Supplementary Information

Antimicrobial activity of silver sulfide quantum dots functionalized with highly conjugated Schiff bases in a one-step synthesis

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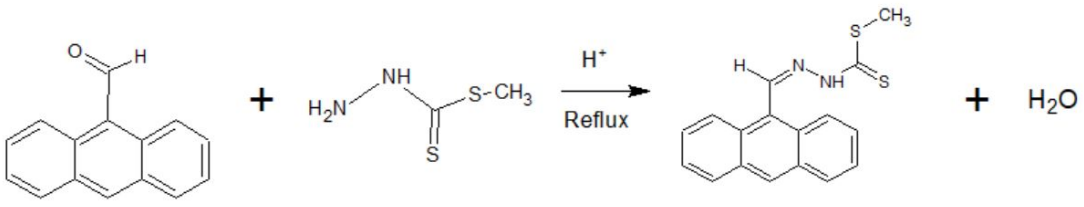
Synthesis of Schiff bases

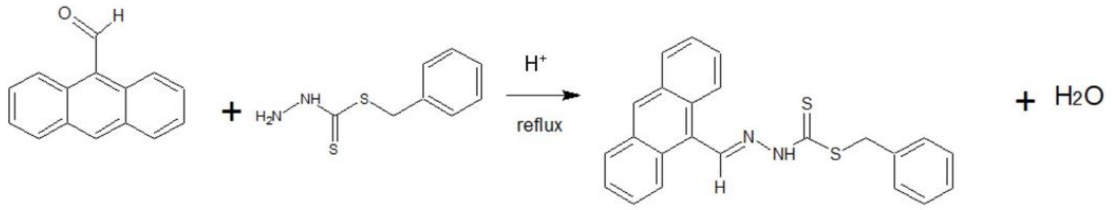
Synthesis of methyl (2Z)-2-[(anthracen-9-yl)methylidene]hydrazine-1-carbodithioate (**9-9anSM**)



S-Methyldithiocarbazate (0.1185 g, 1.64 mmol) was dissolved in hot absolute ethanol (10 mL) and was then added to a hot solution of 9-anthracenecarboxaldehyde (0.2 g, 1.64 mmol) in the same solvent (10 mL). Glacial acetic acid was also added as a catalyst. A colour change from clear to a dark orange was observed. The stirred reaction mixture was kept under reflux for 45 minutes after which a bright orange precipitate formed. The reaction progress was monitored on TLC plates every 5 minutes. The mixture was then left to stand overnight, to maximise crystal precipitation. The crystals were then filtered, washed with cold ethanol, recrystallised from absolute ethanol and dried in a desiccator containing anhydrous silica. Yield: 0.2902 g, 96%; m.p. 232-234 °C; IR (ν_{max}, cm^{-1}): 3147 ν(N-H), 1551 ν(C=N), 2976 ν(C-H), 968 ν(C=S);

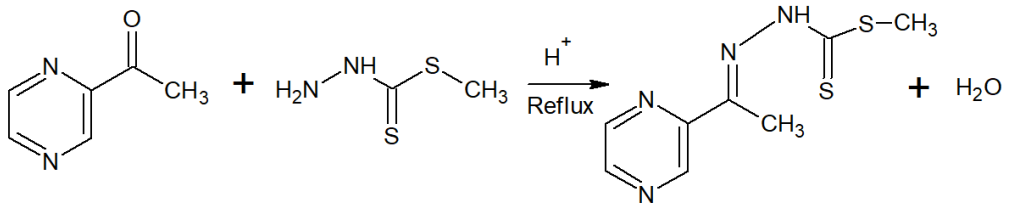
^{1}H NMR (DMSO-d_6) δH: 13.46 (s, 1H, -NH), 9.59 (s, 1H, -C=N), 8.79 (t, 3H), 8.20 (d, 2H), 7.60-7.71 (m, 4H) (Ar-H), 2.61 (s, 3H, -SCH_3).

