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A Review on Active Compounds: Chemistry Behind Tea, Coffee, Chocolate

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Abstract: This review synthesizes current scientific understanding of the principal active chemical constituents found in tea, coffee, and cocoa or chocolate, emphasizing their biochemical activities, production-related chemical transformations, comparative chemistry, and sustainable or green chemistry implications. These three globally consumed plant-derived beverages share several bioactive chemical families that contribute not only to their unique sensory profiles but also to diverse physiological effects in humans.

Tea, derived from the leaves of Camellia sinensis, is particularly rich in polyphenolic catechins, including epigallocatechin-3-gallate (EGCG), which play major roles in antioxidant and anti-inflammatory mechanisms. Alongside these, L-theanine and caffeine contribute to the neuroactive and psychostimulant properties of tea, influencing cognitive performance, relaxation, and metabolic regulation. Chemical modifications during fermentation or oxidation, such as in black and oolong teas, lead to complex products like theaflavins and thearubigins, significantly altering their bioavailability and physiological potency. Coffee, one of the most widely traded commodities, contains caffeine, chlorogenic acids, trigonelline, and roasting-derived compounds such as melanoidins and diterpenes (cafestol and kahweol). These constituents exhibit both beneficial and dose-dependent effects on cardiovascular, metabolic, and neurological health. The brewing method, degree of roasting, and bean variety critically determine the chemical profile and antioxidant capacity of coffee, intertwining sensory quality with potential health outcomes. Cocoa and dark chocolate, derived from Theobroma cacao, contain abundant flavanols (catechin, epicatechin), proanthocyanidins, and methylxanthines, primarily theobromine with minor caffeine content. Post-harvest fermenting, drying, and roasting steps induce profound structural and quantitative changes in these polyphenols, influencing their absorption and physiological activity. While moderate cocoa consumption supports vascular function and endothelial health, heavy processing can diminish its beneficial compounds.Comparative analysis reveals that polyphenols and methylxanthines across tea, coffee, and cocoa form overlapping chemical frameworks, sharing similar structural motifs and biological mechanisms involving reactive oxygen species scavenging, nitric oxide regulation, and adenosine receptor modulation. However, their in vivo effects depend on complex interactions between molecular structure, food matrix, processing, and individual genetic or microbiome-related factors. Furthermore, the review identifies promising green-chemistry strategies to enhance sustainability and bioactive preservation. These include water- or enzyme-assisted extraction, recycling of processing by-products such as coffee pulp or cocoa husks, and energy-efficient roasting technologies. Together, these insights provide an integrative chemical foundation to guide future studies on health impacts, processing optimization, and circular utilization of tea, coffee, and cocoa resources.

Keywords: Tea, Coffee, Cocoa, caffeine, Polyphenols, Methylxanthines, Chlorogenic acids ,Flavanols L-theanine, EGCG, Green chemistry.

I. INTRODUCTION

Tea, coffee, and cocoa are among the most widely consumed beverages and food products worldwide, valued not only for their sensory appeal but also for their physiological and health-promoting effects. The chemical composition of these commodities is dominated by secondary metabolites that determine their flavor, aroma, color, and biological activity. Tea (Camellia sinensis) primarily contains polyphenolic catechins such as epigallocatechin-3-gallate (EGCG), along with the amino acid L-theanine and caffeine, all of which contribute to its antioxidant, neuroactive, and metabolic functions. Coffee, derived from Coffea species, is characterized by a complex mixture of caffeine, chlorogenic acids, trigonelline, and roasting-derived compounds such as melanoidins and diterpenes. These molecules play vital roles in defining coffee's sensory profile and its reported cardiovascular and metabolic effects. Similarly, cocoa and chocolate, obtained from Theobroma cacao, are rich in flavanols such as catechin and epicatechin, proanthocyanidins, and methylxanthines like theobromine and caffeine, which are associated with vascular and neurocognitive benefits.

Despite extensive studies on each of these products individually, there remains a need for a comprehensive review that integrates their chemistry, processing transformations, and biological activities. Understanding the similarities and differences in their active compounds can provide insight into shared chemical mechanisms and guide the development of health-optimized and sustainable processing techniques. Furthermore, agricultural and industrial practices such as fermentation, roasting, and brewing significantly influence the concentration and bioavailability of key bioactive compounds. Recognizing these chemical transformations is essential for optimizing product quality and nutritional benefits.

This review aims to systematically examine the active chemical constituents of tea, coffee, and cocoa, explore their biochemical and health-related effects, analyze the impact of production and processing on compound stability, and identify comparative chemical patterns across the three. The paper also highlights emerging directions in green chemistry, focusing on sustainable extraction methods, waste valorization, and eco-friendly production strategies that preserve bioactive content. By integrating findings from recent analytical, biochemical, and processing studies, this work provides a unified chemical perspective that supports both scientific understanding and industrial application of these globally significant natural products.

II. CHEMICAL COMPOSITION

A. Overview:

Tea, coffee, and cocoa come from distinct plants but share key bioactive chemicals—polyphenols, alkaloids like caffeine and theobromine, amino acids, sugars, minerals, lipids, and aromatics—that drive their flavor, scent, and health effects. Each has a unique profile: tea rich in catechins, coffee in chlorogenic acids, cocoa in flavanols. Harvesting processes like fermentation, roasting, and alkalization transform these, breaking down compounds, creating new ones, and softening bitter notes into smoother tastes and aromas. In short, the plant supplies the raw ingredients; processing crafts the final cup.

B. Tea: Principal Compounds and Their Chemistry

Tea is chemically rich, but a few groups of compounds stand out as the main contributors to its taste, aroma, and biological effects. Tea's chemistry is dominated by polyphenols (especially flavan-3-ols known as catechins) followed by stimulating alkaloids like caffeine, the calming amino acid L-theanine, and a huge variety of volatile molecules that give each tea its signature fragrance. Minerals, sugars, and other small components round out the overall profile.

In green tea in particular, catechins form the backbone of its chemistry. The most abundant and widely discussed is EGCG (−-epigallocatechin-3-gallate), but green tea also contains EGC (−-epigallocatechin), EC (−-epicatechin) and ECG (−-epicatechin-3-gallate). EGCG is widely cited as the major bioactive tea constituent.

