Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic Supplementary Information

Impact of the Zinc complexation of polytopic polyaza ligands on the interaction with double and single stranded DNA/RNA and antimicrobial activity

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Table S1.- Crystallographic data of the "supercomplex" $\{[Zn_2\mathbf{PYPOD}Cl]_2Na(ClO_4)\}^{6+}$.

Formula	$C_{66}H_{106}Cl_9N_{22}NaO_{30}Zn_4$
Formula weight	2291.33
Crystal system	Orthorhombic
Space group	Pbcn
Cell *a* / Å *b* / Å *c* / Å *V* / Å^3	 13.1143(2) 18.5283(2) 38.6732(5) 9397.2(2)
Z	8
T / K	293(2)
size / mm	0.80 × 0.34 × 0.06
F_{000}	4720
density / g.cm^{-3}	1.620
R(int)	0.1013
θ_{max} / deg. θ_{min} / deg.	27.498 3.045
reflections - collected - unique	 58315 10672
*R*1 - all - $F^2 > 2\sigma_{F2}$	 0.1386 0.0669
*wR*2 - all - $F^2 > 2\sigma_{F2}$	 0.2313 0.1978
GoF - all - $F^2 > 2\sigma_{F2}$	 1.045 1.047
- parameters - constraints - restraints	596 0 50

Table S2.- Selected distances and angles of the complex $[Zn_2\mathbf{PYPOD}Cl]^{3+}$

distances	Zn1 – N1	2.090(5)	Zn2 – N10	2.232(4)
	Zn1 – N2	2.285(5)	Zn2 – N6	2.244(4)
	Zn1 – N3	2.182(5)	Zn2 – N7	2.065(4)
	Zn1 – N4	2.209(5)	Zn2 – N8	2.257(4)
	Zn1 – N5	2.196(4)	Zn2 – N9	2.237(4)
	Zn1 – Cl5	2.356(2)	Zn2 – N11	2.086(4)
angles	N1 – Zn1 – N2	76.2(2)	N10 – Zn2 – N6	159.19(15)
	N1 – Zn1 – N3	78.1(2)	N10 – Zn2 – N8	80.20(14)
	N1 – Zn1 – N4	91.00(19)	N10 – Zn2 – N9	81.45(16)
	N1 – Zn1 – N5	172.07(17)	N6 – Zn2 – N8	100.08(14)
	N1 – Zn1 – Cl5	93.89(15)	N7 – Zn2 – N10	92.69(14)
	N2 – Zn1 – Cl5	107.79(17)	N7 – Zn2 – N6	107.76(14)
	N3 – Zn1 – N2	146.5(2)	N7 – Zn2 – N8	77.65(15)
	N3 – Zn1 – N4	81.0(2)	N7 – Zn2 – N9	77.82(16)
	N3 – Zn1 – N5	101.2(2)	N7 – Zn2 – N11	173.84(15)
	N3 – Zn1 – Cl5	94.95(17)	N9 – Zn2 – N6	106.09(15)
	N4 – Zn1 – N2	78.4(2)	N9 – Zn2 – N8	148.46(15)
	N4 – Zn1 – Cl5	172.90(14)	N11 – Zn2 – N10	81.35(15)
	N5 – Zn1 – N2	101.39(18)	N11 – Zn2 – N6	78.09(15)
	N5 – Zn1 – N4	81.09(17)	N11 – Zn2 – N8	99.68(15)
	N5 – Zn1 – Cl5	94.05(12)	N11 – Zn2 – N9	102.65(16)

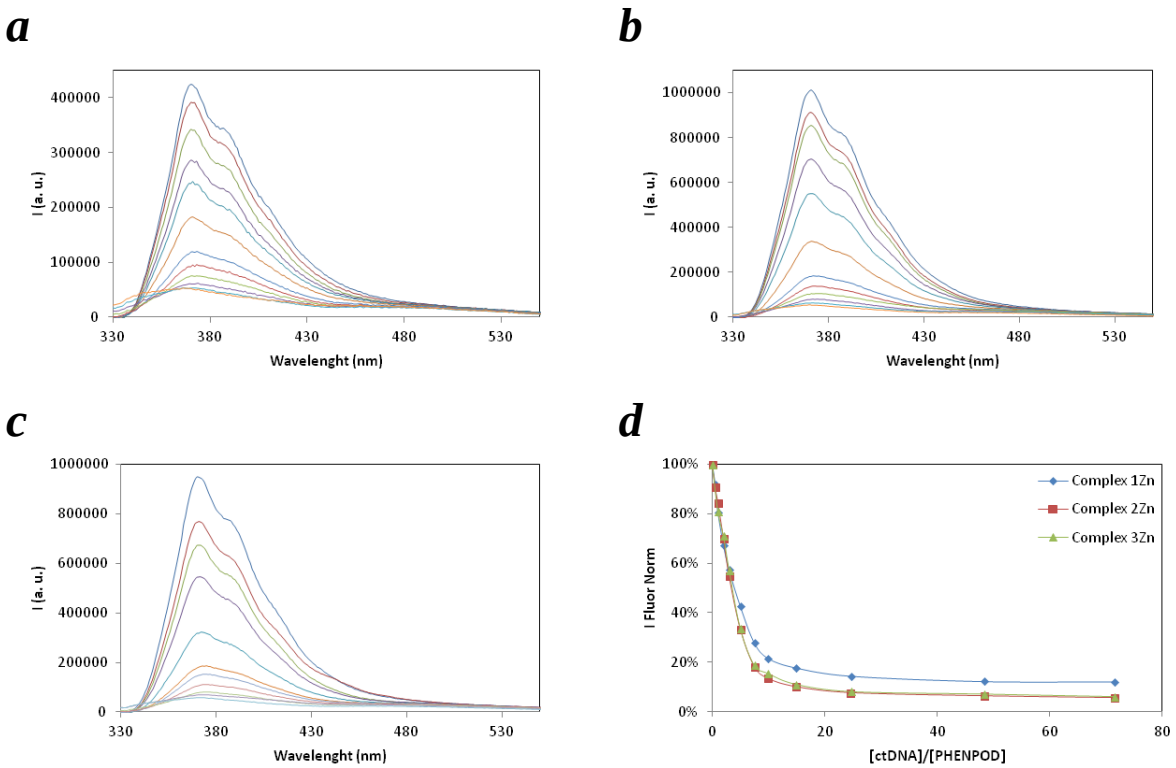

Figure S1.- Fluorescence titrations of (a) Zn**PHENPOD**, (b) Zn_2**PHENPOD** and (c) Zn_3**PHENPOD** with Calf Thymus DNA (ctDNA) at pH 7.4 in cacodylate buffer 0.05 M. (d) Plot of the fluorescence intensity normalized *vs.* metal complex [ctDNA]/[Zn_x**PHENPOD**].

