

## Rationally designed Protein A surface molecularly imprinted magnetic nanoparticles for the capture and detection of *Staphylococcus aureus*

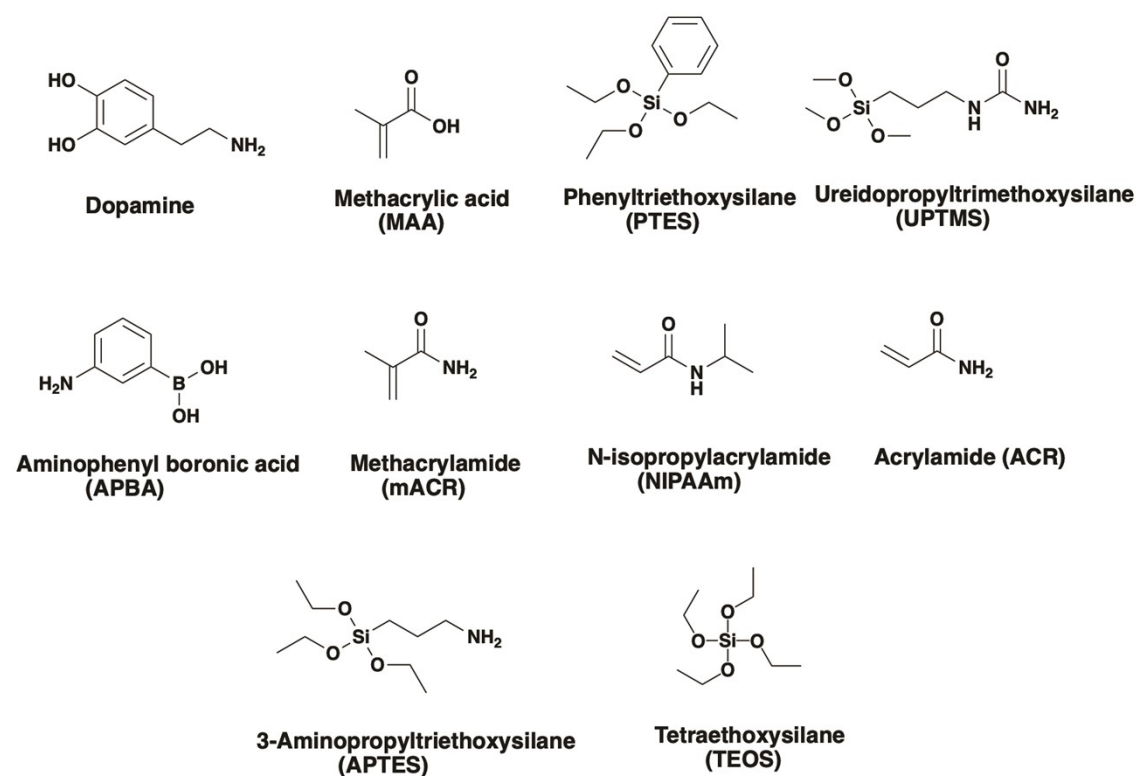
(Supplementary Information)

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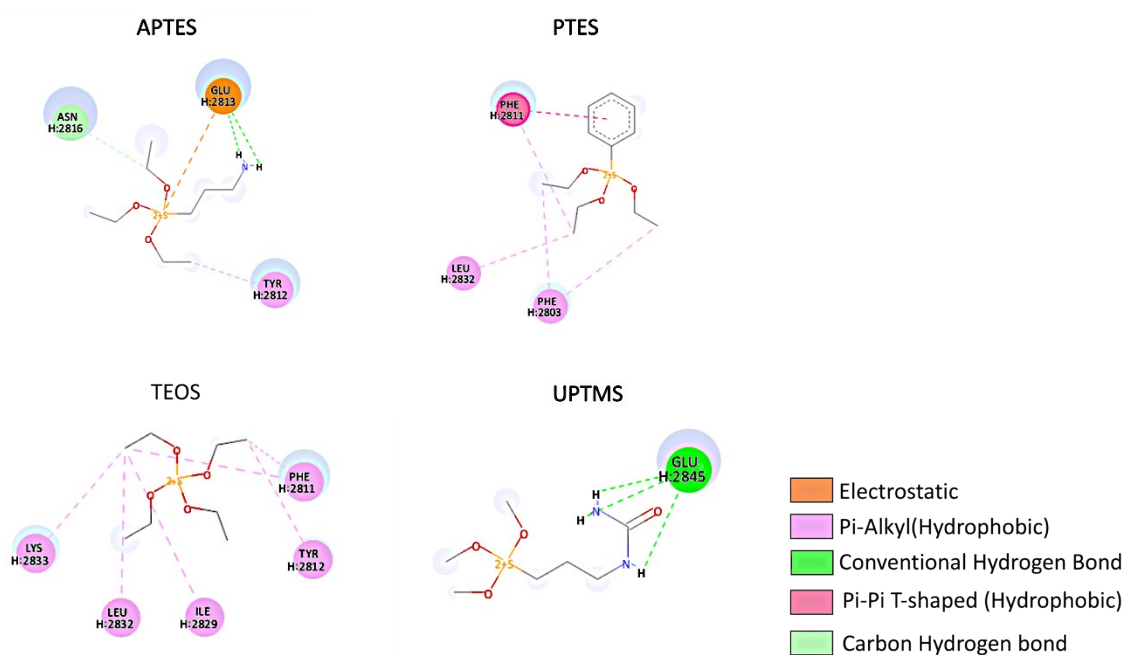
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**Fig. S1** Complete set of monomers used for monomer screening using molecular docking.