These compounds are responsible for antioxidant activity and astringency (i.e., slightly bitter taste of tea).During oxidation (the process used to make oolong and black tea's), many catechins polymerise to form theaflavins and thearubigins, compounds that shape the colour and taste of black tea. In essence, catechins define much of what makes tea "tea"—both in chemistry and in physiological effects.

Thus, Tea is composite of Catechins, particularly epigallocatechin gallate (EGCG), which dominate green tea's polyphenols, imparting antioxidant properties and astringency; oxidation in black and oolong teas converts them to theaflavins and thearubigins for color and taste. Caffeine (20-50 mg per cup) provides stimulation, synergizing with L-theanine for calm alertness and umami notes, while volatiles like terpenes and esters yield floral or grassy aromas. Minerals such as potassium and manganese, alongside sugars and acids, enhance complexity.

C. Coffee: Principal Compounds and Their Chemistry

Coffee beans are incredibly complex chemically. Long before they become the beverage we drink, they already contain a dense mix of alkaloids, phenolic esters, lipids, proteins, and sugars. Once roasting begins, these components react to produce the stimulating effects, bitterness, acidity, and rich aroma that define coffee. Every compound group plays a distinct role in shaping what ends up in the cup.

Chlorogenic acids are the dominant phenolic compounds in green coffee beans. Structurally, they're esters formed between caffeic acid, ferulic acid, and quinic acid, with 5-CQA (5-caffeoylquinic acid) being the most abundant form. CGAs influence both the health-related properties of coffee - especially its antioxidant capacity - and its sensory characteristics, contributing to the drink's characteristic bitterness and acidity. During roasting, CGAs don't remain intact. They break down or transform into other compounds, decreasing in total amount but giving rise to molecules that influence roasted flavor and perceived acidity.

This is why darker roasts often taste less acidic and less phenolic compared to lighter roasts.

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Caffeine is the best-known stimulant in coffee and is present at levels significantly higher than in tea on a per-cup basis. It contributes to coffee's wakefulness-promoting properties and its characteristic bitterness.

Thus, Coffee consists of Chlorogenic acids (e.g., 5-caffeoylquinic acid) which prevail in green beans, fueling antioxidant effects and bitterness that diminish during roasting into flavor precursors; caffeine (80-120 mg per 8 oz cup) and trigonelline drive stimulation and toasty aromas via thermal degradation. Diterpenes cafestol and kahweol add body in unfiltered brews, with lipids, proteins, and sugars sparking Maillard reactions for nutty, caramel volatiles like furans and pyrazines.

Caffeine content varies widely depending on the coffee species, roast level, grind size, brewing method, extraction time, water temperature & serving size. However, major nutrition and analytical sources typically cite these average values:

●Brewed coffee: ~80–120 mg per 8 oz (≈240 mL)
(Many commonly used estimates land near ~95 mg)

●Brewed black tea: ~20–50 mg per cup

D. Cocoa and Chocolate: Principal Compounds and Their Chemistry as

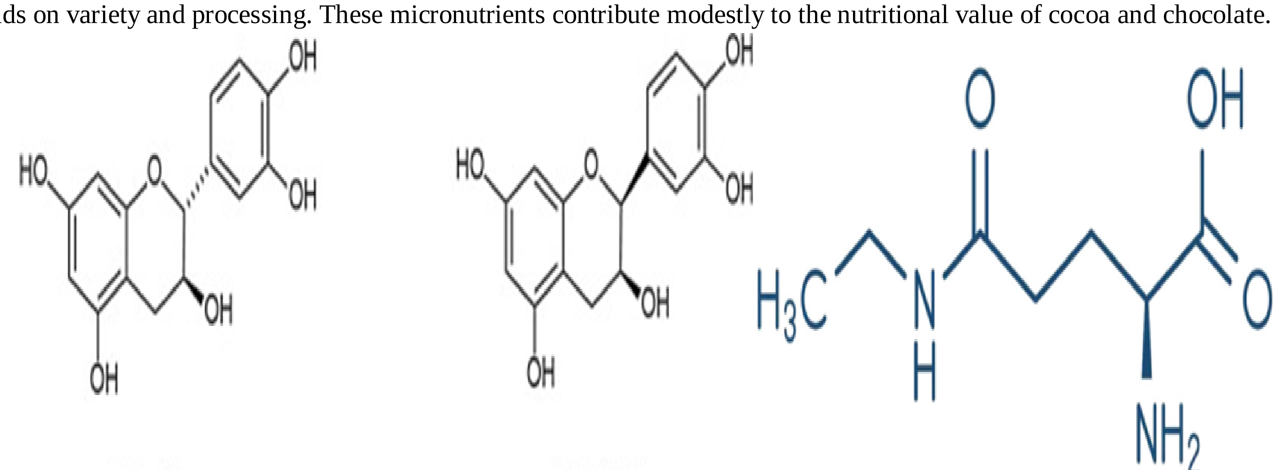
Cocoa and chocolate have a chemical profile that sets them apart from both tea and coffee. They are exceptionally rich in flavanols, larger polyphenolic structures called procyanidins, distinctive methylxanthines especially theobromine and a specialized fat known as cocoa butter. Together, these compounds shape chocolate's taste, texture, and physiological effects.

Raw cocoa beans contain high levels of monomeric flavanols, mainly (−)-epicatechin and (+)-catechin, as well as oligomeric procyanidins (which are essentially chains of these flavanol units).These polyphenols are responsible for much of cocoa's antioxidant capacity and contribute to the characteristic bitterness and astringency of unprocessed cocoa. Products with higher percentages of cocoa solids such as dark chocolate, naturally retain more of these bioactive compounds.Processing steps like fermentation, roasting, and alkalization can decrease flavanol levels, so how chocolate is made greatly influences its final chemical profile.

In contrast to coffee - which is dominated by caffeine - cocoa's primary methylxanthine is theobromine. Caffeine is also present, but in much smaller amounts.Theobromine acts as a mild stimulant in humans, generally less intense than caffeine, and contributes to cocoa's mood and alertness effects. The balance between theobromine and caffeine is one of the chemical traits that makes cocoa physiologically distinct from both tea and coffee.

Cocoa butter is one of the most defining features of chocolate. It is a unique fat composed mainly of the triglycerides of stearic acid, palmitic acid, and oleic acid.This specific combination is what gives chocolate its luxurious, smooth texture and the famous "melt-in-the-mouth" experience - solid at room temperature, yet melting just below human body temperature. Cocoa butter also influences chocolate's snap, gloss, and overall sensory quality.

