Supporting information

Tetra- and pentacyclic triterpene acids from the ancient anti-inflammatory remedy frankincense as inhibitors of microsomal prostaglandin E2 synthase-1

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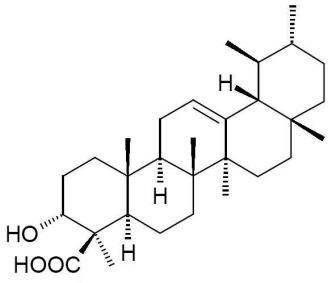
Content:

Isolation and structure elucidation of the triterpene acids

1. Preparation of boswellic acids

Boswellic acids (**1** – **4**) were synthesized according to J. Jauch and J. Bergmann, *Eur. J. Org. Chem.* **2003**, 4752-4756.



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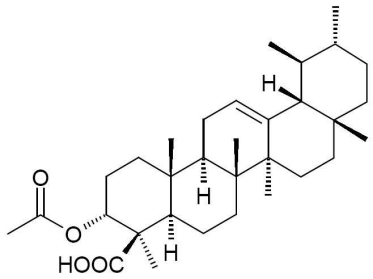

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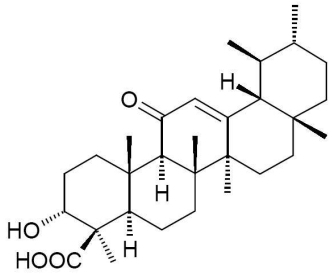

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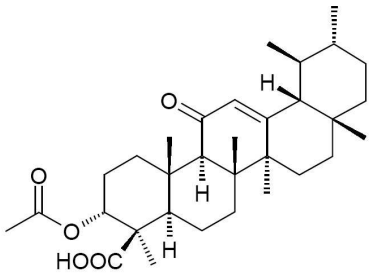


4

Fig. S1. Structures of boswellic acids **1-4**. β-Boswellic acid (**1**), 11-keto-β-boswellic acid (**2**), 3-*O*-acteyl-β-boswellic acid (**3**), and 3-*O*-acteyl-11-keto-β-boswellic acid (**4**).

2. Extraction and isolation of the compounds 5 – 11 from *Boswellia papyrifera*.

The compounds described below were isolated according to the general procedures (see main manuscript) and according to Fig. S2.

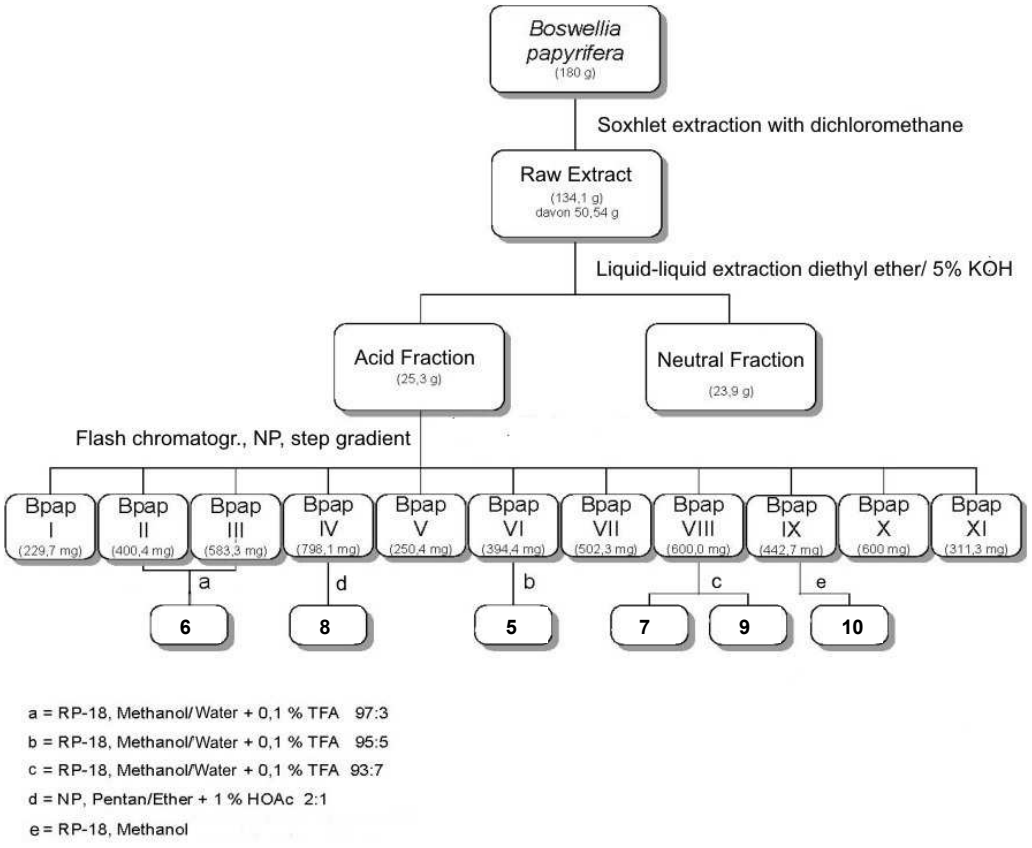


Fig. S2. Isolation of compounds **5** to **10**.