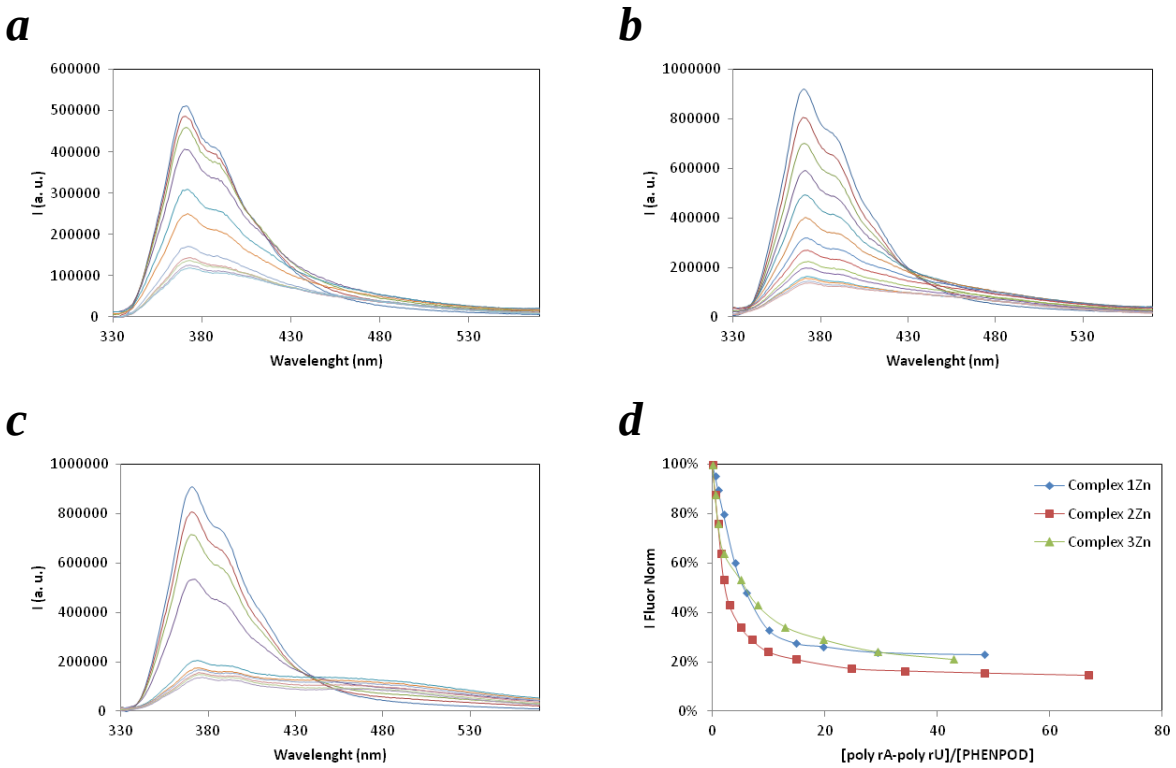

Figure S2.- Fluorescence titrations of (a) Zn**PHENPOD**, (b) Zn_2**PHENPOD** and (c) Zn_3**PHENPOD** with poly rA-poly rU at pH 7.4 in cacodylate buffer 0.05 M. (d) Plot of the fluorescence intensity normalized *vs.* metal complex [poly rA-poly rU]/[Zn_x**PHENPOD**].

