

Supplementary Material

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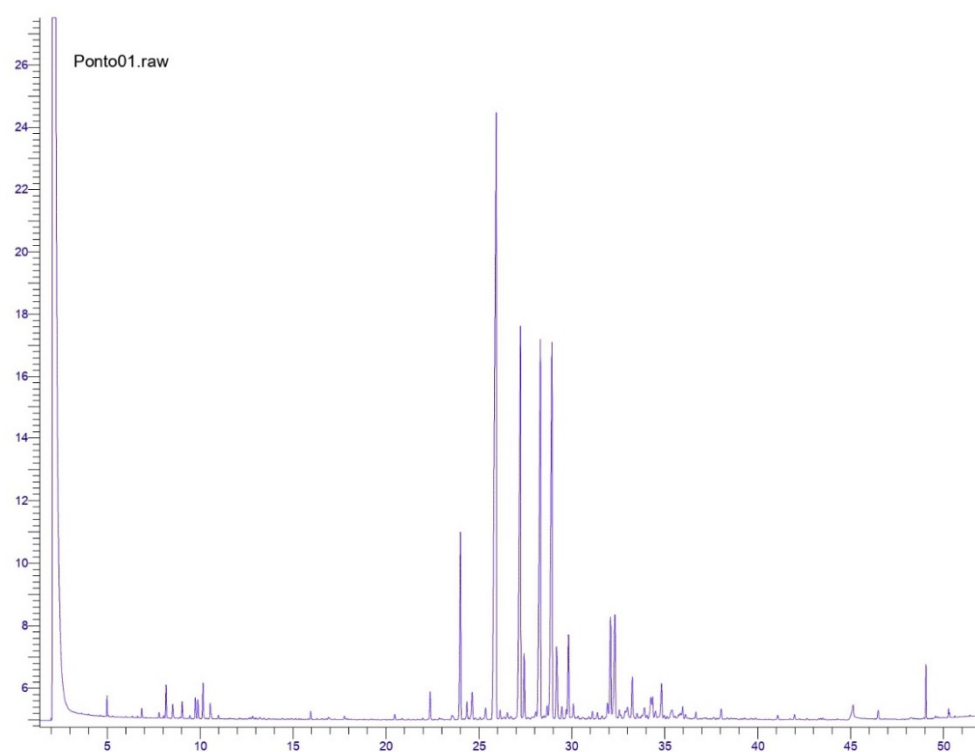


Figure S1 – GC-FID chromatogram of the essential oil of dry leaves from *Vernonanthura tweediana*, Pomerode, SC-Brazil.

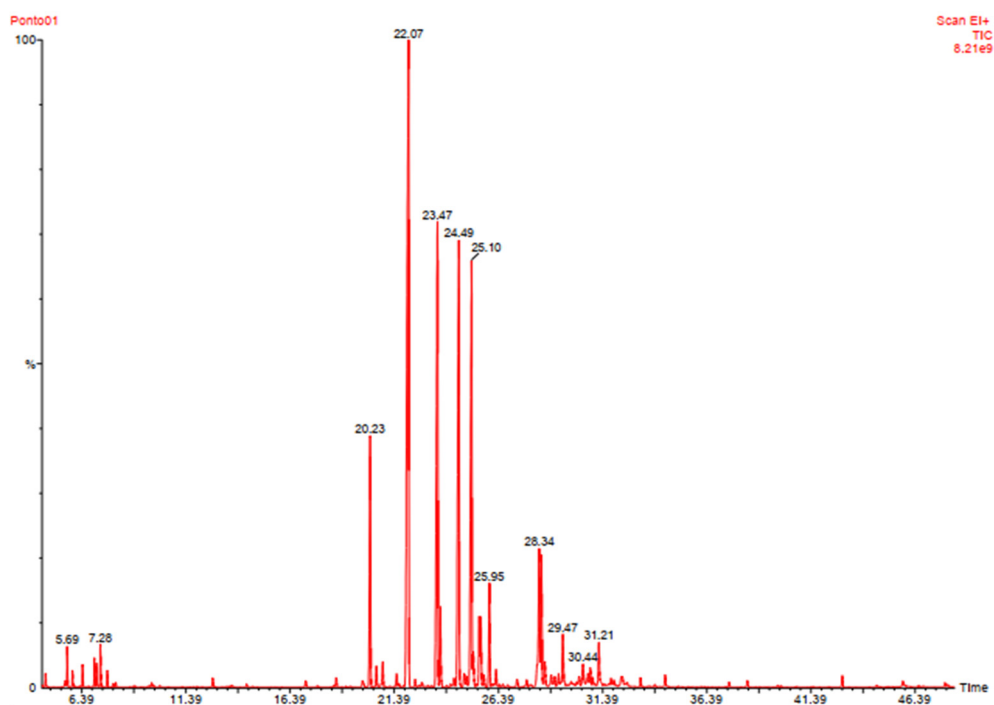
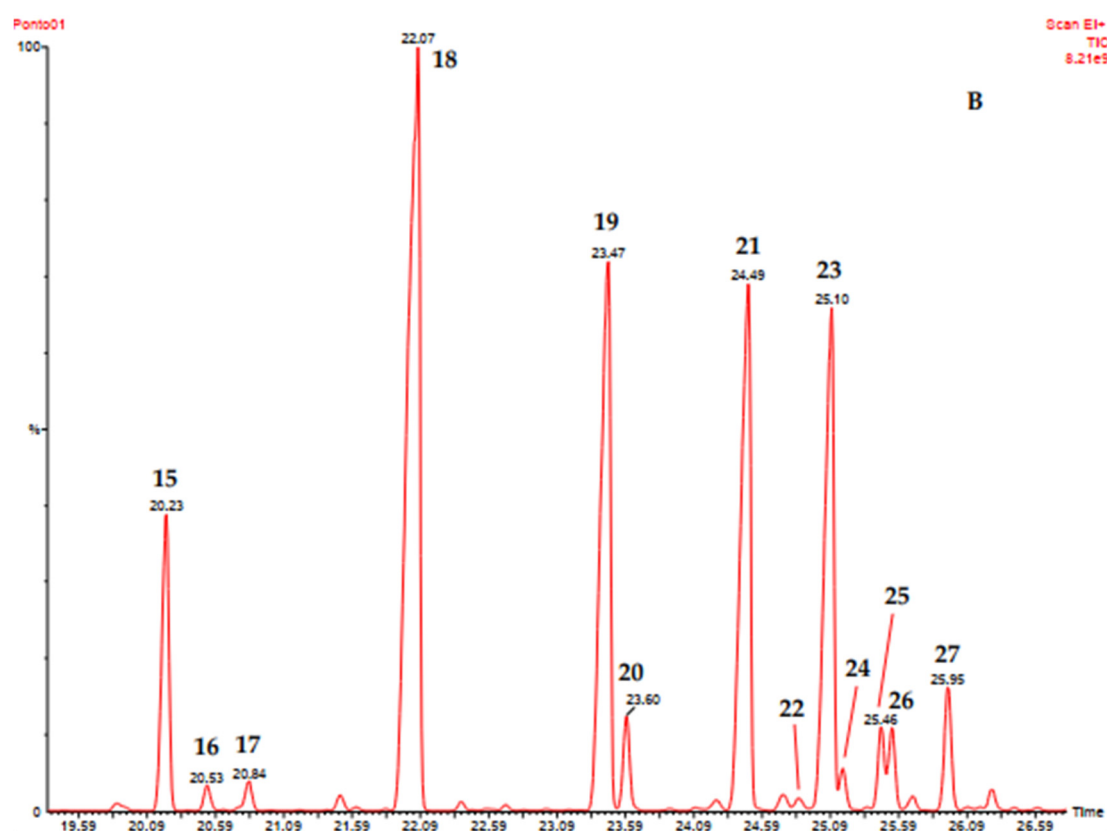
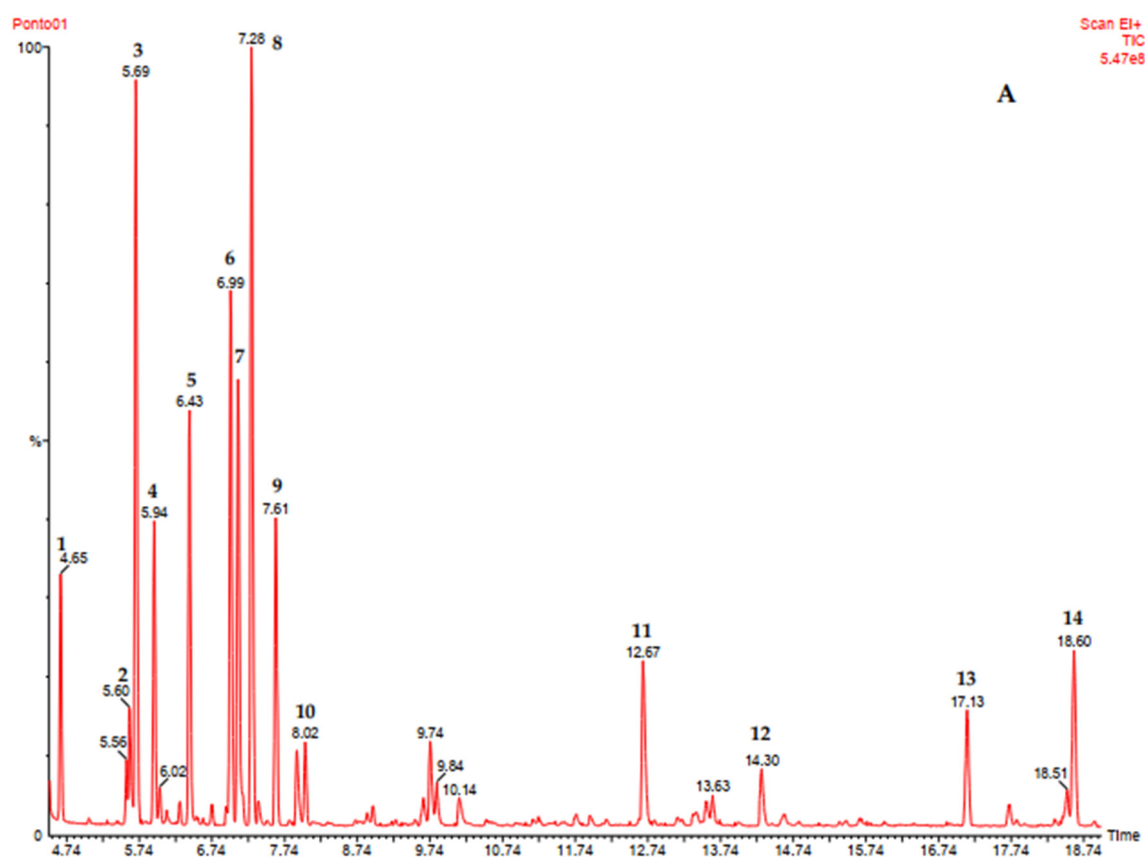


Figure S2 – GC-MS chromatogram of the essential oil of dry leaves from *Vernonia tweediana*, Pomerode, SC-Brazil.



