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"Predicting the Future of Curly Hair Formulations: A Novel Digitally Personalized Approach to Diversity in Hair Care"

Bruna Conrado [1], Cyrus Andriolo [1] , Gizele Freitas [1] , Beatriz Ferreira [1] and Deborah Barros [2]

[1] Hair Application Domain, L'Oréal Brasil Research and Innovation; [2] Evaluation Intelligence, L'Oréal Brasil Research and Innovation

1. Introduction

The global hair care market is constantly evolving, driven by an increasing consumer demand for personalized and sustainable products. This is particularly true within the curly hair segment, projected to represent over 40% of the population by 2030 [1]. Historically, many hair care products often rely on a "one-size-fits-all" approach, which fails to address the unique needs and the heterogeneity of curly hair, with its diverse curl patterns, textures and porosities.

Most mainstream solutions for defining and managing curls often rely on silicone and acrylate-based formulations. While silicones provide excellent smoothness, definition and shine because of their high affinity to the hair surface, this effect is often temporary and disappears in the days following application. Consequently, consumers frequently reapply these products daily, which often creates a build-up effect, weighing down the curls and making the hair appear dull and heavy. Additionally, constant reapplication of product can lead to a more time-consuming and frustrating hair care routine.

Therefore it's important the research for solutions exploring alternative raw materials that can deliver lasting curl definition and at the same time minimize the build-up perception. These attributes are determinant to answer to these critical tensions in the curly consumer journey and delight consumers.

In addition to the consumer high performance expectations, it is key to reduce further the environmental impact of new formulas. Therefore sustainability is a filter of choice for these alternative raw material solutions, like biodegradability impact, for example. Creating sustainable innovations is crucial for the future of the planet and also has been a growing concern among consumers, particularly Gen Z, that prioritizes eco-friendly and tailor-made products when deciding which products to buy [2].

This scenario poses a significant challenge and opportunity for the cosmetics industry: how can we effectively formulate products that resonate with the future of curly hair care, balancing performance, consumer centricity, and sustainability?

To take this next step within the numerous variety of raw materials alternatives available, we decided to focus on the chemical category of carboxylic acids due to the type of affinity with the hair fiber and potential speciafically for curly hair. Given the complexity of this research on the variety of attributes and also predictivity of results, we took this opportunity as example applying a novel digitally personalized approach with a new robust and decision-oriented method to select the best ingredients for lasting curl definition.

The choice to focus on carboxylic acids in this study was based on the chemical knowledge of this category of raw materials and hair fiber science. It has been documented that raw materials that influence the pH and internal keratin structure can affect visual and cosmetic properties of the hair [3]. This suggests a potential for exploring ingredients that interact with the hair fiber through pH-mediated mechanisms. Carboxylic acids have been explored in recent literature due to their unique mechanism of interaction with keratin, through a combination of hydrogen bonding, ionic interactions, and covalent bonding [5], leading to improved curl retention and definition. Additonally, many of these acids are derived from natural sources and offer biodegradability.

However, the specific performance of carboxylic acids in curl definition can vary depending on multiple factors such as the acid's structure, pKa and molecular weight, all which can greatly affect their affinity to the hair fiber itself. Therefore, a systematic and innovative approach to identifying the best carboxylic acid blends for curl definition is crucial to developing the new generation of curl products. Presented with this chemical challenge, the creation of a predictive method becomes key.

Focused on the creation of this new systematic method, the present research represents the second step in our ongoing initiative to address this challenge. The first phase of this project focused was on developing a machine learning algorithm to predict consumer perception of curl definition, based on *in vitro* measurements using RUMBA® [3].

Now, building upon the previous work, we introduced a novel 3-step method to design sustainable curly hair formulations, leveraging our previously developed Curl Definition Score algorithm. This approach integrates in vitro testing, ingredient screening, and consumer validation to identify and optimize formulations with alternative raw materials, specifically for delivering performance to curly hair. Our primary objective is to demonstrate the efficacy of this predictive interdisciplinary method in creating high-performing, sustainable, and consumer-centric hair care solutions.

