

SMILE: Smell Maximisation In Low-cost Eau de parfum

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ABSTRACT

Despite the growing economic importance of the fragrance industry, perfume formulation remains largely guided by empirical knowledge and iterative trial-and-error approaches. The structured design of fragrances, typically organised into top, middle, and base notes through the blending of perfume raw materials, is therefore time-consuming, costly, and difficult to generalise. Existing computational approaches have begun to address this challenge, but are commonly limited to small ingredient sets or require extensive sensory data that are not always available. This work proposes a computer-aided optimisation framework for Eau de Parfum formulation that simultaneously maximises perceived olfactory intensity and minimises formulation cost. The resulting optimisation problem is formulated to preserve the structural balance of top, middle, and base notes inherent to the perfume pyramid. Application of the framework to a fruity-floral Eau de Parfum formulation demonstrates a substantial increase in perceived intensity alongside a reduction in total formulation cost of approximately 64%. The proposed approach is intended as a decision-support tool for perfumers, enabling rapid exploration of cost-intensity trade-offs once a candidate ingredient set has been defined. The framework offers a step towards more systematic, data-driven perfume engineering and provides a foundation for future extensions incorporating ingredient selection and sensory constraints.

Keywords: Optimisation, Industry 4.0, Perfume engineering, Formulation chemistry

INTRODUCTION

In 2017, the global Flavours and Fragrances industry was valued at over 26 billion US dollars, with projections indicating that it will exceed 36 billion US dollars by 2029 [1]. This industry spans a wide range of products, including fine fragrances, shampoos, candles, detergents, and fabric softeners [2]. Despite this sustained economic growth and the increasing interest in perfume engineering as a formal discipline, the literature still reports a notable lack of innovative, scientifically grounded tools for perfume formulation [3]. As a result, the design of fragrances remains largely dependent on empirical expertise and iterative trial-and-error procedures, which are time-consuming, costly, and difficult to generalise [4],

[5]. Perfumes are complex mixtures of volatile compounds, typically dissolved in ethanol, water, or other carrier matrices, and are conventionally structured into top, middle, and base notes. In perfumery, the term notes refers to layers of scent that evaporate at different rates and collectively define the temporal evolution of a fragrance. Top notes consist of highly volatile compounds that dominate the initial sensory impression but dissipate rapidly. Middle notes, often described as the “heart” of the perfume, emerge shortly after application and establish its core olfactory character. Base notes comprise low-volatility compounds that persist for several hours and frequently act as fixatives by retarding the evaporation of more volatile constituents. The persistence and perceived intensity of each note are governed by

thermodynamic behaviour, mass-transfer phenomena, and psychophysical response mechanisms [2]. Carles conceptualised the perfumes structure as a pyramid divided into top, middle, and base notes, proposing typical proportions of 15–25%, 30–40%, and 45–55%, respectively [6]. These proportions were postulated to govern perfume tenacity, that is, the balanced evolution of odour intensity during evaporation.

The top, middle, and base notes described above are achieved by blending chemical ingredients known as perfume raw materials (PRMs), each contributing specific olfactory and volatilisation characteristics to the overall composition. Perfumers typically rely on experience-based heuristics to select and combine these PRMs, refining formulations through repeated sensory evaluation until the desired olfactory profile is achieved. This empirical methodology limits reproducibility and scalability, particularly given that modern cosmetic products often comprise more than 15 ingredients and may include up to 50 PRMs.

In recent years, several studies have tried to address these limitations through computational and data-driven approaches. Rodrigues et al. developed a machine learning-driven framework linking molecular structure to human olfactory perception, combining generative neural networks, odour-intensity prediction, thermodynamic modelling, and optimisation to reproduce target olfactory experiences from experimental data [3]. Viena Santana et al. proposed a systematic computational strategy for perfume formulation, employing deep learning trained on high-fidelity simulations alongside a meta-heuristic optimisation scheme to design compositions that achieve a desired odour spectrum while minimising undesirable notes [7]. Similarly, Zhang et al. introduced an optimisation-based framework for cosmetic formulation using a hierarchy of sensorial and product-property models, combined with iterative model substitution and generalised disjunctive programming, and demonstrated its applicability through a perfume design case study [8].

