Electronic Supplementary Information (ESI)

DNA-Responsive Disassembly of AuNP Aggregates: Influence of Nonbase-paired regions and Colorimetric DNA Detection by Exonuclease III Aided Amplification

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Table S1 DNA sequence used in this study

name	Oligonucleotides sequence (5'-3')
5´SH-A0DNA1	TTGACGTTACCCTTAGC
5´SH-A13DNA1	AAAAAAAAAATCATTGACGTTACCCTTAGC
5´SH-A23DNA1	AAAAAAAAAAAAAAAAAAAATCATTGACGTTACCCTTAGC
5´SH-A33DNA1	AAAAAAAAAAAAAAAAAAAAAAAAAAAAATCATTGACGTTACCCTTAGC
3´SH-A10DNA2	CTTCGATCCTGTAAAAAAAAA
Linker-G12	ACAGGATCGAAGAAATGGTCAATGGGGTAACGTCAA
linker-G0	ACAGGATCGAAGGGGTAACGTCAAGTCGC
linker-G4	ACAGGATCGAAGAAATGGGTAACGTCAAGTCGC
linker-G6	ACAGGATCGAAGAAATGGGGGTAACGTCAAGTCGC
linker-G8	ACAGGATCGAAGAAATGGTCGGGTAACGTCAAGTCGC
linker-G12	ACAGGATCGAAGAAATGGTCAATGGGGTAACGTCAAGTCGC
linker-G16	ACAGGATCGAAGAAATGGTCAATGAGGAGGGTAACGTCAAGTCGC
linker-G20 (linker)	ACAGGATCGAAGAAATGGTCAATGAGGAAACGGGGTAACGTCAAGTCGC
Target-G12	TTGACGTTACCCCATTGACCATTTCTTCGATCCTG
target-G0	GCGACTTGACGTTACCCCTTCGATCCTGTATAAA
target-G4	GCGACTTGACGTTACCCATTTCTTCGATCCTGTATAAA
target-G6	GCGACTTGACGTTACCCCCATTTCTTCGATCCTGTATAAA
target-G8	GCGACTTGACGTTACCCGACCATTTCTTCGATCCTGTATAAA
target-G12	GCGACTTGACGTTACCCCATTGACCATTTCTTCGATCCTGTATAAA
target-G16	GCGACTTGACGTTACCCTCCTCATTGACCATTTCTTCGATCCTGTATAAA
target-G20 (target)	GCGACTTGACGTTACCCCGTTTCCTCATTGACCATTTCTTCGATCCTGTATAAA
linker-O4	ACAGGATCGAAGGGGTAACGTCAAGTCG
linker-O6	ACAGGATCGAAGGGGTAACGTCAAGTCGCA
linker-O8	ACAGGATCGAAGGGGTAACGTCAAGTCGCAAA
linker-O10	ACAGGATCGAAGGGGTAACGTCAAGTCGCAAACC
linker-O12	ACAGGATCGAAGGGGTAACGTCAAGTCGCAAACCGA
linker-O14	ACAGGATCGAAGGGGTAACGTCAAGTCGCAAACCGACG
linker-O16	ACAGGATCGAAGGGGTAACGTCAAGTCGCAAACCGACGAC
target-O4	CGACTTGACGTTACCCCTTCGATCCTGTATAAA
target-O6	TGCGACTTGACGTTACCCCTTCGATCCTGTATAAA
target-O8	TTTGCGACTTGACGTTACCCCTTCGATCCTGTATAAA
target-O10	GGTTTGCGACTTGACGTTACCCCTTCGATCCTGTATAAA
target-O12	TCGGTTTGCGACTTGACGTTACCCCTTCGATCCTGTATAAA
target-O14	CGTCGGTTTGCGACTTGACGTTACCCCTTCGATCCTGTATAAA
target-O16	GTCGTCGGTTTGCGACTTGACGTTACCCCTTCGATCCTGTATAAA
T2	GCGACTTGACG**A**TACCCCGTT**A**CCTCATTGACCATTTCTTCGATCCTGTATAAA
T3	GCGACTTGACG**AA**ACC**G**CGTTTCCTCATTGACCATTTCTTCGATCCTGTATAAA

The inserted sequences in linker DNA (i.e., oligomer F_a) are gaps (linker-G0 to linker-G24) and the overhanging sequences at the 3' termini of linker DNA are overhangs (linker-O4 to linker-O20) are highlighted by an underline. The target (i.e.,

oligomer F_d) for relevant gaps (target-G0 to target-G20) and overhangs (target-O4 to target-O16) are also highlighted by an underline. Five protruding bases (GTCGC) at the 3' termini of each linker with gap (linker G0 to G24) are used to prevent linker DNA from digestion of the exonuclease III. The boldface portion (T2, T3) symbolizes the mutant base.

