Protein Binding for Detection of Small Changes on Nanoparticle Surface

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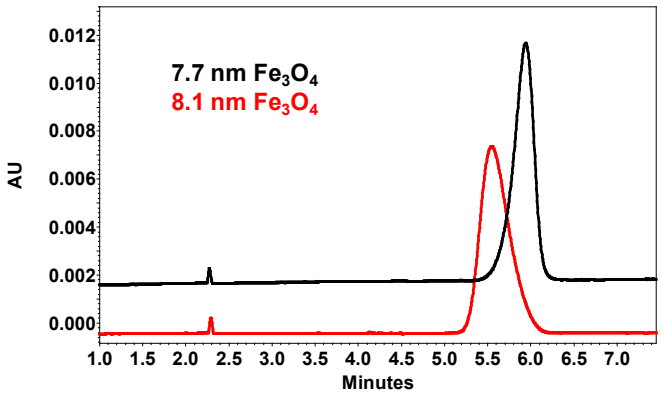
Supporting information

Figure S1. The electropherograms of PAA-Fe_3O_4 nanoparticles for zeta-potential measurement and calculation.



$$\xi = \frac{\mu_e \bullet \eta}{\varepsilon} = \frac{\mu_e \bullet \eta}{\varepsilon_0 \bullet \varepsilon_r} = \frac{\mu_e \bullet 8.90E-4}{8.854187817E-12 \bullet 78.4}$$

Figure S2. The mass spectrum of standard PAA obtained by ESI-LTQ-MS. The A series PAA is shown in regular front, while the B series PAA is in italic. The m/z range 680-850 is selectively shown to display details.

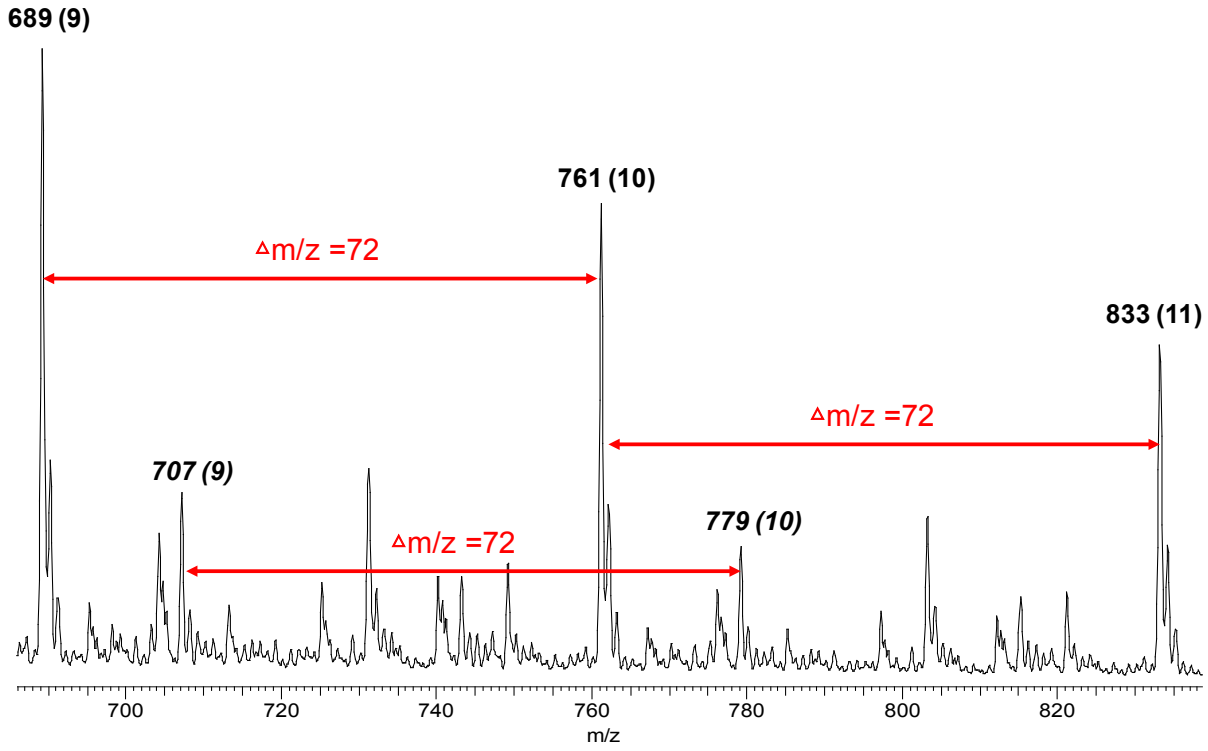


Figure S3. a) The intensity ratio of PAA series (a/b) measured on an Agilent 6210 multi-mode liquid chromatography-time of flight-mass spectrometer (LC-TOF-MS). Sample ionization was performed under the conditions of ESI and atmospheric-pressure chemical ionization. The ratio changes with heating duration; b) the mass spectra for hydrolyzed PAA obtained by ESI-TOF-MS. Four time points are selectively shown to demonstrate the trend.