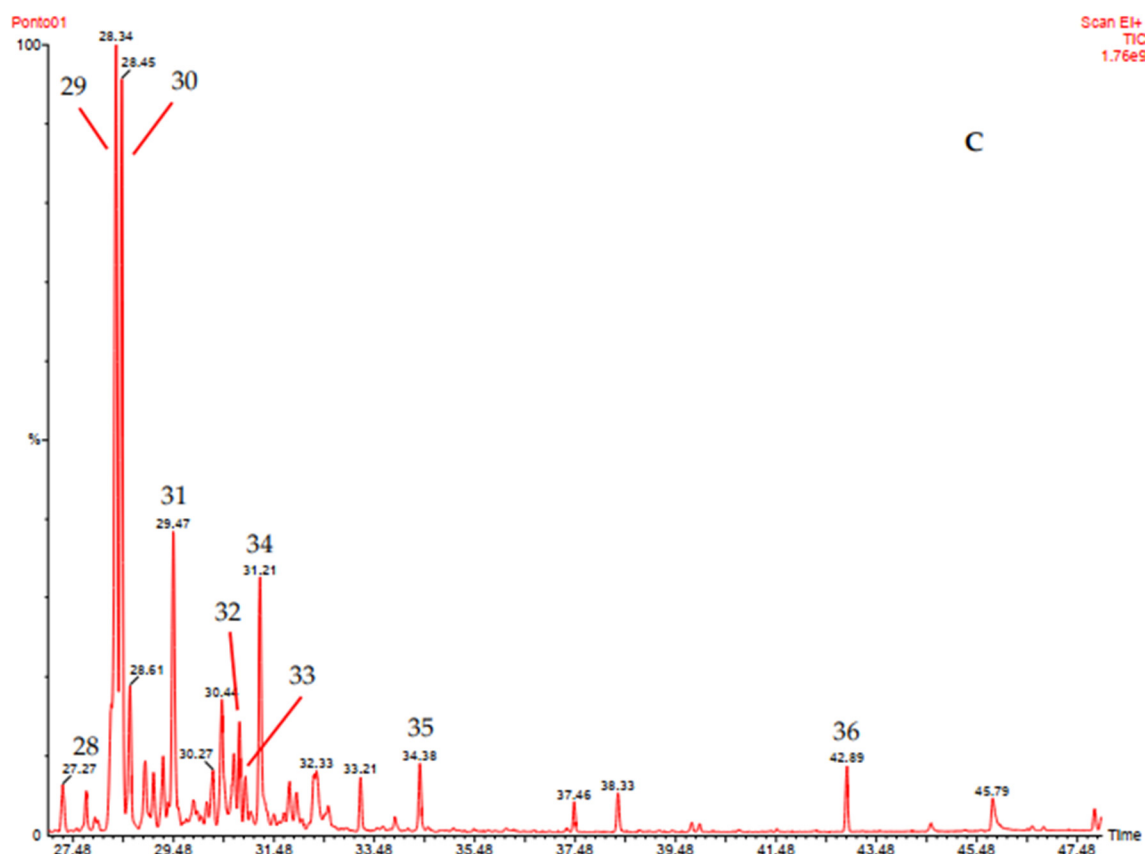
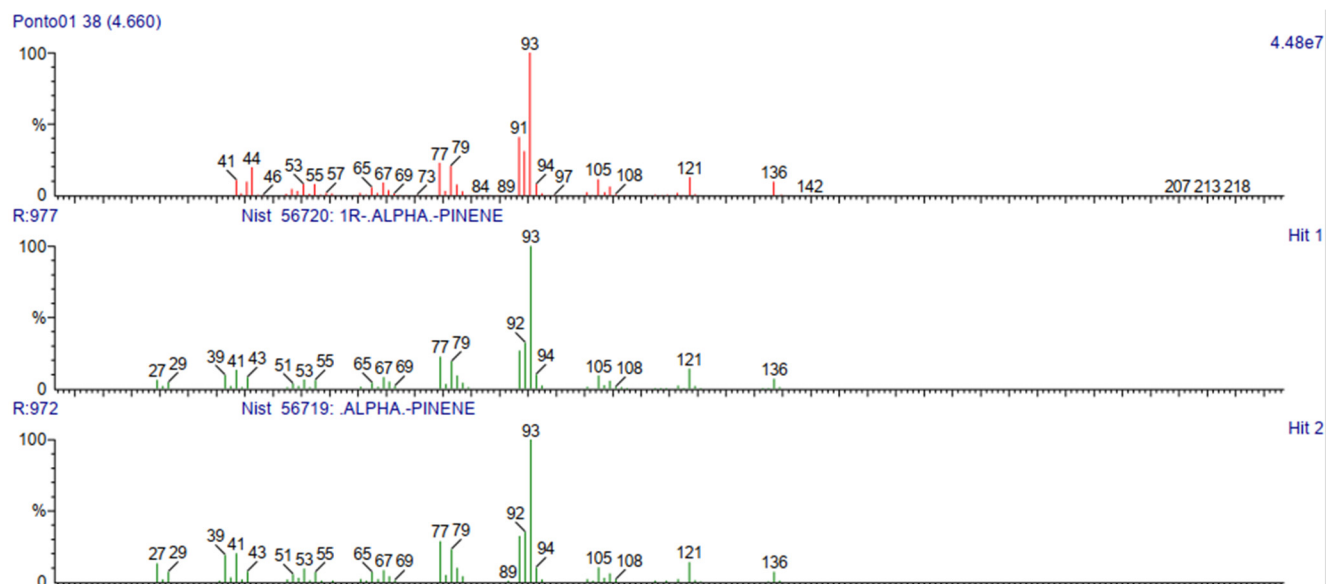


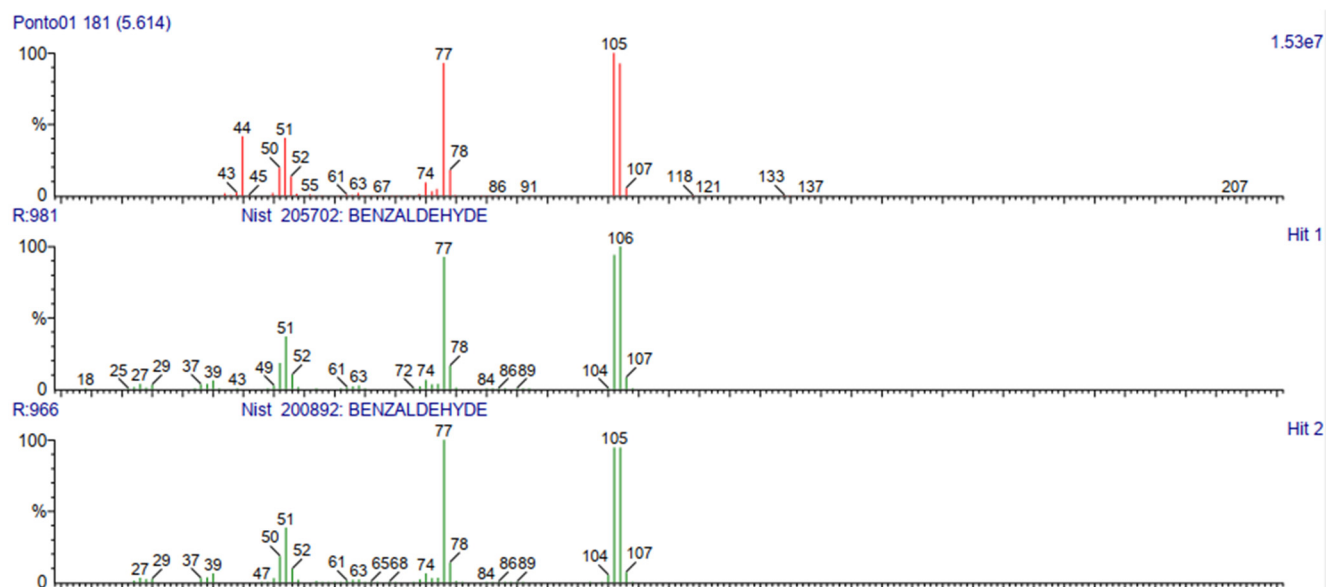
Figure S3 – A. Expanded GC-MS chromatogram of the essential oil from dried leaves from *Vernonanthura tweediana* (4.65 – 18.80 min). Identified peaks are assigned with the entries 1-14; B. Expanded GC-MS chromatogram of the essential oil of dry leaves from *Vernonanthura tweediana* (19.59 – 25.95 min). Identified peaks are assigned with the entries 15-27; C. Expanded GC-MS chromatogram of the essential oil of dry leaves from *Vernonanthura tweediana* (27.20 – 47.88 min). Identified peaks are assigned with the entries 28 – 36.

MS Data - Spectra of the constituents and the MS spectra of the identified compound from the NIST library. For each spectrum, the two main hits are given.

Entry 1: α -pinene.

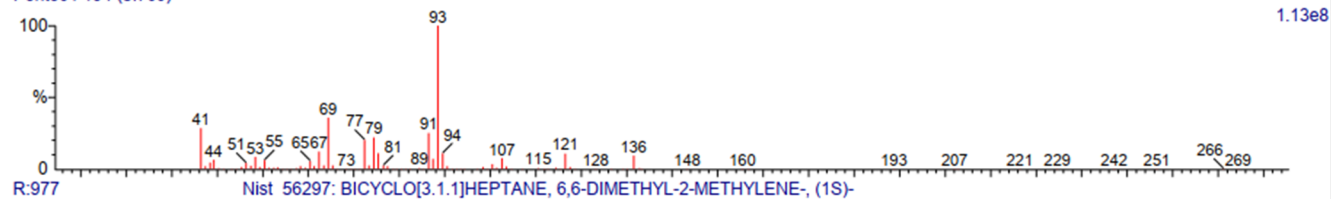


Entry 2: benzaldehyde.



Entry 3: β -pinene.

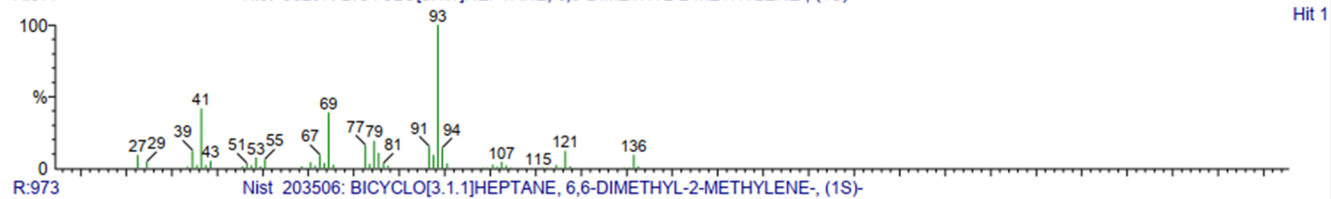
Ponto01 194 (5.700)



1.13e8

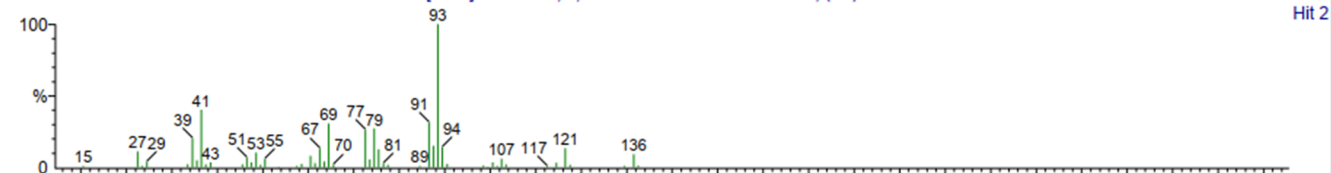
R:977 Nist 56297: BICYCLO[3.1.1]HEPTANE, 6,6-DIMETHYL-2-METHYLENE-, (1S)-

Hit 1



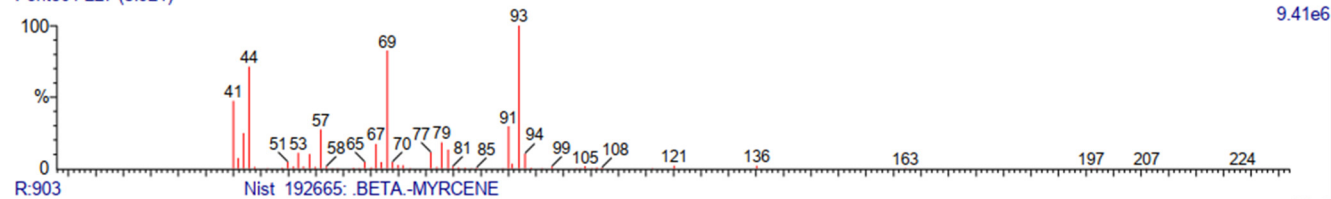
R:973 Nist 203506: BICYCLO[3.1.1]HEPTANE, 6,6-DIMETHYL-2-METHYLENE-, (1S)-

Hit 2



Entry 4: β -myrcene.

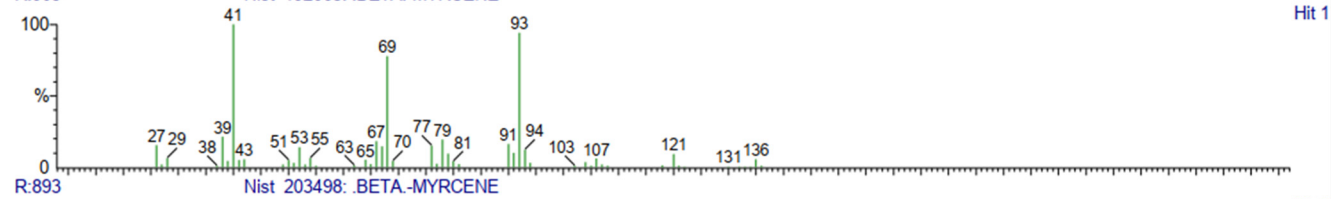
Ponto01 227 (5.921)



9.41e6

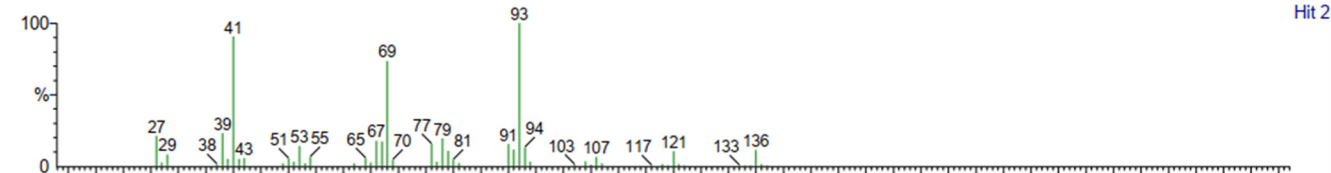
R:903 Nist 192665: BETA-MYRCENE

Hit 1



R:893 Nist 203498: BETA-MYRCENE

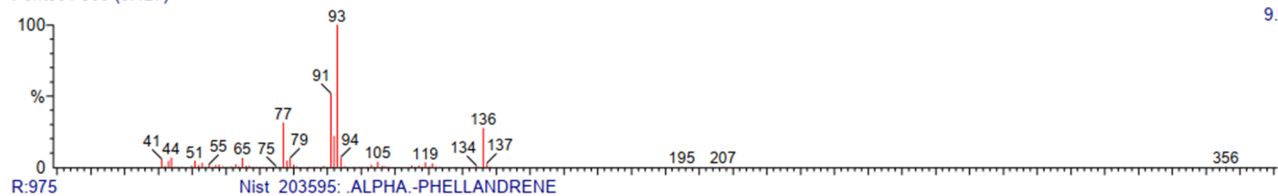
Hit 2



Entry 5: α -phellandrene.

