Croda_Hair Growth - Final Report

A. Croda_Hair Growth - Formulation-ready report

(with detailed chemistry and expected performance)

1. Executive Summary

Hair loss and follicular miniaturization remain major unmet needs in hair-growth therapeutics, even with established active ingredients such as minoxidil. While minoxidil delivers proven benefit through KATP/cAMP signalling, overall hair-growth responsiveness is limited by pathway saturation, inflammation, oxidative stress, and follicular dormancy.

This study applies an AI-driven small-molecule discovery and synergy-screening pipeline to identify novel hair-growth enhancers and synergistic ingredient combinations that are formulation-compatible with minoxidil-based topical systems. Using multi-stage chemical filtering, QSAR modelling, molecular docking, deep-learning bioactivity prediction, and combination-effect modelling, we prioritised a focused set of formulation-ready candidates.

Key outcomes include:

- • Identification of baicalin analogues as the strongest overall balance between predicted dermal papilla (DP) proliferation (+46%) and WNT/β-catenin activation.
- • Recognition of adenosine derivatives and caffeine-like metabolic stimulants as low-risk, scalable candidates suitable for over-the-counter hair-growth products.
- • A ranked shortlist of synergistic ingredient combinations optimised for follicle proliferation, anti-inflammatory performance, scalp microbiome alignment, and topical formulation feasibility.

Objectives

1. **Discover novel hair-growth enhancers suitable for topical scalp delivery.**
2. **Evaluate compatibility and synergy with minoxidil (hero ingredient).**
3. **Reduce early-stage wet-lab burden by replacing large screening programs with AI-based prioritisation.**
4. **Deliver a formulation-ready, decision-support output for hair-growth R&D.**

2. Method

Step 1 — Hair Growth Biology Mapping

Define core biological mechanisms of hair growth:
• dermal papilla proliferation
• WNT/β-catenin activation

• cAMP signalling
• catagen inhibition
• inflammation & oxidative stress control
• scalp microbiome balance
• follicular penetration & delivery

Establish biological targets, pathway nodes, and measurable readouts.

Step 2 — Prepare the Candidate Library (Data → Molecules).

Research begins by constructing a comprehensive small-molecule library relevant to hair-growth biology. Literature mining queries include “hair growth,” “dermal papilla proliferation,” “WNT activation,” “cAMP signalling,” and “inflammation + hair follicle” across scientific publications, GEO datasets, GRAS listings, EU CosIng/INCI registry, patent databases, and internal ingredient sources.

Compound names are standardized into SMILES strings using cheminformatics engines (PubChem / RDKit), followed by physicochemical descriptor generation and chemical-space filtering to retain topical-delivery-appropriate molecules.

Step 2 — Safety and ADMET Filtering.

All candidate molecules undergo silico screening for topical-use suitability. ADMET and toxicity classifiers are applied to identify compounds with irritation risk, phototoxicity, mutagenicity, or scalp barrier disruption concerns. Compounds failing these criteria are removed, producing a safe, formulation-viable subset for further analysis.

Step 3 — Ligand-Based Hair-Growth Bioactivity Scoring. (QSAR)

Surviving candidates are evaluated using ligand-based QSAR models trained on known hair-growth data sources. Predictive models estimate activity on endpoints relevant to follicle biology, including:
• DP proliferation,
• WNT/β-catenin signalling,
• cAMP elevation,
• VEGF/IGF-1 upregulation,
• inflammatory cytokine suppression.

Each compound receives a quantitative growth-potential score to prioritise molecules before structural docking.

Step 4 — Hero ingredient compatibility (Rule-Based Filtering).

To maintain formulation suitability, compounds are screened for chemical compatibility with minoxidil. Rule-based filtering flags:

• strong oxidants,
• strong acids/bases,
• unstable reactive groups,
• peroxide or quinone systems,
• chelators affecting minoxidil stability,
• solubility incompatibilities in hydroalcoholic vehicles.

The output is a list of molecules that can coexist with minoxidil in real formulation environments.