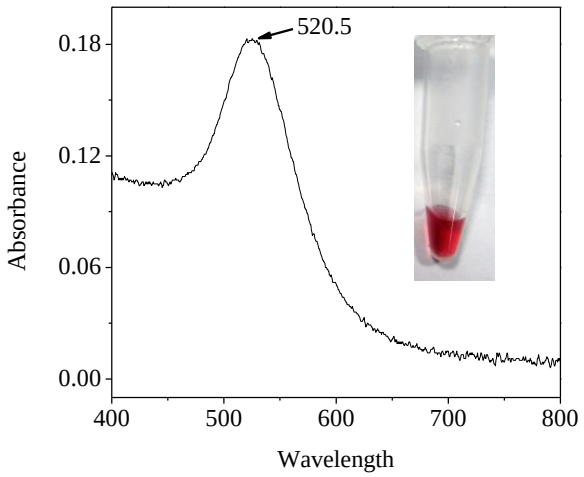

Fig. S1 The UV-vis absorption spectra of DNA-AuNPs. Inset: the photograph. The AuNPs were dispersed in 0.01M PB buffer (pH 7.2) containing 0.5 M NaCl and 0.01% SDS. The solution of DNA-AuNPs was stable during all experiments.

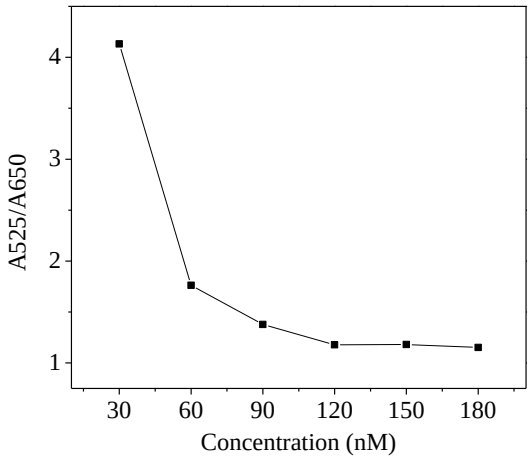

Fig. S2. Relationship between the concentration of linker DNA and the degree of AuNP aggregation.

Optimization of the linker DNA concentration. In practical applications, both a high degree of nanoparticles aggregation and rapid rate of DNA-responsive disassembly of AuNPs are desired. Therefore, it was important to find an appropriate ratio between linker DNA and functionalized AuNPs so that any displacement of linker DNA could result in the disassembly of AuNPs in an efficient manner. If the linker DNA was excessive, oligomer F_d might hybridize with the excessive oligomer F_a which could not disassemble AuNPs, resulting in a reduced sensitivity. However, if the linker DNA was insufficient, linker DNA was not enough to assemble AuNPs. Thus, tests were performed to ensure that these two characteristics were exhibited at acceptable levels. As shown in Fig. S1, the absorbance ratio of 525 nm over 650 nm increased with an increasing concentration of the target from 0 nM to 100 nM, indicating that the addition of the linker increased the degree of nanoparticle aggregation. When the concentration of target was higher than 100 nM, the degree of aggregation changed no longer with further increasing concentration of target. Therefore, 100 nM linker DNA was chosen as the best condition to assemble AuNPs.

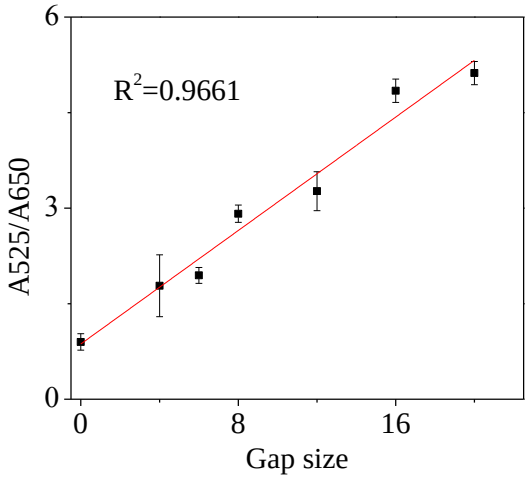

Fig. S3. The effect of gap size on disassembly of AuNPs in the presence of *both target and exonuclease III* monitored by the absorbance ration of 525 nm over 650 nm. [Target] = 40 nM, [Exonuclease III] = 60 U.

Optimization of the linker DNA length. Fig. S2 shows the absorbance ratio increased with the length of the gap size in the presence of both target and exonuclease III and no plateau was observed, which was a bit different to that merely in the presence of target (Fig. 3). This might be attributed that the relative high steric hindrance in the crowed three-dimensional space inhibited the enzyme activity. A shorter gap size prevented the exonuclease III from entering the crowded AuNP aggregate networks, substantially inhibiting the digestion of linker DNA. If increased the gap size, the interparticle distance became larger, decreasing the steric effect. Therefore, exonuclease III could freely access the AuNP aggregate networks so as to improve the disassembly kinetics of AuNPs. In this experiment, a 20 gap nucleotide was chosen because the selectivity became worse when the gap size was further increased.[1]

Supporting reference:

(1) Q. Q. Li, G. Y. Luan, Q. P. Guo and J. X. Liang, *Nucleic Acids Res.*, 2002, **30**, e5.