Supporting Information

Nonionic nontoxic antimicrobial polymers: Indole-grafted poly(vinyl alcohol) with pendant alkyl or ether groups

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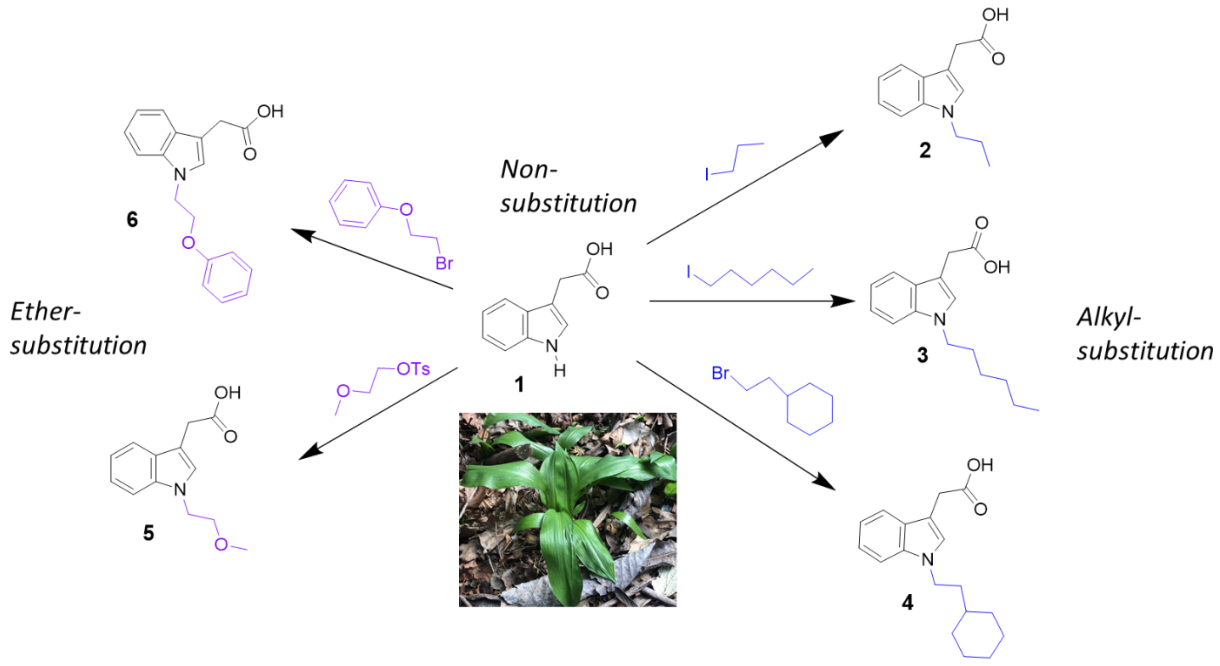

Scheme S1. Synthesis of grafting agents **2-6** from indole-3-acetic acid (**1**), which widely exists in nature, such as wild garlic (the plant shown in the scheme).

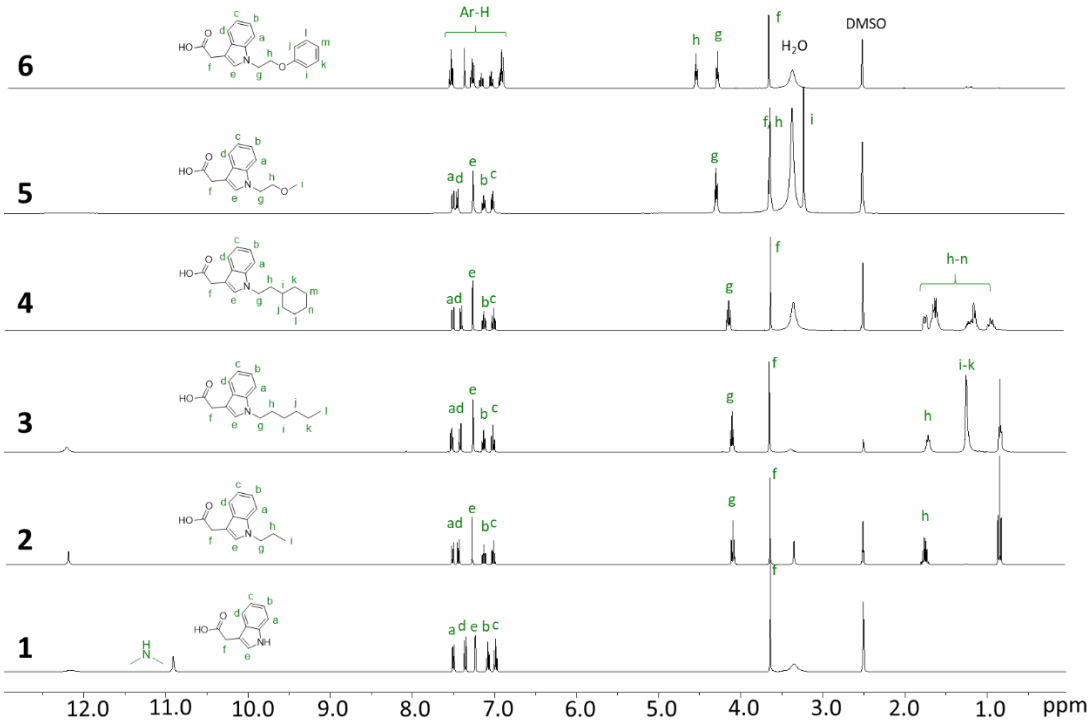

Figure S1. ^{1}H NMR spectra of indole carboxylic acids with different *N*-substituents (**1-6**) in DMSO-d_6.

