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Solubility Analysis of Endodontic Irrigants within the Root Canal System: A Computational Modeling Approach

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Abstract

Introduction: Endodontic irrigation solutions play an important role in the success of root canal treatment because they are able to clean debris, dissolve necrotic tissue, and reduce the number of bacteria. However, the effectiveness of irrigation materials can be affected by temperature factors during clinical procedures. **Purpose:** This study aims to analyse the effect of temperature on the solubility of several endodontic irrigation materials using the COSMO-RS computational modelling method as a predictive approach. **Methods:** This study is an analytical observational study endodontic irrigation). Chemical structure data were obtained from the PubChem database and analysed using COSMO-RS software **Results:** The results showed that increasing the temperature from 36ºC to 37ºC significantly increased the solubility of all irrigation materials. CHX had the highest solubility, followed by EDTA and MTAD. **Conclusion:** Increasing temperature has been shown to increase the solubility of endodontic irrigants, while the COSMO-RS computational method effectively predicts solubility before laboratory testing.

Key Words: Endodontic irrigation solution; solubility; COSMO-RS; temperature

Introduction

Endodontic infection is a biofilm-mediated disease that develops within the complex anatomical structure of the root canal system. The root canal harbors dental pulp tissue and exhibits extensive morphological variations, including lateral canals, isthmuses, and apical ramifications, which collectively create anatomical niches that facilitate microbial persistence and limit effective debridement. Once established, intracanal biofilms demonstrate high resistance to host defense mechanisms and antimicrobial agents, leading to progressive periapical inflammation and potential treatment failure if not adequately eliminated.[1,2]

The primary objective of root canal treatment is the complete elimination of microbial infection through chemomechanical debridement, followed by three-dimensional obturation of the canal space. Although mechanical instrumentation is essential for shaping and enlarging the canal system, it is insufficient to achieve complete disinfection due to the presence of inaccessible anatomical complexities. Consequently, chemical irrigation remains a critical determinant of treatment success, acting as the main mechanism for biofilm disruption, tissue dissolution, and smear layer removal.[1,3]

Sodium hypochlorite (NaOCl) is widely recognized as the gold-standard irrigant due to its broad-spectrum antimicrobial activity and ability to dissolve organic tissue. Ethylenediaminetetraacetic acid (EDTA) is primarily used for inorganic smear layer removal, while chlorhexidine (CHX) provides substantivity against residual microbial populations. Recent evidence indicates that NaOCl-based protocols remain superior in microbial reduction compared to alternative irrigants; however, their clinical effectiveness is influenced by concentration, exposure time, and activation method.[4,5]

The effectiveness of endodontic irrigants is determined not only by their chemical composition but also by physicochemical factors such as temperature, pH, viscosity, and surface tension. Among these variables, temperature is a critical parameter that can modify solution behavior, including solubility and molecular diffusion. An increase in temperature enhances the kinetic energy of molecules, thereby strengthening solute–solvent interactions and accelerating the rate of dissolution.[6,7]

The temperature within the oral cavity and root canal system generally ranges between 36°C and 37°C. Although the difference is relatively small, it may still influence the physicochemical properties of irrigating solutions. Several studies have reported that heating sodium hypochlorite (NaOCl) enhances its antimicrobial activity and organic tissue dissolution capacity.[8] In addition, chelating agents such as EDTA have been shown to exhibit improved efficiency in calcium ion release from dentin under elevated temperature conditions.[9] Other studies have also demonstrated that temperature variations can alter the surface tension of irrigant solutions, thereby improving penetration into dentinal tubules and enhancing interaction with dentinal structures.[10]

From a thermodynamic perspective, the solubility of a substance is strongly dependent on system energy. An increase in temperature enhances solubility by increasing Gibbs free energy dynamics and molecular interactions between solute and solvent.[11] Although numerous studies have investigated the effect of temperature on the antimicrobial activity and physicochemical properties of irrigants, research specifically comparing the solubility of different endodontic irrigants under physiological temperature conditions (36°C–37°C) remains limited. Furthermore, comparative data regarding chlorhexidine digluconate (CHX), EDTA, and MTAD in terms of temperature-dependent solubility have not been systematically explored using modern computational or predictive approaches.

