

Electronic Supplementary Information for

Catechol-Cation adhesion on the silica surfaces: molecular dynamics simulations

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Table S1 Force field parameters for silica

<i>Atom</i>	σ (nm)	ε (kJ·mol ⁻¹)	<i>Charge</i> (e)
Si	0.415	0.389	+1.1, +0.725 ^a
O (bulk)	0.347	0.226	-0.55
O (silanol)	0.347	0.510	-0.675, -0.9 ^a
H	0.1085	0.063	+0.40
Na ⁺	0.317	0.393	+1.0
<i>Bonds</i>	r_0 (nm)	K_r (kJ·mol ⁻¹ ·nm ⁻²)	
Si-O	0.168	238488	
O-H	0.0945	414216	
<i>Angles</i>	θ_0 (°)	K_θ (kJ·mol ⁻¹ ·rad ⁻²)	
O-Si-O	109.5	836.8	
Si-O-Si	149.0	836.8	
Si-O-H	115.0	418.4	

^a Sodium siloxide groups require +0.725e for Si and -0.9e for O.

Table S2. The amounts of sodium and chlorine ions in each simulation system

System	0%-0.2		0%-0.5		9%-0.2		9%-0.5		18%-0.2		18%-0.5	
	Na ⁺	Cl ⁻	Na ⁺	Cl ⁻	Na ⁺	Cl ⁻	Na ⁺	Cl ⁻	Na ⁺	Cl ⁻	Na ⁺	Cl ⁻
TLC	16	20	41	45	19	16	44	41	26	16	51	41
TAC	16	20	41	45	19	16	44	41	26	16	51	41
THC	16	20	41	45	19	16	44	41	29	16	54	41

Table S3. Global free energy minimum of siderophore analogues adhesion on silica surfaces

estimated by umbrella sampling^a

System		PMF (kJ·mol ⁻¹)	
Surfaces	Siderophore	Concentration (M)	
	analogues	0.2	0.5
0% ionization	TLC	-1.9±0.2	-2.3±0.2
	TAC	-5.1±0.5	-4.3±0.4
	THC	-3.8±0.4	-3.7±0.3
9% ionization	TLC	-11.1±0.6	-5.5±0.5
	TAC	-16.4±0.8	-9.2±0.5
	THC	-21.9±1.0	-19.0±1.2
18% ionization	TLC	-27.7±1.2	-15.6±1.0
	TAC	-23.7±0.6	-12.1±0.2
	THC	-10.2±0.5	-6.2±0.4

^a Lower values correspond to stronger adhesion.

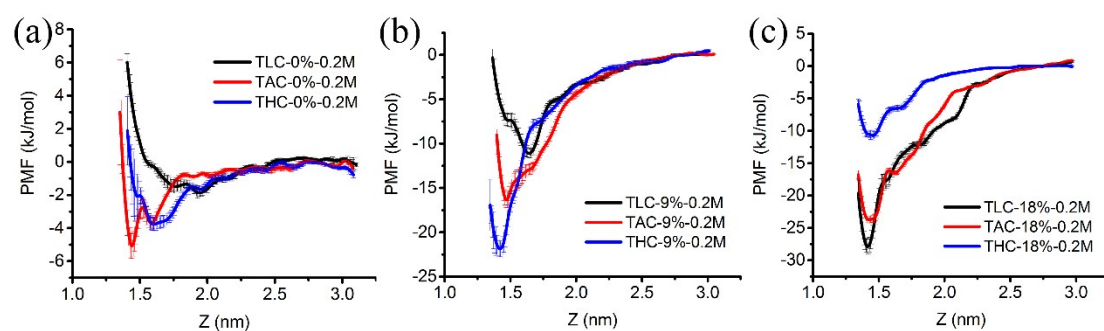


Figure S1. PMF profiles for the adhesion of TLC, TAC and THC onto silica surfaces under 0.2M NaCl solutions. Effect of cationic amino acids on their adhesion on silica surfaces are shown.

