J. Mex. Chem. Soc. **2025**, *69*(2)
Regular Issue

ISSN-e 2594-0317

Phytochemical Profile and Insecticidal Potential of Leaf Essential Oil of *Psidium guajava* Growing in North Central Nigeria

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Received March 29th, 2024; Accepted July 15th, 2024.

DOI for the article: http://dx.doi.org/10.29356/jmcs.v69i2.2245

Supplementary Information

J. Mex. Chem. Soc. **2025**, *69*(2)
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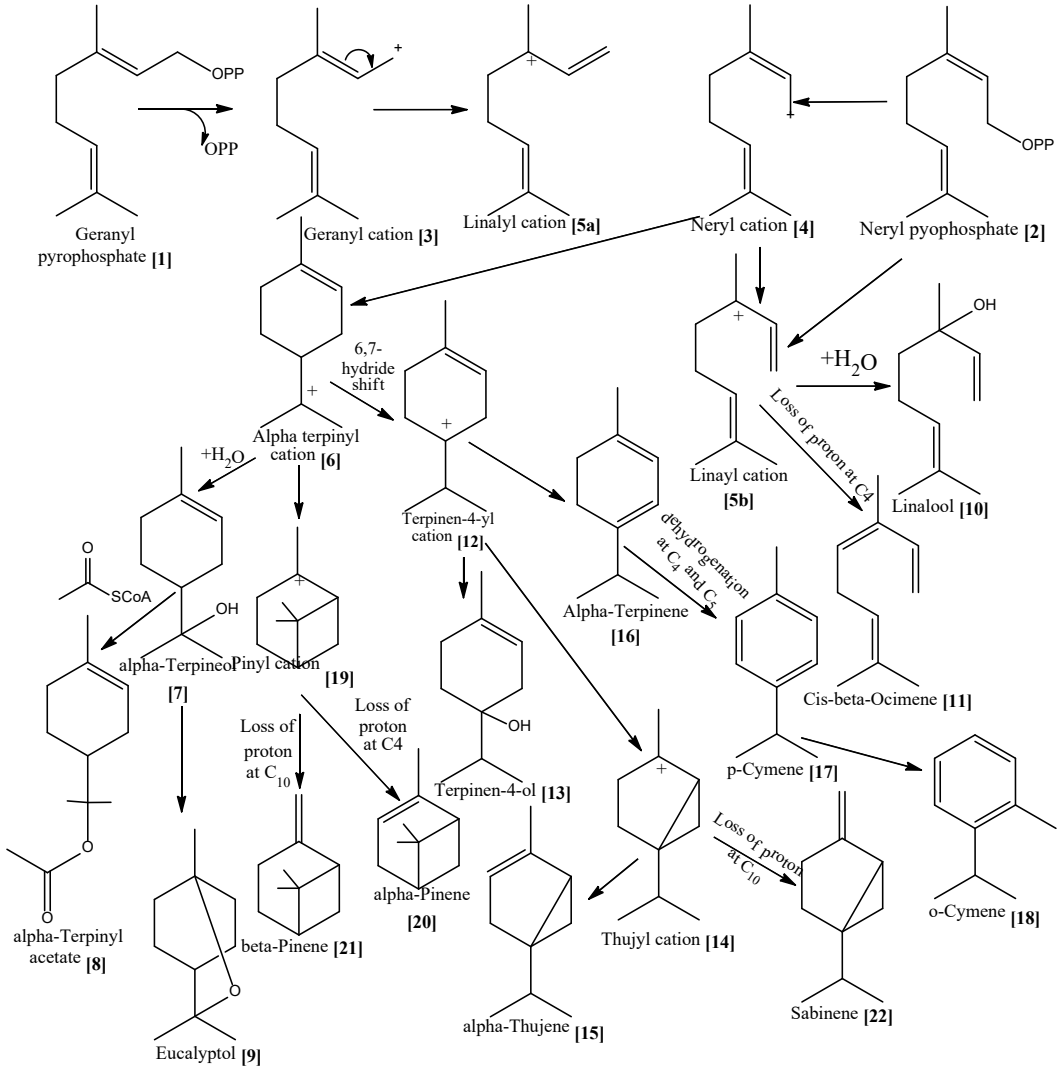
Reaction mechanism 1