Synthesis of Benzyl (2E)-2-[(anthracen-9-yl)methylidene]hydrazine-1-carbodithioate] (**9-9anSB**)



S-Benzyldithiocarbazate (0.1923 g, 0.97 mmol) was dissolved in hot absolute ethanol (10 mL) and was then added to a hot solution of 9-anthracenecarboxaldehyde (0.2 g, 0.97 mmol) in the same solvent (10 mL). Glacial acetic acid was also added as a catalyst. A colour change to a pale orange was observed. The stirred reaction mixture was kept under reflux for three minutes after which a bright yellow-orange precipitate formed. The reaction progress was monitored on TLC plates every 5 minutes. The mixture was then left to stand overnight, to maximise crystal precipitation. The crystals were then filtered, washed with cold ethanol, recrystallised from absolute ethanol and dried in a desiccator containing anhydrous silica. Yield: 0.3085 g, 82%; m.p. 208-210 °C; IR (ν_{max}, cm^{-1}): 3080 ν(N-H), 2857 ν(C-H), 1552 ν(C=N), 956 ν(C=S); ^{1}H NMR (DMSO-d_6) δH: 13.51 (s, 1H, -NH), 9.58 (s, 1H, -C=N), 8.73 (d, 2H), 8.18 (d, 2H), 7.58-7.68 (m, 4H), 7.45 (d, 2H), 7.34 (t, 2H), 7.27 (t, 1H) (Ar-H), 4.59 (s, 2H, -SCH_2).

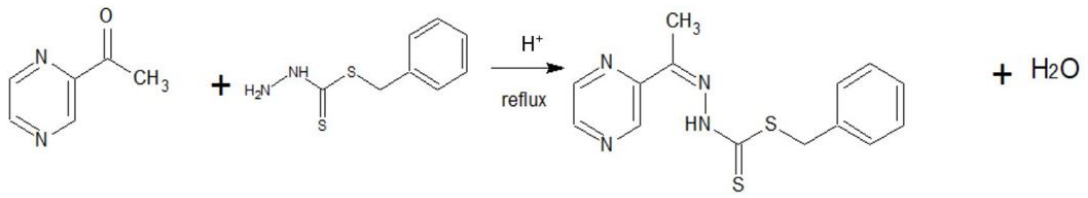
Synthesis of methyl (2E)-2-[1-(pyrazin-2-yl)ethylidene]hydrazine-1-carbodithioate (**AcpySM**)



The synthesis of acetylpyrazine of *S*-methyldithiocarbazate was based on the procedures reported by Hamid *et al*. [96]. S-Methyldithiocarbazate (0.2 g, 1.64 mmol) was dissolved in hot absolute ethanol (10 mL) and was then added to a hot solution of acetylpyrazine (0.2 g,

1.64 mmol) in the same solvent (10 mL). Glacial acetic acid was also added as a catalyst. A colour change from clear to a pale yellow was observed. The stirred reaction mixture was kept under reflux for 30 minutes after which a pale yellow precipitate was formed. The reaction progress was monitored on TLC plates every 5 minutes. The mixture was then left to stand overnight, to maximise crystal precipitation. The crystals were then filtered, washed with cold ethanol, recrystallised from absolute ethanol and dried in a desiccator containing anhydrous silica. Yield: 0.2593 g, 93% (Lit. yield 94%); m.p. 180-183 °C (Lit. m.p. 180-183 °C); IR (ν_{max}, cm^{-1}): 3445 ν(O-H), 3080 ν(N-H), 2948 ν(C-H), 1608 ν(C=N), 956 ν(C=S); ^{1}H NMR (DMSO-d_6) δH: 10.08 (s, 1H, -NH), 8.55-8.56 (s, 3H) (Ar-H), 2.69 (s, 3H, -SCH_3), 2.43 (s, 3H).

Synthesis of Benzyl 2-[1-(pyrazin-2-yl)ethylidene]hydrazine-1-carbodithioate (**AcpySB**)



The synthesis of AcpySbn was based on the procedures reported by Hamid *et al.* [96]. *S*-Benzyldithiocarbazate (0.3248 g, 1.64 mmol) was dissolved in hot absolute ethanol (10 mL) and was then added to a hot solution of acetylpyrazine (0.2 g, 1.64 mmol) in the same solvent (10 mL). Glacial acetic acid was also added as a catalyst. A colour change to a pale yellow was observed. The stirred reaction mixture was kept under reflux for 15 minutes after which a pale yellow precipitate formed. The reaction progress was monitored on TLC plates every 5 minutes. The mixture was then left to stand overnight, to maximise crystal precipitation. The crystals were then filtered, washed with cold ethanol, recrystallised from absolute ethanol and dried in a desiccator containing anhydrous silica. Yield: 0.356 g, 72% (Lit. yield 47%); m.p. 170-172 °C (Lit. [96] m.p. 168-170 °C); IR (ν_{max}, cm^{-1}): 3455 ν(O-H), 3178 ν(N-H), 1610 ν(C=N), 2965 ν(C-H), 961 ν(C=S); ^{1}H NMR (DMSO-d_6) δH: 9.37 (s, 1H, -NH), 8.51-8.57 (s, 3H), 7.33-7.64 (m, 5H) (Ar-H), 2.43 (s, 2H, -SCH_2), 2.17 (s, 3H, -CH_3).