Parallel to experimental and clinical developments, computational modeling has emerged as a powerful approach to investigate irrigation dynamics. Computational fluid dynamics (CFD) enables detailed simulation of irrigant flow behavior, wall shear stress distribution, and apical penetration within anatomically realistic root canal models. Recent CFD studies demonstrate that irrigation efficacy is strongly influenced by canal geometry, needle design, and insertion depth, emphasizing the importance of hydrodynamic optimization for improving debridement efficiency and safety.[12] In addition, thermodynamic modeling approaches, particularly COSMO-RS (Conductor-like Screening Model for Real Solvents), provide molecular-level prediction of solubility and interaction behavior of chemical irrigants, offering a novel framework for understanding solution behavior under clinically relevant conditions. Despite these advances, integration between physicochemical modeling and endodontic irrigation research remains limited.

Although substantial progress has been made in both experimental and computational endodontics, several critical gaps remain. First, most studies focus on antimicrobial efficacy and flow dynamics independently, with limited integration between physicochemical solubility behavior and intracanal fluid mechanics. Second, current irrigation models are predominantly based on simplified anatomical assumptions that do not fully capture the complexity of real root canal systems. Third, there is a lack of predictive computational frameworks capable of simultaneously evaluating irrigant solubility, stability, and hydrodynamic performance under clinically relevant conditions. These limitations restrict the development of optimized, evidence-based irrigation protocols.[3,12] Proper irrigation, indicates that the higher the ability of an irrigating solution to dissolve organic tissue, the more effective the chemical debridement process of the root canal becomes, provided that tissue toxicity and the safety of periapical tissues are appropriately considered.[2]

To address these limitations, this study introduces a computational modeling framework that integrates thermodynamic prediction (COSMO-RS) with endodontic irrigant analysis to evaluate solubility behavior under controlled conditions. The present study does not incorporate computational fluid dynamics (CFD) or intracanal hydrodynamic simulation; rather, it focuses exclusively on molecular-level solubility prediction without coupling to fluid flow modeling within the root canal environment.

Unlike conventional studies that focus solely on antimicrobial or hydrodynamic performance, this approach enables a molecular-level assessment of irrigant behavior, providing fundamental physicochemical insights into solubility and solute–solvent interactions. These findings may contribute to a better understanding of irrigant performance under clinically relevant conditions, although without directly simulating the anatomical or hydrodynamic complexity of the root canal system. This study aims to analyze the solubility behavior of selected endodontic irrigants using a COSMO-RS-based computational modeling approach and to evaluate their physicochemical performance in relation to their potential effectiveness in root canal disinfection protocols.

Methods

Study Design

This study was an analytical computational (in silico) modeling study designed to evaluate the solubility behavior of endodontic irrigants using thermodynamic predictions. The COSMO-RS method was employed to simulate molecular interactions and estimate solubility parameters under controlled theoretical conditions. This approach was selected due to its capability to predict molecular interactions based on thermodynamic parameters without requiring in vitro experimentation.

Study Variables

The independent variable in this study was the type of endodontic irrigant solution, while the dependent variable was the solubility behavior of the irrigants in the root canal environment. The solvent environment was defined as biological fluids commonly found in the root canal, including saliva, gingival crevicular fluid (GCF), pulpal fluid, and blood.

Dataset Selection

This study included eight commonly used endodontic irrigant compounds, namely sodium hypochlorite (NaOCl), ethylenediaminetetraacetic acid (EDTA), chlorhexidine digluconate (CHX), hydroxyethylidene bisphosphonate (HEBP), iodine potassium iodide (IKI), MTAD, Tetraclean, and QMix. The compounds were selected as a curated chemical dataset based on their clinical relevance in endodontic irrigation and the availability of validated molecular structures. Molecular structures were retrieved from the PubChem database and converted into Simplified Molecular Input Line Entry System (SMILES) notation for computational modelling using COSMO-RS.

Inclusion and Exclusion Criteria

The inclusion criteria comprised irrigant compounds that were structurally representable within the COSMO-RS computational framework and could be converted into valid molecular input formats (SMILES notation) for thermodynamic modeling. Compounds were included based on their clinical relevance in endodontic irrigation and the availability of retrievable molecular or representable chemical structures from the PubChem database. Compounds lacking a definable or computable molecular structure suitable for COSMO-RS input were excluded.