Despite their conceptual advances, these approaches suffer from several limitations. They typically focus on formulations containing a small number of PRMs (often three to four ingredients) or investigate the evaporation or performance of individual PRMs in isolation. Moreover, their application generally requires prior knowledge of odour detection thresholds for each ingredient, which are not always available or reliable. These constraints significantly limit their applicability to real-world cosmetic formulations, which are considerably more complex. Moreover, to the best of the authors' knowledge, the literature does not currently report any work aimed at mathematically optimising commercial perfume formulation.

In this work, an alternative optimisation framework for perfume formulation is proposed. Each PRM is

characterised by its own odour intensity, reflecting differences in sensory experience between compounds. Consequently, two PRMs present at the same concentration will not necessarily be perceived at the same intensity level. The perceived odour strength is modelled explicitly in terms of olfactory intensity, based on a sigmoidal relationship between sensory response and the logarithm of stimulus concentration, consistent with established psychophysical models such as Hill's law, and the strongest-component model is employed to evaluate the overall intensity of the formulation [9], [10]. The approach integrates molecular property prediction, olfactory intensity modelling, and constrained numerical optimisation within a unified workflow. PRMs are characterised according to olfactory note classification, vapour-liquid equilibrium behaviour, intrinsic odour intensity, and economic cost, allowing for a quantitative assessment of their contribution to overall perfume performance. Olfactory intensities are computed from predicted gas-phase concentrations using established psychophysical models, while cost considerations are incorporated through a normalised economic metric. Crucially, the optimisation problem is formulated to preserve the structural balance of top, middle, and base notes inherent to the perfume pyramid, as illustrated in Figure 1, enabling the rational design of realistic Eau de Parfum formulations with industrial relevance.

METHODOLOGY

The workflow of the current work is summarised in Figure 1. The proposed workflow begins with the selection of fragrance molecules, followed by the collection of key molecular characteristics, including olfactory note classification and economic information. These data were found through web scraping. In particular, molecules identifiers, molecular weights (MW_i), note type and character were found on Scent Tree, OQEMA Flavour & Fragrance Ingredients and The Good Scent Company. Commercial pricing data for each molecule were retrieved from Sigma-Aldrich, FluoroChem, Perfumer's Apprentice, and Pell Wall. To incorporate economic considerations, the cost per mole of each molecule was normalised between 10^{-3} and 1, generating a dimensionless cost metric suitable for inclusion in the optimisation problem. Moreover, parameters needed to characterise PRMs intensities were retrieved by Wakayama et al [9]. The selected molecules were then combined into fragrance formulations following a predefined Eau de Parfum composition, comprising 75 wt% ethanol, 20 wt% PRMs, and 5 wt% water. In this study, the initial composition was defined to mimic a realistic fragrance pyramid, wherein molecules are categorised as top, middle, or base notes. Each molecule was initially assigned a weight fraction corresponding to its contribution to the total perfume

