










Supplementary Materials

Antibacterial activity of the GC-MS characterized essential oil from the leaves of *Crassocephalum crepidiodes* from North Central Nigeria

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Scheme 2. Propose reaction mechanism for the biogenesis of sesquiterpenoids in the oil [1,2].

Figure S1. GC-MS chromatogram of the oil

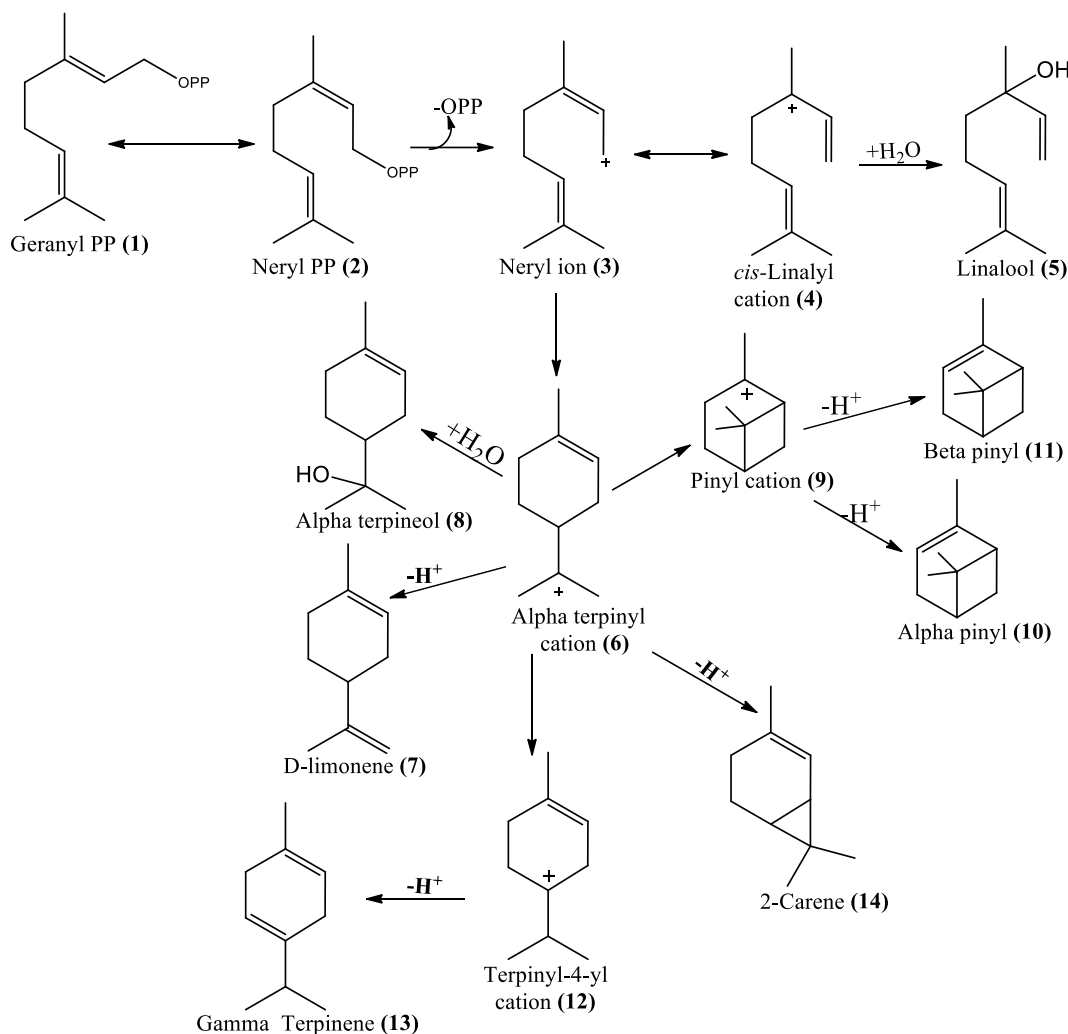
1. Propose reaction scheme for the biogenesis of monoterpenoids in the oil

