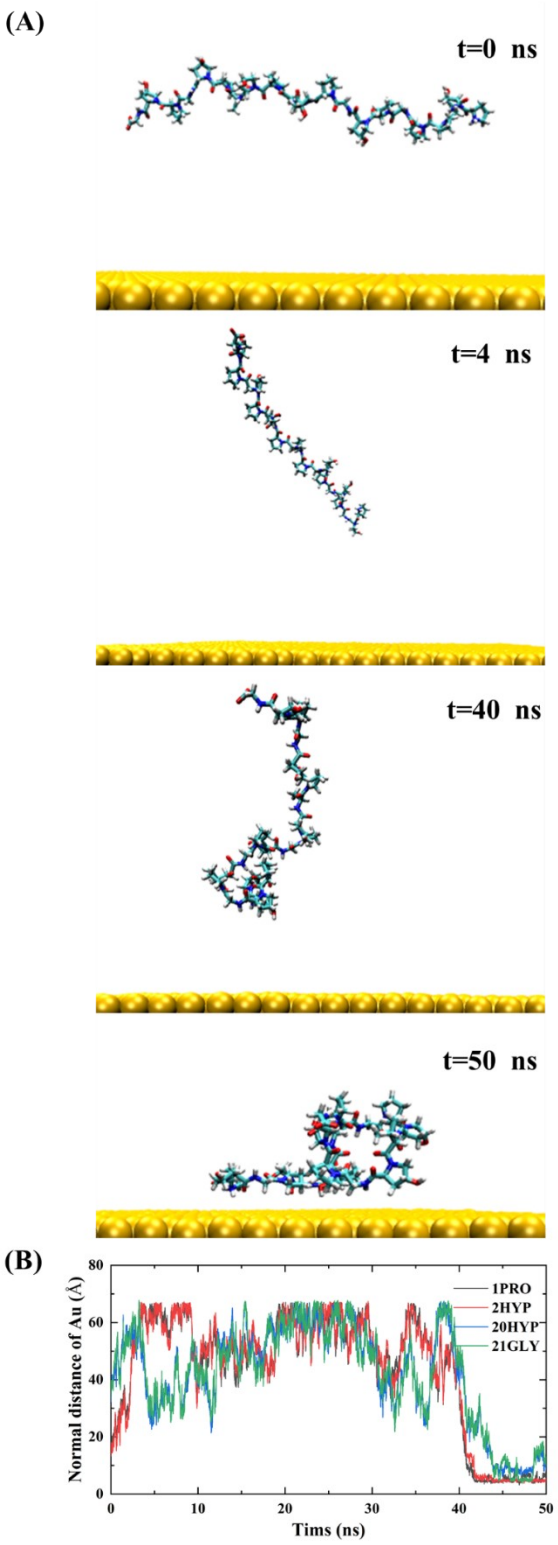


**Figure S9.** A typically trajectory of the MD simulation of PPG-8 on the gold surface: (A) Representative snapshot of the dynamics simulations process (B) The minimum normal distance of the four representative residues in the PPG on the gold surface from initiation to adsorption.

