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INTEGRATIVE IN SILICO ANALYSIS OF COMMERCIAL SOAP INGREDIENTS REVEALS POTENTIAL MODULATORS OF HUMAN MELANOGENESIS PATHWAYS

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ABSTRACT

Commercial soaps widely sold in African markets contain diverse chemical ingredient that may interact with biological pathways in the skin. However, the potential molecular effects of these compounds on melanogenesis and skin physiology remain insufficiently explored, particularly in populations with darker skin types. This study applied an integrative bioinformatics approach to evaluate the chemical composition of commonly used soaps sold in Kaduna markets and to predict their potential interactions with proteins involved in pigmentation regulation and skin signaling pathways. A total of fifteen (15) commercial soap products, comprising both locally manufactured and imported brands, were surveyed. Ingredient profiling identified forty-three (43) unique compounds including surfactants, fatty acids, fragrances, preservatives, pigments, and conditioning agents. Chemical structures of the identified compounds were retrieved from the PubChem database and subjected to target prediction analysis using Swiss Target Prediction. Sixteen compounds generated predicted protein targets, yielding 375 potential human protein interactions associated with enzymes, receptors, kinases, and oxidoreductases involved in skin biology. Pathway enrichment analysis using the KEGG database revealed significant associations with melanogenesis, tyrosine metabolism, MAPK signaling, PI3K–Akt signaling, and Wnt signaling pathways. These pathways play critical roles in melanocyte regulation, pigment synthesis, and cellular responses to environmental stress. In addition, toxicity and safety profiling using ProTox-3.0 indicated that most compounds fall within low to moderate predicted toxicity classes, although a few ingredients demonstrated potential irritation or sensitization alerts. Overall, this study highlights the usefulness of computational toxicology and systems bioinformatics approaches for evaluating cosmetic ingredients and provides preliminary insights into how soap constituents may influence pigmentation-related pathways and skin health in darker skin populations.

Keywords: Bioinformatics; Melanogenesis; Soap ingredients; Skin pigmentation; Computational toxicology

INTRODUCTION

Commercial soaps widely patronized in African markets encompass a heterogeneous array of chemical constituents, including surfactants, fragrances, preservatives, and plant-derived bioactive compounds (Kunatsa & Katerere, 2021; Olajuyigbe et al., 2017). These products are widely used for routine skin cleansing and cosmetic purposes across varied population, notably within sub-Saharan African communities and among individuals of African descent. Despite their widespread use, the molecular effects of their constituent compounds on melanogenesis pathways remain poorly characterized.

This study holds significant implications for individuals demonstrating increased dermal pigmentation, where melanogenesis is integral to the regulation of cutaneous homeostasis and photoprotection (Solano, 2020; Zamudio Díaz et al., 2024). Highly pigmented skin classifications, such as Fitzpatrick phototypes V–VI, are distinguished by elevated constitutive levels of eumelanin, an augmented size and greater abundance of melanosomal organelles, and enhanced tyrosinase enzymatic activity when compared to less pigmented skin types (Hida et al., 2020; Markiewicz & Idowu, 2020; Wang et al., 2024). These inherent biological adaptations provide superior protection against DNA damage induced by ultraviolet (UV) radiation, the genesis of reactive oxygen species (ROS), and associated dermatological sequelae, including solar erythema, accelerated cutaneous senescence, and epidermal neoplasia (D'Mello et al., 2016; Zamudio Díaz et al., 2024). Eumelanin effectively absorbs and disperses UV wavelengths, converting incident energy into thermal efflux and shielding epidermal keratinocytes, thereby contributing to a reduced prevalence of UV-related pathologies within darker-skinned populations (Del Bino et al., 2018; Solano, 2020).

Eumelanin effectively absorbs and scatters UV wavelengths, dissipating energy as heat and shielding keratinocytes, thereby contributing to lower incidence of UV-related pathologies in darker-skinned populations [4,8].

Nevertheless, any dysregulation of melanogenesis, either via inhibition or uncontrolled stimulation, can compromise this delicate homeostatic mechanism, potentially precipitating pigmentary irregularities such as hypo- or hyperpigmentation, which carry substantial cosmetic and psychosocial implications within black communities (Benn et al., 2016; Pollock et al., 2021). Furthermore, exogenous compounds present in personal care products, including various soaps, are capable of modulating key enzymes involved in pigment production (e.g., tyrosinase, TRP-1, DCT) or upstream molecular signaling cascades (e.g., MC1R-mediated pathways); however, the extent of these interactions remains largely uncharacterized for ubiquitous soap components (D. K. Lee et al., 2023; Pillaiyar et al., 2017).

Availability of large data in public repositories, advances in computational bioinformatics and cheminformatics allow for the comprehensive assessment of molecular interactions between chemical agents and proteins, alongside the modulation of biological pathways, on an extensive scale (Y. Lee et al., 2025; Xu et al., 2025; Zheng, 2025). In silico approaches, including molecular docking, network pharmacology, and pathway enrichment analysis, offer efficient means to predict bioactivity and prioritize compounds for experimental validation, particularly when

empirical data on complex mixtures like commercial soaps are limited (Mazri et al., 2025).

This study aims to perform an integrative in silico analysis of bioactive compounds in commercial soaps widely used in African markets, with the goal of predicting their potential modulatory effects on human melanogenesis pathways, particularly in the context of darker skin phenotypes where melanin plays a critical role in pigmentation homeostasis and photoprotection. Specifically, we seek to curate soap ingredient profiles, screen compounds for melanogenesis-relevant bioactivity using cheminformatics, predict target protein and interactions with key proteins (e.g., TYR, TYRP1, DCT, MITF) via SwissTargetPrediction and network pathway analysis, evaluate pathway-level perturbations, and identify potential modulators that may influence melanin balance or inform safer cosmetic formulations for black populations.

MATERIALS AND METHODS

To systematically investigate the potential effects of bioactive ingredients, present in commercial soaps on human melanogenesis, an integrative bioinformatics workflow was developed (Figure 1). This workflow combines chemical informatics, molecular target analysis, and systems biology approaches to predict how compounds commonly found in soaps may interact with key proteins involved in melanin biosynthesis. The approach provides a computational framework for evaluating dermatological safety and biochemical implications of cosmetic products widely used in local markets.