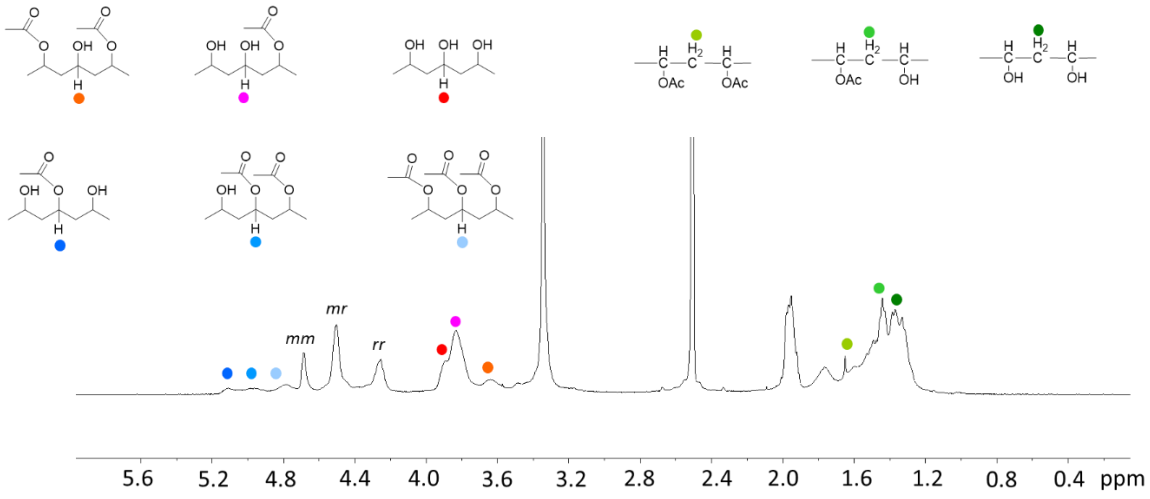

Figure S2. Zoomed-in ^{1}H NMR spectrum of PVA in DMSO-d_6.

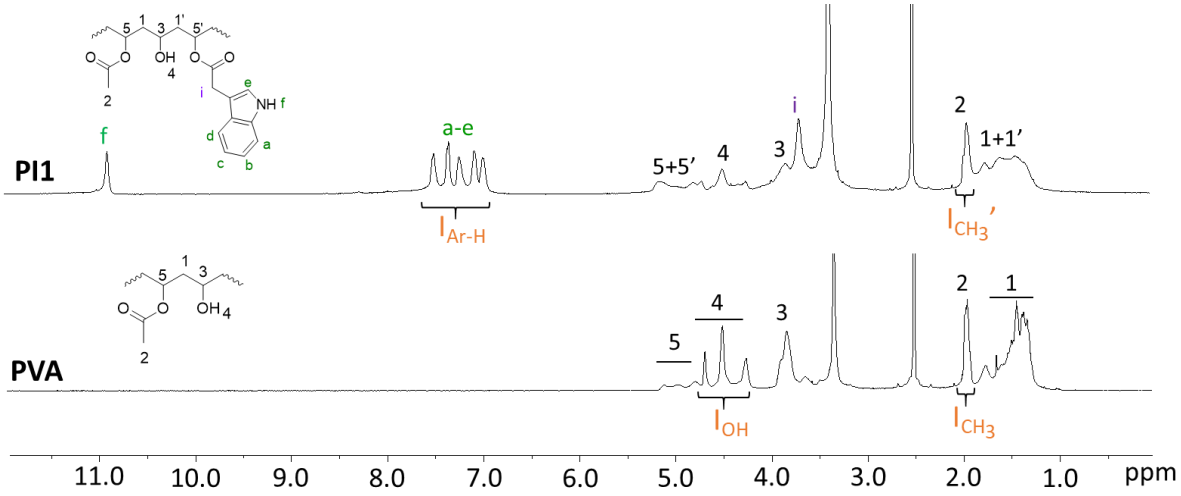

Figure S3. ^{1}H NMR spectra of PVA and indole-based PVA (**PI1**). The integrals for the calculation of OH conversion (p_{OH}) are marked. The p_{OH} value of **PI1** was calculated according to the equation below and the result is shown in Table 1. The integrals of the two spectra are normalized to make $I_{CH3}=I_{CH3'}$ (suppose that the methyl groups did not change before and after the grafting reaction).

$$pOH = \frac{I_{Ar-H}/5}{I_{CH_3}'} / \frac{I_{OH}}{I_{CH_3}}$$

The p_{OH} values of **PI2-5** were calculated using the same equation as above.