Ponto01 303 (6.427)

9.59e7



Hit 1



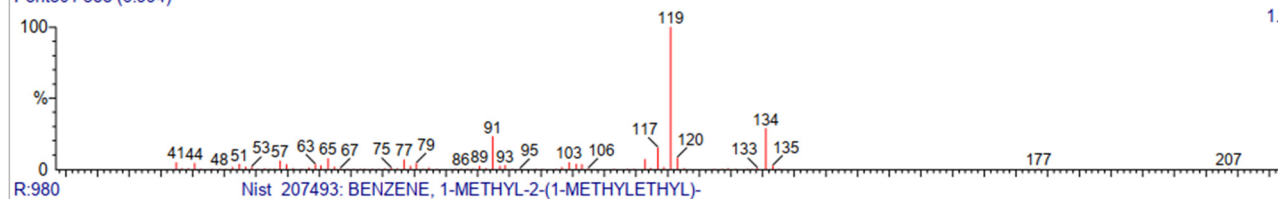
Hit 2



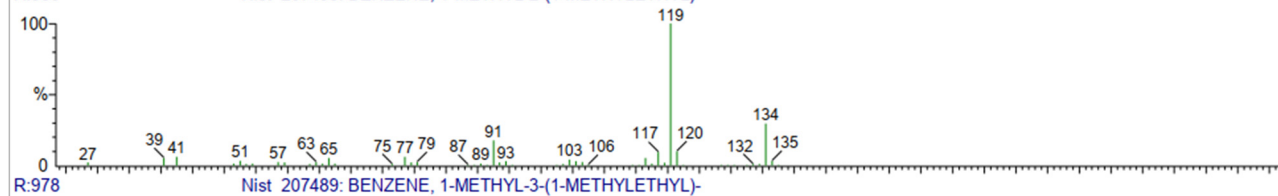
Entry 6: *ortho* or *para*-cymene.

Ponto01 388 (6.994)

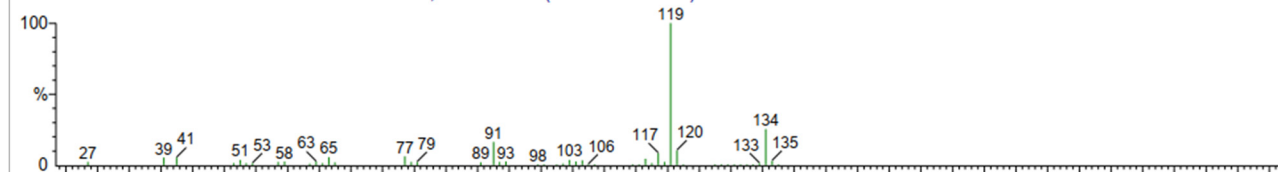
1.44e8



Hit 1



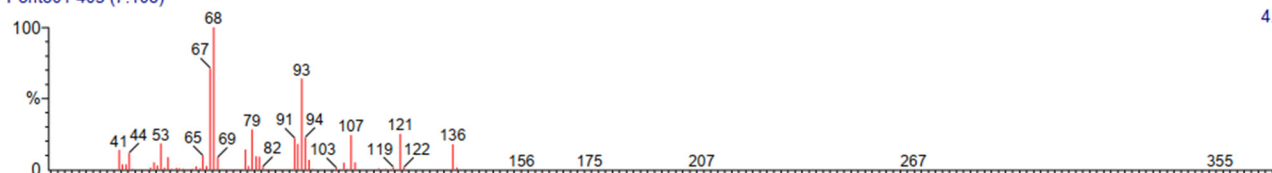
Hit 2



Entry 7: limonene.

Ponto01 405 (7.108)

4.96e7



R:971

Nist 29585: D-LIMONENE

Hit 1



R:963

Nist 198852: D-LIMONENE

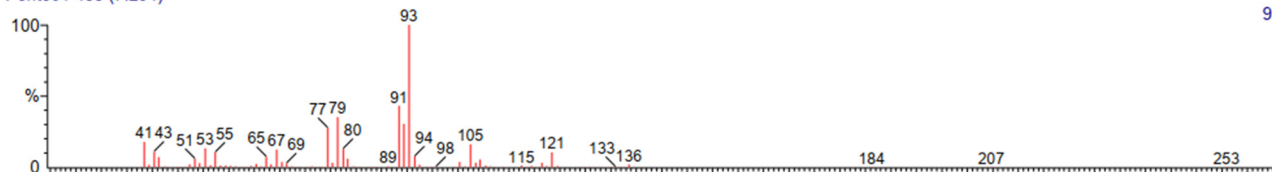
Hit 2



Entry 8: Z- β -ocimene (Alit. 1032).

Ponto01 433 (7.294)

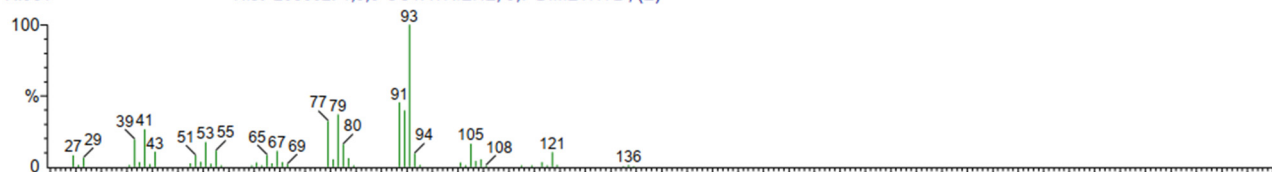
9.60e7



R:981

Nist 203602: 1,3,6-OCTATRIENE, 3,7-DIMETHYL-, (E)-

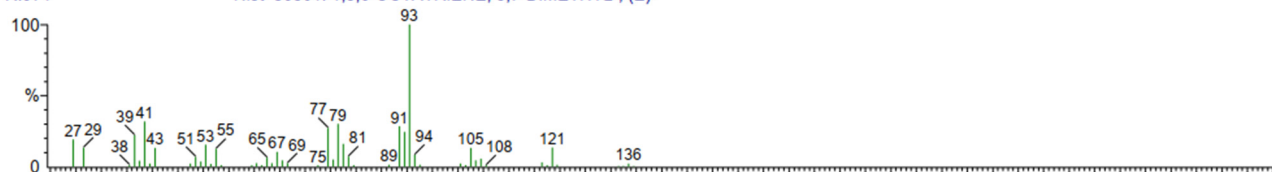
Hit 1



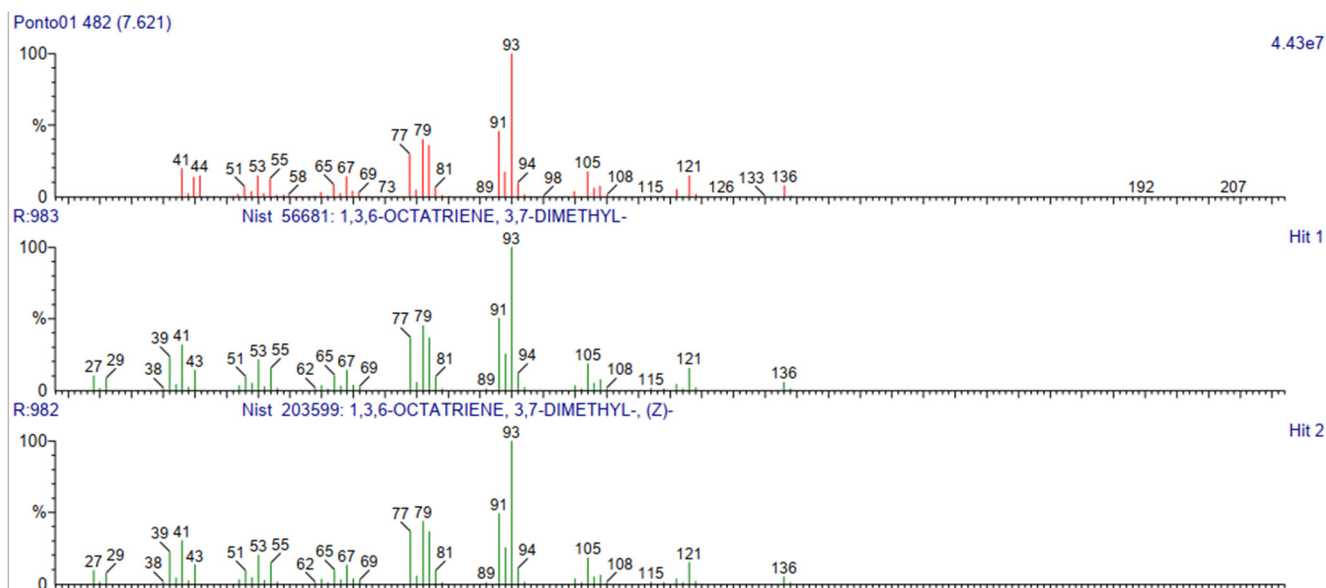
R:971

Nist 56301: 1,3,6-OCTATRIENE, 3,7-DIMETHYL-, (E)-

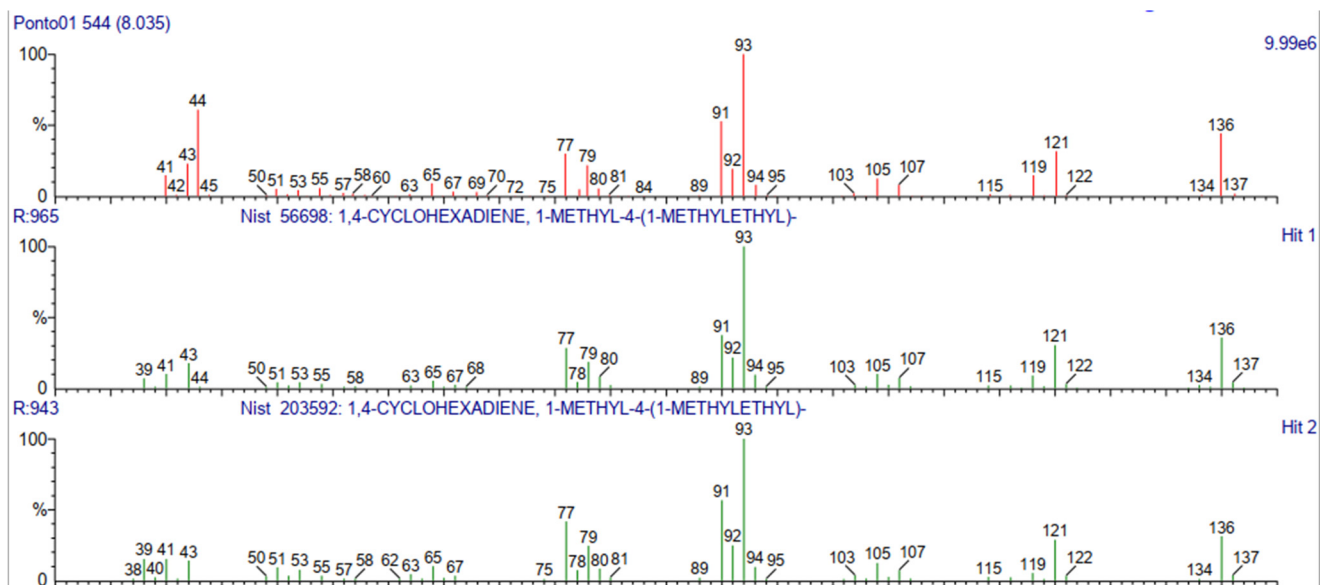
Hit 2



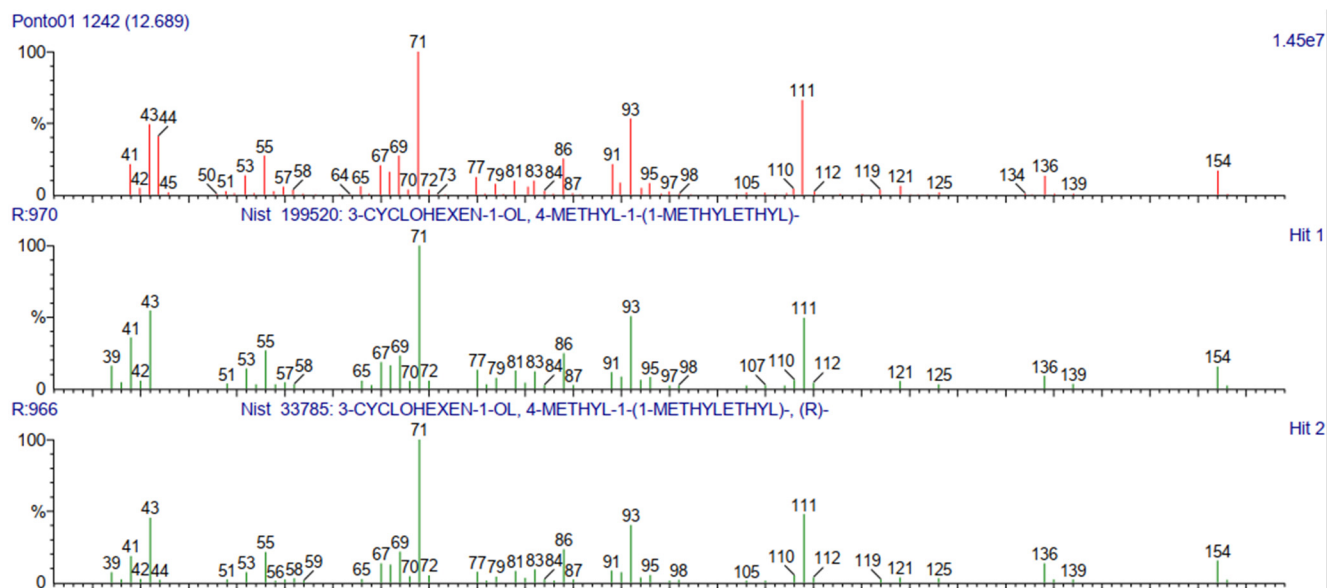
Entry 9: *E*- β -ocimene (A_{lit.} 1044).



