Electronic Supplementary Information

Delavatine A, a structurally unusual cyclopenta[de]isoquinoline alkaloid from

Incarvillea delavayi

Zhongyin Zhang, Fan Yang, Jian-Jun Fu, Yun-Heng Shen, Weiwei He, and Wei-Dong Zhang

a Department of Phytochemistry, School of Pharmacy, Second Military Medical University, Shanghai 200433, P. R. China. shenyunheng@hotmail.com, wdzhangy@hotmail.com

b School of Pharmacy, East China University of Science and Technology, 130 Meilong Road, Shanghai 200237, China.
Contents:

Figure S1. Fitting curves for measuring IC$_{50}$ values.

Figure S2. The positive HR-ESI-MS spectrum of delavatine A.

Figure S3. The $^1$H NMR spectrum of delavatine A (600 MHz, CDCl$_3$).

Figure S4. The $^{13}$C and DEPT NMR spectra of delavatine A (150 MHz, CDCl$_3$).

Figure S5. The $^1$H-$^1$H COSY NMR spectrum of delavatine A (600 MHz, CDCl$_3$).

Figure S6. The HSQC spectrum of delavatine A (600 MHz, CDCl$_3$).

Figure S7. The HMBC spectrum of delavatine A (600 MHz, CDCl$_3$).

Figure S8. The NOESY spectrum of delavatine A (600 MHz, CDCl$_3$).
Figure S1. Fitting curves for measuring IC$_{50}$ value of Delavatine A (1) and Celastrol. Delavatine A was tested with concentrations in the range of 0–13.87 μg/mL (0–50 μM), and the control compound celastrol was tested with concentrations in the range of 0–4.51 μg/mL (0–10 μM).
Figure S2. The positive HR-ESI-MS spectrum of delavatine A.

**Elemental Composition Report**

**Multiple Mass Analysis: 2 mass(es) processed**
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0  Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

<table>
<thead>
<tr>
<th>Mass</th>
<th>RA</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>Score</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>278.1546</td>
<td>100.00</td>
<td>278.1545</td>
<td>0.1</td>
<td>0.4</td>
<td>10.5</td>
<td>1</td>
<td>C19 H20 N O</td>
</tr>
</tbody>
</table>
Figure S3. The $^1$H NMR spectrum of delavatine A (600 MHz, CDCl$_3$).
Figure S4. The $^{13}$C and DEPT NMR spectra of delavatine A (150 MHz, CDCl$_3$).
Figure S5. The $^1$H-$^1$H COSY NMR spectrum of delavatine A (600 MHz, CDCl$_3$).
Figure S6. The HSQC spectrum of delavatine A (600 MHz, CDCl$_3$).
Figure S7. The HMBC spectrum of delavatine A (600 MHz, CDCl$_3$).
Figure S8. The NOESY spectrum of delavatine A (600 MHz, CDCl$_3$).