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Using artificial intelligence to predict the final color of leucite-reinforced ceramic restorations

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Abstract

Objectives: The aim of this study was to evaluate the accuracy of machine learning regression models in predicting the final color of leucite-reinforced glass CAD/CAM ceramic veneer restorations based on substrate shade, ceramic shade, thickness and translucency.

Methods: Leucite-reinforced glass ceramics in four different shades were sectioned in thicknesses of 0.3, 0.5, 0.7, and 1.2 mm. The CIELab coordinates of each specimen were obtained over four different backgrounds (black, white, A1, and A3) interposed with an experimental translucent resin cement using a calibrated spectrophotometer. The color change (CIEDE2000) values, as well as all the CIELab values for each one of the experimental groups, were submitted to 28 different regression models. Each regression model was adjusted according to the weights of each dependent variable to achieve the best-fitting model.

Results: Different substrates, ceramic shades, and thicknesses influenced the *L*, *a*, and *b* of the final restoration. Of all variables, the substrate influenced the final ceramic shade most, followed by the ceramic thickness and the *L*, *a*, and *b* of the ceramic. The decision tree regression model had the lowest mean absolute error and highest accuracy to predict the shade of the ceramic restoration according to the substrate shade, ceramic shade and thickness.

Clinical Significance: The machine learning regression model developed in the study can help clinicians predict the final color of the ceramic veneers made with leucite-reinforced glass CAD/CAM ceramic HT and LT when cemented with translucent cements, based on the color of the substrate and ceramic thicknesses.

KEYWORDS
artificial intelligence, CIEDE2000, CIELab, color science, dental ceramics, spectrophotometer

1 | INTRODUCTION

Dental ceramics are constantly developing and are essential materials for restorative dental treatments.[1] For conventional feldspathic ceramics, the dental technician constructs a ceramic restoration by condensing and sintering layers of ceramic powder with different shades and opacities to mimic the natural tooth structure. However, this approach is becoming rare since computer-aid design and computer-aid manufacturing (CAD/CAM) can produce monolithic ceramic restorations with similar optical properties but higher mechanical properties.[2–4]

IPS Empress CAD (Ivoclar Vivadent, Schaan, Liechtenstein) is a leucite-reinforced ceramic that presents a higher leucite volume as its crystalline phase, resulting in improved mechanical properties.[5] The material is processed using the hot-pressing or CAD/CAM techniques.

The mechanical strength and excellent optical properties make leucite-reinforced ceramics suitable for veneers and anterior crowns.[6]

The chairside CAD/CAM dentistry is an extraordinary achievement that allows the dentist to select and handle ceramic materials. Consequently, the final results depend on the dentist's skills with these materials.[7–17] Considerable research has been devoted to color-matching CAD/CAM ceramic materials. However, most laboratory studies are hard to translate due to the vast number of clinical variables.[18–38]

Visual shade selection is the traditional and most common method used for shade evaluation in dentistry, but it still presents many limitations.[35,39–43] Instrumental color measurement has increased in popularity over the years.[44,45] Different spectrophotometers, colorimeters, and imaging systems have been used in dentistry for shade evaluation.[46,47] Instrumental measurement provides objective and quantitative data, reducing the visual method's subjectivity. However, there is no method to combine the CIELab coordinates (*L*, *a*, and *b*)[30,48] obtained from the tooth substrate and ceramic to predict the best ceramic type, shade, and thickness.

Artificial intelligence (AI) can optimize and accelerate the translation of in-vitro studies. The use of AI in materials science has significantly advanced in recent years, spurred by the desire to accelerate the creation of new materials.[49–51] Conventional methods for exploring potential product designs and material formulations are inefficient, requiring either fractional factorial designs that do not adequately model the interactions of design factors or requiring too much time. However, AI excels at modeling interactions without an exhaustive full-factorial study. In a previous study,[52] the authors were able to predict the depth of cure (DOC) of resin-based composites based on spectrophotometric parameters of the light curing units. Using AI, it was possible to show that the composite and light-curing unit radiant exposure are the most critical factors in determining the composites' depth of cure. This model can predict if the composite and curing light will pass the ISO 4049 standard tests, saving time and resources in materials research and development. Likewise, understanding the variables that influence the CIELab of ceramic restorations would extend the use of spectrophotometers in dentistry, and it can lead to the development of AI models for creating software-assisted shade selection.[53,54]

Thus, the specific aims of the study were to: 1—Evaluate the *L*, *a*, and *b* of monolithic ceramics with different thicknesses, shades, and translucencies, cemented on white, black, A1, and A3 substrates with a translucent resin cement. 2—Explore machine learning regression models to assist in the shade selection of ceramic restorations based on the color coordinate parameters (*L*, *a*, and *b*). The hypotheses tested in this study are: H_1—There will be significant differences in the *L*, *a*, and *b* color coordinates of monolithic ceramics with different thicknesses, shades, and translucencies cemented on white, black, A1, and A3 substrates with translucent resin cement. H_2—The regression model created using the color coordinate parameters (*L*, *a*, and *b*) from the substrate and ceramic and the thickness of the ceramic will predict the final color of the ceramic restoration.

2 | MATERIALS AND METHODS

Leucite-reinforced glass–ceramics blocks (IPS Empress CAD, C14, Ivoclar Vivadent, Schaan Liechtenstein) (Figure 1) in four different shades (HT—A1, A3; LT—A1, A3) were used in this study. The blocks were bonded to dressing sticks (Buehler, Lake Bluff, IL) to allow precise cuts without chipping the specimens during the section. The assembly was mounted in a precision diamond saw machine (Isomet, Buehler, Lake Bluff, IL with the Buehler's Isomet diamond blade 15 LC, dimensions: four inches (102 mm), thickness: 0.012 in (0.3 mm) Buehler, Lake Bluff, IL) and the blocks were sectioned under water cooling at 400 rpm. Specimens ($n = 5$) perpendicular to the long axis of the blocks were obtained with thicknesses of 0.3, 0.5, 0.7, and 1.2 mm. The accuracy of the final thickness was determined with a digital caliper (Mitutoyo Corp, Kawasaki, Japan) with an accuracy of ±0.05 mm. The glaze was not applied to avoid high reflection luster that could affect shade measurement. A pilot study showed that samples prepared following this protocol present similar superficial rugosity to the samples milled in the CEREC MC XL milling machine (according to the ISO 25178—Geometric Product Specifications—Surface texture, Sa = 18.56 ± 1.7 μm for the Isomet 15LC Diamond Saw and Sa = 17.57 ± 1.8 μm for the CEREC MCXL milling machine, $p = 0.832$).