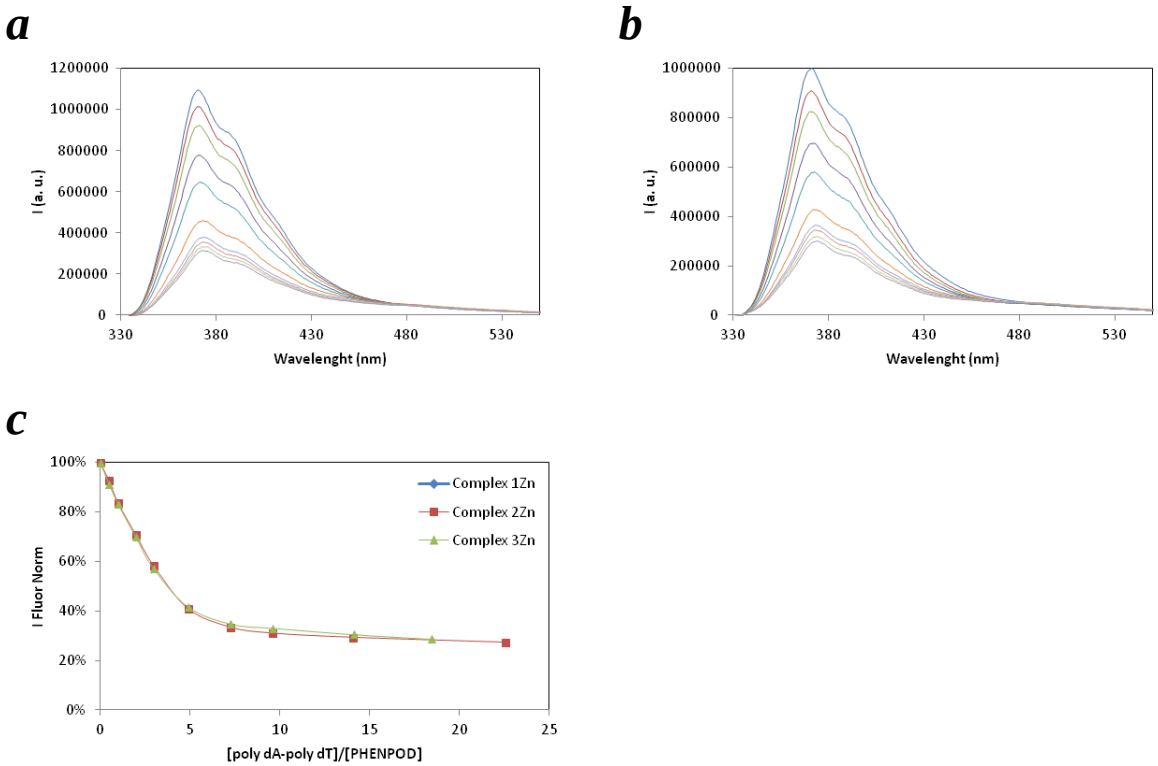

Figure S3.- Fluorescence titrations of (a) Zn_2**PHENPOD** and (b) Zn_3**PHENPOD** with poly dA-poly dT at pH 7.4 in cacodylate buffer 0.05 M. (c) Plot of the fluorescence intensity normalized *vs.* metal complex [poly dA-poly dT]/[Zn_x**PHENPOD**].

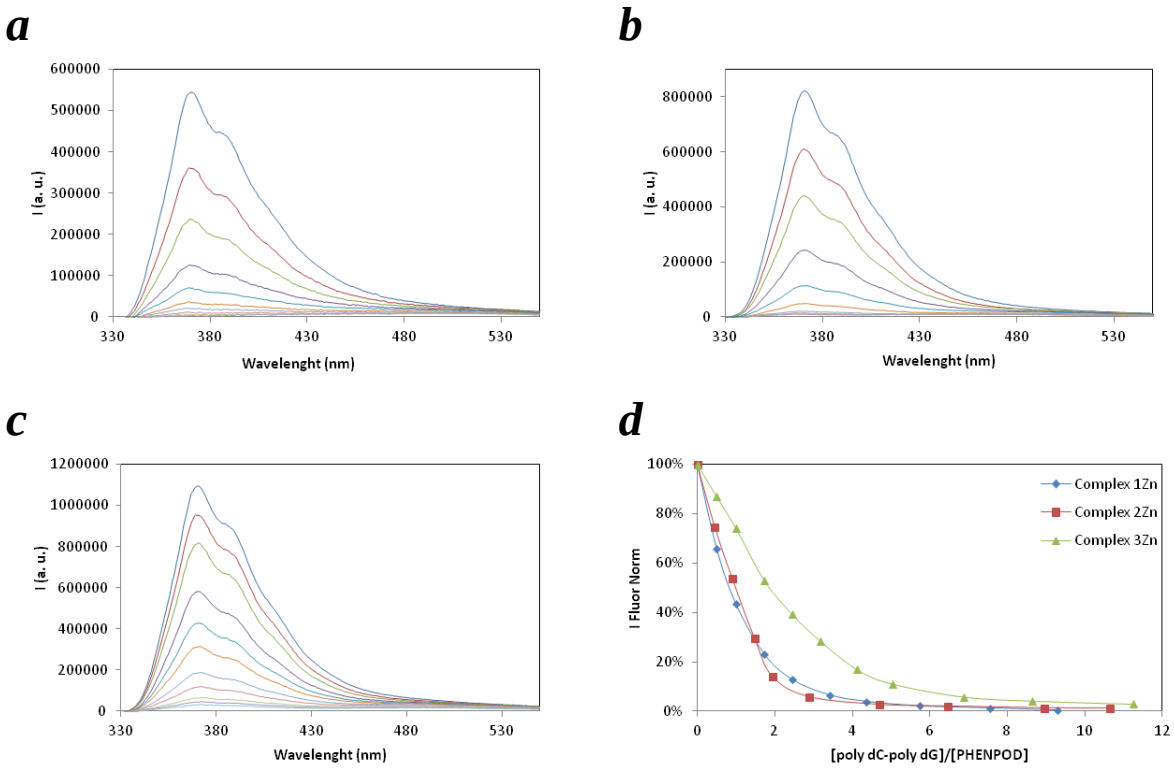

Figure S4.- Fluorescence titrations of (a) Zn**PHENPOD**, (b) Zn_2**PHENPOD** and (c) Zn_3**PHENPOD** with poly dG-poly dC at pH 7.4 in cacodylate buffer 0.05 M. (d) Plot of the fluorescence intensity normalized *vs.* metal complex [poly dG-poly dC]/[Zn_x**PHENPOD**].