Data Acquisition Procedure

The molecular structures of all irrigants were obtained from the PubChem database and converted into SMILES format. Each SMILES structure was then imported into COSMO-RS software to generate molecular surface charge distributions and thermodynamic properties. Solubility calculations were performed using the “solubility in pure solvent” module, with water (H_2O) defined as a surrogate solvent representing the dominant aqueous phase of the physiological oral environment. This approach was used as an approximation of the intraoral and intracanal conditions, where irrigants are primarily in contact with aqueous biological fluids. The output was presented in both numerical form and graphical representation.

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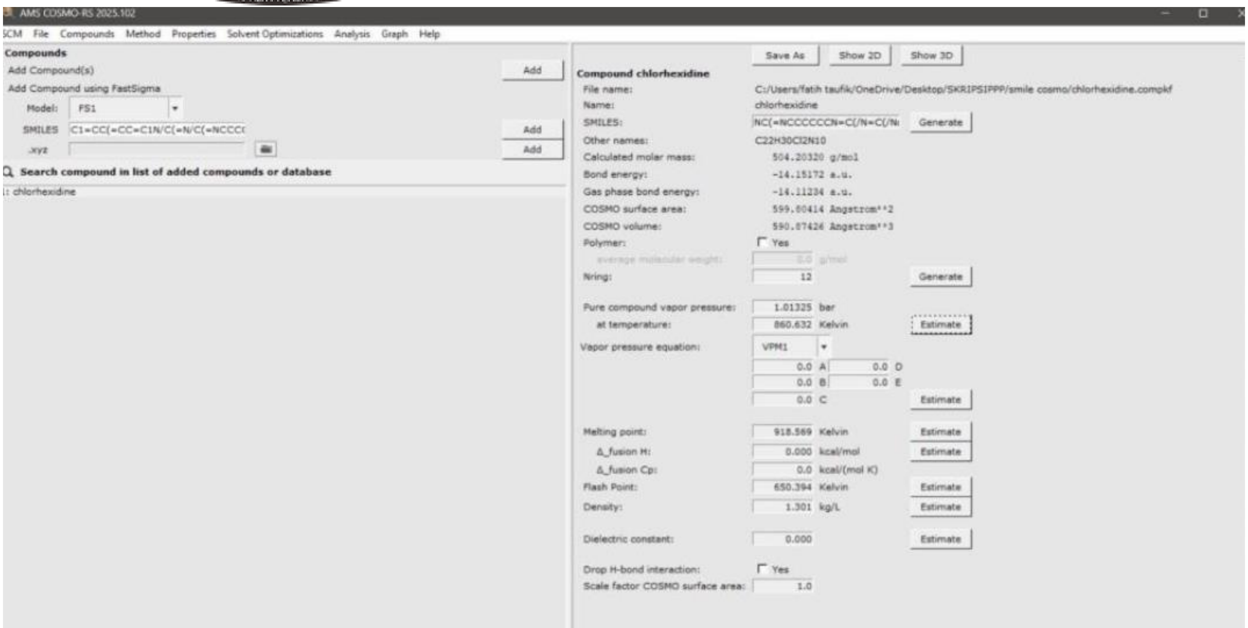

Figure 1. COSMO-RS interface after SMILES input

Data Processing and Analysis

The resulting solubility data were exported and organized using Microsoft Excel for initial tabulation and data management. Subsequent statistical analysis was performed using IBM SPSS Statistics version 29 to evaluate differences among irrigant groups. Computational modeling was carried out using COSMO-RS in the corresponding Amsterdam Modeling Suite (AMS) 2025. Molecular structures retrieved in SMILES format. Solubility predictions were performed under two defined physiological temperature conditions, namely 36°C and 37°C, representing the range of intraoral and intracanal body temperature fluctuations. The COSMO-RS solubility in pure solvent function was applied to estimate thermodynamic solubility behavior based on chemical potential differences between solute and solvent.

Statistical Analysis

Bivariate analysis was performed to evaluate differences between irrigant groups. Independent sample t-tests were used for comparisons between two groups, while one-way analysis of variance (ANOVA) was applied for comparisons involving more than two groups. When ANOVA results indicated statistically significant differences, post hoc analysis was conducted using Tamhane's test due to the assumption of unequal variances among groups. A significance level of $p < 0.05$ was considered statistically significant.

Results

Selection of endodontic irrigants was performed based on the chemical structures of each root canal irrigating solution, obtained from the PubChem database (https://pubchem.ncbi.nlm.nih.gov/), ensuring structural validity for computational analysis (Table 1).

