Supplementary material

A new coumarin from *Murraya alata* activates TRPV1 channel

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Abstract

One new coumarin, muralatin R, was isolated from the leaves of *Murraya alata* Drake (Rutaceae). Its structure was elucidated by extensive analysis of the NMR and MS data, along with the specific rotation comparison. Muralatin R was found to be capable of activating the transient receptor potential vanilloid 1 (TRPV1) channel through desensitization mechanism. The results supply reference for clarification of the therapeutic basis and mechanism of action of *Murraya* plants for treating psychogenic pain or somatoform pain disorders.

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**Table S1.** The NMR data for muralatin R (in CDCl$_3$, $\delta$ in ppm)

**Figure S1.** HRESIMS spectrum for muralatin R.

**Figure S2.** Elemental composition report for muralatin R.

**Figure S3.** $^1$H NMR spectrum for muralatin R in CDCl$_3$.

**Figure S4.** $^{13}$C NMR spectrum for muralatin R in CDCl$_3$.

**Figure S5.** HSQC spectrum for muralatin R in CDCl$_3$.

**Figure S6.** HMBC spectrum for muralatin R in CDCl$_3$.

**Figure S7.** IR spectrum for muralatin R.

**Figure S8.** UV spectrum for muralatin R.
| Position | Muralatin R | $\delta_H$ (J in Hz) | $\delta_C$, type |
|----------|------------|----------------------|-----------------|
| 2        |            | 160.8, C             |                 |
| 3        | 6.22, d (9.7) | 113.4, CH           |                 |
| 4        | 7.89, d (9.7) | 138.6, CH           |                 |
| 5        |            | 148.3, C             |                 |
| 6        |            | 141.7, C             |                 |
| 7        |            | 155.9, C             |                 |
| 8        |            | 115.1, C             |                 |
| 9        |            | 149.0, C             |                 |
| 10       |            | 109.3, C             |                 |
| 1'       | 3.20, dd (13.4, 11.0); 2.98, brd (13.4) | 23.3, CH₂ |                 |
| 2'       | 5.14, brd (11.0) | 78.4, CH           |                 |
| 3'       |            | 72.2, C              |                 |
| 4'       | 1.27, s    | 25.3, CH₃            |                 |
| 5'       | 1.31, s    | 26.2, CH₃            |                 |
| 1''      |            | 172.3, C             |                 |
| 2''      | 2.00, dd (14.8, 6.7); 1.86, dd (14.8, 7.4) | 43.0, CH₂ |                 |
| 3''      | 1.78, m    | 25.1, CH             |                 |
| 4''      | 0.62, d (6.5) | 22.0, CH₃         |                 |
| 5''      | 0.69, d (6.5) | 22.0, CH₃         |                 |
| 5-OCH₃   | 3.94, s    | 61.7, CH₃            |                 |
| 6-OCH₃   | 3.81, s    | 60.8, CH₃            |                 |
| 7-OCH₃   | 3.98, s    | 61.1, CH₃            |                 |
Figure S1. HRESIMS spectrum for muralatin R.
Figure S2. Elemental composition report for muralatin R.
Figure S3. $^1$H NMR spectrum for muralatin R in CDCl$_3$.

Figure S4. $^{13}$C NMR spectrum for muralatin R in CDCl$_3$. 
Figure S5. HSQC spectrum for muralatin R in CDCl₃.

Figure S6. HMBC spectrum for muralatin R in CDCl₃.
Figure S7. IR spectrum for muralatin R.

Figure S8. UV spectrum for muralatin R.