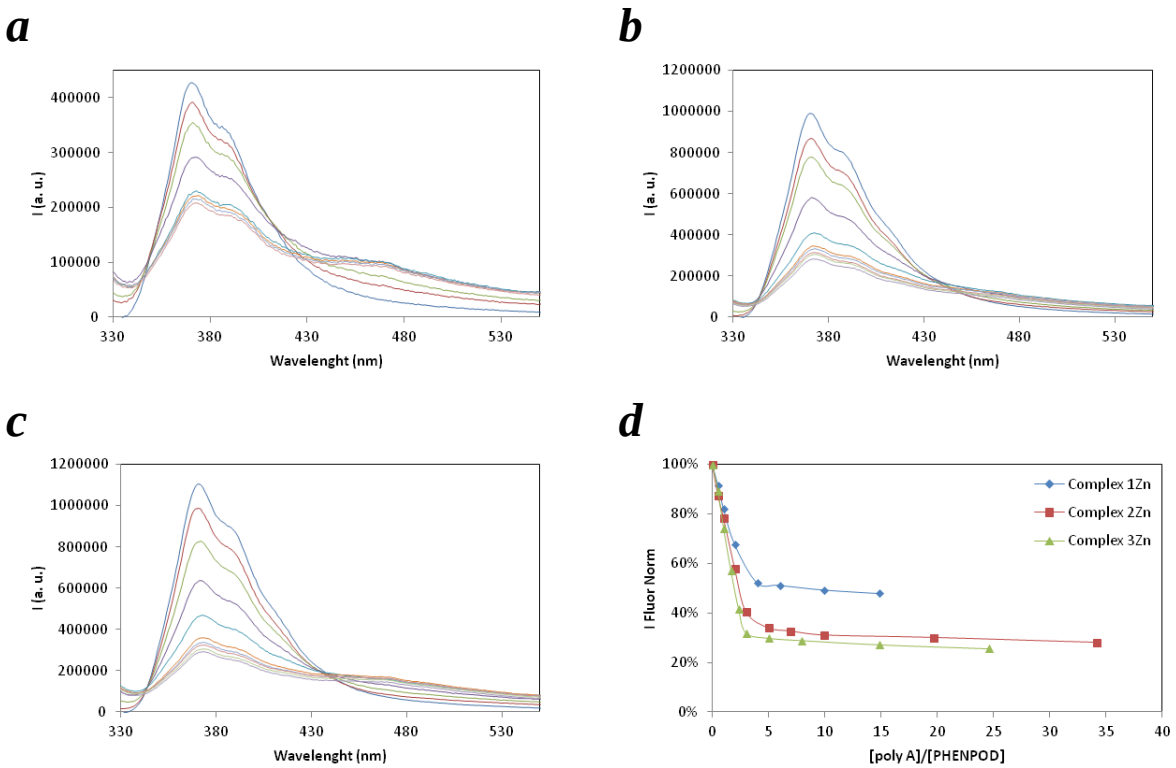

Figure S5.- Fluorescence titrations of (a) Zn**PHENPOD**, (b) Zn_2**PHENPOD** and (c) Zn_3**PHENPOD** with poly dA at pH 7.4 in cacodylate buffer 0.05 M with poly dA. (d) Plot of the fluorescence intensity normalized *vs.* metal complex [poly A]/[Zn_x**PHENPOD**].

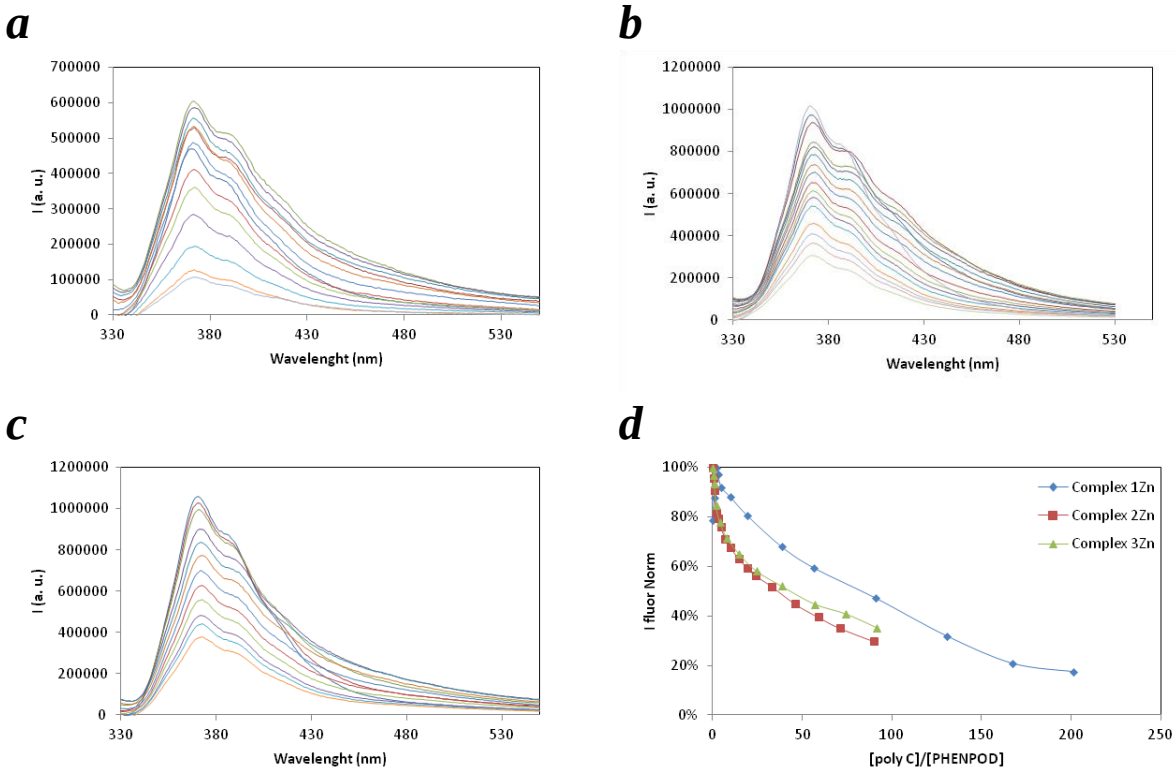

Figure S6.- Fluorescence titrations of (a) Zn**PHENPOD**, (b) Zn_2**PHENPOD** and (c) Zn_3**PHENPOD** with poly dA at pH 7.4 in cacodylate buffer 0.05 M with poly dC. (d) Plot of the fluorescence intensity normalized *vs.* metal complex [poly dC]/[Zn_x**PHENPOD**].

