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CHEMICAL PROFILING OF FLOWERS FROM THE PAULOWNIA TOMENTOSA × P. FORTUNEI HYBRID (SHAN-TONG) GROWN IN UZBEKISTAN (FERGANA VALLEY)

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Abstract: Recent reviews and primary studies show that Paulownia flowers are rich in flavonoids (including prenylated/C-geranylated types), phenylpropanoid glycosides, terpenoids, lignans/iridoids, polysaccharides, and volatile components. For the hybrid Shan-Tong (P. tomentosa × P. fortunei), steam-distilled flower oil contains >30 constituents with lanostane-type derivatives predominating; in P. fortunei flowers, newly described C-geranylated flavonoids (paulownione D–G) have been isolated and structurally confirmed. Building on these advances, we propose a harmonized sampling–extraction–fractionation–identification workflow (GC-MS, HPLC-DAD-MS/MS, HR-MS, and 1D/2D-NMR) tailored to Uzbekistan's Fergana Valley. We also outline testable hypotheses on climate-driven variation and provide a 6-month workplan from field sampling to manuscript.

Keywords: Paulownia, Shan-Tong hybrid, C-geranylated flavonoids, prenylflavonoids, verbascoside, volatile oil, GC-MS, HPLC-MS, NMR.

Introduction. Paulownia species are increasingly studied for bioactive metabolites across multiple classes. Authoritative reviews for P. tomentosa and related taxa list flavonoids (including prenylated/C-geranylated), lignans, phenolic glycosides, terpenoids, phenolic acids, and more. In 2023, a comprehensive review consolidated the chemical composition and health-related prospects of Paulownia flowers; in 2024, a dedicated study reported the volatile profile of Shan-Tong flower oil. These data motivate a region-specific chemical survey under local agronomic conditions.

Notable leads from literature. (i) Shan-Tong flower essential oil (steam distillation; ~0.013% v/w) comprised ~31 compounds with 3-acetoxy-7,8-epoxylanostan-11-ol as a major constituent. (ii) P. fortunei flowers yielded four new C-geranylated flavonoids (paulownione D–G), expanding the characteristic Paulownia prenyl/C-geranyl chemotype. (iii) C-geranylated/prenylated flavonoids such as diplacone and mimulone frequently underpin the genus' reported bioactivities (antioxidant, anti-inflammatory, antibacterial/antiproliferative), warranting marker-guided assays.

Objectives. Establish a full chemical profile of Shan-Tong flowers grown in the Fergana Valley (volatiles, phenolics/flavonoids—including prenyl/C-geranyl types—phenylpropanoid glycosides, iridoids, polysaccharides, and lipid fractions).

Isolate structurally interesting constituents and confirm structures (HR-MS; 1D/2D-NMR).

Quantify key markers and explore seasonal/site effects.

Screen core bioactivities (DPPH/ABTS, antibacterial MIC; optional MTT).

Materials and Methods (fit for Uzbek field and lab conditions)

1) Sampling and Post-harvest Handling

Sites: ≥3–5 plantations across Andijan/Fergana; n = 10–15 trees per site.

Timing: early full bloom (day 2–3), 08:00–10:00 to preserve volatiles.

Drying: shade pre-dry (2–3 h), then 40 °C convection under reduced pressure or lyophilization; fix one method across the study for comparability.

2) Volatile Fraction → GC-MS

SPME route: PDMS/DVB fiber, 40 °C, 30 min exposure; injector 250 °C, splitless; EI, m/z 40–500; NIST library match (≥85% score).

Steam-distillation route: collect essential oil; record yield (v/w).

Targeted confirmation: search for 3-acetoxy-7,8-epoxylanostan-11-ol and related lanostane-type signals reported for Shan-Tong.

3) Phenolics/Flavonoids → HPLC-DAD-MS/MS

Extraction: 70–80% EtOH (or MeOH):water, 1:20–30 (w:v), ultrasound 30–45 min at 25–30 °C; filter (0.45 µm); concentrate.

Partition (optional): water/EtOAc to enrich low-MW phenolics; Sephadex LH-20 for polymeric phenols if needed.