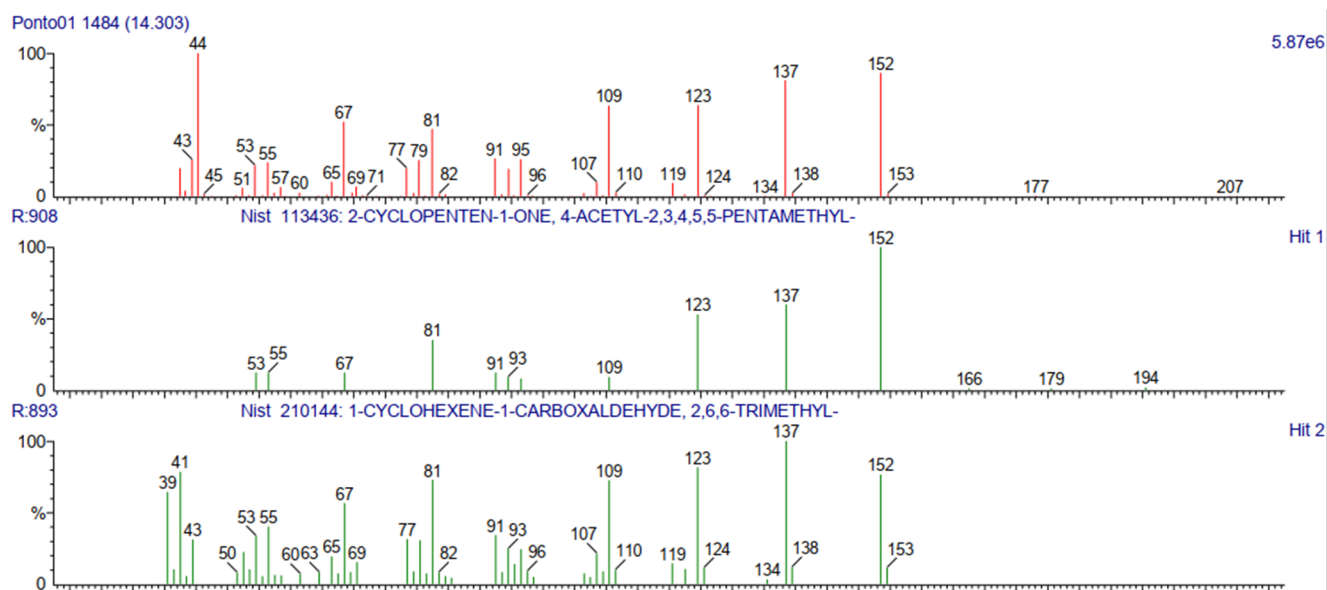
Entry 10: γ -terpinene.



Entry 11: terpinen-4-ol.

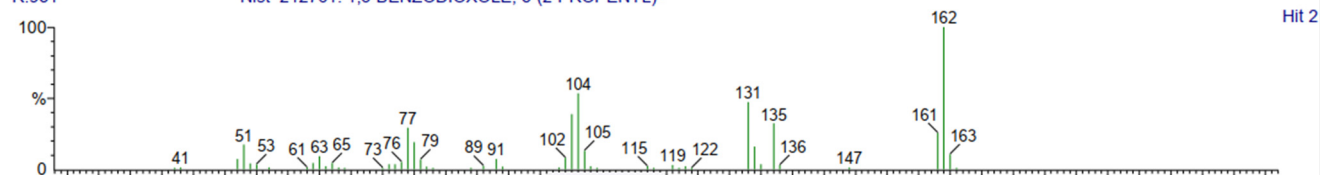
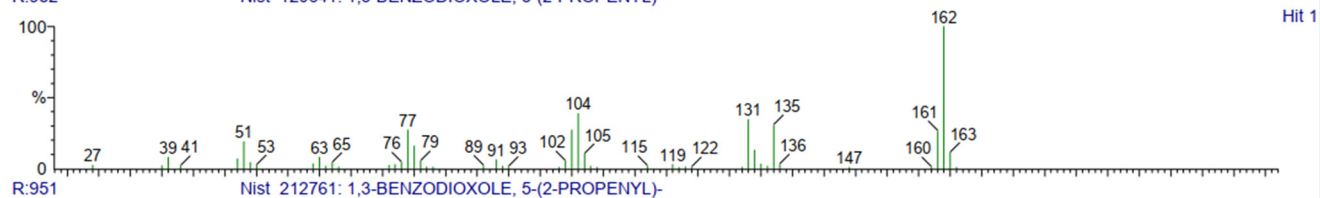
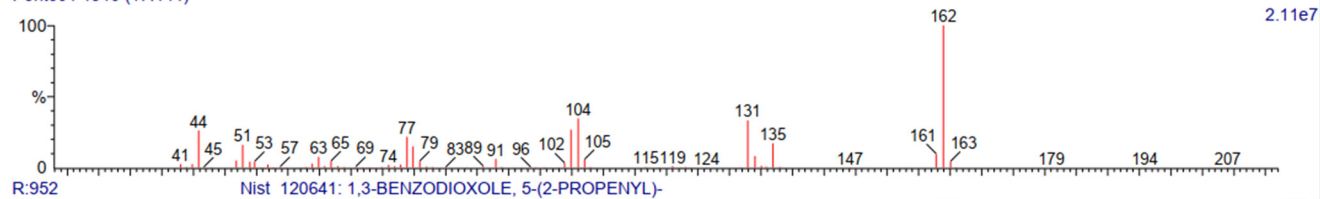


Entry 12: β -cyclocitral.



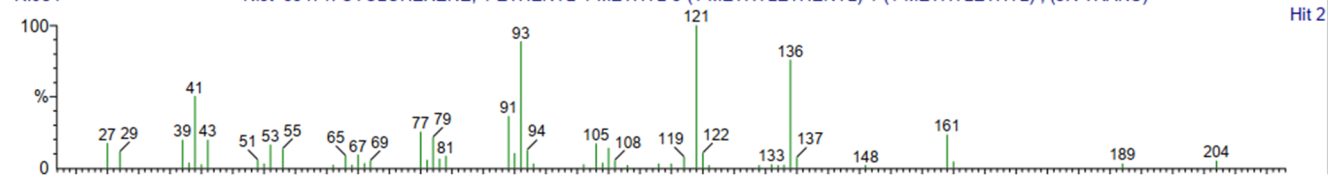
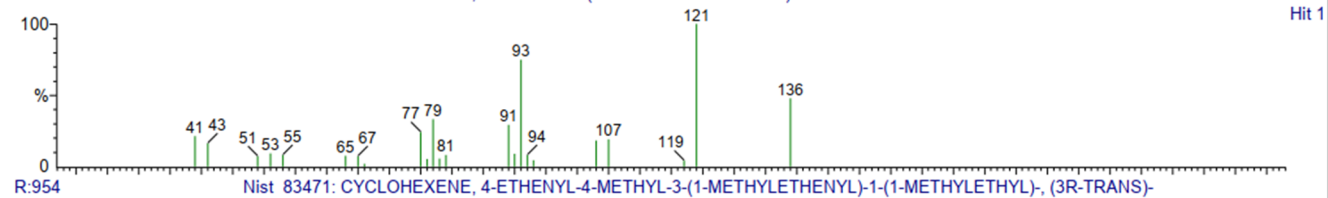
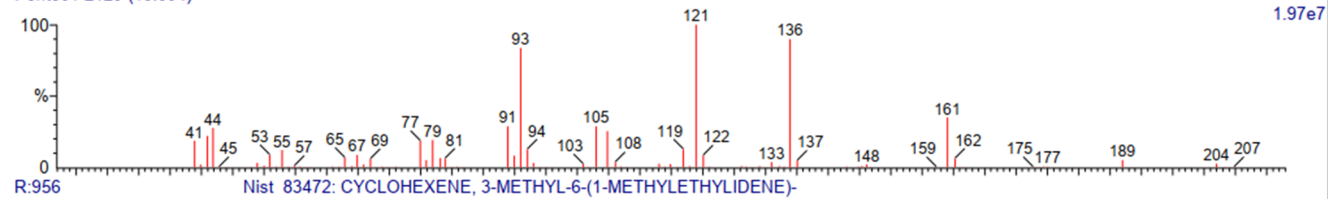
Entry 13: safrole.

Ponto01 1910 (17.144)



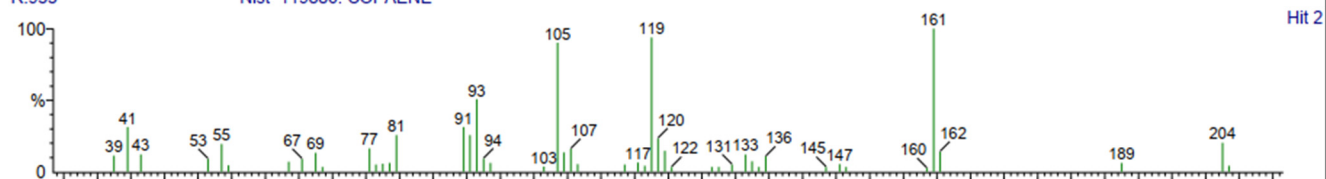
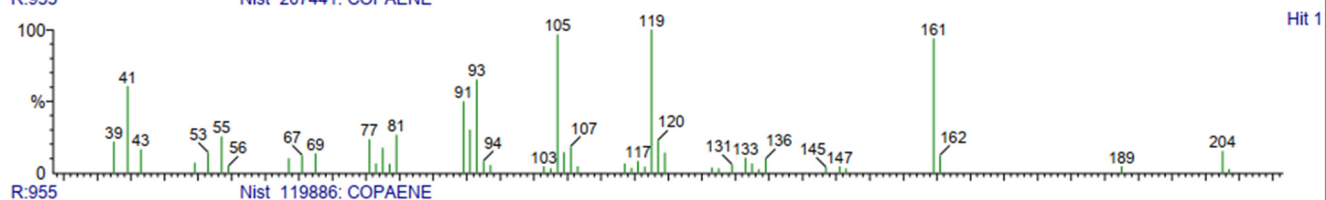
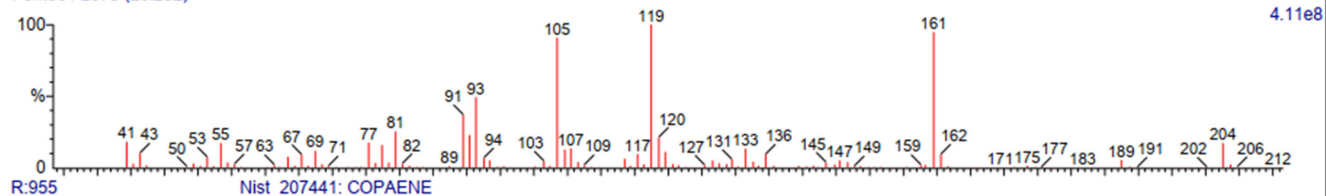
Entry 14: δ -elemene.

Ponto01 2129 (18.604)



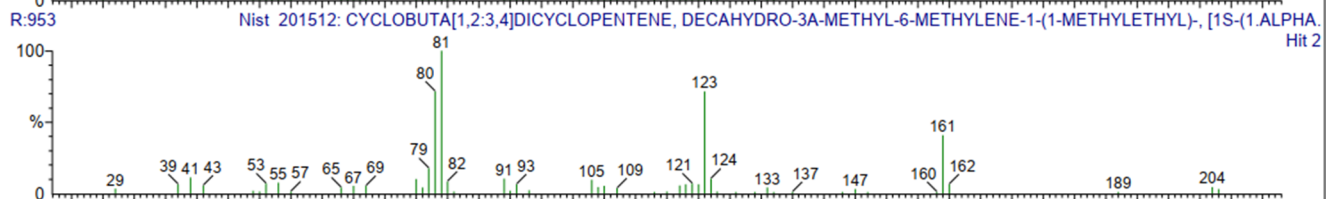
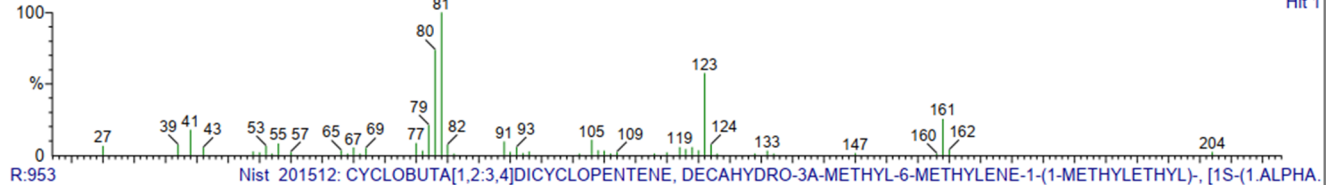
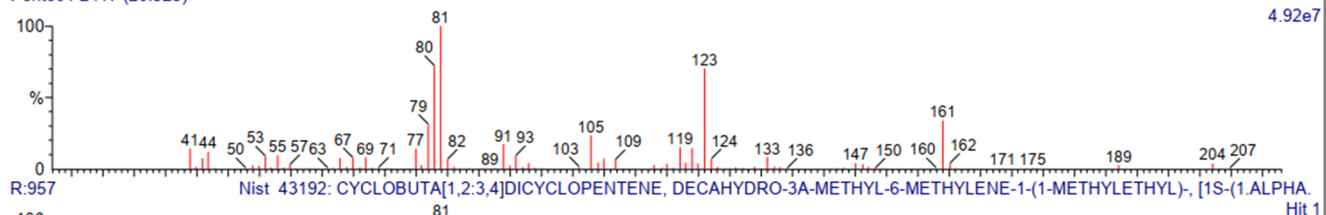
Entry 15: α -copaene.

