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An Evidence-Bounded Product-Development Case Study of a Matcha–Ayurvedic Sachet

Aradhvi Jain
Aradhvijain.17@gmail.com

ABSTRACT

Under academic pressure, high-caffeine, high-sugar energy products are being used more and more frequently by adolescents, which is associated with sleep disturbances, cardiovascular symptoms and decreased well-being. We have proposed a formulation in the following paper that includes a single serve matcha delivery system, 6 Ayurvedic botanicals (Amla, Triphala, Tulsi, Shankhpushpi, Brahmi, Gotu kola), an inulin fibre based and a citrate electrolyte layer. The new formulation is designed as a result of literature survey and cheminformatics screening of 16 marker compounds representing the three signature molecule profiles of matcha against heterogeneous benchmarks, and market, regulatory and ethical considerations. The closest chemical analogues to the matcha were triphala catechins (Tanimoto=0.45), and selected markers exhibited low levels of chemical similarity to caffeine (all ≤0.10), which are not detected by the screen. There is no analytical verification of the nominal caffeine target and the benchmarks are not for safety or efficacy. The validation on the formulation through efficacy, stability, and regulatory testing needs to be performed on future studies.

Keywords: *functional food; adolescent caffeine intake; matcha; L-theanine; Ayurvedic botanicals; cheminformatics; product development; responsible marketing*

1. INTRODUCTION

Adolescents frequently consume stimulants including energy drinks, colas, coffee, caffeine tablets, and drinks with high caffeine and added sugars under exam pressure to stay up longer than usual to study (Pettit & DeBarr, 2011; Riera-Sampol et al., 2022; Buchanan et al., 2018; Hammond & Reid, 2017). Reviews of energy-drink use in young people report associations with sleep disturbances, anxiety, cardiovascular symptoms and other adverse outcomes (Ajibo et al., 2024; Seifert et al., 2011). A conservative caffeine reference of 2.5 mg/kg/day is adopted for comparison, rather than treated as evidence that a formulated product is safe (Ruxton, 2014). Late caffeine, meant to extend study time, works against sleep, which is when learning is consolidated (Owens, 2014), and sleep onset is already delayed during adolescence (Carskadon & Tarokh, 2014). The design question is whether a conceptual no-added-sugar sachet can be transparently specified against caffeine-intake guidance without implying established safety or benefits for adolescents. Matcha may have caffeine and l-theanine, but literature on the effects of the caffeine-l-theanine combination on attention and mood is mixed and does not prove efficacy for the proposed sachet (Payne et al., 2025; Gerolymos et al., 2026; Anas Sohail et al., 2021). Evidence for Ayurvedic botanicals is largely adult-based, though there is strongest evidence for Bacopa

monnieri (Pase et al., 2012; Kongkeaw et al., 2013), mixed results for Centella asiatica (Puttarak et al., 2017), one placebo-controlled Tulsi stress study (Saxena et al., 2012), and primarily traditional/preclinical support for Shankhpushpi (Sharma et al., 2022).

Matcha is a source of caffeine, L-theanine, catechins (mainly EGCG) and other polyphenols (Sokary et al., 2022; Khan & Mukhtar, 2018). Studies have assessed L-theanine's role in relaxation (Williams et al., 2020; Hidese et al., 2019), stress and attention (Williams et al., 2020; Hidese et al., 2019; Dashwood & Visioli, 2025), often in combination with caffeine (Owen et al., 2008; Haskell et al., 2007; Giesbrecht et al., 2010; Camfield et al., 2014), but the evidence remains limited: a 2025 meta-analysis showed small-to-moderate, heterogeneous effects on attention/reaction time (Payne et al., 2025), and a 2026 meta-analysis of 31 trials was similarly cautious (Gerolymos et al., 2026). No studies provide evidence of efficacy for a novel 12-component formulation of matcha, or in adolescents specifically, and the cited matcha drink/bar and older-adult studies do not directly establish whether L-theanine counteracts caffeine-related sleep effects (Dietz et al., 2017; Uchida et al., 2024).

The acute vigilance/reaction-time effect of caffeine is well established in adults (Wikoff et al., 2017), but lower per-kg exposure thresholds, greater vulnerability, and the developmental significance of sleep in adolescents (Carskadon & Tarokh, 2014; O'Callaghan et al., 2018) argue for caution, particularly since evening caffeine increases sleep latency and decreases sleep quality (Snel & Lorist, 2011). Accordingly, this paper adopts the more conservative value of 2.5 mg/kg/day (~125 mg/day for a 50 kg person; Ruxton, 2014) over EFSA's ~3 mg/kg/day.