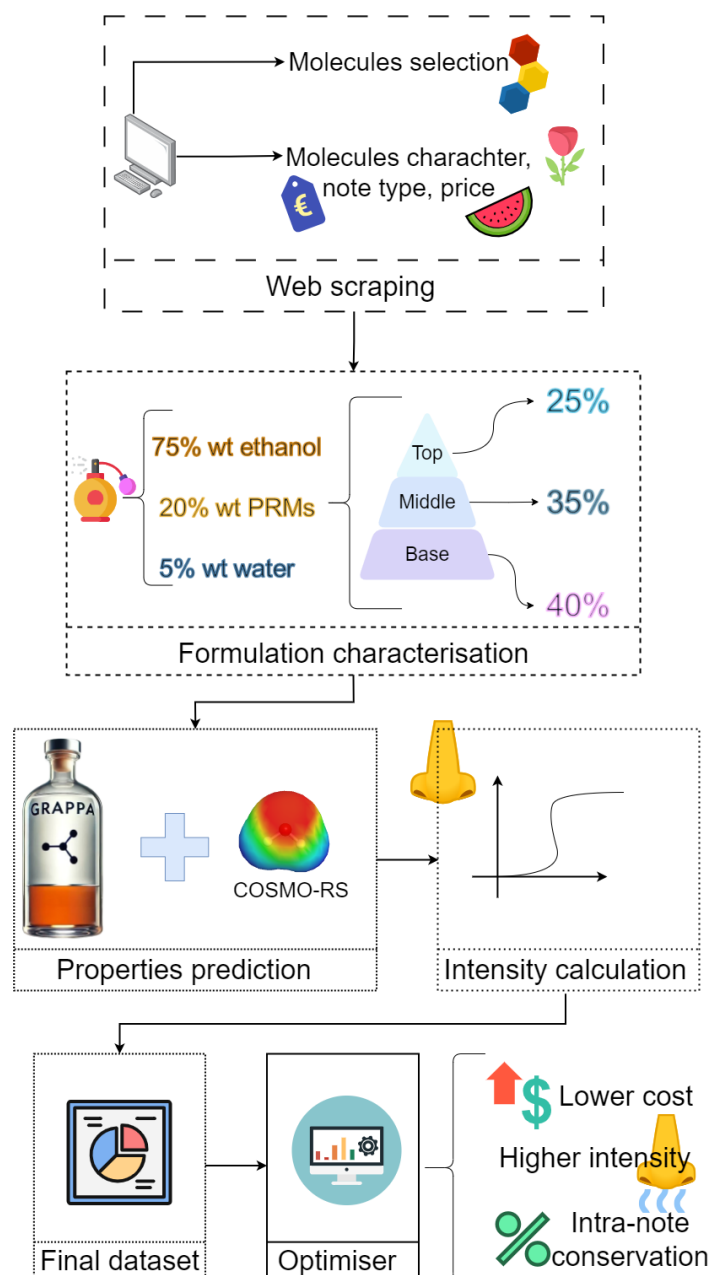


Figure 1. Schematic overview of the workflow adopted in this study. The process begins with web scraping to select and characterise PRMs. The selected molecules are then assembled into an Eau de Parfum formulation following predefined note-distribution constraints. Once the formulation is defined, relevant vapour-liquid equilibrium properties are predicted and used to calculate olfactory intensities. Finally, the molar fractions of the PRMs are optimised to maximise fragrance intensity while minimising formulation cost and preserving the relative proportions of top, middle, and base notes.

fraction. The relative distribution of weight fractions within each note category was determined to preserve intranote balance, reflecting the perfumer’s approach of proportionally blending molecules within top, middle, and base notes to achieve the characteristic volatility and olfactory structure of the formulation (e.g. among 20%wt PRMs, 25% wt of top notes, 35% wt of middle notes and

40% wt of base notes)

Once the formulation is fully characterised, its vapour-liquid equilibrium properties were predicted. Activity coefficients (γ_i) at 36 °C (corresponding to human skin temperature) were calculated using COSMOTerm [11] (version 24.00), while vapour pressures (P_i^0) were estimated using GRAPPA [12]. COSMOTerm was

Table 1: Characterisation of the formulation developed for the current work, along with optimisation results. First, molecule identifiers and notes are reported. Then, activity coefficients, normalised costs, initial molar fraction and intensities are presented. Finally, optimised molar fractions and intensities are presented.