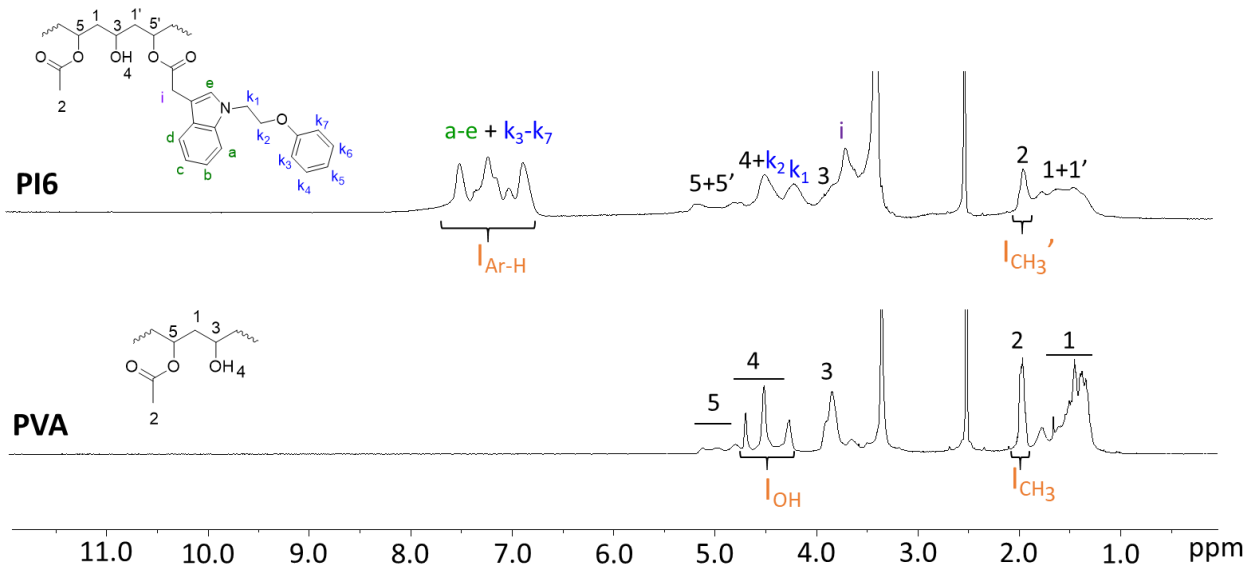

Figure S4. ^{1}H NMR spectra of PVA and indole-based PVA (**PI6**). The integrals for the calculation of OH conversion (p_{OH}) are marked. The p_{OH} value of **PI6** was calculated according to the equation below and the result is shown in Table 1. The integrals of the two spectra are normalized to make $I_{CH3}=I_{CH3'}$ (suppose that the methyl groups did not change before and after the grafting reaction).

$$pOH = \frac{I_{Ar-H}/10}{I_{CH_3}'} / \frac{I_{OH}}{I_{CH_3}}$$

Table S1. Solubility of **PI1-6** at room temperature with the concentration 1 mg/mL. + means soluble, (+) means partially soluble and – means insoluble.

Solvent	**PI1**	**PI2**	**PI3**	**PI4**	**PI5**	**PI6**
Chloroform	–	+	+	+	+	+
THF	(+)	(+)	+	+	+	+
DMF	+	+	+	+	+	+
DMSO	+	+	+	+	+	+
DMAc	+	+	+	+	+	+
Water	–	–	–	–	–	–
Ethanol	(+)	(+)	(+)	(+)	(+)	(+)

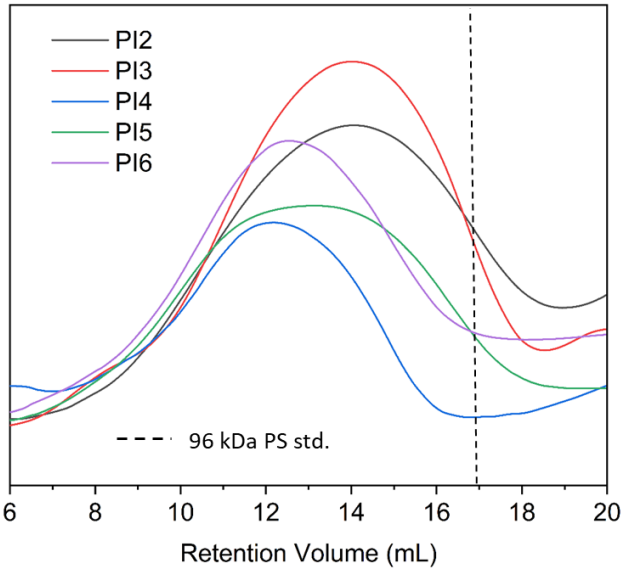

Figure S5. GPC chromatograms in chloroform of the refractive index of **PI2-6**. The retention volume of a polystyrene standard (PS, M_n ~96 KDa) was indicated as the dashed line.

