Aptamer Based Electrostatic-stimuli Responsive

Surfaces for On-demand Binding/Unbinding of a Specific Ligand

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Supplementary information

S1 - Bootstrap resampling:

For each sample (30 data for average height difference), we treated it as the whole population, and resampled the data following the replacement rule of bootstrap algorithm, i.e. we picked up a data from those 30 data randomly, then put back the data in the pool to allow another data pick-up. Such resampling is repeated for many times, in our case, the resampling times N = 1000. The 1000 resampling data generated a new distribution, and we could perform statistical analysis on it. The benefit for application of bootstrap resampling method is no specific distribution assumption needed to post on the data set, and the new resampled distribution can have much more data than the original data set, thus keeps the statistical analysis more stable and robust.

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Supplementary Table 1 Statistical results of confidence intervals for height difference under nonelectrical field conditions based on normal distribution assumption and bootstrap resampling

			Average	Lower bound	Higher bound	Standard deviation
Objective group	Alkanethiol	Normal distribution	-1.66	-1.74	-1.58	0.14
		Bootstrap	-1.66	-1.73	-1.58	-
	Alkanethiol + Aptamer	Normal distribution	-0.53	-0.61	-0.45	0.14
		Bootstrap	-0.53	-0.60	-0.46	-
	Alkanethiol + Aptamer + Thrombin	Normal distribution	1.40	1.30	1.50	0.18
		Bootstrap	1.40	1.32	1.48	-
Control group	Alkanethiol + poly(A)	Normal distribution	-0.92	-1.04	-0.80	0.21
		Bootstrap	-0.92	-1.02	-0.82	-
	Alkanethiol + poly(A) + Thrombin	Normal distribution	-0.89	-1.06	-0.73	0.30
		Bootstrap	-0.89	-1.03	-0.76	-
	Alkanethiol + Aptamer + γ-Thrombin	Normal distribution	-0.55	-0.64	-0.46	0.16
		Bootstrap	-0.55	-0.62	-0.48	-

Supplementary Table 2 Statistical results of confidence intervals for height difference under electrical field application based on normal distribution assumption and bootstrap resampling

		Average	Lower bound	Higher bound	Standard deviation
0mV	Normal distribution	1.43	1.33	1.54	0.18

	Bootstrap	1.43	1.34	1.52	-
100mV	Normal distribution	-0.55	-0.67	-0.43	0.21
	Bootstrap	-0.55	-0.66	-0.45	-
300mV	Normal distribution	-0.53	-0.63	-0.42	0.18
	Bootstrap	-0.53	-0.61	-0.44	-
-100mV	Normal distribution	1.41	1.33	1.50	0.14
	Bootstrap	1.41	1.32	1.51	-
-300mV	Normal distribution	-1.63	-1.77	-1.50	0.25
	Bootstrap	-1.63	-1.74	-1.51	-

S2- Molecular dynamics simulation videos

S2 (a): The video shows the spontaneous dissociation of thrombin from aptamer as observed in the MD simulation using the electric field of 0.5 Vnm^{-1} . The thrombin aptamer is position restrained throughout the simulation to mimic the experimental condition where the aptamer is bound to the gold electrode surface through a thiol linker. 2 ns of a 5 ns simulation is shown only. Video is rendered using VMD ¹.

S2 (b): 3 ns video of a 5 ns simulation of the thrombin-aptamer complex under the influence of a -1.0 Vnm⁻¹ is provided. The thrombin does not dissociate but its secondary structure changes due to the stress induced by the high electric field. Video is rendered using VMD¹.

References

1. Humphrey, W., Dalke, A. & Schulten, K. VMD: Visual molecular dynamics. *Journal of Molecular Graphics* **14**, 33-38 (1996).