Cocoa and dark chocolate supply appreciable amounts of magnesium, copper, iron and potassium, although the exact content depends on variety and processing. These micronutrients contribute modestly to the nutritional value of cocoa and chocolate.



Catechin Epicatechin

L-Theanine

Fig 1: Chemical structures of compounds present in tea, coffee and cocoa

Commodity	Compound Class	Representative Examples	Functional Role(s)	Typical Range/ Processing Sensitivity
Tea	Flavan-3-ols (catechins)	EGCG, EGC, EC, ECG	Major antioxidants; contribute bitterness/astringency; implicated in many bioactivities	High in green tea; oxidized to theaflavins/thearubigins in black tea (loss/transform with fermentation).
	Amino acids	L-theanine	Umami taste; neuromodulatory/relaxation effects (synergy with caffeine)	Varies with cultivar & shade-growth (higher in shaded tea).
	Methylxanthines	Caffeine	CNS stimulant; bitter note	Brewed tea ≈ 20–50 mg per 8-oz cup (varies).
	Volatiles	Terpenes, norisoprenoids, aldehydes	Aroma (floral, green, roasted notes)	Highly process dependent (withering, rolling, drying).
Coffee	Chlorogenic acids (CGA)	5-CQA (5-O-caffeoylquinic acid), 4-CQA, diCQA	Antioxidant, acid/bitterness contributors; health-linked bioactives	Green beans: g/100 g level; brews: very wide (common 50–200 mg/100 mL). Degrades/isomerizes with roasting.
	Alkaloids	Caffeine, trigonelline	Stimulant (caffeine); trigonelline -> nicotinic acid + aroma precursors on roasting	Brewed coffee ≈ 80–120 mg per 8-oz cup (typical ≈95 mg), extraction-dependent.
	Diterpenes (lipid)	Cafestol, kahweol	Influence serum lipids; contribute to mouthfeel	Present in oily/unfiltered brews; reduced by paper filtering.
	Maillard/ volailes	Pyrazines, furans, aldehydes	Roasted aroma and flavor	Generated during roasting; diversity and abundance rise with roast.
Cocoa / Chocolate	Flavanols & procyanidins	(−)-Epicatechin, (+)-Catechin, procyanidin oligomers	Antioxidant activity; vascular effects (endothelial function)	Highest in unalkalized dark cocoa; reduced by fermentation, roasting, Dutch processing.
	Methylxanthines	Theobromine, caffeine (minor)	Mild stimulant, diuretic, bronchodilator; major psychopharm. in cocoa = theobromine	Dark chocolate: higher theobromine content; varies by cocoa % and processing.
	Lipids (cocoa butter)	Triglycerides with stearic/palmitic/oleic acids	Texture, melting point, mouthfeel	Relatively stable to roasting; determines chocolate physical properties.

Table 1: Various Compounds present and their functional roles

III. HEALTH & BIOCHEMICAL EFFECTS

A. Overview:

Besides coffee and tea, chocolate provides bioactive compounds that benefit health and longevity through biochemical pathways. Key ones are methylxanthines (caffeine, theobromine, theophylline) and polyphenols (catechins, flavanols, chlorogenic acids). They influence neuron signaling, metabolism, vascular function, free radical balance, and inflammation for real health effects.

B. Methylxanthines and Neurological Effects:

Caffeine (in coffee and tea) and theobromine (in cocoa) block adenosine receptors that signal sleep and relaxation. Caffeine boosts alertness, focus, memory, mood, reaction time, learning, and cognition by ramping up dopamine and norepinephrine. Theobromine is milder, offering a slight mood lift and relaxation with fewer crashes.
In short, coffee hits hard and fast, while chocolate gives a gentler, calmer boost.

C. Effects on Cardiovascular Function:

Tea catechins and cocoa flavanols boost heart health mainly by increasing nitric oxide (NO), which widens blood vessels and lowers blood pressure. They also fight atherosclerosis by stopping LDL oxidation, improving blood lipids, and making vessels more elastic. Moderate caffeine helps cardiac output and blood flow, but too much can raise blood pressure and heart rate in sensitive people.

D. Metabolic and Anti-Diabetic Properties

Polyphenols in tea, coffee, and cocoa act as strong metabolic regulators—they boost insulin sensitivity, improve glucose uptake, slow carb absorption, and tweak lipid metabolism. Plus, coffee's chlorogenic acid binds to glucose in the intestines, cutting down how much gets absorbed and lowering diabetes risk.

E. Antioxidant & Anti-Inflammatory Effects

Tea catechins (like EGCG), cocoa flavanols, and coffee polyphenols are powerful antioxidants that neutralize free radicals, cut chronic inflammation, protect DNA and cell membranes, and slow age-related oxidative damage. Since chronic oxidative stress drives cancer, skin aging, neurodegenerative diseases like Parkinson’s and Alzheimer’s, and heart disease, these compounds offer strong long-term protection.

F. Effects on Gut Microbiota

(Microbiota are a diverse community of microbe species that live in and on all multicellular organisms, including plants, and can be commensal, mutualistic, or pathogenic.)
Several new studies attribute polyphenols as prebiotic-like substances, which support the growth of good bacteria in the gut, such as Bifidobacterium and Lactrobacillus.
With a healthier microbiome, the body has the benefits of the immune system balance, better digestion, lowered risk of inflammation, improved mood through the so-called brain-gut axis.

G. Possible Risks and Safety Considerations

Even when talking about natural compounds, effects will depend on the dose:

Table 2: Compounds and their health effects

Compound	Possible Risks When Excessive
Caffeine	Anxiety, insomnia, palpitations, dehydration, addiction
Theobromine	Nausea, sweating, fast heartbeat (in very high doses)
Tea polyphenols	Reduced iron absorption if taken with meals
Chocolate products	High sugar & fat in commercial chocolate reduces benefits

H. Neuroprotective and Cognitive-Enhancing Effects

Long-term consumption of polyphenols and methylxanthines from tea, coffee, and cocoa offers neuroprotection by mitigating oxidative stress, inhibiting protein aggregation, and elevating brain-derived neurotrophic factor (BDNF) to enhance memory and synaptic plasticity. Regular intake correlates with reduced risks of Alzheimer's and Parkinson's diseases through antioxidant and anti-inflammatory mechanisms.