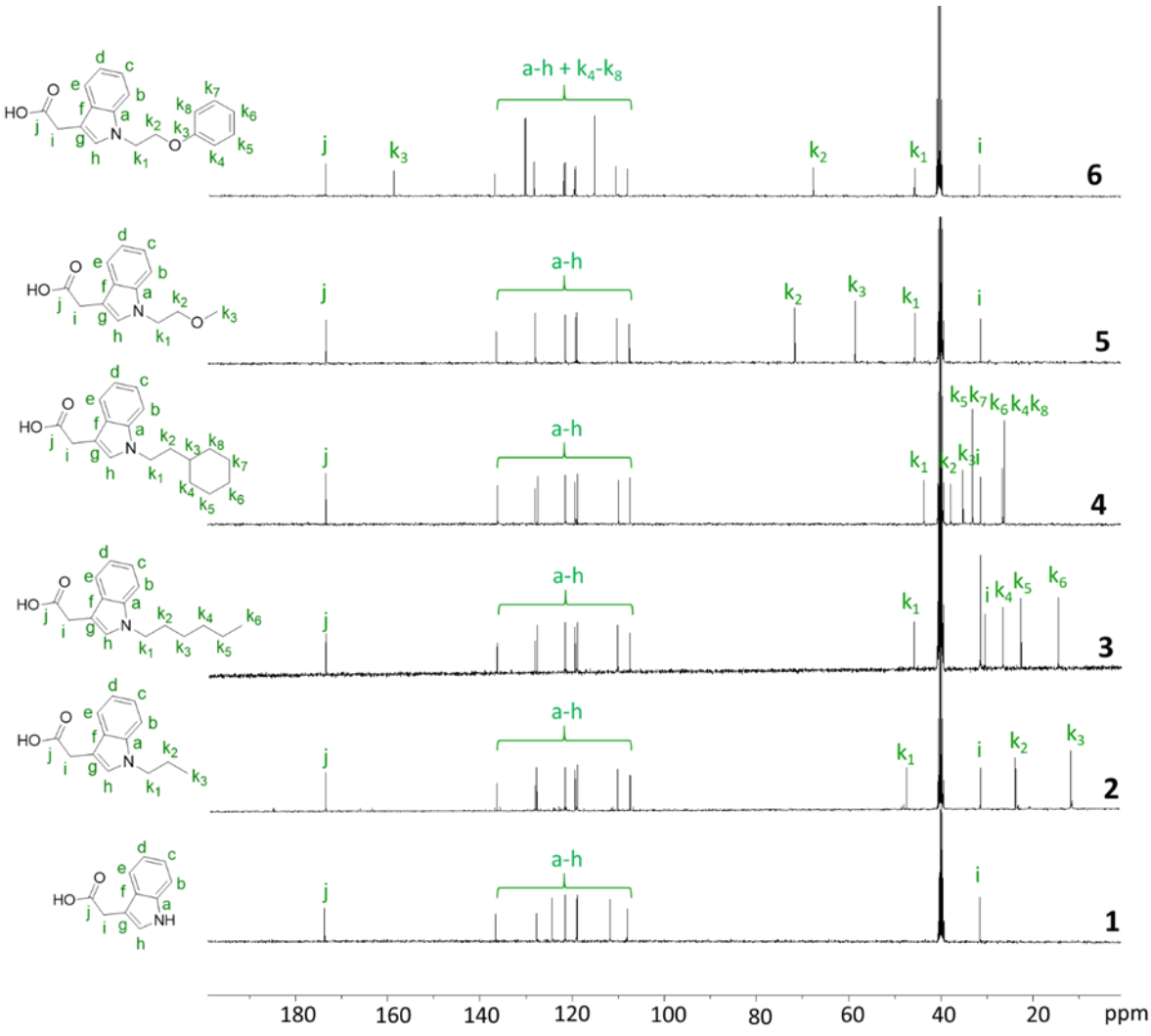

Figure S6. ^{13}C NMR spectra of indole-based carboxylic acid agents **1-6** in DMSO-d_6.