CAS	Name	Note	Note type	γ_i	Norm.cost	x_i^0	Ψ_i^0	x_i^{opt}	Ψ_i^{opt}
103-45-7	2-Phenylethyl Acetate	Floral	Middle	4.38	0.029	0.0027	0.0018	0.0099	0.0178
105-54-4	Ethyl Butanoate	Fruit	Top	2.85	0.157	0.0059	16.633	0.0083	20.754
6259-76-3	Hexyl Salicylate	Floral	Base	14.22	0.001	0.0023	0.0152	0.0094	0.1186
103-37-7	Benzyl Butyrate	Fruit	Middle	5.43	0.084	0.0045	$3.31 \cdot 10^{-6}$	$1 \cdot 10^{-6}$	$1.69 \cdot 10^{-16}$
10339-55-6	Ethyl Linalool	Floral	Middle	1.34	0.134	0.0018	0.0042	$1 \cdot 10^{-6}$	$8.26 \cdot 10^{-8}$
105-87-3	Geranyl Acetate	Floral	Middle	6.17	0.066	0.0011	$2.32 \cdot 10^{-6}$	0.0037	$7.11 \cdot 10^{-5}$
7452-79-1	Ethyl 2-Methylbutyrate	Fruit	Middle	2.90	0.088	0.0011	19.615	0.0064	39.246
103-60-6	Phenirac	Fruit	Middle	6.30	0.122	0.0010	$1.05 \cdot 10^{-13}$	$1 \cdot 10^{-6}$	$4.47 \cdot 10^{-28}$
118-58-1	Benzyl Salicylate	Floral	Base	9.36	0.058	0.0044	0.0044	$1 \cdot 10^{-6}$	$3.59 \cdot 10^{-9}$
122-40-7	Alpha-Amylcinnamaldehyde	Floral	Middle	6.31	0.123	0.0015	$1.72 \cdot 10^{-7}$	$1 \cdot 10^{-6}$	$8.41 \cdot 10^{-17}$
140-11-4	Benzyl Acetate	Floral	Middle	3.73	0.144	0.0019	0.0005	$1 \cdot 10^{-6}$	$1.09 \cdot 10^{-11}$
101-84-8	Diphenyloxide	Floral	Base	7.81	0.020	0.0030	0.0001	0.0099	0.0019
103-05-9	Benzyl tert-Butanol	Floral	Middle	1.02	1.000	0.0013	$1.39 \cdot 10^{-6}$	$1 \cdot 10^{-6}$	$2.60 \cdot 10^{-13}$
123-92-2	Isoamyl Acetate	Fruit	Top	3.07	0.259	0.0053	3.3286	$1 \cdot 10^{-6}$	0.0003
24851-98-7	Methyl Dihydrojasmonate	Floral	Middle	3.10	0.240	0.0016	$1.45 \cdot 10^{-9}$	$1 \cdot 10^{-6}$	$2.99 \cdot 10^{-18}$
106-25-2	Nerol	Floral	Middle	1.41	0.170	0.0029	$6.87 \cdot 10^{-6}$	$1 \cdot 10^{-6}$	$1.53 \cdot 10^{-12}$
120-72-9	Indole	Floral	Base	0.58	0.056	0.0033	$4.89 \cdot 10^{-5}$	$1 \cdot 10^{-6}$	$1.51 \cdot 10^{-11}$
57378-68-4	Delta-Damascone	Floral	Base	2.17	0.147	0.0039	0.0285	$1 \cdot 10^{-6}$	$2.86 \cdot 10^{-7}$
63500-71-0	Florosa Q	Floral	Base	0.58	0.032	0.0044	$6.16 \cdot 10^{-5}$	0.0020	$1.48 \cdot 10^{-5}$
78-70-6	Linalool	Floral	Top	1.01	0.011	0.0072	0.1569	0.01	0.2617

additionally employed to predict the pure-component densities of PRMs at ambient temperature, allowing all cost data to be expressed on a consistent molar basis, as supplier prices can be reported either by mass or by volume.

Optimisation problem formulation

The contribution of each molecule was quantified through its intensity Ψ_i :

$$\Psi_i = \frac{I_{max,i}}{1 + e^{(-X_i - C_i/D_i)}} \quad (1)$$

Where X_i is the logarithm of the concentration of the i th PRM in the gas phase ($\mu\text{g/L}$ air) and $I_{max,i}$, C_i , and D_i are parameters specific to each PRM: $I_{max,i}$ is the odour intensity at saturated gas concentration, C_i is the value of X_i when Ψ_i is $I_{max,i}/2$, and D_i is the steepness of the function. These parameters were retrieved by Wakayama et al [9]. Considering the ideal gas law, $X_i = P_i/RT$, where P_i (Pa) is the equilibrium partial pressure, R is the ideal gas constant ($\text{L Pa K}^{-1} \text{mol}^{-1}$), and T is the temperature (K). From Raoult's law $P_i = \gamma_i x_i P_i^0$, where x_i is the i th molecule molar fraction. Therefore, X_i is a function of the x_i as follows:

$$X_i = \log\left(\frac{\gamma_i x_i P_i^0}{RT} MW_i 10^3\right) \quad (2)$$

The objective function was defined as a weighted combination of total perceptual intensity and economic cost:

$$x_i^* = \operatorname{argmin}\left(-\sum_{i=1}^N \Psi_i(x_i) + \lambda \sum_{i=1}^N c_i x_i\right) \quad (3)$$