I. Anti-Obesity Effects and Adipocyte Regulation

Active compounds in green tea, coffee, and cocoa promote fat metabolism. EGCG in green tea enhances thermogenesis and energy expenditure, chlorogenic acids in coffee favor lipid oxidation, and cocoa flavanols suppress appetite while theobromine inhibits adipocyte hypertrophy.

J. Anti-Cancer Properties

Polyphenols from tea and cocoa flavanols exert anti-cancer effects by suppressing tumor proliferation, inhibiting angiogenesis, inducing apoptosis, and protecting DNA from oxidative damage. Evidence links black and green teas to decreased risks of breast, prostate, and colon cancers.

K. Effects on the Immune System

Bioactives modulate immunity by reducing chronic inflammation via cytokine regulation, enhancing T-cells and macrophages, fostering gut microbiome health, and countering oxidative stress. Cocoa polyphenols particularly aid in combating infections.

L. Antimicrobial and Antiviral Effects

Tea catechins disrupt microbial growth in pathogens like E. coli, S. aureus, and H. pylori by targeting cell membranes and replication. Cocoa compounds exhibit antiviral activity against influenza strains, warranting further investigation.

M. Hormonal Regulation

Caffeine induces acute adrenaline and cortisol surges for energy, while polyphenols improve insulin sensitivity. Dark chocolate elevates serotonin and endorphins for mood enhancement, and tea's L-theanine reduces cortisol to promote relaxation.

N. Dental and Oral Health Effects

Catechins, caffeine, and theobromine combat oral pathogens, reduce caries and periodontal disease, strengthen enamel (with theobromine potentially outperforming fluoride), alleviate inflammation, and improve breath freshness.

O. Detoxification and Liver Protection

Tea and coffee activate hepatic phase I/II enzymes, reduce fat accumulation, shield against oxidative damage, lower non-alcoholic fatty liver disease (NAFLD) risk, and attenuate liver inflammation.

IV. CHEMICAL PROCESSES & PRODUCTION

A. Coffee – Chemical Process and Production

Processing and Chemistry Overview

Coffee chemistry centers on roasting, where Maillard and caramelization reactions between sugars and amino acids generate volatile compounds that define aroma and color. Emerging green methods, such as cold plasma treatments and eco-friendly solvents, enable bioactive and caffeine extraction from byproducts without harsh chemicals.

Tea processing emphasizes controlled enzymatic oxidation. Green tea inactivates enzymes via steaming or pan-firing to retain catechins and antioxidants, while oolong and black teas undergo partial or complete oxidation, yielding theaflavins and thearubigins that alter flavor and hue.

Changes arise primarily from physical factors like temperature, time, and moisture, bypassing chemical additives.

Cocoa processing begins with microbial fermentation of pulp sugars into ethanol and acids, which penetrate beans and initiate biochemical shifts. Drying and roasting then produce flavor precursors that evolve into chocolate's signature aroma via Maillard reactions.

1) Major Steps in Production:

a) Harvesting and Fermentation:

After harvesting, coffee cherries are fermented to remove the mucilage (sticky pulp).Fermentation involves microbial activity (yeasts, bacteria) that breaks down sugars and pectins. This step influences the acidity and final aroma of coffee.

b) Roasting (Main Chemical Step):

enzymes

Pectin ----------------------> Simple sugars + Organic acids

Roasting is where most chemical reactions occur — typically between 180°C–240°C for 10–15 minutes.

Key chemical reactions:

- Maillard Reaction

Between amino acids and reducing sugars → produces melanoidins (brown pigments) and volatile aromatic compounds.

- Caramelization

Breakdown of sugars at high temperature → caramel-like flavors and browning.

Fig 2: Key chemical reactions for coffee

2) Decomposition of Trigonelline

Converts into nicotinic acid (vitamin B_3) and volatile compounds contributing to aroma.

3) Degradation of Chlorogenic Acid

Produces caffeic acid, quinic acid, and antioxidants.

- Brewing:

When hot water passes through ground coffee:

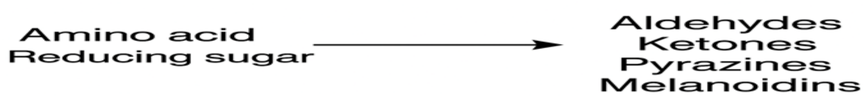


Fig 3: Chemical reaction for degeradation of amino acids

- Caffeine, acids, and aroma oils are extracted (mostly polar compounds).
- Extraction depends on temperature, grind size, and time.
- pH of brewed coffee: 4.5–5.0 (mildly acidic).

B. Tea – Chemical Process and Production

1) Overview

All teas (green, oolong, black) come from Camellia sinensis. The difference lies in the level of oxidation (fermentation) of tea leaves after harvesting.

2) Steps in Tea Production:

a) Withering

- Fresh leaves lose moisture (up to 50–60%).
- Enzymatic activity begins, proteins and lipids break down, releasing volatile precursors.

b) Rolling

- Cell walls are broken, releasing enzymes like polyphenol oxidase (PPO).
- These enzymes start oxidation of polyphenols.

c) Oxidation / Fermentation (Main Chemical Step)

- Green Tea: Heating (pan-firing or steaming) inactivates PPO → no oxidation → catechins remain intact.
- Black Tea: Leaves are left to oxidize (2–3 hours). Catechins oxidize to form complex polyphenols.

Major oxidation reactions:

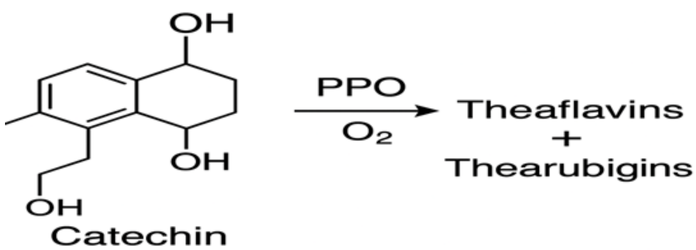


Fig 4: Oxidation reaction of compounds present in tea and coffee

- Theaflavins: contribute golden color and briskness.
- Thearubigins: responsible for dark color and body.

d) Firing / Drying

- Heated at 80–90°C to stop oxidation and remove moisture.
- Formation of volatile terpenes and aldehydes adds aroma.