Six botanicals with known phytochemical effects (including the three-fruit combination "Triphala" that contains Amla) were chosen as contributing ingredients, but not additional stimulants. Amla (Phyllanthus emblica) is rich in hydrolysable tannins, gallic acid, ellagic acid and ascorbic acid, providing an antioxidant layer (Saini et al., 2021; Husain et al., 2019). Triphala is primarily characterised by hydrolysable tannins, including gallic-acid derivatives; catechins are not established here as its dominant constituents (Peterson et al., 2017; Thallada et al., 2026). Tulsi (Ocimum tenuiflorum) provides eugenol and associated volatiles, based on one double-blind placebo-controlled study with a standardised extract for general stress (Saxena et al., 2012; Cohen, 2014), non-applicable for other extracts and adolescents. Shankhpushpi (Convolvulus pluricaulis), an ancient medhya rasayana, provides limited human data with commercial products with inconsistent content from four plant sources (Sethiya et al., 2013; Sharma et al., 2022), explicitly experimental. Brahmi is most researched: extracts with bacosides showed positive effects in specific memory domains in randomised studies, usually after weeks of administration to adults or elderly patients (Pase et al., 2012; Kongkeaw et al., 2013; Calabrese et al., 2008). Gotu kola contributes triterpenoids (asiaticoside, asiatic acid, madecassoside), showing mixed results (Puttarak et al., 2017; Gray et al., 2017; Bandopadhyay et al., 2023). There are two important reservations: the phytochemical composition may vary in dependence on species, cultivation, harvesting, extraction, and storage conditions; thus, standardisation is necessary (Osman et al., 2023; Kellogg et al., 2019); moreover, some herbal ingredients may be potentially dangerous due to their interaction with drugs.

Functional beverages target energy, cognition, stress, hydration and gut health, with botanical positioning now mainstream (Nazir et al., 2019; Maleš et al., 2022; Todorova et al., 2021). Digitally-reached younger consumers favour recognisable plant-derived ingredients, reduced sugar and transparency (Priporas et al., 2017; Qutteina et al., 2019), raising minors-related marketing concerns (Buchanan et al., 2018; Kent et al., 2019); existing teas and other no-added-sugar low-caffeine products mean that uniqueness cannot be established without a systematic market audit. The conceptual contribution is instead the explicit documentation of design assumptions, dose positioning and ethical constraints.

This paper formulates and critically evaluates a conceptual model of a matcha formulation intended for occasional use by older adolescents. The product is first formulated from published human evidence, with each ingredient assigned an explicit functional role. Marker compounds from constituent botanicals are then compared cheminformatically against matcha's signature molecules to interrogate the stated structural rationale, and ingredient amounts are positioned against heterogeneous typical-use ranges and, where relevant, intake guidance; these comparisons do not establish formulation safety, with specific attention to adolescent caffeine guidance. Finally, the product's market positioning, regulatory status, and the ethical implications of marketing a caffeinated product to minors are examined.

2. METHODS

2.1 EVIDENCE-BASED FORMULATION

Ingredients were organised into proposed design roles (matcha anchor/alertness, polyphenol, exploratory calm-related botanical, longer-term cognition-related botanical, and fibre/electrolyte base); these roles are hypotheses, not demonstrated effects with each botanical candidate required to meet three criteria: a documented marker compound/class, at least one human study or systematic review (or explicit exploratory designation), and availability as a standardised extract. Literature was searched in PubMed and Google with the following Latin botanical names and concepts: cognition, memory, stress, antioxidant effects and safety. Dates of search, the number of searches performed and the number of items selected were not documented, reducing the ability to repeat the study. The nominal range of 30–45 mg of caffeine in 1.5 g of matcha is based on the assumed caffeine concentration which is between 20–30 mg/g. No batch specific assay was done. The concept uses botanical doses, with some below range for adults; the volume of water used to reconstitute is suggested to be about 300 mL; bulk is inulin.

2.2 CHEMINFORMATIC SCREENING

Three (EGCG, caffeine, L-theanine) out of sixteen marker compounds (three from matcha and thirteen from the constituents of the botanics) were canonicalised to SMILES and handled by RDKit. Molecular weight, topological polar surface area (TPSA), hydrogen-bond donor/acceptor counts, Lipinski violations and quantitative estimate of drug-likeness (QED) were documented; XLogP entries are reported property values whose provenance requires clarification; structural similarity used Tanimoto coefficients over Morgan fingerprints (radius 2, 2048 bits); drug-likeness used QED. The reported non-chiral Morgan

fingerprints do not distinguish catechin and epicatechin stereochemistry; the selected markers cannot test for undeclared ingredients or prove biological equivalence.

2.3 COMPOSITIONAL DOSE–SAFETY SCREEN

Per serving quantities were reported as a percentage of the 5000 mg total dose and compared with the following class-specific reference quantities: typical dose of botanical, mineral UL, matcha culinary-serving, inulin GI-tolerance guide, and 2.5 mg/kg/day (125 mg/day at illustrative BW of 50 kg) for caffeine (including from all dietary sources). Upper limit of typical adult use botanicals is not a toxicological upper limit and no adolescent use combined-formulation safety upper limit was found. The mineral content of the tables submitted depends on citrate salt forms, which are not independently validated.

2.4 MARKET, REGULATORY AND ETHICAL ANALYSIS

Market positioning was conducted on the basis of secondary data such as categorisation analysis of energy drinks, literature research on adolescent energy drink consumption and illustrative compositions of competitors represented by caffeine and sugar per serving. Rubio et al. (2022) addresses energy drinks and does not substantiate all tea, coffee, tablet and sports-drink values in the illustrative figure. Regulatory discussion considered possible Food Safety and Standards Authority of India (FSSAI) classifications and European Food Safety Authority (EFSA) caffeine guidance. The applicable classification, permitted claims, age restrictions and any per-serving caffeine rule were not independently established from regulatory clauses.