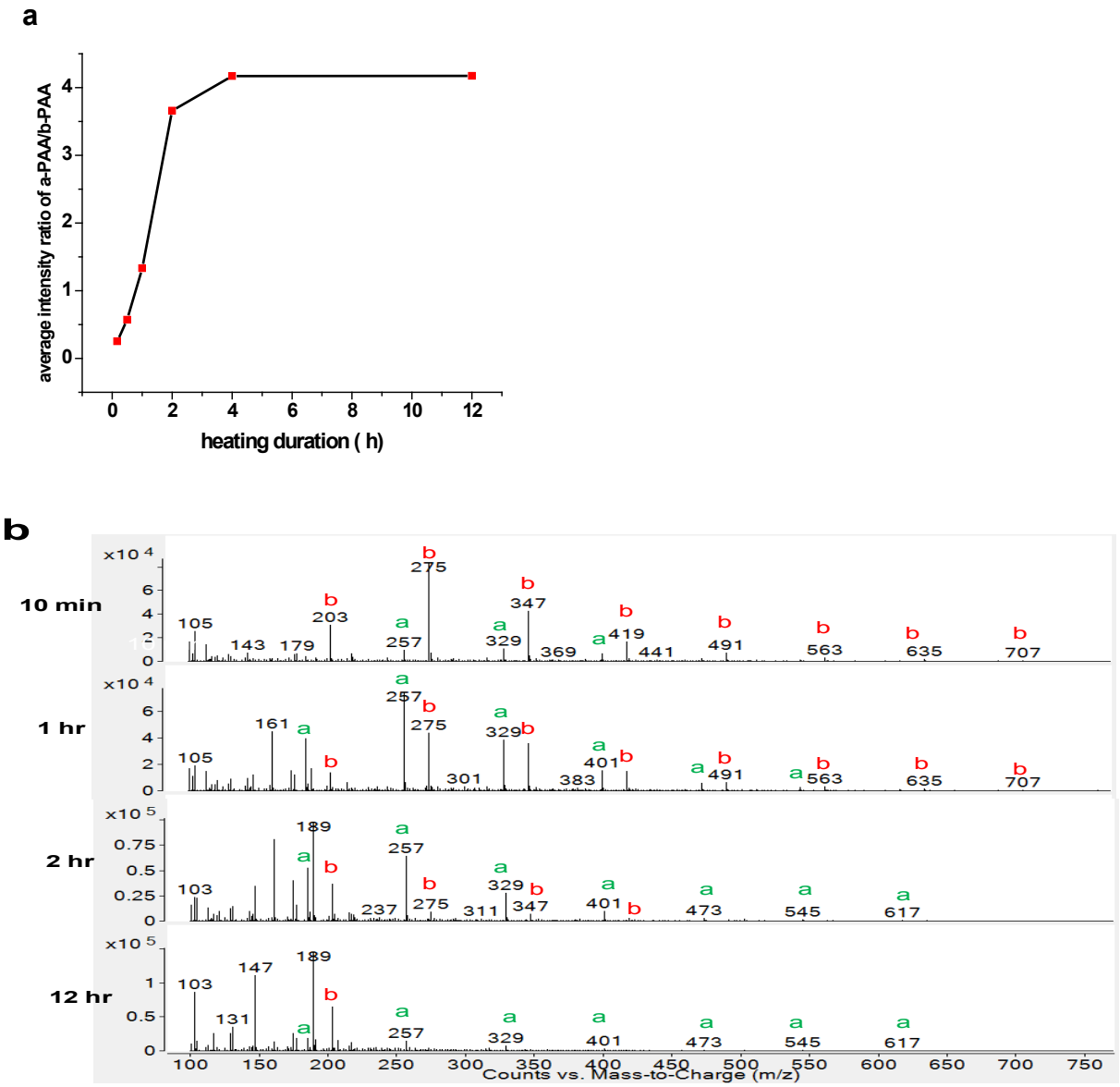


Figure S4. a) 1H NMR spectra for standard and hydrolyzed PAA; b) HSQC and c) COSY NMR spectra for standard PAA.

