

Supporting Information:

Computational design of peptide-Au cluster probe for sensitive detection of $\alpha_{IIb}\beta_3$ Integrin

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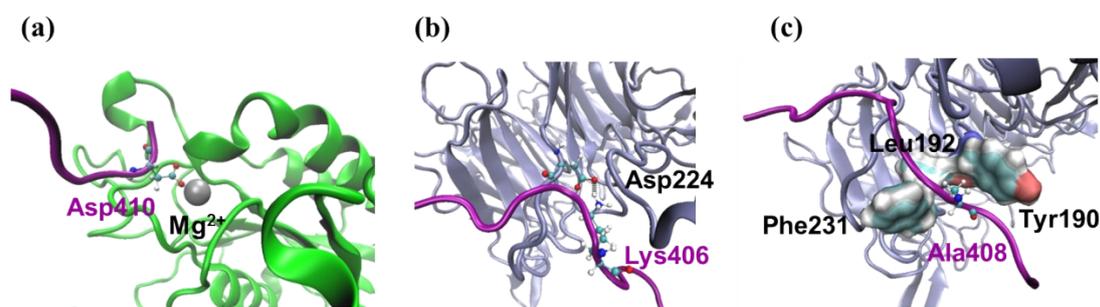


Figure S1. The original binding modes of γ C peptide. (a) The electrostatic interaction between Asp410 of γ C peptide and MIDAS Mg^{2+} ion. (b) The salt bridge formed by Lys406 of γ C peptide and Asp224 of α subunit in integrin. (c) The hydrophobic interaction between Ala408 of γ C peptide and Phe231/Leu192/Tyr190 of α subunit in integrin.

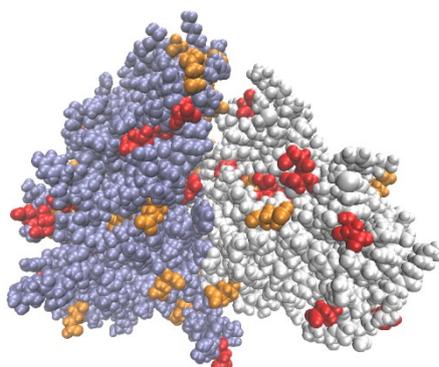


Figure S2. The distribution of the negatively charged residues around the binding site of γ C peptide. Asp and Glu are shown in red and orange, respectively.

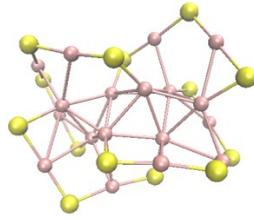


Figure S3. The structure of Au₁₈ cluster encapsulated by 14 sulfur atoms. Au, S atoms are in pink and yellow respectively.

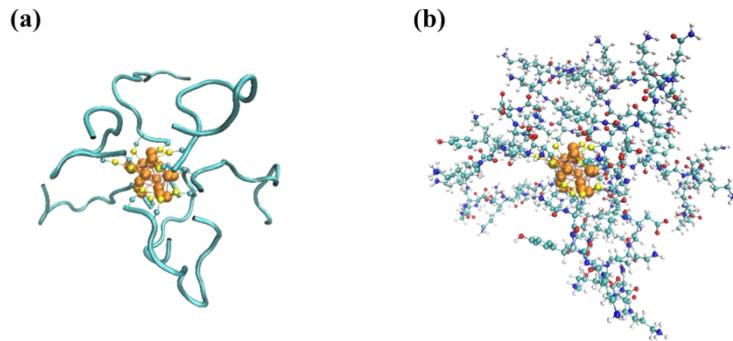


Figure S4. The structure of Au₁₈Peptide₇ probe. Au₁₈ is displayed in CPK representation and the coating peptides are in NewCartoon representation (a) and in CPK representation (b). Au, S, C, N, O, H atoms are in orange, yellow, cyan, blue, red, and white respectively.

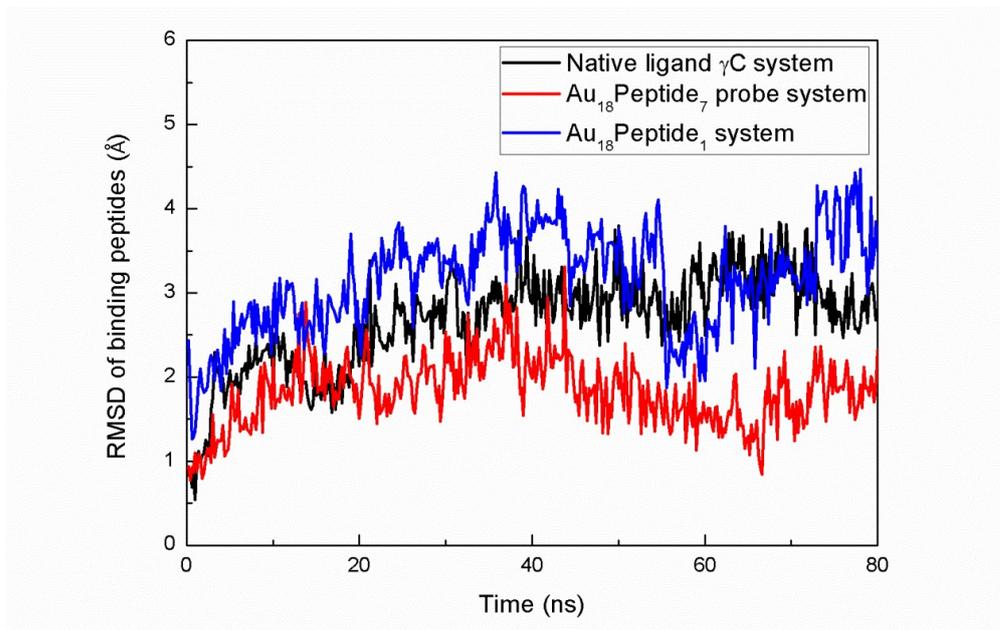


Figure S5. The RMSD of binding motif of γ C peptide (black) and Peptide⁷ of Au₁₈Peptide₇ (red) and of Au₁₈Peptide₁ (blue) bound to $\alpha_{11b}\beta_3$ integrin.