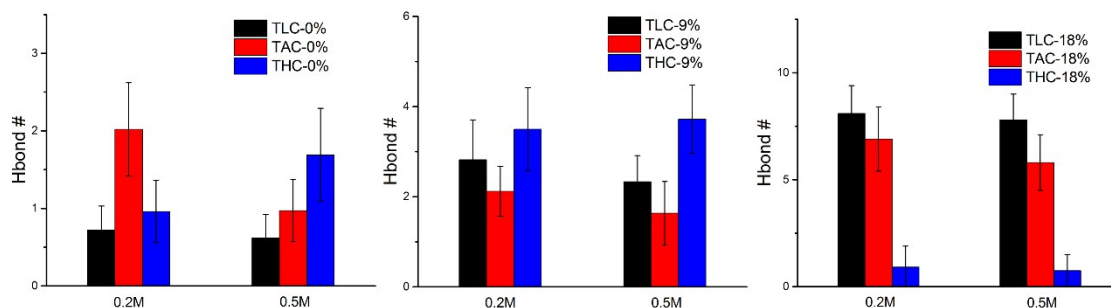


Figure S2. Average numbers and standard deviations of H-bonds formed between siderophore analogues and silica.

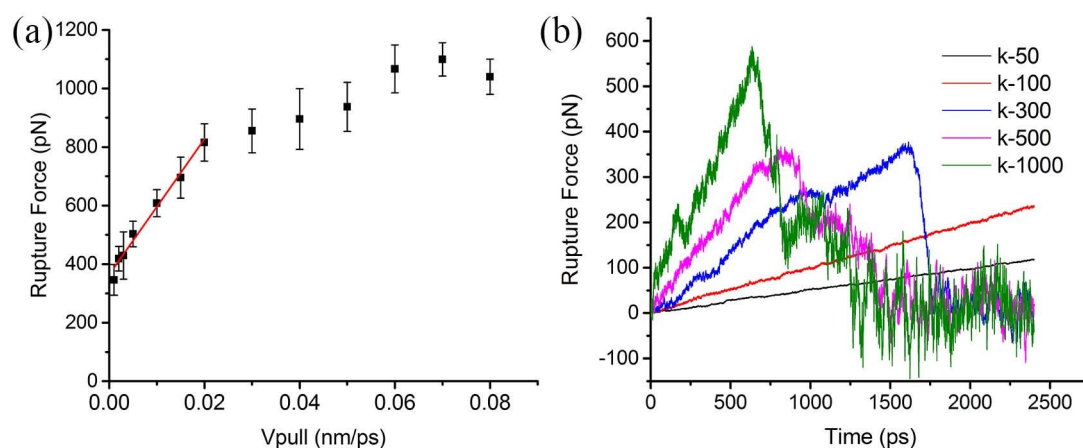


Figure S3. Assessment of pulling velocity and spring constant for the adhesion of TLC onto the silica surface (18% silanol ionization) under 0.2M NaCl solutions. (a) Computed rupture force as a function of pulling velocity V_{pull} . The error bars give an estimated uncertainty. The red line shows a linear fit to the computed forces for V_{pull} less than 0.02 nm·ps⁻¹. (b) Influence of different spring constants on the pulling force under the pulling velocity of 0.001 nm·ps⁻¹.