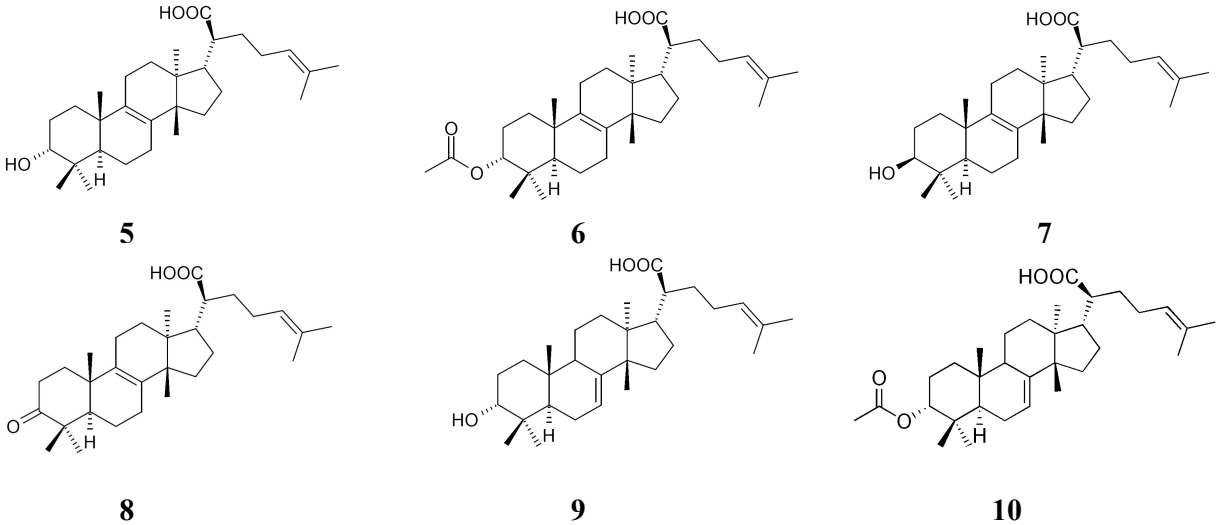


Fig. S3. Structures of the isolated compounds **5** to **10**. 3-α-hydroxy-8,24-diene-tirucallic acid (**5**), 3α-acetoxy-8,24-diene-tirucallic acid (**6**), 3-β-hydroxy-8,24-diene-tirucallic acid (**7**), 3-oxo-8,24-diene-tirucallic acid (**8**), 3-α-hydroxy-7,24-diene-tirucallic acid (**9**), and 3α-acetoxy-7,24-diene-tirucallic acid (**10**).

Data for **5**:

^{1}H-NMR ($(CD_3)_2CO$, 500.13 MHz): δ [ppm] = 5.12 (t, *J* = 7.2 Hz, 1H, H-24), 3.36 (t, *J* = 2.7 Hz, 1H, H-3), 2.26 (dt, *J* = 4.8 Hz, 10.4 Hz, 1H, H-20), 2.14-2.07 (m, 3H, H-7α, H-17, H-11α), 2.03–1.88 (m, 6H, H-2β, H-7β, H-11β, H-16β, H-22β, H-23β), 1.73-1.70 (m, 1H, H-5), 1.65 (s, 3H, H-26), 1.65-1.59 (m, 5H, H-1β, H-2α, H-6α, H-12β, H-15α), 1.58 (s, 3H, H-27), 1.56-1.40 (m, 5H, H-1α, H-6β, H-12α, H-16α, H-22α), 1.29-1.20 (m, 1H, H-15β), 1.06-1.02 (m, 1H, H-23α), 0.97 (s, 3H, H-18), 0.95 (s, 3H, H-29), 0.90 (s, 3H, H-30), 0.87 (s, 3H, H-19), 0.84 (s, 3H, H-28)

^{13}C-NMR ($(CD_3)_2CO$, 125.76 MHz): δ [ppm] = 178.5 (C-21, COOH), 136.6 (C-9, >C=C<), 134.7 (C-8, >C=C<), 133.2 (C-25, H>C=<u>C</u><), 125.8 (C-24, H><u>C</u>=C<), 76.4 (C-3, HO>CH-), 49.4 (C-20, HOOC>CH-), 48.6 (C-17, >CH-), 46.4 (C-5, >CH-), 45.7 (C-13, >C<), 39.3 (C-4, >C<), 38.9 (C-10, >C<), 34.4 (C-22, $-CH_2-$), 31.5 (C-1, $-CH_2-$), 29.8 (C-29, $-CH_3$), 29.1 (C-7, $-CH_2-$), 28.5 (C-16, $-CH_2-$), 27.9 (C-2, $-CH_2-$), 27.7 (C-23, $-CH_2-$), 26.8 (C-26, $-CH_3$), 25.7 (C-30, $-CH_3$), 23.7 (C-28, $-CH_3$), 23.0 (C-11, $-CH_2-$), 21.4 (C-18, $-CH_3$), 20.5 (C-6, $-CH_2-$), 18.7 (C-27, $-CH_3$), 17.1 (C-19, $-CH_3$)

MS (CI, 150 eV): m/z (%) = 456 (40) [M]+, 423 (100), 281 (8), 187 (8)
HRMS (CI, 150 eV): calculated for $C_{30}H_{48}O_3$ 456.3603; found:456.3599

Data for **6**:

^{1}H-NMR ($(CD_3)_2CO$, 500.13 MHz): δ [ppm] = 5.31 (t, *J* = 7.2 Hz, 1H, H-24), 4.61 (t, *J* = 2.7 Hz, 1H, H-3), 2.27 (dt, *J* = 4.4 Hz, 10.6 Hz, 1H, H-20), 2.17-2.09 (m, 2H, H-7α, H-17), 2.00 (s, 3H, H-32), 1.98–1.89 (m, 5H, H-2β, H-7β, H-11β, H-16β, H-23α), 1.66 (s, 3H, H-26), 1.65-1.59 (m, 5H, H-2α, H-5, H-6α, H-12α, H-15α), 1.58 (s, 3H, H-27), 1.56-1.37 (m, 5H, H-1α, H-1β,H-6β, H-12β, H-16α, H-22α), 1.29-1.27 (m, 1H, H-15β), 1.01 (s, 3H, H-18), 0.93 (s, 3H, H-29) 0.91 (s, 3H, H-30), 0.88 (s, 3H, H-19), 0.87 (s, 3H, H-28).