Where c_i is the normalised cost of the molecule and λ is a tunable parameter balancing the importance of cost minimisation against intensity maximisation. In this case, $\lambda = 1$. The optimisation was subject to multiple equality constraints to ensure the structural integrity of the perfume formulation. Specifically, the sum of molar fractions within each note category (top, middle and base) was constrained to match the initial total fraction of that note type, reflecting the intranote balance inherent to the perfume pyramid:

$$\sum_{i \in \text{Top}} x_i = \sum_{i \in \text{Top}} x_i^0 = 0.0183, \quad (4)$$

$$\sum_{i \in \text{Middle}} x_i = \sum_{i \in \text{Middle}} x_i^0 = 0.0200 \quad (5)$$

$$\sum_{i \in \text{Base}} x_i = \sum_{i \in \text{Base}} x_i^0 = 0.0216 \quad (6)$$

The rationale for these constraints is as follows. The

initial molar fractions x_i^0 are derived from the target weight fractions of the perfume pyramid by converting each molecule's assigned weight fraction using its molecular weight and density. Consequently, the sums $\sum_{i \in \text{Top}} x_i^0$, $\sum_{i \in \text{Middle}} x_i^0$, and $\sum_{i \in \text{Base}} x_i^0$ encode the desired note-category proportions at the molar level. Enforcing Equations (4)–(6) as equality constraints during optimisation ensures that the total molar amount of each note category remains unchanged. The optimiser may therefore freely redistribute molar fractions among molecules within a note category, favouring those with higher intensity or lower cost, while the total molar amount of each note category, and hence the overall molar proportion of top, middle, and base notes in the Eau de Parfum, is held constant.

Additionally, target intensity constraints were imposed for specific olfactory categories, such as floral and fruity molecules, to ensure the final composition retained desired sensory characteristics:

$$\sum_{i \in \text{Floral}} \Psi_i(x_i) = \Psi_{\text{Floral}}^{\text{target}} \quad (7)$$

$$\sum_{i \in \text{Fruit}} \Psi_i(x_i) = \Psi_{\text{Fruit}}^{\text{target}} \quad (8)$$

Where $\Psi_{\text{Floral}}^{\text{target}} = 0.4$ and $\Psi_{\text{Fruit}}^{\text{target}} = 60$. It is important to note that, from a psychophysical perspective, olfactory intensities are not strictly additive, and summing individual component intensities does not represent the true perceptual intensity of a fragrance. Nevertheless, the use of summed intensities is an easy and convenient mathematical construct within the optimisation framework, enabling the enforcement of compositional constraints on specific olfactory families. The optimisation problem was solved numerically using the Sequential Least Squares Programming (SLSQP) algorithm implemented in SciPy optimize minimize. x_i bounds ranged from 10^{-6} to 10^{-2} . Given the low concentration regime, infinite dilution conditions were assumed; accordingly, variations in X_i in Equation (2) arise solely from changes in x_i , while γ_i is kept constant.

Convergence was monitored using a 10^{-6} tolerance on the objective function, and the final solution was verified by computing the molar fractions of each note type to confirm they remained conserved within a 10^{-6} difference, thereby ensuring that the perfume pyramid structure was maintained.

RESULTS

Table 1 compares the initial and optimised compositions of the fragrance formulation in terms of molar fraction and olfactory intensity. A clear redistribution of material is observed following optimisation, reflecting the objective function, which maximises the sum of olfactory intensities while reducing economic cost. Molecules characterised by high initial intensities (Ψ_i^0) and relatively

low normalised costs are preferentially selected and assigned increased molar fractions. In particular, Ethyl 2-methylbutyrate, Diphenyl oxide, Linalool, and Hexyl salicylate exhibit substantial increases in molar fraction and corresponding olfactory intensity after optimisation. Among these, Ethyl 2-methylbutyrate emerges as a dominant contributor, with its optimised intensity ($\Psi_i^{\text{opt}} \approx 39.2$) significantly exceeding its initial value, while remaining economically efficient. Under the strongest component model, the perceived intensity of a perfume is governed primarily by the molecule with the highest individual intensity contribution. According to this criterion, the optimised formulation is strongly dominated by Ethyl 2-methylbutyrate, whose intensity far exceeds that of all other components. Compared to the initial formulation, where the maximum individual intensity is substantially lower, the optimisation therefore leads to a pronounced increase in overall perceived perfume intensity.

