

SUPPORTING INFORMATION

Designing antibacterial polymeric systems: (co)poly(2-oxazoline) conjugates with acyclic and macrocyclic polyamino polycarboxylic chelators

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Complexometric titration procedures:

Ca ions trapping ability was studied by complexometric titration in the presence of murexide as an indicator. Samples were dissolved in water (5 mg mL⁻¹) and their pH was adjusted to 4-5, 7 and 12 with the use of NaOH solution. Then CaCl₂ was added (an equimolar amount of Ca ions relative to the DOTA or DTPA molecules in the conjugate) and the solutions were stirred for 24 hours. After this time, 0.15 mL of NaOH (5 mol L⁻¹) and 0.15 mL of murexide solution in a mixture of water:ethanol 1:1 v/v (2.5 mg mL⁻¹) were added to the solution. Titrations were performed with 0.01 M EDTA solution until the color changed from slightly pink to light purple, according to the complexometric titration procedure for the determination of Ca ions ^{1,2}. Based on the volume loss of an EDTA solution of known concentration, the amount of free Ca ions in the solution was calculated. The titration error was 4 % and it was determined by titrating reference solution of CaCl₂ of known concentration, without the addition of polymers and chelating compounds.

Mg ions trapping ability was studied by complexometric titration in an ammonium buffer environment, in the presence of eriochrome black T as an indicator. Samples were dissolved in water (5 mg mL⁻¹) and their pH was adjusted to 7 and 12 with the use of NaOH solution. Then MgCl₂·6H₂O was added (an equimolar amount of Mg ions relative to the DOTA or DTPA molecules in the conjugate) and the solutions were stirred for 24 hours. After this time, 1 mL of ammonium buffer and 0.15 mL of eriochrome black T (solution in MeOH, 5 mg mL⁻¹) were added to the solution. Titrations were performed with 0.01 M EDTA solution until the color changed from pink to purple, according to th

complexometric titration procedure for the determination of Mg ions ¹. Based on the volume loss of an EDTA solution of known concentration, the amount of free Mg ions in the solution was calculated. The titration error was 0.5 % and it was determined by titrating reference solution of MgCl₂ of known concentration, without the addition of polymers and chelating compounds.

Fe ions trapping ability was studied by complexometric titration in the presence of 5-sulfosalicylic acid dihydrate as an indicator. Samples were dissolved in water (5 mg mL⁻¹) and their pH was 3-4. Then FeCl₃·6H₂O was added (an equimolar amount of Fe ions relative to the DOTA or DTPA molecules in the conjugate) and the solutions were stirred for 24 hours. After this time, 0.15 mL of 5-sulfosalicylic acid dihydrate solution in EtOH (16 mg mL⁻¹) were added to the solution. Titrations were performed with 0.01 M EDTA solution until the color changed from brown to bright yellow, according to the complexometric titration procedure for the determination of Fe ions ³. Based on the volume loss of an EDTA solution of known concentration, the amount of free Fe ions in the solution was calculated. The titration error was 2 % and it was determined by titrating reference solution of FeCl₃ of known concentration, without the addition of polymers and chelating compounds.

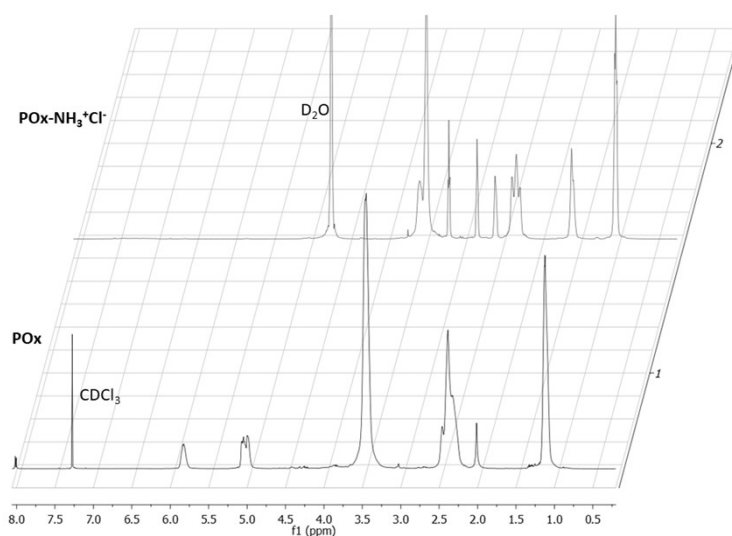


Fig. S1. ¹H NMR of POx (CDCl₃) and POx-NH₃⁺Cl⁻ (D₂O).