Ponto01 2373 (20.232)



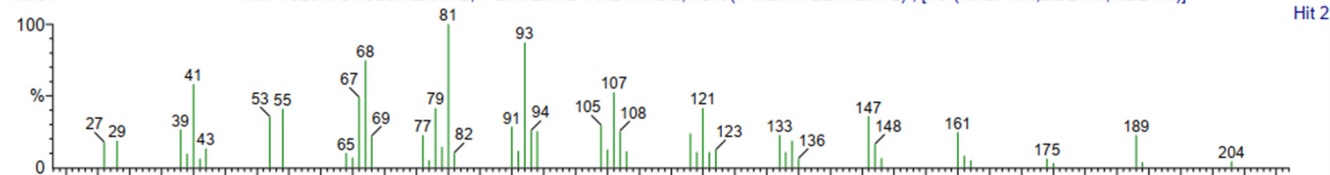
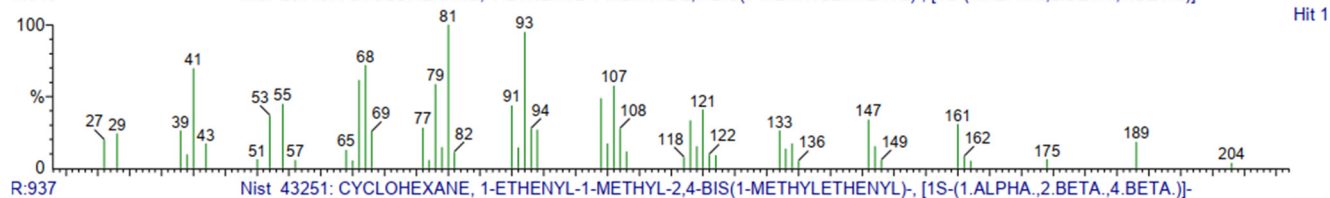
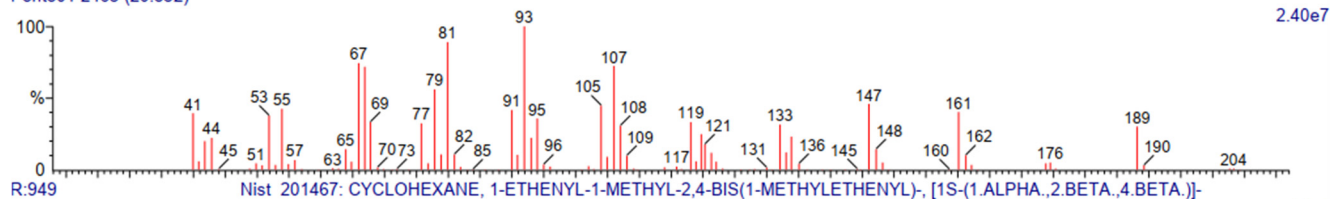
Entry 16: β -bourbonene.

Ponto01 2417 (20.525)



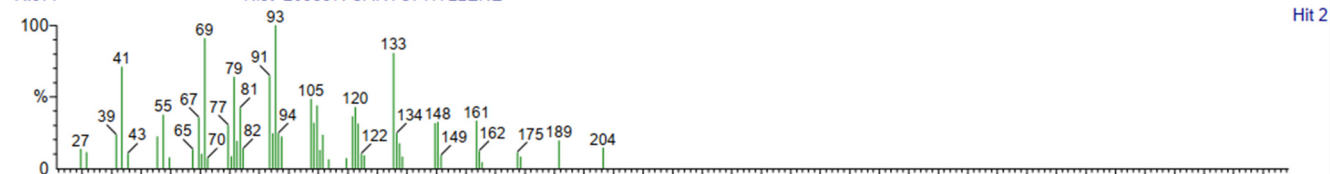
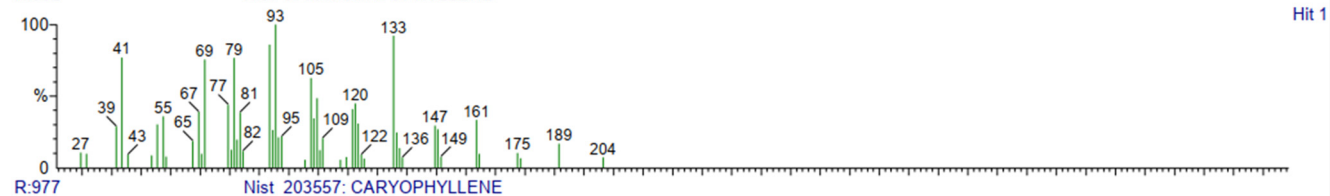
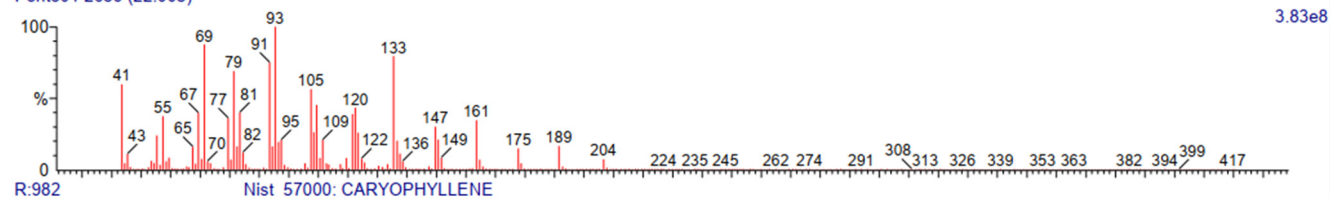
Entry 17: β -elemene.

Ponto01 2463 (20.832)

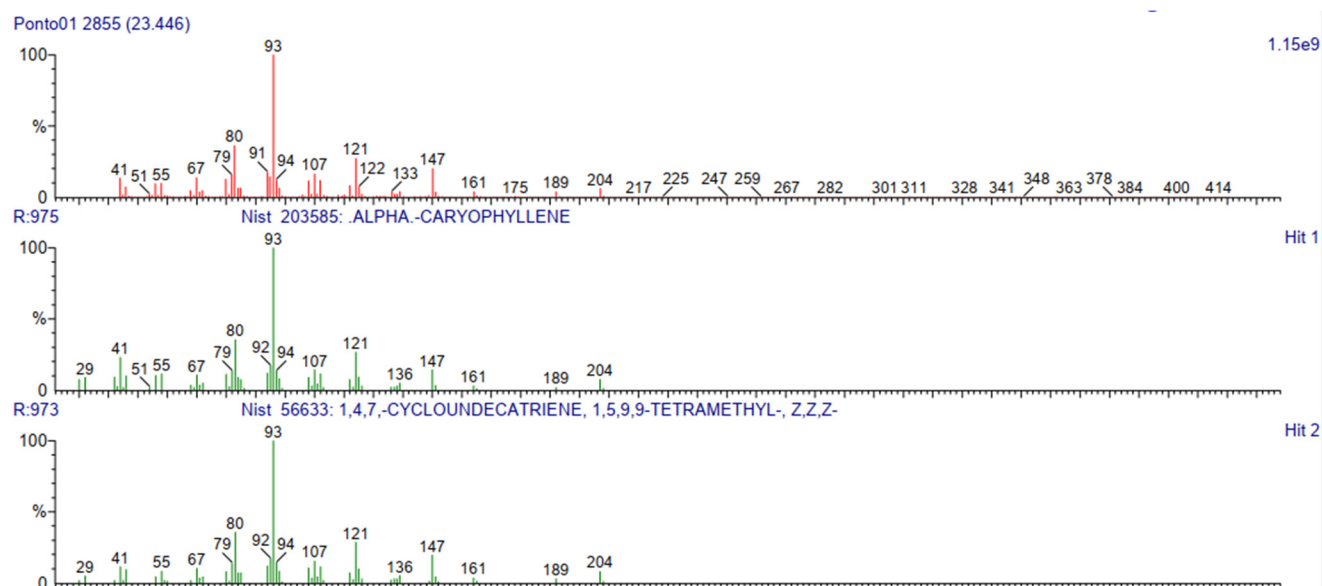


Entry 18: β -caryophyllene.

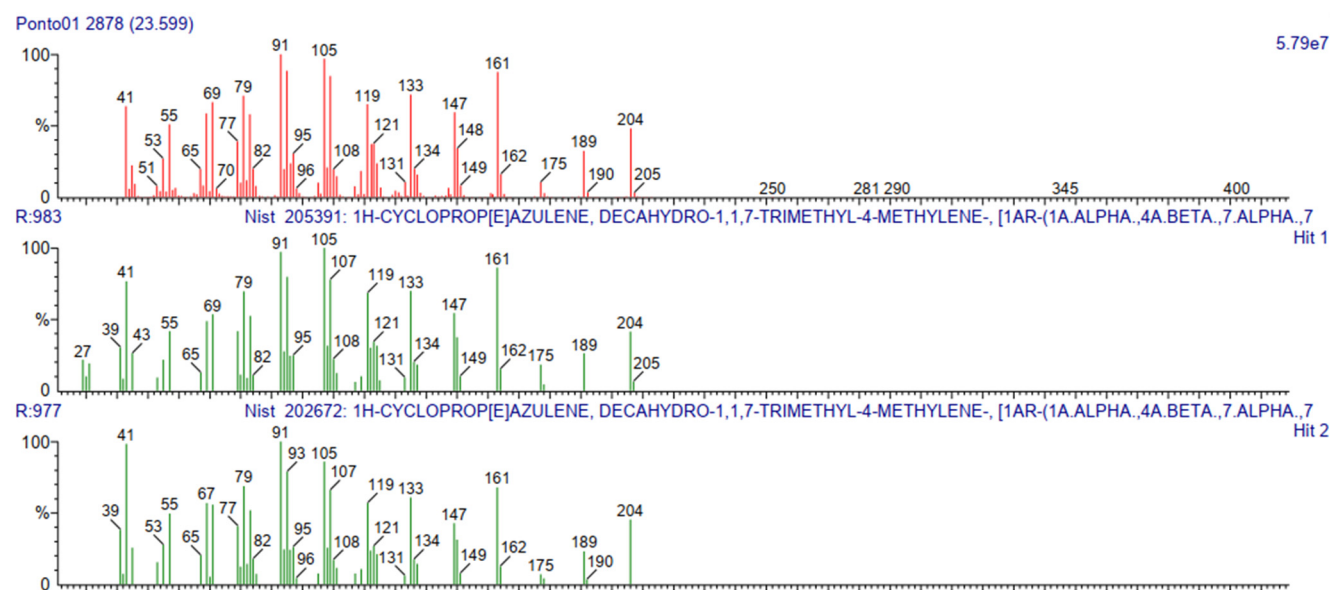
Ponto01 2639 (22.005)



Entry 19: α -caryophyllene.



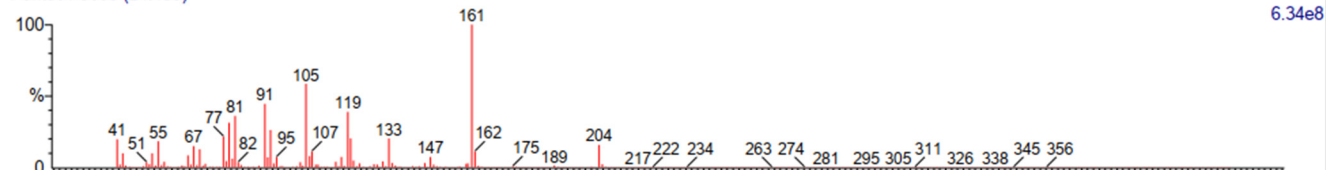
Entry 20: *allo*-aromadendrene.



Entry 21: germacrene D.

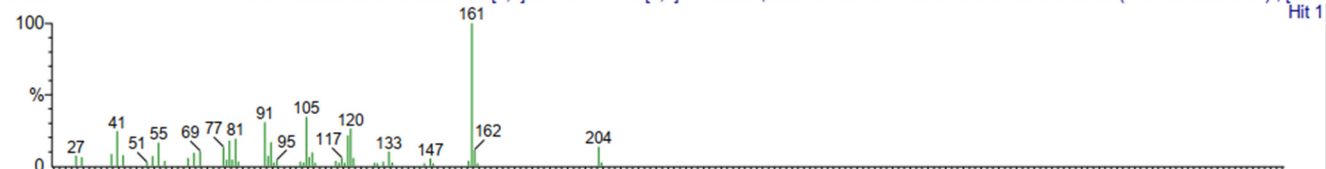
Ponto01 3006 (24.453)

6.34e8



R:967 Nist 119824: 1H-CYCLOPENTA[1,3]CYCLOPROPA[1,2]BENZENE, OCTAHYDRO-7-METHYL-3-METHYLENE-4-(1-METHYLETHYL)-, [3AS-

Hit 1



R:946 Nist 119825: 1,6-CYCLODECAADIENE, 1-METHYL-5-METHYLENE-8-(1-METHYLETHYL)-, [S-(E,E)]-

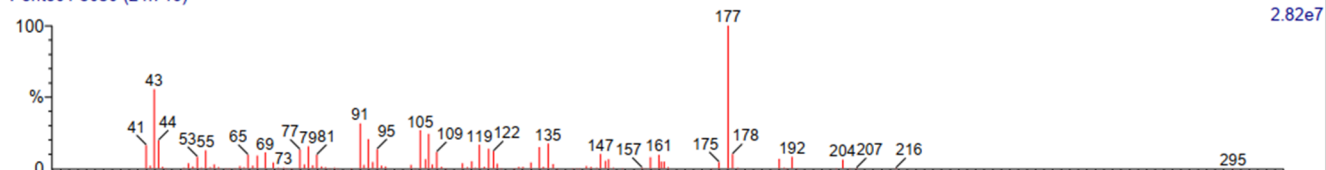
Hit 2



Entry 22: *E*- β -ionone.