Chromatography: C18 (100×2.1 mm, 1.7 µm), A = H_2O+0.1% HCOOH, B = ACN+0.1% HCOOH; 5→95% B over 25 min; DAD 254/280/330 nm; ESI±, m/z 100–1200.

Quantification: external calibration (e.g., luteolin, apigenin, quercetin, rutin, verbascoside), 7-point curves ($R^2 > 0.995$).

4) Prenyl/C-geranylated Flavonoids (Targeted Panel & Isolation)

Markers to monitor: diplacone, mimulone, paulownione D–G (plus known geranyl congeners).

Enrichment: $CHCl_3$/n-BuOH extracts → silica gel gradient (hexane/EtOAc/MeOH) → LH-20 → semi-prep HPLC.

ID: HR-ESI-MS; ^1H, ^{13}C, HSQC, HMBC (structure checks against literature spectra).

5) Polysaccharides (if flower matrix is investigated)

Hot-water extraction (80–90 °C) → ethanol precipitation (4 vol) → dialysis (MWCO 3.5–8 kDa) → lyophilization.

Monosaccharide profile: 2 M TFA hydrolysis → PMP-HPLC or HPAEC-PAD. (Useful for total profile completeness, though the main novelty is expected in prenyl/C-geranyl phenolics.)

6) Bioactivity Screens (fit-for-purpose)

Antioxidant: DPPH/ABTS (IC_{50}).

Antibacterial: MIC vs. reference strains; include MRSA for comparability with diplacone/mimulone literature.

Cytotoxicity (optional): MTT on HEK293/HepG2 for extract safety profiling.

7) QA/QC and Statistics

LOD/LOQ: $3.3\sigma/S$ and $10\sigma/S$; recovery 80–120% via matrix spikes; precision RSD ≤ 15%.

Replicates: $n \geq 3$ per site; use one-way or two-way ANOVA (site × time), Tukey post-hoc; visualize with volcano/heatmaps of marker panels.

Expected Findings and Working Hypotheses

Composition classes: We expect flavonoids (including prenyl/C-geranyl), phenylpropanoid glycosides (e.g., verbascoside), terpenoids, lignans/iridoids, polysaccharides, and a characteristic volatile profile, in line with Paulownia flower literature.

Chemotaxonomic anchors: C-geranylated flavonoids (paulownione series; diplacone/mimulone) are high-value markers for Shan-Tong profiling and will guide isolation priorities.

Volatiles: Expect a lanostane-rich essential-oil fingerprint similar to the 2024 Shan-Tong report; Fergana environmental conditions may shift relative abundances—worth documenting across sites and harvests.

Bioactivity linkage: If diplacone/mimulone are present at meaningful levels, antibacterial (incl. MRSA) and antiproliferative readouts are plausible, justifying targeted bioassays.

Six-Month Workplan (deliverables aligned)

Month 1: Finalize SOPs; site permissions; pilot harvest; stability checks for drying protocols.

Month 2: Optimize solvent/ultrasound extraction; begin GC-MS SPME/SD runs.

Month 3: HPLC-DAD-MS/MS screening; set marker panels; start semi-prep fractions.

Month 4: HR-MS + 1D/2D-NMR on priority fractions; spectral assignment package.

Month 5: DPPH/ABTS, MIC (incl. MRSA), optional MTT; complete QA/QC (recoveries, precision).

Month 6: Statistics, figures, supplementary datasets (chromatograms/spectra), manuscript draft.

Practical Reporting Template (abbreviated)

Sampling log: GPS/site, date, phenophase, drying method/time.

Volatiles: yield (v/w), top-10 constituents (% TIC), Kovats indices, match factors.

Phenolics: target list with RT, $[M\pm H]^{+/-}$, MS/MS ions; calibration plots; µg/g DW.

Isolates: purity (HPLC), full MS/NMR data; dereplication notes.

Bioassays: IC_{50}/MIC with controls; statistics; effect sizes.

QA/QC: spike recoveries, blanks, duplicates, RSDs.

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