Electronic Supplementary Material (ESI) for Soft Matter.

Supplementary Information

A multi-spectroscopic approach to investigate the interactions between Gramicidin A and silver nanoparticles

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Ag content through ICP analysis and determination of D-AgNPs concentrations in the colloidal samples.

Table S1: ICP data

[Ag] (ppm)[a]	[Ag] (M)	$[Ag]_0$ (M)[b]	[AgNPs] (M)
0.25856	$2.396*10^{-6}$	$9.588*10^{-4}$	$1.8*10^{-7}$

[a] Obtained from ICP measurements.
[b] [Ag] in the AgNP initial solution.

Determination of AgNP concentration

(a) Volume of one silver atom (V_{Ag}) :

$$V_{Ag} = \frac{4}{3}\pi r_{Ag}^{3}$$

r_{Ag} : metallic radius of a silver atom (in m)

(b) Volume of one silver nanoparticle ($V_{particle}$) :

$$V_{particle} = \frac{4}{3}\pi r_{particle}^{3}$$

$r_{particle}$: average radius obtained from TEM analysis (in m)

(c) Number of silver atoms for particle (N_{atoms}) :

$$N_{atoms} = \frac{V_{particle}}{V_{Ag}}$$

(d) AgNPs concentration ([AgNPs]) :

$$[AgNPs] = \frac{[Ag]_0}{N_{atoms}}$$

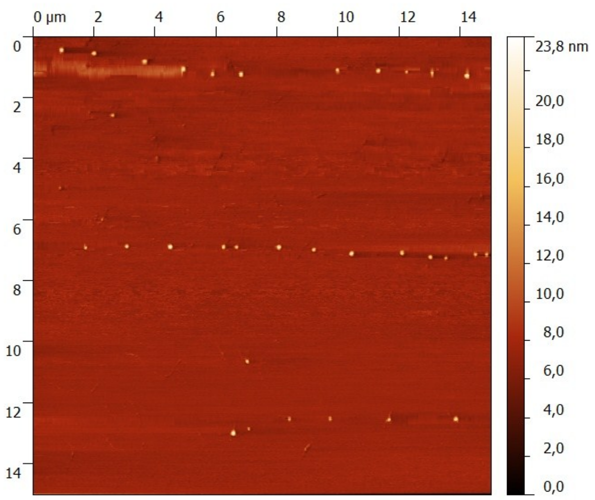

Figure S1: AFM image of D-AgNPs (15x15 µm).

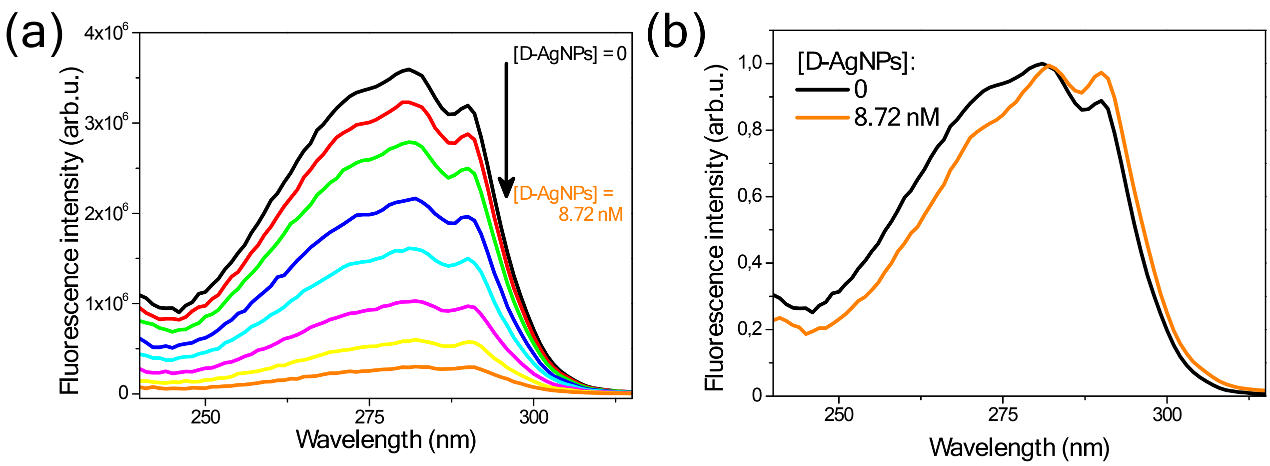

Figure S2: (a) Excitation spectra (λ_{em}= 335 nm) of GramA in EtOH in the presence of increasing concentrations of D-AgNPs (0 to 8.72 nM); (b) normalized excitation spectra of GramA (black line) and GramA + 8.72 nM of D-AgNPs (orange line).