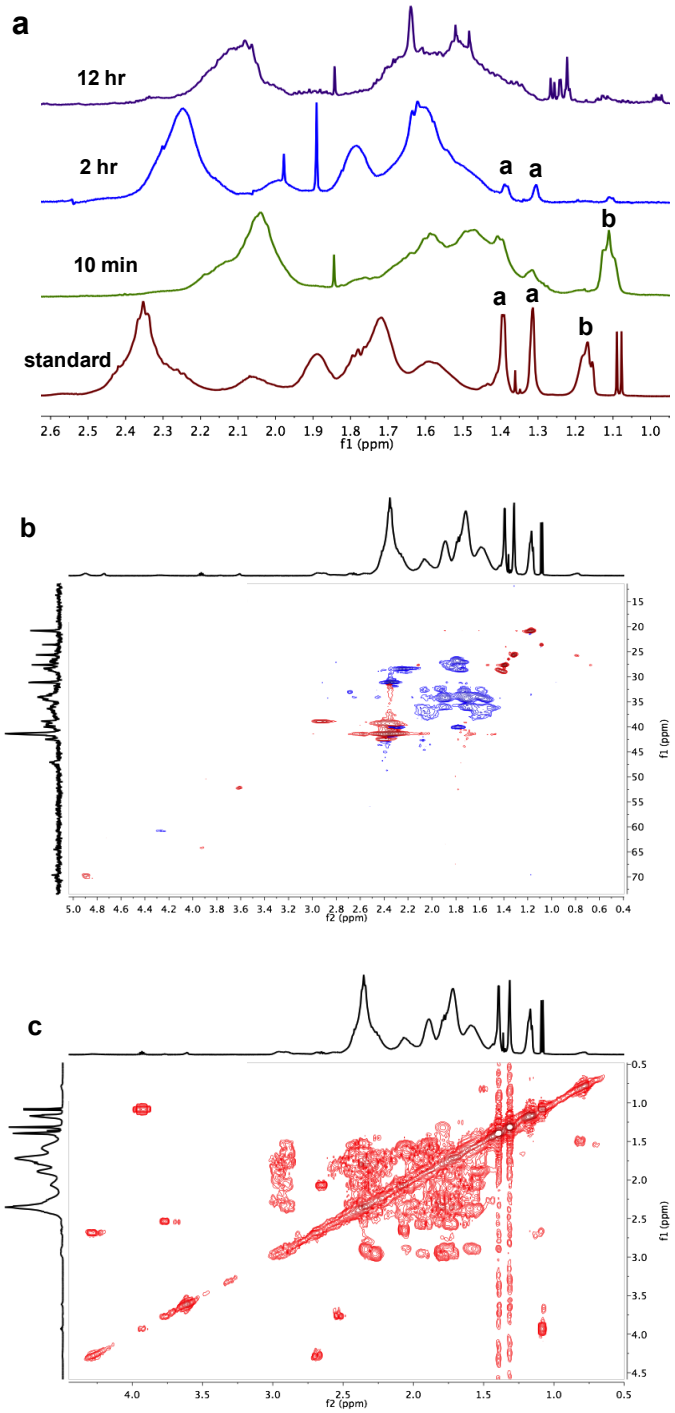


Figure S5. a) The eletropherograms and b) the affinity curve fitted by Hill equation for the interaction between calmodulin (CaM) and 7.7 nm PAA-Fe_3O_4 NPs measured by affinity capillary electrophoresis in 17.5 mM phosphate buffer.

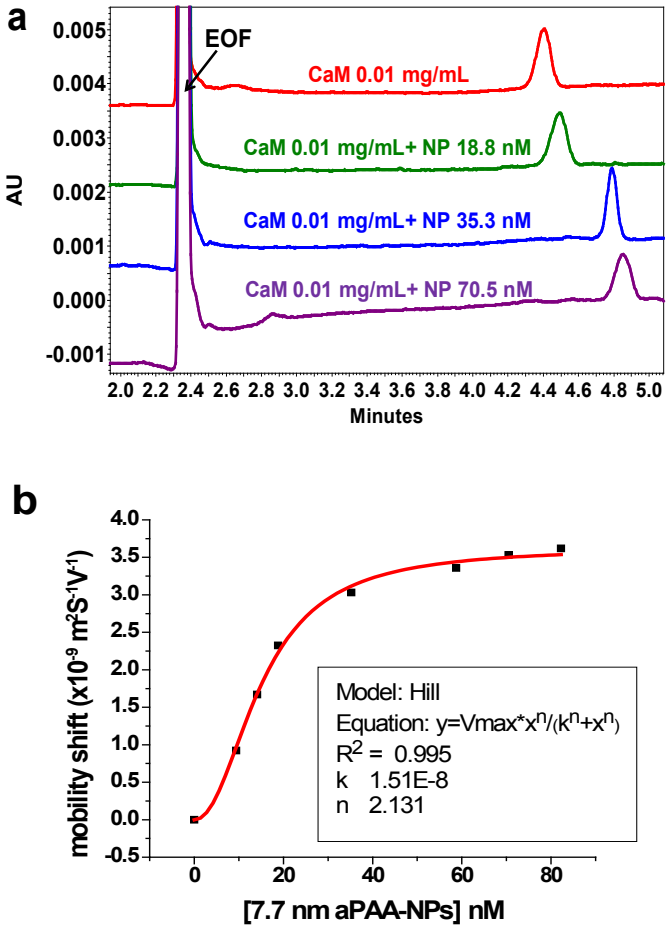


Table S1. Calculated energy of HGA and HGB to the default binding cavity of calmodulin.

polymer fragment	binding free energy (kcal/mol)	vdw energy (kcal/mol)	electrostatic energy (kcal/mol)
Head group A	-3.79	-6.34	+0.76
Head group B	-1.52	-3.59	-0.02

Table S2: Calculated binding free energy of HGA and HGB to selected proteins.

polymer fragment	Binding free energy (kcal/mol)		
	Cytochrome c	**Myoglobin**	**HSA site 2**
Head group A (HGA)	-8.29~ -10.1	-5.42~ -6.46	-8.4~ -9.28
Head group B (HGB)	-6.14~ -7.88	-3.34~ -4.64	-6.24~ -7.34