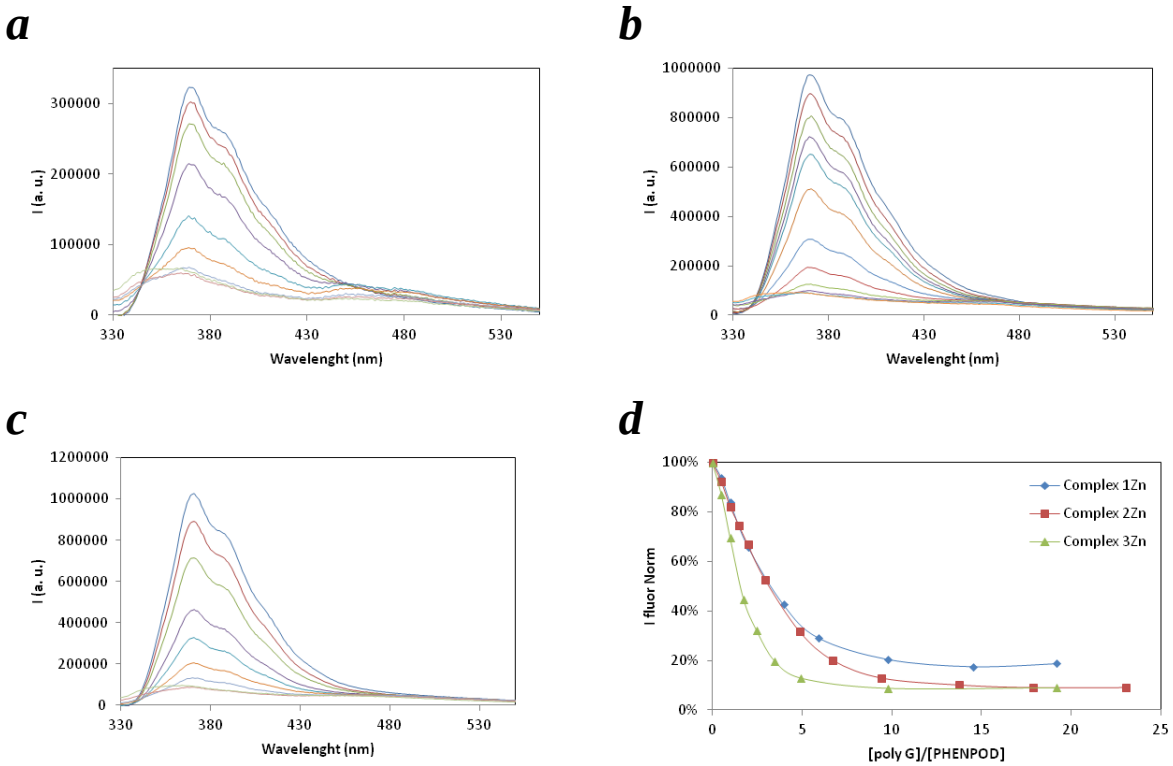

Figure S7.- Fluorescence titrations of (a) Zn**PHENPOD**, (b) Zn_2**PHENPOD** and (c) Zn_3**PHENPOD** with poly dA at pH 7.4 in cacodylate buffer 0.05 M with poly dG. (d) Plot of the fluorescence intensity normalized *vs.* metal complex [poly dG]/[Zn_x**PHENPOD**].

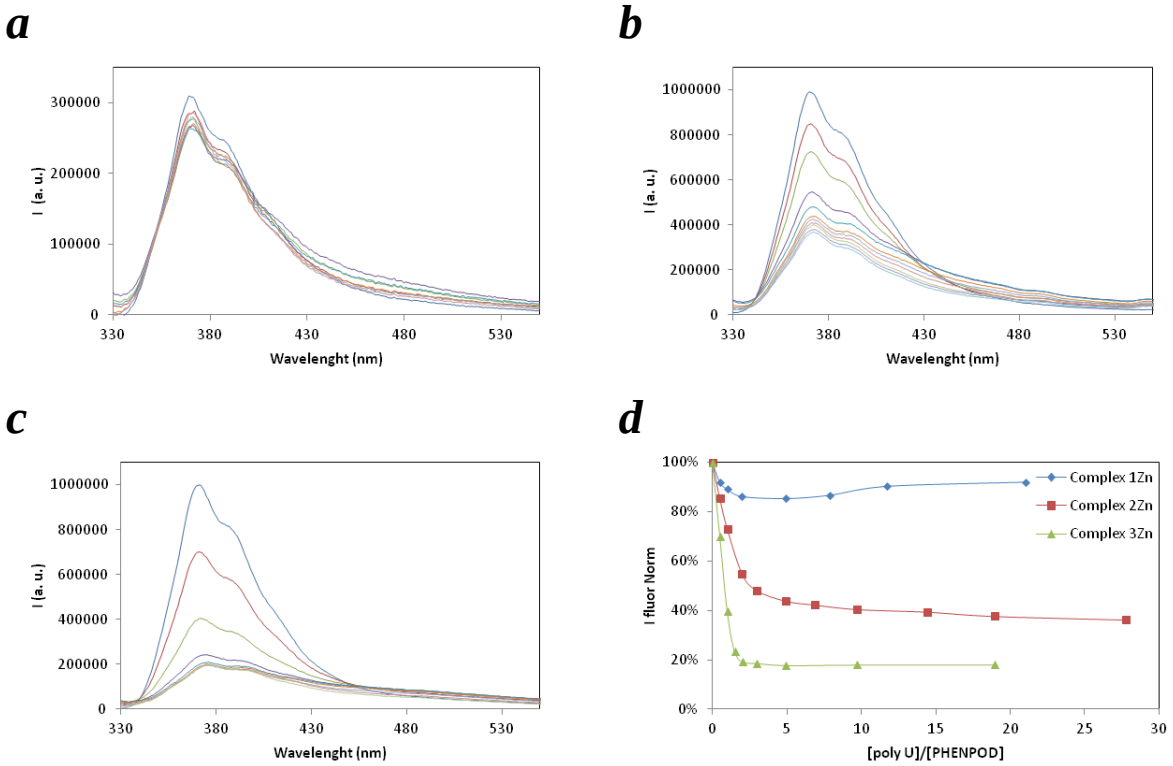

Figure S8.- Fluorescence titrations of (a) Zn**PHENPOD**, (b) Zn_2**PHENPOD** and (c) Zn_3**PHENPOD** with poly U at pH 7.4 in cacodylate buffer 0.05 M. (d) Plot of the fluorescence intensity normalized *vs.* metal complex [poly U]/[Zn_x**PHENPOD**].

