Supporting Information

Functionalized silver nanocapsules with improved antibacterial activity using silica shell modified by quaternary ammonium polyethyleneimine as bacterial cell-targeting agent

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RESULTS AND DISCUSSION

The dosage of silver nitrate. In the preparation of Ag@MSN, silver nitrate was used as silver resource, and its dosage affected the formation of silver core and final silver content of Ag@MSN. To optimize the appropriate dosage of silver nitrate, 1, 2, 3, 4, 5, 6, and 7 mL of silver nitrate were used respectively to synthesize Ag@MSN. And the obtained Ag@MSNs were evaluated for their silver contents, particle sizes, and antibacterial activities against *Pseudomonas syringae pv. Lachrymans*. The ICP-OES results indicated that the silver contents of Ag@MSN-1–7 were 1.34%, 2.43%, 3.49%, 4.08%, 4.36%, 4.44%, and 5.14%, respectively. The TEM images are presented in **Figure S1** and **Figure 4A** (5 mL of silver nitrate), which shows that with increase of the dosages of silver nitrate, the forming probabilities of core-shell Ag@MSN increased, but the particle diameters of Ag@MSN decreased (from 160 to 74 nm). The forming probabilities of core-shell Ag@MSN were close to 100% when silver nitrate was used more than 4 mL. As shown in **Table S1**, the control efficacies of Ag@MSNs against *Pseudomonas syringae pv. Lachrymans* at concentrations of 50 and 100 mg/L are 100%; and the order of the control efficacies of Ag@MSN-1–7 at concentration of 25 mg/L was Ag@MSN-7 > Ag@MSN-6 > Ag@MSN-5 > Ag@MSN-4 > Ag@MSN-3 > Ag@MSN-2 > Ag@MSN-1. The results indicated that the antibacterial activities of Ag@MSNs were associated with their silver contents closely. Moreover, when silver nitrate was used more than 4 mL, there was no significant difference on antibacterial activities. Therefore, 5 mL of silver nitrate was the optimum dosage for the preparation of Ag@MSN which possessed relatively low dosage of silver nitrate and remarkable antibacterial activities.

The molecular weight of PEI. The molecular weight of PEI is an important factor affecting biological activity. High molecular weight of QPEI will result in high charge density, which is conducive to the interaction of QPEI with negatively charged bacterial cell membrane.[1] However, as we mentioned previously, high molecular weight QPEI tends to form micelles to decrease its antibacterial activity. The previous work showed that QPEI with molecular weight of 25000 exhibited higher antibacterial activity and lower hemolytic activity than that with molecular weights of 1300 and 750000.[2] In the market, PEI with molecular weight of 600, 1800, 10000, and 70000 (50% aqueous solution) are widely available. Therefore, considering the above factors and convenience of synthesis, PEI with molecular weight of 10000 was chosen to conjugate with Ag@MSN in this work.

The quaternization reagent. In the quaternization reaction, two groups of quaternization reagent are frequently used, one group is haloalkanes (such as bromohexane and iodopropane) [2-8] and another group is propylene oxide and benzyl chloride.[9, 10] In this study, when haloalkanes were used as quaternization reagent, heating was necessary and bromohexane and iodopropane would react with silver core of Ag@MSN-PEI in the quaternization reaction. In contrast, propylene oxide and benzyl chloride would not react with silver core and the reaction conditions would be relatively mild. Consequently, propylene oxide and benzyl chloride were used as the quaternization reagent in this work.

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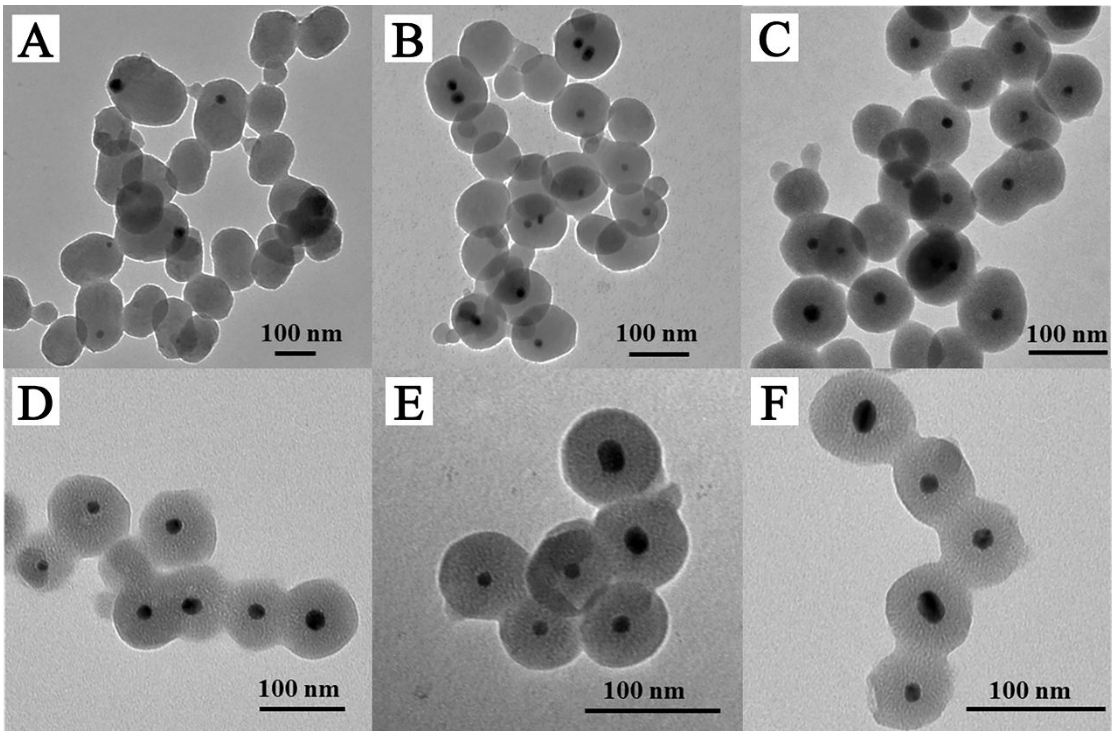

Figure S1. TEM images of Ag@MSN-1 (A), Ag@MSN-2 (B), Ag@MSN-3 (C), Ag@MSN-4 (D), Ag@MSN-6 (E), and Ag@MSN-7 (F).

Table S1. Silver contents, particle sizes, and antimicrobial activities against *Pseudomonas syringae pv. Lachrymans* of Ag@MSNs.

Ag@MSN	Usage of silver nitrate (mL)	Actual contents of Ag (%)	Particle diameter (nm)	Control efficacy of Ag@MSN at different concentrations (mg/L)		
				100	50	25
Ag@MSN-1	1	1.34	160	100%	100%	30.10 ± 3.26% f [a)]
Ag@MSN-2	2	2.43	120	100%	100%	57.20 ± 0.94% e
Ag@MSN-3	3	3.49	105	100%	100%	66.85 ± 1.33% d
Ag@MSN-4	4	4.18	95	100%	100%	84.67 ± 0.43% c
Ag@MSN-5	5	4.36	90	100%	100%	90.13 ± 0.70% b
Ag@MSN-6	6	4.44	80	100%	100%	91.80 ± 0.53% ab
Ag@MSN-7	7	5.14	74	100%	100%	94.16 ± 0.24% a

[a)] Values marked with letters are significantly different according to the Duncan test ($P < 0.05$).