SUPPLEMENTARY MATERIAL

New Xanthone from the roots of *Swertia cordata* (G. Don) Clarke

Devendra Mishra^{a*}, Shivani Joshi^b, Shweta Mishra^c, Mukesh Lal Sah^d, Sama Ajay^e and Arun K. Shaw^e

^aDepartment of Applied Chemistry, Birla Institute of Applied Sciences, Bhimtal, Nainital, Uttarakhand, India, ^bDepartment of Chemistry, University of Minnesota, MN. USA, ^cDepartment of Chemistry, Surajmal College of Engineering and Management, Kichha, Nainital, Uttarakhand, India, ^dDepartment of Pharmaceutical Sciences, Kumaun University, Nainital, Uttarakhand, India, Division of Medicinal and Process Chemistry, CSIR-Central Drug Research Institute, Lucknow, Uttar Pradesh, India.

Abstract: The chloroform extract of *Swertia cordata* (G. Don) roots was subjected to column chromatography, afforded two (One new and one known) xanthones. Both the compounds were isolated for the first time from *Swertia cordata*. The structures of the isolated compounds were established on the basis of melting point, 1D (¹H NMR & ¹³C NMR) and 2D (¹H-¹H COSY, HSQC, and HMBC) NMR spectroscopy, in addition to high resolution mass spectrometry..

Keywords: *Swertia cordata*; xanthones; HRMS; ¹H NMR; ¹³C NMR, HSQC, HMBC.

Corresponding Author: Dr. Devendra Mishra

Department of Applied Chemistry, Birla Institute of Applied Sciences, Bhimtal, Nainital-263002, Uttarakhand, India.

Tel.No.+919456322348

Email: mishra.d123@gmail.com

SUPPLEMENTARY MATERIAL

Figure S1. HRMS (ESI) spectrum of S5.

Figure S2. IR spectrum of S5

Figure S3. ^1H NMR (400 MHz, CDCl_3) of S5.

Figure S4. ^{13}C NMR (400 MHz, CDCl_3) of S5.

Figure S5. ^1H - ^1H COSY spectrum of S5.

Figure S6. HSQC spectrum of S5.

Figure S7. HMBC spectrum of S5.

Figure S8. HRMS (ESI) spectrum of S6.

Figure S9. ^1H NMR (400 MHz, CDCl_3) of S6.

Figure S10. ^{13}C NMR (400 MHz, CDCl_3) of S6.

Figure S11. HMBC correlations of S5.

Figure S12. ^1H NMR expansion of S5.

Figure S13. ^1H NMR expansion of S5.

Table S1. ^1H NMR & ^{13}C NMR data of S5.

Sample Name	Dr. SHAW/AJAY	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	DeV-55-194.d	ACQ Method	ISO-DEC.m	Comment		Acquired Time	1/23/2015 11:06:53 AM

Figure S1. HRMS of S5

PERKIN ELMER

Figure S2. IR Spectrum of S5

11:41 CODE-

X: 4 scans, 4.0 cm^{-1} , flat, smooth, abex

SAIF No-6905

Figure S3 . ¹H NMR (400 MHz) of S5

Figure S4. ^{13}C NMR (400MHz, CDCl_3) of S5

DEV-S5

Figure S5. H-H COSY of S5

DEV-55

Figure S6 . HSQC of S5

DEV-55

Figure S7. HMBC Spectrum of S5

DEV-S6 #21 RT: 0.21 AV: 1 SB: 8 0.02-0.11 NL: 5.88E4
T: FTMS + c ESI Full ms [100.00-2000.00]

Figure S8 HRMS of S6

Figure S 9 ¹H NMR (400 MHz, CDCl₃) of 56

DEV-56

Current Data Parameters
NAME Dev-S6
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150114
Time 5.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 201.48
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6304993 MHz
NUC1 13C
P1 9.00 usec
PLW1 61.09999847 W

===== CHANNEL f2 =====
SFO2 400.1621006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 13.10000038 W
PLW12 0.26705000 W
PLW13 0.21630999 W

F2 - Processing parameters
SI 32768
SF 100.6203986 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

Figure S10. ¹³C NMR (400 MHz CDCl₃) of S6

Figure 11

Selected HMBC Correlations of S5

Table 1 ^1H NMR and ^{13}C NMR data of S5

Position	^1H NMR (400 MHz, CDCl_3) δ ppm	^{13}C NMR (400 MHz, CDCl_3) δ ppm
1	-	158.0
2	-	116.1
3	7.8 (dd, $J=1.4$)	104.3
4	-	93.2
4a	-	148.6
5	-	167.1
6	6.6 (d, $J=2.2$)	97.9
7	6.4 (d, $J=2.2$)	-
8	-	163.7
8a	-	124.0
9	-	181.2
9a	-	117.2
1- OH	12.8 (s)	-
5- OMe	4.0 (s)	56.8
8- OMe	3.8 (s)	56.2

Figure S12. ¹H NMR expansion of S5.

Figure S13. ¹H NMR expansion of 5S.