The eucalyptol synthase facilitated the transformations of geranyl (**1**) and neryl (**2**) pyrophosphates to geranyl (**3**) and neryl (**4**) cations. Isomerization of both cations formed the transoid (**5a**) and cisoid (**5b**) linalyl cations, respectively. Hydration of the ion (**5b**) formed linalool (**10**). Loss of proton from (**5b**) at C_4 formed cis-β-ocimene (**11**). Electrophilic attack of the ion (**4**) on the C_6-C_7 double bond produced α-terpinyl cation (**6**). Hydration of (**6**) formed α-terpineol (**7**) and subsequent acetylation of α-terpineol formed alpha-terpinyl acetate (**8**). 6,7-Hydride shift of the ion (**6**) formed terpinen-4-yl cation (**12**). Subsequent hydration of the latter formed terpinen-4-ol (**13**) in the oil from the leaves of morning harvest. Deprotonation of the ion (**12**) at C_1 formed α-terpinene (**16**). Dehydrogenation of (**16**) at C_4 and C_5 and subsequent isomerization formed o-cymene (**18**) via p-cymene (**17**). Electrophilic attack of the ion (**12**) on C_2-C_3 double bond formed thujyl cation (**14**). Deprotonation of the ion (**14**) at C_{10} formed sabinene. Deprotonation of the ion (**14**) at C_4 formed α-thujene in the leaf oil of the morning harvest.

Folding of the α-terpinyl cation (**6**) towards the C_2-C_3 double bond followed by its electrophilic attack via C_2 produced pinyl cation (**19**). Deprotonation of the latter at C_4 and C_{10} formed α-pinene (**20**) and β-pinene (**21**), respectively [Scheme S1].



Scheme S1. Biogenesis of Eucalyptol Synthase Mediated Monoterpenoids in the Oils [31,32,34].

