**Table S****1** **Similarity results of GC chromatographic fingerprint of 10 batches of RAC**

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Samples | RAC01 | RAC02 | RAC03 | RAC04 | RAC05 | RAC06 | RAC07 | RAC08 | RAC09 | RAC10 |
| RAC01 | 1 | - | - | - | - | - | - | - | - | - |
| RAC02 | 0.975 | 1 | - | - | - | - | - | - | - | - |
| RAC03 | 0.983 | 0.992 | 1 | - | - | - | - | - | - | - |
| RAC04 | 0.877 | 0.938 | 0.903 | 1 | - | - | - | - | - | - |
| RAC05 | 0.761 | 0.855 | 0.807 | 0.977 | 1 | - | - | - | - | - |
| RAC06 | 0.797 | 0.877 | 0.835 | 0.986 | 0.995 | 1 | - | - | - | - |
| RAC07 | 0.985 | 0.994 | 0.986 | 0.941 | 0.853 | 0.878 | 1 | - | - | - |
| RAC08 | 0.946 | 0.983 | 0.961 | 0.983 | 0.927 | 0.943 | 0.986 | 1 | - | - |
| RAC09 | 0.84 | 0.895 | 0.909 | 0.864 | 0.834 | 0.838 | 0.874 | 0.883 | 1 | - |
| RAC10 | 0.697 | 0.803 | 0.752 | 0.953 | 0.995 | 0.985 | 0.8 | 0.887 | 0.808 | 1 |
| Reference | **0.931** | **0.978** | **0.961** | **0.984** | **0.939** | **0.952** | **0.975** | **0.995** | **0.923** | **0.904** |

**Table S2** **Relative percentage content and total relative percentage content of common components in 10 batches of RAC**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| NO. | RT. | CAS | Components | RAC01 | RAC02 | RAC03 | RAC04 | RAC05 | RAC06 | RAC07 | RAC08 | RAC09 | RAC10 |
| 1 | 4.50 | 3691-12-1 | α-guaiene | 0.14 | 0.14 | 0.25 | 0.14 | 0.14 | 0.13 | 0.28 | 0.23 | 0.22 | 0.17 |
| 2 | 5.02 | 68269-87-4 | modhephene | 0.40 | 0.51 | 0.68 | 0.48 | 0.45 | 0.42 | 0.76 | 0.61 | 0.62 | 0.46 |
| 3 | 5.17 | 1000373-94-1 | berkheyaradulene | 0.44 | 0.61 | 0.87 | 0.63 | 0.55 | 0.54 | 0.85 | 0.71 | 0.74 | 0.52 |
| 4 | 5.79 | 61262-67-7 | longifolene-(v4) | 0.59 | 0.50 | 0.86 | 0.55 | 0.49 | 0.46 | 0.91 | 0.69 | 0.80 | 0.68 |
| 5 | 5.97 | 87-44-5 | caryophyllene | 0.51 | 0.58 | 1.02 | 0.58 | 0.53 | 0.52 | 1.05 | 0.96 | 0.80 | 0.61 |
| 6 | 6.48 | 29873-99-2 | γ-elemene | 1.86 | 2.59 | 2.83 | 2.91 | 2.73 | 2.76 | 5.26 | 5.37 | 3.85 | 2.23 |
| 7 | 7.17 | 6753-98-6 | humulene | 0.35 | 0.42 | 0.53 | 0.40 | 0.39 | 0.41 | 0.64 | 0.79 | 0.58 | 0.42 |
