Supporting Information

Triterpenoids with Antiplatelet Aggregation Activity from the Roots of

*Ilex pubescens*

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**Fig. S1** HRESIMS spectrum of compound 1.

<table>
<thead>
<tr>
<th>m/z</th>
<th>Theo. Mass</th>
<th>Delta (ppm)</th>
<th>RDB equiv.</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>455.31601</td>
<td>455.31668</td>
<td>-1.48</td>
<td>8.5</td>
<td>C29 H43 O4</td>
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</tbody>
</table>

**Fig. S2** IR spectrum of compound 1.
Fig. S3 $^1$H NMR spectrum of compound 1 (500 MHz, pyridine-$d_5$).

Fig. S4 $^{13}$C NMR spectrum of compound 1 (125 MHz, pyridine-$d_5$).
Fig. S5 $^1$H-$^1$H COSY spectrum of compound 1 (500 MHz, pyridine-\textit{d}_5).

Fig. S6 HSQC spectrum of compound 1 (500 MHz, pyridine-\textit{d}_5).
Fig. S7 HMBC spectrum of compound 1 (500 MHz, pyridine-$d_5$).

Fig. S8 NOESY spectrum of compound 1 (500 MHz, pyridine-$d_5$).
Fig. S9 HRESIMS spectrum of compound 2.

<table>
<thead>
<tr>
<th>Formula</th>
<th>Mass (Da)</th>
<th>Calc. Mass (Da)</th>
<th>Adduct</th>
<th>Found at Mass (Da)</th>
<th>Error (ppm)</th>
<th>Error (mDa)</th>
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<tbody>
<tr>
<td>C35H54O9</td>
<td>618.3768</td>
<td>663.37389</td>
<td>-HCOO</td>
<td>663.37527</td>
<td>2.1</td>
<td>1.4</td>
</tr>
</tbody>
</table>

Fig. S10 IR spectrum of compound 2.
Fig. S11 $^1$H NMR spectrum of compound 2 (500 MHz, pyridine-$d_5$).

Fig. S12 $^{13}$C NMR spectrum of compound 2 (125 MHz, pyridine-$d_5$).
Fig. S13 $^1$H–$^1$H COSY spectrum of compound 2 (500 MHz, pyridine-$d_5$).

Fig. S14 HSQC spectrum of compound 2 (500 MHz, pyridine-$d_5$).
Fig. S15 HMBC spectrum of compound 2 (500 MHz, pyridine-$d_5$).

Fig. S16 NOESY spectrum of compound 2 (500 MHz, pyridine-$d_5$).
Fig. S17 HRESIMS spectrum of compound 3.

Fig. S18 IR spectrum of compound 3.
Fig. S19 $^1$H NMR spectrum of compound 3 (500 MHz, pyridine-$d_5$).

Fig. S20 $^{13}$C NMR spectrum of compound 3 (125 MHz, pyridine-$d_5$).
Fig. S21 $^1$H-$^1$H COSY spectrum of compound 3 (500 MHz, pyridine-$d_5$).

Fig. S22 HSQC spectrum of compound 3 (500 MHz, pyridine-$d_5$).
Fig. S23 HMBC spectrum of compound 3 (500 MHz, pyridine-$d_5$).

Fig. S24 NOESY spectrum of compound 3 (500 MHz, pyridine-$d_5$).
Fig. S26 HRESIMS spectrum of compound 4.

Fig. S27 IR spectrum of compound 4.
**Fig. S28** $^1$H NMR spectrum of compound 4 (500 MHz, pyridine-$d_5$).

**Fig. S29** $^{13}$C NMR spectrum of compound 4 (125 MHz, pyridine-$d_5$).
Fig. S30 $^1$H-$^1$H COSY spectrum of compound 4 (500 MHz, pyridine-$d_5$).

Fig. S31 HSQC spectrum of compound 4 (500 MHz, pyridine-$d_5$).
Fig. S32 HMBC spectrum of compound 4 (500 MHz, pyridine-$d_5$).

Fig. S33 NOESY spectrum of compound 4 (500 MHz, pyridine-$d_5$).
**Fig. S34** HRESIMS spectrum of compound 5.

**Fig. S35** IR spectrum of compound 5.
Fig. S36 $^1$H NMR spectrum of compound 5 (500 MHz, pyridine-$d_5$).

Fig. S37 $^{13}$C NMR spectrum of compound 5 (125 MHz, pyridine-$d_5$).
Fig. S38 $^1$H-1H COSY spectrum of compound 5 (500 MHz, pyridine-$d_5$).

Fig. S39 HSQC spectrum of compound 5 (500 MHz, pyridine-$d_5$).
Fig. S40 HMBC spectrum of compound 5 (500 MHz, pyridine-$d_5$).

Fig. S41 NOESY spectrum of compound 5 (500 MHz, pyridine-$d_5$).
Fig. S42 HRESIMS spectrum of compound 6.

Fig. S43 IR spectrum of compound 6.
\[ ^1H \text{NMR spectrum of compound 6 (500 MHz, pyridine-}d_5) . \]

\[ ^{13}C \text{NMR spectrum of compound 6 (125 MHz, pyridine-}d_5) . \]

**Fig. S45** \[ ^{13}C \text{NMR spectrum of compound 6 (125 MHz, pyridine-}d_5) . \]
Fig. S46 $^1\text{H}-^1\text{H}$ COSY spectrum of compound 6 (500 MHz, pyridine-$d_5$).

Fig. S47 HSQC spectrum of compound 6 (500 MHz, pyridine-$d_5$).
Fig. S48 HMBC spectrum of compound 6 (500 MHz, pyridine-$d_5$).

Fig. S49 NOESY spectrum of compound 6 (500 MHz, pyridine-$d_5$).
Fig. S50 HRESIMS spectrum of compound 7.

Fig. S51 IR spectrum of compound 7.
Fig. S52 \(^1\)H NMR spectrum of compound 7 (500 MHz, pyridine-\(d_5\)).

Fig. S53 \(^{13}\)C NMR spectrum of compound 7 (125 MHz, pyridine-\(d_5\)).
Fig. S54 ¹H-¹H COSY spectrum of compound 7 (500 MHz, pyridine-d₅).

Fig. S55 HSQC spectrum of compound 7 (500 MHz, pyridine-d₅).
Fig. S56 HMBC spectrum of compound 7 (500 MHz, pyridine-$d_5$).

Fig. S57 NOESY spectrum of compound 7 (500 MHz, pyridine-$d_5$).
Fig. 1 Structures of compounds 1-15.
Fig. 2 Key $^1$H-$^1$H COSY, HMBC and NOESY correlations of compounds 1-4.
Fig. 3 Key $^1$H-$^1$H COSY, HMBC and NOESY correlations of compounds 5-7.
Fig. 4 Dose-Response curves of active compounds.