Scheme 1 shows the isomerization of geranyl pyrophosphate (1) to neryl pyrophosphate (2) followed by formation neryl carbocation (3) from neryl pyrophosphates (2) after the compound was deionized by divalent metal ions in the leaves of the plant. The reactions were aided by D-limonene synthase. The neryl cation isomerized to cis-linalyl cation (4) that subsequently hydrated to form linalool (5). The ion (4) formed α -terpinyl cation (6) by electro-

philic attack on the C₆-C₇ double bond of the ion. The intermediate cation (6) gave D-limonene (7) and α -terpineol (8) via D-limonene synthase catalysed deprotonation at C₈ and hydration processes respectively. Electrophilic attack on the C₂-C₃ double bond of the folded terpinyl cation at C₂ gave pinyl cation (9) that as well produced α -pinene (10) and β -pinene (11) by deprotonation. The synthase catalysed the 6,7-hydrate shift of the α -terpinyl cation to form

terpinen-4-yl cation (**12**) and the ion (**12**) was deprotonated at C₅ to form γ -terpinene (**13**) in the oil. Formation of carbanion at C₂ and subsequent

electrophilic attack of the cation on the carbanion gave 2-carene (**14**) [1,2].



Scheme 1. Proposed reaction mechanism for the biogenesis of monoterpenoids in the oil [1,2].

2. Proposed mechanism for the biogenesis of sesquiterpenoids in the oil

Scheme 2 shows how the β -caryophyllene synthase aided the ionization of E, E-farnesyl pyrophosphate (**15**) to E, E-farnesyl cation (**16**) after the divalent metal ions in the leaves trapped the pyrophosphate ions. Isomerization of the E, E-farnesyl (**16**) formed E, E-nerolidyl cation (**17**). Loss of proton by the ion (**17**) at C₄ formed α -farnesene (**18**) in the oil. Electrophilic addition of the cation (**17**) towards C₁₀-C₁₁ double bond at C₁₁ formed humullyl cation (**18**).

Markovnikoff's addition of the cation (**18**) on the C₂-C₃ double bond via C₂ formed caryophyllyl cation (**19**). The cation (**19**) lost a proton at C₁₅ to form β -caryophyllene (**20**) in the oil. Electrophilic attack of

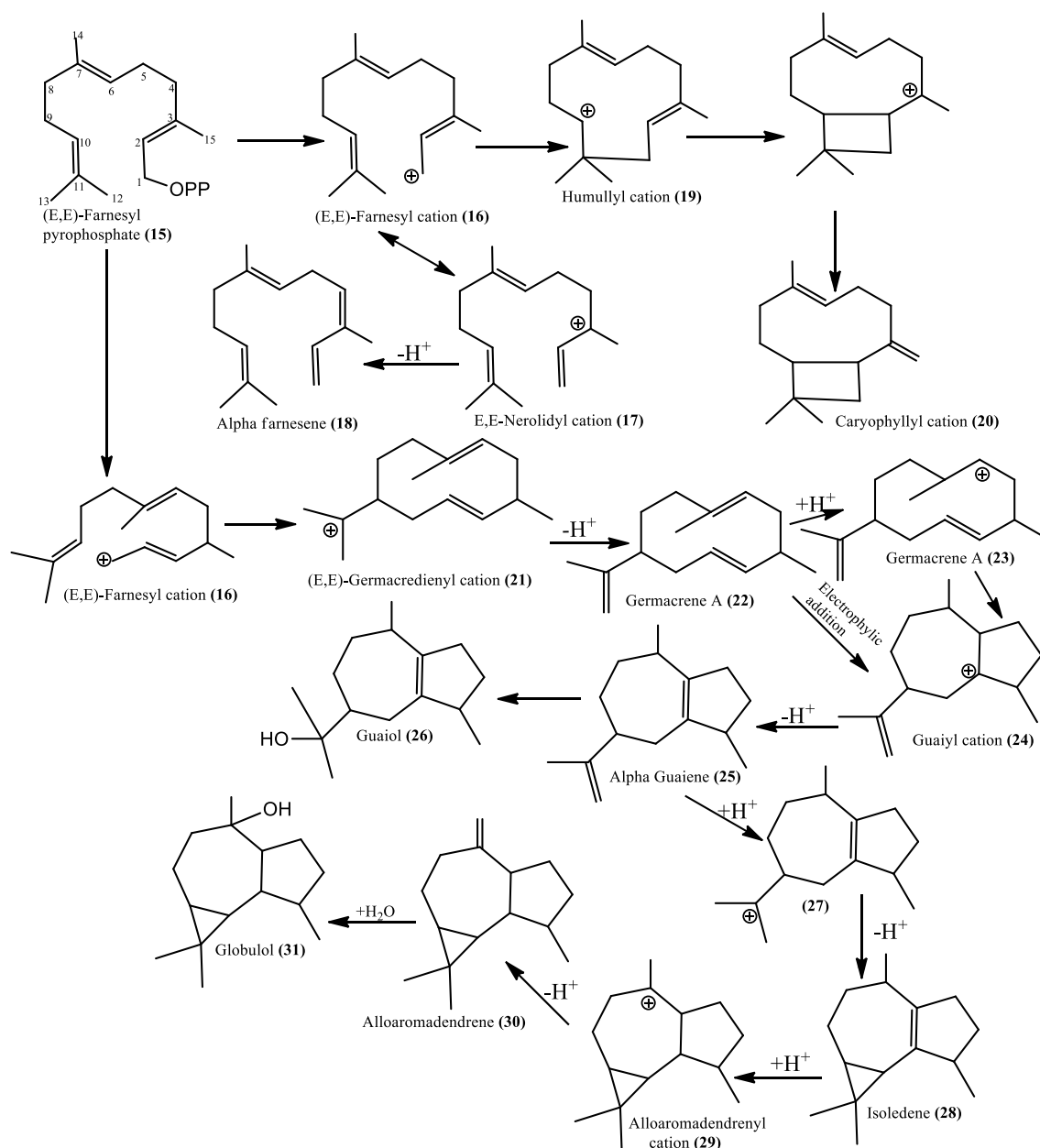
the E, E-farnesyl cation on the C₁₀-C₁₁ double bond via C₁₀ produced E, E-germacradienyl cation (**21**). Loss of proton by the ion (**21**) at C₁₂ produced germacrene A (**22**). Addition of proton to the C₆-C₇ double bond of the compound (**22**)