3. RESULTS

3.1 COMPOSITION

The single-serve formula is a 5000 mg powder mixed in ~300 mL cool water with a nominal caffeine estimate of approximately 40 mg, not an assayed amount through five functional layers - matcha anchor, antioxidant, calm-focus, cognitive-support, and hydration/fiber base (Table 1; Figure 1). Matcha (30%) is the only source of caffeine, being calculated back from the 40 mg target as opposed to being adjusted post-hoc; as such, caffeine, L-theanine, and EGCG scale together in natural leaf proportion. Amla and Triphala (accounting for 55% of the combined botanical weight, within six botanicals that together make up 29% of the serving) strengthen the polyphenols pillar; Tulsi and Shankhpushpi make up for the calm-focus layer together with matcha's L-theanine; Brahmi (Bacopa monnieri) and Gotu kola (Centella asiatica) were included for exploratory longer-term cognition-related rationales, but the proposed occasional-use instructions do not support an expectation of their effects, which have generally been studied after repeated dosing in adults. Citrates account for 19.4% of sachet mass; the previously estimated elemental sodium amount of ~150 mg is inconsistent with 380 mg sodium citrate, and reliable elemental amounts cannot be specified until the exact salt forms are identified. If studying is done in a sedentary position, no hydration benefits have been proven and inulin (980 mg) is a prebiotic filler that

does not absorb quickly as carbohydrates. There is no sweetener added but the matcha bitterness and astringency of Amla, Triphala and Tulsi leaves are yet to be resolved in terms of sensory attributes.

Table 1. The composition of the study sachet used (5 g).

Editorial Note: The original formulation does not specify the precise forms of citrate salts for sodium, potassium, and magnesium and elemental amounts cannot be verified.

Ingredient	**mg/serving**	**% of serving**	**Functional layer**
Matcha powder (ceremonial grade)	1500	30.0	Anchor — caffeine (~40 mg), L-theanine, EGCG
Inulin	980	19.6	Fibre base / bulking agent, prebiotic
Amla extract	500	10.0	Antioxidant (gallic/ellagic acids, tannins)
Sodium citrate	380	7.6	Hydration (≈150 mg elemental Na)
Magnesium citrate	350	7.0	Hydration (≈50 mg elemental Mg)
Triphala extract	300	6.0	Antioxidant — contributes catechins
Potassium citrate	240	4.8	Hydration (≈100 mg elemental K)
Tulsi extract	200	4.0	Exploratory calm rationale (no efficacy shown) (eugenol, volatiles)
Gotu kola extract (10% triterpenes)	150	3.0	Exploratory cognition rationale (no efficacy shown)
Brahmi extract (20% bacosides)	150	3.0	Exploratory cognition rationale (no efficacy shown)
Shankhpushpi extract	150	3.0	Exploratory calm rationale (no efficacy shown) (exploratory)

Natural flavour + steviol glycosides	100	2.0	Palatability, no added sugar
Total	5000	100.0	

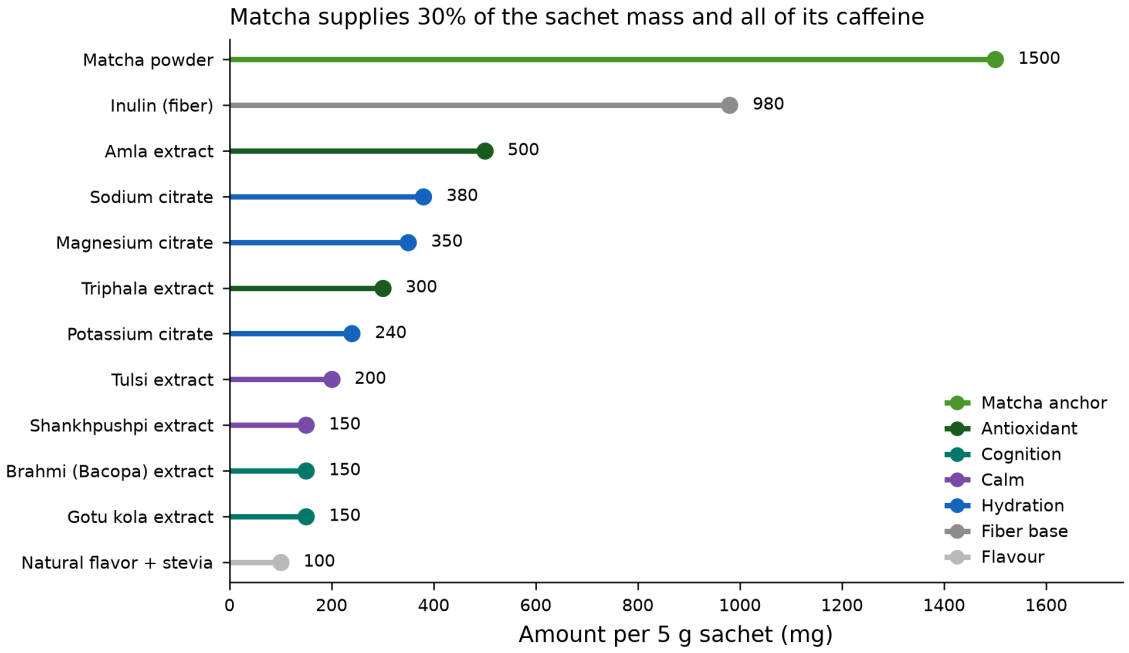


Figure 1. Matcha 30% (sole caffeine source) combined 1450 mg (six botanical extracts); citrate electrolyte layer 19.4% (970 mg); the remainder is balanced with inulin.