^{13}C-NMR ($(CD_3)_2CO$, 125.76 MHz): δ [ppm] = 178,3 (C-21, COOH), 171,5 (C-31, >C=O), 136.3 (C-9, >C=C<), 134.9 (C-8, >C=C<),133.2 (C-25, H>C=<u>C</u><), 125.8 (C-24, H><u>C</u>=C<), 79.1 (C-3, HO>CH-), 51.4 (C-14, >C<), 49.4 (C-20, HOOC>CH-), 48.6 (C-17, >CH-), 47.8 (C-5, >CH-), 45.7 (C-13, >C<), 38.9 (C-10, >C<), 38.5 (C-4, >C<), 34.4 (C-22, $-CH_2-$), 32.2 (C-1, $-CH_2-$), 29.1 (C-28, $-CH_3$), 28.8 (C-7, $-CH_2-$), 28.5 (C-16, $-CH_2-$), 27.7 (C-23, $-CH_2-$), 26.8 (C-26, $-CH_3$), 25.8 (C-30, $-CH_3$), 25.0 (C-2, $-CH_2-$), 23.2 (C-29, $-CH_3$), 23.0 (C-11, $-CH_2-$), 22.1 (C-32, $-CH_3$), 21.3 (C-18, $-CH_3$), 20.3 (C-6, $-CH_2-$), 18.7 (C-27, $-CH_3$), 17.2 (C-19, $-CH_3$).

MS (CI, 150 eV): m/z (%) = 498 (70) [M]+, 483 (12), 439 (84), 423 (100), 343 (24), 281 (20), 189 (16), 95 (12).
HRMS (CI, 150 eV): calculated for $C_{32}H_{50}O_4$: 498.3709; found: 498.3702

Data for **7**:
^{1}H-NMR ($(CD_3)_2SO$, 500.13 MHz): δ [ppm] = 5.07 (t, *J* = 6.5 Hz, 1H, H-24), 3.0 (dd, *J* = 5.2 Hz, 10.8 Hz, 1H, H-3), 2.15-2.04 (m, 2H, H-7α, H-20), 1.92–1.81 (m, 6H, H-7β, H-11α, H-11β, H-17, H-22α, H-23α), 1.67-1.63 (m, 2H, H-1β, H-6β), 1.63 (s, 3H, H-26),1.53 (s, 3H, H-27), 1.51-1.01 (m, 13H, H-1α, H-2α, H-2β, H-5, H-12α, H-12β, H-15α, H-15β, H-16α, H-22β), 0.90 (s, 3H, H-29), 0.89 (s, 3H, H-18), 0.82 (s, 3H, H-30), 0.74 (s, 3H, H-19), 0.69 (s, 3H, H-28)

^{13}C-NMR ($(CD_3)_2SO$, 125.76 MHz): δ [ppm] = 176.8 (C-21, COOH), 133.8 (C-9, >C=C<), 132.4 (C-8, >C=C<), 131.0 (C-25, H>C=C<), 123.7 (C-24, H>C=C<), 76.6 (C-3, HO>CH-), 50.5 (C-5, >CH-), 48.9 (C-14, >C<), 47.2 (C-20, HOOC>CH-), 46.2 (C-17, >CH-), 43.3 (C-13, >C<), 38.5 (C-4, >C<), 36.7 (C-10, >C<), 34.7 (C-1, -CH_2-), 32.1 (C-16, -CH_2-), 28.8 (C-15, -CH_2-), 28.2 (C-12, -CH_2-), 28.1 (C-29, -CH_3), 27.5 (C-2, -CH_2-), 27.1 (C-7, -CH_2-), 26.2 (C-22, -CH_2-), 25.4 (C-23, -CH_3), 25.4 (C-26, -CH_3), 24.1 (C-30, -CH_3), 20.7 (C-11, -CH_2-), 19.9 (C-18, -CH_3), 18.4 (C-6, -CH_2-), 17.4 (C-27, -CH_3), 15.9 (C-28, -CH_3), 15.4 (C-19, -CH_3).

Data for **8**:
^{1}H-NMR ($(CD_3)_2CO$, 500.13 MHz): δ [ppm] = 5.13 (t, *J* = 7.2 Hz, 1H, H-24), 2.56-2.40 (m, 2H, H-2α, H-2β), 2.27 (dt, *J* = 4.7 Hz, 10.5 Hz, 1H, H-20), 2.20-2.09 (m, 3H, H-7β, H-11β, H-17), 2.03-1.90 (5H, H-1β, H-7α, H-11α, H-16β, H-23α), 1.76-1.67 (m, 3H, H-5, H-6β, H-12β), 1.66 (s, 3H, H-26), 1.64-1.60 (m, 2H, H-1α, H-15α), 1.58 (s, 3H, H-27), 1.57-1.38 (m, 4H, H-6β, H-12β, H-16α, H-22α), 1.32-1.27 (m, 1H, H-15β), 1.06 (s, 6H, H-18, H-29), 1.02 (s, 3H, H-28), 0.93 (s, 3H, H-30), 0.86 (s, 3H, H-19)

^{13}C-NMR ($(CD_3)_2CO$, 125.76 MHz): δ [ppm] = 217.8 (C-3, >C=O), 178.3 (C-21, COOH), 136.2 (C-8, >C=C<), 134.8 (C-9, >C=C<), 133.2 (C-25, H>C=C<), 125.8 (C-24, H>C=C<), 53.3 (C-5, >CH-), 51.5 (C-14, >C<), 49.4 (C-20, HOOC>CH-), 48.7 (C-17, >CH-), 48.6 (C-10 >C<), 45.7 (C-13, >C<), 38.9 (C-4, >C<), 37.1 (C-1, -CH_2-), 35.9 (C-2, -CH_2-), 34.4 (C-22, -CH_2-), 29.2 (C-7, -CH_2-), 28.5 (C-16, -CH_2-), 28.0 (C-29, -CH_3), 27.7 (C-23, -CH_2-), 26.8 (C-26, -CH_3), 25.6 (C-30, -CH_3), 22.9 (C-11, -CH_2-), 22.4 (C-18, -CH_3), 21.9 (C-6, -CH_2-), 21.1 (C-18, -CH_3), 18.7 (C-27, -CH_3), 17.2 (C-19, -CH_3)