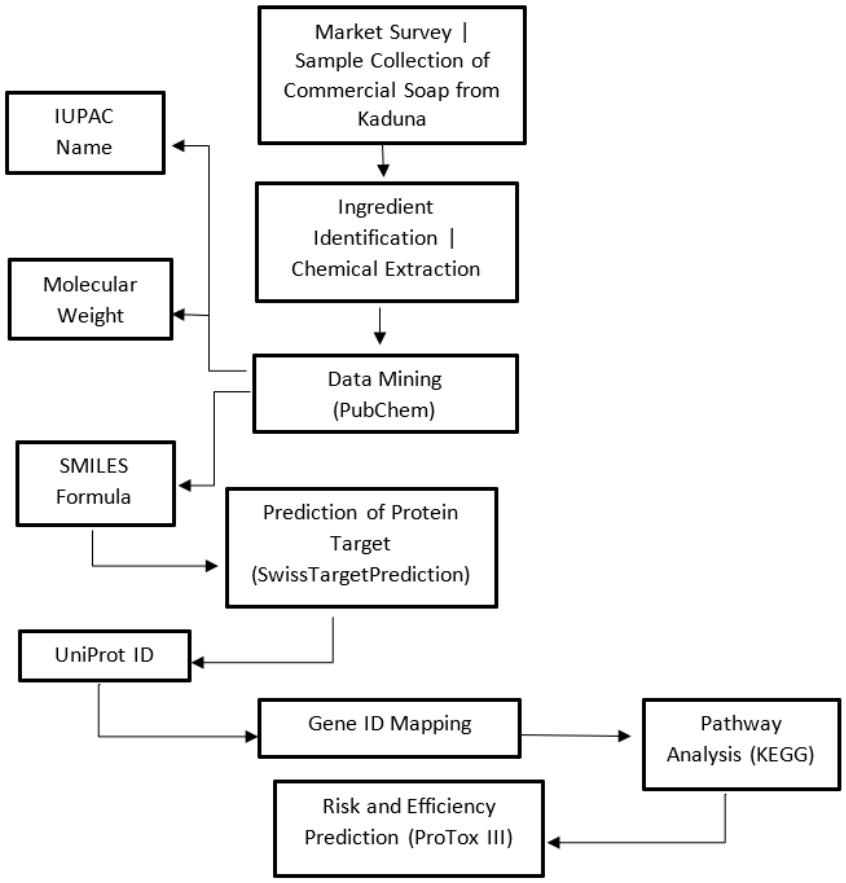


Figure 1: Computational Workflow for Evaluating the Effects of Commercial Soap Ingredients on Human Melanogenesis Pathways

Sample Collection

A market survey and sample selection were conducted and fifteen (15) commonly used commercial soap brands sold in Kaduna markets (coordinates: 10.52090°N, 7.45019°E and 10.51743°N, 7.42846°E) were identified and catalogued. The ingredient lists from product labels are then extracted and mapped to known chemical compounds using PubChem. This step enables the identification and standardization of chemical structures that will be used in subsequent computational analyses**.** Therefore, for each query, the top relevant record was selected based on matching molecular formula and structure. Key outputs noted and retrieved included the compound name, IUPAC name, molecular weight, and SMILES formula. These data will enable functional group classification (e.g., fatty acids, fragrances, alkaline compounds) and provided molecular descriptors such as SMILES formula for downstream target prediction and pathway analysis.

Protein Target Prediction

A computational target prediction analysis using SwissTargetPrediction was performed to identify putative human protein interactors for the characterized soap-derived compounds, based on their molecular resemblance to established bioactive entities. This *in silico* approach enabled the identification of potential interactions between these formulation constituents and proteins implicated in melanogenesis. These findings offer enhanced insight into the prospective molecular mechanisms through which these compounds may modulate cutaneous pigmentation pathways.

The input data is the SMILE formula of the previous analysis retrieved from PubChem for the individual chemical constituent identified.

Pathway Analysis using KEGG

The predicted protein target from the SwissTargetPrediction analysis, were further noted and their UniProt IDs were mapped to their respective gene names with aid of the "Retrieve/ID Mapping" tool of UniProt. Using the mapped genes, the pathways enrichment analysis was carried out using KEGG Mapper. The "Color" from KEGG option was selected, followed by choosing "hsa" (Homo sapiens) under search mode to align with the human-focused study; and the "Exec" was clicked to initiate pathway development.

Risk and Efficiency Prediction Using ProTox-3.0

Risk and efficiency prediction of identified compounds was conducted using the ProTox-3.0 to evaluate potential toxicological profiles, including hepatotoxicity, carcinogenicity, mutagenicity, and skin-related adverse effects. The platform also provided toxicity class estimates and predicted LD_{50} values, allowing preliminary assessment of the safety and functional suitability of soap-derived compounds for topical exposure.

RESULTS AND DISCUSSION

Characterization of Retrieved Compounds

A total of 15 commercial soap products were identified and selected from major retail outlets and open markets in Kaduna State, Nigeria (See Supplementary material 1). The sampled products comprised both locally produced and foreign-manufactured soaps that are widely used by consumers for daily skin cleansing and cosmetic purposes. The selection criteria were based on market availability, frequency of consumer purchase, and diversity of formulation types, including medicated soaps, moisturizing soaps, antibacterial soaps, and cosmetic beauty soaps. Ingredient lists were obtained from product labels and manufacturer information, allowing the compilation of a comprehensive catalogue of chemical constituents present in each product. In total, multiple classes of ingredients were identified, which can be categorized into eight (8) including oil and fatty acids, fragrances, alkaline agents, vitamins, plant/animal extracts, organic compounds, and inorganic compounds and skin-conditioning agents (Supplementary Table S1). Additionally, across all the soap sample the primary saponifiable base was fats and oils, while fragrances aid in the sensory acceptance and can in some individual prompt irritations. Alkaline components noted include Na and or K. Vitamins and animal/plant extracts are considered as bioactive or "conditioning" ingredients often associated with antioxidant, moisturizing, or soothing effects. However, a manual grouping of the entire ingredient resulted to the identification of a total of forty-three (43) unique bioactive compounds. These compounds chemical information including molecular weight, IUPAC name, and SMILES structure were subsequently retrieved for PubChem (Table 1). Here, compound such as Allantoin (158.12 g/mol), Ca_2CO_3 (100.09 g/mol), Coumarin (146.14 g/mol), Glycerin (92.09 g/mol), Hydroquinone (110.11g/mol) and Sodium Palmitate (278.41 g/mol), among other were identified and the SMILE structures presented in table 1.