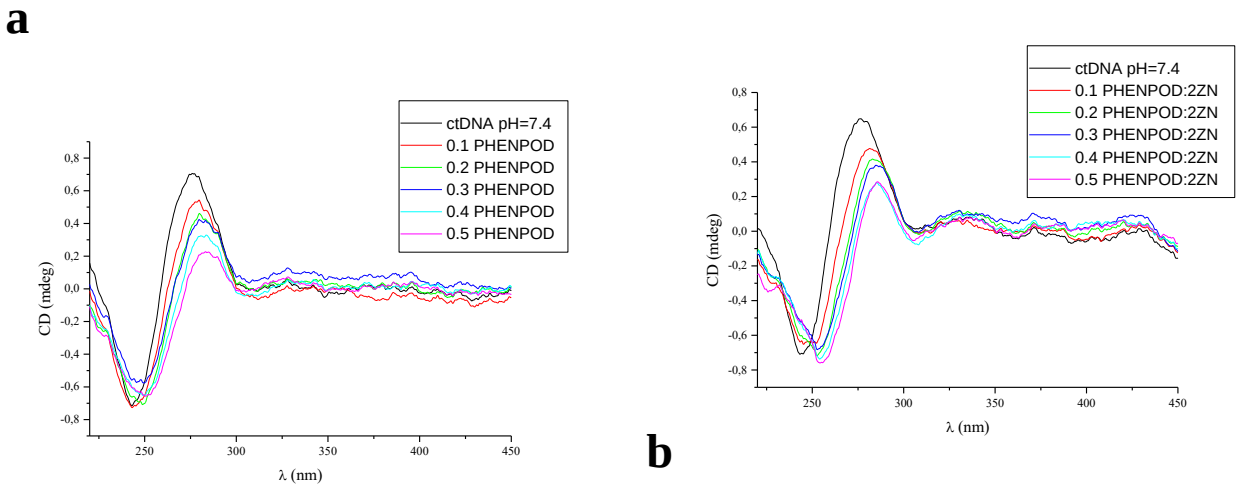

Figure S9. CD titration of *ctDNA* (c = 1.0 × 10^{-5} mol dm^{-3}) with (a) **PHENPOD** and (b) Zn_2**PHENPOD** at molar ratios r = [compound] / [polynucleotide] (buffer sodium cacodylate, I = 0.05 mol dm^{-3}) at pH 7.4.

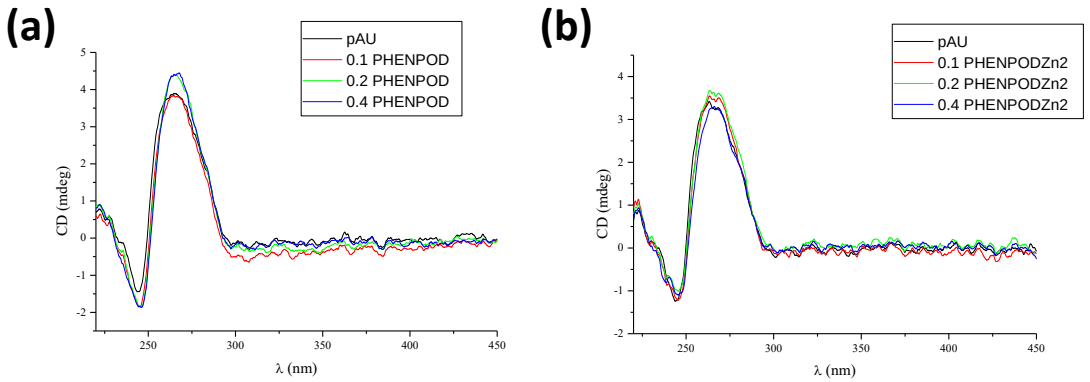

Figure S10. CD titration of poly rA-poly rU (c = 1.0 × 10^{-5} M) with (a) **PHENPOD** and (b) Zn_2**PHENPOD** at molar ratios r = [compound] / [polynucleotide] (buffer sodium cacodylate, I = 0.05 M) at pH 7.4.

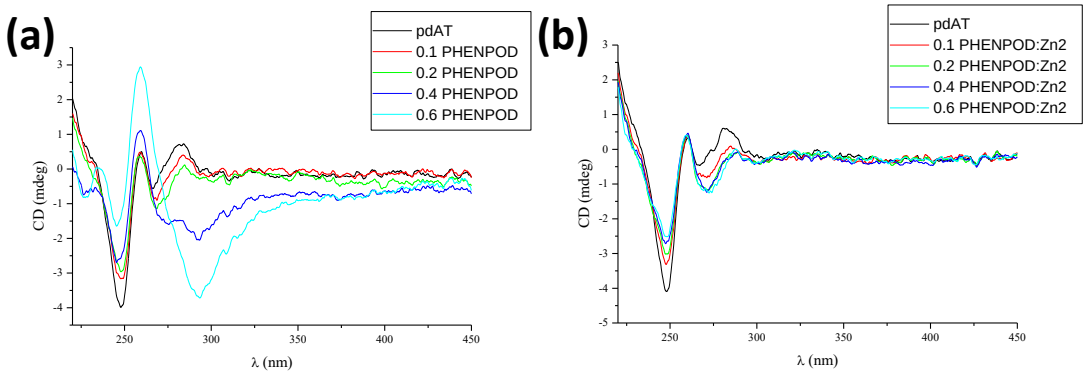

Figure S11. CD titration of poly dA-poly dT ($c = 1.0 \times 10^{-5}$ M) with (a) **PHENPOD** and (b) Zn_2**PHENPOD** at molar ratios r = [compound] / [polynucleotide] (buffer sodium cacodylate, I = 0.05 M) at pH 7.4.

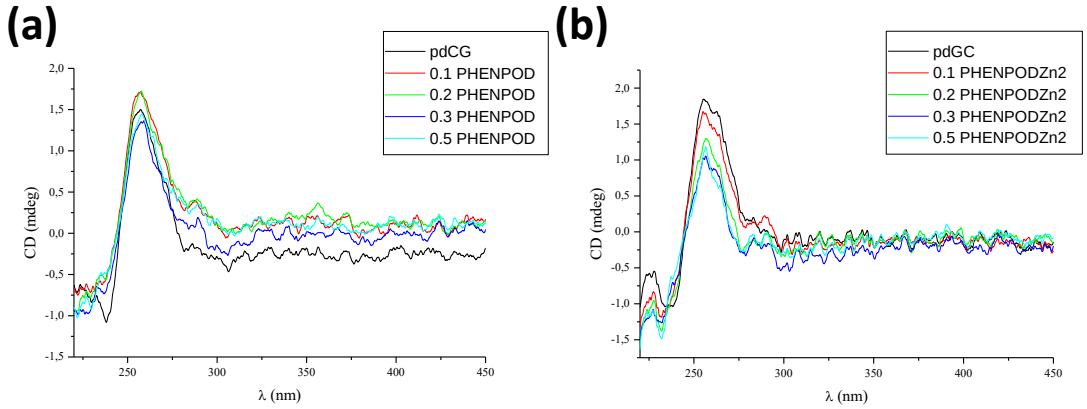

Figure S12. CD titration of poly dG-poly dC ($c = 1.0 \times 10^{-5}$ M) with (a) **PHENPOD** and (b) Zn_2**PHENPOD** at molar ratios r = [compound] / [polynucleotide] (buffer sodium cacodylate, I = 0.05 M) at pH 7.4.

