SUPPLEMENTARY MATERIAL

A new antifungal Eudesmanolide Glycoside Isolated from *Sphaeranthus indicus* Linn. (Family-Compositae)

Bhuwan B. Mishra,^{1,2*} Navneet Kishore³ and Vinod K. Tiwari^{1*}

¹Department of Chemistry, Centre of Advanced study, Institute of Science, Banaras Hindu University, Varanasi-221005, India

²Center of Innovative and Applied Bioprocessing, Mohali-160071, Punjab, India

³Department of Plant Science, Plant Sciences Complex, University of Pretoria, Pretoria-0002, South Africa

*Corresponding authors. E-mail: bbmchem@gmail.com, tiwari_chem@yahoo.co.in

Abstract

A new antifungal eudesmanolide glycoside 11,13-dihydro-3-*O*-(β -digitoxopyranose)-7 α -hydroxy eudasman-6,12-olide (**2**) in addition to known compounds **1** and **3**, has been isolated from *Sphaeranthus indicus* Linn. Its structure was determined by spectral analysis (UV, IR, 1D & 2D NMR and Mass spectrum).

Keywords: *Sphaeranthus indicus*; Eudesmanolide; Glycoside; Anti-fungal activity.

Table of Contents

1. Table S1. The 300 MHz ^1H NMR and 75 MHz ^{13}C NMR spectrum data for compound 2 in CD_3OD using TMS as internal reference.	S-3
2. ^1H NMR spectra of Compound 2	S-4
3. ^{13}C NMR spectra of Compound 2	S-5
4. ^1H NMR spectra of Compound 3	S-6
5. ^{13}C NMR spectra of Compound 3	S-7

Table S1. The 300 MHz ^1H NMR and 75 MHz ^{13}C NMR spectrum data for compound **2** in CD_3OD using TMS as internal reference.

C	δC	δH
1	24.2	1.95 (2H, <i>m</i>)
2	35.2	1.85 (2H, <i>m</i>)
3	75.9	4.12 (1H, <i>d</i> , $J = 2.0$ Hz)
4	139.2	-
5	133.8	-
6	81.5	5.00 (1H, <i>d</i> , $J = 1.0$ Hz)
7	77.9	-
8	25.4	1.70 (2H, <i>m</i>)
9	35.8	1.45 (2H, <i>m</i>)
10	34.7	-
11	49.2	2.79 (1H, <i>q</i> , $J = 7.2$ Hz)
12	178.2	-
13	14.8	1.14 (3H, <i>d</i> , $J = 7.2$ Hz)
14	15.5	1.94 (3H, <i>s</i>)
15	24.2	1.01(3H, <i>s</i>)
1'	95.5	4.75 (1H, <i>dd</i> , $J = 12.1, 2.0$ Hz)
2' α	34.9	1.81 (1H, <i>ddd</i> , $J = 14, 3.2$ Hz)
2' β	-	2.93 (1H, <i>ddd</i> , $J = 14.3, 12.1, 2.5$ Hz)
3'	65.2	4.21 (1H, <i>q</i> , $J = 3.0$ Hz)
4'	65.2	3.43 (1H, <i>dd</i> , $J = 9.5, 3.0$ Hz)
5'	65.2	3.83 (1H, <i>dq</i> , $J = 9.5, 6.2$ Hz)
6'	18.6	1.32 (3H, <i>d</i> , $J = 6.2$ Hz)

C:\WINNMR98\COMMON\DEFAULT.ALS
AM-2 1H Mr. B.B. Mishra

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : R.C.P.BIPIN

DFILE C:\WINNMR98\COMMO
COMNT AM-2 1H_Mr. B.B.
DATIM Fri Oct 09 12:09:
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 48
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 19.7 c
SLVNT CD3OD
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 17

Spectrum 1. 300 MHz ¹H NMR of compound 2 in CD₃OD

C:\WINNMR98\Data\AM-2_13C1BCM_E5.als
 AM-2 13C Mr. B.B. Mishra

JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University
 VARANASI-221005

Operator : R.C.P.BIPIN

DFILE C:\WINNMR98\Data\
 COMNT AM-2 13C Mr.
 DATIM Fri May 29 04:01:
 OBNUC 13C
 EXMOD BCM
 OBFRQ 75.45 MHz
 OBSET 124.00 KHz
 OBFIN 1840.0 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 4000
 ACQTM 1.606 sec
 PD 1.394 sec
 PW1 6.0 us
 IRNUC 1H
 CTEMP 22.7 c
 SLVNT CD3OD
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 26

Spectrum 2.75 MHz ^{13}C NMR of compound 2 in CD_3OD

C:\WINNMR98\COMMON\DEFAULT.ALS
AM-3 1H Mr. B.B. Mishra

Spectrum 3. 300 MHz ^1H NMR of compound **3** in $\text{DMSO}-d_6$

C:\WINNMR98\Data\AM-3_13C1BCM_E1.als
AM-3 13C Mr. B.B. Mishra

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : R.C.P.BIPIN

DFILE C:\WINNMR98\Data\
COMNT AM-3 13C Mr. B.B
DATIM Tue Dec 30 18:56:
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 1600
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 20.1 c
SLVNT DMSO
EXREF 39.50 ppm
BF 0.20 Hz
RGAIN 23

Spectrum 4. 75 MHz ¹³C NMR of compound **3** in DMSO-*d*₆