SUPPLEMENTARY MATERIAL

New ent-Kaurane Diterpenoid Dimer from *Pulicaria inuloides*.

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Abstract:

A new naturally occurring ent-kaurane diterpenoid dimer, 15β, 15′β-oxybis (ent-kaur-16-en-19-oic acid) (1) along with six known compounds, 15β-hydroxy-ent-kaur-16-en-19-oic acid (2), 15β-hydroxy-ent-kaur-16-en-19-oate-β-D-glucopyranoside (3), 6-hydroxykaempferol-3, 7-dimethyl ether (4), quercetatin 3, 7, 3′-trimethyl ether (5), β-sitosterol (6) and β-sitosterol glucoside (daucosterol) (7) were isolated from the aerial parts of *Pulicaria inuloides* DC. Compounds 2–5 were isolated for the first time from genus *Pulicaria*. The structures of compounds 1–7 were established on the basis of extensive 1D- and 2D-NMR spectroscopic techniques in combination with ESI-MS. The antimicrobial activity of the isolated compounds was evaluated against *Staphylococcus aureus*, *Escherichia coli* and *Candida albicans*. Sulphorhodamine B cytotoxic assay against HepG2 (liver cancer) cell line and ABTS antioxidant assay were carried out.

**Key words: P. inuloides; Asteraceae; ent-kaurane; antimicrobial; antioxidant; cytotoxicity**
Figure S1. $^1$H NMR spectrum of compound 1 in CD$_3$OD

Figure S2. APT spectrum of compound 1 in CD$_3$OD

Figure S3. HMQC NMR spectrum of compound 1 in CD$_3$OD

Figure S4. HMBC NMR spectrum of compound 1 in CD$_3$OD.

Figure S5. $^1$H NMR spectrum of compound 1 in DMSO-$d_6$

Figure S6. APT spectrum of compound 1 in DMSO-$d_6$

Figure S7. ESI-MS$^-$ spectrum of compound 1

Figure S8. NOESY spectrum of compound 2 in CD$_3$OD.

Table S1. Results of antimicrobial activity of compounds 2-5
Figure S1. $^1$H NMR spectrum of compound 1 in CD$_3$OD
Figure S2. APT spectrum of compound 1 in CD$_3$OD
Figure S3. HMQC NMR spectrum of compound 1 in CD$_3$OD
Figure S4. HMBC NMR spectrum of compound 1 in CD$_3$OD
Figure S5. $^1$H NMR spectrum of compound 1 in DMSO-$d_6$
Figure S6. APT spectrum of compound 1 in DMSO-d6
Figure S7. ESI-MS$^-$ spectrum of compound 1
Figure S8. NOESY spectrum of compound 2 in CD$_3$OD.
Table S1: Results of antimicrobial activity of compounds 2-5

| Compound (mg/mL) | E. coli |  | S. aureus |  | C. Albicans |  |
|-----------------|---------|---|-----------|---|-------------|---|
|                 | Diameter of inhibition zone (in mm) | % Activity index | Diameter of inhibition zone (in mm) | % Activity index | Diameter of inhibition zone (in mm) | % Activity index |
| 2               | 8       | 34.8 | NA        | ---- | NA          | ---- |
| 3               | 6       | 26.1 | NA        | ---- | 7           | 26.9 |
| 4               | 9       | 39.1 | 16        | 76.2 | 15          | 57.7 |
| 5               | 11      | 47.8 | 20        | 95.2 | 18          | 69.2 |
| Ampicillin      | 23      | 100 | 21        | 100 | NA          | ---- |
| Colitrimazole   | NA      | ---- | NA        | ---- | 26          | 100 |

- NA: No Activity