An experimental translucent resin-based cement with a refractive index of 1.5229 (Table 1) was produced without photoinitiators to simulate the cementation of the ceramic veneer on the substrate without bonding the specimens together. This simulation mimicked the refractive index changes and the light propagation through ceramic, cement, and substrate interfaces.

Four different substrates were used: white background; black background; IPS Empress LT A1 CAD/CAM block; IPS Empress LT A3 CAD/CAM block. For reference, the CIELab coordinates of backgrounds were black ($L = 22.06$, $a = 0.33$, $b = 0.30$), white ($L = 97.29$, $a = -0.06$, $b = 2.39$), IPS Empress LT A1 ($L = 71.29$, $a = 0.99$, $b = 10.87$), and IPS Empress LT A3 ($L = 64.30$, $a = 2.13$, $b = 14.82$).

The color parameters of each specimen were obtained with a D65 illuminant over the different backgrounds interposed with the translucent resin cement using a calibrated spectrophotometer (CM-700d, Konica Minolta, Tokyo, Japan) with a target mask with a sensor-opening diameter of 3 mm (SAV). The CIE 1931 2° Standard Colorimetric Observer was used to calculate color coordinate values for each specimen. The sensor opening of the spectrophotometer was placed in the center of each specimen, and three measurements were collected in both SCI (specular component included) and SCE (specular component excluded) modes. The CIELab coordinates (*L*, *a*, and *b*) from the specimens were used to evaluate color change (ΔE_{00}) from the substrate to the surface of the veneer according to the CIEDE2000 formula: $\Delta E_{00} = [(\Delta L/K_L\ S_L)^2 + (\Delta C/K_C\ S_C)^2 + (\Delta H/K_H\ S_H)^2 + R_T\ (\Delta C/K_C\ S_C)\ (\Delta H/K_H\ S_H)]^{0.5}$, where ΔL, ΔC, and ΔH are the differences in lightness, chroma and hue, and Rt is a function (the so-called rotation function) that accounts for the interaction between chroma and hue differences in the blue region. Weighting functions, S_L, S_C, and S_H adjust the total color difference for variation in the location of the color difference pair in *L*, *a*, and *b* coordinates, and the

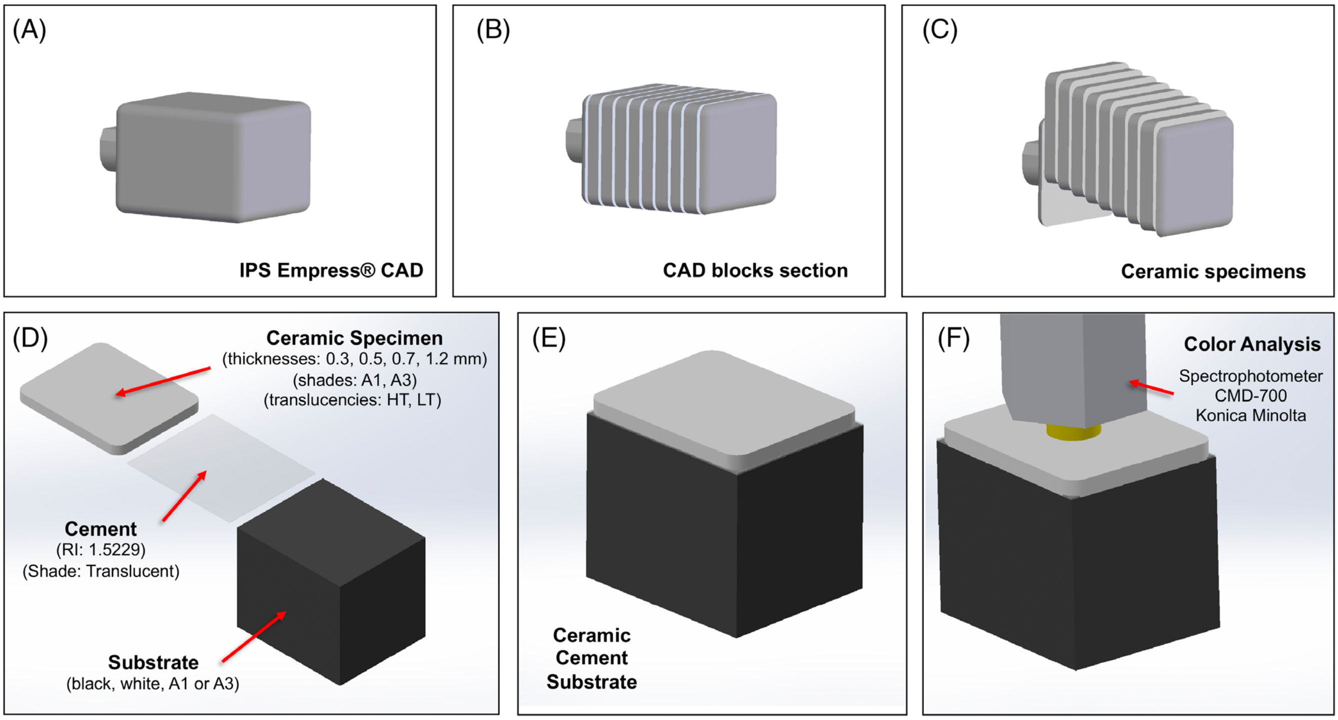

FIGURE 1 Experimental setup. (A) IPS Empress CAD block, (B) sectioning of the blocks, (C) ceramic specimens, (D, E) specimen assembly and evaluation according to different thicknesses, shades, and translucencies interposed by a translucent cement over different backgrounds and (F) spectrophotometric analysis using the CMD-700 Konica Minolta

TABLE 1 Chemical products used in experimental resin cement composition

Material	Chemical	Refractive Index	Concentration (wt%)	Manufacturer
Monomer	Bis-GMA[a]	1.540	26.0	Sigma Aldrich, St. Louis, MO, USA.
Monomer	Bis-EMA 10[a]	1.5112	23.4	Esstech Inc., Essington, PA, USA.
Monomer	TEGDMA[a]	1.459	2.6	Esstech Inc., Essington, PA, USA.
Filler Particle	16 nm fumed silica	1.535	2.0	Evonik Industries AG, Essen, Germany.
Filler Particle	7.5 μm $BaBSiO_2$[b]	1.553	50.0	Esstech Inc., Essington, PA, USA.