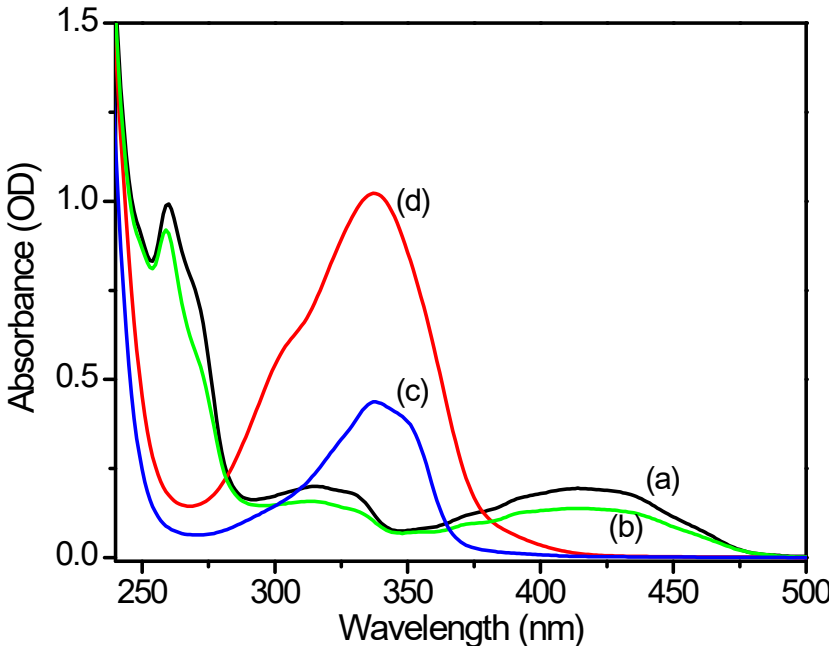
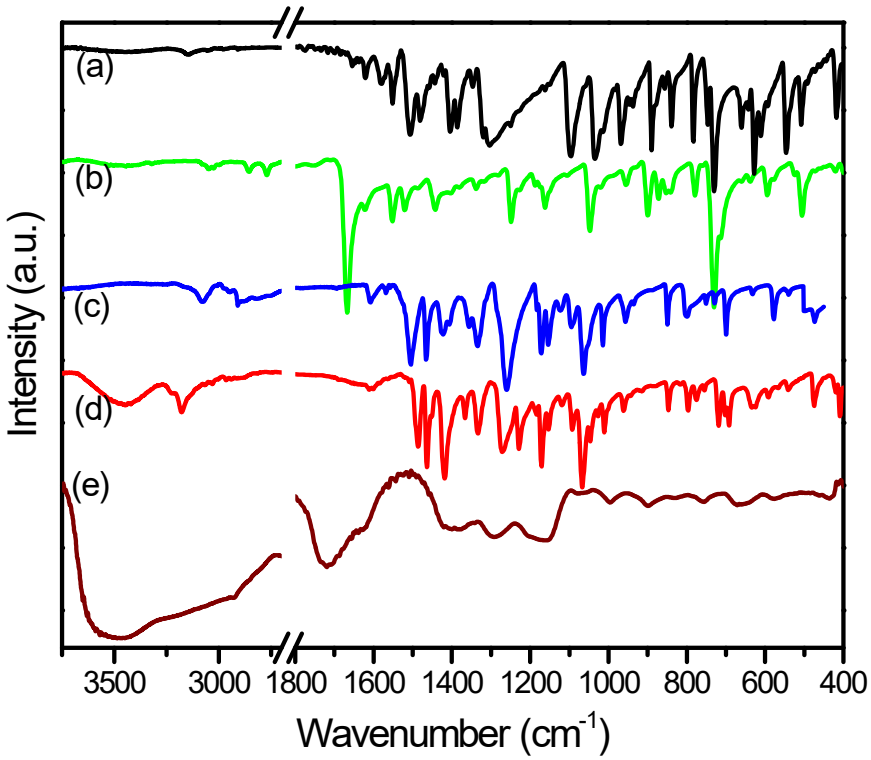


Fig. S1. UV-vis absorption spectra of Schiff bases; (a) **9anSM**, (b) **9anSB**, (c) **AcpySM**, and (d) **AcpySB**.



Fig, S2. FTIR spectra of Schiff bases; (a) **9anSM**, (b) **9anSB**, (c) **AcpySM**, and (d) **AcpySB**, and (e) TGA.