3.2 STRUCTURAL SIMILARITY TO MATCHA (FIGURE 2; SUPPLEMENTARY TABLE B2)

Of sixteen markers, Triphala's catechin/epicatechin was the highest in comparison to EGCG (Tanimoto 0.45), Amla's gallic acid (0.28), chebulagic acid (0.25), quercetin (0.19) and ellagic acid (0.18). All declared markers scored ≤0.10; this is against caffeine (max: scopoletin, 0.10), but does not exclude undeclared stimulants, or give evidence of stimulant effects. The similarity with L-theanine was consistently low (≤0.11).

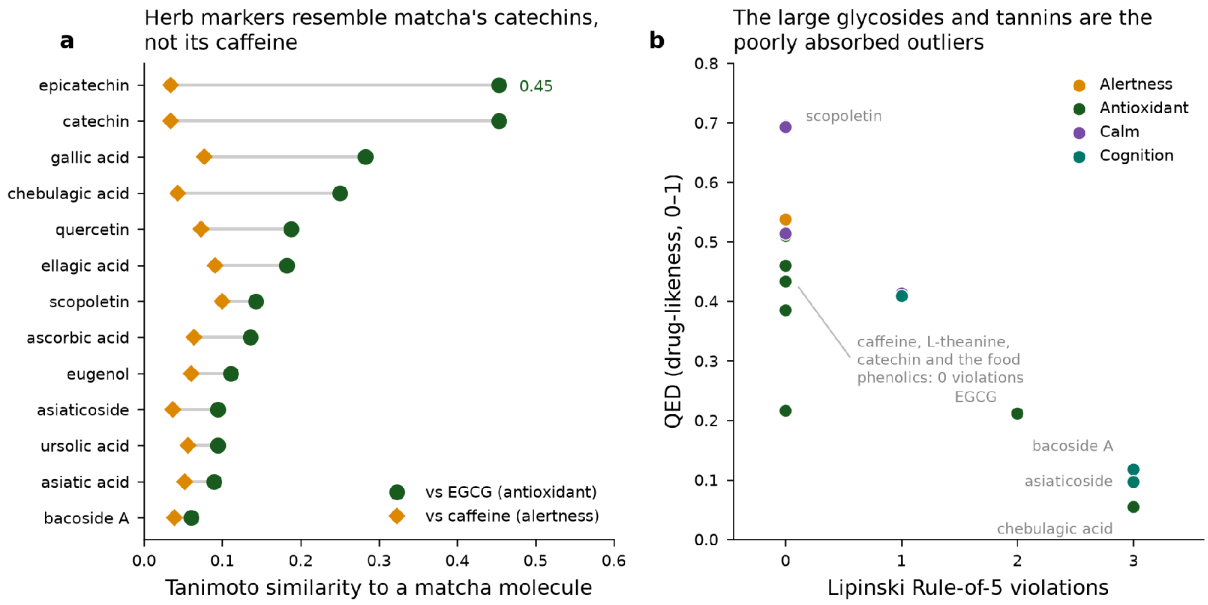


Figure 2. Cheminformatic screening of sixteen marker compounds. (A) Morgan fingerprint (radius 2, 2048 bits) Tanimoto similarity to EGCG (circles)/caffeine (diamonds): Triphala catechins reach 0.45 versus EGCG; none exceed 0.10 versus caffeine. (B) Lipinski violations versus QED: ten compounds show zero violations; chebulagic acid, bacoside A, asiaticoside each carry three violations, QED below 0.12; EGCG carries two.

3.3 PHYSICOCHEMICAL PROFILE (FIGURE 2B; SUPPLEMENTARY TABLE B1)

Molecular weights ranged from 164 Da (eugenol) to 959 Da (asiaticoside); XLogP ranged from −3.6 (L-theanine) to +7.3 (ursolic acid). Ten of 16 compounds were compliant with Lipinski's Rule of Five (0 violations) and QED >0.50; bacoside A, asiaticoside and chebulagic acid had 3 violations each with QED <0.12 which do not indicate bioavailability, clinical efficacy or delayed effects. The originally reported mean XLogP of ≈0.5 has not been supported by a clearly specified calculation; lipophilic (ursolic acid 7.3, asiatic acid 5.7) Tulsi/Gotu kola triterpenes.

3.4 DOSE-POSITIONING COMPARISON (FIGURE 3; SUPPLEMENTARY TABLE C1).

This original plot does not provide a safety clearance; it is designed to compare different types of benchmarks (typical adult dose and dietary reference values). The 40 mg of caffeine used was approximately 32% of the conservative level for the daily dose for adolescents (125 mg, or 2.5 mg/kg for a 50 kg person). The highest proportions were for matcha (75% of the 1-2 g typical food serving) and Amla and Brahmi (both at 50% of the reference ceilings). The mineral percentages for the original minerals are provisional as the citrate hydration states and exact forms of the salts are not known. The three botanicals (Triphala, Tulsi and Shankhpushpi) are outside the lower bounds of the manuscript's

self-described typical use ranges; comparisons are not intended to suggest efficacy or safety.