[a]Bisphenol A diglycidyldimethacrylate (Bis-GMA); Ethoxylated bisphenol A diglycidyldimethacrylate (Bis-EMA 10); Triethylene glycol dimethacrylate (TEGDMA);
[b]Barium Borosilicate ($BaBSiO_2$).

parametric factors K_L, K_C, and K_H are correction terms for the experimental conditions, which were set to 1. Differences in each inherent color parameter were also determined as ΔL, Δa, and Δb by subtracting each specimen from the substrate color coordinate parameter value ($+a =$ red, $-a =$ green; $+b =$ yellow, $-b =$ blue; $+L =$ white, $-L =$ black).

Data were entered into statistical analysis software (Stata/MP 17, StataCorp, College Station, TX, USA) and was checked for normality using Shapiro–Wilk's test and for variance homoscedasticity using Levene's test. Statistical analyses were performed according to the different experimental designs with a level of significance of $\alpha = 0.05$. A power analysis was conducted to determine the sample size for each experiment to provide a power of at least 0.8 at a significance level of 0.5 ($\beta = 0.2$). A three-way analysis of variance (ANOVA) was performed to detect differences in the color coordinates *L*, *a*, and *b* and where the independent variables were the substrates (Black, LT A3, LT A1, and White), the ceramic shades (IPS Empress LT A3, IPS Empress HT A3, IPS Empress LT A1, and IPS Empress HT A1) and the ceramic thicknesses (0.3, 0.5, 0.7, and 1.2 mm). A pairwise comparison was performed using Tukey's test. The descriptive statistical analysis was plotted using Origin Pro (OriginLab Co, Northampton, MA, USA).

The dataset containing all variables was organized into a Jupyter Notebook (www.jupyter.org). The dataset was split into train and test datasets using a 70/30 ratio. Twenty-eight supervised learning regression models were imported from the scikit-learn API (www.scikit-learn.org). All models' mean absolute error (MAE) and the accuracy (R^2 score) were calculated. The regression models with the lowest MAE and higher R^2 score were pre-selected for hyperparameter tuning using exhaustive grid search cross-validation (GridSearchCV, Scikit-learn). Also, the best model feature importance was used to calculate the coefficient of the importance of each one of the variables. The ΔL, Δa, Δb, and ΔE_{00} were calculated by comparing the test dataset to compute for the error between the real data and the machine learning data.

3 | RESULTS

Figure 2 shows the CIELab values for the substrates and ceramics blocks used in this study. For the *L* value, it can be noticed that the Black background had the lowest *L* value as the White background had the higher *L* value. The A1 shade had higher *L* values than the A3 shade for the ceramic blocks, regardless of the translucency (LT or HT). For the same shade color (A1 or A3), the LT ceramics had higher *L* values than the HT ceramics.

For the *a* values, it was noted that the ceramic block IPS Empress HT A1 presented a negative *a* value, which makes it have a greenish aspect. The White background also presented a negative *a* value, but very close to 0. The black background presented a positive *a* value, which makes it have a reddish aspect. The ceramic IPS Empress LT A3 presented the highest *a* value followed by IPS Empress HT A3 and IPS Empress LT A1, respectively.

For the *b* values, all substrates presented a positive *b* value. The White background has a higher *b* value than the black background. The A3 ceramic A3 has a higher *b* value than the A1 ceramic. The LT ceramics have a higher *b* value than the HT ceramics.

Table 2 shows the ΔE_{00}, *L*, *a*, and *b*, and values of the different ceramic restorations with different thicknesses cemented on the different substrates. For the *L* values, significant differences were found among all variables (substrate vs. ceramic type vs. thickness, $df = 27$, $F = 54.87$, $p < 0.001$). According to the pairwise comparison, for the same ceramic type and thickness, the differences were found for all substrate shades ($df = 3$, $F = 5.1 \times 10^5$, $p < 0.001$), where the *L* final of the restoration follows white > A1 > A3 > black for the different backgrounds.

Within the same background, the influence of the different ceramic shades and thicknesses are statistically significant ($df = 9$, $F = 208.19$, $p < 0.001$). However, when the pairwise comparison was performed, the color of the background and the color of the ceramic dictated if the *L* of the final restorations was going to be higher or lower than the background. For the white background, when using different ceramics, the thinner the ceramic the higher the *L* of the final restoration. The inverse is true for the black background, the thinner the ceramic, the lower the *L* of the final restoration. For the A1 and A3 backgrounds, the influence of the thickness on the *L* of the final restoration depends on the differences on *L* values of the ceramic restoration and the background. Hence the higher the difference between *L* of the ceramic and *L* of the substrate the higher is the influence of the thickness on the final *L*. For A1 and A3 backgrounds restored with IPS Empress LT A1 and IPS Empress LT A3, respectively, no differences were found in the *L* of the final restoration among all different thicknesses. The same pattern was found for the *a* and *b* values. However, it is important to notice that the *L*, *a*, and *b* values will influence the final color independently, but an alteration of the axis (*L*, *a*, or *b*) can significantly influence the ΔE_{00} and, subsequently, the final color of the restoration.