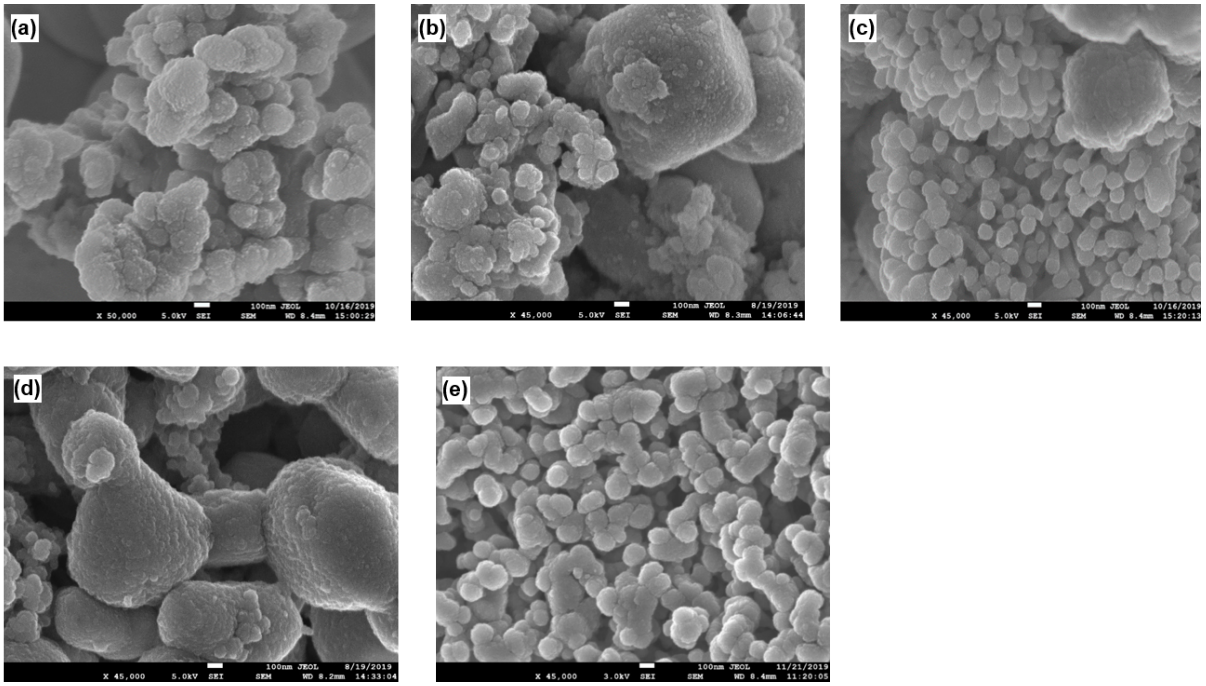


Fig. S3. SEM images of (a) **9anSM**-Ag_2S QDs, (b) **9anSB**-Ag_2S QDs, (c) **AcpySM**-Ag_2S QDs, and (d) **AcpySB**-Ag_2S QDs, and (e)TGA.

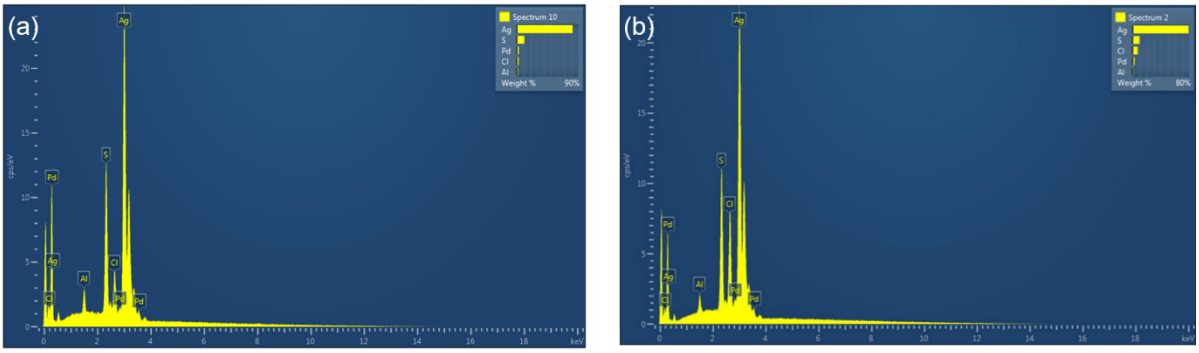


Fig. S4. SEM-EDX spectra for (a) **9anSM**-Ag_2S QDs and (b)TGA-Ag_2S QDs.