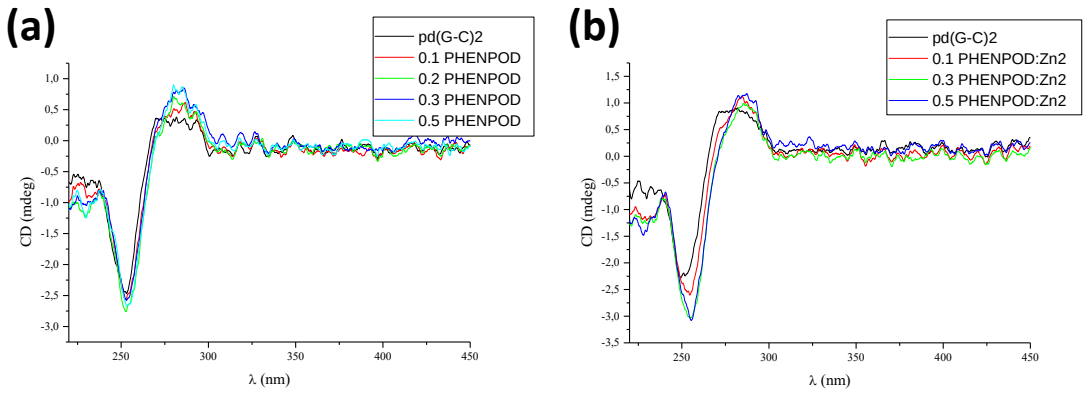

Figure S13. CD titration of poly d(G-C)$_2$ (c = 1.0 × 10^{-5} M) with (a) **PHENPOD** and (b) Zn$_2$**PHENPOD** at molar ratios r = [compound] / [polynucleotide] (buffer sodium cacodylate, I = 0.05 M) at pH 7.4.

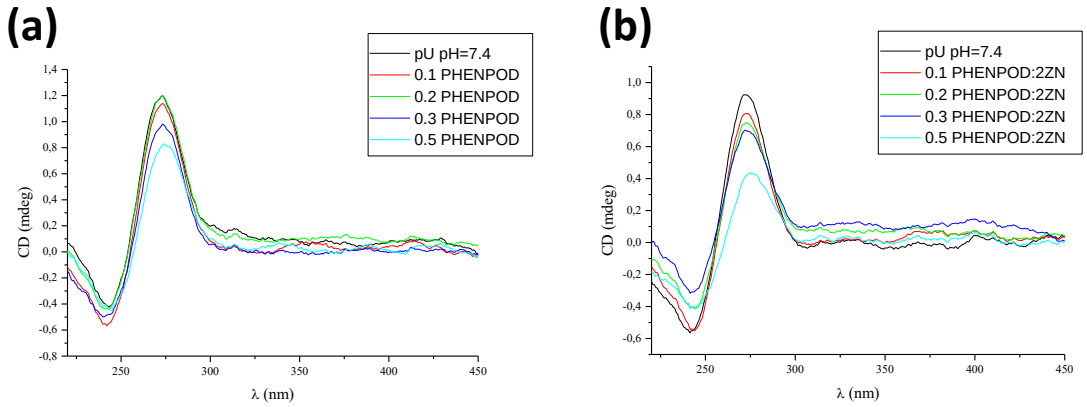

Figure S14. CD titration of poly dU (c = 1.0 × 10^{-5} M) with (a) **PHENPOD** and (b) Zn$_2$**PHENPOD** at molar ratios r = [compound] / [polynucleotide] (buffer sodium cacodylate, I = 0.05 M) at pH 7.4.

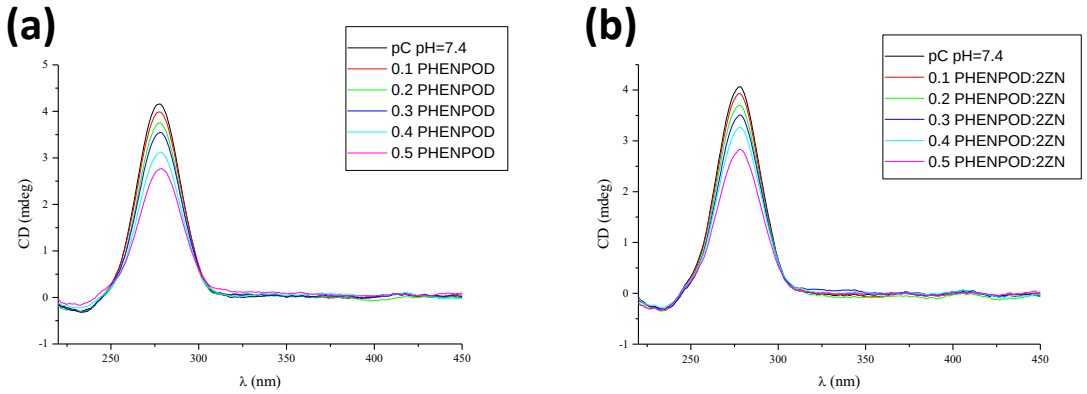

Figure S15. CD titration of poly dC (c = 1.0 × 10^{-5} M) with (a) **PHENPOD** and (b) Zn_2**PHENPOD** at molar ratios r = [compound] / [polynucleotide] (buffer sodium cacodylate, I = 0.05 M) at pH 7.4.