MS (CI, 150 eV): m/z (%) = 455 (8) [M]+, 439 (8), 297 (4), 204 (76), 174 (100), 138 (12)
HRMS (CI, 150 eV): calculated for $C_{30}H_{46}O_3$: 454.3447; found: 454.3450

Data for **9**:
^{1}H-NMR ($(CD_3)_2CO$, 500.13 MHz): δ [ppm] = 5.28 (dd, *J* = 2.9Hz, 6.4Hz, 1H, H-7), 5.12 (t, *J* = 7.2 Hz, 1H, H-24), 3.4 (t, *J* = 2.4 Hz, 1H, H-3), 2.35-2.26 (m, 2H, H-9, H-20), 2.02–1.70 (m, 8H, H-2β, H-5, H-6α, H-6β, H-11α, H-16β, H-17, H-23α, H-12β), 1.64-1.60 (m, 1H, H-1α), 1.66 (s, 3H, H-26),1.56 (s, 3H, H-27), 1.56-1.49 (m, 6H, H-2α, H-11β, H-12α, H-15α, H-15β, H-22α), 1.31-1.26 (m, 2H, H-1β, H-16α), 1.01 (s, 3H, H-30), 0.93 (s, 3H, H-19), 0.91 (s, 3H, H-29), 0.90 (s, 3H, H-28), 0.80 (s, 3H, H-18)

^{13}C-NMR ($(CD_3)_2CO$, 125.76 MHz): δ [ppm] = 178.2 (C-21, COOH), 147.7 (C-8, H>C=<u>C</u><), 133.2 (C-25, H>C=<u>C</u><), 125.8 (C-24, H><u>C</u>=C<), 120.2 (C-7, H><u>C</u>=C<), 76.7 (C-3, HO>CH-), 52.8 (C-14, >C<), 51.5 (C-17, >CH-), 50.4 (C-9, >CH-), 49.2 (C-20, HOOC>CH-), 46.2 (C-5, >CH-), 45.1 (C-13, >C<), 39.1 (C-4, >C<), 36.5 (C-10, >C<), 35.3 (C-15, -CH_2-), 34.3 (C-22, -CH_2-), 33.1 (C-1, -CH_2-), 32.3 (C-12, -CH_2-), 29.5 (C-29, -CH_3), 28.8 (C-16, -CH_2-), 27.8 (C-23, -CH_2-), 27.5 (C-2, -CH_2-), 26.8 (C-26, -CH_3), 25.7 (C-6, -CH_2-), 23.2 (C-28 -CH_3), 23.1 (C-19, -CH_3), 19.1 (C-11, -CH_2-), 18.7 (C-27, -CH_3), 14.5 (C-18, -CH_3).

Data for **10**:
^{1}H-NMR ($(CD_3)_2CO$, 500.13 MHz): δ [ppm] = 5.26 (m, 1H, H-7), 5.09 (t, *J* = 7.0 Hz, 1H, H-24), 4.67 (br. s, 1H, H-3), 2.31 (m, 1H, H-9), 2.29 (m, 1H, H-20), 2.06 (s, 3H, H-32), 2.06-1.74 (m, 9 H, H-2β, H-5, H-6α, H-6β, H-16β, H-17, H-23α, H-23β, H-12β), 1.67 (s, 3H, H-26), 1.58 (s, 3H, H-27) , 1.64-1.42 (m, 8H, H-2α, H-22α, H-22β, H-15α, H-15β, H-11α, H-11β, H-12α), 1.33-1.31 (m, 3H, H-1α, H-1β, H-16α), 0.97 (s, 3H, H-30), 0.96, (s, 3H, H.-28), 0.94 (s, 3H, H-19), 0.83 (s, 3H, H-29), 0.74 (s, 3H, H-18)

^{13}C-NMR ($(CD_3)_2CO$, 125.76 MHz): δ [ppm] = 183.0 (C-21, COOH), 170.8 (C-31, >C=O), 145.6 (C-8, H>C=<u>C</u><), 132.2 (C-25, H>C=<u>C</u><), 123.6 (C-24, H><u>C</u>=C<), 118.2 (C-7, H><u>C</u>=C<), 78.3 (C-3, HO>CH-), 51.1 (C-14, >C<), 49.9 (C-17, >CH-), 48.3 (C-9, >CH-), 47.5 (C-20, HOOC>CH-), 45.6 (C-5, >CH-), 43.3 (C-13, >C<), 36.6 (C-4, >C<), 34.7 (C-10, >C<), 33.4 (C-15, -CH_2-), 32.2 (C-22, -CH_2-), 32.0 (C-1, -CH_2-), 29.9 (C-12, -CH_2-), 27.2 (C-29, -CH_3), 27.1 (C-16, -CH_2-), 26.1 (C-23, -CH_2-), 22.9 (C-2, -CH_2-), 25.7 (C-26, -CH_3), 23.8 (C-6, -CH_2-), 21.6 (C-19, -CH_3), 21.4 (C-28 -CH_3), 21.3 (C-32, -CH_3), 17.6 (C-11, -CH_2-), 17.5 (C-27, -CH_3), 12.8 (C-18, -CH_3)

3. Extraction and isolation of the compounds 11 – 14 from *Boswellia socotrana*

The compounds **11** – **14** described below were isolated according to the general procedures (see main manuscript) and according to Fig. S4.

