Supporting Information

Designing nanoparticle-containing polymeric substrate for detecting cancer cells by computer simulations

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Fig. S1 Time sequence of snapshots illustrating the typical processes of the normal cell (a, c, e) or the cancer cell (b, d, f) leaving the polymeric substrate when adding the shear flow, where $\sigma = 1.56 \text{ } mm^{-2}$ and $\varepsilon = 7.5 \text{ } kJ/mol$. (a)-(b) $a_{CL} = 1 \text{ } k_BT/r_c$, (c)-(d) $a_{CL} = 5 \text{ } k_BT/r_c$, (e)-(f) $a_{CL} = 10 \text{ } k_BT/r_c$.



Fig. S2 The equilibrated snapshots of the nanoparticles in the polymer layer under different a_{CL} : (a) $a_{CL} = 1 k_B T/r_c$, (b) $a_{CL} = 3 k_B T/r_c$, (c) $a_{CL} = 5 k_B T/r_c$, (d) $a_{CL} = 7 k_B T/r_c$, (e) $a_{CL} = 10 k_B T/r_c$.



Fig. S3 (a) The number of receptors around the nanoparticle as a function of interaction parameter ε under different cases. (b) The averaged nanoparticle-cell interaction energy divided by the number of receptors) as a function of ε , where the blue line is the linearly fitted function.



Fig. S4 The settling time of different cells in the substrate as a function of interaction parameter ε . The settling time of 24.0 μ s indicates that the cells do not spontaneously leave the substrate in the simulation (without shear flow). When $\varepsilon = 2.5 \text{ kJ/mol}$, the cells could just weakly attach onto the substrate, thus we take the settling time as zero.