The report should be submitted until December 4th 6 p.m.

The results of MICs and checkerboard will be uploaded soon.

Fill the below tables for each **essential oil** (from page 3 to 5) completely and use both tables and total ion chromatograms (TICs) for your report.

Please access the site for CAS registry number search engine.

(**http://webbook.nist.gov/chemistry/cas-ser.html**)

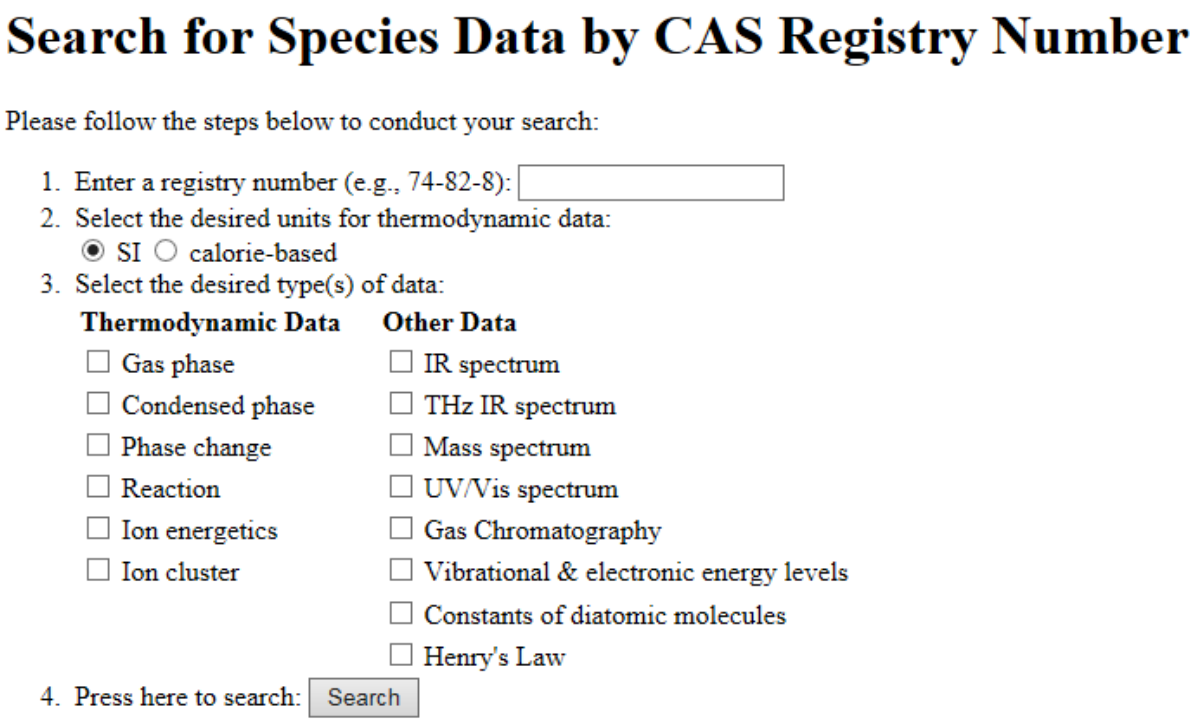
Enter a CAS registry number with hyphen sign and determine the compound names.

If there is a complexed name rather than the simple one, check "**Other names**" section to find a common name whose suffix may be –ol or –ene.

Note that most of terpenoid compounds have –ol or –ene as a suffix.

Note that a semicolon, not a comma, divides the listed names in "Other names" section.

Following figures describe the above procedure.



Search for Species Data by CAS Registry Number

Please follow the steps below to conduct your search:

1. Enter a registry number (e.g., 74-82-8):
2. Select the desired units for thermodynamic data:
   ◉ SI ○ calorie-based
3. Select the desired type(s) of data:

Thermodynamic Data	Other Data
☐ Gas phase	☐ IR spectrum
☐ Condensed phase	☐ THz IR spectrum
☐ Phase change	☐ Mass spectrum
☐ Reaction	☐ UV/Vis spectrum
☐ Ion energetics	☐ Gas Chromatography
☐ Ion cluster	☐ Vibrational & electronic energy levels
	☐ Constants of diatomic molecules
	☐ Henry's Law

4. Press here to search: Search

At first, you will encounter this main page of the website.

Search for Species Data by CAS Registry Number

Please follow the steps below to conduct your search:

1. Enter a registry number (e.g., 74-82-8): 7212-44-4
2. Select the desired units for thermodynamic data:
   ◉ SI ○ calorie-based
3. Select the desired type(s) of data:

Thermodynamic Data	Other Data
☐ Gas phase	☐ IR spectrum
☐ Condensed phase	☐ THz IR spectrum
☐ Phase change	☐ Mass spectrum
☐ Reaction	☐ UV/Vis spectrum
☐ Ion energetics	☐ Gas Chromatography
☐ Ion cluster	☐ Vibrational & electronic energy levels
	☐ Constants of diatomic molecules
	☐ Henry's Law

4. Press here to search: Search

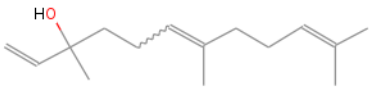
Enter a CAS registry number with hyphen sign.

1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-

- **Formula:** $C_{15}H_{26}O$
- **Molecular weight:** 222.3663
- **IUPAC Standard InChI:**
  - InChI=1S/C15H26O/c1-6-15(5,16)12-8-11-14(4)10-7-9-13(2)3/h6,9,11,16H,1,7-8,10,12H2,2-5H3
  - Download the identifier in a file.