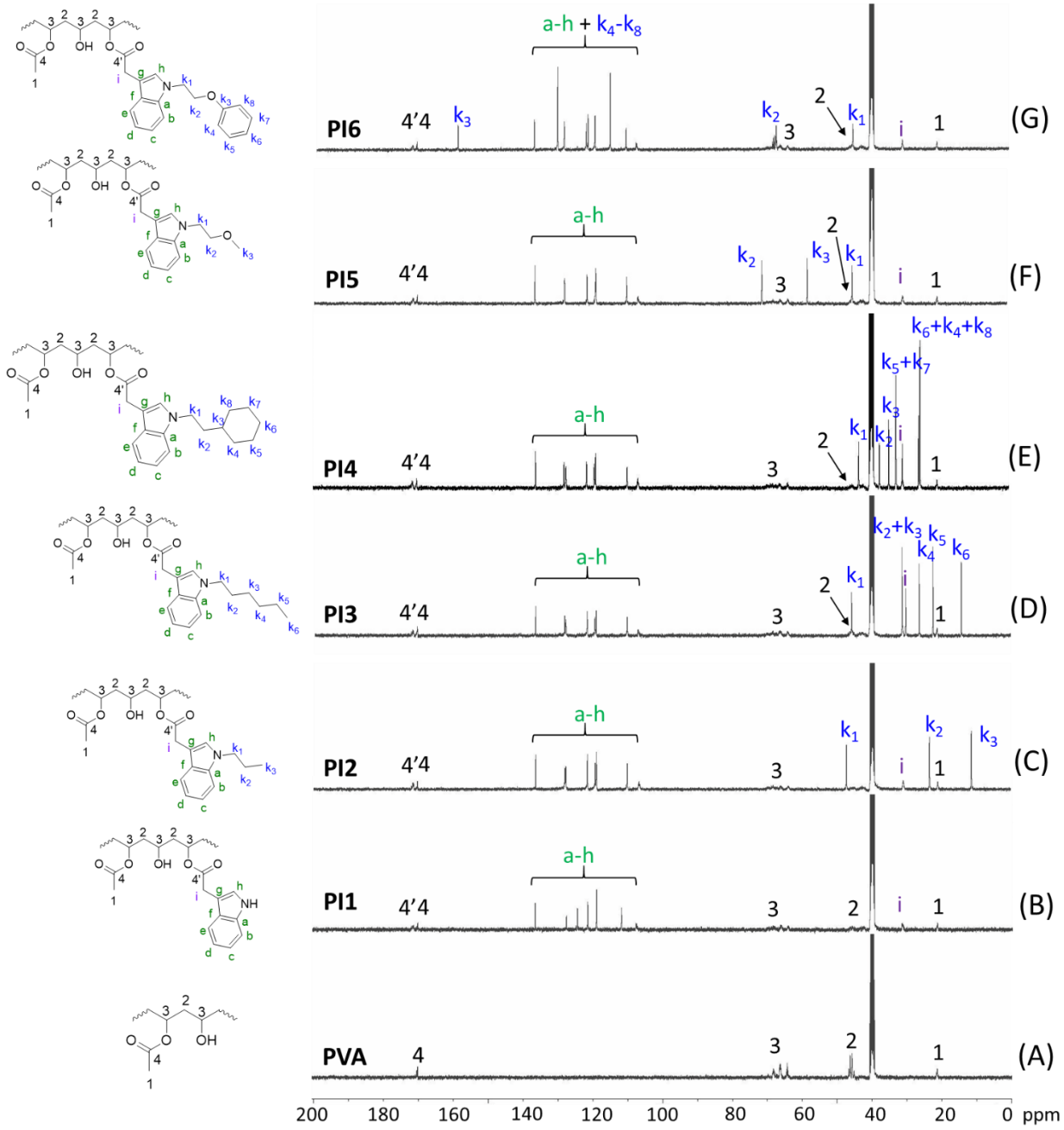

Figure S7. ^{13}C NMR spectra of (A) initial PVA and (B-G) indole-based **PI1-6** in DMSO-d_6.

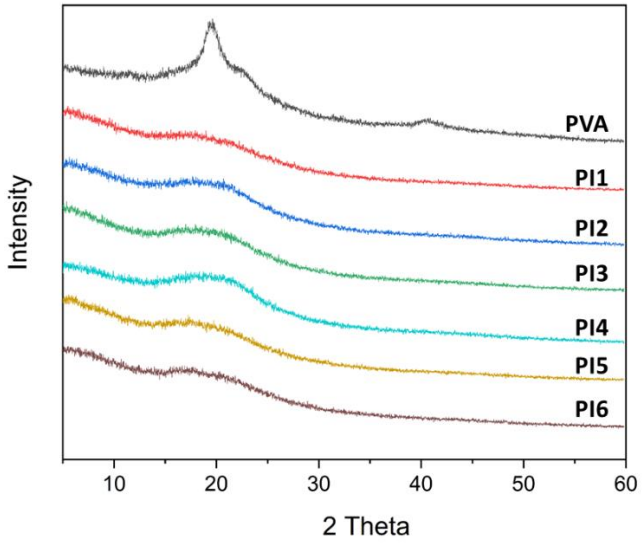

Figure S8. WAXD patterns of initial PVA and indole-grafted PVAs (**PI1-6**).

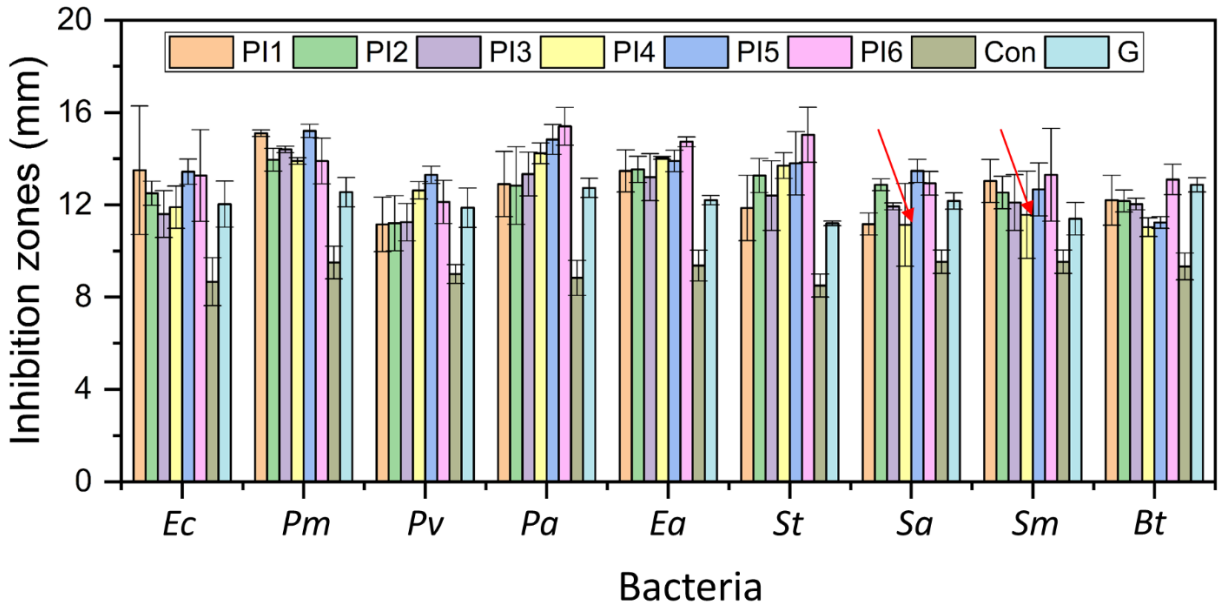

Figure S9. Inhibition zone of **PI1-6**. Pure DMF was used as negative control (marked as Con in the figure). Gentamicin (G) was used as positive control (10 µg per disk). The only two cases where the zones of inhibition did not show significant difference compared to negative control are indicated by red arrows (*p* values ≥ 0.05, Table S1, ESI). Bacteria: *Escherichia coli* (*Ec*), *Proteus mirabilis* (*Pm*), *Proteus vulgaris* (*Pv*), *Pseudomonas aeruginosa* (*Pa*), *Enterobacter*