Table 1: Chemical Characterization of Identified Soap Ingredients showing Compound Names, Molecular Weights, and SMILES Structural Representations of the 43 Catalogued Ingredients

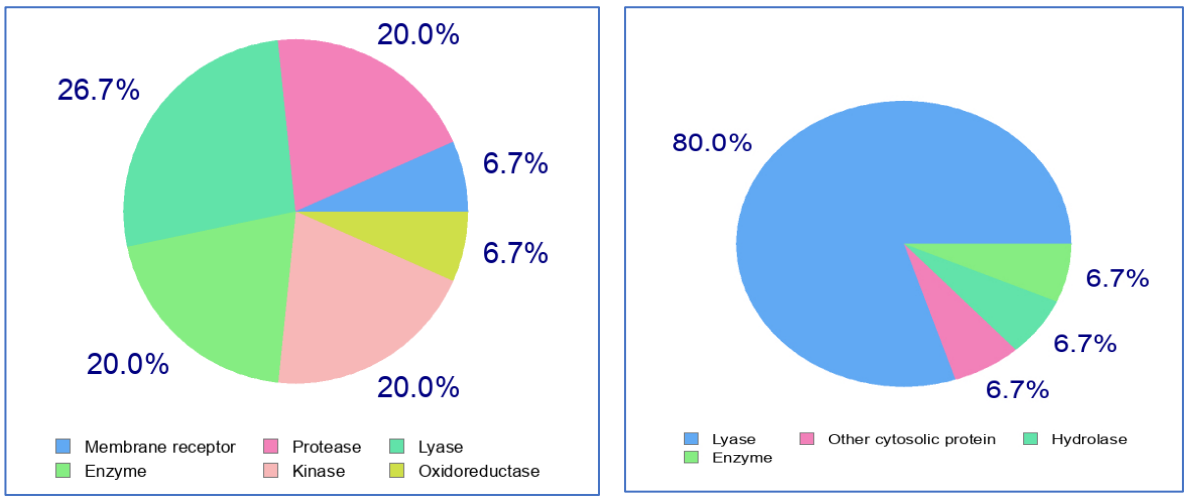
S/N	Compound Name	Numbers of Appearances	IUPAC Name	Molecular Weight (g/mol)	SMILE
1	Allantoin	1	(2,5-dioxoimidazolidin-4-yl)urea	158.12	C1(C(=O)NC(=O)N1)NC(=O)N
2	Alpha-Isomethyl Iononez	1	3-methyl-4-(2,6,6-trimethylcyclohex-2-en-1-yl)but-3-en-2-one	206.32	CC1=CCCC(C1/C=C(\C)/C(=O)C)IC
3	Butylated Hydroxytoluene (BHT)	3	2,6-ditert-butyl-4-methylpheno	220.35	CC1=CC(=C(C(=C1)CIIC)O)CIIC
4	Calcium Carbonate	1	Calcium carbonate	100.09	C(=O)([O-])[O-].[Ca+2]
5	Chloroxylenol (PCMX)	1	4-chloro-3,5-dimethylphenol	156.61	CC1=CC(=CC(=C1Cl)C)O
6	Citric Acid	1	2-hydroxypropane-1,2,3-tricarboxylic acid	192.12	C(C(=O)O)C(CC(=O)O)(C(=O)O)O
7	Citronellol	1	3,7-dimethyloct-6-en-1-ol	156.26	CC(CCC=CIC)CCO
8	Cocamidopropyl Betaine	2	2-[3-(dodecanoylamino)propyl-dimethylazaniumyl]acetate	342.5	CCCCCCCCCCCC(=O)NCCC[N+]IICC(=O)[O-]
9	Coumarin	1	chromen-2-one	146.14	C1=CC=C2C(=C1)C=CC(=O)O2
10	EDTA Disodium	3	2-[2-[bis(carboxymethyl)amino]ethyl-(carboxylatomethyl)amino]acetate	336.21	C(CN(CC(=O)[O-])CC(=O)[O-])N(CC(=O)O)CC(=O)O.[Na+].[Na+]
11	EDTA(Ethylenediaminetetraacetic Acid)	4	2-[2-[bis(carboxymethyl)amino]ethyl-(carboxymethyl)amino]acetic acid	292.24	C(CN(CC(=O)O)CC(=O)O)N(CC(=O)O)CC(=O)O

S/N	Compound Name	Numbers of Appearances	IUPAC Name	Molecular Weight (g/mol)	SMILE
12	Glycerin	9	propane-1,2,3-triol	92.09	C(C(CO)O)O
13	Hansa-Yellow Color	1	2-[(4-methyl-2-nitrophenyl) 61 ioxide 61]-3-oxo-N-phenylbutanamide	340.33	CC1=CC(=C(C=C1)N=NC(C(=O)C)C(=O)NC2=CC=CC=C2)[N+](=O)[O-
14	Hexyl Cinnamal	1	2-benzylideneoctanal	216.32	CCCCCC/C(=C/C1=CC=CC=C1)/C=O
15	Hydroquinone	1	benzene-1,4-diol	110.11	C1=CC(=CC=C1O)O
16	Iron Oxide (Red – CI 77491)	1	Oxo (oxoferriooxy)iron	159.69	O=[Fe]O[Fe]=O
17	Iron Oxide (Yellow – CI 77492)	1	iron(3+) trihydroxide	106.87	[OH-].[OH-].[OH-].[Fe+3]
18	Ketoconazole	1	1-[4-[4-[[(2S,4R)-2-(2,4-dichlorophenyl)-2-(61ioxide61e-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]piperazin-1-yl]ethanone	531.4	CC(=O)N1CCN(CC1)C2=CC=C(C=C2)OC[CH]3CO[C](O3)(CN4C=CN=C4)C5=C(C=C(C=C5)Cl)Cl
19	Kopcinol	2	4-butylbenzene-1,3-diol	166.22	CCCCC1=C(C=C(C=C1)O)O
20	Lauric Acid	2	dodecanoic acid	200.32	CCCCCCCCCCCC(=O)O
21	Limonene	1	1-methyl-4-prop-1-en-2-ylcyclohexene	136.23	CC1=CCC(CC1)C(=C)C
22	Linalool	1	3,7-dimethylocta-1,6-dien-3-ol	154.25	CC(=CCCCI(C=C)O)C
23	Menthol	1	5-methyl-2-propan-2-ylcyclohexan-1-ol	156.26	CC1CCC(C(C1)O)CIC
24	Pigment-Red 5	1	N-(5-chloro-2,4-dimethoxyphenyl)-4-[[5-(diethylsulfamoyl)-2-methoxyphenyl]diazenyl]-3-hydroxynaphthalene-2-carboxamide	627.1	CCN(CC)S(=O)(=O)C1=CC(=C(C=C1)OC)N=NC2=C(C(=CC3=CC=CC=C32)C(=O)NC4=CC(=C(C=C4OC)OC)Cl)O
25	Propylene Glycol	1	propane-1,2-diol	76.09	CC(CO)O
26	Sodium Chloride	5	Sodium chloride	58.44	[Na+].[Cl-]
27	Sodium Isethionate	1	sodium;2-hydroxyethanesulfonate	148.12	C(CS(=O)(=O)[O-])O.[Na+]
28	Sodium Laureth Sulfate (SLES)	1	Sodium 2-dodecoxyethyl sulfate	332.43	CCCCCCCCCCCCOCCOS(=O)(=O)[O-].[Na+]
29	Sodium Lauroyl Isethionate	1	sodium;2-dodecanoyloxyethanesulfonate	330.42	CCCCCCCCCCCC(=O)OCCS(=O)(=O)[O-].[Na+]
30	Sodium Lauryl Sulphate (SLS)	3	Sodium dodecyl sulfate	288.38	CCCCCCCCCCCCOS(=O)(=O)[O-].[Na+]
31	Sodium Metabisulfite	1		190.11	[O-]S(=O)S(=O)(=O)[O-].[Na+].[Na+]
32	Sodium Palmitate	5	Sodium hexadecanoate	278.41	CCCCCCCCCCCCCCCCC(=O)[O-].[Na+]
33	Sodium Stearate	1	Sodium octadecanoate	306.5	CCCCCCCCCCCCCCCCCCC(=O)[O-].[Na+]
34	Sorbitol	1	(2R,3R,4R,5S)-hexane-1,2,3,4,5,6-hexol	182.17	C([CH]([CH]([CH]([CH](CO)O)O)O)O)O
35	Stearic Acid	1	octadecanoic acid	284.5	CCCCCCCCCCCCCCCCCC(=O)O
36	Talc	1	Trimagnesium 61 ioxide(oxo)silane hydroxy-oxido-oxosilane	379.27	O[Si](=O)[O-].O[Si](=O)[O-].[O-][Si](=O)[O-].[O-][Si](=O)[O-].[Mg+2].[Mg+2].[Mg+2]