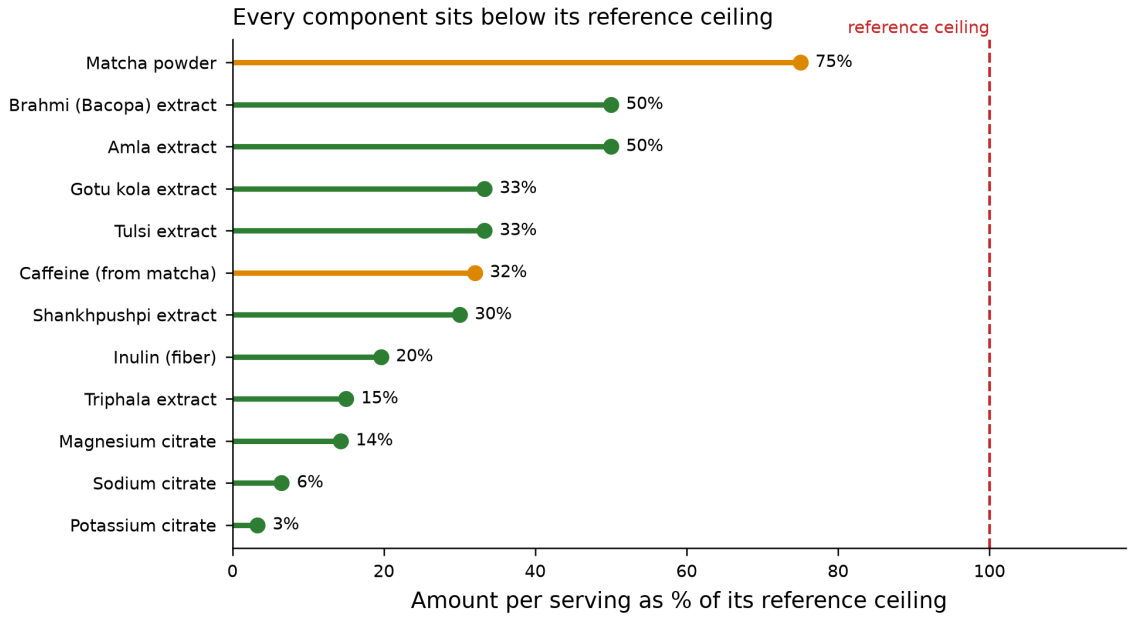


Figure 3. Botanicals (typical doses), minerals (elemental limits/upper intakes), matcha (culinary serving), inulin (GI-tolerance guide), caffeine (2.5 mg/kg/day × 50 kg = 125 mg/day) original per-serving amounts vs. heterogeneous reference benchmarks (not validated safety ceilings). Orange: matcha anchor/caffeine contribution and dashed line: ceiling

3.5 Market positioning (Figure 4)

The caffeine/sugar map was used to put the concept in a low-caffeine, no-added-sugar area distinct from energy drinks (80-160 mg caffeine / 250 mL, 27-54 g sugar), caffeine tablets (100-200 mg, no hydration/flavour), coffee/tea/matcha (unstandardised) and nootropic drinks (premium, poorly justified ingredients). One large energy drink contains more than the 125 mg adolescent daily reference intake, and one standard energy drink plus one cola reaches the 125 mg adolescent daily reference intake.