2. Materials and Methods

Leveraging our previously developed Curl Definition Score algorithm (CDS) [3], we screened 5 biobased carboxylic acids, analyzing their impact on curl definition and combing force. This process was carried out not only to generate new data to refine our existing algorithm, but also to allow us to identify the best actives and incorporate an optimal blend into a specialized leave-in emulsion, in order to achieve exceptional curl-defining properties.

To achieve this, the present work defined a method consisting of 3 main steps: Algorithm Creation, Design of Experiment (DoE) and In Vitro/Vivo Characterization. A step-by-step detailing of this method can be seen in the flowchart in Figure 1.

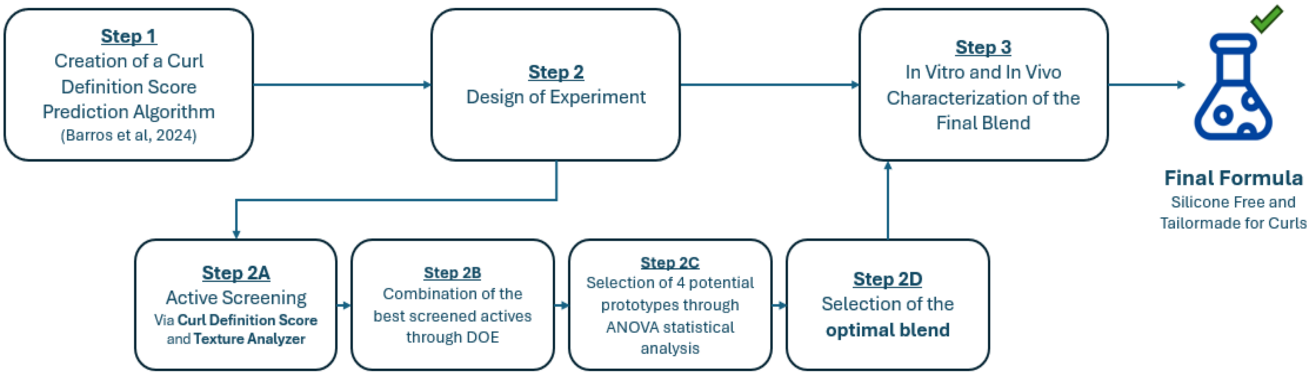


Figure 1. Flowchart of the proposed 3-step method.

We further characterize this innovative blend through Differential Scanning Calorimetry (DSC) and X-Ray Fluorescent Spectroscopy (XRF) tests, gaining insights into its impact on hair structure. Finally, demonstrating our consumer-centric approach, we conduct an extensive quantitative consumer study to compare the performance of this new formulation against a market-leading silicone-based leave-in product.

2.1 Ingredients and Manufacturing

Natural Caucasian Type I and Type III (according to the nomenclature by De La Mettrie et al [4]) were used for this study. The hair swatches are standardized at 2.7 g and 27 cm, and were supplied by International Hair Importers (IHIP). A commercially available silicone-based product for curly hair was sourced from a local store and used as a benchmark for all the tests performed in the study.

For the raw material screening step, a 200 g aqueous solution of each active was manufactured in the lab with a RW 20 Overhead Stirrer, provided by IKA. Rotation was kept between 100-200 rpm, to accommodate for good dispersion of the raw materials.

For the optimization step, the best actives of the screening phase were incorporated in a leave-in emulsion already optimized for the curly consumer (referred as Curl Cream). 200 g of each prototype were manufactured in the overhead stirrer, with rotation kept between 200-800 rpm and emulsification occurring between 60-80°C.

2.2 Ingredient Screening and Prototype Optmization

For Step 2A, 5 biobased carboxylic acids were selected as potential candidates for the formulation. These ingredients were chosen based on known or predicted benefits for curly hair, such as curls definition and moisturizing properties. [5-7].

Aqueous solutions were prepared by dissolving each individual acid in water, at different concentrations and pH ranges, in order to have a first assessment of their impact on curl definition. The general design of the screening can be seen in Table 1.

Table 1. Design of Experiments Matrix of the screening phase of potential actives

Active Ingredient Category	pH	Concentration (%w.t)
Carboxylic Acids	2, 3.5 and 4.5	3%

For Step 2B, the optimal pH and the most performing acids were chosen, and each of them were incorporated in a oil-in-water emulsion, identified by the name of Curl Cream (CC). The impact of the acids and their blends on the cream were explored in an Optimization Design of Experiment (DOE).

