# Analysis of frankincense essential oil compositions by GC-MS

## 1 Instruments and reagents

GC-MS3100 gas chromatograph/mass spectrometer (EAST & WEST ANALYTICAL INSTRUMENTS, INC); Equity-5 (30m×0.25mm×0.25um) silica capillary column; 1 μL micro injector;

Sample: frankincense essential oil

## 2 Analysis conditions

**MS conditions:** EI source; ion source temperature: 200℃; electron energy: 70eV; scanning mode: full scan; scanning range: 28.5u～400u; scanning period: 0.6 s; interface temperature: 250 ℃; multiplier high voltage: 1200 V.

**GC conditions:** Equity-5 (30m×0.25mm×0.25um) silica capillary column; injection port temperature: 250 ℃; split sampling; sample volume: 0.08 μL; column flow: 1 mL/min; split ratio: 70:1; precolumn pressure: 50 kPa; purge rate: 2ml/min; column temperature program: hold at 50℃ for 1min, ramp up to 250 ° C at 5 °C/min and then hold for 10 min.

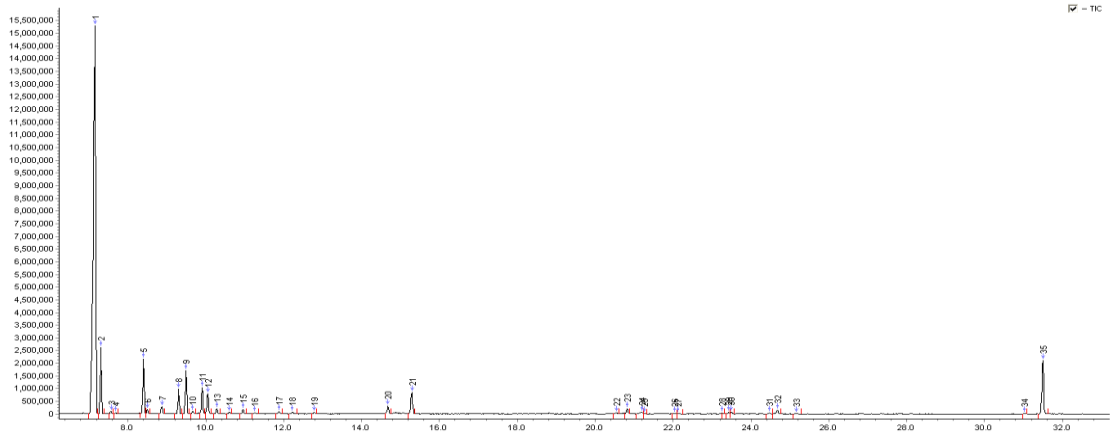

Figure 1 TIC chromatogram of frankincense essential oil

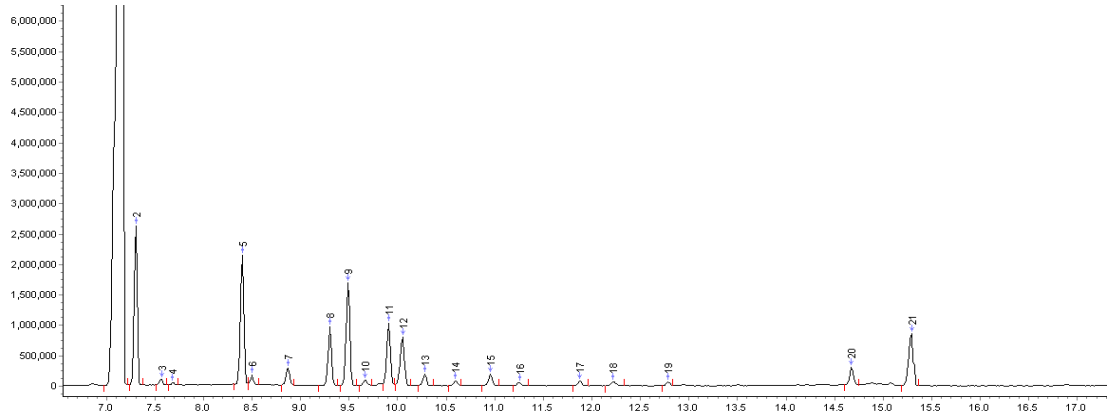

Figure 2 Partially magnified chromatogram

Table 1 Analysis results of frankincense essential oil composition

| Peak No. | Retention time, min | Name | CAS No | Molecular formula | relative amount, % | similarity degree, % |
|---|---|---|---|---|---|---|
| 1 | 7.15 | 1-Isopropyl-4-methylbicyclo[3.1.0]hex-2-ene | 58037-87-9 | $C_{10}H_{16}$ | 64.41 | 95 |
| 2 | 7.30 | Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl-, (1R)- | 7785-70-8 | $C_{10}H_{16}$ | 5.43 | 93 |
| 3 | 7.55 | Bicyclo[3.1.0]hex-2-ene, 4-methylene-1-(1-methylethyl)- **（2,4(10)-Thujadiene）** | 36262-09-6 | $C_{10}H_{14}$ | 0.21 | 83 |
| 4 | 7.68 | 4-Carene, (1S,3R,6R)-(-)- | 5208-49-1 | $C_{10}H_{16}$ | 0.06 | 74 |
| 5 | 8.40 | Phellandrene | 555-10-2 | $C_{10}H_{16}$ | 4.92 | 90 |
| 6 | 8.50 | beta-Pinene | 127-91-3 | $C_{10}H_{16}$ | 0.29 | 83 |
| 7 | 8.86 | 1,6-Octadiene, 7-methyl-3-methylene- **（Myrcene）** | 123-35-3 | $C_{10}H_{16}$ | 0.67 | |
| 8 | 9.30 | 1,3-Cyclohexadiene, 2-methyl-5-(1-methylethyl)- | 99-83-2 | $C_{10}H_{16}$ | 2.14 | 91 |
| 9 | 9.49 | 3-Carene | 13466-78-9 | $C_{10}H_{16}$ | 4.14 | |
| 10 | 9.66 | Cyclohexene, 1-methyl-4-(1-methylethylidene)- | 586-62-9 | $C_{10}H_{16}$ | 0.21 | 85 |
| 11 | 9.91 | Benzene, 1-methyl-4-(1-methylethyl)- **（p-Cymene）** | 99-87-6 | $C_{10}H_{14}$ | 2.40 | 90 |