Table 1. Endodontic Irrigants

No.	Endodontic Irrigant	Structure	SMILES
1.	*Sodium hypochlorite*	NaOCl	[O-]Cl.[Na+]
2.	*Ethylenediaminetetraacetic acid*	$C_{10}H_{16}N_2O_8$	C(CN(CC(=O)O)CC(=O)O)N(CC(=O)O)CC(=O)O
3.	*Chlorhexidine digluconate*	$C_{34}H_{54}Cl_2N_{10}O_{14}$	C1=CC(=CC=C1N/C(=N/C(=NCCCCCCN=C(/N=C(/NC2=CC=C(C=C2)Cl)\N)N)N)/N)Cl.C(O)[C@@H](O)[C@@H](O)[C@H](O)[C@@H](O)C(=O)O.C(O)[C@@H](O)[C@@H](O)[C@H](O)[C@@H](O)C(=O)O
4.	*Hydroxyethylidene Bisphosphonate*	$C_2H_8O_7P_2$	CC(O)(P(=O)(O)O)P(=O)(O)O
5.	*Iodine potassium iodide*	I_2K^-	[K+].[I-].[I-]
6.	*MTAD*	$C_3H_3N_3O_2$	C1=CN=C(N1)[N+](=O)[O-]
7.	*Tetraclean*	$C_{46}H_{58}Cl_2N_4O_{18}$	CCO.C[C@@H]1[C@H]2[C@@H]([C@H]3[C@@H](C(=O)C(=C([C@]3(C(=O)C2=C(C4=C1C=CC=C4O)O)O)O)C(=O)N)N(C)C)O.C[C@@H]1[C@H]2[C@@H]([C@H]3[C@@H](C(=O)C(=C([C@]3(C(=O)C2=C(C4=C1C=CC=C4O)O)O)O)C(=O)N)N(C)C)O.O.Cl.Cl
8.	QMix	$C_{34}H_{54}Cl_2N_{10}O_{14}$	C1=CC(=CC=C1N/C(=N/C(=NCCCCCCN=C(/N=C(/NC2=CC=C(C=C2)Cl)\N)N)N)/N)Cl.C(O)[C@@H](O)[C@@H](O)[C@H](O)[C@@H](O)C(=O)O.C(O)[C@@H](O)[C@@H](O)[C@H](O)[C@@H](O)C(=O)O
		$C_{12}H_7Cl_3O_2$	C1=CC(=C(C=C1Cl)O)OC2=C(C=C(C=C2)Cl)Cl
		$C_{10}H_{16}N_2O_8$	C(CN(CC(=O)O)CC(=O)O)N(CC(=O)O)CC(=O)O

The data analysis demonstrated a statistically significant effect of root canal irrigant type on differences in temperature-dependent solubility behavior, particularly among chlorhexidine (CHX), ethylenediaminetetraacetic acid (EDTA), and MTAD. Based on the results of the independent t-test (Table 2), all irrigants exhibited p-values < 0.05, indicating statistically significant differences in solubility between the temperatures of 36°C and 37°C.

Table 2. T-test results comparing the solubility of endodontic irrigants at 36°C and 37°C

Endodontic Irrigant	Temperature (celcius)	Mean (±SD)	Nilai p
CHX	36°	0,140x10^{-5} (0,5x10^{-8})	<0,002*
	37°	0,142x10^{-5} (0,8x10^{-8})	
EDTA	36°	0,402x10^{-3} (0,279x10^{-5})	<0,001*
	37°	0,412x10^{-3} (0,3384x10^{-5})	
MTAD	36°	1,180x10^{-2} (0,495x10^{-2})	<0,001*
	37°	1,0192 (0,597x10^{-2})	

*Significant T-Test p<0,05

Furthermore, one-way ANOVA analysis (Table 3) revealed statistically significant differences in the solubility of all tested endodontic irrigants. The parameter expressed as mol/L solution showed a significance value of p = 0.001 (p<0.05), confirming significant intergroup differences among the endodontic irrigant categories. Post-hoc analysis using Tamhane's test further demonstrated statistically significant pairwise differences in solubility among the three irrigants (CHX, EDTA, and MTAD) across all evaluated parameters, indicating distinct physicochemical behavior between each irrigant group.

