

Supporting Information

Grafting Nitrilotriacetic Groups onto Carboxylic Acid-Terminated Self-Assembled Monolayers on Gold Surfaces for Immobilization of Histidine-Tagged Proteins

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Table S1. IR peak assignment of the SAMs before and after the coupling.

Table S2. XPS peak assignment of the SAMs before and after the coupling.

Table S3. Comparison between the experimentally determined atomic percentages from XPS data and the theoretical values calculated for different coverages in the SAM of *C15-COOH*.

Table S4. Comparison between the experimentally determined atomic percentages from XPS data and the theoretical values calculated for different coverages in the SAM of *EG3-COOH*.

Table S5. Comparison between the experimentally determined atomic percentages from XPS data and the theoretical values calculated for different coverages in the SAM of *EG5-COOH*.

Figure S1. SPR signals on non-specific adsorption of GFPs on COOH-terminated SAMs of (a) C15-COOH, (b) EG3-COOH, and (c) EG5-COOH. Each set of the experiments (indicated by the numbers) was performed with a different flow rate and a different concentration of the GFP protein solution (1: 5 $\mu\text{L}/\text{min}$ and 0.01 mg/mL, 2: 5 $\mu\text{L}/\text{min}$ and 0.1 mg/mL, 3: 20 $\mu\text{L}/\text{min}$ and 0.1 mg/mL, 4: 10 $\mu\text{L}/\text{min}$ and 0.1 mg/mL).

Table S1. IR Peak Assignment of the SAMs before and after the Coupling.

Band Frequency (cm ⁻¹)				
C15-COOH	C15-NTA	EG3-COOH	EG3-NTA	Mode
		EG5-COOH	EG5-NTA	
		2930 sh	2934 sh	$\nu_a(\text{CH}_2)$ of EG
2917	2918	2918	2918	$\nu_s(\text{CH}_2)$ of alkyl
		2870	2872	$\nu_a(\text{CH}_2)$ of EG
2848	2849	2856 sh	2856 sh	$\nu_s(\text{CH}_2)$ of alkyl
1738	1721	1750	1748	$\nu(\text{C=O})$ free
1718				$\nu(\text{C=O})$ hydrogen bonded
	1677 sh		1670	Amide I
	1550		1554	Amide II
1470	1407	1465	1355	$\delta(\text{CH}_2)$
		1133	1133	$\nu(\text{C-O})$

Table S2. XPS Peak Assignment of the SAMs before and after the Coupling.

Binding Energy (eV)				
EG3-COOH	C15-NTA	EG3-NTA	EG5-NTA	Core level
	856	856	856	Ni 2p _{3/2}
763	763	763	763	Au 4s
643	643	643	643	Au 4p _{1/2}
547	547	547	547	Au 4p _{3/2}
531	531	531	531	O 1s
	402	402	402	N 1s
354	354	354	354	Au 4d _{3/2}
336	336	336	336	Au 4d _{5/2}
284.6	284.6	284.6	284.6	C 1s
89	89	89	89	Au 4f ₅
85	85	85	85	Au 4f ₇

Table S3. Comparison between the Experimentally Determined Atomic Percentages from XPS Data and the Theoretical Values Calculated for Different Coverages in the SAM of *C15-COOH*.

	50% theoretical	30% theoretical	25% theoretical	20% theoretical	Experimental
%C	72.41	76.00	77.08	78.26	89.42
%O	18.96	16.39	15.62	14.78	6.02
%S	3.45	3.72	4.17	4.35	2.36
%N	3.45	2.40	2.08	1.74	1.50
%Ni	1.72	1.20	1.04	0.87	0.70
N/S	1	0.65	0.50	0.40	0.63

Table S4. Comparison between the Experimentally Determined Atomic Percentages from XPS Data and the Theoretical Values Calculated for Different Coverages in the SAM of *EG3-COOH*.

	50% theoretical	30% theoretical	25% theoretical	20% theoretical	experimental
%C	66.66	68.75	69.35	70.00	85.07
%O	26.38	25.31	25	24.67	11.96
%S	2.27	3.10	3.22	3.33	2.40
%N	2.27	1.87	1.61	1.33	1.20
%Ni	1.13	0.94	0.80	0.67	0.40
N/S	1	0.60	0.50	0.40	0.49

Table S5. Comparison between the Experimentally Determined Atomic Percentages from XPS Data and the Theoretical Values Calculated for Different Coverages in the SAM of *EG5-COOH*.

	50% theoretical	30% theoretical	25% theoretical	20% theoretical	experimental
%C	66.66	68.43	68.92	69.44	68.04
%O	27.38	26.56	26.35	26.11	26.81
%S	2.38	2.63	2.70	2.78	3.26
%N	2.38	1.58	1.35	1.11	1.53
%Ni	1.19	0.79	0.67	0.55	0.35
N/S	1	0.60	0.50	0.40	0.47

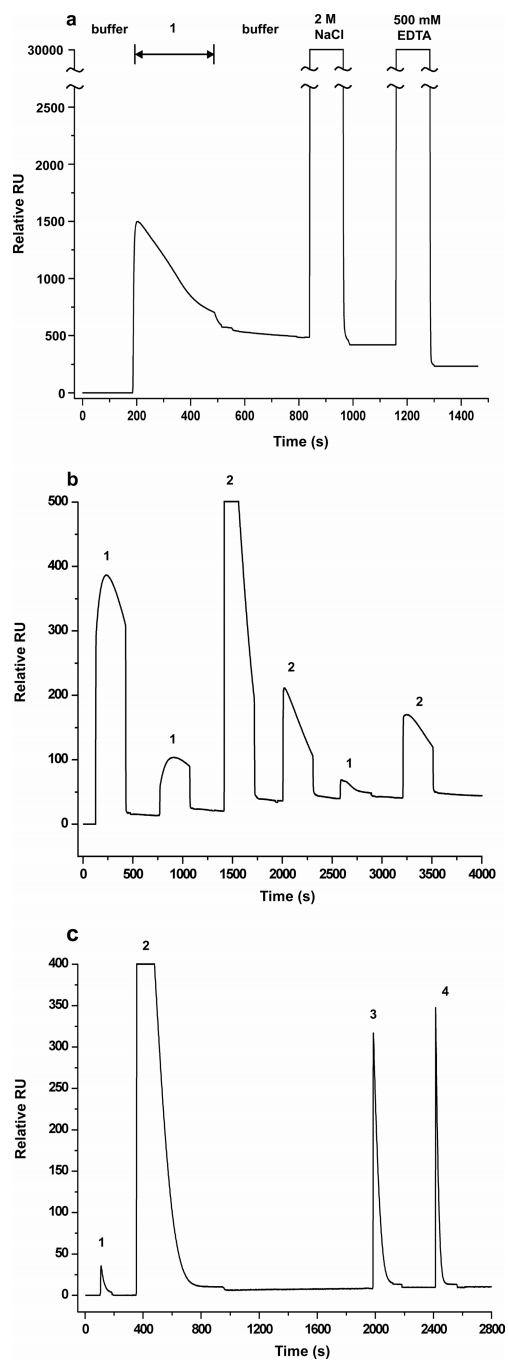


Figure S1