Figure S5

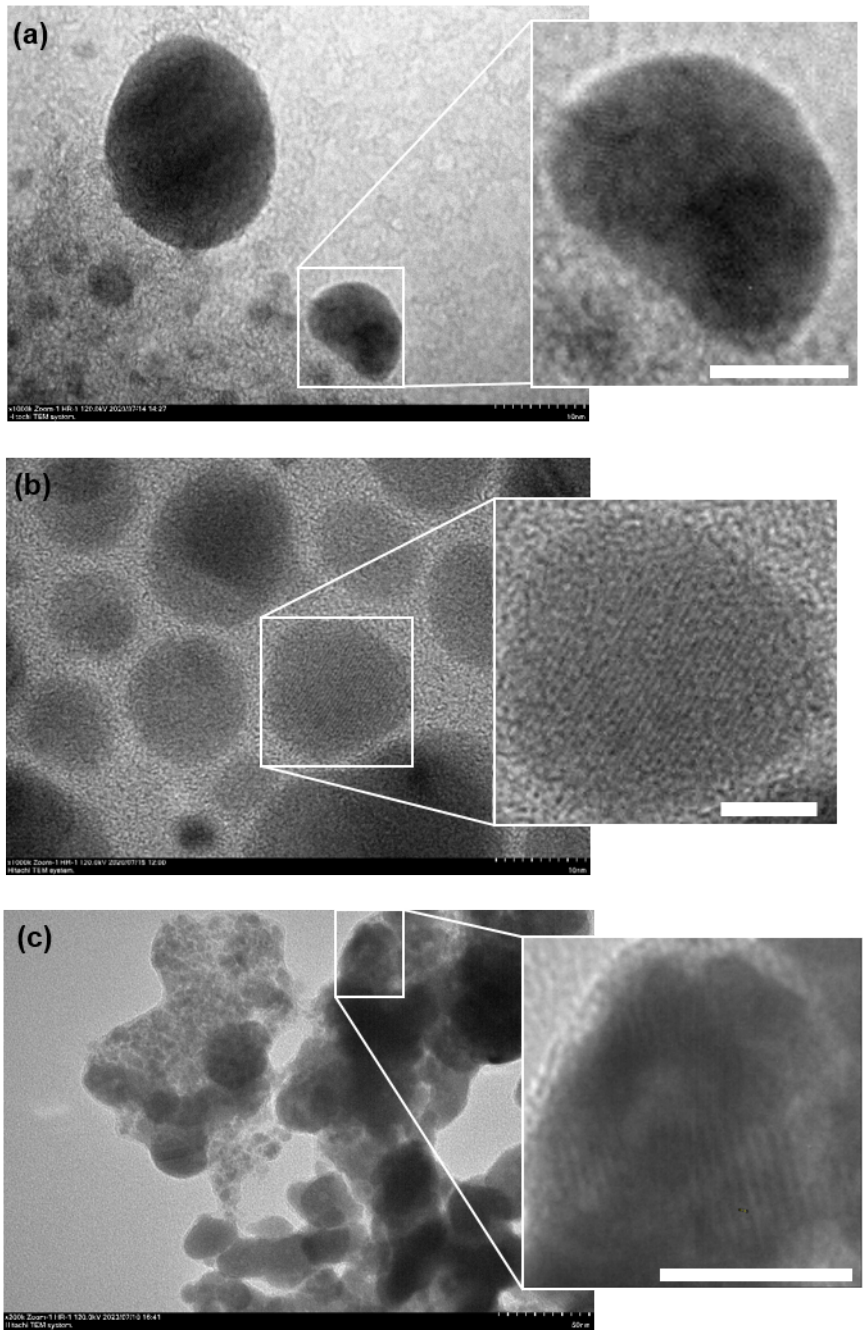


Fig. S5. The HRTEM images of (A) **9anSM-**Ag_2S QDs, (B) **9anSB**-Ag_2S QDs, and (C) **AcpySM-**Ag_2S QDs.