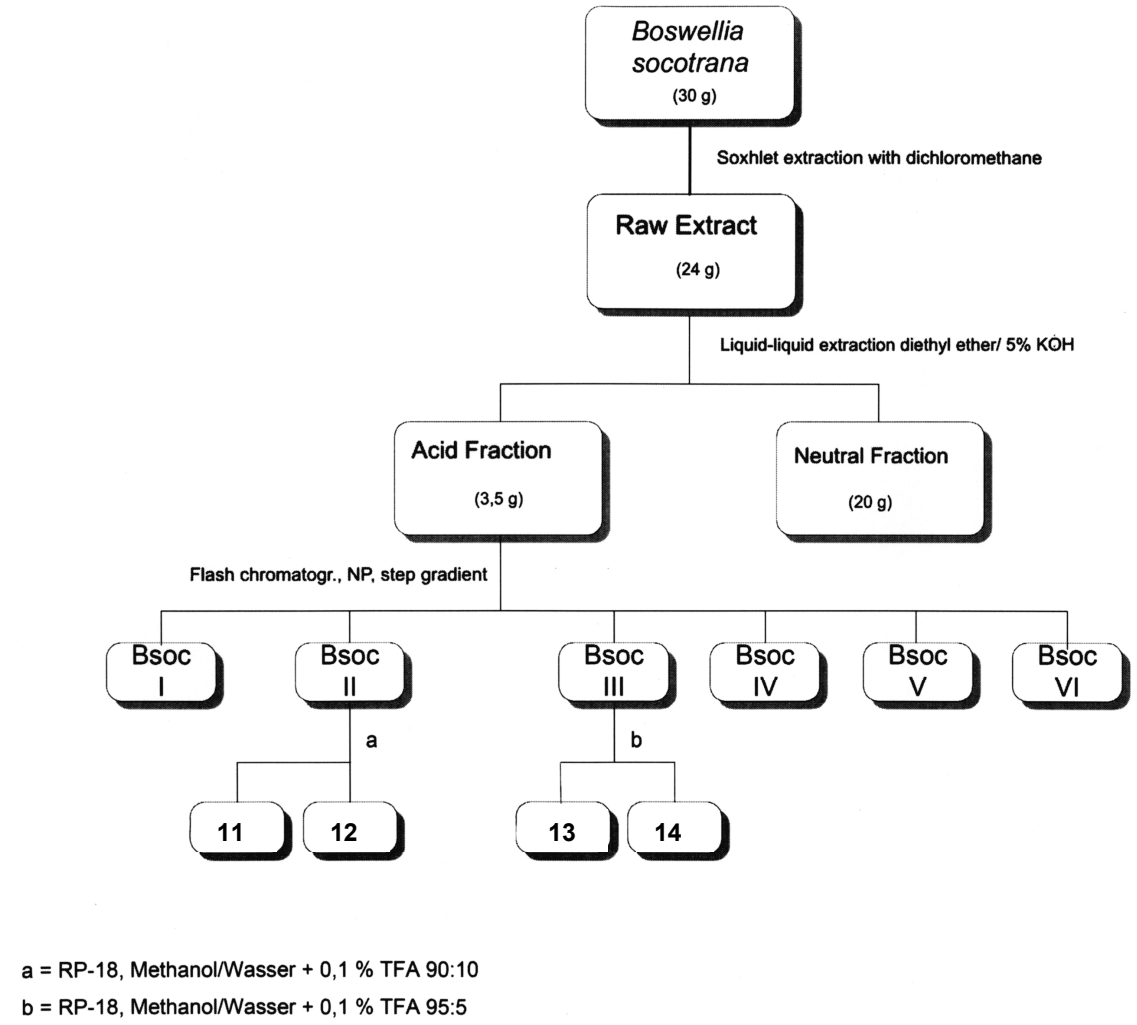


Fig. S4. Isolation of compounds **11** - **14**.

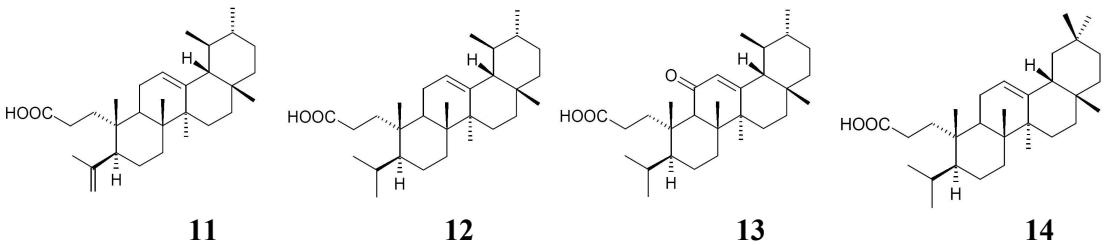


Fig. S5. Structures of compounds **11**-**14**. Roburic acid (**11**), 4,(23)-dihydro-roburic acid (**12**), 4,(23)-dihydro-11-keto-roburic acid (**13**), and 4,(23)-dihydro-nyctanthic acid (**14**).