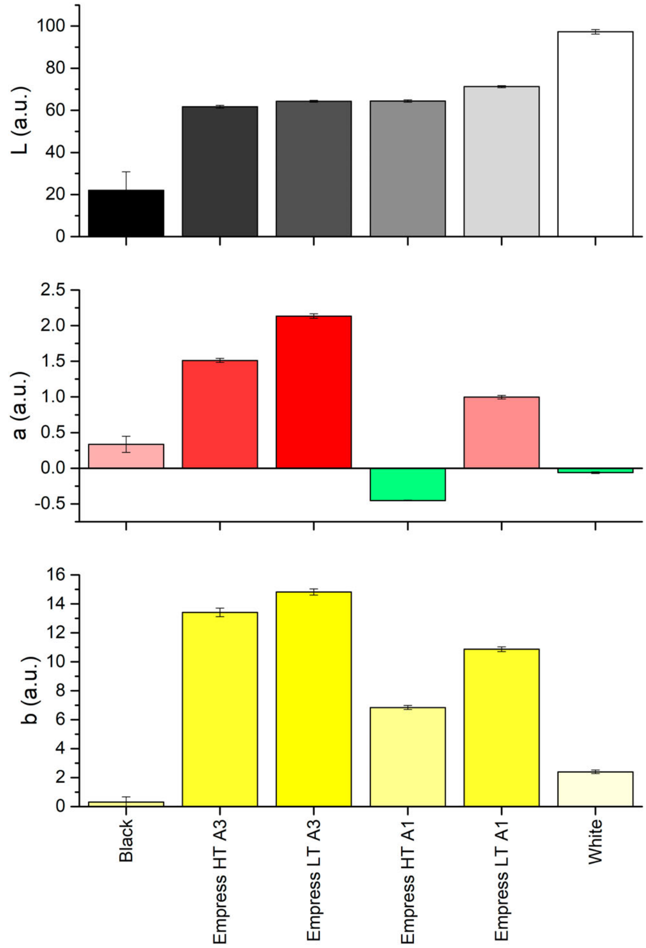

FIGURE 2 CIE *L*, *a*, and *b* color coordinates for the substrates (Black, Empress LT A3, Empress LT A1, and White) and ceramic blocks (Empress HT A3, Empress LT A3, Empress HT A1, and Empress LT A1) used to fabricate the specimens in this study

The decision tree regressor was the best model of all regression models with the lowest mean absolute error (0.226 ± 0.012) and the highest R^2 score (0.997 ± 0.001). All models' results and the best model hyperparameters tuning can be found in the GitHub repository. Figure 3A shows the feature importance of each one of the variables in predicting the final color of the ceramic restoration. The *L* of the substrate (L_{sub}) ranks as the most important feature influencing 60.39 ± 1.37% on the final color of the restoration. The thickness of the restoration is the second most important feature influencing 16.06 ± 0.56%, followed by the *a* of the substrate (a_{sub}). All other features combined account for 10.20 ± 0.45% of the final color of the restoration. Figure 3B shows the error in the ΔL, Δa, Δb, and ΔE_{00} when comparing the real-world data and the predicted data using the decision tree regression model. The machine learning regression model had an average ΔE_{00} error of 0.382 ± 0.316. However, it is important to notice that there are two outlier points above the 1.77 threshold, which suggests that from 634 entries on the testing data set, the regression model regression model could not predict the shade

TABLE 2 ΔE_{00}, *L*, *a*, and *b* values for the ceramic specimens (Empress HT A1, Empress LT A1, Empress HT A3, and Empress LT A3) with different thicknesses (0.3, 0.5, 0.7, and 1.2 mm) cemented over different substrates (Black, A3, A1, and White) used in this study