Table 3. ANOVA test results for the solubility of all endodontic irrigants

	Mean (±SD)	Nilai p
mol/L Solution of all endodontic irrigants	0,33723 (0,484)	0,001*

*Significant One-way Anova test p<0,05

Table 4. Tamhane's post-hoc test results for the mol/L solution parameter

Endodontic Irrigant	CHX	EDTA	MTAD
CHX	-	0,001*	0,001*
EDTA	0,001*	-	0,001*
MTAD	0,001*	0,001*	-

*Tamhane's post-hoc test p<0,05

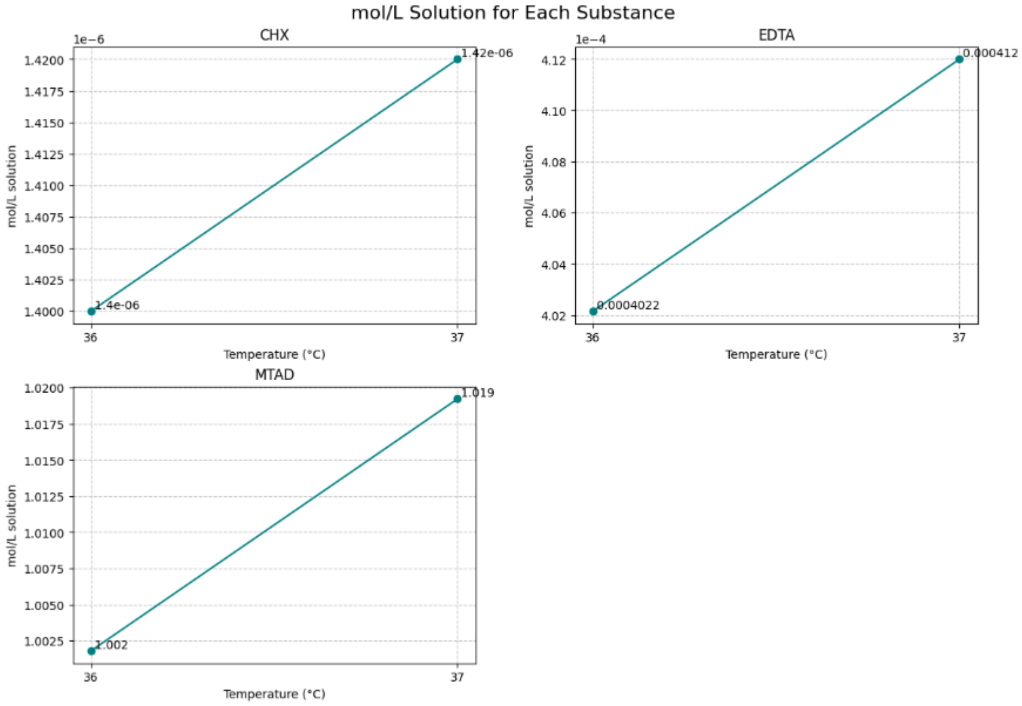

Figure 2. Solubility Graph of mol/L Solution

The results demonstrated a statistically significant increase in solubility for all tested endodontic irrigants when the temperature was elevated from 36°C to 37°C ($p < 0.05$). For chlorhexidine digluconate (CHX), the mole fraction increased from 2.160 to 2.1895 ($p = 0.001$), accompanied by significant increases in both mol/L solvent and mol/L solution parameters ($p = 0.002$). These findings indicate improved solubility of CHX at higher temperatures, which may enhance its antimicrobial efficacy. For ethylenediaminetetraacetic acid (EDTA), the mole fraction increased from 0.619×10^{-5} to 0.634×10^{-5} ($p = 0.001$), with statistically significant increases observed in both mol/L solvent and mol/L solution parameters. Although the magnitude of change was relatively small, the results confirm that EDTA solubility is still influenced by temperature variations. Similarly, for MTAD, the mole fraction increased from 0.0164 to 0.0167 ($p = 0.001$), alongside significant increases in both concentration-related parameters. These findings suggest that MTAD solubility is also temperature-dependent, although current literature remains limited regarding its direct thermodynamic behavior under physiological temperature variation.

All irrigant data presented in Tables 2 and 4 correspond to irrigant solutions that could be represented and processed within COSMO-RS, whereas other solutions could not be read or analyzed by the COSMO-RS software.

