## Electronic Supplementary Information

# Surface conformations of anti-ricin aptamer and its affinity to ricin determined by atomic force microscopy and surface plasmon resonance

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### S1. Statistics of aptamer activity on Au(111) surface with and without CD modification

The AFM topography and recognition images of aptamers on Au(111) surface and CD modified Au(111) surface were used to do statistic study. For Au surfaces with or without CD modification, ten pairs of topography and recognition images were used to compare the aptamer morphology and activity. Each AFM image is in an area of 1500 nm by 1500 nm. The surface modification with CD may change the surface distribution and the orientations of aptamers on the substrate, subsequently the active residues on aptamer may not be available to the ricin molecules in solution. Therefore, the aptamers that lost activity could not show recognition

signals. The aptamer with topography image but without recognition image indicates the influence on that particular aptamer molecule. In Fig. S1, CD 1 column showed the total amount of aptamers that have topography images on CD modified Au (111) surface. The CD 2 column showed the total amount of aptamers that have recognition images with their corresponding topography images. The Au 1 column showed the total amount of aptamers that have topography images on Au (111) surface without CD. The Au 2 column showed the total amount of aptamers that have recognition images with their corresponding topography images on Au (111) surface without CD. The recognition ratio of aptamers on Au(111) surface with CD modification is 643:848=75.8%, while the recognition ratio of aptamers on Au(111) surface without CD modification is 1019:1089=93.6%.

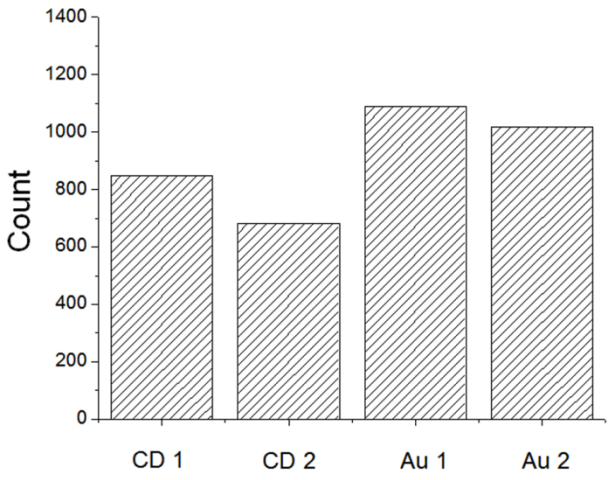


**Fig. S1.** The histograms of aptamer images on Au(111) surface with and without CD modification. CD 1: 848 molecules of aptamers showed topography images on CD modified Au (111) surface.. CD 2: 643 aptamers showed recognition images on CD modified Au (111) surface. Au 1: 1089 aptamers showed topography images on Au (111) surface without CD modification. Au 2: 1019 aptamers showed recognition images on Au (111) surface without CD modification.

**S2. Aptamer conformations on Au(111) surface**

The eleven selected areas from Fig. 2 are enlarged and compared with the simulated aptamer folding conformations. Fig. S2 shows the area number 1 to 7 and their corresponding simulated structures on gold surface. The aptamer 1 and 2 in Fig. S2a both showed rod-shaped topography images. On the contrary, the recognition images showed strong signals in the middle and weak signals on the two ends of each structure. The top-view and side-view (rotated 90 degree from top-view) showed that the position of ricin binding site in these two aptamer conformations are pointing to the solution, so it can easily contact ricin molecule on the AFM tip. Based on the same method, the topography images and recognition images of aptamer 3 and 4 in Fig. S2b showed more significant difference. In Fig. S2c, the recognition signal of aptamer 5 has a more similar shape with its topography image, but the simulated aptamer structure suggests that the recognition signal should be much smaller. This inconsistency between experiment and simulation was mainly caused by the fluctuation during the tip scanning. In Fig. S2d, the aptamer folding structure was supposed to be almost perpendicular to the gold surface, so it showed round shapes in both topography and recognition images. In Fig. S2e, the binding site for ricin was not facing up to the solution, so the binding was blocked by other parts of the aptamer, and the recognition signal was significantly reduced.

