Supplementary Material (ESI) for Chemical Communications

The effect of DNA aptamer configuration on the sensitivity of detection thrombin at surface by acoustic method

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Supporting information

Kinetics analysis of the aptamer binding to a solid support

The time-dependent changes of the frequency and the resistance can be expressed as:

$$-\Delta f_S\,(t) = -(\Delta f_S)_{max}\,[1-\exp(-kt)] \qquad (1)$$
$$\Delta R_m\,(t) = (\Delta R_m)_{max}\,[1-C_R\exp(-kt) + (C_R-1)\exp(-2kt)] \qquad (2)$$

Thus, changes of the frequency could be approximated by first order reaction, while those of R_m are characterized by second order reaction. The fit of frequency changes using Eq. (1) allows to determine $(\Delta f_S)_{max}$ and k. The fit of resistance changes by means of Eq. (2) and using the k value determined from the fit of frequency changes results in $(\Delta R_m)_{max}$ and C_R. The parameter C_R indicates the contribution of viscous forces. If C_R is close to unity, the contribution of viscous forces is relatively low and the first order kinetics holds also for resistance changes. At equilibrium conditions the values $(\Delta f_S)_{max}$, $(\Delta R_m)_{max}$ and C_R can be used for estimation of shear modulus G (see Lucklum et al.[1]). However, as it has been pointed[1], the shear modulus of the layer remains error sensitive, therefore we restricted only by analysis of the kinetics of Δf_S and ΔR_m. The example of the kinetics of the changes of resonant frequency and motional resistance for the layers with highest and lowest $\Delta R_m/\Delta f_S$ ratio, i.e. for BF and BFH aptamers, respectively are shown on Fig. 1S.

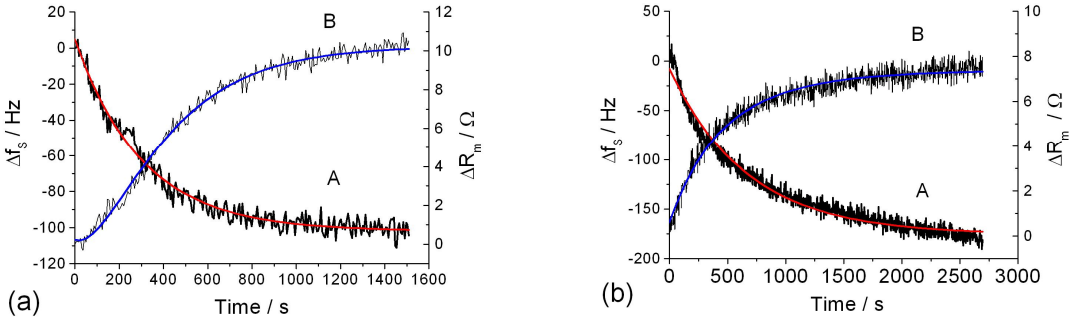

Fig.1S**.** The kinetics of the changes of resonant frequency, Δf_S, (A) and motional resistance, ΔR_m (B) and the fit (full lines) by equations (1) and (2) for frequency and resistance changes, respectively, following of addition of: (a) – BF aptamers, (b) – BFH aptamers at the time t=0. The fit has been performed by least square method using OriginPro version 7.5 (Microcal Software Inc., USA).

Also the fit of the corresponding curves using Eqs. (1) and (2) are presented. As expected the time course of the frequency changes is well fitted by first order reaction, while second order fit holds for changes of resistance. At the same time for most rigid layer, BFH, the C_R value was 1.2±0.5, which is close to the properties of rigid neutravidin layer[1]. Thus, for this layer also the changes of resistance could be close to the first order reaction kinetics. At the same time, for most flexible aptamers the C_R value was higher (1.85±0.3), which suggest substantial contribution of viscous effect. The C_R values for BFA and BFF

aptamers were 1.0±0.3 and 1.4±0.2, respectively. The results obtained are in agreement with those based on analysis of relative changes of resistance and suggest decreased viscoelastic contribution for aptamer layers composed of rigid supporting part (Table 2). The decay times $\tau = 1/k$ estimated according to Eq. (1) for all aptamers studied are shown in Table 2. It is interesting that the decay time for BF aptamers is larger in comparison with those of BFA aptamers. This may be caused by a more rigid support for this aptamer that facilitates faster ordering of the oligonucleotides at the surface, in comparison with more random BF aptamer configuration. The decay time of BFA aptamers is comparable to those of BFF configuration. Significantly larger decay time for aptamer heterodimers (BFH) may be connected with larger length of this configuration in comparison with other aptamers. Due to the increased length, more extensive interactions with neighboring aptamers can be expected, which could cause extension of the decay time.

Reference

1 R. Lucklum, S. Doerner, T. Schneider, B. Schlatt-Masuth, T. Jacobs and P. Hauptmann, *IEEE Int. Freq. Contr. Symp. Proceedings*, 2006, 528.

Table 1. The nucleotide sequences of aptamers analyzed. The underlined nucleotides in the sequence of BFH aptamers indicate differences in composition of binding sites of the heterodimer. BF is conventional single stranded aptamers. BFA, BFF and BFH aptamers contains except biotinylated strand also second strand.

Aptamer	Strand No.	The nucleotide sequence in 5' to 3' direction
BF	1	GGT TGG TGT GGT TGG $(A)_9(T)_{18}$-BIOTIN
BFA	1	GGT TGG TGT GGT TGG $(A)_9(T)_{18}$-BIOTIN
	2	$(A)_{18}$
BFF	1	GGT TGG TGT GGT TGG $(A)_9(T)_{18}$-BIOTIN
	2	$(A)_{18}(G)_9$ GGT TGG TGT GGT TGG
BFH	1	GGT TGG **TG**T GG**T** TGG $(A)_9(T)_{18}$-BIOTIN
	2	$(A)_{18}(G)_{21}$ GGT **A**GG G**CA** GGT TGG

Table 2. The properties of the biosensor based on various aptamers configurations. Mw is molecular weight of aptamers, τ is the decay time, Δf_S and ΔR_m are changes of series resonant frequency and motional resistance, respectively following adsorption of aptamers onto the neutravidin layer, K_D is the dissociation constant, LOD is limit of detection of the thrombin. The aptamer abbreviations are identical with those presented on Fig. 1. The results are mean±S.D. obtained from five independent experiments in each series.

Apta-mer	Mw, kDa	τ, min	$-\Delta f_S$, Hz	ΔR_m, Ω	$\Delta R_m/\Delta f$ Ω/Hz	Δm/Mw, 10^{-3} nM	K_D, nM	LOD, nM
BF	13.6	3.4±2.4	64±11	8.9 ± 3.9	0.14±0.06	6.6±1.1	110 ± 43	3.9
BFA	19.1	1.7±0.9	115±22	6.0 ± 2.9	0.05±0.03	8.3±1.6	7,3 ± 2,1	1.6
BFF	26.9	1.4±0.5	79±16	4.5 ± 1.3	0.06±0.02	4.1±0.8	8,6 ± 1,8	3.6
BFH	30.9	12±6	180±12	6.5 ± 1.6	0.04±0.01	8.1±0.5	2.3±0.7	0.4