Discussion

Endodontic irrigants play a crucial role in the success of root canal treatment due to their ability to remove debris, dissolve necrotic tissue, and reduce the bacterial load within the root canal system. One of the key factors influencing the effectiveness of irrigating solutions is temperature.[8,13] Increased solubility is associated with faster chemical interactions with surrounding tissues, where elevated temperature enhances the dissolution capacity of substances in a solvent medium. In general, liquids at higher temperatures dissolve solutes more efficiently compared to those at lower temperatures. Additionally, increased solute concentration may contribute to changes in solution viscosity, which can further influence fluid dynamics and penetration within confined anatomical structures.[8,14,15]

These findings are consistent with previous studies reporting that temperature elevation can enhance the antimicrobial efficacy of chlorhexidine digluconate (CHX) in root canal irrigation. This effect may be reflected by higher mole fraction values of CHX, indicating increased solute availability and concentration-dependent antimicrobial activity. Therefore, the present study aims to evaluate the effect of physiological oral cavity temperature variations (36°C and 37°C) on the solubility of three commonly used endodontic irrigants, namely chlorhexidine digluconate (CHX), ethylenediaminetetraacetic acid (EDTA), and a mixture of tetracycline, acid, and detergent (MTAD).[6,10]

The results of this study are consistent with thermodynamic principles stating that an increase in temperature raises the kinetic energy of solvent molecules, thereby enhancing solute–solvent interactions and accelerating the dissolution process. Recent studies support this mechanism. For instance, it has been reported that heating EDTA at physiological temperatures enhances calcium ion release from dentin, thereby improving its effectiveness compared to room temperature conditions.[7,8] Other studies have shown that temperature variations can modify the surface tension of irrigant solutions, including EDTA and MTAD, which in turn influences their penetration into dentinal structures. Furthermore, temperature differences have been shown to affect irrigant diffusion within dentinal tubules and improve interactions with bioceramic-based sealers.[9,16]

The clinical implications of these findings should be interpreted within the context of physiological temperature variations in the oral cavity, which typically range between 36°C and 37°C. Within this narrow physiological range, even minor temperature fluctuations may influence the thermodynamic behavior of irrigant solubility, as demonstrated by the computational model. It is important to distinguish these physiological conditions from external heating protocols, such as warm vertical compaction or pre-heated irrigant delivery systems, which have been reported in previous studies to further enhance irrigant reactivity. The present study, however, specifically evaluates solubility behavior under physiological temperature conditions rather than externally induced thermal modification.

The clinical implications of the present findings should be interpreted cautiously, as irrigant selection in endodontic therapy is primarily determined by the targeted tissue substrate, antimicrobial spectrum, and the specific phase of treatment, rather than solubility behavior alone. The observed temperature-dependent variations in solubility may influence the physicochemical availability, diffusion capacity, and interaction dynamics of irrigants, which could indirectly contribute to their overall clinical performance. However, these effects should be regarded as supporting physicochemical modifiers rather than primary determinants in clinical decision-making. Chlorhexidine digluconate (CHX), MTAD, and EDTA retain their established clinical indications based on their intrinsic biological functions, including antimicrobial substantivity and smear layer removal capability. Therefore, solubility variations induced by physiological temperature changes should be interpreted as modulatory physicochemical phenomena that may complement but do not dictate the selection of irrigants in evidence-based endodontic practice.[11,17]

A limitation of this study is that several irrigant compounds could not be processed using the COSMO-RS software. Future studies are recommended to perform direct experimental validation on a wider range of endodontic irrigant solutions to better evaluate and compare their solubility behavior under physiological conditions. The findings of this study are expected to serve as a reference for clinicians, researchers, and academics in selecting the most appropriate irrigant based on specific clinical indications.

Conclusion

Computational modeling using COSMO-RS demonstrated that temperature exerts a significant influence on the solubility behavior of endodontic irrigants. An increase in temperature enhances solubility, primarily driven by increased kinetic energy of solvent molecules, which strengthens solute–solvent interactions and promotes more efficient dissolution processes. Among the irrigants evaluated, chlorhexidine digluconate (CHX) exhibited the highest solubility profile compared with EDTA and MTAD, suggesting superior thermodynamic favorability under the studied conditions.

These findings highlight the applicability of COSMO-RS-based computational modeling as a reliable predictive tool for assessing the physicochemical behavior of endodontic irrigants. Such an approach may support the rational selection and optimization of irrigating solutions in root canal therapy by providing molecular-level insights that are difficult to obtain through conventional experimental methods.

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