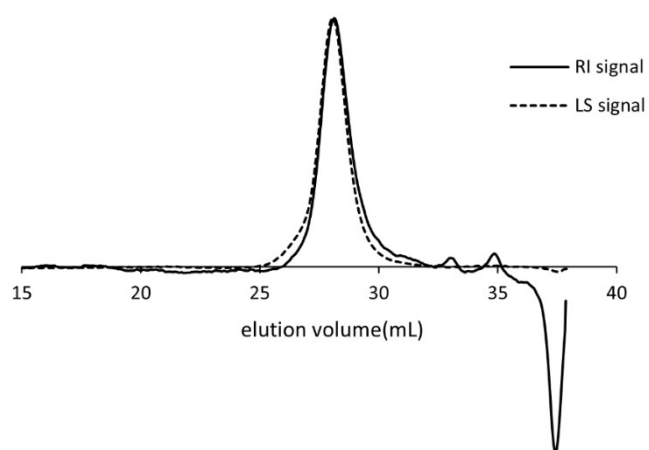


Fig. S2. SEC RI and LS signal of POx (DMF).

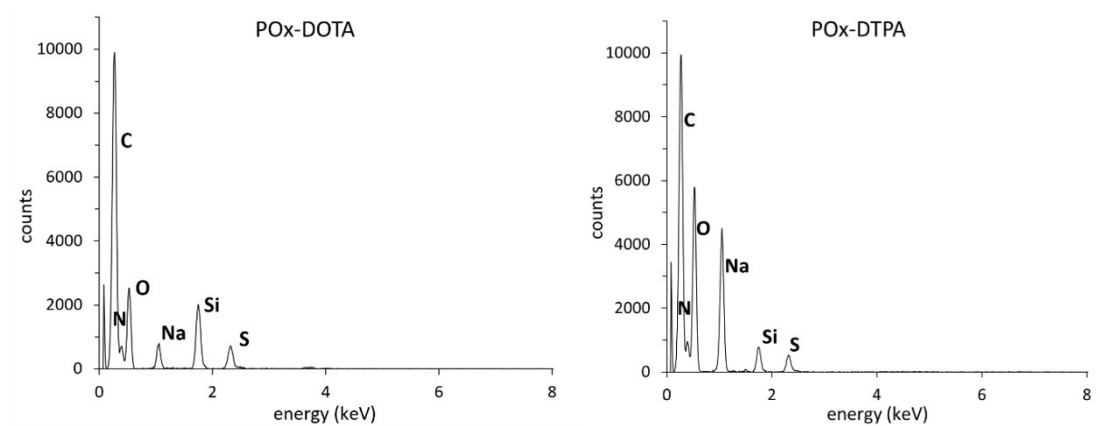


Fig. S3. The EDX curves of pure POx-DOTA and POx-DTPA, non-complexed with Ca^{2+} , Mg^{2+} or Fe^{3+} .