aerogenes (*Ea*), *Salmonella typhimurium* (*St*), *Staphylococcus aureus* (*Sa*), and *Streptococcus mutans* (*Sm*), and *Bacillus thuringiensis* (*Bt*). The error bars stand for standard deviations.

Table S2. *p* values to identify the "significant difference" between **PI1-6** and control (Con). Numbers in black color indicate significant difference ($p<0.05$), and numbers in blue color indicate no significant difference ($p\geq0.05$)

	p value					
	PI1-Con	**PI2**-Con	**PI3**-Con	**PI4**-Con	**PI5**-Con	**PI6**-Con
Ec	0.048	0.005	0.025	0.016	0.002	0.023
Pm	0.008	0.018	0.011	0.013	0.009	0.036
Pv	0.014	0.013	0.003	0.000	0.000	0.001
Pa	0.011	0.020	0.003	0.000	0.000	0.001
Ea	0.003	0.001	0.005	0.000	0.001	0.000
Se	0.018	0.001	0.013	0.000	0.003	0.001
Sa	0.015	0.001	0.001	0.211	0.001	0.001
Sm	0.005	0.003	0.028	0.146	0.012	0.034
Bt	0.005	0.003	0.002	0.014	0.006	0.002

Table S3. *p* values to identify the "significant difference" between **PI1-6** and gentamicin (G). Numbers in black color indicate no significant difference ($p \geq 0.05$), the numbers in red color indicate significantly lower ($p < 0.05$), and the numbers in green indicate significantly higher ($p < 0.05$).

	p value					
	PI1-G	**PI2**-G	**PI3**-G	**PI4**-G	**PI5**-G	**PI6**-G
Ec	0.439	0.513	0.626	0.873	0.101	0.391
Pm	0.031	0.133	0.057	0.010	0.033	0.246
Pv	0.358	0.393	0.329	0.159	0.022	0.707
Pa	0.854	0.925	0.373	0.013	0.009	0.007
Ea	0.078	0.019	0.169	0.000	0.004	0.000
Se	0.461	0.035	0.242	0.002	0.031	0.005
Sa	0.042	0.048	0.351	0.383	0.021	0.100
Sm	0.072	0.119	0.435	0.893	0.893	0.235
Bt	0.362	0.097	0.021	0.003	0.002	0.606

Table S4. *p* values to identify the "significant difference" between **PI2-6** and **PI1**. Numbers in black color indicate no significant difference ($p \geq 0.05$), the numbers in red color indicate significantly lower ($p < 0.05$), and the numbers in green indicate significantly higher ($p < 0.05$).

p value					
	PI2-PI1	**PI3-PI1**	**PI4-PI1**	**PI5-PI1**	**PI6-PI1**
Ec	0.574	0.329	0.398	0.969	0.911
Pm	0.088	0.038	0.014	0.698	0.232
Pv	0.954	0.893	0.054	0.013	0.243
Pa	0.961	0.682	0.193	0.097	0.057
Ea	0.919	0.751	0.341	0.501	0.078
Se	0.203	0.678	0.105	0.165	0.041
Sa	0.005	0.056	0.976	0.004	0.020
Sm	0.498	0.350	0.293	0.690	0.845
Bt	0.963	0.808	0.155	0.206	0.285

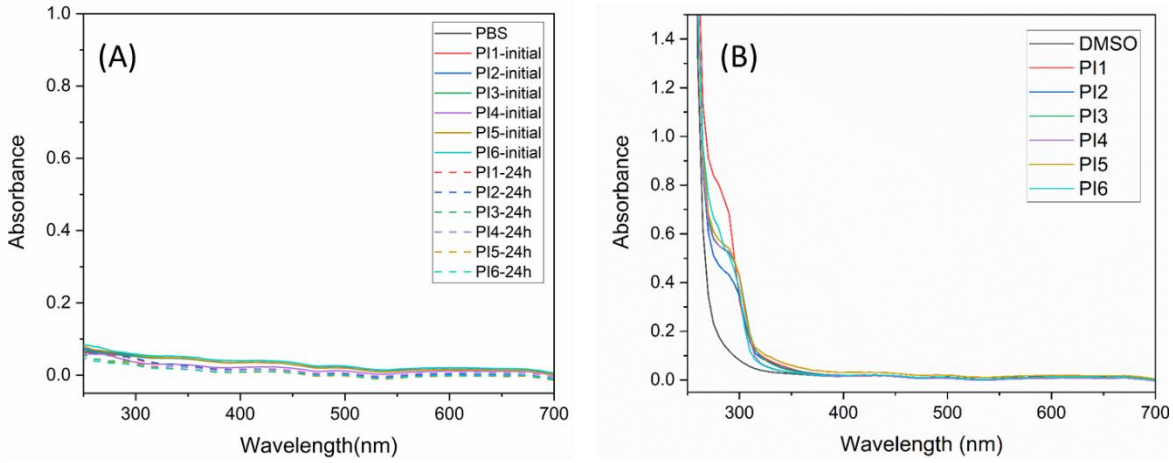

Figure S10. UV-vis absorbance spectra of (A) **PI1-6** in PBS solution (100 μg/mL). **PIX-initial** (X=1-6) were the initial results and **PIX-24h** (X=1-6) were the results after 24 h at 37 °C, and (B) **PI1-6** in DMSO (25 μg/mL) shown as references.