InChITRUST CERTIFIED 2011

- **IUPAC Standard InChIKey:** FQTLCLSUCSAZDY-UHFFFAOYSA-N
- **CAS Registry Number:** 7212-44-4
- **Chemical structure:**



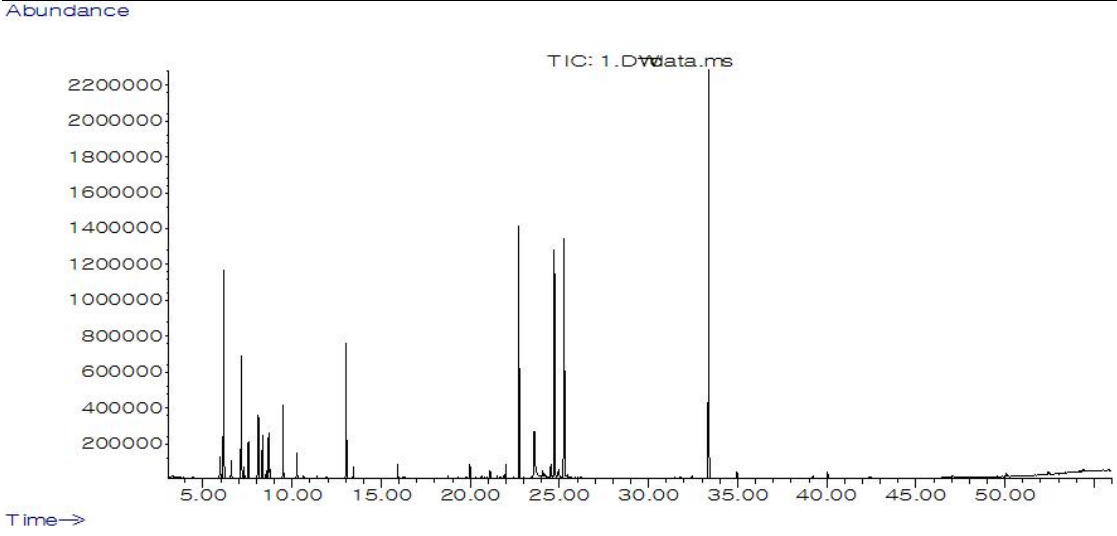
This structure is also available as a 2d Mol file or as a computed 3d SD file
The 3d structure may be viewed using Java or Javascript.

- **Stereoisomers:**
  - Nerolidol
  - 1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (E)-
  - Nerolidol isomer
  - β-Nerolidol
  - +/--trans-Nerolidol
  - β-Nerolidol
- **Other names:** Nerolidol; 3,7,11-Trimethyl-1,6,10-dodecatrien-3-ol; 3,7,11-Trimethyldodeca-1,6,10-trien-3-ol; 3-Hydroxy-3,7,11-trimethyl-dodecatriene-3-ol; FCI 119b; 3,7,11-trimethyl-1,6,10-dodecatrien-3-ol (nerolidol); 3,7,11-trimethyldodeca-1,6,10-trien-3-ol,mixed isomers

Check and determine the name of interesting compound.

