

RESEARCH MONOGRAPH . COMPOUND PROFILE

Theobromine

*The principal methylxanthine in cacao
with milder CNS effects than caffeine and
stronger peripheral vasodilation.*

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ABSTRACT

Theobromine (3,7-dimethylxanthine; CAS 83-67-0) is the principal methylxanthine in cacao (*Theobroma cacao*), with smaller amounts in tea. The compound has milder CNS effects than caffeine but stronger peripheral cardiovascular effects (vasodilation, modest blood pressure reduction). Mechanism is the same general class as caffeine (adenosine antagonism, PDE inhibition) but with different relative potencies at the various adenosine receptor subtypes. Pharmacokinetics: plasma half-life 7 to 12 hours (longer than caffeine). Doses are typically 200 to 700 mg from supplements or chocolate. The compound is also notable for toxicity in dogs and other non-human mammals due to slower metabolism.

1. 1. Compound Identification

Theobromine is described as methylxanthine. The principal methylxanthine in cacao with milder CNS effects than caffeine and stronger peripheral vasodilation.

1.1. 1.1 Class summary

Methylxanthine

1.2. 1.2 Subtitle

The principal methylxanthine in cacao with milder CNS effects than caffeine and stronger peripheral vasodilation.

2. 2. Abstract

Theobromine (3,7-dimethylxanthine; CAS 83-67-0) is the principal methylxanthine in cacao (*Theobroma cacao*), with smaller amounts in tea. The compound has milder CNS effects than caffeine but stronger peripheral cardiovascular effects (vasodilation, modest blood pressure reduction). Mechanism is the same general class as caffeine (adenosine antagonism, PDE inhibition) but with different relative potencies at the various adenosine receptor subtypes. Pharmacokinetics: plasma half-life 7 to 12 hours (longer than caffeine). Doses are typically 200 to 700 mg from supplements or chocolate. The compound is also notable for toxicity in dogs and other non-human mammals due to slower metabolism.

3. Mechanism of Action

Adenosine antagonist; milder CNS effects than caffeine, stronger peripheral vasodilation.

The mechanistic profile described above represents the consensus position from peer-reviewed literature where available; for compounds with sparse formal characterization, this section reflects vendor-grade reports and structurally-related class pharmacology and should be interpreted with appropriate caution.

4. 4. Pharmacokinetics and Routes of Administration

Pharmacokinetic data are summarized within the abstract for compounds with formal Phase 1 records. Compounds without published human pharmacokinetic studies are noted as such; investigators should treat the absence of data as a research limitation.

5. 5. Reported Research Dose Ranges

200 to 700 mg from supplements.

Doses are scaled from clinical use where the compound is approved as a medicine, from Phase 2/3 trials where development advanced, or from rodent dose-response data scaled by allometric assumptions where the compound has no human clinical record. Investigators should treat dose ranges from research-chemical-grade vendors as starting points for their own pharmacokinetic and tolerability characterization rather than validated dosing recommendations.

6. Sourcing and Quality Verification

Investigators should obtain analytical confirmation of identity (mass spectrometry; for peptides, additionally amino acid analysis or N-terminal sequencing) and purity (HPLC area-percent, ideally greater than 95 percent) on every lot. Vendor certificates of analysis vary in quality; third-party analytical confirmation through independent laboratories (e.g., Janoshik Analytical, Anabolic Lab) is the gold standard for research-grade peptides and small molecules.

For compounds with established pharmaceutical-grade marketing in any jurisdiction, sourcing from the marketed product (where legal and accessible) provides the highest quality assurance.

7. 7. Reconstitution and Handling

Peptides should be reconstituted in bacteriostatic water or sterile water for injection in the volume appropriate to the desired concentration; lyophilized peptides should be allowed to come to room temperature before reconstitution to minimize precipitation. Reconstituted peptides should be stored refrigerated and used within the timeframe specified by the manufacturer (typically 14 to 30 days for bacteriostatic water reconstitutions, shorter for sterile water).

Small molecules: storage conditions vary by compound; consult the certificate of analysis for the specific product. Most are stable at room temperature in dry, dark conditions; oxidation-sensitive compounds (e.g., catecholamine precursors) require cool storage and protection from light.

8. 8. Stack Interaction Considerations

Investigators combining this compound with other research substances should consider receptor-level interactions (additive effects at shared targets), enzyme-level interactions (CYP-mediated drug-drug interactions where applicable), and pharmacodynamic interactions (additive sedation, additive serotonergic activity, additive hemodynamic effects).

The stack interaction section in published monographs of well-characterized compounds is necessarily incomplete for any specific combination; investigators should treat novel combinations with elevated caution and titrate gradually.

9. 9. References

1. Smit HJ. Theobromine and the pharmacology of cocoa. Handb Exp Pharmacol 2011.

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