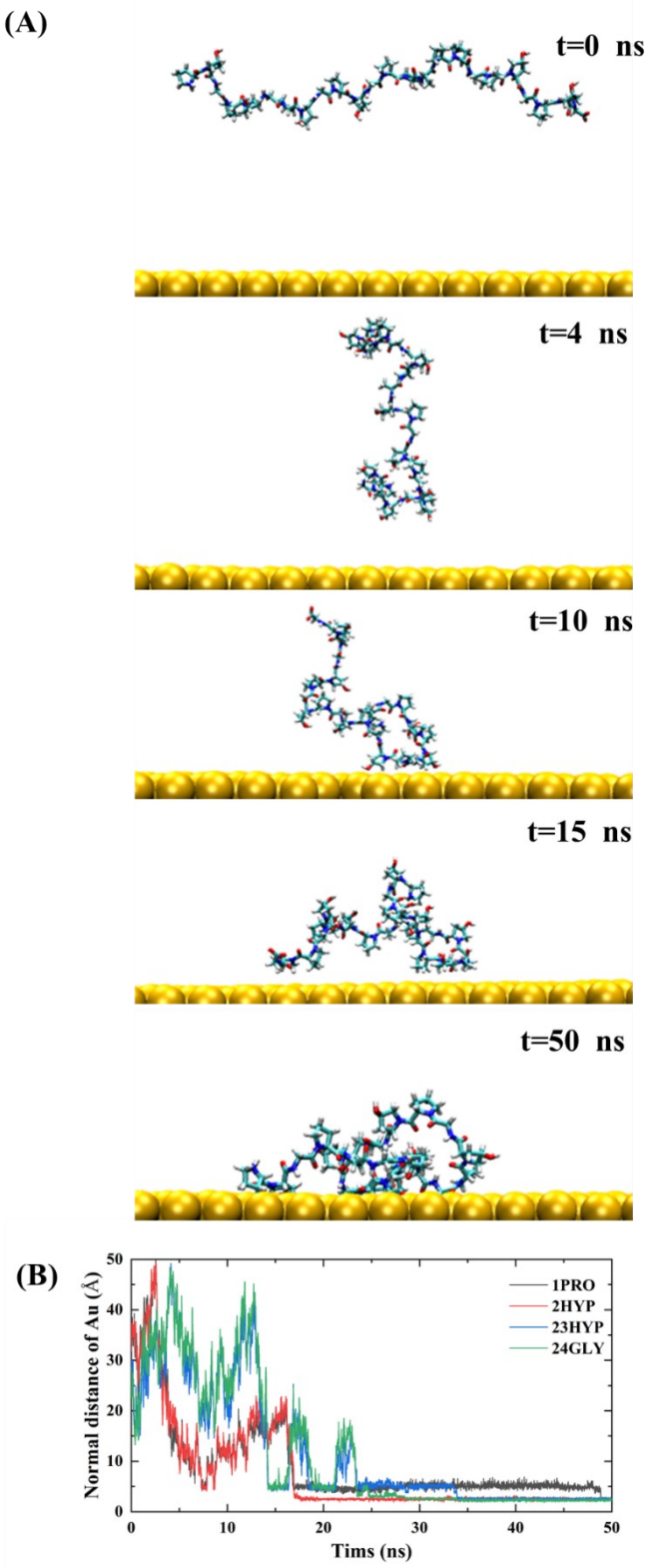


**Figure S10.** A typically trajectory of the MD simulation of PPG-9 on the gold surface: (A) Representative snapshot of the dynamics simulations process (B) The minimum normal distance of the four representative residues in the PPG on the gold surface from initiation to adsorption.

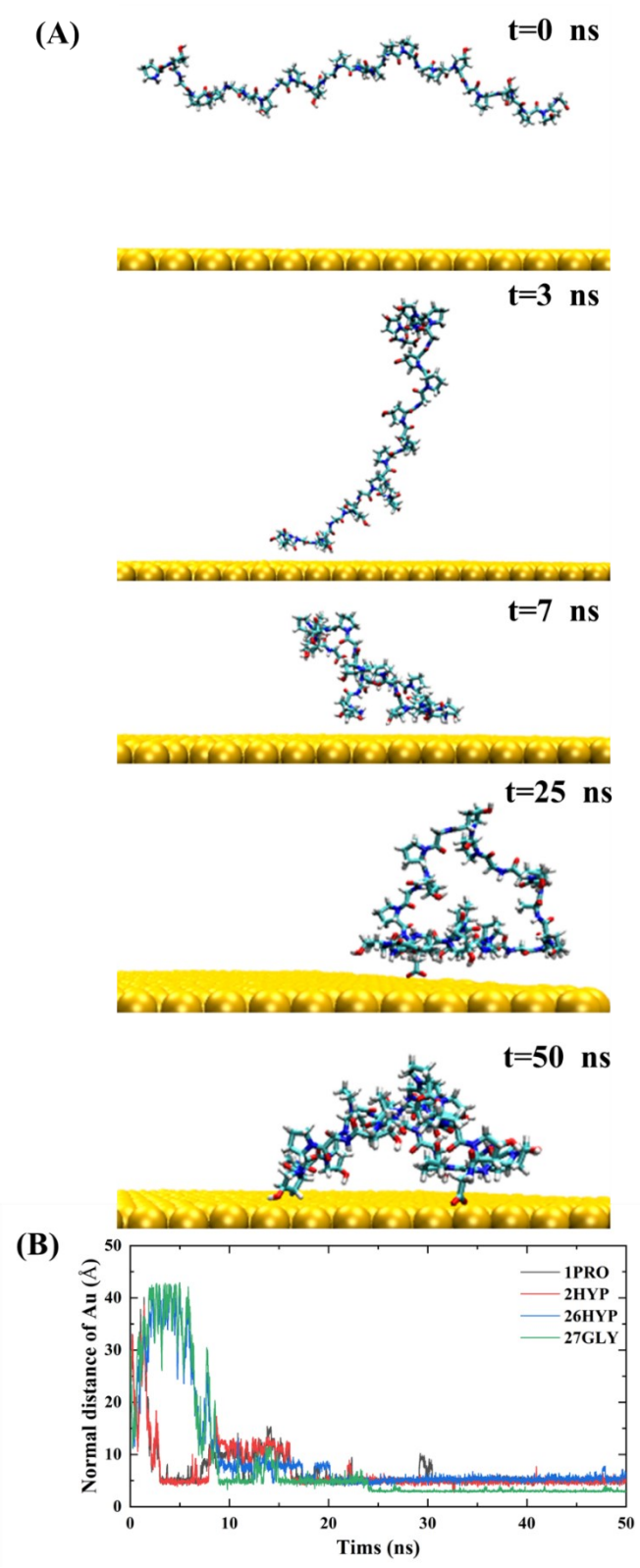


**Figure S11.** A typically trajectory of the MD simulation of PPG-10 on the gold surface: (A) Representative snapshot of the dynamics simulations process (B) The minimum normal distance of the four representative residues in the PPG on the gold surface from initiation to adsorption.