Step 5 — Docking

Shortlisted molecules undergo docking simulations against biological targets associated with hair-growth regulation, including:
• K_ATP channel complex (Kir6.2/SUR2B),
• GSK3β (WNT regulation),
• PDE1A (cAMP turnover),
• TGFBR1 (catagen signalling),
• TRPV1/MT1 (neuroendocrine influence).

Docking outputs—binding energies and pose confidence—feed into downstream predictive models

Step 6 — Hair-Growth Activity Prediction (Deep Learning).

Docking data alone is insufficient to predict functional outcomes; therefore, deep-learning models integrate chemical, structural, and transcriptomic information to estimate hair-growth efficacy metrics. These models output predicted:
• DP proliferation change,
• WNT activation magnitude,
• IL-8/NF-κB suppression scores,
• follicle elongation potential.

This produces a ranked shortlist of 20–40 high-value compounds.

Step 7 — Optional Wet-Lab Validation and Feedback Learning.

Top candidates can be validated by wet-lab assays such as:
• dermal papilla proliferation (MTT/EdU),
• ex vivo follicle elongation culture,
• WNT/β-catenin protein quantification,
• cAMP signalling assays,
• inflammatory cytokine ELISA,
• scalp microbiome antifungal testing.

Experimental data feed back into the model to refine predictions and optimise performance specific to hair-growth biology and formulation rules.

Step 8 — Safety and synergy prediction

Model dual and triple-compound interactions:
- DP proliferation synergy
- WNT+cAMP activation complementarity
- inflammatory + antioxidant pairing

Predict irritation avoidance and safe concentration ranges.

Step 9 — Validation of safety and synergy prediction

3. Results

3.1 Compounds Ranking Table (Model Output)

Rank	Compound	Bioactivity	Toxicity filtered list for topical products				
		DTIGN Kir6.2 – EC50	Skin Irritation	Sensitization	Ames (Mutagenicity)	Dermal Absorption	Status
1	Minoxidil	5.77	Low	Low	Negative	Moderate	Pass
2	Adenosine	5.19	Very low	Very low	Negative	Low	Pass
3	Piroctone Olamine	05.04	Low	Low	Negative	Moderate	Pass
4	Baicalin	4.84	Low	Very low	Negative	Low	Pass

5	Caffeine	<4.0	Low	Low	Negative	High	Pass

3.2 Compound Synergy reports

Decagon					DeepDDI					GraphSynergy			
A	**B**	**Predicted Adverse Interaction**	**Risk Probability**	**Interpretation**	**Pair**	**Interaction Type**	**Mechanism**	**Severity**	**Action**	**A**	**B**	**Synergy Score**	**Interaction Class**
Minoxidil	Caffeine	None	0.08	Safe	Minoxidil + Caffeine	No interaction	Distinct pathways	None	Pass	Minoxidil	Caffeine	0.42	Additive
Minoxidil	Niacinamide	Mild irritation	0.22	Acceptable	Minoxidil + Niacinamide	Additive vasodilation	Local blood flow	Mild	Monitor	Minoxidil	Niacinamide	0.55	Mild synergy
Minoxidil	Baicalin	None	0.05	Safe	Minoxidil + Baicalin	No interaction	Orthogonal	None	Pass	Minoxidil	Baicalin	0.60	Synergy
Minoxidil	Piroctone Olamine	Scalp sensitivity	0.31	Monitor	Minoxidil + Piroctone Olamine	Absorption enhancement	Follicular penetration	Moderate	Control dose	Minoxidil	Piroctone Olamine	0.48	Additive
Caffeine	Niacinamide	None	0.06	Safe	Caffeine + Niacinamide	No interaction	Distinct signaling	None	Pass	Caffeine	Niacinamide	0.50	Additive
Caffeine	Baicalin	None	0.04	Safe	Caffeine + Baicalin	No interaction	Orthogonal	None	Pass	Caffeine	Baicalin	0.62	Synergy
Caffeine	Piroctone Olamine	None	0.09	Safe	Niacinamide + Baicalin	Synergistic anti-inflammatory	NF-κB + cytokines	Beneficial	Promote	Niacinamide	Baicalin	0.68	Strong synergy
Niacinamide	Baicalin	None	0.03	Safe	Baicalin + Piroctone Olamine	Additive anti-inflammatory	COX-2 + NF-κB	Beneficial	Promote	Baicalin	Piroctone Olamine	0.65	Strong synergy
Niacinamide	Piroctone Olamine	Mild erythema	0.25	Acceptable									
Baicalin	Piroctone Olamine	None	0.07	Safe									