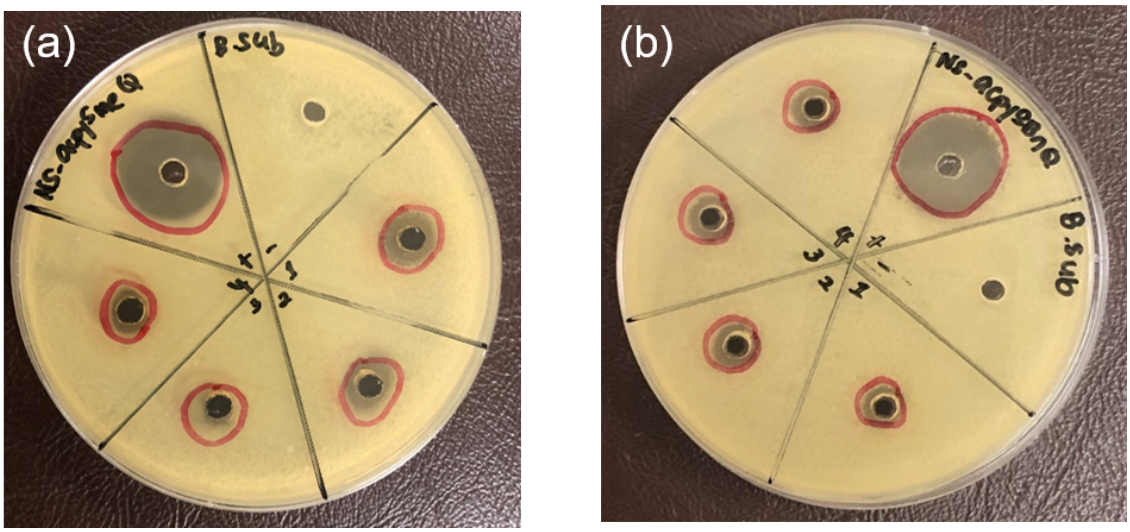


Fig. S6. The representative images of growth inhibition zones of *B. subtilis* nurtured with (a) **AcpySM**-Ag_2S and (b) **AcpySB**-Ag_2S.