C. Cocoa / Chocolate – Chemical Process and Production

1) Overview

Cocoa beans from Theobroma cacao undergo fermentation, drying, roasting, and conching.
Each step drives a set of chemical transformations responsible for chocolate's flavor, color, and texture.

2) Major Steps:

a) Fermentation:

- It takes 5–7 days. Yeasts, lactic acid bacteria, and acetic acid bacteria convert sugars to acids and alcohols:

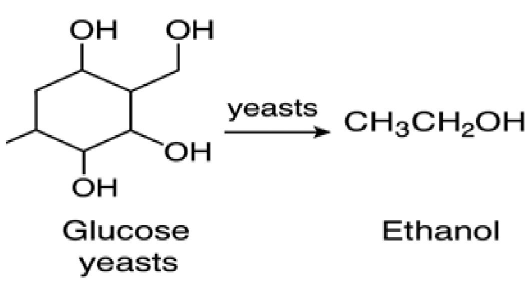


Fig 5 : Fermentation of glucose into ethanol

Acids diffuse into the beans, killing the embryo and activating enzymes that break down proteins and polyphenols.

- Polyphenols oxidize and polymerize → reduction of bitterness and astringency.

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- Precursors for flavor compounds are formed.

b) Drying:
- Reduces moisture content (from 60% to 7%).
- Stops microbial activity.
- Non-enzymatic browning (mild Maillard reaction) may start

c) Roasting (Main Chemical Step):
- Performed at 120–150°C.
- Maillard reactions between amino acids and sugars produce pyrazines, aldehydes, and esters — key aroma molecules.
- Caramelization of sugars deepens color and flavor.
- Acids volatilize, reducing sourness.

Important reaction:

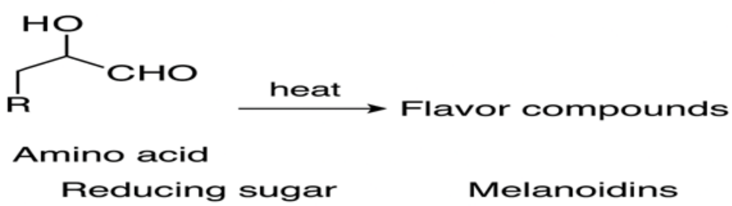

Fig 6: Action of heat on amino acids

d) Grinding & Conching:
- Roasted nibs are ground into a paste (chocolate liquor).
- Conching (mixing at 60–80°C) smooths texture and allows oxidation of residual volatiles.
- Addition of sugar, milk, and cocoa butter finalizes flavor.

V. ACTIVE COMPOUNDS: CHEMISTRY AND NATURAL PRODUCT ORIGINS

A. Tea: Catechins and EGCG
Green tea from Camellia sinensis contains high levels of polyphenolic catechins, particularly epigallocatechin-3-gallate (EGCG), a flavan-3-ol with multiple hydroxyl groups and a gallate ester. EGCG supports antioxidant, anti-inflammatory, and cancer-preventive effects through the plant's phenylpropanoid pathway. Its concentrations vary by cultivar, harvest timing, and processing, with green tea methods minimizing oxidation to preserve catechins. The compound's polarity suits extraction in aqueous ethanol, while its heat sensitivity requires gentle conditions.

B. Coffee: Caffeine and Chlorogenic Acids (CGAs)
Coffee beans from Coffea species feature methylxanthines like caffeine—synthesized from xanthosine—and chlorogenic acids (CGAs), mainly caffeoylquinic acids, which provide strong antioxidant properties in raw beans. Roasting partially breaks down CGAs, generating new derivatives. Both compounds exhibit moderate polarity, dissolving well in water or ethanol. Spent coffee grounds emerge as a sustainable source for CGA recovery and industrial applications.

C. Cocoa/Chocolate: Theobromine and Flavan-3-ols
Cocoa from Theobroma cacao is abundant in methylxanthines (primarily theobromine, plus minor caffeine) and flavan-3-ols like (-)-epicatechin and procyanidins, underpinning its health benefits.

Theobromine shares structural similarities with caffeine but has unique substitution patterns affecting bioactivity. Fermentation, drying, and roasting significantly reduce flavanol content, emphasizing the need for optimized processing. By-products such as pod husks and shells offer potential for eco-friendly extraction of these bioactives.

VI. PRINCIPLES OF GREEN EXTRACTION APPLIED TO THESE NATURAL PRODUCTS

Green extraction (conceptualized alongside the 12 principles) aims to minimize or eliminate hazardous solvents, lower energy consumption, increase selectivity/yield, and valorize waste streams. Practical green extraction routes include:

1) Ultrasound-assisted extraction (UAE): Enhances mass transfer, lowers temperature and solvent use; widely effective for CGAs and flavanols; preserves thermolabile EGCG.
2) Microwave-assisted extraction (MAE): Rapid heating and shorter extraction times; reported to increase methylxanthine yields from cocoa byproducts.
3) Supercritical CO_2 ($scCO_2$): Non-toxic, tunable solvent for nonpolar to mildly polar compounds (often used with cosolvents for polar species); excellent for defatting and selective methylxanthine/fat removal from cocoa/coffee residues. $scCO_2$ leaves no solvent residues and can be energy-efficient when integrated with heat recovery.
4) Natural deep eutectic solvents (NADES) and ionic liquids (ILs): Designer polar solvents with tunable properties; NADES + UAE/MAE combinations enrich CGAs and methylxanthines while reducing volatile organic solvent use; ionic liquids with MAE have shown increased CGA yields in lab studies (careful solvent selection and recyclability are essential).

Comprehensive comparisons demonstrate that UAE (with ethanol/water or NADES) and MAE often outperform conventional maceration in yield, time and energy consumption for these classes of compounds. Valorization of residues (SCG, cocoa husk) using these technologies reduces waste and creates circular economy opportunities.

VII. REPRESENTATIVE GREEN WORKFLOWS

A. For Tea (EGCG-rich extracts)

1) Feedstock: Freshly milled green tea leaves or matcha.
2) Solvent: 50–70% ethanol in water (food-grade), or NADES when biocompatible formulations are desired.
3) Method: Low-temperature UAE (room temp to 40°C) with optimized sonication time (5–30 min) and solid:liquid ratios; optional MAE for rapid scaling.
4) Purification: Adsorption on food-grade resins or membrane filtration (ultrafiltration/nanofiltration) rather than repeated liquid-liquid extractions.
5) Rationale: Lower temperatures protect EGCG; ethanol/water is safe and recyclable; adsorption/membrane steps avoid large solvent volumes.