B. Market Intelligence Report for Croda

1. Trend Signal Timeline

#	Trend	2022	2023	2024	Evaluation
1	Anti-hair fall (classic claims)	🟢	🟢	🟡	Mature
2	Hair growth serums (leave-on)	🟡	🟢	🟢	Growing
3	Scalp-first / skinification	🟡	🟢	🟢	Strong
4	Hair growth + peptides	🟡	🟡	🟢	Emerging
5	Hair growth + botanical actives	🟢	🟢	🟡	Stable
6	Hair growth + scalp barrier repair	⚪	🟡	🟢	Emerging
7	Hair growth + microbiome / postbiotic	⚪	⚪	🟡	Early signal

Source:

Trend 1-5:
Mintel GNPD – *Hair Care Product Launches* (EU, US, ASEAN), 2022–202
Innova Market Insights – *Top Trends in Hair & Scalp Care*, 2023–2024
Euromonitor – *Hair Care: Global Industry Overview*, 2024
Trend 6:
WGSN Beauty – *Skinification of Hair & Scalp*, 2023–2025
Innova Market Insights – *Barrier Care Beyond Skin*, 2024
CosmeticsDesign Europe – Editorial synthesis, 2023
Trend 7:
Innova Market Insights – *Microbiome Beauty Trends*, 2023–2024
Mintel – *Scalp Care & Microbiome*, 2024
WGSN Beauty – *Postbiotic Actives in Personal Care*, 2024–2026

2. Industry trend reports

#	Sub-category	Competitive intensity	Key brands
1	Hair growth + caffeine / niacinamide	🔴 Overcrowded	L'Oréal, The Ordinary, Alpecin

2	Hair growth + peptide complex	🔴 Overcrowded	Kérastase, Vichy, DS Laboratories
3	Hair growth + botanical actives	🟡 Emerging	Yves Rocher, Aveda, Phyto
4	Hair growth + scalp barrier repair	🟢 Underserved	Very few
5	Hair growth + microbiome / postbiotic	🟢 Underserved	Gallinée (limited), niche brands
6	Hair growth + bond repair / hair strength	🟡 Emerging	Olaplex (adjacent), K18 (adjacent)

Source:

Mintel GNPD – Claim & ingredient tagging, 2022–2024
Innova Claims Database – Hair care sub-claims
Brand websites / INCI disclosures (manual verification)

3. Competitor Claim Saturation Map

#	Claim	# SKU in the market	Evaluation
1	Anti-hair fall / reduces hair loss	150+	🔴 Saturated
2	Strengthens hair roots	120+	🔴 Saturated
3	Promotes hair growth	90+	🔴 Saturated
4	Thickening / increases hair density	70+	🟡 Medium
5	Scalp health / scalp care	60+	🟡 Medium
6	Hair growth + botanical actives	40+	🟡 Medium
7	Hair growth + peptides	25+	🟡 Medium
8	Hair growth + scalp barrier repair	8	🟢 White space

9	Hair growth + microbiome / postbiotic	5	🟢 White space
10	Hair growth + clinical / follicle vitality claim	6	🟢 White space

Source:

Mintel GNPD – Claim tagging & SKU count
Innova Claims Database – Cross-validation
Manual SKU normalization (remove shampoo-only SKUs)

4. Hero Ingredient Crowding Matrix

#	Ingredient	# Brands Used	Evaluation
1	Caffeine	40+	🔴 Commodity
2	Minoxidil	25 - 30 (OTC / pharma)	❌ Regulatory heavy
3	Niacinamide	30+	🔴 Overused
4	Piroctone olamine	8 - 12	🟡 Crowded
5	Adenosine	6 - 10 (mainly JP/KR)	🟡 Crowded
6	Baicalin	2 - 4	🟢 White space
7	Biotin	25+	🔴 Commodity
8	Peptide complexes	15+	🟡 Crowded
9	Botanical extracts (anti-hair fall)	20+	🟡 Crowded
10	Scalp barrier lipids / ceramides	<5	🟢 Opportunity
11	Microbiome / postbiotic actives	<5	🟢 White space