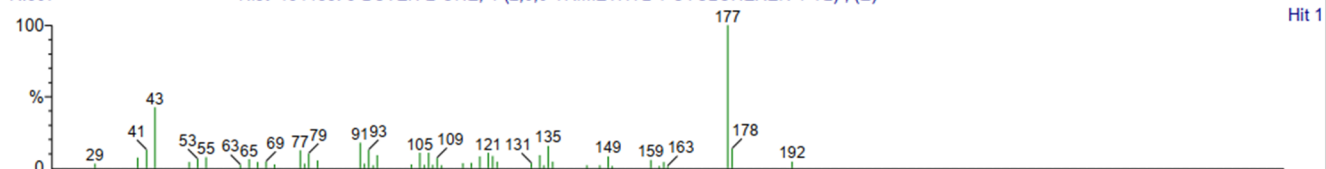
Ponto01 3050 (24.746)

2.82e7



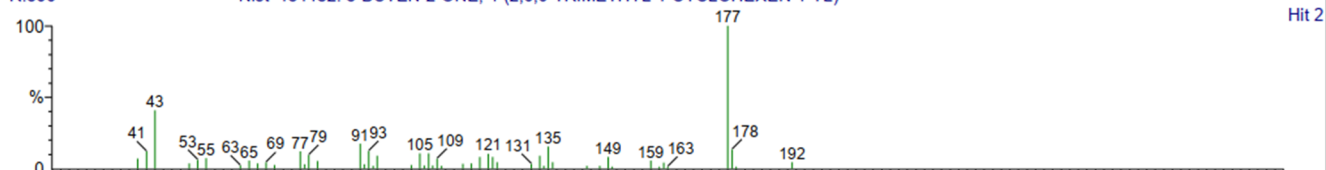
R:897 Nist 131153: 3-BUTEN-2-ONE, 4-(2,6,6-TRIMETHYL-1-CYCLOHEXEN-1-YL)-, (E)-

Hit 1



R:896 Nist 131152: 3-BUTEN-2-ONE, 4-(2,6,6-TRIMETHYL-1-CYCLOHEXEN-1-YL)-

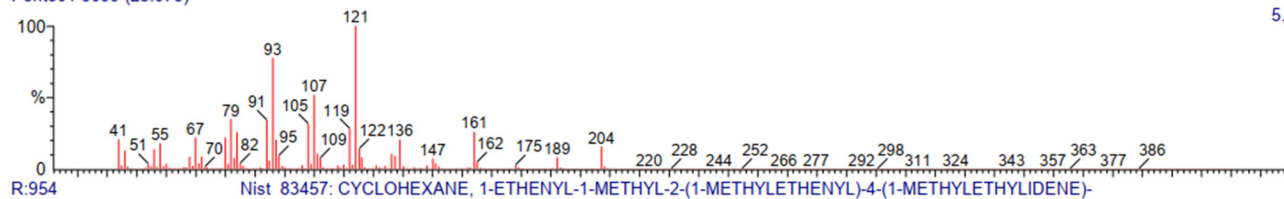
Hit 2



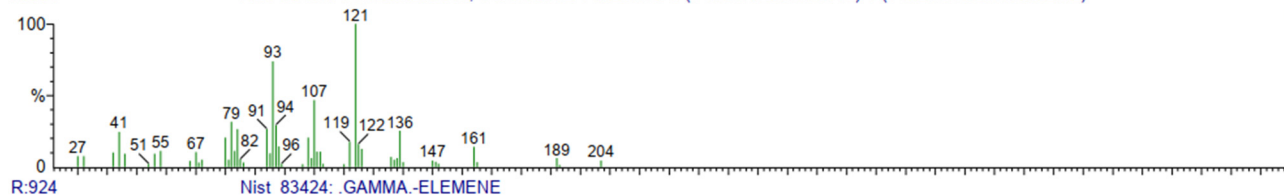
Entry 23: bicyclogermacrene. The identification was based on AI and literature [16].

Ponto01 3099 (25.073)

5.59e8



Hit 1

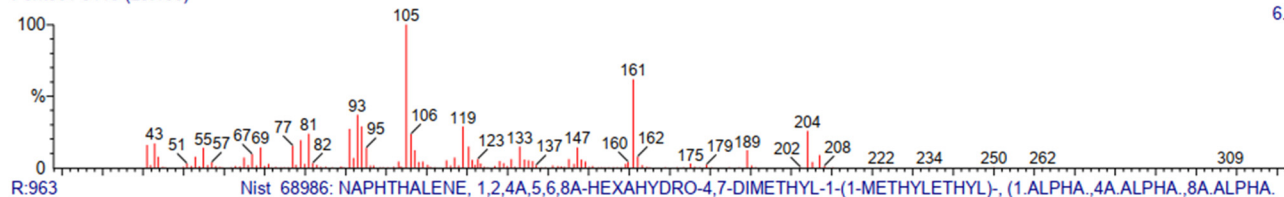


Hit 2

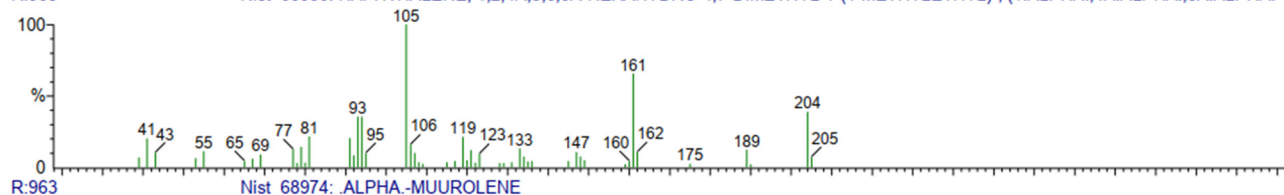
Entry 24: α -muurolene.

Ponto01 3115 (25.180)

6.35e7



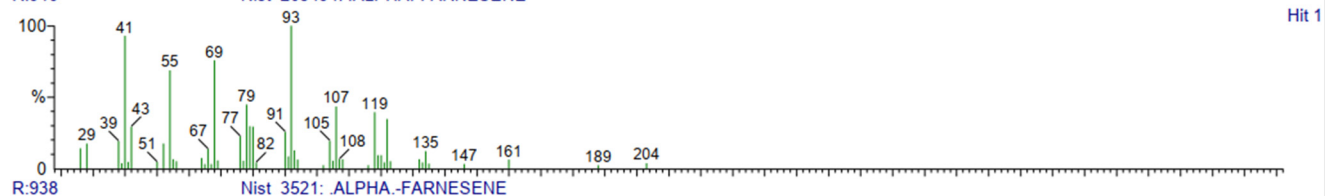
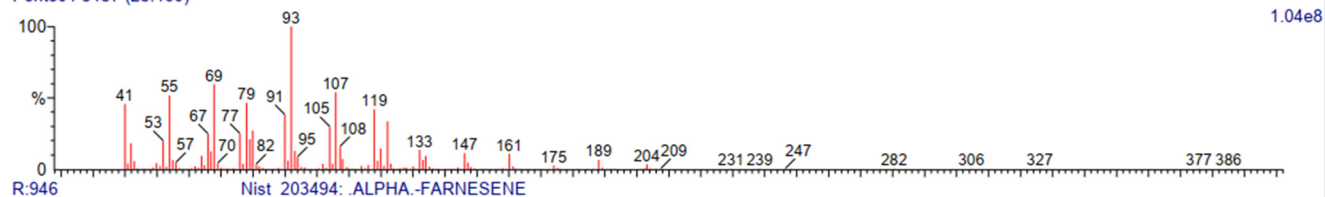
Hit 1



Hit 2

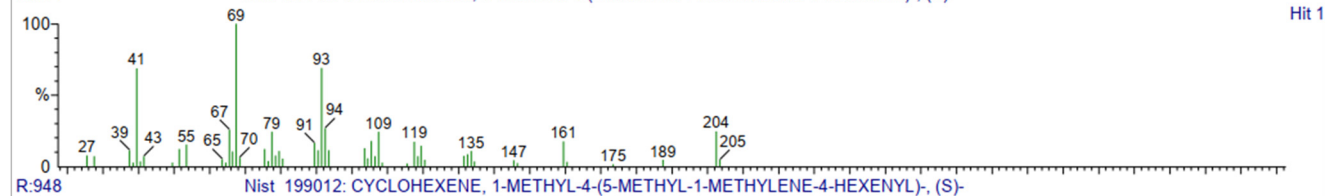
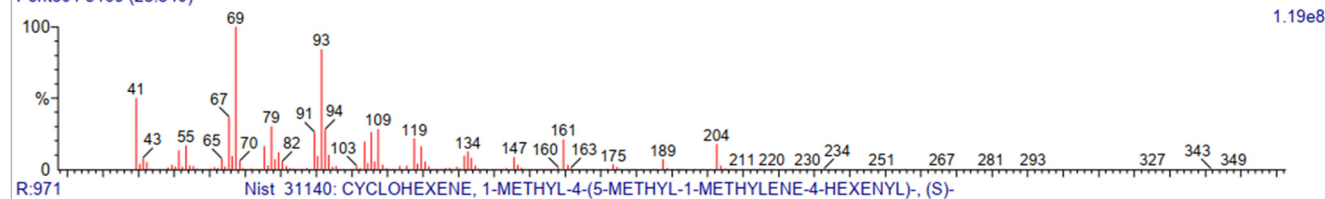
Entry 25: *E,E*- α -farnesene.

Ponto01 3157 (25.460)



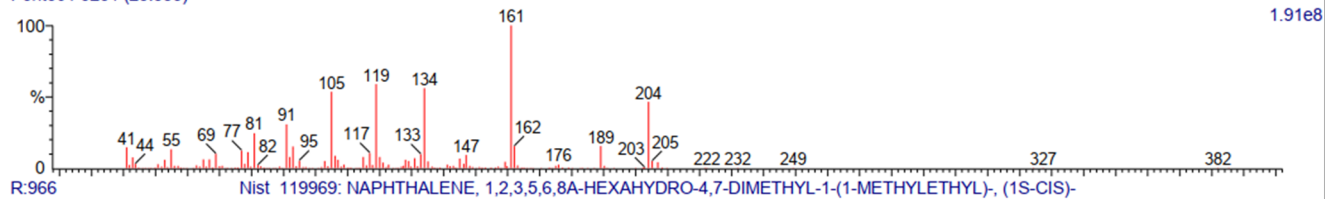
Entry 26: β -bisabolene.

Ponto01 3169 (25.540)

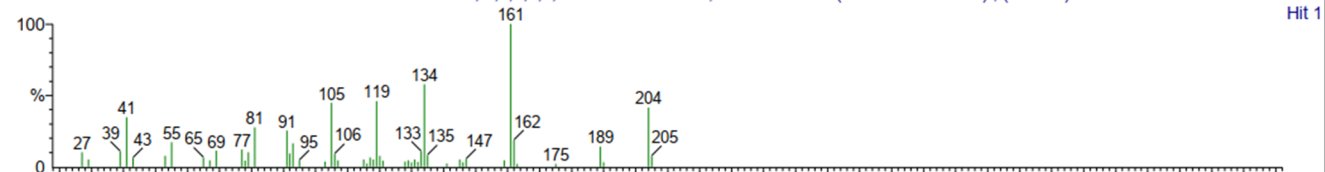


Entry 27: δ -cadinene.