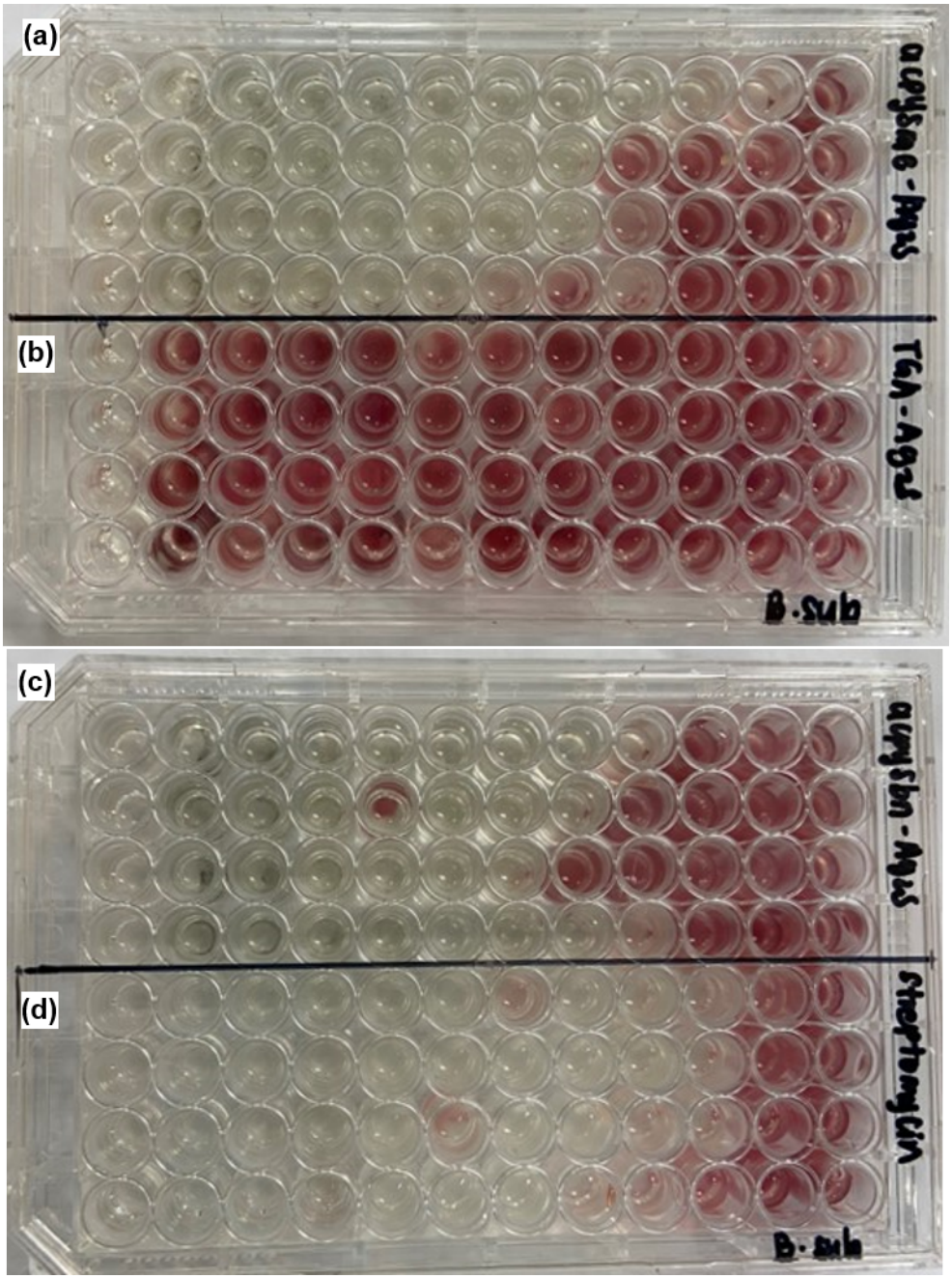


Fig. S7. The representative images of microbroth dilution method to determine the lowest concentration of (a) **AcpySM**-Ag_2S QDs, (b) streptomycin, (c) **AcpySB**-Ag_2S QDs, and (d) TGA-Ag_2S QDs to inhibit *B. subtilis* bacterial strain.

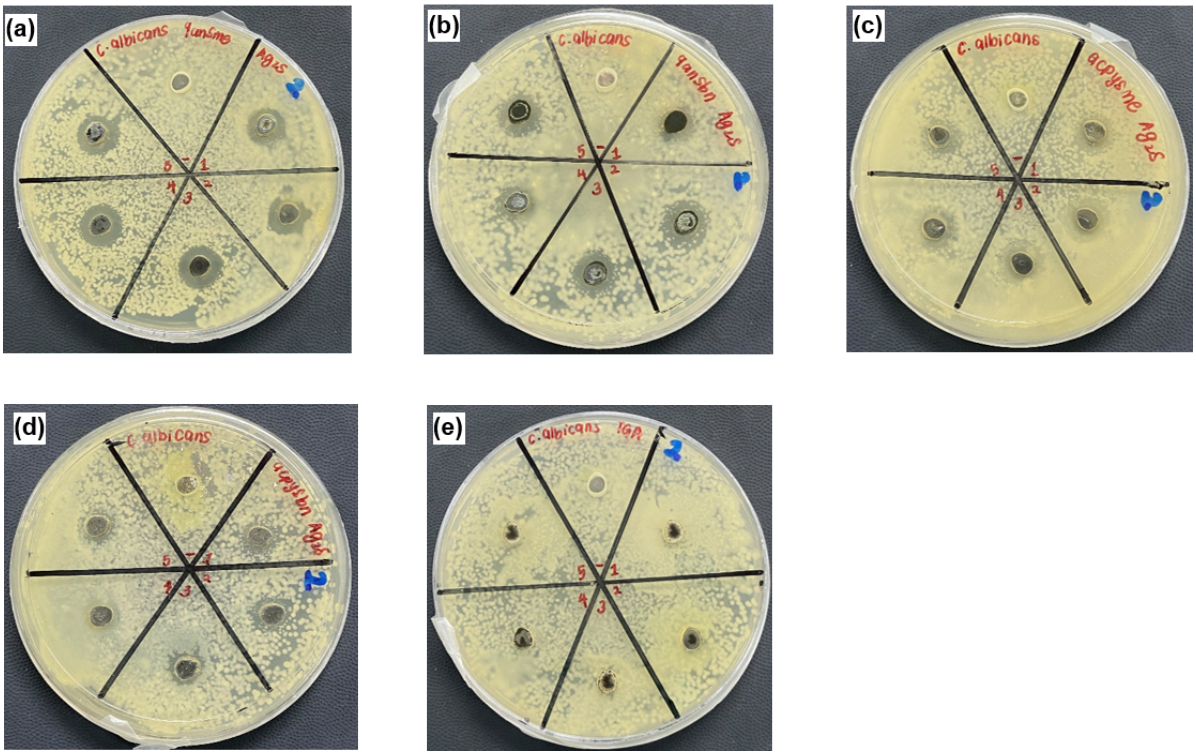


Fig. S8. The representative images of growth inhibition zones of *C. albicans* nurtured with (a) **9anSM**-Ag_2S QDs, (b) **9anSB**-Ag_2S QDs, (c) **AcpySM**-Ag_2S QDs, (d) **AcpySB**-Ag_2S, and (d) TGA-Ag_2S QDs to inhibit.