In order to thoroughly explore the potential of these acids and their respective combinations, the general matrix of the optimization was built to obtain a wide range of experimental points, resulting in 9 different formulations. The formulations contained an acid concentration varying from 0-4%, and could contain and acid by itself or a blend of two different acids.

2.3 Machine Learning and Predictive Modeling

The raw data obtained from the RUMBA and Texture Analyzer equipments was compiled and analyzed using an internal machine learning software. A total of 6 algorithms were explored by the software to determine the best fit for the datasets, which comprised of: Supply Vector Method, Random Forest, Neural Network, Linear Regression and Polynomial Regression (2nd and 8th degree).

The internal software is able to choose the best numerical method fit based on the calculation of the Root Mean Squared Error (RMSE). Alongside the numerical fit, the internal software also applies an analysis of variance (ANOVA) in order to correlate the impact of actives concentrations on Curl Definition Score and Combing Force. The internal software then generates a list of potential formulas with the prediction of the highest Curl Definition Scores and Combing Forces. Of this list, the top four potential formulas were chosen to be tested in Step 2C. The formula with the best experimental result was then chosen as the optimal blend, and proceeded to Step 3, In Vitro and In Vivo testing.

All the tests involving image processing and output analysis were carried out in an Intel Core i5 2.6GHz computer, with 15GB RAM and 8 processors.

2.4 In Vitro Testing

Curl Pattern Type III and Type I hair swatches were treated with 0.41g of each prototype/product. The application technique was standardized across all samples to minimize variability. Each condition was tested in triplicate to account for potential variations. Following application, the treated hair swatches were placed in a controlled oven set to standard room temperature and pressure and allowed to completely dry.

Curl Definition was quantified in Type III swatches, using RUMBA® polarization imaging provided by Bossa Nova Technologies, to obtain the outputs of Alignment, Volume and Standard Deviation (STDev). Calculation of the Curl Definiton Score was done according to the method proposed by Barros et al [3].

Combing Force was quantified in Type I swatches, using a Texture Analyzer from Stable Mycro Systems. Combing force was measure in terms of Force (g) required for the hair combing rig to pass through the full length of the swatch. Calculations were done according to the method provided by the supplier.

The contribution to hair integrity of the acids incorporated within the Curl Cream (CC)was assessed by measuring Ca^{2+} content inside the fiber via X-Ray Fluorescence Spectroscopy, and by measuring the temperature and enthalpy of denaturation via Differential Scanning Calorimetry (DSC). Both methods were performed as described by Zhang et al [7]. The combination of these results were analyzed to assess internal fiber efficacy through the bonding mechanism of the final blend of actives.

2.4 Consumer Study

The top-performing blend identified by the Curl Definition Score algorithm was chosen for the consumer evaluation step.. A quantitative Learning-Use-Deprivation study was conducted with consumers as described by Morizet et al [8], to compare the new formulation against the commercial benchmark. Participants with curly hair used both products and evaluated them based on curl definition, lasting performance, combing ease, and perceived convenience. Statistical ANOVA and t-tests were performed to determine significant differences between the prototype and the benchmark.

3. Results

3.1 Step 2A - Screening of Active Ingredients

Results of Curl Definition Score can be seen in Figure 2.