S/N	Compound Name	Numbers of Appearances	IUPAC Name	Molecular Weight (g/mol)	SMILE
37	Tetra Sodium Etidronate	8	Tetrasodium 1,1-diphosphonato ethanol	293.96	CC(O)(P(=O)([O-])[O-])P(=O)([O-])[O-].[Na+].[Na+].[Na+].[Na+]
38	TetraSodium EDTA	4	TetraSodium 2-[2-[bis(carboxylatomethyl)amino]ethyl-(carboxylatomethyl)amino]acetate	380.17	C(CN(CC(=O)[O-])CC(=O)[O-])N(CC(=O)[O-])CC(=O)[O-].[Na+].[Na+].[Na+].[Na+]
39	Titanium Dioxide	9	Dioxo titanium	79.866	O=[Ti]=O
40	Vitamin C	1	(2R)-2-[(1S)-1,2-dihydroxyethyl]-3,4-dihydroxy-2H-furan-5-one	176.12	C([CH]([CH]1C(=C(C(=O)O1)O)O)O)O
41	Vitamin E	5	(2R)-2,5,7,8-tetramethyl-2-[(4R,8R)-4,8,12-trimethyltridecyl]-3,4-dihydrochromen-6-ol	430.7	CC1=C(C2=C(CC[C](O2)ICCC[CH]ICCC[CH]ICCCCIC)C(=C1O)C)C
42	Vitamin E Acetate	1	[(2R)-2,5,7,8-tetramethyl-2-[(4R,8R)-4,8,12-trimethyltridecyl]-3,4-dihydrochromen-6-yl] acetate	472.7	CC1=C(C(=C(C2=C1O[C](CC2)ICCC[CH]ICCC[CH]ICCCCIC)C)OC(=O)C)C
43	Zinc Oxide	1	Zinc oxygen(2-)	81.4	[O-2].[Zn+2]

Prediction and Identification of Melanogenesis-Related Targets

To explore potential biological interactions, the chemical structures of the identified compounds were subjected to target prediction analysis using SwissTargetPrediction. Here, only 16 out of the 43 SMILE structure yielded protein target predictions. Thus, 375 unique protein targets with probability scores ≥ 0.1 were included for subsequent analysis. The analysis predicted several probable human protein targets based on structural similarity to known bioactive molecules. Among the predicted targets were proteins associated with pigmentation regulation and melanocyte signaling pathways. Notably, the following classes of protein were identified such as enzymes, membrane receptors, kinases, lyases, proteases and oxidoreductases (Figure 2, Table 2 and Supplementary Table S2). Other predicted targets included AQP3, which is associated with skin barrier regulation and hydration; MAPK family kinases linked to inflammatory signaling; and tyrosinase family enzymes (TYR, TYRP1, DCT) involved in melanin biosynthesis. Compounds such as Allantoin and lauric acid repeatedly showed predicted interactions with these melanin and inflammation related proteins. These predictions provided a preliminary indication that some soap ingredients may have the potential to interact with pigmentation-related molecular targets, thereby warranting further structural interaction analysis through pathway enrichment.



(a) (b)

Figure 2: Classification and Distribution of Predicted Protein Associated with Various Compounds from some Soap Constituent. Several compounds showed Predicted Interactions with proteins Linked to Melanogenesis and Pigment Regulation, including Enzymes as shown in (a) Allantoin and (b) Coumarin.

Table 2: Some Swiss Target Prediction Tool Prediction of Protein Targets for some Identified Compounds within Range of Probability Score 0.8 - 1.0

S/N	Ligands	Target Name	UniProt ID	Target Class	Probability Score
1	Ketoconazole	Thromboxane-A synthase	P24557	Cytochrome P450	1
		Alpha-2a adrenergic receptor	P08913	Family A G protein-coupled receptor	1
		Serotonin 1b (5-HT1b) receptor (by homology)	P28222	Family A G protein-coupled receptor	1
		Cytochrome P450 11B1	P15538	Cytochrome P450	1
2	Butylated Hydroxytoluene	Carbonic anhydrase II	P00918	Lyase	0.98
		GABA-A receptor; alpha-1/beta-2/gamma-2	P14867	Ligand-gated ion channel	0.62
3	Coumarin	Carbonic anhydrase I	P00915	Lyase	0.86
		Carbonic anhydrase XIII (by homology)	Q8N1Q1	Lyase	0.86
4	Hydroquinone	Carbonic anhydrase II	P00918	Lyase	1
		Carbonic anhydrase III	P07451	Lyase	1
		Carbonic anhydrase XII	O43570	Lyase	1
5	Lauric Acid	Free fatty acid receptor 1	O14842	Family A G protein-coupled receptor	0.94
6	Menthol	Transient receptor potential cation channel subfamily M member 8	Q7Z2W7	Voltage-gated ion channel	0.94

KEGG Pathway Analysis of Predicted Targets

The 375 unique proteins predicted were mapped to their respective genes. With these genes pathway enrichment analysis using the KEGG pathway database identified significant associations with signaling pathways involved in pigmentation regulation, melanogenesis, inflammation, and cellular responses. Prominent pathways included melanogenesis, tyrosine metabolism, Phenylalanine metabolism, MAPK signaling, PI3K-Akt signaling, Wnt signaling, Notch signaling, Hedgehog signaling pathway, GnRH signaling pathway, Melanoma, and estrogen signaling (Figure 3). These results provide systems-level insight into how soap-derived compounds may influence pigment regulation networks in skin cells.