Source:

1. Caffeine

Mintel GNPD – Hair Loss & Scalp Care Products (2022–2024)
Innova Market Insights – Top Functional Ingredients in Hair Care
Euromonitor – Hair Care Ingredients Benchmarking

2. Minoxidil

FDA OTC Monograph – Hair Loss Products
EMA / MHRA – Minoxidil topical classifications
IQVIA – OTC Hair Loss Market

3. Niacinamide

Mintel GNPD – Multifunctional Ingredients in Hair & Scalp Care
CosmeticsDesign Europe – Ingredient trend articles

4. Piroctone Olamine

EU CosIng database
Mintel GNPD – Anti-dandruff actives
Cosmetics & Toiletries Journal – Dandruff actives reviews

5. Adenosine

Shiseido research publications
Journal of Dermatology (JP/KR clinical studies)
Mintel GNPD – Asia hair care innovation

6. Baicalin

PubMed – Baicalin & hair follicle inflammation
Mintel GNPD – Botanical actives (hair care)
Innova – Emerging botanical actives

7. Biotin

Euromonitor – Hair Supplements & Topicals
Mintel GNPD – “Biotin” keyword analysis

8. Peptide Complexes

INCI listings (e.g. Acetyl Tetrapeptide-3, Copper peptides)
Supplier marketing (DSM, BASF, Croda, Lucas Meyer)
Mintel GNPD – Peptides in hair care

9. Botanical extracts (anti-hair fall)

Mintel GNPD – Botanical actives
Innova – Plant-based hair care
Euromonitor – Natural positioning in hair care

10. Scalp barrier lipids / ceramides

Mintel GNPD – Barrier repair in scalp care
CosmeticsDesign – “Skinification of scalp” articles

11. Microbiome / Postbiotic actives — 🟢 White space (<5 brands)

CosmeticsDesign Europe – Microbiome in hair care
Gallinée case studies
Mintel – Microbiome beauty trend

5. Ingredient Availability

#	Ingredient	Function role	# Suppliers	Regions	Regulatory fit	Cost fit @ $10/kg	Availability risk
1	Procapil™ (Croda)	Anti-hair fall, follicle support	1 (Croda)	US / EU / ASEAN	Cosmetic ✔	🟡 Medium	🟡 Medium (single-source)
2	Apiscalp™ (Croda)	Scalp health, soothing	1 (Croda)	US / EU / ASEAN	Cosmetic ✔	🟡 Medium	🟡 Medium (single-source)
3	Caffeine	Microcirculation support	10+	Global	Cosmetic ✔	🟢 Low	🟢 Low
4	Niacinamide	Scalp conditioning	10+	Global	Cosmetic ✔	🟢 Low	🟢 Low

5	Peptide complexes	Hair root signaling	5–7	US / EU	Cosmetic ✔	🟡 Medium	🟡 Medium
6	Botanical extracts (saw palmetto, ginseng)	Anti-hair fall support	8–10	US / EU / ASEAN	Cosmetic ✔	🟢 Low	🟢 Low
7	Scalp barrier lipids / ceramides	Barrier repair	3–5	US / EU	Cosmetic ✔	🟡 Medium	🟡 Medium
8	Microbiome / postbiotic actives	Scalp balance	2–3	EU / US	Cosmetic ✔	🔴 High	🔴 High
9	Minoxidil	Hair regrowth	5–6 (OTC)	US / EU	Drug / OTC	🔴 High	🔴 High (regulatory)
10	Silicone-based film formers	Sensory / slip	10+	Global	Cosmetic ✔	🟢 Low	❌ Excluded
11	Piroctone Olamine	Anti-dandruff, scalp microbiome balance	5–7	US / EU / ASEAN	Cosmetic ✔	🟢 Low	🟢 Low

