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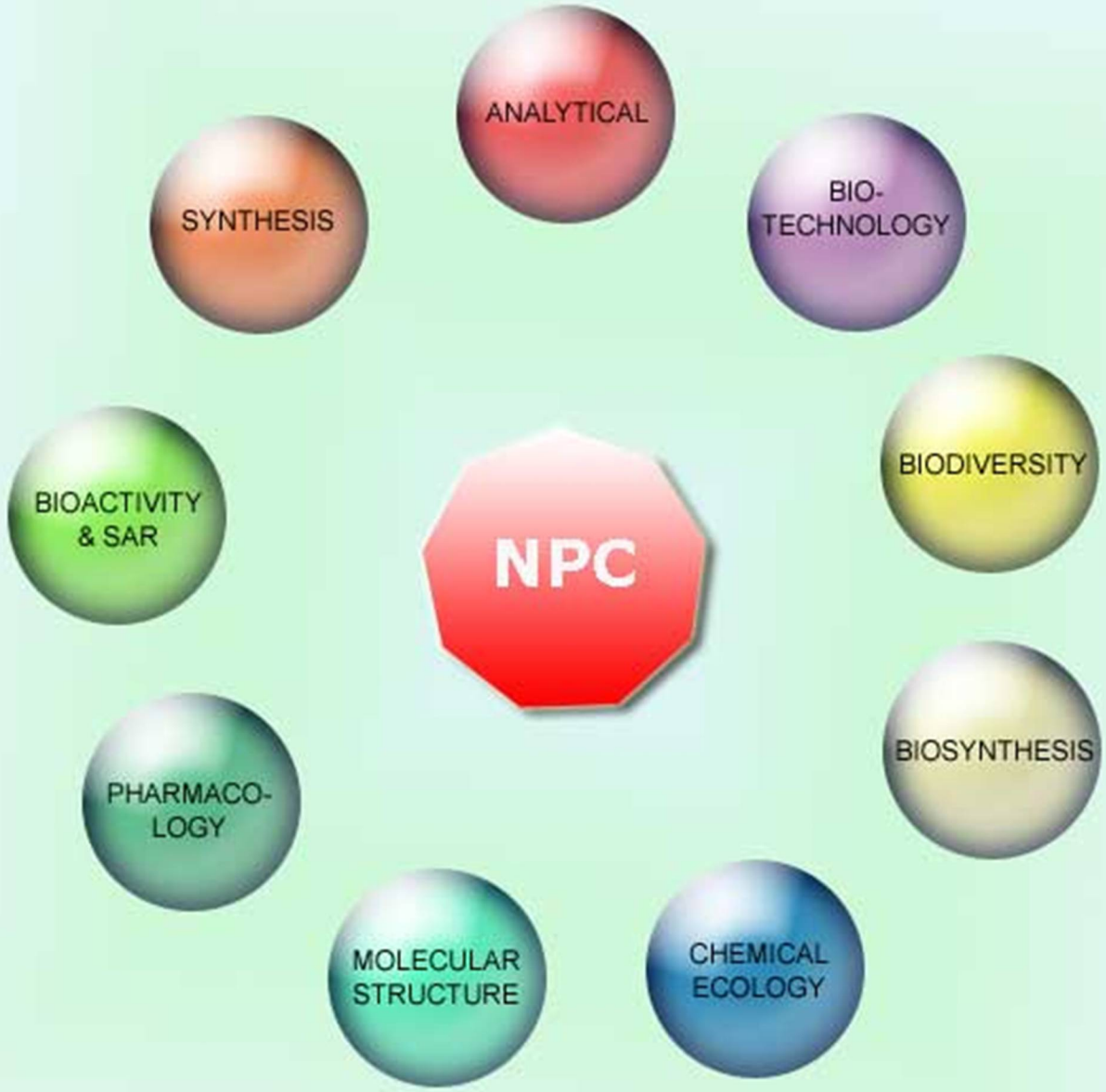