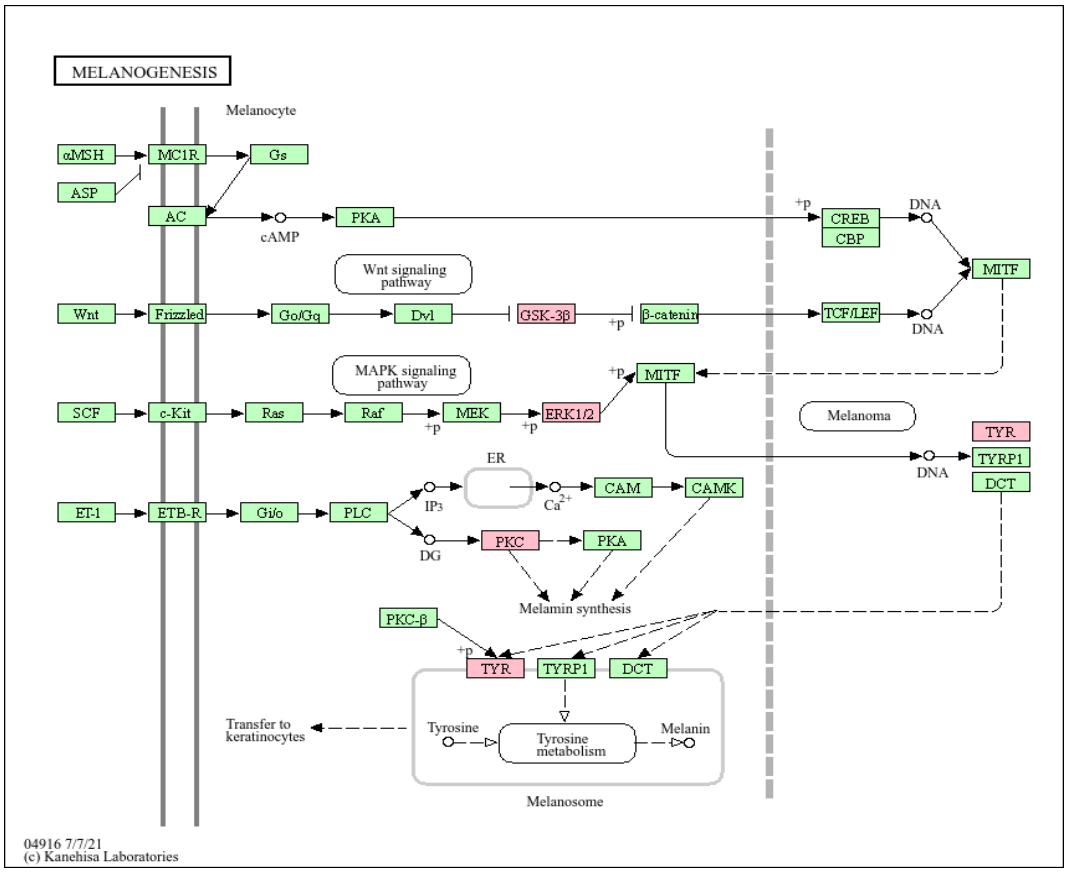


Figure 3: KEGG Pathway Enrichment Analysis of Predicted Protein Targets Associated with Melanogenesis and Related Signaling Pathways

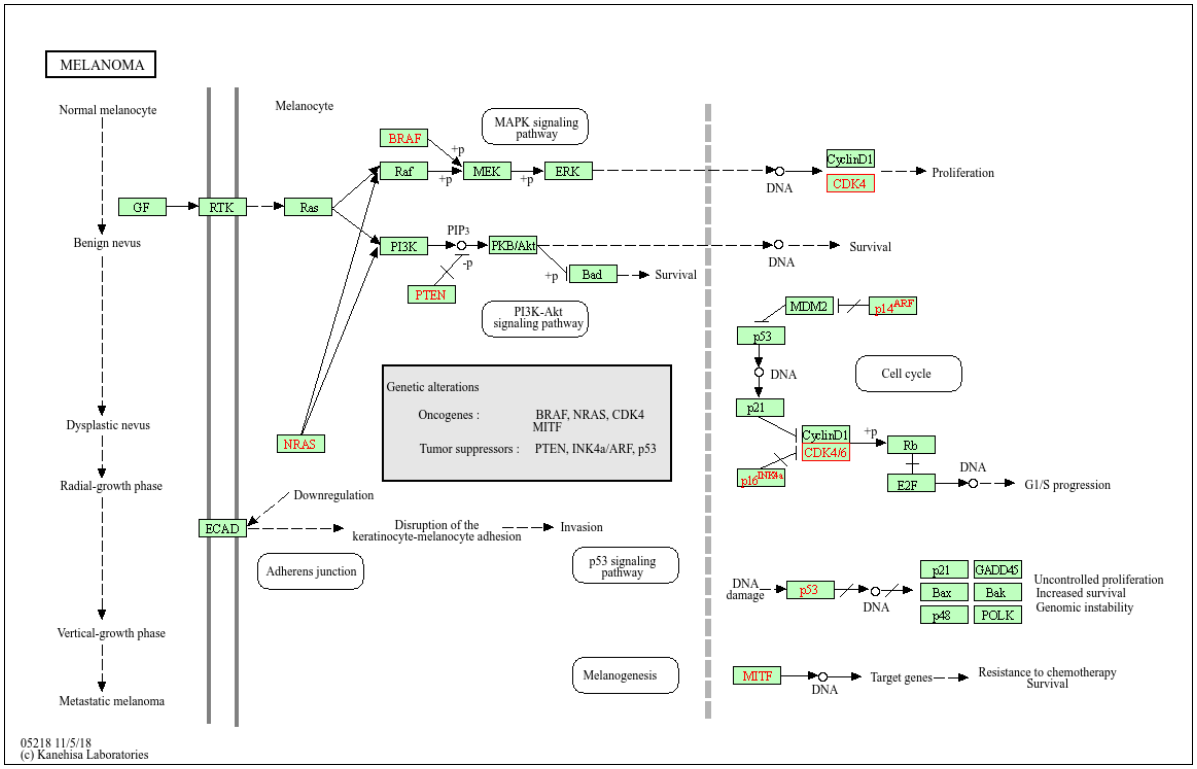


Figure 4: KEGG Pathway Analysis Highlighting Melanoma and Associated Regulatory Signaling Pathways Targeted by Identified Soap Ingredients