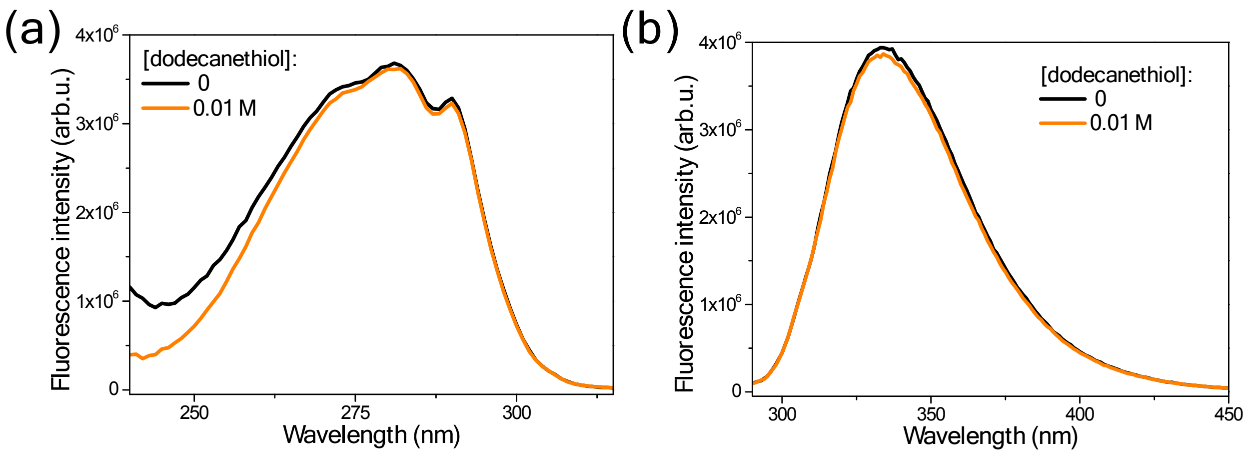

Figure S3: (a) Excitation spectra (λ_{em}= 335 nm) of GramA (black line) and GramA + 0.01 M of dodecanethiol (orange line); (b) emission spectra (λ_{exc}= 280 nm) of GramA (black line) and GramA + 0.01 M of dodecanethiol (orange line).

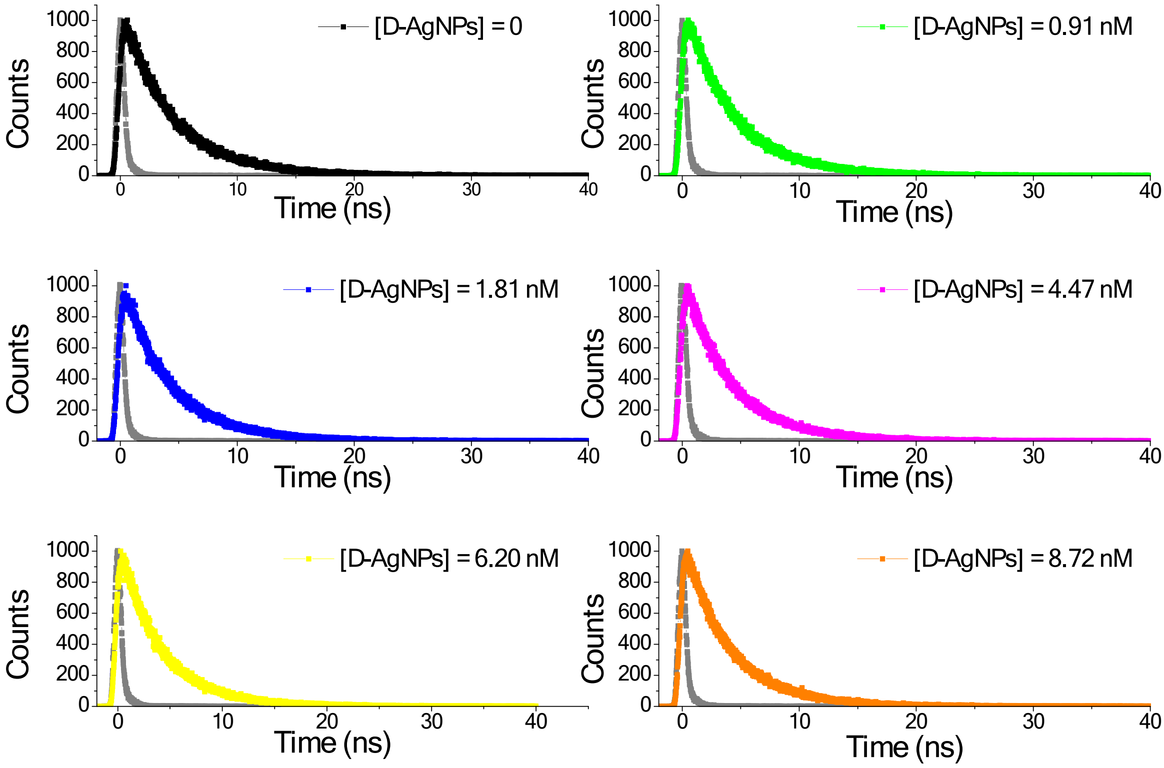

Figure S4: Fluorescence decay kinetics of GramA in EtOH solution in the presence of increasing amounts of D-AgNPs.