Substrate	Ceramic	Thickness	ΔE_{00}	*L*	*a*	*b*
Black	Empress HT A1	0.3	18.94 ± 0.75 Bd	37.93 ± 0.86 Bd	−0.46 ± 0.02 Aa	−5.15 ± 0.52 Cc
		0.5	24.6 ± 1.09 Bc	44.51 ± 1.22 Bc	−0.89 ± 0.05 Ab	−5.61 ± 0.43 Dd
		0.7	26.23 ± 0.41 Cb	46.57 ± 0.45 Bb	−1.06 ± 0.04 Ac	−4.32 ± 0.39 Db
		1.2	32.41 ± 0.82 Ca	53.24 ± 0.82 Ca	−1.33 ± 0.04 Ad	−2.5 ± 0.17 Da
	Empress LT A1	0.3	22.95 ± 0.57 Ad	42.83 ± 0.7 Ad	−0.79 ± 0.04 Ca	−4.63 ± 0.38 Bd
		0.5	28.22 ± 0.59 Ac	48.78 ± 0.67 Ac	−1.06 ± 0.03 Bb	−3.91 ± 0.48 Cc
		0.7	33.73 ± 0.74 Ab	54.59 ± 0.72 Ab	−1.18 ± 0.01 Bc	−2.09 ± 0.08 Cb
		1.2	40.82 ± 0.81 Aa	61.33 ± 0.72 Aa	−1.19 ± 0.02 Bc	1.14 ± 0.09 Ca
	Empress HT A3	0.3	18.03 ± 0.88 Dd	37.02 ± 1.09 Cd	−0.64 ± 0.09 Ba	−4.22 ± 0.62 Ad
		0.5	23.42 ± 0.68 Cc	43.61 ± 0.74 Cc	−0.88 ± 0.04 Ab	−3.19 ± 0.28 Bc
		0.7	26.35 ± 0.57 Cb	46.92 ± 0.62 Bb	−1.19 ± 0.05 Bc	−2.56 ± 0.25 Bb
		1.2	32.54 ± 0.86 Ca	53.52 ± 0.86 Ca	−1.2 ± 0.04 Bc	0.63 ± 0.3 Ba
	Empress LT A3	0.3	18.45 ± 0.62 Cd	37.62 ± 0.76 Bd	−0.58 ± 0.07 Ba	−3.96 ± 0.24 Ad
		0.5	22.69 ± 0.39 Dc	42.97 ± 0.43 Dc	−0.93 ± 0.04 Ab	−1.76 ± 0.23 Ac
		0.7	28.33 ± 0.64 Bb	49.21 ± 0.67 Cb	−0.99 ± 0.03 Ab	−0.21 ± 0.19 Ab
		1.2	36.18 ± 0.32 Ba	56.96 ± 0.31 Ba	−1.08 ± 0.05 Bc	3.92 ± 0.24 Aa
A3	Empress HT A1	0.3	2.76 ± 0.17 Bc	65.35 ± 0.28 Ba	1.78 ± 0.03 Ba	10.73 ± 0.25 Ca
		0.5	4.38 ± 0.53 Aab	65.93 ± 0.55 Ba	1.5 ± 0.06 Bb	8.51 ± 0.58 Db
		0.7	4.16 ± 0.25 Bb	65.1 ± 0.29 Ba	1.31 ± 0.03 Cc	8.62 ± 0.36 Cb[a]
		1.2	4.67 ± 0.32 Ba	65.13 ± 0.56 Ba	0.99 ± 0.05 Cd[a]	8.03 ± 0.36 Dc
	Empress LT A1	0.3	4.67 ± 0.41 Ac	67.48 ± 0.4 Ac	1.38 ± 0.07 Ca	8.91 ± 0.4 Da[a]
		0.5	4.65 ± 0.29 Ac	67.62 ± 0.37 Ac	1.34 ± 0.05 Ca	9.08 ± 0.3 Ca[a]
		0.7	5.21 ± 0.23 Ab	68.33 ± 0.27 Ab	1.17 ± 0.06 Db	8.73 ± 0.17 Ca
		1.2	6.06 ± 0.26 Aa	69.84 ± 0.34 Aa	0.84 ± 0.05 Dc	8.8 ± 0.17 Ca
	Empress HT A3	0.3	2.11 ± 0.31 Ca	65.11 ± 0.39 Ba	1.87 ± 0.04 Aa	11.66 ± 0.36 Bc[a]
		0.5	1.83 ± 0.38 Bab	64.71 ± 0.65 Cab	1.84 ± 0.06 Aa	12.07 ± 0.55 Bb[a]
		0.7	1.69 ± 0.36 Cab	64.26 ± 0.53 Cbc	1.73 ± 0.08 Bb	12.27 ± 0.63 Bab[a]
		1.2	1.58 ± 0.27 Cb	63.8 ± 0.48 Cc	1.73 ± 0.07 Bb	12.57 ± 0.66 Ba
	Empress LT A3	0.3	1.54 ± 0.23 Da	65.05 ± 0.3 Ba	1.86 ± 0.05 Ab	12.58 ± 0.36 Ab[a]
		0.5	1.3 ± 0.26 Ca	64.81 ± 0.38 Ca	1.81 ± 0.07 Ab	12.91 ± 0.32 Ab[a]
		0.7	0.83 ± 0.12 Db	64.8 ± 0.3 Bca	1.94 ± 0.04 Aa	13.72 ± 0.17 Aa[a]
		1.2	0.66 ± 0.19 Db	64.74 ± 0.32 Ba	1.88 ± 0.05 Aa	14.08 ± 0.16 Aa
A1	Empress HT A1	0.3	1.55 ± 0.25 Ac	71.08 ± 0.2 Ba	0.84 ± 0.05 Ba	8.68 ± 0.37 Da
		0.5	2.01 ± 0.2 Abc	70.91 ± 0.29 Ba	0.78 ± 0.05 Ba	8.08 ± 0.32 Db
		0.7	2.13 ± 0.17 Bb	69.37 ± 0.35 Bb	0.71 ± 0.07 Cb	8.77 ± 0.33 Da[a]
		1.2	3.03 ± 0.23 Ba	67.88 ± 0.35 Bc	0.65 ± 0.02 Cb	8.85 ± 0.15 Da
	Empress LT A1	0.3	1.46 ± 0.16 Aa	72.16 ± 0.24 Aa	0.71 ± 0.02 Ca	9.04 ± 0.14 Cb[a]
		0.5	1.34 ± 0.16 Ca	71.93 ± 0.26 Aa	0.71 ± 0.09 Ca	9.15 ± 0.22 Cb[a]
		0.7	1.24 ± 0.18 Ca	71.81 ± 0.11 Aa	0.72 ± 0.04 Ca	9.22 ± 0.24 Cb
		1.2	1.04 ± 0.24 Ca	72.1 ± 0.34 Aa	0.7 ± 0.07 Ca	9.79 ± 0.21 Ca
	Empress HT A3	0.3	1.64 ± 0.38 Ac	69.41 ± 0.5 Da	0.93 ± 0.06 Ad	10.38 ± 0.99 Bd
		0.5	1.48 ± 0.72 BCc	69.59 ± 0.82 Ca	1.14 ± 0.13 Ac	11.85 ± 0.53 Bc[a]
		0.7	2.22 ± 0.37 Bb	68.73 ± 0.44 Cb	1.25 ± 0.02 Bb	12.35 ± 0.26 Bb[a]
		1.2	4.06 ± 0.41 Aa	66.71 ± 0.43 Cc	1.53 ± 0.11 Ba	13.68 ± 0.47 Ba
	Empress LT A3	0.3	0.92 ± 0.36 Bd	70.19 ± 0.43 Ca	0.98 ± 0.1 Ad	11.3 ± 0.34 Ad
		0.5	1.91 ± 0.25 ABc	69.42 ± 0.29 Cb	1.13 ± 0.1 Ac	12.77 ± 0.2 Ac[a]

(Continues)

TABLE 2 (Continued)

Substrate	Ceramic	Thickness	ΔE_{00}	*L*	*a*	*b*
		0.7	2.93 ± 0.15 Ab	68.59 ± 0.17 Cc	1.35 ± 0.1 Ab	14.05 ± 0.2 Ab[a]
		1.2	4.03 ± 0.52 Aa	67.25 ± 0.49 Cd	1.75 ± 0.06 Aa	14.63 ± 0.64 Aa
White	Empress HT A1	0.3	4.05 ± 0.2 Cd	94.77 ± 0.38 Aa	−0.01 ± 0.02 Bd	6.95 ± 0.17 Dd
		0.5	6.6 ± 0.08 Dc	91.57 ± 0.22 Ab	0.24 ± 0.02 Dc	9.52 ± 0.08 Dc
		0.7	8.72 ± 0.4 Db	88.54 ± 0.83 Ac	0.43 ± 0.03 Db	11.38 ± 0.2 Db
		1.2	12.25 ± 0.27 Da	83.57 ± 0.5 Bd	1.02 ± 0.04 Da[a]	14.35 ± 0.21 Da
	Empress LT A1	0.3	5.82 ± 0.12 Bd	94.25 ± 0.16 Aa	0.01 ± 0.05 Bd	9.39 ± 0.18 Cd
		0.5	7.93 ± 0.13 Cc	91.86 ± 0.16 Ab	0.51 ± 0.03 Cc	11.91 ± 0.19 Cc
		0.7	10.1 ± 0.15 Cb	88.93 ± 0.49 Ac	0.98 ± 0.02 Cb	14.29 ± 0.12 Cb
		1.2	12.95 ± 0.15 Ca	84.69 ± 0.18 Ad	2 ± 0.05 Ca	16.91 ± 0.25 Ca
	Empress HT A3	0.3	7.44 ± 0.38 Ad	93.04 ± 0.35 Ba	0.34 ± 0.04 Ad	11.56 ± 0.52 Bd[a]
		0.5	10.09 ± 0.2 Bc	90.57 ± 0.31 Bb	0.94 ± 0.08 Bc	15.21 ± 0.26 Bc
		0.7	12.41 ± 0.24 Bb	87.14 ± 0.36 Bc	1.64 ± 0.09 Bb	17.82 ± 0.29 Bb
		1.2	16.85 ± 0.41 Ba	80.07 ± 0.59 Cd	3.11 ± 0.1 Ba	21.68 ± 0.68 Ba
	Empress LT A3	0.3	7.89 ± 0.33 Ad	92.79 ± 0.39 Ba	0.37 ± 0.05 Ad	12.23 ± 0.43 Ad[a]
		0.5	11.42 ± 0.19 Ac	88.72 ± 0.4 Cb	1.25 ± 0.03 Ac	16.81 ± 0.18 Ac
		0.7	13.8 ± 0.15 Ab	85.87 ± 0.25 Cc	2.01 ± 0.05 Ab	19.99 ± 0.19 Ab
		1.2	18.37 ± 0.24 Aa	78.22 ± 0.45 Dd	3.77 ± 0.14 Aa	23.51 ± 0.26 Aa