B. For Coffee (CGA and caffeine)

1) Feedstock: Spent coffee grounds (valorization) or green beans.
2) Solvent: Aqueous ethanol or NADES; simple ethanol enables food-grade extracts.
3) Method: UAE or pressurized liquid extraction (PLE) for high CGA yield; MAE can be used for faster throughput. Use lower temperatures to preserve CGAs.
4) Purification: Resins or preparative chromatography if high purity is required; otherwise concentrate and spray-dry for nutraceutical powders.
5) Rationale: UAE maximizes yield with low solvent and energy use; valorizing SCG reduces waste streams.

C. For Cocoa (flavanols and theobromine)

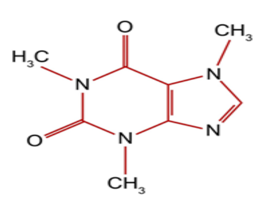

Fig 7: Structure of flavanols in cocoa

1) Feedstock: Cocoa nibs, shells or pod husk (valorization).
2) Solvent: Ethanol/water or moderate polarity NADES; $scCO_2$ for defatting step with subsequent polar extraction for flavanols.
3) Method: $scCO_2$ extraction to remove fat and nonpolar impurities (recoverable CO_2), followed by UAE/MAE for flavanols and theobromine from defatted material.
4) Purification: Adsorption/desorption and membrane concentration; encapsulation for stability (green encapsulants).
5) Rationale: Combined $scCO_2$ + UAE preserves flavanols, reduces solvent residues, and produces clean extracts from agro-waste.

VIII. ENVIRONMENTAL AND ECONOMIC CONSIDERATIONS

Green methods reduce volatile organic solvent use and can lower energy consumption via shorter processing times, but trade-offs exist: equipment ($scCO_2$, MAE reactors) requires capital investment, and solvent recycling or NADES recovery strategies must be designed. Life-cycle assessment and techno-economic analysis are recommended when scaling to ensure net environmental benefit. Valorizing residues creates additional revenue streams and reduces disposal impacts.

IX. CHALLENGES AND RESEARCH GAPS

1) Scalability: Many green extraction studies are lab-scale; scalable continuous processes, energy recovery and solvent recycling need demonstration.
2) Solvent recovery & toxicity: NADES/ILs require validated recovery and toxicity profiles for food use.
3) Compound stability: EGCG and some flavanols are oxidation-sensitive; process conditions and downstream storage/encapsulation must be optimized.
4) Standardization: Variability in feedstock (cultivar, processing) complicates reproducible extract composition; robust process controls are needed.

X. CONCLUSIONS AND RECOMMENDATIONS

Applying green chemistry to extraction and processing of bioactives from tea, coffee and cocoa is both feasible and beneficial.Here are some practical steps for researchers and industries.

1) Prioritize low-temperature, solvent-efficient techniques (UAE, MAE) with food-grade solvents (ethanol/water, NADES where food-safe).
2) Use $scCO_2$ for defatting or nonpolar separation steps when solvent-free extracts are required.
3) Valorize agro-residues (spent coffee grounds) as feedstocks to improve economics and reduce waste.
4) Integrate purification techniques that minimize solvent exchange (resins, membranes) and design for solvent recycling.

XI. SUGGESTED EXPERIMENTAL PROTOCOL — EGCG EXTRACT VIA UAE (BENCH SCALE)

1) Materials: green tea leaves (2 g), ethanol 50% v/v (40 mL food grade), ultrasound bath (40 kHz).
2) Procedure: Add leaves + solvent to 50 mL tube; sonicate at 35°C for 15 min; cool; centrifuge 5 min at 3000×g; collect supernatant; repeat once; combine extracts; concentrate under reduced pressure at ≤40°C; purify on food-grade macroporous resin and elute with 70% ethanol; dry under vacuum or spray-dry with maltodextrin if powder desired.

XII. COMPARATIVE CHEMISTRY

A. *Botanical Origin and Processing:*

Tea from Camellia sinensis leaves undergoes oxidation to yield catechins in green varieties or theaflavins/thearubigins in black/oolong teas. Coffee seeds from Coffea seeds transform via roasting, sparking Maillard reactions among phenolics, sugars, and proteins for aroma. Cocoa from Theobroma cacao seeds relies on fermentation and roasting to reshape polyphenols and generate flavor precursors.

B. *Chemical Composition and Molecular Families of Active Compounds:*

Tea emphasizes catechins like EGCG, water-soluble antioxidants prone to polymerization. Coffee features chlorogenic acids that degrade during roasting into melanoidins, sustaining antioxidant capacity. Cocoa prioritizes epicatechin, procyanidins, and theobromine, modulated by its lipid-rich matrix for altered solubility and absorption.

C. *Concentrations and Serving Context*

A typical 240 mL serving of coffee delivers the most caffeine (approximately 80–120 mg), while tea provides between 20–50 mg per serving. Cocoa generally contains less caffeine but a higher concentration of theobromine. Polyphenol content varies with processing: green tea retains high levels of monomeric catechins, green coffee beans have abundant chlorogenic acids which diminish after roasting, and cocoa flavanol content depends on fermentation and alkalization treatments.

Aspect	Tea	Coffee	Cocoa
Primary Polyphenol	Catechins/EGCG	Chlorogenic acids	Flavanols/Procyanidins
Main Alkaloid	Caffeine (20-50 mg/240 mL)	Caffeine (80-120 mg/240 mL)	Theobromine
Processing Impact	Oxidation forms polymers	Roasting yields melanoidins/volatiles	Fermentation reduces flavanols

Table 2: Comparison of chemical processing of tea, coffee and cocoa

D. Processing Effects and Chemical Reactivity

1) Tea – Oxidation

Enzymatic oxidation during withering converts catechins into theaflavins and thearubigins, which influence tea's color, taste, astringency, and antioxidant properties.

2) Coffee – Roasting and Maillard Chemistry

Roasting reduces chlorogenic acids but generates volatile aroma compounds and melanoidins through Maillard reactions. Even though CGAs decline, melanoidins and other fragments help maintain antioxidant capacity.