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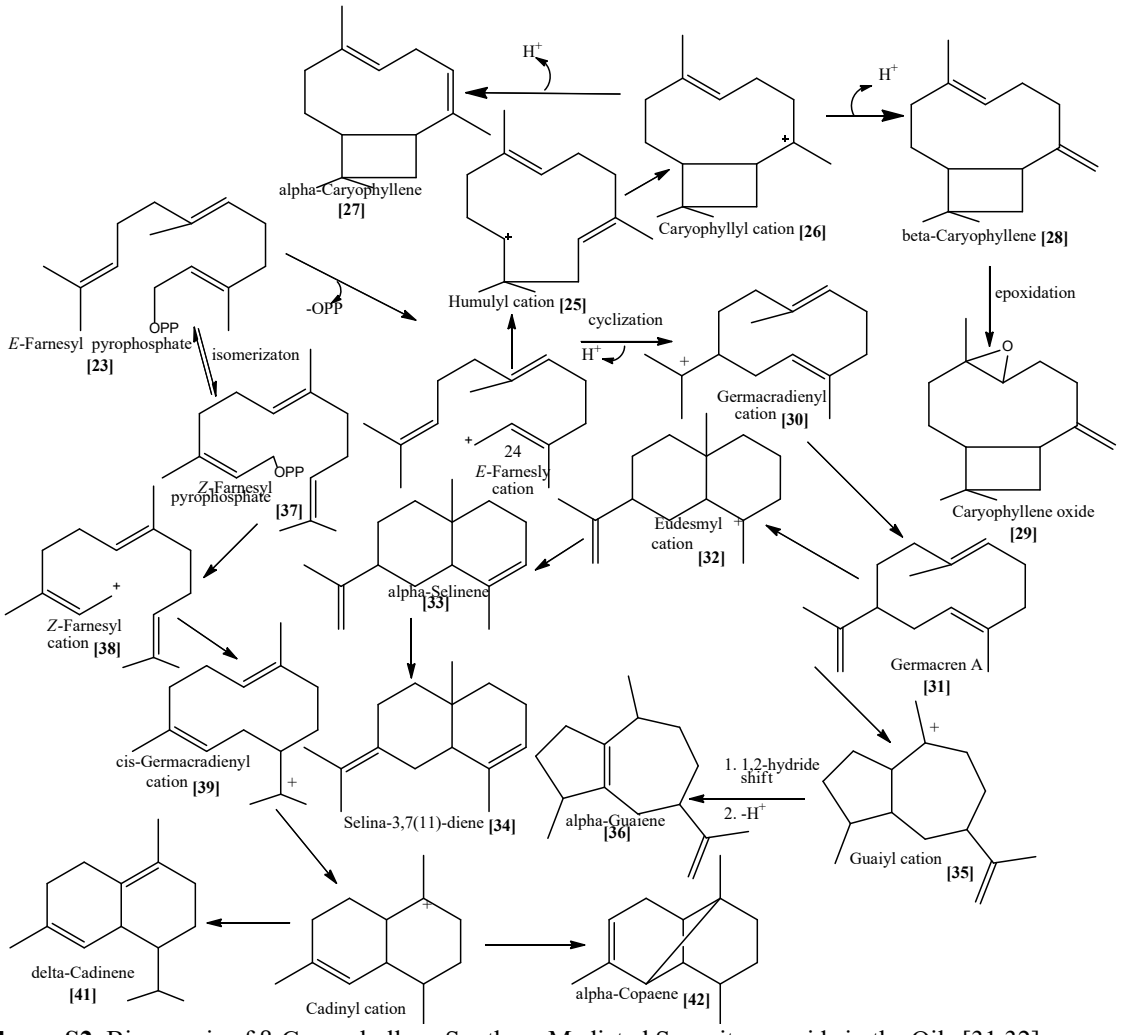
β-Caryophyllene synthase mediated the ionization of *E*-farnesyl pyrophosphate (**23**) to form *E*-farnesyl cation (**24**). Electrophilic attack of the ion (**24**) on its C_{10}-C_{11} double bond via C_{11} formed humulyl cation (**25**). Subsequent electrophilic attack of the ion (**25**) on C_2-C_3 double bond via C_2 formed caryophyllyl cation (**26**). Deprotonation of the ion (**26**) at C_4 and C_{15} formed α-caryophyllene (**27**) and β-caryophyllene (**28**), respectively. Epoxidation of (**28**) at C_6-C_7 double bond formed caryophyllene oxide (**29**). Electrophilic attack of farnesyl cation (**24**) on the C_{10}-C_{11} double bond via C_{10} formed germacradienyl cation (**30**). Deprotonation of the ion (**30**) at C_{13} formed germacrene A (**31**). Protonation of (**31**) at C_6 followed by electrophilic attack of the cation on the C_2-C_3 double bond via C_2 formed eudesmyl cation (**32**). Deprotonation of the ion (**32**) at C_4 formed α-selinene (**33**). Protonation of the compound (**33**) at C_{13} and subsequent deprotonation of the cation at C_{10} formed Selina-3,7(11)-diene (**34**). Addition of proton to germacrene A at C_3 and ensuing electrophilic attack of the cation on the C_6-C_7 double bond via C_6 formed guaiyl cation (**35**). 1,2-Hydride shift of the ion (**35**) from C_6 to C_7 and subsequent deprotonation at C_2 formed α-guaiene (**36**). Isomerization of *E*-farnesyl pyrophosphate (**23**) formed *Z*-farnesyl pyrophosphate (**37**). Ionization of the latter formed *Z*-farnesyl cation (**38**). Electrophilic attack of the ion (**38**) on the C_{10}-C_{11} bond via C_{10} formed the *Z*-germacradienyl cation (**39**). 1,3-Hydride shift from C_1 to C_{10} and subsequent electrophilic attack of the cation on the C_6-C_7 double bond via C_6 formed cadinyl cation (**40**). Deprotonation of the ion (**40**) at C_6 formed δ-cadinene (**41**). Electrophilic attack of the cation (**40**) on the C_2-C_3 double bond followed by deprotonation at C_4 formed α-copaene (**42**).



Scheme S2. Biogenesis of β-Caryophyllene Synthase Mediated Sesquiterpenoids in the Oils [31,32]