Polymer-Iodine Complexes: A Study on Interaction and Antimicrobial Effects of Selected Poly(2-alkyl-2-oxazolines)

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Introduction

Iodine is a potent, broad-spectrum disinfectant, but its low water solubility and volatility limit its application. Complexation with water-soluble polymers, forming iodophors, improves iodine's stability and usability. While PVP-based iodophors are widely used, poly(2-oxazolines) (POZs) offer a promising alternative due to their biocompatibility, tunable hydrophilicity, and structural flexibility. This study explores iodine complexation with PMOZ, PEOZ, and PPOZ versus PVP using advanced physicochemical and modelling methods to reveal mechanisms influencing complex formation and antimicrobial potential.

Methods

- UV-Vis spectroscopy
- Viscometry
- Partitioning (Using Chamber)
- Antimicrobial analyses

Results

Iodophors were prepared using PVP, PMOZ, PEOZ, and PPOZ at varying [polymer]:[iodine] ratios (1:1, 5:1, 10:1) in I_2/KI solution. UV-Vis spectra (Figure 1) showed bathochromic shifts and increased peak intensity for PVP, PEOZ, and especially PPOZ, indicating strong complexation and intense colouration. PMOZ showed no spectral shift or visible colour change, suggesting weak iodine interaction.

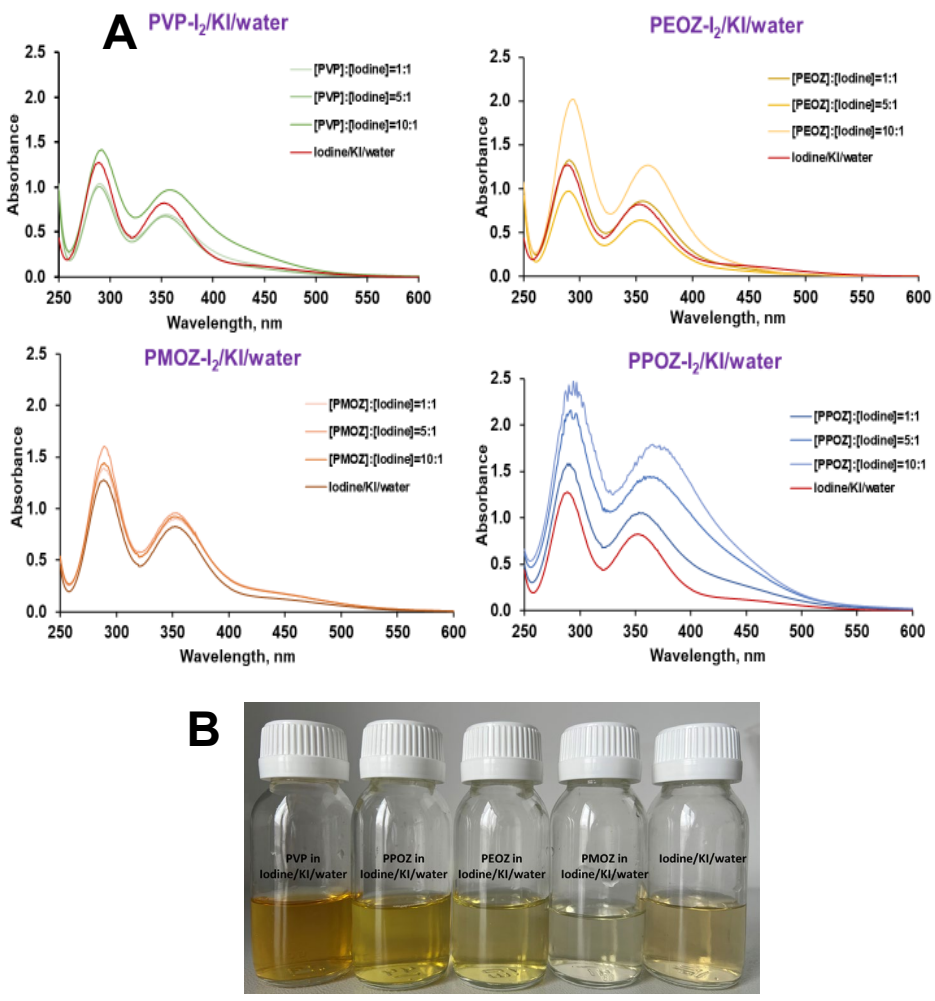

Figure 1. A) UV–vis spectra of PVP-iodine, PEOZ-iodine, PMOZ-iodine, and PPOZ-iodine solutions with molar ratio [polymer]:[iodine] = 1:1, 5:1, 10:1 and 0.04 mg/mL iodine solution. B) photo insert