Source:

EU CosIng (Anti-dandruff actives)
Supplier catalogs (BASF, Clariant, Symrise)
Mintel GNPD – anti-dandruff ingredient usage

6. Ingredient-Level Regulatory

Ingredient	Regulatory Decision	Market Scope	Reasoning (Rule Triggered)	Recommendation
Procapil™ (Croda)	🟢 APPROVED	EU / US / ASEAN	Cosmetic active, INCI-clear, no drug claims	Keep
Apiscalp™ (Croda)	🟢 APPROVED	EU / US / ASEAN	Cosmetic soothing active, scalp health	Keep
Caffeine	🟢 APPROVED	Global	Widely accepted cosmetic active	Keep
Niacinamide	🟢 APPROVED	Global	Cosmetic conditioning, barrier support	Keep
Peptide complexes	🟡 CONDITIONAL	EU / US	INCI varies, some peptides need safety dossier	Require peptide-level validation

Botanical extracts	🟢 APPROVED	EU / US / ASEAN	Traditional cosmetic botanicals	Keep
Scalp lipids / ceramides	🟡 CONDITIONAL	EU / US	Usage level & source-dependent	Check % + origin
Postbiotic actives	🔴 HIGH RISK	EU / US	Novel cosmetic actives, unclear status in ASEAN	Optional / R&D only
Minoxidil	❌ BLOCKED (Cosmetic route)	EU / ASEAN	Classified as Drug	Exclude from cosmetic SKU
Minoxidil	⚠️ CONDITIONAL	US	OTC Drug	Separate OTC product only
Silicones	❌ EXCLUDED	All	Business constraint (brief)	Exclude
Piroctone Olamine	🟢 APPROVED	EU / US / ASEAN	Cosmetic anti-dandruff active	Keep

Source:

EU CosIng (Anti-dandruff actives)
Supplier catalogs (BASF, Clariant, Symrise)
Mintel GNPD – anti-dandruff ingredient usage

7. Claim Subtantiation

Overall Ranking						
Rank	**API(s) & Strength**	**Dosage Form**	**Regulatory Fit**	**Claim Strength**	**Business Fit**	**Overall Verdict**
1	Caffeine 0.1–1%	Gel	🟢 Cosmetic	🟡 Medium	🟢 High	⭐ Best hero active
2	Piroctone Olamine 0.1–1%	Cream	🟢 Cosmetic	🟡 Medium	🟢 High	⭐ Strong support active
3	Minoxidil 2–5%	Gel / Cream	🔴 Drug / OTC	🔴 High	🔴 Low	❌ Excluded
4	Minoxidil + Piroctone	Cream	🔴 Drug / OTC	🔴 Very high	🔴 Low	❌ Excluded

Detailed Claim Substantial					
Rank	**Ingredient(s)**	**Allowed Cosmetic Claims**	**Claim Status**	**Evidence Type**	**Notes**
1	Caffeine	Helps reduce appearance of hair fall	🟢	Literature + in-vitro	Commodity but safe
		Energizes scalp / scalp vitality	🟢	PDE1A inhibition (non-public)	Avoid enzyme naming
		Supports healthier-looking hair growth	🟡	Indirect biological rationale	Wording control
2	Piroctone Olamine	Maintains healthy scalp balance	🟢	Microbiome / anti-fungal data	Strong scalp story
		Helps reduce hair fall linked to scalp imbalance	🟡	Indirect inflammation link	Support claim only
		Supports scalp conditions for hair growth	🟡	Environment-based	Not growth claim
3	Minoxidil	Promotes hair regrowth	🔴	Drug clinical data	Cosmetic forbidden
4	Minoxidil combos	Increases hair growth (cm/month)	🔴	Drug	Exclude entirely

Source:

EU CosIng (Anti-dandruff actives)
Supplier catalogs (BASF, Clariant, Symrise)
Mintel GNPD – anti-dandruff ingredient usage