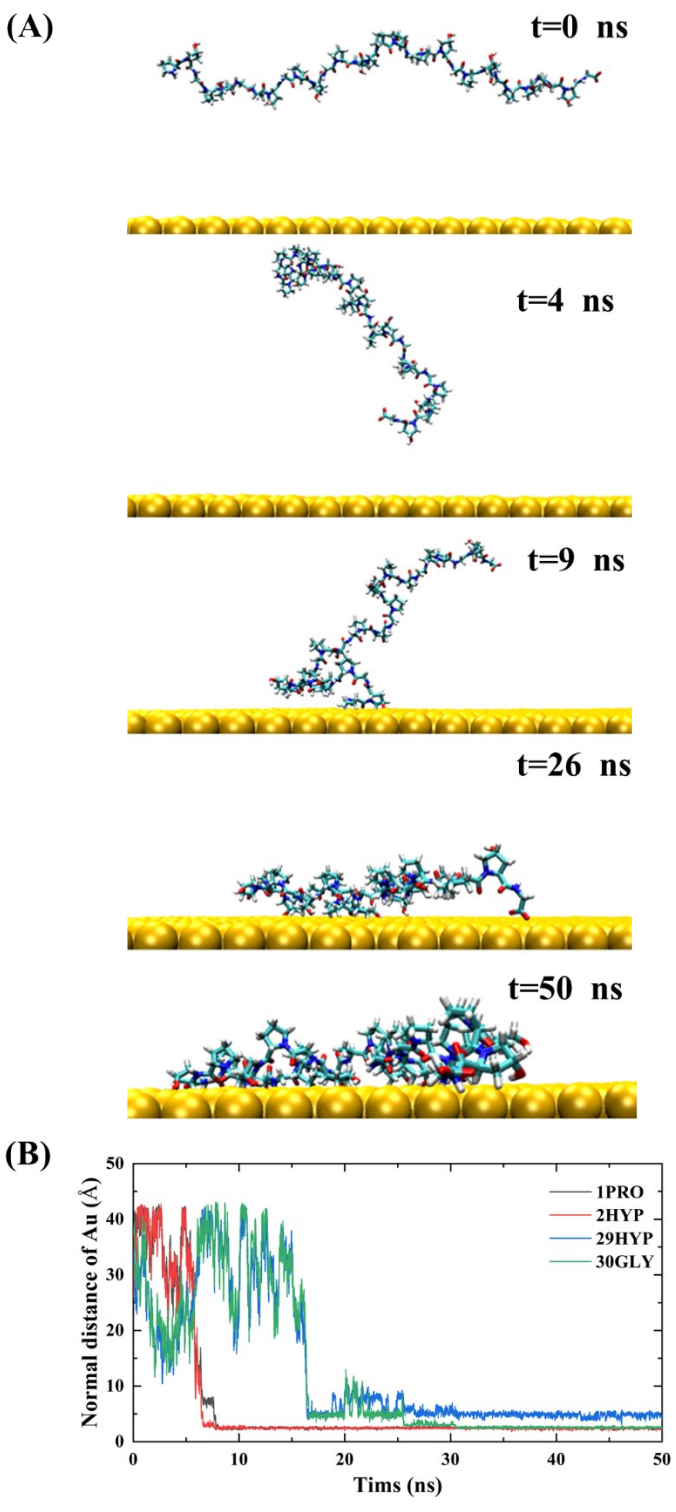


**Table S2.** In the 30 simulated trajectories, the number of times the following residues entered the first and second water layers as anchoring residues

| | **N-terminal** | **C- terminal** |
|---|---|---|
| **second water layer** | 14 | 16 |
| **first water layer** | 11 | 19 |

**Figure S12.** RDF for the interaction of the O atoms of water with gold.

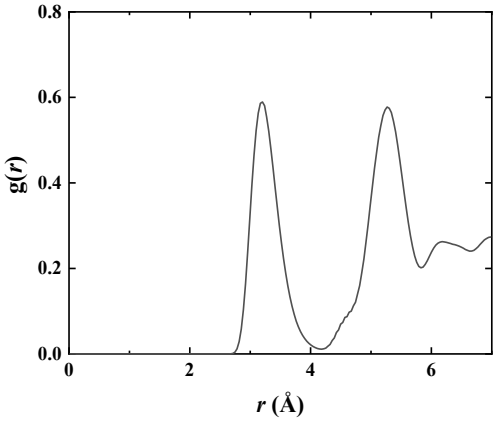


**Figure S13.** RDFs for the interaction of the backbone atoms of collagen systems containing 1-10 PPG units (i.e. O, N, C, and CA) with gold.