Table S2: Fluorescence decay times (obtained through nonlinear least-squares error minimization analysis) of GramA in the presence of increasing amounts of D-AgNPs.

D-AgNPs concentration (nM)	**τ_i GramA at 335 nm (ns)**		**ChiSQ**	$\bar{\tau}_{w.a.}$ **(ns)**
--	4.38 ± 0.01 (95%)	1.2 ± 0.1 (5%)	1.0773	4.22
0.91	4.23 ± 0.01 (95%)	1.2 ± 0.1 (5%)	0.9811	4.08
1.81	4.26 ± 0.01 (92%)	0.4 ± 0.1 (8%)	1.0430	3.95
4.47	4.07 ± 0.01 (95%)	0.7 ± 0.1 (5%)	1.0518	3.90
6.20	4.07 ± 0.01 (94%)	0.78 ± 0.01 (6%)	1.0621	3.87
8.72	3.98 ± 0.01 (94%)	0.74 ± 0.08 (6%)	0.9813	3.78

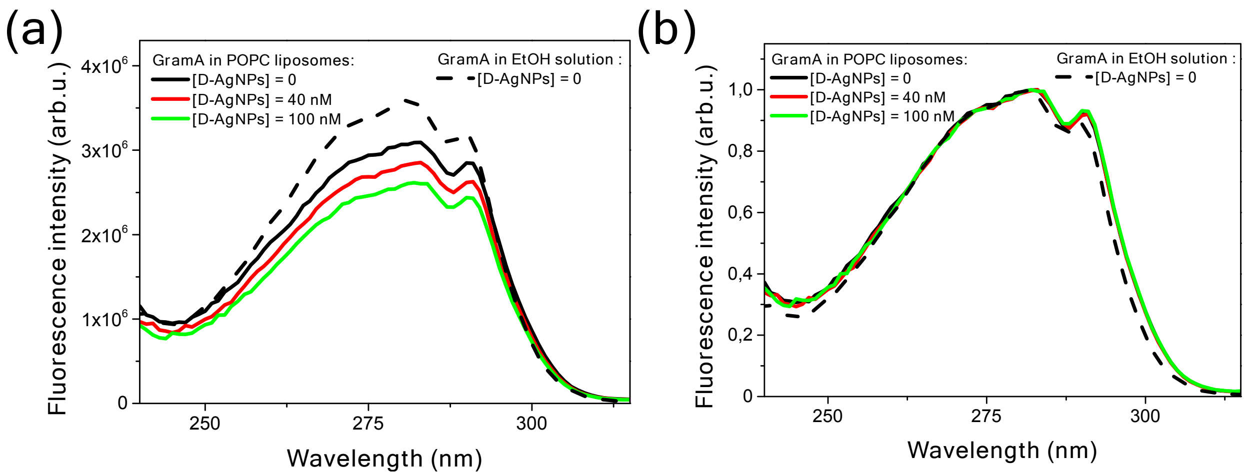

Figure S5: (a) Excitation spectra (λ_{em}= 335 nm) and (b) normalized excitation spectra of GramA into POPC bilayers without D-AgNPs (black solid line) and with increasing concentrations of D-AgNPs (red line: [D-AgNPs] = 40 nM; green line: [D-AgNPs] = 100 nM). For reference, GramA emission spectrum in EtOH is also reported (black dashed line).