| 8 | 7.41 | 451-55-8 | γ-curcumene | 0.18 | 0.35 | 0.57 | 0.29 | 0.28 | 0.28 | 1.01 | 0.42 | 0.55 | 0.25 |
| 9 | 8.17 | 17066-67-0 | β-selinene | 0.50 | 0.57 | 0.45 | 0.67 | 0.60 | 0.72 | 0.90 | 0.94 | 1.08 | 0.58 |
| 10 | 9.23 | 20307-83-9 | β-sesquiphellandrene | 0.43 | 0.62 | 0.47 | 0.63 | 0.56 | 0.83 | 0.90 | 0.49 | 0.78 | 0.51 |
| 11 | 9.57 | 4630-7-3 | valencene | 0.60 | 0.72 | 0.82 | 0.78 | 0.78 | 1.07 | 1.95 | 1.53 | 1.41 | 0.7 |
| 12 | 23.04 | 639-99-6 | elemol | 2.68 | 2.61 | 3.95 | 0.35 | 0.67 | 2.24 | 1.40 | 3.61 | 0.87 | 1.66 |
| 13 | 25.34 | 6989-21-5 | atractylon | 7.20 | 6.91 | 7.93 | 8.28 | 12.59 | 14.96 | 24.96 | 15.36 | 16.73 | 9.71 |
| 14 | 31.07 | 23811-08-7 | hinesol | 5.70 | 7.08 | 9.57 | 3.03 | 1.82 | 11.18 | 2.70 | 2.46 | 1.79 | 6.47 |
| 15 | 33.55 | 473-15-4 | β-eudesmol | 25.86 | 19.40 | 22.87 | 4.96 | 7.87 | 1.32 | 12.87 | 14.92 | 7.31 | 25.2 |
| 16 | 44.97 | 55290-63-6 | atractylodin | 12.86 | 15.77 | 14.85 | 21.23 | 17.31 | 20.50 | 15.32 | 12.67 | 21.58 | 18.29 |
| Total relative content % | | | | **88.36** | **88.99** | **86.60** | **79.75** | **70.98** | **85.02** | **88.94** | **88.13** | **82.05** | **89.96** |

**Table S3** **Chemical composition and gene targets of RAC**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| NO. | PubChem CID | Components | Canonical Smiles | Gene Targets |
| 1 | 5317844 | α-guaiene | CC1CCC(CC2=C1CCC2C)C(=C)C | PPARA, CNR2, CXCR3, MAOB, NR1I3 |
| 2 | 188073 | modhephene | CC1CCC23C1(CCC2)C(=CC3(C)C)C | PPARA, CNR2, NR1I3, FAAH, TRPV1, AR, CYP19A1, ESR1, CHRM2, SLC6A2, SLC6A4, CYP2C19 |
| 3 | 14034017 | berkheyaradulene | CC1CCC2(C13CCCC3(C=C2C)C)C | PPARA, CNR2, NR1I3, FAAH, TRPV1, AR, CYP19A1, ESR1, CHRM2, SLC6A2, SLC6A4, CYP2C19 |
| 4 | 570529 | longifolene-(v4) | CC1(CC=CC2(C3C1CC2(CC3)C)C)C | PPARA, CNR2, AR, CYP19A1, ESR1, CHRM2, SLC6A2, SLC6A4, CYP2C19, NR1I3, FAAH, TRPV1, ACHE |
| 5 | 5281515 | caryophyllene | CC1=CCCC(=C)C2CC(C2CC1)(C)C | PPARA, CNR2, FAAH, TRPV1 |
| 6 | 12309452 | γ-elemene | CC(=C1CCC(C(C1)C(=C)C)(C)C=C)C | PPARA, CNR2, CXCR3, NR1H3 |
| 7 | 5281520 | humulene | CC1=CCC(C=CCC(=CCC1)C)(C)C | PPARA, CNR2, GLI2, GLI1, MAOB, TRPV1 |