at C₆, followed by C₇ - C₆ hydride shift formed an intermediate cation (**23**). Electrophilic attack on the C₂-C₃ double bond of the ion (**23**) at C₂ formed guaiyl cation (**24**). Loss of proton of the ion (**24**) at C₂ produced α -guaiene (**25**). Hydration of the compound at C₁₁-C₁₂ double bond of the compound (**25**) gave guaiol (**26**) in the oil.

Protonation of the C₁₁-C₁₂ double bond of α-guaiene formed an intermediate cation (27).

Formation of carbanion by deprotonation at C₁ of the ion (27) followed by electrophilic addition of the cation on the carbanion formed isolekene (28).

Protonation of the double bond in the isolekene followed by 6,7-hydride shift formed alloaromadendryl cation (29). Loss of proton by the ion (29) at C₁₅ formed alloaromadendrene (30) in the oil. Hydration of the cation (30) produced globulol (31) in the oil.



Scheme 2. Propose reaction mechanism for the biogenesis of sesquiterpenoids in the oil [1,2].

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		Sample Information
Analyzed by	: Ronald Ibia	
Analyzed	: 17/10/2023 05:29:04AM	
Sample Type	: Unknown	
Level #	: 1	
Sample Name	: EBL	
Sample ID	: EBL	
IS Amount	: 11 µl	
Sample Amount	: 1	
Dilution Factor	: 1	
Vial #	: 11	
Injection Volume	: 0.10	
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Org. Data File	: C:\GCMSolution\Plant extract\EBL_QGD	
Method File	: C:\GCMSolution\Plant extract\Essential Oil.iqm	
Org. Method File	: C:\GCMSolution\Plant extract\Essential Oil.iqm	
Report File	:	
Tuning File	: C:\GCMSolution\System1\Tune 1\A12.102023.A2nd.gct	
[Comment]		
EBL		
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Modified	: 17/10/2023 06:03:45 AM	

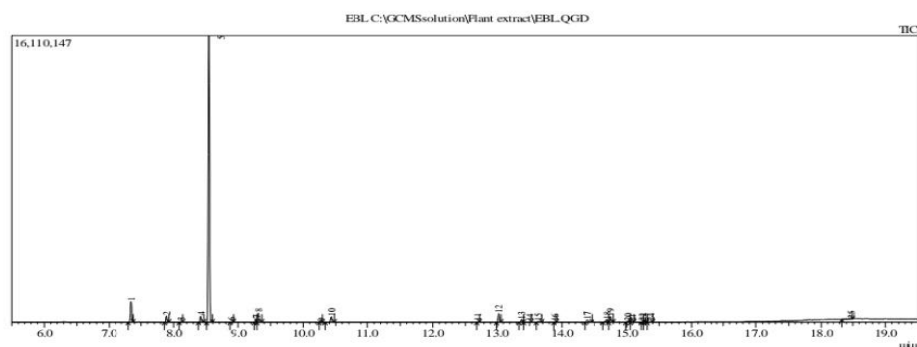


Figure S1. GC-MS chromatogram of the oil

References

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