
ABSTRACT

The East Indian Sandalwood, *Santalum album* L., a tropical woody tree, deposits sesquiterpenoid rich essential oil in the heartwood. In view of its century-old traditional uses in perfumery and healthcare this investigation in prospecting of phenylpropanoid and terpenoids from *in vitro* tissues, in comparison to the *in vivo* trees, was undertaken to throw light on the phytochemistry of the healthcare molecules, explore *in vitro* tissues as alternate avenues for the supply and profiling of metabolites as a pre-requisite towards future sesquiterpenoid biosynthetic studies in this plant.

Important phenylpropanoid enzymes i.e., phenylalanine ammonia lyase (PAL), cinnamyl alcohol dehydrogenase (CAD) and lignin peroxidases (POX) and their products, i.e., phenolic, hydroxycinnamic and benzoic acid, flavonoid, anthocyanin and lignin contents showed concomitant increase with lignification/ vascularization as visualized with histochemical analyses. HPLC analysis revealed identities and quantities of 20 phenolics, whereas LC-MS analysis identified ~52 phenylpropanoids through out development.

Differential accumulation of terpenoid biosynthetic pathway enzymes, i.e., DXP synthase, HMGR reductase and sesquiterpene synthase and metabolites i.e., sesquiterpenoid hydrocarbons and alcohols, photosynthetic pigments and farnesylated intermediates were evident from GC and HPTLC analyses. A putative sesquiterpene synthase (~60 kDa) was partially purified from leaves. GC-MS/ MS studies revealed the presence of ~47 volatile constituents in sandalwood. The fragrant sandalwood oil constituent, β -santalol was isolated from somatic embryos and characterized by ^{13}C -NMR, ESI-MS, LC-APCI-MS, MALDI-ToF, GC-MS/ MS and FTIR analyses whereas the bioactive constituent α -santalol, bulk-purified from sandalwood oil by HPTLC, RLCCC and column chromatography.

Tissue extracts rich in terpenoids and phenylpropanoids revealed antimicrobial, antioxidant, α -amylase inhibition, anti-tyrosinase and neuroprotective potentials *in vitro*. Sandalwood oil and α -santalol showed strong *in vivo* antioxidant and anti-hyperglycemic potentials.

Homology-based cloning using degenerate primers, yielded partial clones of a housekeeping gene (actin), a phenylpropanoid gene (CAD) and 4 terpenoid biosynthetic pathway genes (DXP synthase, FPP synthase, monoterpene synthase and sesquiterpene synthase), that showed homology and phylogenetic relationships with other plant genes. Homology-based modeling revealed their protein structure-function relationships, i.e., catalytic sites, domains and motifs. Structures were validated by Ramachandran plots. Transcriptional profiling by sqRT-PCR revealed higher expression levels of five transcripts in callus and young tree.

Keywords: Sandalwood, *Santalum album* L., prospecting, phenylpropanoid, sesquiterpenoid, santalol, terpene synthase, bioactivity.