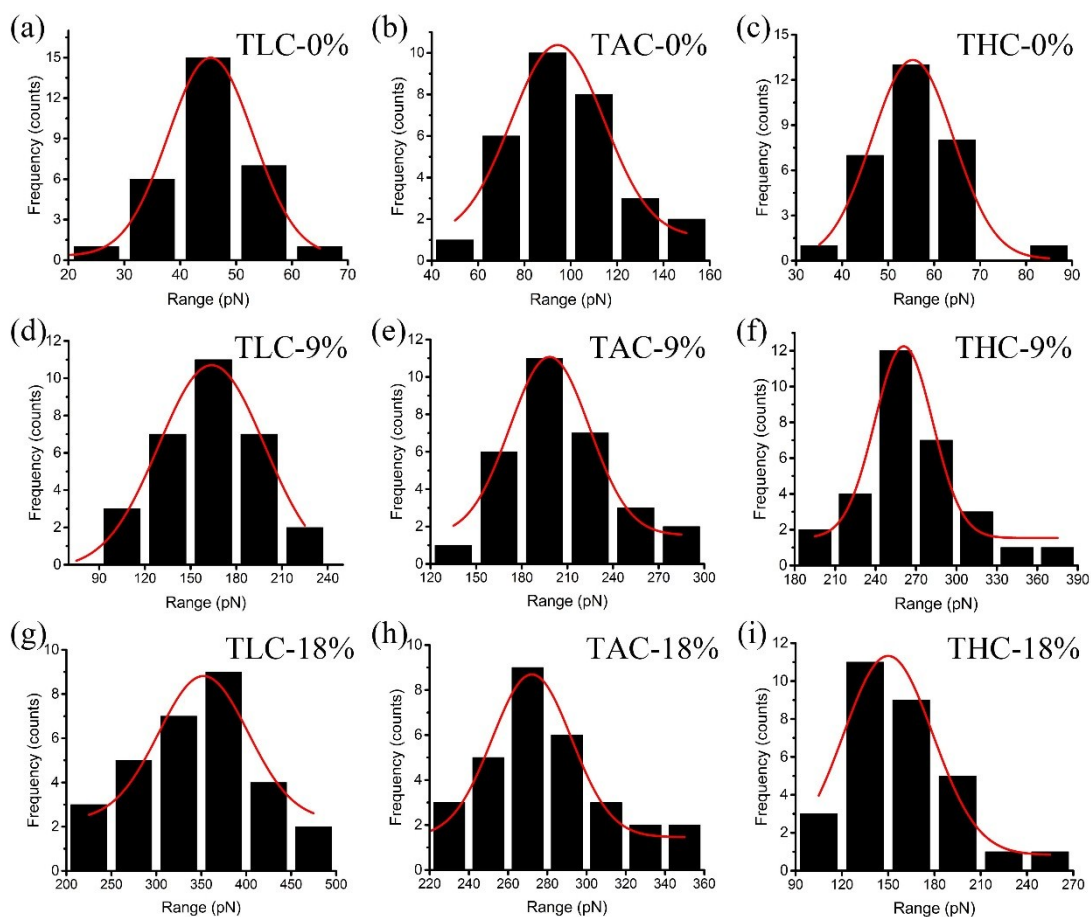


Figure S4. The histograms for rupture forces of TLC, TAC and THC onto silica surfaces for 0% (a)-(c), 9% (d)-(f) and 18% (g)-(i) silanol ionization under 0.2M NaCl solution. Each red line corresponds to a Gaussian fit.