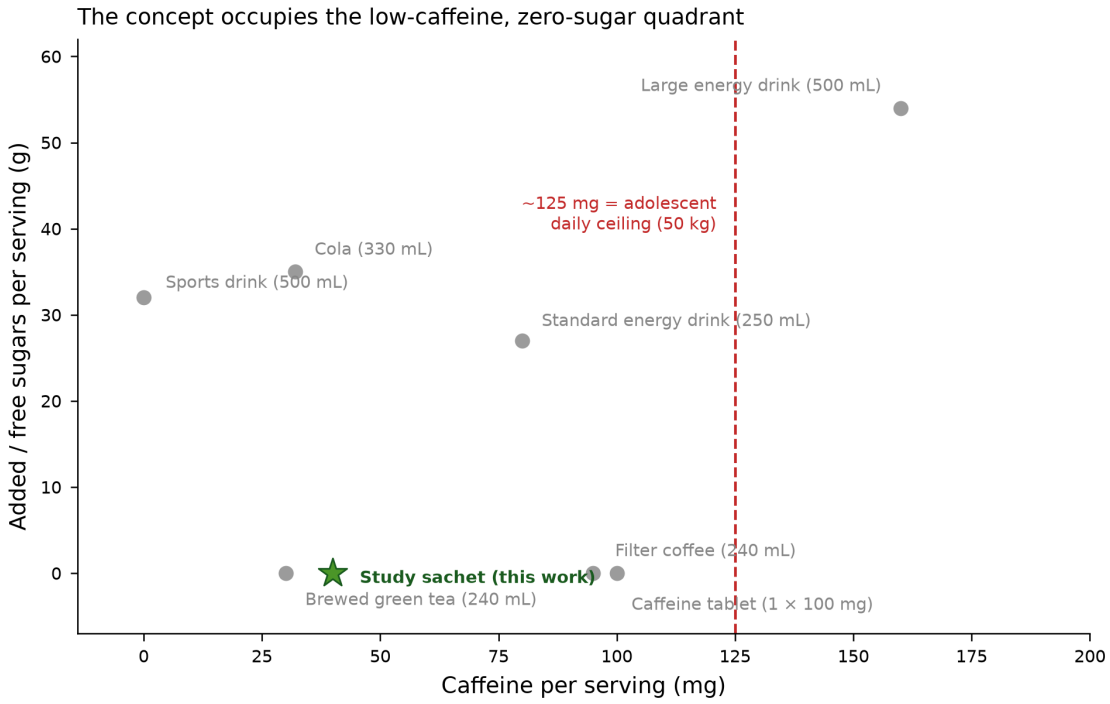


Figure 4. Caffeine vs. added/free sugar per serving. The composition/exposure analysis of comparator products was derived from published data; the study sachet is a proposed sub-50 mg-caffeine, no-added-sugar design, not demonstrated to occupy a unique market segment. Based on the conservative daily reference for adolescents (50 kg) of ~125 mg, the dashed line indicates that one large energy drink goes over the daily reference, while one standard energy drink plus one cola is at the daily reference.

4. DISCUSSION

The concept illustrates a documented approach to setting a preliminary caffeine target and describing the selected ingredients. However, the market map is illustrative rather than a comprehensive competitor audit, the heterogeneous dose benchmarks do not establish safety, and the structural screen describes selected declared molecules rather than testing for adulteration (Gurley et al., 2014; Jagim et al., 2023).

All the limitations of the work, however, are design and market ones, rather than clinical ones, for which the results are addressed. The dose–safety screen tests compositional reasonableness only. All reference limits for the six botanicals are adult or traditional-use values; no adolescent-specific thresholds exist, and this substitution is a material limitation rather than a technicality, given differences in body mass, metabolism and developmental stage. Structural similarity is also not biological equivalence: A Tanimoto score of 0.45 between catechin and EGCG does not necessarily mean that the two share same target, same concentration, same effect, nor same Absorption, Distribution, Metabolism, Excretion and Toxicity (ADMET) properties, and the cheminformatic efforts were limited to 2D structure/physicochemical description; no Absorption, Distribution, Metabolism, Excretion and Toxicity (ADMET) modelling,

bioavailability modelling, or modelling for matrix effect or toxicity modelling was attempted, and PubChem GHS flags are for concentrated-reagent exposure, not dietary-level 9 exposure. The markers themselves stand in for idealised single molecules rather than the variable, multi-species commercial extracts (four source species for Shankhpushpi alone) a manufacturer would actually procure, so botanical content will vary with origin, harvesting, extraction and storage in ways the screen cannot capture.

Evidence quality across the botanicals is similarly uneven: Brahmi reasonably cumulative, Gotu kola mixed, Tulsi supported by a single standardised-extract trial, Shankhpushpi exploratory with an unresolved species-identity problem, and all of it adult-derived, with no adolescent efficacy or safety data behind caffeine, L-theanine, matcha, or any botanical at the doses and populations used here. The nominal 40 mg caffeine target is a design constraint but not analytically capped or audited, but 2.5 mg/kg/day is the maximum reference dose for daily intake from all sources, and individual caffeine sensitivity differs, and caffeine may adversely affect sleep in a dose- and timing-dependent manner even at lower intakes (Snel & Lorist, 2011). In other words, while the dose is capped, the risk still persists.

There are similar constraints in the market analysis, manufacturing and regulatory assessment. There are no consumer surveys, willingness-to-pay studies, taste tests, or competitor product audits; positioning is based on secondary sources, while the Figure 4 competitors are only illustrative; there are no supplier quotes, and therefore cost per serving is just an estimation. The available documentation does not establish validated manufacturing or stability testing of the finished product; dissolution rate, sensory acceptability, moisture sensitivity, shelf life, blending and microbial safety have not been proven by bench-scale formulation alone. The regulatory assessment is limited to one jurisdictional frame (FSSAI in tandem with EFSA caffeine guidance); in other jurisdictions, the classification, permitted caffeine content, labeling, and underage access restrictions are very different.

Four elements of the approach are nonetheless worth retaining: fixing the caffeine target first and deriving matcha mass from it, rather than the reverse; using cheminformatic screening to describe the declared marker set without claiming that it detects hidden stimulants; treating Rule-of-Five/QED profiles as descriptive heuristics rather than a basis for predicting cognitive effects; and integrating regulatory/ethical review to narrow use-occasion and eliminate unsupported claims rather than treating this as a marketing afterthought. Countervailing weaknesses include unresolved palatability (matcha bitterness compounded by Amla/Triphala/Tulsi astringency), undetermined stability of three hygroscopic component classes, exposure to tightening regulation of youth-targeted caffeine products, and a premium-price structure (ceremonial-grade matcha plus six standardised extracts) untested against a discretionary, price-sensitive segment.

On regulatory and ethical grounds, the product would likely fall under FSSAI's health-supplement/nutraceutical/botanical-food categories, permitting no disease-related or unsubstantiated cognitive claims, requiring a "CONTAINS CAFFEINE" declaration, and without a verified classification, specific regulatory clause or established 40 mg/serving permission for this formulation. Restrictions on marketing caffeinated botanical mixtures to minors require formal regulatory review. Ethically, marketing any caffeinated product to an academically stressed, potentially

sleep-deprived adolescent population risks exploiting that vulnerability regardless of dose (Murphy et al., 2020; Kent et al., 2019); a harm-reduction rationale would depend on unverified substitution of higher-caffeine products rather than introducing an additional caffeine occasion. An adult (18+) target population would not be subject to all the concerns of being marketed to a minor, but only if the targeting of adult audiences to sleep-optimized messages, which are generally not enduring, and the reduction of such messages when considering commercial pressure, can be shown to be present at the concept stage.