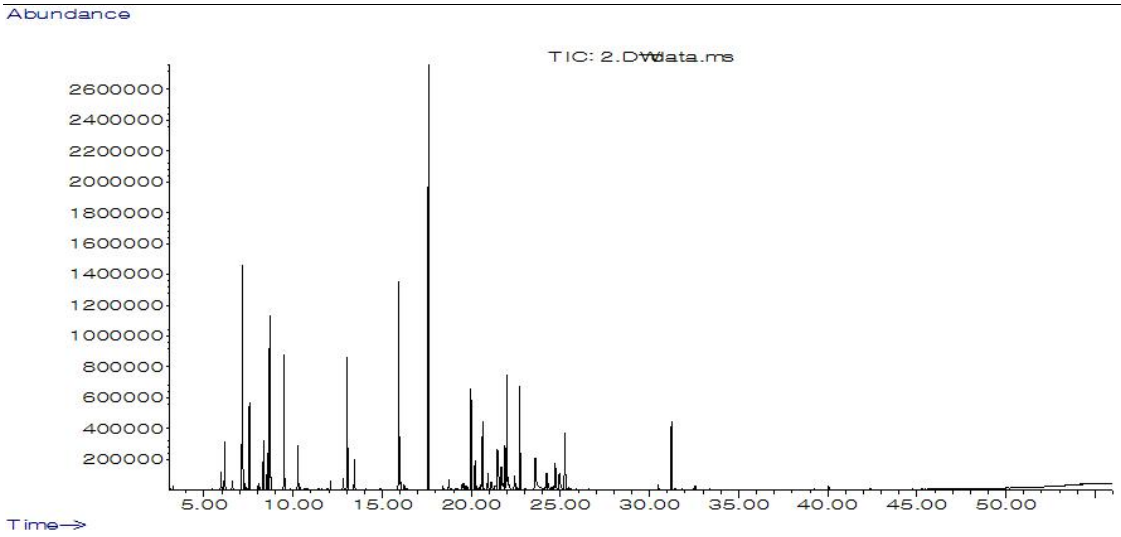
Cryptomeria japonica

Compounds	Relative proportion (%)	Retention time	CAS Registry Number
	19.36	33.37	020070-61-5
	12.18	34.70	000473-15-4
	10.93	22.72	000639-99-6
	10.61	24.71	001209-71-8
	9.84	6.16	000080-56-8
	5.71	13.03	000098-55-5
	5.53	7.15	003387-41-5
	3.05	8.11	013466-78-9
	3.01	9.48	000099-85-4
	2.02	8.68	000138-86-3
	1.97	8.34	000099-86-5
	1.64	7.54	000123-35-3
	1.18	5.96	002867-05-2
	1.06	10.26	000586-62-9
	0.98	6.58	000079-92-5
	0.72	19.97	000470-40-6
	0.67	21.99	000483-76-1
	0.63	15.92	005655-61-8
	0.57	7.30	000127-91-3
	0.38	24.97	019912-62-0
	0.38	21.11	023986-74-5
	0.38	8.74	000555-10-2
	0.35	24.92	003856-25-5



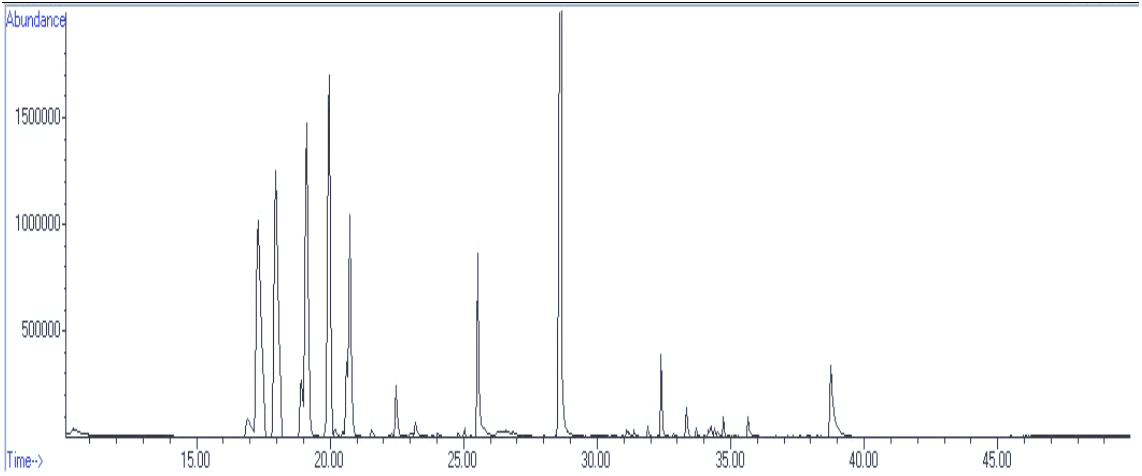
Chamaecyparis obtusa

Compounds	Relative proportion (%)	Retention time	CAS Registry Number
	15.67	17.59	000079-92-5
	8.96	7.15	000099-85-4
	7.69	15.93	005655-61-8
	6.60	8.68	000138-86-3
	4.75	9.49	000099-85-4
	4.71	13.03	000562-74-3
	4.47	21.99	000483-76-1
	4.03	19.97	000470-40-6
	3.91	22.72	000123-35-3
	3.27	7.54	000123-35-3
	2.72	25.25	051317-08-9
	2.69	31.22	003564-54-3
	2.62	20.63	023986-74-5
	1.92	6.16	007785-26-4
	1.90	8.34	000099-86-5
	1.57	21.47	022567-17-5
	1.54	10.26	000098-55-5
	1.06	24.71	001209-71-8
	1.04	21.67	001461-03-6
	0.72	24.22	000077-53-2
	0.42	18.75	000515-13-9
	0.35	12.10	000076-22-2
	0.30	19.56	000087-44-5
	0.29	7.30	000127-91-3
	0.27	19.48	000546-28-1
	0.18	8.05	000099-83-2



Abies holophylla

Compounds	Relative proportion (%)	Retention time	CAS Registry Number
	20.91	28.624	005655-61-8
	14.99	17.958	000079-92-5
	14.41	17.304	000080-56-8
	13.90	19.953	000498-15-7
	13.37	19.119	000123-35-3
	9.14	20.736	003387-41-5
	4.79	25.527	000507-70-0
	3.33	38.757	000515-69-5
	2.09	18.921	018172-67-3
	1.66	32.400	000087-44-5
	1.41	22.474	029050-33-7



GC/MS condition

Column: HP5-MS

Carrier gas: He

Temperature: injector 250℃, detector 300℃

Oven temperature:

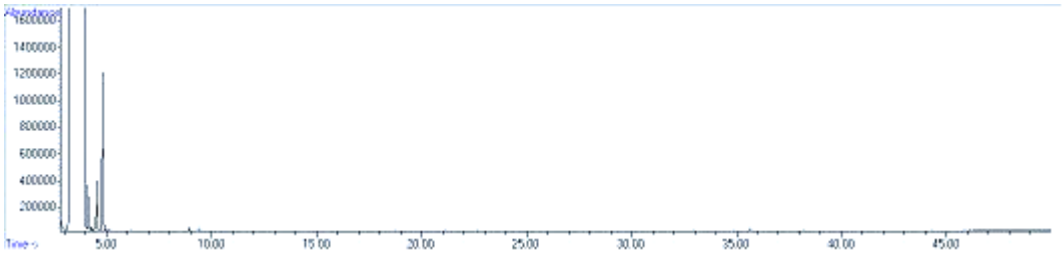
Initial temperature at 35℃ during 10 min
increasing temperature with 8℃/min by 120℃
increasing temperature with 4℃/min by 200℃
Increasing temperature with 8℃/min by 280℃
Final temperature at 330℃ (10 min)