8. Compliance

Overall Compliance					
Rank	**API(s) & Strength**	**Regulatory Classification**	**Claim Compliance**	**IP / Patent Risk**	**Overall Compliance Verdict**
1	Minoxidil 2–5% + Piroctone Olamine 0.1–1%	🔴 Drug / OTC (Minoxidil)	🔴 Not cosmetic	🟡 Combo patents exist	❌ BLOCKED
2	Minoxidil 2–5%	🔴 Drug / OTC	🔴 Not cosmetic	🟡 Mature drug IP	❌ BLOCKED
3	Caffeine 0.1–1%	🟢 Cosmetic	🟡 Wording-sensitive	🔴 Commodity	✅ APPROVED
4	Piroctone Olamine 0.1–1%	🟢 Cosmetic	🟡 Support-only	🟡 Moderate	✅ APPROVED (support)

Detailed Compliance Breakdown		
1. Minoxidil 2–5% + Piroctone Olamine 0.1–1%		
Dimension	Status	Explanation
Regulatory	🔴	Minoxidil = drug (EU Medicinal Product, US OTC monograph)
Cosmetic legality	❌	Not allowed in cosmetic products
Claim risk	🔴	“increased 5 cm/month” = drug-level efficacy
IP / Patent	🟡	Combination formulations patented historically
Croda fit	❌	Outside Croda Beauty portfolio
Recommendation	❌ Exclude from Vecura cosmetic pipeline	
2. Minoxidil 2–5% (Gel)		
Dimension	Status	Explanation
Regulatory	🔴	OTC drug (US), medicinal product (EU)
Claims	🔴	Hair regrowth claims are drug-only
IP	🟡	API off-patent, but formulation patents remain
Business risk	🔴	Regulatory + pharmacovigilance burden

Recommendation	❌ Hard stop	
3. Caffeine 0.1–1%		
Dimension	Status	Explanation
Regulatory	🟢	Cosmetic ingredient (EU CosIng / US / ASEAN)
Claim allowance	🟡	No direct regrowth claims
Allowed claims	🟢	“Helps reduce hair fall”, “energizes scalp”
IP / Patent	🔴	Commodity, no exclusivity
Business fit	🟢	Scalable, low risk
Recommendation	✅ Hero cosmetic active	

Claim Compliance Matrix			
Claim Type	**Caffeine**	**Piroctone Olamine**	**Minoxidil**
Reduces hair fall	🟢	🟡	🔴
Promotes hair growth	🟡	🔴	🔴
Increases hair density	🟡	🔴	🔴
cm/month growth	🔴	🔴	🔴
Scalp health	🟢	🟢	🟡

Source:

EU Regulation (EC) No 1223/2009
Commission Regulation (EU) No 655/2013
ASEAN Cosmetic Directive (ACD)
FDA OTC Drug Monographs (M032)
EU Borderline Manual

9. Final Recommendation to Croda

✅ STRONG FIT FOR

- Topical hair growth serum / tonic
- Anti–hair loss scalp treatment
- Scalp health–focused ingredient system (multi-active)

⚠ **WATCH OUT**

- Scalp irritation risk at higher Minoxidil or penetration-enhancer levels
- Polyphenol stability and color drift in leave-on formulations
- Sensory balance (greasiness / residue) with multi-active systems

➡ **NEXT STEPS**

- In vitro dermal papilla cell assay (proliferation, Wnt markers)
- Combination screening (Minoxidil + polyphenol / Piroctone Olamine)
- Short-term scalp tolerance & efficacy study (4–8 weeks)

APPENDIX - Data Sources & Citation Index

Project: Hair Growth Ingredient Discovery & Formulation Intelligence
Partner: Croda – Consumer Beauty
Markets: EU, US, ASEAN

1. Market & Trend Intelligence Sources

1.1 Industry Trend Reports

Source	Coverage	Usage in Report
Mintel GNPD – Beauty & Personal Care	Global	Trend Signal Timeline, Claim Saturation
WGSN Beauty	EU / US	Emerging scalp-first & skinification trends
Innova Market Insights	Global	Ingredient trend validation
Euromonitor – Beauty & Personal Care	Global	Category growth & maturity assessment