| 8 | 6428861 | γ-curcumene | CC1=CC=C(CC1)C(C)CCC=C(C)C | PTGS2, SLC6A2 |
| 9 | 28237 | β-selinene | CC(=C)C1CCC2(CCCC(=C)C2C1)C | CHRM3, CHRM1, PTGS2, GABRA2, RXRA, CHRM2, ADRA1B, GABRA1, CHRNA7, GABRA6 |
| 10 | 12315492 | β-sesquiphellandrene | CC(CCC=C(C)C)C1CCC(=C)C=C1 | PTGS2, SLC6A2, GABRA1 |
| 11 | 9855795 | valencene | CC1CCC=C2C1(CC(CC2)C(=C)C)C | PPARA, CNR2, CYP19A1, AR, ESR1, CHRM2, ACHE, SLC6A2, SLC6A4, CYP2C19, NR1H3, BCHE, PTPN1, NR1I3, FAAH, TRPV1, ESR2 |
| 12 | 92138 | elemol | CC(=C)C1CC(CCC1(C)C=C)C(C)(C)O | UGT2B7, HSD11B1, PTGS1, NR1H3, CYP19A1, SLC6A4, AR, CYP17A1, NR3C2, NR1I3, PABPC1, SLC10A2, SAE1, AKR1B10, BCHE, SHBG, ICMT, GRM5, ABHD6, HSD17B2, GCGR, CNR2, HRH3, PSEN2, SLC18A3 |
| 13 | 3080635 | atractylon | CC1=COC2=C1CC3C(=C)CCCC3(C2)C | ADRA1A, ADRA1B, ADRB1, ADRB2, AKR1C3, APP, AR, CHRM1, CHRM2, CHRM3, CHRM4, CHRM5, CHRNA7, CTSB, CTSD, CTSL, CTSS, CYP19A1, DRD1, DRD2, DRD4, EPHX2, FKBP1A, HSD11B1, HTR2A, HTR2C, IMPDH2, MGLL, MTNR1A, MTNR1B, NOS2, NOS3, OPRM1, P2RX7, PABPC1, PAR1, PDE3A, PDE4D, PIK3CA, PIK3CG, PRKDC, PTPN1, RAPGEF4, RXRA, S1PR1, S1PR3, SCN5A, SIGMAR1, SLC5A7, SLC6A3, SLC6A4, TBXAS1, TRPA1 |
| 14 | 10878761 | hinesol | CC1CCC=C(C12CCC(C2)C(C)(C)O)C | ACHE, AKR1B10, AR, ATP12A, BCHE, CES2, CHRM2, CYP17A1, CYP19A1, CYP2C19, CYP51A1, DHCR7, ESR1, ESR2, FABP1, FABP3, FABP4, FABP5, G6PD, GABRA1, GABRA2, GABRA3, GABRA5, GABRA6, GRIA2, HMGCR, HSD11B1, NPC1L1, NR1H3, NR1I3, NR3C1, PPARA, PPARD, PREP, PTGER2, PTGES, PTPN1, PTPN11, PTPN2, PTPN6, RORA, RORC, SCD, SERPINA6, SHBG, SLC6A2, SLC6A4, SQLE, SREBF2, TERT, TOP1, UGT2B7 |
| 15 | 91457 | β-eudesmol | CC12CCCC(=C)C1CC(CC2)C(C)(C)O | UGT2B7, HSD11B1, PTGS1, NR1H3, CYP19A1, NR1I3, CYP17A1, SLC6A4, SAE1, AKR1B10, BCHE, CNR2, AR, SHBG, ESR1, CHRM2, ACHE, SLC6A2, CYP2C19, TRPM8, PTPN1, HMGCR, GCGR, ABHD6, PER2, GABRA1, CHRNA7, UBA2 |
| 16 | 5321047 | atractylodin | CC=CC#CC#CC=CC1=CC=CO1 | GRM5, CYP11B1, CYP11B2, TNNC1, SLC6A3, CTSC, CTSF, CTSK, CTSS, CTSV, CTSL, CTSB, TLR9, TRPA1, HCRTR1, ADORA1, ADORA2A, CDC25B, SLC6A4, FLT3, HSD17B2, AR, ESR1, CYP19A1 |