SUPPLEMENTARY MATERIAL

An antibacterial isovaleronitrile diglycoside from *Detarium microcarpum*. Guill. Perr. (Fabaceae)

William F. Feudjou\textsuperscript{a,e}, Arnaud M. Mbock\textsuperscript{b}, Blandine M. O. Wache\textsuperscript{a}, Valerie T. Sielinou\textsuperscript{a}, Racéline K. Gounoue\textsuperscript{b}, Pierre Mkounga\textsuperscript{a}, Bruno N. Lenta\textsuperscript{c}, Théophile Dimo\textsuperscript{b}, Fabrice B. Fekam\textsuperscript{d}, Norbert Sewald\textsuperscript{f} and Augustin Ephrem Nkengfack\textsuperscript{a*}

\textsuperscript{a}Department of Organic Chemistry, University of Yaoundé I, P. O. Box 812 Yaoundé, Cameroon,
\textsuperscript{b}Department of Animal Biology and Physiology, University of Yaoundé I, P. O. Box 812 Yaoundé, Cameroon,
\textsuperscript{c}Department of Chemistry, University of Yaoundé I, Higher Teacher Training college, P. O. Box 47 Yaoundé, Cameroon,
\textsuperscript{d}Department of Biochemistry, University of Yaoundé I, P. O. Box 812 Yaoundé, Cameroon,
\textsuperscript{e}Laboratory of Phytochemistry, Centre for Research on Medicinal Plants and Traditional Medicine, Institute of Medical Research and Medicinal Plants Studies, P.O. Box 13033, Yaounde, Cameroon,
\textsuperscript{f}Department of Chemistry, Bielefeld University, P.O. Box 100131, 33501 Bielefeld, Germany,
*Corresponding author: ankengf@yahoo.fr

ABSTRACT

A new isovaleronitrile diglycoside, named microcarposide (1), together with six known compounds, lupeol (2), betulinic acid (3), β-sitosterol glucoside (4), methyl gallate (5), luteolin (6), and epicatechin (7), were isolated from the methanolic extract of the fruits of *Detarium microcarpum* Guill. Perr. The structures of the compounds were determined by extensive analysis of 1D- and 2D- \textsuperscript{1}H and \textsuperscript{13}C NMR spectroscopic data in conjunction with mass spectrometry and by comparison with data reported in the literature. Compound 1 was characterized as (2R)-2-[(6"-O-β-L-rhamnopyranosyl-β-D-glucopyranosyl) oxy]-3-methylbutanenitrile. Some of the isolated compounds were evaluated for their antibacterial activities against several microorganisms; only compound 1 was active against *Salmonella typhi*, *S. enteritidis* and *S. typhimurium* with minimum inhibition concentration (MIC) values of 153.4, 76.7 and 76.7 μM, respectively.

Key words: Fabaceae, *Detarium microcarpum*, Isovaleronitrile diglycoside, microcarposide, antibacterial activity
FIGURES

Figure S1: ESI-MS of compound 1

Figure S2: IR spectrum of compound 1
**Figure S3:** $^{13}$C NMR (125MHz, DMSO) spectrum of compound 1

**Figure S4:** $^1$H NMR (500MHz, DMSO) spectrum of compound 1
Figure S5: $^1$H NMR (500MHz, DMSO) extended spectrum of compound 1

Figure S6: HMQC spectrum of compound 1 (DMSO)
Figure S7: HMBC spectrum of compound 1 (DMSO)

Figure S8: Extended HMBC spectrum of compound 1 (DMSO)
**Figure S9:** Extended HMBC spectrum of compound 1 (DMSO)

**Figure S10:** Extended HMBC spectrum of compound 1 (DMSO)
Figure S11: DEPT 135 spectrum of compound 1

Figure S12: COSY spectrum of compound 1
Figure S13 – Absolute configuration of heterodendrin and epiheterodendrin

TABLES

Table S1: Antibacterial activities of compounds 1-5.

| Compounds | Parameters | ST  | STM  | SE  |
|-----------|------------|-----|------|-----|
| 1         | MIC (μM)   | 153.5 | 76.7 | 76.7 |
|           | MBC (μM)   | 306.8 | 153.5 | 153.5 |
|           | MBC/MIC    | 2 | 2 | 2 |
| 2         | MIC (μM)   | >293.1 | >293.1 | >293.1 |
|           | MBC (μM)   | >293.1 | >293.1 | >293.1 |
|           | MBC/MIC    | / | / | / |
| 3         | MIC (μM)   | >273.9 | >273.9 | >273.9 |
|           | MBC (μM)   | >273.9 | >273.9 | >273.9 |
|           | MBC/MIC    | / | / | / |
| 4         | MIC (μM)   | >216.8 | >216.8 | >216.8 |
|           | MBC (μM)   | >216.8 | >216.8 | >216.8 |
|           | MBC/MIC    | / | / | / |
| 5         | MIC (μM)   | >678.8 | >678.8 | >678.8 |
|           | MBC (μM)   | >678.8 | >678.8 | >678.8 |
|           | MBC/MIC    | / | / | / |
| RD        | MIC (μM)   | 1.5 | 1.5 | 3 |
|           | MBC (μM)   | 6 | 6 | 12 |
|           | MBC/MIC    | 4 | 4 | 4 |

Compound 1 (1); lupeol (2); betulinic acid (3); β-sitosterol glucoside (4); methyl gallate (5); (RD) ciprofloxacin.