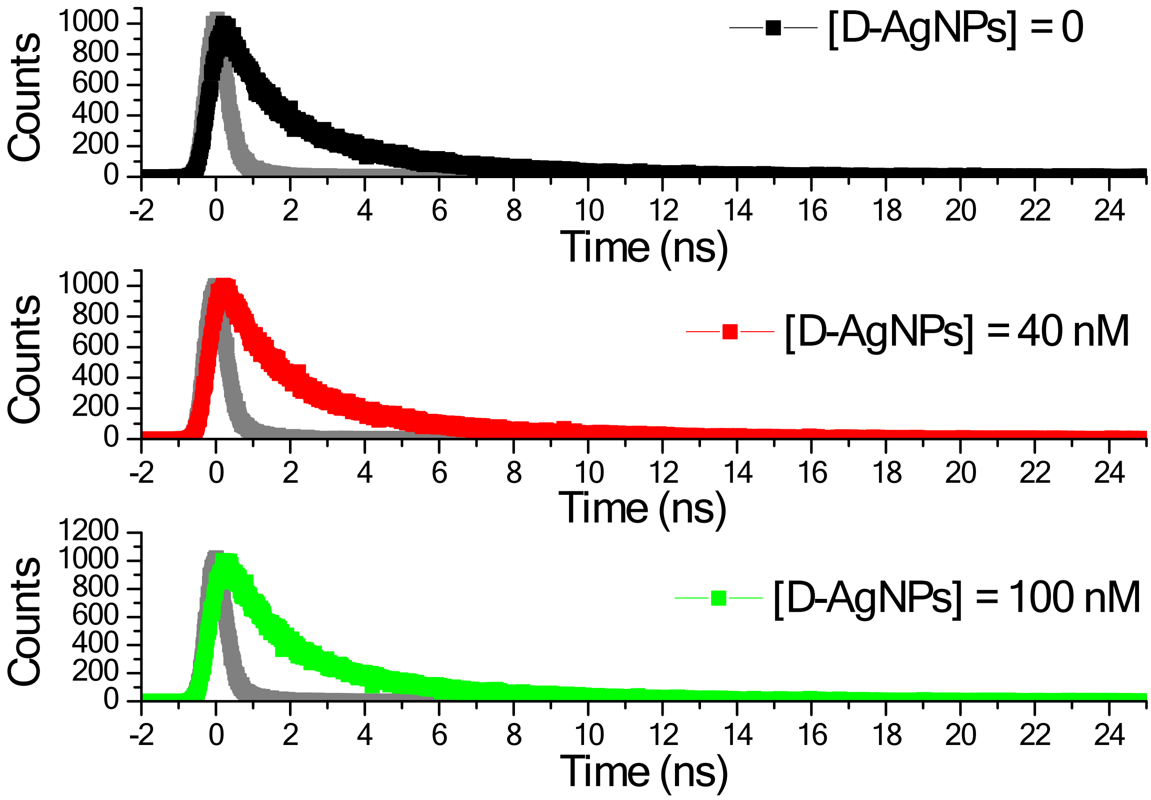

Figure S6: Fluorescence decay kinetics of GramA in POPC liposomes in the presence of increasing amounts of D-AgNPs.

Table S3: Fluorescence decay times (obtained through nonlinear least-squares error minimization analysis) of GramA in POPC liposomes in the presence of increasing amounts of D-AgNPs.

D-AgNPs concentration (nM)	**τ_i GramA at 335 nm (ns)**		**ChiSQ**	**$\bar{\tau}_{w.a.}$ (ns)**
--	3.54 ± 0.02 (69%)	0.74 ± 0.02 (31%)	1.0074	2.67
40	3.69 ± 0.02 (65%)	0.86 ± 0.02 (35%)	0.9701	2.70
100	3.67 ± 0.02 (63%)	1.01 ± 0.02 (37%)	1.0562	2.68

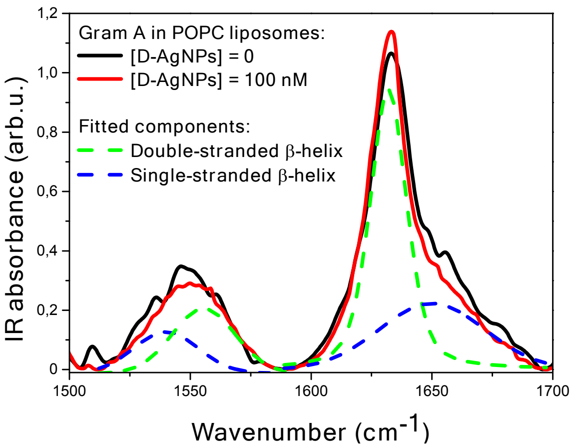

Figure S7: Normalized ATR-FTIR spectra in the amide I and II region (1500-1700 cm^{-1}) of POPC liposomes containing GramA (black line) and POPC liposomes containing GramA and D-AgNPs (red line). Dashed lines show the curve fitting results for the black curve for double stranded helix contribution (green dashed line) and single stranded helix contribution (blue dashed line).

Table S4: Curve fitting results for amide I and II bands of GramA in POPC from the ATR-FTIR spectra.

Literature assignments					
	Single-stranded	Double-stranded		Single-stranded	Double-stranded
Amide I	≈1650 cm^{-1}	≈1630 cm^{-1}	Amide II	≈1540 cm^{-1}	≈1560 cm^{-1}
Curve-fitting results (areas in percentage) for experimental results					
GramA	45%	55%		46%	54%
+ 100 nM D-AgNPs	36%	64%		40%	60%