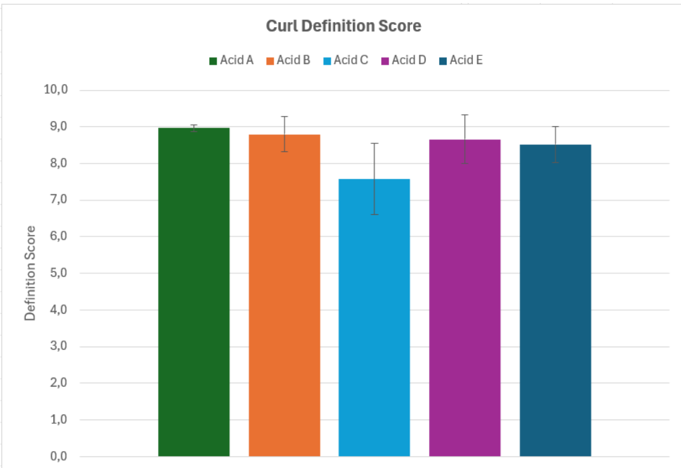
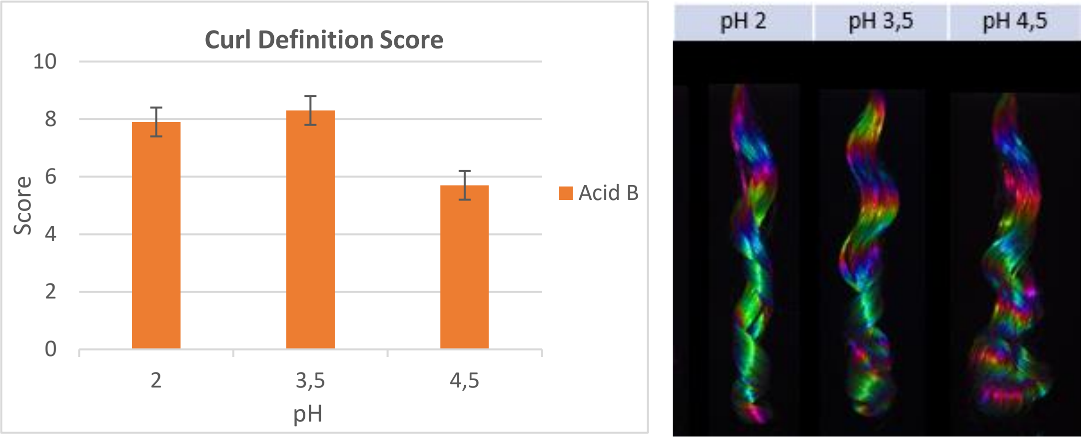


Figure 2. Curl Definition Score (CDS) of the 5 evaluated acids in aqueous solution.

As can be inferred from the graph, all acids presented statistically similar values, with the exception of Acid C. Acid B presented the second most higher value of curl definition, followed by acids D and E.

Parallel to this study, and in a manner of preparations for the optimization step, all acids were individually incorporated into the Curl Cream (CC) to assess their impact on the physicochemical stability. Incorporation of Acid D and E demonstrated instability and consequently deprioritized in the study.

The assessment of the optimal pH on the CDS can be seen in Figure 3, illustrated by the case of Acid B. A combined analysis of the graph and the images provided by the RUMBA demonstrates that the optimal pH of operation was found to be 3.5.



(**a**) (**b**)

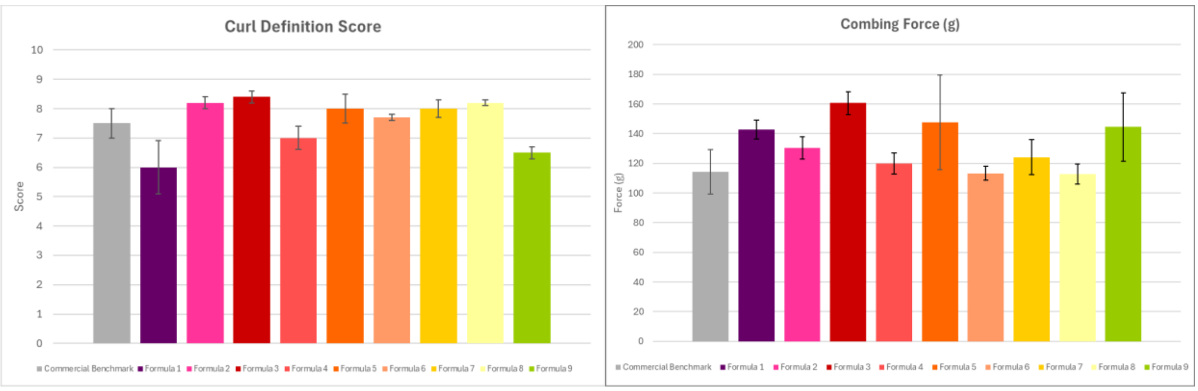
Figure 3. (a) Curl Definition Score and (b) RUMBA images of Acid B at 3%.