Conversely, several molecules are effectively excluded from the optimised formulation, with their molar fractions reduced to the imposed lower bound. This behaviour is particularly evident for compounds exhibiting extremely low initial intensities, such as Benzyl butyrate, Phenirac, Alpha-amylcinnamaldehyde, Ethyl linalool, Methyl dihydrojasmonate, and Benzyl salicylate. Despite some of these molecules having moderate or even low normalised costs, their negligible olfactory contributions render their inclusion unjustifiable within the optimisation framework. In addition, molecules associated with comparatively high costs and modest intensities, such as Benzyl tert-butanol and Isoamyl acetate, are strongly penalised and largely removed from the formulation. In addition to the objective function, explicit constraints were imposed on the summed olfactory intensities of fruity and floral components, as defined in Equations (7) and (8). The target floral and fruity intensities were set to $\Psi_{\text{Floral}}^{\text{target}} = 0.4$ and $\Psi_{\text{Fruit}}^{\text{target}} = 60$, respectively, compared to initial summed values of approximately 0.21 for floral notes and 39.6 for fruity notes. Following optimisation, both constraints are satisfied exactly, with optimised floral and fruity intensities of 0.400 and 60.0, respectively.

Under this formulation, the total summed intensity increases from 39.8 in the initial composition to 60.4 after optimisation. However, the actual perceived intensity of the perfume remains governed by the strongest component model and is therefore dominated by Ethyl 2-methylbutyrate.

Beyond sensory performance, the optimisation yields a substantial economic benefit. The total normalised cost of the formulation (calculated as $\sum_{i=1}^N c_i x_i$) is reduced from 0.00762 in the initial composition to 0.00279 after optimisation, corresponding to a cost reduction of approximately 64%. Importantly, this reduction is achieved simultaneously with an increase in overall perceived intensity, as dictated by the strongest component

model. Lastly, the influence of the cost–intensity trade-off parameter λ in the objective function was also examined. For the results presented above, $\lambda = 1$ was used, corresponding to equal weighting of intensity maximisation and cost minimisation. When λ was set to 0, such that only olfactory intensity was maximised, the optimiser selected a substantially larger number of molecules, including high-cost components. Although this intensity-only optimisation still reduced the total normalised cost from approximately 0.007 to 0.005, the reduction was markedly smaller than in the $\lambda = 1$ case. This comparison highlights that λ acts as a tunable formulation parameter, allowing the optimisation to prioritise either maximal intensity or economic efficiency depending on the desired design objective. The sensitivity of the optimisation to λ was further explored by increasing its value to 100, thereby strongly prioritising cost minimisation. In this specific case, no substantial changes in the optimised formulation were observed relative to the $\lambda = 1$ solution. This behaviour arises from the limited number of candidate components and, more importantly, from the presence of strict compositional constraints, including the perfume pyramid structure and the imposed floral and fruity intensity targets. These constraints must be satisfied simultaneously, which necessarily enforces the inclusion of certain molecules regardless of the cost penalty applied. This outcome reflects a limitation of the formulation space defined by the modeller rather than a failure of the optimisation strategy itself. In practical perfumery, expert knowledge would guide the initial selection and balancing of ingredients, preventing excessive dominance of individual components while ensuring that structural and sensory requirements are met without reliance on extreme parameter tuning.

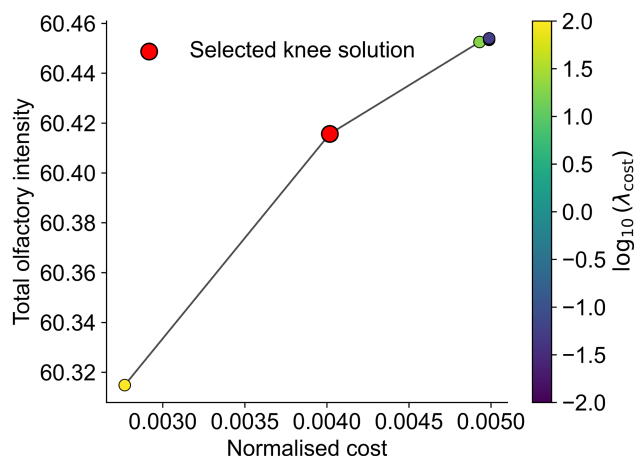


Figure 2. Pareto front: intensity–cost trade-off.