Note: Upper case letters shows difference between Ceramic according to the same susbtrate and thickness. Lower case shows differences between Thickness according to the same substrate and ceramic.
[a]No statistical differences were found between Substrates according to the same Ceramic and Thickness.

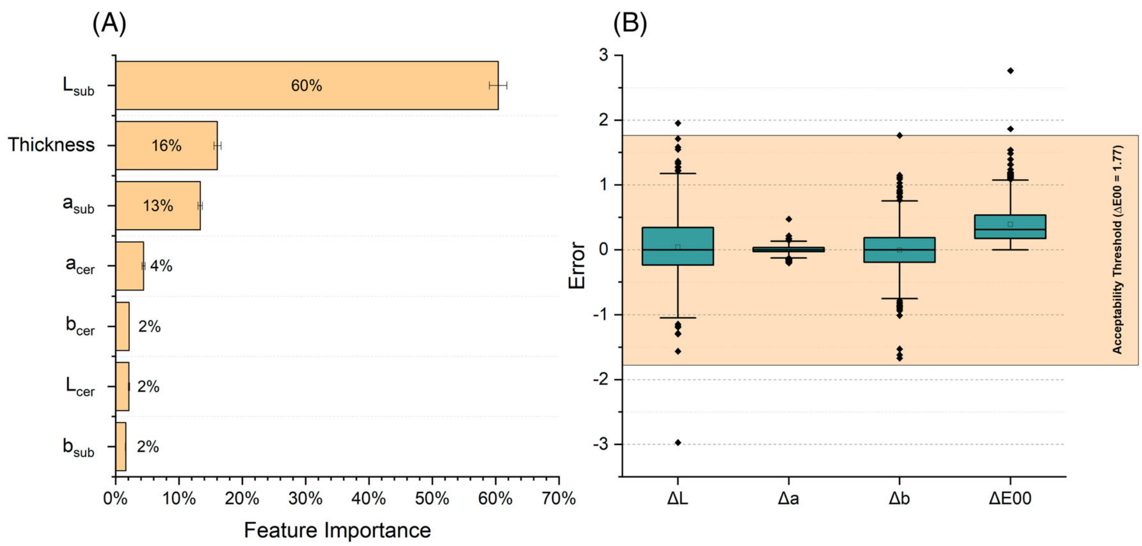

FIGURE 3 Summary of the Decision Tree Regressor results. (A) The relative importance of each independent variable to predict the final color of the ceramic restoration. (B) The measuring error to the predicted target value. The ΔL, Δa, Δb, and ΔE_{00} is obtained by the difference between the predicted result and the real measured data. The orange area represents the limit boundaries within the ΔE_{00} acceptability threshold (1.77)

within the acceptability threshold on two occasions. The complete model regression coding and deployment can be found in the GitHub repository (https://github.com/drmateusrocha/Predict-Color-Ceramic-Restorations).

4 | DISCUSSION

This study confirmed that the color of the substrate and the ceramic restorative material shade and thickness significantly influence the final color of the restoration.[18,20,24,25] Thus, the first research hypothesis was accepted. From all variables, the substrate influences the final color of the restoration the most, followed by the ceramic thickness and the *L*, *a*, and *b* of the ceramic.

In a previous study,[17] the authors evaluated leucite-based 0.6 mm ceramic veneers cemented using seven different resin cement shades on dies of nine different substrate shades. None of the 63 combinations of cement and substrate shade resulted in an acceptable match with the target shade. Interestingly, they observed no color difference between veneers cemented with a translucent cement or cemented with a high chroma cement on the same substrate color. They considered that the substrate color was the dominant factor when cementing thin veneers, and an opaque ceramic should be incorporated to improve shade matching.

Also, another study[37] demonstrated no difference in the color matching of IPS Empress CAD veneers milled from different blocks (multichromatic and high or low translucency) with the same thicknesses (axial reduction of 0.8 mm) cemented over a discolored substrate (A4). Different cement opacities or different ceramic translucencies could not mask a discolored substrate. In the present study, the final *L* of the ceramic is affected by the ceramic material's translucency. When substrate A3 was considered, IPS Empress LT A1 significantly increased the *L* value of the final ceramic compared to the other ceramics. Interestingly, when the regression model developed in this study was applied to a similar scenario (substrate A4, IPS Empress CAD, and target final shade A1), a low translucency ceramic veneer would need a minimum thickness of 1.1 mm to achieve a final restoration shade below the acceptability threshold (1.77). Besides that, the regression model predicted that a 0.8 mm low translucency ceramic veneer would not mask a discolored substrate A4. Thus, the second research hypothesis was accepted.

In this study, for A1 and A3 backgrounds restored with IPS Empress LT A1 and IPS Empress LT A3, respectively, no differences were found in the *L* of the final restoration among all different thicknesses. However, the ceramic thickness influenced the final color when higher color differences between the substrate and the final ceramic were present. The interesting finding is that the difference between the ceramic shade and the dental substrate does not assume a linear correlation. While exploring the different regression models, it was found that the difference between the substrate and the ceramic shade assumes a sigmoid function. This means that the smaller the color differences between the substrate and the ceramic shades, the lower is the influence of the ceramic thickness on the restoration final color. Thus, when the ceramic shade is properly selected, minor discrepancies in the ceramic thickness will not be visually perceptible. However, when clinicians aim to use a whiter ceramic to mask dark substrates, the minimum ceramic thickness is fundamental to achieve an acceptable outcome.