3) Cocoa – Fermentation and Alkalisation

Fermentation reduces native polyphenols and forms flavor precursors, while alkalization (Dutch processing) further decreases flavanol content but reduces bitterness. Minimally processed dark cocoa maintains the highest flavanol levels.

E. Bioavailability and Metabolic Fate

1) Tea Catechins

Catechins are partly absorbed in the small intestine and circulate mainly as conjugated forms. Gallated catechins like EGCG show lower absorption but may have notable effects in the gut.

2) Coffee CGAs

Only a small fraction of CGAs is absorbed directly. Most are broken down by intestinal microbes into smaller phenolic acids, which become the main circulating metabolites.

3) Cocoa Flavanols and Procyanidins

Cocoa epicatechin is well absorbed, whereas larger procyanidins are metabolized by intestinal microbes into bioactive phenolic acids. Cocoa's fat matrix also influences absorption and transport of these compounds.

F. Sensory Profiles and Functional Implications

Chemical differences explain the distinct taste, aroma, and mouthfeel of tea, coffee, and cocoa. Coffee's aroma is dominated by volatiles formed during roasting. Tea offers flavors ranging from floral to grassy to earthy depending on oxidation. Cocoa combines roasted notes with richness from cocoa butter. The polyphenols contribute bitterness and astringency, which affect consumer preference. Although all possess antioxidant properties in vitro, their differing metabolic fates result in unique physiological effects.

G. *Methylxanthine Alkaloid Profiles*

Tea and coffee primarily contain caffeine, with tea delivering less per serving despite similar dry-weight levels in leaves. Coffee features high caffeine plus chlorogenic acids, while cocoa is theobromine-dominant with moderate caffeine. Caffeine drives CNS stimulation in tea/coffee; theobromine in cocoa offers milder CNS effects but stronger cardiac/smooth-muscle actions.

H. *Polyphenols and Antioxidant Characteristics*

Tea is rich in flavan-3-ols for radical scavenging and metal chelation. Coffee's key polyphenols—chlorogenic and hydroxycinnamic acids—retain antioxidant activity post-roasting. Cocoa provides flavan-3-ols and procyanidins with anti-inflammatory benefits.

I. *Macronutrient Composition and Nutritional Relevance*

Tea infusions are low-calorie, mainly polyphenols, caffeine, amino acids, and trace minerals. Coffee adds carbohydrates, lipids, and diterpenes like cafestol/kahweol. Cocoa is energy-dense due to high fat (cocoa butter), with lipids enhancing flavanol/sugar/protein delivery.

J. *Coffee: Green Chemistry and Natural Processing*

Green chemistry in coffee includes using cold plasma technology, which modifies ground coffee beans without solvents or additives, reducing chemical waste and improving desirable aroma compounds such as aldehydes, furans, and pyrazine compounds. Sustainable valorization methods also convert coffee byproducts (pulp, husk, silverskin, spent grounds) into value-added products using biological and chemical green processes, such as composting and biogas production. Natural extraction methods like deep eutectic solvents enable caffeine extraction from coffee pulp with less environmental impact.
Key natural processes in coffee are given below:

- Use of indigenous biological controls for pests instead of synthetic pesticides.
- Biological fermentation and traditional sun-drying of green beans.
- Valorization of coffee waste for energy and soil improvement.

K. *Cocoa: Natural Processing and Sustainability*

Cocoa bean processing relies on natural fermentation, where the beans and pulp are piled and covered with banana leaves to kickstart anaerobic fermentation by indigenous yeasts and bacteria. This process breaks down sugars into ethanol and acids, producing unique chocolate flavors and allowing natural microbial succession. Sun drying is used after fermentation for moisture reduction with minimal energy use.

L. *Cocoa processing stages:*

- Natural fermentation (5–7 days) with indigenous microorganisms.
- Sun drying for preservation and quality.
- Biochemical changes during fermentation and drying that develop flavor precursors.

M. *Tea: Green Chemistry Innovations and Natural Methods*

Tea processing, especially for green tea, uses natural enzyme deactivation (pan-firing or steaming) to prevent oxidation and preserve polyphenols. This avoids chemical additives and conserves the antioxidant properties of catechins and other phenolic compounds. Green chemistry is also seen in the use of phytochemicals in tea for nanoparticle synthesis and stabilization, replacing hazardous chemicals with natural tea extracts.

N. *Traditional tea production steps:*

- Withering (moisture reduction with minimal energy).
- Steaming or pan-firing to deactivate enzymes naturally and preserve color.
- Oxidation/fermentation for black tea, controlled by natural microbial and enzymatic activity

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REFERENCES

[1] Anastas PT, Warner JC. Green Chemistry: Theory and Practice. 1998. (ACS summary of 12 principles). American Chemical Society

[2] Chemat F, Vian MA, Cravotto G. “Green Extraction of Natural Products: Concept and Principles.” Int J Mol Sci. 2012. (Foundational green extraction review). Green Extraction of Natural Products

[3] Nagle DG, Ferreira D, Zhou YD. “Epigallocatechin-3-gallate (EGCG) — review.” PMC/NCBI review. (EGCG chemistry and bioactivity).https://pmc.ncbi.nlm.nih.gov/articles/PMC2903211/?utm

[4] Capasso L. “Epigallocatechin Gallate (EGCG): Pharmacological Properties” Molecules 2025review. https://www.mdpi.com/1420-3049/30/3/654?utm

[5] Ramadan M. “Optimizing Chlorogenic Acid Extraction From Spent Coffee Grounds” (Systematic review, 2025). https://pmc.ncbi.nlm.nih.gov/articles/PMC12203399/?utm

[6] Syakfanaya AM, et al. “NADES-UAE for caffeine and CGA enrichment.” Pharmacognosy Journal 2019. https://www.phcogj.com/article/825?utm

[7] González-Alejo FA, et al. “Supercritical Fluid Extraction of Fat and Caffeine with Theobromine Retention in the Cocoa Shell.” Processes 2019. https://www.mdpi.com/2227-9717/7/6/385?utm

[8] Belwal T., et al. “Bioactive Compounds from Cocoa Husk: Extraction” Frontiers/PMC 2022. https://pmc.ncbi.nlm.nih.gov/articles/PMC8947495/?utm