Pareto Front results

To further investigate the trade-off between olfactory performance and formulation cost, a Pareto-front

analysis was performed by sweeping the cost regularisation parameter, λ_{cost} , over a logarithmically spaced grid and solving the constrained optimisation problem for each value.

In addition to the original note-fraction constraints (Equations (7)–(8)), soft constraints were introduced on the total floral and fruit intensities, allowing them to vary within 0.8–1.5 times their respective initial values. The resulting solutions define Pareto curves describing the compromise between total olfactory intensity and normalised cost.

An automatic knee-selection criterion based on the normalised intensity–cost trade-off was then applied to identify an optimal balance between performance and cost. The selected solution ($\lambda_{\text{cost}} \approx 43.3$) yields a substantial increase in total intensity (from ≈ 39.8 to ≈ 60.4) alongside a marked reduction in normalised cost (from ≈ 0.0071 to ≈ 0.0040), while satisfying all constraints exactly. The floral and fruit intensities increase from 0.21 to 0.51 and from 39.6 to 59.9, respectively. This Pareto-selected formulation closely aligns with the previously reported optimisation case corresponding to $\lambda = 100$, both in terms of the selected molecules (seven components are retained with non-negligible contributions) and the overall composition profile, with most remaining components pushed towards their lower bounds. Moreover, inspection of the Pareto front indicates diminishing returns in total intensity for normalised costs above approximately 0.003–0.004, suggesting that further cost increases yield only marginal performance gains.

CONCLUSIONS AND PERSPECTIVES

In this work, a systematic optimisation framework for Eau de Parfum formulation has been proposed, aimed at simultaneously maximising olfactory intensity and minimising economic cost. By coupling physicochemical property prediction, intensity modelling, and constrained numerical optimisation, the methodology provides a quantitative tool capable of redistributing PRMs in a cost-efficient manner while preserving the structural integrity of the fragrance pyramid. The results demonstrate that significant gains in perceived intensity can be achieved alongside substantial reductions in formulation cost, highlighting the potential of optimisation-based approaches to support perfume engineering and formulation design. It should be emphasised that, in the present study, fragrance molecules were initially selected in a simplified manner, based primarily on their fruity and floral character, with olfactory intensities computed a posteriori. This led to a pronounced imbalance in intrinsic intensity across the candidate set, whereby a small number of molecules exhibited markedly higher intensity contributions than others. As a consequence, the optimiser was naturally driven towards selecting and amplifying

these dominant components, in accordance with both the objective function and the model of olfactory perception. While this behaviour is fully consistent with the mathematical formulation of the problem, it does not reflect the typical workflow of a professional perfumer, who would usually pre-select ingredients with broadly comparable olfactory strength in order to achieve a balanced sensory profile. From this perspective, the proposed framework is not intended to replace the creative expertise of the perfumer, but rather to act as a decision-support tool that accelerates and rationalises the formulation process. When applied to a candidate set already curated by a perfumer, based on experience, artistic intent, and desired olfactory balance, the optimisation tool can rapidly identify cost-intensity trade-offs and suggest optimal molar fractions that respect both sensory constraints and economic targets. In this sense, the methodology offers a means to formalise and streamline stages of formulation refinement that are traditionally addressed through iterative trial-and-error experimentation. Future work will focus on extending the optimisation framework to include a preliminary selection stage, in which candidate molecules are dynamically pooled and screened based on their intensity-to-cost ratios. Such an approach would enable the optimiser not only to determine optimal molar fractions, but also to identify the most promising subset of ingredients from a larger candidate library. The integration of molecule selection and composition optimisation within a unified framework would represent a significant step towards fully computer-aided perfume formulation, with the potential to further enhance efficiency, reduce development costs, and support innovation in fragrance design.

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