The result confirms that the pH has a significant effect on curl definition, potentially caused by the availability of the species in solution. Since Acid B is a dicarboxyllic acid, at pH 2 and 3.5, the acid is below its pKa2, which allows it to be present in the general form of H_2B^-. At pH 4.5, however, the acid has likely lost its two protons, and is present in a species with might negative charge (HB^{2-}). It is possible that this increased negative charge leads to a repulsion between the molecules of the acid, and also between the negatively charged sites of keratin, which in hand could explain the lower curl definition at this condition.

3.2 Step 2B – Optimization DOE

Building upon the results found in Step 2A, Acid A and Acid B were selected as potential actives, and proceeded to an Optimazation DOE, with concentration intervals calculated by our internal software, as previously discussed in Section 2. .

Results of Curl Definition Score and Combing Force can be seen in Figure 4. The color maps in Figure 5 illustrate the correlation of the ingredients's concentration with Curl Definition and Combing Force.



(**a**) (**b**)

Figure 4. (a) CDS and (b) Combing Force results for the Optimization DOE formulas at pH 3.5.

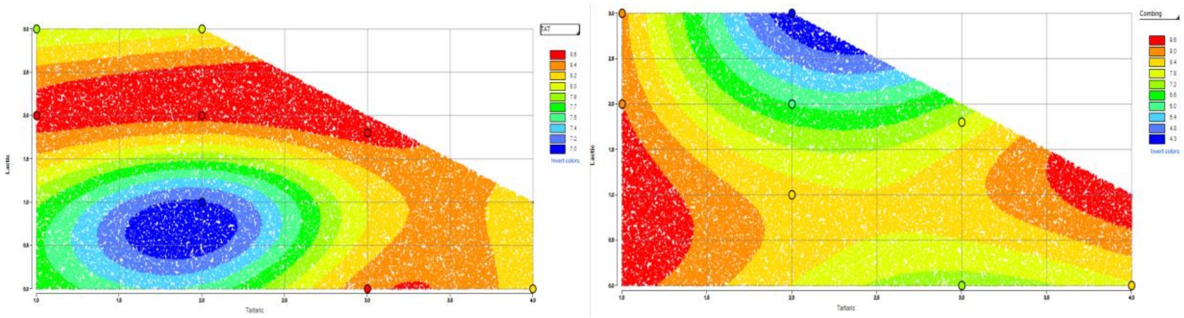


Figure 5. Color map depicting the impact of the concentration of Acid A and Acid B on (a) Curl Definition Score (CDS) and (b) Combing Force (expressed in 1/Force(g)) for the formulas at pH 3.5. Red represents a higher numerical amount and blue the lowest.

Conjoint analysis of Figures 4 and 5 allows us to understand the impact of the two acids of the performance of the formula. It is possible to see that higher concentrations (>3%) of both Acid A and Acid B result in higher values of Curl Definition, in the range of 8-8.6.

On the other hand, however, it is possible to see from Figure 5b that higher amounts of acids result in a unfavorable combing capacity (lower [1/F(g)] values translate to less favorable combing). Combing capacity significantly decreases for a concentration of Acid A > 2% and for Acid B > 3% thus indicating that, for cosmeticity purposes, a lower amount is recommended.

3.3 Step 2C and 2D – Selection of Top Prototypes and Identification of Optimal Blend

With the data found in Step 2B, the internal software predicted four potential prototypes that could potentially achieve combing and curl definition superior results compared to the commercial benchmark. Figure 6 shows the experimental results for CDS and Combing Force versus the commercial benchmark. Table 2 demonstrates the values of CDS and Combing Force predicted by the internal algorithm in comparison to the real experimental values, in order to assess the accuracy of the method.

