SUPPLEMENTARY MATERIAL

A new rearranged tricyclic abietane diterpenoid from *Salvia chloroleuca* Rech. f. & Allen

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Abstract

Phytochemical investigation of the roots of *Salvia chloroleuca* led to the isolation and identification of a new rearranged abietane diterpenoid (**1**). Its structure was elucidated by interpretation of its 1D and 2D NMR spectra and completed by the analysis of the HR-ESIMS data. Compound (**1**) is the second report of a rearranged tricyclic abietane diterpenoid with an acetal functionality between C-2 and C-11. A plausible biosynthetic pathway of **1** was also proposed.

Fig. S1. Key HMBC correlations of **1**

¹H NMR spectrum of Compound 1

Dr Takmar (3-B)2

Current Data Parameters
NAME Dr Monsef 3
EXPNO 19
PROCNO 1

F2 - Acquisition Parameters
Date 20120206
Time 14.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT MeOD
NS 12
DS 0
SWH 9014.423 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 181
DW 55.467 usec
DE 6.50 usec
TE 293.9 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 4.00 usec
PL1 3.00 dB
SFO1 500.1335009 MHz

F2 - Processing parameters
SI 16384
SF 500.1300083 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 30.00

Expanded ¹H NMR spectrum of Compound 1

^{13}C NMR spectrum of Compound 1

(3-8) 2
Dr Takmar

Current Data Parameters
NAME Dr Monsef 3
EXPNO 23
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120207
Time 17.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT MeOD
NS 1930
DS 0
SWH 34090.910 Hz
FIDRES 1.040372 Hz
AQ 0.4806473 sec
RG 1820
DW 14.667 usec
DE 6.50 usec
TE 296.1 K
D1 2.50000000 sec
d11 0.03000000 sec
DELTA 2.40000010 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ^{13}C
P1 9.00 usec
PL1 2.50 dB
SFO1 125.7726799 MHz

===== CHANNEL f2 =====
PCPDPRG2 waitz16
NUC2 ^1H
PCPD2 90.00 usec
PL12 18.50 dB
PL13 18.50 dB
PL2 -1.00 dB
SFO2 500.1335009 MHz

F2 - Processing parameters
SI 16384
SF 125.7576115 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

Expanded ^{13}C NMR spectrum of Compound 1

DEPT-135 spectrum of Compound 1

DEPT-90 spectrum of Compound 1

COSY spectrum of Compound 1

HSQC spectrum of Compound 1

Expanded HSQC spectrum of Compound 1

HMBC spectrum of Compound 1

Expanded HMBC spectrum of Compound 1

Expanded HMBC spectrum of Compound 1

NOESY spectrum of Compound 1

HRMS spectrum of Compound 1

IR spectrum of Compound 1

Date: Sun Jan 05 23:08:14 1997

Dr. Takmar

Scans: 4

Resolution: 4.000

RP-HPLC chromatogram picture of compound 1