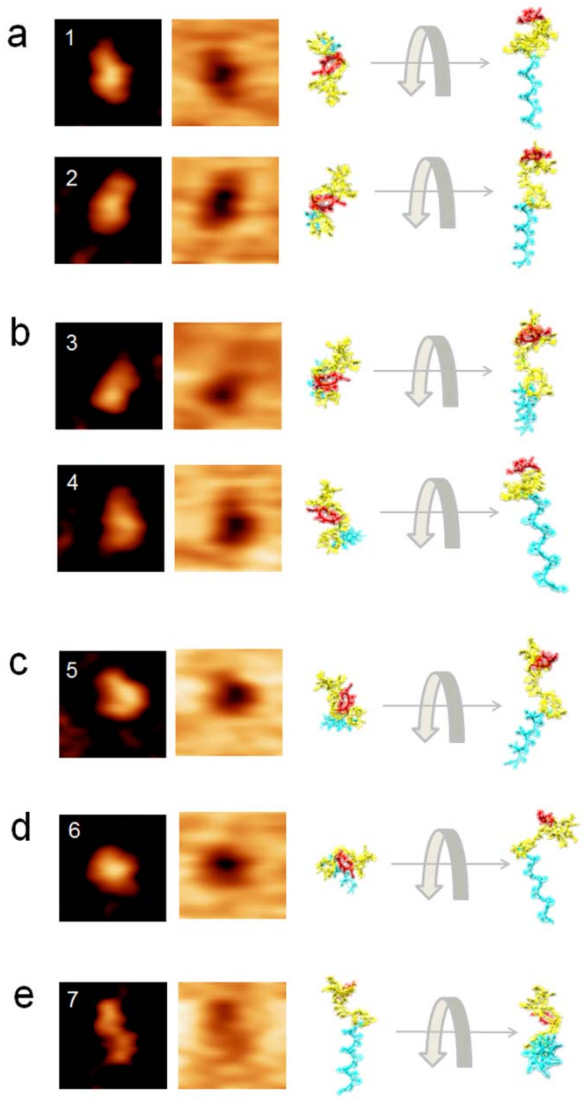


**Fig. S2.** The enlarged AFM topography and recognition images of individual aptamer molecule on Au(111) surface. Image size 25 nm × 25 nm. The numbers 1 to 7 are corresponding to the same numbers in Fig. 2. (a) The similar conformations with rod-shaped topography images and round-shaped recognition images in the middle. (b) The similar conformations with recognition signals in only one side of the topography images. (c) The topography and recognition images are similar because of the experimental errors. (d) The topography images and recognition images are similar due to the aptamer orientation. (e) The binding site for ricin was blocked by special aptamer orientation.

In the selected areas 9, 10, and 11 from Fig. 2, some topography images of the aptamers are larger than others. Therefore, aggregations of two or three aptamer molecules may exist. The AFM topography images cannot provide resolutions high enough to distinguish the possible aggregations of molecules in such small size. However, the recognition images showed clear signals of the small binding sites and in turn proved the aggregations. Fig. S2 showed the comparisons of the experimental images of and simulated folding structures of the representative aptamer aggregations. For area 9, the two aptamer molecules had some parts of the structures overlaid in the topography image, and look like one large molecule. However, the recognition image clearly shows two recognition spots, one is large and another is small. The other parts of the two aptamers show much weaker recognition signals. Therefore the two aptamers can be distinguished with the help of the simulated aptamer folding structures. The predicted binding sites for ricin (highlighted in red) in the two simulated structures agree with the positions of the two recognition spots. The same method was used to check the right part of the selected area 10. The topography images of right side and left side are very similar, but the recognition images show the difference. The right side is the aggregation of two aptamer molecules with two recognition spots, but the left side only shows on recognition spot. Therefore, the recognition signals determine the number of aptamers in the topography images. In the selected area 11, the topography image seems a continuous molecule, but the two recognition spots obviously show that they are two aptamer molecules.

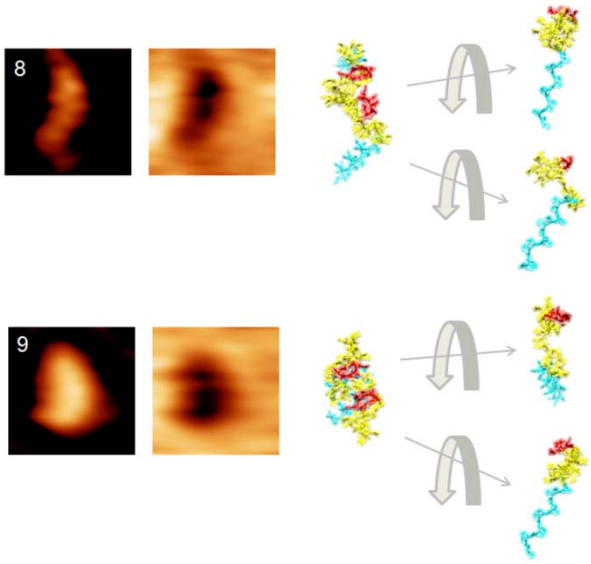


**Fig. S3.** The enlarged AFM topography and recognition images of aggregated aptamers on Au(111) surface. Image size 30 nm × 30 nm. The numbers 8 and 9 are corresponding to the same number in Fig. 2. The topography images in 8 and 9 cannot provide enough information for the aggregation. Their corresponding recognition images distinguished the two aptamer molecules in close contacts.