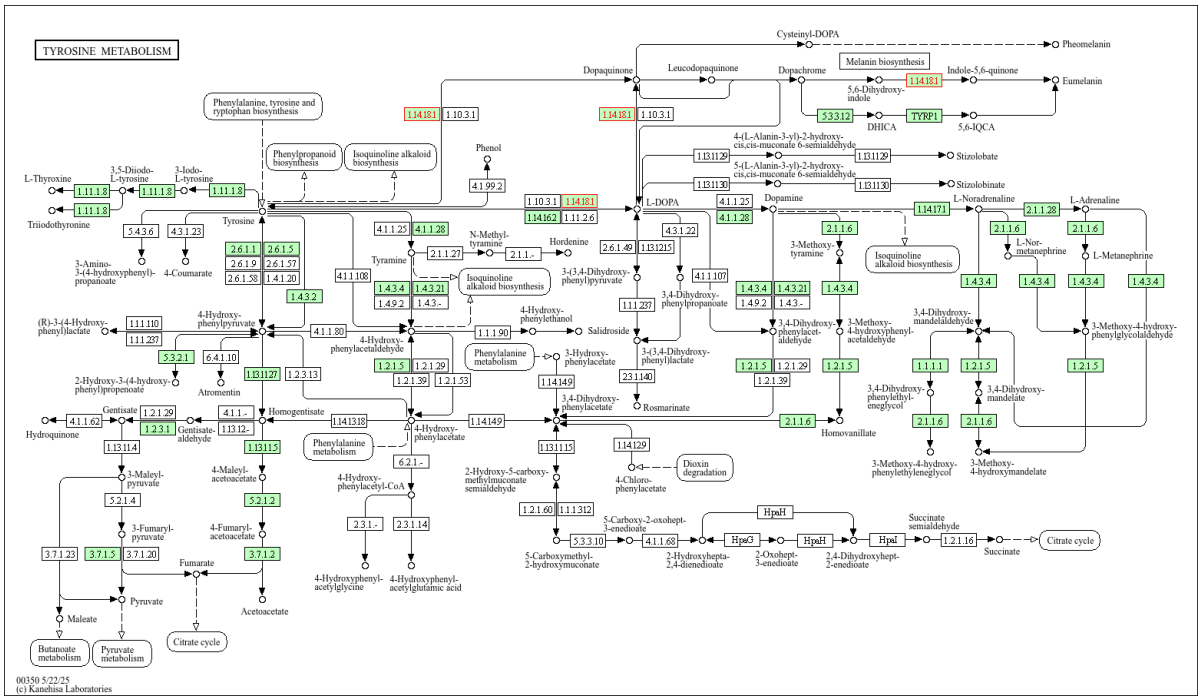


Figure 5: Functional Enrichment of Predicted Targets showing KEGG Pathways Involved in Tyrosine Metabolism, Cellular Signaling, and Metabolic Regulation

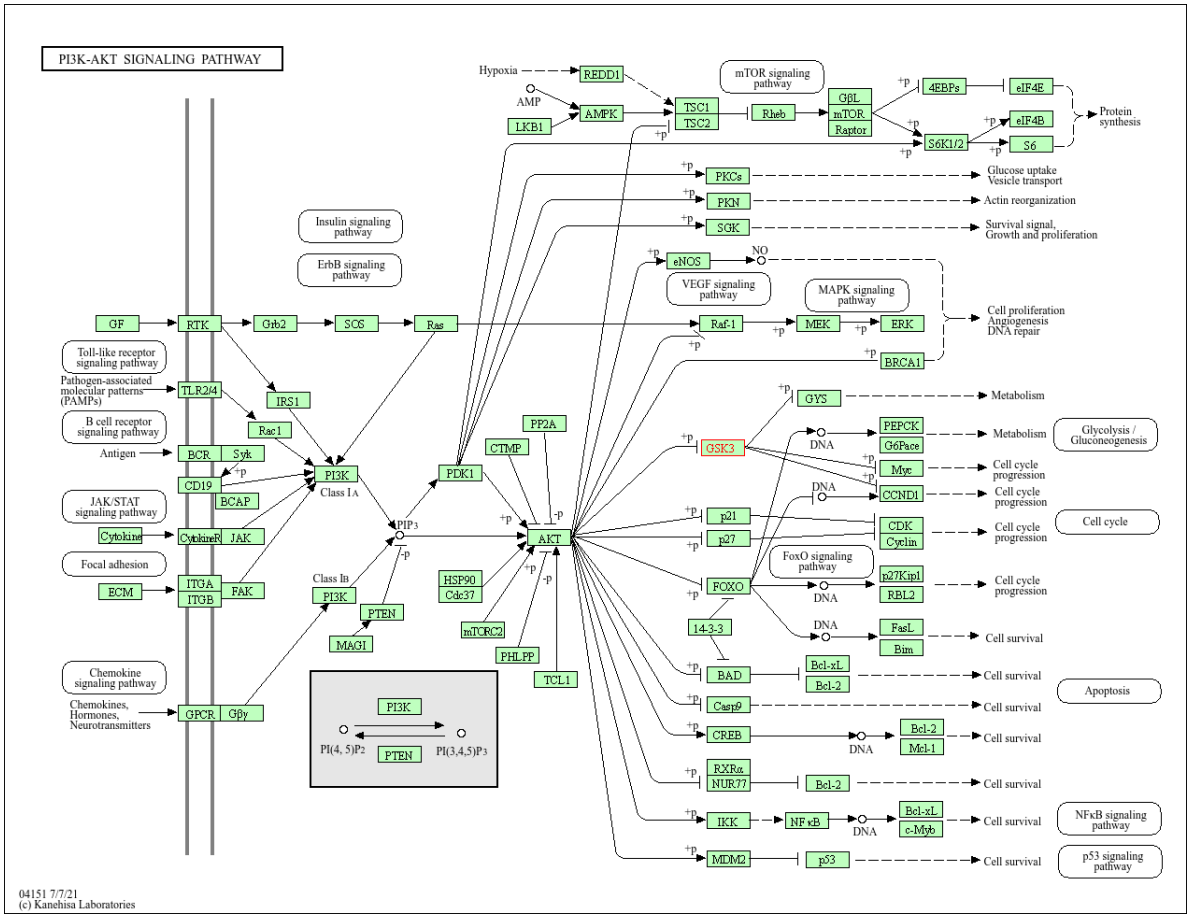


Figure 6: KEGG Pathway Enrichment Analysis of Predicted Protein TARGETS associated with P13K-AKT Pathways