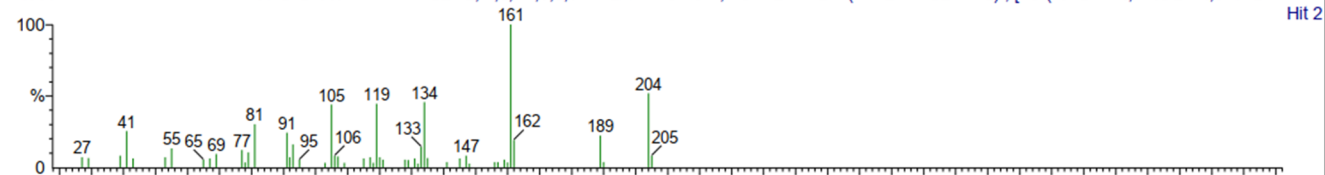
Ponto01 3231 (25.953)



R:966 Nist 119969: NAPHTHALENE, 1,2,3,5,6,8A-HEXAHYDRO-4,7-DIMETHYL-1-(1-METHYLETHYL)-, (1S-CIS)-

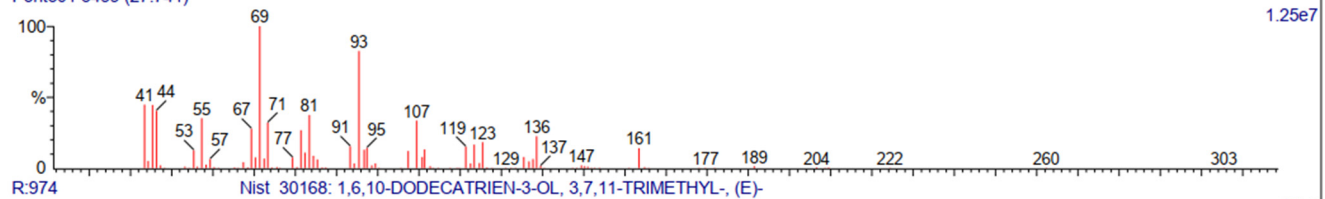


R:965 Nist 212733: NAPHTHALENE, 1,2,4A,5,8,8A-HEXAHYDRO-4,7-DIMETHYL-1-(1-METHYLETHYL)-, [1S-(1ALPHA.,4A.BETA.,8A.ALPH

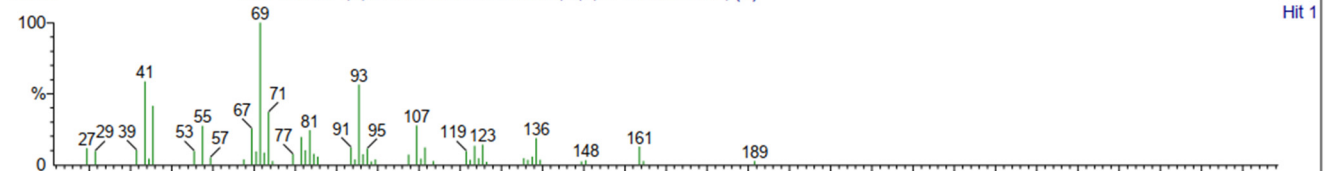


Entry 28: *E*-nerolidol.

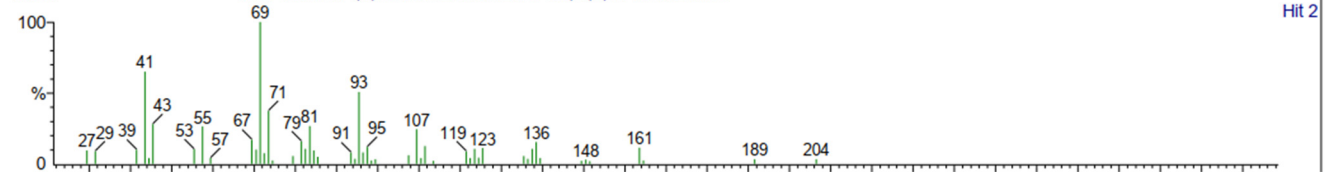
Ponto01 3499 (27.741)



R:974 Nist 30168: 1,6,10-DODECATRIEN-3-OL, 3,7,11-TRIMETHYL-, (E)-



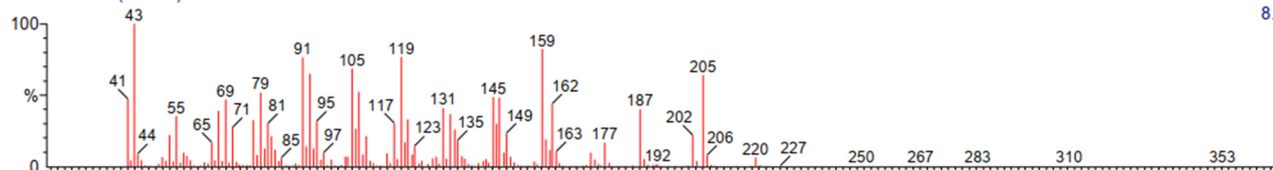
R:960 Nist 199011: 1,6,10-DODECATRIEN-3-OL, 3,7,11-TRIMETHYL-



Entry 29: spathulenol.

Ponto01 3587 (28.327)

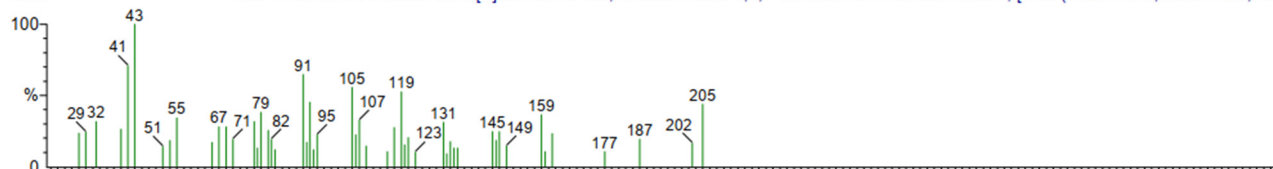
8.90e7



R:963

Nist 193210: 1H-CYCLOPROP[E]AZULEN-7-OL, DECAHYDRO-1,1,7-TRIMETHYL-4-METHYLENE-, [1AR-(1A.ALPHA.,4A.ALPHA.,7.BET

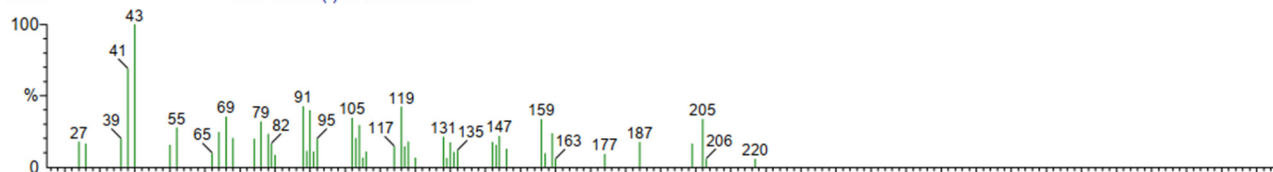
Hit 1



R:957

Nist 5917: (-)-SPATHULENOL

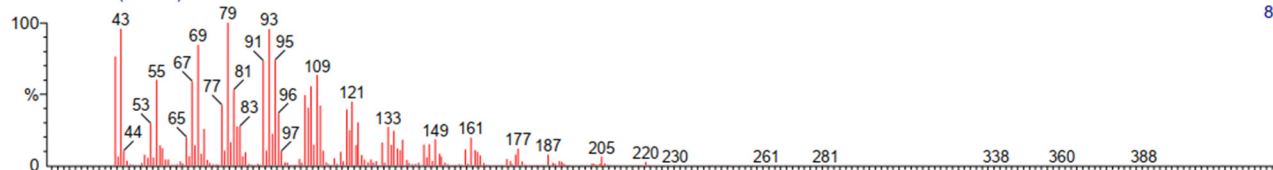
Hit 2



Entry 30: caryophyllene oxide.

Ponto01 3604 (28.441)

8.22e7



R:963

Nist 193197: CARYOPHYLLENE OXIDE

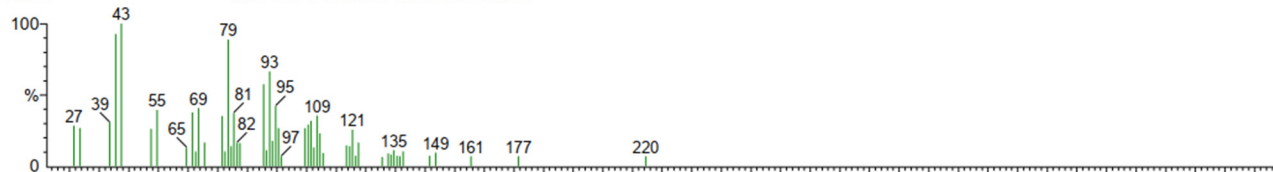
Hit 1



R:924

Nist 5854: CARYOPHYLLENE OXIDE

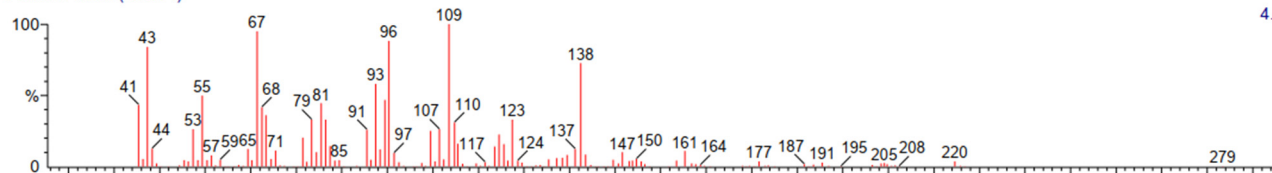
Hit 2



Entry 31: humulene-1,2-epoxide.

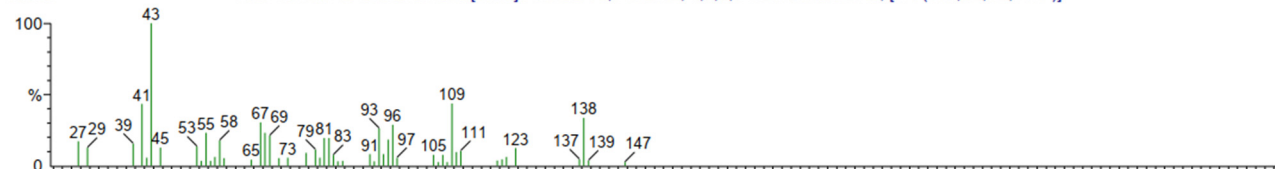
Ponto01 3759 (29.474)

4.93e7



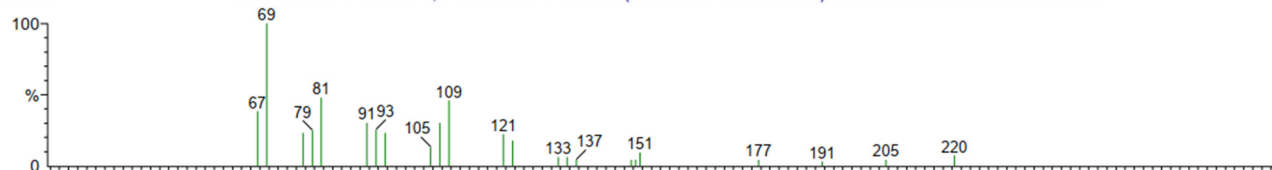
R:888 Nist 10120: 12-OXABICYCLO[9.1.0]DODECA-3,7-DIENE, 1,5,5,8-TETRAMETHYL-, [1R-(1R*,3E,7E,11R*)]-

Hit 1



R:829 Nist 30974: 1-FORMYL-2,2-DIMETHYL-3-TRANS-(3-METHYL-BUT-2-ENYL)-6-METHYLIDENE-CYCLOHEXANE

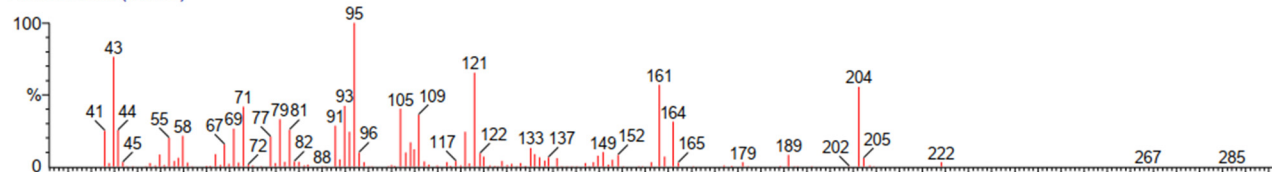
Hit 2



Entry 32: It was assigned as τ -muurolol by the fact that α -cadinol is in entry 33.

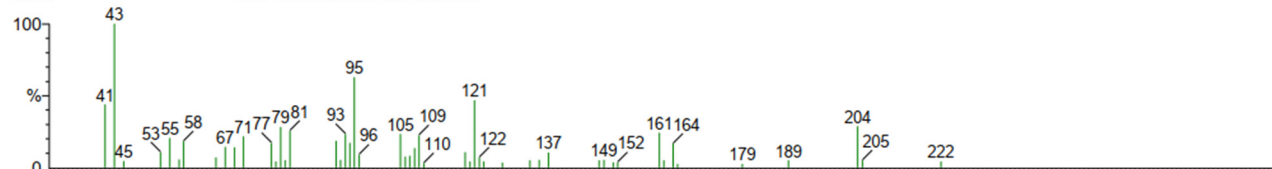
Ponto01 3958 (30.802)

2.24e7



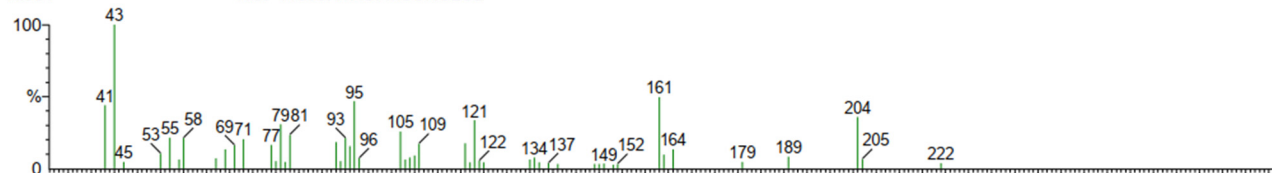
R:939 Nist 9521: ALPHA-CADINOL

Hit 1



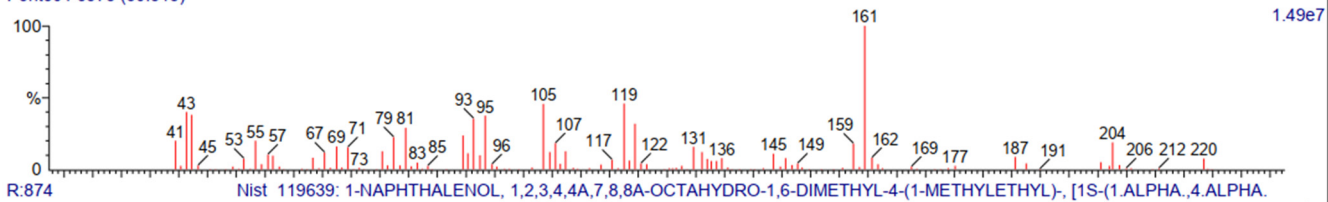
R:931 Nist 11663: TAU-MUUROLOL

Hit 2



Entry 33: α -muurolol.