[9] Alvarez-Yanamango E., et al. “A Comprehensive Review of Green Extraction Methods and Encapsulation of Theobromine from Cocoa Bean Shells” Food Engineering Reviews 2025. https://www.researchgate.net/publication/394878138_A_Comprehensive_Review_of_the_Development_of_Green_Extraction_Methods_and_Encapsulation_of_Theobromine_from_Cocoa_Bean_Shells_for_Nutraceutical_Applications?utm

[10] Akpabli-Tsigbe NDK, et al. “Ultrasonic-assisted extraction of bioactive caffeoylquinic acids” PMC Khan N, Mukhtar H. Tea polyphenols for health promotion. https://pmc.ncbi.nlm.nih.gov/articles/PMC3220617/?utm. Wang Q, et al. Coffee, tea, and cocoa in obesity prevention. https://pmc.ncbi.nlm.nih.gov/articles/PMC11061710/?utm Makiso MU, et al. Bioactive compounds in coffee and their role in lowering the risk of disease. Katz DL, et al. Cocoa and Chocolate in Human Health and Disease.https://pmc.ncbi.nlm.nih.gov/articles/PMC4696435/?utm Hermund DB, et al. Fate of flavonoids and theobromine in cocoa beans during roasting. AOCS / DTU (2024–2025). Aocs Online Library+1

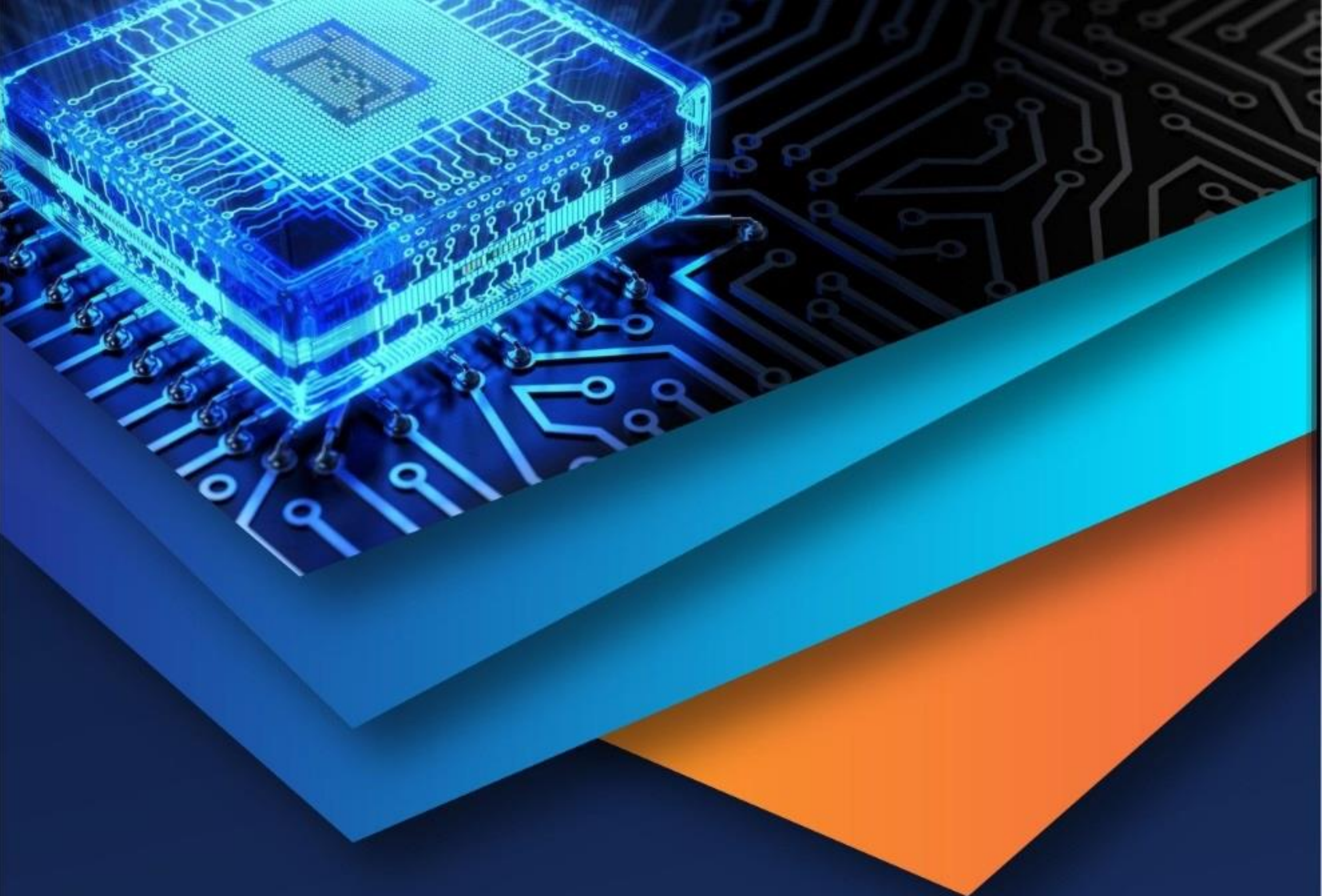
[11] Harvard T.H. Chan / Mayo Clinic / EFIC pages on typical caffeine amounts (for cup-level estimates). Wang Q., et al. (2024). Coffee, tea, and cocoa in obesity prevention. https://pmc.ncbi.nlm.nih.gov/articles/PMC11061710/?utm

[12] Yashin A., et al. (2013). Antioxidant and antiradical activity of coffee. https://pmc.ncbi.nlm.nih.gov/articles/PMC4665516/?utm

[13] Del Rio D., et al. (2010). Bioavailability of coffee chlorogenic acids and green tea flavan-3-ols. PMC — human metabolic fate and conjugation. https://pmc.ncbi.nlm.nih.gov/articles/PMC3257704/?utm

[14] La Mantia A., et al. (2023). Effect of cocoa roasting on chocolate polyphenols. PMC - processing impacts on cocoa polyphenols. https://pmc.ncbi.nlm.nih.gov/articles/PMC9952295/?utm

[15] Jalil A. M. M., & Ismail A. (2008). Polyphenols in cocoa and cocoa products. PMC - cocoa polyphenols and processing losses. https://pmc.ncbi.nlm.nih.gov/articles/PMC6245372/?utm



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