**Table S1** Surface composition (in atomic percentage) of nanoparticles at different steps of molecular imprinting.

	Carbon	Oxygen	Silicon	Iron
$\text{Fe}_3\text{O}_4$	36.413	48.368	--	15.219
$\text{Fe}_3\text{O}_4@\text{SiO}_2$	17.282	53.741	3.811	25.165
APTES coating	17.998	60.73	3.999	17.272
Glutaraldehyde functionalization	28.13	52.061	3.479	16.33
MIP	22.21	53.256	3.775	20.758
NIP	18.833	48.487	4.931	27.749



**Fig. S2** 2D-diagram representing interaction between selected monomers and the Protein

A

**Table S2** The fitting parameters for Langmuir, Freundlich and Hill equation model

Model	Parameters	MMIPs	MNIP
Langmuir isotherm	Equation	$C_e/q_e = 1/(q_{max}K_L) + C_e/q_{max}$	
		$C_e/q_e = 0.17C_e - 0.50$	
	$q_{max}$ (mg g <sup>-1</sup> )	5.74	
	$K_L$ (mL mg <sup>-1</sup> )	-0.34	
	$R^2$	0.92	
Freundlich isotherm	Equation	$\ln q_e = (1/n)\ln C_e + \ln K_f$	
		$\ln q_e = 0.50\ln C_e + 1.16$	$\log q_e = 0.64\ln C_e - 1.59$
	$K_f$ (mg g <sup>-1</sup> )	3.18	0.09
	$n_f$	1.99	0.76
	$R^2$	0.94	0.82
Hill isotherm	Equation	$q_e = q_{max} * x^n / (k^n + x^n)$	
	$q_{max}$	10.93	
	$K_d$ (mg mL <sup>-1</sup> )	9.33	
	$n$	15.21	
	$R^2$	0.99	

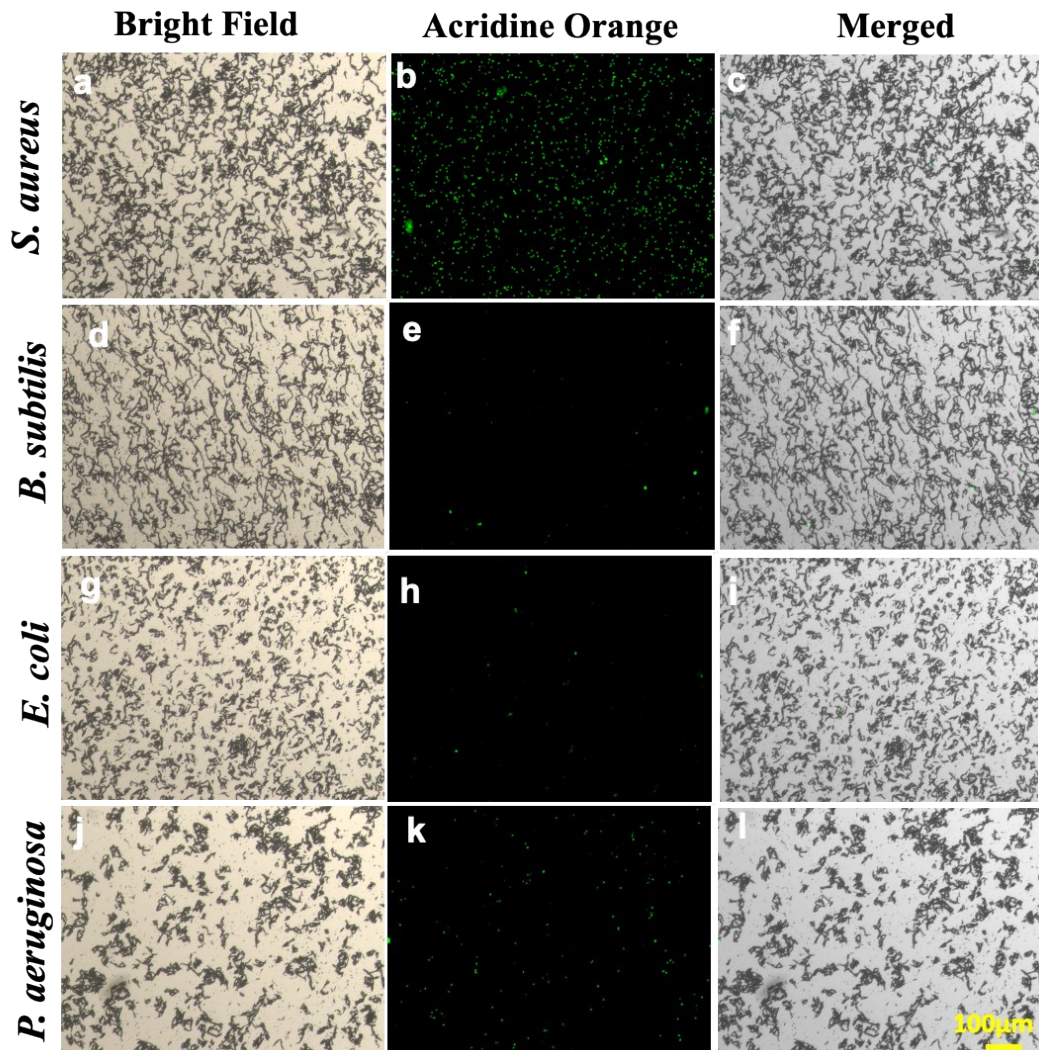


Fig. 53 Fluorescence microscope images of different bacteria treated with MIP. a), b) and c) show bright field, fluorescence, and merged image of *S. aureus* treated with MIP. d), e) and f) show bright field, fluorescence, and merged image of treated *B. subtilis* with MIP. g), h) and i) show bright field, Fluorescence, and merged image of treated *E. coli* with MIP. j), k) and l) showed bright field, Fluorescence, and merged image of treated *P. aeruginosa* with MIP.