Volume 7. Issue 2. Pages 143-282. 2012
ISSN 1934-578X (printed); ISSN 1555-9475 (online)
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NPC Natural Product Communications

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NPC Natural Product Communications

2012
Vol. 7
No. 2
193 - 194

Eucleanal: A New Napthalene Derivative from *Euclea divinorum*

Margaret Mwihaki Ng'ang'a[a], Hidayat Hussain*[,b,c], Sumesh Chhabra*[,a], Caroline Langat-Thoruwa[a], Karsten Krohn[b,]*, Javid Hussain[b], Ahmed Al-Harrasi[b] and Ivan Robert Green[d]

[a]*Department of Chemistry*, *Kenyatta University*, *P.O. Box 43844-00100*, *Nairobi*, *Kenya*

[b]*Department of Biological Sciences and Chemistry*, *College of Arts and Sciences*, *University of Nizwa*, *Birkat Al-Mouz*, *Nizwa 616*, *Sultanate of Oman*

[c]*Department Chemistry*, *Universität Paderborn*, *Warburger Straße 100*, *33098 Paderborn*, *Germany*

[d]*Department of Chemistry*, *University of the Western Cape*, *P/Bag X17*, *Bellville*, *7530*, *South Africa*

Hidayat110@gmail.com; k.krohn@upb.de

Received: March 3rd, 2011; Accepted: December 30th, 2011

A new naphthalene derivative, named eucleanal (**1**), was isolated from *Euclea divinorum* Hiern., and its structure elucidated by detailed spectroscopic (^{1}H, ^{13}C NMR, COSY, HMQC, HMBC) and HREIMS analysis.

Key words: *Euclea divinorum*, Ebenaceae, Eucleanal, NMR, Structure elucidation.

The African continent is endowed with a world-renowned biodiversity, with a rich multitude of food plants used as herbs, health foods and for therapeutic purposes [1]. In the course of phytochemical studies of medicinal plants from Africa and Pakistan [2-9], we investigated leaves of *Euclea divinorum* Hiern. (Ebenaceae) and here report on the structure elucidation of a new naphthalene derivative, named eucleanal (**1**).

Eucleanal (**1**) was obtained as red solid from CH_2Cl_2/EtOEt, with a melting point of 218-220°C. The IR spectrum showed absorption peaks at 1580 and 1420 cm^{-1}, suggesting the presence of a benzene ring, and at 3390 and 1630 cm^{-1}, indicated the presence of a hydroxyl and carbonyl group, respectively. The UV–visible spectrum exhibited absorption maxima at (λ_{max}, $CHCl_3$) 234 and 345 nm. The molecular formula of eucleanal (**1**) was assigned $C_{12}H_{10}O_3$ on the basis of the HREIMS, with a molecular peak at *m/z* 202.0640, and ^{1}H and ^{13}C NMR spectral analyses. The ^{1}H NMR spectrum in $CDCl_3$ revealed the presence of an aldehydic proton at δ 10.06, a hydroxyl proton at δ 9.43 and a 3-proton singlet at δ 4.10 for a methoxy group attached to an aromatic nucleus. In addition, the ^{1}H NMR spectrum revealed the presence of five aromatic signals at δ 7.82 (1H, d, *J* = 1.5 Hz, H-7), 7.58 (1H, dd, *J* = 1.5, 8.5 Hz, H-2), 7.44 (1H, t, *J* = 8.5 Hz, H-3), 7.30 (1H, d, *J* = 1.5 Hz, H-5), and 6.97 (1H, dd, *J* = 1.5, 8.5 Hz, H-4). From the correlation spectroscopy (COSY), it was evident that two protons (δ 7.82 and 7.30) were coupled to each other via *meta* coupling (*J* = 1.5 Hz), while the remaining three protons (δ 7.58, 7.44, and 6.97) were correlated to each other via *ortho* (*J* = 8.5 Hz) as well as *meta* coupling (*J* = 1.5 Hz). Based on this information, it was evident that compound **1** has a monosubstituted A ring and a disubstituted B ring.