The iodine-binding ability of PVP, PMOZ, PEOZ, and PPOZ was evaluated using a two-chamber Ussing system with spectrophotometric quantification at 352 nm. All iodophors showed partition coefficients (PC) >1, confirming iodine retention in the donor cell due to polymer binding (Figure 2). The binding affinity followed the trend: PEOZ ≈ PPOZ > PMOZ > PVP. Higher PC values indicate stronger iodine-polymer interaction, with PEOZ and PPOZ demonstrating the highest affinity.

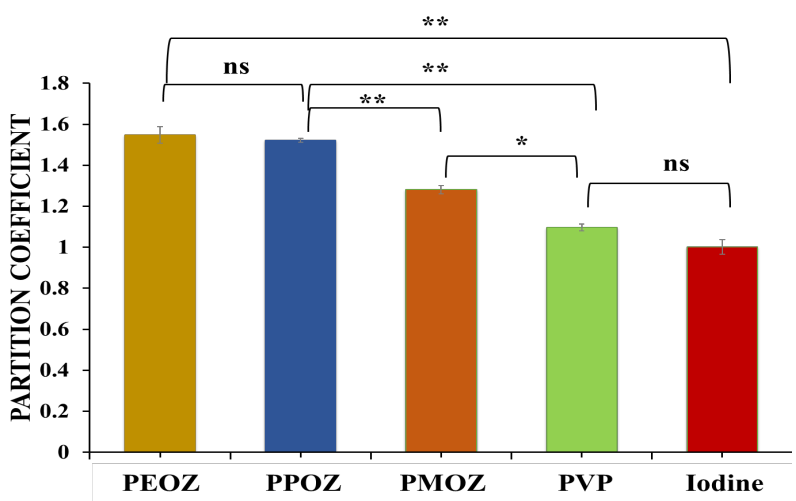

Figure 2. Comparative analysis of the partition coefficient values for pure iodine and iodophors PVP, PPOZ, PEOZ and PMOZ. A statistically significant difference is given as: ***- p < 0.001; ** - p <0.01; * - p <0.05 and no statistically significant difference – p> 0.05

Results

All polymers showed reduced intrinsic viscosity in iodine/KI/water, confirming polymer–iodine complexation and chain compaction. The effect was strongest for PPOZ and PEOZ. Huggins constants further indicated reduced solvent quality and increased compactness of iodophor structures.

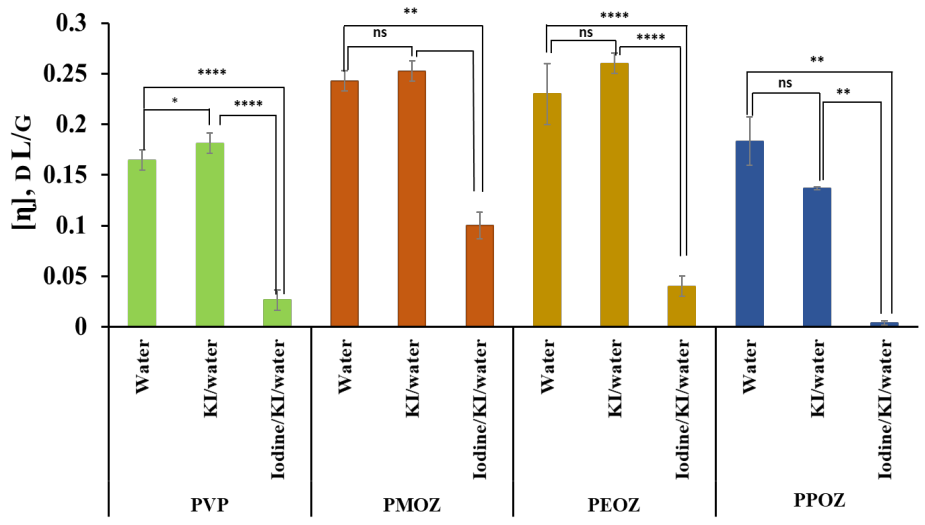

Figure 3. Intrinsic viscosity values in three different solvents for four polymers. All values are the means ± standard deviations of triplicate experiments. Statistically significant differences are given as: **** - p < 0.0001; *** - p < 0.001; ** - p < 0.01; * - p < 0.05.

