SUPPLEMENTARY MATERIAL

A new Isoquinoline alkaloid with anti-microbial properties from *Berberis jaeschkeana* Schneid. Var. *jaeschkeana*

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Abstract

One new isoquinoline alkaloid named Berberidione (**1**) along with four new source alkaloids berberine (**2**), palmatine (**3**), jatrorrhizine (**4**), chondrofoline (**5**) and three new source non alkaloids syringic acid (**6**), β -sitosterol (**7**) and stigmasterol (**8**) were isolated and characterized from different fractions of *Berberis jaeschkeana* Schneid var. *jaeschkeana*. All the structure were determined from 1D and 2D spectroscopic data. Crude extract, sub-fractions and isolated compounds showed excellent anti-microbial properties. The toxicity level for the alkaloids was found to be very low on THP-1 cells.

Keywords: *Berberis Jaeschkeana*, Berberidione, Anti-microbial.

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H NMR spectrum of Compound 1

```

NAME          D166801
EXPNO         1
PROCNO        1
Date_         20120904
Time          20.14
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zg30
TD            32564
SOLVENT       CDC13
NS            16
DS            2
SWH           8223.685 Hz
FIDRES        0.252539 Hz
AQ            1.9799412 sec
RG            406
DW            60.800 usec
DE            6.50 usec
TE            296.1 K
D1            2.00000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            9.40 usec
PL1           -4.00 dB
PL1W          19.93825150 W
SFO1          400.1324710 MHz
SI            32768
SF            400.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

ALAMZEB
 BUV
 @proton CDC13

¹³C NMR spectrum of Compound 1

```

NAME           D166801
EXPNO           2
PROCNO          1
Date_           20120904
Time            22.35
INSTRUM         spect
PROBHD          5 mm QNP 1H/13
PULPROG         deptqgppsp.2
TD              32768
SOLVENT          CDC13
NS              3072
DS               4
SWH             24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6816244 sec
RG              2050
DW              20.800 usec
DE              6.50 usec
TE              296.0 K
CNST2           145.0000000
CNST12          1.5000000
D1              2.00000000 sec
D2              0.00344828 sec
D12             0.00002000 sec
D16             0.00020000 sec
D28             0.50000000 sec
TD0             1
    
```

```

===== CHANNEL f1 =====
NUC1             13C
P1               7.00 usec
P12              2000.00 usec
PL0              120.00 dB
PL1              -2.60 dB
PL0W             0.00000000 W
PL1W             61.34123230 W
SFO1            100.6228298 MHz
SP2              8.66 dB
SPNAM2           Crp60comp.4
SPOAL2           0.500
SPOFFS2          0.00 Hz
    
```

```

===== CHANNEL f2 =====
CPDPRG2          waltz16
NUC2             1H
P0               15.00 usec
P3               10.00 usec
P4               20.00 usec
PCPD2            80.00 usec
PL2              -4.00 dB
PL12             14.06 dB
PL13             120.00 dB
PL2W            19.93825150 W
PL12W            0.31166428 W
PL13W            0.00000000 W
SFO2            400.1316005 MHz
    
```

===== GRADIENT CHANNEL =====

ALAMZEB
 BUV
 @deptq135 CDC13

HMBC spectrum of Compound 1

ALAMZEB
 BUV
 @HMBC_AIG CDC13

NAME D166801
 EXPNO 3
 PROCNO 1
 Date_ 20120904
 Time 22.36
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG hmbcetgpl3nd
 TD 4096
 SOLVENT CDC13
 NS 16
 DS 16
 SWH 8012.820 Hz
 FIDRES 1.956255 Hz
 AQ 0.2556404 sec
 RG 2050
 DW 62.400 usec
 DE 6.50 usec
 TE 295.9 K
 CNST6 120.0000000
 CNST7 170.0000000
 CNST13 10.0000000
 CNST30 0.5981157
 D0 0.00000300 sec
 D1 1.50000000 sec
 D6 0.05000000 sec
 D16 0.00020000 sec
 IN0 0.00002235 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.40 usec
 P2 18.80 usec
 PL1 -4.00 dB
 PL1W 19.93825150 W
 SFO1 400.1324008 MHz

===== CHANNEL f2 =====
 NUC2 13C
 P3 7.00 usec
 P24 2000.00 usec
 PL2 -3.00 dB
 PL2W 67.25932312 W
 SFO2 100.6228138 MHz
 SP7 8.26 dB
 SPNAM7 Crp60comp.4
 SPOAL7 0.500
 SPOFFS7 0.00 Hz

===== GRADIENT CHANNEL =====
 GPNAM1 SMSQ10.100
 GPNAM3 SMSQ10.100
 GPNAM4 SMSQ10.100
 GPNAM5 SMSQ10.100
 GPNAM6 SMSQ10.100
 GPZ1 80.00 %
 GPZ3 14.00 %
 GPZ4 0.00 %

HSQC spectrum of Compound 1

ALAMZEB
BUV
@HSQC CDC13