Taken together, these constraints mean no claim of efficacy, safety, or commercial viability is established by this paper. The work instead demonstrates a method including evidence-based formulation, computational structural characterisation, preliminary dose-positioning comparison, and regulatory-ethical positioning that yields a defensible concept bounded strictly by its evidence: composition, dose and design rationale are claimed, not efficacy. Progression to an actual product would require sensory acceptability, stability, cost, regulatory clearance, and properly supervised human evaluation, in that order.

5. CONCLUSION AND FUTURE WORK

The paper suggests the concept of 5 g sachet formulation containing matcha (40 mg of caffeine, 6 Ayurvedic extract and citrate electrolytes and inulin fibre) and uses pediatric guidelines to calculate dose of caffeine and scales the amount of matcha accordingly for occasional use in the adolescent. The highest similarity reported for EGCG was found in a maximum of 16 botanical markers using cheminformatics, and the similarity to caffeine was highest at 0.10. These descriptive data cannot detect adulteration, are not intended to prove cognition benefits or safety. The amount of caffeine and combined-formulation safety have yet to be tested. The illustrative market and regulatory analyses highlight constraints and do not create a niche or regulatory permission – at this stage, no niche or permission is proven here. Key next steps include sensory evaluation, ingredient sourcing and costing, analytical methods validation and regulatory consultations before proceeding to human studies. What is important about this project is not the specific formulation of the sachet, but rather the importance of making explicit dose assumptions and setting clear limits on computational evidence to support preliminary product design, without evidence of safety or efficacy.

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APPENDICES

Appendix A: Formulation and preparation

Composition: as Table 1. Total mass 5000 mg per single-serve sachet; caffeine nominally approximately 40 mg (not analytically verified; estimated variation depends on matcha source), sourced entirely from 1500 mg ceremonial-grade matcha powder.

Preparation (bench prototype, non-consumption): weigh each component on a balance readable to 0.001 g in descending mass order. Pre-blend the four smallest components (natural flavour/steviol glycosides 100 mg, and the three 150 mg extracts) with an equal mass of inulin to aid distribution, then add the remaining inulin, the citrate salts, Triphala, Amla and finally matcha. Blend by geometric dilution — combining equal volumes at each step — rather than by adding small components to the full batch. Sieve to break agglomerates and blend again. Fill into moisture-barrier sachets under low humidity and seal immediately.

Intended reconstitution (as designed, not as tested): one sachet in approximately 300 mL cool water, stirred or shaken until dispersed. Proposed occasional use only; no consumption study or safety evaluation was carried out. Any future use recommendation requires regulatory and safety review.

Draft label mock-up:

MATCHA–BOTANICAL SACHET (concept) (concept) Matcha + botanical blend (no efficacy claim) Dissolve 1 sachet in 300 mL cool water. ── Not intended for evening study use ── CONTAINS CAFFEINE: ~40 mg per sachet (about one cup of green tea) Ingredients: Matcha powder, inulin, Amla extract, sodium citrate, magnesium citrate, Triphala extract, potassium citrate, Tulsi extract, Gotu kola extract (10% triterpenes), Brahmi extract (20% bacosides), Shankhpushpi extract, natural lemon-mint flavour, steviol glycosides. * NOT for daily use. Maximum 1 sachet per day. * Not proposed for individuals under 18, during pregnancy or lactation, for caffeine-sensitive individuals, or for those taking medication (possible herb-drug interactions). * Sleep beats stimulants: 7-9 hours of rest does more for memory than any all-nighter. No added sugar. Vegan. Not intended to diagnose, treat, cure or prevent any disease.

Appendix B — Cheminformatic descriptor and similarity tables

Table B1. Physicochemical descriptors of the sixteen marker compounds (PubChem structures, RDKit descriptors). MW = molecular weight (Da); TPSA = topological polar surface area (Å²); HBD/HBA = hydrogen-bond donors/acceptors; Ro5 = Lipinski Rule-of-Five violations; QED = Quantitative Estimate of Drug-likeness.

Compound	**Ingredient**	**Pillar**	**Formula**	**MW**	**XLogP**	**TPSA**	**HBD**	**HBA**	**Ro5**	**QED**
caffeine	matcha (ingredient)	Alertness	C8H10N4O2	194.2	-0.1	58.4	0	3	0	0.538
epigallocatechin gallate	matcha (ingredient)	Antioxidant	C22H18O11	458.4	1.2	197.0	8	11	2	0.212
ascorbic acid	Amla	Antioxidant	C6H8O6	176.1	-1.6	107.0	4	6	0	0.385
ellagic acid	Amla	Antioxidant	C14H6O8	302.2	1.1	134.0	4	8	0	0.216
gallic acid	Amla	Antioxidant	C7H6O5	170.1	0.7	98.0	4	5	0	0.46
catechin	Triphala	Antioxidant	C15H14O6	290.3	0.4	110.0	5	6	0	0.51
chebulagic acid	Triphala	Antioxidant	C41H30O27	954.7	0.4	447.0	13	27	3	0.055
epicatechin	Triphala	Antioxidant	C15H14O6	290.3	0.4	110.0	5	6	0	0.51
quercetin	Triphala	Antioxidant	C15H10O7	302.2	1.5	127.0	5	7	0	0.434
L-theanine	matcha (ingredient)	Calm	C7H14N2O3	174.2	-3.6	92.4	3	4	0	0.514