Main Compounds in Essential oil Fractions

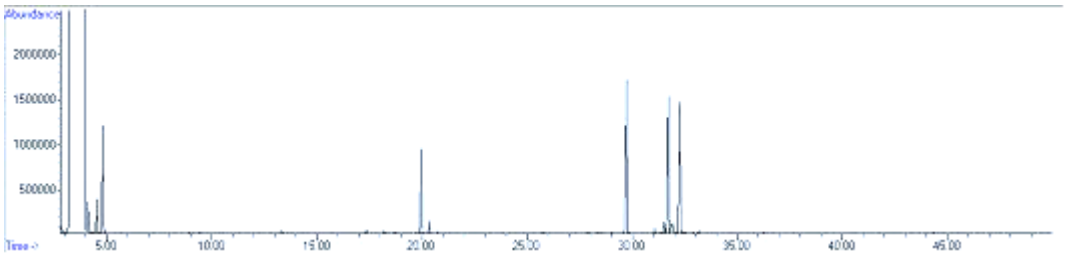
Cryptomeria japonica

Fraction	Main Compound	Retention Time
1	-	-
2	Terpinen-4-ol	19.976
	Elemol	29.743
	γ-Eudesmol	31.723
	β-Eudesmol	32.289
3	Terpinen-4-ol	19.947
	Bornyl acetate	22.905
4	Nezukol	41.805
5	Kaurene	40.329
	δ-Cadinene	28.953

Fraction 1



Fraction 2



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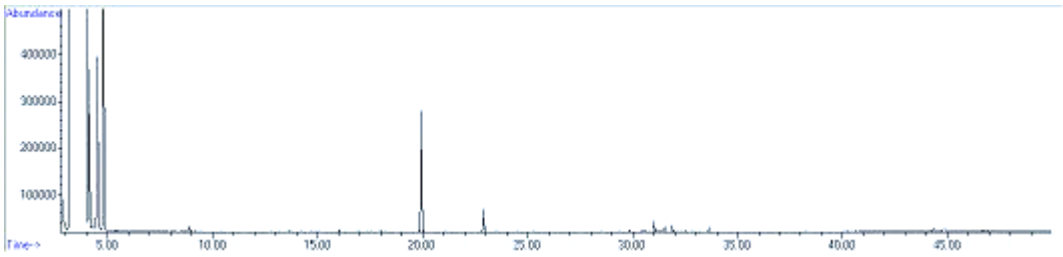

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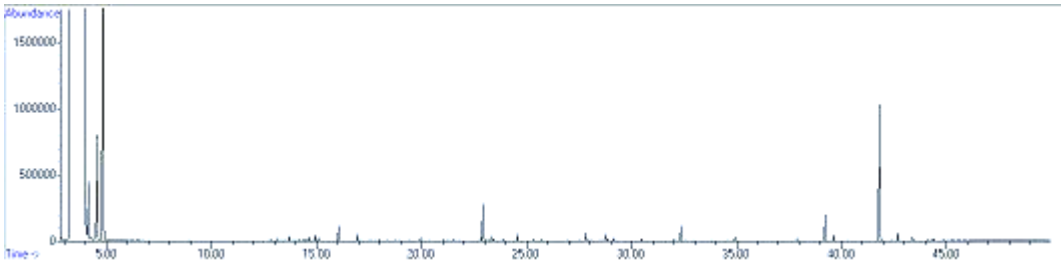

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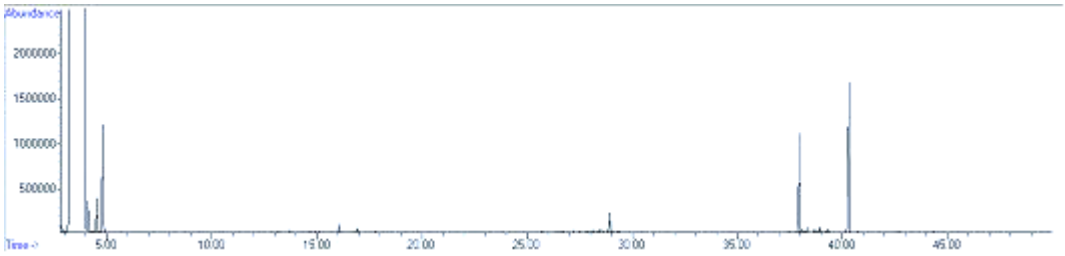
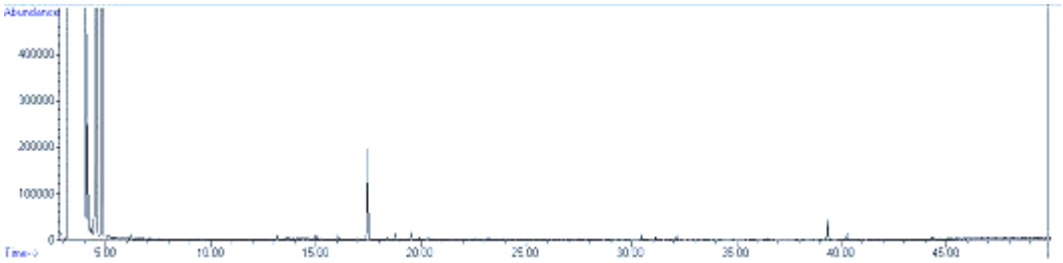