```

NAME          D166801
EXPNO         4
PROCNO        1
Date_         20120905
Time          0.41
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       hsqcedetgppsp.3
TD            1024
SOLVENT       CDC13
NS            16
DS            16
SWH           8012.820 Hz
FIDRES        7.825020 Hz
AQ            0.0639476 sec
RG            2050
DW            62.400 usec
DE            6.50 usec
TE            295.7 K
CNST2         145.0000000
D0            0.00000300 sec
D1            1.00000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D21           0.00360000 sec
IN0           0.00003000 sec
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            9.40 usec
P2           18.80 usec
P28           0.00 usec
PL1           -4.00 dB
PL1W          19.93825150 W
SFO1          400.1324008 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2       garp4
NUC2          13C
P3            7.00 usec
P14           500.00 usec
P31           1900.00 usec
PCPD2         70.00 usec
PL0           120.00 dB
PL2           -3.00 dB
PL12          15.00 dB
PL0W           0.00000000 W
PL2W          67.25932312 W
PL12W         1.06598854 W
SFO2          100.6214217 MHz
SP3           8.26 dB
SP18          14.46 dB
SPNAM3        Crp60,0.5,20.1
SPNAM18       Crp60_xfilt.2
SPOAL3        0.500
SPOAL18       0.500
SPOFFS3       0.00 Hz
  
```

COSY spectrum of Compound 1

ALAMZEB
 BUV
 @COSY CDC13

NAME D166801
 EXPNO 5
 PROCNO 1
 Date_ 20120905
 Time 1.56
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG cosygcgpmfzf.ptg
 TD 2048
 SOLVENT CDC13
 NS 8
 DS 8
 SWH 8012.820 Hz
 FIDRES 3.912510 Hz
 AQ 0.1278452 sec
 RG 2050
 DW 62.400 usec
 DE 6.50 usec
 TE 295.7 K
 D0 0.00000300 sec
 D1 1.00000000 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 IN0 0.00012495 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.40 usec
 PL1 -4.00 dB
 PL1W 19.93825150 W
 SFO1 400.1324008 MHz

===== GRADIENT CHANNEL =====
 GPNAM1 SMSQ10.100
 GPNAM2 SMSQ10.100
 GPNAM3 SMSQ10.100
 GPNAM4 SMSQ10.100
 GPNAM5 SMSQ10.100
 GPZ1 16.00 %
 GPZ2 12.00 %
 GPZ3 40.00 %
 GPZ4 27.13 %
 GPZ5 23.17 %
 P16 1000.00 usec
 ND0 1
 TD 128
 SFO1 400.1324 MHz
 FIDRES 62.520687 Hz
 SW 20.000 ppm
 FMODE QF
 SI 1024
 SF 400.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40
 SI 1024
 MC2 QF
 SF 400.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

BUV_120905175403 #89 RT: 1.11 AV: 1 NL: 2.58E7

T: FTMS {1,1} + p ESI Full lock ms [75.00-1200.00]

UV spectrum of Compound 1

Survey Scan

HMBC NMR Correlations of Compound 1

Table S1. ^{13}C and ^1H and data of Berberidione (**1**) (CDCl_3 , δ in ppm, J in Hz)

C.No	δ_{C}	δ_{H} (mult, J Hz)
1	107.07	7.53, (s)
2	146.96	---
3	151.01	---
4	107.27	6.68, (s)
4a	133.75	---
5	28.42	2.94, (t, 6.8)
6	40.28	3.57, (dt, 6.8, 2.8)
8	170.32	---
8a	119.05	---
9	107.97	7.41, (s)
10	146.63	---
11	141.65	---
12	139.71	---
12a	142.01	---
13	---	---
13a	166.64	---
13b	122.37	---
-O-CH ₂ -O-	101.43	6.03, (s)
10-OMe	56.50	3.97, (s)