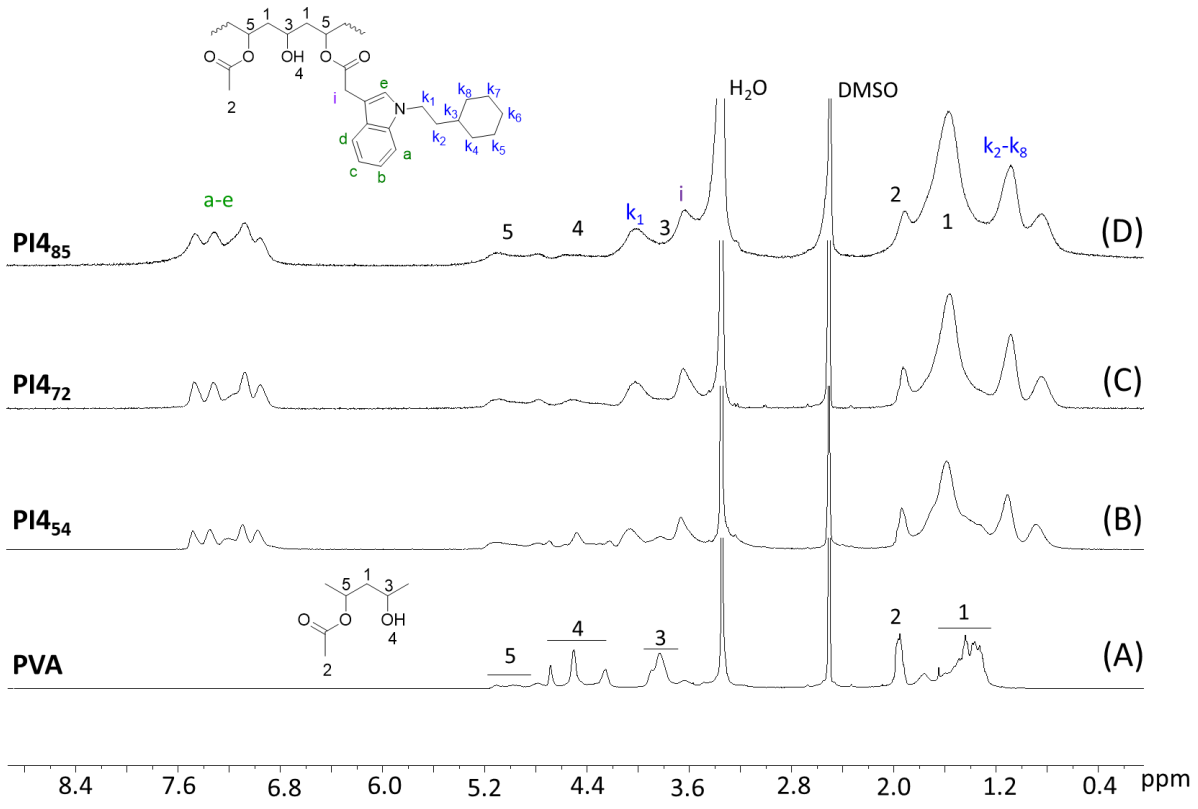

Figure S11. ^{1}H NMR spectra of (A) PVA, (B) **PI4$_{54}$**, (C) **PI4$_{72}$** and (D) **PI4$_{85}$** in DMSO-d$_6$.

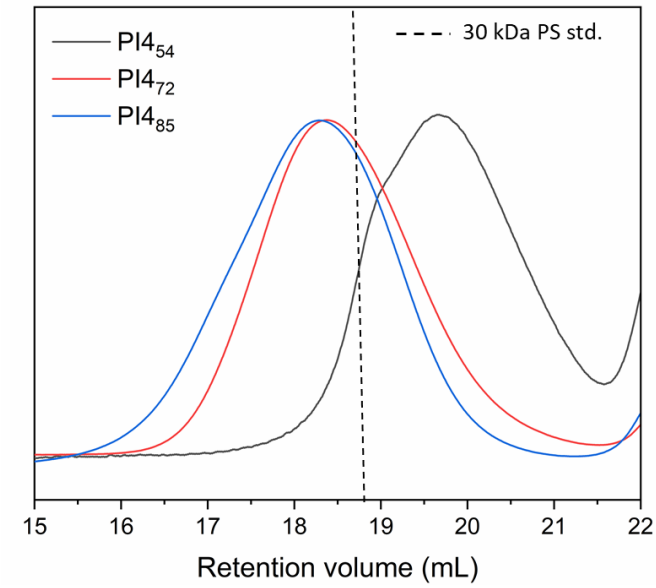

Figure S12.GPC chromatograms in THF of the refractive index of **PI4$_{54}$**, **PI4$_{72}$** and **PI4$_{85}$**. The retention volume of a polystyrene standard (PS, M_n ~30 KDa) was indicated as the dashed line.