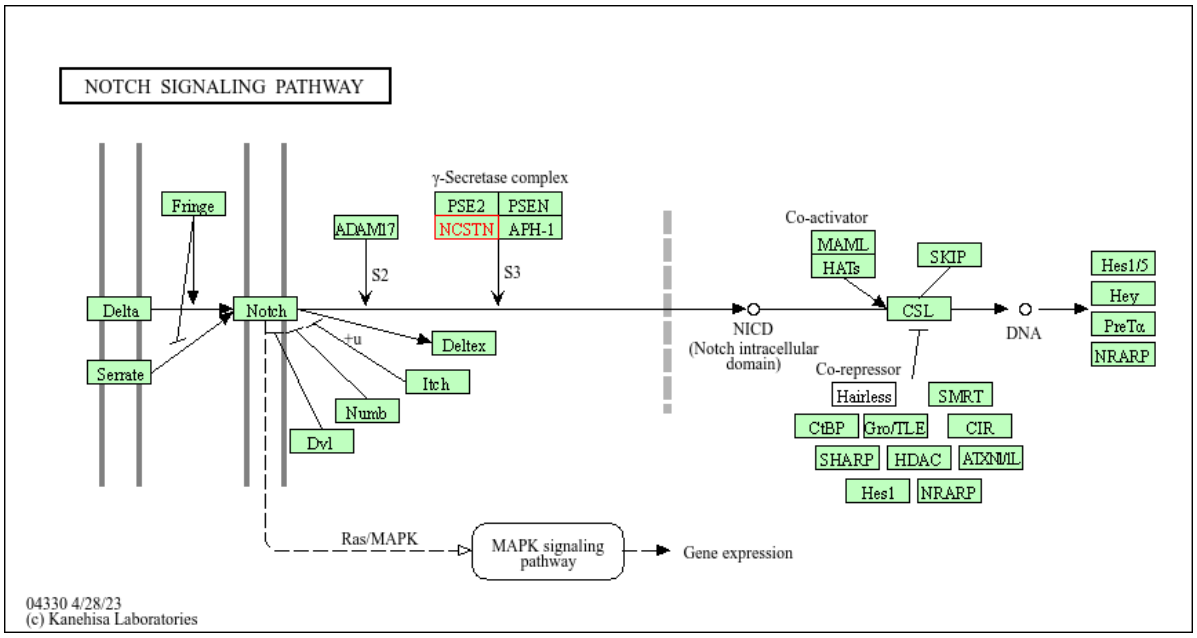


Figure 7: KEGG Pathway Enrichment Analysis of Predicted Protein Targets Associated with Notch Pathway

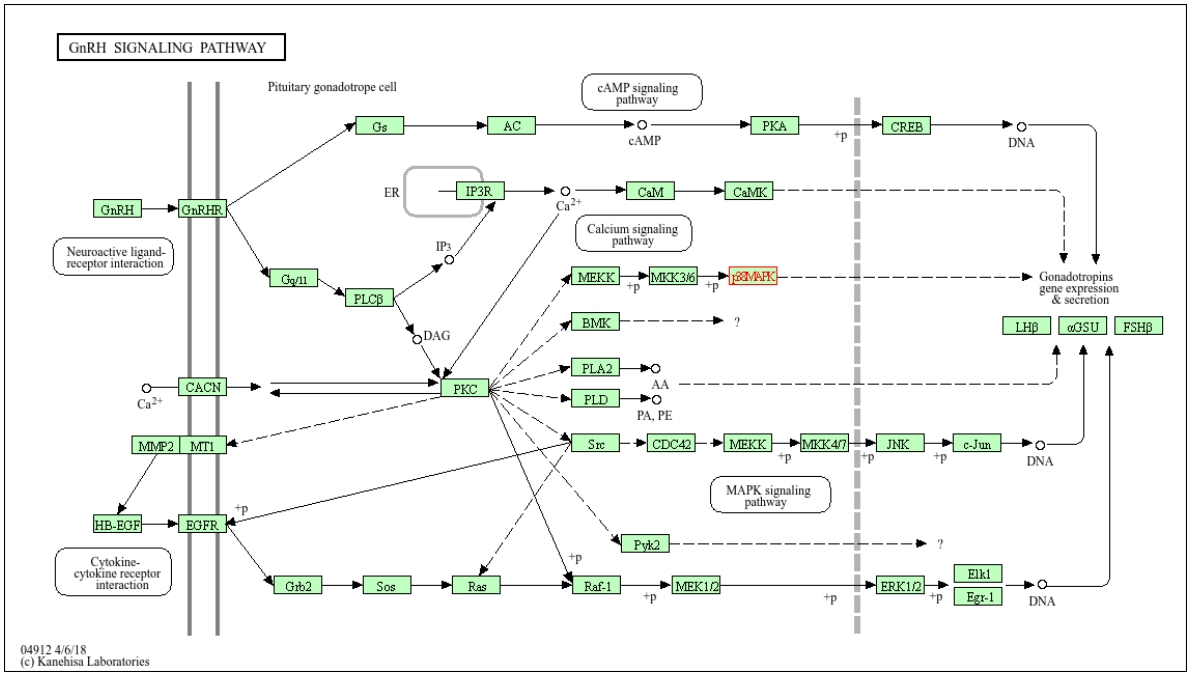


Figure 8: KEGG Pathway Enrichment Analysis of Predicted Protein Targets Associated with GnRH Pathway