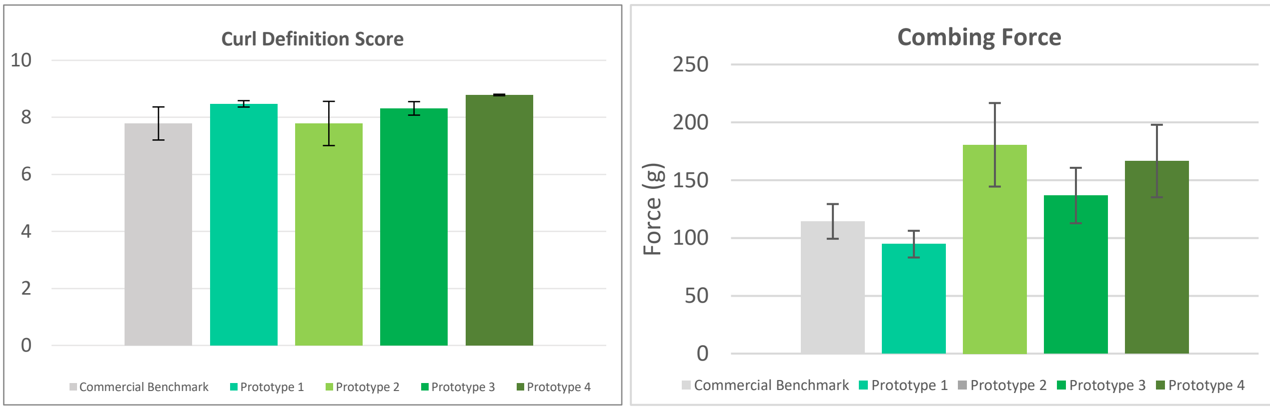


Figure 6. (a) Curl Definition Score and (b) Combing Force results Top 4 prototypes at pH 3.5, in comparison to the commercia benchmark.

Table 2. List of Top Prototypes and their relative error (%) calculated with predictive and experimental results, as generated by the internal software and in-vitro empirical data

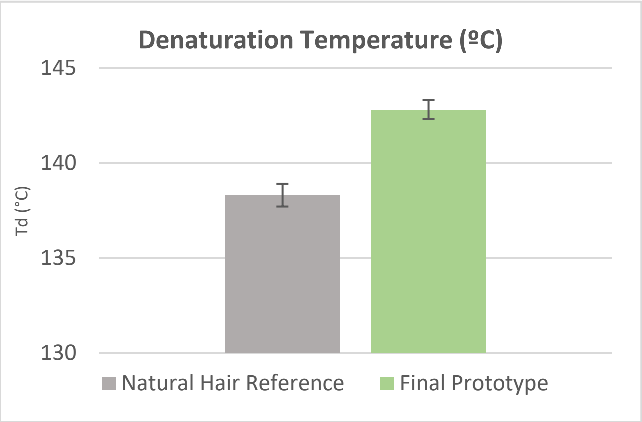
Prototype	Relative Error of Combing Force (%)	Relative Error for CDS (%)
1	12.15%	12,88%
2	67.02%	2,49%
3	16.88%	5,88%
4	14.06%	1,59%

By combining the data present in Table 3 and Figure 6, we are able to draw to main conclusions: 1) the internal software was able to predict the Curl Definition Score with great accuracy, at a margin of error below 15%; 2) the accuracy was not satisfactory for combing force (error 12-67%), indicating a non trivial impact of the acids on the cosmeticity of the formula.

Furthermore, by analyzing both graphs in conjunction, it is possible to infer that the only prototype that achieved superior results against the benchmark is Prototype 1, with a statistically lower combing force (equivalent to higher 1/F(g) value) and curl definition comparable to the benchmark. Thus, Prototype 1 was chosen as the Optimal Blend, which then proceeded to In Vitro and Vivo Characterization.

3.4 In Vitro Results (DSC and X-Ray Fluorescent Microscopy)

Results for DSC and XRF can be seen in Figures 6 and 7, respectively.



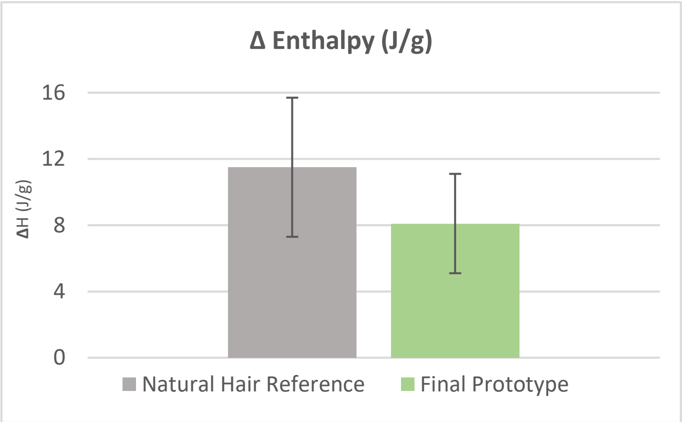


Figure 6. (a) Denaturation Temperature and (b) Enthalpy of Denaturation of the final formula in comparison to natural untreated hair (Reference).