The masking ability of 0.5 and 1 mm IPS Empress CAD restorations cemented with four different cement shades on a discolored resin substrate (A3.5) has been reported.[20] Their results agree with the present study's result as they found a significant difference in the *L* value between the different thicknesses evaluated. Considering a similar scenario (substrate A3.5, IPS Empress CAD, translucent cement, and final shade A1), the application of the regression model developed in this study indicated that a low translucency A1 IPS Empress CAD ceramic with a minimum thickness of 1.1 mm would be needed to produce a final restoration below of the acceptability threshold. The predicted final shade agreed with their results. It is important to notice that this study only tested the thicknesses of 0.5 and 1 mm. The IPS Empress CAD low translucency ceramic resulted in a color difference above the acceptability threshold in both thicknesses evaluated. A natural and satisfactory result is quite challenging when restoring a tooth presenting a discolored substrate with monolithic restorations.[25] An increased ceramic opacity can reduce the light transmission and improve the ceramic's ability to mask a dark substrate. This approach usually results in an unnatural appearance and the loss of the optical blend of the ceramic veneer with the substrate.[11]

One of the main advantages of a monolithic restoration fabricated by a CAD/CAM system is the time efficiency, as the restoration can be delivered in one clinical session. Another advantage is the higher chipping fracture resistance of monolithic restorations compared to porcelain-veneered restorations.[4] Monolithic CAD/CAM restorations are highly influenced by the substrate shade and the thickness and type of ceramic. The influence of the thickness on the restoration's final appearance depends on the type of CAD/CAM ceramic material.[36] Due to the vast number of available CAD/CAM materials, the generalizability of these results is limited.

Digital dentistry has been successful when determining the restorations' shape and position.[27] Nevertheless, the selection of the restoration's shade still relies on the dentist and dental technician's experience and ability. Color matching was a problem in the past, and despite the advances achieved by dentistry, it is still a major issue today.[40] The color of teeth is determined by a visual method, using shade guides comparisons, or by instrumental measurement.[41,47] Several researchers have addressed this field, seeking results that would allow more shade predictability while selecting the CAD/CAM material. Shade guides do not match natural teeth and other shade guides. The visual method is considerably affected by the type of shade guide,[15] the light conditions,[9] and the operator variables.[13,43] Finally, the reproducibility of the selected shade is impaired as the ceramic systems may not match the dentist's shade guide.[10]

Recent studies have investigated intraoral scanner applicability for shade selection.[16] The intraoral scanners' accuracy for color matching is inferior compared to a reference spectrophotometer.[44] However, color measurement is a recent feature added to intraoral scanners and surely will receive further improvement. Ideally, the development of software using a regression model to assist the dentist with shade matching integrated into the intraoral scanner software could provide immediate feedback during the tooth preparation resulting in more conservative and precise tooth preparations.

Since 1931, the International Commission on Illumination (CIE), has published recommendations on the specification of basic colorimetry standards.[22,23] The CIE system uses three coordinates to determine a particular color in a color space. Over the years, different color formulas have been used in the industry: CIE 76 (ΔE_{ab}), CIE 94 (ΔE_{94}), CMC (ΔE_{CMC}) and CIEDE2000 (ΔE_{00}).[21] For color measurement in dentistry, two formulae are recommended for calculating ΔE: CIE 76 (ΔE_{ab}) and CIEDE2000 (ΔE_{00}).[48]

The CIEDE2000 is more complex than the anterior formulas and includes a rotation function and weighting functions to reduce discrepancies and errors that occur due to the nonuniformity of the CIELab color space for small color differences under reference conditions.[35,47] Recent research seems to agree that the CIEDE2000 is superior to its predecessors when representing color differences as human eyes see them.[30,42,43] Ideally, the color difference formula should correspond to the visual judgment of an average observer. Better color difference formulae provide better indicators of clinically and visually perceptible and unacceptable color differences between tooth colors.[42]

The objective data obtained from the instrumental color measurement are not practically and clinically meaningful without establishing thresholds for perceptibility and acceptability.[29] These thresholds are essential to guide the selection of esthetic dental materials and interpreting clinical research and laboratory research.[35] Perceptibility is the color difference between two objects that can be identified by 50% of observers under controlled conditions, with the other 50% of observers noticing no difference. A color difference at or below the 50:50% perceptibility threshold is considered a nearly perfect color match. Acceptability is the difference in color considered acceptable by 50% of observers, while the other 50% considering it unacceptable. If a color difference is above the 50:50% acceptability threshold, the color match is considered unacceptable. In dentistry, an unacceptable dental esthetics outcome results in replacement or correction of the restoration.

Acceptability and perceptibility values vary among color difference formulas. Recent literature has focused on establishing the CIEDE2000 formula thresholds for dental materials.[19,28,35,39] A relevant multi-center study[35] determined that the CIEDE2000 perceptibility threshold and the acceptability threshold values were 0.81 (0.34–1.28) and 1.77 (1.23–2.37), respectively. Although the present study used this reference as the threshold, the results should be interpreted with caution since the geometric configuration of the spectrophotometer used in this study was d:8° while these reference threshold values were obtained using a 0°/45° spectrophotometer.

The color measurement geometry defines the geometric conditions under which the object is illuminated and viewed. The geometry of the light source relative to the object is defined by the angular size, which varies with the distance between the light source and the object.[12] Nevertheless, it could be argued that the use of a spectrophotometer with d:8° illuminant/observer angle is unusual for clinical dentistry or even color research in dentistry, and most perceptibility and acceptability studies used a recommended illuminant/observer of 0° or 0°/45° (CIE) spectrophotometer. While there is some debate about what the best measurement geometry uses for clinical application, the existing instrument geometries are somewhat extreme; for example, a direct geometry such as 0°/45° emulates a real-world viewing environment where the object is viewed with a black or dark surround with an overhead light at 0° and is viewed at 45° by an observer. The color we see (or measure) under these conditions is specific to this measurement geometry. This type of illumination and viewing is rarely experienced in the real world, where, in most environments, the illumination usually comes from multiple directions, either directly or indirectly (diffuse).[26]

Thus, the reference perceptibility and acceptability threshold in this study would be unfeasible, restricting visual and instrumental comparisons. However, this is only true for gonioapparent colors (pertaining to a change in appearance with illumination angle or viewing angle).[26] The color we see (or measure) under these conditions is specific to this measurement geometry. For most diffuse objects (i.e., enamel and dentin after preparation), instrument geometry does not play a large role in altering the measured color. In fact, to rule out influences of the substrate surface on the final color, measure the true color of the substrate and generate a clean dataset for real color regression model application, the use of a d:8° spectrophotometer is essential.