Table 1– Comparative table of Huggins constants (k_H) for different solvents and polymers.

Polymer	Water	KI/water	Iodine/KI/water
	k_H	k_H	k_H
PVP	1,48±0,34	1,52 ± 0,39	>100
PMOZ	1,12±0,12	1,02±0,03	9,98±2,87
PEOZ	1,49±0,70	1,04 ± 0,65	>100
PPOZ	2,25±1,52	3,73±0,09	>100

All iodophors showed activity against *S. aureus*, *B. subtilis*, *E. coli*, and *C. albicans*. The most potent was [PPOZ]-iodine (10:1), with the lowest MBCs: 4.88×10^{-5} mg/mL for *S. aureus* and *B. subtilis*, and 9.7×10^{-5} mg/mL for *E. coli*. For *C. albicans*, [PVP]-iodine (1:1) showed the best result: 1.6×10^{3} mg/mL ($p < 0.0001$).

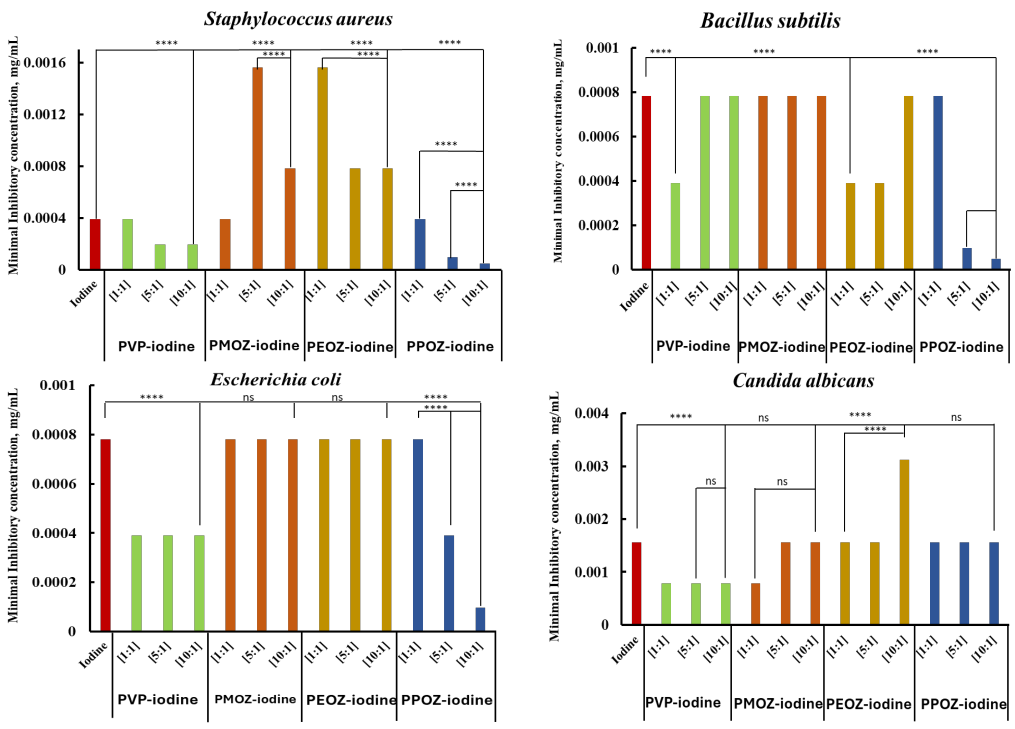

Figure 4. Minimal Bactericidal Concentrations of iodophors based on PVP, PMOZ, PEOZ, and PPOZ against Staphylococcus aureus, Bacillus subtilis, Escherichia coli and Candida albicans. Statistical significance compared to a positive control (pure iodine) was evaluated via a one-way ANOVA test (****- p < 0.0001; and no statistically significant difference – p> 0.05).

Conclusion

Based on UV-vis and partition coefficient data, PPOZ and PEOZ showed the highest iodine-binding efficiency, correlating with more substantial bathochromic shifts and higher k_H values. These polymers also formed compact iodine complexes and exhibited superior antimicrobial activity. In contrast, PMOZ showed minimal binding and weak bioactivity. Structural features explain the observed differences in interaction and efficacy.

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