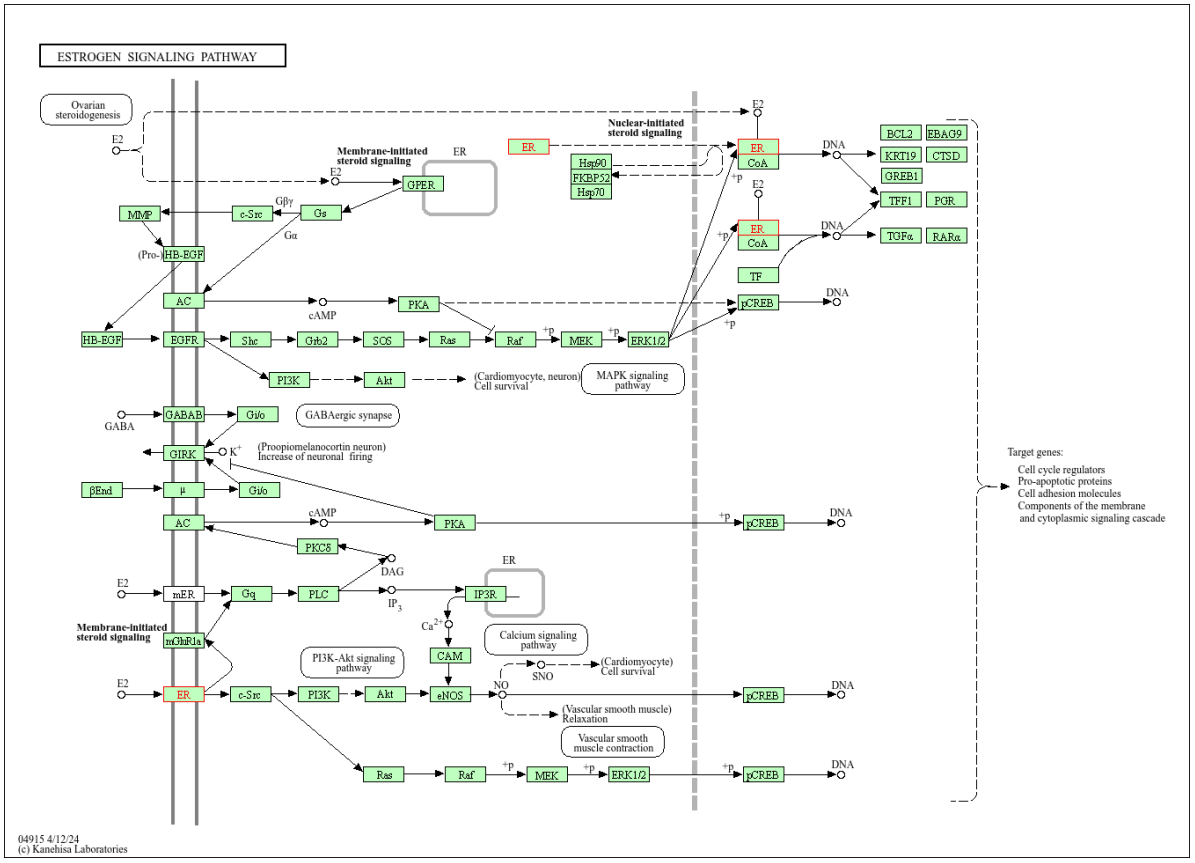


Figure 9: KEGG Pathway Enrichment Analysis of Predicted Protein Targets Associated with Estrogen Pathway

Toxicity and Safety Prediction using ProTox-3.0

The toxicological profiles of the identified compounds were evaluated using the computational toxicity prediction platform ProTox-3.0. The analysis generated predicted toxicity classes, LD_{50} values, and potential toxicological endpoints including hepatotoxicity, carcinogenicity, mutagenicity, and skin irritation potential, for compound such as Coumarin, Hexyl Cinnamal, Hydroquinone, Ketoconazole and N-Butylresorcinol (Kopcinol), among others (see Supplementary Material S2). The results indicated that most of the compounds fell within moderate to low predicted toxicity classes, although a few ingredients exhibited predicted alerts associated with irritant or sensitization potential. These findings provide a preliminary safety assessment of the evaluated compounds and highlight the importance of computational screening in identifying

ingredients that may require further dermatological evaluation for safe cosmetic formulation.

Discussion

The present study applied an integrative bioinformatics approach to evaluate the potential biological interactions of ingredients present in commercial soaps commonly sold in Kaduna markets and their possible implications for melanogenesis regulation and skin health in darker skin populations. The *in-silico* analysis of 43 unique bioactive compounds from 15 commercial soaps commonly used in Nigeria revealed a diverse chemical profile, including surfactants (e.g., Sodium Laureth Sulfate, Sodium Lauryl Sulphate), preservatives (e.g., EDTA variants), fragrances (e.g., Coumarin, Hexyl Cinnamal), and potential modulators such as Hydroquinone, Lauric Acid, Allantoin, and Butylated Hydroxytoluene (BHT). SwissTargetPrediction identified 375 protein targets (probability ≥0.1) for 16 compounds, with enrichment in melanogenesis-related proteins, including tyrosinase (TYR), tyrosinase-related protein 1 (TYRP1), and dopachrome tautomerase (DCT), as well as upstream regulators like MITF and associated signaling pathways (e.g., MC1R/cAMP, MAPK, PI3K-Akt, Wnt, Notch) (D'Mello et al., 2016; Pillaiyar et al., 2017). KEGG pathway enrichment confirmed significant associations with melanogenesis, tyrosine metabolism, MAPK signaling, and melanoma-related networks, suggesting that certain soap ingredients may perturb melanin biosynthesis and pigmentation homeostasis.

These findings are particularly relevant for individuals with darker skin phenotypes (Fitzpatrick types V–VI), prevalent in African populations, where higher eumelanin content and larger melanosomes provide superior photoprotection against UV-induced damage, reducing risks of photoaging and skin cancer (Brar et al., 2025; Solano, 2020). Interference with melanin production, whether through the suppression of tyrosinase-related enzymes or subsequent cellular signaling pathways, has the potential to compromise dermatological defenses. Such disruptions could exacerbate conditions characterized by either reduced or excessive pigmentation, which frequently carry substantial psychosocial implications, particularly within populations of African descent (Benn et al., 2016). Notably, Hydroquinone, detected in one product, is a well-established tyrosinase inhibitor that suppresses melanogenesis but poses risks of exogenous ochronosis, irritant dermatitis, and permanent blue-black pigmentation with prolonged use, especially concerning in darker skin where such effects are more pronounced and harder to treat (Pillaiyar et al., 2017; Zolghadri et al., 2023). Coumarin and related fragrances showed predicted interactions with pigmentation-linked targets, consistent with some coumarin derivatives modulating melanogenesis through pathways like PKA/CREB or GSK3β/β-catenin (Kim et al., 2023). Lauric acid and Allantoin also emerged as recurrent hits for melanin/inflammation-related proteins, aligning with evidence that fatty acids influence tyrosinase degradation or stability, potentially affecting eumelanin/pheomelanin balance (Ando et al., 2004).

ProTox-3.0 predictions indicated moderate to low toxicity for most compounds, though alerts for skin irritation/sensitization in fragrances (e.g., Coumarin, Hexyl Cinnamal) and Hydroquinone underscore the need for caution in daily topical exposure via soaps (Banerjee et al., 2024). This results reveals that common cosmetic ingredients present in cleansing formulations distributed within African markets may inadvertently influence melanogenesis. This warrants further empirical validation, including *in vitro* cellular assays involving melanocytes, to assess the potential for adverse effects on pigmentary stability and intrinsic photoprotection within highly pigmented populations. Prioritizing the development of innocuous product compositions, specifically through the exclusion of documented melanin-reducing compounds such as Hydroquinone, could significantly enhance dermatological safety and mitigate undesired alterations in dermal coloration.

CONCLUSION

This study used a bioinformatics approach to investigate the chemical ingredients present in commonly used soaps sold in Kaduna and to predict their potential effects on skin pigmentation pathways. A total of 43 compounds were identified, and computational analyses suggested that some of these ingredients may interact with proteins involved in melanogenesis and skin signaling pathways, including those related to tyrosine metabolism, MAPK, and PI3K–Akt signaling.

Toxicity prediction further indicated that most compounds fall within low to moderate safety risk categories, although a few ingredients showed potential irritation or sensitization alerts. Overall, the findings highlight the value of computational screening for assessing cosmetic product safety and suggest that certain soap ingredients may influence pigmentation-related pathways, emphasizing the need for further experimental validation, particularly for populations with darker skin types.

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