Data for **11**:

^{1}H-NMR ($(CD_3)_2CO$, 500.13 MHz): δ [ppm] = 5.21 (dd, *J* = 3.0 Hz, 4.2 Hz, 1H, H-12), 4.88 (br. s, 1H, H-24), 4.73 (br. s, 1H, H-24), 2.43-2.36 (ddd, *J* = 4.7 Hz, 11.4 Hz, 15.9 Hz, 1H, H-2α), 2.24-2.17 (ddd, *J* = 6.3 Hz, 11.5 Hz, 15.4 Hz, 1H, H-2β), 2.11-2.06 (m, 3H, H-5, H-11β, H-16α), 2.02-1.81 (m, 4H, H-6β, H-9, H-11α, H-15β), 1.78 (s, 3H, H-23), 1.68-1.55 (m, 2H, H-1α, H-7α), 1.46-1.29 (m, 8H, H-6α, H-7β, H-18, H-19, H-21α, H-21β, H-22α, H-22β), 1.17 (s, 3H, H-27, 1.11 (s, 3H, H-26), 1.09-1.04 (m, 1H, H-15α), 0.99 (s, 3H, H-25), 0.94-0.88 (m, 5H, H-16β, H-20, H-30), 0.84 (m, 6H, H-28, H-29)

^{13}C-NMR ($(CD_3)_2CO$, 125.76 MHz): δ [ppm] = 175.9 (C-3, COOH), 149.5 (C-4, >$\underline{C}$=CH_2), 141.4 (C-13, >$\underline{C}$=C<$_H$), 126.5 (C-12, >C=$\underline{C}$<$_H$), 114.9 (C-24, >C=$\underline{C}H_2$), 61.1 (C-18, >CH-), 51.9 (C-5, >CH-), 44.5 (C-8, C-14, >C<), 43.3 (C-22, -CH_2-), 41.6 (C-19, >CH-), 41.4 (C-20, >CH-), 40.8 (C-10, > C<), 39.6 (C-9, >CH-), 36.1 (C-1, -CH_2-), 35.5 (C-17, >C<), 33.4 (C-7, -CH_2-), 32.9 (C-21, -CH_2-), 30.26 (C-28, CH_3), 29.8 (C-2, -CH_2-), 29.7 (C-16, -CH_2), 28.3 (C-15, -CH_2-), 26.4 (C-6, -CH_2-), 25.3 (C-11, -CH_2-), 25.0 (C-23, -CH_3), 24.7 (C-27, -CH_3), 22.7 (C-30, -CH_3), 21.2 (C-25, -CH_3), 19.0 (C-29, -CH_3), 18.5 (C-26, -CH_3)

Data for **12**:

^{1}H-NMR ($(CD_3)_2CO$, 500.13 MHz): δ [ppm] = 5.21 (t, *J* = 3.6 Hz, 1H, H-12), 2.19 (t, *J* = 8.4 Hz, 2H, H-1β, H-2α), 2.09-2.06 (m, 1H, H-6α), 2.00-1.82 (m, 5H, H-4, H-9, H-11α, H-11β, H-15β), 1.73-1.67 (m, 2H, H-1α, H-2β), 1.59-1.52 (m, 2H, H-6β, H-7α), 1.46-1.29 (m, 8H, H-6α, H-7β, H-18, H-19, H-21α, H-21β, H-22α, H-22β), 1.15 (br. s, 4H, H-5, H-27), 1.08 (s, 3H, H-26), 1.06-1.04 (m, 1H, H-15α), 0.97 (s, 3H, H-25), 0.95 (br. s, 3H, H-23), 0.94-0.92 (d, *J* = 8.3 Hz, 4H, H-30, H-20), 0.86 (d, *J* = 6.8 Hz, 3H, H-24), 0.83 (d, *J* = 5.7 Hz, 6H, H-28, H-29)

^{13}C-NMR ($(CD_3)_2CO$, 125.76 MHz): δ [ppm] = 175.9 (C-3, COOH, aus HMBC), 141.4 (C-13, >$\underline{C}$=C<$_H$), 126.7 (C-12, >C=$\underline{C}$<$_H$), 61.1 (C-18, >CH-), 49.4 (C-5, >CH-), 44.5 (C-8, C-14, >C<), 43.3 (C-22, -CH_2-), 41.7 (C-10, > C<), 41.6 (C-19, >CH-), 41.4 (C-20, >CH-), 39.6 (C-9, >CH-), 35.5 (C-17, >C<), 35.1 (C-1, -CH_2-), 33.8 (C-7, -CH_2-), 32.9 (C-21, -CH_2-), 30.26 (C-28, CH_3), 29.8 (C-2, -CH_2-), 29.7 (C-16, -CH_2), 28.3 (C-15, -CH_2-), 26.8 (C-4, >C<), 26.1 (C-23, -CH_3), 25.4 (C-11, -CH_2-), 24.5 (C-27, -CH_3), 22.6 (C-30, -CH_3), 21.0 (C-25, -CH_3), 20.3 (C-24, -CH_3), 19.9 (C-6, -CH_2-), 19.0 (C-29, -CH_3), 18.6 (C-26, -CH_3)

Data for **13**:

^{1}H-NMR ($(CD_3)_2CO$, 500.13 MHz): δ [ppm] = 5.50 (s, 1H, H-12), 2.76-2.72 (m, H-1β, H-9), 2.24-2.09 (m, 3H, H-2α, H-2β, H-16α), 2.00-1.47 (m, 10H, H-1α, H-4, H-6α, H-7β, H-15β, H-

18, H-19, H-21α, H-21β, H-22α), 1.40 (s, 3H, H-27), 1.39-1.37 (m, 1H, H-7α), 1.29-1.26 (m, 1H, H-15α), 1.21-1.20 (d, 6H, H-25, H-26), 1.14-1.11 (m, 2H, H-5, H-6β), 1.05 (s, 1H, H-16β), 0.98-0.91 (m, 7H, H-20, H-23, H-30), 0.86-0.85 (m, 6H, H-24, H-28), 0.83 (d, *J* = 6.4 Hz, 3H, H-29)