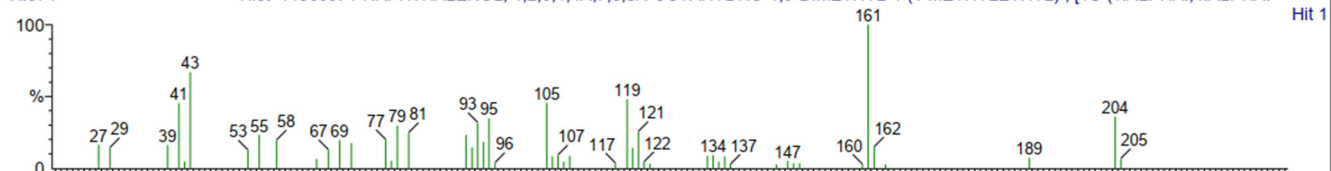
Ponto01 3975 (30.915)



R:874

Nist 119639: 1-NAPHTHALENOL, 1,2,3,4,4A,7,8,8A-OCTAHYDRO-1,6-DIMETHYL-4-(1-METHYLETHYL)-, [1S-(1-ALPHA.,4-ALPHA.

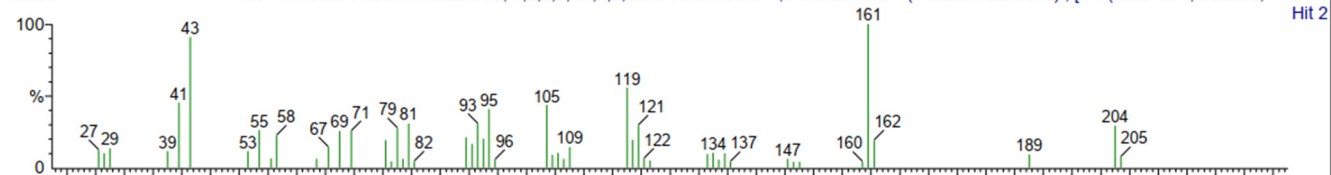
Hit 1



R:869

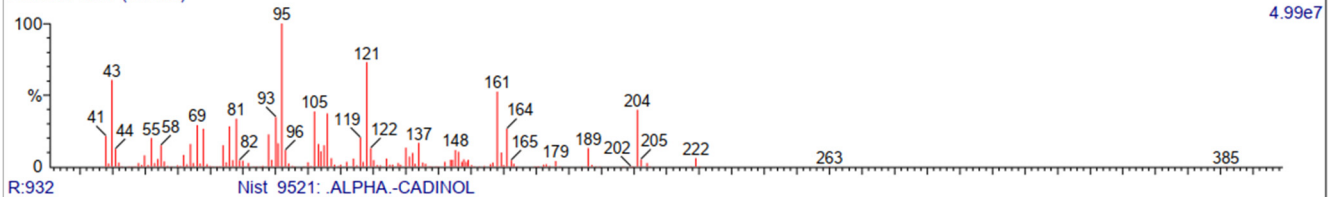
Nist 119638: 1-NAPHTHALENOL, 1,2,3,4,4A,7,8,8A-OCTAHYDRO-1,6-DIMETHYL-4-(1-METHYLETHYL)-, [1R-(1-ALPHA.,4-BETA.,

Hit 2



Entry 34: α -cadinol

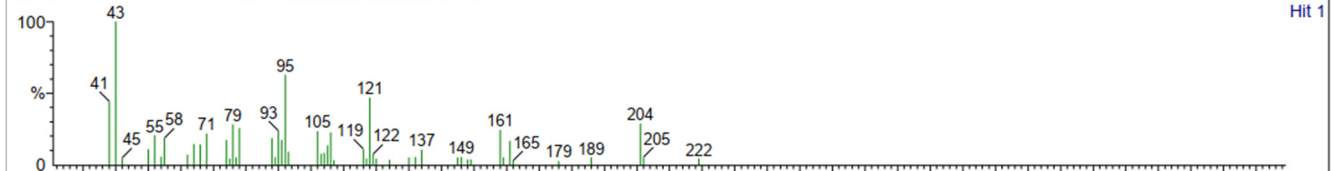
Ponto01 4017 (31.195)



R:932

Nist 9521: ALPHA-CADINOL

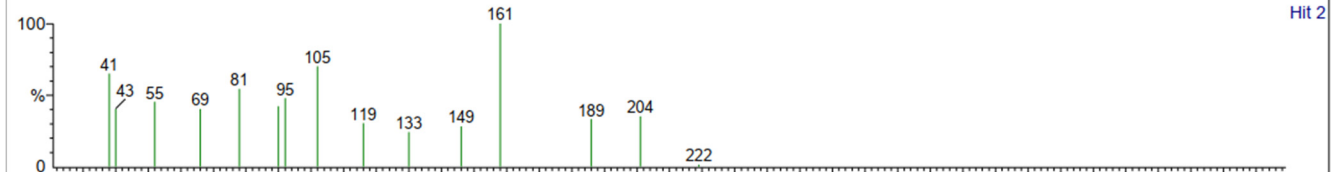
Hit 1



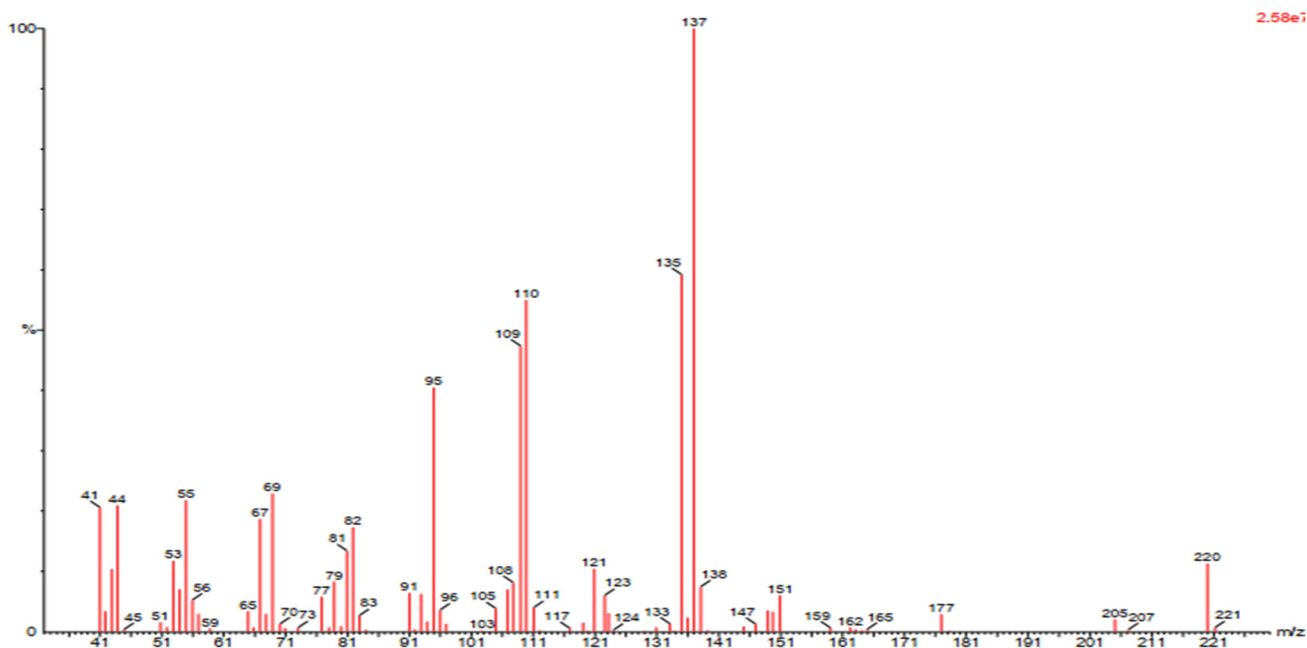
R:920

Nist 119818: DIHYDRO-CIS-ALPHA-COPAENE-8-OL

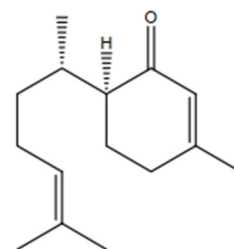
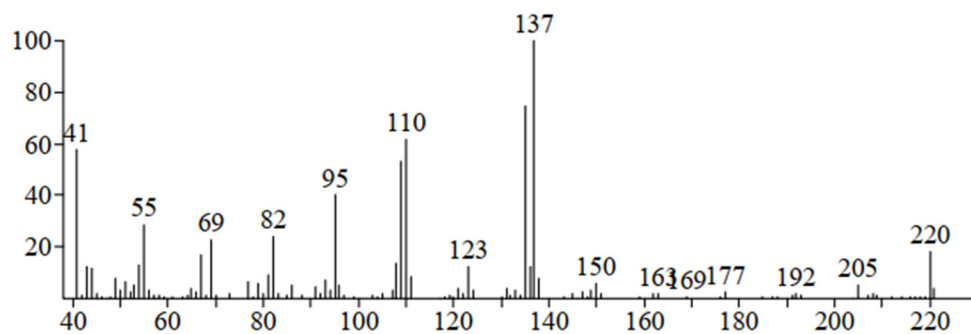
Hit 2



Entry 35: 6*R*,7*R*-bisabolone (AI_{lit} 1740). Retention time 34.38 min.

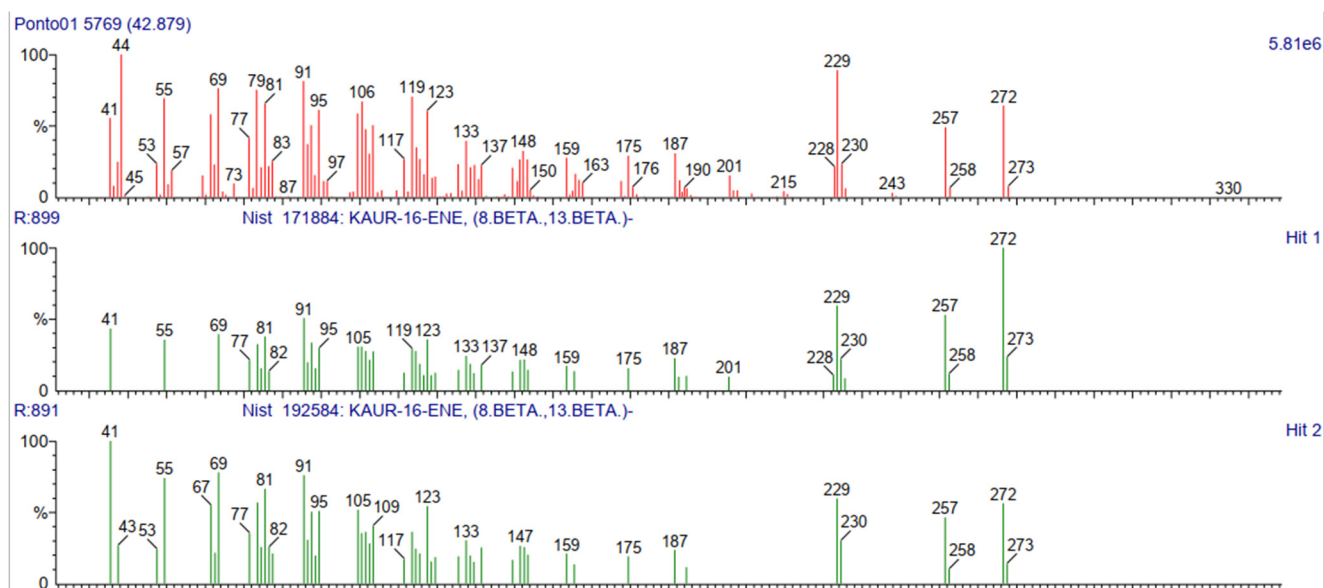


RT: 38.24 AI: 1740 KI: 1742 **Bisabolone <(6*R*,7*R*)>**
 CAS#: 72441-71-5 MF: C₁₅H₂₄O FW: 220 MSD LIB#: 138
 CN: 2-cyclohexen-1-one, 6-(1,5-dimethyl-4-hexenyl)-3-methyl-, (R-(R*,R*))-
 Synonyms: α-oxobisabolene
 Source: Amyris, comm. oil, Haiti ex Harold Bussenins; 0.30% *Amyris balsamifera*,
 Phytochem 28:1909(1989)



Mass spectrum of 6*R*,7*R*-bisabolone from literature [16].

Entry 36: kaur-16-ene



Reference

- [16] Adams, R.P. Identification of essential oils components by gas chromatography, mass spectroscopy. 4th ed.; Allured Publishing: Carol Stream, USA, 2017; 809 pp.