A d:8°spectrophotometer uses an integrating sphere with a powdery white coating that reflects nearly 100% of the light energy.[45] A calibrated light source illuminates the inside of the sphere, which diffusely illuminates the sample (placed on the outside port of the sphere) from all directions, and the detector views the sample from a near-normal angle of 8°. This geometry correlates best with colors seen in diffuse viewing environments, and it has advantages over direct geometry in that it is less sensitive to variations in the sample surface. It is also much less sensitive to other appearance attributes such as visual texture, the directionality of the surface, and nonuniformity in surface color, which, depending on what is being measured, can be either an advantage or disadvantage.

Clinically, after the tooth preparation, the tooth surface can affect the clinician's ability to determine the true substrate color due to roughness produced by the prepping burs. The use of a 0°/45° spectrophotometer will be too sensitive to the prep roughness. Perhaps the most serious disadvantage of the 0°/45° spectrophotometer is that the substrate surface roughness is eliminated when the resin cement infiltrates the substrate during the bonding procedure. Thus, all potential differences in the substrate roughness during the substrate shade measurement can generate co-founder during the machine learning training.

There will always be some interaction between the surface morphology of a specimen and the efflux optics of an instrument. CAD/CAM restorations usually are polished using different polishing systems or glazed by applying a glaze paste or spray. Previous studies have compared the effect of polishing, glazing, the combination of both techniques, and their application in different phases of manufacturing ceramic restorations.[32,33] Different surface-finishing protocols result in different surface roughness and, consequently, other optical properties. Surface texture influences the light reflection, affecting the translucency and shade of ceramic restorations, the rougher the ceramic surface, the lower the ceramic material's translucency.[8] In the present study, the samples' superficial rugosity was similar to the restorations' rugosity of samples obtained from the CEREC MC XL milling machine in a pilot study. Thus, this regression model is to assist with the true color values of ceramic restoration. Further investigation is needed to account for the variations in the surface roughness and gloss of different materials on the perceptibility and acceptability thresholds.

The shades from Vita Classic "A" group were selected in to train the machine learning as this group represents the most frequently selected shades for ceramic restorations.[14] Although the regression model can extrapolate to predict the shades on the B, C and D vita color groups, further studies need to be conducted to validate the regression model in different clinical scenarios. Also, the increase of database and software development can tune the regression model using machine learning.

Ideally, the use of translucent cements should be preferred as the influence of the cement on the final color of the restoration may be unpredictable. Many studies have investigated the coupling medium's effect on the ceramic restorations' final color.[50–52] The cement characteristics influence high translucent ceramics' shade more than low translucent ceramics' shade.[50] Also, cement shade has a higher effect on the final appearance of thinner ceramics.[52] Color and translucency of ceramic discs of 1.0 mm in thickness over white and black backgrounds have been evaluated when interposed with glycerin (refractive index = 1.48) or air (refractive index = 1.00029).[51] Color comparisons could not be performed when the coupling medium was not the same as it significantly affected the color perception. In this study, an experimental cement without photoinitiators was used as a coupling medium to mimic a conventional cement's optical properties. It also allowed the multiple uses of the samples and substrates, consequently reducing the variation within the study and reducing the number of samples needed. Further research should be undertaken to evaluate the influence of different cements under the present study's conditions. Further data collection is required to support the applicability of the regression model for other dental ceramics (i.e., lithium disilicate and zirconium oxide).

The ability to use data to make better predictions lies at the core of the current AI revolution. A key aspect of many models—like supervised learning—is the focus on prediction. A key issue for designers of new prediction tools is how to evaluate whether the model is an improvement on the status quo—for instance, whether a shade selection software can outperform current human visual shade selection. From all 28 regression models tested, the decision tree regressor was the model that produced the lowest error and highest accuracy in predicting the restoration final color. A decision tree regression is a tree of questions that must be answered in a sequence to produce a predicted regression. A decision tree regression is a tree of questions that must be answered in a sequence to produce a predicted regression model. Figure 3 shows that the L_{sub} and the thickness are the most important features in determining the restoration color. This exemplifies the importance of the clinician understanding the limitation of using leucite-reinforced ceramic in discolored teeth/substrate as it might not mask dark substrates. Also, the results emphasize the importance of whitening/bleaching treatment to facilitate substrate masking when the desired final color is too discrepant from the initial substrate shade. Lastly, the model results highlight the importance of the preparation depth to accommodate a minimum ceramic thickness capable of masking the substrate and achieving the desired final color.

Although this research focused on the use of regression models, other studies[53,54] found that other AI methods, such as Principal Component Analysis and Artificial Neural Networks, are also suitable for the prediction of color restorations. However, more comprehensive AI modeling using deep learning is suggested since all AI models studied this far have a high risk of overfitting and might not be extrapolated to all clinical scenarios. Further research should be focused on expanding the machine learning model by adding more data and features (substrate shades, ceramics shades, ceramic translucencies, ceramic types, and cement shades); developing an intuitive interface to facilitate the use of the regression model by dentists and dental technicians and integrating it with the intra-oral scanner software to provide immediate feedback regarding the ideal preparation depth and ceramic material thickness.

5 | CONCLUSION

Within the limitations of this current study, it was concluded that:

- Different substrates, ceramic shades, and ceramic thicknesses influence the *L*, *a*, and *b* coordinates of the final restoration. The influence of the ceramic thickness on the final color depends on the difference between ΔE_{00} of the substrate and the ceramic.
- The decision tree regression model developed in the study was able to predict the *L*, *a*, and *b* of the ceramic restorations made with IPS Empress CAD HT and LT, based on the CIELab of the substrate and different ceramic thicknesses. Of all variables, the substrate *L* value influenced the final ceramic shade the most, followed by the ceramic thickness.

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DATA AVAILABILITY STATEMENT

If the data are available from the corresponding author on request, please mention that "The data sets used and/or analyzed during the current study are available from the corresponding author on reasonable request.

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