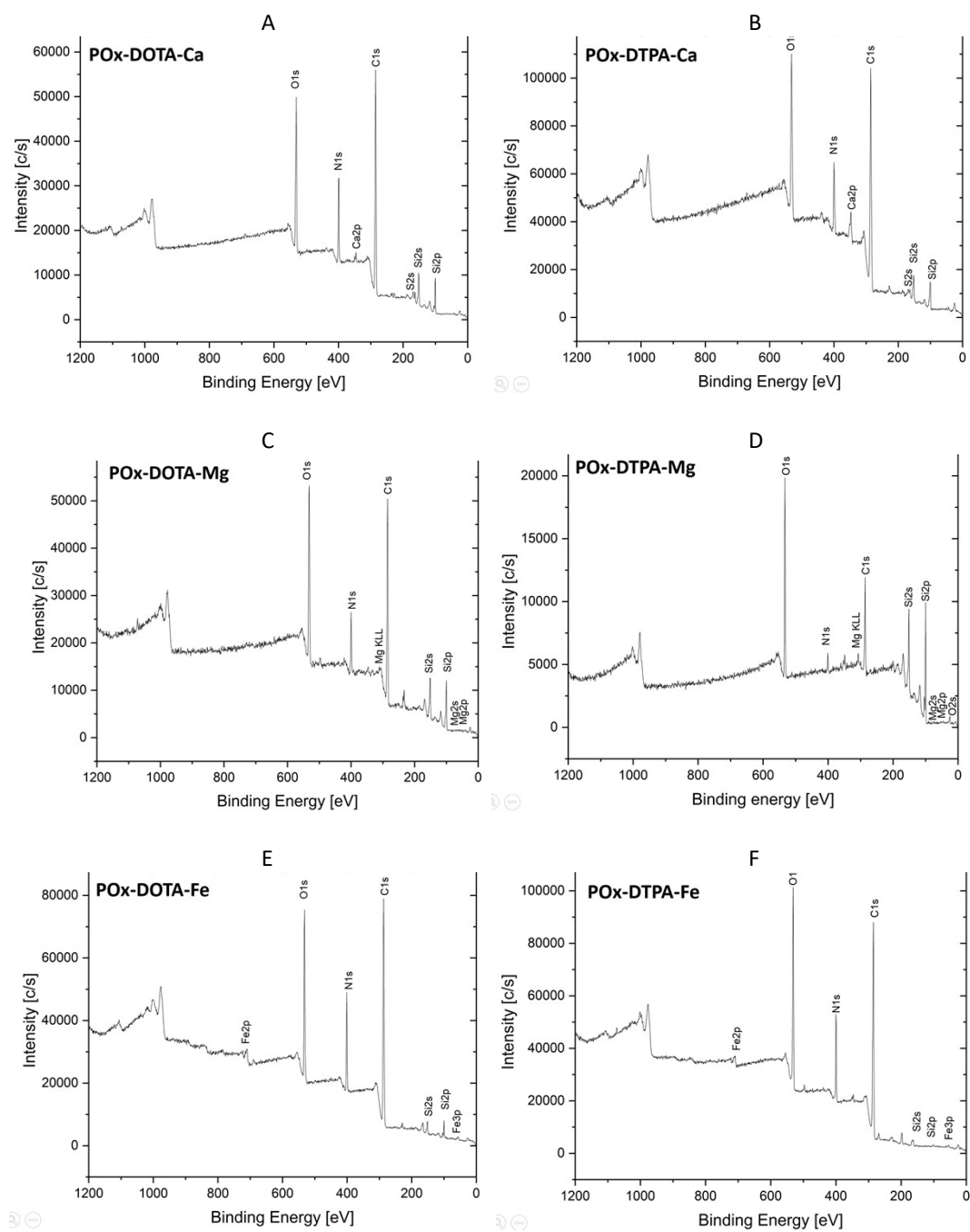


Fig. S4. XPS survey photoemission spectra of POx-DOTA-Ca (A), POx-DTPA-Ca (B), POx-DOTA-Mg (C), POx-DTPA-Mg (D), POx-DOTA-Fe (E) and POx-DTPA-Fe (F).

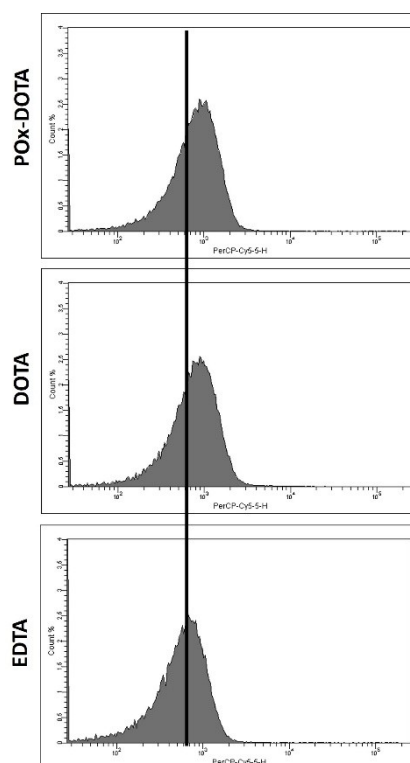


Fig. S5. Flow cytometry analysis of Trypan Blue staining of *E. coli* treated with DOTA and EDTA.

SUPPORTING INFORMATION REFERENCES

- 1 O. Gjems, *Analyst*, 1960, **85**, 738–744.
- 2 J. C. H. Van Schouwenburg, *Anal. Chem.*, 1960, **32**, 709–711.
- 3 J. Kozak, J. Paluch, M. Kozak, M. Duracz, M. Wieczorek and P. Koscielniak, *Molecules*, 2020, **25**, 1533.