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### Volatiles Composition of Fresh Aroma and Hydrodistilled Volatile Oil of *Chrysopogon Zizanioides* Roots Growing In Egypt Along With the Cytotoxic Activities of the Hydrodistilled Oil

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**Supplementary material**



**Figure S1: The cell viability profiles of A549 and HePG2 with *C. zizanioides* oil treatments.**

**Table S1: Composition of the volatile aroma of the fresh sample aroma (FSA) analyzed by headspace (HS) and the hydrodistilled oil (HDO)**

|  |  |  |
| --- | --- | --- |
|  | Relative contents, % |  |
| KI | Components | HS | HDO | Chemical class |
| 1008 | o-Cymene | 0.19 | - | Monoterpene |
| 1017 | limonene | 0.18 | 0.21 |
| 1046 | γ-Terpinene | 0.09 | - |
| 1228 | Carvone | - | 7.07 | Oxygenated monoterpenes |
| 1239 | Carveol | - | 0.64 |
| 1332 | Phenethyl alcohol, 2-(1-hydroxyethyl)-α-methyl | 0.57 | - |
| 1344 | α-Cubebene | 0.01 | - | Sesquiterepnes(non-oxygneated) |
| 1361 | Cyclosativene | 3.30 | - |
| 1365 | Ylangene | 0.66 | - |
| 1375 | longipinene | 1.53 | - |
| 1378 | α-Cubebene | 0.67 | - |
| 1393 | β-Cubebene | 0.55 | - |
| 1398 | α-bergamotene | 0.42 | - |
| 1404 | Cedr-8(15)-ene | 3.80 | - |
| 1408 | α-Gurjunene | 1.95 | - |
| 1414 | Caryophyllene | - | 0.18 |
| 1416 | α-Copaene | 1.37 | - |
| 1422 | cis-muurola-4(14),5-diene | 0.77 | - |
| 1430 | α-Guaiene | 0.08 |  0.94 |
| 1433 | Aristol-9-ene | 2.16 | - |
| 1437 | Sativene | 11.52 | - |
| 1442 | Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl | 14.17 | - |
| 1446 | allo-Aromadendrene | 4.94 | - |
| 1456 | Acoradiene | 0.98 | - |
| 1458 | β-ylangene | 0.30 | - |
| 1460 | Neoisolongifolene, 8,9-dehydro- | 0.16 | - |
| 1469 | 1-Isopropyl-4,7-dimethyl-1,2,4a,5,6,8a- | 3.51 | - |
| 1474 | δ-Guaiene | 1.03 | - |
| 1478 | (gamma.-Muurolene) | 0.73 | - |
| 1479 | δ-Selinene | 2.07 | - |
| 1482 | eremophilene | 1.51 | - |
| 1486 | Germacrene D | 0.22 | - |
| 1488 | 4,5-di-epi-aristolochene | 1.16 | - |
| 1495 | δ-Cadinene | 1.80 | - |
| 1496 | α-Muurolene) | 0.36 | 0.39 |
| 1502 | 3-Carene, 4-acetyl | - | 0.12 |
| 1504 | α-(Z,E)-Farnesene | 0.04 | - |
| 1507 | (-)-delta.-Panasinsine | 2.30 | - |
| 1510 | Valencene | 9.41 | - |
| 1522 | Isodaucene | - | 0.15 |
| 1523 | -selinene | 0.78 | - |
| 1531 | α-Bulnesene | 0.39 | - |
| 1538 | β-Vatirenene | 1.99 | - |
| 1548 | Aristolene | 0.58 | - |
| 1549 | α -Curcumene | - | 0.21 |
| 1565 | longifolene | 2.44 | - |
| 1638 | á-Vatirenene | - | 0.48 |