Chamaecyparis obtusa

Fraction	Main Compound	Retention Time
1	-	-
2	Terpinen-4-ol	19.947
	Elemol	29.686
	α-Eudesmol	32.215
3	Terpinen-4-ol	19.935
4	Bornyl acetate	22.905
5	Bornyl acetate	22.917
	2-Carene	24.588
6	δ-Cadinene	28.959
	Thujopsene	27.014
	β-Cubebene	27.643
	γ-Cadinene	28.868
	Beyerene	38.154

Fraction 1



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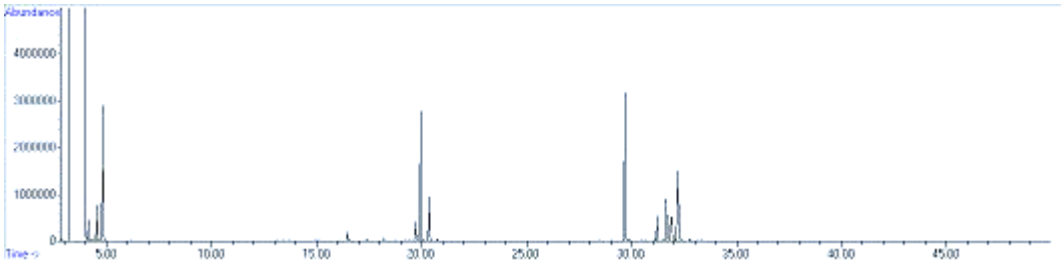

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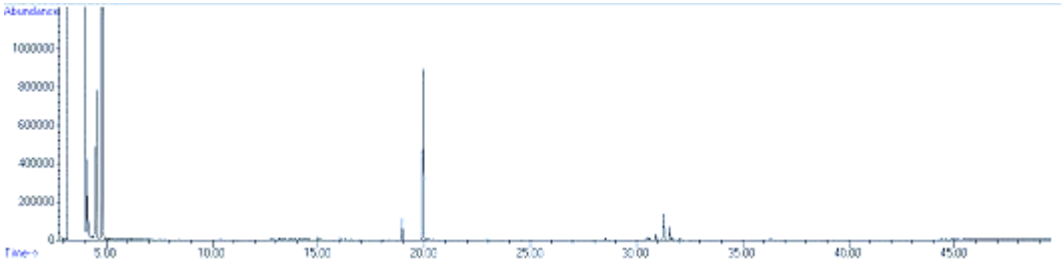

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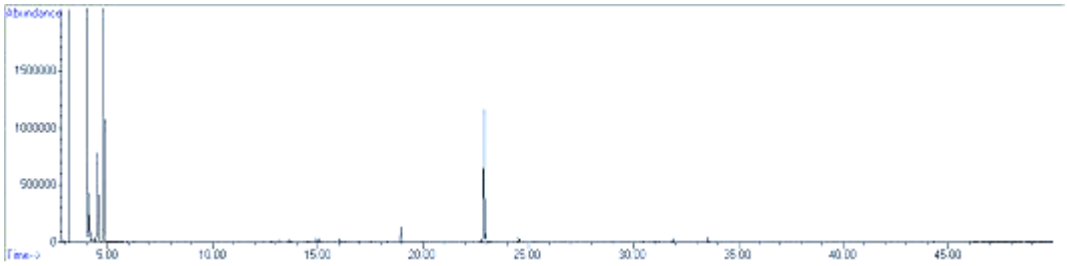
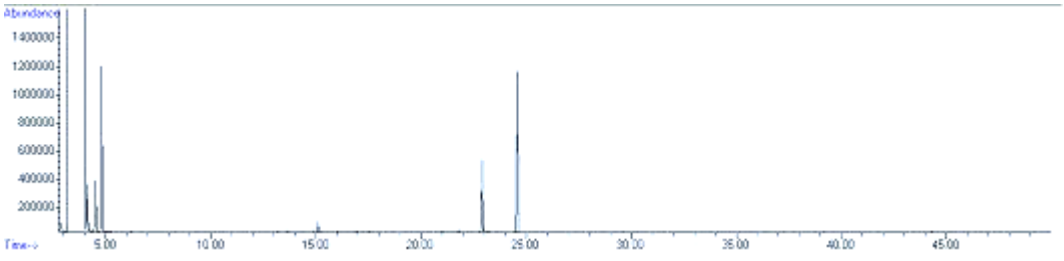
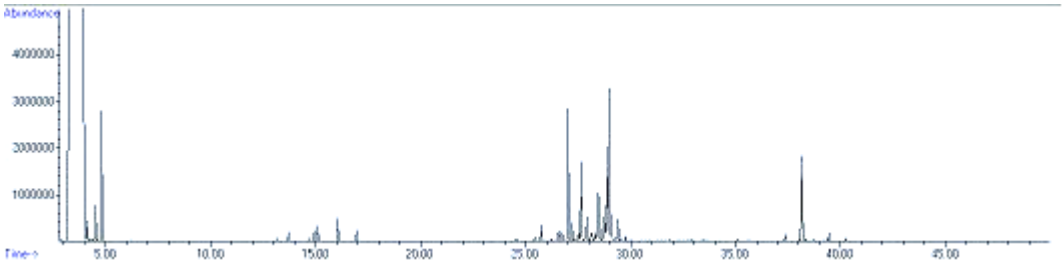