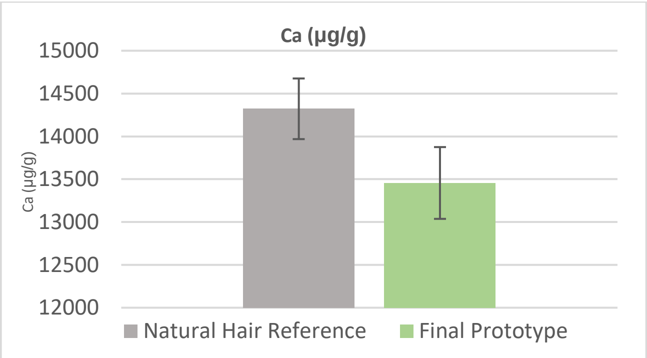


Figure 7. Ca^{2+} dosage of the final formula in comparison to natural untreated hair (Reference), via X-Ray Fluorescent Microscopy (XRF).

As can be inferred from the graphs, DSC analysis revealed that the final formula was able to increase the denaturation temperature in 3.5°C, and reduce enthalpy of denaturation by approximately 3,4 J/g. Additionally, Ca^{2+} dosage revealed a significant decrease of 866 µg/g.

3.5 In Vivo Results

Table 3 demonstrates the Learning-Use-Deprivation study consumer results with Final Prototype usage. The data in this table reveals the favorable scores achieved on definition and lasting performance (Long Lasting Curl Definition & Gives the right volume to hair), and perceived convenience (Makes routine easier).

Table 3. Consumer perception of Final Formula versus Commercial Benchmark for important curly hair attributes, according to TopBox percentage.

Attribute	Final Formula (% of Agreement)	Commercial Benchmark (% of Agreement)
Long Lasting Curl Definition	86%	78%
Makes routine easier	86%	79%
Gives the right volume to hair	97%	93%

4. Discussion

This research presents a novel 3-step methodology for developing high-performing curly hair formulations, leveraging predictive modeling and in vitro testing. This approach successfully identified an optimal blend of biobased carboxylic acids that outperformed a silicone-based commercial benchmark in both in vitro and in vivo consumer tests, addressing the increasing demand for novel technologies in hair care.

The success of the predictive model in accurately estimating Curl Definition Score demonstrates its potential as a valuable tool for efficient raw material screening and formulation optimization. However, the model's lower accuracy in predicting combing force (12-67% error) highlights the complex interplay between ingredient interactions and resulting physical properties, suggesting the need for refinement of the model. The successful identification of Prototype 1 as the optimal blend, despite the discrepancy in combing force prediction, confirms the value of combining the model with empirical data on most promising prototypes.

In vitro results provide further insights into the mechanism of action of the acid blend. The observed increase in denaturation temperature (3.5°C) and decrease in enthalpy of denaturation (3.4 J/g) indicate an interaction between the carboxylic acids and the keratin structure, potentially bringing protective benefits to the hair fiber. The significant decrease in Ca^{2+} (Figure 7)with the final formula suggests a potential strengthening of the hair fiber, which could contribute to improved and long lasting curl definition.

The consumer study results reinforce the in vitro findings, with participants reporting significantly improved lasting curl definition and convenience ($p<0.05$) compared to the silicone-based benchmark. This positive consumer feedback demonstrates the effectiveness and predictiveness of the 3-step methodology.

5. Conclusion

This study demonstrates the potential of hybrid predictive methods with in vitro and in vivo testing to design sustainable and effective curly hair formulations. Our numerical method enabled efficient ingredient screening and formulation optimization based on measurable physical properties and consumer feedback. The resulting silicone-free prototype outperformed a market benchmark, showcasing the potential of this approach for developing innovative and inclusive hair care solutions. This research is a key step towards personalized and sustainable cosmetics.

Finally, while this study focuses on curly hair, this methodology could be adapted to other hair types and cosmetic categories, opening up exciting possibilities for developing personalized formulations based on individual needs and characteristics. Further research could investigate the applicability of this approach to skincare, makeup, and other personal care products, potentially leading to more effective, sustainable, and personalized cosmetic solutions.

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