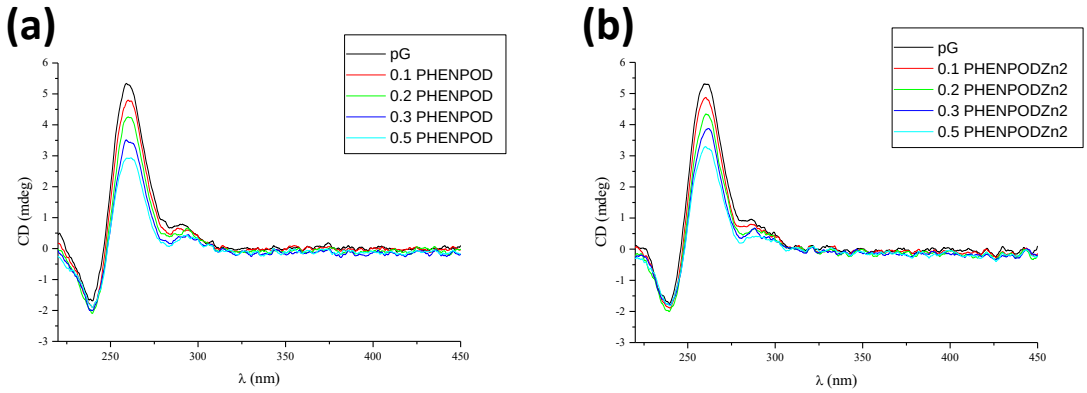

Figure S16. CD titration of poly dC (c = 1.0 × 10^{-5} M) with (a) **PHENPOD** and (b) Zn_2**PHENPOD** at molar ratios r = [compound] / [polynucleotide] (buffer sodium cacodylate, I = 0.05 M) at pH 7.4.

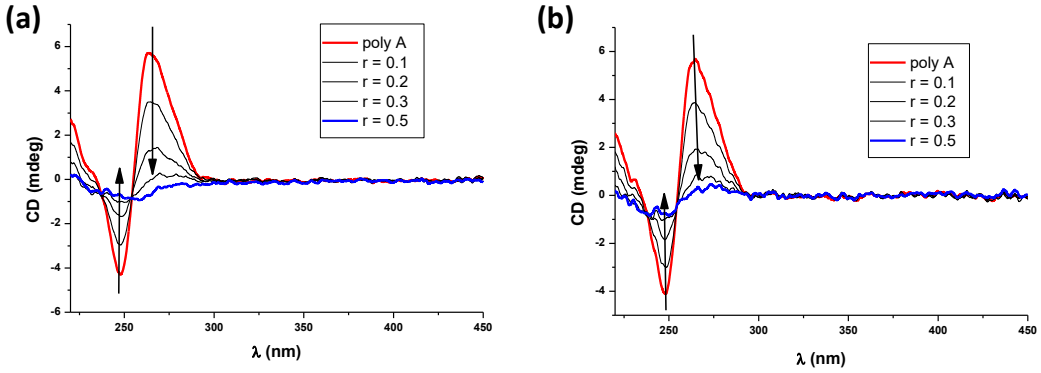

Figure S17. CD titration of poly dA (c = 1.0 × 10^{-5} M) with (a) **PHENPOD** and (b) Zn_2**PHENPOD** at molar ratios r = [compound] / [polynucleotide] (buffer sodium cacodylate, I = 0.05 M) at pH 7.4.

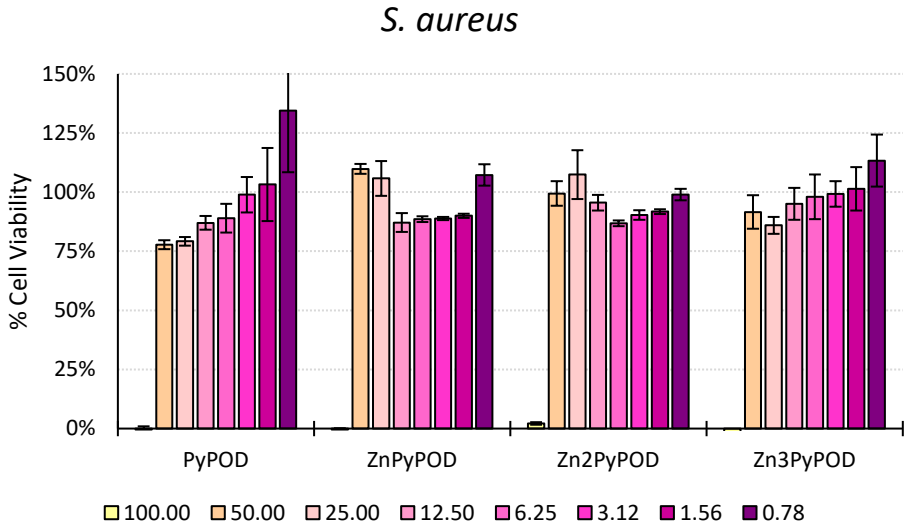

Figure S18. Cell viability analysis based on the optical density at 600 nm for **PYPOD**, Zn**PYPOD**, Zn_2**PYPOD** and Zn_3**PYPOD** in *S. aureus*. Bottom legend represents the concentration in µM.

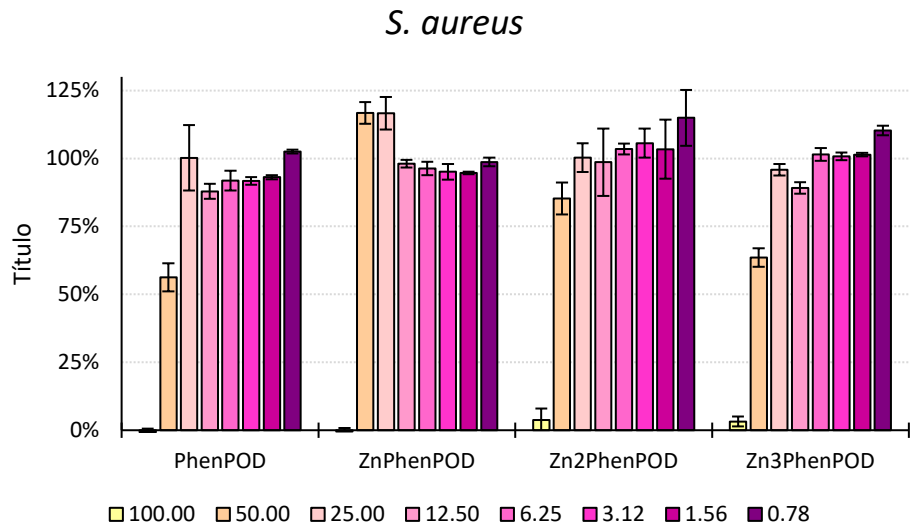

Figure S19. Cell viability analysis based on the optical density at 600 nm for **PHENPOD**, Zn**PHENPOD**, Zn_2**PHENPOD** and Zn_3**PHENPOD** in *S. aureus*. Bottom legend represents the concentration in μM.