Fraction 5



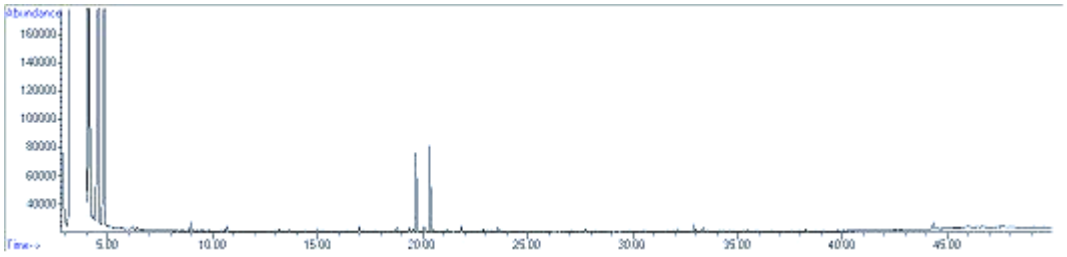
Fraction 6



Abies holophylla

Fraction	Main Compound	Retention Time
1	Borneol	19.707
	α-Terpineol	20.359
2	Borneol	19.718
3	α-Bisabolol	32.827
	Nerolidol	29.875
4	bornyl acetate	22.905
5	bornyl acetate	22.945
6	β-Myrcene	13.693
	Caryophyllene	26.596
	α-Humulene	27.494

Fraction 1



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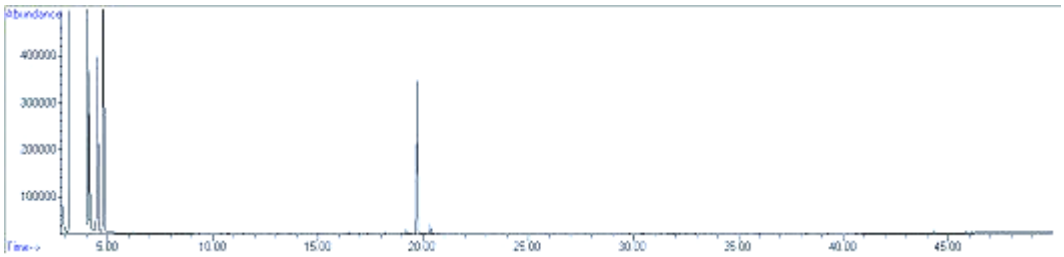

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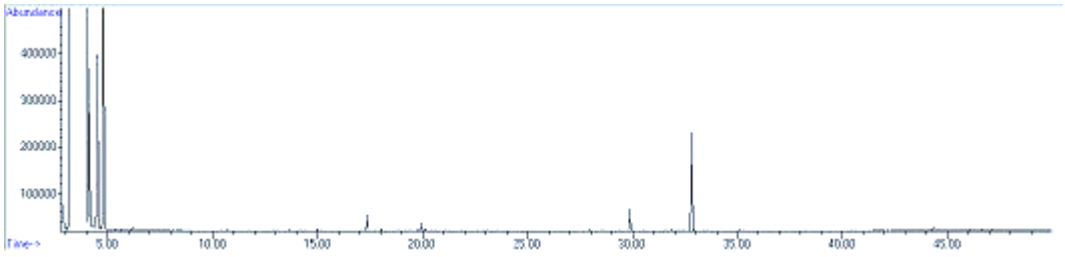

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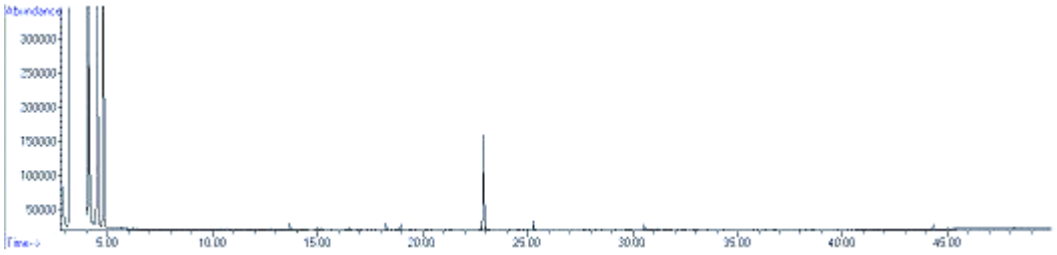