^{13}C-NMR ($(CD_3)_2CO$, 125.76 MHz): δ [ppm] = 200.0 (C-11, >C=O), 176.2 (C-3, COOH), 165.6 (C-13, >$\underline{C}$=C<$_H$), 132.3 (C-12, >C=$\underline{C}$<$_H$), 60.7 (C-18, >CH-), 53.8 (C-9, >CH-), 49.2 (C-5, >CH-), 46.6 (C-10, C-14, >C<), 45.9 (C-8, >C<), 42.7 (C-22, -CH_2-), 41.1 (C-20, >CH-), 40.9 (C-19, >CH-), 35.7 (C-17, >C<), 35.4 (C-1, -CH_2-), 32.6 (from DEPT 135, C-7, -CH_2-), 30.37 (from DEPT 135, C-2, -CH_2-), 30.2 (C-28, -CH_3), 29.2 (C-16, -CH_2-), 28.9 (C-15, -CH_2-), 26.1 (C-4, >C<), 26.0 (C-23, -CH_3), 22.4 (C-30, -CH_3), 21.8 (C-27, -CH_3), 20.7 (C-25, -CH_3), 20.3 (C-24, -CH_3), 19.9 (C-26, -CH_3), 19.2 (C-6, -CH_2-), 18.8 (C-29, -CH_3)

MS (EI, 70 eV): m/z (%) = 456 (4), 273 (28), 193 (20), 155 (28), 137 (30), 91 (100)

HRMS (EI, 70 eV): calculated for $C_{30}H_{48}O_3$: 456.3603; found: 456.3600

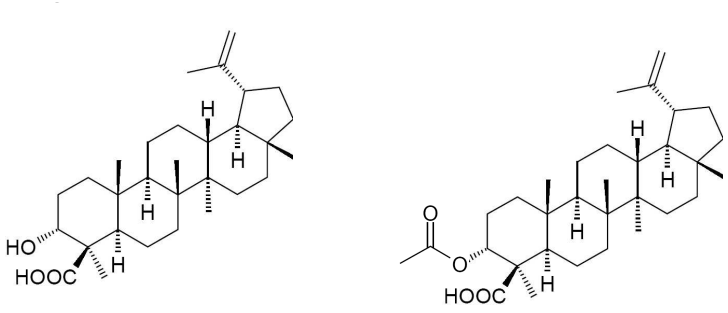
Data for **14**:
^{1}H-NMR ($(CD_3)_2CO$, 500.13 MHz): δ [ppm] = 5.24 (t, *J* = 3.4 Hz, 1H, H-12), 2.18 (m, 2H, H-1β, H-2α), 2.10-2.06 (m, 1H, H-6α), 2.00-1.66 (m, 8H, H-1α, H-2β, H-4, H-9, H-11α, H-11β, H-15β, H-18, H-19β), 1.56-1.22 (m, 6H, H-6α, H-7α, H-7β, H-21α, H-22α, H-22β), 1.20 (s, 3H, H-27), 1.13-1.11 (m, 2H, H-5, H-6β, H-21β), 1.05 (m, 5H, H-15α, H-19α, H-26), 0.96 (s, 3H, H-25), 0.94 (s, 3H, H-23), 0.89 (d, 6H, H-29, H-30), 0.87 (s, 3H, H-28), 0.86-0.84 (d, 4H, H-16β, H-24)

^{13}C-NMR ($(CD_3)_2CO$, 125.76 MHz): δ [ppm] = 176.1 (C-3, COOH), 146.8 (C-13, >$\underline{C}$=C<$_H$), 123.9 (C-12, >C=$\underline{C}$<$_H$), 49.4 (C-5, >CH-), 49.2 (C-18, >CH-), 48.6 C-19, >CH-), 44.1 (C-14, >C<), 41.5 (C-8, C-10 >C<), 39.6 (C-9, >CH-), 38.7 (C-22, -CH_2-), 36.4 (C-21, -CH_2-), 34.9 (C-1, -CH_2-), 34.6 (C-30, -CH_3), 34.3 (C-17, >C<), 33.4 (C-7, -CH_2-), 32.7 (C-20, >C<), 29.8 (C-28, CH_3), 29.7 (C-2, -CH_2-), 28.6 (C-16, -CH_2), 27.9 (C-15, -CH_2-), 27.2 (C-27, -CH_3), 26.8 (C-4, >C<), 26.2 (C-23, -CH_3), 25.5 (C-11, -CH_2-), 24.9 (C-29, -CH_3), 20.8 (C-25, -CH_3), 20.3 (C-24, -CH_3), 19.9 (C-6, -CH_2-), 18.40 (C-26, -CH_3)

MS (EI, 70 eV): m/z (%) = 442 (24) [M]+, 427 (16), 218 (100), 203 (40), 91 (44)
HRMS (EI, 70 eV): calculated for $C_{30}H_{50}O_2$: 442.3810; found: 442.3780

4. Isolation of luepolic acids 15 and 16 from *Boswellia serrata*

Lupeolic acids 15 and 16 were isolated from *Boswellia serrata* according to G. Culioli, C. Mathe, P. Archier, C. Vieillescazes, *Phytochem*. **2003**, *62*, 537-541 and according to K. Belsner, B. Buchele, U. Werz, T. Simmet, *Magnetic Resonance in Chemistry* 2003;41:629-32.



15 **16**

Fig. S6. Structures of lupeolic acids **15** and **16**. Lupeolic acid (**15**) and 3-*O*-acetyl-lupeolic acid (**16**).

3. Extraction and isolation of the compound 17 from *Boswellia carterii*

Compound **17** described below was isolated according to the general procedures and according to Fig. S7.