Applied to

- Trend Signal Timeline (2022–2024)
- Industry Trend Reports table
- Market maturity classification (Mature / Growing / Emerging)

1.2 Competitor & Product Intelligence

Source	Coverage	Usage
Mintel GNPD SKU database	Global	Claim saturation counts
Brand official websites (L'Oréal, Vichy, Kérastase, The Ordinary, Alpecin, DS Labs, Aveda, Phyto)	EU / US	Claim wording & hero ingredient mapping

Retail platforms (Sephora, Boots, Watsons, Amazon)	EU / US / ASEAN	SKU count & positioning

Applied to

- Competitor Claim Saturation Map
- Hero Ingredient Crowding Matrix

1.3 Consumer Signal Sources

Source	Coverage	Usage
Consumer surveys (internal / partner-provided)	Variable	Pain point validation
Social listening summaries (Reddit, TikTok, Instagram – qualitative)	Global	Signal confirmation only

⚠️ *Used directionally, not as quantitative proof*

2. Biology & Target Mapping Sources

2.1 Pathway & Disease Biology

Source	Type	Usage
Reactome	Pathway DB	WNT/β-catenin, TGF-β, cytokine pathways
KEGG	Pathway DB	Hair follicle signaling context
Open Targets Platform	Target–disease	Hair loss relevance scoring
TTD (Therapeutic Target Database)	Target DB	Validation of druggable proteins

2.2 Biomarkers & Assays

Source	Type	Usage
PubChem BioAssay	Assay DB	EC50 / IC50 endpoints
FDA Biomarker Table	Regulatory	Biomarker relevance validation
PubMed	Literature	Mechanism & assay justification

3. Compound & Ingredient Intelligence

3.1 Compound Libraries

Source	Type	Usage
PubChem	Chemical DB	SMILES, descriptors
DrugBank	Drug DB	Pharmacology-backed expansion
GRAS Database	Safety	Human exposure screening
EU CosIng	Regulatory	Cosmetic eligibility
INCI Database	Regulatory	Commercial readiness
Croda Internal Catalog	Partner DB	Proprietary ingredients
Vecurate (internal)	Aggregated	Unified compound layer

3.2 Cheminformatics & Filtering

Tool	Function
RDKit	Fingerprints, logP, MW, TPSA, rule-based filtering

4. AI / In-silico Modeling Sources

4.1 Ligand-Based & Structure-Based Models

Model / Tool	Purpose
ChemProp	QSAR bioactivity prediction
AutoDock Vina	Docking
GNINA	CNN-based docking
DiffDock	Diffusion docking
DTIGN	Structure-based activity prediction
Decagon	Polypharmacy side-effect prediction
DeepDDI	Drug–drug interaction
GraphSynergy	Mechanistic synergy prediction

5. Regulatory & Compliance Sources

5.1 Cosmetic & Drug Regulation

Source	Jurisdiction
EU Regulation (EC) No 1223/2009	EU Cosmetics
Commission Regulation (EU) No 655/2013	Claims
ASEAN Cosmetic Directive (ACD)	ASEAN
FDA OTC Drug Monographs (M032)	US
EU Borderline Manual	EU

6. IP & Patent Intelligence

Source	Usage
Google Patents	Prior-art & formulation density
EPO Espacenet	Patent landscape sanity check
USPTO Public Search	US filing trends

⚠️ *Used for IP awareness, not freedom-to-operate opinions*

7. Formulation & Manufacturing References

Source	Purpose
Medisca Formulation Database	Dosage form inspiration
USP <795>	Beyond-use dating
Reaxys	Retrosynthesis feasibility
MolPort	Vendor availability & pricing
ISO 16128	Natural origin & sustainability

8. Environmental & Sustainability Signals

Source	Usage
Supplier disclosures (where available)	CO_2 qualitative assessment
Academic LCA literature (generic)	Directional footprint estimates
Industry best practices	Risk flagging

⚠️ *CO_2 values are indicative, not certified LCA*

9. Scope & Disclaimer

- All sources are **public or partner-provided**
- Outputs are **decision-support**, not regulatory or legal opinions
- Quantitative claims require **experimental validation**