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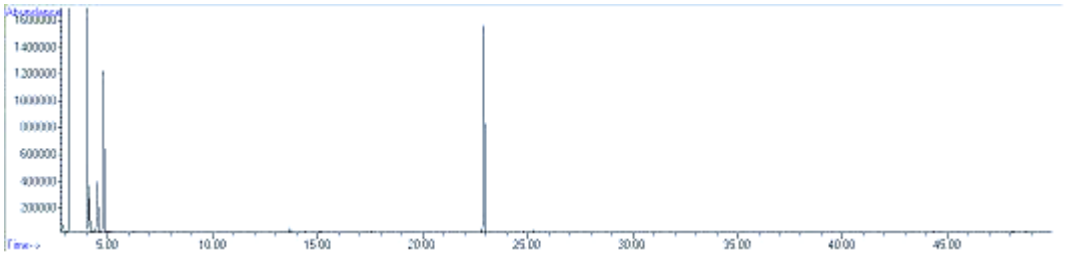
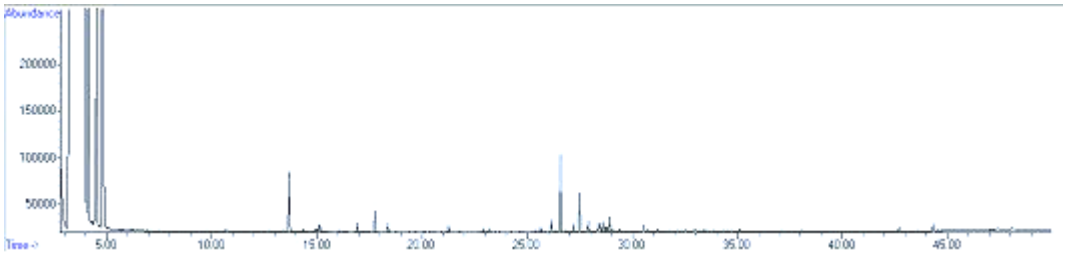
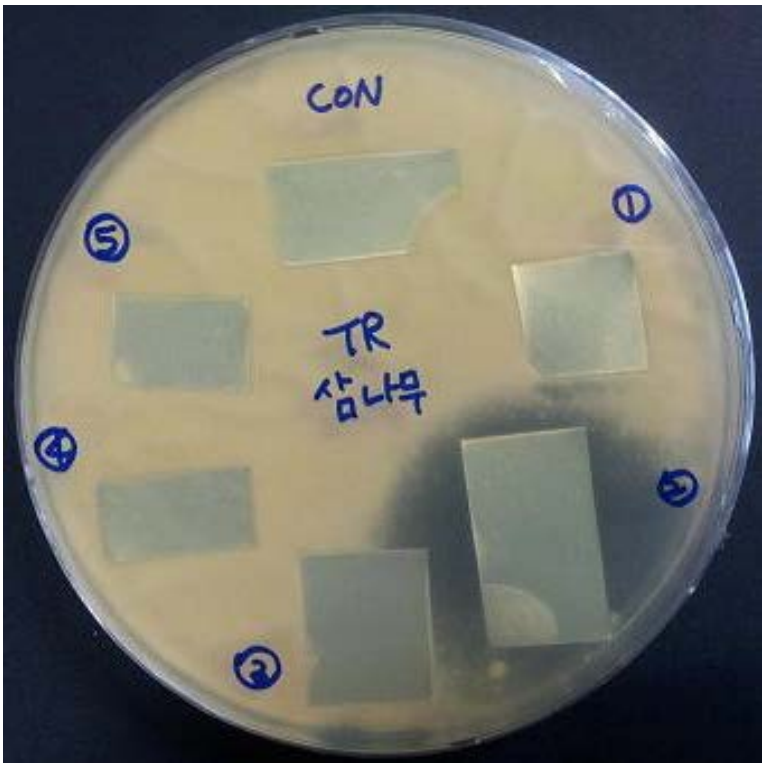
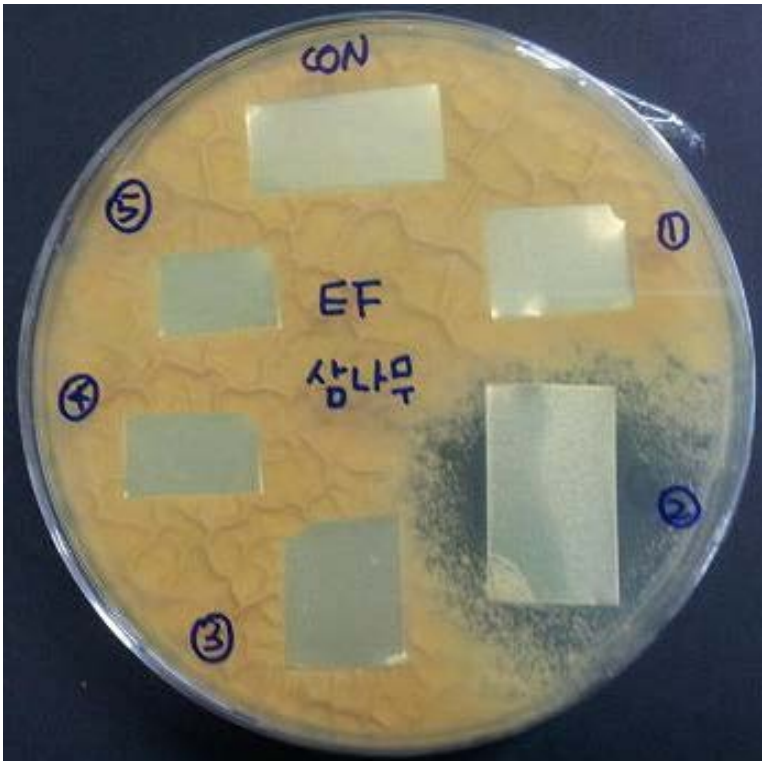