| 1504 | sesquicineole | 0.60 | - | Ethers |
| 1631 | Ledene oxide-(II) | - | 0.27 |
| 1640 | Aromadendrene oxide-(2) | - | 0.88 |
| 1656 | ç-Gurjunenepoxide-(2) | - | 2.25 |
| 1686 | Aristolene epoxide | - | 3.05 |
| 1764 | Aromadendrene oxide-(1) | - | 0.33 |
| 1772 | Calarene epoxide | - | 1.65 |
| 1792 | 4,6,6-Trimethyl-2-(3-methylbuta 1,3 dienyl)oxatricyclo[5.1.0.0(2,4)]octane | 0.70 | - |
| 1532 | Eudesm-4(14)-en-11-ol | - | 3.39 | Alcohols |
| 1544 | β-Eudesmol | 1.85 | - |
| 1570 | (cis-Eudesm-6-en-11-ol) | 0.52 | - |
| 1571 | Germacrene D-4-ol | 0.6 | - |
| 1596 | Selina-6-en-4-ol | 0.94 | - |
| 1600 | Humulane-1,6-dien-3-ol | 2.13 | - |
| 1602 | Cubenol | - | 0.16 |
| 1605 | (Selin-6-en-4.alpha.-ol) | 0.04 | - |
| 1613 | (Junenol) | 0.42 | - |
| 1620 | allo-Khusiol | - | 0.61 |
| 1639 | Delta cadinol | - | 0.68 |
| 1642 | Eudesm-7(11)-en-4-ol | - | 3.7 |
| 1643 | Cubenol | - | 0.65 |
| 1645 | Cedr-8(15)-en-9-ol | - | 0.47 |
| 1648 | tau.-Cadinol | - | 6.26 |
| 1677 | Zizanol | - | 3 |
| 1710 | Aristol-1(10)-en-9-ol | - | 2.33 |
| 1712 | Cedr-8-en-13-ol | 5.74 | 1.97 |
| 1714 | 4,11(13)-Eudesmadien-12-ol | - | 0.34 |
| 1718 | (Khusimol) | 0.21 | 16.48 |
| 1735 | à-Vetivol | - | 1.06 |
| 1736 | Valerenol | - | 0.74 |
| 1752 | Aristol-1(10)-en-9-ol | - | 12.51 |
| 1760 | lanceol | 2.29 | - |
| 1770 | α-Muurolene-14-ol | - | 0.2 |
| 1774 | Cyclocopacamphenol | - |  7.69 |
| 1776 | beta-Costol | - |  0.6 |
| 1856 | Isovalencenal | - | 2.49 | Aldehydes |
| 1607 | 2H-Benzocyclohepten-2-one,3,4,4a,5,6,7,8,9-octahydro-4amethyl-,(S)- | - | 0.21 | Ketons |
| 1606 | Khusimone | - | 2.06 |
| 1669 | Epizizanone | - | 2.02 |
| 1700 | Oplopanone | 0.29 | - |
| 1780 | ((-)-.beta.-Vetivone) | 0.85 | - |
| 1789 | Nootkatone | - | 0.44 |
| 1801 | Aristol-9-en-8-one | 0.98 | - |
| 1842 | (-)-á-Vetivone | - | 3.39 |
| Relative contents % | Monoterpenes | 0.46 | 0.21 |  |
| Oxygenated monoterpenes | 0.57 | 7.71 |
| Sesquiterpenes (non-oxygenated) | 79.69 | 2.47 |
| Sesquiterpenes (ether) | 1.30 | 8.43 |
| Sesquiterpenes (alcohol) | 14.14 | 63.44 |
| Sesquiterpenes (aldehyde) | - | 2.49 |
| Sesquiterpenes (ketones) | 2.11 | 8.12 |
| Identified compounds | 98.27 | 92.87 |
| Un-identified compounds | 1.73 | 7.13 |

**Table S2: Cytotoxicity profile with IC50 values of *C. zizanioides* oil sample and doxorubicin**

|  |  |
| --- | --- |
| **Cell line** | **IC50 (µg/ml)** |
| Oil sample | Doxorubicin  |
| A549 | 32.16 ± 1.19 | 28.30 ± 0.08 |
| HePG2 | 37.63 ± 1.02 | 21.60 ± 0.07 |