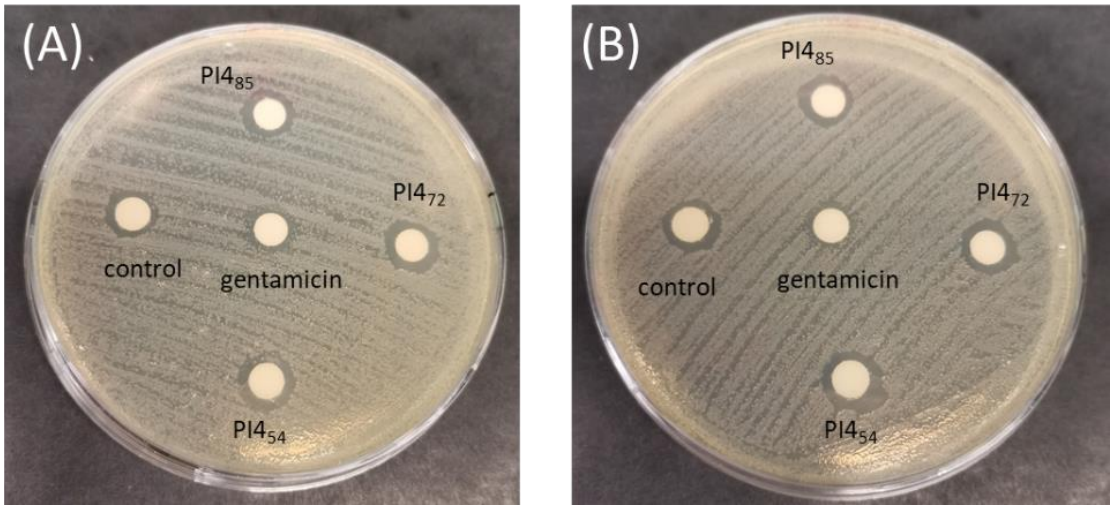

Figure S13. Plate images of disk diffusion test of **PI4$_{54}$**, **PI4$_{72}$** and **PI4$_{85}$**. Pure DMF and gentamicin (10 µg per disk) were used as negative and positive controls, respectively. Bacteria: *Escherichia coli* ATCC 8739 (A) and *Pseudomonas fluorescens* PCL 1701 (B).

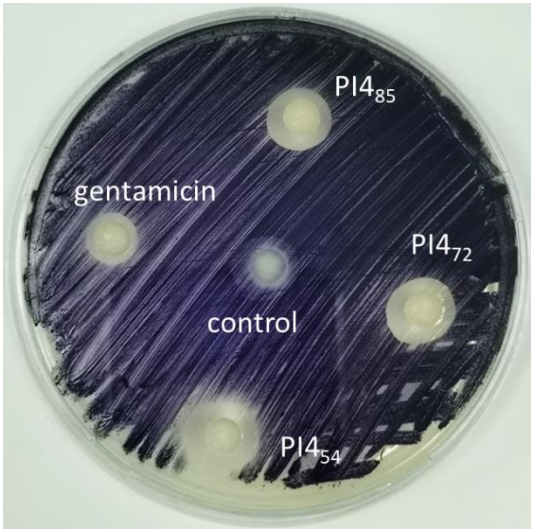

Figure S14. Photos of the plate diffusion assay of the tested samples for anti-QS evaluations. The pigment inhibition can be observed and measured by the turbid halo.

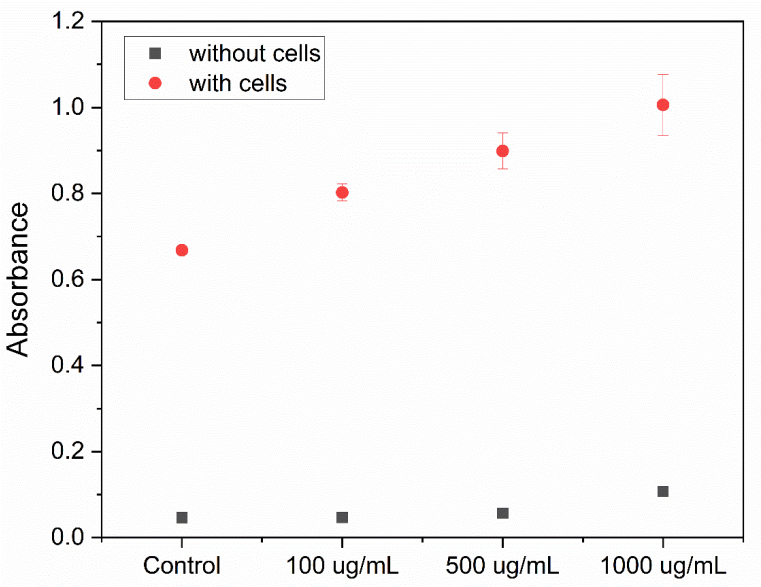

Figure S15. UV absorbance at 600 nm of **PI1** at three concentrations (100, 500 and 1000 µg/mL) in MTT assay. The control indicated with black dot represents the background, and the control indicated with red dot represents the negative control, corresponding to 100% of cell viability.