Fraction 6

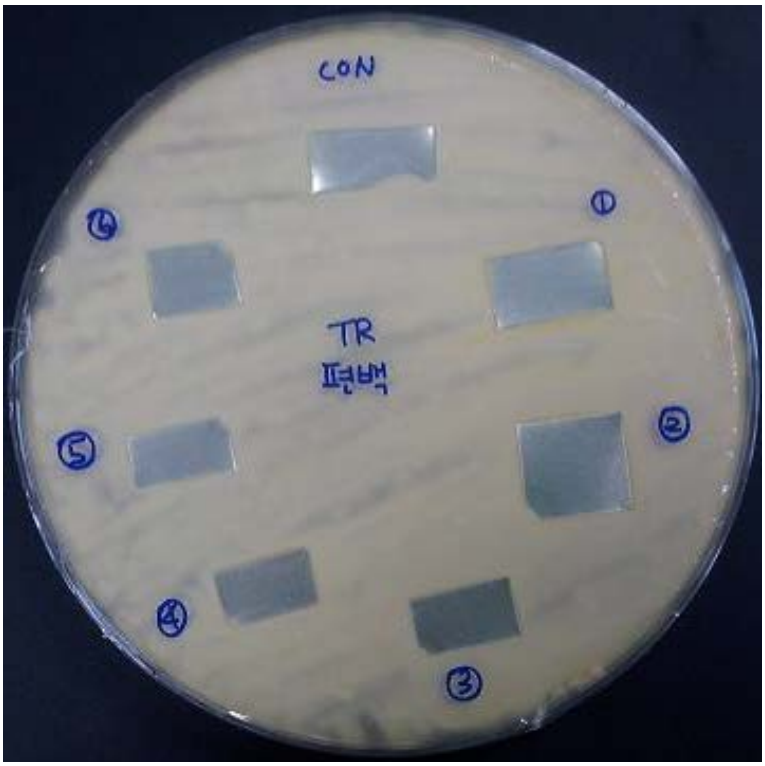
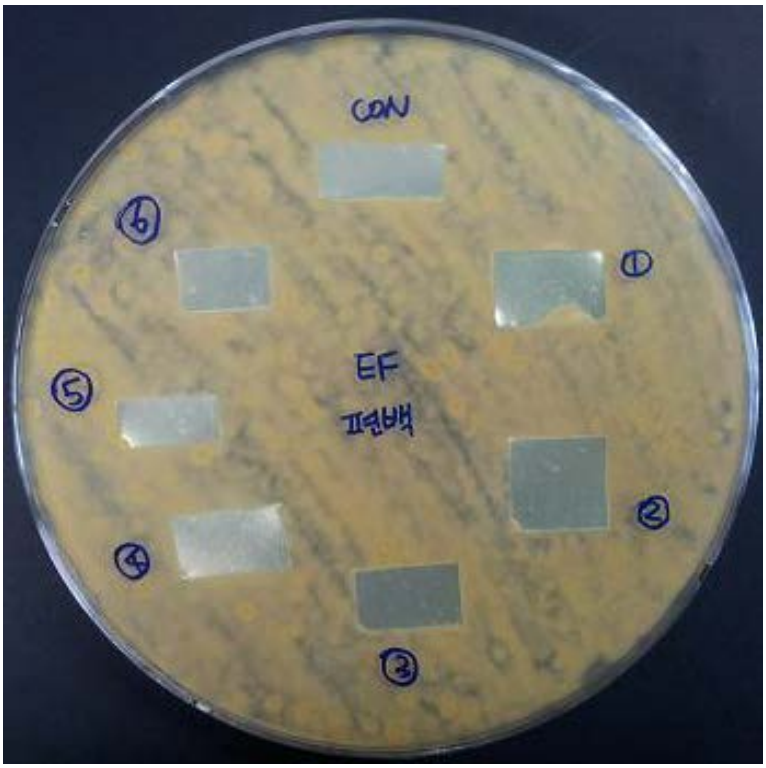


Antifungal activity by TLC bioassay

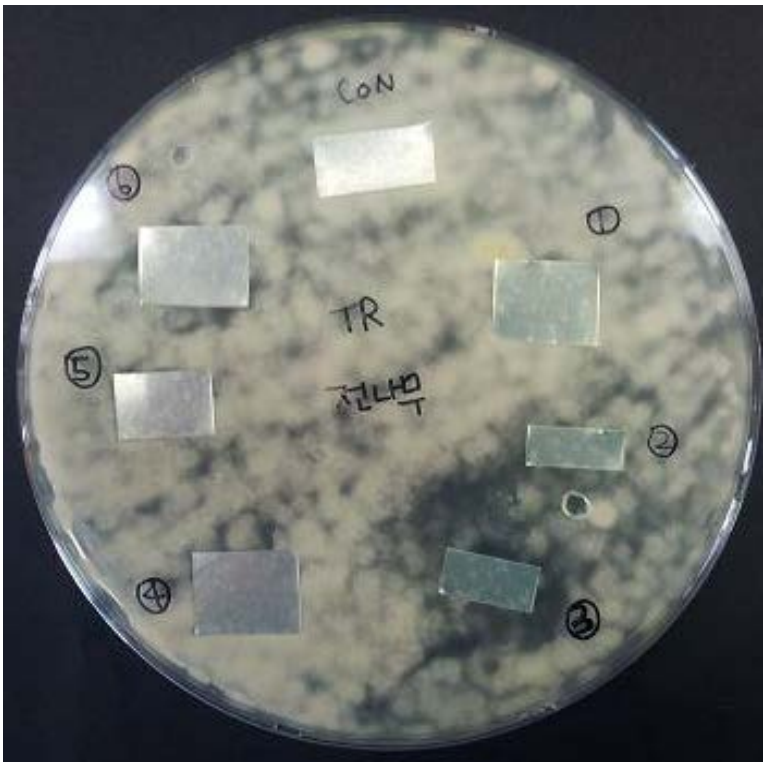
Cryptomeria japonica

Trichophyton rubrum

Epidermophyton floccosum


Chamaecyparis obtusa

Trichophyton rubrum

Epidermophyton floccosum


Abies holophylla

Trichophyton rubrum

Epidermophyton floccosum