scopoletin	Shankhpushpi	Calm	C10H8O4	192.2	1.5	55.8	1	4	0	0.695
eugenol	Tulsi	Calm	C10H12O2	164.2	2.0	29.5	1	2	0	0.693
ursolic acid	Tulsi	Calm	C30H48O3	456.7	7.3	57.5	2	3	1	0.414
bacoside A	Brahmi	Cognition	C41H68O13	769.0	2.8	216.0	8	13	3	0.118
asiatic acid	Gotu kola	Cognition	C30H48O5	488.7	5.7	98.0	4	5	1	0.409
asiaticoside	Gotu kola	Cognition	C48H78O19	959.1	0.1	315.0	12	19	3	0.097

Table B2. Tanimoto similarity of each botanical marker compound to matcha's three signature molecules (Morgan fingerprints, radius 2, 2048 bits), sorted by similarity to EGCG.

Interpretation: The listed botanical ranges describe typical adult use rather than safety ceilings; all comparisons marked “YES” in the original source should not be read as evidence of safety. Elemental mineral estimates are provisional.

Compound	**Ingredient**	**Pillar**	**EGCG (antioxidant)**	**caffeine (alertness)**	**L-theanine (calm)**
catechin	Triphala	Antioxidant	0.453	0.034	0.017
epicatechin	Triphala	Antioxidant	0.453	0.034	0.017
gallic acid	Amla	Antioxidant	0.283	0.077	0.105
chebulagic acid	Triphala	Antioxidant	0.25	0.043	0.054
quercetin	Triphala	Antioxidant	0.188	0.073	0.035
ellagic acid	Amla	Antioxidant	0.182	0.091	0.043
scopoletin	Shankhpushpi	Calm	0.143	0.1	0.058
ascorbic acid	Amla	Antioxidant	0.136	0.064	0.087
eugenol	Tulsi	Calm	0.111	0.06	0.06
ursolic acid	Tulsi	Calm	0.094	0.056	0.07

asiaticoside	Gotu kola	Cognition	0.094	0.037	0.057
asiatic acid	Gotu kola	Cognition	0.089	0.052	0.08
bacoside A	Brahmi	Cognition	0.06	0.039	0.039

Appendix C — Dose–safety percentage table

Table C1. Per-serving amounts against reference ceilings. Minerals are compared on an elemental basis. Caffeine (40 mg, from matcha) is 32% of the 125 mg conservative adolescent reference (2.5 mg/kg/day × 50 kg) and is not listed separately below as it is contained within the matcha row.

Ingredient	**Sachet (mg)**	**Elemental (mg)**	**Reference range**	**Basis**	**% of serving**	**% of ceiling**	Safety established?
Matcha powder	1500	1500	1–2 g typical culinary serving	typical matcha serving	30.0	75.0	Not established
Amla extract	500	500	500–1000 mg/day	typical supplement dose	10.0	50.0	Not established
Triphala extract	300	300	500–2000 mg/day	typical supplement dose	6.0	15.0	Not established
Tulsi extract	200	200	300–600 mg/day	typical supplement dose	4.0	33.3	Not established
Shankhpushpi extract	150	150	~250–500 mg/day	traditional/typical dose	3.0	30.0	Not established
Brahmi (Bacopa) extract	150	150	150–300 mg/day	clinical-study dose	3.0	50.0	Not established
Gotu kola extract	150	150	60–450 mg/day	typical supplement dose	3.0	33.3	Not established
Sodium citrate	380	150	Na limit <2300 mg/day	daily dietary limit (Na)	7.6	6.5	Not established

Potassium citrate	240	100	K AI 2300–3000 mg/day	adequate intake (K)	4.8	3.3	Not established
Magnesium citrate	350	50	Mg suppl. UL 350 mg/day	supplemental UL, elemental (NIH)	7.0	14.3	Not established
Natural flavor + stevia	100	100	flavor/sweetener q.s.	self-limiting	2.0	—	—
Inulin (fiber)	980	980	well tolerated <5 g/serving	GI-tolerance guide	19.6	19.6	Not established

Appendix D — Data and reproducibility

- Structures and properties: PubChem, resolved by canonical CID (16/16 resolved).
- Descriptors, fingerprints, similarity: RDKit; Morgan fingerprints radius 2, 2048 bits; Tanimoto coefficient.
- Caffeine reference: 2.5 mg/kg/day (Ruxton, 2014) applied to a 50 kg adolescent; EFSA guidance (~3 mg/kg/day) noted for comparison.
- Accompanying data files: tanimoto_to_matcha.csv (similarity matrix), dose_safety_check.csv (dose–safety screen).
- Figures: fig1_composition.png, fig2_cheminformatics.png, fig3_dose_safety.png, fig4_positioning.png.