The ^{13}C NMR spectrum and DEPT experiments displayed twelve signals attributed to one methoxy, one aldehyde, 5 methine and five quaternary carbons. The positions of attachment for the aldehydic, methoxy and hydroxyl carbons in rings A and B were confirmed from the HMBC correlations: CHO to C-1; H-2 to C-1, C-3, C-4, C-9, and CHO; H-3 to C-1, C-2, C-4, and C-10; H-4 to C-2, C-3, C-5, and C-10. Similarly HMBC correlations of H-5 to C-4, C-6, C-7, and C-10; H-7 to C-5, C-6, C-8, and C-9 confirmed the regiochemistry in ring B. Consequently, the structure was established to be 8-hydroxy-6-methoxy-1-naphthaldehyde (**1**), named eucleanal, after the producing organism, *Euclea divinorum.*

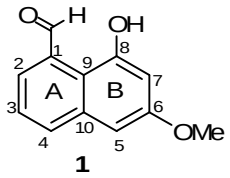

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Figure 1: Structure of eucleanal (**1**).

Experimental

General: IR, Nicolet-510P spectrophotometer; MS, MAT 8200 and Micromass LCT mass spectrometers; NMR, Bruker AMX-500; CC, silica gel (70–230 and 230–400 mesh; E-Merck, Darmstadt, Germany), and Sephadex LH-20 (Amersham Biosciences AB, Uppsala, Sweden).

Plant material: The plants of *Euclea divinorum* Hiern. (Ebenaceae) were collected from the Masai land in the Kajiado district of the Rift valley province in December 2004 and authenticated by Mr Simon Mathenge (Plant taxonomist), Department of Botany, University of Nairobi. A voucher specimen (MM/12/04) is deposited in Nairobi University herbarium, Chiromo Campus.

Extraction and isolation: The air-dried leaves of *E. divinorum* (1.25 kg) were ground and extracted sequentially to afford crude extracts of light petroleum (23 g), dichloromethane (28 g), ethyl acetate (33 g), and methanol (52 g). The ethyl acetate crude extract (33 g) was subjected to VLC using light petroleum, light petroleum: CH_2Cl_2, CH_2Cl_2: MeOH in gradient elution, which afforded 60 fractions (FVC_{1-60}). Preparative TLC of FVC_{27-35} (1.6 g) using dichloromethane: ethyl acetate (9:1) as the solvent system gave 4 fractions (F_{A-D}). Re-crystallization of the 3rd fraction (F_C) (0.05 g) using light petroleum: acetone (9:1) afforded red crystals of eucleanal (**2**, 3.0 mg).

Eucleanal (**1**)

Red solid.
MP: 218-220°C.
IR (CH_2Cl_2): 3390, 1630, 1580, 1420 cm^{-1}.
UV ($CHCl_3$) λ_{max} (log ε): 234 (2.78), 345 (3.55) nm.
^{1}H NMR (500 MHz, $CDCl_3$): δ 10.06, 9.43, 7.82 (1H, d, *J* = 1.5 Hz, H-7), 7.58 (1H, dd, *J* = 1.5, 8.5 Hz, H-2), 7.44 (1H, t, *J* = 8.5 Hz, H-3), 7.30 (1H, d, *J* = 1.5 Hz, H-5), 6.97 (1H, dd, *J* = 1.5, 8.5 Hz, H-4), 4.10 (3H, s, OMe).
^{13}C NMR (125 MHz, $CDCl_3$): δ 192.1 (-CHO), 158.6 (C-6), 155.8 (C-8), 143.6 (C-2), 136.1 (C-4), 135.4 (C-10), 130.1 (C-1), 126.9 (C-3), 123.4 (C-9), 107.1 (C-7), 106.8 (C-5), 56.4 (-OCH_3).
MS (EI, 230°C) *m/z* (%): 202.0640 (24) $[M]^+$.
HREIMS: *m/z* 202.0630 (Calcd. 202.0630 for $C_{12}H_{10}O_3$).

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Natural Product Communications
2012
Volume 7, Number 2

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