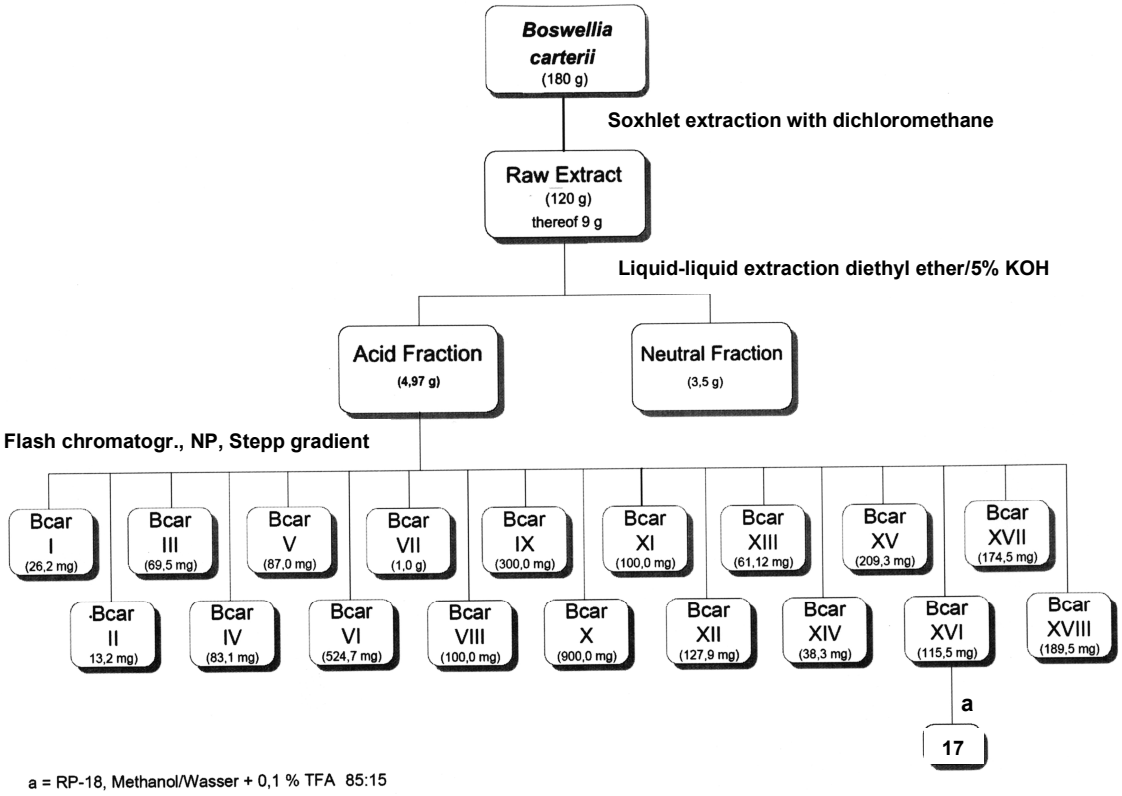
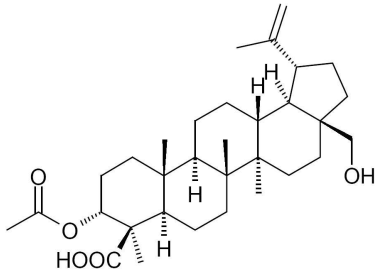


Fig. S7. Isolation of compound 17.



17

Fig. S8. Structure of 3-*O*-acetyl-28-hydroxy-lupeolic acid (**17**).

Data for 17:

^{1}H-NMR ($(CD_3)OD$, 500.13 MHz): δ [ppm] = 5.24 (t, *J* = 2.7 Hz, 1H, H-3), 4.69 (dd, *J* = 2.2 Hz, 1H, H-29), 4.58 (dd, *J* = 2.2 Hz, 1.4 Hz, 1H, H-29), 3.77-3.74 (dd, *J* = 1.3 Hz, 11.1 Hz, 1H, H-28), 3.29 (s, 1H, H-28), 2.43 (dt, *J* = 5.9 Hz, 11.1 Hz, 1H, H-19), 2.21-2.13 (m, 1H, H-2β), 2.08 (s, 3H, H-32), 1.99-1.90 (m, xH, H-6β, H-16β, H-21β, H-22β), 1.83-1.70 (m, 4H, H-6α, H-12β, H-13, H-15β), 1.70 (s, 3H, H-30), 1.66-1.37 (m, 9H, H-1β, H-2α, H-5, H-7α, H-

7β, H-9, H-11β, H-18, H-21α), 1.26-1.20 (m, 2H, H-11α, H-16α), 1.17 (s, 3H, H-23), 1.16-1.13 (m, 1H, H-1α), 1.11 (s, 3H, H-26), 1.10-1.06 (m, 2H, H-12α, H-15α), 1.05 (s, 3H, H-27), 1.03-1.00 (m, 1H, H-22α), 0.84 (s, 3H, H-25)

^{13}C-NMR ($(CD_3)OD$, 125.76 MHz): δ [ppm] = 179.8 (C-24, COOH), 172.4 (C-31, >C=O), 151.9 (C-20, >C=$C<H_2$), 110.3 (C-29, >C=C=$C<H_2$), 75.3 (C-3, $_{AcO}$>CH-), 60.4 (C-28, -CH_2-OH), 51.8 (C-5, >CH-), 51.1 (C-9, >CH-), 50.0 (C-18, >CH-), 47.8 (C-4, >C<), 43.9 (C-14, >C<), 42.2 (C-8, >C<), 38.9 (C-10, >C<), 38.8 (C-13, >CH-), 35.8 (C-1, -CH_2-), 35.4 (C-7, -CH_2-), 35.1 (C-22, -CH_2-), 30.9 (C-21, -CH_2-), 30.7 (C-17, >C<), 30.4 (C-16, -CH_2-), 28.2 (C-15, -CH_2-), 26.7 (C-12, -CH_2-), 24.8 (C-2, -CH_2-), 24.3 (C-23, -CH_3), 22.2 (C-11, -CH_2-), 21.1 (C-32, -CH_3), 20.8 (C-6, -CH_2-), 19.3 (C-30, -CH_3), 16.5 (C-26, -CH_3), 15.2 (C-27, -CH_3), 14.1 (C-25, -CH_3)

MS (CI, 150 eV): m/z (%) = 483 (100), 434 (40), 380 (80), 334 (28), 203 (16), 175 (16)

MS (ESI –): 513 $[M–1]^-$ (100)