| 12 | 10.05 | D-Limonene | 5989-27-5 | $C_{10}H_{16}$ | 2.11 | 88 |
| 13 | 10.28 | 1,3,6-Octatriene, 3,7-dimethyl-, (E)- | 3779-61-1 | $C_{10}H_{16}$ | 0.43 | 91 |
| 14 | 10.60 | 1,3,6-Octatriene, 3,7-dimethyl-, (Z)- | 3338-55-4 | $C_{10}H_{16}$ | 0.17 | 81 |

| Peak No. | Retention time, min | Name | CAS No | Molecular formula | relative amount, % | similarity degree, % |
|---|---|---|---|---|---|---|
| 15 | 10.95 | 1,4-Cyclohexadiene, 1-methyl-4-(1-methylethyl)- | 99-85-4 | $C_{10}H_{16}$ | 0.47 | 85 |
| 16 | 11.26 | 5-Isopropyl-2-methylbicyclo[3.1.0]hexan-2-ol cis-Sabinenehydrate | 15826-82-1 | $C_{10}H_{18}O$ | 0.12 | 82 |
| 17 | 11.87 | 2-Carene | 554-61-0 | $C_{10}H_{16}$ | 0.18 | 86 |
| 18 | 12.22 | Terpineol, cis- | 7299-41-4 | $C_{10}H_{18}O$ | 0.20 | 80 |
| 19 | 12.78 | Thujone | 546-80-5 | $C_{10}H_{16}O$ | 0.16 | 86 |
| 20 | 14.67 | 1-Methyl-4-isopropyl-1-cyclohexen-4-ol （**4-Terpineol**） | 562-74-3 | $C_{10}H_{18}O$ | 0.76 | 84 |
| 21 | 15.28 | Anisole, p-allyl- | 140-67-0 | $C_{10}H_{12}O$ | 2.61 | 92 |
| 22 | 20.55 | Tricyclo[4.4.0.0(2,7)]dec-3-ene, 8-isopropyl-1,3-dimethyl- | 3856-25-5 | $C_{15}H_{24}$ | 0.10 | 74 |
| 23 | 20.82 | Cyclobuta[1,2:3,4]dicyclopentene, decahydro-3a-methyl-6-methylene-1-(1-methylethyl)-, | 5208-59-3 | $C_{15}H_{24}$ | 0.46 | 88 |
| 24 | 21.19 | Benzene, 1,2-dimethoxy-4-(2-propenyl)- | 93-15-2 | $C_{11}H_{14}O_2$ | 0.26 | 84 |
| 25 | 21.26 | Humulen-(v1) | N/A | $C_{15}H_{24}$ | 0.03 | 74 |
| 26 | 22.04 | Germacrene D | 23986-74-5 | $C_{15}H_{24}$ | 0.04 | 76 |
| 27 | 22.12 | Bicyclo[3.1.1]hept-2-ene, 2,6-dimethyl-6-(4-methyl-3-pentenyl)- | 17699-05-7 | $C_{15}H_{24}$ | 0.04 | 78 |
| 28 | 23.43 | Naphthalene, 1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)- | 483-75-0 | $C_{15}H_{24}$ | 0.04 | 80 |
| 29 | 23.50 | Isocaryophillene | N/A | $C_{15}H_{24}$ | 0.05 | 81 |
| 30 | 24.48 | Cadina-1(10),4-diene | 483-76-1 | $C_{15}H_{24}$ | 0.09 | 70 |
| 31 | 24.68 | VERIDIFLOROL | N/A | $C_{15}H_{26}O$ | 0.55 | 68 |
| 32 | 25.17 | Benzene, 1,2,3-trimethoxy-5-(2-propenyl)- | 487-11-6 | $C_{12}H_{16}O_3$ | 0.07 | 81 |
| 33 | 31.03 | Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)- （**3-Thujene**） | 2867-05-2 | $C_{10}H_{16}$ | 0.05 | 76 |
| 34 | 31.50 | Isopropyl Myristate | 110-27-0 | $C_{17}H_{34}O_2$ | 6.14 | 88 |