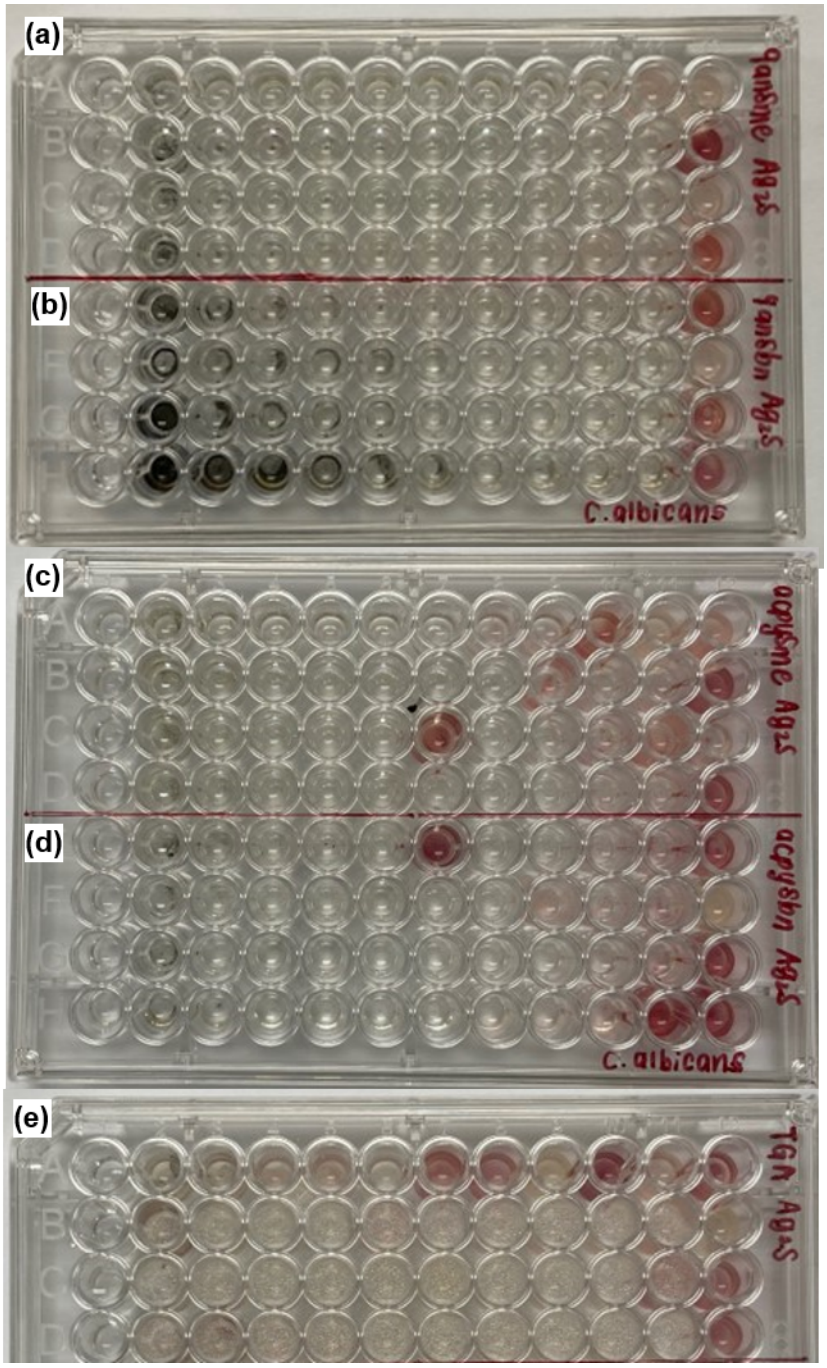


Fig. S9. The images of microbroth dilution method to determine the lowest concentration of (a) **9anSM**-Ag_2S QDs, (b) **9anSB**-Ag_2S QDs, (c) **AcpySM**-Ag_2S QDs, (d) **AcpySB**-Ag_2S, and (d) TGA-Ag_2S QDs to inhibit *C. albicans*.

Table S1. Total mortality of brine shrimp larvae (*A. salina* L.) by Schiff bases-Ag_2S QDs and TGA-Ag_2S QDs.

Sample		Total mortality of brine shrimp (*A. salina*) larvae (%)				
		0 µg/mL (control)	10 µg/mL	100 µg/mL	1000 µg/mL	10,000 µg/mL
Schiff bases-Ag_2S QDs	9anSM-Ag_2S	0	0	0	3.3	5.1
	9anSB-Ag_2S	0	0	0	5.7	19.3
	AcpySM-Ag_2S	0	0	0	7.5	19.7
	AcpySB-Ag_2S	0	3.3	13.3	19.8	39.5
TGA-Ag_2S QDs		0	0	0	0	2.3