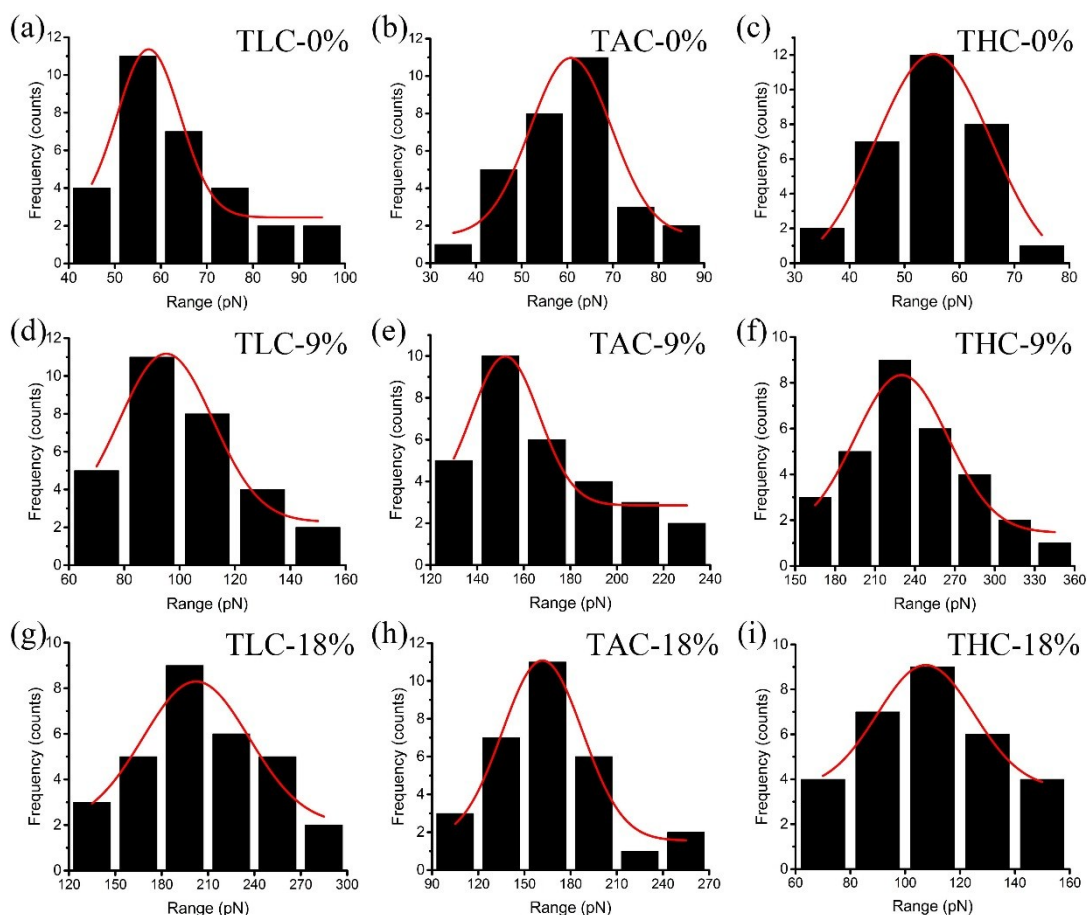


Figure S5. The histograms for rupture forces of TLC, TAC and THC onto the silica surface for (a)-(c) 0%, (d)-(f) 9% and (g)-(i) 18% silanol ionization under 0.5M NaCl solutions. Every red line corresponds to a Gaussian fit.

Table S4 Rupture forces of siderophore analogues adhered on silica surfaces estimated by SMD and derivatives of the PMF from umbrella sampling.

System		Rupture Force (pN)			
Surfaces	Siderophore analogues	SMD		Derivatives of the PMF	
		Concentration (M)		Concentration (M)	
		0.2	0.5	0.2	0.5
0% ionization	TLC	46±7	57±9	26±2	38±4
	TAC	94±20	60±9	60±5	42±4
	THC	55±10	55±8	34±3	32±3
9% ionization	TLC	163±34	95±17	98±7	54±4
	TAC	198±33	152±15	125±10	92±8
	THC	260±29	230±35	184±16	130±13
18% ionization	TLC	352±50	202±34	228±20	147±14
	TAC	272±40	162±26	198±17	100±8
	THC	150±29	108±18	95±7	68±5

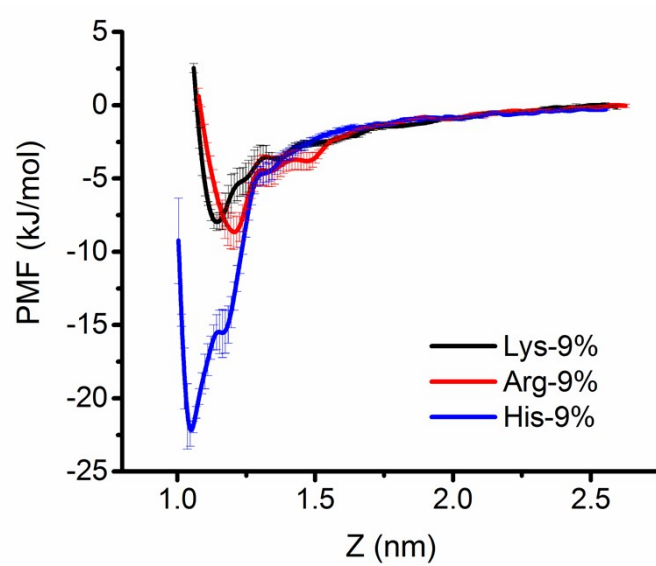


Figure S6. PMF profiles for the adhesion of Lys, Arg and His amino acids onto the silica surface (9% silanol ionization) under 0.2M NaCl solution. Adhesions of three single cationic amino acids on the negatively charged silica surface are shown above.